



## Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 04:37 PM UTC

PDB ID : 4A0W / pdb\_00004a0w  
EMDB ID : EMD-1962  
Title : model built against symmetry-free cryo-EM map of TRiC-ADP-AlFx  
Authors : Cong, Y.; Schroder, G.F.; Meyer, A.S.; Jakana, J.; Ma, B.; Dougherty, M.T.; Schmid, M.F.; Reissmann, S.; Levitt, M.; Ludtke, S.L.; Frydman, J.; Chiu, W.  
Deposited on : 2011-09-13  
Resolution : 13.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

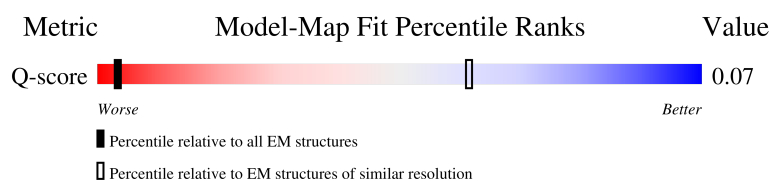
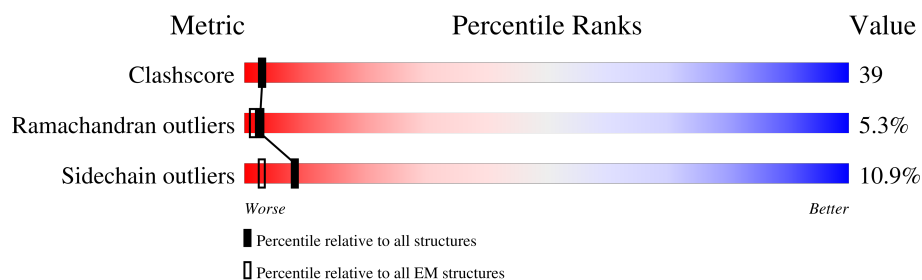
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.90 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                       | 62 ( 13.40 - 14.30 )                                     |

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     | 513    | <div> <div>17%</div> <div>43%</div> <div>45%</div> <div>11%</div> <div>.</div> </div> |
| 1   | B     | 513    | <div> <div>15%</div> <div>46%</div> <div>42%</div> <div>11%</div> <div>.</div> </div> |
| 1   | C     | 513    | <div> <div>13%</div> <div>41%</div> <div>45%</div> <div>9%</div> <div>.</div> </div>  |
| 1   | D     | 513    | <div> <div>19%</div> <div>42%</div> <div>46%</div> <div>11%</div> <div>.</div> </div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 513    |                  |
| 1   | F     | 513    |                  |
| 1   | G     | 513    |                  |
| 1   | H     | 513    |                  |
| 1   | I     | 513    |                  |
| 1   | J     | 513    |                  |
| 1   | K     | 513    |                  |
| 1   | L     | 513    |                  |
| 1   | M     | 513    |                  |
| 1   | N     | 513    |                  |
| 1   | O     | 513    |                  |
| 1   | P     | 513    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

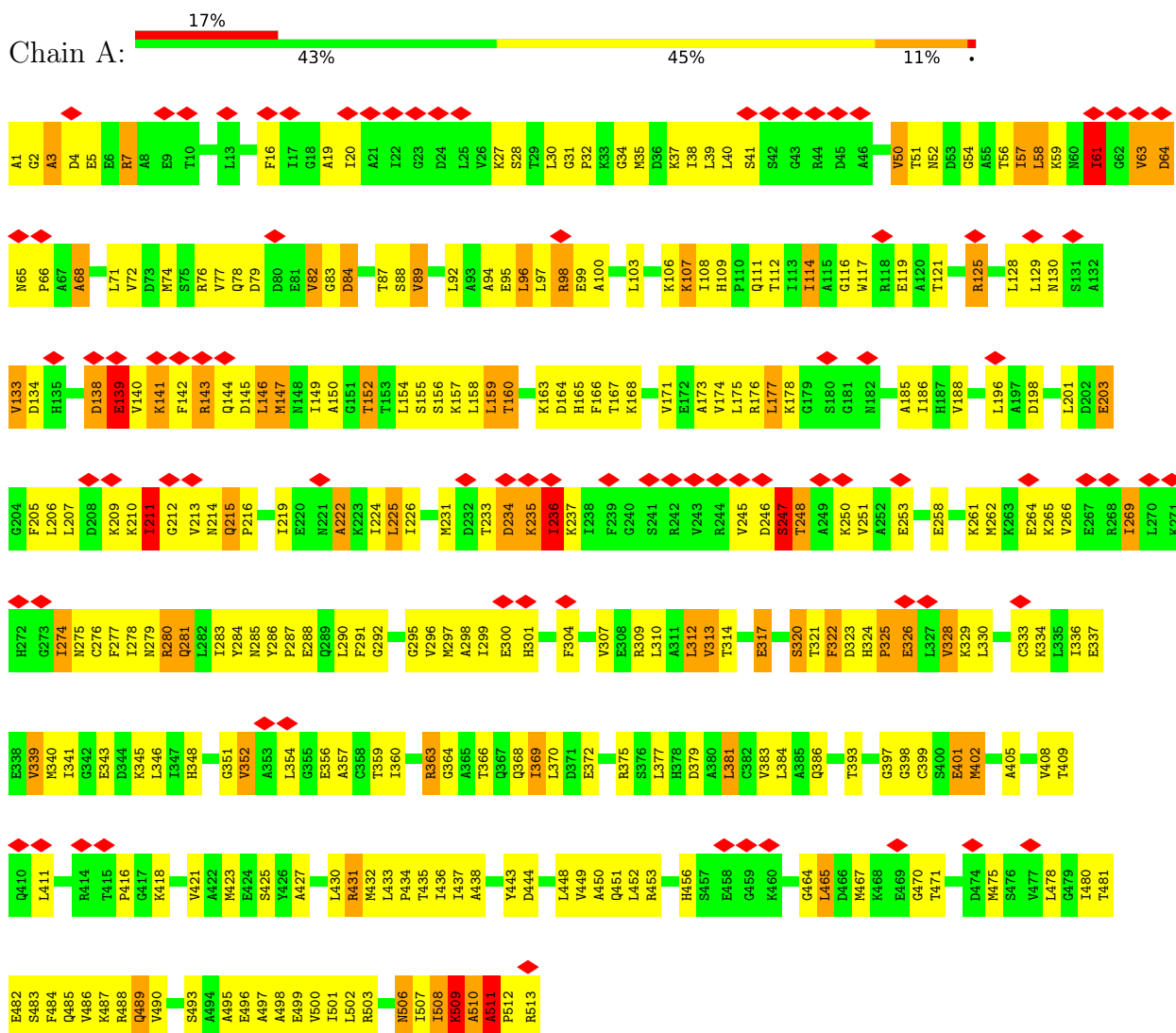
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | B     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | C     | 490      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3673  | 2295 | 645 | 714 | 19 |         |       |
| 1   | D     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | E     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | F     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | G     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | H     | 492      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3693  | 2308 | 649 | 717 | 19 |         |       |
| 1   | I     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | J     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | K     | 491      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3681  | 2299 | 646 | 717 | 19 |         |       |
| 1   | L     | 490      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3676  | 2296 | 645 | 716 | 19 |         |       |
| 1   | M     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |
| 1   | N     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3700  | 2312 | 650 | 719 | 19 |         |       |
| 1   | O     | 490      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3676  | 2296 | 645 | 716 | 19 |         |       |
| 1   | P     | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3855  | 2409 | 679 | 748 | 19 |         |       |

### 3 Residue-property plots

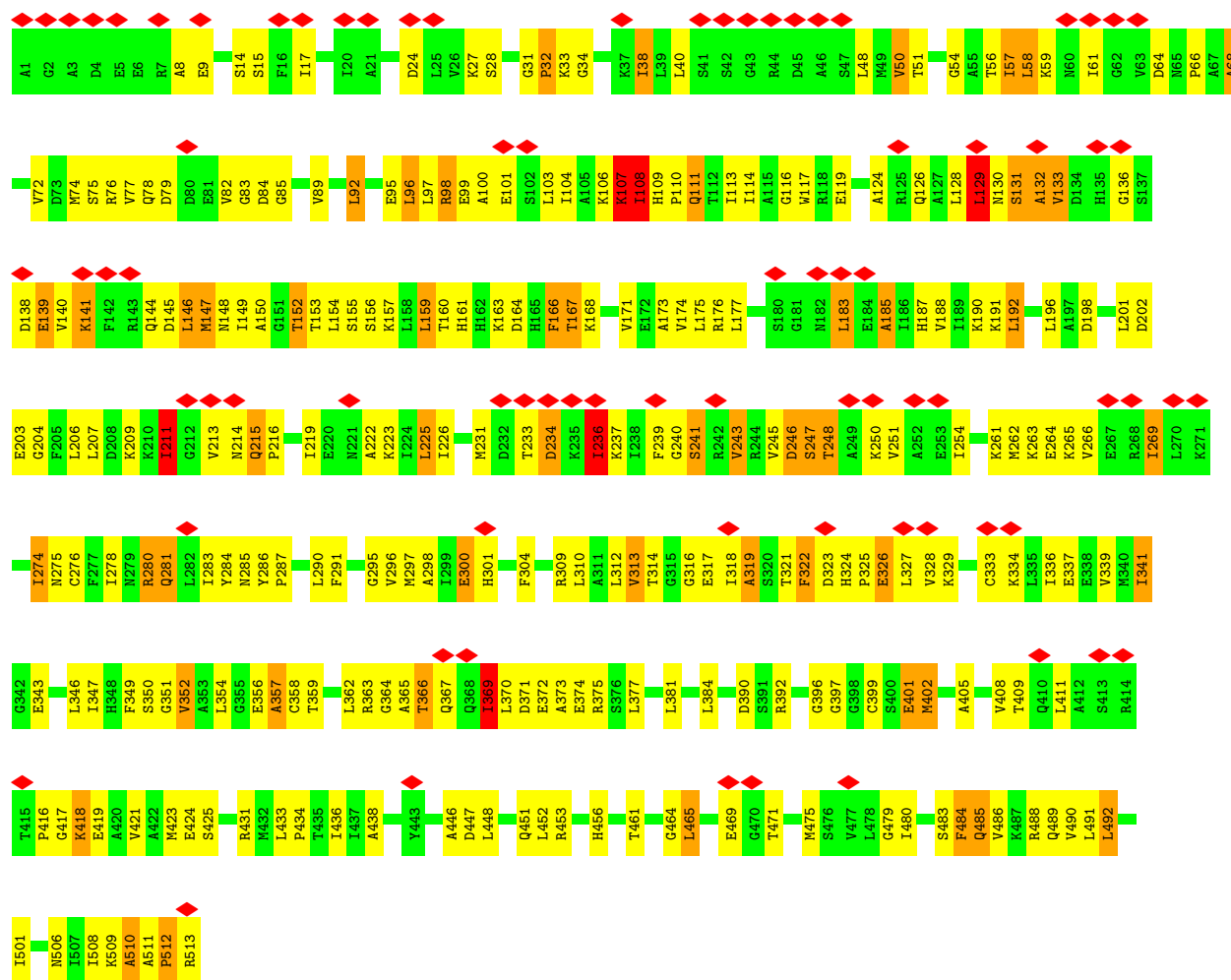
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: T-COMPLEX PROTEIN 1 SUBUNIT BETA

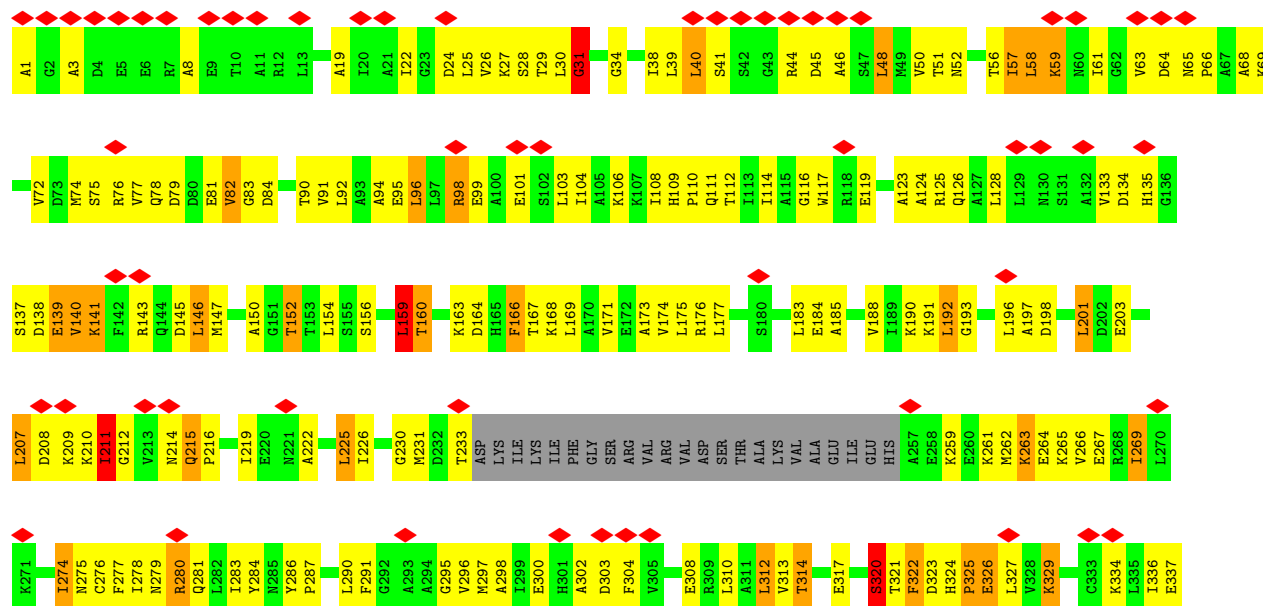
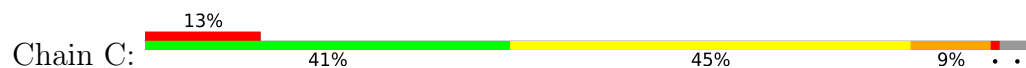


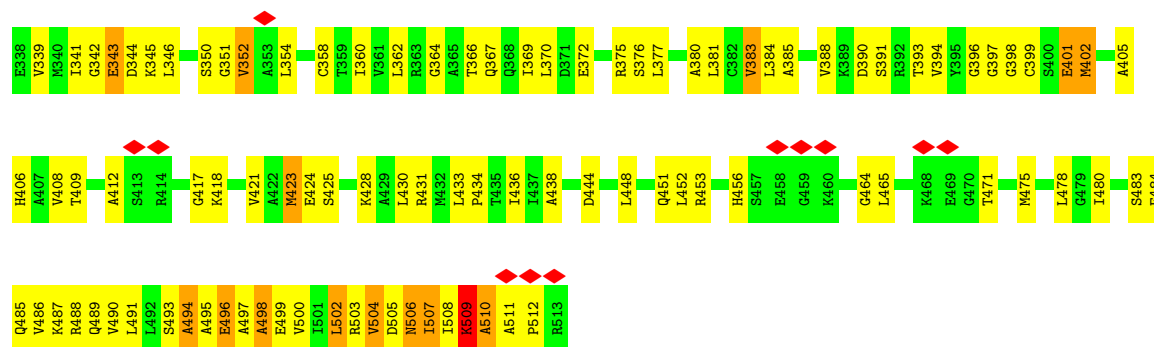
#### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



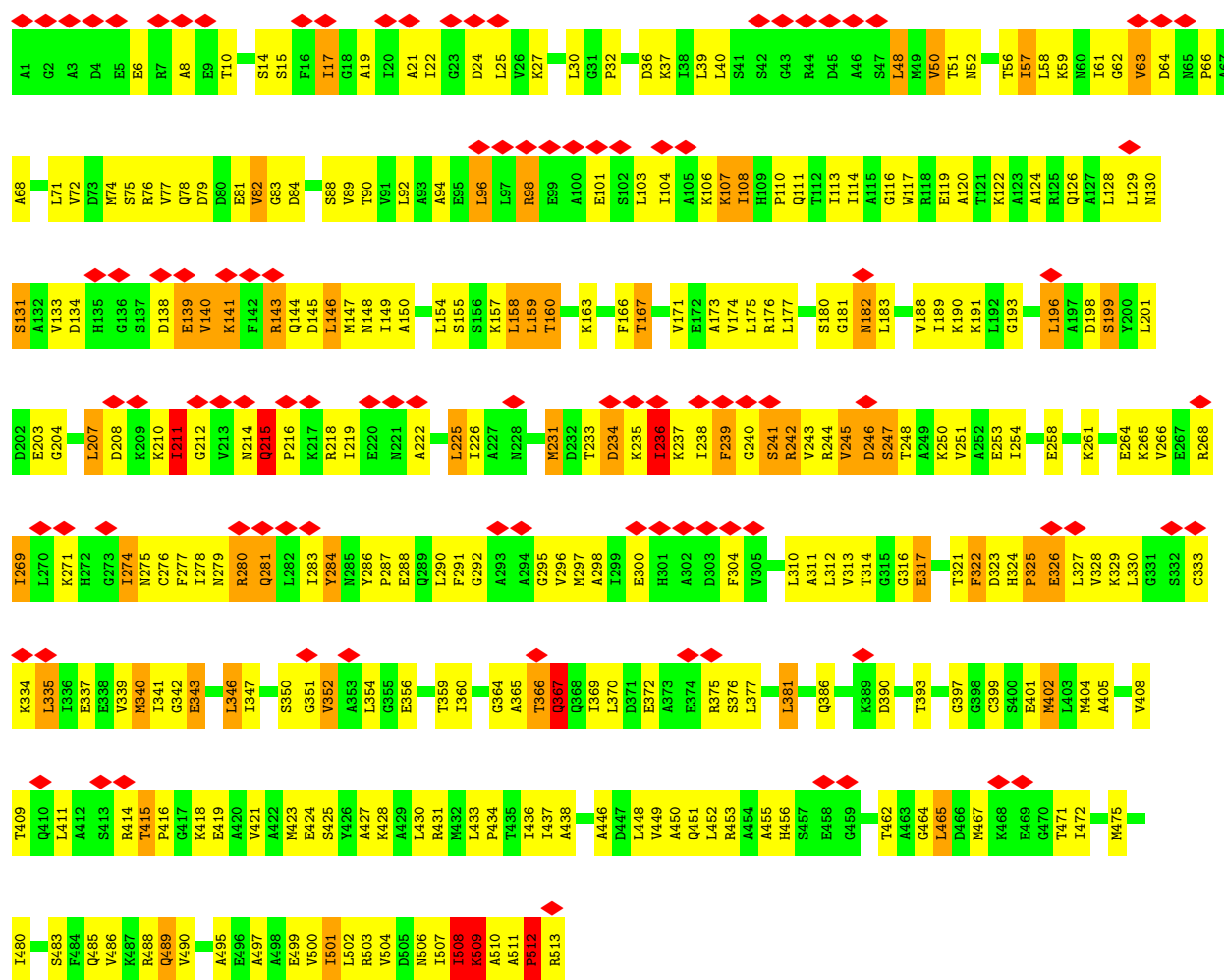
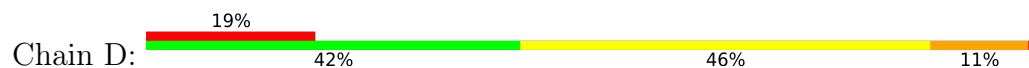


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

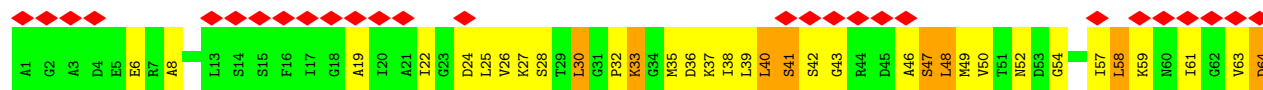
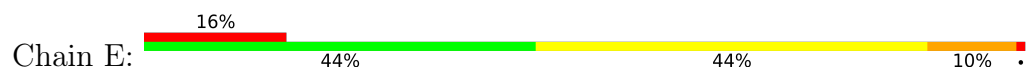


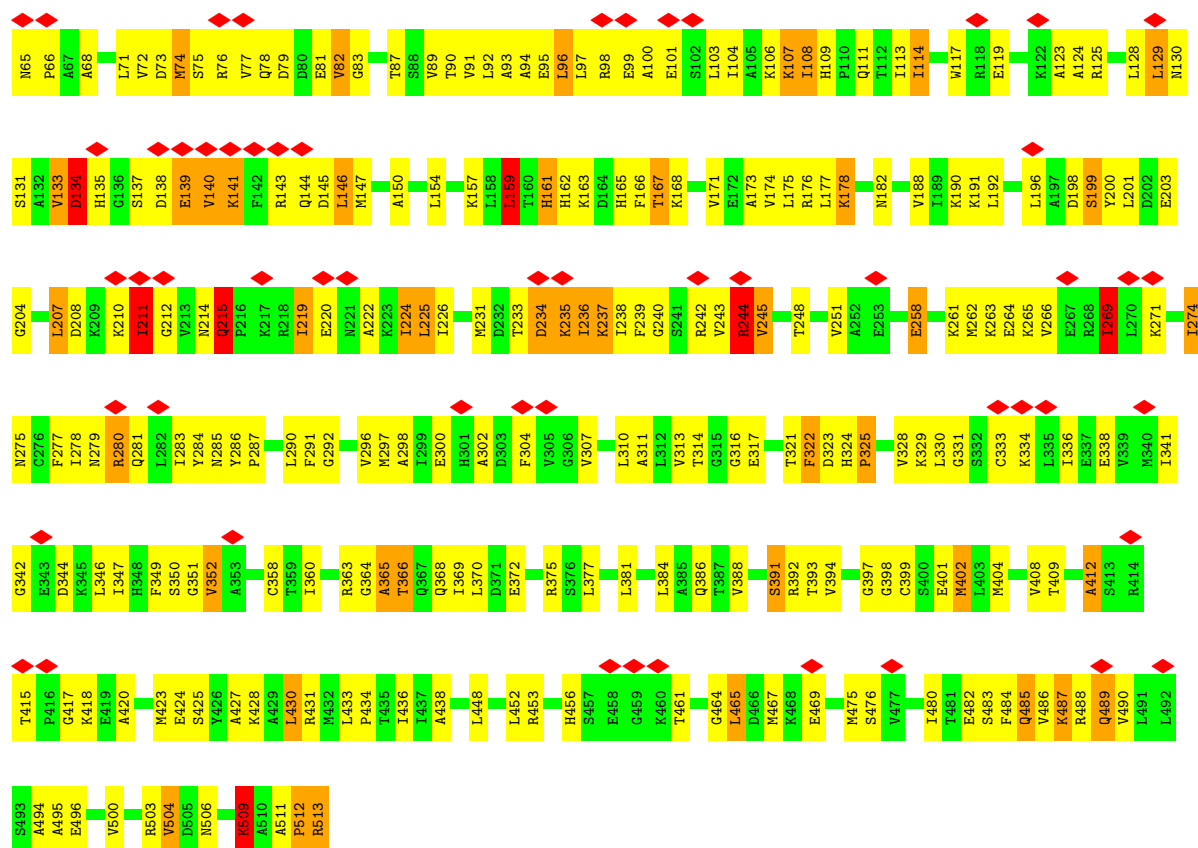


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

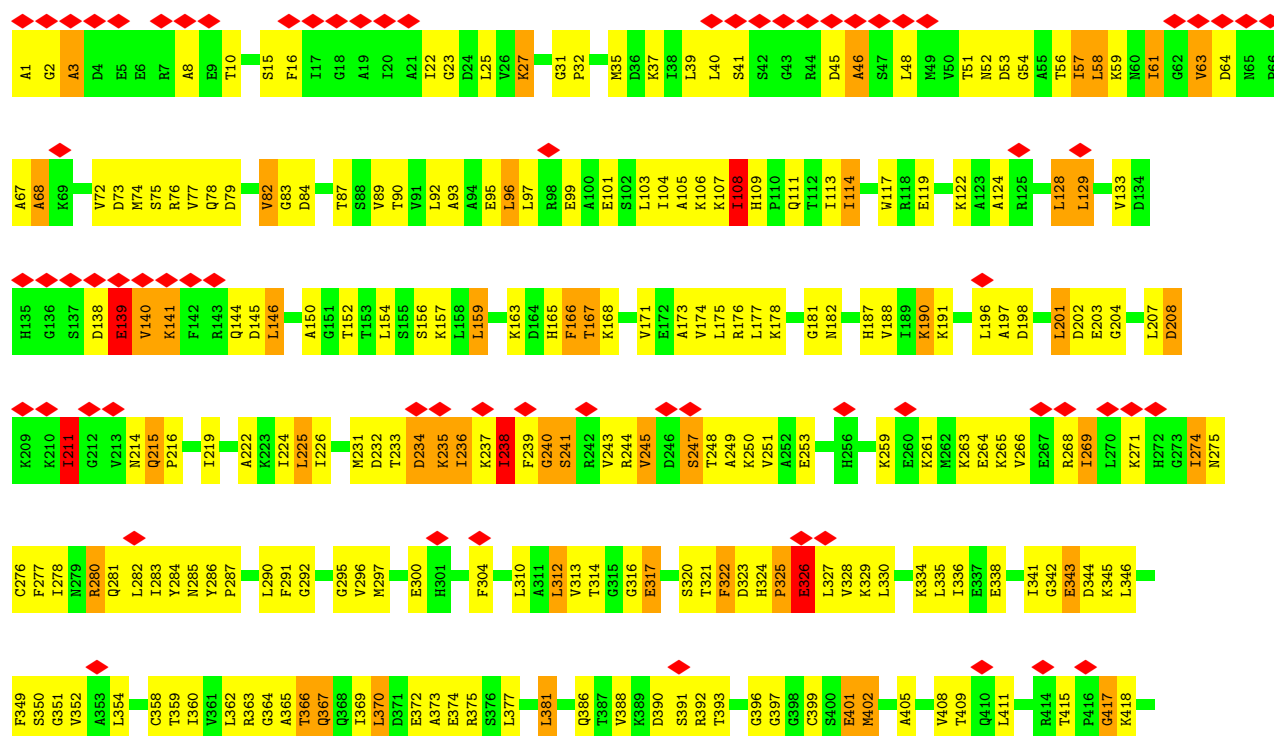
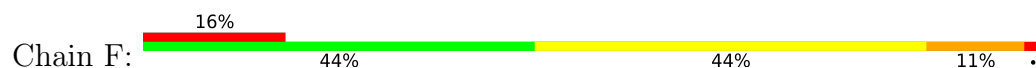


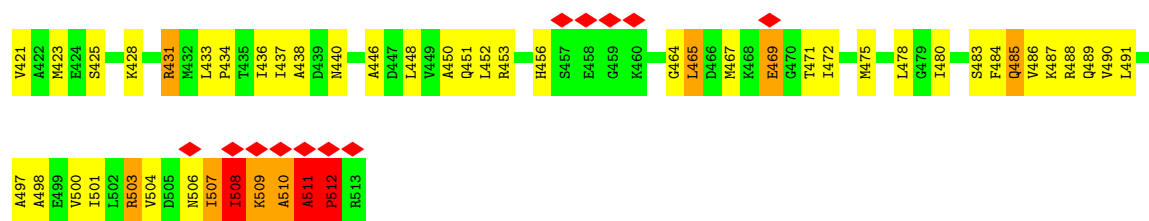
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



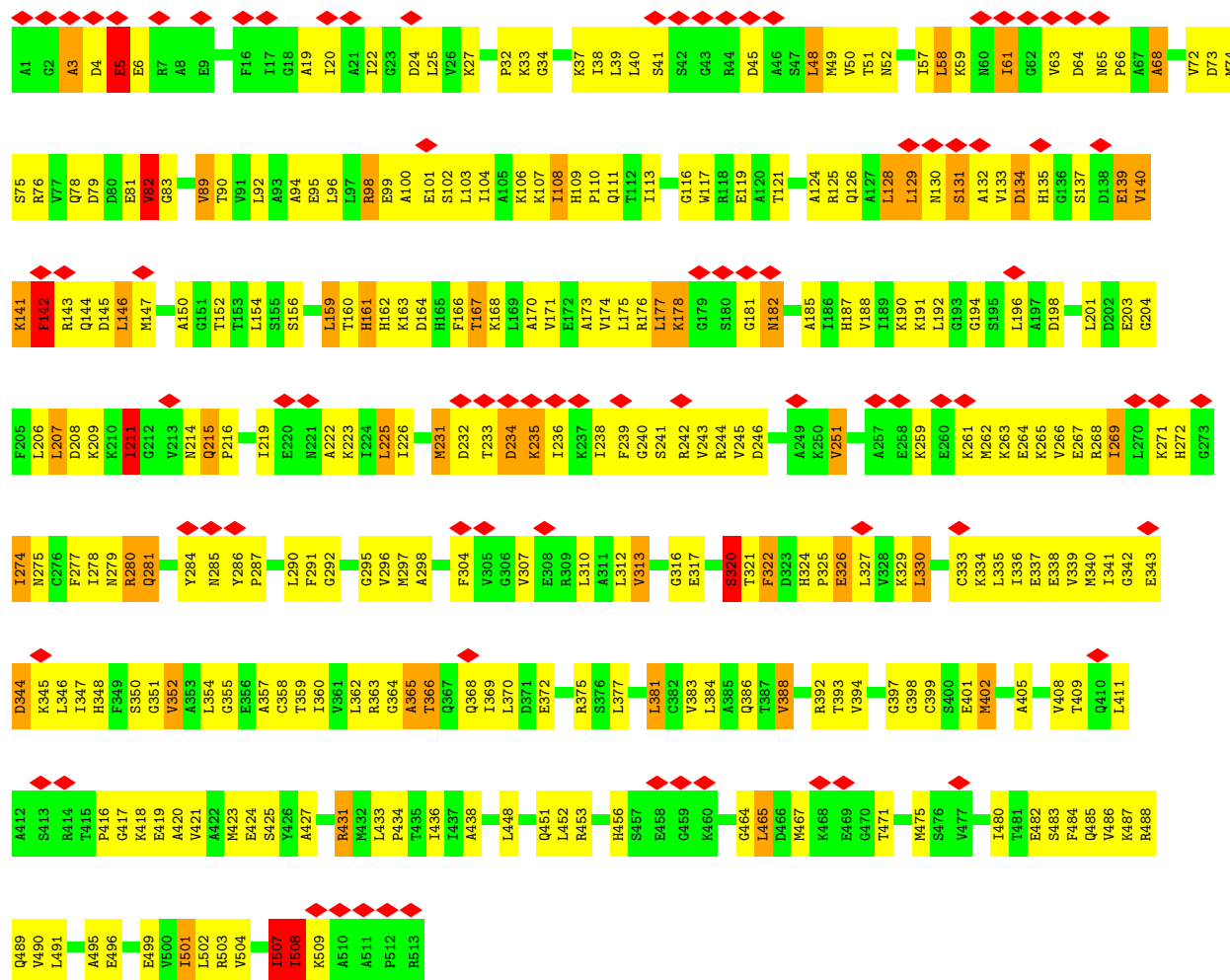
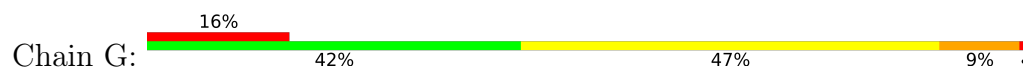


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

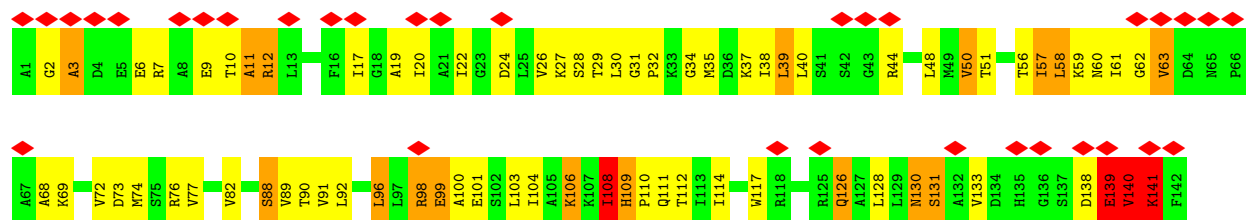
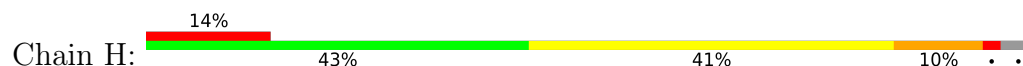


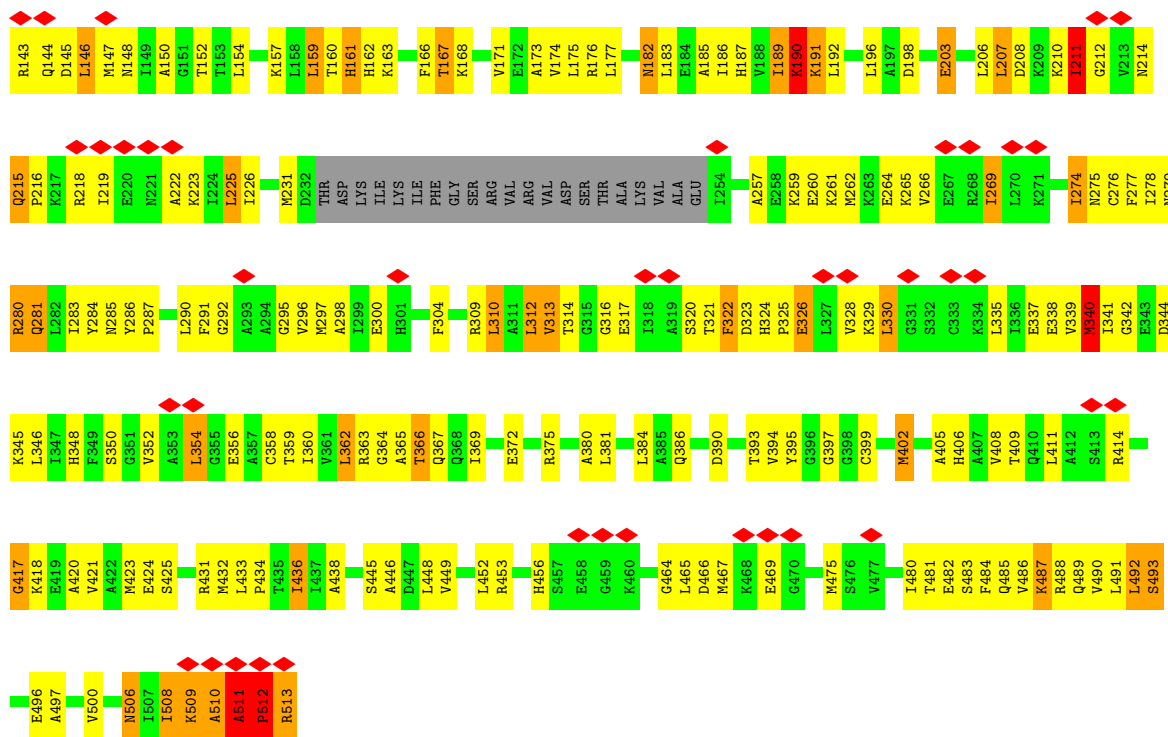


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

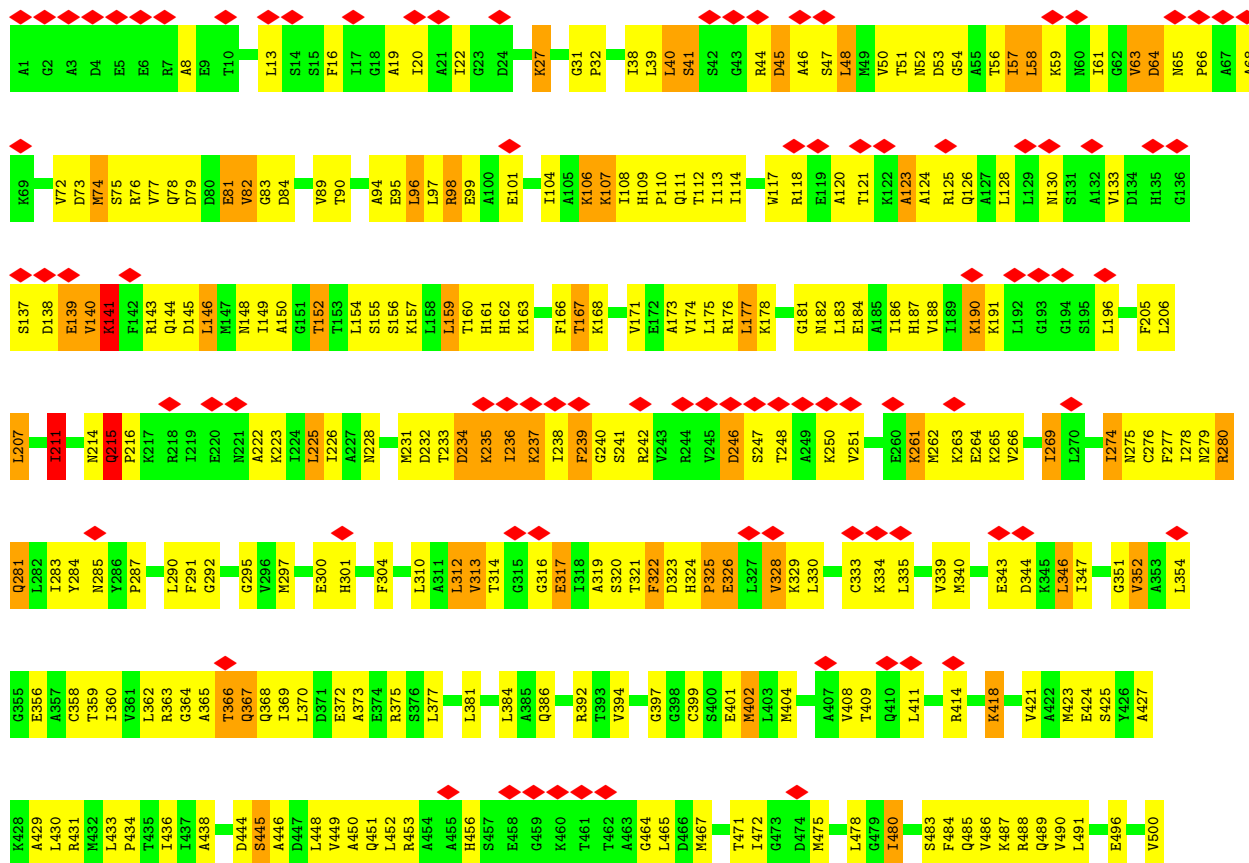
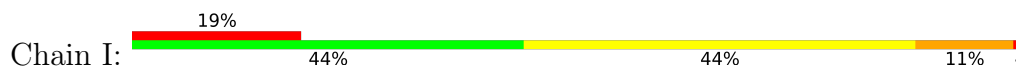


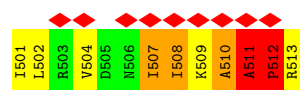
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



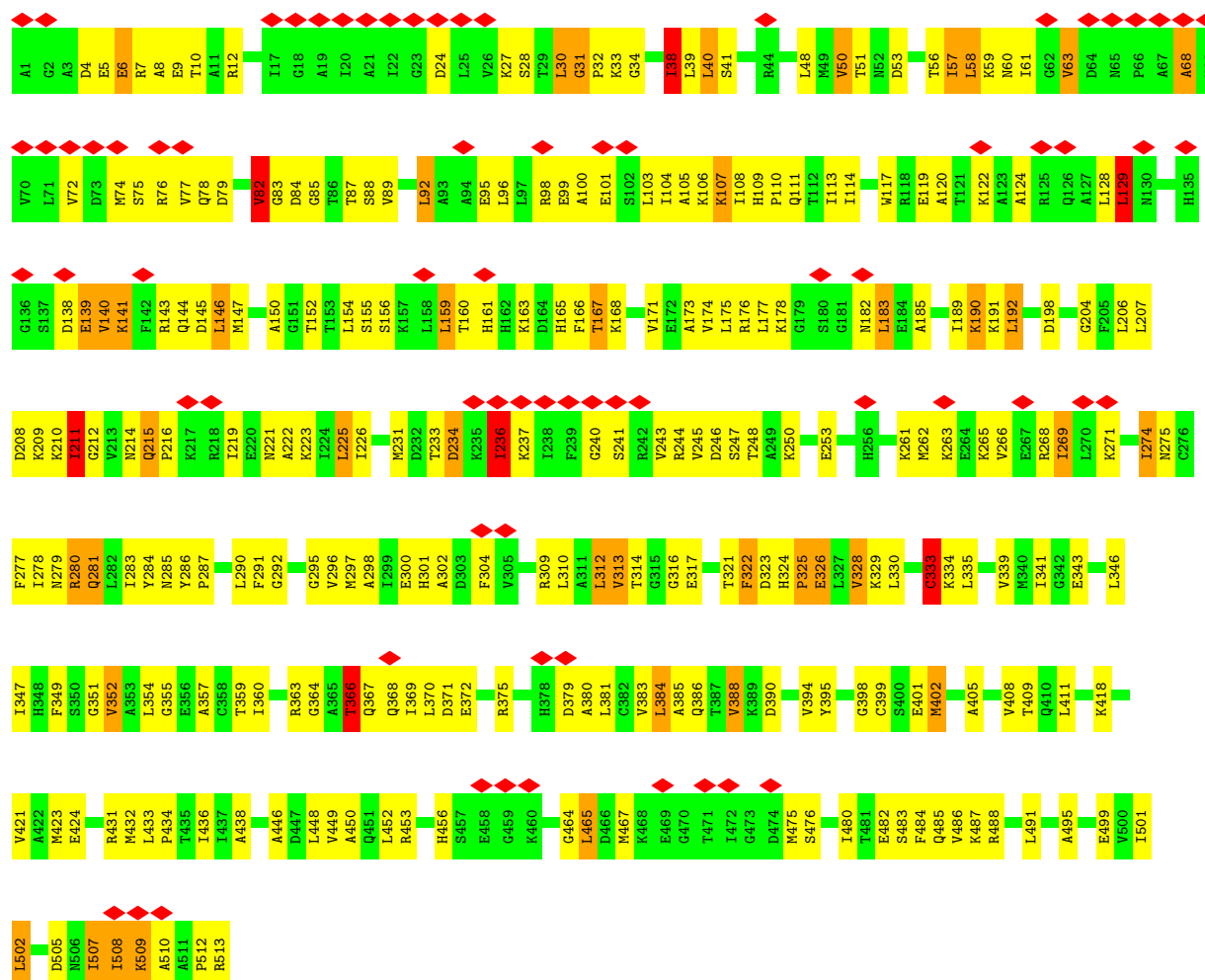


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

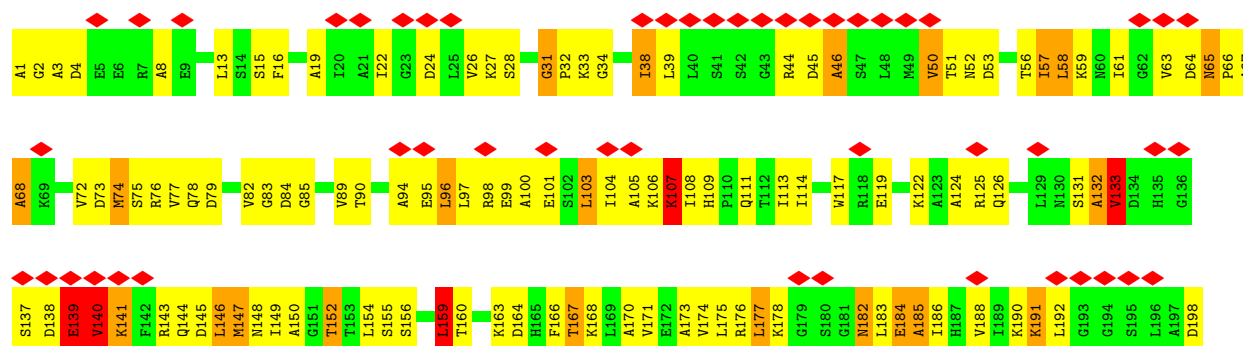




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

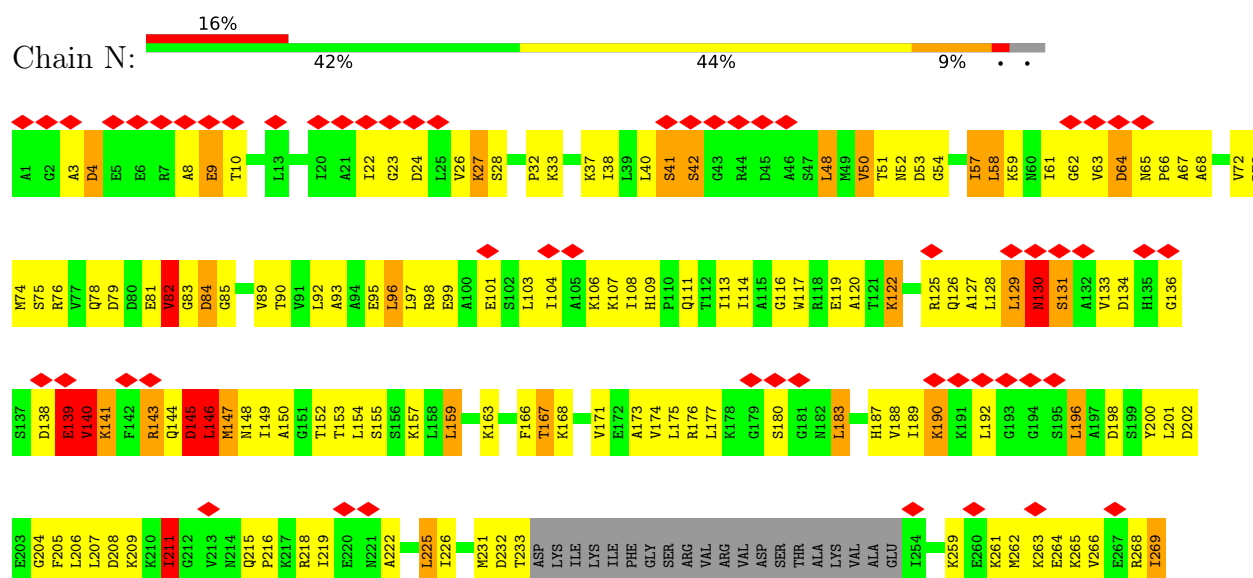


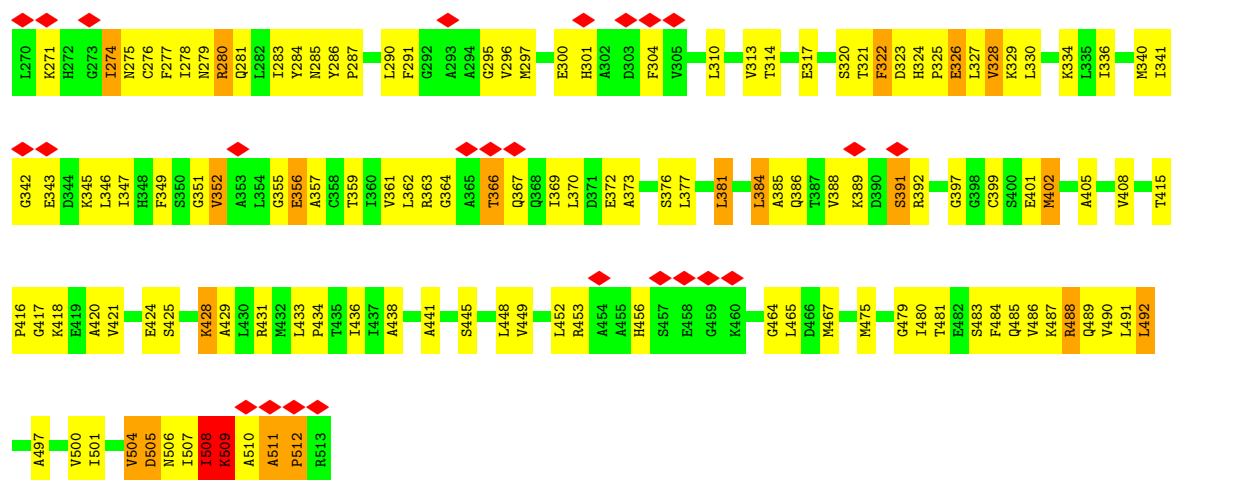


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

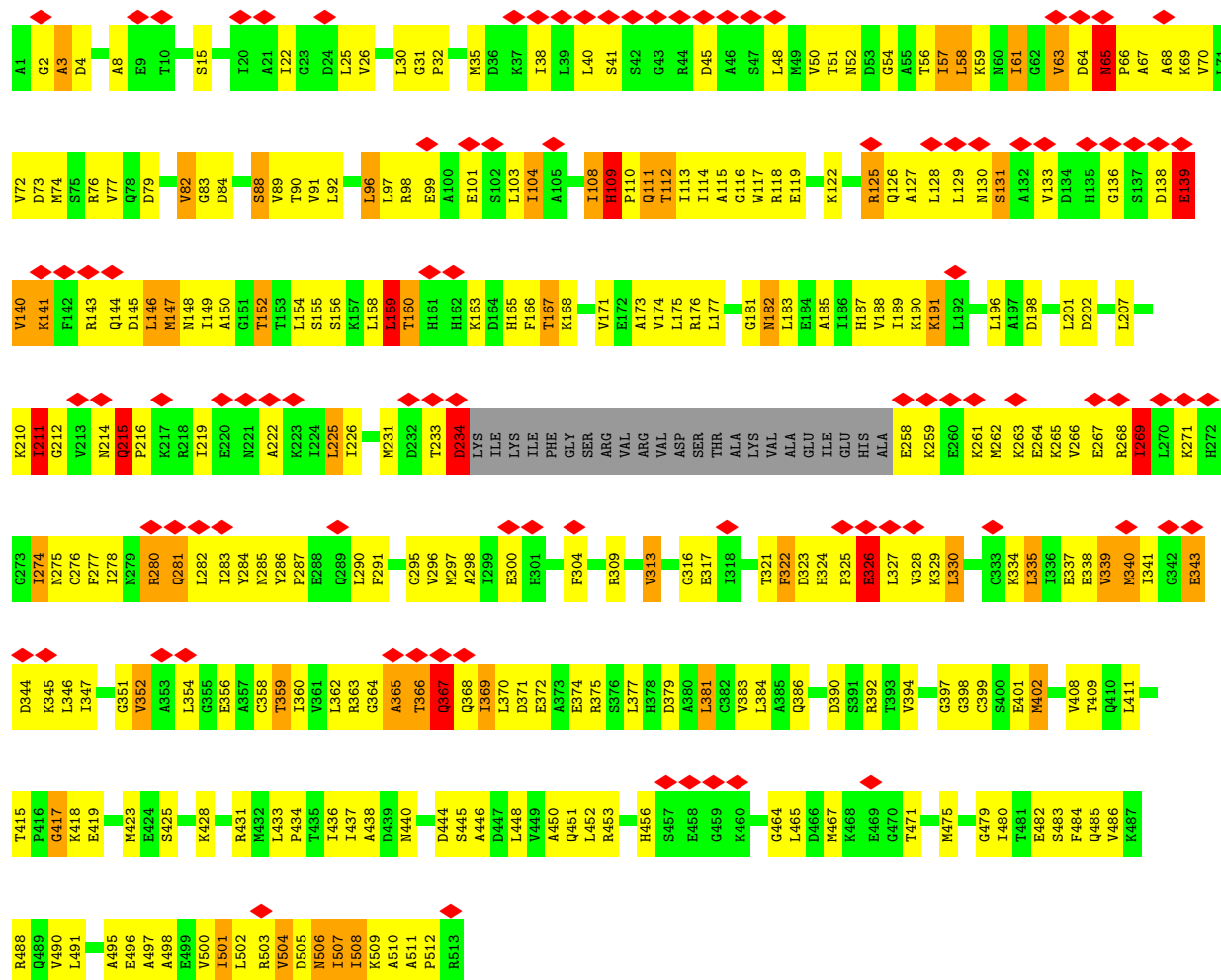


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



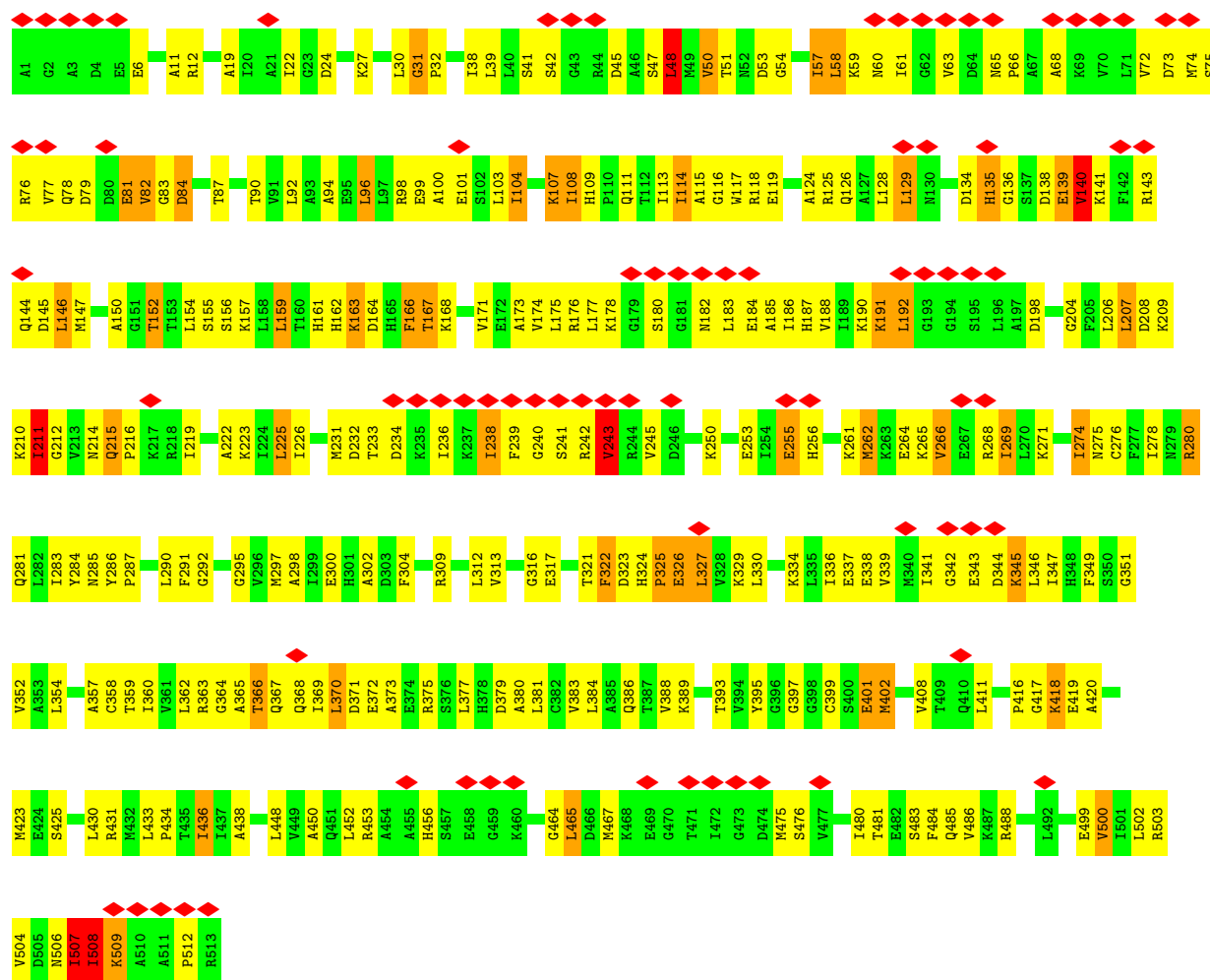


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, C1           | Depositor |
| Number of particles used             | 16495               | Depositor |
| Resolution determination method      | Not provided        |           |
| CTF correction method                | EACH MICROGRAPH     | Depositor |
| Microscope                           | JEOL 3200FSC        | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 18                  | Depositor |
| Minimum defocus (nm)                 | 1200                | Depositor |
| Maximum defocus (nm)                 | 3000                | Depositor |
| Magnification                        | 50000               | Depositor |
| Image detector                       | KODAK SO-163 FILM   | Depositor |
| Maximum map value                    | 1.502               | Depositor |
| Minimum map value                    | -1.026              | Depositor |
| Average map value                    | 0.057               | Depositor |
| Map value standard deviation         | 0.237               | Depositor |
| Recommended contour level            | 1                   | Depositor |
| Map size ( $\text{\AA}$ )            | 345.6, 345.6, 345.6 | wwPDB     |
| Map dimensions                       | 144, 144, 144       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.4, 2.4, 2.4       | 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     | 0.75         | 1/3896 (0.0%)  | 1.20        | 21/5249 (0.4%)   |
| 1   | B     | 0.74         | 0/3896         | 1.22        | 19/5249 (0.4%)   |
| 1   | C     | 0.72         | 0/3711         | 1.19        | 18/5000 (0.4%)   |
| 1   | D     | 0.75         | 0/3896         | 1.20        | 14/5249 (0.3%)   |
| 1   | E     | 0.77         | 0/3896         | 1.23        | 19/5249 (0.4%)   |
| 1   | F     | 0.76         | 0/3896         | 1.23        | 22/5249 (0.4%)   |
| 1   | G     | 0.77         | 0/3896         | 1.25        | 25/5249 (0.5%)   |
| 1   | H     | 0.76         | 0/3732         | 1.21        | 21/5028 (0.4%)   |
| 1   | I     | 0.76         | 1/3896 (0.0%)  | 1.24        | 19/5249 (0.4%)   |
| 1   | J     | 0.75         | 0/3896         | 1.19        | 18/5249 (0.3%)   |
| 1   | K     | 0.73         | 0/3719         | 1.19        | 19/5011 (0.4%)   |
| 1   | L     | 0.76         | 0/3714         | 1.18        | 14/5004 (0.3%)   |
| 1   | M     | 0.77         | 3/3896 (0.1%)  | 1.17        | 13/5249 (0.2%)   |
| 1   | N     | 0.72         | 0/3739         | 1.19        | 10/5038 (0.2%)   |
| 1   | O     | 0.75         | 0/3714         | 1.25        | 26/5004 (0.5%)   |
| 1   | P     | 0.73         | 0/3896         | 1.23        | 20/5249 (0.4%)   |
| All | All   | 0.75         | 5/61289 (0.0%) | 1.21        | 298/82575 (0.4%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | M     | 507 | ILE  | CA-C  | 6.79 | 1.59        | 1.52     |
| 1   | M     | 148 | ASN  | CA-C  | 6.47 | 1.55        | 1.52     |
| 1   | M     | 509 | LYS  | CA-C  | 5.76 | 1.61        | 1.52     |
| 1   | I     | 510 | ALA  | CA-C  | 5.71 | 1.55        | 1.52     |
| 1   | A     | 509 | LYS  | N-CA  | 5.10 | 1.52        | 1.46     |

All (298) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 339 | VAL  | N-CA-C | 10.95 | 121.78      | 110.72   |
| 1   | O     | 505 | ASP  | N-CA-C | 9.52  | 121.26      | 111.07   |
| 1   | D     | 107 | LYS  | N-CA-C | 9.46  | 124.77      | 113.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 512 | PRO  | N-CA-CB | -8.93 | 93.88       | 103.25   |
| 1   | I     | 45  | ASP  | N-CA-C  | -8.62 | 102.34      | 113.12   |
| 1   | N     | 488 | ARG  | CB-CA-C | -8.51 | 97.51       | 110.88   |
| 1   | A     | 235 | LYS  | N-CA-C  | 8.35  | 120.38      | 111.28   |
| 1   | A     | 510 | ALA  | N-CA-C  | 8.23  | 122.89      | 109.72   |
| 1   | B     | 138 | ASP  | N-CA-C  | 8.20  | 120.22      | 111.28   |
| 1   | M     | 63  | VAL  | N-CA-C  | 8.10  | 118.88      | 110.62   |
| 1   | F     | 511 | ALA  | CA-C-N  | 7.97  | 129.80      | 119.84   |
| 1   | F     | 511 | ALA  | C-N-CA  | 7.97  | 129.80      | 119.84   |
| 1   | E     | 63  | VAL  | N-CA-C  | 7.95  | 118.75      | 110.72   |
| 1   | J     | 508 | ILE  | N-CA-C  | 7.93  | 119.22      | 108.11   |
| 1   | H     | 7   | ARG  | N-CA-C  | 7.87  | 119.86      | 111.28   |
| 1   | B     | 239 | PHE  | N-CA-C  | 7.81  | 119.87      | 111.36   |
| 1   | A     | 138 | ASP  | N-CA-C  | 7.77  | 119.75      | 111.28   |
| 1   | B     | 269 | ILE  | N-CA-C  | 7.73  | 117.84      | 110.42   |
| 1   | N     | 63  | VAL  | N-CA-C  | 7.72  | 118.49      | 110.62   |
| 1   | M     | 243 | VAL  | N-CA-C  | 7.70  | 119.94      | 108.46   |
| 1   | L     | 63  | VAL  | N-CA-C  | 7.67  | 117.79      | 110.42   |
| 1   | C     | 211 | ILE  | CB-CA-C | -7.67 | 102.15      | 111.97   |
| 1   | I     | 269 | ILE  | N-CA-C  | 7.62  | 117.73      | 110.42   |
| 1   | H     | 339 | VAL  | N-CA-C  | 7.61  | 118.83      | 108.17   |
| 1   | D     | 243 | VAL  | N-CA-C  | 7.58  | 117.70      | 110.42   |
| 1   | N     | 504 | VAL  | N-CA-C  | 7.58  | 117.70      | 110.42   |
| 1   | O     | 136 | GLY  | N-CA-C  | 7.54  | 117.08      | 110.21   |
| 1   | F     | 243 | VAL  | N-CA-C  | 7.52  | 120.43      | 108.85   |
| 1   | E     | 240 | GLY  | N-CA-C  | -7.51 | 105.37      | 115.36   |
| 1   | F     | 84  | ASP  | N-CA-C  | 7.50  | 119.53      | 111.36   |
| 1   | H     | 63  | VAL  | N-CA-C  | 7.47  | 118.24      | 110.62   |
| 1   | P     | 236 | ILE  | N-CA-C  | 7.43  | 118.20      | 110.62   |
| 1   | E     | 243 | VAL  | N-CA-C  | 7.43  | 118.57      | 108.17   |
| 1   | G     | 508 | ILE  | N-CA-C  | 7.39  | 124.72      | 109.34   |
| 1   | I     | 63  | VAL  | N-CA-C  | 7.37  | 118.14      | 110.62   |
| 1   | C     | 63  | VAL  | N-CA-C  | 7.36  | 118.13      | 110.62   |
| 1   | J     | 63  | VAL  | N-CA-C  | 7.36  | 118.12      | 110.62   |
| 1   | A     | 63  | VAL  | N-CA-C  | 7.35  | 118.11      | 110.62   |
| 1   | F     | 509 | LYS  | N-CA-C  | 7.32  | 119.87      | 108.96   |
| 1   | A     | 147 | MET  | N-CA-CB | -7.30 | 101.11      | 112.13   |
| 1   | G     | 243 | VAL  | N-CA-C  | 7.28  | 118.36      | 108.17   |
| 1   | P     | 508 | ILE  | CB-CA-C | -7.27 | 99.37       | 111.29   |
| 1   | P     | 63  | VAL  | N-CA-C  | 7.24  | 118.00      | 110.62   |
| 1   | C     | 61  | ILE  | N-CA-C  | 7.21  | 118.50      | 108.12   |
| 1   | K     | 61  | ILE  | N-CA-C  | 7.18  | 118.46      | 108.12   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | J     | 243 | VAL  | N-CA-C   | 7.14  | 118.17      | 108.17   |
| 1   | F     | 63  | VAL  | N-CA-C   | 7.14  | 117.93      | 110.72   |
| 1   | D     | 240 | GLY  | N-CA-C   | -7.13 | 105.39      | 115.30   |
| 1   | O     | 506 | ASN  | N-CA-C   | 7.06  | 118.98      | 111.28   |
| 1   | E     | 333 | CYS  | N-CA-C   | 7.05  | 120.15      | 110.06   |
| 1   | G     | 6   | GLU  | N-CA-C   | 7.04  | 120.72      | 109.24   |
| 1   | C     | 376 | SER  | N-CA-C   | 7.01  | 118.58      | 111.07   |
| 1   | E     | 239 | PHE  | N-CA-C   | 7.01  | 118.92      | 111.28   |
| 1   | N     | 84  | ASP  | N-CA-C   | 7.00  | 118.70      | 111.14   |
| 1   | M     | 269 | ILE  | N-CA-C   | 6.99  | 117.13      | 110.42   |
| 1   | D     | 235 | LYS  | N-CA-C   | 6.98  | 118.89      | 111.28   |
| 1   | D     | 340 | MET  | CB-CA-C  | -6.95 | 102.92      | 111.82   |
| 1   | L     | 61  | ILE  | N-CA-C   | 6.95  | 118.13      | 108.12   |
| 1   | J     | 61  | ILE  | N-CA-C   | 6.93  | 118.09      | 108.12   |
| 1   | F     | 107 | LYS  | N-CA-C   | 6.92  | 120.96      | 111.54   |
| 1   | O     | 445 | SER  | N-CA-C   | 6.88  | 118.77      | 111.28   |
| 1   | E     | 368 | GLN  | N-CA-C   | -6.87 | 103.79      | 111.28   |
| 1   | B     | 240 | GLY  | N-CA-C   | -6.86 | 105.77      | 115.30   |
| 1   | F     | 235 | LYS  | N-CA-C   | 6.81  | 118.59      | 111.03   |
| 1   | G     | 142 | PHE  | N-CA-C   | 6.81  | 118.36      | 111.07   |
| 1   | G     | 211 | ILE  | CB-CA-C  | -6.76 | 103.32      | 111.97   |
| 1   | O     | 367 | GLN  | N-CA-C   | 6.74  | 116.76      | 107.73   |
| 1   | K     | 383 | VAL  | N-CA-C   | 6.74  | 116.89      | 110.42   |
| 1   | C     | 494 | ALA  | N-CA-C   | -6.74 | 105.03      | 113.18   |
| 1   | L     | 511 | ALA  | CA-C-N   | 6.71  | 126.97      | 119.32   |
| 1   | L     | 511 | ALA  | C-N-CA   | 6.71  | 126.97      | 119.32   |
| 1   | O     | 285 | ASN  | N-CA-C   | 6.71  | 118.59      | 111.28   |
| 1   | H     | 269 | ILE  | N-CA-C   | 6.65  | 116.80      | 110.42   |
| 1   | J     | 240 | GLY  | N-CA-C   | -6.64 | 106.07      | 115.30   |
| 1   | F     | 211 | ILE  | CB-CA-C  | -6.62 | 103.49      | 111.97   |
| 1   | P     | 508 | ILE  | N-CA-C   | 6.59  | 123.04      | 109.34   |
| 1   | O     | 365 | ALA  | N-CA-C   | 6.55  | 118.08      | 111.07   |
| 1   | P     | 61  | ILE  | N-CA-C   | 6.55  | 117.55      | 108.12   |
| 1   | C     | 193 | GLY  | N-CA-C   | 6.54  | 119.99      | 110.63   |
| 1   | F     | 166 | PHE  | CA-CB-CG | 6.54  | 120.34      | 113.80   |
| 1   | G     | 235 | LYS  | N-CA-C   | 6.53  | 119.39      | 111.82   |
| 1   | C     | 498 | ALA  | N-CA-C   | -6.52 | 104.17      | 111.28   |
| 1   | N     | 145 | ASP  | N-CA-C   | -6.51 | 104.19      | 111.28   |
| 1   | H     | 354 | LEU  | N-CA-C   | 6.51  | 118.03      | 111.07   |
| 1   | L     | 512 | PRO  | N-CA-C   | 6.49  | 123.42      | 113.75   |
| 1   | I     | 61  | ILE  | N-CA-C   | 6.46  | 117.43      | 108.12   |
| 1   | P     | 507 | ILE  | N-CA-C   | 6.46  | 119.62      | 108.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 504 | VAL  | N-CA-C   | 6.42  | 117.37      | 108.89   |
| 1   | I     | 44  | ARG  | N-CA-C   | 6.40  | 120.38      | 111.74   |
| 1   | B     | 161 | HIS  | N-CA-C   | -6.38 | 104.55      | 112.72   |
| 1   | B     | 243 | VAL  | N-CA-C   | 6.38  | 117.05      | 107.80   |
| 1   | B     | 61  | ILE  | N-CA-C   | 6.38  | 117.30      | 108.12   |
| 1   | G     | 507 | ILE  | CA-C-N   | 6.37  | 133.44      | 121.97   |
| 1   | G     | 507 | ILE  | C-N-CA   | 6.37  | 133.44      | 121.97   |
| 1   | O     | 61  | ILE  | N-CA-C   | 6.37  | 117.95      | 108.46   |
| 1   | D     | 63  | VAL  | N-CA-C   | 6.36  | 116.52      | 110.42   |
| 1   | G     | 368 | GLN  | N-CA-C   | -6.36 | 104.35      | 111.28   |
| 1   | E     | 285 | ASN  | N-CA-C   | 6.31  | 118.16      | 111.28   |
| 1   | H     | 109 | HIS  | CA-C-N   | 6.30  | 126.50      | 119.32   |
| 1   | H     | 109 | HIS  | C-N-CA   | 6.30  | 126.50      | 119.32   |
| 1   | O     | 211 | ILE  | CB-CA-C  | -6.29 | 103.92      | 111.97   |
| 1   | H     | 506 | ASN  | CA-CB-CG | 6.28  | 118.88      | 112.60   |
| 1   | E     | 211 | ILE  | CB-CA-C  | -6.26 | 103.95      | 111.97   |
| 1   | A     | 211 | ILE  | CB-CA-C  | -6.25 | 103.97      | 111.97   |
| 1   | O     | 269 | ILE  | N-CA-C   | 6.22  | 116.39      | 110.42   |
| 1   | K     | 511 | ALA  | CA-C-N   | 6.22  | 127.61      | 119.84   |
| 1   | K     | 511 | ALA  | C-N-CA   | 6.22  | 127.61      | 119.84   |
| 1   | I     | 445 | SER  | N-CA-C   | 6.21  | 118.05      | 111.28   |
| 1   | F     | 61  | ILE  | N-CA-C   | 6.21  | 117.06      | 108.12   |
| 1   | J     | 161 | HIS  | N-CA-C   | -6.20 | 105.62      | 113.43   |
| 1   | K     | 285 | ASN  | N-CA-C   | 6.16  | 117.99      | 111.28   |
| 1   | O     | 313 | VAL  | N-CA-C   | 6.16  | 116.33      | 110.42   |
| 1   | B     | 313 | VAL  | N-CA-C   | 6.13  | 116.31      | 110.42   |
| 1   | F     | 240 | GLY  | N-CA-C   | -6.13 | 106.62      | 115.27   |
| 1   | D     | 211 | ILE  | CB-CA-C  | -6.13 | 104.12      | 111.97   |
| 1   | H     | 285 | ASN  | N-CA-C   | 6.12  | 117.96      | 111.28   |
| 1   | D     | 242 | ARG  | N-CA-CB  | -6.11 | 100.16      | 110.49   |
| 1   | G     | 63  | VAL  | N-CA-C   | 6.10  | 116.84      | 110.62   |
| 1   | L     | 211 | ILE  | CB-CA-C  | -6.08 | 104.19      | 111.97   |
| 1   | O     | 211 | ILE  | N-CA-CB  | 6.08  | 117.66      | 110.55   |
| 1   | C     | 211 | ILE  | N-CA-CB  | 6.08  | 117.66      | 110.55   |
| 1   | B     | 147 | MET  | N-CA-CB  | -6.06 | 102.98      | 112.13   |
| 1   | B     | 285 | ASN  | N-CA-C   | 6.06  | 117.88      | 111.28   |
| 1   | C     | 327 | LEU  | N-CA-C   | 6.05  | 117.87      | 111.28   |
| 1   | N     | 130 | ASN  | CA-CB-CG | 6.04  | 118.64      | 112.60   |
| 1   | N     | 285 | ASN  | N-CA-C   | 6.03  | 117.85      | 111.28   |
| 1   | C     | 509 | LYS  | N-CA-C   | 6.02  | 123.61      | 110.80   |
| 1   | G     | 161 | HIS  | N-CA-C   | -5.99 | 105.22      | 113.18   |
| 1   | B     | 211 | ILE  | CB-CA-C  | -5.97 | 104.08      | 112.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | M     | 280 | ARG  | CB-CA-C   | -5.97 | 103.46      | 111.88   |
| 1   | P     | 285 | ASN  | N-CA-C    | 5.96  | 117.77      | 111.28   |
| 1   | O     | 234 | ASP  | CA-CB-CG  | 5.95  | 118.55      | 112.60   |
| 1   | F     | 285 | ASN  | N-CA-C    | 5.91  | 117.72      | 111.28   |
| 1   | H     | 211 | ILE  | CB-CA-C   | -5.91 | 104.41      | 111.97   |
| 1   | E     | 235 | LYS  | N-CA-C    | 5.88  | 118.64      | 111.82   |
| 1   | A     | 61  | ILE  | N-CA-C    | 5.87  | 118.64      | 108.95   |
| 1   | J     | 313 | VAL  | N-CA-C    | 5.87  | 116.06      | 110.42   |
| 1   | J     | 333 | CYS  | N-CA-C    | 5.87  | 118.87      | 107.71   |
| 1   | C     | 211 | ILE  | CA-CB-CG1 | 5.87  | 120.38      | 110.40   |
| 1   | G     | 240 | GLY  | N-CA-C    | -5.87 | 107.14      | 115.30   |
| 1   | N     | 211 | ILE  | CB-CA-C   | -5.87 | 104.46      | 111.97   |
| 1   | G     | 333 | CYS  | N-CA-C    | 5.86  | 117.96      | 108.41   |
| 1   | P     | 42  | SER  | N-CA-C    | 5.85  | 117.46      | 111.14   |
| 1   | H     | 487 | LYS  | N-CA-C    | 5.84  | 117.73      | 111.36   |
| 1   | J     | 507 | ILE  | N-CA-C    | 5.84  | 121.06      | 113.07   |
| 1   | E     | 269 | ILE  | N-CA-C    | 5.83  | 116.01      | 110.42   |
| 1   | O     | 63  | VAL  | N-CA-C    | 5.82  | 116.56      | 110.62   |
| 1   | A     | 508 | ILE  | CA-C-O    | -5.82 | 115.00      | 121.17   |
| 1   | M     | 48  | LEU  | N-CA-C    | 5.82  | 118.59      | 108.76   |
| 1   | A     | 444 | ASP  | CA-CB-CG  | 5.81  | 118.41      | 112.60   |
| 1   | A     | 511 | ALA  | N-CA-C    | 5.81  | 122.65      | 109.81   |
| 1   | O     | 503 | ARG  | N-CA-C    | 5.81  | 118.56      | 111.82   |
| 1   | L     | 383 | VAL  | N-CA-C    | 5.81  | 116.58      | 110.72   |
| 1   | A     | 285 | ASN  | N-CA-C    | 5.80  | 117.60      | 111.28   |
| 1   | K     | 63  | VAL  | N-CA-C    | 5.78  | 116.51      | 110.62   |
| 1   | K     | 133 | VAL  | N-CA-C    | 5.78  | 121.35      | 109.34   |
| 1   | L     | 285 | ASN  | N-CA-C    | 5.78  | 117.58      | 111.28   |
| 1   | C     | 31  | GLY  | CA-C-N    | 5.77  | 125.90      | 119.32   |
| 1   | C     | 31  | GLY  | C-N-CA    | 5.77  | 125.90      | 119.32   |
| 1   | J     | 107 | LYS  | N-CA-CB   | -5.77 | 103.69      | 112.28   |
| 1   | I     | 285 | ASN  | N-CA-C    | 5.76  | 117.56      | 111.28   |
| 1   | G     | 61  | ILE  | N-CA-C    | 5.76  | 116.42      | 108.12   |
| 1   | M     | 285 | ASN  | N-CA-C    | 5.76  | 117.56      | 111.28   |
| 1   | C     | 510 | ALA  | N-CA-C    | 5.76  | 118.68      | 110.10   |
| 1   | H     | 29  | THR  | N-CA-C    | 5.74  | 117.54      | 111.28   |
| 1   | M     | 64  | ASP  | N-CA-C    | 5.71  | 117.47      | 108.96   |
| 1   | J     | 38  | ILE  | N-CA-C    | 5.70  | 115.93      | 110.74   |
| 1   | I     | 235 | LYS  | N-CA-C    | 5.67  | 117.32      | 111.03   |
| 1   | H     | 511 | ALA  | CA-C-N    | 5.67  | 126.92      | 119.84   |
| 1   | H     | 511 | ALA  | C-N-CA    | 5.67  | 126.92      | 119.84   |
| 1   | I     | 239 | PHE  | N-CA-C    | 5.66  | 117.45      | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 333 | CYS  | N-CA-C    | 5.65  | 118.11      | 110.88   |
| 1   | P     | 266 | VAL  | N-CA-C    | 5.64  | 116.29      | 110.82   |
| 1   | E     | 64  | ASP  | N-CA-C    | 5.63  | 117.53      | 109.14   |
| 1   | F     | 507 | ILE  | N-CA-C    | 5.63  | 121.05      | 109.34   |
| 1   | K     | 149 | ILE  | N-CA-C    | 5.63  | 116.36      | 110.62   |
| 1   | J     | 60  | ASN  | N-CA-C    | 5.62  | 117.41      | 111.28   |
| 1   | K     | 414 | ARG  | N-CA-C    | 5.62  | 117.41      | 111.28   |
| 1   | A     | 333 | CYS  | N-CA-C    | 5.62  | 118.08      | 110.88   |
| 1   | F     | 503 | ARG  | N-CA-C    | 5.59  | 118.31      | 111.82   |
| 1   | M     | 509 | LYS  | N-CA-CB   | -5.59 | 103.62      | 112.63   |
| 1   | B     | 510 | ALA  | N-CA-C    | 5.58  | 116.74      | 108.60   |
| 1   | L     | 327 | LEU  | N-CA-C    | 5.57  | 117.36      | 111.28   |
| 1   | F     | 64  | ASP  | N-CA-C    | 5.57  | 117.44      | 109.14   |
| 1   | N     | 147 | MET  | N-CA-C    | -5.57 | 106.07      | 112.86   |
| 1   | G     | 484 | PHE  | N-CA-C    | 5.56  | 117.34      | 111.28   |
| 1   | G     | 82  | VAL  | N-CA-CB   | 5.56  | 120.40      | 111.23   |
| 1   | H     | 31  | GLY  | CA-C-N    | 5.55  | 125.22      | 119.56   |
| 1   | H     | 31  | GLY  | C-N-CA    | 5.55  | 125.22      | 119.56   |
| 1   | N     | 64  | ASP  | N-CA-C    | 5.52  | 117.36      | 109.14   |
| 1   | A     | 313 | VAL  | N-CA-C    | 5.51  | 116.25      | 110.62   |
| 1   | J     | 285 | ASN  | N-CA-C    | 5.51  | 117.28      | 111.28   |
| 1   | G     | 365 | ALA  | N-CA-C    | 5.49  | 117.34      | 111.36   |
| 1   | B     | 107 | LYS  | N-CA-C    | 5.48  | 122.47      | 110.80   |
| 1   | D     | 501 | ILE  | N-CA-C    | 5.48  | 115.72      | 110.74   |
| 1   | P     | 211 | ILE  | CB-CA-C   | -5.48 | 104.96      | 111.97   |
| 1   | C     | 166 | PHE  | CA-CB-CG  | 5.46  | 119.26      | 113.80   |
| 1   | A     | 107 | LYS  | N-CA-CB   | -5.45 | 105.64      | 113.65   |
| 1   | E     | 487 | LYS  | N-CA-C    | 5.45  | 117.30      | 111.36   |
| 1   | G     | 135 | HIS  | N-CA-C    | 5.45  | 118.91      | 111.39   |
| 1   | O     | 125 | ARG  | CB-CA-C   | -5.45 | 101.75      | 110.79   |
| 1   | G     | 285 | ASN  | N-CA-C    | 5.44  | 117.21      | 111.28   |
| 1   | O     | 211 | ILE  | CA-CB-CG1 | 5.43  | 119.64      | 110.40   |
| 1   | A     | 64  | ASP  | N-CA-C    | 5.41  | 117.02      | 108.96   |
| 1   | O     | 65  | ASN  | CA-CB-CG  | 5.41  | 118.01      | 112.60   |
| 1   | K     | 503 | ARG  | CB-CA-C   | -5.40 | 101.83      | 110.79   |
| 1   | P     | 166 | PHE  | CA-CB-CG  | 5.39  | 119.19      | 113.80   |
| 1   | P     | 507 | ILE  | CA-C-N    | 5.39  | 131.68      | 121.97   |
| 1   | P     | 507 | ILE  | C-N-CA    | 5.39  | 131.68      | 121.97   |
| 1   | J     | 31  | GLY  | CA-C-N    | 5.39  | 125.21      | 119.28   |
| 1   | J     | 31  | GLY  | C-N-CA    | 5.39  | 125.21      | 119.28   |
| 1   | I     | 64  | ASP  | N-CA-C    | 5.38  | 116.98      | 108.96   |
| 1   | K     | 107 | LYS  | N-CA-CB   | -5.37 | 105.75      | 113.65   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | I     | 211 | ILE  | N-CA-CB  | 5.37  | 116.83      | 110.55   |
| 1   | H     | 39  | LEU  | N-CA-CB  | -5.37 | 101.66      | 110.68   |
| 1   | L     | 330 | LEU  | CA-C-N   | -5.37 | 118.00      | 121.65   |
| 1   | L     | 330 | LEU  | C-N-CA   | -5.37 | 118.00      | 121.65   |
| 1   | D     | 149 | ILE  | N-CA-C   | 5.36  | 116.09      | 110.62   |
| 1   | O     | 417 | GLY  | CA-C-N   | 5.36  | 128.00      | 120.28   |
| 1   | O     | 417 | GLY  | C-N-CA   | 5.36  | 128.00      | 120.28   |
| 1   | K     | 211 | ILE  | CB-CA-C  | -5.36 | 105.11      | 111.97   |
| 1   | J     | 211 | ILE  | CB-CA-C  | -5.35 | 105.12      | 111.97   |
| 1   | L     | 84  | ASP  | N-CA-C   | 5.35  | 116.91      | 109.31   |
| 1   | H     | 313 | VAL  | N-CA-C   | 5.35  | 115.55      | 110.42   |
| 1   | I     | 313 | VAL  | N-CA-C   | 5.33  | 116.06      | 110.62   |
| 1   | G     | 4   | ASP  | CA-C-N   | 5.30  | 131.66      | 121.54   |
| 1   | G     | 4   | ASP  | C-N-CA   | 5.30  | 131.66      | 121.54   |
| 1   | I     | 511 | ALA  | CA-C-N   | 5.29  | 126.46      | 119.84   |
| 1   | I     | 511 | ALA  | C-N-CA   | 5.29  | 126.46      | 119.84   |
| 1   | O     | 109 | HIS  | CA-CB-CG | 5.29  | 119.09      | 113.80   |
| 1   | K     | 185 | ALA  | N-CA-C   | 5.28  | 117.30      | 110.65   |
| 1   | O     | 63  | VAL  | CB-CA-C  | -5.28 | 105.02      | 112.14   |
| 1   | K     | 31  | GLY  | CA-C-N   | 5.27  | 124.94      | 119.56   |
| 1   | K     | 31  | GLY  | C-N-CA   | 5.27  | 124.94      | 119.56   |
| 1   | E     | 224 | ILE  | N-CA-C   | 5.27  | 115.55      | 108.17   |
| 1   | G     | 313 | VAL  | N-CA-C   | 5.26  | 115.47      | 110.42   |
| 1   | H     | 330 | LEU  | CA-C-N   | -5.26 | 118.07      | 121.65   |
| 1   | H     | 330 | LEU  | C-N-CA   | -5.26 | 118.07      | 121.65   |
| 1   | A     | 5   | GLU  | N-CA-C   | 5.25  | 118.11      | 109.76   |
| 1   | B     | 108 | ILE  | N-CA-CB  | 5.24  | 119.87      | 111.23   |
| 1   | F     | 313 | VAL  | N-CA-C   | 5.24  | 115.45      | 110.42   |
| 1   | C     | 512 | PRO  | N-CA-C   | 5.23  | 119.43      | 111.11   |
| 1   | A     | 142 | PHE  | N-CA-C   | 5.23  | 116.98      | 111.28   |
| 1   | E     | 509 | LYS  | N-CA-C   | 5.22  | 121.93      | 110.80   |
| 1   | P     | 163 | LYS  | N-CA-C   | 5.22  | 116.97      | 111.28   |
| 1   | L     | 138 | ASP  | N-CA-C   | 5.22  | 116.97      | 111.28   |
| 1   | M     | 61  | ILE  | N-CA-C   | 5.22  | 117.26      | 108.81   |
| 1   | C     | 185 | ALA  | N-CA-C   | 5.21  | 118.78      | 111.74   |
| 1   | B     | 109 | HIS  | CA-C-N   | 5.21  | 125.01      | 119.28   |
| 1   | B     | 109 | HIS  | C-N-CA   | 5.21  | 125.01      | 119.28   |
| 1   | K     | 269 | ILE  | N-CA-C   | 5.21  | 115.42      | 110.42   |
| 1   | M     | 94  | ALA  | N-CA-C   | 5.20  | 116.95      | 111.28   |
| 1   | I     | 149 | ILE  | N-CA-C   | 5.20  | 115.92      | 110.62   |
| 1   | G     | 107 | LYS  | N-CA-CB  | -5.19 | 104.69      | 113.15   |
| 1   | D     | 327 | LEU  | N-CA-C   | 5.19  | 116.94      | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 166 | PHE  | CA-CB-CG  | 5.19  | 118.99      | 113.80   |
| 1   | P     | 47  | SER  | N-CA-C    | 5.18  | 116.68      | 108.96   |
| 1   | E     | 182 | ASN  | CB-CA-C   | -5.18 | 110.62      | 116.63   |
| 1   | B     | 185 | ALA  | N-CA-C    | 5.17  | 118.72      | 111.74   |
| 1   | P     | 345 | LYS  | N-CA-C    | 5.17  | 117.72      | 110.23   |
| 1   | G     | 5   | GLU  | N-CA-CB   | -5.16 | 101.77      | 110.49   |
| 1   | J     | 248 | THR  | N-CA-C    | 5.16  | 118.03      | 111.69   |
| 1   | D     | 158 | LEU  | N-CA-C    | 5.16  | 116.90      | 111.28   |
| 1   | F     | 508 | ILE  | N-CA-C    | 5.16  | 120.06      | 109.34   |
| 1   | O     | 149 | ILE  | N-CA-C    | 5.15  | 115.88      | 110.62   |
| 1   | I     | 510 | ALA  | N-CA-C    | 5.15  | 116.98      | 108.48   |
| 1   | K     | 323 | ASP  | N-CA-C    | -5.15 | 106.77      | 113.16   |
| 1   | G     | 383 | VAL  | CB-CA-C   | -5.15 | 105.38      | 111.97   |
| 1   | E     | 365 | ALA  | N-CA-C    | 5.15  | 116.89      | 111.28   |
| 1   | E     | 61  | ILE  | N-CA-C    | 5.14  | 115.31      | 108.11   |
| 1   | P     | 327 | LEU  | N-CA-C    | 5.14  | 116.89      | 111.28   |
| 1   | J     | 30  | LEU  | N-CA-C    | 5.14  | 117.68      | 110.23   |
| 1   | M     | 240 | GLY  | N-CA-C    | -5.12 | 108.18      | 115.30   |
| 1   | F     | 238 | ILE  | CA-C-N    | 5.12  | 127.15      | 120.28   |
| 1   | F     | 238 | ILE  | C-N-CA    | 5.12  | 127.15      | 120.28   |
| 1   | A     | 222 | ALA  | N-CA-C    | 5.11  | 117.63      | 110.23   |
| 1   | F     | 512 | PRO  | CA-N-CD   | -5.11 | 104.85      | 112.00   |
| 1   | P     | 60  | ASN  | N-CA-C    | 5.10  | 116.84      | 111.28   |
| 1   | B     | 484 | PHE  | N-CA-C    | 5.09  | 116.83      | 111.28   |
| 1   | C     | 506 | ASN  | N-CA-C    | 5.09  | 116.81      | 108.52   |
| 1   | E     | 417 | GLY  | N-CA-C    | 5.09  | 120.22      | 110.86   |
| 1   | A     | 363 | ARG  | CA-C-N    | -5.08 | 117.55      | 121.82   |
| 1   | A     | 363 | ARG  | C-N-CA    | -5.08 | 117.55      | 121.82   |
| 1   | K     | 382 | CYS  | N-CA-C    | 5.08  | 116.66      | 111.03   |
| 1   | F     | 190 | LYS  | CB-CA-C   | -5.07 | 100.21      | 109.54   |
| 1   | H     | 30  | LEU  | N-CA-C    | 5.07  | 117.58      | 110.23   |
| 1   | I     | 237 | LYS  | N-CA-CB   | 5.06  | 117.65      | 110.16   |
| 1   | L     | 85  | GLY  | N-CA-C    | -5.06 | 101.19      | 113.18   |
| 1   | A     | 4   | ASP  | N-CA-C    | -5.06 | 99.09       | 107.99   |
| 1   | O     | 30  | LEU  | N-CA-C    | 5.06  | 117.56      | 110.23   |
| 1   | M     | 149 | ILE  | N-CA-C    | 5.04  | 115.81      | 110.72   |
| 1   | M     | 327 | LEU  | N-CA-C    | 5.03  | 116.77      | 111.28   |
| 1   | E     | 133 | VAL  | N-CA-C    | 5.03  | 117.99      | 112.96   |
| 1   | I     | 211 | ILE  | CA-CB-CG1 | 5.03  | 118.95      | 110.40   |
| 1   | K     | 327 | LEU  | N-CA-C    | 5.02  | 116.75      | 111.28   |
| 1   | P     | 31  | GLY  | CA-C-N    | 5.02  | 125.04      | 119.32   |
| 1   | P     | 31  | GLY  | C-N-CA    | 5.02  | 125.04      | 119.32   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 333 | CYS  | N-CA-C | 5.01 | 119.12      | 112.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3855  | 0        | 3970     | 327     | 0            |
| 1   | B     | 3855  | 0        | 3970     | 325     | 0            |
| 1   | C     | 3673  | 0        | 3778     | 326     | 0            |
| 1   | D     | 3855  | 0        | 3970     | 323     | 0            |
| 1   | E     | 3855  | 0        | 3970     | 292     | 0            |
| 1   | F     | 3855  | 0        | 3970     | 343     | 0            |
| 1   | G     | 3855  | 0        | 3970     | 330     | 0            |
| 1   | H     | 3693  | 0        | 3795     | 312     | 0            |
| 1   | I     | 3855  | 0        | 3970     | 330     | 0            |
| 1   | J     | 3855  | 0        | 3970     | 298     | 0            |
| 1   | K     | 3681  | 0        | 3782     | 325     | 0            |
| 1   | L     | 3676  | 0        | 3777     | 306     | 0            |
| 1   | M     | 3855  | 0        | 3970     | 291     | 0            |
| 1   | N     | 3700  | 0        | 3802     | 312     | 0            |
| 1   | O     | 3676  | 0        | 3777     | 317     | 0            |
| 1   | P     | 3855  | 0        | 3970     | 297     | 0            |
| All | All   | 60649 | 0        | 62411    | 4856    | 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 39.

All (4856) 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:O:146:LEU:HD12 | 1:O:171:VAL:HG13 | 1.25                     | 1.16              |
| 1:B:146:LEU:HD12 | 1:B:171:VAL:HG13 | 1.24                     | 1.12              |
| 1:L:146:LEU:HD12 | 1:L:171:VAL:HG13 | 1.31                     | 1.09              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:VAL:HB   | 1:A:290:LEU:HD21 | 1.35                     | 1.08              |
| 1:D:266:VAL:HB   | 1:D:290:LEU:HD21 | 1.32                     | 1.08              |
| 1:P:266:VAL:HB   | 1:P:290:LEU:HD21 | 1.36                     | 1.05              |
| 1:O:266:VAL:HB   | 1:O:290:LEU:HD21 | 1.38                     | 1.05              |
| 1:J:146:LEU:HD12 | 1:J:171:VAL:HG13 | 1.37                     | 1.04              |
| 1:I:211:ILE:H    | 1:I:211:ILE:HD12 | 1.24                     | 1.03              |
| 1:D:146:LEU:HD21 | 1:D:150:ALA:HB3  | 1.39                     | 1.03              |
| 1:L:364:GLY:HA3  | 1:L:370:LEU:HD11 | 1.41                     | 1.03              |
| 1:N:146:LEU:HD11 | 1:N:168:LYS:HA   | 1.37                     | 1.02              |
| 1:G:32:PRO:HD2   | 1:G:467:MET:HE1  | 1.38                     | 1.01              |
| 1:D:146:LEU:HD12 | 1:D:171:VAL:HG13 | 1.39                     | 1.00              |
| 1:E:266:VAL:HB   | 1:E:290:LEU:HD21 | 1.43                     | 1.00              |
| 1:N:127:ALA:HB1  | 1:N:491:LEU:HD13 | 1.42                     | 1.00              |
| 1:L:157:LYS:HB3  | 1:L:159:LEU:HD13 | 1.44                     | 0.99              |
| 1:M:146:LEU:HD12 | 1:M:171:VAL:HG13 | 1.40                     | 0.98              |
| 1:A:146:LEU:HD12 | 1:A:171:VAL:HG13 | 1.47                     | 0.97              |
| 1:H:146:LEU:HD21 | 1:H:150:ALA:HB3  | 1.46                     | 0.96              |
| 1:B:341:ILE:HG22 | 1:B:363:ARG:HH21 | 1.30                     | 0.96              |
| 1:D:188:VAL:HB   | 1:D:377:LEU:HD22 | 1.46                     | 0.96              |
| 1:M:39:LEU:HA    | 1:O:509:LYS:HZ3  | 1.30                     | 0.96              |
| 1:F:511:ALA:HB1  | 1:F:512:PRO:HD2  | 1.47                     | 0.95              |
| 1:G:146:LEU:HD12 | 1:G:171:VAL:HG13 | 1.47                     | 0.95              |
| 1:H:146:LEU:HD12 | 1:H:171:VAL:HG13 | 1.48                     | 0.94              |
| 1:O:211:ILE:H    | 1:O:211:ILE:HD12 | 1.30                     | 0.93              |
| 1:A:146:LEU:HD22 | 1:A:168:LYS:HA   | 1.46                     | 0.93              |
| 1:J:402:MET:HE3  | 1:J:453:ARG:HG2  | 1.50                     | 0.92              |
| 1:M:63:VAL:HG11  | 1:O:2:GLY:HA3    | 1.48                     | 0.92              |
| 1:K:146:LEU:HD21 | 1:K:150:ALA:HB3  | 1.49                     | 0.92              |
| 1:A:92:LEU:HD11  | 1:A:433:LEU:HD21 | 1.51                     | 0.92              |
| 1:E:211:ILE:HD11 | 1:E:297:MET:HG3  | 1.52                     | 0.92              |
| 1:F:106:LYS:HE2  | 1:F:113:ILE:HD11 | 1.49                     | 0.92              |
| 1:D:79:ASP:HA    | 1:D:83:GLY:CA    | 2.01                     | 0.91              |
| 1:G:402:MET:HE3  | 1:G:453:ARG:HG2  | 1.51                     | 0.91              |
| 1:H:446:ALA:HB2  | 1:P:108:ILE:HG21 | 1.52                     | 0.91              |
| 1:K:269:ILE:HG23 | 1:K:274:ILE:HG21 | 1.52                     | 0.91              |
| 1:C:402:MET:HE3  | 1:C:453:ARG:HG2  | 1.51                     | 0.91              |
| 1:H:211:ILE:HD11 | 1:H:297:MET:HG3  | 1.50                     | 0.91              |
| 1:C:38:ILE:HD13  | 1:H:508:ILE:HA   | 1.52                     | 0.91              |
| 1:E:173:ALA:HB2  | 1:E:360:ILE:HD11 | 1.50                     | 0.91              |
| 1:E:146:LEU:HD22 | 1:E:168:LYS:HA   | 1.53                     | 0.90              |
| 1:O:38:ILE:HG22  | 1:O:50:VAL:HB    | 1.52                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:140:VAL:HA   | 1:O:175:LEU:HD22 | 1.53                     | 0.90              |
| 1:M:402:MET:HE3  | 1:M:453:ARG:HG2  | 1.51                     | 0.90              |
| 1:P:402:MET:HE3  | 1:P:453:ARG:HG2  | 1.54                     | 0.90              |
| 1:C:146:LEU:HD12 | 1:C:171:VAL:HG13 | 1.52                     | 0.90              |
| 1:F:266:VAL:HB   | 1:F:290:LEU:HD21 | 1.54                     | 0.89              |
| 1:I:269:ILE:HG23 | 1:I:274:ILE:CG2  | 2.03                     | 0.89              |
| 1:N:146:LEU:HD23 | 1:N:150:ALA:HB3  | 1.54                     | 0.89              |
| 1:C:79:ASP:HA    | 1:C:83:GLY:CA    | 2.02                     | 0.89              |
| 1:H:171:VAL:HG12 | 1:H:384:LEU:HG   | 1.55                     | 0.89              |
| 1:F:369:ILE:O    | 1:F:372:GLU:HG2  | 1.73                     | 0.89              |
| 1:P:146:LEU:HD22 | 1:P:168:LYS:HA   | 1.54                     | 0.89              |
| 1:P:211:ILE:HD11 | 1:P:297:MET:HG3  | 1.53                     | 0.89              |
| 1:D:507:ILE:HG23 | 1:H:39:LEU:HD23  | 1.51                     | 0.88              |
| 1:J:211:ILE:HD11 | 1:J:297:MET:HG3  | 1.53                     | 0.88              |
| 1:B:146:LEU:HD21 | 1:B:150:ALA:HB3  | 1.55                     | 0.88              |
| 1:B:269:ILE:HG23 | 1:B:274:ILE:CG2  | 2.02                     | 0.88              |
| 1:B:79:ASP:HA    | 1:B:83:GLY:CA    | 2.04                     | 0.88              |
| 1:K:159:LEU:H    | 1:K:159:LEU:HD13 | 1.37                     | 0.88              |
| 1:G:146:LEU:HD23 | 1:G:147:MET:H    | 1.37                     | 0.88              |
| 1:I:146:LEU:HD12 | 1:I:171:VAL:HG13 | 1.56                     | 0.88              |
| 1:N:27:LYS:HD3   | 1:N:28:SER:N     | 1.88                     | 0.88              |
| 1:E:38:ILE:H     | 1:G:508:ILE:HD13 | 1.37                     | 0.87              |
| 1:H:402:MET:HE3  | 1:H:453:ARG:HG2  | 1.56                     | 0.87              |
| 1:F:245:VAL:HG11 | 1:F:250:LYS:HB3  | 1.55                     | 0.87              |
| 1:A:27:LYS:HA    | 1:A:436:ILE:HD11 | 1.55                     | 0.87              |
| 1:P:32:PRO:HA    | 1:P:155:SER:O    | 1.75                     | 0.86              |
| 1:B:106:LYS:HB3  | 1:I:446:ALA:HB2  | 1.57                     | 0.86              |
| 1:I:124:ALA:HA   | 1:I:491:LEU:HD13 | 1.57                     | 0.86              |
| 1:J:146:LEU:HD21 | 1:J:150:ALA:HB3  | 1.57                     | 0.86              |
| 1:J:82:VAL:HG21  | 1:J:483:SER:HB3  | 1.56                     | 0.86              |
| 1:C:38:ILE:HG21  | 1:H:508:ILE:HG23 | 1.58                     | 0.85              |
| 1:H:140:VAL:HA   | 1:H:175:LEU:HD22 | 1.56                     | 0.85              |
| 1:E:402:MET:HE3  | 1:E:453:ARG:HG2  | 1.55                     | 0.85              |
| 1:E:79:ASP:HA    | 1:E:83:GLY:CA    | 2.06                     | 0.85              |
| 1:J:40:LEU:HB2   | 1:J:48:LEU:HD21  | 1.57                     | 0.85              |
| 1:P:38:ILE:HG22  | 1:P:50:VAL:HB    | 1.57                     | 0.85              |
| 1:N:183:LEU:HD21 | 1:N:381:LEU:HD11 | 1.57                     | 0.85              |
| 1:K:192:LEU:HG   | 1:K:366:THR:HG21 | 1.57                     | 0.85              |
| 1:E:146:LEU:HD21 | 1:E:167:THR:HG23 | 1.58                     | 0.85              |
| 1:M:269:ILE:HG23 | 1:M:274:ILE:HG22 | 1.57                     | 0.85              |
| 1:N:32:PRO:HD2   | 1:N:467:MET:HE1  | 1.59                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:ILE:HG23 | 1:C:499:GLU:HG3  | 1.59                     | 0.84              |
| 1:B:402:MET:HE3  | 1:B:453:ARG:HG2  | 1.58                     | 0.84              |
| 1:L:233:THR:HG21 | 1:L:261:LYS:HE2  | 1.59                     | 0.84              |
| 1:E:37:LYS:HB3   | 1:G:508:ILE:HG23 | 1.57                     | 0.84              |
| 1:M:192:LEU:HG   | 1:M:366:THR:HG21 | 1.59                     | 0.84              |
| 1:C:146:LEU:HD23 | 1:C:147:MET:H    | 1.42                     | 0.84              |
| 1:J:146:LEU:HD23 | 1:J:147:MET:H    | 1.42                     | 0.84              |
| 1:K:67:ALA:HB2   | 1:K:507:ILE:HG21 | 1.58                     | 0.84              |
| 1:N:211:ILE:HD11 | 1:N:297:MET:HG3  | 1.60                     | 0.84              |
| 1:I:266:VAL:HB   | 1:I:290:LEU:HD21 | 1.60                     | 0.84              |
| 1:B:108:ILE:HD12 | 1:B:108:ILE:H    | 1.40                     | 0.83              |
| 1:F:138:ASP:O    | 1:F:139:GLU:HB2  | 1.78                     | 0.83              |
| 1:N:146:LEU:HD22 | 1:N:147:MET:H    | 1.43                     | 0.83              |
| 1:L:211:ILE:HD11 | 1:L:297:MET:HG3  | 1.58                     | 0.83              |
| 1:N:402:MET:HE3  | 1:N:453:ARG:HG2  | 1.59                     | 0.83              |
| 1:M:100:ALA:HA   | 1:M:103:LEU:HD13 | 1.59                     | 0.83              |
| 1:O:70:VAL:HG11  | 1:O:506:ASN:HB3  | 1.57                     | 0.83              |
| 1:K:402:MET:HE3  | 1:K:453:ARG:HG2  | 1.60                     | 0.83              |
| 1:L:266:VAL:HB   | 1:L:290:LEU:HD21 | 1.58                     | 0.83              |
| 1:F:417:GLY:HA3  | 1:O:450:ALA:HB1  | 1.58                     | 0.83              |
| 1:N:82:VAL:O     | 1:N:386:GLN:HG3  | 1.77                     | 0.83              |
| 1:P:103:LEU:HG   | 1:P:113:ILE:HD13 | 1.59                     | 0.83              |
| 1:E:25:LEU:HG    | 1:G:509:LYS:O    | 1.77                     | 0.82              |
| 1:E:214:ASN:O    | 1:E:215:GLN:HG2  | 1.78                     | 0.82              |
| 1:J:266:VAL:HB   | 1:J:290:LEU:HD21 | 1.59                     | 0.82              |
| 1:B:269:ILE:HG23 | 1:B:274:ILE:HG21 | 1.61                     | 0.82              |
| 1:I:402:MET:HE3  | 1:I:453:ARG:HG2  | 1.62                     | 0.82              |
| 1:N:38:ILE:HG22  | 1:N:50:VAL:HB    | 1.61                     | 0.82              |
| 1:I:369:ILE:O    | 1:I:372:GLU:HB3  | 1.78                     | 0.82              |
| 1:L:402:MET:HE3  | 1:L:453:ARG:HG2  | 1.60                     | 0.82              |
| 1:A:203:GLU:CD   | 1:A:203:GLU:H    | 1.88                     | 0.82              |
| 1:N:283:ILE:HG22 | 1:N:300:GLU:HG3  | 1.61                     | 0.82              |
| 1:N:266:VAL:HB   | 1:N:290:LEU:HD21 | 1.60                     | 0.82              |
| 1:F:211:ILE:HD11 | 1:F:297:MET:HG3  | 1.62                     | 0.82              |
| 1:I:269:ILE:HG23 | 1:I:274:ILE:HG21 | 1.59                     | 0.82              |
| 1:G:211:ILE:HD11 | 1:G:297:MET:HG3  | 1.62                     | 0.82              |
| 1:A:245:VAL:HG11 | 1:A:250:LYS:HB3  | 1.60                     | 0.81              |
| 1:A:32:PRO:HD2   | 1:A:467:MET:HE1  | 1.60                     | 0.81              |
| 1:C:48:LEU:HD12  | 1:C:48:LEU:H     | 1.41                     | 0.81              |
| 1:C:211:ILE:H    | 1:C:211:ILE:CD1  | 1.92                     | 0.81              |
| 1:M:146:LEU:HD21 | 1:M:150:ALA:HB3  | 1.62                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:65:ASN:H     | 1:O:65:ASN:HD22  | 1.26                     | 0.81              |
| 1:O:402:MET:HE3  | 1:O:453:ARG:HG2  | 1.61                     | 0.81              |
| 1:A:265:LYS:O    | 1:A:269:ILE:HB   | 1.79                     | 0.81              |
| 1:C:283:ILE:HG22 | 1:C:300:GLU:HG3  | 1.62                     | 0.81              |
| 1:H:269:ILE:HG23 | 1:H:274:ILE:CG2  | 2.10                     | 0.81              |
| 1:M:207:LEU:HD22 | 1:M:208:ASP:H    | 1.45                     | 0.81              |
| 1:K:269:ILE:HG23 | 1:K:274:ILE:CG2  | 2.11                     | 0.81              |
| 1:J:245:VAL:HG21 | 1:J:250:LYS:HD3  | 1.62                     | 0.81              |
| 1:P:146:LEU:HD12 | 1:P:171:VAL:HG13 | 1.61                     | 0.81              |
| 1:B:211:ILE:HD11 | 1:B:297:MET:HG3  | 1.63                     | 0.81              |
| 1:D:140:VAL:HA   | 1:D:175:LEU:HD22 | 1.62                     | 0.81              |
| 1:I:140:VAL:HA   | 1:I:175:LEU:HD22 | 1.62                     | 0.81              |
| 1:A:433:LEU:O    | 1:A:436:ILE:HG22 | 1.80                     | 0.81              |
| 1:H:372:GLU:HG3  | 1:H:375:ARG:NH2  | 1.96                     | 0.81              |
| 1:K:211:ILE:HD11 | 1:K:297:MET:HG3  | 1.63                     | 0.81              |
| 1:L:448:LEU:HD21 | 1:L:465:LEU:HD12 | 1.61                     | 0.81              |
| 1:E:372:GLU:HA   | 1:E:375:ARG:NH1  | 1.96                     | 0.81              |
| 1:K:138:ASP:O    | 1:K:139:GLU:HB2  | 1.80                     | 0.81              |
| 1:C:166:PHE:CZ   | 1:C:198:ASP:HB3  | 2.16                     | 0.80              |
| 1:F:475:MET:SD   | 1:F:480:ILE:HB   | 2.21                     | 0.80              |
| 1:I:146:LEU:HD21 | 1:I:150:ALA:HB3  | 1.63                     | 0.80              |
| 1:P:283:ILE:HG22 | 1:P:300:GLU:HG3  | 1.62                     | 0.80              |
| 1:P:448:LEU:HD21 | 1:P:465:LEU:HD12 | 1.63                     | 0.80              |
| 1:L:146:LEU:HD23 | 1:L:147:MET:H    | 1.44                     | 0.80              |
| 1:N:146:LEU:HB3  | 1:N:171:VAL:HG11 | 1.64                     | 0.80              |
| 1:G:78:GLN:OE1   | 1:G:489:GLN:HB2  | 1.81                     | 0.80              |
| 1:H:399:CYS:SG   | 1:H:464:GLY:HA3  | 2.22                     | 0.80              |
| 1:L:402:MET:SD   | 1:L:456:HIS:HB2  | 2.21                     | 0.80              |
| 1:O:79:ASP:HA    | 1:O:83:GLY:CA    | 2.12                     | 0.80              |
| 1:K:146:LEU:HD13 | 1:K:168:LYS:HA   | 1.64                     | 0.80              |
| 1:K:159:LEU:HD23 | 1:K:163:LYS:HG2  | 1.62                     | 0.80              |
| 1:K:448:LEU:HD21 | 1:K:465:LEU:HD12 | 1.62                     | 0.80              |
| 1:L:269:ILE:HG23 | 1:L:274:ILE:HG21 | 1.64                     | 0.80              |
| 1:I:163:LYS:HA   | 1:I:166:PHE:CD1  | 2.17                     | 0.79              |
| 1:M:442:GLY:O    | 1:O:109:HIS:HB3  | 1.81                     | 0.79              |
| 1:P:206:LEU:HD11 | 1:P:346:LEU:HD23 | 1.62                     | 0.79              |
| 1:L:133:VAL:HG11 | 1:L:394:VAL:HA   | 1.63                     | 0.79              |
| 1:A:176:ARG:HH12 | 1:A:201:LEU:HD21 | 1.46                     | 0.79              |
| 1:D:402:MET:HE3  | 1:D:453:ARG:HG2  | 1.63                     | 0.79              |
| 1:N:163:LYS:HA   | 1:N:166:PHE:CD1  | 2.17                     | 0.79              |
| 1:G:364:GLY:HA3  | 1:G:370:LEU:HD13 | 1.65                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:188:VAL:HG11 | 1:B:377:LEU:HD22 | 1.63                     | 0.79              |
| 1:K:154:LEU:HD22 | 1:K:167:THR:HB   | 1.65                     | 0.79              |
| 1:B:108:ILE:CD1  | 1:I:446:ALA:HB3  | 2.13                     | 0.79              |
| 1:G:245:VAL:HG21 | 1:G:251:VAL:HG22 | 1.63                     | 0.79              |
| 1:L:265:LYS:O    | 1:L:269:ILE:HB   | 1.83                     | 0.79              |
| 1:B:448:LEU:HD21 | 1:B:465:LEU:HD12 | 1.62                     | 0.78              |
| 1:G:133:VAL:HG23 | 1:G:134:ASP:H    | 1.45                     | 0.78              |
| 1:P:146:LEU:HD21 | 1:P:167:THR:HG23 | 1.65                     | 0.78              |
| 1:L:163:LYS:HA   | 1:L:166:PHE:CD1  | 2.18                     | 0.78              |
| 1:M:206:LEU:HD11 | 1:M:346:LEU:HD23 | 1.64                     | 0.78              |
| 1:O:269:ILE:HG23 | 1:O:274:ILE:CG2  | 2.13                     | 0.78              |
| 1:P:152:THR:OG1  | 1:P:480:ILE:HG23 | 1.83                     | 0.78              |
| 1:P:324:HIS:O    | 1:P:329:LYS:HG2  | 1.83                     | 0.78              |
| 1:A:154:LEU:HD22 | 1:A:167:THR:HB   | 1.66                     | 0.78              |
| 1:I:106:LYS:HZ3  | 1:I:106:LYS:HB3  | 1.48                     | 0.78              |
| 1:O:448:LEU:HD21 | 1:O:465:LEU:HD12 | 1.65                     | 0.78              |
| 1:E:233:THR:HG21 | 1:E:261:LYS:HE2  | 1.66                     | 0.78              |
| 1:F:402:MET:HE3  | 1:F:453:ARG:HG2  | 1.63                     | 0.78              |
| 1:G:124:ALA:HB1  | 1:G:491:LEU:HD13 | 1.65                     | 0.78              |
| 1:H:324:HIS:O    | 1:H:329:LYS:HG2  | 1.84                     | 0.78              |
| 1:K:148:ASN:HA   | 1:K:479:GLY:O    | 1.82                     | 0.78              |
| 1:N:109:HIS:NE2  | 1:N:111:GLN:HB2  | 1.98                     | 0.78              |
| 1:A:211:ILE:HD11 | 1:A:297:MET:HG3  | 1.65                     | 0.78              |
| 1:M:38:ILE:HG21  | 1:O:507:ILE:HG13 | 1.63                     | 0.78              |
| 1:K:283:ILE:HG22 | 1:K:300:GLU:HG3  | 1.65                     | 0.78              |
| 1:L:79:ASP:HA    | 1:L:83:GLY:CA    | 2.14                     | 0.78              |
| 1:F:32:PRO:HD2   | 1:F:467:MET:HE1  | 1.63                     | 0.78              |
| 1:I:433:LEU:O    | 1:I:436:ILE:HG22 | 1.83                     | 0.78              |
| 1:P:188:VAL:CG1  | 1:P:377:LEU:HD21 | 2.13                     | 0.78              |
| 1:M:269:ILE:HG23 | 1:M:274:ILE:CG2  | 2.13                     | 0.78              |
| 1:M:283:ILE:HG22 | 1:M:300:GLU:HG3  | 1.64                     | 0.78              |
| 1:B:508:ILE:O    | 1:G:37:LYS:HD2   | 1.83                     | 0.78              |
| 1:H:189:ILE:HG13 | 1:H:206:LEU:HD12 | 1.66                     | 0.78              |
| 1:O:108:ILE:HG22 | 1:O:109:HIS:H    | 1.46                     | 0.78              |
| 1:A:246:ASP:O    | 1:A:247:SER:HB3  | 1.84                     | 0.77              |
| 1:C:146:LEU:HD22 | 1:C:168:LYS:HA   | 1.63                     | 0.77              |
| 1:J:402:MET:SD   | 1:J:456:HIS:HB2  | 2.23                     | 0.77              |
| 1:B:59:LYS:HZ1   | 1:B:76:ARG:HB2   | 1.48                     | 0.77              |
| 1:D:245:VAL:HG11 | 1:D:250:LYS:HB3  | 1.66                     | 0.77              |
| 1:E:415:THR:O    | 1:E:420:ALA:HB2  | 1.84                     | 0.77              |
| 1:I:126:GLN:O    | 1:I:130:ASN:HB2  | 1.84                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:119:GLU:HB3  | 1:G:423:MET:HE3  | 1.64                     | 0.77              |
| 1:P:163:LYS:HA   | 1:P:166:PHE:CD1  | 2.19                     | 0.77              |
| 1:P:204:GLY:HA3  | 1:P:349:PHE:O    | 1.84                     | 0.77              |
| 1:K:146:LEU:HD12 | 1:K:171:VAL:HG13 | 1.66                     | 0.77              |
| 1:N:226:ILE:HD12 | 1:N:317:GLU:HG3  | 1.67                     | 0.77              |
| 1:K:399:CYS:SG   | 1:K:464:GLY:HA3  | 2.25                     | 0.77              |
| 1:A:79:ASP:HA    | 1:A:83:GLY:HA3   | 1.66                     | 0.77              |
| 1:C:109:HIS:CE1  | 1:C:111:GLN:HB2  | 2.20                     | 0.77              |
| 1:D:283:ILE:HG22 | 1:D:300:GLU:HG3  | 1.65                     | 0.77              |
| 1:G:27:LYS:HB2   | 1:G:436:ILE:CD1  | 2.13                     | 0.77              |
| 1:F:417:GLY:CA   | 1:O:450:ALA:HB1  | 2.14                     | 0.77              |
| 1:H:269:ILE:HG23 | 1:H:274:ILE:HG21 | 1.66                     | 0.77              |
| 1:L:383:VAL:HG23 | 1:L:384:LEU:HD22 | 1.66                     | 0.77              |
| 1:L:504:VAL:HG22 | 1:P:369:ILE:HD11 | 1.64                     | 0.77              |
| 1:O:154:LEU:HD22 | 1:O:167:THR:HB   | 1.67                     | 0.77              |
| 1:B:433:LEU:O    | 1:B:436:ILE:HG22 | 1.84                     | 0.77              |
| 1:C:169:LEU:HD11 | 1:C:201:LEU:HG   | 1.67                     | 0.77              |
| 1:C:79:ASP:HA    | 1:C:83:GLY:HA2   | 1.67                     | 0.76              |
| 1:O:211:ILE:H    | 1:O:211:ILE:CD1  | 1.97                     | 0.76              |
| 1:G:265:LYS:O    | 1:G:269:ILE:HB   | 1.85                     | 0.76              |
| 1:K:266:VAL:HB   | 1:K:290:LEU:HD21 | 1.66                     | 0.76              |
| 1:K:163:LYS:HA   | 1:K:166:PHE:CD1  | 2.20                     | 0.76              |
| 1:O:438:ALA:CB   | 1:O:448:LEU:HG   | 2.15                     | 0.76              |
| 1:C:418:LYS:HA   | 1:L:453:ARG:NH2  | 1.99                     | 0.76              |
| 1:I:89:VAL:HG12  | 1:I:490:VAL:HB   | 1.68                     | 0.76              |
| 1:O:67:ALA:HB2   | 1:O:508:ILE:H    | 1.49                     | 0.76              |
| 1:C:78:GLN:NE2   | 1:C:486:VAL:HA   | 2.00                     | 0.76              |
| 1:B:146:LEU:HD23 | 1:B:147:MET:H    | 1.50                     | 0.76              |
| 1:D:248:THR:O    | 1:D:251:VAL:HG12 | 1.85                     | 0.76              |
| 1:M:82:VAL:HA    | 1:M:386:GLN:HG3  | 1.66                     | 0.76              |
| 1:B:154:LEU:HD22 | 1:B:167:THR:HB   | 1.67                     | 0.76              |
| 1:L:324:HIS:HB2  | 1:L:329:LYS:NZ   | 2.00                     | 0.76              |
| 1:O:408:VAL:HA   | 1:O:411:LEU:HD12 | 1.66                     | 0.76              |
| 1:F:140:VAL:HA   | 1:F:175:LEU:HD22 | 1.67                     | 0.76              |
| 1:I:211:ILE:H    | 1:I:211:ILE:CD1  | 1.97                     | 0.76              |
| 1:B:59:LYS:CE    | 1:B:76:ARG:HB2   | 2.14                     | 0.76              |
| 1:D:372:GLU:HG3  | 1:D:375:ARG:NH1  | 2.00                     | 0.76              |
| 1:E:265:LYS:O    | 1:E:269:ILE:HB   | 1.86                     | 0.76              |
| 1:H:325:PRO:O    | 1:H:326:GLU:HG3  | 1.86                     | 0.76              |
| 1:J:128:LEU:HD23 | 1:J:394:VAL:HG11 | 1.66                     | 0.76              |
| 1:L:152:THR:OG1  | 1:L:480:ILE:HG23 | 1.85                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:159:LEU:HD11 | 1:L:372:GLU:OE2  | 1.85                     | 0.76              |
| 1:N:188:VAL:CG1  | 1:N:377:LEU:HD22 | 2.15                     | 0.76              |
| 1:I:38:ILE:HG22  | 1:I:50:VAL:HB    | 1.65                     | 0.76              |
| 1:C:402:MET:SD   | 1:C:456:HIS:HB2  | 2.26                     | 0.75              |
| 1:M:128:LEU:HD13 | 1:M:488:ARG:HG2  | 1.69                     | 0.75              |
| 1:E:150:ALA:HB2  | 1:E:384:LEU:HD21 | 1.67                     | 0.75              |
| 1:N:269:ILE:HG23 | 1:N:274:ILE:HG21 | 1.68                     | 0.75              |
| 1:N:325:PRO:O    | 1:N:326:GLU:HG2  | 1.86                     | 0.75              |
| 1:A:437:ILE:HB   | 1:A:465:LEU:HD12 | 1.69                     | 0.75              |
| 1:D:324:HIS:O    | 1:D:329:LYS:HG2  | 1.87                     | 0.75              |
| 1:J:27:LYS:HD2   | 1:J:436:ILE:HD11 | 1.69                     | 0.75              |
| 1:M:59:LYS:HE2   | 1:M:76:ARG:HB2   | 1.66                     | 0.75              |
| 1:E:79:ASP:HA    | 1:E:83:GLY:HA3   | 1.69                     | 0.75              |
| 1:I:79:ASP:HA    | 1:I:83:GLY:CA    | 2.15                     | 0.75              |
| 1:O:325:PRO:O    | 1:O:326:GLU:HG3  | 1.85                     | 0.75              |
| 1:P:119:GLU:HB3  | 1:P:423:MET:HE3  | 1.68                     | 0.75              |
| 1:P:146:LEU:HD12 | 1:P:171:VAL:CG1  | 2.16                     | 0.75              |
| 1:A:324:HIS:HB2  | 1:A:329:LYS:NZ   | 2.02                     | 0.75              |
| 1:B:108:ILE:HD12 | 1:I:446:ALA:HB3  | 1.69                     | 0.75              |
| 1:I:372:GLU:HG3  | 1:I:375:ARG:NH2  | 2.01                     | 0.75              |
| 1:J:192:LEU:HG   | 1:J:343:GLU:OE1  | 1.85                     | 0.75              |
| 1:J:245:VAL:HG11 | 1:J:250:LYS:HB3  | 1.67                     | 0.75              |
| 1:N:24:ASP:O     | 1:N:27:LYS:HD2   | 1.86                     | 0.75              |
| 1:L:79:ASP:HA    | 1:L:83:GLY:HA3   | 1.68                     | 0.75              |
| 1:N:188:VAL:HG11 | 1:N:377:LEU:HD22 | 1.68                     | 0.75              |
| 1:A:79:ASP:HA    | 1:A:83:GLY:CA    | 2.16                     | 0.75              |
| 1:G:204:GLY:O    | 1:G:359:THR:HB   | 1.87                     | 0.75              |
| 1:H:58:LEU:HB3   | 1:H:72:VAL:CG1   | 2.16                     | 0.75              |
| 1:J:92:LEU:H     | 1:J:92:LEU:HD13  | 1.52                     | 0.75              |
| 1:O:163:LYS:HA   | 1:O:166:PHE:CD1  | 2.21                     | 0.75              |
| 1:C:497:ALA:HB1  | 1:C:500:VAL:HB   | 1.69                     | 0.75              |
| 1:J:58:LEU:HB3   | 1:J:72:VAL:HG13  | 1.67                     | 0.75              |
| 1:L:146:LEU:HD12 | 1:L:171:VAL:CG1  | 2.12                     | 0.75              |
| 1:A:354:LEU:HD23 | 1:A:356:GLU:H    | 1.51                     | 0.75              |
| 1:F:324:HIS:O    | 1:F:328:VAL:HG23 | 1.87                     | 0.75              |
| 1:D:89:VAL:HG12  | 1:D:490:VAL:HB   | 1.69                     | 0.74              |
| 1:I:324:HIS:O    | 1:I:329:LYS:HG2  | 1.87                     | 0.74              |
| 1:P:208:ASP:O    | 1:P:209:LYS:HG3  | 1.87                     | 0.74              |
| 1:K:214:ASN:O    | 1:K:215:GLN:HB2  | 1.87                     | 0.74              |
| 1:P:250:LYS:O    | 1:P:253:GLU:HG2  | 1.86                     | 0.74              |
| 1:A:146:LEU:HD22 | 1:A:168:LYS:CA   | 2.17                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:214:ASN:O    | 1:A:215:GLN:HB2  | 1.86                     | 0.74              |
| 1:B:324:HIS:HB2  | 1:B:329:LYS:NZ   | 2.03                     | 0.74              |
| 1:B:27:LYS:HA    | 1:B:436:ILE:HD11 | 1.67                     | 0.74              |
| 1:B:364:GLY:HA3  | 1:B:370:LEU:HD13 | 1.68                     | 0.74              |
| 1:F:402:MET:SD   | 1:F:456:HIS:HB2  | 2.28                     | 0.74              |
| 1:M:124:ALA:O    | 1:M:128:LEU:HG   | 1.87                     | 0.74              |
| 1:E:483:SER:O    | 1:E:486:VAL:HG22 | 1.88                     | 0.74              |
| 1:K:206:LEU:HD21 | 1:K:346:LEU:HD23 | 1.68                     | 0.74              |
| 1:K:325:PRO:O    | 1:K:326:GLU:HG3  | 1.86                     | 0.74              |
| 1:N:146:LEU:HD11 | 1:N:168:LYS:CA   | 2.15                     | 0.74              |
| 1:F:324:HIS:O    | 1:F:329:LYS:HG2  | 1.88                     | 0.74              |
| 1:B:369:ILE:O    | 1:B:372:GLU:HB3  | 1.87                     | 0.74              |
| 1:F:433:LEU:O    | 1:F:436:ILE:HG22 | 1.86                     | 0.74              |
| 1:P:265:LYS:O    | 1:P:269:ILE:HB   | 1.87                     | 0.74              |
| 1:D:510:ALA:HB2  | 1:H:57:ILE:HG12  | 1.69                     | 0.74              |
| 1:J:283:ILE:HG22 | 1:J:300:GLU:HG3  | 1.68                     | 0.74              |
| 1:O:51:THR:HG21  | 1:O:56:THR:HB    | 1.68                     | 0.74              |
| 1:G:145:ASP:OD1  | 1:G:171:VAL:HB   | 1.87                     | 0.73              |
| 1:O:79:ASP:HA    | 1:O:83:GLY:HA3   | 1.68                     | 0.73              |
| 1:L:103:LEU:HG   | 1:L:113:ILE:HD13 | 1.70                     | 0.73              |
| 1:L:401:GLU:HG2  | 1:L:433:LEU:HD22 | 1.69                     | 0.73              |
| 1:A:269:ILE:HG23 | 1:A:274:ILE:HG21 | 1.70                     | 0.73              |
| 1:H:92:LEU:HD11  | 1:H:433:LEU:HD21 | 1.69                     | 0.73              |
| 1:K:32:PRO:HA    | 1:K:155:SER:O    | 1.88                     | 0.73              |
| 1:P:79:ASP:HA    | 1:P:83:GLY:HA3   | 1.69                     | 0.73              |
| 1:E:269:ILE:HG23 | 1:E:274:ILE:HG21 | 1.71                     | 0.73              |
| 1:L:214:ASN:O    | 1:L:215:GLN:HB2  | 1.88                     | 0.73              |
| 1:P:139:GLU:O    | 1:P:140:VAL:HB   | 1.87                     | 0.73              |
| 1:N:127:ALA:CB   | 1:N:491:LEU:HD13 | 2.17                     | 0.73              |
| 1:B:214:ASN:O    | 1:B:215:GLN:HB2  | 1.87                     | 0.73              |
| 1:H:101:GLU:O    | 1:H:104:ILE:HG12 | 1.88                     | 0.73              |
| 1:L:188:VAL:CG1  | 1:L:377:LEU:HD22 | 2.19                     | 0.73              |
| 1:N:500:VAL:O    | 1:N:504:VAL:HG23 | 1.89                     | 0.73              |
| 1:C:399:CYS:SG   | 1:C:464:GLY:HA3  | 2.28                     | 0.73              |
| 1:C:401:GLU:HG2  | 1:C:433:LEU:HD22 | 1.71                     | 0.73              |
| 1:H:324:HIS:HB2  | 1:H:329:LYS:NZ   | 2.04                     | 0.73              |
| 1:A:38:ILE:HG22  | 1:A:50:VAL:HB    | 1.69                     | 0.73              |
| 1:A:226:ILE:HG12 | 1:A:278:ILE:HG23 | 1.71                     | 0.73              |
| 1:C:146:LEU:HD12 | 1:C:171:VAL:CG1  | 2.19                     | 0.73              |
| 1:G:146:LEU:HD12 | 1:G:171:VAL:CG1  | 2.17                     | 0.73              |
| 1:J:204:GLY:O    | 1:J:359:THR:HB   | 1.89                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:163:LYS:HA   | 1:H:166:PHE:CD1  | 2.24                     | 0.72              |
| 1:I:79:ASP:HA    | 1:I:83:GLY:HA3   | 1.71                     | 0.72              |
| 1:K:159:LEU:HD12 | 1:K:369:ILE:HG23 | 1.71                     | 0.72              |
| 1:C:433:LEU:O    | 1:C:436:ILE:HG22 | 1.89                     | 0.72              |
| 1:K:106:LYS:HE2  | 1:K:418:LYS:NZ   | 2.03                     | 0.72              |
| 1:A:146:LEU:HD21 | 1:A:167:THR:HG23 | 1.71                     | 0.72              |
| 1:O:32:PRO:HA    | 1:O:155:SER:C    | 2.14                     | 0.72              |
| 1:O:214:ASN:O    | 1:O:215:GLN:HB2  | 1.89                     | 0.72              |
| 1:F:74:MET:O     | 1:F:77:VAL:HG12  | 1.90                     | 0.72              |
| 1:B:313:VAL:HG22 | 1:B:357:ALA:HB3  | 1.71                     | 0.72              |
| 1:J:399:CYS:SG   | 1:J:464:GLY:HA3  | 2.29                     | 0.72              |
| 1:O:70:VAL:CG1   | 1:O:506:ASN:HB3  | 2.20                     | 0.72              |
| 1:B:191:LYS:HE2  | 1:B:346:LEU:HD11 | 1.72                     | 0.72              |
| 1:B:283:ILE:HG22 | 1:B:300:GLU:HG3  | 1.69                     | 0.72              |
| 1:J:59:LYS:HE2   | 1:J:76:ARG:HB2   | 1.72                     | 0.72              |
| 1:K:192:LEU:HA   | 1:K:366:THR:HG21 | 1.71                     | 0.72              |
| 1:P:214:ASN:O    | 1:P:215:GLN:HB2  | 1.87                     | 0.72              |
| 1:F:324:HIS:ND1  | 1:F:325:PRO:HD3  | 2.05                     | 0.72              |
| 1:E:188:VAL:HG21 | 1:E:377:LEU:HD13 | 1.72                     | 0.72              |
| 1:G:145:ASP:O    | 1:G:171:VAL:HG11 | 1.90                     | 0.72              |
| 1:H:27:LYS:HG3   | 1:H:436:ILE:HD11 | 1.69                     | 0.72              |
| 1:H:214:ASN:O    | 1:H:215:GLN:HB2  | 1.88                     | 0.72              |
| 1:K:103:LEU:HG   | 1:K:113:ILE:HD13 | 1.72                     | 0.72              |
| 1:P:399:CYS:SG   | 1:P:464:GLY:HA3  | 2.30                     | 0.72              |
| 1:I:214:ASN:O    | 1:I:215:GLN:HB2  | 1.90                     | 0.72              |
| 1:C:497:ALA:CB   | 1:C:500:VAL:HB   | 2.20                     | 0.72              |
| 1:D:63:VAL:HG22  | 1:E:513:ARG:HD3  | 1.72                     | 0.71              |
| 1:E:248:THR:O    | 1:E:251:VAL:HG12 | 1.89                     | 0.71              |
| 1:L:146:LEU:HD23 | 1:L:147:MET:N    | 2.04                     | 0.71              |
| 1:N:265:LYS:O    | 1:N:269:ILE:HB   | 1.89                     | 0.71              |
| 1:A:141:LYS:HG2  | 1:A:144:GLN:HB2  | 1.73                     | 0.71              |
| 1:A:163:LYS:HG3  | 1:A:166:PHE:CG   | 2.25                     | 0.71              |
| 1:B:163:LYS:HA   | 1:B:166:PHE:CD1  | 2.24                     | 0.71              |
| 1:J:103:LEU:HG   | 1:J:113:ILE:HD13 | 1.72                     | 0.71              |
| 1:K:233:THR:HG21 | 1:K:261:LYS:HE2  | 1.71                     | 0.71              |
| 1:N:507:ILE:O    | 1:N:508:ILE:HB   | 1.89                     | 0.71              |
| 1:O:114:ILE:HA   | 1:O:117:TRP:CE3  | 2.25                     | 0.71              |
| 1:B:79:ASP:HA    | 1:B:83:GLY:HA3   | 1.70                     | 0.71              |
| 1:F:111:GLN:HA   | 1:F:114:ILE:HD12 | 1.70                     | 0.71              |
| 1:L:324:HIS:HB2  | 1:L:329:LYS:HZ3  | 1.55                     | 0.71              |
| 1:E:140:VAL:HA   | 1:E:175:LEU:HD22 | 1.73                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:219:ILE:HD11 | 1:K:336:ILE:HB   | 1.72                     | 0.71              |
| 1:B:146:LEU:CD2  | 1:B:147:MET:H    | 2.04                     | 0.71              |
| 1:E:324:HIS:O    | 1:E:329:LYS:HG2  | 1.90                     | 0.71              |
| 1:G:399:CYS:SG   | 1:G:464:GLY:HA3  | 2.30                     | 0.71              |
| 1:L:226:ILE:HD13 | 1:L:307:VAL:HG13 | 1.72                     | 0.71              |
| 1:N:146:LEU:HD13 | 1:N:147:MET:N    | 2.06                     | 0.71              |
| 1:O:475:MET:SD   | 1:O:480:ILE:HB   | 2.31                     | 0.71              |
| 1:C:74:MET:O     | 1:C:77:VAL:HG12  | 1.90                     | 0.71              |
| 1:C:214:ASN:O    | 1:C:215:GLN:HB2  | 1.90                     | 0.71              |
| 1:D:133:VAL:HG23 | 1:D:134:ASP:H    | 1.52                     | 0.71              |
| 1:H:324:HIS:O    | 1:H:328:VAL:HG13 | 1.90                     | 0.71              |
| 1:I:32:PRO:HD2   | 1:I:467:MET:HE1  | 1.73                     | 0.71              |
| 1:J:214:ASN:O    | 1:J:215:GLN:HB2  | 1.88                     | 0.71              |
| 1:L:146:LEU:HD21 | 1:L:150:ALA:HB3  | 1.73                     | 0.71              |
| 1:A:146:LEU:HD12 | 1:A:171:VAL:CG1  | 2.19                     | 0.71              |
| 1:A:402:MET:HE3  | 1:A:453:ARG:HG2  | 1.72                     | 0.71              |
| 1:G:125:ARG:HA   | 1:G:128:LEU:CD1  | 2.21                     | 0.71              |
| 1:A:78:GLN:OE1   | 1:A:489:GLN:HG3  | 1.91                     | 0.71              |
| 1:D:399:CYS:SG   | 1:D:464:GLY:HA3  | 2.30                     | 0.71              |
| 1:I:106:LYS:HB3  | 1:I:106:LYS:NZ   | 2.05                     | 0.71              |
| 1:I:324:HIS:HB2  | 1:I:329:LYS:NZ   | 2.06                     | 0.71              |
| 1:J:398:GLY:HA2  | 1:J:401:GLU:OE1  | 1.90                     | 0.71              |
| 1:O:82:VAL:HG13  | 1:O:83:GLY:H     | 1.56                     | 0.71              |
| 1:P:74:MET:O     | 1:P:77:VAL:HG12  | 1.91                     | 0.71              |
| 1:C:124:ALA:HA   | 1:C:491:LEU:HD13 | 1.72                     | 0.71              |
| 1:F:216:PRO:CG   | 1:F:295:GLY:HA2  | 2.21                     | 0.71              |
| 1:F:216:PRO:HG2  | 1:F:295:GLY:HA2  | 1.73                     | 0.71              |
| 1:H:139:GLU:O    | 1:H:140:VAL:HB   | 1.91                     | 0.71              |
| 1:P:114:ILE:HD11 | 1:P:502:LEU:HB2  | 1.71                     | 0.71              |
| 1:B:145:ASP:O    | 1:B:171:VAL:HG11 | 1.91                     | 0.70              |
| 1:D:214:ASN:O    | 1:D:215:GLN:HB2  | 1.91                     | 0.70              |
| 1:D:510:ALA:N    | 1:H:39:LEU:HD13  | 2.06                     | 0.70              |
| 1:B:92:LEU:HD11  | 1:B:433:LEU:HD21 | 1.72                     | 0.70              |
| 1:B:190:LYS:HD2  | 1:B:190:LYS:C    | 2.16                     | 0.70              |
| 1:H:108:ILE:HG23 | 1:H:109:HIS:H    | 1.55                     | 0.70              |
| 1:K:160:THR:HG23 | 1:K:164:ASP:HB3  | 1.73                     | 0.70              |
| 1:L:501:ILE:O    | 1:L:502:LEU:HB2  | 1.91                     | 0.70              |
| 1:O:32:PRO:HB2   | 1:O:467:MET:HE1  | 1.73                     | 0.70              |
| 1:A:411:LEU:HB3  | 1:A:423:MET:SD   | 2.32                     | 0.70              |
| 1:C:31:GLY:O     | 1:C:156:SER:HA   | 1.90                     | 0.70              |
| 1:D:324:HIS:HB2  | 1:D:329:LYS:NZ   | 2.06                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:28:SER:HB2   | 1:M:35:MET:HG2   | 1.73                     | 0.70              |
| 1:O:146:LEU:HD21 | 1:O:150:ALA:HB3  | 1.72                     | 0.70              |
| 1:O:496:GLU:O    | 1:O:500:VAL:HG13 | 1.92                     | 0.70              |
| 1:B:475:MET:SD   | 1:B:480:ILE:HB   | 2.30                     | 0.70              |
| 1:C:133:VAL:HG11 | 1:C:393:THR:O    | 1.91                     | 0.70              |
| 1:F:265:LYS:O    | 1:F:269:ILE:HB   | 1.91                     | 0.70              |
| 1:G:369:ILE:O    | 1:G:372:GLU:HB2  | 1.91                     | 0.70              |
| 1:B:416:PRO:HG2  | 1:B:419:GLU:OE1  | 1.90                     | 0.70              |
| 1:E:146:LEU:HD23 | 1:E:147:MET:H    | 1.57                     | 0.70              |
| 1:E:146:LEU:HD12 | 1:E:171:VAL:CG1  | 2.21                     | 0.70              |
| 1:F:399:CYS:SG   | 1:F:464:GLY:HA3  | 2.32                     | 0.70              |
| 1:H:417:GLY:HA2  | 1:P:453:ARG:HH21 | 1.57                     | 0.70              |
| 1:K:163:LYS:O    | 1:K:166:PHE:HB2  | 1.91                     | 0.70              |
| 1:K:438:ALA:HB2  | 1:K:448:LEU:HG   | 1.73                     | 0.70              |
| 1:L:178:LYS:NZ   | 1:L:388:VAL:HG11 | 2.07                     | 0.70              |
| 1:C:101:GLU:O    | 1:C:104:ILE:HG12 | 1.91                     | 0.70              |
| 1:E:399:CYS:SG   | 1:E:464:GLY:HA3  | 2.31                     | 0.70              |
| 1:H:145:ASP:OD1  | 1:H:171:VAL:HB   | 1.92                     | 0.70              |
| 1:L:109:HIS:CE1  | 1:L:111:GLN:HB2  | 2.26                     | 0.70              |
| 1:M:352:VAL:HG22 | 1:M:355:GLY:H    | 1.56                     | 0.70              |
| 1:B:174:VAL:HG11 | 1:B:384:LEU:HB2  | 1.73                     | 0.70              |
| 1:B:265:LYS:HE2  | 1:B:322:PHE:CE1  | 2.26                     | 0.70              |
| 1:H:484:PHE:CE2  | 1:H:488:ARG:HD3  | 2.26                     | 0.70              |
| 1:K:313:VAL:HG13 | 1:K:352:VAL:HB   | 1.73                     | 0.70              |
| 1:P:411:LEU:HB3  | 1:P:423:MET:CE   | 2.22                     | 0.70              |
| 1:D:364:GLY:HA3  | 1:D:370:LEU:HD13 | 1.73                     | 0.70              |
| 1:H:88:SER:O     | 1:H:92:LEU:HD13  | 1.91                     | 0.70              |
| 1:M:27:LYS:HG3   | 1:M:436:ILE:CG1  | 2.21                     | 0.70              |
| 1:B:325:PRO:O    | 1:B:326:GLU:HG2  | 1.92                     | 0.70              |
| 1:M:214:ASN:O    | 1:M:215:GLN:HB2  | 1.90                     | 0.70              |
| 1:M:236:ILE:HG13 | 1:M:237:LYS:H    | 1.56                     | 0.70              |
| 1:O:89:VAL:HG12  | 1:O:490:VAL:HB   | 1.73                     | 0.70              |
| 1:A:146:LEU:HD23 | 1:A:147:MET:H    | 1.57                     | 0.69              |
| 1:A:258:GLU:OE2  | 1:A:284:TYR:HE2  | 1.75                     | 0.69              |
| 1:D:446:ALA:HB2  | 1:K:418:LYS:HD3  | 1.72                     | 0.69              |
| 1:E:119:GLU:OE1  | 1:E:423:MET:HE1  | 1.91                     | 0.69              |
| 1:H:310:LEU:O    | 1:H:314:THR:HG22 | 1.92                     | 0.69              |
| 1:J:233:THR:HG21 | 1:J:261:LYS:HE2  | 1.71                     | 0.69              |
| 1:J:475:MET:SD   | 1:J:480:ILE:HB   | 2.31                     | 0.69              |
| 1:H:133:VAL:HG22 | 1:H:395:TYR:CE2  | 2.27                     | 0.69              |
| 1:H:341:ILE:HD11 | 1:H:348:HIS:CE1  | 2.27                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:82:VAL:HG21  | 1:J:483:SER:CB   | 2.21                     | 0.69              |
| 1:K:58:LEU:HB3   | 1:K:72:VAL:CG1   | 2.21                     | 0.69              |
| 1:K:186:ILE:HG22 | 1:K:377:LEU:HD21 | 1.74                     | 0.69              |
| 1:L:324:HIS:O    | 1:L:329:LYS:HG2  | 1.92                     | 0.69              |
| 1:N:233:THR:HG21 | 1:N:261:LYS:HE2  | 1.74                     | 0.69              |
| 1:P:92:LEU:HD11  | 1:P:433:LEU:HD21 | 1.74                     | 0.69              |
| 1:K:343:GLU:HG3  | 1:K:344:ASP:N    | 2.06                     | 0.69              |
| 1:F:214:ASN:O    | 1:F:215:GLN:HB2  | 1.90                     | 0.69              |
| 1:J:58:LEU:HB3   | 1:J:72:VAL:CG1   | 2.21                     | 0.69              |
| 1:P:109:HIS:CE1  | 1:P:111:GLN:HB2  | 2.28                     | 0.69              |
| 1:H:112:THR:HG21 | 1:H:418:LYS:HD2  | 1.74                     | 0.69              |
| 1:M:139:GLU:O    | 1:M:140:VAL:HB   | 1.91                     | 0.69              |
| 1:M:226:ILE:HG12 | 1:M:278:ILE:HG23 | 1.74                     | 0.69              |
| 1:O:174:VAL:HG11 | 1:O:384:LEU:HB2  | 1.75                     | 0.69              |
| 1:O:325:PRO:C    | 1:O:326:GLU:HG3  | 2.17                     | 0.69              |
| 1:B:399:CYS:SG   | 1:B:464:GLY:HA3  | 2.33                     | 0.69              |
| 1:D:512:PRO:HB3  | 1:H:60:ASN:CG    | 2.18                     | 0.69              |
| 1:E:30:LEU:CD1   | 1:E:30:LEU:H     | 2.04                     | 0.69              |
| 1:J:269:ILE:HG23 | 1:J:274:ILE:CG2  | 2.23                     | 0.69              |
| 1:B:236:ILE:HG22 | 1:B:237:LYS:H    | 1.58                     | 0.69              |
| 1:E:59:LYS:HE2   | 1:E:76:ARG:HB2   | 1.74                     | 0.69              |
| 1:G:216:PRO:HG2  | 1:G:295:GLY:HA2  | 1.74                     | 0.69              |
| 1:J:216:PRO:HG2  | 1:J:295:GLY:HA2  | 1.75                     | 0.69              |
| 1:K:192:LEU:HB2  | 1:K:343:GLU:CD   | 2.17                     | 0.69              |
| 1:O:96:LEU:HD13  | 1:O:97:LEU:N     | 2.07                     | 0.69              |
| 1:A:92:LEU:HG    | 1:A:433:LEU:HD11 | 1.74                     | 0.69              |
| 1:A:174:VAL:HG12 | 1:A:381:LEU:HD22 | 1.75                     | 0.69              |
| 1:B:59:LYS:NZ    | 1:B:76:ARG:HB2   | 2.08                     | 0.69              |
| 1:B:265:LYS:HZ2  | 1:B:287:PRO:HG3  | 1.56                     | 0.69              |
| 1:E:146:LEU:HD12 | 1:E:171:VAL:HG13 | 1.73                     | 0.69              |
| 1:E:433:LEU:O    | 1:E:436:ILE:HG22 | 1.93                     | 0.69              |
| 1:F:236:ILE:HG22 | 1:F:237:LYS:H    | 1.58                     | 0.69              |
| 1:H:39:LEU:O     | 1:H:48:LEU:HA    | 1.92                     | 0.69              |
| 1:H:74:MET:O     | 1:H:77:VAL:HG12  | 1.93                     | 0.69              |
| 1:H:325:PRO:C    | 1:H:326:GLU:HG3  | 2.16                     | 0.69              |
| 1:K:139:GLU:O    | 1:K:140:VAL:HB   | 1.93                     | 0.69              |
| 1:M:188:VAL:CG1  | 1:M:377:LEU:HD21 | 2.23                     | 0.69              |
| 1:A:139:GLU:OE2  | 1:A:178:LYS:HD3  | 1.93                     | 0.69              |
| 1:B:146:LEU:HD12 | 1:B:171:VAL:CG1  | 2.11                     | 0.69              |
| 1:D:404:MET:HE3  | 1:D:430:LEU:HG   | 1.75                     | 0.69              |
| 1:I:411:LEU:HB3  | 1:I:423:MET:SD   | 2.33                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:219:ILE:HD11 | 1:L:336:ILE:HB   | 1.73                     | 0.69              |
| 1:M:109:HIS:CE1  | 1:M:111:GLN:HB2  | 2.28                     | 0.69              |
| 1:C:191:LYS:HZ1  | 1:C:346:LEU:HD21 | 1.56                     | 0.69              |
| 1:C:269:ILE:HG23 | 1:C:274:ILE:CG2  | 2.23                     | 0.69              |
| 1:I:177:LEU:HG   | 1:I:186:ILE:HD11 | 1.75                     | 0.69              |
| 1:O:65:ASN:O     | 1:O:508:ILE:HB   | 1.93                     | 0.69              |
| 1:P:171:VAL:HA   | 1:P:174:VAL:HG22 | 1.75                     | 0.69              |
| 1:A:19:ALA:HB1   | 1:A:94:ALA:HA    | 1.75                     | 0.68              |
| 1:A:114:ILE:HG21 | 1:A:502:LEU:HB2  | 1.74                     | 0.68              |
| 1:F:58:LEU:HB3   | 1:F:72:VAL:CG1   | 2.23                     | 0.68              |
| 1:J:364:GLY:HA3  | 1:J:370:LEU:HD13 | 1.75                     | 0.68              |
| 1:M:216:PRO:HG2  | 1:M:295:GLY:HA2  | 1.74                     | 0.68              |
| 1:N:59:LYS:HE2   | 1:N:76:ARG:HB2   | 1.73                     | 0.68              |
| 1:O:166:PHE:CZ   | 1:O:198:ASP:HB3  | 2.28                     | 0.68              |
| 1:P:324:HIS:HB2  | 1:P:329:LYS:NZ   | 2.08                     | 0.68              |
| 1:B:269:ILE:HG23 | 1:B:274:ILE:HG22 | 1.75                     | 0.68              |
| 1:B:317:GLU:HB2  | 1:B:329:LYS:HG2  | 1.75                     | 0.68              |
| 1:C:269:ILE:HG23 | 1:C:274:ILE:HG21 | 1.74                     | 0.68              |
| 1:L:146:LEU:CD2  | 1:L:147:MET:H    | 2.06                     | 0.68              |
| 1:P:129:LEU:HD22 | 1:P:129:LEU:N    | 2.08                     | 0.68              |
| 1:H:486:VAL:O    | 1:H:490:VAL:HG13 | 1.93                     | 0.68              |
| 1:J:316:GLY:O    | 1:J:330:LEU:HB2  | 1.93                     | 0.68              |
| 1:M:59:LYS:HE2   | 1:M:76:ARG:CB    | 2.23                     | 0.68              |
| 1:A:269:ILE:HG23 | 1:A:274:ILE:CG2  | 2.24                     | 0.68              |
| 1:K:316:GLY:O    | 1:K:330:LEU:HB2  | 1.94                     | 0.68              |
| 1:N:183:LEU:CD2  | 1:N:381:LEU:HD11 | 2.24                     | 0.68              |
| 1:E:74:MET:O     | 1:E:77:VAL:HG12  | 1.94                     | 0.68              |
| 1:E:283:ILE:HG22 | 1:E:300:GLU:HG3  | 1.73                     | 0.68              |
| 1:I:317:GLU:HB3  | 1:I:329:LYS:HD3  | 1.74                     | 0.68              |
| 1:L:159:LEU:HD23 | 1:L:163:LYS:CD   | 2.23                     | 0.68              |
| 1:A:78:GLN:NE2   | 1:A:486:VAL:HA   | 2.09                     | 0.68              |
| 1:B:402:MET:SD   | 1:B:456:HIS:HB2  | 2.33                     | 0.68              |
| 1:F:178:LYS:HE2  | 1:F:388:VAL:HG21 | 1.75                     | 0.68              |
| 1:F:508:ILE:HG22 | 1:F:509:LYS:H    | 1.58                     | 0.68              |
| 1:G:99:GLU:CD    | 1:G:425:SER:HB2  | 2.19                     | 0.68              |
| 1:G:214:ASN:O    | 1:G:215:GLN:HB2  | 1.92                     | 0.68              |
| 1:G:398:GLY:HA2  | 1:G:401:GLU:OE1  | 1.94                     | 0.68              |
| 1:J:96:LEU:HD11  | 1:J:117:TRP:HZ2  | 1.58                     | 0.68              |
| 1:J:216:PRO:CG   | 1:J:295:GLY:HA2  | 2.23                     | 0.68              |
| 1:L:92:LEU:HD11  | 1:L:433:LEU:HD21 | 1.75                     | 0.68              |
| 1:N:448:LEU:HD21 | 1:N:465:LEU:HD12 | 1.75                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:324:HIS:O    | 1:O:329:LYS:HG2  | 1.94                     | 0.68              |
| 1:G:146:LEU:HD21 | 1:G:167:THR:HG23 | 1.75                     | 0.68              |
| 1:G:418:LYS:HB2  | 1:N:449:VAL:HG11 | 1.75                     | 0.68              |
| 1:K:171:VAL:HG12 | 1:K:384:LEU:HG   | 1.74                     | 0.68              |
| 1:F:54:GLY:HA3   | 1:F:87:THR:HG21  | 1.75                     | 0.68              |
| 1:J:59:LYS:CE    | 1:J:76:ARG:HB2   | 2.24                     | 0.68              |
| 1:J:63:VAL:HG21  | 1:K:1:ALA:HA     | 1.75                     | 0.68              |
| 1:A:159:LEU:HG   | 1:A:163:LYS:HD3  | 1.75                     | 0.68              |
| 1:A:188:VAL:HG11 | 1:A:377:LEU:HD22 | 1.75                     | 0.68              |
| 1:E:38:ILE:O     | 1:G:508:ILE:HG21 | 1.92                     | 0.68              |
| 1:I:434:PRO:HB3  | 1:I:452:LEU:CD2  | 2.24                     | 0.68              |
| 1:J:341:ILE:HG23 | 1:J:363:ARG:NH2  | 2.09                     | 0.68              |
| 1:N:152:THR:OG1  | 1:N:480:ILE:HG23 | 1.94                     | 0.68              |
| 1:O:365:ALA:O    | 1:O:366:THR:HB   | 1.92                     | 0.68              |
| 1:F:59:LYS:HE2   | 1:F:76:ARG:HB2   | 1.75                     | 0.68              |
| 1:H:189:ILE:O    | 1:H:190:LYS:HB3  | 1.92                     | 0.68              |
| 1:J:74:MET:O     | 1:J:77:VAL:HG12  | 1.94                     | 0.68              |
| 1:M:433:LEU:O    | 1:M:436:ILE:HG22 | 1.94                     | 0.68              |
| 1:O:316:GLY:O    | 1:O:330:LEU:HB2  | 1.94                     | 0.68              |
| 1:A:369:ILE:O    | 1:A:372:GLU:HB3  | 1.94                     | 0.67              |
| 1:D:145:ASP:OD1  | 1:D:171:VAL:HB   | 1.94                     | 0.67              |
| 1:L:161:HIS:CD2  | 1:L:162:HIS:H    | 2.13                     | 0.67              |
| 1:M:399:CYS:SG   | 1:M:464:GLY:HA3  | 2.34                     | 0.67              |
| 1:O:265:LYS:HE2  | 1:O:322:PHE:CE2  | 2.30                     | 0.67              |
| 1:A:325:PRO:O    | 1:A:328:VAL:HG23 | 1.95                     | 0.67              |
| 1:F:27:LYS:CB    | 1:F:436:ILE:HD11 | 2.23                     | 0.67              |
| 1:F:146:LEU:HD13 | 1:F:168:LYS:HA   | 1.76                     | 0.67              |
| 1:K:58:LEU:HB3   | 1:K:72:VAL:HG13  | 1.76                     | 0.67              |
| 1:O:483:SER:O    | 1:O:486:VAL:HG22 | 1.94                     | 0.67              |
| 1:P:99:GLU:HG2   | 1:P:425:SER:HB2  | 1.75                     | 0.67              |
| 1:P:128:LEU:CD2  | 1:P:488:ARG:HG2  | 2.25                     | 0.67              |
| 1:B:190:LYS:HE2  | 1:B:371:ASP:OD1  | 1.94                     | 0.67              |
| 1:C:219:ILE:HD11 | 1:C:336:ILE:HB   | 1.76                     | 0.67              |
| 1:H:283:ILE:HG22 | 1:H:300:GLU:HG3  | 1.76                     | 0.67              |
| 1:J:145:ASP:O    | 1:J:171:VAL:HG11 | 1.94                     | 0.67              |
| 1:O:74:MET:O     | 1:O:77:VAL:HG12  | 1.94                     | 0.67              |
| 1:C:163:LYS:O    | 1:C:166:PHE:HB2  | 1.94                     | 0.67              |
| 1:D:504:VAL:HG21 | 1:H:38:ILE:HG12  | 1.76                     | 0.67              |
| 1:K:171:VAL:O    | 1:K:174:VAL:HG22 | 1.94                     | 0.67              |
| 1:L:475:MET:SD   | 1:L:480:ILE:HB   | 2.35                     | 0.67              |
| 1:M:101:GLU:O    | 1:M:104:ILE:HG12 | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:324:HIS:O    | 1:N:328:VAL:HG22 | 1.95                     | 0.67              |
| 1:B:159:LEU:HD23 | 1:B:163:LYS:HG2  | 1.75                     | 0.67              |
| 1:D:418:LYS:HG3  | 1:K:450:ALA:HB2  | 1.75                     | 0.67              |
| 1:E:38:ILE:HG22  | 1:E:50:VAL:HB    | 1.76                     | 0.67              |
| 1:H:157:LYS:HB3  | 1:H:159:LEU:HD11 | 1.77                     | 0.67              |
| 1:H:411:LEU:O    | 1:H:414:ARG:HB3  | 1.95                     | 0.67              |
| 1:I:166:PHE:HD2  | 1:I:362:LEU:HD22 | 1.58                     | 0.67              |
| 1:N:159:LEU:HG   | 1:N:163:LYS:CD   | 2.24                     | 0.67              |
| 1:D:402:MET:SD   | 1:D:456:HIS:HB2  | 2.34                     | 0.67              |
| 1:H:177:LEU:HD11 | 1:H:186:ILE:HD11 | 1.76                     | 0.67              |
| 1:O:58:LEU:HB3   | 1:O:72:VAL:HG13  | 1.77                     | 0.67              |
| 1:O:511:ALA:N    | 1:O:512:PRO:HD3  | 2.09                     | 0.67              |
| 1:A:317:GLU:HB2  | 1:A:329:LYS:HG2  | 1.74                     | 0.67              |
| 1:A:483:SER:O    | 1:A:486:VAL:HG22 | 1.94                     | 0.67              |
| 1:C:266:VAL:HB   | 1:C:290:LEU:HD21 | 1.74                     | 0.67              |
| 1:F:188:VAL:CG2  | 1:F:377:LEU:HD21 | 2.25                     | 0.67              |
| 1:H:145:ASP:O    | 1:H:171:VAL:HG11 | 1.94                     | 0.67              |
| 1:I:438:ALA:CB   | 1:I:448:LEU:HG   | 2.24                     | 0.67              |
| 1:J:146:LEU:CD2  | 1:J:147:MET:H    | 2.08                     | 0.67              |
| 1:F:511:ALA:CB   | 1:F:512:PRO:HD2  | 2.23                     | 0.67              |
| 1:O:269:ILE:HG23 | 1:O:274:ILE:HG21 | 1.76                     | 0.67              |
| 1:B:452:LEU:HD13 | 1:B:465:LEU:HD13 | 1.75                     | 0.67              |
| 1:D:6:GLU:HB3    | 1:D:10:THR:OG1   | 1.95                     | 0.67              |
| 1:F:508:ILE:HG22 | 1:F:509:LYS:N    | 2.09                     | 0.67              |
| 1:J:38:ILE:H     | 1:J:38:ILE:HD12  | 1.60                     | 0.67              |
| 1:N:324:HIS:HB2  | 1:N:329:LYS:NZ   | 2.09                     | 0.67              |
| 1:B:192:LEU:HB3  | 1:B:343:GLU:OE2  | 1.95                     | 0.67              |
| 1:B:512:PRO:HB3  | 1:G:39:LEU:HB3   | 1.76                     | 0.67              |
| 1:J:265:LYS:HE2  | 1:J:322:PHE:CE1  | 2.30                     | 0.67              |
| 1:K:204:GLY:O    | 1:K:359:THR:HB   | 1.95                     | 0.67              |
| 1:N:139:GLU:O    | 1:N:140:VAL:HB   | 1.95                     | 0.67              |
| 1:O:145:ASP:O    | 1:O:171:VAL:HG11 | 1.95                     | 0.67              |
| 1:D:448:LEU:HD21 | 1:D:465:LEU:HD12 | 1.76                     | 0.66              |
| 1:G:207:LEU:O    | 1:G:347:ILE:HG22 | 1.94                     | 0.66              |
| 1:G:325:PRO:O    | 1:G:326:GLU:HG2  | 1.95                     | 0.66              |
| 1:H:58:LEU:HB3   | 1:H:72:VAL:HG13  | 1.74                     | 0.66              |
| 1:L:174:VAL:HG11 | 1:L:384:LEU:HB2  | 1.76                     | 0.66              |
| 1:G:171:VAL:HG12 | 1:G:384:LEU:HG   | 1.76                     | 0.66              |
| 1:J:51:THR:HG21  | 1:J:56:THR:HB    | 1.77                     | 0.66              |
| 1:K:59:LYS:HE2   | 1:K:76:ARG:HB2   | 1.76                     | 0.66              |
| 1:M:497:ALA:O    | 1:M:500:VAL:HG22 | 1.96                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:146:LEU:HD23 | 1:P:147:MET:H    | 1.59                     | 0.66              |
| 1:P:402:MET:SD   | 1:P:456:HIS:HB2  | 2.35                     | 0.66              |
| 1:A:82:VAL:HG13  | 1:A:83:GLY:H     | 1.58                     | 0.66              |
| 1:B:124:ALA:HA   | 1:B:491:LEU:HD13 | 1.78                     | 0.66              |
| 1:D:446:ALA:CB   | 1:K:418:LYS:HD3  | 2.24                     | 0.66              |
| 1:H:32:PRO:HD2   | 1:H:467:MET:CE   | 2.25                     | 0.66              |
| 1:H:191:LYS:HG2  | 1:H:341:ILE:CG2  | 2.25                     | 0.66              |
| 1:I:32:PRO:HA    | 1:I:155:SER:O    | 1.95                     | 0.66              |
| 1:I:128:LEU:HD22 | 1:I:484:PHE:CE2  | 2.29                     | 0.66              |
| 1:L:138:ASP:O    | 1:L:139:GLU:HB2  | 1.94                     | 0.66              |
| 1:C:372:GLU:HG3  | 1:C:375:ARG:CZ   | 2.25                     | 0.66              |
| 1:F:324:HIS:HB2  | 1:F:329:LYS:NZ   | 2.11                     | 0.66              |
| 1:G:101:GLU:O    | 1:G:104:ILE:HG12 | 1.94                     | 0.66              |
| 1:G:146:LEU:HD23 | 1:G:147:MET:N    | 2.09                     | 0.66              |
| 1:J:101:GLU:O    | 1:J:104:ILE:HG12 | 1.96                     | 0.66              |
| 1:J:146:LEU:HD12 | 1:J:171:VAL:CG1  | 2.19                     | 0.66              |
| 1:J:324:HIS:HB2  | 1:J:329:LYS:NZ   | 2.09                     | 0.66              |
| 1:L:316:GLY:O    | 1:L:330:LEU:HB2  | 1.96                     | 0.66              |
| 1:M:503:ARG:HH11 | 1:M:503:ARG:HG3  | 1.61                     | 0.66              |
| 1:A:163:LYS:HA   | 1:A:166:PHE:CD1  | 2.30                     | 0.66              |
| 1:C:111:GLN:O    | 1:C:114:ILE:HB   | 1.95                     | 0.66              |
| 1:H:38:ILE:HD12  | 1:H:48:LEU:HD22  | 1.78                     | 0.66              |
| 1:H:130:ASN:O    | 1:H:131:SER:HB3  | 1.93                     | 0.66              |
| 1:I:52:ASN:HD21  | 1:I:157:LYS:HD3  | 1.59                     | 0.66              |
| 1:I:74:MET:O     | 1:I:77:VAL:HG12  | 1.94                     | 0.66              |
| 1:I:146:LEU:CD1  | 1:I:171:VAL:HG13 | 2.24                     | 0.66              |
| 1:K:100:ALA:HA   | 1:K:103:LEU:HD22 | 1.77                     | 0.66              |
| 1:L:216:PRO:HG2  | 1:L:295:GLY:HA2  | 1.77                     | 0.66              |
| 1:M:166:PHE:CE1  | 1:M:198:ASP:HB3  | 2.31                     | 0.66              |
| 1:P:79:ASP:HA    | 1:P:83:GLY:CA    | 2.24                     | 0.66              |
| 1:A:397:GLY:HA3  | 1:A:475:MET:HE3  | 1.78                     | 0.66              |
| 1:C:39:LEU:HD12  | 1:C:57:ILE:HD11  | 1.76                     | 0.66              |
| 1:D:269:ILE:HG23 | 1:D:274:ILE:HG21 | 1.75                     | 0.66              |
| 1:F:452:LEU:HD13 | 1:F:465:LEU:HD13 | 1.78                     | 0.66              |
| 1:K:324:HIS:O    | 1:K:329:LYS:HG2  | 1.96                     | 0.66              |
| 1:O:59:LYS:HE2   | 1:O:76:ARG:HB2   | 1.78                     | 0.66              |
| 1:A:164:ASP:O    | 1:A:167:THR:HG22 | 1.95                     | 0.66              |
| 1:A:324:HIS:HB2  | 1:A:329:LYS:HZ3  | 1.59                     | 0.66              |
| 1:D:265:LYS:O    | 1:D:269:ILE:HB   | 1.96                     | 0.66              |
| 1:F:16:PHE:HA    | 1:F:97:LEU:HD23  | 1.77                     | 0.66              |
| 1:F:511:ALA:HB1  | 1:F:512:PRO:CD   | 2.22                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:390:ASP:HB3  | 1:H:485:GLN:OE1  | 1.96                     | 0.66              |
| 1:I:59:LYS:HE2   | 1:I:76:ARG:HB2   | 1.78                     | 0.66              |
| 1:I:483:SER:O    | 1:I:486:VAL:HG22 | 1.96                     | 0.66              |
| 1:N:204:GLY:HA3  | 1:N:349:PHE:O    | 1.95                     | 0.66              |
| 1:P:269:ILE:HG23 | 1:P:274:ILE:HG21 | 1.77                     | 0.66              |
| 1:C:211:ILE:H    | 1:C:211:ILE:HD12 | 1.61                     | 0.66              |
| 1:C:369:ILE:O    | 1:C:372:GLU:HB3  | 1.96                     | 0.66              |
| 1:C:448:LEU:HD21 | 1:C:465:LEU:HD12 | 1.77                     | 0.66              |
| 1:F:32:PRO:HD2   | 1:F:467:MET:CE   | 2.25                     | 0.66              |
| 1:G:146:LEU:CD2  | 1:G:147:MET:H    | 2.06                     | 0.66              |
| 1:L:411:LEU:HB3  | 1:L:423:MET:SD   | 2.36                     | 0.66              |
| 1:N:146:LEU:HD22 | 1:N:147:MET:N    | 2.11                     | 0.66              |
| 1:O:111:GLN:HA   | 1:O:114:ILE:HG12 | 1.78                     | 0.66              |
| 1:O:398:GLY:HA2  | 1:O:401:GLU:OE1  | 1.96                     | 0.66              |
| 1:B:213:VAL:HG11 | 1:F:304:PHE:CE1  | 2.31                     | 0.66              |
| 1:F:101:GLU:O    | 1:F:104:ILE:HG12 | 1.95                     | 0.66              |
| 1:G:438:ALA:HB2  | 1:G:448:LEU:HG   | 1.76                     | 0.66              |
| 1:I:324:HIS:ND1  | 1:I:325:PRO:HD3  | 2.11                     | 0.66              |
| 1:O:233:THR:O    | 1:O:234:ASP:HB3  | 1.94                     | 0.66              |
| 1:C:171:VAL:HG12 | 1:C:384:LEU:HG   | 1.78                     | 0.65              |
| 1:H:96:LEU:HD11  | 1:H:117:TRP:HZ2  | 1.61                     | 0.65              |
| 1:J:206:LEU:HD11 | 1:J:346:LEU:HD21 | 1.78                     | 0.65              |
| 1:K:192:LEU:HA   | 1:K:366:THR:CG2  | 2.27                     | 0.65              |
| 1:L:402:MET:SD   | 1:L:453:ARG:HA   | 2.36                     | 0.65              |
| 1:E:402:MET:SD   | 1:E:456:HIS:HB2  | 2.37                     | 0.65              |
| 1:J:433:LEU:O    | 1:J:436:ILE:HG22 | 1.96                     | 0.65              |
| 1:M:188:VAL:HG13 | 1:M:377:LEU:HD21 | 1.78                     | 0.65              |
| 1:N:101:GLU:O    | 1:N:104:ILE:HG12 | 1.96                     | 0.65              |
| 1:N:154:LEU:HD22 | 1:N:167:THR:HB   | 1.79                     | 0.65              |
| 1:O:130:ASN:O    | 1:O:131:SER:HB3  | 1.95                     | 0.65              |
| 1:P:408:VAL:HA   | 1:P:411:LEU:HD12 | 1.79                     | 0.65              |
| 1:P:411:LEU:HB3  | 1:P:423:MET:HE2  | 1.77                     | 0.65              |
| 1:B:51:THR:HG21  | 1:B:56:THR:HB    | 1.78                     | 0.65              |
| 1:B:154:LEU:HD23 | 1:B:163:LYS:HG3  | 1.78                     | 0.65              |
| 1:D:141:LYS:HG2  | 1:D:144:GLN:HB2  | 1.77                     | 0.65              |
| 1:L:452:LEU:HD13 | 1:L:465:LEU:HD13 | 1.79                     | 0.65              |
| 1:O:35:MET:HE1   | 1:O:440:ASN:HB2  | 1.77                     | 0.65              |
| 1:A:434:PRO:HB3  | 1:A:452:LEU:CD2  | 2.26                     | 0.65              |
| 1:E:139:GLU:HG2  | 1:E:140:VAL:HG23 | 1.79                     | 0.65              |
| 1:L:43:GLY:O     | 1:L:44:ARG:HG2   | 1.95                     | 0.65              |
| 1:M:112:THR:HG21 | 1:M:418:LYS:NZ   | 2.10                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:411:LEU:HB3  | 1:O:423:MET:SD   | 2.37                     | 0.65              |
| 1:P:6:GLU:HB3    | 1:P:11:ALA:HB2   | 1.79                     | 0.65              |
| 1:C:159:LEU:HG   | 1:C:163:LYS:HG2  | 1.78                     | 0.65              |
| 1:E:145:ASP:OD1  | 1:E:171:VAL:HB   | 1.96                     | 0.65              |
| 1:F:188:VAL:HG23 | 1:F:360:ILE:O    | 1.96                     | 0.65              |
| 1:B:59:LYS:HE2   | 1:B:76:ARG:HB2   | 1.78                     | 0.65              |
| 1:G:33:LYS:N     | 1:G:33:LYS:HD2   | 2.11                     | 0.65              |
| 1:N:146:LEU:CD2  | 1:N:147:MET:H    | 2.08                     | 0.65              |
| 1:N:150:ALA:HB2  | 1:N:384:LEU:HD11 | 1.78                     | 0.65              |
| 1:P:27:LYS:HB2   | 1:P:436:ILE:HD11 | 1.77                     | 0.65              |
| 1:A:511:ALA:O    | 1:F:25:LEU:HG    | 1.97                     | 0.65              |
| 1:B:372:GLU:O    | 1:B:375:ARG:HB3  | 1.96                     | 0.65              |
| 1:F:128:LEU:O    | 1:F:129:LEU:HD22 | 1.97                     | 0.65              |
| 1:J:341:ILE:HD12 | 1:J:346:LEU:HD23 | 1.78                     | 0.65              |
| 1:L:32:PRO:HD2   | 1:L:467:MET:HE1  | 1.78                     | 0.65              |
| 1:L:99:GLU:HG2   | 1:L:425:SER:HB2  | 1.79                     | 0.65              |
| 1:A:379:ASP:O    | 1:A:383:VAL:HG23 | 1.97                     | 0.65              |
| 1:B:216:PRO:CG   | 1:B:295:GLY:HA2  | 2.27                     | 0.65              |
| 1:C:418:LYS:HA   | 1:L:453:ARG:CZ   | 2.26                     | 0.65              |
| 1:C:483:SER:O    | 1:C:486:VAL:HG22 | 1.97                     | 0.65              |
| 1:D:74:MET:O     | 1:D:77:VAL:HG12  | 1.96                     | 0.65              |
| 1:F:438:ALA:HB2  | 1:F:448:LEU:HG   | 1.78                     | 0.65              |
| 1:I:31:GLY:O     | 1:I:156:SER:HA   | 1.96                     | 0.65              |
| 1:M:163:LYS:HA   | 1:M:166:PHE:CD1  | 2.32                     | 0.65              |
| 1:N:369:ILE:O    | 1:N:372:GLU:HB3  | 1.97                     | 0.65              |
| 1:P:483:SER:O    | 1:P:486:VAL:HG22 | 1.96                     | 0.65              |
| 1:C:394:VAL:HG21 | 1:C:487:LYS:HG3  | 1.78                     | 0.65              |
| 1:I:124:ALA:HA   | 1:I:491:LEU:CD1  | 2.27                     | 0.65              |
| 1:O:146:LEU:HD23 | 1:O:147:MET:N    | 2.11                     | 0.65              |
| 1:O:152:THR:OG1  | 1:O:480:ILE:HG23 | 1.97                     | 0.65              |
| 1:A:74:MET:O     | 1:A:77:VAL:HG12  | 1.96                     | 0.65              |
| 1:B:141:LYS:HG2  | 1:B:144:GLN:HB2  | 1.79                     | 0.65              |
| 1:C:219:ILE:HD12 | 1:C:275:ASN:HB3  | 1.78                     | 0.65              |
| 1:D:325:PRO:C    | 1:D:326:GLU:HG3  | 2.22                     | 0.65              |
| 1:E:163:LYS:HA   | 1:E:166:PHE:CD1  | 2.32                     | 0.65              |
| 1:F:82:VAL:CG2   | 1:F:485:GLN:HG2  | 2.27                     | 0.65              |
| 1:G:79:ASP:HA    | 1:G:82:VAL:O     | 1.97                     | 0.65              |
| 1:H:216:PRO:CG   | 1:H:295:GLY:HA2  | 2.27                     | 0.65              |
| 1:J:140:VAL:HA   | 1:J:175:LEU:HD22 | 1.79                     | 0.65              |
| 1:J:324:HIS:ND1  | 1:J:325:PRO:HD3  | 2.11                     | 0.65              |
| 1:K:38:ILE:HG22  | 1:K:50:VAL:HB    | 1.79                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:140:VAL:HA   | 1:L:175:LEU:HD22 | 1.79                     | 0.65              |
| 1:P:276:CYS:HA   | 1:P:297:MET:O    | 1.96                     | 0.65              |
| 1:B:159:LEU:HD13 | 1:B:159:LEU:H    | 1.61                     | 0.64              |
| 1:C:160:THR:HA   | 1:C:163:LYS:HB3  | 1.79                     | 0.64              |
| 1:O:146:LEU:HD12 | 1:O:171:VAL:CG1  | 2.15                     | 0.64              |
| 1:A:145:ASP:O    | 1:A:171:VAL:HG11 | 1.97                     | 0.64              |
| 1:C:418:LYS:HD3  | 1:L:450:ALA:HB1  | 1.77                     | 0.64              |
| 1:E:154:LEU:HD21 | 1:E:163:LYS:NZ   | 2.12                     | 0.64              |
| 1:I:438:ALA:HB2  | 1:I:448:LEU:HG   | 1.77                     | 0.64              |
| 1:J:128:LEU:O    | 1:J:129:LEU:HB3  | 1.97                     | 0.64              |
| 1:J:236:ILE:HG23 | 1:J:237:LYS:N    | 2.12                     | 0.64              |
| 1:O:112:THR:HG22 | 1:O:418:LYS:HE3  | 1.77                     | 0.64              |
| 1:D:324:HIS:ND1  | 1:D:325:PRO:HD3  | 2.12                     | 0.64              |
| 1:F:41:SER:HB3   | 1:F:45:ASP:OD2   | 1.97                     | 0.64              |
| 1:F:108:ILE:CD1  | 1:O:446:ALA:HB3  | 2.28                     | 0.64              |
| 1:H:492:LEU:HD13 | 1:H:492:LEU:C    | 2.22                     | 0.64              |
| 1:I:128:LEU:HD22 | 1:I:484:PHE:CZ   | 2.32                     | 0.64              |
| 1:N:134:ASP:OD1  | 1:N:392:ARG:HA   | 1.98                     | 0.64              |
| 1:N:433:LEU:O    | 1:N:436:ILE:HG22 | 1.96                     | 0.64              |
| 1:P:84:ASP:OD1   | 1:P:383:VAL:HG22 | 1.98                     | 0.64              |
| 1:P:265:LYS:HE2  | 1:P:322:PHE:CE1  | 2.33                     | 0.64              |
| 1:B:512:PRO:HB3  | 1:G:39:LEU:HD13  | 1.79                     | 0.64              |
| 1:C:216:PRO:CG   | 1:C:295:GLY:HA2  | 2.28                     | 0.64              |
| 1:F:176:ARG:NE   | 1:F:358:CYS:HB2  | 2.13                     | 0.64              |
| 1:O:372:GLU:HG3  | 1:O:375:ARG:NH1  | 2.12                     | 0.64              |
| 1:P:190:LYS:HA   | 1:P:362:LEU:O    | 1.97                     | 0.64              |
| 1:A:146:LEU:HD21 | 1:A:150:ALA:HB3  | 1.80                     | 0.64              |
| 1:B:146:LEU:HD23 | 1:B:147:MET:N    | 2.13                     | 0.64              |
| 1:B:341:ILE:HG22 | 1:B:363:ARG:NH2  | 2.10                     | 0.64              |
| 1:F:483:SER:O    | 1:F:486:VAL:HG22 | 1.97                     | 0.64              |
| 1:J:63:VAL:CG2   | 1:K:1:ALA:HA     | 2.27                     | 0.64              |
| 1:K:99:GLU:HG2   | 1:K:425:SER:CB   | 2.28                     | 0.64              |
| 1:L:209:LYS:CE   | 1:L:302:ALA:HA   | 2.28                     | 0.64              |
| 1:L:397:GLY:HA3  | 1:L:475:MET:HE3  | 1.80                     | 0.64              |
| 1:P:146:LEU:HD22 | 1:P:168:LYS:CA   | 2.28                     | 0.64              |
| 1:P:269:ILE:HG23 | 1:P:274:ILE:CG2  | 2.28                     | 0.64              |
| 1:B:38:ILE:HG23  | 1:B:50:VAL:HB    | 1.80                     | 0.64              |
| 1:B:106:LYS:HB3  | 1:I:446:ALA:CB   | 2.28                     | 0.64              |
| 1:E:188:VAL:HG11 | 1:E:377:LEU:HD22 | 1.79                     | 0.64              |
| 1:F:402:MET:SD   | 1:F:453:ARG:HA   | 2.37                     | 0.64              |
| 1:I:38:ILE:HG21  | 1:N:506:ASN:ND2  | 2.12                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:119:GLU:O    | 1:J:122:LYS:HB3  | 1.97                     | 0.64              |
| 1:N:216:PRO:HG2  | 1:N:295:GLY:HA2  | 1.78                     | 0.64              |
| 1:P:59:LYS:HE2   | 1:P:76:ARG:HB2   | 1.79                     | 0.64              |
| 1:G:78:GLN:NE2   | 1:G:486:VAL:HA   | 2.12                     | 0.64              |
| 1:I:74:MET:SD    | 1:I:74:MET:C     | 2.81                     | 0.64              |
| 1:M:39:LEU:HD22  | 1:O:3:ALA:HB3    | 1.79                     | 0.64              |
| 1:N:219:ILE:HD12 | 1:N:275:ASN:HB3  | 1.80                     | 0.64              |
| 1:N:317:GLU:OE1  | 1:N:329:LYS:HD2  | 1.98                     | 0.64              |
| 1:P:188:VAL:HG11 | 1:P:377:LEU:HD21 | 1.79                     | 0.64              |
| 1:D:475:MET:SD   | 1:D:480:ILE:HB   | 2.38                     | 0.64              |
| 1:I:183:LEU:O    | 1:I:184:GLU:HG3  | 1.97                     | 0.64              |
| 1:J:138:ASP:O    | 1:J:139:GLU:HB2  | 1.98                     | 0.64              |
| 1:L:216:PRO:CG   | 1:L:295:GLY:HA2  | 2.28                     | 0.64              |
| 1:A:231:MET:HB2  | 1:A:284:TYR:H    | 1.63                     | 0.64              |
| 1:A:250:LYS:O    | 1:A:253:GLU:HG2  | 1.97                     | 0.64              |
| 1:D:160:THR:HA   | 1:D:163:LYS:HB3  | 1.80                     | 0.64              |
| 1:E:482:GLU:OE1  | 1:E:487:LYS:HE3  | 1.98                     | 0.64              |
| 1:H:146:LEU:HD12 | 1:H:171:VAL:CG1  | 2.25                     | 0.64              |
| 1:H:324:HIS:ND1  | 1:H:325:PRO:HD3  | 2.12                     | 0.64              |
| 1:H:402:MET:SD   | 1:H:453:ARG:HA   | 2.38                     | 0.64              |
| 1:L:497:ALA:O    | 1:L:500:VAL:HG22 | 1.97                     | 0.64              |
| 1:O:114:ILE:HA   | 1:O:117:TRP:CZ3  | 2.33                     | 0.64              |
| 1:P:222:ALA:HA   | 1:P:275:ASN:OD1  | 1.97                     | 0.64              |
| 1:B:89:VAL:HG12  | 1:B:490:VAL:HB   | 1.79                     | 0.64              |
| 1:G:364:GLY:HA3  | 1:G:370:LEU:CD1  | 2.28                     | 0.64              |
| 1:G:433:LEU:O    | 1:G:436:ILE:HG22 | 1.98                     | 0.64              |
| 1:I:248:THR:O    | 1:I:251:VAL:HG12 | 1.98                     | 0.64              |
| 1:K:210:LYS:HE2  | 1:K:212:GLY:O    | 1.97                     | 0.64              |
| 1:O:324:HIS:ND1  | 1:O:325:PRO:HD3  | 2.12                     | 0.64              |
| 1:A:82:VAL:HA    | 1:A:386:GLN:CD   | 2.23                     | 0.63              |
| 1:A:364:GLY:HA3  | 1:A:370:LEU:CD1  | 2.28                     | 0.63              |
| 1:B:418:LYS:HG3  | 1:I:450:ALA:HB2  | 1.80                     | 0.63              |
| 1:C:208:ASP:O    | 1:C:209:LYS:HG3  | 1.98                     | 0.63              |
| 1:D:58:LEU:HB3   | 1:D:72:VAL:CG1   | 2.28                     | 0.63              |
| 1:K:146:LEU:CD1  | 1:K:171:VAL:HG13 | 2.26                     | 0.63              |
| 1:O:231:MET:HG3  | 1:O:283:ILE:HG13 | 1.80                     | 0.63              |
| 1:O:324:HIS:HB2  | 1:O:329:LYS:NZ   | 2.13                     | 0.63              |
| 1:P:173:ALA:CB   | 1:P:360:ILE:HD11 | 2.28                     | 0.63              |
| 1:P:245:VAL:HG11 | 1:P:250:LYS:HB2  | 1.81                     | 0.63              |
| 1:B:192:LEU:HD23 | 1:B:366:THR:HG22 | 1.79                     | 0.63              |
| 1:B:446:ALA:CB   | 1:I:107:LYS:HB2  | 2.28                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:246:ASP:O    | 1:D:247:SER:HB3  | 1.98                     | 0.63              |
| 1:K:99:GLU:HG2   | 1:K:425:SER:HB2  | 1.81                     | 0.63              |
| 1:K:190:LYS:HB2  | 1:K:370:LEU:HD21 | 1.79                     | 0.63              |
| 1:A:109:HIS:CE1  | 1:A:111:GLN:HB2  | 2.33                     | 0.63              |
| 1:A:418:LYS:HD3  | 1:M:450:ALA:HB2  | 1.79                     | 0.63              |
| 1:B:48:LEU:HD21  | 1:F:506:ASN:CG   | 2.22                     | 0.63              |
| 1:B:130:ASN:O    | 1:B:131:SER:HB2  | 1.97                     | 0.63              |
| 1:D:79:ASP:HA    | 1:D:83:GLY:HA3   | 1.78                     | 0.63              |
| 1:F:236:ILE:HG22 | 1:F:237:LYS:N    | 2.13                     | 0.63              |
| 1:G:58:LEU:HB3   | 1:G:72:VAL:HG11  | 1.81                     | 0.63              |
| 1:M:59:LYS:HE3   | 1:M:73:ASP:HA    | 1.79                     | 0.63              |
| 1:N:99:GLU:HG2   | 1:N:425:SER:HB2  | 1.80                     | 0.63              |
| 1:A:89:VAL:HB    | 1:A:490:VAL:HG23 | 1.80                     | 0.63              |
| 1:B:145:ASP:OD1  | 1:B:171:VAL:HB   | 1.99                     | 0.63              |
| 1:B:513:ARG:HG3  | 1:G:45:ASP:OD2   | 1.99                     | 0.63              |
| 1:C:451:GLN:NE2  | 1:C:471:THR:HA   | 2.13                     | 0.63              |
| 1:L:206:LEU:HD21 | 1:L:346:LEU:HD23 | 1.78                     | 0.63              |
| 1:L:390:ASP:HB3  | 1:L:485:GLN:OE1  | 1.97                     | 0.63              |
| 1:M:65:ASN:HA    | 1:M:510:ALA:CB   | 2.28                     | 0.63              |
| 1:P:231:MET:HG3  | 1:P:283:ILE:HG13 | 1.81                     | 0.63              |
| 1:P:369:ILE:O    | 1:P:372:GLU:HB3  | 1.98                     | 0.63              |
| 1:B:483:SER:O    | 1:B:486:VAL:HG22 | 1.99                     | 0.63              |
| 1:E:141:LYS:HG2  | 1:E:144:GLN:HB2  | 1.80                     | 0.63              |
| 1:H:138:ASP:O    | 1:H:139:GLU:HB2  | 1.97                     | 0.63              |
| 1:I:123:ALA:HA   | 1:I:126:GLN:HE21 | 1.64                     | 0.63              |
| 1:I:188:VAL:HG13 | 1:I:377:LEU:HD21 | 1.80                     | 0.63              |
| 1:J:82:VAL:HA    | 1:J:386:GLN:CB   | 2.29                     | 0.63              |
| 1:C:58:LEU:HB3   | 1:C:72:VAL:HG11  | 1.79                     | 0.63              |
| 1:F:163:LYS:HG3  | 1:F:166:PHE:CE2  | 2.34                     | 0.63              |
| 1:K:133:VAL:HA   | 1:K:393:THR:O    | 1.99                     | 0.63              |
| 1:K:438:ALA:CB   | 1:K:448:LEU:HG   | 2.27                     | 0.63              |
| 1:L:146:LEU:HD21 | 1:L:167:THR:HG23 | 1.80                     | 0.63              |
| 1:M:146:LEU:HD21 | 1:M:150:ALA:CB   | 2.28                     | 0.63              |
| 1:P:401:GLU:HG2  | 1:P:433:LEU:HD22 | 1.80                     | 0.63              |
| 1:A:435:THR:OG1  | 1:M:107:LYS:HE2  | 1.99                     | 0.63              |
| 1:B:324:HIS:ND1  | 1:B:325:PRO:HD3  | 2.13                     | 0.63              |
| 1:G:78:GLN:HG3   | 1:G:83:GLY:CA    | 2.29                     | 0.63              |
| 1:G:401:GLU:HG2  | 1:G:433:LEU:HD22 | 1.81                     | 0.63              |
| 1:H:146:LEU:CD2  | 1:H:147:MET:H    | 2.12                     | 0.63              |
| 1:I:211:ILE:HD11 | 1:I:297:MET:HG3  | 1.80                     | 0.63              |
| 1:I:399:CYS:SG   | 1:I:464:GLY:HA3  | 2.39                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:145:ASP:OD1  | 1:J:171:VAL:HB   | 1.99                     | 0.63              |
| 1:K:141:LYS:HG2  | 1:K:144:GLN:HB2  | 1.81                     | 0.63              |
| 1:N:32:PRO:HD2   | 1:N:467:MET:CE   | 2.29                     | 0.63              |
| 1:P:219:ILE:HD12 | 1:P:275:ASN:HB3  | 1.80                     | 0.63              |
| 1:C:79:ASP:HA    | 1:C:83:GLY:HA3   | 1.80                     | 0.63              |
| 1:F:108:ILE:HD13 | 1:O:444:ASP:OD2  | 1.99                     | 0.63              |
| 1:G:324:HIS:HB2  | 1:G:329:LYS:NZ   | 2.14                     | 0.63              |
| 1:H:274:ILE:O    | 1:H:296:VAL:HG22 | 1.98                     | 0.63              |
| 1:K:51:THR:HG21  | 1:K:56:THR:HB    | 1.80                     | 0.63              |
| 1:M:280:ARG:CD   | 1:M:304:PHE:HB2  | 2.29                     | 0.63              |
| 1:O:64:ASP:HB3   | 1:O:66:PRO:HD2   | 1.81                     | 0.63              |
| 1:B:111:GLN:HA   | 1:B:114:ILE:CG1  | 2.29                     | 0.63              |
| 1:I:367:GLN:OE1  | 1:I:369:ILE:HB   | 1.99                     | 0.63              |
| 1:L:145:ASP:OD1  | 1:L:171:VAL:HB   | 1.98                     | 0.63              |
| 1:M:74:MET:O     | 1:M:77:VAL:HG12  | 1.99                     | 0.63              |
| 1:N:146:LEU:CD1  | 1:N:168:LYS:HA   | 2.20                     | 0.63              |
| 1:A:7:ARG:CZ     | 1:A:509:LYS:HE3  | 2.29                     | 0.62              |
| 1:A:402:MET:SD   | 1:A:456:HIS:HB2  | 2.39                     | 0.62              |
| 1:D:145:ASP:O    | 1:D:171:VAL:HG11 | 1.99                     | 0.62              |
| 1:D:316:GLY:C    | 1:D:317:GLU:HG2  | 2.23                     | 0.62              |
| 1:E:434:PRO:HB3  | 1:E:452:LEU:CD2  | 2.29                     | 0.62              |
| 1:F:269:ILE:HG23 | 1:F:274:ILE:HG21 | 1.80                     | 0.62              |
| 1:H:402:MET:SD   | 1:H:456:HIS:HB2  | 2.39                     | 0.62              |
| 1:I:27:LYS:CA    | 1:I:436:ILE:HD11 | 2.28                     | 0.62              |
| 1:B:438:ALA:HB2  | 1:B:448:LEU:HG   | 1.81                     | 0.62              |
| 1:C:484:PHE:CE2  | 1:C:488:ARG:HD3  | 2.35                     | 0.62              |
| 1:D:245:VAL:O    | 1:D:246:ASP:HB2  | 1.98                     | 0.62              |
| 1:I:159:LEU:HD23 | 1:I:160:THR:N    | 2.13                     | 0.62              |
| 1:I:402:MET:SD   | 1:I:456:HIS:HB2  | 2.39                     | 0.62              |
| 1:L:209:LYS:HE3  | 1:L:302:ALA:HA   | 1.81                     | 0.62              |
| 1:H:51:THR:HA    | 1:H:375:ARG:NH2  | 2.13                     | 0.62              |
| 1:H:483:SER:O    | 1:H:486:VAL:HG22 | 1.99                     | 0.62              |
| 1:H:497:ALA:O    | 1:H:500:VAL:HG22 | 1.99                     | 0.62              |
| 1:I:58:LEU:HB3   | 1:I:72:VAL:HG11  | 1.79                     | 0.62              |
| 1:J:204:GLY:HA3  | 1:J:349:PHE:O    | 1.99                     | 0.62              |
| 1:K:313:VAL:HG22 | 1:K:357:ALA:HB3  | 1.82                     | 0.62              |
| 1:N:146:LEU:HD13 | 1:N:147:MET:H    | 1.63                     | 0.62              |
| 1:O:280:ARG:HD2  | 1:O:304:PHE:HB2  | 1.80                     | 0.62              |
| 1:B:128:LEU:CD1  | 1:B:488:ARG:HG2  | 2.30                     | 0.62              |
| 1:B:326:GLU:HG3  | 1:B:327:LEU:N    | 2.15                     | 0.62              |
| 1:D:411:LEU:O    | 1:D:414:ARG:HB3  | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:434:PRO:HB3  | 1:H:452:LEU:CD2  | 2.30                     | 0.62              |
| 1:H:448:LEU:HD11 | 1:H:465:LEU:HD11 | 1.81                     | 0.62              |
| 1:I:108:ILE:HD12 | 1:I:418:LYS:HE3  | 1.81                     | 0.62              |
| 1:I:188:VAL:CG1  | 1:I:377:LEU:HD21 | 2.29                     | 0.62              |
| 1:I:265:LYS:HE2  | 1:I:322:PHE:CE1  | 2.34                     | 0.62              |
| 1:I:325:PRO:C    | 1:I:326:GLU:HG3  | 2.23                     | 0.62              |
| 1:O:399:CYS:SG   | 1:O:464:GLY:HA3  | 2.39                     | 0.62              |
| 1:H:22:ILE:HD12  | 1:H:90:THR:HG22  | 1.80                     | 0.62              |
| 1:H:417:GLY:HA2  | 1:P:453:ARG:NH2  | 2.13                     | 0.62              |
| 1:I:99:GLU:HB2   | 1:I:425:SER:HB2  | 1.81                     | 0.62              |
| 1:O:343:GLU:HG3  | 1:O:344:ASP:N    | 2.14                     | 0.62              |
| 1:A:141:LYS:CG   | 1:A:144:GLN:HB2  | 2.29                     | 0.62              |
| 1:D:191:LYS:HZ1  | 1:D:346:LEU:HD21 | 1.65                     | 0.62              |
| 1:E:24:ASP:O     | 1:E:27:LYS:HG2   | 1.98                     | 0.62              |
| 1:F:224:ILE:HD11 | 1:F:336:ILE:CD1  | 2.30                     | 0.62              |
| 1:G:372:GLU:O    | 1:G:375:ARG:HB3  | 2.00                     | 0.62              |
| 1:H:82:VAL:HA    | 1:H:386:GLN:HG3  | 1.81                     | 0.62              |
| 1:N:96:LEU:HD13  | 1:N:97:LEU:N     | 2.14                     | 0.62              |
| 1:N:399:CYS:SG   | 1:N:464:GLY:HA3  | 2.39                     | 0.62              |
| 1:B:213:VAL:HG11 | 1:F:304:PHE:HE1  | 1.63                     | 0.62              |
| 1:G:233:THR:HG21 | 1:G:261:LYS:HE2  | 1.82                     | 0.62              |
| 1:G:274:ILE:O    | 1:G:296:VAL:HG22 | 1.99                     | 0.62              |
| 1:I:448:LEU:HD21 | 1:I:465:LEU:HD12 | 1.81                     | 0.62              |
| 1:J:146:LEU:HD23 | 1:J:147:MET:N    | 2.12                     | 0.62              |
| 1:M:110:PRO:HA   | 1:M:113:ILE:HD12 | 1.82                     | 0.62              |
| 1:A:58:LEU:HB3   | 1:A:72:VAL:HG13  | 1.81                     | 0.62              |
| 1:B:245:VAL:HG11 | 1:B:250:LYS:HB3  | 1.81                     | 0.62              |
| 1:E:244:ARG:O    | 1:E:245:VAL:HG22 | 1.99                     | 0.62              |
| 1:G:59:LYS:HE2   | 1:G:76:ARG:HB2   | 1.82                     | 0.62              |
| 1:H:265:LYS:HE2  | 1:H:322:PHE:CE1  | 2.35                     | 0.62              |
| 1:J:92:LEU:HD12  | 1:J:433:LEU:HD21 | 1.81                     | 0.62              |
| 1:K:324:HIS:HB2  | 1:K:329:LYS:NZ   | 2.14                     | 0.62              |
| 1:L:154:LEU:HD21 | 1:L:163:LYS:NZ   | 2.15                     | 0.62              |
| 1:B:101:GLU:O    | 1:B:104:ILE:HG12 | 2.00                     | 0.62              |
| 1:B:183:LEU:HD11 | 1:B:381:LEU:HD11 | 1.82                     | 0.62              |
| 1:D:334:LYS:CD   | 1:D:351:GLY:HA3  | 2.30                     | 0.62              |
| 1:E:146:LEU:HD22 | 1:E:168:LYS:CA   | 2.27                     | 0.62              |
| 1:H:141:LYS:HG3  | 1:H:144:GLN:HB2  | 1.82                     | 0.62              |
| 1:K:79:ASP:HA    | 1:K:83:GLY:HA2   | 1.80                     | 0.62              |
| 1:L:32:PRO:HA    | 1:L:156:SER:HA   | 1.82                     | 0.62              |
| 1:L:438:ALA:HB2  | 1:L:448:LEU:HG   | 1.81                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:183:LEU:HB2  | 1:M:381:LEU:HD21 | 1.82                     | 0.62              |
| 1:A:146:LEU:CD1  | 1:A:171:VAL:HG13 | 2.25                     | 0.62              |
| 1:B:99:GLU:HG2   | 1:B:425:SER:HB2  | 1.81                     | 0.62              |
| 1:D:138:ASP:O    | 1:D:139:GLU:HB2  | 1.99                     | 0.62              |
| 1:E:173:ALA:CB   | 1:E:360:ILE:HD11 | 2.27                     | 0.62              |
| 1:F:35:MET:HE1   | 1:F:440:ASN:HB2  | 1.81                     | 0.62              |
| 1:G:171:VAL:CG1  | 1:G:384:LEU:HG   | 2.29                     | 0.62              |
| 1:G:177:LEU:HD12 | 1:G:177:LEU:O    | 2.00                     | 0.62              |
| 1:P:452:LEU:HD13 | 1:P:465:LEU:HD13 | 1.82                     | 0.62              |
| 1:B:27:LYS:CA    | 1:B:436:ILE:HD11 | 2.30                     | 0.61              |
| 1:E:412:ALA:HB1  | 1:E:424:GLU:HB3  | 1.81                     | 0.61              |
| 1:F:57:ILE:HG23  | 1:F:58:LEU:HD22  | 1.81                     | 0.61              |
| 1:F:108:ILE:HD11 | 1:O:446:ALA:HB3  | 1.81                     | 0.61              |
| 1:H:341:ILE:HG23 | 1:H:363:ARG:NH2  | 2.15                     | 0.61              |
| 1:I:188:VAL:HG23 | 1:I:360:ILE:O    | 2.00                     | 0.61              |
| 1:P:176:ARG:NE   | 1:P:358:CYS:HB2  | 2.15                     | 0.61              |
| 1:P:325:PRO:C    | 1:P:326:GLU:HG3  | 2.24                     | 0.61              |
| 1:A:317:GLU:CB   | 1:A:329:LYS:HG2  | 2.29                     | 0.61              |
| 1:C:108:ILE:HB   | 1:L:446:ALA:HB2  | 1.82                     | 0.61              |
| 1:E:128:LEU:HD22 | 1:E:484:PHE:CZ   | 2.35                     | 0.61              |
| 1:E:222:ALA:HA   | 1:E:275:ASN:HB2  | 1.83                     | 0.61              |
| 1:I:138:ASP:O    | 1:I:139:GLU:HB2  | 2.00                     | 0.61              |
| 1:M:324:HIS:HB2  | 1:M:329:LYS:NZ   | 2.15                     | 0.61              |
| 1:P:316:GLY:O    | 1:P:330:LEU:HB2  | 1.99                     | 0.61              |
| 1:A:177:LEU:HG   | 1:A:186:ILE:HD11 | 1.82                     | 0.61              |
| 1:C:207:LEU:HD11 | 1:C:209:LYS:HE3  | 1.82                     | 0.61              |
| 1:D:312:LEU:O    | 1:D:354:LEU:HD22 | 1.99                     | 0.61              |
| 1:I:106:LYS:HE2  | 1:I:418:LYS:HA   | 1.80                     | 0.61              |
| 1:K:19:ALA:HB1   | 1:K:94:ALA:HA    | 1.82                     | 0.61              |
| 1:L:154:LEU:HD21 | 1:L:163:LYS:HZ2  | 1.65                     | 0.61              |
| 1:N:78:GLN:HE22  | 1:N:489:GLN:HE21 | 1.48                     | 0.61              |
| 1:N:79:ASP:HA    | 1:N:83:GLY:HA2   | 1.82                     | 0.61              |
| 1:B:78:GLN:NE2   | 1:B:486:VAL:HA   | 2.15                     | 0.61              |
| 1:B:171:VAL:HG12 | 1:B:384:LEU:HG   | 1.82                     | 0.61              |
| 1:D:79:ASP:HA    | 1:D:83:GLY:HA2   | 1.80                     | 0.61              |
| 1:D:313:VAL:HG13 | 1:D:352:VAL:HB   | 1.82                     | 0.61              |
| 1:F:82:VAL:C     | 1:F:386:GLN:HG3  | 2.26                     | 0.61              |
| 1:F:96:LEU:HD22  | 1:F:96:LEU:C     | 2.25                     | 0.61              |
| 1:G:452:LEU:HD13 | 1:G:465:LEU:HD13 | 1.82                     | 0.61              |
| 1:L:171:VAL:O    | 1:L:174:VAL:HG22 | 2.01                     | 0.61              |
| 1:M:434:PRO:HB3  | 1:M:452:LEU:CD2  | 2.30                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:189:ILE:HG22 | 1:N:190:LYS:H    | 1.64                     | 0.61              |
| 1:C:109:HIS:NE2  | 1:C:111:GLN:HB2  | 2.15                     | 0.61              |
| 1:D:210:LYS:HE2  | 1:D:212:GLY:O    | 2.00                     | 0.61              |
| 1:D:449:VAL:CG1  | 1:K:417:GLY:HA3  | 2.31                     | 0.61              |
| 1:G:143:ARG:HA   | 1:G:143:ARG:HE   | 1.65                     | 0.61              |
| 1:H:57:ILE:HD13  | 1:H:57:ILE:C     | 2.26                     | 0.61              |
| 1:H:59:LYS:HE2   | 1:H:76:ARG:HB2   | 1.83                     | 0.61              |
| 1:I:32:PRO:HD2   | 1:I:467:MET:CE   | 2.30                     | 0.61              |
| 1:J:146:LEU:CD1  | 1:J:171:VAL:HG13 | 2.24                     | 0.61              |
| 1:K:183:LEU:HD13 | 1:K:381:LEU:HG   | 1.81                     | 0.61              |
| 1:M:484:PHE:CE2  | 1:M:488:ARG:HD3  | 2.35                     | 0.61              |
| 1:A:206:LEU:HD11 | 1:A:346:LEU:HD23 | 1.83                     | 0.61              |
| 1:G:402:MET:SD   | 1:G:456:HIS:HB2  | 2.41                     | 0.61              |
| 1:I:121:THR:O    | 1:I:125:ARG:HG2  | 2.01                     | 0.61              |
| 1:L:188:VAL:HG11 | 1:L:377:LEU:HD22 | 1.82                     | 0.61              |
| 1:D:188:VAL:CB   | 1:D:377:LEU:HD22 | 2.25                     | 0.61              |
| 1:L:369:ILE:O    | 1:L:372:GLU:HB3  | 2.01                     | 0.61              |
| 1:M:216:PRO:CG   | 1:M:295:GLY:HA2  | 2.30                     | 0.61              |
| 1:M:431:ARG:NH2  | 1:M:434:PRO:HG2  | 2.16                     | 0.61              |
| 1:A:368:GLN:OE1  | 1:C:509:LYS:HE3  | 2.00                     | 0.61              |
| 1:H:345:LYS:C    | 1:H:346:LEU:HD12 | 2.26                     | 0.61              |
| 1:J:84:ASP:OD1   | 1:J:383:VAL:HG22 | 2.00                     | 0.61              |
| 1:M:258:GLU:OE2  | 1:M:284:TYR:HE2  | 1.84                     | 0.61              |
| 1:M:325:PRO:C    | 1:M:326:GLU:HG3  | 2.26                     | 0.61              |
| 1:A:39:LEU:HD12  | 1:A:57:ILE:HG13  | 1.82                     | 0.61              |
| 1:A:159:LEU:HD23 | 1:A:160:THR:N    | 2.15                     | 0.61              |
| 1:B:131:SER:HA   | 1:B:461:THR:HG21 | 1.82                     | 0.61              |
| 1:B:176:ARG:CZ   | 1:B:358:CYS:HB2  | 2.30                     | 0.61              |
| 1:D:159:LEU:HG   | 1:D:163:LYS:HB2  | 1.82                     | 0.61              |
| 1:F:316:GLY:O    | 1:F:330:LEU:HB2  | 2.01                     | 0.61              |
| 1:G:37:LYS:O     | 1:G:50:VAL:HA    | 2.00                     | 0.61              |
| 1:G:381:LEU:C    | 1:G:381:LEU:HD12 | 2.26                     | 0.61              |
| 1:I:95:GLU:O     | 1:I:98:ARG:HD2   | 2.01                     | 0.61              |
| 1:L:64:ASP:CB    | 1:L:512:PRO:HA   | 2.31                     | 0.61              |
| 1:L:188:VAL:HA   | 1:L:360:ILE:O    | 2.00                     | 0.61              |
| 1:M:166:PHE:CZ   | 1:M:198:ASP:HB3  | 2.36                     | 0.61              |
| 1:O:146:LEU:HD23 | 1:O:147:MET:H    | 1.65                     | 0.61              |
| 1:O:339:VAL:O    | 1:O:340:MET:HB2  | 2.01                     | 0.61              |
| 1:A:225:LEU:HD13 | 1:A:329:LYS:CE   | 2.31                     | 0.61              |
| 1:B:171:VAL:O    | 1:B:174:VAL:HG22 | 2.01                     | 0.61              |
| 1:B:397:GLY:HA3  | 1:B:475:MET:HE3  | 1.83                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:27:LYS:CB    | 1:C:436:ILE:HD11 | 2.30                     | 0.61              |
| 1:C:146:LEU:HD23 | 1:C:147:MET:N    | 2.13                     | 0.61              |
| 1:C:211:ILE:HD11 | 1:C:297:MET:HG3  | 1.83                     | 0.61              |
| 1:D:452:LEU:HD13 | 1:D:465:LEU:HD13 | 1.81                     | 0.61              |
| 1:F:89:VAL:HG12  | 1:F:490:VAL:HB   | 1.83                     | 0.61              |
| 1:J:367:GLN:CG   | 1:J:369:ILE:HB   | 2.31                     | 0.61              |
| 1:K:106:LYS:HE2  | 1:K:418:LYS:HZ1  | 1.62                     | 0.61              |
| 1:K:166:PHE:CZ   | 1:K:198:ASP:HB3  | 2.36                     | 0.61              |
| 1:L:485:GLN:HB3  | 1:L:489:GLN:HE22 | 1.64                     | 0.61              |
| 1:N:483:SER:O    | 1:N:486:VAL:HG22 | 2.01                     | 0.61              |
| 1:O:117:TRP:HE1  | 1:O:498:ALA:HB3  | 1.65                     | 0.61              |
| 1:P:206:LEU:HD21 | 1:P:346:LEU:HB3  | 1.83                     | 0.61              |
| 1:B:446:ALA:HB1  | 1:I:107:LYS:HB2  | 1.82                     | 0.60              |
| 1:C:225:LEU:HA   | 1:C:329:LYS:HD3  | 1.83                     | 0.60              |
| 1:I:225:LEU:HD12 | 1:I:226:ILE:N    | 2.16                     | 0.60              |
| 1:J:160:THR:HA   | 1:J:163:LYS:HB2  | 1.83                     | 0.60              |
| 1:M:397:GLY:O    | 1:M:465:LEU:HD23 | 2.00                     | 0.60              |
| 1:O:54:GLY:O     | 1:O:58:LEU:HD23  | 2.00                     | 0.60              |
| 1:B:191:LYS:CE   | 1:B:346:LEU:HD11 | 2.30                     | 0.60              |
| 1:F:165:HIS:O    | 1:F:168:LYS:HB3  | 2.01                     | 0.60              |
| 1:H:19:ALA:HB3   | 1:H:98:ARG:NH2   | 2.16                     | 0.60              |
| 1:I:475:MET:SD   | 1:I:480:ILE:HB   | 2.41                     | 0.60              |
| 1:L:176:ARG:NH2  | 1:L:360:ILE:HG12 | 2.16                     | 0.60              |
| 1:M:146:LEU:HD13 | 1:M:167:THR:O    | 2.00                     | 0.60              |
| 1:A:325:PRO:C    | 1:A:326:GLU:HG3  | 2.26                     | 0.60              |
| 1:B:225:LEU:HD11 | 1:B:324:HIS:CE1  | 2.36                     | 0.60              |
| 1:I:63:VAL:O     | 1:I:513:ARG:HD2  | 2.00                     | 0.60              |
| 1:L:317:GLU:HB2  | 1:L:329:LYS:HD3  | 1.83                     | 0.60              |
| 1:N:189:ILE:HG22 | 1:N:190:LYS:N    | 2.16                     | 0.60              |
| 1:A:475:MET:SD   | 1:A:480:ILE:HB   | 2.41                     | 0.60              |
| 1:B:110:PRO:O    | 1:B:113:ILE:HB   | 2.01                     | 0.60              |
| 1:B:203:GLU:OE2  | 1:B:350:SER:HB2  | 2.00                     | 0.60              |
| 1:C:140:VAL:HA   | 1:C:175:LEU:HD22 | 1.82                     | 0.60              |
| 1:D:39:LEU:O     | 1:D:48:LEU:HA    | 2.02                     | 0.60              |
| 1:D:133:VAL:HB   | 1:D:393:THR:O    | 2.01                     | 0.60              |
| 1:E:159:LEU:HG   | 1:E:163:LYS:CD   | 2.31                     | 0.60              |
| 1:K:65:ASN:ND2   | 1:K:66:PRO:HD3   | 2.16                     | 0.60              |
| 1:K:171:VAL:HG12 | 1:K:384:LEU:CG   | 2.31                     | 0.60              |
| 1:O:497:ALA:O    | 1:O:500:VAL:HG22 | 2.01                     | 0.60              |
| 1:C:265:LYS:HZ2  | 1:C:287:PRO:HG3  | 1.66                     | 0.60              |
| 1:D:39:LEU:HD13  | 1:E:513:ARG:OXT  | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:5:GLU:O      | 1:J:6:GLU:HB2    | 2.00                     | 0.60              |
| 1:K:32:PRO:HG2   | 1:K:467:MET:HE1  | 1.83                     | 0.60              |
| 1:L:204:GLY:O    | 1:L:359:THR:HB   | 2.01                     | 0.60              |
| 1:L:399:CYS:SG   | 1:L:464:GLY:HA3  | 2.41                     | 0.60              |
| 1:M:32:PRO:HD2   | 1:M:467:MET:HE1  | 1.83                     | 0.60              |
| 1:O:145:ASP:OD1  | 1:O:171:VAL:HB   | 2.01                     | 0.60              |
| 1:P:499:GLU:O    | 1:P:503:ARG:HG2  | 2.01                     | 0.60              |
| 1:E:137:SER:OG   | 1:E:388:VAL:HA   | 2.01                     | 0.60              |
| 1:F:106:LYS:CG   | 1:O:446:ALA:HB2  | 2.32                     | 0.60              |
| 1:H:28:SER:O     | 1:H:34:GLY:HA2   | 2.02                     | 0.60              |
| 1:H:37:LYS:O     | 1:H:50:VAL:HA    | 2.01                     | 0.60              |
| 1:I:223:LYS:HB2  | 1:I:274:ILE:HA   | 1.84                     | 0.60              |
| 1:J:192:LEU:HG   | 1:J:343:GLU:CD   | 2.27                     | 0.60              |
| 1:K:146:LEU:HD12 | 1:K:171:VAL:HG22 | 1.83                     | 0.60              |
| 1:K:475:MET:SD   | 1:K:480:ILE:HB   | 2.41                     | 0.60              |
| 1:M:112:THR:HG21 | 1:M:418:LYS:HZ1  | 1.67                     | 0.60              |
| 1:N:122:LYS:O    | 1:N:125:ARG:HG2  | 2.01                     | 0.60              |
| 1:P:380:ALA:O    | 1:P:384:LEU:HD23 | 2.01                     | 0.60              |
| 1:C:159:LEU:HD23 | 1:C:160:THR:N    | 2.15                     | 0.60              |
| 1:D:369:ILE:O    | 1:D:372:GLU:HB3  | 2.02                     | 0.60              |
| 1:F:145:ASP:O    | 1:F:171:VAL:HG11 | 2.01                     | 0.60              |
| 1:F:265:LYS:HE2  | 1:F:322:PHE:CE1  | 2.37                     | 0.60              |
| 1:G:483:SER:O    | 1:G:486:VAL:HG22 | 2.01                     | 0.60              |
| 1:I:228:ASN:OD1  | 1:I:319:ALA:HB3  | 2.01                     | 0.60              |
| 1:J:269:ILE:HG23 | 1:J:274:ILE:HG21 | 1.83                     | 0.60              |
| 1:K:146:LEU:HD12 | 1:K:171:VAL:CG1  | 2.32                     | 0.60              |
| 1:B:274:ILE:O    | 1:B:296:VAL:HG22 | 2.02                     | 0.60              |
| 1:B:324:HIS:HB2  | 1:B:329:LYS:CE   | 2.31                     | 0.60              |
| 1:C:225:LEU:HD13 | 1:C:329:LYS:HE2  | 1.82                     | 0.60              |
| 1:D:276:CYS:HA   | 1:D:297:MET:O    | 2.01                     | 0.60              |
| 1:E:364:GLY:HA3  | 1:E:370:LEU:HD13 | 1.83                     | 0.60              |
| 1:M:366:THR:HG22 | 1:M:370:LEU:CD2  | 2.32                     | 0.60              |
| 1:N:3:ALA:O      | 1:N:4:ASP:HB3    | 2.02                     | 0.60              |
| 1:I:283:ILE:HG22 | 1:I:300:GLU:HG3  | 1.82                     | 0.60              |
| 1:J:79:ASP:HA    | 1:J:83:GLY:HA2   | 1.83                     | 0.60              |
| 1:K:106:LYS:HE2  | 1:K:418:LYS:CE   | 2.32                     | 0.60              |
| 1:N:128:LEU:O    | 1:N:129:LEU:HD22 | 2.01                     | 0.60              |
| 1:O:58:LEU:HB3   | 1:O:72:VAL:CG1   | 2.31                     | 0.60              |
| 1:A:106:LYS:HD2  | 1:A:421:VAL:HG11 | 1.84                     | 0.60              |
| 1:A:265:LYS:HE2  | 1:A:322:PHE:CE1  | 2.37                     | 0.60              |
| 1:B:276:CYS:HA   | 1:B:297:MET:O    | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:284:TYR:O    | 1:C:287:PRO:HD2  | 2.01                     | 0.60              |
| 1:C:452:LEU:HD13 | 1:C:465:LEU:HD13 | 1.82                     | 0.60              |
| 1:D:211:ILE:HD11 | 1:D:297:MET:HG3  | 1.84                     | 0.60              |
| 1:F:390:ASP:HB3  | 1:F:485:GLN:OE1  | 2.01                     | 0.60              |
| 1:G:317:GLU:HB2  | 1:G:329:LYS:HD3  | 1.84                     | 0.60              |
| 1:G:402:MET:SD   | 1:G:453:ARG:HA   | 2.41                     | 0.60              |
| 1:I:276:CYS:HA   | 1:I:297:MET:O    | 2.02                     | 0.60              |
| 1:L:196:LEU:HD12 | 1:L:196:LEU:O    | 2.01                     | 0.60              |
| 1:M:433:LEU:HA   | 1:M:436:ILE:HG22 | 1.83                     | 0.60              |
| 1:N:54:GLY:O     | 1:N:58:LEU:HD23  | 2.01                     | 0.60              |
| 1:N:99:GLU:CD    | 1:N:425:SER:HB2  | 2.27                     | 0.60              |
| 1:A:140:VAL:HA   | 1:A:175:LEU:HD22 | 1.84                     | 0.59              |
| 1:B:324:HIS:HB2  | 1:B:329:LYS:HE2  | 1.84                     | 0.59              |
| 1:D:163:LYS:HD2  | 1:D:166:PHE:HB2  | 1.83                     | 0.59              |
| 1:E:159:LEU:HG   | 1:E:163:LYS:HD3  | 1.84                     | 0.59              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:CG   | 2.32                     | 0.59              |
| 1:G:89:VAL:HB    | 1:G:490:VAL:CG2  | 2.31                     | 0.59              |
| 1:I:51:THR:HG21  | 1:I:56:THR:HB    | 1.84                     | 0.59              |
| 1:I:118:ARG:O    | 1:I:121:THR:HB   | 2.01                     | 0.59              |
| 1:K:109:HIS:CE1  | 1:K:111:GLN:HB2  | 2.36                     | 0.59              |
| 1:M:47:SER:HB2   | 1:M:48:LEU:HD13  | 1.83                     | 0.59              |
| 1:M:274:ILE:O    | 1:M:296:VAL:HG22 | 2.02                     | 0.59              |
| 1:D:269:ILE:HG23 | 1:D:274:ILE:CG2  | 2.31                     | 0.59              |
| 1:F:145:ASP:OD1  | 1:F:171:VAL:HB   | 2.02                     | 0.59              |
| 1:F:274:ILE:O    | 1:F:296:VAL:HG22 | 2.02                     | 0.59              |
| 1:J:325:PRO:C    | 1:J:326:GLU:HG3  | 2.27                     | 0.59              |
| 1:M:402:MET:SD   | 1:M:456:HIS:HB2  | 2.42                     | 0.59              |
| 1:P:280:ARG:HD2  | 1:P:304:PHE:HB2  | 1.84                     | 0.59              |
| 1:B:50:VAL:HG13  | 1:B:375:ARG:NH2  | 2.16                     | 0.59              |
| 1:B:190:LYS:HD2  | 1:B:190:LYS:O    | 2.02                     | 0.59              |
| 1:B:326:GLU:HG3  | 1:B:327:LEU:H    | 1.66                     | 0.59              |
| 1:C:216:PRO:HG2  | 1:C:295:GLY:HA2  | 1.84                     | 0.59              |
| 1:E:30:LEU:H     | 1:E:30:LEU:HD13  | 1.64                     | 0.59              |
| 1:E:210:LYS:HE2  | 1:E:212:GLY:O    | 2.02                     | 0.59              |
| 1:E:398:GLY:HA2  | 1:E:401:GLU:OE1  | 2.02                     | 0.59              |
| 1:F:224:ILE:HD11 | 1:F:336:ILE:HD11 | 1.84                     | 0.59              |
| 1:F:250:LYS:O    | 1:F:253:GLU:HG2  | 2.01                     | 0.59              |
| 1:G:59:LYS:HE2   | 1:G:76:ARG:CB    | 2.32                     | 0.59              |
| 1:L:283:ILE:HG22 | 1:L:300:GLU:HG3  | 1.84                     | 0.59              |
| 1:N:364:GLY:HA3  | 1:N:370:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:431:ARG:NH2  | 1:A:434:PRO:HG2  | 2.17                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:418:LYS:HG3  | 1:I:450:ALA:CA   | 2.32                     | 0.59              |
| 1:G:352:VAL:HG23 | 1:G:355:GLY:H    | 1.66                     | 0.59              |
| 1:I:222:ALA:HA   | 1:I:275:ASN:OD1  | 2.03                     | 0.59              |
| 1:I:324:HIS:O    | 1:I:328:VAL:HG22 | 2.02                     | 0.59              |
| 1:K:101:GLU:O    | 1:K:104:ILE:HG12 | 2.00                     | 0.59              |
| 1:M:401:GLU:HG2  | 1:M:433:LEU:HD22 | 1.83                     | 0.59              |
| 1:M:509:LYS:HG2  | 1:M:509:LYS:O    | 2.01                     | 0.59              |
| 1:A:149:ILE:O    | 1:A:152:THR:HG22 | 2.03                     | 0.59              |
| 1:A:175:LEU:O    | 1:A:178:LYS:HB3  | 2.02                     | 0.59              |
| 1:D:128:LEU:HD21 | 1:D:488:ARG:HG2  | 1.83                     | 0.59              |
| 1:D:284:TYR:O    | 1:D:287:PRO:HD2  | 2.02                     | 0.59              |
| 1:E:101:GLU:O    | 1:E:104:ILE:HG12 | 2.02                     | 0.59              |
| 1:E:236:ILE:HG23 | 1:E:238:ILE:H    | 1.67                     | 0.59              |
| 1:E:269:ILE:HG23 | 1:E:274:ILE:CG2  | 2.32                     | 0.59              |
| 1:E:324:HIS:ND1  | 1:E:325:PRO:HD3  | 2.18                     | 0.59              |
| 1:G:126:GLN:HA   | 1:G:130:ASN:ND2  | 2.17                     | 0.59              |
| 1:G:225:LEU:HD12 | 1:G:226:ILE:N    | 2.18                     | 0.59              |
| 1:G:475:MET:SD   | 1:G:480:ILE:HB   | 2.42                     | 0.59              |
| 1:J:12:ARG:HD3   | 1:J:501:ILE:HG21 | 1.82                     | 0.59              |
| 1:J:324:HIS:O    | 1:J:328:VAL:HG22 | 2.02                     | 0.59              |
| 1:N:402:MET:CE   | 1:N:453:ARG:HG2  | 2.33                     | 0.59              |
| 1:O:233:THR:HG21 | 1:O:261:LYS:HE3  | 1.83                     | 0.59              |
| 1:P:128:LEU:HD22 | 1:P:488:ARG:HG2  | 1.85                     | 0.59              |
| 1:C:137:SER:H    | 1:C:141:LYS:HE3  | 1.68                     | 0.59              |
| 1:C:262:MET:HE1  | 1:C:286:TYR:C    | 2.27                     | 0.59              |
| 1:D:317:GLU:HB3  | 1:D:329:LYS:HD3  | 1.83                     | 0.59              |
| 1:E:190:LYS:HD2  | 1:E:190:LYS:C    | 2.28                     | 0.59              |
| 1:H:231:MET:HB2  | 1:H:284:TYR:H    | 1.66                     | 0.59              |
| 1:I:226:ILE:HG12 | 1:I:278:ILE:HG23 | 1.83                     | 0.59              |
| 1:J:152:THR:HG21 | 1:J:480:ILE:HA   | 1.84                     | 0.59              |
| 1:L:269:ILE:HG23 | 1:L:274:ILE:CG2  | 2.30                     | 0.59              |
| 1:N:58:LEU:HB3   | 1:N:72:VAL:HG11  | 1.85                     | 0.59              |
| 1:O:96:LEU:HD13  | 1:O:96:LEU:C     | 2.27                     | 0.59              |
| 1:O:108:ILE:HG22 | 1:O:109:HIS:HD2  | 1.67                     | 0.59              |
| 1:O:173:ALA:HB2  | 1:O:360:ILE:HD11 | 1.84                     | 0.59              |
| 1:O:190:LYS:HD3  | 1:O:370:LEU:HD23 | 1.84                     | 0.59              |
| 1:O:211:ILE:HD11 | 1:O:297:MET:HG3  | 1.83                     | 0.59              |
| 1:B:484:PHE:HE2  | 1:B:488:ARG:NE   | 1.99                     | 0.59              |
| 1:C:98:ARG:HA    | 1:C:98:ARG:HE    | 1.67                     | 0.59              |
| 1:D:146:LEU:CD2  | 1:D:147:MET:H    | 2.16                     | 0.59              |
| 1:F:58:LEU:HB3   | 1:F:72:VAL:HG11  | 1.85                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:312:LEU:O    | 1:F:354:LEU:HD22 | 2.02                     | 0.59              |
| 1:H:58:LEU:HB3   | 1:H:72:VAL:HG11  | 1.83                     | 0.59              |
| 1:N:206:LEU:HD21 | 1:N:346:LEU:HD22 | 1.85                     | 0.59              |
| 1:O:187:HIS:HB2  | 1:O:309:ARG:NH1  | 2.17                     | 0.59              |
| 1:O:390:ASP:HB3  | 1:O:485:GLN:HE21 | 1.68                     | 0.59              |
| 1:C:163:LYS:HA   | 1:C:166:PHE:CD1  | 2.38                     | 0.59              |
| 1:C:438:ALA:HB2  | 1:C:448:LEU:HG   | 1.84                     | 0.59              |
| 1:F:248:THR:O    | 1:F:251:VAL:HG12 | 2.02                     | 0.59              |
| 1:H:190:LYS:HG2  | 1:H:191:LYS:N    | 2.17                     | 0.59              |
| 1:J:30:LEU:HG    | 1:J:87:THR:O     | 2.03                     | 0.59              |
| 1:J:274:ILE:O    | 1:J:296:VAL:HG22 | 2.03                     | 0.59              |
| 1:K:324:HIS:ND1  | 1:K:325:PRO:HD3  | 2.18                     | 0.59              |
| 1:M:40:LEU:HD22  | 1:M:41:SER:N     | 2.17                     | 0.59              |
| 1:M:128:LEU:CD1  | 1:M:488:ARG:HG2  | 2.31                     | 0.59              |
| 1:P:31:GLY:O     | 1:P:156:SER:HA   | 2.03                     | 0.59              |
| 1:C:114:ILE:HA   | 1:C:117:TRP:CE3  | 2.38                     | 0.59              |
| 1:C:114:ILE:HD12 | 1:C:499:GLU:HG3  | 1.84                     | 0.59              |
| 1:C:143:ARG:NE   | 1:C:143:ARG:HA   | 2.17                     | 0.59              |
| 1:D:245:VAL:CG1  | 1:D:250:LYS:HB3  | 2.33                     | 0.59              |
| 1:F:448:LEU:HD21 | 1:F:465:LEU:HD12 | 1.84                     | 0.59              |
| 1:H:191:LYS:HG2  | 1:H:341:ILE:HG21 | 1.84                     | 0.59              |
| 1:J:32:PRO:HD2   | 1:J:467:MET:HE1  | 1.83                     | 0.59              |
| 1:J:434:PRO:HB3  | 1:J:452:LEU:CD2  | 2.33                     | 0.59              |
| 1:K:59:LYS:HE3   | 1:K:73:ASP:HA    | 1.83                     | 0.59              |
| 1:L:166:PHE:CZ   | 1:L:198:ASP:HB3  | 2.38                     | 0.59              |
| 1:N:219:ILE:HB   | 1:N:275:ASN:HB3  | 1.84                     | 0.59              |
| 1:O:451:GLN:HE22 | 1:O:471:THR:HA   | 1.68                     | 0.59              |
| 1:A:38:ILE:HG12  | 1:C:506:ASN:HD21 | 1.68                     | 0.59              |
| 1:A:478:LEU:HB3  | 1:A:480:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:498:ALA:O    | 1:A:501:ILE:HG22 | 2.02                     | 0.59              |
| 1:B:148:ASN:HA   | 1:B:479:GLY:O    | 2.02                     | 0.59              |
| 1:D:154:LEU:CD2  | 1:D:163:LYS:HG3  | 2.32                     | 0.59              |
| 1:D:173:ALA:O    | 1:D:176:ARG:HG2  | 2.03                     | 0.59              |
| 1:E:225:LEU:HD13 | 1:E:329:LYS:HE2  | 1.85                     | 0.59              |
| 1:F:485:GLN:HB2  | 1:F:489:GLN:OE1  | 2.03                     | 0.59              |
| 1:G:133:VAL:HG23 | 1:G:134:ASP:N    | 2.17                     | 0.59              |
| 1:G:133:VAL:HG12 | 1:G:393:THR:O    | 2.01                     | 0.59              |
| 1:H:9:GLU:HG2    | 1:H:10:THR:N     | 2.17                     | 0.59              |
| 1:I:216:PRO:CG   | 1:I:295:GLY:HA2  | 2.33                     | 0.59              |
| 1:J:95:GLU:OE1   | 1:J:432:MET:HB3  | 2.02                     | 0.59              |
| 1:L:166:PHE:CE1  | 1:L:198:ASP:HB3  | 2.38                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:268:ARG:O    | 1:L:271:LYS:HG2  | 2.03                     | 0.59              |
| 1:N:452:LEU:HD13 | 1:N:465:LEU:HD13 | 1.84                     | 0.59              |
| 1:P:312:LEU:O    | 1:P:354:LEU:HD22 | 2.03                     | 0.59              |
| 1:D:21:ALA:O     | 1:D:25:LEU:HD23  | 2.03                     | 0.58              |
| 1:D:154:LEU:CD2  | 1:D:167:THR:HB   | 2.33                     | 0.58              |
| 1:D:390:ASP:HB2  | 1:D:485:GLN:HE22 | 1.68                     | 0.58              |
| 1:E:219:ILE:HG21 | 1:E:275:ASN:O    | 2.02                     | 0.58              |
| 1:G:146:LEU:CD2  | 1:G:167:THR:HG23 | 2.33                     | 0.58              |
| 1:G:366:THR:HG23 | 1:G:366:THR:O    | 2.03                     | 0.58              |
| 1:I:145:ASP:O    | 1:I:171:VAL:HG11 | 2.03                     | 0.58              |
| 1:J:166:PHE:CZ   | 1:J:198:ASP:HB3  | 2.38                     | 0.58              |
| 1:K:140:VAL:HA   | 1:K:175:LEU:HD22 | 1.85                     | 0.58              |
| 1:L:178:LYS:HZ2  | 1:L:388:VAL:HG11 | 1.67                     | 0.58              |
| 1:P:216:PRO:HG2  | 1:P:295:GLY:HA2  | 1.85                     | 0.58              |
| 1:A:418:LYS:HA   | 1:M:453:ARG:NH2  | 2.17                     | 0.58              |
| 1:B:280:ARG:O    | 1:B:281:GLN:HB3  | 2.03                     | 0.58              |
| 1:C:231:MET:HG3  | 1:C:283:ILE:HG13 | 1.85                     | 0.58              |
| 1:C:345:LYS:C    | 1:C:346:LEU:HD12 | 2.28                     | 0.58              |
| 1:I:163:LYS:O    | 1:I:166:PHE:HB2  | 2.03                     | 0.58              |
| 1:K:66:PRO:HB3   | 1:K:509:LYS:NZ   | 2.18                     | 0.58              |
| 1:N:106:LYS:HG3  | 1:N:418:LYS:NZ   | 2.18                     | 0.58              |
| 1:B:231:MET:HG3  | 1:B:283:ILE:HG13 | 1.84                     | 0.58              |
| 1:C:211:ILE:H    | 1:C:211:ILE:HD13 | 1.68                     | 0.58              |
| 1:C:509:LYS:HD2  | 1:C:509:LYS:N    | 2.17                     | 0.58              |
| 1:E:313:VAL:HG13 | 1:E:352:VAL:HB   | 1.85                     | 0.58              |
| 1:F:51:THR:HG22  | 1:F:53:ASP:H     | 1.67                     | 0.58              |
| 1:K:324:HIS:CG   | 1:K:325:PRO:HD3  | 2.38                     | 0.58              |
| 1:L:186:ILE:CD1  | 1:L:381:LEU:HD21 | 2.34                     | 0.58              |
| 1:N:127:ALA:HB1  | 1:N:491:LEU:CD1  | 2.25                     | 0.58              |
| 1:N:431:ARG:O    | 1:N:434:PRO:HD2  | 2.03                     | 0.58              |
| 1:P:226:ILE:HB   | 1:P:317:GLU:OE2  | 2.03                     | 0.58              |
| 1:C:40:LEU:HD21  | 1:H:2:GLY:HA2    | 1.85                     | 0.58              |
| 1:F:31:GLY:O     | 1:F:156:SER:HB3  | 2.03                     | 0.58              |
| 1:G:326:GLU:HG3  | 1:G:327:LEU:N    | 2.18                     | 0.58              |
| 1:H:126:GLN:O    | 1:H:126:GLN:HG2  | 2.02                     | 0.58              |
| 1:I:235:LYS:O    | 1:I:236:ILE:HG22 | 2.04                     | 0.58              |
| 1:J:82:VAL:HA    | 1:J:386:GLN:HB3  | 1.84                     | 0.58              |
| 1:J:385:ALA:O    | 1:J:388:VAL:HG13 | 2.03                     | 0.58              |
| 1:L:226:ILE:HG12 | 1:L:278:ILE:HG23 | 1.85                     | 0.58              |
| 1:M:483:SER:O    | 1:M:486:VAL:HG22 | 2.04                     | 0.58              |
| 1:P:173:ALA:HB2  | 1:P:360:ILE:HD11 | 1.85                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:372:GLU:HA   | 1:P:375:ARG:NH2  | 2.18                     | 0.58              |
| 1:A:171:VAL:O    | 1:A:174:VAL:HG22 | 2.03                     | 0.58              |
| 1:C:402:MET:SD   | 1:C:453:ARG:HA   | 2.42                     | 0.58              |
| 1:D:431:ARG:O    | 1:D:434:PRO:HD2  | 2.03                     | 0.58              |
| 1:E:59:LYS:HE2   | 1:E:76:ARG:CB    | 2.32                     | 0.58              |
| 1:G:274:ILE:HG23 | 1:G:296:VAL:HG21 | 1.85                     | 0.58              |
| 1:I:96:LEU:O     | 1:I:96:LEU:HD22  | 2.04                     | 0.58              |
| 1:K:146:LEU:HD13 | 1:K:168:LYS:CA   | 2.33                     | 0.58              |
| 1:P:188:VAL:HG13 | 1:P:377:LEU:HD21 | 1.85                     | 0.58              |
| 1:D:39:LEU:HB3   | 1:E:513:ARG:O    | 2.03                     | 0.58              |
| 1:D:408:VAL:HA   | 1:D:411:LEU:HD12 | 1.84                     | 0.58              |
| 1:E:99:GLU:O     | 1:E:103:LEU:HD13 | 2.03                     | 0.58              |
| 1:G:397:GLY:HA3  | 1:G:475:MET:HE3  | 1.84                     | 0.58              |
| 1:K:216:PRO:HG2  | 1:K:295:GLY:HA2  | 1.85                     | 0.58              |
| 1:K:274:ILE:O    | 1:K:296:VAL:HG22 | 2.03                     | 0.58              |
| 1:B:401:GLU:HG2  | 1:B:433:LEU:HD22 | 1.84                     | 0.58              |
| 1:C:145:ASP:O    | 1:C:171:VAL:HG11 | 2.03                     | 0.58              |
| 1:F:146:LEU:HD21 | 1:F:150:ALA:HB3  | 1.85                     | 0.58              |
| 1:F:421:VAL:HB   | 1:O:453:ARG:HH22 | 1.69                     | 0.58              |
| 1:I:32:PRO:HD2   | 1:I:467:MET:SD   | 2.44                     | 0.58              |
| 1:J:143:ARG:HA   | 1:J:143:ARG:HE   | 1.69                     | 0.58              |
| 1:K:322:PHE:HA   | 1:K:324:HIS:CD2  | 2.39                     | 0.58              |
| 1:L:313:VAL:HG13 | 1:L:352:VAL:HB   | 1.86                     | 0.58              |
| 1:P:114:ILE:HD11 | 1:P:502:LEU:CB   | 2.34                     | 0.58              |
| 1:P:146:LEU:CD2  | 1:P:167:THR:HG23 | 2.33                     | 0.58              |
| 1:A:116:GLY:O    | 1:A:119:GLU:HB2  | 2.03                     | 0.58              |
| 1:A:171:VAL:CG1  | 1:A:384:LEU:HG   | 2.33                     | 0.58              |
| 1:B:111:GLN:HA   | 1:B:114:ILE:HG12 | 1.86                     | 0.58              |
| 1:B:185:ALA:HA   | 1:B:309:ARG:CD   | 2.33                     | 0.58              |
| 1:C:324:HIS:ND1  | 1:C:325:PRO:HD3  | 2.18                     | 0.58              |
| 1:D:119:GLU:O    | 1:D:122:LYS:HB3  | 2.03                     | 0.58              |
| 1:G:39:LEU:O     | 1:G:48:LEU:HA    | 2.03                     | 0.58              |
| 1:H:154:LEU:HD21 | 1:H:163:LYS:HZ3  | 1.68                     | 0.58              |
| 1:I:478:LEU:HB3  | 1:I:480:ILE:HD12 | 1.86                     | 0.58              |
| 1:J:92:LEU:HA    | 1:J:95:GLU:OE2   | 2.03                     | 0.58              |
| 1:K:483:SER:O    | 1:K:486:VAL:HG22 | 2.03                     | 0.58              |
| 1:L:274:ILE:O    | 1:L:296:VAL:HG22 | 2.03                     | 0.58              |
| 1:M:145:ASP:OD1  | 1:M:171:VAL:HB   | 2.04                     | 0.58              |
| 1:N:27:LYS:HD3   | 1:N:28:SER:H     | 1.66                     | 0.58              |
| 1:N:269:ILE:HG23 | 1:N:274:ILE:CG2  | 2.32                     | 0.58              |
| 1:O:89:VAL:HA    | 1:O:490:VAL:HG23 | 1.86                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:341:ILE:HG23 | 1:O:363:ARG:NH2  | 2.19                     | 0.58              |
| 1:P:41:SER:O     | 1:P:45:ASP:HB2   | 2.04                     | 0.58              |
| 1:A:114:ILE:HA   | 1:A:117:TRP:CE3  | 2.38                     | 0.58              |
| 1:B:390:ASP:CB   | 1:B:485:GLN:HE22 | 2.17                     | 0.58              |
| 1:D:146:LEU:HD12 | 1:D:171:VAL:CG1  | 2.24                     | 0.58              |
| 1:F:225:LEU:HD11 | 1:F:324:HIS:ND1  | 2.19                     | 0.58              |
| 1:G:160:THR:HA   | 1:G:163:LYS:HB3  | 1.85                     | 0.58              |
| 1:I:171:VAL:HG12 | 1:I:384:LEU:HG   | 1.84                     | 0.58              |
| 1:I:190:LYS:HD2  | 1:I:190:LYS:O    | 2.04                     | 0.58              |
| 1:O:146:LEU:HD11 | 1:O:150:ALA:CB   | 2.34                     | 0.58              |
| 1:O:146:LEU:HD13 | 1:O:167:THR:O    | 2.02                     | 0.58              |
| 1:B:57:ILE:HG23  | 1:B:58:LEU:HD22  | 1.86                     | 0.58              |
| 1:B:140:VAL:HA   | 1:B:175:LEU:HD22 | 1.86                     | 0.58              |
| 1:C:133:VAL:HG23 | 1:C:134:ASP:H    | 1.68                     | 0.58              |
| 1:E:404:MET:HE3  | 1:E:430:LEU:HD11 | 1.86                     | 0.58              |
| 1:F:284:TYR:O    | 1:F:287:PRO:HD2  | 2.04                     | 0.58              |
| 1:F:325:PRO:C    | 1:F:326:GLU:HG3  | 2.29                     | 0.58              |
| 1:H:108:ILE:HG23 | 1:H:109:HIS:N    | 2.19                     | 0.58              |
| 1:H:154:LEU:HD21 | 1:H:163:LYS:NZ   | 2.19                     | 0.58              |
| 1:I:82:VAL:HA    | 1:I:386:GLN:HG3  | 1.85                     | 0.58              |
| 1:I:106:LYS:CE   | 1:I:418:LYS:HA   | 2.33                     | 0.58              |
| 1:I:171:VAL:O    | 1:I:175:LEU:HG   | 2.03                     | 0.58              |
| 1:I:451:GLN:HE22 | 1:I:471:THR:HA   | 1.69                     | 0.58              |
| 1:J:324:HIS:O    | 1:J:329:LYS:HG2  | 2.03                     | 0.58              |
| 1:M:58:LEU:HB3   | 1:M:72:VAL:HG11  | 1.85                     | 0.58              |
| 1:A:284:TYR:O    | 1:A:287:PRO:HD2  | 2.03                     | 0.57              |
| 1:A:287:PRO:O    | 1:A:291:PHE:HD1  | 1.85                     | 0.57              |
| 1:C:209:LYS:NZ   | 1:C:303:ASP:H    | 2.01                     | 0.57              |
| 1:F:231:MET:HG3  | 1:F:283:ILE:HG13 | 1.85                     | 0.57              |
| 1:I:269:ILE:HG23 | 1:I:274:ILE:HG22 | 1.85                     | 0.57              |
| 1:L:434:PRO:HB3  | 1:L:452:LEU:CD2  | 2.34                     | 0.57              |
| 1:M:24:ASP:O     | 1:M:27:LYS:HB3   | 2.03                     | 0.57              |
| 1:M:48:LEU:HD12  | 1:O:508:ILE:CD1  | 2.34                     | 0.57              |
| 1:M:207:LEU:HD22 | 1:M:208:ASP:N    | 2.18                     | 0.57              |
| 1:N:504:VAL:O    | 1:N:505:ASP:HB2  | 2.04                     | 0.57              |
| 1:O:269:ILE:HG23 | 1:O:274:ILE:HG22 | 1.86                     | 0.57              |
| 1:P:134:ASP:O    | 1:P:135:HIS:HB2  | 2.03                     | 0.57              |
| 1:B:74:MET:O     | 1:B:77:VAL:HG12  | 2.04                     | 0.57              |
| 1:E:109:HIS:CE1  | 1:E:111:GLN:HB2  | 2.39                     | 0.57              |
| 1:G:99:GLU:HG3   | 1:G:425:SER:CB   | 2.34                     | 0.57              |
| 1:L:114:ILE:HA   | 1:L:117:TRP:CE3  | 2.39                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:178:LYS:NZ   | 1:M:388:VAL:HB   | 2.19                     | 0.57              |
| 1:M:475:MET:SD   | 1:M:480:ILE:HB   | 2.44                     | 0.57              |
| 1:O:402:MET:SD   | 1:O:456:HIS:HB2  | 2.45                     | 0.57              |
| 1:P:431:ARG:NH1  | 1:P:453:ARG:HD3  | 2.18                     | 0.57              |
| 1:A:27:LYS:HG3   | 1:A:436:ILE:HG13 | 1.85                     | 0.57              |
| 1:F:27:LYS:CA    | 1:F:436:ILE:HD11 | 2.34                     | 0.57              |
| 1:G:154:LEU:HD22 | 1:G:167:THR:HB   | 1.85                     | 0.57              |
| 1:G:324:HIS:ND1  | 1:G:325:PRO:HD3  | 2.18                     | 0.57              |
| 1:H:89:VAL:HG11  | 1:H:490:VAL:HG11 | 1.86                     | 0.57              |
| 1:I:48:LEU:HD13  | 1:N:508:ILE:HD11 | 1.87                     | 0.57              |
| 1:J:448:LEU:HD21 | 1:J:465:LEU:HD12 | 1.85                     | 0.57              |
| 1:M:503:ARG:HH11 | 1:M:503:ARG:CG   | 2.18                     | 0.57              |
| 1:N:434:PRO:HB3  | 1:N:452:LEU:CD2  | 2.33                     | 0.57              |
| 1:P:216:PRO:CG   | 1:P:295:GLY:HA2  | 2.33                     | 0.57              |
| 1:B:173:ALA:O    | 1:B:176:ARG:HG2  | 2.05                     | 0.57              |
| 1:B:222:ALA:HA   | 1:B:275:ASN:OD1  | 2.04                     | 0.57              |
| 1:D:163:LYS:O    | 1:D:166:PHE:HB2  | 2.04                     | 0.57              |
| 1:G:128:LEU:HD22 | 1:G:129:LEU:HD22 | 1.86                     | 0.57              |
| 1:H:161:HIS:CG   | 1:H:162:HIS:H    | 2.22                     | 0.57              |
| 1:J:206:LEU:HD21 | 1:J:346:LEU:HG   | 1.85                     | 0.57              |
| 1:K:64:ASP:CG    | 1:K:66:PRO:HD2   | 2.30                     | 0.57              |
| 1:K:191:LYS:HE3  | 1:K:191:LYS:HA   | 1.86                     | 0.57              |
| 1:M:63:VAL:HA    | 1:M:513:ARG:HA   | 1.86                     | 0.57              |
| 1:M:133:VAL:HG23 | 1:M:134:ASP:H    | 1.69                     | 0.57              |
| 1:P:82:VAL:HG13  | 1:P:83:GLY:H     | 1.70                     | 0.57              |
| 1:P:163:LYS:O    | 1:P:166:PHE:HB2  | 2.05                     | 0.57              |
| 1:B:100:ALA:HA   | 1:B:103:LEU:HD13 | 1.86                     | 0.57              |
| 1:D:78:GLN:HE21  | 1:D:486:VAL:HA   | 1.69                     | 0.57              |
| 1:F:141:LYS:HG2  | 1:F:144:GLN:HB2  | 1.85                     | 0.57              |
| 1:F:225:LEU:CD1  | 1:F:329:LYS:HE2  | 2.34                     | 0.57              |
| 1:H:99:GLU:O     | 1:H:103:LEU:HD13 | 2.04                     | 0.57              |
| 1:K:226:ILE:HG12 | 1:K:278:ILE:HG23 | 1.86                     | 0.57              |
| 1:D:61:ILE:HG21  | 1:E:513:ARG:HG2  | 1.85                     | 0.57              |
| 1:F:408:VAL:HA   | 1:F:411:LEU:HD12 | 1.87                     | 0.57              |
| 1:J:92:LEU:HB3   | 1:J:433:LEU:HD11 | 1.86                     | 0.57              |
| 1:N:59:LYS:HE3   | 1:N:73:ASP:HA    | 1.85                     | 0.57              |
| 1:N:274:ILE:HG23 | 1:N:296:VAL:HG21 | 1.85                     | 0.57              |
| 1:A:341:ILE:HD11 | 1:A:348:HIS:CE1  | 2.40                     | 0.57              |
| 1:C:203:GLU:OE2  | 1:C:350:SER:HB2  | 2.03                     | 0.57              |
| 1:D:163:LYS:HA   | 1:D:166:PHE:CD1  | 2.38                     | 0.57              |
| 1:E:133:VAL:HG11 | 1:E:393:THR:O    | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:503:ARG:O    | 1:E:504:VAL:HB   | 2.05                     | 0.57              |
| 1:F:128:LEU:C    | 1:F:129:LEU:HD13 | 2.30                     | 0.57              |
| 1:F:452:LEU:HA   | 1:F:472:ILE:HG21 | 1.85                     | 0.57              |
| 1:H:22:ILE:O     | 1:H:26:VAL:HG22  | 2.05                     | 0.57              |
| 1:H:133:VAL:HG21 | 1:H:394:VAL:HA   | 1.86                     | 0.57              |
| 1:H:171:VAL:O    | 1:H:174:VAL:HG22 | 2.04                     | 0.57              |
| 1:I:141:LYS:HG2  | 1:I:144:GLN:HB2  | 1.86                     | 0.57              |
| 1:I:161:HIS:CD2  | 1:I:162:HIS:H    | 2.23                     | 0.57              |
| 1:J:190:LYS:HD3  | 1:J:370:LEU:HD23 | 1.87                     | 0.57              |
| 1:K:126:GLN:NE2  | 1:K:411:LEU:HD11 | 2.20                     | 0.57              |
| 1:P:208:ASP:C    | 1:P:209:LYS:HG3  | 2.29                     | 0.57              |
| 1:P:364:GLY:HA3  | 1:P:370:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:245:VAL:CG1  | 1:A:250:LYS:HB3  | 2.33                     | 0.57              |
| 1:A:248:THR:O    | 1:A:251:VAL:HG12 | 2.04                     | 0.57              |
| 1:D:499:GLU:O    | 1:D:503:ARG:HG2  | 2.05                     | 0.57              |
| 1:G:116:GLY:O    | 1:G:119:GLU:HB2  | 2.05                     | 0.57              |
| 1:G:154:LEU:HD23 | 1:G:163:LYS:HG3  | 1.87                     | 0.57              |
| 1:G:402:MET:CE   | 1:G:453:ARG:HG2  | 2.31                     | 0.57              |
| 1:I:128:LEU:HD11 | 1:I:488:ARG:HB3  | 1.86                     | 0.57              |
| 1:I:452:LEU:HD13 | 1:I:465:LEU:HD13 | 1.86                     | 0.57              |
| 1:K:177:LEU:HD23 | 1:K:186:ILE:HD11 | 1.86                     | 0.57              |
| 1:L:231:MET:HG3  | 1:L:283:ILE:HG13 | 1.87                     | 0.57              |
| 1:M:210:LYS:HE2  | 1:M:212:GLY:O    | 2.05                     | 0.57              |
| 1:M:345:LYS:C    | 1:M:346:LEU:HD12 | 2.30                     | 0.57              |
| 1:N:52:ASN:ND2   | 1:N:157:LYS:HA   | 2.20                     | 0.57              |
| 1:O:163:LYS:O    | 1:O:166:PHE:HB2  | 2.03                     | 0.57              |
| 1:A:210:LYS:HE2  | 1:A:212:GLY:O    | 2.04                     | 0.57              |
| 1:D:159:LEU:HG   | 1:D:163:LYS:CG   | 2.35                     | 0.57              |
| 1:F:173:ALA:HA   | 1:F:176:ARG:CZ   | 2.34                     | 0.57              |
| 1:G:126:GLN:HA   | 1:G:130:ASN:HD22 | 1.69                     | 0.57              |
| 1:G:128:LEU:HD22 | 1:G:129:LEU:CD2  | 2.34                     | 0.57              |
| 1:H:128:LEU:HD11 | 1:H:491:LEU:CD1  | 2.34                     | 0.57              |
| 1:I:40:LEU:HD13  | 1:I:41:SER:H     | 1.69                     | 0.57              |
| 1:K:59:LYS:HE2   | 1:K:76:ARG:CB    | 2.35                     | 0.57              |
| 1:K:341:ILE:HG23 | 1:K:363:ARG:CZ   | 2.34                     | 0.57              |
| 1:N:143:ARG:HA   | 1:N:143:ARG:HE   | 1.69                     | 0.57              |
| 1:N:226:ILE:HG12 | 1:N:278:ILE:HG23 | 1.87                     | 0.57              |
| 1:N:356:GLU:O    | 1:N:356:GLU:HG3  | 2.05                     | 0.57              |
| 1:O:183:LEU:HD11 | 1:O:381:LEU:HD11 | 1.86                     | 0.57              |
| 1:B:108:ILE:HD12 | 1:B:108:ILE:N    | 2.15                     | 0.57              |
| 1:C:92:LEU:HD11  | 1:C:433:LEU:HD21 | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:392:ARG:C    | 1:I:484:PHE:HB2  | 2.30                     | 0.57              |
| 1:K:146:LEU:HD23 | 1:K:148:ASN:H    | 1.70                     | 0.57              |
| 1:M:58:LEU:HB3   | 1:M:72:VAL:CG1   | 2.35                     | 0.57              |
| 1:M:138:ASP:O    | 1:M:139:GLU:HB2  | 2.05                     | 0.57              |
| 1:O:231:MET:HB2  | 1:O:284:TYR:H    | 1.68                     | 0.57              |
| 1:P:24:ASP:O     | 1:P:27:LYS:HG2   | 2.05                     | 0.57              |
| 1:P:188:VAL:HA   | 1:P:360:ILE:O    | 2.05                     | 0.57              |
| 1:P:417:GLY:HA2  | 1:P:420:ALA:HB3  | 1.86                     | 0.57              |
| 1:P:438:ALA:HB2  | 1:P:448:LEU:HG   | 1.86                     | 0.57              |
| 1:A:219:ILE:HD12 | 1:A:275:ASN:HB3  | 1.87                     | 0.56              |
| 1:A:510:ALA:O    | 1:F:25:LEU:HD11  | 2.05                     | 0.56              |
| 1:B:365:ALA:O    | 1:B:366:THR:HG23 | 2.04                     | 0.56              |
| 1:C:313:VAL:HG13 | 1:C:352:VAL:HG21 | 1.87                     | 0.56              |
| 1:D:365:ALA:O    | 1:D:366:THR:HG22 | 2.05                     | 0.56              |
| 1:E:394:VAL:HG21 | 1:E:487:LYS:HG3  | 1.87                     | 0.56              |
| 1:J:245:VAL:C    | 1:J:247:SER:H    | 2.13                     | 0.56              |
| 1:K:32:PRO:HA    | 1:K:156:SER:HA   | 1.86                     | 0.56              |
| 1:N:216:PRO:CG   | 1:N:295:GLY:HA2  | 2.35                     | 0.56              |
| 1:O:61:ILE:HG12  | 1:O:63:VAL:HG23  | 1.87                     | 0.56              |
| 1:B:54:GLY:O     | 1:B:58:LEU:HD23  | 2.05                     | 0.56              |
| 1:D:36:ASP:OD2   | 1:D:158:LEU:HB2  | 2.05                     | 0.56              |
| 1:D:483:SER:O    | 1:D:486:VAL:HG22 | 2.05                     | 0.56              |
| 1:D:508:ILE:O    | 1:D:509:LYS:HB2  | 2.05                     | 0.56              |
| 1:E:106:LYS:HG2  | 1:E:108:ILE:HG12 | 1.86                     | 0.56              |
| 1:E:453:ARG:NH2  | 1:J:418:LYS:HA   | 2.20                     | 0.56              |
| 1:H:417:GLY:CA   | 1:P:453:ARG:HH21 | 2.18                     | 0.56              |
| 1:I:120:ALA:O    | 1:I:123:ALA:HB3  | 2.04                     | 0.56              |
| 1:K:145:ASP:O    | 1:K:171:VAL:HG11 | 2.05                     | 0.56              |
| 1:K:200:TYR:O    | 1:K:361:VAL:HG23 | 2.04                     | 0.56              |
| 1:L:99:GLU:O     | 1:L:103:LEU:HD13 | 2.05                     | 0.56              |
| 1:L:506:ASN:HB3  | 1:P:38:ILE:HG12  | 1.87                     | 0.56              |
| 1:M:51:THR:HG21  | 1:M:56:THR:HB    | 1.87                     | 0.56              |
| 1:M:276:CYS:HA   | 1:M:297:MET:O    | 2.05                     | 0.56              |
| 1:N:326:GLU:HG3  | 1:N:327:LEU:N    | 2.21                     | 0.56              |
| 1:O:101:GLU:O    | 1:O:104:ILE:HG23 | 2.05                     | 0.56              |
| 1:O:154:LEU:HD23 | 1:O:163:LYS:HG3  | 1.86                     | 0.56              |
| 1:O:433:LEU:O    | 1:O:436:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:140:VAL:H    | 1:A:178:LYS:HZ2  | 1.54                     | 0.56              |
| 1:C:434:PRO:HB3  | 1:C:452:LEU:CD2  | 2.35                     | 0.56              |
| 1:D:339:VAL:O    | 1:D:340:MET:HB2  | 2.05                     | 0.56              |
| 1:D:507:ILE:CG2  | 1:H:39:LEU:HD23  | 2.32                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:211:ILE:HD13 | 1:E:215:GLN:HG3  | 1.87                     | 0.56              |
| 1:F:152:THR:OG1  | 1:F:480:ILE:HA   | 2.06                     | 0.56              |
| 1:F:317:GLU:HB3  | 1:F:329:LYS:HD3  | 1.87                     | 0.56              |
| 1:F:431:ARG:NE   | 1:F:431:ARG:HA   | 2.20                     | 0.56              |
| 1:G:78:GLN:HG3   | 1:G:83:GLY:HA2   | 1.87                     | 0.56              |
| 1:G:206:LEU:HD23 | 1:G:348:HIS:HD2  | 1.70                     | 0.56              |
| 1:H:185:ALA:HA   | 1:H:309:ARG:NE   | 2.21                     | 0.56              |
| 1:H:402:MET:HG2  | 1:H:431:ARG:NH2  | 2.20                     | 0.56              |
| 1:K:280:ARG:HD2  | 1:K:304:PHE:HB2  | 1.87                     | 0.56              |
| 1:L:99:GLU:HG2   | 1:L:425:SER:CB   | 2.35                     | 0.56              |
| 1:L:222:ALA:HA   | 1:L:275:ASN:HB2  | 1.86                     | 0.56              |
| 1:M:411:LEU:HB3  | 1:M:423:MET:CE   | 2.35                     | 0.56              |
| 1:N:324:HIS:ND1  | 1:N:325:PRO:HD3  | 2.20                     | 0.56              |
| 1:O:334:LYS:CB   | 1:O:351:GLY:HA3  | 2.35                     | 0.56              |
| 1:P:96:LEU:HD21  | 1:P:117:TRP:HZ2  | 1.70                     | 0.56              |
| 1:A:276:CYS:HA   | 1:A:297:MET:O    | 2.05                     | 0.56              |
| 1:B:251:VAL:HG21 | 1:F:240:GLY:CA   | 2.35                     | 0.56              |
| 1:C:108:ILE:HB   | 1:L:446:ALA:CB   | 2.35                     | 0.56              |
| 1:D:63:VAL:HG22  | 1:E:513:ARG:CD   | 2.35                     | 0.56              |
| 1:E:89:VAL:HG12  | 1:E:490:VAL:HB   | 1.88                     | 0.56              |
| 1:E:226:ILE:HG12 | 1:E:278:ILE:HG23 | 1.87                     | 0.56              |
| 1:E:453:ARG:HH22 | 1:J:418:LYS:HA   | 1.70                     | 0.56              |
| 1:F:58:LEU:HB3   | 1:F:72:VAL:HG13  | 1.87                     | 0.56              |
| 1:F:450:ALA:CB   | 1:O:417:GLY:H    | 2.18                     | 0.56              |
| 1:H:369:ILE:O    | 1:H:372:GLU:HB3  | 2.06                     | 0.56              |
| 1:I:334:LYS:CB   | 1:I:351:GLY:HA3  | 2.36                     | 0.56              |
| 1:M:63:VAL:CG1   | 1:O:2:GLY:HA3    | 2.29                     | 0.56              |
| 1:M:162:HIS:HB3  | 1:M:198:ASP:OD2  | 2.06                     | 0.56              |
| 1:N:27:LYS:HG2   | 1:N:436:ILE:CD1  | 2.36                     | 0.56              |
| 1:N:324:HIS:HB2  | 1:N:329:LYS:HZ3  | 1.69                     | 0.56              |
| 1:P:59:LYS:HE3   | 1:P:73:ASP:HA    | 1.87                     | 0.56              |
| 1:C:27:LYS:HB3   | 1:C:436:ILE:HD11 | 1.88                     | 0.56              |
| 1:D:24:ASP:O     | 1:D:27:LYS:HG2   | 2.05                     | 0.56              |
| 1:F:106:LYS:CE   | 1:F:113:ILE:HD11 | 2.31                     | 0.56              |
| 1:F:146:LEU:HB2  | 1:F:171:VAL:HG21 | 1.88                     | 0.56              |
| 1:F:343:GLU:HG3  | 1:F:344:ASP:H    | 1.71                     | 0.56              |
| 1:K:166:PHE:HE2  | 1:K:363:ARG:O    | 1.88                     | 0.56              |
| 1:K:334:LYS:CG   | 1:K:351:GLY:HA3  | 2.36                     | 0.56              |
| 1:L:157:LYS:HB3  | 1:L:159:LEU:CD1  | 2.28                     | 0.56              |
| 1:L:284:TYR:O    | 1:L:287:PRO:HD2  | 2.05                     | 0.56              |
| 1:N:82:VAL:HB    | 1:N:485:GLN:HB3  | 1.86                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:130:ASN:O    | 1:N:131:SER:HB3  | 2.06                     | 0.56              |
| 1:O:367:GLN:O    | 1:O:370:LEU:HB3  | 2.05                     | 0.56              |
| 1:A:30:LEU:HG    | 1:A:87:THR:O     | 2.06                     | 0.56              |
| 1:C:114:ILE:HG23 | 1:C:499:GLU:CG   | 2.34                     | 0.56              |
| 1:C:152:THR:OG1  | 1:C:480:ILE:HA   | 2.06                     | 0.56              |
| 1:C:154:LEU:CD2  | 1:C:167:THR:HB   | 2.36                     | 0.56              |
| 1:D:128:LEU:O    | 1:D:129:LEU:HB2  | 2.06                     | 0.56              |
| 1:F:411:LEU:HD13 | 1:F:423:MET:HE2  | 1.88                     | 0.56              |
| 1:I:123:ALA:HA   | 1:I:126:GLN:HG2  | 1.88                     | 0.56              |
| 1:K:186:ILE:CG2  | 1:K:377:LEU:HD21 | 2.35                     | 0.56              |
| 1:K:433:LEU:O    | 1:K:436:ILE:HG22 | 2.04                     | 0.56              |
| 1:K:500:VAL:HG12 | 1:K:503:ARG:NH1  | 2.20                     | 0.56              |
| 1:N:99:GLU:CG    | 1:N:425:SER:HB2  | 2.35                     | 0.56              |
| 1:P:154:LEU:CD2  | 1:P:167:THR:HB   | 2.36                     | 0.56              |
| 1:C:40:LEU:HD22  | 1:H:510:ALA:HB2  | 1.88                     | 0.56              |
| 1:D:39:LEU:HD21  | 1:E:511:ALA:HB1  | 1.86                     | 0.56              |
| 1:D:128:LEU:CD2  | 1:D:488:ARG:HG2  | 2.36                     | 0.56              |
| 1:E:131:SER:OG   | 1:E:461:THR:HG21 | 2.06                     | 0.56              |
| 1:F:75:SER:O     | 1:F:78:GLN:HB3   | 2.04                     | 0.56              |
| 1:H:68:ALA:O     | 1:H:72:VAL:HG23  | 2.06                     | 0.56              |
| 1:H:141:LYS:CG   | 1:H:144:GLN:HB2  | 2.36                     | 0.56              |
| 1:J:438:ALA:HB2  | 1:J:448:LEU:HG   | 1.86                     | 0.56              |
| 1:J:508:ILE:O    | 1:J:509:LYS:HB2  | 2.06                     | 0.56              |
| 1:K:209:LYS:HE2  | 1:K:301:HIS:O    | 2.06                     | 0.56              |
| 1:L:186:ILE:HD12 | 1:L:381:LEU:HD11 | 1.87                     | 0.56              |
| 1:N:59:LYS:HE2   | 1:N:76:ARG:CB    | 2.35                     | 0.56              |
| 1:N:207:LEU:O    | 1:N:347:ILE:HG22 | 2.04                     | 0.56              |
| 1:N:280:ARG:HD2  | 1:N:304:PHE:HB2  | 1.88                     | 0.56              |
| 1:N:402:MET:SD   | 1:N:453:ARG:HA   | 2.46                     | 0.56              |
| 1:O:99:GLU:O     | 1:O:103:LEU:HD13 | 2.06                     | 0.56              |
| 1:O:219:ILE:HB   | 1:O:275:ASN:HB3  | 1.86                     | 0.56              |
| 1:A:2:GLY:O      | 1:A:3:ALA:HB2    | 2.05                     | 0.56              |
| 1:B:132:ALA:O    | 1:B:133:VAL:HG22 | 2.06                     | 0.56              |
| 1:D:280:ARG:HD2  | 1:D:304:PHE:HB2  | 1.87                     | 0.56              |
| 1:E:280:ARG:HD2  | 1:E:304:PHE:HB2  | 1.88                     | 0.56              |
| 1:G:146:LEU:CD1  | 1:G:171:VAL:HG13 | 2.29                     | 0.56              |
| 1:G:163:LYS:O    | 1:G:166:PHE:HB2  | 2.06                     | 0.56              |
| 1:G:312:LEU:O    | 1:G:354:LEU:HD22 | 2.06                     | 0.56              |
| 1:K:32:PRO:HG2   | 1:K:467:MET:CE   | 2.36                     | 0.56              |
| 1:K:192:LEU:HB2  | 1:K:343:GLU:OE2  | 2.06                     | 0.56              |
| 1:K:340:MET:HG2  | 1:K:345:LYS:HG2  | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:431:ARG:O    | 1:L:434:PRO:HD2  | 2.06                     | 0.56              |
| 1:M:313:VAL:O    | 1:M:352:VAL:HG23 | 2.06                     | 0.56              |
| 1:N:367:GLN:CG   | 1:N:369:ILE:HB   | 2.36                     | 0.56              |
| 1:P:484:PHE:CE2  | 1:P:488:ARG:HD3  | 2.41                     | 0.56              |
| 1:D:139:GLU:O    | 1:D:140:VAL:HB   | 2.06                     | 0.56              |
| 1:D:254:ILE:HG21 | 1:E:238:ILE:HG13 | 1.88                     | 0.56              |
| 1:F:231:MET:HB2  | 1:F:284:TYR:H    | 1.70                     | 0.56              |
| 1:G:284:TYR:O    | 1:G:287:PRO:HD2  | 2.05                     | 0.56              |
| 1:I:231:MET:HG3  | 1:I:283:ILE:HG13 | 1.87                     | 0.56              |
| 1:N:231:MET:HG3  | 1:N:283:ILE:HG13 | 1.88                     | 0.56              |
| 1:B:284:TYR:O    | 1:B:287:PRO:HD2  | 2.06                     | 0.56              |
| 1:B:452:LEU:HD22 | 1:B:465:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:367:GLN:CD   | 1:C:369:ILE:HB   | 2.31                     | 0.56              |
| 1:D:58:LEU:HB3   | 1:D:72:VAL:HG11  | 1.87                     | 0.56              |
| 1:F:280:ARG:HD2  | 1:F:304:PHE:HB2  | 1.87                     | 0.56              |
| 1:G:226:ILE:HG12 | 1:G:278:ILE:HG23 | 1.88                     | 0.56              |
| 1:L:157:LYS:CB   | 1:L:159:LEU:HD13 | 2.26                     | 0.56              |
| 1:N:138:ASP:O    | 1:N:139:GLU:HB2  | 2.06                     | 0.56              |
| 1:N:287:PRO:O    | 1:N:291:PHE:HD1  | 1.88                     | 0.56              |
| 1:P:338:GLU:OE1  | 1:P:345:LYS:HD3  | 2.06                     | 0.56              |
| 1:B:231:MET:HB2  | 1:B:284:TYR:H    | 1.72                     | 0.55              |
| 1:C:431:ARG:HH21 | 1:C:434:PRO:HG2  | 1.71                     | 0.55              |
| 1:G:326:GLU:HG3  | 1:G:327:LEU:H    | 1.71                     | 0.55              |
| 1:H:433:LEU:O    | 1:H:436:ILE:HG22 | 2.06                     | 0.55              |
| 1:I:431:ARG:HH21 | 1:I:434:PRO:HG2  | 1.71                     | 0.55              |
| 1:J:211:ILE:CD1  | 1:J:297:MET:HG3  | 2.32                     | 0.55              |
| 1:K:401:GLU:OE1  | 1:K:433:LEU:HB3  | 2.06                     | 0.55              |
| 1:M:226:ILE:HD13 | 1:M:307:VAL:HG13 | 1.87                     | 0.55              |
| 1:M:232:ASP:HA   | 1:M:284:TYR:CD1  | 2.41                     | 0.55              |
| 1:O:52:ASN:H     | 1:O:375:ARG:HD3  | 1.71                     | 0.55              |
| 1:O:108:ILE:HG22 | 1:O:109:HIS:CD2  | 2.41                     | 0.55              |
| 1:A:262:MET:HE1  | 1:A:286:TYR:O    | 2.05                     | 0.55              |
| 1:D:218:ARG:HD2  | 1:D:337:GLU:OE1  | 2.06                     | 0.55              |
| 1:E:33:LYS:HA    | 1:E:33:LYS:HE3   | 1.88                     | 0.55              |
| 1:F:59:LYS:HE3   | 1:F:73:ASP:HA    | 1.87                     | 0.55              |
| 1:F:188:VAL:HG22 | 1:F:377:LEU:HD21 | 1.87                     | 0.55              |
| 1:F:204:GLY:HA3  | 1:F:349:PHE:O    | 2.06                     | 0.55              |
| 1:F:431:ARG:HA   | 1:F:431:ARG:CZ   | 2.37                     | 0.55              |
| 1:H:163:LYS:HG3  | 1:H:166:PHE:CG   | 2.41                     | 0.55              |
| 1:I:280:ARG:HD2  | 1:I:304:PHE:HB2  | 1.87                     | 0.55              |
| 1:K:317:GLU:HB2  | 1:K:329:LYS:HD3  | 1.87                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:32:PRO:HD2   | 1:M:467:MET:CE   | 2.36                     | 0.55              |
| 1:O:185:ALA:HA   | 1:O:309:ARG:HE   | 1.70                     | 0.55              |
| 1:O:379:ASP:O    | 1:O:383:VAL:HG23 | 2.06                     | 0.55              |
| 1:P:115:ALA:O    | 1:P:118:ARG:HB3  | 2.05                     | 0.55              |
| 1:D:32:PRO:O     | 1:D:155:SER:HB3  | 2.07                     | 0.55              |
| 1:D:226:ILE:HG12 | 1:D:278:ILE:HG23 | 1.88                     | 0.55              |
| 1:G:269:ILE:HG23 | 1:G:274:ILE:CG2  | 2.36                     | 0.55              |
| 1:I:59:LYS:HE3   | 1:I:73:ASP:HA    | 1.87                     | 0.55              |
| 1:L:159:LEU:HD12 | 1:L:159:LEU:N    | 2.22                     | 0.55              |
| 1:L:274:ILE:HG23 | 1:L:296:VAL:HG21 | 1.87                     | 0.55              |
| 1:L:448:LEU:C    | 1:L:448:LEU:HD13 | 2.31                     | 0.55              |
| 1:N:508:ILE:O    | 1:N:509:LYS:HB2  | 2.04                     | 0.55              |
| 1:O:334:LYS:O    | 1:O:335:LEU:HB2  | 2.06                     | 0.55              |
| 1:P:317:GLU:HB2  | 1:P:329:LYS:HD3  | 1.87                     | 0.55              |
| 1:A:324:HIS:ND1  | 1:A:325:PRO:HD3  | 2.21                     | 0.55              |
| 1:B:312:LEU:O    | 1:B:354:LEU:HD22 | 2.05                     | 0.55              |
| 1:C:262:MET:HE1  | 1:C:286:TYR:O    | 2.07                     | 0.55              |
| 1:D:14:SER:O     | 1:D:17:ILE:HG22  | 2.07                     | 0.55              |
| 1:E:231:MET:HG3  | 1:E:283:ILE:HG13 | 1.87                     | 0.55              |
| 1:F:478:LEU:HB3  | 1:F:480:ILE:HD13 | 1.87                     | 0.55              |
| 1:G:176:ARG:HH22 | 1:G:360:ILE:CG1  | 2.18                     | 0.55              |
| 1:H:12:ARG:HD3   | 1:H:100:ALA:HB1  | 1.88                     | 0.55              |
| 1:H:163:LYS:O    | 1:H:166:PHE:HB2  | 2.06                     | 0.55              |
| 1:I:365:ALA:O    | 1:I:366:THR:HB   | 2.07                     | 0.55              |
| 1:J:146:LEU:HD21 | 1:J:167:THR:HG23 | 1.88                     | 0.55              |
| 1:M:431:ARG:NH1  | 1:M:453:ARG:HD3  | 2.20                     | 0.55              |
| 1:A:397:GLY:O    | 1:A:465:LEU:HG   | 2.06                     | 0.55              |
| 1:B:375:ARG:HH11 | 1:B:375:ARG:HG3  | 1.70                     | 0.55              |
| 1:E:133:VAL:HG21 | 1:E:393:THR:O    | 2.06                     | 0.55              |
| 1:H:99:GLU:HG3   | 1:H:425:SER:CB   | 2.36                     | 0.55              |
| 1:J:231:MET:HB2  | 1:J:284:TYR:H    | 1.71                     | 0.55              |
| 1:K:28:SER:O     | 1:K:34:GLY:HA2   | 2.05                     | 0.55              |
| 1:K:176:ARG:HH21 | 1:K:360:ILE:HG12 | 1.71                     | 0.55              |
| 1:K:276:CYS:HA   | 1:K:297:MET:O    | 2.06                     | 0.55              |
| 1:K:352:VAL:HG22 | 1:K:355:GLY:H    | 1.72                     | 0.55              |
| 1:K:364:GLY:HA3  | 1:K:370:LEU:HD13 | 1.88                     | 0.55              |
| 1:L:334:LYS:HB3  | 1:L:350:SER:O    | 2.07                     | 0.55              |
| 1:M:266:VAL:HB   | 1:M:290:LEU:HD21 | 1.89                     | 0.55              |
| 1:O:397:GLY:HA3  | 1:O:475:MET:HE3  | 1.88                     | 0.55              |
| 1:O:448:LEU:C    | 1:O:448:LEU:HD13 | 2.32                     | 0.55              |
| 1:P:124:ALA:O    | 1:P:128:LEU:HG   | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:54:GLY:O     | 1:A:58:LEU:HD23  | 2.06                     | 0.55              |
| 1:A:226:ILE:HD11 | 1:A:310:LEU:HD12 | 1.88                     | 0.55              |
| 1:F:109:HIS:CE1  | 1:F:111:GLN:HB2  | 2.42                     | 0.55              |
| 1:F:451:GLN:NE2  | 1:F:471:THR:HA   | 2.21                     | 0.55              |
| 1:H:365:ALA:O    | 1:H:366:THR:HB   | 2.05                     | 0.55              |
| 1:H:489:GLN:O    | 1:H:493:SER:HB2  | 2.06                     | 0.55              |
| 1:I:216:PRO:HG2  | 1:I:295:GLY:HA2  | 1.87                     | 0.55              |
| 1:K:451:GLN:HE22 | 1:K:471:THR:HA   | 1.72                     | 0.55              |
| 1:M:317:GLU:HB2  | 1:M:329:LYS:HG2  | 1.87                     | 0.55              |
| 1:N:159:LEU:HG   | 1:N:163:LYS:HD3  | 1.87                     | 0.55              |
| 1:B:152:THR:OG1  | 1:B:480:ILE:HG23 | 2.06                     | 0.55              |
| 1:D:268:ARG:O    | 1:D:271:LYS:HG2  | 2.07                     | 0.55              |
| 1:F:317:GLU:CB   | 1:F:329:LYS:HD3  | 2.37                     | 0.55              |
| 1:G:141:LYS:HG2  | 1:G:144:GLN:HB2  | 1.88                     | 0.55              |
| 1:I:27:LYS:O     | 1:I:436:ILE:HD11 | 2.07                     | 0.55              |
| 1:I:54:GLY:O     | 1:I:58:LEU:HD23  | 2.07                     | 0.55              |
| 1:I:236:ILE:HG23 | 1:I:238:ILE:H    | 1.71                     | 0.55              |
| 1:J:96:LEU:HD11  | 1:J:117:TRP:CZ2  | 2.41                     | 0.55              |
| 1:M:334:LYS:CB   | 1:M:351:GLY:HA3  | 2.36                     | 0.55              |
| 1:N:159:LEU:HG   | 1:N:163:LYS:HD2  | 1.87                     | 0.55              |
| 1:P:324:HIS:HB2  | 1:P:329:LYS:HZ3  | 1.71                     | 0.55              |
| 1:A:171:VAL:HA   | 1:A:174:VAL:HG22 | 1.87                     | 0.55              |
| 1:B:96:LEU:HD13  | 1:B:96:LEU:C     | 2.32                     | 0.55              |
| 1:B:280:ARG:HD2  | 1:B:304:PHE:HB2  | 1.88                     | 0.55              |
| 1:B:324:HIS:HB2  | 1:B:329:LYS:HZ1  | 1.72                     | 0.55              |
| 1:C:92:LEU:CD1   | 1:C:433:LEU:HD21 | 2.36                     | 0.55              |
| 1:H:161:HIS:CD2  | 1:H:162:HIS:H    | 2.24                     | 0.55              |
| 1:H:216:PRO:HG3  | 1:H:295:GLY:HA2  | 1.89                     | 0.55              |
| 1:J:32:PRO:HD2   | 1:J:467:MET:CE   | 2.37                     | 0.55              |
| 1:K:78:GLN:HE22  | 1:K:489:GLN:HB3  | 1.71                     | 0.55              |
| 1:L:59:LYS:HE2   | 1:L:76:ARG:HB2   | 1.89                     | 0.55              |
| 1:M:92:LEU:HG    | 1:M:433:LEU:HD21 | 1.89                     | 0.55              |
| 1:M:119:GLU:HB3  | 1:M:423:MET:HE3  | 1.89                     | 0.55              |
| 1:M:143:ARG:HH22 | 1:M:168:LYS:HE3  | 1.72                     | 0.55              |
| 1:M:431:ARG:HH21 | 1:M:434:PRO:HG2  | 1.72                     | 0.55              |
| 1:N:324:HIS:O    | 1:N:329:LYS:HG2  | 2.07                     | 0.55              |
| 1:O:101:GLU:HA   | 1:O:104:ILE:CG2  | 2.37                     | 0.55              |
| 1:O:185:ALA:HA   | 1:O:309:ARG:NE   | 2.21                     | 0.55              |
| 1:O:188:VAL:CB   | 1:O:377:LEU:HD13 | 2.37                     | 0.55              |
| 1:O:322:PHE:HA   | 1:O:324:HIS:CD2  | 2.42                     | 0.55              |
| 1:O:452:LEU:HD13 | 1:O:465:LEU:HD13 | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:27:LYS:CB    | 1:P:436:ILE:HD11 | 2.37                     | 0.55              |
| 1:P:324:HIS:ND1  | 1:P:325:PRO:HD3  | 2.22                     | 0.55              |
| 1:A:150:ALA:HB1  | 1:A:167:THR:OG1  | 2.06                     | 0.55              |
| 1:A:324:HIS:HB2  | 1:A:329:LYS:CE   | 2.37                     | 0.55              |
| 1:C:114:ILE:CG2  | 1:C:499:GLU:HG3  | 2.33                     | 0.55              |
| 1:C:276:CYS:HA   | 1:C:297:MET:O    | 2.06                     | 0.55              |
| 1:E:75:SER:O     | 1:E:78:GLN:HB3   | 2.07                     | 0.55              |
| 1:G:133:VAL:HB   | 1:G:393:THR:H    | 1.72                     | 0.55              |
| 1:G:222:ALA:HB1  | 1:G:336:ILE:HD12 | 1.89                     | 0.55              |
| 1:G:431:ARG:HA   | 1:G:431:ARG:CZ   | 2.37                     | 0.55              |
| 1:H:312:LEU:O    | 1:H:354:LEU:HD22 | 2.05                     | 0.55              |
| 1:I:108:ILE:CD1  | 1:I:418:LYS:HE3  | 2.36                     | 0.55              |
| 1:I:265:LYS:HZ2  | 1:I:287:PRO:HG3  | 1.70                     | 0.55              |
| 1:I:452:LEU:HD13 | 1:I:465:LEU:CD1  | 2.37                     | 0.55              |
| 1:L:390:ASP:CB   | 1:L:485:GLN:HE22 | 2.20                     | 0.55              |
| 1:N:111:GLN:O    | 1:N:114:ILE:HB   | 2.06                     | 0.55              |
| 1:N:145:ASP:HB3  | 1:N:171:VAL:HG21 | 1.87                     | 0.55              |
| 1:N:149:ILE:O    | 1:N:152:THR:HG22 | 2.05                     | 0.55              |
| 1:C:111:GLN:HA   | 1:C:114:ILE:HG12 | 1.87                     | 0.55              |
| 1:D:334:LYS:O    | 1:D:335:LEU:HB2  | 2.07                     | 0.55              |
| 1:E:104:ILE:O    | 1:E:107:LYS:HB2  | 2.06                     | 0.55              |
| 1:E:364:GLY:HA3  | 1:E:370:LEU:CD1  | 2.37                     | 0.55              |
| 1:F:222:ALA:HA   | 1:F:275:ASN:OD1  | 2.06                     | 0.55              |
| 1:G:190:LYS:HA   | 1:G:362:LEU:O    | 2.06                     | 0.55              |
| 1:G:324:HIS:O    | 1:G:329:LYS:HG2  | 2.07                     | 0.55              |
| 1:J:139:GLU:O    | 1:J:140:VAL:HB   | 2.07                     | 0.55              |
| 1:J:231:MET:HG3  | 1:J:283:ILE:HG13 | 1.88                     | 0.55              |
| 1:L:504:VAL:HG22 | 1:P:369:ILE:CD1  | 2.36                     | 0.55              |
| 1:P:128:LEU:HD21 | 1:P:488:ARG:HG2  | 1.88                     | 0.55              |
| 1:C:58:LEU:HB3   | 1:C:72:VAL:CG1   | 2.38                     | 0.54              |
| 1:E:82:VAL:HG11  | 1:E:485:GLN:HG2  | 1.89                     | 0.54              |
| 1:E:200:TYR:HD2  | 1:E:363:ARG:NH2  | 2.05                     | 0.54              |
| 1:F:139:GLU:HG2  | 1:F:178:LYS:HZ1  | 1.72                     | 0.54              |
| 1:H:397:GLY:HA3  | 1:H:475:MET:HE3  | 1.89                     | 0.54              |
| 1:L:27:LYS:HB2   | 1:L:436:ILE:HG12 | 1.88                     | 0.54              |
| 1:N:32:PRO:HA    | 1:N:155:SER:HB3  | 1.88                     | 0.54              |
| 1:A:209:LYS:HE2  | 1:A:301:HIS:O    | 2.08                     | 0.54              |
| 1:A:213:VAL:HG11 | 1:C:304:PHE:CZ   | 2.42                     | 0.54              |
| 1:B:106:LYS:O    | 1:B:107:LYS:HB3  | 2.07                     | 0.54              |
| 1:C:265:LYS:O    | 1:C:269:ILE:HB   | 2.07                     | 0.54              |
| 1:E:397:GLY:HA3  | 1:E:475:MET:HE3  | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:219:ILE:HD12 | 1:G:275:ASN:HB3  | 1.88                     | 0.54              |
| 1:K:284:TYR:O    | 1:K:287:PRO:HD2  | 2.08                     | 0.54              |
| 1:K:448:LEU:HD13 | 1:K:448:LEU:C    | 2.32                     | 0.54              |
| 1:L:367:GLN:C    | 1:L:369:ILE:H    | 2.14                     | 0.54              |
| 1:N:58:LEU:HB3   | 1:N:72:VAL:CG1   | 2.37                     | 0.54              |
| 1:N:93:ALA:O     | 1:N:96:LEU:HD12  | 2.07                     | 0.54              |
| 1:A:236:ILE:HG23 | 1:A:237:LYS:N    | 2.23                     | 0.54              |
| 1:B:513:ARG:HA   | 1:G:61:ILE:HG12  | 1.89                     | 0.54              |
| 1:D:25:LEU:HG    | 1:E:512:PRO:HD3  | 1.90                     | 0.54              |
| 1:E:163:LYS:O    | 1:E:166:PHE:HB2  | 2.08                     | 0.54              |
| 1:F:497:ALA:O    | 1:F:500:VAL:HG22 | 2.08                     | 0.54              |
| 1:H:146:LEU:HD23 | 1:H:147:MET:N    | 2.22                     | 0.54              |
| 1:I:157:LYS:HB3  | 1:I:159:LEU:HD22 | 1.90                     | 0.54              |
| 1:K:145:ASP:OD1  | 1:K:171:VAL:HB   | 2.07                     | 0.54              |
| 1:L:451:GLN:HE22 | 1:L:471:THR:HA   | 1.71                     | 0.54              |
| 1:O:35:MET:HE1   | 1:O:440:ASN:CB   | 2.37                     | 0.54              |
| 1:P:107:LYS:O    | 1:P:107:LYS:HG2  | 2.08                     | 0.54              |
| 1:A:171:VAL:HG12 | 1:A:384:LEU:HG   | 1.89                     | 0.54              |
| 1:B:324:HIS:O    | 1:B:328:VAL:HG23 | 2.08                     | 0.54              |
| 1:C:84:ASP:OD1   | 1:C:383:VAL:HG13 | 2.07                     | 0.54              |
| 1:E:215:GLN:HB3  | 1:E:292:GLY:HA2  | 1.89                     | 0.54              |
| 1:H:143:ARG:HA   | 1:H:143:ARG:HE   | 1.72                     | 0.54              |
| 1:I:32:PRO:HA    | 1:I:155:SER:C    | 2.32                     | 0.54              |
| 1:I:75:SER:O     | 1:I:78:GLN:HB3   | 2.08                     | 0.54              |
| 1:K:99:GLU:CD    | 1:K:425:SER:HB2  | 2.32                     | 0.54              |
| 1:K:152:THR:OG1  | 1:K:480:ILE:HG23 | 2.07                     | 0.54              |
| 1:L:74:MET:O     | 1:L:77:VAL:HG12  | 2.07                     | 0.54              |
| 1:N:95:GLU:CD    | 1:N:429:ALA:HB1  | 2.32                     | 0.54              |
| 1:O:188:VAL:HB   | 1:O:377:LEU:HD13 | 1.89                     | 0.54              |
| 1:O:207:LEU:O    | 1:O:347:ILE:HG22 | 2.08                     | 0.54              |
| 1:A:58:LEU:HB3   | 1:A:72:VAL:CG1   | 2.37                     | 0.54              |
| 1:A:114:ILE:HA   | 1:A:117:TRP:CZ3  | 2.43                     | 0.54              |
| 1:F:146:LEU:HG   | 1:F:171:VAL:CG1  | 2.38                     | 0.54              |
| 1:G:121:THR:O    | 1:G:125:ARG:HG3  | 2.07                     | 0.54              |
| 1:G:287:PRO:O    | 1:G:291:PHE:HD2  | 1.90                     | 0.54              |
| 1:H:59:LYS:CE    | 1:H:76:ARG:HB2   | 2.37                     | 0.54              |
| 1:H:171:VAL:CG1  | 1:H:384:LEU:HG   | 2.34                     | 0.54              |
| 1:I:146:LEU:HD21 | 1:I:150:ALA:CB   | 2.35                     | 0.54              |
| 1:I:176:ARG:CZ   | 1:I:358:CYS:HB2  | 2.38                     | 0.54              |
| 1:J:110:PRO:HB2  | 1:J:502:LEU:HB3  | 1.88                     | 0.54              |
| 1:J:208:ASP:O    | 1:J:209:LYS:HG3  | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:231:MET:HG3  | 1:K:283:ILE:HG13 | 1.88                     | 0.54              |
| 1:M:96:LEU:HD13  | 1:M:96:LEU:C     | 2.31                     | 0.54              |
| 1:M:231:MET:HG3  | 1:M:283:ILE:HG13 | 1.89                     | 0.54              |
| 1:N:9:GLU:CD     | 1:N:9:GLU:H      | 2.14                     | 0.54              |
| 1:N:99:GLU:OE2   | 1:N:428:LYS:HE2  | 2.08                     | 0.54              |
| 1:O:324:HIS:O    | 1:O:328:VAL:HG13 | 2.06                     | 0.54              |
| 1:P:161:HIS:CD2  | 1:P:162:HIS:H    | 2.26                     | 0.54              |
| 1:E:22:ILE:HD12  | 1:E:90:THR:CG2   | 2.38                     | 0.54              |
| 1:E:108:ILE:HD11 | 1:J:449:VAL:HB   | 1.90                     | 0.54              |
| 1:E:171:VAL:O    | 1:E:174:VAL:HG22 | 2.08                     | 0.54              |
| 1:F:106:LYS:HG3  | 1:O:446:ALA:HB2  | 1.90                     | 0.54              |
| 1:G:226:ILE:HB   | 1:G:317:GLU:OE2  | 2.08                     | 0.54              |
| 1:H:211:ILE:CD1  | 1:H:297:MET:HG3  | 2.32                     | 0.54              |
| 1:H:225:LEU:HD12 | 1:H:226:ILE:N    | 2.22                     | 0.54              |
| 1:I:191:LYS:HE3  | 1:I:346:LEU:HG   | 1.90                     | 0.54              |
| 1:I:488:ARG:HG3  | 1:I:489:GLN:OE1  | 2.07                     | 0.54              |
| 1:K:209:LYS:HD3  | 1:K:300:GLU:O    | 2.08                     | 0.54              |
| 1:L:334:LYS:CG   | 1:L:351:GLY:HA3  | 2.37                     | 0.54              |
| 1:M:27:LYS:HG3   | 1:M:436:ILE:HG13 | 1.90                     | 0.54              |
| 1:O:96:LEU:HD11  | 1:O:498:ALA:CB   | 2.37                     | 0.54              |
| 1:O:108:ILE:HG22 | 1:O:109:HIS:N    | 2.20                     | 0.54              |
| 1:O:154:LEU:HD21 | 1:O:163:LYS:NZ   | 2.23                     | 0.54              |
| 1:A:112:THR:HG21 | 1:A:418:LYS:HD2  | 1.88                     | 0.54              |
| 1:B:160:THR:HA   | 1:B:163:LYS:HB3  | 1.90                     | 0.54              |
| 1:B:431:ARG:HH21 | 1:B:434:PRO:HG2  | 1.73                     | 0.54              |
| 1:C:139:GLU:OE1  | 1:C:140:VAL:HG23 | 2.08                     | 0.54              |
| 1:C:146:LEU:CD2  | 1:C:147:MET:H    | 2.15                     | 0.54              |
| 1:C:325:PRO:C    | 1:C:326:GLU:HG3  | 2.33                     | 0.54              |
| 1:D:462:THR:O    | 1:D:475:MET:HB3  | 2.08                     | 0.54              |
| 1:E:96:LEU:HD13  | 1:E:96:LEU:C     | 2.33                     | 0.54              |
| 1:I:32:PRO:CD    | 1:I:467:MET:HE1  | 2.37                     | 0.54              |
| 1:L:139:GLU:O    | 1:L:140:VAL:HB   | 2.08                     | 0.54              |
| 1:M:82:VAL:HA    | 1:M:386:GLN:CG   | 2.37                     | 0.54              |
| 1:N:146:LEU:HD11 | 1:N:168:LYS:HG3  | 1.90                     | 0.54              |
| 1:O:283:ILE:HG22 | 1:O:300:GLU:HG3  | 1.88                     | 0.54              |
| 1:P:211:ILE:CD1  | 1:P:297:MET:HG3  | 2.34                     | 0.54              |
| 1:C:159:LEU:HD13 | 1:C:372:GLU:OE2  | 2.08                     | 0.54              |
| 1:C:222:ALA:HA   | 1:C:275:ASN:CG   | 2.33                     | 0.54              |
| 1:D:269:ILE:HD13 | 1:D:274:ILE:HG21 | 1.89                     | 0.54              |
| 1:E:159:LEU:O    | 1:E:163:LYS:HB3  | 2.07                     | 0.54              |
| 1:E:310:LEU:O    | 1:E:314:THR:HG22 | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:82:VAL:HG21  | 1:F:485:GLN:HG2  | 1.88                     | 0.54              |
| 1:F:226:ILE:O    | 1:F:329:LYS:HE3  | 2.07                     | 0.54              |
| 1:G:5:GLU:O      | 1:G:5:GLU:HG2    | 2.07                     | 0.54              |
| 1:L:149:ILE:O    | 1:L:152:THR:HG22 | 2.07                     | 0.54              |
| 1:L:462:THR:O    | 1:L:475:MET:HB3  | 2.06                     | 0.54              |
| 1:M:222:ALA:HA   | 1:M:275:ASN:HB2  | 1.89                     | 0.54              |
| 1:N:159:LEU:HB3  | 1:N:369:ILE:CG2  | 2.38                     | 0.54              |
| 1:A:96:LEU:HD21  | 1:A:117:TRP:HZ2  | 1.72                     | 0.54              |
| 1:A:96:LEU:HD21  | 1:A:117:TRP:CZ2  | 2.43                     | 0.54              |
| 1:A:155:SER:HA   | 1:A:160:THR:HG21 | 1.89                     | 0.54              |
| 1:B:110:PRO:O    | 1:B:114:ILE:HG12 | 2.08                     | 0.54              |
| 1:B:334:LYS:CD   | 1:B:351:GLY:HA3  | 2.38                     | 0.54              |
| 1:C:310:LEU:O    | 1:C:314:THR:HG22 | 2.08                     | 0.54              |
| 1:C:329:LYS:HB2  | 1:C:329:LYS:NZ   | 2.23                     | 0.54              |
| 1:D:448:LEU:C    | 1:D:448:LEU:HD13 | 2.33                     | 0.54              |
| 1:E:40:LEU:HD13  | 1:E:41:SER:O     | 2.07                     | 0.54              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:HD21 | 1.89                     | 0.54              |
| 1:G:24:ASP:O     | 1:G:27:LYS:HG2   | 2.08                     | 0.54              |
| 1:G:137:SER:OG   | 1:G:388:VAL:HA   | 2.07                     | 0.54              |
| 1:G:163:LYS:HA   | 1:G:166:PHE:CD1  | 2.43                     | 0.54              |
| 1:I:106:LYS:HZ3  | 1:I:106:LYS:CB   | 2.18                     | 0.54              |
| 1:I:152:THR:OG1  | 1:I:480:ILE:HG23 | 2.07                     | 0.54              |
| 1:J:372:GLU:O    | 1:J:375:ARG:HB3  | 2.08                     | 0.54              |
| 1:K:66:PRO:HB3   | 1:K:509:LYS:HZ3  | 1.73                     | 0.54              |
| 1:K:434:PRO:HB3  | 1:K:452:LEU:CD2  | 2.37                     | 0.54              |
| 1:L:155:SER:HA   | 1:L:160:THR:HG21 | 1.89                     | 0.54              |
| 1:L:345:LYS:C    | 1:L:346:LEU:HD12 | 2.33                     | 0.54              |
| 1:N:448:LEU:HD21 | 1:N:465:LEU:CD1  | 2.37                     | 0.54              |
| 1:O:372:GLU:O    | 1:O:375:ARG:HB3  | 2.07                     | 0.54              |
| 1:P:500:VAL:O    | 1:P:504:VAL:HG22 | 2.08                     | 0.54              |
| 1:B:418:LYS:HG3  | 1:I:450:ALA:CB   | 2.37                     | 0.54              |
| 1:C:280:ARG:HD2  | 1:C:304:PHE:HB2  | 1.90                     | 0.54              |
| 1:E:161:HIS:CG   | 1:E:162:HIS:H    | 2.26                     | 0.54              |
| 1:F:190:LYS:HD3  | 1:F:374:GLU:HB2  | 1.90                     | 0.54              |
| 1:G:203:GLU:HB2  | 1:G:350:SER:HB2  | 1.90                     | 0.54              |
| 1:H:433:LEU:HB2  | 1:H:434:PRO:HD3  | 1.89                     | 0.54              |
| 1:I:154:LEU:HD22 | 1:I:167:THR:HB   | 1.89                     | 0.54              |
| 1:I:366:THR:C    | 1:I:367:GLN:HG3  | 2.32                     | 0.54              |
| 1:J:210:LYS:HE2  | 1:J:212:GLY:O    | 2.08                     | 0.54              |
| 1:J:431:ARG:HH21 | 1:J:434:PRO:HG2  | 1.73                     | 0.54              |
| 1:L:219:ILE:HB   | 1:L:275:ASN:HB3  | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:173:ALA:O    | 1:M:176:ARG:HG2  | 2.07                     | 0.54              |
| 1:O:354:LEU:HD23 | 1:O:356:GLU:H    | 1.73                     | 0.54              |
| 1:P:176:ARG:CD   | 1:P:358:CYS:HB2  | 2.38                     | 0.54              |
| 1:P:187:HIS:O    | 1:P:359:THR:HG23 | 2.08                     | 0.54              |
| 1:A:52:ASN:H     | 1:A:375:ARG:HH11 | 1.55                     | 0.53              |
| 1:A:512:PRO:HG2  | 1:F:57:ILE:HD12  | 1.90                     | 0.53              |
| 1:B:166:PHE:CZ   | 1:B:198:ASP:HB3  | 2.42                     | 0.53              |
| 1:E:369:ILE:O    | 1:E:372:GLU:HB3  | 2.09                     | 0.53              |
| 1:F:232:ASP:HA   | 1:F:284:TYR:CD1  | 2.43                     | 0.53              |
| 1:G:496:GLU:HA   | 1:G:499:GLU:HB3  | 1.90                     | 0.53              |
| 1:I:79:ASP:HA    | 1:I:83:GLY:HA2   | 1.88                     | 0.53              |
| 1:J:209:LYS:HE2  | 1:J:301:HIS:O    | 2.07                     | 0.53              |
| 1:J:411:LEU:HB3  | 1:J:423:MET:CE   | 2.38                     | 0.53              |
| 1:O:317:GLU:HB2  | 1:O:329:LYS:HD3  | 1.89                     | 0.53              |
| 1:P:262:MET:HG3  | 1:P:290:LEU:HD22 | 1.89                     | 0.53              |
| 1:A:82:VAL:HG13  | 1:A:83:GLY:N     | 2.22                     | 0.53              |
| 1:B:219:ILE:HB   | 1:B:275:ASN:HB3  | 1.90                     | 0.53              |
| 1:D:159:LEU:HG   | 1:D:163:LYS:CB   | 2.39                     | 0.53              |
| 1:D:425:SER:O    | 1:D:428:LYS:HG2  | 2.08                     | 0.53              |
| 1:F:106:LYS:HE2  | 1:F:113:ILE:CD1  | 2.33                     | 0.53              |
| 1:F:188:VAL:HG21 | 1:F:377:LEU:HD11 | 1.90                     | 0.53              |
| 1:F:225:LEU:HD12 | 1:F:226:ILE:N    | 2.24                     | 0.53              |
| 1:I:222:ALA:HA   | 1:I:275:ASN:HB2  | 1.91                     | 0.53              |
| 1:J:174:VAL:O    | 1:J:177:LEU:HB3  | 2.08                     | 0.53              |
| 1:K:207:LEU:HB3  | 1:K:347:ILE:CG2  | 2.38                     | 0.53              |
| 1:K:321:THR:O    | 1:K:323:ASP:N    | 2.41                     | 0.53              |
| 1:L:32:PRO:HD2   | 1:L:467:MET:CE   | 2.38                     | 0.53              |
| 1:L:96:LEU:HD13  | 1:L:97:LEU:N     | 2.24                     | 0.53              |
| 1:M:117:TRP:CD1  | 1:M:495:ALA:HA   | 2.43                     | 0.53              |
| 1:M:141:LYS:HG2  | 1:M:144:GLN:HB2  | 1.89                     | 0.53              |
| 1:O:146:LEU:CD2  | 1:O:147:MET:H    | 2.20                     | 0.53              |
| 1:A:211:ILE:HG13 | 1:A:298:ALA:O    | 2.09                     | 0.53              |
| 1:B:266:VAL:HB   | 1:B:290:LEU:HD21 | 1.88                     | 0.53              |
| 1:D:324:HIS:O    | 1:D:328:VAL:HG23 | 2.08                     | 0.53              |
| 1:D:402:MET:HE3  | 1:D:453:ARG:CG   | 2.37                     | 0.53              |
| 1:E:49:MET:HE1   | 1:E:375:ARG:NH2  | 2.23                     | 0.53              |
| 1:E:222:ALA:HB1  | 1:E:336:ILE:HD12 | 1.90                     | 0.53              |
| 1:G:223:LYS:HD3  | 1:G:272:HIS:CE1  | 2.43                     | 0.53              |
| 1:I:231:MET:HB2  | 1:I:284:TYR:H    | 1.72                     | 0.53              |
| 1:I:312:LEU:O    | 1:I:354:LEU:HD22 | 2.08                     | 0.53              |
| 1:J:40:LEU:N     | 1:K:3:ALA:HB2    | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:188:VAL:CG1  | 1:K:377:LEU:HD22 | 2.38                     | 0.53              |
| 1:L:58:LEU:HB3   | 1:L:72:VAL:HG11  | 1.90                     | 0.53              |
| 1:M:99:GLU:HB3   | 1:M:425:SER:HB2  | 1.90                     | 0.53              |
| 1:M:211:ILE:HG13 | 1:M:298:ALA:O    | 2.09                     | 0.53              |
| 1:N:310:LEU:O    | 1:N:314:THR:HG22 | 2.07                     | 0.53              |
| 1:P:159:LEU:HD13 | 1:P:159:LEU:N    | 2.24                     | 0.53              |
| 1:A:233:THR:HG21 | 1:A:261:LYS:HE2  | 1.89                     | 0.53              |
| 1:B:509:LYS:HG3  | 1:G:38:ILE:O     | 2.08                     | 0.53              |
| 1:D:15:SER:OG    | 1:D:501:ILE:HG21 | 2.08                     | 0.53              |
| 1:D:25:LEU:HG    | 1:E:512:PRO:HG3  | 1.91                     | 0.53              |
| 1:E:59:LYS:CE    | 1:E:76:ARG:HB2   | 2.39                     | 0.53              |
| 1:E:99:GLU:HG2   | 1:E:425:SER:HB2  | 1.90                     | 0.53              |
| 1:F:269:ILE:HG23 | 1:F:274:ILE:CG2  | 2.37                     | 0.53              |
| 1:H:317:GLU:HB3  | 1:H:330:LEU:H    | 1.74                     | 0.53              |
| 1:K:216:PRO:CG   | 1:K:295:GLY:HA2  | 2.39                     | 0.53              |
| 1:K:376:SER:O    | 1:K:379:ASP:HB2  | 2.09                     | 0.53              |
| 1:L:231:MET:HB2  | 1:L:284:TYR:H    | 1.74                     | 0.53              |
| 1:N:283:ILE:HG22 | 1:N:300:GLU:CG   | 2.37                     | 0.53              |
| 1:P:108:ILE:HG22 | 1:P:109:HIS:N    | 2.23                     | 0.53              |
| 1:A:128:LEU:O    | 1:A:129:LEU:HB2  | 2.07                     | 0.53              |
| 1:A:280:ARG:HD2  | 1:A:304:PHE:HB2  | 1.91                     | 0.53              |
| 1:C:287:PRO:O    | 1:C:291:PHE:HD1  | 1.91                     | 0.53              |
| 1:D:89:VAL:CG1   | 1:D:490:VAL:HB   | 2.38                     | 0.53              |
| 1:D:512:PRO:O    | 1:D:513:ARG:HB2  | 2.08                     | 0.53              |
| 1:E:204:GLY:HA3  | 1:E:349:PHE:O    | 2.08                     | 0.53              |
| 1:E:242:ARG:HD3  | 1:E:242:ARG:N    | 2.24                     | 0.53              |
| 1:F:82:VAL:HG13  | 1:F:486:VAL:HG12 | 1.90                     | 0.53              |
| 1:G:141:LYS:CG   | 1:G:144:GLN:HB2  | 2.38                     | 0.53              |
| 1:G:216:PRO:CG   | 1:G:295:GLY:HA2  | 2.37                     | 0.53              |
| 1:J:280:ARG:HD2  | 1:J:304:PHE:HB2  | 1.90                     | 0.53              |
| 1:J:433:LEU:HB2  | 1:J:434:PRO:HD3  | 1.91                     | 0.53              |
| 1:K:268:ARG:O    | 1:K:271:LYS:HG2  | 2.09                     | 0.53              |
| 1:M:177:LEU:HG   | 1:M:186:ILE:HD11 | 1.91                     | 0.53              |
| 1:N:154:LEU:HD13 | 1:N:167:THR:OG1  | 2.09                     | 0.53              |
| 1:O:40:LEU:HD23  | 1:O:48:LEU:HG    | 1.89                     | 0.53              |
| 1:O:262:MET:HE1  | 1:O:286:TYR:O    | 2.08                     | 0.53              |
| 1:B:114:ILE:HA   | 1:B:117:TRP:CE3  | 2.43                     | 0.53              |
| 1:B:216:PRO:HG2  | 1:B:295:GLY:HA2  | 1.91                     | 0.53              |
| 1:B:431:ARG:O    | 1:B:434:PRO:HD2  | 2.09                     | 0.53              |
| 1:C:402:MET:HG2  | 1:C:431:ARG:HH22 | 1.74                     | 0.53              |
| 1:F:39:LEU:CD1   | 1:F:57:ILE:HG13  | 2.38                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:310:LEU:O    | 1:F:314:THR:HG22 | 2.08                     | 0.53              |
| 1:G:280:ARG:HD2  | 1:G:304:PHE:HB2  | 1.89                     | 0.53              |
| 1:H:110:PRO:O    | 1:H:114:ILE:HG12 | 2.09                     | 0.53              |
| 1:J:12:ARG:HB2   | 1:J:501:ILE:HG23 | 1.90                     | 0.53              |
| 1:J:274:ILE:HG23 | 1:J:296:VAL:HG21 | 1.91                     | 0.53              |
| 1:K:52:ASN:H     | 1:K:375:ARG:NH2  | 2.06                     | 0.53              |
| 1:K:313:VAL:CG1  | 1:K:352:VAL:HB   | 2.39                     | 0.53              |
| 1:L:143:ARG:NE   | 1:L:143:ARG:HA   | 2.24                     | 0.53              |
| 1:L:163:LYS:O    | 1:L:166:PHE:HB2  | 2.08                     | 0.53              |
| 1:N:438:ALA:HB2  | 1:N:448:LEU:HG   | 1.90                     | 0.53              |
| 1:O:119:GLU:HB3  | 1:O:423:MET:HE3  | 1.89                     | 0.53              |
| 1:O:211:ILE:HG13 | 1:O:298:ALA:O    | 2.09                     | 0.53              |
| 1:O:265:LYS:HE2  | 1:O:322:PHE:CZ   | 2.44                     | 0.53              |
| 1:A:16:PHE:HA    | 1:A:97:LEU:HD23  | 1.90                     | 0.53              |
| 1:B:513:ARG:HG3  | 1:G:45:ASP:CG    | 2.34                     | 0.53              |
| 1:C:159:LEU:HG   | 1:C:163:LYS:CG   | 2.39                     | 0.53              |
| 1:D:22:ILE:HD12  | 1:D:90:THR:CG2   | 2.39                     | 0.53              |
| 1:D:211:ILE:HG13 | 1:D:298:ALA:O    | 2.09                     | 0.53              |
| 1:E:231:MET:HB2  | 1:E:284:TYR:H    | 1.73                     | 0.53              |
| 1:E:334:LYS:HB3  | 1:E:351:GLY:HA3  | 1.91                     | 0.53              |
| 1:F:448:LEU:C    | 1:F:448:LEU:HD13 | 2.33                     | 0.53              |
| 1:G:146:LEU:HB2  | 1:G:171:VAL:HG21 | 1.90                     | 0.53              |
| 1:K:211:ILE:HG12 | 1:K:298:ALA:H    | 1.73                     | 0.53              |
| 1:L:207:LEU:HD11 | 1:L:209:LYS:HE2  | 1.89                     | 0.53              |
| 1:N:274:ILE:O    | 1:N:296:VAL:HG22 | 2.09                     | 0.53              |
| 1:P:101:GLU:O    | 1:P:104:ILE:HG23 | 2.09                     | 0.53              |
| 1:P:185:ALA:HA   | 1:P:309:ARG:CD   | 2.39                     | 0.53              |
| 1:P:334:LYS:CD   | 1:P:351:GLY:HA3  | 2.39                     | 0.53              |
| 1:A:283:ILE:HG22 | 1:A:300:GLU:HG3  | 1.91                     | 0.53              |
| 1:B:418:LYS:HD3  | 1:I:449:VAL:CG1  | 2.38                     | 0.53              |
| 1:C:431:ARG:CZ   | 1:C:431:ARG:HA   | 2.39                     | 0.53              |
| 1:E:203:GLU:HG2  | 1:E:350:SER:HB2  | 1.91                     | 0.53              |
| 1:F:163:LYS:HG3  | 1:F:166:PHE:CD2  | 2.44                     | 0.53              |
| 1:F:274:ILE:HG23 | 1:F:296:VAL:CG2  | 2.39                     | 0.53              |
| 1:G:146:LEU:HD11 | 1:G:150:ALA:CB   | 2.39                     | 0.53              |
| 1:I:140:VAL:HA   | 1:I:175:LEU:CD2  | 2.35                     | 0.53              |
| 1:J:4:ASP:CG     | 1:J:513:ARG:HG2  | 2.33                     | 0.53              |
| 1:J:114:ILE:HD11 | 1:J:502:LEU:HD23 | 1.91                     | 0.53              |
| 1:J:341:ILE:HD12 | 1:J:346:LEU:CD2  | 2.39                     | 0.53              |
| 1:K:496:GLU:O    | 1:K:500:VAL:HG13 | 2.08                     | 0.53              |
| 1:M:79:ASP:O     | 1:M:83:GLY:HA2   | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:146:LEU:CD2  | 1:M:150:ALA:HB3  | 2.35                     | 0.53              |
| 1:M:511:ALA:HB3  | 1:M:512:PRO:HD3  | 1.91                     | 0.53              |
| 1:O:146:LEU:HB2  | 1:O:171:VAL:CG2  | 2.39                     | 0.53              |
| 1:P:159:LEU:HD22 | 1:P:159:LEU:H    | 1.74                     | 0.53              |
| 1:P:284:TYR:O    | 1:P:287:PRO:HD2  | 2.08                     | 0.53              |
| 1:A:345:LYS:C    | 1:A:346:LEU:HD12 | 2.34                     | 0.53              |
| 1:D:82:VAL:HG13  | 1:D:83:GLY:N     | 2.24                     | 0.53              |
| 1:F:27:LYS:HB2   | 1:F:436:ILE:HD11 | 1.91                     | 0.53              |
| 1:F:367:GLN:OE1  | 1:F:369:ILE:HB   | 2.08                     | 0.53              |
| 1:G:259:LYS:O    | 1:G:263:LYS:HG2  | 2.09                     | 0.53              |
| 1:J:79:ASP:HA    | 1:J:83:GLY:CA    | 2.39                     | 0.53              |
| 1:J:284:TYR:O    | 1:J:287:PRO:HD2  | 2.09                     | 0.53              |
| 1:K:13:LEU:HD23  | 1:K:13:LEU:C     | 2.34                     | 0.53              |
| 1:K:65:ASN:HD22  | 1:K:65:ASN:H     | 1.57                     | 0.53              |
| 1:K:89:VAL:HG12  | 1:K:490:VAL:HG23 | 1.91                     | 0.53              |
| 1:M:412:ALA:CB   | 1:M:424:GLU:HB3  | 2.39                     | 0.53              |
| 1:N:89:VAL:HG12  | 1:N:490:VAL:HB   | 1.91                     | 0.53              |
| 1:P:266:VAL:HG21 | 1:P:290:LEU:HD11 | 1.91                     | 0.53              |
| 1:A:434:PRO:HB3  | 1:A:452:LEU:HD23 | 1.91                     | 0.53              |
| 1:A:482:GLU:OE1  | 1:A:487:LYS:HE3  | 2.08                     | 0.53              |
| 1:B:211:ILE:HG12 | 1:B:298:ALA:H    | 1.74                     | 0.53              |
| 1:B:390:ASP:HB2  | 1:B:485:GLN:HE22 | 1.74                     | 0.53              |
| 1:C:372:GLU:O    | 1:C:375:ARG:HB3  | 2.08                     | 0.53              |
| 1:D:451:GLN:HE22 | 1:D:471:THR:HA   | 1.74                     | 0.53              |
| 1:E:37:LYS:HD2   | 1:G:508:ILE:HG12 | 1.91                     | 0.53              |
| 1:F:392:ARG:C    | 1:F:484:PHE:HB2  | 2.33                     | 0.53              |
| 1:H:109:HIS:CE1  | 1:H:111:GLN:HB2  | 2.44                     | 0.53              |
| 1:H:453:ARG:HH22 | 1:P:418:LYS:HG3  | 1.74                     | 0.53              |
| 1:J:322:PHE:HA   | 1:J:324:HIS:CD2  | 2.44                     | 0.53              |
| 1:K:177:LEU:C    | 1:K:177:LEU:HD12 | 2.33                     | 0.53              |
| 1:K:452:LEU:HD13 | 1:K:465:LEU:CD1  | 2.39                     | 0.53              |
| 1:M:231:MET:HB2  | 1:M:284:TYR:H    | 1.73                     | 0.53              |
| 1:N:326:GLU:HG3  | 1:N:327:LEU:H    | 1.73                     | 0.53              |
| 1:O:117:TRP:NE1  | 1:O:498:ALA:HB3  | 2.24                     | 0.53              |
| 1:P:96:LEU:O     | 1:P:96:LEU:HD22  | 2.09                     | 0.53              |
| 1:P:185:ALA:HA   | 1:P:309:ARG:HD3  | 1.91                     | 0.53              |
| 1:P:337:GLU:HG3  | 1:P:339:VAL:HG23 | 1.90                     | 0.53              |
| 1:P:366:THR:O    | 1:P:366:THR:HG22 | 2.09                     | 0.53              |
| 1:A:405:ALA:HB2  | 1:A:430:LEU:HB2  | 1.91                     | 0.52              |
| 1:B:206:LEU:C    | 1:B:206:LEU:HD13 | 2.35                     | 0.52              |
| 1:B:262:MET:HE1  | 1:B:286:TYR:O    | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:449:VAL:HG11 | 1:K:417:GLY:HA3  | 1.91                     | 0.52              |
| 1:F:1:ALA:N      | 1:F:508:ILE:HD12 | 2.25                     | 0.52              |
| 1:F:114:ILE:HA   | 1:F:117:TRP:CZ3  | 2.44                     | 0.52              |
| 1:F:483:SER:HB2  | 1:F:486:VAL:HG13 | 1.91                     | 0.52              |
| 1:G:20:ILE:HB    | 1:G:98:ARG:NH2   | 2.24                     | 0.52              |
| 1:H:402:MET:HG2  | 1:H:431:ARG:HH22 | 1.74                     | 0.52              |
| 1:J:369:ILE:O    | 1:J:372:GLU:HB2  | 2.09                     | 0.52              |
| 1:K:79:ASP:HA    | 1:K:83:GLY:CA    | 2.39                     | 0.52              |
| 1:L:32:PRO:HA    | 1:L:155:SER:O    | 2.09                     | 0.52              |
| 1:N:78:GLN:NE2   | 1:N:489:GLN:HE21 | 2.06                     | 0.52              |
| 1:P:114:ILE:HA   | 1:P:117:TRP:CE3  | 2.44                     | 0.52              |
| 1:A:163:LYS:HG3  | 1:A:166:PHE:HB2  | 1.91                     | 0.52              |
| 1:A:216:PRO:HG2  | 1:A:295:GLY:HA2  | 1.91                     | 0.52              |
| 1:B:149:ILE:O    | 1:B:152:THR:HG22 | 2.08                     | 0.52              |
| 1:B:254:ILE:CG2  | 1:F:238:ILE:HD12 | 2.40                     | 0.52              |
| 1:D:203:GLU:CD   | 1:D:203:GLU:H    | 2.17                     | 0.52              |
| 1:E:114:ILE:HA   | 1:E:117:TRP:CE3  | 2.44                     | 0.52              |
| 1:E:161:HIS:CD2  | 1:E:162:HIS:H    | 2.27                     | 0.52              |
| 1:G:297:MET:CE   | 1:G:347:ILE:HD11 | 2.39                     | 0.52              |
| 1:H:56:THR:HG21  | 1:H:375:ARG:CD   | 2.39                     | 0.52              |
| 1:J:154:LEU:HB3  | 1:J:160:THR:OG1  | 2.08                     | 0.52              |
| 1:L:107:LYS:O    | 1:L:108:ILE:HD13 | 2.10                     | 0.52              |
| 1:M:131:SER:HB2  | 1:M:461:THR:HG21 | 1.91                     | 0.52              |
| 1:M:500:VAL:HA   | 1:M:503:ARG:NH1  | 2.24                     | 0.52              |
| 1:O:364:GLY:HA3  | 1:O:370:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:313:VAL:CG1  | 1:A:352:VAL:HG11 | 2.40                     | 0.52              |
| 1:D:171:VAL:HA   | 1:D:174:VAL:HG22 | 1.92                     | 0.52              |
| 1:D:176:ARG:NH1  | 1:D:201:LEU:HD21 | 2.25                     | 0.52              |
| 1:D:324:HIS:HB2  | 1:D:329:LYS:HZ3  | 1.75                     | 0.52              |
| 1:D:450:ALA:HB2  | 1:K:416:PRO:HB3  | 1.90                     | 0.52              |
| 1:E:394:VAL:HG23 | 1:E:482:GLU:HB2  | 1.91                     | 0.52              |
| 1:F:51:THR:HA    | 1:F:375:ARG:HD2  | 1.91                     | 0.52              |
| 1:H:146:LEU:HB2  | 1:H:171:VAL:HG21 | 1.90                     | 0.52              |
| 1:H:482:GLU:OE1  | 1:H:487:LYS:HE2  | 2.09                     | 0.52              |
| 1:I:110:PRO:HA   | 1:I:113:ILE:HD12 | 1.90                     | 0.52              |
| 1:J:483:SER:O    | 1:J:486:VAL:HG22 | 2.09                     | 0.52              |
| 1:K:402:MET:CE   | 1:K:453:ARG:HG2  | 2.34                     | 0.52              |
| 1:L:280:ARG:HD2  | 1:L:304:PHE:HB2  | 1.90                     | 0.52              |
| 1:M:438:ALA:CB   | 1:M:448:LEU:HG   | 2.40                     | 0.52              |
| 1:N:99:GLU:HG2   | 1:N:425:SER:CB   | 2.39                     | 0.52              |
| 1:O:154:LEU:HD21 | 1:O:163:LYS:HZ2  | 1.73                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:190:LYS:HA   | 1:O:362:LEU:O    | 2.10                     | 0.52              |
| 1:A:431:ARG:O    | 1:A:434:PRO:HD2  | 2.10                     | 0.52              |
| 1:B:226:ILE:HG12 | 1:B:278:ILE:HG23 | 1.92                     | 0.52              |
| 1:C:146:LEU:HD11 | 1:C:150:ALA:CB   | 2.39                     | 0.52              |
| 1:D:231:MET:HB2  | 1:D:284:TYR:H    | 1.73                     | 0.52              |
| 1:E:154:LEU:HD21 | 1:E:163:LYS:HZ2  | 1.73                     | 0.52              |
| 1:I:225:LEU:HD13 | 1:I:329:LYS:HE2  | 1.91                     | 0.52              |
| 1:I:397:GLY:HA3  | 1:I:475:MET:HE3  | 1.90                     | 0.52              |
| 1:M:38:ILE:HG13  | 1:M:38:ILE:O     | 2.07                     | 0.52              |
| 1:O:148:ASN:HA   | 1:O:479:GLY:O    | 2.10                     | 0.52              |
| 1:P:226:ILE:HG12 | 1:P:278:ILE:HG23 | 1.91                     | 0.52              |
| 1:P:402:MET:HE3  | 1:P:453:ARG:CG   | 2.34                     | 0.52              |
| 1:C:27:LYS:HB2   | 1:C:436:ILE:HD11 | 1.92                     | 0.52              |
| 1:C:219:ILE:HB   | 1:C:275:ASN:HB3  | 1.90                     | 0.52              |
| 1:D:146:LEU:CD1  | 1:D:171:VAL:HG13 | 2.28                     | 0.52              |
| 1:D:297:MET:HE1  | 1:D:347:ILE:HD11 | 1.91                     | 0.52              |
| 1:E:171:VAL:HA   | 1:E:174:VAL:HG22 | 1.91                     | 0.52              |
| 1:E:176:ARG:HD2  | 1:E:358:CYS:SG   | 2.50                     | 0.52              |
| 1:F:397:GLY:HA3  | 1:F:475:MET:HE3  | 1.91                     | 0.52              |
| 1:G:408:VAL:HA   | 1:G:411:LEU:HD12 | 1.91                     | 0.52              |
| 1:H:159:LEU:O    | 1:H:163:LYS:HB3  | 2.10                     | 0.52              |
| 1:I:96:LEU:C     | 1:I:96:LEU:HD13  | 2.35                     | 0.52              |
| 1:J:313:VAL:HG13 | 1:J:352:VAL:HG21 | 1.91                     | 0.52              |
| 1:J:505:ASP:O    | 1:J:507:ILE:HG12 | 2.09                     | 0.52              |
| 1:L:99:GLU:CG    | 1:L:425:SER:HB2  | 2.39                     | 0.52              |
| 1:L:438:ALA:CB   | 1:L:448:LEU:HG   | 2.40                     | 0.52              |
| 1:N:48:LEU:HD13  | 1:N:48:LEU:N     | 2.24                     | 0.52              |
| 1:N:231:MET:HB2  | 1:N:284:TYR:H    | 1.75                     | 0.52              |
| 1:B:174:VAL:HG12 | 1:B:381:LEU:HD22 | 1.92                     | 0.52              |
| 1:C:145:ASP:OD1  | 1:C:171:VAL:HB   | 2.10                     | 0.52              |
| 1:F:276:CYS:HA   | 1:F:297:MET:O    | 2.09                     | 0.52              |
| 1:F:334:LYS:CG   | 1:F:351:GLY:HA3  | 2.38                     | 0.52              |
| 1:G:219:ILE:HB   | 1:G:275:ASN:HB3  | 1.92                     | 0.52              |
| 1:I:145:ASP:OD1  | 1:I:171:VAL:HB   | 2.09                     | 0.52              |
| 1:I:159:LEU:HD23 | 1:I:159:LEU:C    | 2.34                     | 0.52              |
| 1:J:84:ASP:CG    | 1:J:85:GLY:H     | 2.18                     | 0.52              |
| 1:K:84:ASP:CG    | 1:K:85:GLY:H     | 2.16                     | 0.52              |
| 1:K:222:ALA:HA   | 1:K:275:ASN:OD1  | 2.09                     | 0.52              |
| 1:L:78:GLN:NE2   | 1:L:486:VAL:HA   | 2.24                     | 0.52              |
| 1:N:52:ASN:OD1   | 1:N:157:LYS:HG2  | 2.09                     | 0.52              |
| 1:P:143:ARG:HA   | 1:P:143:ARG:HE   | 1.75                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:313:VAL:HG22 | 1:P:357:ALA:HB3  | 1.91                     | 0.52              |
| 1:C:57:ILE:HD13  | 1:C:57:ILE:C     | 2.34                     | 0.52              |
| 1:G:83:GLY:H     | 1:G:486:VAL:HG12 | 1.75                     | 0.52              |
| 1:G:130:ASN:O    | 1:G:131:SER:HB2  | 2.09                     | 0.52              |
| 1:G:171:VAL:HA   | 1:G:174:VAL:HG22 | 1.90                     | 0.52              |
| 1:G:171:VAL:O    | 1:G:174:VAL:HG22 | 2.10                     | 0.52              |
| 1:H:338:GLU:HA   | 1:H:346:LEU:O    | 2.10                     | 0.52              |
| 1:I:283:ILE:HG22 | 1:I:300:GLU:CG   | 2.39                     | 0.52              |
| 1:J:104:ILE:HG13 | 1:J:105:ALA:N    | 2.24                     | 0.52              |
| 1:K:365:ALA:C    | 1:K:366:THR:HG23 | 2.35                     | 0.52              |
| 1:M:171:VAL:O    | 1:M:174:VAL:HG22 | 2.09                     | 0.52              |
| 1:P:145:ASP:O    | 1:P:171:VAL:HG11 | 2.09                     | 0.52              |
| 1:P:210:LYS:HE2  | 1:P:212:GLY:O    | 2.10                     | 0.52              |
| 1:P:475:MET:SD   | 1:P:480:ILE:HB   | 2.49                     | 0.52              |
| 1:A:61:ILE:CG2   | 1:A:63:VAL:HG23  | 2.40                     | 0.52              |
| 1:A:159:LEU:CG   | 1:A:163:LYS:HD3  | 2.38                     | 0.52              |
| 1:A:364:GLY:HA3  | 1:A:370:LEU:HD11 | 1.90                     | 0.52              |
| 1:B:171:VAL:O    | 1:B:175:LEU:HG   | 2.10                     | 0.52              |
| 1:F:82:VAL:CG1   | 1:F:486:VAL:HG12 | 2.39                     | 0.52              |
| 1:F:106:LYS:HG2  | 1:O:446:ALA:HB2  | 1.92                     | 0.52              |
| 1:G:187:HIS:O    | 1:G:359:THR:HG23 | 2.10                     | 0.52              |
| 1:G:324:HIS:CG   | 1:G:325:PRO:HD3  | 2.44                     | 0.52              |
| 1:I:89:VAL:HA    | 1:I:490:VAL:HG23 | 1.91                     | 0.52              |
| 1:J:207:LEU:O    | 1:J:347:ILE:HG22 | 2.09                     | 0.52              |
| 1:K:163:LYS:HD2  | 1:K:166:PHE:CG   | 2.45                     | 0.52              |
| 1:L:484:PHE:CE2  | 1:L:488:ARG:HD3  | 2.44                     | 0.52              |
| 1:N:128:LEU:C    | 1:N:129:LEU:HD13 | 2.34                     | 0.52              |
| 1:N:192:LEU:HB2  | 1:N:343:GLU:OE1  | 2.08                     | 0.52              |
| 1:O:171:VAL:O    | 1:O:174:VAL:HG22 | 2.10                     | 0.52              |
| 1:P:32:PRO:CD    | 1:P:467:MET:HE1  | 2.40                     | 0.52              |
| 1:P:38:ILE:CG2   | 1:P:50:VAL:HB    | 2.33                     | 0.52              |
| 1:P:150:ALA:HB1  | 1:P:167:THR:OG1  | 2.10                     | 0.52              |
| 1:P:157:LYS:HB3  | 1:P:159:LEU:CD2  | 2.39                     | 0.52              |
| 1:P:269:ILE:HG12 | 1:P:274:ILE:HG21 | 1.91                     | 0.52              |
| 1:A:74:MET:HG2   | 1:A:493:SER:OG   | 2.10                     | 0.52              |
| 1:A:340:MET:HG2  | 1:A:345:LYS:HG2  | 1.91                     | 0.52              |
| 1:B:219:ILE:HD12 | 1:B:275:ASN:HB3  | 1.91                     | 0.52              |
| 1:C:44:ARG:HH11  | 1:C:44:ARG:HG3   | 1.75                     | 0.52              |
| 1:D:154:LEU:HD21 | 1:D:163:LYS:HZ2  | 1.75                     | 0.52              |
| 1:G:268:ARG:O    | 1:G:271:LYS:HG2  | 2.10                     | 0.52              |
| 1:I:19:ALA:HB1   | 1:I:94:ALA:HA    | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:507:ILE:O    | 1:I:508:ILE:HB   | 2.09                     | 0.52              |
| 1:J:128:LEU:HB3  | 1:J:484:PHE:CE1  | 2.44                     | 0.52              |
| 1:J:146:LEU:HB2  | 1:J:171:VAL:HG21 | 1.92                     | 0.52              |
| 1:K:313:VAL:HG13 | 1:K:352:VAL:CB   | 2.39                     | 0.52              |
| 1:O:392:ARG:C    | 1:O:484:PHE:HB2  | 2.35                     | 0.52              |
| 1:P:507:ILE:HG22 | 1:P:508:ILE:HG23 | 1.91                     | 0.52              |
| 1:A:31:GLY:O     | 1:A:156:SER:HA   | 2.09                     | 0.52              |
| 1:A:219:ILE:HB   | 1:A:275:ASN:HB3  | 1.92                     | 0.52              |
| 1:A:511:ALA:C    | 1:F:25:LEU:HG    | 2.34                     | 0.52              |
| 1:B:219:ILE:HD11 | 1:B:336:ILE:HB   | 1.91                     | 0.52              |
| 1:E:96:LEU:HD13  | 1:E:97:LEU:N     | 2.24                     | 0.52              |
| 1:F:152:THR:HG21 | 1:F:480:ILE:HG23 | 1.92                     | 0.52              |
| 1:G:140:VAL:HA   | 1:G:175:LEU:HD22 | 1.91                     | 0.52              |
| 1:G:313:VAL:HG13 | 1:G:352:VAL:CG1  | 2.40                     | 0.52              |
| 1:J:38:ILE:O     | 1:J:39:LEU:HB2   | 2.10                     | 0.52              |
| 1:J:448:LEU:HD21 | 1:J:465:LEU:CD1  | 2.40                     | 0.52              |
| 1:K:174:VAL:HG21 | 1:K:384:LEU:CB   | 2.40                     | 0.52              |
| 1:K:225:LEU:HD11 | 1:K:324:HIS:ND1  | 2.25                     | 0.52              |
| 1:L:207:LEU:HB3  | 1:L:347:ILE:HG23 | 1.92                     | 0.52              |
| 1:N:146:LEU:CD1  | 1:N:147:MET:H    | 2.23                     | 0.52              |
| 1:O:82:VAL:HG13  | 1:O:83:GLY:N     | 2.22                     | 0.52              |
| 1:O:190:LYS:HD3  | 1:O:370:LEU:CD2  | 2.39                     | 0.52              |
| 1:O:452:LEU:HD13 | 1:O:465:LEU:CD1  | 2.40                     | 0.52              |
| 1:P:58:LEU:HB3   | 1:P:72:VAL:CG1   | 2.40                     | 0.52              |
| 1:A:173:ALA:HB2  | 1:A:360:ILE:HD11 | 1.92                     | 0.51              |
| 1:B:510:ALA:HB3  | 1:G:25:LEU:CG    | 2.39                     | 0.51              |
| 1:D:367:GLN:HG2  | 1:D:369:ILE:H    | 1.74                     | 0.51              |
| 1:G:59:LYS:CE    | 1:G:76:ARG:HB2   | 2.40                     | 0.51              |
| 1:G:99:GLU:HG3   | 1:G:425:SER:HB2  | 1.91                     | 0.51              |
| 1:G:146:LEU:HD21 | 1:G:150:ALA:HB3  | 1.92                     | 0.51              |
| 1:H:280:ARG:HD2  | 1:H:304:PHE:HB2  | 1.91                     | 0.51              |
| 1:H:438:ALA:HB2  | 1:H:448:LEU:HG   | 1.91                     | 0.51              |
| 1:H:496:GLU:O    | 1:H:500:VAL:HG13 | 2.10                     | 0.51              |
| 1:I:187:HIS:O    | 1:I:359:THR:HG23 | 2.09                     | 0.51              |
| 1:I:207:LEU:O    | 1:I:347:ILE:HG22 | 2.10                     | 0.51              |
| 1:I:225:LEU:HD11 | 1:I:324:HIS:ND1  | 2.26                     | 0.51              |
| 1:K:192:LEU:HG   | 1:K:366:THR:CG2  | 2.33                     | 0.51              |
| 1:L:283:ILE:HG22 | 1:L:300:GLU:CG   | 2.40                     | 0.51              |
| 1:M:175:LEU:HD23 | 1:M:178:LYS:HE2  | 1.91                     | 0.51              |
| 1:M:372:GLU:HG2  | 1:M:375:ARG:NH2  | 2.25                     | 0.51              |
| 1:N:431:ARG:NH2  | 1:N:434:PRO:HG2  | 2.25                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:368:GLN:O    | 1:O:371:ASP:HB2  | 2.10                     | 0.51              |
| 1:C:341:ILE:C    | 1:C:343:GLU:H    | 2.19                     | 0.51              |
| 1:C:405:ALA:HA   | 1:C:408:VAL:HG22 | 1.92                     | 0.51              |
| 1:C:448:LEU:C    | 1:C:448:LEU:HD13 | 2.36                     | 0.51              |
| 1:G:485:GLN:HB3  | 1:G:488:ARG:HH21 | 1.75                     | 0.51              |
| 1:G:499:GLU:O    | 1:G:503:ARG:HG3  | 2.10                     | 0.51              |
| 1:H:452:LEU:HD13 | 1:H:465:LEU:HD13 | 1.92                     | 0.51              |
| 1:I:58:LEU:HB3   | 1:I:72:VAL:CG1   | 2.41                     | 0.51              |
| 1:J:192:LEU:HD13 | 1:J:366:THR:OG1  | 2.10                     | 0.51              |
| 1:L:310:LEU:O    | 1:L:313:VAL:HB   | 2.11                     | 0.51              |
| 1:L:431:ARG:HA   | 1:L:431:ARG:CZ   | 2.40                     | 0.51              |
| 1:O:141:LYS:HG2  | 1:O:144:GLN:HB2  | 1.91                     | 0.51              |
| 1:A:509:LYS:H    | 1:F:37:LYS:NZ    | 2.07                     | 0.51              |
| 1:B:438:ALA:CB   | 1:B:448:LEU:HG   | 2.40                     | 0.51              |
| 1:D:103:LEU:HD11 | 1:D:113:ILE:HG13 | 1.93                     | 0.51              |
| 1:E:92:LEU:O     | 1:E:95:GLU:HG2   | 2.11                     | 0.51              |
| 1:F:219:ILE:HB   | 1:F:275:ASN:HB3  | 1.92                     | 0.51              |
| 1:F:431:ARG:O    | 1:F:434:PRO:HD2  | 2.10                     | 0.51              |
| 1:F:500:VAL:HA   | 1:F:503:ARG:HG2  | 1.92                     | 0.51              |
| 1:G:51:THR:HA    | 1:G:375:ARG:HD2  | 1.93                     | 0.51              |
| 1:G:124:ALA:O    | 1:G:128:LEU:HD12 | 2.10                     | 0.51              |
| 1:G:507:ILE:HD12 | 1:G:508:ILE:HG13 | 1.92                     | 0.51              |
| 1:H:262:MET:HE1  | 1:H:286:TYR:O    | 2.11                     | 0.51              |
| 1:I:196:LEU:HD13 | 1:I:196:LEU:C    | 2.35                     | 0.51              |
| 1:I:451:GLN:NE2  | 1:I:471:THR:HA   | 2.25                     | 0.51              |
| 1:J:128:LEU:HD21 | 1:J:487:LYS:HB2  | 1.92                     | 0.51              |
| 1:J:221:ASN:HA   | 1:J:333:CYS:HB2  | 1.93                     | 0.51              |
| 1:J:223:LYS:HB2  | 1:J:274:ILE:HA   | 1.91                     | 0.51              |
| 1:J:287:PRO:O    | 1:J:291:PHE:HD2  | 1.93                     | 0.51              |
| 1:L:96:LEU:HD13  | 1:L:96:LEU:C     | 2.35                     | 0.51              |
| 1:L:152:THR:HG21 | 1:L:481:THR:O    | 2.10                     | 0.51              |
| 1:N:497:ALA:O    | 1:N:501:ILE:HG12 | 2.10                     | 0.51              |
| 1:O:32:PRO:HB2   | 1:O:467:MET:CE   | 2.40                     | 0.51              |
| 1:O:171:VAL:O    | 1:O:175:LEU:HG   | 2.10                     | 0.51              |
| 1:P:171:VAL:CA   | 1:P:174:VAL:HG22 | 2.39                     | 0.51              |
| 1:B:104:ILE:C    | 1:B:106:LYS:H    | 2.18                     | 0.51              |
| 1:B:126:GLN:HE22 | 1:B:411:LEU:HD11 | 1.75                     | 0.51              |
| 1:B:418:LYS:HG3  | 1:I:450:ALA:HA   | 1.91                     | 0.51              |
| 1:B:447:ASP:CA   | 1:I:107:LYS:HG2  | 2.40                     | 0.51              |
| 1:C:274:ILE:HG23 | 1:C:274:ILE:O    | 2.10                     | 0.51              |
| 1:D:366:THR:O    | 1:D:366:THR:HG23 | 2.09                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:171:VAL:HA   | 1:I:174:VAL:HG22 | 1.93                     | 0.51              |
| 1:I:448:LEU:C    | 1:I:448:LEU:HD13 | 2.36                     | 0.51              |
| 1:J:219:ILE:HB   | 1:J:275:ASN:HB3  | 1.91                     | 0.51              |
| 1:J:367:GLN:HG2  | 1:J:369:ILE:HB   | 1.93                     | 0.51              |
| 1:L:39:LEU:O     | 1:L:48:LEU:HA    | 2.11                     | 0.51              |
| 1:L:64:ASP:HB3   | 1:L:512:PRO:HA   | 1.92                     | 0.51              |
| 1:O:66:PRO:HG3   | 1:O:510:ALA:HB3  | 1.93                     | 0.51              |
| 1:O:276:CYS:HA   | 1:O:297:MET:O    | 2.10                     | 0.51              |
| 1:O:345:LYS:C    | 1:O:346:LEU:HD12 | 2.35                     | 0.51              |
| 1:P:219:ILE:HD11 | 1:P:336:ILE:HB   | 1.92                     | 0.51              |
| 1:B:24:ASP:O     | 1:B:27:LYS:HG2   | 2.10                     | 0.51              |
| 1:B:448:LEU:HD13 | 1:B:448:LEU:C    | 2.36                     | 0.51              |
| 1:C:41:SER:HB3   | 1:C:45:ASP:OD2   | 2.11                     | 0.51              |
| 1:D:130:ASN:O    | 1:D:131:SER:HB3  | 2.11                     | 0.51              |
| 1:E:35:MET:HE2   | 1:G:504:VAL:HG12 | 1.92                     | 0.51              |
| 1:F:154:LEU:HD22 | 1:F:167:THR:HB   | 1.92                     | 0.51              |
| 1:F:366:THR:C    | 1:F:367:GLN:HG3  | 2.36                     | 0.51              |
| 1:I:284:TYR:O    | 1:I:287:PRO:HD2  | 2.09                     | 0.51              |
| 1:L:82:VAL:HA    | 1:L:386:GLN:HG3  | 1.92                     | 0.51              |
| 1:M:57:ILE:C     | 1:M:57:ILE:HD13  | 2.35                     | 0.51              |
| 1:N:274:ILE:HG23 | 1:N:296:VAL:CG2  | 2.40                     | 0.51              |
| 1:N:448:LEU:C    | 1:N:448:LEU:HD13 | 2.36                     | 0.51              |
| 1:O:191:LYS:HG2  | 1:O:341:ILE:HG22 | 1.93                     | 0.51              |
| 1:P:147:MET:HE3  | 1:P:168:LYS:HE3  | 1.92                     | 0.51              |
| 1:P:204:GLY:O    | 1:P:359:THR:HB   | 2.11                     | 0.51              |
| 1:A:171:VAL:O    | 1:A:175:LEU:HG   | 2.11                     | 0.51              |
| 1:B:418:LYS:HA   | 1:I:453:ARG:NH2  | 2.25                     | 0.51              |
| 1:C:106:LYS:O    | 1:C:108:ILE:HG23 | 2.11                     | 0.51              |
| 1:C:334:LYS:HD3  | 1:C:351:GLY:HA3  | 1.91                     | 0.51              |
| 1:G:176:ARG:HE   | 1:G:358:CYS:HB2  | 1.76                     | 0.51              |
| 1:G:324:HIS:HB2  | 1:G:329:LYS:HZ3  | 1.74                     | 0.51              |
| 1:I:143:ARG:HA   | 1:I:143:ARG:HE   | 1.75                     | 0.51              |
| 1:J:216:PRO:HG3  | 1:J:295:GLY:HA2  | 1.93                     | 0.51              |
| 1:K:324:HIS:HB2  | 1:K:329:LYS:HZ1  | 1.75                     | 0.51              |
| 1:L:191:LYS:HD2  | 1:L:344:ASP:HB3  | 1.92                     | 0.51              |
| 1:M:171:VAL:HA   | 1:M:174:VAL:HG22 | 1.91                     | 0.51              |
| 1:M:448:LEU:HD21 | 1:M:465:LEU:CD1  | 2.41                     | 0.51              |
| 1:O:166:PHE:HD2  | 1:O:362:LEU:HD22 | 1.76                     | 0.51              |
| 1:O:485:GLN:HA   | 1:O:488:ARG:HG2  | 1.92                     | 0.51              |
| 1:O:501:ILE:O    | 1:O:502:LEU:HD12 | 2.10                     | 0.51              |
| 1:P:19:ALA:HB1   | 1:P:94:ALA:HA    | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:ALA:HA   | 1:A:275:ASN:OD1  | 2.11                     | 0.51              |
| 1:A:274:ILE:O    | 1:A:296:VAL:HG22 | 2.10                     | 0.51              |
| 1:B:128:LEU:HD11 | 1:B:488:ARG:HG2  | 1.93                     | 0.51              |
| 1:B:313:VAL:HG13 | 1:B:352:VAL:HG21 | 1.93                     | 0.51              |
| 1:C:210:LYS:HE2  | 1:C:212:GLY:O    | 2.11                     | 0.51              |
| 1:C:397:GLY:O    | 1:C:465:LEU:HD23 | 2.10                     | 0.51              |
| 1:D:110:PRO:O    | 1:D:113:ILE:HB   | 2.11                     | 0.51              |
| 1:E:431:ARG:HH21 | 1:E:434:PRO:HG2  | 1.75                     | 0.51              |
| 1:G:191:LYS:O    | 1:G:370:LEU:HD21 | 2.11                     | 0.51              |
| 1:G:225:LEU:HG   | 1:G:277:PHE:CD1  | 2.46                     | 0.51              |
| 1:G:338:GLU:OE1  | 1:G:345:LYS:HE3  | 2.10                     | 0.51              |
| 1:H:143:ARG:HG3  | 1:H:143:ARG:O    | 2.10                     | 0.51              |
| 1:I:95:GLU:CD    | 1:I:429:ALA:HA   | 2.35                     | 0.51              |
| 1:I:174:VAL:HG11 | 1:I:384:LEU:HB2  | 1.93                     | 0.51              |
| 1:K:124:ALA:HA   | 1:K:491:LEU:HD13 | 1.93                     | 0.51              |
| 1:K:219:ILE:HB   | 1:K:275:ASN:HB3  | 1.92                     | 0.51              |
| 1:K:231:MET:HB2  | 1:K:284:TYR:H    | 1.75                     | 0.51              |
| 1:K:283:ILE:CG2  | 1:K:300:GLU:HG3  | 2.38                     | 0.51              |
| 1:K:334:LYS:HG3  | 1:K:351:GLY:HA3  | 1.93                     | 0.51              |
| 1:L:159:LEU:HD23 | 1:L:163:LYS:HD3  | 1.92                     | 0.51              |
| 1:L:223:LYS:HB2  | 1:L:274:ILE:HA   | 1.93                     | 0.51              |
| 1:M:319:ALA:HA   | 1:M:329:LYS:HZ1  | 1.76                     | 0.51              |
| 1:N:373:ALA:HA   | 1:N:376:SER:HB2  | 1.92                     | 0.51              |
| 1:N:508:ILE:HG22 | 1:N:509:LYS:HG3  | 1.93                     | 0.51              |
| 1:O:324:HIS:HB2  | 1:O:329:LYS:CE   | 2.40                     | 0.51              |
| 1:B:236:ILE:HG22 | 1:B:237:LYS:N    | 2.25                     | 0.51              |
| 1:B:512:PRO:C    | 1:G:61:ILE:HG21  | 2.36                     | 0.51              |
| 1:C:40:LEU:HD22  | 1:H:510:ALA:CB   | 2.40                     | 0.51              |
| 1:D:114:ILE:HD11 | 1:D:502:LEU:CD1  | 2.40                     | 0.51              |
| 1:D:114:ILE:HD11 | 1:D:502:LEU:HD12 | 1.93                     | 0.51              |
| 1:D:236:ILE:HG23 | 1:D:237:LYS:N    | 2.26                     | 0.51              |
| 1:D:415:THR:HB   | 1:D:419:GLU:HB2  | 1.91                     | 0.51              |
| 1:E:30:LEU:CD1   | 1:E:30:LEU:N     | 2.73                     | 0.51              |
| 1:E:284:TYR:O    | 1:E:287:PRO:HD2  | 2.10                     | 0.51              |
| 1:F:59:LYS:HE2   | 1:F:76:ARG:CB    | 2.40                     | 0.51              |
| 1:F:401:GLU:HG2  | 1:F:433:LEU:HD22 | 1.92                     | 0.51              |
| 1:H:448:LEU:HD13 | 1:H:448:LEU:C    | 2.35                     | 0.51              |
| 1:I:211:ILE:CD1  | 1:I:211:ILE:N    | 2.72                     | 0.51              |
| 1:I:324:HIS:HB2  | 1:I:329:LYS:HZ1  | 1.75                     | 0.51              |
| 1:J:431:ARG:O    | 1:J:434:PRO:HD2  | 2.11                     | 0.51              |
| 1:J:448:LEU:HD13 | 1:J:448:LEU:C    | 2.35                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:131:SER:O    | 1:K:132:ALA:HB3  | 2.11                     | 0.51              |
| 1:L:183:LEU:HD12 | 1:L:381:LEU:HD22 | 1.93                     | 0.51              |
| 1:M:39:LEU:HA    | 1:O:509:LYS:NZ   | 2.15                     | 0.51              |
| 1:M:145:ASP:O    | 1:M:171:VAL:HG11 | 2.11                     | 0.51              |
| 1:M:219:ILE:HB   | 1:M:275:ASN:HB3  | 1.92                     | 0.51              |
| 1:N:163:LYS:HG3  | 1:N:166:PHE:CG   | 2.46                     | 0.51              |
| 1:O:354:LEU:HD21 | 1:O:356:GLU:HB3  | 1.92                     | 0.51              |
| 1:B:163:LYS:O    | 1:B:166:PHE:HB2  | 2.11                     | 0.51              |
| 1:B:187:HIS:HB2  | 1:B:309:ARG:NH1  | 2.25                     | 0.51              |
| 1:B:402:MET:SD   | 1:B:453:ARG:HA   | 2.51                     | 0.51              |
| 1:C:154:LEU:CD2  | 1:C:163:LYS:HG3  | 2.41                     | 0.51              |
| 1:C:209:LYS:HZ1  | 1:C:303:ASP:H    | 1.58                     | 0.51              |
| 1:C:222:ALA:HA   | 1:C:275:ASN:HB2  | 1.92                     | 0.51              |
| 1:C:451:GLN:HE22 | 1:C:471:THR:HA   | 1.76                     | 0.51              |
| 1:D:101:GLU:O    | 1:D:104:ILE:HG12 | 2.10                     | 0.51              |
| 1:G:159:LEU:HD23 | 1:G:160:THR:N    | 2.25                     | 0.51              |
| 1:G:431:ARG:O    | 1:G:434:PRO:HD2  | 2.10                     | 0.51              |
| 1:H:106:LYS:HZ2  | 1:H:418:LYS:HA   | 1.75                     | 0.51              |
| 1:H:399:CYS:SG   | 1:H:475:MET:HB2  | 2.51                     | 0.51              |
| 1:I:334:LYS:CD   | 1:I:351:GLY:HA3  | 2.41                     | 0.51              |
| 1:L:162:HIS:HB3  | 1:L:198:ASP:OD2  | 2.11                     | 0.51              |
| 1:M:59:LYS:CE    | 1:M:76:ARG:HB2   | 2.38                     | 0.51              |
| 1:M:324:HIS:HB2  | 1:M:329:LYS:CE   | 2.41                     | 0.51              |
| 1:O:176:ARG:NE   | 1:O:358:CYS:HB2  | 2.26                     | 0.51              |
| 1:O:211:ILE:CD1  | 1:O:211:ILE:N    | 2.71                     | 0.51              |
| 1:A:324:HIS:HB2  | 1:A:329:LYS:HE2  | 1.92                     | 0.51              |
| 1:A:451:GLN:NE2  | 1:A:471:THR:HA   | 2.26                     | 0.51              |
| 1:B:222:ALA:HA   | 1:B:275:ASN:CG   | 2.36                     | 0.51              |
| 1:B:397:GLY:HA3  | 1:B:475:MET:CE   | 2.41                     | 0.51              |
| 1:C:166:PHE:CE1  | 1:C:198:ASP:HB3  | 2.46                     | 0.51              |
| 1:D:234:ASP:OD2  | 1:E:237:LYS:HE3  | 2.11                     | 0.51              |
| 1:D:313:VAL:HG13 | 1:D:352:VAL:CB   | 2.41                     | 0.51              |
| 1:F:233:THR:O    | 1:F:234:ASP:HB3  | 2.11                     | 0.51              |
| 1:G:108:ILE:HG22 | 1:G:109:HIS:N    | 2.26                     | 0.51              |
| 1:H:187:HIS:O    | 1:H:359:THR:HG23 | 2.11                     | 0.51              |
| 1:H:207:LEU:HD13 | 1:H:208:ASP:N    | 2.26                     | 0.51              |
| 1:H:475:MET:SD   | 1:H:480:ILE:HB   | 2.51                     | 0.51              |
| 1:I:364:GLY:HA3  | 1:I:370:LEU:CD2  | 2.41                     | 0.51              |
| 1:J:265:LYS:O    | 1:J:269:ILE:HB   | 2.11                     | 0.51              |
| 1:K:222:ALA:HA   | 1:K:275:ASN:CG   | 2.36                     | 0.51              |
| 1:L:274:ILE:HG23 | 1:L:296:VAL:CG2  | 2.41                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:343:GLU:H    | 1:L:343:GLU:CD   | 2.19                     | 0.51              |
| 1:M:163:LYS:O    | 1:M:166:PHE:HB2  | 2.10                     | 0.51              |
| 1:N:99:GLU:O     | 1:N:103:LEU:HD13 | 2.11                     | 0.51              |
| 1:B:128:LEU:O    | 1:B:129:LEU:HB2  | 2.11                     | 0.50              |
| 1:B:192:LEU:CD2  | 1:B:366:THR:HG22 | 2.41                     | 0.50              |
| 1:B:310:LEU:O    | 1:B:314:THR:HG22 | 2.10                     | 0.50              |
| 1:C:98:ARG:HE    | 1:C:98:ARG:CA    | 2.24                     | 0.50              |
| 1:C:499:GLU:HG2  | 1:C:503:ARG:HH21 | 1.76                     | 0.50              |
| 1:D:405:ALA:HA   | 1:D:408:VAL:HG22 | 1.93                     | 0.50              |
| 1:E:431:ARG:CZ   | 1:E:431:ARG:HA   | 2.42                     | 0.50              |
| 1:G:40:LEU:HB2   | 1:G:48:LEU:HD23  | 1.94                     | 0.50              |
| 1:G:152:THR:CG2  | 1:G:480:ILE:HG23 | 2.40                     | 0.50              |
| 1:H:128:LEU:HD11 | 1:H:491:LEU:HD12 | 1.92                     | 0.50              |
| 1:H:159:LEU:HG   | 1:H:163:LYS:HD3  | 1.94                     | 0.50              |
| 1:H:324:HIS:HB2  | 1:H:329:LYS:CE   | 2.42                     | 0.50              |
| 1:I:89:VAL:HA    | 1:I:490:VAL:CG2  | 2.41                     | 0.50              |
| 1:J:192:LEU:HD13 | 1:J:366:THR:CG2  | 2.41                     | 0.50              |
| 1:L:111:GLN:O    | 1:L:114:ILE:HB   | 2.12                     | 0.50              |
| 1:M:111:GLN:O    | 1:M:114:ILE:HB   | 2.10                     | 0.50              |
| 1:O:15:SER:OG    | 1:O:501:ILE:HG21 | 2.11                     | 0.50              |
| 1:P:31:GLY:C     | 1:P:156:SER:HA   | 2.36                     | 0.50              |
| 1:P:431:ARG:O    | 1:P:434:PRO:HD2  | 2.10                     | 0.50              |
| 1:A:146:LEU:CD2  | 1:A:147:MET:H    | 2.24                     | 0.50              |
| 1:A:163:LYS:HG3  | 1:A:166:PHE:CB   | 2.40                     | 0.50              |
| 1:D:159:LEU:HG   | 1:D:163:LYS:HG2  | 1.94                     | 0.50              |
| 1:H:99:GLU:HG3   | 1:H:425:SER:HB2  | 1.94                     | 0.50              |
| 1:I:262:MET:SD   | 1:I:290:LEU:HB2  | 2.52                     | 0.50              |
| 1:J:146:LEU:CD2  | 1:J:167:THR:HG23 | 2.41                     | 0.50              |
| 1:J:274:ILE:HG23 | 1:J:296:VAL:CG2  | 2.41                     | 0.50              |
| 1:K:82:VAL:HB    | 1:K:485:GLN:HB3  | 1.93                     | 0.50              |
| 1:L:82:VAL:HG13  | 1:L:83:GLY:N     | 2.25                     | 0.50              |
| 1:L:269:ILE:CG2  | 1:L:274:ILE:HG21 | 2.37                     | 0.50              |
| 1:M:131:SER:CB   | 1:M:461:THR:HG21 | 2.41                     | 0.50              |
| 1:M:324:HIS:HB2  | 1:M:329:LYS:HE2  | 1.92                     | 0.50              |
| 1:M:438:ALA:HB2  | 1:M:448:LEU:HG   | 1.92                     | 0.50              |
| 1:P:231:MET:HB2  | 1:P:284:TYR:H    | 1.77                     | 0.50              |
| 1:B:418:LYS:HE3  | 1:I:446:ALA:O    | 2.11                     | 0.50              |
| 1:C:48:LEU:HG    | 1:H:510:ALA:HB3  | 1.92                     | 0.50              |
| 1:C:69:LYS:HD3   | 1:C:510:ALA:HB3  | 1.91                     | 0.50              |
| 1:C:75:SER:O     | 1:C:78:GLN:HB3   | 2.11                     | 0.50              |
| 1:D:433:LEU:O    | 1:D:436:ILE:HG22 | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:334:LYS:HD2  | 1:F:351:GLY:HA3  | 1.94                     | 0.50              |
| 1:F:469:GLU:HG2  | 1:F:471:THR:OG1  | 2.11                     | 0.50              |
| 1:G:207:LEU:HD22 | 1:G:208:ASP:N    | 2.26                     | 0.50              |
| 1:G:269:ILE:HG23 | 1:G:274:ILE:HG21 | 1.92                     | 0.50              |
| 1:G:334:LYS:CD   | 1:G:351:GLY:HA3  | 2.42                     | 0.50              |
| 1:H:106:LYS:NZ   | 1:H:418:LYS:HA   | 2.26                     | 0.50              |
| 1:H:211:ILE:HB   | 1:H:215:GLN:OE1  | 2.10                     | 0.50              |
| 1:H:286:TYR:HB2  | 1:H:287:PRO:HD3  | 1.94                     | 0.50              |
| 1:H:312:LEU:HD22 | 1:H:354:LEU:HD22 | 1.93                     | 0.50              |
| 1:I:171:VAL:O    | 1:I:174:VAL:HG22 | 2.11                     | 0.50              |
| 1:I:372:GLU:HG3  | 1:I:375:ARG:HH21 | 1.73                     | 0.50              |
| 1:K:154:LEU:HD23 | 1:K:163:LYS:HG3  | 1.92                     | 0.50              |
| 1:K:287:PRO:O    | 1:K:291:PHE:HD1  | 1.94                     | 0.50              |
| 1:L:101:GLU:O    | 1:L:104:ILE:HG12 | 2.12                     | 0.50              |
| 1:L:108:ILE:HG22 | 1:L:109:HIS:N    | 2.26                     | 0.50              |
| 1:M:48:LEU:HG    | 1:O:506:ASN:ND2  | 2.27                     | 0.50              |
| 1:N:173:ALA:O    | 1:N:176:ARG:HG2  | 2.11                     | 0.50              |
| 1:P:166:PHE:CZ   | 1:P:198:ASP:HB3  | 2.47                     | 0.50              |
| 1:P:176:ARG:HD2  | 1:P:358:CYS:HB2  | 1.93                     | 0.50              |
| 1:D:58:LEU:HB3   | 1:D:72:VAL:HG13  | 1.93                     | 0.50              |
| 1:D:334:LYS:HD3  | 1:D:351:GLY:HA3  | 1.92                     | 0.50              |
| 1:E:190:LYS:HD2  | 1:E:190:LYS:O    | 2.11                     | 0.50              |
| 1:F:146:LEU:HG   | 1:F:171:VAL:HG11 | 1.92                     | 0.50              |
| 1:F:261:LYS:O    | 1:F:264:GLU:HG2  | 2.12                     | 0.50              |
| 1:F:268:ARG:O    | 1:F:271:LYS:HG2  | 2.11                     | 0.50              |
| 1:G:50:VAL:HG11  | 1:G:372:GLU:HG2  | 1.94                     | 0.50              |
| 1:H:166:PHE:CZ   | 1:H:198:ASP:HB3  | 2.47                     | 0.50              |
| 1:I:160:THR:HA   | 1:I:163:LYS:HB3  | 1.94                     | 0.50              |
| 1:I:206:LEU:C    | 1:I:206:LEU:HD12 | 2.36                     | 0.50              |
| 1:I:452:LEU:HA   | 1:I:472:ILE:HG21 | 1.93                     | 0.50              |
| 1:I:510:ALA:O    | 1:I:511:ALA:HB2  | 2.11                     | 0.50              |
| 1:L:146:LEU:CD2  | 1:L:167:THR:HG23 | 2.41                     | 0.50              |
| 1:M:343:GLU:HG2  | 1:M:344:ASP:N    | 2.25                     | 0.50              |
| 1:N:23:GLY:O     | 1:N:27:LYS:HB3   | 2.12                     | 0.50              |
| 1:N:441:ALA:HB2  | 1:N:467:MET:HG2  | 1.94                     | 0.50              |
| 1:O:163:LYS:HD2  | 1:O:166:PHE:CG   | 2.47                     | 0.50              |
| 1:P:59:LYS:CE    | 1:P:76:ARG:HB2   | 2.41                     | 0.50              |
| 1:A:146:LEU:CD2  | 1:A:167:THR:HG23 | 2.39                     | 0.50              |
| 1:A:211:ILE:HG12 | 1:A:298:ALA:H    | 1.77                     | 0.50              |
| 1:C:133:VAL:HG21 | 1:C:393:THR:H    | 1.77                     | 0.50              |
| 1:C:171:VAL:O    | 1:C:174:VAL:HG22 | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:LEU:HD11 | 1:D:324:HIS:ND1  | 2.27                     | 0.50              |
| 1:F:139:GLU:O    | 1:F:140:VAL:HB   | 2.12                     | 0.50              |
| 1:G:225:LEU:HD21 | 1:G:324:HIS:CE1  | 2.46                     | 0.50              |
| 1:H:359:THR:HG22 | 1:H:360:ILE:N    | 2.27                     | 0.50              |
| 1:H:431:ARG:O    | 1:H:434:PRO:HD2  | 2.10                     | 0.50              |
| 1:J:110:PRO:CB   | 1:J:502:LEU:HB3  | 2.42                     | 0.50              |
| 1:L:117:TRP:HD1  | 1:L:495:ALA:HB1  | 1.75                     | 0.50              |
| 1:O:146:LEU:HD11 | 1:O:150:ALA:HB3  | 1.93                     | 0.50              |
| 1:O:231:MET:HE1  | 1:O:265:LYS:HD3  | 1.92                     | 0.50              |
| 1:P:115:ALA:O    | 1:P:119:GLU:HG2  | 2.12                     | 0.50              |
| 1:P:280:ARG:HG3  | 1:P:304:PHE:HB2  | 1.94                     | 0.50              |
| 1:A:159:LEU:CD1  | 1:A:163:LYS:HD3  | 2.42                     | 0.50              |
| 1:B:216:PRO:HG3  | 1:B:295:GLY:HA2  | 1.94                     | 0.50              |
| 1:C:27:LYS:HA    | 1:C:30:LEU:HD13  | 1.92                     | 0.50              |
| 1:C:452:LEU:HD13 | 1:C:465:LEU:CD1  | 2.41                     | 0.50              |
| 1:D:239:PHE:HB3  | 1:D:241:SER:H    | 1.77                     | 0.50              |
| 1:D:372:GLU:O    | 1:D:375:ARG:HG2  | 2.12                     | 0.50              |
| 1:E:96:LEU:HD21  | 1:E:117:TRP:CZ2  | 2.47                     | 0.50              |
| 1:G:245:VAL:HG11 | 1:G:251:VAL:HG22 | 1.93                     | 0.50              |
| 1:H:222:ALA:HA   | 1:H:275:ASN:OD1  | 2.12                     | 0.50              |
| 1:H:340:MET:O    | 1:H:340:MET:HE3  | 2.12                     | 0.50              |
| 1:J:236:ILE:HG23 | 1:J:237:LYS:H    | 1.75                     | 0.50              |
| 1:J:280:ARG:O    | 1:J:281:GLN:HB3  | 2.12                     | 0.50              |
| 1:K:99:GLU:CG    | 1:K:425:SER:HB2  | 2.42                     | 0.50              |
| 1:K:170:ALA:O    | 1:K:173:ALA:HB3  | 2.12                     | 0.50              |
| 1:M:324:HIS:O    | 1:M:329:LYS:HG3  | 2.12                     | 0.50              |
| 1:N:146:LEU:HD21 | 1:N:167:THR:HG23 | 1.93                     | 0.50              |
| 1:N:206:LEU:HD13 | 1:N:206:LEU:C    | 2.37                     | 0.50              |
| 1:N:402:MET:SD   | 1:N:456:HIS:HB2  | 2.51                     | 0.50              |
| 1:O:79:ASP:HA    | 1:O:83:GLY:HA2   | 1.93                     | 0.50              |
| 1:A:32:PRO:CD    | 1:A:467:MET:HE1  | 2.36                     | 0.50              |
| 1:A:324:HIS:O    | 1:A:329:LYS:HG3  | 2.12                     | 0.50              |
| 1:B:318:ILE:O    | 1:B:318:ILE:HG22 | 2.11                     | 0.50              |
| 1:C:106:LYS:NZ   | 1:C:108:ILE:HD11 | 2.26                     | 0.50              |
| 1:C:222:ALA:HA   | 1:C:275:ASN:OD1  | 2.12                     | 0.50              |
| 1:D:211:ILE:HD13 | 1:D:215:GLN:OE1  | 2.12                     | 0.50              |
| 1:G:129:LEU:HD13 | 1:G:129:LEU:N    | 2.27                     | 0.50              |
| 1:H:185:ALA:HA   | 1:H:309:ARG:CD   | 2.40                     | 0.50              |
| 1:H:226:ILE:HA   | 1:H:278:ILE:O    | 2.11                     | 0.50              |
| 1:H:509:LYS:HB2  | 1:H:509:LYS:NZ   | 2.26                     | 0.50              |
| 1:J:100:ALA:HA   | 1:J:103:LEU:HD22 | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:287:PRO:O    | 1:L:291:PHE:HD1  | 1.95                     | 0.50              |
| 1:L:317:GLU:OE1  | 1:L:329:LYS:HD2  | 2.11                     | 0.50              |
| 1:L:452:LEU:HD22 | 1:L:465:LEU:HD11 | 1.92                     | 0.50              |
| 1:M:146:LEU:CD2  | 1:M:147:MET:H    | 2.24                     | 0.50              |
| 1:M:191:LYS:NZ   | 1:M:346:LEU:HD11 | 2.26                     | 0.50              |
| 1:M:397:GLY:HA3  | 1:M:475:MET:HE3  | 1.94                     | 0.50              |
| 1:M:402:MET:HE3  | 1:M:453:ARG:CG   | 2.35                     | 0.50              |
| 1:O:48:LEU:H     | 1:O:48:LEU:HD12  | 1.77                     | 0.50              |
| 1:O:117:TRP:HD1  | 1:O:495:ALA:HB1  | 1.77                     | 0.50              |
| 1:P:22:ILE:HD12  | 1:P:90:THR:CG2   | 2.42                     | 0.50              |
| 1:A:364:GLY:HA3  | 1:A:370:LEU:HD13 | 1.94                     | 0.50              |
| 1:B:418:LYS:HD3  | 1:I:449:VAL:HG12 | 1.92                     | 0.50              |
| 1:C:59:LYS:CE    | 1:C:76:ARG:HB2   | 2.41                     | 0.50              |
| 1:D:79:ASP:HA    | 1:D:83:GLY:N     | 2.26                     | 0.50              |
| 1:D:342:GLY:C    | 1:D:343:GLU:HG2  | 2.36                     | 0.50              |
| 1:E:96:LEU:O     | 1:E:96:LEU:HD22  | 2.12                     | 0.50              |
| 1:F:203:GLU:HG3  | 1:F:350:SER:HB2  | 1.92                     | 0.50              |
| 1:G:211:ILE:CD1  | 1:G:297:MET:HG3  | 2.38                     | 0.50              |
| 1:G:508:ILE:O    | 1:G:508:ILE:HG22 | 2.12                     | 0.50              |
| 1:H:402:MET:HE2  | 1:H:402:MET:O    | 2.12                     | 0.50              |
| 1:I:173:ALA:O    | 1:I:176:ARG:HG2  | 2.12                     | 0.50              |
| 1:I:232:ASP:HA   | 1:I:284:TYR:CD1  | 2.47                     | 0.50              |
| 1:J:152:THR:HG23 | 1:J:480:ILE:HG12 | 1.92                     | 0.50              |
| 1:J:352:VAL:HG22 | 1:J:355:GLY:H    | 1.77                     | 0.50              |
| 1:K:232:ASP:HA   | 1:K:284:TYR:HB2  | 1.94                     | 0.50              |
| 1:K:452:LEU:HD13 | 1:K:465:LEU:HD13 | 1.93                     | 0.50              |
| 1:M:146:LEU:CD1  | 1:M:171:VAL:HG13 | 2.28                     | 0.50              |
| 1:M:411:LEU:HB3  | 1:M:423:MET:SD   | 2.51                     | 0.50              |
| 1:N:163:LYS:O    | 1:N:166:PHE:HB2  | 2.11                     | 0.50              |
| 1:N:475:MET:SD   | 1:N:480:ILE:HB   | 2.52                     | 0.50              |
| 1:O:31:GLY:O     | 1:O:156:SER:HA   | 2.12                     | 0.50              |
| 1:O:59:LYS:HE3   | 1:O:73:ASP:HA    | 1.94                     | 0.50              |
| 1:O:182:ASN:HD22 | 1:O:182:ASN:N    | 2.10                     | 0.50              |
| 1:A:39:LEU:HD22  | 1:C:1:ALA:C      | 2.37                     | 0.50              |
| 1:A:138:ASP:O    | 1:A:139:GLU:HB2  | 2.10                     | 0.50              |
| 1:A:209:LYS:HB2  | 1:A:299:ILE:HG23 | 1.94                     | 0.50              |
| 1:A:431:ARG:CZ   | 1:A:431:ARG:HA   | 2.42                     | 0.50              |
| 1:B:337:GLU:HG3  | 1:B:339:VAL:HG23 | 1.93                     | 0.50              |
| 1:B:485:GLN:HB2  | 1:B:489:GLN:HE22 | 1.76                     | 0.50              |
| 1:D:154:LEU:HD22 | 1:D:167:THR:HB   | 1.93                     | 0.50              |
| 1:E:219:ILE:HB   | 1:E:275:ASN:HB3  | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:391:SER:C    | 1:E:392:ARG:HG3  | 2.36                     | 0.50              |
| 1:F:51:THR:HA    | 1:F:375:ARG:HH11 | 1.77                     | 0.50              |
| 1:F:487:LYS:HA   | 1:F:490:VAL:HG12 | 1.94                     | 0.50              |
| 1:G:78:GLN:HG3   | 1:G:83:GLY:HA3   | 1.94                     | 0.50              |
| 1:H:312:LEU:HD22 | 1:H:354:LEU:CD2  | 2.42                     | 0.50              |
| 1:H:324:HIS:HB2  | 1:H:329:LYS:HZ1  | 1.75                     | 0.50              |
| 1:H:394:VAL:HG21 | 1:H:487:LYS:HG3  | 1.94                     | 0.50              |
| 1:H:511:ALA:HB3  | 1:H:512:PRO:HD2  | 1.93                     | 0.50              |
| 1:J:163:LYS:HA   | 1:J:166:PHE:CD1  | 2.47                     | 0.50              |
| 1:K:265:LYS:HE2  | 1:K:322:PHE:CE1  | 2.47                     | 0.50              |
| 1:K:274:ILE:HG23 | 1:K:296:VAL:CG2  | 2.41                     | 0.50              |
| 1:L:119:GLU:HG3  | 1:L:423:MET:HE3  | 1.93                     | 0.50              |
| 1:M:265:LYS:HE2  | 1:M:322:PHE:CZ   | 2.47                     | 0.50              |
| 1:N:352:VAL:HG23 | 1:N:355:GLY:H    | 1.77                     | 0.50              |
| 1:O:65:ASN:H     | 1:O:65:ASN:ND2   | 2.00                     | 0.50              |
| 1:P:274:ILE:O    | 1:P:274:ILE:HG23 | 2.12                     | 0.50              |
| 1:A:89:VAL:HB    | 1:A:490:VAL:CG2  | 2.42                     | 0.49              |
| 1:A:496:GLU:HA   | 1:A:499:GLU:HB3  | 1.94                     | 0.49              |
| 1:B:452:LEU:HD13 | 1:B:465:LEU:CD1  | 2.42                     | 0.49              |
| 1:C:334:LYS:HD3  | 1:C:351:GLY:CA   | 2.42                     | 0.49              |
| 1:D:502:LEU:C    | 1:D:502:LEU:HD13 | 2.37                     | 0.49              |
| 1:D:506:ASN:O    | 1:H:37:LYS:HD2   | 2.11                     | 0.49              |
| 1:E:226:ILE:HD12 | 1:E:317:GLU:HG3  | 1.94                     | 0.49              |
| 1:F:163:LYS:O    | 1:F:163:LYS:HG2  | 2.11                     | 0.49              |
| 1:F:287:PRO:O    | 1:F:291:PHE:HD1  | 1.95                     | 0.49              |
| 1:F:448:LEU:HD11 | 1:F:465:LEU:HD11 | 1.92                     | 0.49              |
| 1:G:146:LEU:HD22 | 1:G:168:LYS:HA   | 1.93                     | 0.49              |
| 1:G:335:LEU:HD21 | 1:G:337:GLU:OE1  | 2.11                     | 0.49              |
| 1:I:154:LEU:CD2  | 1:I:163:LYS:HG3  | 2.42                     | 0.49              |
| 1:J:334:LYS:CD   | 1:J:351:GLY:HA3  | 2.41                     | 0.49              |
| 1:K:341:ILE:HG23 | 1:K:363:ARG:NH2  | 2.27                     | 0.49              |
| 1:M:187:HIS:O    | 1:M:359:THR:HG23 | 2.11                     | 0.49              |
| 1:N:166:PHE:CE1  | 1:N:198:ASP:HB3  | 2.47                     | 0.49              |
| 1:O:146:LEU:HB2  | 1:O:171:VAL:HG21 | 1.94                     | 0.49              |
| 1:O:433:LEU:O    | 1:O:437:ILE:HG12 | 2.12                     | 0.49              |
| 1:A:372:GLU:HG3  | 1:A:375:ARG:CZ   | 2.42                     | 0.49              |
| 1:B:32:PRO:HA    | 1:B:155:SER:HB3  | 1.94                     | 0.49              |
| 1:C:188:VAL:HG11 | 1:C:377:LEU:HD22 | 1.94                     | 0.49              |
| 1:C:502:LEU:HD22 | 1:C:502:LEU:H    | 1.77                     | 0.49              |
| 1:E:274:ILE:O    | 1:E:274:ILE:HG23 | 2.13                     | 0.49              |
| 1:F:2:GLY:O      | 1:F:3:ALA:HB2    | 2.10                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:176:ARG:HH12 | 1:F:201:LEU:HD21 | 1.77                     | 0.49              |
| 1:G:32:PRO:O     | 1:G:156:SER:HA   | 2.12                     | 0.49              |
| 1:G:324:HIS:HB2  | 1:G:329:LYS:HE2  | 1.94                     | 0.49              |
| 1:H:22:ILE:HD12  | 1:H:90:THR:CG2   | 2.42                     | 0.49              |
| 1:H:174:VAL:HA   | 1:H:177:LEU:HD12 | 1.94                     | 0.49              |
| 1:H:438:ALA:CB   | 1:H:448:LEU:HG   | 2.42                     | 0.49              |
| 1:K:176:ARG:NH2  | 1:K:360:ILE:HG12 | 2.27                     | 0.49              |
| 1:M:204:GLY:O    | 1:M:359:THR:HB   | 2.11                     | 0.49              |
| 1:N:259:LYS:O    | 1:N:263:LYS:HG2  | 2.12                     | 0.49              |
| 1:O:82:VAL:HA    | 1:O:386:GLN:HG3  | 1.93                     | 0.49              |
| 1:P:39:LEU:HD12  | 1:P:57:ILE:HD11  | 1.94                     | 0.49              |
| 1:P:57:ILE:HG23  | 1:P:58:LEU:HD23  | 1.93                     | 0.49              |
| 1:P:96:LEU:HD21  | 1:P:117:TRP:CZ2  | 2.47                     | 0.49              |
| 1:A:38:ILE:O     | 1:A:38:ILE:HG13  | 2.12                     | 0.49              |
| 1:A:222:ALA:HA   | 1:A:275:ASN:CG   | 2.37                     | 0.49              |
| 1:B:27:LYS:CB    | 1:B:436:ILE:HD11 | 2.43                     | 0.49              |
| 1:B:202:ASP:HB2  | 1:B:359:THR:O    | 2.12                     | 0.49              |
| 1:C:222:ALA:HA   | 1:C:275:ASN:CB   | 2.42                     | 0.49              |
| 1:D:287:PRO:O    | 1:D:291:PHE:HD1  | 1.95                     | 0.49              |
| 1:E:171:VAL:CG1  | 1:E:384:LEU:HG   | 2.42                     | 0.49              |
| 1:F:171:VAL:O    | 1:F:174:VAL:HG22 | 2.12                     | 0.49              |
| 1:K:263:LYS:O    | 1:K:266:VAL:HG12 | 2.11                     | 0.49              |
| 1:L:171:VAL:O    | 1:L:175:LEU:HG   | 2.11                     | 0.49              |
| 1:M:225:LEU:HD13 | 1:M:329:LYS:CE   | 2.43                     | 0.49              |
| 1:M:402:MET:HG2  | 1:M:431:ARG:HH22 | 1.76                     | 0.49              |
| 1:N:57:ILE:HG23  | 1:N:58:LEU:CD2   | 2.42                     | 0.49              |
| 1:N:421:VAL:O    | 1:N:424:GLU:HG2  | 2.13                     | 0.49              |
| 1:O:394:VAL:HG23 | 1:O:482:GLU:HB2  | 1.94                     | 0.49              |
| 1:O:425:SER:O    | 1:O:428:LYS:HG2  | 2.13                     | 0.49              |
| 1:A:143:ARG:HA   | 1:A:143:ARG:HE   | 1.77                     | 0.49              |
| 1:A:159:LEU:N    | 1:A:159:LEU:HD22 | 2.27                     | 0.49              |
| 1:A:485:GLN:HG3  | 1:A:488:ARG:HH21 | 1.76                     | 0.49              |
| 1:B:111:GLN:O    | 1:B:114:ILE:HB   | 2.12                     | 0.49              |
| 1:C:78:GLN:NE2   | 1:C:489:GLN:HB2  | 2.27                     | 0.49              |
| 1:C:425:SER:O    | 1:C:428:LYS:HG2  | 2.12                     | 0.49              |
| 1:C:452:LEU:HD11 | 1:C:456:HIS:HE1  | 1.77                     | 0.49              |
| 1:D:61:ILE:HG12  | 1:E:513:ARG:HG2  | 1.94                     | 0.49              |
| 1:E:59:LYS:HE3   | 1:E:73:ASP:HA    | 1.92                     | 0.49              |
| 1:E:207:LEU:HD13 | 1:E:208:ASP:N    | 2.27                     | 0.49              |
| 1:E:341:ILE:HG23 | 1:E:363:ARG:NH2  | 2.26                     | 0.49              |
| 1:G:322:PHE:HA   | 1:G:324:HIS:CD2  | 2.47                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:451:GLN:HE22 | 1:G:471:THR:HA   | 1.76                     | 0.49              |
| 1:H:405:ALA:HA   | 1:H:408:VAL:HG22 | 1.94                     | 0.49              |
| 1:I:39:LEU:HD12  | 1:I:57:ILE:HG13  | 1.94                     | 0.49              |
| 1:J:192:LEU:O    | 1:J:192:LEU:HD12 | 2.12                     | 0.49              |
| 1:J:313:VAL:HG22 | 1:J:357:ALA:HB3  | 1.94                     | 0.49              |
| 1:J:334:LYS:HD2  | 1:J:351:GLY:HA3  | 1.93                     | 0.49              |
| 1:J:408:VAL:HA   | 1:J:411:LEU:HD12 | 1.95                     | 0.49              |
| 1:J:438:ALA:CB   | 1:J:448:LEU:HG   | 2.42                     | 0.49              |
| 1:K:185:ALA:CB   | 1:K:357:ALA:HA   | 2.42                     | 0.49              |
| 1:N:192:LEU:HG   | 1:N:366:THR:CG2  | 2.43                     | 0.49              |
| 1:P:157:LYS:HB3  | 1:P:159:LEU:HD22 | 1.94                     | 0.49              |
| 1:P:222:ALA:HA   | 1:P:275:ASN:CG   | 2.37                     | 0.49              |
| 1:P:379:ASP:O    | 1:P:383:VAL:HG23 | 2.12                     | 0.49              |
| 1:P:438:ALA:CB   | 1:P:448:LEU:HG   | 2.42                     | 0.49              |
| 1:A:2:GLY:HA2    | 1:A:513:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:334:LYS:CB   | 1:A:351:GLY:HA3  | 2.42                     | 0.49              |
| 1:A:506:ASN:HB3  | 1:F:35:MET:HE2   | 1.94                     | 0.49              |
| 1:B:75:SER:O     | 1:B:78:GLN:HB3   | 2.13                     | 0.49              |
| 1:B:141:LYS:CG   | 1:B:144:GLN:HB2  | 2.43                     | 0.49              |
| 1:C:166:PHE:CD2  | 1:C:362:LEU:HD22 | 2.47                     | 0.49              |
| 1:C:381:LEU:C    | 1:C:381:LEU:HD23 | 2.38                     | 0.49              |
| 1:G:139:GLU:O    | 1:G:140:VAL:HB   | 2.12                     | 0.49              |
| 1:H:216:PRO:HG2  | 1:H:295:GLY:HA2  | 1.94                     | 0.49              |
| 1:I:215:GLN:HG3  | 1:I:292:GLY:HA2  | 1.94                     | 0.49              |
| 1:I:239:PHE:O    | 1:I:241:SER:N    | 2.45                     | 0.49              |
| 1:I:343:GLU:HG3  | 1:I:344:ASP:H    | 1.76                     | 0.49              |
| 1:J:38:ILE:HD13  | 1:J:39:LEU:H     | 1.77                     | 0.49              |
| 1:J:111:GLN:HA   | 1:J:114:ILE:HG12 | 1.94                     | 0.49              |
| 1:K:59:LYS:CE    | 1:K:76:ARG:HB2   | 2.42                     | 0.49              |
| 1:M:99:GLU:O     | 1:M:102:SER:HB2  | 2.12                     | 0.49              |
| 1:M:373:ALA:O    | 1:M:377:LEU:HB2  | 2.12                     | 0.49              |
| 1:O:116:GLY:O    | 1:O:119:GLU:HB2  | 2.12                     | 0.49              |
| 1:P:32:PRO:HD2   | 1:P:467:MET:HE1  | 1.93                     | 0.49              |
| 1:P:171:VAL:O    | 1:P:174:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:312:LEU:O    | 1:A:312:LEU:HD22 | 2.13                     | 0.49              |
| 1:D:64:ASP:CG    | 1:D:66:PRO:HD2   | 2.37                     | 0.49              |
| 1:E:198:ASP:O    | 1:E:199:SER:HB3  | 2.12                     | 0.49              |
| 1:E:438:ALA:HB2  | 1:E:448:LEU:HG   | 1.94                     | 0.49              |
| 1:F:124:ALA:HA   | 1:F:491:LEU:HD13 | 1.95                     | 0.49              |
| 1:F:146:LEU:HD21 | 1:F:150:ALA:CB   | 2.42                     | 0.49              |
| 1:F:175:LEU:HA   | 1:F:178:LYS:HD2  | 1.95                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:370:LEU:O    | 1:F:370:LEU:HD13 | 2.13                     | 0.49              |
| 1:F:381:LEU:O    | 1:F:381:LEU:HD22 | 2.11                     | 0.49              |
| 1:I:27:LYS:C     | 1:I:436:ILE:HD11 | 2.36                     | 0.49              |
| 1:I:145:ASP:OD2  | 1:I:175:LEU:HD11 | 2.12                     | 0.49              |
| 1:J:110:PRO:O    | 1:J:113:ILE:HB   | 2.12                     | 0.49              |
| 1:J:177:LEU:HD13 | 1:J:177:LEU:C    | 2.38                     | 0.49              |
| 1:K:412:ALA:CB   | 1:K:424:GLU:HB3  | 2.43                     | 0.49              |
| 1:L:187:HIS:HB3  | 1:L:359:THR:HG23 | 1.94                     | 0.49              |
| 1:N:67:ALA:HB1   | 1:N:507:ILE:HG21 | 1.95                     | 0.49              |
| 1:N:108:ILE:HG22 | 1:N:109:HIS:N    | 2.27                     | 0.49              |
| 1:N:114:ILE:HA   | 1:N:117:TRP:CE3  | 2.47                     | 0.49              |
| 1:N:284:TYR:O    | 1:N:287:PRO:HD2  | 2.12                     | 0.49              |
| 1:P:116:GLY:O    | 1:P:119:GLU:HB2  | 2.12                     | 0.49              |
| 1:B:364:GLY:HA3  | 1:B:370:LEU:CD1  | 2.39                     | 0.49              |
| 1:B:434:PRO:HB3  | 1:B:452:LEU:CD2  | 2.42                     | 0.49              |
| 1:B:451:GLN:HE22 | 1:B:471:THR:HA   | 1.78                     | 0.49              |
| 1:D:190:LYS:HD2  | 1:D:190:LYS:O    | 2.12                     | 0.49              |
| 1:E:35:MET:CE    | 1:G:504:VAL:HG12 | 2.43                     | 0.49              |
| 1:F:82:VAL:HG11  | 1:F:486:VAL:HA   | 1.94                     | 0.49              |
| 1:G:397:GLY:HA3  | 1:G:475:MET:CE   | 2.43                     | 0.49              |
| 1:H:108:ILE:CG2  | 1:H:109:HIS:N    | 2.75                     | 0.49              |
| 1:H:277:PHE:CE2  | 1:H:279:ASN:HB2  | 2.47                     | 0.49              |
| 1:J:209:LYS:HE2  | 1:J:302:ALA:HA   | 1.93                     | 0.49              |
| 1:K:107:LYS:HD2  | 1:K:107:LYS:O    | 2.13                     | 0.49              |
| 1:K:177:LEU:C    | 1:K:177:LEU:CD1  | 2.85                     | 0.49              |
| 1:K:192:LEU:O    | 1:K:343:GLU:HB3  | 2.13                     | 0.49              |
| 1:K:431:ARG:O    | 1:K:434:PRO:HD2  | 2.12                     | 0.49              |
| 1:M:159:LEU:HD22 | 1:M:159:LEU:N    | 2.28                     | 0.49              |
| 1:M:236:ILE:HG13 | 1:M:237:LYS:N    | 2.24                     | 0.49              |
| 1:N:96:LEU:HD13  | 1:N:96:LEU:C     | 2.37                     | 0.49              |
| 1:N:211:ILE:CD1  | 1:N:297:MET:HG3  | 2.37                     | 0.49              |
| 1:N:392:ARG:HG3  | 1:N:484:PHE:CD2  | 2.47                     | 0.49              |
| 1:O:111:GLN:HA   | 1:O:114:ILE:CG1  | 2.42                     | 0.49              |
| 1:B:225:LEU:HD11 | 1:B:324:HIS:ND1  | 2.27                     | 0.49              |
| 1:C:51:THR:HG21  | 1:C:56:THR:HB    | 1.95                     | 0.49              |
| 1:C:274:ILE:O    | 1:C:296:VAL:HG22 | 2.13                     | 0.49              |
| 1:D:150:ALA:O    | 1:D:154:LEU:HD13 | 2.12                     | 0.49              |
| 1:E:138:ASP:O    | 1:E:139:GLU:HB2  | 2.12                     | 0.49              |
| 1:E:277:PHE:O    | 1:E:298:ALA:HA   | 2.12                     | 0.49              |
| 1:F:114:ILE:HA   | 1:F:117:TRP:CE3  | 2.47                     | 0.49              |
| 1:F:163:LYS:HA   | 1:F:166:PHE:CD1  | 2.48                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:500:VAL:O    | 1:F:504:VAL:HG22 | 2.12                     | 0.49              |
| 1:G:99:GLU:CG    | 1:G:425:SER:HB2  | 2.42                     | 0.49              |
| 1:J:484:PHE:CE2  | 1:J:488:ARG:HD3  | 2.48                     | 0.49              |
| 1:K:274:ILE:HG23 | 1:K:296:VAL:HG21 | 1.94                     | 0.49              |
| 1:L:111:GLN:HA   | 1:L:114:ILE:HG12 | 1.94                     | 0.49              |
| 1:L:368:GLN:HE22 | 1:M:507:ILE:HD11 | 1.77                     | 0.49              |
| 1:N:171:VAL:O    | 1:N:174:VAL:HG22 | 2.12                     | 0.49              |
| 1:N:340:MET:HG2  | 1:N:345:LYS:HG2  | 1.95                     | 0.49              |
| 1:O:226:ILE:HB   | 1:O:317:GLU:OE2  | 2.13                     | 0.49              |
| 1:P:32:PRO:HD2   | 1:P:467:MET:SD   | 2.52                     | 0.49              |
| 1:P:185:ALA:HB1  | 1:P:357:ALA:HB1  | 1.95                     | 0.49              |
| 1:A:484:PHE:CE2  | 1:A:488:ARG:HD3  | 2.48                     | 0.49              |
| 1:B:14:SER:O     | 1:B:17:ILE:HG22  | 2.13                     | 0.49              |
| 1:B:263:LYS:O    | 1:B:266:VAL:HG12 | 2.13                     | 0.49              |
| 1:C:116:GLY:O    | 1:C:119:GLU:HB2  | 2.13                     | 0.49              |
| 1:C:265:LYS:HE2  | 1:C:322:PHE:CE1  | 2.48                     | 0.49              |
| 1:D:402:MET:SD   | 1:D:453:ARG:HA   | 2.53                     | 0.49              |
| 1:E:19:ALA:HB1   | 1:E:94:ALA:HA    | 1.94                     | 0.49              |
| 1:E:54:GLY:O     | 1:E:58:LEU:HD23  | 2.13                     | 0.49              |
| 1:E:392:ARG:C    | 1:E:484:PHE:HB2  | 2.37                     | 0.49              |
| 1:G:125:ARG:HA   | 1:G:128:LEU:HD11 | 1.95                     | 0.49              |
| 1:G:159:LEU:HG   | 1:G:163:LYS:HG2  | 1.95                     | 0.49              |
| 1:G:343:GLU:HG3  | 1:G:344:ASP:N    | 2.28                     | 0.49              |
| 1:G:502:LEU:HD23 | 1:G:502:LEU:O    | 2.12                     | 0.49              |
| 1:H:32:PRO:HD2   | 1:H:467:MET:HE1  | 1.94                     | 0.49              |
| 1:H:266:VAL:HB   | 1:H:290:LEU:HD21 | 1.94                     | 0.49              |
| 1:I:146:LEU:HD13 | 1:I:167:THR:O    | 2.12                     | 0.49              |
| 1:I:334:LYS:HB3  | 1:I:351:GLY:HA3  | 1.94                     | 0.49              |
| 1:K:509:LYS:O    | 1:K:510:ALA:HB2  | 2.11                     | 0.49              |
| 1:M:188:VAL:CG2  | 1:M:377:LEU:HD21 | 2.43                     | 0.49              |
| 1:N:146:LEU:CG   | 1:N:147:MET:H    | 2.26                     | 0.49              |
| 1:N:176:ARG:HH12 | 1:N:201:LEU:HD11 | 1.77                     | 0.49              |
| 1:O:22:ILE:HD12  | 1:O:90:THR:CG2   | 2.43                     | 0.49              |
| 1:P:448:LEU:HD13 | 1:P:448:LEU:C    | 2.37                     | 0.49              |
| 1:C:123:ALA:O    | 1:C:126:GLN:HG2  | 2.13                     | 0.49              |
| 1:C:324:HIS:HB2  | 1:C:329:LYS:NZ   | 2.28                     | 0.49              |
| 1:C:345:LYS:O    | 1:C:346:LEU:HD12 | 2.12                     | 0.49              |
| 1:C:496:GLU:O    | 1:C:497:ALA:HB3  | 2.12                     | 0.49              |
| 1:D:106:LYS:C    | 1:D:107:LYS:HG2  | 2.38                     | 0.49              |
| 1:E:128:LEU:HD11 | 1:E:488:ARG:HD3  | 1.95                     | 0.49              |
| 1:E:262:MET:HE2  | 1:E:286:TYR:O    | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:96:LEU:HD11  | 1:F:498:ALA:HB1  | 1.94                     | 0.49              |
| 1:G:22:ILE:HD12  | 1:G:90:THR:CG2   | 2.42                     | 0.49              |
| 1:I:166:PHE:CD2  | 1:I:362:LEU:HD22 | 2.42                     | 0.49              |
| 1:J:40:LEU:H     | 1:K:3:ALA:HB2    | 1.77                     | 0.49              |
| 1:L:159:LEU:HD23 | 1:L:163:LYS:HD2  | 1.92                     | 0.49              |
| 1:L:385:ALA:O    | 1:L:388:VAL:HG12 | 2.13                     | 0.49              |
| 1:L:431:ARG:HH21 | 1:L:434:PRO:HG2  | 1.77                     | 0.49              |
| 1:M:96:LEU:O     | 1:M:96:LEU:HD22  | 2.13                     | 0.49              |
| 1:N:265:LYS:HE2  | 1:N:322:PHE:CE1  | 2.48                     | 0.49              |
| 1:O:32:PRO:CB    | 1:O:467:MET:HE1  | 2.41                     | 0.49              |
| 1:O:103:LEU:CD2  | 1:O:113:ILE:HG21 | 2.43                     | 0.49              |
| 1:O:173:ALA:O    | 1:O:176:ARG:HG2  | 2.13                     | 0.49              |
| 1:O:381:LEU:O    | 1:O:381:LEU:HD22 | 2.12                     | 0.49              |
| 1:P:192:LEU:HB2  | 1:P:366:THR:OG1  | 2.12                     | 0.49              |
| 1:A:341:ILE:HG23 | 1:A:363:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:287:PRO:O    | 1:B:291:PHE:HD2  | 1.96                     | 0.48              |
| 1:E:108:ILE:HA   | 1:J:446:ALA:CB   | 2.43                     | 0.48              |
| 1:F:396:GLY:HA3  | 1:F:480:ILE:HG22 | 1.95                     | 0.48              |
| 1:F:397:GLY:HA3  | 1:F:475:MET:CE   | 2.43                     | 0.48              |
| 1:G:225:LEU:HG   | 1:G:277:PHE:CE1  | 2.48                     | 0.48              |
| 1:G:369:ILE:HA   | 1:G:372:GLU:CD   | 2.38                     | 0.48              |
| 1:I:159:LEU:HG   | 1:I:163:LYS:HG2  | 1.94                     | 0.48              |
| 1:I:452:LEU:HD22 | 1:I:465:LEU:HD11 | 1.95                     | 0.48              |
| 1:K:32:PRO:CG    | 1:K:467:MET:HE1  | 2.43                     | 0.48              |
| 1:L:92:LEU:CD1   | 1:L:433:LEU:HD21 | 2.40                     | 0.48              |
| 1:M:27:LYS:HG3   | 1:M:436:ILE:HG12 | 1.93                     | 0.48              |
| 1:M:366:THR:HG22 | 1:M:370:LEU:HD22 | 1.95                     | 0.48              |
| 1:M:390:ASP:CB   | 1:M:485:GLN:HE22 | 2.26                     | 0.48              |
| 1:N:27:LYS:HG2   | 1:N:436:ILE:HD11 | 1.94                     | 0.48              |
| 1:N:233:THR:CG2  | 1:N:261:LYS:HE2  | 2.43                     | 0.48              |
| 1:O:26:VAL:HG23  | 1:O:91:VAL:HG22  | 1.94                     | 0.48              |
| 1:O:173:ALA:CB   | 1:O:360:ILE:HD11 | 2.43                     | 0.48              |
| 1:P:431:ARG:HH21 | 1:P:434:PRO:HG2  | 1.78                     | 0.48              |
| 1:P:485:GLN:HG2  | 1:P:488:ARG:HH21 | 1.78                     | 0.48              |
| 1:A:108:ILE:CD1  | 1:M:445:SER:HB2  | 2.43                     | 0.48              |
| 1:A:506:ASN:ND2  | 1:F:440:ASN:HA   | 2.28                     | 0.48              |
| 1:B:38:ILE:CG2   | 1:B:50:VAL:HB    | 2.43                     | 0.48              |
| 1:B:79:ASP:HA    | 1:B:83:GLY:HA2   | 1.93                     | 0.48              |
| 1:C:154:LEU:HD22 | 1:C:167:THR:HB   | 1.93                     | 0.48              |
| 1:D:159:LEU:H    | 1:D:159:LEU:HD22 | 1.78                     | 0.48              |
| 1:D:452:LEU:HD13 | 1:D:465:LEU:CD1  | 2.42                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:117:TRP:HD1  | 1:E:495:ALA:HB1  | 1.77                     | 0.48              |
| 1:E:287:PRO:O    | 1:E:291:PHE:HD1  | 1.96                     | 0.48              |
| 1:F:274:ILE:HG23 | 1:F:296:VAL:HG21 | 1.94                     | 0.48              |
| 1:F:323:ASP:C    | 1:F:325:PRO:HD2  | 2.38                     | 0.48              |
| 1:G:424:GLU:O    | 1:G:427:ALA:HB3  | 2.13                     | 0.48              |
| 1:H:511:ALA:HB3  | 1:H:512:PRO:CD   | 2.43                     | 0.48              |
| 1:I:123:ALA:HA   | 1:I:126:GLN:CG   | 2.43                     | 0.48              |
| 1:I:146:LEU:HD23 | 1:I:148:ASN:H    | 1.78                     | 0.48              |
| 1:N:141:LYS:CE   | 1:N:144:GLN:HB2  | 2.43                     | 0.48              |
| 1:A:32:PRO:HD2   | 1:A:467:MET:CE   | 2.37                     | 0.48              |
| 1:A:334:LYS:HB3  | 1:A:351:GLY:HA3  | 1.96                     | 0.48              |
| 1:B:146:LEU:HD13 | 1:B:167:THR:O    | 2.12                     | 0.48              |
| 1:C:117:TRP:HE1  | 1:C:498:ALA:HB3  | 1.76                     | 0.48              |
| 1:C:171:VAL:CG1  | 1:C:384:LEU:HG   | 2.42                     | 0.48              |
| 1:C:211:ILE:CD1  | 1:C:211:ILE:N    | 2.69                     | 0.48              |
| 1:C:475:MET:SD   | 1:C:480:ILE:HB   | 2.53                     | 0.48              |
| 1:D:37:LYS:HZ2   | 1:E:509:LYS:HA   | 1.79                     | 0.48              |
| 1:D:57:ILE:HD11  | 1:E:513:ARG:OXT  | 2.12                     | 0.48              |
| 1:D:117:TRP:CD1  | 1:D:495:ALA:HB1  | 2.48                     | 0.48              |
| 1:E:503:ARG:HG3  | 1:E:504:VAL:N    | 2.26                     | 0.48              |
| 1:F:226:ILE:HG12 | 1:F:278:ILE:HG23 | 1.94                     | 0.48              |
| 1:G:110:PRO:HA   | 1:G:113:ILE:HD12 | 1.94                     | 0.48              |
| 1:G:417:GLY:HA2  | 1:G:420:ALA:HB3  | 1.95                     | 0.48              |
| 1:H:452:LEU:HD11 | 1:H:456:HIS:HE1  | 1.78                     | 0.48              |
| 1:I:280:ARG:O    | 1:I:281:GLN:HB3  | 2.13                     | 0.48              |
| 1:I:486:VAL:O    | 1:I:490:VAL:HG12 | 2.13                     | 0.48              |
| 1:J:12:ARG:HD3   | 1:J:501:ILE:CG2  | 2.43                     | 0.48              |
| 1:J:28:SER:O     | 1:J:34:GLY:HA2   | 2.13                     | 0.48              |
| 1:M:188:VAL:HA   | 1:M:360:ILE:O    | 2.11                     | 0.48              |
| 1:M:390:ASP:HB2  | 1:M:485:GLN:HE22 | 1.77                     | 0.48              |
| 1:N:52:ASN:HD21  | 1:N:157:LYS:HA   | 1.78                     | 0.48              |
| 1:O:139:GLU:HG3  | 1:O:140:VAL:N    | 2.28                     | 0.48              |
| 1:O:263:LYS:O    | 1:O:267:GLU:HG2  | 2.13                     | 0.48              |
| 1:P:373:ALA:O    | 1:P:377:LEU:HB2  | 2.13                     | 0.48              |
| 1:A:225:LEU:HD11 | 1:A:324:HIS:CE1  | 2.49                     | 0.48              |
| 1:A:313:VAL:HG22 | 1:A:357:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:369:ILE:O    | 1:A:372:GLU:CB   | 2.62                     | 0.48              |
| 1:A:372:GLU:HG3  | 1:A:375:ARG:NH2  | 2.28                     | 0.48              |
| 1:D:222:ALA:HA   | 1:D:275:ASN:HB2  | 1.96                     | 0.48              |
| 1:E:108:ILE:HD12 | 1:J:446:ALA:O    | 2.12                     | 0.48              |
| 1:E:130:ASN:O    | 1:E:131:SER:HB2  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:145:ASP:O    | 1:E:171:VAL:HG11 | 2.14                     | 0.48              |
| 1:F:219:ILE:HD11 | 1:F:336:ILE:HB   | 1.96                     | 0.48              |
| 1:G:334:LYS:CB   | 1:G:351:GLY:HA3  | 2.43                     | 0.48              |
| 1:I:163:LYS:HA   | 1:I:166:PHE:HD1  | 1.76                     | 0.48              |
| 1:J:380:ALA:O    | 1:J:384:LEU:HD22 | 2.12                     | 0.48              |
| 1:K:13:LEU:HD21  | 1:K:511:ALA:O    | 2.13                     | 0.48              |
| 1:K:45:ASP:O     | 1:K:46:ALA:HB2   | 2.12                     | 0.48              |
| 1:K:99:GLU:O     | 1:K:103:LEU:HD13 | 2.12                     | 0.48              |
| 1:K:154:LEU:CD2  | 1:K:163:LYS:HG3  | 2.44                     | 0.48              |
| 1:K:154:LEU:HD13 | 1:K:167:THR:OG1  | 2.13                     | 0.48              |
| 1:K:233:THR:O    | 1:K:234:ASP:HB3  | 2.13                     | 0.48              |
| 1:K:309:ARG:O    | 1:K:313:VAL:HG23 | 2.13                     | 0.48              |
| 1:M:141:LYS:HE2  | 1:M:144:GLN:CG   | 2.44                     | 0.48              |
| 1:M:280:ARG:HD2  | 1:M:304:PHE:HB2  | 1.95                     | 0.48              |
| 1:M:431:ARG:CZ   | 1:M:431:ARG:HA   | 2.43                     | 0.48              |
| 1:N:92:LEU:HD11  | 1:N:433:LEU:HD21 | 1.96                     | 0.48              |
| 1:N:232:ASP:HA   | 1:N:284:TYR:CD1  | 2.48                     | 0.48              |
| 1:O:284:TYR:CE2  | 1:O:286:TYR:HD2  | 2.31                     | 0.48              |
| 1:P:219:ILE:HB   | 1:P:275:ASN:HB3  | 1.94                     | 0.48              |
| 1:B:116:GLY:O    | 1:B:119:GLU:HB2  | 2.14                     | 0.48              |
| 1:E:284:TYR:CE2  | 1:E:286:TYR:HD2  | 2.32                     | 0.48              |
| 1:F:452:LEU:HD13 | 1:F:465:LEU:CD1  | 2.43                     | 0.48              |
| 1:G:41:SER:HB3   | 1:G:45:ASP:OD2   | 2.14                     | 0.48              |
| 1:G:448:LEU:HD21 | 1:G:465:LEU:HD12 | 1.95                     | 0.48              |
| 1:H:61:ILE:HG13  | 1:H:62:GLY:N     | 2.28                     | 0.48              |
| 1:H:183:LEU:CD1  | 1:H:186:ILE:HD12 | 2.43                     | 0.48              |
| 1:H:226:ILE:HG12 | 1:H:278:ILE:HG23 | 1.95                     | 0.48              |
| 1:I:431:ARG:O    | 1:I:434:PRO:HD2  | 2.13                     | 0.48              |
| 1:J:109:HIS:CE1  | 1:J:111:GLN:HB2  | 2.48                     | 0.48              |
| 1:J:341:ILE:HG23 | 1:J:363:ARG:CZ   | 2.43                     | 0.48              |
| 1:K:22:ILE:HD12  | 1:K:90:THR:CG2   | 2.43                     | 0.48              |
| 1:L:64:ASP:CG    | 1:L:66:PRO:HD2   | 2.39                     | 0.48              |
| 1:L:226:ILE:HA   | 1:L:278:ILE:O    | 2.14                     | 0.48              |
| 1:L:452:LEU:HD11 | 1:L:456:HIS:HE1  | 1.77                     | 0.48              |
| 1:M:57:ILE:HD13  | 1:M:57:ILE:O     | 2.14                     | 0.48              |
| 1:M:203:GLU:H    | 1:M:203:GLU:CD   | 2.21                     | 0.48              |
| 1:N:107:LYS:O    | 1:N:107:LYS:HG2  | 2.13                     | 0.48              |
| 1:N:125:ARG:C    | 1:N:127:ALA:H    | 2.21                     | 0.48              |
| 1:N:510:ALA:C    | 1:N:512:PRO:HD2  | 2.38                     | 0.48              |
| 1:O:202:ASP:HB2  | 1:O:359:THR:HG22 | 1.94                     | 0.48              |
| 1:B:79:ASP:HA    | 1:B:83:GLY:N     | 2.29                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:334:LYS:CB   | 1:B:351:GLY:HA3  | 2.43                     | 0.48              |
| 1:C:39:LEU:CD1   | 1:C:57:ILE:HD11  | 2.40                     | 0.48              |
| 1:C:380:ALA:O    | 1:C:384:LEU:HD23 | 2.14                     | 0.48              |
| 1:E:27:LYS:CB    | 1:E:436:ILE:HD11 | 2.44                     | 0.48              |
| 1:E:203:GLU:CG   | 1:E:350:SER:HB2  | 2.43                     | 0.48              |
| 1:E:322:PHE:HA   | 1:E:324:HIS:CD2  | 2.48                     | 0.48              |
| 1:F:96:LEU:HD13  | 1:F:97:LEU:N     | 2.28                     | 0.48              |
| 1:F:411:LEU:HB3  | 1:F:423:MET:SD   | 2.53                     | 0.48              |
| 1:G:59:LYS:HE3   | 1:G:73:ASP:HA    | 1.95                     | 0.48              |
| 1:G:82:VAL:HG22  | 1:G:386:GLN:HB3  | 1.94                     | 0.48              |
| 1:G:110:PRO:O    | 1:G:113:ILE:HB   | 2.13                     | 0.48              |
| 1:H:51:THR:HG23  | 1:H:375:ARG:CZ   | 2.44                     | 0.48              |
| 1:H:284:TYR:O    | 1:H:287:PRO:HD2  | 2.13                     | 0.48              |
| 1:I:45:ASP:O     | 1:I:47:SER:N     | 2.43                     | 0.48              |
| 1:I:96:LEU:HD13  | 1:I:97:LEU:N     | 2.29                     | 0.48              |
| 1:I:366:THR:O    | 1:I:366:THR:HG23 | 2.13                     | 0.48              |
| 1:L:145:ASP:O    | 1:L:171:VAL:HG11 | 2.13                     | 0.48              |
| 1:M:48:LEU:HD12  | 1:O:508:ILE:HD11 | 1.95                     | 0.48              |
| 1:M:152:THR:OG1  | 1:M:480:ILE:HA   | 2.13                     | 0.48              |
| 1:M:265:LYS:HZ2  | 1:M:287:PRO:HG3  | 1.78                     | 0.48              |
| 1:N:75:SER:O     | 1:N:78:GLN:HB3   | 2.14                     | 0.48              |
| 1:O:38:ILE:HD12  | 1:O:48:LEU:HD22  | 1.95                     | 0.48              |
| 1:O:126:GLN:OE1  | 1:O:411:LEU:HD11 | 2.13                     | 0.48              |
| 1:P:82:VAL:HG13  | 1:P:83:GLY:N     | 2.28                     | 0.48              |
| 1:P:431:ARG:CZ   | 1:P:431:ARG:HA   | 2.43                     | 0.48              |
| 1:A:28:SER:HB2   | 1:A:35:MET:SD    | 2.53                     | 0.48              |
| 1:A:411:LEU:CB   | 1:A:423:MET:SD   | 3.02                     | 0.48              |
| 1:A:452:LEU:HD11 | 1:A:456:HIS:CE1  | 2.49                     | 0.48              |
| 1:A:508:ILE:HB   | 1:F:37:LYS:HZ1   | 1.78                     | 0.48              |
| 1:C:433:LEU:HB2  | 1:C:434:PRO:HD3  | 1.96                     | 0.48              |
| 1:C:434:PRO:HB3  | 1:C:452:LEU:HD22 | 1.96                     | 0.48              |
| 1:D:111:GLN:HG2  | 1:H:35:MET:CE    | 2.43                     | 0.48              |
| 1:D:222:ALA:HA   | 1:D:275:ASN:OD1  | 2.14                     | 0.48              |
| 1:E:448:LEU:HD21 | 1:E:465:LEU:CD1  | 2.44                     | 0.48              |
| 1:F:177:LEU:C    | 1:F:177:LEU:HD13 | 2.39                     | 0.48              |
| 1:F:510:ALA:O    | 1:F:511:ALA:CB   | 2.61                     | 0.48              |
| 1:G:164:ASP:O    | 1:G:167:THR:HG22 | 2.14                     | 0.48              |
| 1:G:266:VAL:HB   | 1:G:290:LEU:HD21 | 1.95                     | 0.48              |
| 1:I:52:ASN:ND2   | 1:I:157:LYS:HD3  | 2.27                     | 0.48              |
| 1:J:9:GLU:HG3    | 1:J:10:THR:N     | 2.29                     | 0.48              |
| 1:J:146:LEU:HD11 | 1:J:150:ALA:CB   | 2.43                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:122:LYS:O    | 1:K:125:ARG:HG2  | 2.13                     | 0.48              |
| 1:L:431:ARG:NH2  | 1:L:434:PRO:HG2  | 2.28                     | 0.48              |
| 1:M:190:LYS:HA   | 1:M:362:LEU:O    | 2.14                     | 0.48              |
| 1:N:219:ILE:HD11 | 1:N:336:ILE:HB   | 1.94                     | 0.48              |
| 1:N:222:ALA:HA   | 1:N:275:ASN:HB2  | 1.95                     | 0.48              |
| 1:O:284:TYR:O    | 1:O:287:PRO:HD2  | 2.14                     | 0.48              |
| 1:P:99:GLU:HG2   | 1:P:425:SER:CB   | 2.43                     | 0.48              |
| 1:P:143:ARG:HA   | 1:P:143:ARG:NE   | 2.28                     | 0.48              |
| 1:P:146:LEU:CD2  | 1:P:147:MET:H    | 2.26                     | 0.48              |
| 1:A:2:GLY:O      | 1:A:3:ALA:CB     | 2.62                     | 0.48              |
| 1:A:95:GLU:HA    | 1:A:98:ARG:HD2   | 1.96                     | 0.48              |
| 1:A:496:GLU:HA   | 1:A:499:GLU:CB   | 2.44                     | 0.48              |
| 1:B:106:LYS:CB   | 1:I:446:ALA:HB2  | 2.37                     | 0.48              |
| 1:B:274:ILE:HG23 | 1:B:296:VAL:CG2  | 2.44                     | 0.48              |
| 1:C:211:ILE:HG13 | 1:C:298:ALA:H    | 1.79                     | 0.48              |
| 1:C:398:GLY:HA2  | 1:C:401:GLU:CD   | 2.39                     | 0.48              |
| 1:D:188:VAL:HA   | 1:D:360:ILE:O    | 2.14                     | 0.48              |
| 1:D:418:LYS:NZ   | 1:D:418:LYS:HB3  | 2.29                     | 0.48              |
| 1:E:52:ASN:HB3   | 1:E:157:LYS:HG2  | 1.96                     | 0.48              |
| 1:E:487:LYS:HA   | 1:E:490:VAL:HG12 | 1.94                     | 0.48              |
| 1:F:226:ILE:HG12 | 1:F:278:ILE:CG2  | 2.43                     | 0.48              |
| 1:G:99:GLU:O     | 1:G:102:SER:HB2  | 2.13                     | 0.48              |
| 1:H:6:GLU:HB3    | 1:H:11:ALA:HB1   | 1.95                     | 0.48              |
| 1:K:392:ARG:C    | 1:K:484:PHE:HB2  | 2.38                     | 0.48              |
| 1:M:431:ARG:O    | 1:M:434:PRO:HD2  | 2.14                     | 0.48              |
| 1:N:148:ASN:HA   | 1:N:479:GLY:O    | 2.13                     | 0.48              |
| 1:O:58:LEU:HD12  | 1:O:72:VAL:HG22  | 1.95                     | 0.48              |
| 1:P:65:ASN:CG    | 1:P:66:PRO:HD3   | 2.38                     | 0.48              |
| 1:P:238:ILE:O    | 1:P:240:GLY:N    | 2.46                     | 0.48              |
| 1:B:160:THR:HG23 | 1:B:164:ASP:HB3  | 1.94                     | 0.48              |
| 1:C:24:ASP:O     | 1:C:27:LYS:HG2   | 2.14                     | 0.48              |
| 1:C:317:GLU:CD   | 1:C:329:LYS:HG3  | 2.39                     | 0.48              |
| 1:D:190:LYS:HD2  | 1:D:190:LYS:C    | 2.39                     | 0.48              |
| 1:D:283:ILE:HG22 | 1:D:300:GLU:CG   | 2.42                     | 0.48              |
| 1:D:489:GLN:HE21 | 1:D:489:GLN:H    | 1.62                     | 0.48              |
| 1:F:372:GLU:HB2  | 1:F:375:ARG:HH21 | 1.79                     | 0.48              |
| 1:G:277:PHE:O    | 1:G:298:ALA:HA   | 2.14                     | 0.48              |
| 1:H:211:ILE:HG12 | 1:H:298:ALA:H    | 1.78                     | 0.48              |
| 1:M:51:THR:HG22  | 1:M:53:ASP:O     | 2.14                     | 0.48              |
| 1:M:225:LEU:HD11 | 1:M:324:HIS:CE1  | 2.47                     | 0.48              |
| 1:M:334:LYS:HB2  | 1:M:351:GLY:HA3  | 1.95                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:434:PRO:HB3  | 1:M:452:LEU:HD22 | 1.95                     | 0.48              |
| 1:N:261:LYS:O    | 1:N:264:GLU:HG2  | 2.13                     | 0.48              |
| 1:O:57:ILE:HG23  | 1:O:58:LEU:CD2   | 2.44                     | 0.48              |
| 1:O:145:ASP:OD2  | 1:O:175:LEU:HD11 | 2.13                     | 0.48              |
| 1:O:259:LYS:O    | 1:O:262:MET:HB3  | 2.13                     | 0.48              |
| 1:A:188:VAL:CG1  | 1:A:377:LEU:HD22 | 2.43                     | 0.48              |
| 1:C:114:ILE:HD12 | 1:C:499:GLU:HA   | 1.96                     | 0.48              |
| 1:C:364:GLY:HA3  | 1:C:370:LEU:HD13 | 1.96                     | 0.48              |
| 1:D:254:ILE:CG2  | 1:E:238:ILE:HG13 | 2.44                     | 0.48              |
| 1:G:176:ARG:HD2  | 1:G:358:CYS:SG   | 2.54                     | 0.48              |
| 1:I:188:VAL:CG2  | 1:I:377:LEU:HD21 | 2.44                     | 0.48              |
| 1:I:206:LEU:HD12 | 1:I:206:LEU:O    | 2.14                     | 0.48              |
| 1:J:40:LEU:CD1   | 1:J:40:LEU:C     | 2.87                     | 0.48              |
| 1:K:106:LYS:HE2  | 1:K:418:LYS:HE2  | 1.94                     | 0.48              |
| 1:K:173:ALA:HB1  | 1:K:360:ILE:CD1  | 2.43                     | 0.48              |
| 1:L:58:LEU:HB3   | 1:L:72:VAL:CG1   | 2.44                     | 0.48              |
| 1:L:323:ASP:C    | 1:L:325:PRO:HD2  | 2.39                     | 0.48              |
| 1:M:226:ILE:HA   | 1:M:278:ILE:O    | 2.14                     | 0.48              |
| 1:N:208:ASP:O    | 1:N:209:LYS:HG3  | 2.13                     | 0.48              |
| 1:N:232:ASP:HA   | 1:N:284:TYR:HB2  | 1.96                     | 0.48              |
| 1:O:222:ALA:HA   | 1:O:275:ASN:OD1  | 2.13                     | 0.48              |
| 1:B:96:LEU:HD13  | 1:B:97:LEU:N     | 2.29                     | 0.47              |
| 1:B:326:GLU:CG   | 1:B:327:LEU:H    | 2.23                     | 0.47              |
| 1:B:418:LYS:CG   | 1:I:450:ALA:HA   | 2.43                     | 0.47              |
| 1:C:125:ARG:HG2  | 1:C:128:LEU:HD12 | 1.96                     | 0.47              |
| 1:C:188:VAL:HG21 | 1:C:377:LEU:HD13 | 1.96                     | 0.47              |
| 1:D:421:VAL:O    | 1:D:424:GLU:HG2  | 2.14                     | 0.47              |
| 1:E:177:LEU:C    | 1:E:177:LEU:HD13 | 2.39                     | 0.47              |
| 1:E:324:HIS:O    | 1:E:328:VAL:HG23 | 2.13                     | 0.47              |
| 1:E:475:MET:SD   | 1:E:480:ILE:HB   | 2.54                     | 0.47              |
| 1:F:176:ARG:CZ   | 1:F:358:CYS:HB2  | 2.44                     | 0.47              |
| 1:F:485:GLN:HB3  | 1:F:488:ARG:HH21 | 1.79                     | 0.47              |
| 1:G:100:ALA:HA   | 1:G:103:LEU:HD13 | 1.95                     | 0.47              |
| 1:I:114:ILE:HA   | 1:I:117:TRP:CE3  | 2.49                     | 0.47              |
| 1:J:40:LEU:HB2   | 1:J:48:LEU:CD2   | 2.37                     | 0.47              |
| 1:J:117:TRP:O    | 1:J:120:ALA:HB3  | 2.14                     | 0.47              |
| 1:K:24:ASP:O     | 1:K:27:LYS:HG2   | 2.14                     | 0.47              |
| 1:L:133:VAL:HG12 | 1:L:395:TYR:CE2  | 2.49                     | 0.47              |
| 1:L:222:ALA:HA   | 1:L:275:ASN:CB   | 2.44                     | 0.47              |
| 1:M:35:MET:N     | 1:M:35:MET:SD    | 2.86                     | 0.47              |
| 1:N:187:HIS:O    | 1:N:359:THR:HG23 | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:337:GLU:OE2  | 1:O:339:VAL:HG22 | 2.14                     | 0.47              |
| 1:P:38:ILE:HG22  | 1:P:50:VAL:CB    | 2.35                     | 0.47              |
| 1:P:82:VAL:HG13  | 1:P:486:VAL:HG12 | 1.96                     | 0.47              |
| 1:P:173:ALA:HA   | 1:P:176:ARG:CZ   | 2.43                     | 0.47              |
| 1:A:225:LEU:HG   | 1:A:277:PHE:CD1  | 2.49                     | 0.47              |
| 1:A:497:ALA:O    | 1:A:500:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:150:ALA:HB1  | 1:C:167:THR:OG1  | 2.14                     | 0.47              |
| 1:C:274:ILE:HG23 | 1:C:296:VAL:CG2  | 2.44                     | 0.47              |
| 1:D:32:PRO:HA    | 1:D:155:SER:HB3  | 1.96                     | 0.47              |
| 1:D:71:LEU:HD12  | 1:D:497:ALA:HB1  | 1.95                     | 0.47              |
| 1:D:163:LYS:HE3  | 1:D:376:SER:OG   | 2.13                     | 0.47              |
| 1:E:313:VAL:HG13 | 1:E:352:VAL:CB   | 2.44                     | 0.47              |
| 1:F:154:LEU:HD21 | 1:F:163:LYS:NZ   | 2.29                     | 0.47              |
| 1:F:163:LYS:HA   | 1:F:166:PHE:CE1  | 2.49                     | 0.47              |
| 1:G:124:ALA:CB   | 1:G:491:LEU:HD13 | 2.41                     | 0.47              |
| 1:G:176:ARG:NE   | 1:G:358:CYS:HB2  | 2.29                     | 0.47              |
| 1:G:324:HIS:HB2  | 1:G:329:LYS:CE   | 2.43                     | 0.47              |
| 1:H:341:ILE:HG23 | 1:H:363:ARG:CZ   | 2.44                     | 0.47              |
| 1:I:22:ILE:HD12  | 1:I:90:THR:CG2   | 2.44                     | 0.47              |
| 1:I:64:ASP:CG    | 1:I:66:PRO:HD2   | 2.39                     | 0.47              |
| 1:I:274:ILE:HG23 | 1:I:274:ILE:O    | 2.14                     | 0.47              |
| 1:I:404:MET:HE3  | 1:I:430:LEU:CD1  | 2.44                     | 0.47              |
| 1:J:128:LEU:HD23 | 1:J:394:VAL:CG1  | 2.41                     | 0.47              |
| 1:M:192:LEU:H    | 1:M:192:LEU:HD12 | 1.79                     | 0.47              |
| 1:O:191:LYS:NZ   | 1:O:346:LEU:HD13 | 2.29                     | 0.47              |
| 1:O:335:LEU:HD21 | 1:O:337:GLU:OE1  | 2.13                     | 0.47              |
| 1:A:57:ILE:HG23  | 1:A:58:LEU:CD2   | 2.44                     | 0.47              |
| 1:C:112:THR:HG21 | 1:C:418:LYS:HD2  | 1.96                     | 0.47              |
| 1:C:261:LYS:O    | 1:C:264:GLU:HG2  | 2.14                     | 0.47              |
| 1:C:509:LYS:HA   | 1:C:509:LYS:CE   | 2.44                     | 0.47              |
| 1:E:108:ILE:HD13 | 1:J:446:ALA:HA   | 1.95                     | 0.47              |
| 1:E:159:LEU:HD13 | 1:E:159:LEU:H    | 1.79                     | 0.47              |
| 1:E:175:LEU:O    | 1:E:178:LYS:HG2  | 2.14                     | 0.47              |
| 1:H:27:LYS:HG3   | 1:H:436:ILE:CD1  | 2.43                     | 0.47              |
| 1:H:189:ILE:HG22 | 1:H:190:LYS:N    | 2.29                     | 0.47              |
| 1:H:196:LEU:C    | 1:H:196:LEU:HD13 | 2.40                     | 0.47              |
| 1:K:58:LEU:HB3   | 1:K:72:VAL:HG11  | 1.95                     | 0.47              |
| 1:L:182:ASN:CG   | 1:L:183:LEU:H    | 2.22                     | 0.47              |
| 1:L:310:LEU:O    | 1:L:314:THR:HG22 | 2.13                     | 0.47              |
| 1:L:334:LYS:HD2  | 1:L:351:GLY:HA3  | 1.96                     | 0.47              |
| 1:L:364:GLY:HA3  | 1:L:370:LEU:CD1  | 2.28                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:61:ILE:HG13  | 1:N:62:GLY:N     | 2.30                     | 0.47              |
| 1:N:177:LEU:C    | 1:N:177:LEU:HD13 | 2.39                     | 0.47              |
| 1:P:146:LEU:CD1  | 1:P:171:VAL:HG13 | 2.37                     | 0.47              |
| 1:P:341:ILE:HG23 | 1:P:363:ARG:NH2  | 2.30                     | 0.47              |
| 1:B:28:SER:O     | 1:B:34:GLY:HA2   | 2.14                     | 0.47              |
| 1:B:108:ILE:HG13 | 1:I:444:ASP:CG   | 2.39                     | 0.47              |
| 1:B:177:LEU:HD13 | 1:B:177:LEU:C    | 2.39                     | 0.47              |
| 1:B:433:LEU:HA   | 1:B:436:ILE:HG22 | 1.95                     | 0.47              |
| 1:D:51:THR:HG21  | 1:D:56:THR:HB    | 1.95                     | 0.47              |
| 1:D:146:LEU:HD23 | 1:D:148:ASN:H    | 1.80                     | 0.47              |
| 1:D:166:PHE:CZ   | 1:D:198:ASP:HB3  | 2.49                     | 0.47              |
| 1:D:250:LYS:O    | 1:D:253:GLU:HG2  | 2.13                     | 0.47              |
| 1:E:324:HIS:HB2  | 1:E:329:LYS:NZ   | 2.30                     | 0.47              |
| 1:F:51:THR:HG21  | 1:F:56:THR:HB    | 1.96                     | 0.47              |
| 1:F:247:SER:C    | 1:F:249:ALA:H    | 2.22                     | 0.47              |
| 1:G:81:GLU:HB3   | 1:G:485:GLN:HG3  | 1.95                     | 0.47              |
| 1:G:274:ILE:HG23 | 1:G:296:VAL:CG2  | 2.44                     | 0.47              |
| 1:H:24:ASP:O     | 1:H:27:LYS:HB3   | 2.15                     | 0.47              |
| 1:I:434:PRO:HB3  | 1:I:452:LEU:HD23 | 1.96                     | 0.47              |
| 1:J:38:ILE:HD12  | 1:J:38:ILE:N     | 2.24                     | 0.47              |
| 1:J:40:LEU:HD13  | 1:J:41:SER:N     | 2.29                     | 0.47              |
| 1:J:233:THR:O    | 1:J:234:ASP:HB3  | 2.14                     | 0.47              |
| 1:K:207:LEU:HD13 | 1:K:208:ASP:N    | 2.29                     | 0.47              |
| 1:L:67:ALA:HB2   | 1:L:507:ILE:HB   | 1.96                     | 0.47              |
| 1:L:188:VAL:HG12 | 1:L:377:LEU:HD22 | 1.94                     | 0.47              |
| 1:L:488:ARG:HG3  | 1:L:489:GLN:OE1  | 2.14                     | 0.47              |
| 1:M:263:LYS:O    | 1:M:267:GLU:HG2  | 2.14                     | 0.47              |
| 1:M:411:LEU:HD13 | 1:M:423:MET:HE2  | 1.96                     | 0.47              |
| 1:N:269:ILE:CG2  | 1:N:274:ILE:HG21 | 2.41                     | 0.47              |
| 1:N:452:LEU:HD13 | 1:N:465:LEU:CD1  | 2.44                     | 0.47              |
| 1:O:324:HIS:HB2  | 1:O:329:LYS:HE2  | 1.95                     | 0.47              |
| 1:P:402:MET:SD   | 1:P:453:ARG:HA   | 2.55                     | 0.47              |
| 1:A:274:ILE:HG23 | 1:A:296:VAL:HG21 | 1.96                     | 0.47              |
| 1:B:248:THR:O    | 1:B:251:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:64:ASP:CG    | 1:C:66:PRO:HD2   | 2.39                     | 0.47              |
| 1:C:92:LEU:O     | 1:C:95:GLU:HG2   | 2.14                     | 0.47              |
| 1:D:369:ILE:HG23 | 1:D:372:GLU:OE1  | 2.15                     | 0.47              |
| 1:D:402:MET:CE   | 1:D:453:ARG:HG2  | 2.40                     | 0.47              |
| 1:D:500:VAL:HG12 | 1:H:369:ILE:HD11 | 1.97                     | 0.47              |
| 1:E:32:PRO:HD2   | 1:E:467:MET:CE   | 2.44                     | 0.47              |
| 1:E:52:ASN:CB    | 1:E:157:LYS:HG2  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:64:ASP:CG    | 1:E:66:PRO:HD2   | 2.40                     | 0.47              |
| 1:E:146:LEU:CD2  | 1:E:147:MET:H    | 2.25                     | 0.47              |
| 1:E:365:ALA:O    | 1:E:366:THR:HG23 | 2.15                     | 0.47              |
| 1:F:159:LEU:HB3  | 1:F:372:GLU:CD   | 2.39                     | 0.47              |
| 1:F:334:LYS:HD3  | 1:F:335:LEU:N    | 2.30                     | 0.47              |
| 1:F:381:LEU:HD22 | 1:F:381:LEU:C    | 2.40                     | 0.47              |
| 1:G:59:LYS:HZ1   | 1:G:75:SER:HB3   | 1.79                     | 0.47              |
| 1:H:159:LEU:HD23 | 1:H:163:LYS:HD3  | 1.97                     | 0.47              |
| 1:K:114:ILE:HA   | 1:K:117:TRP:CZ3  | 2.49                     | 0.47              |
| 1:K:175:LEU:O    | 1:K:178:LYS:HG2  | 2.15                     | 0.47              |
| 1:K:192:LEU:CG   | 1:K:366:THR:HG21 | 2.36                     | 0.47              |
| 1:K:343:GLU:HG3  | 1:K:344:ASP:HB2  | 1.95                     | 0.47              |
| 1:L:210:LYS:HE2  | 1:L:212:GLY:O    | 2.15                     | 0.47              |
| 1:L:277:PHE:O    | 1:L:298:ALA:HA   | 2.15                     | 0.47              |
| 1:L:506:ASN:CB   | 1:P:38:ILE:HG12  | 2.45                     | 0.47              |
| 1:L:509:LYS:HG3  | 1:L:510:ALA:N    | 2.29                     | 0.47              |
| 1:M:226:ILE:HG12 | 1:M:278:ILE:CG2  | 2.42                     | 0.47              |
| 1:N:82:VAL:HA    | 1:N:386:GLN:CD   | 2.39                     | 0.47              |
| 1:O:210:LYS:HE2  | 1:O:212:GLY:O    | 2.14                     | 0.47              |
| 1:A:51:THR:HA    | 1:A:375:ARG:HD2  | 1.96                     | 0.47              |
| 1:A:499:GLU:O    | 1:A:502:LEU:HB3  | 2.15                     | 0.47              |
| 1:A:508:ILE:O    | 1:A:509:LYS:CG   | 2.62                     | 0.47              |
| 1:B:89:VAL:CG1   | 1:B:490:VAL:HB   | 2.42                     | 0.47              |
| 1:C:385:ALA:O    | 1:C:388:VAL:HG12 | 2.15                     | 0.47              |
| 1:E:37:LYS:HZ2   | 1:G:507:ILE:HG22 | 1.80                     | 0.47              |
| 1:E:133:VAL:HG23 | 1:E:134:ASP:OD1  | 2.14                     | 0.47              |
| 1:E:146:LEU:HD21 | 1:E:167:THR:CG2  | 2.38                     | 0.47              |
| 1:F:201:LEU:HD22 | 1:F:202:ASP:N    | 2.29                     | 0.47              |
| 1:F:434:PRO:HB3  | 1:F:452:LEU:CD2  | 2.45                     | 0.47              |
| 1:G:52:ASN:H     | 1:G:375:ARG:HH11 | 1.62                     | 0.47              |
| 1:H:448:LEU:HD11 | 1:H:465:LEU:CD1  | 2.44                     | 0.47              |
| 1:I:154:LEU:O    | 1:I:157:LYS:HB2  | 2.15                     | 0.47              |
| 1:J:82:VAL:HG11  | 1:J:483:SER:HB2  | 1.97                     | 0.47              |
| 1:J:379:ASP:O    | 1:J:383:VAL:HG23 | 2.14                     | 0.47              |
| 1:K:13:LEU:HD11  | 1:K:513:ARG:HB3  | 1.95                     | 0.47              |
| 1:K:31:GLY:C     | 1:K:156:SER:HA   | 2.39                     | 0.47              |
| 1:K:198:ASP:O    | 1:K:363:ARG:HB2  | 2.14                     | 0.47              |
| 1:L:74:MET:HE3   | 1:L:493:SER:OG   | 2.15                     | 0.47              |
| 1:L:209:LYS:NZ   | 1:L:303:ASP:H    | 2.11                     | 0.47              |
| 1:M:111:GLN:HA   | 1:M:114:ILE:HG12 | 1.97                     | 0.47              |
| 1:M:509:LYS:O    | 1:M:509:LYS:CG   | 2.63                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:27:LYS:HD3   | 1:N:27:LYS:C     | 2.37                     | 0.47              |
| 1:N:280:ARG:HG3  | 1:N:304:PHE:CA   | 2.45                     | 0.47              |
| 1:N:504:VAL:HG12 | 1:N:506:ASN:H    | 1.80                     | 0.47              |
| 1:O:96:LEU:O     | 1:O:96:LEU:HD22  | 2.15                     | 0.47              |
| 1:P:242:ARG:C    | 1:P:243:VAL:HG23 | 2.39                     | 0.47              |
| 1:P:433:LEU:HB2  | 1:P:434:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:71:LEU:O     | 1:A:74:MET:HB3   | 2.14                     | 0.47              |
| 1:B:40:LEU:HD13  | 1:B:40:LEU:C     | 2.40                     | 0.47              |
| 1:B:128:LEU:HD13 | 1:B:488:ARG:HG2  | 1.94                     | 0.47              |
| 1:B:154:LEU:HD22 | 1:B:167:THR:CB   | 2.43                     | 0.47              |
| 1:B:159:LEU:CD2  | 1:B:163:LYS:HG2  | 2.41                     | 0.47              |
| 1:C:57:ILE:HG23  | 1:C:58:LEU:HD22  | 1.96                     | 0.47              |
| 1:C:78:GLN:HE22  | 1:C:489:GLN:HB2  | 1.80                     | 0.47              |
| 1:C:150:ALA:O    | 1:C:154:LEU:HD13 | 2.15                     | 0.47              |
| 1:C:265:LYS:NZ   | 1:C:287:PRO:HG3  | 2.29                     | 0.47              |
| 1:C:402:MET:HE1  | 1:C:406:HIS:HB2  | 1.97                     | 0.47              |
| 1:C:412:ALA:HA   | 1:C:423:MET:HG2  | 1.96                     | 0.47              |
| 1:C:497:ALA:CA   | 1:C:500:VAL:HB   | 2.44                     | 0.47              |
| 1:D:32:PRO:HD2   | 1:D:467:MET:CE   | 2.45                     | 0.47              |
| 1:D:159:LEU:H    | 1:D:159:LEU:CD2  | 2.27                     | 0.47              |
| 1:D:226:ILE:HA   | 1:D:278:ILE:O    | 2.14                     | 0.47              |
| 1:D:316:GLY:O    | 1:D:317:GLU:HG2  | 2.15                     | 0.47              |
| 1:D:433:LEU:HB2  | 1:D:434:PRO:HD3  | 1.96                     | 0.47              |
| 1:E:81:GLU:O     | 1:E:82:VAL:HB    | 2.15                     | 0.47              |
| 1:E:124:ALA:O    | 1:E:128:LEU:HG   | 2.14                     | 0.47              |
| 1:E:485:GLN:HB2  | 1:E:489:GLN:HE22 | 1.79                     | 0.47              |
| 1:F:93:ALA:O     | 1:F:96:LEU:HD12  | 2.14                     | 0.47              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:CD2  | 2.44                     | 0.47              |
| 1:F:451:GLN:HE22 | 1:F:471:THR:HA   | 1.77                     | 0.47              |
| 1:G:117:TRP:HD1  | 1:G:495:ALA:HB1  | 1.80                     | 0.47              |
| 1:G:140:VAL:HG22 | 1:G:178:LYS:NZ   | 2.29                     | 0.47              |
| 1:G:206:LEU:HD23 | 1:G:348:HIS:CD2  | 2.49                     | 0.47              |
| 1:H:146:LEU:HD23 | 1:H:147:MET:H    | 1.79                     | 0.47              |
| 1:H:485:GLN:HE21 | 1:H:488:ARG:HH21 | 1.63                     | 0.47              |
| 1:I:59:LYS:HE2   | 1:I:76:ARG:CB    | 2.42                     | 0.47              |
| 1:I:225:LEU:HG   | 1:I:277:PHE:CD1  | 2.49                     | 0.47              |
| 1:I:263:LYS:O    | 1:I:266:VAL:HG12 | 2.15                     | 0.47              |
| 1:J:146:LEU:HB2  | 1:J:171:VAL:CG2  | 2.45                     | 0.47              |
| 1:J:263:LYS:O    | 1:J:266:VAL:HG12 | 2.15                     | 0.47              |
| 1:K:2:GLY:O      | 1:K:3:ALA:HB3    | 2.13                     | 0.47              |
| 1:K:146:LEU:HD12 | 1:K:171:VAL:CG2  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:231:MET:HG2  | 1:K:279:ASN:HD22 | 1.80                     | 0.47              |
| 1:L:146:LEU:HB2  | 1:L:171:VAL:HG21 | 1.96                     | 0.47              |
| 1:L:261:LYS:O    | 1:L:264:GLU:HG2  | 2.15                     | 0.47              |
| 1:L:433:LEU:O    | 1:L:436:ILE:HG22 | 2.14                     | 0.47              |
| 1:L:433:LEU:HB2  | 1:L:434:PRO:HD3  | 1.97                     | 0.47              |
| 1:L:508:ILE:HG23 | 1:L:509:LYS:N    | 2.29                     | 0.47              |
| 1:M:124:ALA:HA   | 1:M:491:LEU:HD13 | 1.97                     | 0.47              |
| 1:M:222:ALA:HA   | 1:M:275:ASN:OD1  | 2.15                     | 0.47              |
| 1:M:268:ARG:O    | 1:M:271:LYS:HG2  | 2.14                     | 0.47              |
| 1:M:324:HIS:O    | 1:M:328:VAL:HG23 | 2.15                     | 0.47              |
| 1:M:405:ALA:HA   | 1:M:408:VAL:HG22 | 1.96                     | 0.47              |
| 1:N:141:LYS:HE2  | 1:N:144:GLN:HB2  | 1.97                     | 0.47              |
| 1:O:143:ARG:HA   | 1:O:143:ARG:HE   | 1.79                     | 0.47              |
| 1:O:160:THR:HA   | 1:O:163:LYS:HB3  | 1.96                     | 0.47              |
| 1:O:397:GLY:HA3  | 1:O:475:MET:CE   | 2.45                     | 0.47              |
| 1:B:510:ALA:HB3  | 1:G:25:LEU:HD11  | 1.95                     | 0.47              |
| 1:C:124:ALA:CA   | 1:C:491:LEU:HD13 | 2.41                     | 0.47              |
| 1:D:78:GLN:NE2   | 1:D:486:VAL:HA   | 2.29                     | 0.47              |
| 1:D:107:LYS:O    | 1:D:108:ILE:HB   | 2.15                     | 0.47              |
| 1:D:452:LEU:HA   | 1:D:472:ILE:HG21 | 1.95                     | 0.47              |
| 1:E:159:LEU:HG   | 1:E:163:LYS:HD2  | 1.96                     | 0.47              |
| 1:E:261:LYS:O    | 1:E:264:GLU:HG2  | 2.15                     | 0.47              |
| 1:F:173:ALA:O    | 1:F:176:ARG:HG2  | 2.14                     | 0.47              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:HG   | 1.95                     | 0.47              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:HD11 | 1.96                     | 0.47              |
| 1:G:92:LEU:HD11  | 1:G:433:LEU:HD21 | 1.97                     | 0.47              |
| 1:G:146:LEU:HD11 | 1:G:150:ALA:HB3  | 1.97                     | 0.47              |
| 1:G:206:LEU:HD21 | 1:G:346:LEU:HB3  | 1.96                     | 0.47              |
| 1:H:174:VAL:HG12 | 1:H:381:LEU:HD22 | 1.96                     | 0.47              |
| 1:I:287:PRO:O    | 1:I:291:PHE:HD2  | 1.97                     | 0.47              |
| 1:J:111:GLN:O    | 1:J:114:ILE:HB   | 2.15                     | 0.47              |
| 1:J:421:VAL:O    | 1:J:424:GLU:HG2  | 2.15                     | 0.47              |
| 1:L:32:PRO:CA    | 1:L:156:SER:HA   | 2.45                     | 0.47              |
| 1:N:116:GLY:O    | 1:N:119:GLU:HB2  | 2.15                     | 0.47              |
| 1:N:136:GLY:HA2  | 1:N:391:SER:O    | 2.15                     | 0.47              |
| 1:N:448:LEU:HD11 | 1:N:465:LEU:HD11 | 1.96                     | 0.47              |
| 1:O:196:LEU:C    | 1:O:196:LEU:HD13 | 2.39                     | 0.47              |
| 1:O:334:LYS:CG   | 1:O:351:GLY:HA3  | 2.45                     | 0.47              |
| 1:P:483:SER:HB2  | 1:P:486:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:64:ASP:CG    | 1:A:66:PRO:HD2   | 2.40                     | 0.47              |
| 1:A:399:CYS:HA   | 1:A:456:HIS:NE2  | 2.29                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:312:LEU:HD13 | 1:B:354:LEU:CD2  | 2.45                     | 0.47              |
| 1:D:207:LEU:HD13 | 1:D:208:ASP:N    | 2.29                     | 0.47              |
| 1:D:509:LYS:HE2  | 1:H:63:VAL:HG21  | 1.97                     | 0.47              |
| 1:E:503:ARG:O    | 1:E:504:VAL:CB   | 2.63                     | 0.47              |
| 1:G:175:LEU:O    | 1:G:178:LYS:HD2  | 2.15                     | 0.47              |
| 1:G:215:GLN:HE21 | 1:G:292:GLY:N    | 2.13                     | 0.47              |
| 1:H:287:PRO:O    | 1:H:291:PHE:HD1  | 1.98                     | 0.47              |
| 1:I:57:ILE:HG23  | 1:I:58:LEU:HD22  | 1.97                     | 0.47              |
| 1:I:211:ILE:HB   | 1:I:215:GLN:OE1  | 2.14                     | 0.47              |
| 1:I:322:PHE:HA   | 1:I:324:HIS:CD2  | 2.48                     | 0.47              |
| 1:J:31:GLY:O     | 1:J:156:SER:HA   | 2.15                     | 0.47              |
| 1:J:110:PRO:HA   | 1:J:113:ILE:HD12 | 1.97                     | 0.47              |
| 1:K:399:CYS:SG   | 1:K:464:GLY:CA   | 3.01                     | 0.47              |
| 1:L:57:ILE:C     | 1:L:57:ILE:HD13  | 2.40                     | 0.47              |
| 1:N:326:GLU:CG   | 1:N:327:LEU:H    | 2.26                     | 0.47              |
| 1:A:450:ALA:HB2  | 1:M:108:ILE:HD13 | 1.96                     | 0.47              |
| 1:B:164:ASP:O    | 1:B:167:THR:HG22 | 2.15                     | 0.47              |
| 1:B:283:ILE:CG2  | 1:B:300:GLU:HG3  | 2.40                     | 0.47              |
| 1:C:201:LEU:HD23 | 1:C:360:ILE:HG12 | 1.95                     | 0.47              |
| 1:C:438:ALA:CB   | 1:C:448:LEU:HG   | 2.44                     | 0.47              |
| 1:D:57:ILE:HG23  | 1:D:58:LEU:HD22  | 1.96                     | 0.47              |
| 1:I:57:ILE:HG23  | 1:I:58:LEU:CD2   | 2.45                     | 0.47              |
| 1:I:117:TRP:O    | 1:I:120:ALA:HB3  | 2.15                     | 0.47              |
| 1:J:75:SER:O     | 1:J:78:GLN:HB3   | 2.15                     | 0.47              |
| 1:J:146:LEU:HD13 | 1:J:167:THR:O    | 2.13                     | 0.47              |
| 1:K:15:SER:HB3   | 1:K:501:ILE:CG2  | 2.45                     | 0.47              |
| 1:K:57:ILE:HD13  | 1:K:57:ILE:C     | 2.40                     | 0.47              |
| 1:K:89:VAL:HG12  | 1:K:490:VAL:CG2  | 2.45                     | 0.47              |
| 1:K:448:LEU:HD22 | 1:K:451:GLN:HE21 | 1.79                     | 0.47              |
| 1:L:280:ARG:O    | 1:L:281:GLN:HB3  | 2.15                     | 0.47              |
| 1:L:352:VAL:HG23 | 1:L:355:GLY:H    | 1.78                     | 0.47              |
| 1:M:163:LYS:HA   | 1:M:166:PHE:HD1  | 1.80                     | 0.47              |
| 1:N:82:VAL:HB    | 1:N:485:GLN:CB   | 2.44                     | 0.47              |
| 1:N:276:CYS:HA   | 1:N:297:MET:O    | 2.15                     | 0.47              |
| 1:O:127:ALA:HB3  | 1:O:491:LEU:CD1  | 2.45                     | 0.47              |
| 1:P:32:PRO:HD2   | 1:P:467:MET:CE   | 2.45                     | 0.47              |
| 1:P:57:ILE:HD13  | 1:P:57:ILE:C     | 2.39                     | 0.47              |
| 1:P:154:LEU:HD22 | 1:P:167:THR:HB   | 1.96                     | 0.47              |
| 1:P:186:ILE:HG21 | 1:P:381:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:265:LYS:HZ2  | 1:A:287:PRO:HG3  | 1.79                     | 0.46              |
| 1:A:448:LEU:C    | 1:A:448:LEU:HD13 | 2.40                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:226:ILE:HG12 | 1:B:278:ILE:CG2  | 2.45                     | 0.46              |
| 1:C:231:MET:CG   | 1:C:283:ILE:HG13 | 2.45                     | 0.46              |
| 1:D:509:LYS:N    | 1:H:39:LEU:HD22  | 2.31                     | 0.46              |
| 1:K:31:GLY:O     | 1:K:156:SER:HA   | 2.15                     | 0.46              |
| 1:K:174:VAL:HG11 | 1:K:384:LEU:HB2  | 1.97                     | 0.46              |
| 1:K:369:ILE:O    | 1:K:372:GLU:HB3  | 2.13                     | 0.46              |
| 1:L:469:GLU:OE1  | 1:L:469:GLU:HA   | 2.14                     | 0.46              |
| 1:M:63:VAL:HG11  | 1:O:2:GLY:CA     | 2.33                     | 0.46              |
| 1:O:103:LEU:HD21 | 1:O:113:ILE:HG21 | 1.96                     | 0.46              |
| 1:P:134:ASP:O    | 1:P:135:HIS:CB   | 2.62                     | 0.46              |
| 1:A:166:PHE:CZ   | 1:A:198:ASP:HB3  | 2.50                     | 0.46              |
| 1:A:222:ALA:HA   | 1:A:275:ASN:HB2  | 1.96                     | 0.46              |
| 1:A:234:ASP:CG   | 1:A:235:LYS:H    | 2.23                     | 0.46              |
| 1:B:92:LEU:HD11  | 1:B:433:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:233:THR:HG21 | 1:C:261:LYS:HE2  | 1.97                     | 0.46              |
| 1:C:334:LYS:HB3  | 1:C:351:GLY:HA3  | 1.97                     | 0.46              |
| 1:E:38:ILE:O     | 1:E:38:ILE:HG13  | 2.15                     | 0.46              |
| 1:E:107:LYS:HG2  | 1:E:107:LYS:O    | 2.15                     | 0.46              |
| 1:E:233:THR:O    | 1:E:234:ASP:HB3  | 2.15                     | 0.46              |
| 1:F:82:VAL:HG23  | 1:F:485:GLN:OE1  | 2.16                     | 0.46              |
| 1:F:216:PRO:HG2  | 1:F:295:GLY:CA   | 2.44                     | 0.46              |
| 1:F:222:ALA:HA   | 1:F:275:ASN:HB2  | 1.97                     | 0.46              |
| 1:G:19:ALA:HB1   | 1:G:94:ALA:CB    | 2.45                     | 0.46              |
| 1:H:40:LEU:HB2   | 1:H:48:LEU:CD2   | 2.45                     | 0.46              |
| 1:H:133:VAL:HG22 | 1:H:395:TYR:CD2  | 2.50                     | 0.46              |
| 1:I:394:VAL:HG21 | 1:I:487:LYS:HG3  | 1.97                     | 0.46              |
| 1:J:402:MET:HG2  | 1:J:431:ARG:HH22 | 1.80                     | 0.46              |
| 1:K:174:VAL:HG21 | 1:K:384:LEU:HB3  | 1.96                     | 0.46              |
| 1:N:159:LEU:HB3  | 1:N:369:ILE:HG22 | 1.97                     | 0.46              |
| 1:N:341:ILE:HG23 | 1:N:363:ARG:HH21 | 1.79                     | 0.46              |
| 1:O:431:ARG:HH21 | 1:O:434:PRO:HG3  | 1.80                     | 0.46              |
| 1:P:65:ASN:ND2   | 1:P:66:PRO:HD3   | 2.30                     | 0.46              |
| 1:P:283:ILE:HG22 | 1:P:300:GLU:CG   | 2.38                     | 0.46              |
| 1:P:343:GLU:HG3  | 1:P:344:ASP:H    | 1.80                     | 0.46              |
| 1:A:27:LYS:CA    | 1:A:436:ILE:HD11 | 2.37                     | 0.46              |
| 1:A:401:GLU:HG2  | 1:A:433:LEU:HD22 | 1.96                     | 0.46              |
| 1:B:146:LEU:O    | 1:B:147:MET:HB2  | 2.15                     | 0.46              |
| 1:C:146:LEU:HD22 | 1:C:168:LYS:CA   | 2.40                     | 0.46              |
| 1:C:324:HIS:O    | 1:C:329:LYS:HB2  | 2.15                     | 0.46              |
| 1:D:57:ILE:C     | 1:D:57:ILE:HD13  | 2.41                     | 0.46              |
| 1:D:116:GLY:O    | 1:D:119:GLU:HB2  | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:100:ALA:HA   | 1:E:103:LEU:HD22 | 1.96                     | 0.46              |
| 1:E:431:ARG:O    | 1:E:434:PRO:HD2  | 2.16                     | 0.46              |
| 1:F:187:HIS:O    | 1:F:359:THR:HG23 | 2.15                     | 0.46              |
| 1:F:204:GLY:HA3  | 1:F:350:SER:HA   | 1.96                     | 0.46              |
| 1:H:313:VAL:HG13 | 1:H:352:VAL:CG2  | 2.44                     | 0.46              |
| 1:I:38:ILE:HG21  | 1:N:506:ASN:HD22 | 1.81                     | 0.46              |
| 1:K:4:ASP:HB3    | 1:K:508:ILE:HG23 | 1.98                     | 0.46              |
| 1:K:15:SER:HB3   | 1:K:501:ILE:HG22 | 1.96                     | 0.46              |
| 1:L:159:LEU:HD12 | 1:L:159:LEU:H    | 1.80                     | 0.46              |
| 1:M:146:LEU:HD22 | 1:M:147:MET:H    | 1.80                     | 0.46              |
| 1:O:177:LEU:HD13 | 1:O:177:LEU:C    | 2.40                     | 0.46              |
| 1:P:57:ILE:HG23  | 1:P:58:LEU:CD2   | 2.45                     | 0.46              |
| 1:P:58:LEU:HB3   | 1:P:72:VAL:HG11  | 1.97                     | 0.46              |
| 1:P:146:LEU:HD21 | 1:P:150:ALA:HB3  | 1.97                     | 0.46              |
| 1:A:176:ARG:HH22 | 1:A:360:ILE:CG1  | 2.29                     | 0.46              |
| 1:A:372:GLU:O    | 1:A:375:ARG:HB3  | 2.16                     | 0.46              |
| 1:B:15:SER:HB3   | 1:B:501:ILE:HG21 | 1.97                     | 0.46              |
| 1:B:27:LYS:HB2   | 1:B:436:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:322:PHE:HA   | 1:B:324:HIS:CD2  | 2.51                     | 0.46              |
| 1:C:216:PRO:HG2  | 1:C:295:GLY:CA   | 2.45                     | 0.46              |
| 1:D:39:LEU:HD21  | 1:E:511:ALA:CB   | 2.46                     | 0.46              |
| 1:D:246:ASP:O    | 1:D:247:SER:CB   | 2.64                     | 0.46              |
| 1:D:274:ILE:HG23 | 1:D:274:ILE:O    | 2.15                     | 0.46              |
| 1:D:390:ASP:CB   | 1:D:485:GLN:HE22 | 2.29                     | 0.46              |
| 1:F:15:SER:CB    | 1:F:501:ILE:HG23 | 2.44                     | 0.46              |
| 1:F:171:VAL:HA   | 1:F:174:VAL:HG22 | 1.96                     | 0.46              |
| 1:I:13:LEU:O     | 1:I:16:PHE:HB3   | 2.15                     | 0.46              |
| 1:L:141:LYS:O    | 1:L:145:ASP:HB2  | 2.15                     | 0.46              |
| 1:O:364:GLY:HA3  | 1:O:370:LEU:HD13 | 1.98                     | 0.46              |
| 1:A:215:GLN:HG3  | 1:A:292:GLY:HA2  | 1.97                     | 0.46              |
| 1:A:402:MET:HG2  | 1:A:431:ARG:HH22 | 1.81                     | 0.46              |
| 1:C:190:LYS:O    | 1:C:190:LYS:HD2  | 2.14                     | 0.46              |
| 1:C:231:MET:HB2  | 1:C:284:TYR:H    | 1.81                     | 0.46              |
| 1:C:283:ILE:CG2  | 1:C:300:GLU:HG3  | 2.41                     | 0.46              |
| 1:D:25:LEU:HD22  | 1:D:25:LEU:N     | 2.31                     | 0.46              |
| 1:D:154:LEU:HD21 | 1:D:163:LYS:NZ   | 2.31                     | 0.46              |
| 1:E:283:ILE:HG22 | 1:E:300:GLU:CG   | 2.41                     | 0.46              |
| 1:F:111:GLN:HA   | 1:F:114:ILE:CD1  | 2.42                     | 0.46              |
| 1:G:222:ALA:HA   | 1:G:275:ASN:HB2  | 1.97                     | 0.46              |
| 1:H:274:ILE:O    | 1:H:274:ILE:HG23 | 2.15                     | 0.46              |
| 1:H:397:GLY:HA3  | 1:H:475:MET:CE   | 2.46                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:57:ILE:C     | 1:I:57:ILE:HD13  | 2.40                     | 0.46              |
| 1:J:268:ARG:O    | 1:J:271:LYS:HG2  | 2.15                     | 0.46              |
| 1:K:428:LYS:C    | 1:K:428:LYS:HD3  | 2.41                     | 0.46              |
| 1:L:146:LEU:HD13 | 1:L:167:THR:O    | 2.15                     | 0.46              |
| 1:M:219:ILE:HD11 | 1:M:336:ILE:HB   | 1.97                     | 0.46              |
| 1:A:52:ASN:CG    | 1:A:157:LYS:HG2  | 2.40                     | 0.46              |
| 1:B:85:GLY:HA2   | 1:B:153:THR:OG1  | 2.16                     | 0.46              |
| 1:C:367:GLN:NE2  | 1:C:369:ILE:HD12 | 2.30                     | 0.46              |
| 1:E:224:ILE:HD11 | 1:E:349:PHE:HE2  | 1.80                     | 0.46              |
| 1:G:225:LEU:HD13 | 1:G:329:LYS:CE   | 2.44                     | 0.46              |
| 1:G:405:ALA:HA   | 1:G:408:VAL:HG22 | 1.98                     | 0.46              |
| 1:H:99:GLU:HG3   | 1:H:425:SER:HB3  | 1.97                     | 0.46              |
| 1:H:274:ILE:HG23 | 1:H:296:VAL:CG2  | 2.46                     | 0.46              |
| 1:I:188:VAL:HG22 | 1:I:377:LEU:HD21 | 1.98                     | 0.46              |
| 1:J:57:ILE:C     | 1:J:57:ILE:HD13  | 2.40                     | 0.46              |
| 1:L:209:LYS:NZ   | 1:L:302:ALA:HA   | 2.30                     | 0.46              |
| 1:M:448:LEU:HA   | 1:M:451:GLN:HE21 | 1.80                     | 0.46              |
| 1:N:122:LYS:CD   | 1:N:125:ARG:HE   | 2.28                     | 0.46              |
| 1:N:367:GLN:HG2  | 1:N:369:ILE:HB   | 1.97                     | 0.46              |
| 1:O:431:ARG:NH1  | 1:O:453:ARG:HD3  | 2.30                     | 0.46              |
| 1:P:117:TRP:HB3  | 1:P:499:GLU:OE2  | 2.15                     | 0.46              |
| 1:B:297:MET:CE   | 1:B:347:ILE:HD11 | 2.46                     | 0.46              |
| 1:B:324:HIS:CG   | 1:B:325:PRO:HD3  | 2.51                     | 0.46              |
| 1:C:111:GLN:HA   | 1:C:114:ILE:CG1  | 2.46                     | 0.46              |
| 1:C:124:ALA:CB   | 1:C:491:LEU:HB3  | 2.46                     | 0.46              |
| 1:C:137:SER:O    | 1:C:388:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:367:GLN:HG2  | 1:C:369:ILE:H    | 1.80                     | 0.46              |
| 1:D:117:TRP:HD1  | 1:D:495:ALA:HB1  | 1.81                     | 0.46              |
| 1:D:177:LEU:HD13 | 1:D:177:LEU:C    | 2.41                     | 0.46              |
| 1:E:82:VAL:HG13  | 1:E:83:GLY:N     | 2.31                     | 0.46              |
| 1:E:269:ILE:CG2  | 1:E:274:ILE:HG21 | 2.41                     | 0.46              |
| 1:E:402:MET:HG2  | 1:E:431:ARG:HH22 | 1.81                     | 0.46              |
| 1:F:431:ARG:HH21 | 1:F:434:PRO:HG2  | 1.79                     | 0.46              |
| 1:G:160:THR:HG23 | 1:G:164:ASP:HB3  | 1.96                     | 0.46              |
| 1:G:208:ASP:O    | 1:G:209:LYS:HG3  | 2.16                     | 0.46              |
| 1:G:231:MET:C    | 1:G:284:TYR:HB2  | 2.40                     | 0.46              |
| 1:G:269:ILE:HG12 | 1:G:274:ILE:HG21 | 1.97                     | 0.46              |
| 1:G:418:LYS:H    | 1:N:453:ARG:NH1  | 2.14                     | 0.46              |
| 1:H:390:ASP:HB2  | 1:H:485:GLN:HE22 | 1.80                     | 0.46              |
| 1:I:27:LYS:HA    | 1:I:436:ILE:HD11 | 1.97                     | 0.46              |
| 1:I:101:GLU:O    | 1:I:104:ILE:HG12 | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:192:LEU:HD22 | 1:J:366:THR:HG21 | 1.98                     | 0.46              |
| 1:J:206:LEU:C    | 1:J:206:LEU:HD13 | 2.41                     | 0.46              |
| 1:J:402:MET:SD   | 1:J:453:ARG:HA   | 2.55                     | 0.46              |
| 1:K:74:MET:O     | 1:K:77:VAL:HG12  | 2.16                     | 0.46              |
| 1:K:226:ILE:HA   | 1:K:278:ILE:O    | 2.15                     | 0.46              |
| 1:L:143:ARG:HA   | 1:L:143:ARG:HE   | 1.81                     | 0.46              |
| 1:L:208:ASP:O    | 1:L:209:LYS:HG3  | 2.16                     | 0.46              |
| 1:M:177:LEU:O    | 1:M:177:LEU:HD13 | 2.16                     | 0.46              |
| 1:N:41:SER:OG    | 1:N:42:SER:N     | 2.47                     | 0.46              |
| 1:N:397:GLY:HA3  | 1:N:475:MET:HE3  | 1.97                     | 0.46              |
| 1:O:59:LYS:CE    | 1:O:76:ARG:HB2   | 2.45                     | 0.46              |
| 1:O:158:LEU:C    | 1:O:160:THR:H    | 2.23                     | 0.46              |
| 1:P:81:GLU:O     | 1:P:386:GLN:NE2  | 2.49                     | 0.46              |
| 1:A:37:LYS:O     | 1:A:50:VAL:HA    | 2.15                     | 0.46              |
| 1:A:176:ARG:HH22 | 1:A:360:ILE:HG13 | 1.80                     | 0.46              |
| 1:B:492:LEU:O    | 1:B:492:LEU:HD13 | 2.16                     | 0.46              |
| 1:C:57:ILE:HD13  | 1:C:57:ILE:O     | 2.15                     | 0.46              |
| 1:C:154:LEU:HD23 | 1:C:163:LYS:HG3  | 1.98                     | 0.46              |
| 1:C:485:GLN:O    | 1:C:489:GLN:HG2  | 2.16                     | 0.46              |
| 1:D:59:LYS:HZ1   | 1:D:76:ARG:N     | 2.14                     | 0.46              |
| 1:F:57:ILE:HD13  | 1:F:57:ILE:C     | 2.41                     | 0.46              |
| 1:G:162:HIS:HB3  | 1:G:198:ASP:OD2  | 2.16                     | 0.46              |
| 1:G:225:LEU:HD11 | 1:G:324:HIS:ND1  | 2.30                     | 0.46              |
| 1:H:191:LYS:HG3  | 1:H:192:LEU:N    | 2.31                     | 0.46              |
| 1:H:219:ILE:HB   | 1:H:275:ASN:HB3  | 1.96                     | 0.46              |
| 1:I:408:VAL:HA   | 1:I:411:LEU:HD12 | 1.98                     | 0.46              |
| 1:J:51:THR:HG22  | 1:J:53:ASP:O     | 2.15                     | 0.46              |
| 1:L:276:CYS:HA   | 1:L:297:MET:O    | 2.16                     | 0.46              |
| 1:M:141:LYS:HE2  | 1:M:144:GLN:HG2  | 1.97                     | 0.46              |
| 1:M:159:LEU:HG   | 1:M:163:LYS:HD2  | 1.97                     | 0.46              |
| 1:N:501:ILE:HA   | 1:N:504:VAL:HG23 | 1.97                     | 0.46              |
| 1:O:52:ASN:HB2   | 1:O:375:ARG:HH11 | 1.81                     | 0.46              |
| 1:O:274:ILE:HG23 | 1:O:274:ILE:O    | 2.15                     | 0.46              |
| 1:P:177:LEU:C    | 1:P:177:LEU:HD13 | 2.41                     | 0.46              |
| 1:P:226:ILE:HG12 | 1:P:278:ILE:CG2  | 2.46                     | 0.46              |
| 1:A:16:PHE:HA    | 1:A:97:LEU:CD2   | 2.45                     | 0.46              |
| 1:A:219:ILE:HD12 | 1:A:275:ASN:CB   | 2.46                     | 0.46              |
| 1:A:384:LEU:HD22 | 1:A:384:LEU:N    | 2.31                     | 0.46              |
| 1:D:82:VAL:CG1   | 1:D:83:GLY:N     | 2.78                     | 0.46              |
| 1:D:89:VAL:HA    | 1:D:490:VAL:HG21 | 1.98                     | 0.46              |
| 1:D:233:THR:O    | 1:D:234:ASP:HB3  | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:405:ALA:HA   | 1:J:408:VAL:HG22 | 1.97                     | 0.46              |
| 1:L:431:ARG:CZ   | 1:L:453:ARG:HD3  | 2.45                     | 0.46              |
| 1:M:478:LEU:HB3  | 1:M:480:ILE:HD12 | 1.97                     | 0.46              |
| 1:O:225:LEU:HD11 | 1:O:324:HIS:ND1  | 2.30                     | 0.46              |
| 1:P:150:ALA:O    | 1:P:154:LEU:HD13 | 2.16                     | 0.46              |
| 1:P:176:ARG:CZ   | 1:P:358:CYS:HB2  | 2.46                     | 0.46              |
| 1:P:395:TYR:HE2  | 1:P:476:SER:HG   | 1.64                     | 0.46              |
| 1:A:163:LYS:CG   | 1:A:166:PHE:HB2  | 2.46                     | 0.46              |
| 1:A:334:LYS:CD   | 1:A:351:GLY:HA3  | 2.46                     | 0.46              |
| 1:C:117:TRP:HD1  | 1:C:495:ALA:CB   | 2.29                     | 0.46              |
| 1:C:188:VAL:CG2  | 1:C:377:LEU:HD13 | 2.46                     | 0.46              |
| 1:C:226:ILE:HG12 | 1:C:278:ILE:CG2  | 2.45                     | 0.46              |
| 1:D:130:ASN:O    | 1:D:131:SER:CB   | 2.64                     | 0.46              |
| 1:D:143:ARG:HA   | 1:D:143:ARG:HE   | 1.80                     | 0.46              |
| 1:D:421:VAL:HB   | 1:K:453:ARG:HH12 | 1.81                     | 0.46              |
| 1:E:103:LEU:HG   | 1:E:113:ILE:HD13 | 1.97                     | 0.46              |
| 1:F:25:LEU:HD22  | 1:F:25:LEU:N     | 2.31                     | 0.46              |
| 1:G:82:VAL:HG11  | 1:G:483:SER:CB   | 2.45                     | 0.46              |
| 1:G:159:LEU:HB3  | 1:G:369:ILE:HG23 | 1.97                     | 0.46              |
| 1:I:188:VAL:HG21 | 1:I:377:LEU:HD11 | 1.98                     | 0.46              |
| 1:J:452:LEU:HD13 | 1:J:465:LEU:HD13 | 1.98                     | 0.46              |
| 1:K:39:LEU:HD12  | 1:K:57:ILE:HG13  | 1.98                     | 0.46              |
| 1:M:250:LYS:HE2  | 1:M:253:GLU:OE1  | 2.16                     | 0.46              |
| 1:N:176:ARG:HH12 | 1:N:201:LEU:HD21 | 1.81                     | 0.46              |
| 1:N:313:VAL:HG13 | 1:N:352:VAL:HB   | 1.97                     | 0.46              |
| 1:O:438:ALA:HB2  | 1:O:448:LEU:HG   | 1.94                     | 0.46              |
| 1:A:438:ALA:HB2  | 1:A:448:LEU:HG   | 1.96                     | 0.45              |
| 1:B:411:LEU:HB3  | 1:B:423:MET:HE3  | 1.98                     | 0.45              |
| 1:C:207:LEU:HD13 | 1:C:208:ASP:N    | 2.30                     | 0.45              |
| 1:D:111:GLN:O    | 1:D:114:ILE:HB   | 2.16                     | 0.45              |
| 1:D:141:LYS:CG   | 1:D:144:GLN:HB2  | 2.45                     | 0.45              |
| 1:D:274:ILE:O    | 1:D:296:VAL:HG22 | 2.16                     | 0.45              |
| 1:D:431:ARG:HH21 | 1:D:434:PRO:HG2  | 1.81                     | 0.45              |
| 1:E:99:GLU:CB    | 1:E:425:SER:HB2  | 2.45                     | 0.45              |
| 1:E:196:LEU:C    | 1:E:196:LEU:HD13 | 2.41                     | 0.45              |
| 1:E:311:ALA:HA   | 1:E:314:THR:CG2  | 2.46                     | 0.45              |
| 1:E:448:LEU:HD13 | 1:E:448:LEU:C    | 2.41                     | 0.45              |
| 1:F:1:ALA:H1     | 1:F:508:ILE:HD12 | 1.81                     | 0.45              |
| 1:F:159:LEU:HB3  | 1:F:372:GLU:OE2  | 2.16                     | 0.45              |
| 1:G:262:MET:HE1  | 1:G:286:TYR:O    | 2.16                     | 0.45              |
| 1:G:448:LEU:C    | 1:G:448:LEU:HD13 | 2.41                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:189:ILE:CG1  | 1:H:206:LEU:HD12 | 2.43                     | 0.45              |
| 1:J:317:GLU:HB2  | 1:J:329:LYS:HD3  | 1.98                     | 0.45              |
| 1:J:431:ARG:HA   | 1:J:431:ARG:CZ   | 2.46                     | 0.45              |
| 1:L:262:MET:SD   | 1:L:290:LEU:HB2  | 2.56                     | 0.45              |
| 1:L:396:GLY:O    | 1:L:475:MET:HG2  | 2.16                     | 0.45              |
| 1:L:431:ARG:NH1  | 1:L:453:ARG:HD3  | 2.31                     | 0.45              |
| 1:O:451:GLN:NE2  | 1:O:471:THR:HA   | 2.31                     | 0.45              |
| 1:P:287:PRO:O    | 1:P:291:PHE:HD1  | 1.98                     | 0.45              |
| 1:P:386:GLN:HG2  | 1:P:389:LYS:HG3  | 1.98                     | 0.45              |
| 1:B:431:ARG:NH2  | 1:B:434:PRO:HG2  | 2.30                     | 0.45              |
| 1:B:510:ALA:HB3  | 1:G:25:LEU:HG    | 1.97                     | 0.45              |
| 1:C:38:ILE:HG13  | 1:C:38:ILE:O     | 2.15                     | 0.45              |
| 1:C:176:ARG:NE   | 1:C:358:CYS:HB2  | 2.31                     | 0.45              |
| 1:D:154:LEU:HD21 | 1:D:167:THR:HB   | 1.98                     | 0.45              |
| 1:D:204:GLY:HA3  | 1:D:350:SER:HA   | 1.98                     | 0.45              |
| 1:D:405:ALA:HA   | 1:D:408:VAL:CG2  | 2.47                     | 0.45              |
| 1:H:511:ALA:O    | 1:H:513:ARG:N    | 2.49                     | 0.45              |
| 1:I:487:LYS:HA   | 1:I:490:VAL:HG12 | 1.98                     | 0.45              |
| 1:K:402:MET:HE2  | 1:K:402:MET:O    | 2.16                     | 0.45              |
| 1:K:402:MET:HG2  | 1:K:431:ARG:HH22 | 1.81                     | 0.45              |
| 1:L:512:PRO:O    | 1:L:513:ARG:HB3  | 2.16                     | 0.45              |
| 1:N:154:LEU:HD21 | 1:N:163:LYS:NZ   | 2.32                     | 0.45              |
| 1:O:313:VAL:HG13 | 1:O:352:VAL:CB   | 2.46                     | 0.45              |
| 1:O:402:MET:CE   | 1:O:453:ARG:HG2  | 2.41                     | 0.45              |
| 1:P:171:VAL:O    | 1:P:175:LEU:HG   | 2.15                     | 0.45              |
| 1:P:269:ILE:CG2  | 1:P:274:ILE:HG21 | 2.46                     | 0.45              |
| 1:A:28:SER:O     | 1:A:34:GLY:HA2   | 2.16                     | 0.45              |
| 1:A:107:LYS:O    | 1:A:107:LYS:HG2  | 2.17                     | 0.45              |
| 1:B:57:ILE:HG23  | 1:B:58:LEU:CD2   | 2.45                     | 0.45              |
| 1:B:319:ALA:HA   | 1:B:329:LYS:HZ1  | 1.81                     | 0.45              |
| 1:B:452:LEU:HD11 | 1:B:456:HIS:CE1  | 2.51                     | 0.45              |
| 1:C:99:GLU:O     | 1:C:103:LEU:HD13 | 2.17                     | 0.45              |
| 1:D:366:THR:O    | 1:D:367:GLN:HB3  | 2.17                     | 0.45              |
| 1:F:219:ILE:HD12 | 1:F:275:ASN:HB3  | 1.98                     | 0.45              |
| 1:F:341:ILE:HG23 | 1:F:363:ARG:NH2  | 2.30                     | 0.45              |
| 1:G:27:LYS:HB2   | 1:G:436:ILE:HD12 | 1.97                     | 0.45              |
| 1:G:232:ASP:HA   | 1:G:284:TYR:CD1  | 2.51                     | 0.45              |
| 1:H:57:ILE:HD13  | 1:H:57:ILE:O     | 2.15                     | 0.45              |
| 1:I:65:ASN:CG    | 1:I:66:PRO:HD3   | 2.41                     | 0.45              |
| 1:I:154:LEU:HD21 | 1:I:163:LYS:HG3  | 1.99                     | 0.45              |
| 1:I:485:GLN:HE22 | 1:I:488:ARG:NH2  | 2.15                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:216:PRO:HG2  | 1:J:295:GLY:CA   | 2.45                     | 0.45              |
| 1:J:277:PHE:CE2  | 1:J:279:ASN:HB2  | 2.51                     | 0.45              |
| 1:J:452:LEU:HD13 | 1:J:465:LEU:CD1  | 2.46                     | 0.45              |
| 1:K:114:ILE:HA   | 1:K:117:TRP:CE3  | 2.51                     | 0.45              |
| 1:M:39:LEU:HD12  | 1:M:57:ILE:HD11  | 1.97                     | 0.45              |
| 1:M:103:LEU:HD21 | 1:M:113:ILE:HG21 | 1.98                     | 0.45              |
| 1:N:222:ALA:HA   | 1:N:275:ASN:CG   | 2.41                     | 0.45              |
| 1:O:58:LEU:CB    | 1:O:72:VAL:HG13  | 2.44                     | 0.45              |
| 1:O:122:LYS:O    | 1:O:125:ARG:HB2  | 2.15                     | 0.45              |
| 1:P:317:GLU:CB   | 1:P:329:LYS:HD3  | 2.46                     | 0.45              |
| 1:P:365:ALA:O    | 1:P:366:THR:CB   | 2.64                     | 0.45              |
| 1:P:369:ILE:O    | 1:P:372:GLU:CB   | 2.64                     | 0.45              |
| 1:B:129:LEU:HD12 | 1:B:129:LEU:HA   | 1.73                     | 0.45              |
| 1:B:150:ALA:O    | 1:B:154:LEU:HD13 | 2.16                     | 0.45              |
| 1:B:209:LYS:HE2  | 1:B:301:HIS:O    | 2.16                     | 0.45              |
| 1:D:82:VAL:HB    | 1:D:485:GLN:HB2  | 1.97                     | 0.45              |
| 1:D:311:ALA:HA   | 1:D:314:THR:HG22 | 1.98                     | 0.45              |
| 1:F:52:ASN:HD21  | 1:F:157:LYS:HA   | 1.80                     | 0.45              |
| 1:H:417:GLY:HA3  | 1:P:450:ALA:HA   | 1.98                     | 0.45              |
| 1:I:367:GLN:OE1  | 1:I:370:LEU:HG   | 2.17                     | 0.45              |
| 1:I:367:GLN:CD   | 1:I:369:ILE:HB   | 2.41                     | 0.45              |
| 1:J:114:ILE:HA   | 1:J:117:TRP:CE3  | 2.51                     | 0.45              |
| 1:J:226:ILE:HG12 | 1:J:278:ILE:CG2  | 2.47                     | 0.45              |
| 1:K:119:GLU:HB3  | 1:K:423:MET:SD   | 2.56                     | 0.45              |
| 1:K:232:ASP:HA   | 1:K:284:TYR:CD1  | 2.52                     | 0.45              |
| 1:M:106:LYS:HD3  | 1:M:108:ILE:HG13 | 1.99                     | 0.45              |
| 1:M:485:GLN:HB3  | 1:M:489:GLN:HE22 | 1.80                     | 0.45              |
| 1:N:79:ASP:HA    | 1:N:83:GLY:CA    | 2.46                     | 0.45              |
| 1:N:146:LEU:C    | 1:N:148:ASN:N    | 2.75                     | 0.45              |
| 1:O:4:ASP:HB3    | 1:O:509:LYS:CE   | 2.46                     | 0.45              |
| 1:O:32:PRO:O     | 1:O:155:SER:O    | 2.34                     | 0.45              |
| 1:O:41:SER:HB3   | 1:O:45:ASP:OD2   | 2.17                     | 0.45              |
| 1:P:99:GLU:O     | 1:P:103:LEU:HD13 | 2.16                     | 0.45              |
| 1:A:107:LYS:O    | 1:A:108:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:159:LEU:N    | 1:A:159:LEU:CD2  | 2.80                     | 0.45              |
| 1:A:277:PHE:CE2  | 1:A:279:ASN:HB2  | 2.51                     | 0.45              |
| 1:B:27:LYS:HB2   | 1:B:436:ILE:CD1  | 2.47                     | 0.45              |
| 1:B:371:ASP:O    | 1:B:374:GLU:HB3  | 2.16                     | 0.45              |
| 1:B:396:GLY:HA3  | 1:B:480:ILE:HG22 | 1.97                     | 0.45              |
| 1:B:492:LEU:HD13 | 1:B:492:LEU:C    | 2.42                     | 0.45              |
| 1:C:286:TYR:HB2  | 1:C:287:PRO:HD3  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:334:LYS:CB   | 1:E:351:GLY:HA3  | 2.47                     | 0.45              |
| 1:E:433:LEU:HB2  | 1:E:434:PRO:HD3  | 1.98                     | 0.45              |
| 1:F:207:LEU:O    | 1:F:208:ASP:CB   | 2.65                     | 0.45              |
| 1:G:226:ILE:HG12 | 1:G:278:ILE:CG2  | 2.47                     | 0.45              |
| 1:G:507:ILE:HB   | 1:G:508:ILE:H    | 1.59                     | 0.45              |
| 1:H:203:GLU:HG2  | 1:H:350:SER:OG   | 2.15                     | 0.45              |
| 1:H:259:LYS:O    | 1:H:262:MET:HB3  | 2.16                     | 0.45              |
| 1:H:324:HIS:HB2  | 1:H:329:LYS:HE2  | 1.98                     | 0.45              |
| 1:I:324:HIS:HB2  | 1:I:329:LYS:CE   | 2.45                     | 0.45              |
| 1:I:431:ARG:CZ   | 1:I:453:ARG:HD3  | 2.45                     | 0.45              |
| 1:J:313:VAL:HG13 | 1:J:352:VAL:CG2  | 2.47                     | 0.45              |
| 1:L:205:PHE:HA   | 1:L:359:THR:OG1  | 2.16                     | 0.45              |
| 1:L:233:THR:O    | 1:L:234:ASP:HB3  | 2.17                     | 0.45              |
| 1:L:506:ASN:ND2  | 1:P:38:ILE:HG12  | 2.31                     | 0.45              |
| 1:M:64:ASP:C     | 1:M:66:PRO:HD2   | 2.42                     | 0.45              |
| 1:M:146:LEU:O    | 1:M:147:MET:HB2  | 2.17                     | 0.45              |
| 1:M:171:VAL:O    | 1:M:175:LEU:HG   | 2.17                     | 0.45              |
| 1:M:367:GLN:CD   | 1:M:369:ILE:HD12 | 2.42                     | 0.45              |
| 1:N:219:ILE:CD1  | 1:N:275:ASN:HB3  | 2.46                     | 0.45              |
| 1:N:222:ALA:HA   | 1:N:275:ASN:OD1  | 2.16                     | 0.45              |
| 1:N:313:VAL:HG13 | 1:N:352:VAL:CG1  | 2.47                     | 0.45              |
| 1:O:309:ARG:O    | 1:O:313:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:185:ALA:HA   | 1:B:309:ARG:HG2  | 1.98                     | 0.45              |
| 1:D:204:GLY:O    | 1:D:359:THR:HB   | 2.16                     | 0.45              |
| 1:E:27:LYS:CD    | 1:E:436:ILE:HD11 | 2.47                     | 0.45              |
| 1:F:57:ILE:HD13  | 1:F:57:ILE:O     | 2.17                     | 0.45              |
| 1:G:341:ILE:O    | 1:G:343:GLU:N    | 2.46                     | 0.45              |
| 1:H:146:LEU:CD1  | 1:H:171:VAL:HG13 | 2.34                     | 0.45              |
| 1:H:380:ALA:O    | 1:H:384:LEU:HD23 | 2.17                     | 0.45              |
| 1:I:138:ASP:O    | 1:I:139:GLU:CB   | 2.64                     | 0.45              |
| 1:I:222:ALA:HA   | 1:I:275:ASN:CG   | 2.41                     | 0.45              |
| 1:J:78:GLN:HE21  | 1:J:82:VAL:HG12  | 1.82                     | 0.45              |
| 1:J:99:GLU:O     | 1:J:103:LEU:HD13 | 2.16                     | 0.45              |
| 1:L:32:PRO:HA    | 1:L:155:SER:C    | 2.41                     | 0.45              |
| 1:L:154:LEU:HD22 | 1:L:167:THR:HB   | 1.98                     | 0.45              |
| 1:N:392:ARG:HG3  | 1:N:484:PHE:CG   | 2.51                     | 0.45              |
| 1:A:451:GLN:HE22 | 1:A:471:THR:HA   | 1.81                     | 0.45              |
| 1:A:509:LYS:H    | 1:F:37:LYS:HZ1   | 1.65                     | 0.45              |
| 1:B:96:LEU:O     | 1:B:96:LEU:HD22  | 2.16                     | 0.45              |
| 1:C:19:ALA:HB1   | 1:C:94:ALA:HA    | 1.98                     | 0.45              |
| 1:C:164:ASP:O    | 1:C:167:THR:HG22 | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:277:PHE:O    | 1:C:298:ALA:HA   | 2.17                     | 0.45              |
| 1:C:320:SER:HB2  | 1:C:321:THR:H    | 1.61                     | 0.45              |
| 1:D:509:LYS:HG2  | 1:H:63:VAL:HG21  | 1.97                     | 0.45              |
| 1:E:171:VAL:O    | 1:E:175:LEU:HG   | 2.16                     | 0.45              |
| 1:E:211:ILE:HG12 | 1:E:298:ALA:H    | 1.82                     | 0.45              |
| 1:E:313:VAL:O    | 1:E:352:VAL:HG23 | 2.17                     | 0.45              |
| 1:E:313:VAL:CG1  | 1:E:352:VAL:HB   | 2.45                     | 0.45              |
| 1:F:188:VAL:CG1  | 1:F:377:LEU:HD21 | 2.47                     | 0.45              |
| 1:F:222:ALA:HA   | 1:F:275:ASN:CG   | 2.41                     | 0.45              |
| 1:G:194:GLY:HA2  | 1:G:364:GLY:O    | 2.16                     | 0.45              |
| 1:G:211:ILE:HG23 | 1:G:298:ALA:O    | 2.17                     | 0.45              |
| 1:G:363:ARG:O    | 1:G:370:LEU:HD11 | 2.16                     | 0.45              |
| 1:H:152:THR:HG21 | 1:H:480:ILE:HA   | 1.98                     | 0.45              |
| 1:I:236:ILE:HG12 | 1:I:237:LYS:H    | 1.81                     | 0.45              |
| 1:K:159:LEU:HD12 | 1:K:369:ILE:CG2  | 2.44                     | 0.45              |
| 1:L:206:LEU:HD11 | 1:L:346:LEU:HD23 | 1.99                     | 0.45              |
| 1:L:209:LYS:HZ1  | 1:L:303:ASP:H    | 1.64                     | 0.45              |
| 1:M:119:GLU:HA   | 1:M:119:GLU:OE1  | 2.16                     | 0.45              |
| 1:M:313:VAL:HG22 | 1:M:357:ALA:HB3  | 1.98                     | 0.45              |
| 1:O:4:ASP:HB3    | 1:O:509:LYS:NZ   | 2.31                     | 0.45              |
| 1:O:277:PHE:O    | 1:O:298:ALA:HA   | 2.17                     | 0.45              |
| 1:P:284:TYR:CE2  | 1:P:286:TYR:CD1  | 3.05                     | 0.45              |
| 1:A:159:LEU:HG   | 1:A:163:LYS:CD   | 2.45                     | 0.45              |
| 1:B:433:LEU:HB2  | 1:B:434:PRO:HD3  | 1.98                     | 0.45              |
| 1:C:402:MET:HE3  | 1:C:453:ARG:CG   | 2.35                     | 0.45              |
| 1:C:431:ARG:O    | 1:C:434:PRO:HD2  | 2.16                     | 0.45              |
| 1:E:146:LEU:CD1  | 1:E:171:VAL:HG13 | 2.45                     | 0.45              |
| 1:E:235:LYS:O    | 1:E:237:LYS:N    | 2.47                     | 0.45              |
| 1:F:22:ILE:HD12  | 1:F:90:THR:CG2   | 2.47                     | 0.45              |
| 1:G:215:GLN:HE21 | 1:G:292:GLY:CA   | 2.30                     | 0.45              |
| 1:G:265:LYS:HE2  | 1:G:322:PHE:CE1  | 2.51                     | 0.45              |
| 1:I:65:ASN:ND2   | 1:I:66:PRO:HD3   | 2.32                     | 0.45              |
| 1:I:76:ARG:O     | 1:I:79:ASP:HB3   | 2.16                     | 0.45              |
| 1:I:404:MET:HE3  | 1:I:430:LEU:HD11 | 1.98                     | 0.45              |
| 1:J:219:ILE:HD12 | 1:J:275:ASN:HB3  | 1.98                     | 0.45              |
| 1:L:31:GLY:O     | 1:L:156:SER:HA   | 2.17                     | 0.45              |
| 1:L:222:ALA:HA   | 1:L:275:ASN:CG   | 2.42                     | 0.45              |
| 1:M:140:VAL:HA   | 1:M:175:LEU:HD22 | 1.98                     | 0.45              |
| 1:N:64:ASP:C     | 1:N:66:PRO:HD2   | 2.41                     | 0.45              |
| 1:N:140:VAL:HA   | 1:N:175:LEU:HD13 | 1.99                     | 0.45              |
| 1:O:500:VAL:O    | 1:O:504:VAL:HG22 | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:57:ILE:C     | 1:A:57:ILE:HD13  | 2.41                     | 0.45              |
| 1:B:222:ALA:HA   | 1:B:275:ASN:HB2  | 1.99                     | 0.45              |
| 1:C:163:LYS:HD2  | 1:C:166:PHE:CG   | 2.52                     | 0.45              |
| 1:D:96:LEU:O     | 1:D:96:LEU:HD22  | 2.17                     | 0.45              |
| 1:F:79:ASP:HA    | 1:F:83:GLY:HA2   | 1.98                     | 0.45              |
| 1:F:103:LEU:O    | 1:F:106:LYS:HB3  | 2.16                     | 0.45              |
| 1:G:233:THR:O    | 1:G:234:ASP:HB3  | 2.17                     | 0.45              |
| 1:G:431:ARG:NH2  | 1:G:434:PRO:HG2  | 2.32                     | 0.45              |
| 1:I:123:ALA:O    | 1:I:126:GLN:HG2  | 2.17                     | 0.45              |
| 1:I:402:MET:HE3  | 1:I:453:ARG:CG   | 2.40                     | 0.45              |
| 1:K:171:VAL:O    | 1:K:175:LEU:HG   | 2.17                     | 0.45              |
| 1:L:75:SER:O     | 1:L:78:GLN:HB3   | 2.16                     | 0.45              |
| 1:M:448:LEU:HD13 | 1:M:448:LEU:C    | 2.41                     | 0.45              |
| 1:N:183:LEU:O    | 1:N:183:LEU:HD23 | 2.16                     | 0.45              |
| 1:N:274:ILE:HG23 | 1:N:274:ILE:O    | 2.17                     | 0.45              |
| 1:O:165:HIS:O    | 1:O:168:LYS:HB3  | 2.17                     | 0.45              |
| 1:O:268:ARG:O    | 1:O:271:LYS:HG2  | 2.17                     | 0.45              |
| 1:O:366:THR:HG23 | 1:O:367:GLN:HG3  | 1.98                     | 0.45              |
| 1:P:226:ILE:HA   | 1:P:278:ILE:O    | 2.16                     | 0.45              |
| 1:A:432:MET:O    | 1:A:435:THR:HB   | 2.17                     | 0.45              |
| 1:A:452:LEU:HD13 | 1:A:465:LEU:HD22 | 1.98                     | 0.45              |
| 1:B:211:ILE:HG13 | 1:B:298:ALA:O    | 2.17                     | 0.45              |
| 1:B:274:ILE:O    | 1:B:274:ILE:HG23 | 2.16                     | 0.45              |
| 1:B:313:VAL:CG2  | 1:B:357:ALA:HB3  | 2.45                     | 0.45              |
| 1:B:402:MET:HG3  | 1:B:452:LEU:HG   | 1.99                     | 0.45              |
| 1:C:325:PRO:O    | 1:C:326:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:343:GLU:HG3  | 1:C:344:ASP:H    | 1.81                     | 0.45              |
| 1:D:261:LYS:O    | 1:D:264:GLU:HG2  | 2.17                     | 0.45              |
| 1:D:451:GLN:NE2  | 1:D:471:THR:HA   | 2.32                     | 0.45              |
| 1:E:146:LEU:HD12 | 1:E:171:VAL:HG11 | 1.99                     | 0.45              |
| 1:E:431:ARG:NH2  | 1:E:434:PRO:HG2  | 2.32                     | 0.45              |
| 1:F:99:GLU:HG3   | 1:F:425:SER:CB   | 2.47                     | 0.45              |
| 1:F:225:LEU:HG   | 1:F:277:PHE:CD1  | 2.52                     | 0.45              |
| 1:F:225:LEU:HD13 | 1:F:329:LYS:HE2  | 1.99                     | 0.45              |
| 1:G:226:ILE:HA   | 1:G:278:ILE:O    | 2.17                     | 0.45              |
| 1:G:365:ALA:O    | 1:G:366:THR:HG22 | 2.17                     | 0.45              |
| 1:H:231:MET:HG3  | 1:H:283:ILE:HG13 | 1.99                     | 0.45              |
| 1:H:453:ARG:CZ   | 1:P:417:GLY:H    | 2.30                     | 0.45              |
| 1:I:408:VAL:HG21 | 1:I:427:ALA:HA   | 1.98                     | 0.45              |
| 1:I:433:LEU:HB2  | 1:I:434:PRO:HD3  | 1.99                     | 0.45              |
| 1:J:114:ILE:HD13 | 1:J:117:TRP:CZ3  | 2.52                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:141:LYS:HD2  | 1:J:144:GLN:HB2  | 1.98                     | 0.45              |
| 1:J:262:MET:HE1  | 1:J:286:TYR:O    | 2.17                     | 0.45              |
| 1:K:313:VAL:O    | 1:K:352:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:337:GLU:HG3  | 1:M:339:VAL:HG23 | 1.99                     | 0.45              |
| 1:N:209:LYS:HE2  | 1:N:301:HIS:O    | 2.17                     | 0.45              |
| 1:O:57:ILE:C     | 1:O:57:ILE:HD13  | 2.42                     | 0.45              |
| 1:O:222:ALA:HA   | 1:O:275:ASN:HB2  | 1.98                     | 0.45              |
| 1:O:371:ASP:O    | 1:O:374:GLU:HB3  | 2.17                     | 0.45              |
| 1:P:173:ALA:O    | 1:P:176:ARG:HG2  | 2.17                     | 0.45              |
| 1:P:186:ILE:HG21 | 1:P:381:LEU:CD1  | 2.47                     | 0.45              |
| 1:P:255:GLU:HG3  | 1:P:256:HIS:N    | 2.30                     | 0.45              |
| 1:P:268:ARG:O    | 1:P:271:LYS:HG2  | 2.17                     | 0.45              |
| 1:P:286:TYR:HB2  | 1:P:287:PRO:HD3  | 1.98                     | 0.45              |
| 1:B:381:LEU:HD13 | 1:B:381:LEU:C    | 2.42                     | 0.44              |
| 1:C:146:LEU:HD21 | 1:C:167:THR:HG23 | 1.99                     | 0.44              |
| 1:C:259:LYS:O    | 1:C:262:MET:HB3  | 2.17                     | 0.44              |
| 1:C:323:ASP:C    | 1:C:325:PRO:HD2  | 2.42                     | 0.44              |
| 1:C:487:LYS:O    | 1:C:490:VAL:HG12 | 2.17                     | 0.44              |
| 1:D:146:LEU:HD23 | 1:D:147:MET:N    | 2.32                     | 0.44              |
| 1:D:203:GLU:HG2  | 1:D:350:SER:HB2  | 1.99                     | 0.44              |
| 1:E:438:ALA:CB   | 1:E:448:LEU:HG   | 2.47                     | 0.44              |
| 1:H:257:ALA:O    | 1:H:260:GLU:HB3  | 2.16                     | 0.44              |
| 1:I:191:LYS:CE   | 1:I:346:LEU:HG   | 2.47                     | 0.44              |
| 1:I:354:LEU:HG   | 1:I:356:GLU:H    | 1.82                     | 0.44              |
| 1:K:206:LEU:HD21 | 1:K:346:LEU:HB3  | 1.98                     | 0.44              |
| 1:K:345:LYS:C    | 1:K:346:LEU:HD12 | 2.42                     | 0.44              |
| 1:K:431:ARG:HH21 | 1:K:434:PRO:HG2  | 1.81                     | 0.44              |
| 1:L:51:THR:HG21  | 1:L:56:THR:OG1   | 2.17                     | 0.44              |
| 1:L:159:LEU:CD1  | 1:L:159:LEU:H    | 2.30                     | 0.44              |
| 1:M:114:ILE:HA   | 1:M:117:TRP:HE3  | 1.82                     | 0.44              |
| 1:M:215:GLN:HG3  | 1:M:292:GLY:HA2  | 1.98                     | 0.44              |
| 1:M:402:MET:CE   | 1:M:453:ARG:HG2  | 2.35                     | 0.44              |
| 1:N:117:TRP:O    | 1:N:120:ALA:HB3  | 2.17                     | 0.44              |
| 1:P:231:MET:HE1  | 1:P:265:LYS:HD3  | 1.99                     | 0.44              |
| 1:A:201:LEU:CD2  | 1:A:360:ILE:HG12 | 2.47                     | 0.44              |
| 1:B:168:LYS:O    | 1:B:171:VAL:HG22 | 2.17                     | 0.44              |
| 1:C:171:VAL:HA   | 1:C:174:VAL:HG22 | 1.98                     | 0.44              |
| 1:D:146:LEU:HB2  | 1:D:171:VAL:HG21 | 1.98                     | 0.44              |
| 1:D:225:LEU:HD11 | 1:D:324:HIS:CE1  | 2.52                     | 0.44              |
| 1:D:280:ARG:O    | 1:D:281:GLN:HB3  | 2.17                     | 0.44              |
| 1:E:384:LEU:HD22 | 1:E:384:LEU:N    | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:415:THR:HG21 | 1:F:423:MET:SD   | 2.58                     | 0.44              |
| 1:F:485:GLN:HG3  | 1:F:489:GLN:HE22 | 1.83                     | 0.44              |
| 1:G:106:LYS:HD2  | 1:G:113:ILE:HD11 | 1.99                     | 0.44              |
| 1:G:317:GLU:OE2  | 1:G:329:LYS:HE3  | 2.17                     | 0.44              |
| 1:G:431:ARG:HH21 | 1:G:434:PRO:HG2  | 1.83                     | 0.44              |
| 1:I:168:LYS:O    | 1:I:171:VAL:HG22 | 2.17                     | 0.44              |
| 1:J:154:LEU:HD23 | 1:J:163:LYS:HB3  | 1.99                     | 0.44              |
| 1:K:188:VAL:HG21 | 1:K:362:LEU:HD12 | 2.00                     | 0.44              |
| 1:L:211:ILE:CD1  | 1:L:297:MET:HG3  | 2.40                     | 0.44              |
| 1:L:280:ARG:HG3  | 1:L:304:PHE:HB2  | 1.98                     | 0.44              |
| 1:M:113:ILE:HG23 | 1:M:422:ALA:HB1  | 1.99                     | 0.44              |
| 1:M:146:LEU:HB2  | 1:M:171:VAL:HG21 | 1.99                     | 0.44              |
| 1:N:122:LYS:HD2  | 1:N:125:ARG:HE   | 1.82                     | 0.44              |
| 1:O:261:LYS:O    | 1:O:264:GLU:HG2  | 2.17                     | 0.44              |
| 1:O:338:GLU:OE1  | 1:O:345:LYS:HE2  | 2.17                     | 0.44              |
| 1:P:75:SER:O     | 1:P:78:GLN:HB3   | 2.17                     | 0.44              |
| 1:P:96:LEU:HD22  | 1:P:96:LEU:C     | 2.42                     | 0.44              |
| 1:P:114:ILE:HA   | 1:P:117:TRP:CZ3  | 2.51                     | 0.44              |
| 1:P:129:LEU:N    | 1:P:129:LEU:CD2  | 2.80                     | 0.44              |
| 1:A:2:GLY:HA2    | 1:A:513:ARG:HH11 | 1.83                     | 0.44              |
| 1:A:39:LEU:CD1   | 1:A:57:ILE:HG13  | 2.46                     | 0.44              |
| 1:A:159:LEU:HG   | 1:A:163:LYS:HB3  | 1.99                     | 0.44              |
| 1:A:225:LEU:HD13 | 1:A:329:LYS:HE3  | 2.00                     | 0.44              |
| 1:B:261:LYS:O    | 1:B:264:GLU:HG2  | 2.16                     | 0.44              |
| 1:B:286:TYR:HB2  | 1:B:287:PRO:HD3  | 1.98                     | 0.44              |
| 1:B:356:GLU:O    | 1:B:357:ALA:HB2  | 2.17                     | 0.44              |
| 1:C:431:ARG:NH1  | 1:C:453:ARG:HD3  | 2.32                     | 0.44              |
| 1:C:452:LEU:HD11 | 1:C:456:HIS:CE1  | 2.52                     | 0.44              |
| 1:D:40:LEU:HB2   | 1:D:48:LEU:HD23  | 1.99                     | 0.44              |
| 1:D:124:ALA:O    | 1:D:128:LEU:HG   | 2.18                     | 0.44              |
| 1:D:323:ASP:C    | 1:D:325:PRO:HD2  | 2.42                     | 0.44              |
| 1:D:446:ALA:CA   | 1:K:418:LYS:HD3  | 2.46                     | 0.44              |
| 1:F:326:GLU:HB2  | 1:F:327:LEU:H    | 1.57                     | 0.44              |
| 1:G:57:ILE:HG23  | 1:G:58:LEU:HD22  | 1.99                     | 0.44              |
| 1:G:434:PRO:HB3  | 1:G:452:LEU:CD2  | 2.47                     | 0.44              |
| 1:H:280:ARG:O    | 1:H:281:GLN:HB3  | 2.17                     | 0.44              |
| 1:H:367:GLN:HG3  | 1:H:369:ILE:HB   | 1.99                     | 0.44              |
| 1:L:59:LYS:HE3   | 1:L:73:ASP:HA    | 2.00                     | 0.44              |
| 1:L:174:VAL:HG11 | 1:L:384:LEU:CB   | 2.46                     | 0.44              |
| 1:L:206:LEU:HD23 | 1:L:348:HIS:CD2  | 2.53                     | 0.44              |
| 1:M:438:ALA:O    | 1:M:441:ALA:HB3  | 2.16                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:415:THR:OG1  | 1:N:420:ALA:HA   | 2.18                     | 0.44              |
| 1:O:115:ALA:O    | 1:O:118:ARG:HB3  | 2.17                     | 0.44              |
| 1:O:402:MET:SD   | 1:O:453:ARG:HA   | 2.57                     | 0.44              |
| 1:P:100:ALA:HA   | 1:P:103:LEU:HD13 | 1.99                     | 0.44              |
| 1:P:161:HIS:CG   | 1:P:162:HIS:H    | 2.35                     | 0.44              |
| 1:A:51:THR:HG21  | 1:A:56:THR:HB    | 1.98                     | 0.44              |
| 1:A:108:ILE:HG21 | 1:M:444:ASP:CG   | 2.42                     | 0.44              |
| 1:B:196:LEU:C    | 1:B:196:LEU:HD13 | 2.42                     | 0.44              |
| 1:B:321:THR:O    | 1:B:323:ASP:N    | 2.51                     | 0.44              |
| 1:D:321:THR:O    | 1:D:323:ASP:N    | 2.51                     | 0.44              |
| 1:E:28:SER:HB2   | 1:E:35:MET:HG2   | 2.00                     | 0.44              |
| 1:E:226:ILE:HD13 | 1:E:307:VAL:HG13 | 2.00                     | 0.44              |
| 1:F:314:THR:HG23 | 1:F:316:GLY:H    | 1.83                     | 0.44              |
| 1:F:450:ALA:HB1  | 1:O:417:GLY:H    | 1.82                     | 0.44              |
| 1:H:6:GLU:HB3    | 1:H:11:ALA:CB    | 2.46                     | 0.44              |
| 1:H:56:THR:HG21  | 1:H:375:ARG:HD2  | 1.98                     | 0.44              |
| 1:I:225:LEU:HD12 | 1:I:225:LEU:C    | 2.42                     | 0.44              |
| 1:I:225:LEU:HG   | 1:I:277:PHE:CE1  | 2.53                     | 0.44              |
| 1:I:225:LEU:CD1  | 1:I:329:LYS:HE2  | 2.47                     | 0.44              |
| 1:J:269:ILE:HG23 | 1:J:274:ILE:HG22 | 1.98                     | 0.44              |
| 1:K:166:PHE:CE2  | 1:K:363:ARG:O    | 2.70                     | 0.44              |
| 1:K:274:ILE:O    | 1:K:274:ILE:HG23 | 2.17                     | 0.44              |
| 1:L:166:PHE:CE1  | 1:L:198:ASP:CB   | 3.00                     | 0.44              |
| 1:L:222:ALA:HA   | 1:L:275:ASN:OD1  | 2.17                     | 0.44              |
| 1:L:274:ILE:O    | 1:L:274:ILE:HG23 | 2.17                     | 0.44              |
| 1:L:341:ILE:HG23 | 1:L:363:ARG:CZ   | 2.47                     | 0.44              |
| 1:P:145:ASP:OD1  | 1:P:171:VAL:HB   | 2.17                     | 0.44              |
| 1:A:309:ARG:O    | 1:A:313:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:317:GLU:HB3  | 1:C:329:LYS:HG3  | 1.99                     | 0.44              |
| 1:C:398:GLY:HA2  | 1:C:401:GLU:OE1  | 2.18                     | 0.44              |
| 1:C:399:CYS:SG   | 1:C:464:GLY:CA   | 3.03                     | 0.44              |
| 1:E:30:LEU:H     | 1:E:30:LEU:HD12  | 1.82                     | 0.44              |
| 1:F:67:ALA:HB2   | 1:F:507:ILE:HG21 | 1.99                     | 0.44              |
| 1:F:128:LEU:HD22 | 1:F:128:LEU:HA   | 1.79                     | 0.44              |
| 1:G:68:ALA:O     | 1:G:72:VAL:HG23  | 2.17                     | 0.44              |
| 1:I:20:ILE:N     | 1:I:98:ARG:HH22  | 2.15                     | 0.44              |
| 1:I:27:LYS:CB    | 1:I:436:ILE:HD11 | 2.47                     | 0.44              |
| 1:I:109:HIS:HB3  | 1:I:112:THR:OG1  | 2.17                     | 0.44              |
| 1:I:431:ARG:C    | 1:I:434:PRO:HD2  | 2.43                     | 0.44              |
| 1:J:68:ALA:O     | 1:J:72:VAL:HG23  | 2.17                     | 0.44              |
| 1:K:394:VAL:HG23 | 1:K:482:GLU:HB2  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:372:GLU:HG3  | 1:L:375:ARG:NH2  | 2.31                     | 0.44              |
| 1:M:146:LEU:HD23 | 1:M:148:ASN:H    | 1.82                     | 0.44              |
| 1:N:22:ILE:HD12  | 1:N:90:THR:CG2   | 2.47                     | 0.44              |
| 1:N:51:THR:HG22  | 1:N:53:ASP:H     | 1.82                     | 0.44              |
| 1:N:65:ASN:N     | 1:N:66:PRO:HD2   | 2.33                     | 0.44              |
| 1:N:159:LEU:HD22 | 1:N:159:LEU:N    | 2.32                     | 0.44              |
| 1:N:219:ILE:HG21 | 1:N:275:ASN:O    | 2.17                     | 0.44              |
| 1:N:222:ALA:HA   | 1:N:275:ASN:CB   | 2.48                     | 0.44              |
| 1:P:334:LYS:HD3  | 1:P:351:GLY:HA3  | 1.98                     | 0.44              |
| 1:A:145:ASP:OD1  | 1:A:171:VAL:HB   | 2.17                     | 0.44              |
| 1:A:274:ILE:O    | 1:A:274:ILE:HG23 | 2.16                     | 0.44              |
| 1:C:108:ILE:HB   | 1:L:446:ALA:CA   | 2.48                     | 0.44              |
| 1:C:174:VAL:O    | 1:C:177:LEU:HB3  | 2.18                     | 0.44              |
| 1:C:452:LEU:HD22 | 1:C:465:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:280:ARG:HG3  | 1:D:304:PHE:HB2  | 1.99                     | 0.44              |
| 1:E:191:LYS:HD2  | 1:E:344:ASP:HB3  | 1.99                     | 0.44              |
| 1:E:483:SER:HB2  | 1:E:486:VAL:HG13 | 2.00                     | 0.44              |
| 1:F:52:ASN:ND2   | 1:F:157:LYS:HA   | 2.33                     | 0.44              |
| 1:F:109:HIS:NE2  | 1:F:111:GLN:HB2  | 2.33                     | 0.44              |
| 1:G:192:LEU:N    | 1:G:192:LEU:HD12 | 2.33                     | 0.44              |
| 1:H:225:LEU:HD12 | 1:H:225:LEU:C    | 2.42                     | 0.44              |
| 1:H:276:CYS:HA   | 1:H:297:MET:O    | 2.18                     | 0.44              |
| 1:J:165:HIS:O    | 1:J:168:LYS:HB3  | 2.17                     | 0.44              |
| 1:J:198:ASP:C    | 1:J:363:ARG:HB2  | 2.43                     | 0.44              |
| 1:J:323:ASP:C    | 1:J:325:PRO:HD2  | 2.42                     | 0.44              |
| 1:J:324:HIS:HB2  | 1:J:329:LYS:CE   | 2.47                     | 0.44              |
| 1:K:109:HIS:NE2  | 1:K:111:GLN:HB2  | 2.33                     | 0.44              |
| 1:K:191:LYS:HZ2  | 1:K:346:LEU:HD11 | 1.83                     | 0.44              |
| 1:K:206:LEU:HD11 | 1:K:346:LEU:HD23 | 1.99                     | 0.44              |
| 1:K:226:ILE:HG12 | 1:K:278:ILE:CG2  | 2.47                     | 0.44              |
| 1:K:415:THR:HG23 | 1:K:416:PRO:HD2  | 2.00                     | 0.44              |
| 1:K:433:LEU:HB2  | 1:K:434:PRO:HD3  | 2.00                     | 0.44              |
| 1:L:22:ILE:O     | 1:L:26:VAL:HG22  | 2.18                     | 0.44              |
| 1:L:265:LYS:HE2  | 1:L:322:PHE:CE1  | 2.53                     | 0.44              |
| 1:N:128:LEU:O    | 1:N:129:LEU:HD13 | 2.17                     | 0.44              |
| 1:N:189:ILE:CG2  | 1:N:190:LYS:H    | 2.30                     | 0.44              |
| 1:N:366:THR:H    | 1:N:370:LEU:HD22 | 1.83                     | 0.44              |
| 1:N:510:ALA:O    | 1:N:511:ALA:HB3  | 2.18                     | 0.44              |
| 1:O:143:ARG:HA   | 1:O:143:ARG:NE   | 2.33                     | 0.44              |
| 1:A:96:LEU:HD22  | 1:A:96:LEU:C     | 2.43                     | 0.44              |
| 1:A:96:LEU:HD22  | 1:A:96:LEU:O     | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:41:SER:HB3   | 1:C:45:ASP:CG    | 2.42                     | 0.44              |
| 1:D:176:ARG:HH22 | 1:D:360:ILE:HG13 | 1.82                     | 0.44              |
| 1:F:245:VAL:CG1  | 1:F:250:LYS:HB3  | 2.37                     | 0.44              |
| 1:H:146:LEU:HD13 | 1:H:167:THR:O    | 2.17                     | 0.44              |
| 1:H:261:LYS:O    | 1:H:265:LYS:HG3  | 2.17                     | 0.44              |
| 1:H:421:VAL:O    | 1:H:424:GLU:HG2  | 2.17                     | 0.44              |
| 1:I:109:HIS:CE1  | 1:I:111:GLN:HB2  | 2.53                     | 0.44              |
| 1:I:191:LYS:NZ   | 1:I:346:LEU:HG   | 2.31                     | 0.44              |
| 1:I:226:ILE:HA   | 1:I:278:ILE:O    | 2.17                     | 0.44              |
| 1:L:119:GLU:CG   | 1:L:423:MET:HE3  | 2.48                     | 0.44              |
| 1:O:110:PRO:O    | 1:O:113:ILE:HB   | 2.18                     | 0.44              |
| 1:P:211:ILE:HG12 | 1:P:298:ALA:H    | 1.82                     | 0.44              |
| 1:A:159:LEU:HD22 | 1:A:159:LEU:H    | 1.82                     | 0.44              |
| 1:A:393:THR:HB   | 1:A:481:THR:OG1  | 2.18                     | 0.44              |
| 1:A:513:ARG:NE   | 1:F:63:VAL:HG11  | 2.33                     | 0.44              |
| 1:B:251:VAL:HG21 | 1:F:240:GLY:HA2  | 1.98                     | 0.44              |
| 1:C:28:SER:O     | 1:C:34:GLY:HA2   | 2.18                     | 0.44              |
| 1:D:415:THR:HA   | 1:D:416:PRO:HD3  | 1.93                     | 0.44              |
| 1:D:433:LEU:O    | 1:D:437:ILE:HG12 | 2.17                     | 0.44              |
| 1:E:166:PHE:CZ   | 1:E:198:ASP:HB3  | 2.53                     | 0.44              |
| 1:F:341:ILE:C    | 1:F:343:GLU:H    | 2.26                     | 0.44              |
| 1:F:438:ALA:CB   | 1:F:448:LEU:HG   | 2.45                     | 0.44              |
| 1:G:143:ARG:HA   | 1:G:143:ARG:NE   | 2.32                     | 0.44              |
| 1:H:112:THR:CG2  | 1:H:418:LYS:HD2  | 2.44                     | 0.44              |
| 1:H:215:GLN:HE21 | 1:H:292:GLY:N    | 2.16                     | 0.44              |
| 1:H:372:GLU:HG3  | 1:H:375:ARG:HH22 | 1.81                     | 0.44              |
| 1:H:406:HIS:O    | 1:H:409:THR:HG22 | 2.17                     | 0.44              |
| 1:I:173:ALA:HA   | 1:I:176:ARG:CZ   | 2.48                     | 0.44              |
| 1:J:110:PRO:HB3  | 1:J:502:LEU:CG   | 2.48                     | 0.44              |
| 1:J:222:ALA:HA   | 1:J:275:ASN:HB2  | 1.99                     | 0.44              |
| 1:K:32:PRO:HA    | 1:K:156:SER:CA   | 2.48                     | 0.44              |
| 1:K:334:LYS:HD3  | 1:K:335:LEU:N    | 2.33                     | 0.44              |
| 1:K:431:ARG:NH2  | 1:K:434:PRO:HG2  | 2.32                     | 0.44              |
| 1:M:207:LEU:HB3  | 1:M:347:ILE:CG2  | 2.48                     | 0.44              |
| 1:O:154:LEU:HD13 | 1:O:167:THR:OG1  | 2.18                     | 0.44              |
| 1:P:51:THR:HG22  | 1:P:53:ASP:O     | 2.18                     | 0.44              |
| 1:A:133:VAL:HG13 | 1:A:134:ASP:H    | 1.82                     | 0.44              |
| 1:A:158:LEU:HD23 | 1:A:369:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:31:GLY:O     | 1:B:156:SER:HA   | 2.17                     | 0.44              |
| 1:B:64:ASP:CG    | 1:B:66:PRO:HD2   | 2.43                     | 0.44              |
| 1:C:38:ILE:HG21  | 1:H:508:ILE:HG12 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:LEU:C     | 1:C:96:LEU:HD22  | 2.43                     | 0.44              |
| 1:C:163:LYS:HA   | 1:C:166:PHE:HD1  | 1.83                     | 0.44              |
| 1:D:146:LEU:CD2  | 1:D:147:MET:N    | 2.80                     | 0.44              |
| 1:E:244:ARG:O    | 1:E:245:VAL:HG13 | 2.17                     | 0.44              |
| 1:F:82:VAL:HA    | 1:F:386:GLN:CD   | 2.43                     | 0.44              |
| 1:F:362:LEU:HD11 | 1:F:377:LEU:HD22 | 1.99                     | 0.44              |
| 1:F:431:ARG:C    | 1:F:434:PRO:HD2  | 2.43                     | 0.44              |
| 1:G:453:ARG:HH21 | 1:N:417:GLY:HA2  | 1.83                     | 0.44              |
| 1:H:26:VAL:CG2   | 1:H:91:VAL:HG22  | 2.47                     | 0.44              |
| 1:H:96:LEU:O     | 1:H:96:LEU:HD22  | 2.18                     | 0.44              |
| 1:H:210:LYS:HE2  | 1:H:212:GLY:O    | 2.18                     | 0.44              |
| 1:H:352:VAL:HG13 | 1:H:352:VAL:O    | 2.18                     | 0.44              |
| 1:I:146:LEU:HD13 | 1:I:168:LYS:HA   | 1.99                     | 0.44              |
| 1:I:163:LYS:HD2  | 1:I:166:PHE:CG   | 2.53                     | 0.44              |
| 1:N:52:ASN:HD21  | 1:N:157:LYS:HG2  | 1.83                     | 0.44              |
| 1:N:205:PHE:HA   | 1:N:359:THR:OG1  | 2.18                     | 0.44              |
| 1:N:449:VAL:HG12 | 1:N:453:ARG:NH2  | 2.33                     | 0.44              |
| 1:O:52:ASN:H     | 1:O:375:ARG:CD   | 2.31                     | 0.44              |
| 1:P:159:LEU:HD23 | 1:P:163:LYS:CD   | 2.48                     | 0.44              |
| 1:A:269:ILE:CG2  | 1:A:274:ILE:HG21 | 2.44                     | 0.43              |
| 1:C:65:ASN:ND2   | 1:C:66:PRO:HD3   | 2.33                     | 0.43              |
| 1:C:431:ARG:NH2  | 1:C:434:PRO:HG2  | 2.32                     | 0.43              |
| 1:D:408:VAL:HG23 | 1:D:427:ALA:HB1  | 2.00                     | 0.43              |
| 1:F:52:ASN:HD21  | 1:F:157:LYS:HG2  | 1.82                     | 0.43              |
| 1:F:59:LYS:CE    | 1:F:76:ARG:HB2   | 2.43                     | 0.43              |
| 1:F:176:ARG:NH1  | 1:F:201:LEU:HD21 | 2.33                     | 0.43              |
| 1:G:416:PRO:HB2  | 1:G:419:GLU:OE1  | 2.17                     | 0.43              |
| 1:H:133:VAL:HG21 | 1:H:394:VAL:CA   | 2.47                     | 0.43              |
| 1:H:190:LYS:HA   | 1:H:362:LEU:O    | 2.18                     | 0.43              |
| 1:H:431:ARG:HH21 | 1:H:434:PRO:HG2  | 1.83                     | 0.43              |
| 1:I:154:LEU:HD13 | 1:I:167:THR:OG1  | 2.18                     | 0.43              |
| 1:J:50:VAL:HG13  | 1:J:375:ARG:HH21 | 1.83                     | 0.43              |
| 1:J:225:LEU:HD11 | 1:J:324:HIS:CE1  | 2.53                     | 0.43              |
| 1:J:236:ILE:CG2  | 1:J:237:LYS:N    | 2.81                     | 0.43              |
| 1:K:95:GLU:CD    | 1:K:429:ALA:HB1  | 2.43                     | 0.43              |
| 1:K:104:ILE:HG13 | 1:K:105:ALA:N    | 2.32                     | 0.43              |
| 1:K:310:LEU:O    | 1:K:310:LEU:HD13 | 2.18                     | 0.43              |
| 1:L:149:ILE:HG21 | 1:L:387:THR:OG1  | 2.18                     | 0.43              |
| 1:M:28:SER:O     | 1:M:34:GLY:HA2   | 2.18                     | 0.43              |
| 1:M:404:MET:CE   | 1:M:430:LEU:HD11 | 2.48                     | 0.43              |
| 1:N:146:LEU:HD21 | 1:N:168:LYS:HA   | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:163:LYS:HG3  | 1:N:166:PHE:HB2  | 2.00                     | 0.43              |
| 1:N:268:ARG:O    | 1:N:271:LYS:HG2  | 2.17                     | 0.43              |
| 1:O:326:GLU:HB2  | 1:O:327:LEU:H    | 1.67                     | 0.43              |
| 1:P:232:ASP:HA   | 1:P:284:TYR:HB2  | 1.99                     | 0.43              |
| 1:B:154:LEU:HD23 | 1:B:163:LYS:CG   | 2.45                     | 0.43              |
| 1:D:75:SER:O     | 1:D:78:GLN:HB3   | 2.18                     | 0.43              |
| 1:D:88:SER:O     | 1:D:92:LEU:HD13  | 2.17                     | 0.43              |
| 1:D:286:TYR:HB2  | 1:D:287:PRO:HD3  | 2.00                     | 0.43              |
| 1:E:25:LEU:HD22  | 1:E:25:LEU:N     | 2.32                     | 0.43              |
| 1:E:274:ILE:O    | 1:E:296:VAL:HG22 | 2.18                     | 0.43              |
| 1:E:321:THR:O    | 1:E:323:ASP:N    | 2.51                     | 0.43              |
| 1:E:381:LEU:HD13 | 1:E:381:LEU:C    | 2.43                     | 0.43              |
| 1:G:64:ASP:CG    | 1:G:66:PRO:HD2   | 2.43                     | 0.43              |
| 1:I:280:ARG:O    | 1:I:281:GLN:CB   | 2.66                     | 0.43              |
| 1:J:222:ALA:HA   | 1:J:275:ASN:OD1  | 2.18                     | 0.43              |
| 1:K:99:GLU:HG2   | 1:K:425:SER:HB3  | 1.98                     | 0.43              |
| 1:K:146:LEU:HD13 | 1:K:167:THR:O    | 2.17                     | 0.43              |
| 1:K:226:ILE:HD13 | 1:K:307:VAL:HG13 | 1.99                     | 0.43              |
| 1:K:354:LEU:HD22 | 1:K:356:GLU:CB   | 2.48                     | 0.43              |
| 1:L:19:ALA:HB1   | 1:L:94:ALA:HA    | 2.00                     | 0.43              |
| 1:L:313:VAL:HG13 | 1:L:352:VAL:CG1  | 2.48                     | 0.43              |
| 1:M:82:VAL:CA    | 1:M:386:GLN:HG3  | 2.42                     | 0.43              |
| 1:M:188:VAL:HB   | 1:M:360:ILE:HB   | 2.00                     | 0.43              |
| 1:M:269:ILE:HG23 | 1:M:274:ILE:HG21 | 1.97                     | 0.43              |
| 1:N:163:LYS:HG3  | 1:N:166:PHE:CB   | 2.48                     | 0.43              |
| 1:N:200:TYR:O    | 1:N:361:VAL:HB   | 2.17                     | 0.43              |
| 1:N:438:ALA:CB   | 1:N:448:LEU:HG   | 2.48                     | 0.43              |
| 1:O:226:ILE:HG12 | 1:O:278:ILE:CG2  | 2.48                     | 0.43              |
| 1:O:324:HIS:CG   | 1:O:325:PRO:HD3  | 2.52                     | 0.43              |
| 1:O:364:GLY:HA3  | 1:O:370:LEU:CD2  | 2.47                     | 0.43              |
| 1:O:369:ILE:O    | 1:O:372:GLU:CB   | 2.65                     | 0.43              |
| 1:P:233:THR:HG21 | 1:P:261:LYS:HE2  | 1.99                     | 0.43              |
| 1:A:173:ALA:O    | 1:A:176:ARG:HG2  | 2.18                     | 0.43              |
| 1:B:216:PRO:HG2  | 1:B:295:GLY:CA   | 2.48                     | 0.43              |
| 1:B:405:ALA:HA   | 1:B:408:VAL:HG22 | 2.00                     | 0.43              |
| 1:C:369:ILE:HG23 | 1:C:372:GLU:OE1  | 2.18                     | 0.43              |
| 1:E:219:ILE:HD13 | 1:E:219:ILE:H    | 1.83                     | 0.43              |
| 1:E:394:VAL:CG2  | 1:E:482:GLU:HB2  | 2.48                     | 0.43              |
| 1:E:431:ARG:NH1  | 1:E:453:ARG:HD3  | 2.33                     | 0.43              |
| 1:F:236:ILE:CG2  | 1:F:237:LYS:H    | 2.28                     | 0.43              |
| 1:G:170:ALA:O    | 1:G:173:ALA:HB3  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:146:LEU:HD23 | 1:H:148:ASN:H    | 1.83                     | 0.43              |
| 1:H:148:ASN:O    | 1:H:152:THR:HG23 | 2.18                     | 0.43              |
| 1:K:27:LYS:O     | 1:K:436:ILE:HD11 | 2.18                     | 0.43              |
| 1:K:164:ASP:O    | 1:K:167:THR:HG22 | 2.19                     | 0.43              |
| 1:L:146:LEU:HD11 | 1:L:150:ALA:CB   | 2.47                     | 0.43              |
| 1:L:334:LYS:CD   | 1:L:351:GLY:HA3  | 2.49                     | 0.43              |
| 1:M:116:GLY:O    | 1:M:119:GLU:HB2  | 2.18                     | 0.43              |
| 1:N:226:ILE:HA   | 1:N:278:ILE:O    | 2.18                     | 0.43              |
| 1:O:117:TRP:HZ2  | 1:O:498:ALA:HB1  | 1.84                     | 0.43              |
| 1:O:159:LEU:HD22 | 1:O:159:LEU:N    | 2.33                     | 0.43              |
| 1:O:274:ILE:O    | 1:O:296:VAL:HG22 | 2.19                     | 0.43              |
| 1:P:145:ASP:C    | 1:P:171:VAL:HG21 | 2.43                     | 0.43              |
| 1:A:51:THR:HA    | 1:A:375:ARG:HH11 | 1.84                     | 0.43              |
| 1:A:154:LEU:CD2  | 1:A:167:THR:HB   | 2.41                     | 0.43              |
| 1:B:176:ARG:HH12 | 1:B:201:LEU:HD21 | 1.82                     | 0.43              |
| 1:B:274:ILE:HG23 | 1:B:296:VAL:HG21 | 2.00                     | 0.43              |
| 1:C:177:LEU:C    | 1:C:177:LEU:HD13 | 2.44                     | 0.43              |
| 1:D:52:ASN:CB    | 1:D:157:LYS:HG2  | 2.48                     | 0.43              |
| 1:D:265:LYS:HE2  | 1:D:322:PHE:CE1  | 2.54                     | 0.43              |
| 1:G:188:VAL:HB   | 1:G:377:LEU:HD13 | 2.01                     | 0.43              |
| 1:G:225:LEU:HD13 | 1:G:329:LYS:HE2  | 2.00                     | 0.43              |
| 1:G:274:ILE:O    | 1:G:274:ILE:HG23 | 2.17                     | 0.43              |
| 1:G:402:MET:HE2  | 1:G:402:MET:O    | 2.18                     | 0.43              |
| 1:G:431:ARG:C    | 1:G:434:PRO:HD2  | 2.43                     | 0.43              |
| 1:I:125:ARG:HA   | 1:I:128:LEU:HD12 | 2.00                     | 0.43              |
| 1:I:146:LEU:HB2  | 1:I:171:VAL:HG21 | 2.00                     | 0.43              |
| 1:I:205:PHE:HA   | 1:I:359:THR:OG1  | 2.18                     | 0.43              |
| 1:I:421:VAL:O    | 1:I:424:GLU:HG2  | 2.18                     | 0.43              |
| 1:J:163:LYS:HA   | 1:J:166:PHE:HD1  | 1.82                     | 0.43              |
| 1:K:215:GLN:HG3  | 1:K:292:GLY:HA2  | 2.00                     | 0.43              |
| 1:L:280:ARG:HG2  | 1:L:302:ALA:O    | 2.19                     | 0.43              |
| 1:M:321:THR:O    | 1:M:323:ASP:N    | 2.52                     | 0.43              |
| 1:P:30:LEU:HD11  | 1:P:87:THR:O     | 2.17                     | 0.43              |
| 1:B:233:THR:O    | 1:B:234:ASP:HB3  | 2.18                     | 0.43              |
| 1:B:254:ILE:HG21 | 1:F:238:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:230:GLY:HA2  | 1:C:279:ASN:HD21 | 1.83                     | 0.43              |
| 1:D:215:GLN:HE21 | 1:D:292:GLY:N    | 2.17                     | 0.43              |
| 1:D:438:ALA:CB   | 1:D:448:LEU:HG   | 2.49                     | 0.43              |
| 1:E:38:ILE:HD12  | 1:E:48:LEU:HD22  | 1.99                     | 0.43              |
| 1:E:486:VAL:O    | 1:E:490:VAL:HG12 | 2.19                     | 0.43              |
| 1:F:111:GLN:O    | 1:F:114:ILE:HB   | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:365:ALA:O    | 1:F:366:THR:HG23 | 2.18                     | 0.43              |
| 1:F:433:LEU:HA   | 1:F:436:ILE:HG22 | 2.01                     | 0.43              |
| 1:G:19:ALA:HB1   | 1:G:94:ALA:HA    | 2.00                     | 0.43              |
| 1:G:58:LEU:HB3   | 1:G:72:VAL:CG1   | 2.49                     | 0.43              |
| 1:G:261:LYS:O    | 1:G:264:GLU:HG2  | 2.17                     | 0.43              |
| 1:G:499:GLU:HG2  | 1:G:503:ARG:HG3  | 1.99                     | 0.43              |
| 1:H:159:LEU:CD2  | 1:H:163:LYS:HD3  | 2.49                     | 0.43              |
| 1:H:431:ARG:CZ   | 1:H:431:ARG:HA   | 2.49                     | 0.43              |
| 1:I:99:GLU:CB    | 1:I:425:SER:HB2  | 2.46                     | 0.43              |
| 1:I:242:ARG:NH1  | 1:I:242:ARG:HB3  | 2.34                     | 0.43              |
| 1:I:265:LYS:O    | 1:I:269:ILE:HG13 | 2.18                     | 0.43              |
| 1:J:40:LEU:H     | 1:K:3:ALA:CB     | 2.31                     | 0.43              |
| 1:J:57:ILE:HD13  | 1:J:57:ILE:O     | 2.18                     | 0.43              |
| 1:K:365:ALA:O    | 1:K:366:THR:HG23 | 2.19                     | 0.43              |
| 1:L:284:TYR:CE2  | 1:L:286:TYR:HD1  | 2.37                     | 0.43              |
| 1:M:154:LEU:HD21 | 1:M:163:LYS:NZ   | 2.34                     | 0.43              |
| 1:M:159:LEU:HG   | 1:M:163:LYS:CD   | 2.48                     | 0.43              |
| 1:M:287:PRO:O    | 1:M:291:PHE:HD2  | 2.01                     | 0.43              |
| 1:N:192:LEU:HG   | 1:N:366:THR:HG21 | 1.99                     | 0.43              |
| 1:A:68:ALA:O     | 1:A:72:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:82:VAL:HA    | 1:A:386:GLN:NE2  | 2.34                     | 0.43              |
| 1:A:512:PRO:HD3  | 1:F:39:LEU:HD21  | 1.99                     | 0.43              |
| 1:B:95:GLU:HA    | 1:B:98:ARG:HD2   | 2.01                     | 0.43              |
| 1:B:246:ASP:O    | 1:B:247:SER:HB2  | 2.19                     | 0.43              |
| 1:B:280:ARG:O    | 1:B:281:GLN:CB   | 2.66                     | 0.43              |
| 1:C:79:ASP:CA    | 1:C:83:GLY:HA2   | 2.44                     | 0.43              |
| 1:D:82:VAL:HA    | 1:D:386:GLN:HG3  | 2.01                     | 0.43              |
| 1:D:313:VAL:CG1  | 1:D:352:VAL:HB   | 2.48                     | 0.43              |
| 1:D:381:LEU:HD22 | 1:D:381:LEU:O    | 2.18                     | 0.43              |
| 1:E:103:LEU:CD2  | 1:E:113:ILE:HD13 | 2.49                     | 0.43              |
| 1:F:99:GLU:HG3   | 1:F:425:SER:HB2  | 2.00                     | 0.43              |
| 1:F:446:ALA:CB   | 1:O:418:LYS:HG2  | 2.48                     | 0.43              |
| 1:G:394:VAL:HG23 | 1:G:482:GLU:HB2  | 1.99                     | 0.43              |
| 1:H:183:LEU:HD13 | 1:H:381:LEU:HD11 | 2.01                     | 0.43              |
| 1:I:433:LEU:HA   | 1:I:436:ILE:HG22 | 2.01                     | 0.43              |
| 1:J:38:ILE:HB    | 1:J:48:LEU:HD22  | 2.00                     | 0.43              |
| 1:J:159:LEU:HB2  | 1:J:163:LYS:HG3  | 2.01                     | 0.43              |
| 1:J:191:LYS:HE3  | 1:J:346:LEU:HD22 | 2.00                     | 0.43              |
| 1:K:173:ALA:HB1  | 1:K:360:ILE:HD11 | 1.99                     | 0.43              |
| 1:K:206:LEU:HD13 | 1:K:206:LEU:C    | 2.44                     | 0.43              |
| 1:K:381:LEU:O    | 1:K:381:LEU:HD22 | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:158:LEU:O    | 1:L:158:LEU:HG   | 2.19                     | 0.43              |
| 1:N:225:LEU:HD11 | 1:N:324:HIS:ND1  | 2.34                     | 0.43              |
| 1:P:154:LEU:HD21 | 1:P:163:LYS:NZ   | 2.33                     | 0.43              |
| 1:P:508:ILE:HD12 | 1:P:509:LYS:HD3  | 1.99                     | 0.43              |
| 1:A:99:GLU:HG2   | 1:A:425:SER:HB2  | 2.00                     | 0.43              |
| 1:A:222:ALA:HA   | 1:A:275:ASN:CB   | 2.48                     | 0.43              |
| 1:A:224:ILE:HD11 | 1:A:336:ILE:HD11 | 1.99                     | 0.43              |
| 1:C:506:ASN:O    | 1:C:507:ILE:HG13 | 2.18                     | 0.43              |
| 1:F:96:LEU:HD23  | 1:F:117:TRP:HZ2  | 1.84                     | 0.43              |
| 1:G:128:LEU:HD23 | 1:G:488:ARG:HG2  | 2.01                     | 0.43              |
| 1:I:123:ALA:HA   | 1:I:126:GLN:NE2  | 2.31                     | 0.43              |
| 1:I:265:LYS:HZ2  | 1:I:287:PRO:CG   | 2.32                     | 0.43              |
| 1:I:334:LYS:HD3  | 1:I:351:GLY:HA3  | 2.01                     | 0.43              |
| 1:I:483:SER:HB2  | 1:I:486:VAL:HG13 | 2.00                     | 0.43              |
| 1:J:106:LYS:O    | 1:J:108:ILE:HG13 | 2.18                     | 0.43              |
| 1:J:341:ILE:CD1  | 1:J:346:LEU:HD23 | 2.46                     | 0.43              |
| 1:K:321:THR:C    | 1:K:323:ASP:H    | 2.26                     | 0.43              |
| 1:L:103:LEU:O    | 1:L:106:LYS:HB2  | 2.18                     | 0.43              |
| 1:L:280:ARG:O    | 1:L:281:GLN:CB   | 2.67                     | 0.43              |
| 1:L:448:LEU:HD21 | 1:L:465:LEU:CD1  | 2.39                     | 0.43              |
| 1:N:149:ILE:HB   | 1:N:481:THR:HG23 | 2.01                     | 0.43              |
| 1:N:266:VAL:CB   | 1:N:290:LEU:HD21 | 2.38                     | 0.43              |
| 1:N:313:VAL:HG22 | 1:N:357:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:196:LEU:HD13 | 1:A:196:LEU:C    | 2.43                     | 0.43              |
| 1:A:226:ILE:HD13 | 1:A:307:VAL:HG13 | 2.01                     | 0.43              |
| 1:B:334:LYS:HD3  | 1:B:351:GLY:HA3  | 2.00                     | 0.43              |
| 1:B:508:ILE:H    | 1:G:37:LYS:HZ2   | 1.66                     | 0.43              |
| 1:B:511:ALA:N    | 1:B:512:PRO:HD3  | 2.33                     | 0.43              |
| 1:C:26:VAL:HG23  | 1:C:91:VAL:HG22  | 2.00                     | 0.43              |
| 1:C:65:ASN:CG    | 1:C:66:PRO:HD3   | 2.44                     | 0.43              |
| 1:C:133:VAL:HG21 | 1:C:393:THR:O    | 2.19                     | 0.43              |
| 1:C:329:LYS:HB2  | 1:C:329:LYS:HZ3  | 1.83                     | 0.43              |
| 1:D:196:LEU:HD22 | 1:D:196:LEU:HA   | 1.85                     | 0.43              |
| 1:E:262:MET:HG2  | 1:E:290:LEU:HD22 | 2.01                     | 0.43              |
| 1:E:496:GLU:O    | 1:E:500:VAL:HG13 | 2.18                     | 0.43              |
| 1:F:92:LEU:O     | 1:F:95:GLU:HG2   | 2.18                     | 0.43              |
| 1:F:145:ASP:OD2  | 1:F:175:LEU:HD11 | 2.18                     | 0.43              |
| 1:G:181:GLY:O    | 1:G:182:ASN:CB   | 2.67                     | 0.43              |
| 1:H:59:LYS:NZ    | 1:H:76:ARG:HB2   | 2.34                     | 0.43              |
| 1:H:141:LYS:HA   | 1:H:141:LYS:HD2  | 1.71                     | 0.43              |
| 1:I:496:GLU:O    | 1:I:500:VAL:HG22 | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:154:LEU:HD22 | 1:J:167:THR:HB   | 2.01                     | 0.43              |
| 1:J:173:ALA:HA   | 1:J:176:ARG:CZ   | 2.49                     | 0.43              |
| 1:J:215:GLN:HA   | 1:J:292:GLY:HA2  | 2.00                     | 0.43              |
| 1:J:310:LEU:O    | 1:J:314:THR:HG22 | 2.19                     | 0.43              |
| 1:K:57:ILE:HD13  | 1:K:57:ILE:O     | 2.19                     | 0.43              |
| 1:K:402:MET:SD   | 1:K:456:HIS:HB2  | 2.58                     | 0.43              |
| 1:L:173:ALA:HA   | 1:L:176:ARG:CZ   | 2.48                     | 0.43              |
| 1:M:274:ILE:O    | 1:M:274:ILE:HG23 | 2.18                     | 0.43              |
| 1:N:501:ILE:HA   | 1:N:504:VAL:CG2  | 2.49                     | 0.43              |
| 1:O:38:ILE:HD12  | 1:O:48:LEU:CD2   | 2.48                     | 0.43              |
| 1:A:59:LYS:HE2   | 1:A:76:ARG:HB2   | 2.01                     | 0.43              |
| 1:A:139:GLU:O    | 1:A:141:LYS:N    | 2.52                     | 0.43              |
| 1:B:163:LYS:HD2  | 1:B:166:PHE:CG   | 2.54                     | 0.43              |
| 1:C:192:LEU:HB3  | 1:C:366:THR:HG22 | 2.00                     | 0.43              |
| 1:C:269:ILE:HG12 | 1:C:274:ILE:HG21 | 2.01                     | 0.43              |
| 1:D:32:PRO:HA    | 1:D:155:SER:CB   | 2.49                     | 0.43              |
| 1:D:231:MET:HB3  | 1:D:265:LYS:HZ3  | 1.84                     | 0.43              |
| 1:F:259:LYS:O    | 1:F:263:LYS:HG2  | 2.19                     | 0.43              |
| 1:G:50:VAL:HG22  | 1:G:375:ARG:NH1  | 2.34                     | 0.43              |
| 1:G:159:LEU:HG   | 1:G:163:LYS:CG   | 2.48                     | 0.43              |
| 1:G:266:VAL:HG13 | 1:G:267:GLU:N    | 2.34                     | 0.43              |
| 1:H:313:VAL:HG13 | 1:H:352:VAL:HB   | 2.00                     | 0.43              |
| 1:H:366:THR:HG23 | 1:H:366:THR:O    | 2.19                     | 0.43              |
| 1:H:431:ARG:HD3  | 1:H:453:ARG:NH1  | 2.33                     | 0.43              |
| 1:H:445:SER:O    | 1:H:449:VAL:HG23 | 2.19                     | 0.43              |
| 1:I:19:ALA:HB1   | 1:I:94:ALA:CA    | 2.49                     | 0.43              |
| 1:I:225:LEU:HD13 | 1:I:329:LYS:CE   | 2.49                     | 0.43              |
| 1:I:277:PHE:CE2  | 1:I:279:ASN:HB2  | 2.54                     | 0.43              |
| 1:J:24:ASP:O     | 1:J:27:LYS:HG2   | 2.19                     | 0.43              |
| 1:J:390:ASP:HB2  | 1:J:485:GLN:HE22 | 1.84                     | 0.43              |
| 1:J:431:ARG:NH2  | 1:J:434:PRO:HG2  | 2.33                     | 0.43              |
| 1:K:27:LYS:HB2   | 1:K:436:ILE:CD1  | 2.49                     | 0.43              |
| 1:K:74:MET:SD    | 1:K:77:VAL:HG12  | 2.59                     | 0.43              |
| 1:L:61:ILE:HG23  | 1:L:63:VAL:HG23  | 2.01                     | 0.43              |
| 1:L:141:LYS:HG2  | 1:L:144:GLN:HB2  | 2.00                     | 0.43              |
| 1:N:277:PHE:CE2  | 1:N:279:ASN:HB2  | 2.53                     | 0.43              |
| 1:O:158:LEU:O    | 1:O:160:THR:N    | 2.52                     | 0.43              |
| 1:O:226:ILE:HG12 | 1:O:278:ILE:HG23 | 2.01                     | 0.43              |
| 1:O:266:VAL:HB   | 1:O:290:LEU:CD2  | 2.29                     | 0.43              |
| 1:P:209:LYS:NZ   | 1:P:302:ALA:HA   | 2.34                     | 0.43              |
| 1:A:158:LEU:HD13 | 1:C:504:VAL:HG21 | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:ALA:HA   | 1:A:309:ARG:HE   | 1.84                     | 0.43              |
| 1:B:110:PRO:HA   | 1:B:113:ILE:HD12 | 2.00                     | 0.43              |
| 1:B:448:LEU:HA   | 1:B:451:GLN:HE21 | 1.84                     | 0.43              |
| 1:D:74:MET:HE2   | 1:D:77:VAL:CG1   | 2.49                     | 0.43              |
| 1:D:297:MET:CE   | 1:D:347:ILE:HD11 | 2.49                     | 0.43              |
| 1:F:74:MET:HE2   | 1:F:77:VAL:CG1   | 2.49                     | 0.43              |
| 1:F:236:ILE:CG2  | 1:F:237:LYS:N    | 2.82                     | 0.43              |
| 1:F:283:ILE:HG22 | 1:F:300:GLU:HG3  | 1.99                     | 0.43              |
| 1:F:321:THR:O    | 1:F:323:ASP:N    | 2.51                     | 0.43              |
| 1:G:191:LYS:HZ1  | 1:G:346:LEU:HD21 | 1.84                     | 0.43              |
| 1:H:59:LYS:HE3   | 1:H:73:ASP:HA    | 2.01                     | 0.43              |
| 1:J:183:LEU:O    | 1:J:183:LEU:HG   | 2.19                     | 0.43              |
| 1:K:373:ALA:HA   | 1:K:376:SER:HB3  | 2.00                     | 0.43              |
| 1:L:193:GLY:HA3  | 1:L:343:GLU:OE2  | 2.19                     | 0.43              |
| 1:L:203:GLU:CD   | 1:L:203:GLU:H    | 2.26                     | 0.43              |
| 1:M:405:ALA:HA   | 1:M:408:VAL:CG2  | 2.48                     | 0.43              |
| 1:N:183:LEU:HD23 | 1:N:183:LEU:C    | 2.44                     | 0.43              |
| 1:O:82:VAL:HG21  | 1:O:485:GLN:HG3  | 2.00                     | 0.43              |
| 1:O:334:LYS:HB3  | 1:O:351:GLY:HA3  | 2.01                     | 0.43              |
| 1:P:211:ILE:HD13 | 1:P:215:GLN:CB   | 2.49                     | 0.43              |
| 1:P:215:GLN:HE21 | 1:P:292:GLY:N    | 2.17                     | 0.43              |
| 1:A:7:ARG:NH2    | 1:A:509:LYS:HG3  | 2.34                     | 0.42              |
| 1:B:390:ASP:HB3  | 1:B:485:GLN:HE22 | 1.84                     | 0.42              |
| 1:C:146:LEU:HD11 | 1:C:150:ALA:HB3  | 2.01                     | 0.42              |
| 1:C:188:VAL:CG1  | 1:C:377:LEU:HD22 | 2.50                     | 0.42              |
| 1:C:402:MET:HG2  | 1:C:431:ARG:NH2  | 2.34                     | 0.42              |
| 1:D:110:PRO:O    | 1:D:114:ILE:HG12 | 2.18                     | 0.42              |
| 1:D:198:ASP:O    | 1:D:199:SER:HB3  | 2.19                     | 0.42              |
| 1:E:258:GLU:O    | 1:E:261:LYS:HB2  | 2.18                     | 0.42              |
| 1:E:269:ILE:HG12 | 1:E:274:ILE:HG21 | 2.00                     | 0.42              |
| 1:F:274:ILE:O    | 1:F:274:ILE:HG23 | 2.19                     | 0.42              |
| 1:G:176:ARG:NH1  | 1:G:201:LEU:HD21 | 2.34                     | 0.42              |
| 1:H:26:VAL:HG23  | 1:H:91:VAL:HG22  | 2.01                     | 0.42              |
| 1:H:173:ALA:HA   | 1:H:176:ARG:NE   | 2.33                     | 0.42              |
| 1:H:341:ILE:HD11 | 1:H:348:HIS:NE2  | 2.33                     | 0.42              |
| 1:I:74:MET:O     | 1:I:74:MET:SD    | 2.77                     | 0.42              |
| 1:I:233:THR:O    | 1:I:234:ASP:HB3  | 2.18                     | 0.42              |
| 1:I:485:GLN:HE22 | 1:I:488:ARG:HH21 | 1.67                     | 0.42              |
| 1:K:171:VAL:HG12 | 1:K:384:LEU:CD1  | 2.49                     | 0.42              |
| 1:L:24:ASP:O     | 1:L:27:LYS:HG2   | 2.19                     | 0.42              |
| 1:L:161:HIS:CG   | 1:L:162:HIS:H    | 2.37                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:206:LEU:C    | 1:M:206:LEU:HD13 | 2.44                     | 0.42              |
| 1:M:433:LEU:HB2  | 1:M:434:PRO:HD3  | 2.00                     | 0.42              |
| 1:O:189:ILE:HG22 | 1:O:190:LYS:N    | 2.33                     | 0.42              |
| 1:P:57:ILE:HD13  | 1:P:57:ILE:O     | 2.19                     | 0.42              |
| 1:A:437:ILE:CB   | 1:A:465:LEU:HD12 | 2.44                     | 0.42              |
| 1:A:465:LEU:N    | 1:A:465:LEU:HD23 | 2.34                     | 0.42              |
| 1:B:421:VAL:O    | 1:B:424:GLU:HG2  | 2.19                     | 0.42              |
| 1:C:211:ILE:HG23 | 1:C:298:ALA:O    | 2.19                     | 0.42              |
| 1:D:159:LEU:CD2  | 1:D:159:LEU:N    | 2.82                     | 0.42              |
| 1:D:453:ARG:NH2  | 1:K:417:GLY:HA2  | 2.33                     | 0.42              |
| 1:E:297:MET:CE   | 1:E:347:ILE:HD11 | 2.49                     | 0.42              |
| 1:F:96:LEU:HD22  | 1:F:96:LEU:O     | 2.19                     | 0.42              |
| 1:F:284:TYR:CE2  | 1:F:286:TYR:HD1  | 2.37                     | 0.42              |
| 1:H:269:ILE:HG23 | 1:H:274:ILE:HG22 | 1.97                     | 0.42              |
| 1:H:312:LEU:HD23 | 1:H:312:LEU:HA   | 1.84                     | 0.42              |
| 1:H:466:ASP:HB3  | 1:H:469:GLU:HB3  | 2.01                     | 0.42              |
| 1:I:316:GLY:C    | 1:I:317:GLU:HG2  | 2.44                     | 0.42              |
| 1:J:263:LYS:HA   | 1:J:266:VAL:HG12 | 2.02                     | 0.42              |
| 1:J:367:GLN:HG2  | 1:J:369:ILE:H    | 1.84                     | 0.42              |
| 1:L:59:LYS:HE3   | 1:L:72:VAL:O     | 2.19                     | 0.42              |
| 1:L:114:ILE:HA   | 1:L:117:TRP:CZ3  | 2.53                     | 0.42              |
| 1:L:207:LEU:CD1  | 1:L:209:LYS:HE2  | 2.48                     | 0.42              |
| 1:M:197:ALA:O    | 1:M:198:ASP:HB2  | 2.19                     | 0.42              |
| 1:N:64:ASP:CG    | 1:N:66:PRO:HD2   | 2.44                     | 0.42              |
| 1:N:198:ASP:C    | 1:N:363:ARG:HB2  | 2.44                     | 0.42              |
| 1:O:483:SER:HB2  | 1:O:486:VAL:HG13 | 2.01                     | 0.42              |
| 1:P:81:GLU:O     | 1:P:82:VAL:HB    | 2.19                     | 0.42              |
| 1:P:231:MET:CG   | 1:P:283:ILE:HG13 | 2.48                     | 0.42              |
| 1:A:100:ALA:O    | 1:A:103:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:107:LYS:C    | 1:A:108:ILE:HG13 | 2.45                     | 0.42              |
| 1:A:185:ALA:HA   | 1:A:309:ARG:NE   | 2.34                     | 0.42              |
| 1:B:32:PRO:HA    | 1:B:155:SER:CB   | 2.48                     | 0.42              |
| 1:B:433:LEU:C    | 1:B:436:ILE:HG22 | 2.45                     | 0.42              |
| 1:B:506:ASN:O    | 1:B:508:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:22:ILE:HD12  | 1:C:90:THR:CG2   | 2.49                     | 0.42              |
| 1:C:38:ILE:CG2   | 1:H:508:ILE:HG12 | 2.50                     | 0.42              |
| 1:C:406:HIS:O    | 1:C:409:THR:HG22 | 2.19                     | 0.42              |
| 1:E:154:LEU:HD21 | 1:E:163:LYS:HZ3  | 1.81                     | 0.42              |
| 1:E:313:VAL:HG13 | 1:E:352:VAL:CG2  | 2.49                     | 0.42              |
| 1:G:129:LEU:HA   | 1:G:392:ARG:HH22 | 1.83                     | 0.42              |
| 1:H:486:VAL:HG23 | 1:H:487:LYS:N    | 2.33                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:57:ILE:HD13  | 1:I:57:ILE:O     | 2.19                     | 0.42              |
| 1:J:368:GLN:O    | 1:J:371:ASP:HB2  | 2.19                     | 0.42              |
| 1:J:395:TYR:HE2  | 1:J:476:SER:OG   | 2.01                     | 0.42              |
| 1:J:399:CYS:SG   | 1:J:464:GLY:CA   | 3.03                     | 0.42              |
| 1:K:192:LEU:CA   | 1:K:366:THR:HG21 | 2.46                     | 0.42              |
| 1:L:499:GLU:HG2  | 1:L:503:ARG:HE   | 1.84                     | 0.42              |
| 1:M:265:LYS:O    | 1:M:269:ILE:HG13 | 2.19                     | 0.42              |
| 1:M:284:TYR:O    | 1:M:287:PRO:HD2  | 2.19                     | 0.42              |
| 1:N:145:ASP:O    | 1:N:146:LEU:HB3  | 2.20                     | 0.42              |
| 1:O:69:LYS:O     | 1:O:72:VAL:HB    | 2.19                     | 0.42              |
| 1:O:89:VAL:HA    | 1:O:490:VAL:CG2  | 2.50                     | 0.42              |
| 1:O:187:HIS:HB2  | 1:O:309:ARG:HH12 | 1.83                     | 0.42              |
| 1:P:12:ARG:HD2   | 1:P:100:ALA:HB1  | 2.02                     | 0.42              |
| 1:A:320:SER:HB2  | 1:A:321:THR:H    | 1.64                     | 0.42              |
| 1:A:398:GLY:HA2  | 1:A:401:GLU:OE1  | 2.19                     | 0.42              |
| 1:B:78:GLN:HE21  | 1:B:486:VAL:HA   | 1.83                     | 0.42              |
| 1:B:92:LEU:CD1   | 1:B:433:LEU:HD11 | 2.49                     | 0.42              |
| 1:B:108:ILE:HG23 | 1:I:444:ASP:OD2  | 2.18                     | 0.42              |
| 1:B:314:THR:HG23 | 1:B:316:GLY:H    | 1.84                     | 0.42              |
| 1:E:125:ARG:HG2  | 1:E:128:LEU:HD12 | 2.01                     | 0.42              |
| 1:E:277:PHE:CE2  | 1:E:279:ASN:HB2  | 2.53                     | 0.42              |
| 1:E:324:HIS:CG   | 1:E:325:PRO:HD3  | 2.54                     | 0.42              |
| 1:E:511:ALA:HA   | 1:E:512:PRO:HD3  | 1.88                     | 0.42              |
| 1:F:269:ILE:HG12 | 1:F:274:ILE:HG21 | 2.01                     | 0.42              |
| 1:F:487:LYS:HA   | 1:F:487:LYS:HD3  | 1.90                     | 0.42              |
| 1:G:225:LEU:HD12 | 1:G:225:LEU:C    | 2.43                     | 0.42              |
| 1:I:51:THR:HG22  | 1:I:53:ASP:H     | 1.84                     | 0.42              |
| 1:K:140:VAL:HG12 | 1:K:141:LYS:N    | 2.35                     | 0.42              |
| 1:K:173:ALA:HA   | 1:K:176:ARG:CZ   | 2.48                     | 0.42              |
| 1:K:203:GLU:H    | 1:K:203:GLU:CD   | 2.27                     | 0.42              |
| 1:K:397:GLY:HA3  | 1:K:475:MET:HE3  | 1.99                     | 0.42              |
| 1:L:205:PHE:HA   | 1:L:359:THR:CB   | 2.49                     | 0.42              |
| 1:L:216:PRO:HG2  | 1:L:295:GLY:CA   | 2.48                     | 0.42              |
| 1:L:509:LYS:HE2  | 1:L:509:LYS:HA   | 2.01                     | 0.42              |
| 1:M:51:THR:CG2   | 1:M:56:THR:HB    | 2.48                     | 0.42              |
| 1:N:27:LYS:HG2   | 1:N:436:ILE:HD12 | 1.99                     | 0.42              |
| 1:N:82:VAL:C     | 1:N:386:GLN:HG3  | 2.43                     | 0.42              |
| 1:N:146:LEU:CD2  | 1:N:167:THR:HG23 | 2.49                     | 0.42              |
| 1:N:163:LYS:O    | 1:N:163:LYS:HG2  | 2.19                     | 0.42              |
| 1:N:163:LYS:CG   | 1:N:166:PHE:HB2  | 2.49                     | 0.42              |
| 1:N:188:VAL:O    | 1:N:189:ILE:HD13 | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:321:THR:O    | 1:N:323:ASP:N    | 2.52                     | 0.42              |
| 1:O:321:THR:C    | 1:O:323:ASP:H    | 2.27                     | 0.42              |
| 1:P:24:ASP:HA    | 1:P:27:LYS:HD3   | 2.00                     | 0.42              |
| 1:P:222:ALA:HA   | 1:P:275:ASN:HB2  | 2.02                     | 0.42              |
| 1:C:38:ILE:HG21  | 1:H:508:ILE:CG2  | 2.40                     | 0.42              |
| 1:C:82:VAL:HG13  | 1:C:83:GLY:N     | 2.35                     | 0.42              |
| 1:C:183:LEU:O    | 1:C:184:GLU:HG3  | 2.19                     | 0.42              |
| 1:C:197:ALA:O    | 1:C:198:ASP:HB2  | 2.20                     | 0.42              |
| 1:C:280:ARG:HG3  | 1:C:304:PHE:HA   | 2.00                     | 0.42              |
| 1:C:500:VAL:HA   | 1:C:503:ARG:HG2  | 2.02                     | 0.42              |
| 1:C:508:ILE:O    | 1:C:509:LYS:HB2  | 2.20                     | 0.42              |
| 1:D:61:ILE:HG13  | 1:D:62:GLY:N     | 2.34                     | 0.42              |
| 1:D:171:VAL:O    | 1:D:174:VAL:HG22 | 2.20                     | 0.42              |
| 1:E:27:LYS:HB2   | 1:E:436:ILE:HD11 | 2.02                     | 0.42              |
| 1:E:274:ILE:HG23 | 1:E:296:VAL:HG21 | 2.02                     | 0.42              |
| 1:E:434:PRO:HB3  | 1:E:452:LEU:HD23 | 1.99                     | 0.42              |
| 1:F:82:VAL:HB    | 1:F:485:GLN:HG2  | 2.00                     | 0.42              |
| 1:G:117:TRP:CD1  | 1:G:495:ALA:HB1  | 2.55                     | 0.42              |
| 1:I:81:GLU:O     | 1:I:82:VAL:HB    | 2.19                     | 0.42              |
| 1:K:22:ILE:O     | 1:K:26:VAL:HG22  | 2.19                     | 0.42              |
| 1:K:455:ALA:HB2  | 1:K:472:ILE:HD12 | 2.02                     | 0.42              |
| 1:M:104:ILE:HG13 | 1:M:105:ALA:N    | 2.34                     | 0.42              |
| 1:M:324:HIS:ND1  | 1:M:325:PRO:HD3  | 2.35                     | 0.42              |
| 1:N:22:ILE:O     | 1:N:26:VAL:HG22  | 2.19                     | 0.42              |
| 1:O:57:ILE:HG23  | 1:O:58:LEU:HD22  | 2.02                     | 0.42              |
| 1:P:191:LYS:NZ   | 1:P:346:LEU:HD11 | 2.34                     | 0.42              |
| 1:P:326:GLU:HB2  | 1:P:327:LEU:H    | 1.58                     | 0.42              |
| 1:A:219:ILE:HG21 | 1:A:275:ASN:O    | 2.18                     | 0.42              |
| 1:A:237:LYS:O    | 1:A:237:LYS:HD3  | 2.19                     | 0.42              |
| 1:A:418:LYS:CD   | 1:M:450:ALA:HB2  | 2.48                     | 0.42              |
| 1:B:191:LYS:N    | 1:B:362:LEU:O    | 2.49                     | 0.42              |
| 1:B:284:TYR:CE2  | 1:B:286:TYR:CD1  | 3.08                     | 0.42              |
| 1:C:190:LYS:HD2  | 1:C:190:LYS:C    | 2.44                     | 0.42              |
| 1:D:117:TRP:O    | 1:D:120:ALA:HB3  | 2.20                     | 0.42              |
| 1:D:411:LEU:HB3  | 1:D:423:MET:SD   | 2.60                     | 0.42              |
| 1:D:504:VAL:HG21 | 1:H:38:ILE:HG23  | 2.00                     | 0.42              |
| 1:E:133:VAL:HG21 | 1:E:393:THR:H    | 1.85                     | 0.42              |
| 1:E:431:ARG:CZ   | 1:E:453:ARG:HD3  | 2.50                     | 0.42              |
| 1:F:225:LEU:HD12 | 1:F:225:LEU:C    | 2.43                     | 0.42              |
| 1:F:232:ASP:OD1  | 1:F:284:TYR:HD1  | 2.03                     | 0.42              |
| 1:G:245:VAL:HG21 | 1:G:251:VAL:CG2  | 2.42                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:291:PHE:HD1  | 1:G:296:VAL:CG1  | 2.33                     | 0.42              |
| 1:G:317:GLU:CB   | 1:G:329:LYS:HD3  | 2.49                     | 0.42              |
| 1:G:448:LEU:HD11 | 1:G:465:LEU:HD11 | 2.01                     | 0.42              |
| 1:H:17:ILE:O     | 1:H:20:ILE:HG22  | 2.19                     | 0.42              |
| 1:H:420:ALA:HB3  | 1:P:453:ARG:NH2  | 2.34                     | 0.42              |
| 1:I:139:GLU:OE2  | 1:I:140:VAL:HG23 | 2.20                     | 0.42              |
| 1:I:346:LEU:N    | 1:I:346:LEU:HD12 | 2.35                     | 0.42              |
| 1:J:114:ILE:HA   | 1:J:117:TRP:CZ3  | 2.54                     | 0.42              |
| 1:L:57:ILE:HD13  | 1:L:57:ILE:O     | 2.19                     | 0.42              |
| 1:L:232:ASP:HA   | 1:L:284:TYR:HB2  | 2.02                     | 0.42              |
| 1:L:402:MET:HE3  | 1:L:453:ARG:CG   | 2.40                     | 0.42              |
| 1:M:85:GLY:HA2   | 1:M:153:THR:OG1  | 2.19                     | 0.42              |
| 1:N:48:LEU:H     | 1:N:48:LEU:HD22  | 1.84                     | 0.42              |
| 1:N:334:LYS:CD   | 1:N:351:GLY:HA3  | 2.49                     | 0.42              |
| 1:O:287:PRO:O    | 1:O:291:PHE:HD1  | 2.03                     | 0.42              |
| 1:A:7:ARG:HB3    | 1:A:509:LYS:HB2  | 2.02                     | 0.42              |
| 1:A:20:ILE:HB    | 1:A:98:ARG:NH2   | 2.34                     | 0.42              |
| 1:A:431:ARG:C    | 1:A:434:PRO:HD2  | 2.45                     | 0.42              |
| 1:B:326:GLU:CG   | 1:B:327:LEU:N    | 2.80                     | 0.42              |
| 1:C:110:PRO:HB2  | 1:C:502:LEU:HG   | 2.01                     | 0.42              |
| 1:C:262:MET:SD   | 1:C:290:LEU:HB2  | 2.60                     | 0.42              |
| 1:C:444:ASP:OD1  | 1:L:108:ILE:HG13 | 2.19                     | 0.42              |
| 1:D:261:LYS:O    | 1:D:265:LYS:HG3  | 2.20                     | 0.42              |
| 1:E:89:VAL:HA    | 1:E:490:VAL:HG21 | 2.02                     | 0.42              |
| 1:F:96:LEU:CD2   | 1:F:117:TRP:HZ2  | 2.31                     | 0.42              |
| 1:F:106:LYS:HE3  | 1:F:418:LYS:HZ1  | 1.84                     | 0.42              |
| 1:F:390:ASP:HB3  | 1:F:485:GLN:CD   | 2.45                     | 0.42              |
| 1:G:451:GLN:NE2  | 1:G:471:THR:HA   | 2.35                     | 0.42              |
| 1:H:176:ARG:NE   | 1:H:358:CYS:HB2  | 2.34                     | 0.42              |
| 1:K:108:ILE:HG22 | 1:K:109:HIS:N    | 2.33                     | 0.42              |
| 1:L:139:GLU:OE2  | 1:L:178:LYS:HD2  | 2.19                     | 0.42              |
| 1:L:150:ALA:O    | 1:L:154:LEU:HD13 | 2.20                     | 0.42              |
| 1:L:163:LYS:HA   | 1:L:166:PHE:HD1  | 1.79                     | 0.42              |
| 1:M:192:LEU:CG   | 1:M:366:THR:HG21 | 2.41                     | 0.42              |
| 1:O:101:GLU:HA   | 1:O:104:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:32:PRO:HA    | 1:A:155:SER:C    | 2.43                     | 0.42              |
| 1:A:84:ASP:OD2   | 1:A:383:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:206:LEU:HD13 | 1:A:206:LEU:C    | 2.45                     | 0.42              |
| 1:A:334:LYS:HD3  | 1:A:351:GLY:HA3  | 2.01                     | 0.42              |
| 1:B:145:ASP:OD2  | 1:B:175:LEU:HD11 | 2.20                     | 0.42              |
| 1:B:447:ASP:HA   | 1:I:107:LYS:HG2  | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:LEU:HD13 | 1:C:196:LEU:C    | 2.45                     | 0.42              |
| 1:C:312:LEU:HD13 | 1:C:312:LEU:O    | 2.20                     | 0.42              |
| 1:C:341:ILE:O    | 1:C:343:GLU:N    | 2.49                     | 0.42              |
| 1:C:397:GLY:HA3  | 1:C:475:MET:HE3  | 2.01                     | 0.42              |
| 1:D:143:ARG:HG3  | 1:D:143:ARG:O    | 2.19                     | 0.42              |
| 1:F:99:GLU:CG    | 1:F:425:SER:HB2  | 2.49                     | 0.42              |
| 1:G:81:GLU:O     | 1:G:82:VAL:CG2   | 2.68                     | 0.42              |
| 1:G:196:LEU:C    | 1:G:196:LEU:HD13 | 2.44                     | 0.42              |
| 1:H:381:LEU:HD13 | 1:H:381:LEU:C    | 2.45                     | 0.42              |
| 1:I:246:ASP:OD1  | 1:I:250:LYS:HD2  | 2.20                     | 0.42              |
| 1:J:7:ARG:HH21   | 1:N:37:LYS:HD2   | 1.85                     | 0.42              |
| 1:J:324:HIS:CG   | 1:J:325:PRO:HD3  | 2.54                     | 0.42              |
| 1:K:67:ALA:O     | 1:K:68:ALA:HB2   | 2.19                     | 0.42              |
| 1:K:173:ALA:O    | 1:K:176:ARG:HG2  | 2.20                     | 0.42              |
| 1:L:324:HIS:ND1  | 1:L:325:PRO:HD3  | 2.35                     | 0.42              |
| 1:M:404:MET:O    | 1:M:408:VAL:HG22 | 2.20                     | 0.42              |
| 1:N:190:LYS:HA   | 1:N:362:LEU:O    | 2.19                     | 0.42              |
| 1:N:405:ALA:HA   | 1:N:408:VAL:HG22 | 2.02                     | 0.42              |
| 1:O:65:ASN:OD1   | 1:O:510:ALA:HB2  | 2.19                     | 0.42              |
| 1:O:139:GLU:O    | 1:O:141:LYS:N    | 2.52                     | 0.42              |
| 1:P:325:PRO:HA   | 1:P:329:LYS:HG3  | 2.00                     | 0.42              |
| 1:A:203:GLU:HG2  | 1:A:351:GLY:H    | 1.84                     | 0.42              |
| 1:A:323:ASP:C    | 1:A:325:PRO:HD2  | 2.44                     | 0.42              |
| 1:B:106:LYS:O    | 1:B:107:LYS:CB   | 2.66                     | 0.42              |
| 1:B:185:ALA:HA   | 1:B:309:ARG:HD3  | 2.02                     | 0.42              |
| 1:B:223:LYS:HB2  | 1:B:274:ILE:HA   | 2.00                     | 0.42              |
| 1:C:82:VAL:HB    | 1:C:485:GLN:OE1  | 2.20                     | 0.42              |
| 1:C:108:ILE:HB   | 1:L:446:ALA:HA   | 2.02                     | 0.42              |
| 1:D:19:ALA:HB3   | 1:D:98:ARG:HH22  | 1.85                     | 0.42              |
| 1:D:37:LYS:O     | 1:D:50:VAL:HG23  | 2.20                     | 0.42              |
| 1:D:211:ILE:HG12 | 1:D:298:ALA:H    | 1.85                     | 0.42              |
| 1:D:258:GLU:OE2  | 1:D:284:TYR:CE2  | 2.72                     | 0.42              |
| 1:D:372:GLU:HG3  | 1:D:375:ARG:CZ   | 2.48                     | 0.42              |
| 1:E:65:ASN:CG    | 1:E:66:PRO:HD3   | 2.45                     | 0.42              |
| 1:F:45:ASP:O     | 1:F:46:ALA:HB3   | 2.20                     | 0.42              |
| 1:F:203:GLU:CG   | 1:F:350:SER:HB2  | 2.50                     | 0.42              |
| 1:F:405:ALA:HA   | 1:F:408:VAL:HG22 | 2.01                     | 0.42              |
| 1:G:131:SER:HB3  | 1:G:132:ALA:H    | 1.68                     | 0.42              |
| 1:I:51:THR:HA    | 1:I:375:ARG:NH1  | 2.35                     | 0.42              |
| 1:I:226:ILE:HG12 | 1:I:278:ILE:CG2  | 2.50                     | 0.42              |
| 1:I:500:VAL:O    | 1:I:504:VAL:HG12 | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:507:ILE:HG22 | 1:I:508:ILE:N    | 2.35                     | 0.42              |
| 1:J:189:ILE:HG22 | 1:J:190:LYS:N    | 2.34                     | 0.42              |
| 1:J:280:ARG:O    | 1:J:281:GLN:CB   | 2.68                     | 0.42              |
| 1:J:312:LEU:O    | 1:J:354:LEU:HD22 | 2.19                     | 0.42              |
| 1:K:74:MET:O     | 1:K:74:MET:SD    | 2.78                     | 0.42              |
| 1:K:168:LYS:O    | 1:K:171:VAL:HG22 | 2.20                     | 0.42              |
| 1:L:96:LEU:O     | 1:L:96:LEU:HD22  | 2.19                     | 0.42              |
| 1:L:126:GLN:H    | 1:L:126:GLN:HG2  | 1.61                     | 0.42              |
| 1:L:191:LYS:HD3  | 1:L:192:LEU:H    | 1.84                     | 0.42              |
| 1:N:109:HIS:CD2  | 1:N:111:GLN:HB2  | 2.54                     | 0.42              |
| 1:N:324:HIS:CG   | 1:N:325:PRO:HD3  | 2.55                     | 0.42              |
| 1:N:433:LEU:HB2  | 1:N:434:PRO:HD3  | 2.00                     | 0.42              |
| 1:O:198:ASP:O    | 1:O:363:ARG:HB2  | 2.20                     | 0.42              |
| 1:O:431:ARG:HA   | 1:O:431:ARG:CZ   | 2.49                     | 0.42              |
| 1:P:261:LYS:O    | 1:P:264:GLU:HG2  | 2.20                     | 0.42              |
| 1:P:368:GLN:O    | 1:P:371:ASP:HB2  | 2.20                     | 0.42              |
| 1:A:82:VAL:CG1   | 1:A:83:GLY:H     | 2.30                     | 0.42              |
| 1:A:231:MET:HG3  | 1:A:283:ILE:HG13 | 2.02                     | 0.42              |
| 1:B:154:LEU:O    | 1:B:157:LYS:HB2  | 2.20                     | 0.42              |
| 1:C:143:ARG:HA   | 1:C:143:ARG:HE   | 1.84                     | 0.42              |
| 1:C:154:LEU:HD21 | 1:C:167:THR:HB   | 2.02                     | 0.42              |
| 1:C:163:LYS:HD2  | 1:C:166:PHE:CD1  | 2.55                     | 0.42              |
| 1:D:24:ASP:HA    | 1:D:27:LYS:HD3   | 2.01                     | 0.42              |
| 1:D:226:ILE:HG12 | 1:D:278:ILE:CG2  | 2.49                     | 0.42              |
| 1:E:266:VAL:HB   | 1:E:290:LEU:CD2  | 2.30                     | 0.42              |
| 1:F:215:GLN:HG3  | 1:F:292:GLY:HA2  | 2.02                     | 0.42              |
| 1:F:338:GLU:OE2  | 1:F:345:LYS:HE2  | 2.20                     | 0.42              |
| 1:G:163:LYS:HA   | 1:G:166:PHE:HD1  | 1.84                     | 0.42              |
| 1:G:188:VAL:CB   | 1:G:377:LEU:HD13 | 2.50                     | 0.42              |
| 1:G:265:LYS:NZ   | 1:G:287:PRO:HG3  | 2.35                     | 0.42              |
| 1:H:162:HIS:HB3  | 1:H:198:ASP:OD2  | 2.20                     | 0.42              |
| 1:I:280:ARG:HG3  | 1:I:304:PHE:CA   | 2.50                     | 0.42              |
| 1:J:284:TYR:CE2  | 1:J:286:TYR:CD1  | 3.08                     | 0.42              |
| 1:K:75:SER:O     | 1:K:78:GLN:HB2   | 2.20                     | 0.42              |
| 1:K:146:LEU:CD2  | 1:K:147:MET:H    | 2.33                     | 0.42              |
| 1:K:222:ALA:HA   | 1:K:275:ASN:HB2  | 2.02                     | 0.42              |
| 1:O:191:LYS:HD3  | 1:O:344:ASP:HB3  | 2.01                     | 0.42              |
| 1:P:206:LEU:C    | 1:P:206:LEU:HD13 | 2.45                     | 0.42              |
| 1:P:266:VAL:CG2  | 1:P:290:LEU:HD11 | 2.50                     | 0.42              |
| 1:P:280:ARG:HG3  | 1:P:304:PHE:CA   | 2.50                     | 0.42              |
| 1:P:452:LEU:HD13 | 1:P:465:LEU:CD1  | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:452:LEU:HD22 | 1:P:465:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:1:ALA:HB2    | 1:F:61:ILE:HG21  | 2.02                     | 0.41              |
| 1:A:57:ILE:HD13  | 1:A:57:ILE:O     | 2.20                     | 0.41              |
| 1:A:261:LYS:O    | 1:A:264:GLU:HG2  | 2.19                     | 0.41              |
| 1:B:128:LEU:HD22 | 1:B:484:PHE:CZ   | 2.55                     | 0.41              |
| 1:B:146:LEU:CD2  | 1:B:167:THR:HG23 | 2.50                     | 0.41              |
| 1:B:370:LEU:O    | 1:B:373:ALA:HB3  | 2.20                     | 0.41              |
| 1:C:140:VAL:HG12 | 1:C:141:LYS:N    | 2.33                     | 0.41              |
| 1:D:106:LYS:C    | 1:D:107:LYS:CG   | 2.93                     | 0.41              |
| 1:D:245:VAL:HG12 | 1:D:246:ASP:N    | 2.34                     | 0.41              |
| 1:D:280:ARG:HG3  | 1:D:304:PHE:CA   | 2.50                     | 0.41              |
| 1:E:117:TRP:HD1  | 1:E:495:ALA:CB   | 2.32                     | 0.41              |
| 1:F:68:ALA:O     | 1:F:72:VAL:HG23  | 2.20                     | 0.41              |
| 1:F:310:LEU:O    | 1:F:310:LEU:HD13 | 2.20                     | 0.41              |
| 1:G:326:GLU:CG   | 1:G:327:LEU:H    | 2.29                     | 0.41              |
| 1:H:146:LEU:CD2  | 1:H:147:MET:N    | 2.79                     | 0.41              |
| 1:H:191:LYS:HE3  | 1:H:346:LEU:HD13 | 2.02                     | 0.41              |
| 1:I:313:VAL:HG13 | 1:I:352:VAL:HG21 | 2.02                     | 0.41              |
| 1:I:365:ALA:O    | 1:I:366:THR:CB   | 2.67                     | 0.41              |
| 1:I:373:ALA:O    | 1:I:377:LEU:HB2  | 2.20                     | 0.41              |
| 1:J:236:ILE:CD1  | 1:J:237:LYS:H    | 2.33                     | 0.41              |
| 1:J:284:TYR:CE2  | 1:J:286:TYR:HD1  | 2.38                     | 0.41              |
| 1:K:211:ILE:HG13 | 1:K:298:ALA:O    | 2.20                     | 0.41              |
| 1:L:262:MET:HE1  | 1:L:286:TYR:O    | 2.20                     | 0.41              |
| 1:M:222:ALA:HA   | 1:M:275:ASN:CB   | 2.49                     | 0.41              |
| 1:N:219:ILE:HD12 | 1:N:275:ASN:CB   | 2.49                     | 0.41              |
| 1:N:219:ILE:CD1  | 1:N:276:CYS:HB2  | 2.49                     | 0.41              |
| 1:N:510:ALA:O    | 1:N:511:ALA:CB   | 2.68                     | 0.41              |
| 1:O:154:LEU:CD2  | 1:O:163:LYS:HG3  | 2.50                     | 0.41              |
| 1:P:54:GLY:O     | 1:P:58:LEU:HD23  | 2.20                     | 0.41              |
| 1:P:164:ASP:O    | 1:P:167:THR:HG22 | 2.20                     | 0.41              |
| 1:P:345:LYS:C    | 1:P:346:LEU:HD12 | 2.44                     | 0.41              |
| 1:A:171:VAL:CA   | 1:A:174:VAL:HG22 | 2.50                     | 0.41              |
| 1:A:286:TYR:HB2  | 1:A:287:PRO:HD3  | 2.01                     | 0.41              |
| 1:A:508:ILE:HB   | 1:F:37:LYS:NZ    | 2.35                     | 0.41              |
| 1:C:226:ILE:HG12 | 1:C:278:ILE:HG23 | 2.02                     | 0.41              |
| 1:C:263:LYS:O    | 1:C:267:GLU:HG2  | 2.19                     | 0.41              |
| 1:D:96:LEU:HD22  | 1:D:96:LEU:C     | 2.44                     | 0.41              |
| 1:E:211:ILE:CD1  | 1:E:297:MET:HG3  | 2.34                     | 0.41              |
| 1:F:96:LEU:HA    | 1:F:99:GLU:OE2   | 2.20                     | 0.41              |
| 1:F:133:VAL:HB   | 1:F:393:THR:O    | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:448:LEU:HD11 | 1:F:465:LEU:CD1  | 2.50                     | 0.41              |
| 1:H:157:LYS:HB3  | 1:H:159:LEU:CD1  | 2.48                     | 0.41              |
| 1:H:508:ILE:O    | 1:H:508:ILE:HG22 | 2.20                     | 0.41              |
| 1:I:300:GLU:OE2  | 1:I:301:HIS:HB2  | 2.20                     | 0.41              |
| 1:J:141:LYS:HD3  | 1:J:141:LYS:HA   | 1.91                     | 0.41              |
| 1:J:176:ARG:HH22 | 1:J:360:ILE:HG12 | 1.85                     | 0.41              |
| 1:J:231:MET:HE1  | 1:J:265:LYS:HD3  | 2.02                     | 0.41              |
| 1:K:16:PHE:HA    | 1:K:97:LEU:HD23  | 2.01                     | 0.41              |
| 1:K:452:LEU:HD22 | 1:K:465:LEU:HD11 | 2.02                     | 0.41              |
| 1:L:404:MET:HE3  | 1:L:430:LEU:CD1  | 2.50                     | 0.41              |
| 1:M:58:LEU:HD13  | 1:M:58:LEU:HA    | 1.88                     | 0.41              |
| 1:M:112:THR:HG21 | 1:M:418:LYS:HZ2  | 1.83                     | 0.41              |
| 1:M:154:LEU:HD21 | 1:M:163:LYS:HZ2  | 1.84                     | 0.41              |
| 1:M:286:TYR:HB2  | 1:M:287:PRO:HD3  | 2.02                     | 0.41              |
| 1:N:189:ILE:CG2  | 1:N:190:LYS:N    | 2.82                     | 0.41              |
| 1:N:262:MET:HE1  | 1:N:286:TYR:O    | 2.21                     | 0.41              |
| 1:P:225:LEU:HD11 | 1:P:324:HIS:CE1  | 2.55                     | 0.41              |
| 1:P:397:GLY:HA3  | 1:P:475:MET:HE3  | 2.02                     | 0.41              |
| 1:A:280:ARG:HG3  | 1:A:304:PHE:HB2  | 2.02                     | 0.41              |
| 1:B:159:LEU:HD12 | 1:B:372:GLU:CD   | 2.45                     | 0.41              |
| 1:B:392:ARG:HB3  | 1:B:484:PHE:CG   | 2.55                     | 0.41              |
| 1:D:146:LEU:HD13 | 1:D:167:THR:O    | 2.20                     | 0.41              |
| 1:D:191:LYS:NZ   | 1:D:346:LEU:HD21 | 2.32                     | 0.41              |
| 1:E:79:ASP:HA    | 1:E:83:GLY:HA2   | 1.92                     | 0.41              |
| 1:E:128:LEU:C    | 1:E:130:ASN:H    | 2.29                     | 0.41              |
| 1:E:207:LEU:O    | 1:E:347:ILE:HG22 | 2.19                     | 0.41              |
| 1:H:96:LEU:HD11  | 1:H:117:TRP:CZ2  | 2.49                     | 0.41              |
| 1:H:222:ALA:HA   | 1:H:275:ASN:HB2  | 2.00                     | 0.41              |
| 1:H:261:LYS:O    | 1:H:264:GLU:HG2  | 2.20                     | 0.41              |
| 1:I:261:LYS:O    | 1:I:264:GLU:HG2  | 2.20                     | 0.41              |
| 1:I:310:LEU:O    | 1:I:314:THR:HG22 | 2.20                     | 0.41              |
| 1:J:51:THR:CG2   | 1:J:56:THR:HB    | 2.47                     | 0.41              |
| 1:J:138:ASP:O    | 1:J:139:GLU:CB   | 2.67                     | 0.41              |
| 1:J:313:VAL:HG13 | 1:J:352:VAL:CB   | 2.51                     | 0.41              |
| 1:J:324:HIS:HB2  | 1:J:329:LYS:HZ3  | 1.84                     | 0.41              |
| 1:K:183:LEU:HB2  | 1:K:381:LEU:HG   | 2.02                     | 0.41              |
| 1:L:334:LYS:HD2  | 1:L:350:SER:C    | 2.46                     | 0.41              |
| 1:M:40:LEU:HD23  | 1:M:47:SER:O     | 2.20                     | 0.41              |
| 1:M:141:LYS:HG3  | 1:M:144:GLN:H    | 1.85                     | 0.41              |
| 1:N:174:VAL:HG11 | 1:N:384:LEU:CB   | 2.50                     | 0.41              |
| 1:N:341:ILE:C    | 1:N:343:GLU:H    | 2.27                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:397:GLY:HA3  | 1:N:475:MET:CE   | 2.51                     | 0.41              |
| 1:N:438:ALA:O    | 1:N:441:ALA:HB3  | 2.20                     | 0.41              |
| 1:O:339:VAL:O    | 1:O:340:MET:CB   | 2.67                     | 0.41              |
| 1:P:154:LEU:CD2  | 1:P:163:LYS:HG2  | 2.50                     | 0.41              |
| 1:A:35:MET:HG2   | 1:C:505:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:215:GLN:HE21 | 1:A:292:GLY:N    | 2.18                     | 0.41              |
| 1:B:114:ILE:HD13 | 1:B:117:TRP:CZ3  | 2.55                     | 0.41              |
| 1:B:190:LYS:HD3  | 1:B:370:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:261:LYS:O    | 1:B:265:LYS:HG3  | 2.20                     | 0.41              |
| 1:B:399:CYS:SG   | 1:B:464:GLY:CA   | 3.08                     | 0.41              |
| 1:C:337:GLU:HG3  | 1:C:339:VAL:CG2  | 2.50                     | 0.41              |
| 1:D:236:ILE:HG23 | 1:D:237:LYS:H    | 1.83                     | 0.41              |
| 1:D:397:GLY:O    | 1:D:465:LEU:HB2  | 2.21                     | 0.41              |
| 1:F:247:SER:C    | 1:F:249:ALA:N    | 2.79                     | 0.41              |
| 1:F:364:GLY:HA3  | 1:F:370:LEU:CD1  | 2.51                     | 0.41              |
| 1:G:95:GLU:HA    | 1:G:98:ARG:HD2   | 2.02                     | 0.41              |
| 1:G:152:THR:HG21 | 1:G:480:ILE:HG23 | 2.02                     | 0.41              |
| 1:H:225:LEU:HG   | 1:H:277:PHE:CD1  | 2.55                     | 0.41              |
| 1:J:324:HIS:HB2  | 1:J:329:LYS:HE2  | 2.02                     | 0.41              |
| 1:J:452:LEU:CD2  | 1:J:465:LEU:HD21 | 2.50                     | 0.41              |
| 1:K:231:MET:HE1  | 1:K:265:LYS:HD3  | 2.03                     | 0.41              |
| 1:L:159:LEU:HG   | 1:L:369:ILE:HG23 | 2.01                     | 0.41              |
| 1:L:421:VAL:O    | 1:L:424:GLU:HG2  | 2.21                     | 0.41              |
| 1:L:500:VAL:O    | 1:L:504:VAL:HG23 | 2.20                     | 0.41              |
| 1:M:48:LEU:HD22  | 1:M:48:LEU:H     | 1.85                     | 0.41              |
| 1:M:261:LYS:O    | 1:M:264:GLU:HG2  | 2.20                     | 0.41              |
| 1:N:103:LEU:HD21 | 1:N:113:ILE:HG21 | 2.02                     | 0.41              |
| 1:N:130:ASN:O    | 1:N:131:SER:CB   | 2.69                     | 0.41              |
| 1:N:171:VAL:HG12 | 1:N:384:LEU:HD12 | 2.02                     | 0.41              |
| 1:N:385:ALA:O    | 1:N:388:VAL:HG22 | 2.19                     | 0.41              |
| 1:N:445:SER:O    | 1:N:449:VAL:HG23 | 2.21                     | 0.41              |
| 1:O:313:VAL:HG13 | 1:O:352:VAL:HB   | 2.03                     | 0.41              |
| 1:O:394:VAL:CG2  | 1:O:482:GLU:HB2  | 2.50                     | 0.41              |
| 1:P:154:LEU:HD21 | 1:P:167:THR:HB   | 2.02                     | 0.41              |
| 1:P:225:LEU:HD13 | 1:P:329:LYS:CE   | 2.50                     | 0.41              |
| 1:A:108:ILE:HD13 | 1:M:445:SER:N    | 2.36                     | 0.41              |
| 1:A:225:LEU:C    | 1:A:225:LEU:HD12 | 2.44                     | 0.41              |
| 1:A:511:ALA:HA   | 1:A:512:PRO:HD3  | 1.87                     | 0.41              |
| 1:B:191:LYS:HG3  | 1:B:192:LEU:H    | 1.85                     | 0.41              |
| 1:C:109:HIS:HA   | 1:C:110:PRO:HD2  | 1.87                     | 0.41              |
| 1:C:133:VAL:HG23 | 1:C:134:ASP:N    | 2.35                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:58:LEU:HB3   | 1:E:72:VAL:CG1   | 2.50                     | 0.41              |
| 1:E:338:GLU:HA   | 1:E:347:ILE:HA   | 2.03                     | 0.41              |
| 1:F:104:ILE:HG13 | 1:F:105:ALA:N    | 2.35                     | 0.41              |
| 1:F:106:LYS:HZ2  | 1:O:446:ALA:HB1  | 1.86                     | 0.41              |
| 1:F:166:PHE:CD1  | 1:F:198:ASP:HB2  | 2.56                     | 0.41              |
| 1:F:266:VAL:CG2  | 1:F:290:LEU:HD11 | 2.50                     | 0.41              |
| 1:F:362:LEU:HD13 | 1:F:373:ALA:HB1  | 2.02                     | 0.41              |
| 1:F:433:LEU:C    | 1:F:436:ILE:HG22 | 2.46                     | 0.41              |
| 1:F:508:ILE:CG2  | 1:F:509:LYS:N    | 2.82                     | 0.41              |
| 1:G:316:GLY:O    | 1:G:330:LEU:HB2  | 2.21                     | 0.41              |
| 1:H:284:TYR:CE2  | 1:H:286:TYR:CD1  | 3.09                     | 0.41              |
| 1:I:110:PRO:O    | 1:I:113:ILE:HB   | 2.20                     | 0.41              |
| 1:I:191:LYS:O    | 1:I:363:ARG:HA   | 2.20                     | 0.41              |
| 1:I:364:GLY:HA3  | 1:I:370:LEU:HD21 | 2.01                     | 0.41              |
| 1:I:397:GLY:HA3  | 1:I:475:MET:CE   | 2.49                     | 0.41              |
| 1:J:38:ILE:CD1   | 1:J:39:LEU:H     | 2.32                     | 0.41              |
| 1:J:63:VAL:HG22  | 1:K:1:ALA:HA     | 2.02                     | 0.41              |
| 1:J:206:LEU:HD11 | 1:J:346:LEU:CD2  | 2.49                     | 0.41              |
| 1:K:231:MET:HE3  | 1:K:265:LYS:HZ3  | 1.85                     | 0.41              |
| 1:L:24:ASP:HA    | 1:L:27:LYS:HD3   | 2.03                     | 0.41              |
| 1:L:163:LYS:O    | 1:L:163:LYS:HG2  | 2.20                     | 0.41              |
| 1:L:183:LEU:HD22 | 1:L:183:LEU:N    | 2.36                     | 0.41              |
| 1:L:385:ALA:O    | 1:L:389:LYS:HG2  | 2.21                     | 0.41              |
| 1:M:22:ILE:O     | 1:M:26:VAL:HG22  | 2.20                     | 0.41              |
| 1:M:99:GLU:CB    | 1:M:425:SER:HB2  | 2.50                     | 0.41              |
| 1:M:236:ILE:HG23 | 1:M:237:LYS:N    | 2.35                     | 0.41              |
| 1:M:261:LYS:O    | 1:M:265:LYS:HG3  | 2.20                     | 0.41              |
| 1:N:176:ARG:NH1  | 1:N:201:LEU:HD11 | 2.35                     | 0.41              |
| 1:N:192:LEU:HD12 | 1:N:192:LEU:N    | 2.36                     | 0.41              |
| 1:N:489:GLN:HA   | 1:N:492:LEU:HD11 | 2.03                     | 0.41              |
| 1:O:128:LEU:HD23 | 1:O:128:LEU:HA   | 1.79                     | 0.41              |
| 1:O:219:ILE:HD12 | 1:O:275:ASN:HB3  | 2.01                     | 0.41              |
| 1:O:402:MET:HE3  | 1:O:453:ARG:CG   | 2.42                     | 0.41              |
| 1:P:107:LYS:O    | 1:P:107:LYS:CG   | 2.68                     | 0.41              |
| 1:P:219:ILE:HD12 | 1:P:275:ASN:CB   | 2.49                     | 0.41              |
| 1:P:287:PRO:O    | 1:P:290:LEU:HB3  | 2.21                     | 0.41              |
| 1:A:146:LEU:O    | 1:A:147:MET:HB2  | 2.19                     | 0.41              |
| 1:B:174:VAL:HG12 | 1:B:381:LEU:CD2  | 2.51                     | 0.41              |
| 1:D:145:ASP:OD2  | 1:D:175:LEU:HD11 | 2.21                     | 0.41              |
| 1:D:157:LYS:HB3  | 1:D:159:LEU:CD2  | 2.50                     | 0.41              |
| 1:D:245:VAL:O    | 1:D:246:ASP:CB   | 2.67                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:411:LEU:HD13 | 1:D:423:MET:HE2  | 2.01                     | 0.41              |
| 1:E:145:ASP:OD2  | 1:E:175:LEU:HD11 | 2.21                     | 0.41              |
| 1:E:222:ALA:HB1  | 1:E:336:ILE:CD1  | 2.51                     | 0.41              |
| 1:E:330:LEU:N    | 1:E:330:LEU:HD22 | 2.36                     | 0.41              |
| 1:E:408:VAL:HG21 | 1:E:427:ALA:HA   | 2.02                     | 0.41              |
| 1:F:139:GLU:HG2  | 1:F:178:LYS:NZ   | 2.36                     | 0.41              |
| 1:F:282:LEU:HD22 | 1:F:282:LEU:N    | 2.36                     | 0.41              |
| 1:G:128:LEU:CG   | 1:G:488:ARG:HG2  | 2.51                     | 0.41              |
| 1:G:277:PHE:CE2  | 1:G:279:ASN:HB2  | 2.56                     | 0.41              |
| 1:H:99:GLU:CG    | 1:H:425:SER:HB2  | 2.50                     | 0.41              |
| 1:H:140:VAL:HG12 | 1:H:141:LYS:N    | 2.34                     | 0.41              |
| 1:H:225:LEU:HD11 | 1:H:324:HIS:CE1  | 2.55                     | 0.41              |
| 1:H:354:LEU:HD21 | 1:H:356:GLU:HB2  | 2.02                     | 0.41              |
| 1:I:48:LEU:CD1   | 1:N:508:ILE:HD11 | 2.49                     | 0.41              |
| 1:I:99:GLU:HB2   | 1:I:425:SER:CB   | 2.47                     | 0.41              |
| 1:I:222:ALA:HA   | 1:I:275:ASN:CB   | 2.50                     | 0.41              |
| 1:I:431:ARG:NH2  | 1:I:434:PRO:HG2  | 2.34                     | 0.41              |
| 1:J:12:ARG:CD    | 1:J:501:ILE:HG21 | 2.49                     | 0.41              |
| 1:J:146:LEU:HD22 | 1:J:168:LYS:HA   | 2.02                     | 0.41              |
| 1:J:225:LEU:HD13 | 1:J:329:LYS:HE3  | 2.02                     | 0.41              |
| 1:J:394:VAL:HG23 | 1:J:482:GLU:HB2  | 2.02                     | 0.41              |
| 1:J:495:ALA:O    | 1:J:499:GLU:HB2  | 2.21                     | 0.41              |
| 1:K:452:LEU:HD11 | 1:K:456:HIS:CE1  | 2.56                     | 0.41              |
| 1:L:126:GLN:O    | 1:L:127:ALA:HB2  | 2.21                     | 0.41              |
| 1:L:159:LEU:O    | 1:L:161:HIS:N    | 2.53                     | 0.41              |
| 1:L:433:LEU:O    | 1:L:437:ILE:HG12 | 2.21                     | 0.41              |
| 1:M:140:VAL:HG12 | 1:M:141:LYS:N    | 2.35                     | 0.41              |
| 1:M:399:CYS:SG   | 1:M:464:GLY:CA   | 3.06                     | 0.41              |
| 1:N:57:ILE:HG23  | 1:N:58:LEU:HD22  | 2.02                     | 0.41              |
| 1:N:59:LYS:CE    | 1:N:76:ARG:HB2   | 2.47                     | 0.41              |
| 1:N:84:ASP:OD1   | 1:N:84:ASP:N     | 2.50                     | 0.41              |
| 1:N:106:LYS:HG3  | 1:N:418:LYS:HZ2  | 1.83                     | 0.41              |
| 1:N:326:GLU:CG   | 1:N:327:LEU:N    | 2.83                     | 0.41              |
| 1:O:38:ILE:O     | 1:O:38:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:165:HIS:O    | 1:A:168:LYS:HB3  | 2.20                     | 0.41              |
| 1:A:397:GLY:HA3  | 1:A:475:MET:CE   | 2.46                     | 0.41              |
| 1:B:32:PRO:HA    | 1:B:155:SER:C    | 2.45                     | 0.41              |
| 1:B:68:ALA:O     | 1:B:72:VAL:HG23  | 2.21                     | 0.41              |
| 1:B:190:LYS:HD3  | 1:B:370:LEU:CD2  | 2.51                     | 0.41              |
| 1:C:262:MET:CE   | 1:C:286:TYR:HB3  | 2.51                     | 0.41              |
| 1:C:269:ILE:CG2  | 1:C:274:ILE:HG21 | 2.45                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:191:LYS:HG3  | 1:D:193:GLY:H    | 1.85                     | 0.41              |
| 1:D:277:PHE:CE2  | 1:D:279:ASN:HB2  | 2.55                     | 0.41              |
| 1:D:446:ALA:HB2  | 1:K:418:LYS:CD   | 2.44                     | 0.41              |
| 1:D:509:LYS:HG3  | 1:H:61:ILE:HG21  | 2.03                     | 0.41              |
| 1:E:159:LEU:C    | 1:E:159:LEU:CD2  | 2.93                     | 0.41              |
| 1:F:310:LEU:HD13 | 1:F:310:LEU:C    | 2.45                     | 0.41              |
| 1:G:52:ASN:H     | 1:G:375:ARG:NH1  | 2.18                     | 0.41              |
| 1:G:75:SER:O     | 1:G:78:GLN:HB3   | 2.21                     | 0.41              |
| 1:G:82:VAL:HG11  | 1:G:483:SER:OG   | 2.20                     | 0.41              |
| 1:H:187:HIS:NE2  | 1:H:189:ILE:HD11 | 2.36                     | 0.41              |
| 1:H:218:ARG:HG3  | 1:H:337:GLU:HB3  | 2.03                     | 0.41              |
| 1:I:146:LEU:HD12 | 1:I:171:VAL:CG1  | 2.40                     | 0.41              |
| 1:I:146:LEU:CD1  | 1:I:167:THR:O    | 2.68                     | 0.41              |
| 1:J:58:LEU:HD13  | 1:J:58:LEU:HA    | 1.91                     | 0.41              |
| 1:J:173:ALA:O    | 1:J:176:ARG:HG2  | 2.20                     | 0.41              |
| 1:J:309:ARG:O    | 1:J:313:VAL:HG23 | 2.21                     | 0.41              |
| 1:J:346:LEU:HD12 | 1:J:346:LEU:HA   | 1.90                     | 0.41              |
| 1:J:452:LEU:HD11 | 1:J:456:HIS:CE1  | 2.55                     | 0.41              |
| 1:K:45:ASP:O     | 1:K:46:ALA:CB    | 2.69                     | 0.41              |
| 1:K:225:LEU:HD13 | 1:K:226:ILE:N    | 2.35                     | 0.41              |
| 1:L:313:VAL:HG13 | 1:L:352:VAL:CB   | 2.49                     | 0.41              |
| 1:M:76:ARG:HA    | 1:M:79:ASP:HB3   | 2.02                     | 0.41              |
| 1:M:103:LEU:HD23 | 1:M:113:ILE:HD13 | 2.03                     | 0.41              |
| 1:M:448:LEU:HD11 | 1:M:465:LEU:HD11 | 2.03                     | 0.41              |
| 1:P:100:ALA:HA   | 1:P:103:LEU:HD22 | 2.02                     | 0.41              |
| 1:P:373:ALA:O    | 1:P:377:LEU:CB   | 2.68                     | 0.41              |
| 1:A:485:GLN:O    | 1:A:489:GLN:HG2  | 2.20                     | 0.41              |
| 1:D:32:PRO:HD2   | 1:D:467:MET:HE1  | 2.01                     | 0.41              |
| 1:D:57:ILE:HD13  | 1:D:57:ILE:O     | 2.20                     | 0.41              |
| 1:D:231:MET:HB3  | 1:D:265:LYS:NZ   | 2.35                     | 0.41              |
| 1:D:324:HIS:CG   | 1:D:325:PRO:HD3  | 2.56                     | 0.41              |
| 1:E:26:VAL:HG23  | 1:E:91:VAL:CG2   | 2.51                     | 0.41              |
| 1:E:165:HIS:O    | 1:E:168:LYS:HB3  | 2.21                     | 0.41              |
| 1:E:392:ARG:O    | 1:E:484:PHE:HB2  | 2.20                     | 0.41              |
| 1:F:35:MET:CE    | 1:F:440:ASN:HB2  | 2.50                     | 0.41              |
| 1:F:190:LYS:HB2  | 1:F:190:LYS:HE3  | 1.87                     | 0.41              |
| 1:F:239:PHE:HB2  | 1:F:241:SER:H    | 1.85                     | 0.41              |
| 1:F:334:LYS:HD3  | 1:F:335:LEU:CB   | 2.51                     | 0.41              |
| 1:F:433:LEU:O    | 1:F:437:ILE:HG12 | 2.20                     | 0.41              |
| 1:G:452:LEU:HD13 | 1:G:465:LEU:CD1  | 2.49                     | 0.41              |
| 1:H:185:ALA:HA   | 1:H:309:ARG:HD3  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:393:THR:HB   | 1:H:481:THR:OG1  | 2.20                     | 0.41              |
| 1:H:453:ARG:CZ   | 1:P:417:GLY:N    | 2.84                     | 0.41              |
| 1:I:511:ALA:N    | 1:I:512:PRO:HD2  | 2.36                     | 0.41              |
| 1:J:32:PRO:HA    | 1:J:155:SER:O    | 2.21                     | 0.41              |
| 1:J:321:THR:O    | 1:J:323:ASP:N    | 2.53                     | 0.41              |
| 1:K:33:LYS:HB2   | 1:K:440:ASN:OD1  | 2.21                     | 0.41              |
| 1:K:58:LEU:HD12  | 1:K:58:LEU:HA    | 1.89                     | 0.41              |
| 1:K:190:LYS:HA   | 1:K:362:LEU:O    | 2.21                     | 0.41              |
| 1:K:228:ASN:ND2  | 1:K:319:ALA:HB3  | 2.36                     | 0.41              |
| 1:K:277:PHE:O    | 1:K:298:ALA:HA   | 2.21                     | 0.41              |
| 1:K:384:LEU:HD22 | 1:K:384:LEU:N    | 2.36                     | 0.41              |
| 1:L:141:LYS:HE2  | 1:L:144:GLN:HB2  | 2.02                     | 0.41              |
| 1:L:177:LEU:O    | 1:L:177:LEU:HD13 | 2.21                     | 0.41              |
| 1:L:231:MET:CG   | 1:L:283:ILE:HG13 | 2.51                     | 0.41              |
| 1:L:447:ASP:O    | 1:L:451:GLN:HG2  | 2.21                     | 0.41              |
| 1:M:96:LEU:HD13  | 1:M:97:LEU:N     | 2.35                     | 0.41              |
| 1:M:146:LEU:CD2  | 1:M:147:MET:N    | 2.83                     | 0.41              |
| 1:M:207:LEU:HB3  | 1:M:347:ILE:HG23 | 2.02                     | 0.41              |
| 1:M:412:ALA:HB1  | 1:M:424:GLU:HB3  | 2.02                     | 0.41              |
| 1:N:146:LEU:CD1  | 1:N:168:LYS:HG3  | 2.50                     | 0.41              |
| 1:N:266:VAL:HB   | 1:N:290:LEU:CD2  | 2.40                     | 0.41              |
| 1:P:219:ILE:CD1  | 1:P:275:ASN:HB3  | 2.49                     | 0.41              |
| 1:P:317:GLU:OE2  | 1:P:329:LYS:HE3  | 2.20                     | 0.41              |
| 1:A:92:LEU:HD12  | 1:A:92:LEU:N     | 2.36                     | 0.41              |
| 1:A:233:THR:O    | 1:A:234:ASP:HB3  | 2.21                     | 0.41              |
| 1:A:280:ARG:O    | 1:A:281:GLN:CB   | 2.69                     | 0.41              |
| 1:B:222:ALA:HA   | 1:B:275:ASN:CB   | 2.51                     | 0.41              |
| 1:C:490:VAL:O    | 1:C:494:ALA:N    | 2.54                     | 0.41              |
| 1:D:30:LEU:HD12  | 1:D:30:LEU:H     | 1.86                     | 0.41              |
| 1:E:71:LEU:C     | 1:E:71:LEU:HD23  | 2.46                     | 0.41              |
| 1:E:263:LYS:HA   | 1:E:266:VAL:HG12 | 2.02                     | 0.41              |
| 1:F:119:GLU:O    | 1:F:122:LYS:HB3  | 2.20                     | 0.41              |
| 1:F:203:GLU:HG3  | 1:F:351:GLY:H    | 1.86                     | 0.41              |
| 1:F:215:GLN:HE21 | 1:F:292:GLY:N    | 2.19                     | 0.41              |
| 1:F:225:LEU:HG   | 1:F:277:PHE:CE1  | 2.56                     | 0.41              |
| 1:F:266:VAL:HB   | 1:F:290:LEU:CD2  | 2.37                     | 0.41              |
| 1:F:399:CYS:SG   | 1:F:464:GLY:CA   | 3.06                     | 0.41              |
| 1:G:142:PHE:CD1  | 1:G:142:PHE:N    | 2.86                     | 0.41              |
| 1:G:159:LEU:HD22 | 1:G:159:LEU:N    | 2.36                     | 0.41              |
| 1:G:206:LEU:HD13 | 1:G:206:LEU:C    | 2.46                     | 0.41              |
| 1:G:433:LEU:HB2  | 1:G:434:PRO:HD3  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:501:ILE:HD12 | 1:G:501:ILE:HA   | 1.78                     | 0.41              |
| 1:H:2:GLY:O      | 1:H:3:ALA:HB2    | 2.21                     | 0.41              |
| 1:H:10:THR:O     | 1:H:11:ALA:HB2   | 2.21                     | 0.41              |
| 1:H:159:LEU:CG   | 1:H:163:LYS:HD3  | 2.50                     | 0.41              |
| 1:H:168:LYS:O    | 1:H:171:VAL:HG22 | 2.21                     | 0.41              |
| 1:H:316:GLY:O    | 1:H:330:LEU:HB3  | 2.21                     | 0.41              |
| 1:H:411:LEU:HB3  | 1:H:423:MET:CE   | 2.50                     | 0.41              |
| 1:I:139:GLU:HG2  | 1:I:178:LYS:NZ   | 2.36                     | 0.41              |
| 1:I:216:PRO:HG2  | 1:I:295:GLY:CA   | 2.51                     | 0.41              |
| 1:I:431:ARG:NH1  | 1:I:453:ARG:HD3  | 2.36                     | 0.41              |
| 1:J:124:ALA:HB2  | 1:J:491:LEU:CD1  | 2.51                     | 0.41              |
| 1:J:274:ILE:O    | 1:J:274:ILE:HG23 | 2.21                     | 0.41              |
| 1:K:51:THR:HG22  | 1:K:53:ASP:O     | 2.21                     | 0.41              |
| 1:K:103:LEU:O    | 1:K:106:LYS:HB3  | 2.20                     | 0.41              |
| 1:K:231:MET:HG2  | 1:K:279:ASN:ND2  | 2.35                     | 0.41              |
| 1:K:334:LYS:HD2  | 1:K:351:GLY:HA3  | 2.03                     | 0.41              |
| 1:K:485:GLN:HG3  | 1:K:489:GLN:OE1  | 2.21                     | 0.41              |
| 1:L:82:VAL:HG13  | 1:L:83:GLY:H     | 1.86                     | 0.41              |
| 1:L:280:ARG:HG3  | 1:L:304:PHE:CA   | 2.51                     | 0.41              |
| 1:M:211:ILE:HG22 | 1:M:288:GLU:OE1  | 2.21                     | 0.41              |
| 1:M:222:ALA:HA   | 1:M:275:ASN:CG   | 2.46                     | 0.41              |
| 1:O:31:GLY:HA3   | 1:O:437:ILE:HD12 | 2.02                     | 0.41              |
| 1:O:216:PRO:CG   | 1:O:295:GLY:HA2  | 2.51                     | 0.41              |
| 1:O:258:GLU:O    | 1:O:261:LYS:HB2  | 2.20                     | 0.41              |
| 1:O:381:LEU:HD22 | 1:O:381:LEU:C    | 2.45                     | 0.41              |
| 1:P:48:LEU:CD1   | 1:P:48:LEU:N     | 2.84                     | 0.41              |
| 1:P:182:ASN:CG   | 1:P:183:LEU:H    | 2.29                     | 0.41              |
| 1:P:185:ALA:HA   | 1:P:309:ARG:HG2  | 2.03                     | 0.41              |
| 1:P:452:LEU:HD11 | 1:P:456:HIS:HE1  | 1.84                     | 0.41              |
| 1:A:399:CYS:SG   | 1:A:464:GLY:HA3  | 2.61                     | 0.41              |
| 1:A:408:VAL:HG23 | 1:A:427:ALA:HB1  | 2.02                     | 0.41              |
| 1:C:396:GLY:O    | 1:C:475:MET:HE3  | 2.21                     | 0.41              |
| 1:D:82:VAL:CG1   | 1:D:83:GLY:H     | 2.34                     | 0.41              |
| 1:D:402:MET:HB3  | 1:D:456:HIS:CG   | 2.56                     | 0.41              |
| 1:D:455:ALA:HB2  | 1:D:472:ILE:HD12 | 2.03                     | 0.41              |
| 1:F:280:ARG:HG3  | 1:F:304:PHE:CA   | 2.50                     | 0.41              |
| 1:F:480:ILE:N    | 1:F:480:ILE:HD12 | 2.36                     | 0.41              |
| 1:G:82:VAL:HG21  | 1:G:483:SER:HB3  | 2.03                     | 0.41              |
| 1:G:103:LEU:HD21 | 1:G:113:ILE:HG21 | 2.03                     | 0.41              |
| 1:G:320:SER:HB2  | 1:G:321:THR:H    | 1.63                     | 0.41              |
| 1:H:219:ILE:HD12 | 1:H:275:ASN:HB3  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:186:ILE:HG23 | 1:K:360:ILE:HD12 | 2.02                     | 0.41              |
| 1:K:431:ARG:CZ   | 1:K:431:ARG:HA   | 2.51                     | 0.41              |
| 1:L:27:LYS:HA    | 1:L:30:LEU:HD13  | 2.03                     | 0.41              |
| 1:L:219:ILE:HD13 | 1:L:276:CYS:HB2  | 2.03                     | 0.41              |
| 1:M:40:LEU:HD22  | 1:M:41:SER:H     | 1.86                     | 0.41              |
| 1:M:117:TRP:O    | 1:M:120:ALA:HB3  | 2.21                     | 0.41              |
| 1:M:138:ASP:O    | 1:M:139:GLU:CB   | 2.68                     | 0.41              |
| 1:M:150:ALA:O    | 1:M:154:LEU:HD13 | 2.21                     | 0.41              |
| 1:N:397:GLY:O    | 1:N:465:LEU:HD23 | 2.20                     | 0.41              |
| 1:N:431:ARG:HH21 | 1:N:434:PRO:HG2  | 1.86                     | 0.41              |
| 1:O:411:LEU:O    | 1:O:415:THR:HG22 | 2.21                     | 0.41              |
| 1:P:207:LEU:HB3  | 1:P:347:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:117:TRP:HD1  | 1:A:495:ALA:HA   | 1.86                     | 0.40              |
| 1:A:231:MET:C    | 1:A:284:TYR:HB2  | 2.46                     | 0.40              |
| 1:A:398:GLY:HA2  | 1:A:401:GLU:CD   | 2.46                     | 0.40              |
| 1:A:443:TYR:CE2  | 1:A:470:GLY:HA3  | 2.56                     | 0.40              |
| 1:A:449:VAL:HG21 | 1:M:107:LYS:HD2  | 2.02                     | 0.40              |
| 1:B:216:PRO:HG2  | 1:B:295:GLY:C    | 2.45                     | 0.40              |
| 1:C:506:ASN:C    | 1:C:507:ILE:HG13 | 2.45                     | 0.40              |
| 1:D:27:LYS:HB2   | 1:D:436:ILE:HD13 | 2.03                     | 0.40              |
| 1:D:509:LYS:HG2  | 1:H:63:VAL:CG2   | 2.51                     | 0.40              |
| 1:E:30:LEU:HG    | 1:E:87:THR:O     | 2.20                     | 0.40              |
| 1:E:82:VAL:HA    | 1:E:386:GLN:HG3  | 2.03                     | 0.40              |
| 1:E:316:GLY:C    | 1:E:317:GLU:HG2  | 2.46                     | 0.40              |
| 1:E:452:LEU:HD13 | 1:E:465:LEU:HD13 | 2.03                     | 0.40              |
| 1:F:82:VAL:HA    | 1:F:386:GLN:HG3  | 2.03                     | 0.40              |
| 1:F:370:LEU:HD22 | 1:F:370:LEU:HA   | 1.81                     | 0.40              |
| 1:G:89:VAL:HB    | 1:G:490:VAL:HG23 | 2.02                     | 0.40              |
| 1:G:96:LEU:HD23  | 1:G:96:LEU:C     | 2.46                     | 0.40              |
| 1:G:176:ARG:HH22 | 1:G:360:ILE:HG13 | 1.83                     | 0.40              |
| 1:G:185:ALA:HB1  | 1:G:357:ALA:HB1  | 2.03                     | 0.40              |
| 1:G:399:CYS:SG   | 1:G:464:GLY:CA   | 3.06                     | 0.40              |
| 1:G:487:LYS:HA   | 1:G:490:VAL:HG12 | 2.03                     | 0.40              |
| 1:H:231:MET:HE3  | 1:H:265:LYS:HZ3  | 1.87                     | 0.40              |
| 1:I:436:ILE:HG21 | 1:I:436:ILE:HD13 | 1.87                     | 0.40              |
| 1:J:192:LEU:HD12 | 1:J:192:LEU:C    | 2.45                     | 0.40              |
| 1:J:207:LEU:HD22 | 1:J:208:ASP:H    | 1.85                     | 0.40              |
| 1:J:395:TYR:HE2  | 1:J:476:SER:HG   | 1.69                     | 0.40              |
| 1:K:280:ARG:O    | 1:K:281:GLN:CB   | 2.68                     | 0.40              |
| 1:K:280:ARG:O    | 1:K:281:GLN:HB3  | 2.21                     | 0.40              |
| 1:M:226:ILE:HB   | 1:M:317:GLU:OE2  | 2.21                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:152:THR:HG21 | 1:N:481:THR:O    | 2.21                     | 0.40              |
| 1:N:508:ILE:HA   | 1:N:508:ILE:HD13 | 1.72                     | 0.40              |
| 1:O:119:GLU:HG3  | 1:O:419:GLU:HB3  | 2.03                     | 0.40              |
| 1:O:147:MET:SD   | 1:O:168:LYS:HE2  | 2.61                     | 0.40              |
| 1:O:233:THR:HG21 | 1:O:261:LYS:CE   | 2.48                     | 0.40              |
| 1:P:140:VAL:HA   | 1:P:175:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:146:LEU:HD11 | 1:A:150:ALA:CB   | 2.52                     | 0.40              |
| 1:A:205:PHE:HA   | 1:A:359:THR:OG1  | 2.21                     | 0.40              |
| 1:B:92:LEU:CD1   | 1:B:92:LEU:N     | 2.84                     | 0.40              |
| 1:B:312:LEU:HD13 | 1:B:312:LEU:C    | 2.47                     | 0.40              |
| 1:C:112:THR:CG2  | 1:C:418:LYS:HD2  | 2.51                     | 0.40              |
| 1:C:173:ALA:HA   | 1:C:176:ARG:CZ   | 2.51                     | 0.40              |
| 1:C:280:ARG:HG2  | 1:C:302:ALA:O    | 2.21                     | 0.40              |
| 1:C:312:LEU:CD1  | 1:C:312:LEU:C    | 2.95                     | 0.40              |
| 1:C:421:VAL:O    | 1:C:424:GLU:HG2  | 2.21                     | 0.40              |
| 1:D:215:GLN:HG3  | 1:D:292:GLY:HA2  | 2.03                     | 0.40              |
| 1:D:310:LEU:O    | 1:D:313:VAL:HB   | 2.21                     | 0.40              |
| 1:D:322:PHE:HA   | 1:D:324:HIS:CD2  | 2.57                     | 0.40              |
| 1:D:411:LEU:HB3  | 1:D:423:MET:HE2  | 2.03                     | 0.40              |
| 1:E:41:SER:H     | 1:G:3:ALA:HA     | 1.86                     | 0.40              |
| 1:E:58:LEU:HB3   | 1:E:72:VAL:HG11  | 2.02                     | 0.40              |
| 1:E:93:ALA:HA    | 1:E:494:ALA:HB1  | 2.03                     | 0.40              |
| 1:F:171:VAL:O    | 1:F:175:LEU:HG   | 2.22                     | 0.40              |
| 1:G:219:ILE:HD12 | 1:G:275:ASN:CB   | 2.51                     | 0.40              |
| 1:G:421:VAL:O    | 1:G:424:GLU:HG2  | 2.21                     | 0.40              |
| 1:H:191:LYS:HB2  | 1:H:191:LYS:HE2  | 1.78                     | 0.40              |
| 1:H:215:GLN:HG3  | 1:H:292:GLY:HA2  | 2.03                     | 0.40              |
| 1:I:324:HIS:HB2  | 1:I:329:LYS:HE2  | 2.03                     | 0.40              |
| 1:J:209:LYS:CE   | 1:J:302:ALA:HA   | 2.50                     | 0.40              |
| 1:J:211:ILE:HG23 | 1:J:298:ALA:O    | 2.21                     | 0.40              |
| 1:K:64:ASP:C     | 1:K:66:PRO:HD2   | 2.46                     | 0.40              |
| 1:M:38:ILE:HD13  | 1:O:507:ILE:HG13 | 2.02                     | 0.40              |
| 1:M:225:LEU:HD12 | 1:M:225:LEU:C    | 2.46                     | 0.40              |
| 1:N:219:ILE:HD13 | 1:N:276:CYS:HB2  | 2.02                     | 0.40              |
| 1:N:484:PHE:HE2  | 1:N:488:ARG:HE   | 1.65                     | 0.40              |
| 1:O:57:ILE:HD13  | 1:O:57:ILE:O     | 2.21                     | 0.40              |
| 1:O:401:GLU:HG2  | 1:O:433:LEU:HD22 | 2.03                     | 0.40              |
| 1:P:240:GLY:O    | 1:P:241:SER:HB2  | 2.20                     | 0.40              |
| 1:P:321:THR:O    | 1:P:323:ASP:N    | 2.55                     | 0.40              |
| 1:P:393:THR:HB   | 1:P:481:THR:OG1  | 2.22                     | 0.40              |
| 1:A:310:LEU:O    | 1:A:314:THR:HG22 | 2.21                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:337:GLU:HG3  | 1:A:339:VAL:CG2  | 2.51                     | 0.40              |
| 1:C:487:LYS:HA   | 1:C:490:VAL:HG12 | 2.04                     | 0.40              |
| 1:D:81:GLU:OE1   | 1:D:81:GLU:HA    | 2.21                     | 0.40              |
| 1:D:216:PRO:CG   | 1:D:295:GLY:HA2  | 2.51                     | 0.40              |
| 1:D:354:LEU:HD21 | 1:D:356:GLU:HB3  | 2.04                     | 0.40              |
| 1:D:446:ALA:HA   | 1:K:418:LYS:HD3  | 2.02                     | 0.40              |
| 1:E:37:LYS:O     | 1:E:50:VAL:HA    | 2.21                     | 0.40              |
| 1:E:46:ALA:O     | 1:E:47:SER:HB2   | 2.22                     | 0.40              |
| 1:E:280:ARG:HG2  | 1:E:302:ALA:O    | 2.20                     | 0.40              |
| 1:F:27:LYS:HB2   | 1:F:436:ILE:CD1  | 2.51                     | 0.40              |
| 1:G:191:LYS:CE   | 1:G:346:LEU:HD21 | 2.51                     | 0.40              |
| 1:G:226:ILE:HD13 | 1:G:307:VAL:HG13 | 2.03                     | 0.40              |
| 1:H:38:ILE:HG22  | 1:H:50:VAL:HG12  | 2.03                     | 0.40              |
| 1:I:339:VAL:CG1  | 1:I:340:MET:N    | 2.83                     | 0.40              |
| 1:J:177:LEU:HG   | 1:J:381:LEU:HD21 | 2.03                     | 0.40              |
| 1:J:177:LEU:HD21 | 1:J:182:ASN:O    | 2.21                     | 0.40              |
| 1:J:384:LEU:N    | 1:J:384:LEU:HD13 | 2.37                     | 0.40              |
| 1:K:96:LEU:HD12  | 1:K:498:ALA:HB1  | 2.02                     | 0.40              |
| 1:K:418:LYS:NZ   | 1:K:418:LYS:HB3  | 2.36                     | 0.40              |
| 1:L:39:LEU:CD1   | 1:L:57:ILE:HD11  | 2.51                     | 0.40              |
| 1:L:39:LEU:HD13  | 1:L:513:ARG:HH22 | 1.85                     | 0.40              |
| 1:L:215:GLN:HE21 | 1:L:292:GLY:N    | 2.19                     | 0.40              |
| 1:M:39:LEU:HD12  | 1:M:57:ILE:CD1   | 2.52                     | 0.40              |
| 1:M:189:ILE:HG22 | 1:M:190:LYS:N    | 2.35                     | 0.40              |
| 1:N:143:ARG:HA   | 1:N:143:ARG:NE   | 2.35                     | 0.40              |
| 1:O:163:LYS:HA   | 1:O:166:PHE:HD1  | 1.82                     | 0.40              |
| 1:A:125:ARG:H    | 1:A:125:ARG:HG3  | 1.70                     | 0.40              |
| 1:C:50:VAL:HG13  | 1:C:375:ARG:HH21 | 1.87                     | 0.40              |
| 1:C:96:LEU:HD22  | 1:C:96:LEU:O     | 2.22                     | 0.40              |
| 1:C:390:ASP:HB3  | 1:C:485:GLN:CD   | 2.46                     | 0.40              |
| 1:D:19:ALA:HB1   | 1:D:94:ALA:HA    | 2.03                     | 0.40              |
| 1:D:59:LYS:HE2   | 1:D:76:ARG:HB2   | 2.02                     | 0.40              |
| 1:D:193:GLY:HA2  | 1:D:343:GLU:OE2  | 2.22                     | 0.40              |
| 1:D:233:THR:HG21 | 1:D:261:LYS:CE   | 2.51                     | 0.40              |
| 1:E:154:LEU:HD22 | 1:E:167:THR:HB   | 2.02                     | 0.40              |
| 1:E:244:ARG:CG   | 1:E:245:VAL:H    | 2.35                     | 0.40              |
| 1:G:40:LEU:HD13  | 1:G:40:LEU:C     | 2.46                     | 0.40              |
| 1:G:133:VAL:CG2  | 1:G:134:ASP:H    | 2.26                     | 0.40              |
| 1:G:154:LEU:CD2  | 1:G:163:LYS:HG3  | 2.49                     | 0.40              |
| 1:G:214:ASN:O    | 1:G:215:GLN:CB   | 2.66                     | 0.40              |
| 1:G:280:ARG:O    | 1:G:281:GLN:HB3  | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:146:LEU:HD13 | 1:H:168:LYS:HA   | 2.02                     | 0.40              |
| 1:I:106:LYS:CE   | 1:I:418:LYS:HD3  | 2.52                     | 0.40              |
| 1:I:321:THR:O    | 1:I:323:ASP:N    | 2.55                     | 0.40              |
| 1:J:12:ARG:CA    | 1:J:501:ILE:HD12 | 2.52                     | 0.40              |
| 1:J:381:LEU:HD13 | 1:J:381:LEU:C    | 2.47                     | 0.40              |
| 1:K:107:LYS:HE3  | 1:K:107:LYS:HB3  | 1.90                     | 0.40              |
| 1:K:433:LEU:HD12 | 1:K:433:LEU:H    | 1.86                     | 0.40              |
| 1:L:59:LYS:HZ1   | 1:L:76:ARG:N     | 2.20                     | 0.40              |
| 1:L:206:LEU:C    | 1:L:206:LEU:HD13 | 2.46                     | 0.40              |
| 1:L:206:LEU:H    | 1:L:359:THR:HG21 | 1.86                     | 0.40              |
| 1:M:75:SER:O     | 1:M:78:GLN:HB3   | 2.21                     | 0.40              |
| 1:M:367:GLN:C    | 1:M:369:ILE:H    | 2.29                     | 0.40              |
| 1:N:85:GLY:O     | 1:N:153:THR:HG23 | 2.22                     | 0.40              |
| 1:N:325:PRO:O    | 1:N:326:GLU:CG   | 2.65                     | 0.40              |
| 1:N:341:ILE:HG23 | 1:N:363:ARG:NH2  | 2.36                     | 0.40              |
| 1:O:88:SER:O     | 1:O:92:LEU:HD13  | 2.22                     | 0.40              |
| 1:O:280:ARG:O    | 1:O:281:GLN:HB3  | 2.22                     | 0.40              |
| 1:O:317:GLU:OE2  | 1:O:329:LYS:HE3  | 2.22                     | 0.40              |
| 1:O:452:LEU:HD11 | 1:O:456:HIS:CE1  | 2.56                     | 0.40              |
| 1:P:222:ALA:HB1  | 1:P:336:ILE:HD12 | 2.04                     | 0.40              |
| 1:A:163:LYS:O    | 1:A:166:PHE:HB2  | 2.21                     | 0.40              |
| 1:B:204:GLY:HA3  | 1:B:349:PHE:O    | 2.21                     | 0.40              |
| 1:B:291:PHE:HD1  | 1:B:296:VAL:CG1  | 2.35                     | 0.40              |
| 1:B:431:ARG:C    | 1:B:434:PRO:HD2  | 2.47                     | 0.40              |
| 1:B:510:ALA:HB3  | 1:G:25:LEU:CD1   | 2.51                     | 0.40              |
| 1:C:106:LYS:HZ3  | 1:C:108:ILE:HD11 | 1.86                     | 0.40              |
| 1:C:146:LEU:HB2  | 1:C:171:VAL:HG21 | 2.03                     | 0.40              |
| 1:E:39:LEU:HD21  | 1:G:508:ILE:O    | 2.21                     | 0.40              |
| 1:E:237:LYS:HG3  | 1:E:237:LYS:O    | 2.21                     | 0.40              |
| 1:E:418:LYS:HD2  | 1:J:450:ALA:CB   | 2.52                     | 0.40              |
| 1:F:22:ILE:HG13  | 1:F:23:GLY:N     | 2.37                     | 0.40              |
| 1:F:82:VAL:HA    | 1:F:386:GLN:CG   | 2.52                     | 0.40              |
| 1:F:178:LYS:CE   | 1:F:388:VAL:HG21 | 2.48                     | 0.40              |
| 1:F:284:TYR:CE2  | 1:F:286:TYR:CD1  | 3.09                     | 0.40              |
| 1:F:402:MET:HE3  | 1:F:453:ARG:CG   | 2.41                     | 0.40              |
| 1:G:146:LEU:HD13 | 1:G:167:THR:O    | 2.19                     | 0.40              |
| 1:G:173:ALA:O    | 1:G:176:ARG:HG2  | 2.21                     | 0.40              |
| 1:H:69:LYS:O     | 1:H:72:VAL:HB    | 2.22                     | 0.40              |
| 1:H:166:PHE:HZ   | 1:H:363:ARG:O    | 2.05                     | 0.40              |
| 1:H:321:THR:O    | 1:H:323:ASP:N    | 2.54                     | 0.40              |
| 1:H:449:VAL:HG12 | 1:H:453:ARG:NH1  | 2.36                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:63:VAL:HG21  | 1:K:1:ALA:CA     | 2.47                     | 0.40              |
| 1:J:185:ALA:HB1  | 1:J:357:ALA:HB1  | 2.03                     | 0.40              |
| 1:J:250:LYS:HG3  | 1:J:253:GLU:OE1  | 2.22                     | 0.40              |
| 1:K:222:ALA:HA   | 1:K:275:ASN:CB   | 2.52                     | 0.40              |
| 1:L:176:ARG:HH22 | 1:L:360:ILE:HG12 | 1.84                     | 0.40              |
| 1:L:186:ILE:HD12 | 1:L:381:LEU:HD21 | 2.02                     | 0.40              |
| 1:M:431:ARG:C    | 1:M:434:PRO:HD2  | 2.47                     | 0.40              |
| 1:M:433:LEU:CA   | 1:M:436:ILE:HG22 | 2.52                     | 0.40              |
| 1:M:452:LEU:HD11 | 1:M:456:HIS:CE1  | 2.57                     | 0.40              |
| 1:M:500:VAL:O    | 1:M:504:VAL:HB   | 2.22                     | 0.40              |
| 1:N:40:LEU:HD13  | 1:N:40:LEU:C     | 2.47                     | 0.40              |
| 1:N:322:PHE:HA   | 1:N:324:HIS:CD2  | 2.56                     | 0.40              |
| 1:P:59:LYS:HE2   | 1:P:76:ARG:CB    | 2.51                     | 0.40              |
| 1:P:372:GLU:HA   | 1:P:375:ARG:CZ   | 2.50                     | 0.40              |
| 1:P:416:PRO:HB2  | 1:P:419:GLU:OE1  | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 1   | A     | 511/513 (100%) | 459 (90%) | 30 (6%) | 22 (4%)  | 2           | 17 |
| 1   | B     | 511/513 (100%) | 455 (89%) | 27 (5%) | 29 (6%)  | 1           | 14 |
| 1   | C     | 486/513 (95%)  | 442 (91%) | 22 (4%) | 22 (4%)  | 2           | 17 |
| 1   | D     | 511/513 (100%) | 456 (89%) | 22 (4%) | 33 (6%)  | 1           | 12 |
| 1   | E     | 511/513 (100%) | 445 (87%) | 26 (5%) | 40 (8%)  | 1           | 10 |
| 1   | F     | 511/513 (100%) | 461 (90%) | 19 (4%) | 31 (6%)  | 1           | 13 |
| 1   | G     | 511/513 (100%) | 462 (90%) | 25 (5%) | 24 (5%)  | 2           | 16 |
| 1   | H     | 488/513 (95%)  | 437 (90%) | 24 (5%) | 27 (6%)  | 1           | 15 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | I     | 511/513 (100%)  | 453 (89%)  | 27 (5%)  | 31 (6%)  | 1           | 13 |
| 1   | J     | 511/513 (100%)  | 462 (90%)  | 27 (5%)  | 22 (4%)  | 2           | 17 |
| 1   | K     | 487/513 (95%)   | 444 (91%)  | 20 (4%)  | 23 (5%)  | 2           | 16 |
| 1   | L     | 486/513 (95%)   | 435 (90%)  | 28 (6%)  | 23 (5%)  | 2           | 16 |
| 1   | M     | 511/513 (100%)  | 455 (89%)  | 33 (6%)  | 23 (4%)  | 2           | 17 |
| 1   | N     | 489/513 (95%)   | 435 (89%)  | 30 (6%)  | 24 (5%)  | 1           | 16 |
| 1   | O     | 486/513 (95%)   | 445 (92%)  | 18 (4%)  | 23 (5%)  | 2           | 16 |
| 1   | P     | 511/513 (100%)  | 465 (91%)  | 21 (4%)  | 25 (5%)  | 1           | 16 |
| All | All   | 8032/8208 (98%) | 7211 (90%) | 399 (5%) | 422 (5%) | 2           | 15 |

All (422) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ALA  |
| 1   | A     | 82  | VAL  |
| 1   | A     | 84  | ASP  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 234 | ASP  |
| 1   | A     | 236 | ILE  |
| 1   | A     | 247 | SER  |
| 1   | A     | 281 | GLN  |
| 1   | A     | 325 | PRO  |
| 1   | A     | 366 | THR  |
| 1   | A     | 506 | ASN  |
| 1   | A     | 509 | LYS  |
| 1   | A     | 511 | ALA  |
| 1   | B     | 84  | ASP  |
| 1   | B     | 131 | SER  |
| 1   | B     | 141 | LYS  |
| 1   | B     | 215 | GLN  |
| 1   | B     | 234 | ASP  |
| 1   | B     | 236 | ILE  |
| 1   | B     | 241 | SER  |
| 1   | B     | 246 | ASP  |
| 1   | B     | 247 | SER  |
| 1   | B     | 281 | GLN  |
| 1   | B     | 326 | GLU  |
| 1   | B     | 357 | ALA  |
| 1   | B     | 366 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 369 | ILE  |
| 1   | C     | 3   | ALA  |
| 1   | C     | 31  | GLY  |
| 1   | C     | 215 | GLN  |
| 1   | C     | 274 | ILE  |
| 1   | C     | 281 | GLN  |
| 1   | C     | 509 | LYS  |
| 1   | C     | 511 | ALA  |
| 1   | D     | 8   | ALA  |
| 1   | D     | 68  | ALA  |
| 1   | D     | 131 | SER  |
| 1   | D     | 139 | GLU  |
| 1   | D     | 182 | ASN  |
| 1   | D     | 215 | GLN  |
| 1   | D     | 234 | ASP  |
| 1   | D     | 236 | ILE  |
| 1   | D     | 239 | PHE  |
| 1   | D     | 241 | SER  |
| 1   | D     | 242 | ARG  |
| 1   | D     | 244 | ARG  |
| 1   | D     | 246 | ASP  |
| 1   | D     | 247 | SER  |
| 1   | D     | 281 | GLN  |
| 1   | D     | 325 | PRO  |
| 1   | D     | 509 | LYS  |
| 1   | D     | 511 | ALA  |
| 1   | D     | 512 | PRO  |
| 1   | E     | 6   | GLU  |
| 1   | E     | 36  | ASP  |
| 1   | E     | 82  | VAL  |
| 1   | E     | 139 | GLU  |
| 1   | E     | 161 | HIS  |
| 1   | E     | 199 | SER  |
| 1   | E     | 220 | GLU  |
| 1   | E     | 234 | ASP  |
| 1   | E     | 237 | LYS  |
| 1   | E     | 244 | ARG  |
| 1   | E     | 245 | VAL  |
| 1   | E     | 325 | PRO  |
| 1   | E     | 366 | THR  |
| 1   | E     | 504 | VAL  |
| 1   | E     | 509 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 3   | ALA  |
| 1   | F     | 46  | ALA  |
| 1   | F     | 139 | GLU  |
| 1   | F     | 208 | ASP  |
| 1   | F     | 215 | GLN  |
| 1   | F     | 234 | ASP  |
| 1   | F     | 236 | ILE  |
| 1   | F     | 325 | PRO  |
| 1   | F     | 366 | THR  |
| 1   | F     | 510 | ALA  |
| 1   | F     | 511 | ALA  |
| 1   | F     | 512 | PRO  |
| 1   | G     | 5   | GLU  |
| 1   | G     | 34  | GLY  |
| 1   | G     | 82  | VAL  |
| 1   | G     | 141 | LYS  |
| 1   | G     | 182 | ASN  |
| 1   | G     | 215 | GLN  |
| 1   | G     | 234 | ASP  |
| 1   | G     | 326 | GLU  |
| 1   | G     | 342 | GLY  |
| 1   | G     | 366 | THR  |
| 1   | G     | 508 | ILE  |
| 1   | H     | 11  | ALA  |
| 1   | H     | 108 | ILE  |
| 1   | H     | 131 | SER  |
| 1   | H     | 139 | GLU  |
| 1   | H     | 190 | LYS  |
| 1   | H     | 215 | GLN  |
| 1   | H     | 366 | THR  |
| 1   | H     | 511 | ALA  |
| 1   | H     | 512 | PRO  |
| 1   | I     | 41  | SER  |
| 1   | I     | 46  | ALA  |
| 1   | I     | 82  | VAL  |
| 1   | I     | 84  | ASP  |
| 1   | I     | 137 | SER  |
| 1   | I     | 139 | GLU  |
| 1   | I     | 182 | ASN  |
| 1   | I     | 215 | GLN  |
| 1   | I     | 236 | ILE  |
| 1   | I     | 240 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 281 | GLN  |
| 1   | I     | 325 | PRO  |
| 1   | I     | 366 | THR  |
| 1   | I     | 508 | ILE  |
| 1   | I     | 509 | LYS  |
| 1   | I     | 511 | ALA  |
| 1   | I     | 512 | PRO  |
| 1   | J     | 6   | GLU  |
| 1   | J     | 8   | ALA  |
| 1   | J     | 139 | GLU  |
| 1   | J     | 215 | GLN  |
| 1   | J     | 234 | ASP  |
| 1   | J     | 236 | ILE  |
| 1   | J     | 241 | SER  |
| 1   | J     | 281 | GLN  |
| 1   | J     | 325 | PRO  |
| 1   | J     | 509 | LYS  |
| 1   | K     | 46  | ALA  |
| 1   | K     | 68  | ALA  |
| 1   | K     | 133 | VAL  |
| 1   | K     | 137 | SER  |
| 1   | K     | 139 | GLU  |
| 1   | K     | 141 | LYS  |
| 1   | K     | 215 | GLN  |
| 1   | K     | 281 | GLN  |
| 1   | K     | 322 | PHE  |
| 1   | K     | 325 | PRO  |
| 1   | K     | 366 | THR  |
| 1   | K     | 506 | ASN  |
| 1   | K     | 510 | ALA  |
| 1   | K     | 512 | PRO  |
| 1   | L     | 68  | ALA  |
| 1   | L     | 82  | VAL  |
| 1   | L     | 127 | ALA  |
| 1   | L     | 139 | GLU  |
| 1   | L     | 142 | PHE  |
| 1   | L     | 160 | THR  |
| 1   | L     | 215 | GLN  |
| 1   | L     | 281 | GLN  |
| 1   | L     | 325 | PRO  |
| 1   | L     | 368 | GLN  |
| 1   | L     | 508 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 509 | LYS  |
| 1   | M     | 30  | LEU  |
| 1   | M     | 131 | SER  |
| 1   | M     | 139 | GLU  |
| 1   | M     | 141 | LYS  |
| 1   | M     | 159 | LEU  |
| 1   | M     | 215 | GLN  |
| 1   | M     | 246 | ASP  |
| 1   | M     | 416 | PRO  |
| 1   | N     | 4   | ASP  |
| 1   | N     | 8   | ALA  |
| 1   | N     | 131 | SER  |
| 1   | N     | 139 | GLU  |
| 1   | N     | 326 | GLU  |
| 1   | N     | 508 | ILE  |
| 1   | N     | 509 | LYS  |
| 1   | N     | 511 | ALA  |
| 1   | N     | 512 | PRO  |
| 1   | O     | 3   | ALA  |
| 1   | O     | 68  | ALA  |
| 1   | O     | 82  | VAL  |
| 1   | O     | 131 | SER  |
| 1   | O     | 215 | GLN  |
| 1   | O     | 340 | MET  |
| 1   | O     | 366 | THR  |
| 1   | O     | 507 | ILE  |
| 1   | P     | 48  | LEU  |
| 1   | P     | 82  | VAL  |
| 1   | P     | 135 | HIS  |
| 1   | P     | 136 | GLY  |
| 1   | P     | 138 | ASP  |
| 1   | P     | 140 | VAL  |
| 1   | P     | 215 | GLN  |
| 1   | P     | 234 | ASP  |
| 1   | P     | 239 | PHE  |
| 1   | P     | 243 | VAL  |
| 1   | P     | 366 | THR  |
| 1   | P     | 506 | ASN  |
| 1   | P     | 508 | ILE  |
| 1   | P     | 512 | PRO  |
| 1   | A     | 68  | ALA  |
| 1   | A     | 215 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 274 | ILE  |
| 1   | A     | 322 | PHE  |
| 1   | B     | 8   | ALA  |
| 1   | B     | 68  | ALA  |
| 1   | B     | 82  | VAL  |
| 1   | B     | 107 | LYS  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 132 | ALA  |
| 1   | B     | 133 | VAL  |
| 1   | B     | 136 | GLY  |
| 1   | B     | 274 | ILE  |
| 1   | B     | 319 | ALA  |
| 1   | B     | 322 | PHE  |
| 1   | C     | 8   | ALA  |
| 1   | C     | 68  | ALA  |
| 1   | C     | 82  | VAL  |
| 1   | C     | 140 | VAL  |
| 1   | C     | 160 | THR  |
| 1   | C     | 322 | PHE  |
| 1   | C     | 342 | GLY  |
| 1   | C     | 343 | GLU  |
| 1   | C     | 417 | GLY  |
| 1   | C     | 507 | ILE  |
| 1   | D     | 82  | VAL  |
| 1   | D     | 108 | ILE  |
| 1   | D     | 141 | LYS  |
| 1   | D     | 160 | THR  |
| 1   | D     | 181 | GLY  |
| 1   | D     | 274 | ILE  |
| 1   | D     | 322 | PHE  |
| 1   | D     | 508 | ILE  |
| 1   | E     | 68  | ALA  |
| 1   | E     | 123 | ALA  |
| 1   | E     | 129 | LEU  |
| 1   | E     | 135 | HIS  |
| 1   | E     | 140 | VAL  |
| 1   | E     | 274 | ILE  |
| 1   | E     | 322 | PHE  |
| 1   | E     | 331 | GLY  |
| 1   | E     | 342 | GLY  |
| 1   | F     | 8   | ALA  |
| 1   | F     | 68  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 141 | LYS  |
| 1   | F     | 274 | ILE  |
| 1   | F     | 322 | PHE  |
| 1   | F     | 342 | GLY  |
| 1   | F     | 417 | GLY  |
| 1   | F     | 508 | ILE  |
| 1   | G     | 3   | ALA  |
| 1   | G     | 68  | ALA  |
| 1   | G     | 131 | SER  |
| 1   | G     | 134 | ASP  |
| 1   | G     | 139 | GLU  |
| 1   | G     | 236 | ILE  |
| 1   | G     | 274 | ILE  |
| 1   | G     | 322 | PHE  |
| 1   | H     | 161 | HIS  |
| 1   | H     | 274 | ILE  |
| 1   | H     | 322 | PHE  |
| 1   | H     | 417 | GLY  |
| 1   | H     | 506 | ASN  |
| 1   | I     | 8   | ALA  |
| 1   | I     | 141 | LYS  |
| 1   | I     | 234 | ASP  |
| 1   | I     | 246 | ASP  |
| 1   | I     | 247 | SER  |
| 1   | I     | 274 | ILE  |
| 1   | I     | 322 | PHE  |
| 1   | J     | 68  | ALA  |
| 1   | J     | 141 | LYS  |
| 1   | J     | 246 | ASP  |
| 1   | J     | 274 | ILE  |
| 1   | J     | 322 | PHE  |
| 1   | J     | 366 | THR  |
| 1   | K     | 8   | ALA  |
| 1   | K     | 274 | ILE  |
| 1   | K     | 504 | VAL  |
| 1   | K     | 507 | ILE  |
| 1   | L     | 8   | ALA  |
| 1   | L     | 114 | ILE  |
| 1   | L     | 141 | LYS  |
| 1   | L     | 274 | ILE  |
| 1   | L     | 322 | PHE  |
| 1   | L     | 502 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 4   | ASP  |
| 1   | M     | 8   | ALA  |
| 1   | M     | 47  | SER  |
| 1   | M     | 68  | ALA  |
| 1   | M     | 234 | ASP  |
| 1   | M     | 236 | ILE  |
| 1   | M     | 249 | ALA  |
| 1   | M     | 274 | ILE  |
| 1   | M     | 322 | PHE  |
| 1   | M     | 511 | ALA  |
| 1   | N     | 68  | ALA  |
| 1   | N     | 81  | GLU  |
| 1   | N     | 82  | VAL  |
| 1   | N     | 141 | LYS  |
| 1   | N     | 146 | LEU  |
| 1   | N     | 183 | LEU  |
| 1   | N     | 196 | LEU  |
| 1   | N     | 274 | ILE  |
| 1   | N     | 322 | PHE  |
| 1   | O     | 8   | ALA  |
| 1   | O     | 141 | LYS  |
| 1   | O     | 159 | LEU  |
| 1   | O     | 181 | GLY  |
| 1   | O     | 274 | ILE  |
| 1   | P     | 68  | ALA  |
| 1   | P     | 114 | ILE  |
| 1   | P     | 141 | LYS  |
| 1   | P     | 274 | ILE  |
| 1   | P     | 322 | PHE  |
| 1   | P     | 325 | PRO  |
| 1   | A     | 88  | SER  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 416 | PRO  |
| 1   | B     | 32  | PRO  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 417 | GLY  |
| 1   | B     | 512 | PRO  |
| 1   | C     | 141 | LYS  |
| 1   | C     | 159 | LEU  |
| 1   | C     | 325 | PRO  |
| 1   | D     | 183 | LEU  |
| 1   | D     | 335 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 159 | LEU  |
| 1   | E     | 236 | ILE  |
| 1   | E     | 281 | GLN  |
| 1   | F     | 197 | ALA  |
| 1   | F     | 281 | GLN  |
| 1   | F     | 343 | GLU  |
| 1   | G     | 281 | GLN  |
| 1   | H     | 3   | ALA  |
| 1   | H     | 88  | SER  |
| 1   | H     | 130 | ASN  |
| 1   | H     | 141 | LYS  |
| 1   | H     | 182 | ASN  |
| 1   | H     | 281 | GLN  |
| 1   | H     | 340 | MET  |
| 1   | H     | 510 | ALA  |
| 1   | I     | 107 | LYS  |
| 1   | J     | 88  | SER  |
| 1   | J     | 129 | LEU  |
| 1   | K     | 132 | ALA  |
| 1   | K     | 184 | GLU  |
| 1   | L     | 47  | SER  |
| 1   | L     | 181 | GLY  |
| 1   | L     | 182 | ASN  |
| 1   | M     | 140 | VAL  |
| 1   | M     | 325 | PRO  |
| 1   | N     | 133 | VAL  |
| 1   | N     | 180 | SER  |
| 1   | N     | 281 | GLN  |
| 1   | O     | 84  | ASP  |
| 1   | O     | 139 | GLU  |
| 1   | O     | 281 | GLN  |
| 1   | O     | 322 | PHE  |
| 1   | O     | 335 | LEU  |
| 1   | P     | 84  | ASP  |
| 1   | P     | 281 | GLN  |
| 1   | P     | 509 | LYS  |
| 1   | A     | 114 | ILE  |
| 1   | C     | 46  | ALA  |
| 1   | D     | 84  | ASP  |
| 1   | D     | 199 | SER  |
| 1   | D     | 367 | GLN  |
| 1   | E     | 134 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 141 | LYS  |
| 1   | E     | 412 | ALA  |
| 1   | E     | 506 | ASN  |
| 1   | H     | 140 | VAL  |
| 1   | I     | 123 | ALA  |
| 1   | J     | 510 | ALA  |
| 1   | J     | 512 | PRO  |
| 1   | K     | 140 | VAL  |
| 1   | E     | 8   | ALA  |
| 1   | E     | 47  | SER  |
| 1   | E     | 192 | LEU  |
| 1   | F     | 114 | ILE  |
| 1   | F     | 241 | SER  |
| 1   | F     | 326 | GLU  |
| 1   | G     | 320 | SER  |
| 1   | I     | 68  | ALA  |
| 1   | I     | 133 | VAL  |
| 1   | J     | 140 | VAL  |
| 1   | K     | 159 | LEU  |
| 1   | O     | 160 | THR  |
| 1   | C     | 320 | SER  |
| 1   | E     | 41  | SER  |
| 1   | G     | 238 | ILE  |
| 1   | K     | 182 | ASN  |
| 1   | L     | 108 | ILE  |
| 1   | L     | 417 | GLY  |
| 1   | M     | 108 | ILE  |
| 1   | M     | 241 | SER  |
| 1   | M     | 508 | ILE  |
| 1   | N     | 140 | VAL  |
| 1   | O     | 140 | VAL  |
| 1   | O     | 326 | GLU  |
| 1   | E     | 43  | GLY  |
| 1   | E     | 114 | ILE  |
| 1   | E     | 512 | PRO  |
| 1   | F     | 108 | ILE  |
| 1   | I     | 140 | VAL  |
| 1   | A     | 507 | ILE  |
| 1   | F     | 181 | GLY  |
| 1   | F     | 238 | ILE  |
| 1   | G     | 140 | VAL  |
| 1   | G     | 507 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 508 | ILE  |
| 1   | N     | 342 | GLY  |
| 1   | N     | 416 | PRO  |
| 1   | O     | 133 | VAL  |
| 1   | E     | 108 | ILE  |
| 1   | H     | 189 | ILE  |
| 1   | H     | 342 | GLY  |
| 1   | I     | 507 | ILE  |
| 1   | J     | 82  | VAL  |
| 1   | O     | 108 | ILE  |
| 1   | P     | 108 | ILE  |
| 1   | D     | 140 | VAL  |
| 1   | E     | 215 | GLN  |
| 1   | F     | 82  | VAL  |
| 1   | F     | 140 | VAL  |
| 1   | H     | 364 | GLY  |
| 1   | I     | 181 | GLY  |
| 1   | P     | 342 | GLY  |

### 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     | 409/409 (100%) | 359 (88%) | 50 (12%) | 5           | 17 |
| 1   | B     | 409/409 (100%) | 368 (90%) | 41 (10%) | 7           | 24 |
| 1   | C     | 389/409 (95%)  | 344 (88%) | 45 (12%) | 5           | 18 |
| 1   | D     | 409/409 (100%) | 362 (88%) | 47 (12%) | 5           | 18 |
| 1   | E     | 409/409 (100%) | 367 (90%) | 42 (10%) | 7           | 23 |
| 1   | F     | 409/409 (100%) | 364 (89%) | 45 (11%) | 6           | 20 |
| 1   | G     | 409/409 (100%) | 363 (89%) | 46 (11%) | 6           | 19 |
| 1   | H     | 391/409 (96%)  | 348 (89%) | 43 (11%) | 6           | 20 |
| 1   | I     | 409/409 (100%) | 364 (89%) | 45 (11%) | 6           | 20 |
| 1   | J     | 409/409 (100%) | 370 (90%) | 39 (10%) | 8           | 25 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | K     | 390/409 (95%)   | 347 (89%)  | 43 (11%)  | 6           | 20 |
| 1   | L     | 390/409 (95%)   | 350 (90%)  | 40 (10%)  | 7           | 23 |
| 1   | M     | 409/409 (100%)  | 372 (91%)  | 37 (9%)   | 9           | 27 |
| 1   | N     | 392/409 (96%)   | 340 (87%)  | 52 (13%)  | 4           | 14 |
| 1   | O     | 390/409 (95%)   | 349 (90%)  | 41 (10%)  | 6           | 21 |
| 1   | P     | 409/409 (100%)  | 362 (88%)  | 47 (12%)  | 5           | 18 |
| All | All   | 6432/6544 (98%) | 5729 (89%) | 703 (11%) | 8           | 21 |

All (703) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ARG  |
| 1   | A     | 40  | LEU  |
| 1   | A     | 41  | SER  |
| 1   | A     | 50  | VAL  |
| 1   | A     | 57  | ILE  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 65  | ASN  |
| 1   | A     | 89  | VAL  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 98  | ARG  |
| 1   | A     | 121 | THR  |
| 1   | A     | 125 | ARG  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 133 | VAL  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 143 | ARG  |
| 1   | A     | 146 | LEU  |
| 1   | A     | 152 | THR  |
| 1   | A     | 159 | LEU  |
| 1   | A     | 160 | THR  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 203 | GLU  |
| 1   | A     | 207 | LEU  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 236 | ILE  |
| 1   | A     | 247 | SER  |
| 1   | A     | 248 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 269 | ILE  |
| 1   | A     | 280 | ARG  |
| 1   | A     | 288 | GLU  |
| 1   | A     | 312 | LEU  |
| 1   | A     | 317 | GLU  |
| 1   | A     | 320 | SER  |
| 1   | A     | 326 | GLU  |
| 1   | A     | 328 | VAL  |
| 1   | A     | 330 | LEU  |
| 1   | A     | 339 | VAL  |
| 1   | A     | 343 | GLU  |
| 1   | A     | 352 | VAL  |
| 1   | A     | 369 | ILE  |
| 1   | A     | 381 | LEU  |
| 1   | A     | 401 | GLU  |
| 1   | A     | 402 | MET  |
| 1   | A     | 409 | THR  |
| 1   | A     | 431 | ARG  |
| 1   | A     | 465 | LEU  |
| 1   | A     | 489 | GLN  |
| 1   | A     | 503 | ARG  |
| 1   | B     | 9   | GLU  |
| 1   | B     | 33  | LYS  |
| 1   | B     | 38  | ILE  |
| 1   | B     | 50  | VAL  |
| 1   | B     | 57  | ILE  |
| 1   | B     | 58  | LEU  |
| 1   | B     | 92  | LEU  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 98  | ARG  |
| 1   | B     | 108 | ILE  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 146 | LEU  |
| 1   | B     | 152 | THR  |
| 1   | B     | 159 | LEU  |
| 1   | B     | 167 | THR  |
| 1   | B     | 183 | LEU  |
| 1   | B     | 192 | LEU  |
| 1   | B     | 207 | LEU  |
| 1   | B     | 211 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 225 | LEU  |
| 1   | B     | 236 | ILE  |
| 1   | B     | 241 | SER  |
| 1   | B     | 243 | VAL  |
| 1   | B     | 248 | THR  |
| 1   | B     | 280 | ARG  |
| 1   | B     | 300 | GLU  |
| 1   | B     | 333 | CYS  |
| 1   | B     | 341 | ILE  |
| 1   | B     | 352 | VAL  |
| 1   | B     | 367 | GLN  |
| 1   | B     | 369 | ILE  |
| 1   | B     | 401 | GLU  |
| 1   | B     | 402 | MET  |
| 1   | B     | 409 | THR  |
| 1   | B     | 418 | LYS  |
| 1   | B     | 465 | LEU  |
| 1   | B     | 469 | GLU  |
| 1   | B     | 485 | GLN  |
| 1   | B     | 492 | LEU  |
| 1   | C     | 25  | LEU  |
| 1   | C     | 29  | THR  |
| 1   | C     | 40  | LEU  |
| 1   | C     | 48  | LEU  |
| 1   | C     | 52  | ASN  |
| 1   | C     | 57  | ILE  |
| 1   | C     | 58  | LEU  |
| 1   | C     | 59  | LYS  |
| 1   | C     | 81  | GLU  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 98  | ARG  |
| 1   | C     | 135 | HIS  |
| 1   | C     | 138 | ASP  |
| 1   | C     | 139 | GLU  |
| 1   | C     | 146 | LEU  |
| 1   | C     | 152 | THR  |
| 1   | C     | 159 | LEU  |
| 1   | C     | 192 | LEU  |
| 1   | C     | 201 | LEU  |
| 1   | C     | 207 | LEU  |
| 1   | C     | 211 | ILE  |
| 1   | C     | 225 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 263 | LYS  |
| 1   | C     | 269 | ILE  |
| 1   | C     | 280 | ARG  |
| 1   | C     | 308 | GLU  |
| 1   | C     | 312 | LEU  |
| 1   | C     | 314 | THR  |
| 1   | C     | 320 | SER  |
| 1   | C     | 326 | GLU  |
| 1   | C     | 329 | LYS  |
| 1   | C     | 352 | VAL  |
| 1   | C     | 354 | LEU  |
| 1   | C     | 383 | VAL  |
| 1   | C     | 391 | SER  |
| 1   | C     | 401 | GLU  |
| 1   | C     | 402 | MET  |
| 1   | C     | 423 | MET  |
| 1   | C     | 430 | LEU  |
| 1   | C     | 478 | LEU  |
| 1   | C     | 493 | SER  |
| 1   | C     | 496 | GLU  |
| 1   | C     | 502 | LEU  |
| 1   | C     | 504 | VAL  |
| 1   | C     | 509 | LYS  |
| 1   | D     | 17  | ILE  |
| 1   | D     | 48  | LEU  |
| 1   | D     | 50  | VAL  |
| 1   | D     | 57  | ILE  |
| 1   | D     | 96  | LEU  |
| 1   | D     | 98  | ARG  |
| 1   | D     | 126 | GLN  |
| 1   | D     | 143 | ARG  |
| 1   | D     | 146 | LEU  |
| 1   | D     | 159 | LEU  |
| 1   | D     | 167 | THR  |
| 1   | D     | 180 | SER  |
| 1   | D     | 182 | ASN  |
| 1   | D     | 189 | ILE  |
| 1   | D     | 196 | LEU  |
| 1   | D     | 207 | LEU  |
| 1   | D     | 211 | ILE  |
| 1   | D     | 215 | GLN  |
| 1   | D     | 219 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 225 | LEU  |
| 1   | D     | 231 | MET  |
| 1   | D     | 236 | ILE  |
| 1   | D     | 238 | ILE  |
| 1   | D     | 245 | VAL  |
| 1   | D     | 269 | ILE  |
| 1   | D     | 280 | ARG  |
| 1   | D     | 284 | TYR  |
| 1   | D     | 288 | GLU  |
| 1   | D     | 317 | GLU  |
| 1   | D     | 326 | GLU  |
| 1   | D     | 330 | LEU  |
| 1   | D     | 341 | ILE  |
| 1   | D     | 343 | GLU  |
| 1   | D     | 346 | LEU  |
| 1   | D     | 352 | VAL  |
| 1   | D     | 366 | THR  |
| 1   | D     | 367 | GLN  |
| 1   | D     | 381 | LEU  |
| 1   | D     | 401 | GLU  |
| 1   | D     | 402 | MET  |
| 1   | D     | 409 | THR  |
| 1   | D     | 415 | THR  |
| 1   | D     | 465 | LEU  |
| 1   | D     | 489 | GLN  |
| 1   | D     | 508 | ILE  |
| 1   | D     | 509 | LYS  |
| 1   | D     | 512 | PRO  |
| 1   | E     | 30  | LEU  |
| 1   | E     | 33  | LYS  |
| 1   | E     | 40  | LEU  |
| 1   | E     | 42  | SER  |
| 1   | E     | 48  | LEU  |
| 1   | E     | 57  | ILE  |
| 1   | E     | 58  | LEU  |
| 1   | E     | 74  | MET  |
| 1   | E     | 96  | LEU  |
| 1   | E     | 98  | ARG  |
| 1   | E     | 107 | LYS  |
| 1   | E     | 129 | LEU  |
| 1   | E     | 134 | ASP  |
| 1   | E     | 143 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 146 | LEU  |
| 1   | E     | 159 | LEU  |
| 1   | E     | 167 | THR  |
| 1   | E     | 178 | LYS  |
| 1   | E     | 201 | LEU  |
| 1   | E     | 207 | LEU  |
| 1   | E     | 211 | ILE  |
| 1   | E     | 215 | GLN  |
| 1   | E     | 219 | ILE  |
| 1   | E     | 225 | LEU  |
| 1   | E     | 244 | ARG  |
| 1   | E     | 258 | GLU  |
| 1   | E     | 269 | ILE  |
| 1   | E     | 271 | LYS  |
| 1   | E     | 280 | ARG  |
| 1   | E     | 346 | LEU  |
| 1   | E     | 352 | VAL  |
| 1   | E     | 391 | SER  |
| 1   | E     | 402 | MET  |
| 1   | E     | 409 | THR  |
| 1   | E     | 428 | LYS  |
| 1   | E     | 430 | LEU  |
| 1   | E     | 465 | LEU  |
| 1   | E     | 469 | GLU  |
| 1   | E     | 476 | SER  |
| 1   | E     | 485 | GLN  |
| 1   | E     | 489 | GLN  |
| 1   | E     | 513 | ARG  |
| 1   | F     | 10  | THR  |
| 1   | F     | 27  | LYS  |
| 1   | F     | 40  | LEU  |
| 1   | F     | 48  | LEU  |
| 1   | F     | 57  | ILE  |
| 1   | F     | 58  | LEU  |
| 1   | F     | 96  | LEU  |
| 1   | F     | 108 | ILE  |
| 1   | F     | 128 | LEU  |
| 1   | F     | 129 | LEU  |
| 1   | F     | 139 | GLU  |
| 1   | F     | 146 | LEU  |
| 1   | F     | 159 | LEU  |
| 1   | F     | 167 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 182 | ASN  |
| 1   | F     | 191 | LYS  |
| 1   | F     | 196 | LEU  |
| 1   | F     | 201 | LEU  |
| 1   | F     | 211 | ILE  |
| 1   | F     | 225 | LEU  |
| 1   | F     | 235 | LYS  |
| 1   | F     | 238 | ILE  |
| 1   | F     | 244 | ARG  |
| 1   | F     | 245 | VAL  |
| 1   | F     | 247 | SER  |
| 1   | F     | 269 | ILE  |
| 1   | F     | 280 | ARG  |
| 1   | F     | 312 | LEU  |
| 1   | F     | 317 | GLU  |
| 1   | F     | 320 | SER  |
| 1   | F     | 326 | GLU  |
| 1   | F     | 346 | LEU  |
| 1   | F     | 352 | VAL  |
| 1   | F     | 367 | GLN  |
| 1   | F     | 370 | LEU  |
| 1   | F     | 381 | LEU  |
| 1   | F     | 391 | SER  |
| 1   | F     | 401 | GLU  |
| 1   | F     | 402 | MET  |
| 1   | F     | 409 | THR  |
| 1   | F     | 428 | LYS  |
| 1   | F     | 431 | ARG  |
| 1   | F     | 465 | LEU  |
| 1   | F     | 469 | GLU  |
| 1   | F     | 485 | GLN  |
| 1   | G     | 48  | LEU  |
| 1   | G     | 49  | MET  |
| 1   | G     | 58  | LEU  |
| 1   | G     | 65  | ASN  |
| 1   | G     | 74  | MET  |
| 1   | G     | 89  | VAL  |
| 1   | G     | 98  | ARG  |
| 1   | G     | 108 | ILE  |
| 1   | G     | 111 | GLN  |
| 1   | G     | 128 | LEU  |
| 1   | G     | 129 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 142 | PHE  |
| 1   | G     | 146 | LEU  |
| 1   | G     | 159 | LEU  |
| 1   | G     | 161 | HIS  |
| 1   | G     | 167 | THR  |
| 1   | G     | 177 | LEU  |
| 1   | G     | 178 | LYS  |
| 1   | G     | 207 | LEU  |
| 1   | G     | 211 | ILE  |
| 1   | G     | 225 | LEU  |
| 1   | G     | 231 | MET  |
| 1   | G     | 235 | LYS  |
| 1   | G     | 239 | PHE  |
| 1   | G     | 241 | SER  |
| 1   | G     | 242 | ARG  |
| 1   | G     | 244 | ARG  |
| 1   | G     | 246 | ASP  |
| 1   | G     | 251 | VAL  |
| 1   | G     | 269 | ILE  |
| 1   | G     | 280 | ARG  |
| 1   | G     | 310 | LEU  |
| 1   | G     | 320 | SER  |
| 1   | G     | 330 | LEU  |
| 1   | G     | 339 | VAL  |
| 1   | G     | 340 | MET  |
| 1   | G     | 344 | ASP  |
| 1   | G     | 352 | VAL  |
| 1   | G     | 381 | LEU  |
| 1   | G     | 388 | VAL  |
| 1   | G     | 402 | MET  |
| 1   | G     | 409 | THR  |
| 1   | G     | 431 | ARG  |
| 1   | G     | 465 | LEU  |
| 1   | G     | 501 | ILE  |
| 1   | G     | 508 | ILE  |
| 1   | H     | 12  | ARG  |
| 1   | H     | 44  | ARG  |
| 1   | H     | 50  | VAL  |
| 1   | H     | 57  | ILE  |
| 1   | H     | 58  | LEU  |
| 1   | H     | 96  | LEU  |
| 1   | H     | 98  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 99  | GLU  |
| 1   | H     | 106 | LYS  |
| 1   | H     | 108 | ILE  |
| 1   | H     | 126 | GLN  |
| 1   | H     | 139 | GLU  |
| 1   | H     | 140 | VAL  |
| 1   | H     | 141 | LYS  |
| 1   | H     | 146 | LEU  |
| 1   | H     | 159 | LEU  |
| 1   | H     | 160 | THR  |
| 1   | H     | 167 | THR  |
| 1   | H     | 182 | ASN  |
| 1   | H     | 190 | LYS  |
| 1   | H     | 191 | LYS  |
| 1   | H     | 203 | GLU  |
| 1   | H     | 207 | LEU  |
| 1   | H     | 211 | ILE  |
| 1   | H     | 223 | LYS  |
| 1   | H     | 225 | LEU  |
| 1   | H     | 280 | ARG  |
| 1   | H     | 310 | LEU  |
| 1   | H     | 312 | LEU  |
| 1   | H     | 320 | SER  |
| 1   | H     | 326 | GLU  |
| 1   | H     | 335 | LEU  |
| 1   | H     | 340 | MET  |
| 1   | H     | 344 | ASP  |
| 1   | H     | 362 | LEU  |
| 1   | H     | 402 | MET  |
| 1   | H     | 432 | MET  |
| 1   | H     | 436 | ILE  |
| 1   | H     | 492 | LEU  |
| 1   | H     | 493 | SER  |
| 1   | H     | 509 | LYS  |
| 1   | H     | 512 | PRO  |
| 1   | H     | 513 | ARG  |
| 1   | I     | 27  | LYS  |
| 1   | I     | 40  | LEU  |
| 1   | I     | 48  | LEU  |
| 1   | I     | 57  | ILE  |
| 1   | I     | 58  | LEU  |
| 1   | I     | 74  | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 81  | GLU  |
| 1   | I     | 96  | LEU  |
| 1   | I     | 98  | ARG  |
| 1   | I     | 106 | LYS  |
| 1   | I     | 141 | LYS  |
| 1   | I     | 146 | LEU  |
| 1   | I     | 152 | THR  |
| 1   | I     | 159 | LEU  |
| 1   | I     | 167 | THR  |
| 1   | I     | 177 | LEU  |
| 1   | I     | 190 | LYS  |
| 1   | I     | 207 | LEU  |
| 1   | I     | 211 | ILE  |
| 1   | I     | 215 | GLN  |
| 1   | I     | 225 | LEU  |
| 1   | I     | 261 | LYS  |
| 1   | I     | 280 | ARG  |
| 1   | I     | 312 | LEU  |
| 1   | I     | 317 | GLU  |
| 1   | I     | 320 | SER  |
| 1   | I     | 326 | GLU  |
| 1   | I     | 328 | VAL  |
| 1   | I     | 330 | LEU  |
| 1   | I     | 335 | LEU  |
| 1   | I     | 346 | LEU  |
| 1   | I     | 352 | VAL  |
| 1   | I     | 367 | GLN  |
| 1   | I     | 368 | GLN  |
| 1   | I     | 381 | LEU  |
| 1   | I     | 401 | GLU  |
| 1   | I     | 402 | MET  |
| 1   | I     | 409 | THR  |
| 1   | I     | 414 | ARG  |
| 1   | I     | 418 | LYS  |
| 1   | I     | 445 | SER  |
| 1   | I     | 480 | ILE  |
| 1   | I     | 501 | ILE  |
| 1   | I     | 502 | LEU  |
| 1   | I     | 512 | PRO  |
| 1   | J     | 33  | LYS  |
| 1   | J     | 38  | ILE  |
| 1   | J     | 40  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 50  | VAL  |
| 1   | J     | 57  | ILE  |
| 1   | J     | 58  | LEU  |
| 1   | J     | 82  | VAL  |
| 1   | J     | 89  | VAL  |
| 1   | J     | 92  | LEU  |
| 1   | J     | 98  | ARG  |
| 1   | J     | 107 | LYS  |
| 1   | J     | 129 | LEU  |
| 1   | J     | 146 | LEU  |
| 1   | J     | 159 | LEU  |
| 1   | J     | 167 | THR  |
| 1   | J     | 178 | LYS  |
| 1   | J     | 183 | LEU  |
| 1   | J     | 190 | LYS  |
| 1   | J     | 192 | LEU  |
| 1   | J     | 211 | ILE  |
| 1   | J     | 225 | LEU  |
| 1   | J     | 236 | ILE  |
| 1   | J     | 244 | ARG  |
| 1   | J     | 269 | ILE  |
| 1   | J     | 280 | ARG  |
| 1   | J     | 312 | LEU  |
| 1   | J     | 326 | GLU  |
| 1   | J     | 328 | VAL  |
| 1   | J     | 333 | CYS  |
| 1   | J     | 335 | LEU  |
| 1   | J     | 339 | VAL  |
| 1   | J     | 352 | VAL  |
| 1   | J     | 366 | THR  |
| 1   | J     | 384 | LEU  |
| 1   | J     | 388 | VAL  |
| 1   | J     | 402 | MET  |
| 1   | J     | 409 | THR  |
| 1   | J     | 465 | LEU  |
| 1   | J     | 502 | LEU  |
| 1   | K     | 38  | ILE  |
| 1   | K     | 44  | ARG  |
| 1   | K     | 50  | VAL  |
| 1   | K     | 57  | ILE  |
| 1   | K     | 58  | LEU  |
| 1   | K     | 65  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 74  | MET  |
| 1   | K     | 96  | LEU  |
| 1   | K     | 98  | ARG  |
| 1   | K     | 103 | LEU  |
| 1   | K     | 107 | LYS  |
| 1   | K     | 139 | GLU  |
| 1   | K     | 140 | VAL  |
| 1   | K     | 143 | ARG  |
| 1   | K     | 146 | LEU  |
| 1   | K     | 147 | MET  |
| 1   | K     | 152 | THR  |
| 1   | K     | 159 | LEU  |
| 1   | K     | 167 | THR  |
| 1   | K     | 177 | LEU  |
| 1   | K     | 182 | ASN  |
| 1   | K     | 184 | GLU  |
| 1   | K     | 191 | LYS  |
| 1   | K     | 207 | LEU  |
| 1   | K     | 211 | ILE  |
| 1   | K     | 223 | LYS  |
| 1   | K     | 225 | LEU  |
| 1   | K     | 280 | ARG  |
| 1   | K     | 320 | SER  |
| 1   | K     | 326 | GLU  |
| 1   | K     | 330 | LEU  |
| 1   | K     | 352 | VAL  |
| 1   | K     | 381 | LEU  |
| 1   | K     | 391 | SER  |
| 1   | K     | 402 | MET  |
| 1   | K     | 414 | ARG  |
| 1   | K     | 415 | THR  |
| 1   | K     | 428 | LYS  |
| 1   | K     | 478 | LEU  |
| 1   | K     | 504 | VAL  |
| 1   | K     | 507 | ILE  |
| 1   | K     | 509 | LYS  |
| 1   | K     | 513 | ARG  |
| 1   | L     | 40  | LEU  |
| 1   | L     | 44  | ARG  |
| 1   | L     | 50  | VAL  |
| 1   | L     | 57  | ILE  |
| 1   | L     | 65  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 74  | MET  |
| 1   | L     | 96  | LEU  |
| 1   | L     | 98  | ARG  |
| 1   | L     | 119 | GLU  |
| 1   | L     | 125 | ARG  |
| 1   | L     | 126 | GLN  |
| 1   | L     | 133 | VAL  |
| 1   | L     | 139 | GLU  |
| 1   | L     | 142 | PHE  |
| 1   | L     | 146 | LEU  |
| 1   | L     | 152 | THR  |
| 1   | L     | 167 | THR  |
| 1   | L     | 192 | LEU  |
| 1   | L     | 207 | LEU  |
| 1   | L     | 211 | ILE  |
| 1   | L     | 223 | LYS  |
| 1   | L     | 225 | LEU  |
| 1   | L     | 259 | LYS  |
| 1   | L     | 269 | ILE  |
| 1   | L     | 280 | ARG  |
| 1   | L     | 312 | LEU  |
| 1   | L     | 320 | SER  |
| 1   | L     | 330 | LEU  |
| 1   | L     | 343 | GLU  |
| 1   | L     | 352 | VAL  |
| 1   | L     | 367 | GLN  |
| 1   | L     | 401 | GLU  |
| 1   | L     | 402 | MET  |
| 1   | L     | 415 | THR  |
| 1   | L     | 465 | LEU  |
| 1   | L     | 502 | LEU  |
| 1   | L     | 505 | ASP  |
| 1   | L     | 507 | ILE  |
| 1   | L     | 508 | ILE  |
| 1   | L     | 509 | LYS  |
| 1   | M     | 4   | ASP  |
| 1   | M     | 33  | LYS  |
| 1   | M     | 35  | MET  |
| 1   | M     | 40  | LEU  |
| 1   | M     | 48  | LEU  |
| 1   | M     | 57  | ILE  |
| 1   | M     | 58  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 65  | ASN  |
| 1   | M     | 82  | VAL  |
| 1   | M     | 89  | VAL  |
| 1   | M     | 96  | LEU  |
| 1   | M     | 98  | ARG  |
| 1   | M     | 108 | ILE  |
| 1   | M     | 131 | SER  |
| 1   | M     | 139 | GLU  |
| 1   | M     | 140 | VAL  |
| 1   | M     | 143 | ARG  |
| 1   | M     | 146 | LEU  |
| 1   | M     | 159 | LEU  |
| 1   | M     | 167 | THR  |
| 1   | M     | 177 | LEU  |
| 1   | M     | 183 | LEU  |
| 1   | M     | 190 | LYS  |
| 1   | M     | 196 | LEU  |
| 1   | M     | 207 | LEU  |
| 1   | M     | 211 | ILE  |
| 1   | M     | 225 | LEU  |
| 1   | M     | 312 | LEU  |
| 1   | M     | 326 | GLU  |
| 1   | M     | 343 | GLU  |
| 1   | M     | 352 | VAL  |
| 1   | M     | 368 | GLN  |
| 1   | M     | 401 | GLU  |
| 1   | M     | 402 | MET  |
| 1   | M     | 489 | GLN  |
| 1   | M     | 503 | ARG  |
| 1   | M     | 507 | ILE  |
| 1   | N     | 9   | GLU  |
| 1   | N     | 10  | THR  |
| 1   | N     | 27  | LYS  |
| 1   | N     | 33  | LYS  |
| 1   | N     | 41  | SER  |
| 1   | N     | 42  | SER  |
| 1   | N     | 48  | LEU  |
| 1   | N     | 50  | VAL  |
| 1   | N     | 57  | ILE  |
| 1   | N     | 58  | LEU  |
| 1   | N     | 74  | MET  |
| 1   | N     | 82  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 96  | LEU  |
| 1   | N     | 98  | ARG  |
| 1   | N     | 122 | LYS  |
| 1   | N     | 126 | GLN  |
| 1   | N     | 129 | LEU  |
| 1   | N     | 130 | ASN  |
| 1   | N     | 139 | GLU  |
| 1   | N     | 140 | VAL  |
| 1   | N     | 143 | ARG  |
| 1   | N     | 145 | ASP  |
| 1   | N     | 146 | LEU  |
| 1   | N     | 159 | LEU  |
| 1   | N     | 167 | THR  |
| 1   | N     | 190 | LYS  |
| 1   | N     | 196 | LEU  |
| 1   | N     | 202 | ASP  |
| 1   | N     | 211 | ILE  |
| 1   | N     | 215 | GLN  |
| 1   | N     | 218 | ARG  |
| 1   | N     | 225 | LEU  |
| 1   | N     | 269 | ILE  |
| 1   | N     | 280 | ARG  |
| 1   | N     | 320 | SER  |
| 1   | N     | 328 | VAL  |
| 1   | N     | 330 | LEU  |
| 1   | N     | 352 | VAL  |
| 1   | N     | 356 | GLU  |
| 1   | N     | 366 | THR  |
| 1   | N     | 381 | LEU  |
| 1   | N     | 384 | LEU  |
| 1   | N     | 389 | LYS  |
| 1   | N     | 391 | SER  |
| 1   | N     | 401 | GLU  |
| 1   | N     | 402 | MET  |
| 1   | N     | 428 | LYS  |
| 1   | N     | 487 | LYS  |
| 1   | N     | 492 | LEU  |
| 1   | N     | 505 | ASP  |
| 1   | N     | 508 | ILE  |
| 1   | N     | 509 | LYS  |
| 1   | O     | 25  | LEU  |
| 1   | O     | 57  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 58  | LEU  |
| 1   | O     | 65  | ASN  |
| 1   | O     | 88  | SER  |
| 1   | O     | 96  | LEU  |
| 1   | O     | 98  | ARG  |
| 1   | O     | 104 | ILE  |
| 1   | O     | 109 | HIS  |
| 1   | O     | 111 | GLN  |
| 1   | O     | 112 | THR  |
| 1   | O     | 129 | LEU  |
| 1   | O     | 138 | ASP  |
| 1   | O     | 139 | GLU  |
| 1   | O     | 146 | LEU  |
| 1   | O     | 147 | MET  |
| 1   | O     | 152 | THR  |
| 1   | O     | 159 | LEU  |
| 1   | O     | 167 | THR  |
| 1   | O     | 182 | ASN  |
| 1   | O     | 191 | LYS  |
| 1   | O     | 201 | LEU  |
| 1   | O     | 211 | ILE  |
| 1   | O     | 215 | GLN  |
| 1   | O     | 225 | LEU  |
| 1   | O     | 234 | ASP  |
| 1   | O     | 269 | ILE  |
| 1   | O     | 280 | ARG  |
| 1   | O     | 282 | LEU  |
| 1   | O     | 326 | GLU  |
| 1   | O     | 330 | LEU  |
| 1   | O     | 343 | GLU  |
| 1   | O     | 352 | VAL  |
| 1   | O     | 359 | THR  |
| 1   | O     | 367 | GLN  |
| 1   | O     | 369 | ILE  |
| 1   | O     | 381 | LEU  |
| 1   | O     | 402 | MET  |
| 1   | O     | 409 | THR  |
| 1   | O     | 501 | ILE  |
| 1   | O     | 508 | ILE  |
| 1   | P     | 48  | LEU  |
| 1   | P     | 50  | VAL  |
| 1   | P     | 57  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 58  | LEU  |
| 1   | P     | 81  | GLU  |
| 1   | P     | 96  | LEU  |
| 1   | P     | 98  | ARG  |
| 1   | P     | 104 | ILE  |
| 1   | P     | 107 | LYS  |
| 1   | P     | 125 | ARG  |
| 1   | P     | 126 | GLN  |
| 1   | P     | 129 | LEU  |
| 1   | P     | 139 | GLU  |
| 1   | P     | 140 | VAL  |
| 1   | P     | 144 | GLN  |
| 1   | P     | 146 | LEU  |
| 1   | P     | 152 | THR  |
| 1   | P     | 159 | LEU  |
| 1   | P     | 167 | THR  |
| 1   | P     | 178 | LYS  |
| 1   | P     | 180 | SER  |
| 1   | P     | 184 | GLU  |
| 1   | P     | 191 | LYS  |
| 1   | P     | 192 | LEU  |
| 1   | P     | 207 | LEU  |
| 1   | P     | 211 | ILE  |
| 1   | P     | 223 | LYS  |
| 1   | P     | 225 | LEU  |
| 1   | P     | 238 | ILE  |
| 1   | P     | 243 | VAL  |
| 1   | P     | 255 | GLU  |
| 1   | P     | 262 | MET  |
| 1   | P     | 269 | ILE  |
| 1   | P     | 280 | ARG  |
| 1   | P     | 326 | GLU  |
| 1   | P     | 352 | VAL  |
| 1   | P     | 367 | GLN  |
| 1   | P     | 370 | LEU  |
| 1   | P     | 388 | VAL  |
| 1   | P     | 401 | GLU  |
| 1   | P     | 402 | MET  |
| 1   | P     | 418 | LYS  |
| 1   | P     | 430 | LEU  |
| 1   | P     | 436 | ILE  |
| 1   | P     | 465 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 500 | VAL  |
| 1   | P     | 507 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | ASN  |
| 1   | A     | 111 | GLN  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 214 | ASN  |
| 1   | A     | 348 | HIS  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 410 | GLN  |
| 1   | A     | 451 | GLN  |
| 1   | A     | 506 | ASN  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 162 | HIS  |
| 1   | B     | 182 | ASN  |
| 1   | B     | 187 | HIS  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 386 | GLN  |
| 1   | B     | 406 | HIS  |
| 1   | B     | 451 | GLN  |
| 1   | B     | 489 | GLN  |
| 1   | C     | 65  | ASN  |
| 1   | C     | 126 | GLN  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 348 | HIS  |
| 1   | C     | 367 | GLN  |
| 1   | C     | 386 | GLN  |
| 1   | C     | 410 | GLN  |
| 1   | D     | 65  | ASN  |
| 1   | D     | 126 | GLN  |
| 1   | D     | 182 | ASN  |
| 1   | D     | 281 | GLN  |
| 1   | D     | 386 | GLN  |
| 1   | D     | 410 | GLN  |
| 1   | D     | 451 | GLN  |
| 1   | D     | 485 | GLN  |
| 1   | D     | 489 | GLN  |
| 1   | E     | 65  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 78  | GLN  |
| 1   | E     | 182 | ASN  |
| 1   | E     | 214 | ASN  |
| 1   | E     | 215 | GLN  |
| 1   | E     | 489 | GLN  |
| 1   | F     | 135 | HIS  |
| 1   | F     | 182 | ASN  |
| 1   | F     | 187 | HIS  |
| 1   | F     | 386 | GLN  |
| 1   | F     | 410 | GLN  |
| 1   | F     | 451 | GLN  |
| 1   | F     | 489 | GLN  |
| 1   | G     | 65  | ASN  |
| 1   | G     | 187 | HIS  |
| 1   | G     | 214 | ASN  |
| 1   | G     | 348 | HIS  |
| 1   | G     | 410 | GLN  |
| 1   | G     | 451 | GLN  |
| 1   | H     | 60  | ASN  |
| 1   | H     | 78  | GLN  |
| 1   | H     | 126 | GLN  |
| 1   | H     | 161 | HIS  |
| 1   | H     | 348 | HIS  |
| 1   | H     | 386 | GLN  |
| 1   | H     | 410 | GLN  |
| 1   | H     | 485 | GLN  |
| 1   | H     | 489 | GLN  |
| 1   | I     | 65  | ASN  |
| 1   | I     | 126 | GLN  |
| 1   | I     | 161 | HIS  |
| 1   | I     | 182 | ASN  |
| 1   | I     | 214 | ASN  |
| 1   | I     | 368 | GLN  |
| 1   | I     | 410 | GLN  |
| 1   | I     | 451 | GLN  |
| 1   | I     | 485 | GLN  |
| 1   | I     | 489 | GLN  |
| 1   | J     | 161 | HIS  |
| 1   | J     | 214 | ASN  |
| 1   | J     | 348 | HIS  |
| 1   | J     | 410 | GLN  |
| 1   | K     | 52  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 65  | ASN  |
| 1   | K     | 78  | GLN  |
| 1   | K     | 126 | GLN  |
| 1   | K     | 165 | HIS  |
| 1   | K     | 182 | ASN  |
| 1   | K     | 272 | HIS  |
| 1   | K     | 410 | GLN  |
| 1   | K     | 451 | GLN  |
| 1   | K     | 489 | GLN  |
| 1   | L     | 126 | GLN  |
| 1   | L     | 144 | GLN  |
| 1   | L     | 161 | HIS  |
| 1   | L     | 162 | HIS  |
| 1   | L     | 165 | HIS  |
| 1   | L     | 182 | ASN  |
| 1   | L     | 214 | ASN  |
| 1   | L     | 348 | HIS  |
| 1   | L     | 368 | GLN  |
| 1   | L     | 386 | GLN  |
| 1   | L     | 410 | GLN  |
| 1   | L     | 451 | GLN  |
| 1   | L     | 489 | GLN  |
| 1   | M     | 52  | ASN  |
| 1   | M     | 130 | ASN  |
| 1   | M     | 161 | HIS  |
| 1   | M     | 165 | HIS  |
| 1   | M     | 214 | ASN  |
| 1   | M     | 386 | GLN  |
| 1   | M     | 410 | GLN  |
| 1   | M     | 451 | GLN  |
| 1   | M     | 489 | GLN  |
| 1   | N     | 78  | GLN  |
| 1   | N     | 275 | ASN  |
| 1   | N     | 368 | GLN  |
| 1   | N     | 386 | GLN  |
| 1   | N     | 485 | GLN  |
| 1   | N     | 489 | GLN  |
| 1   | O     | 65  | ASN  |
| 1   | O     | 109 | HIS  |
| 1   | O     | 182 | ASN  |
| 1   | O     | 214 | ASN  |
| 1   | O     | 281 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 348 | HIS  |
| 1   | O     | 386 | GLN  |
| 1   | O     | 410 | GLN  |
| 1   | O     | 451 | GLN  |
| 1   | O     | 485 | GLN  |
| 1   | O     | 506 | ASN  |
| 1   | P     | 52  | ASN  |
| 1   | P     | 65  | ASN  |
| 1   | P     | 78  | GLN  |
| 1   | P     | 144 | GLN  |
| 1   | P     | 161 | HIS  |
| 1   | P     | 214 | ASN  |
| 1   | P     | 368 | GLN  |
| 1   | P     | 386 | GLN  |
| 1   | P     | 451 | GLN  |
| 1   | P     | 485 | GLN  |

### 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 ⓘ

There are no chain breaks in this entry.

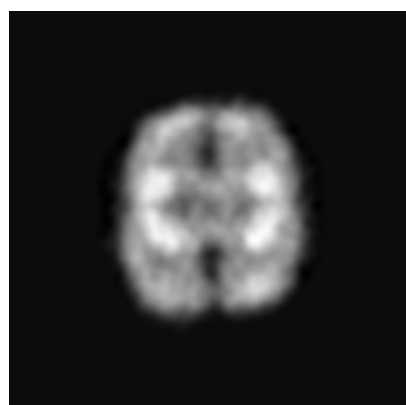
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1962. These allow visual inspection of the internal detail of the map and identification of artifacts.

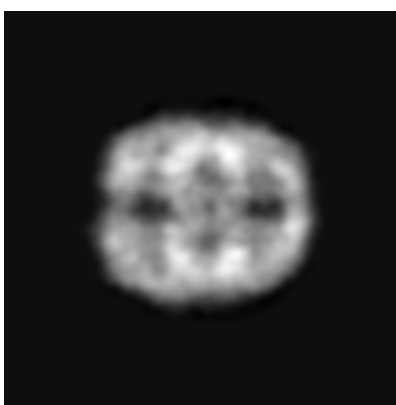
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y



Z

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

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

#### 6.2.1 Primary map



X Index: 72



Y Index: 72

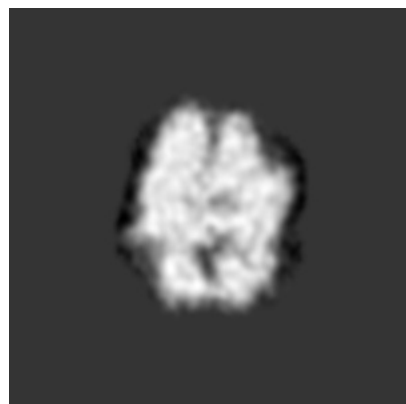


Z Index: 72

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: 94



Y Index: 51

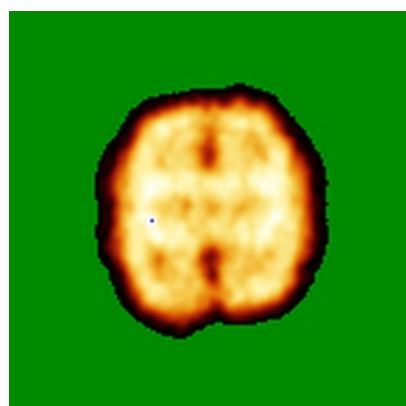


Z Index: 81

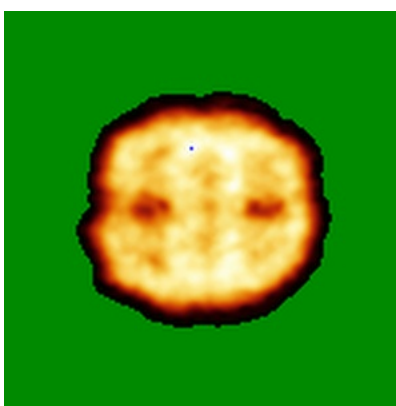
The images above show the largest variance slices of the map in three orthogonal directions.

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

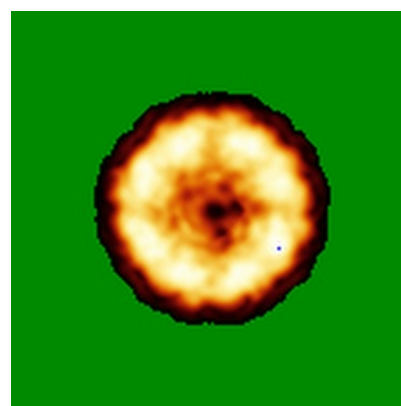
### 6.4.1 Primary map



X



Y

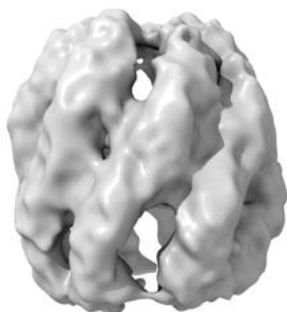


Z

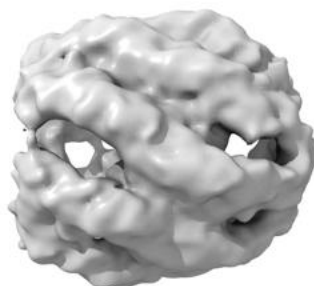
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

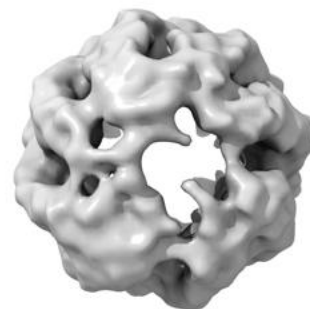
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

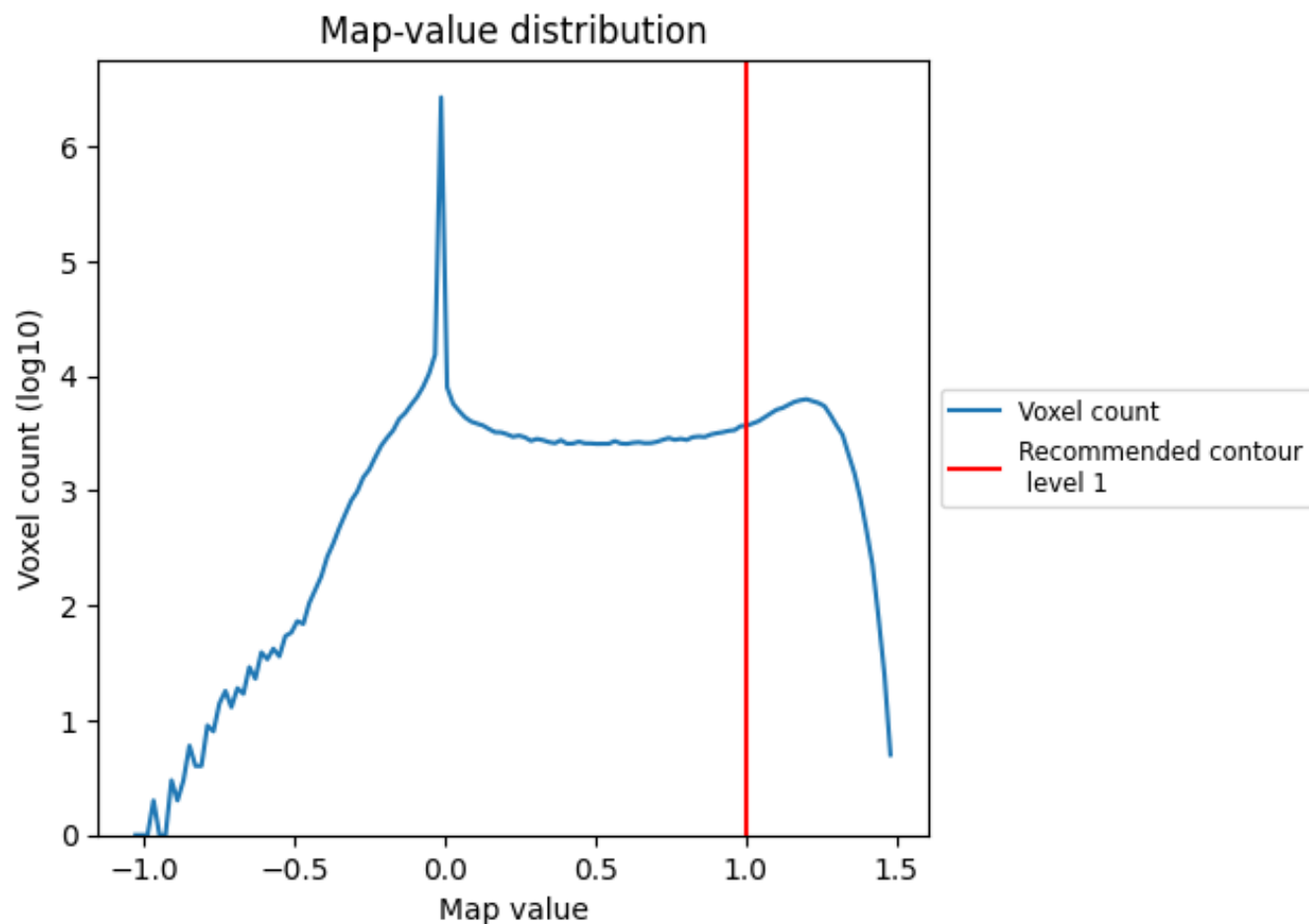
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

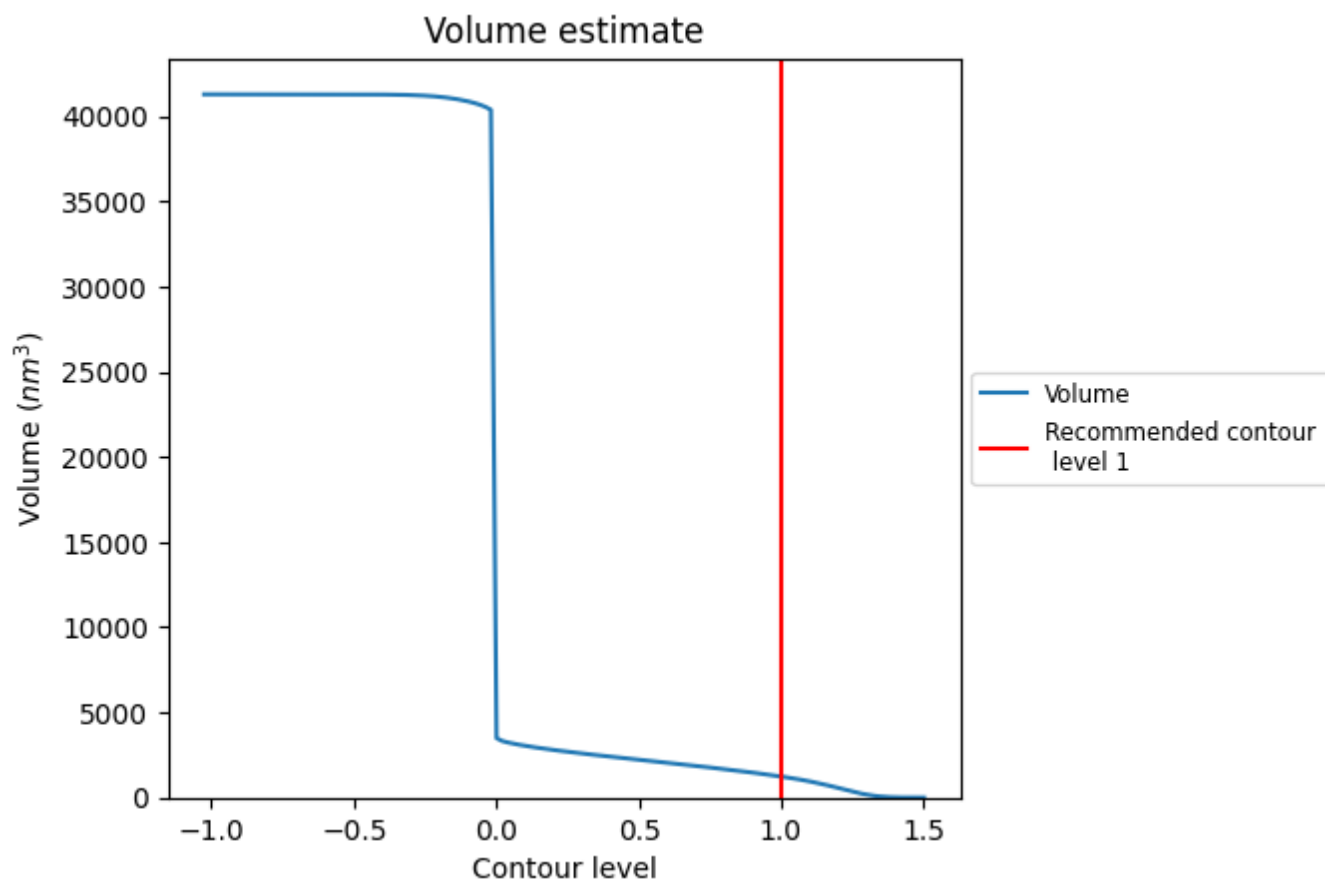
This section contains the results of statistical analysis of the map.

### 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.

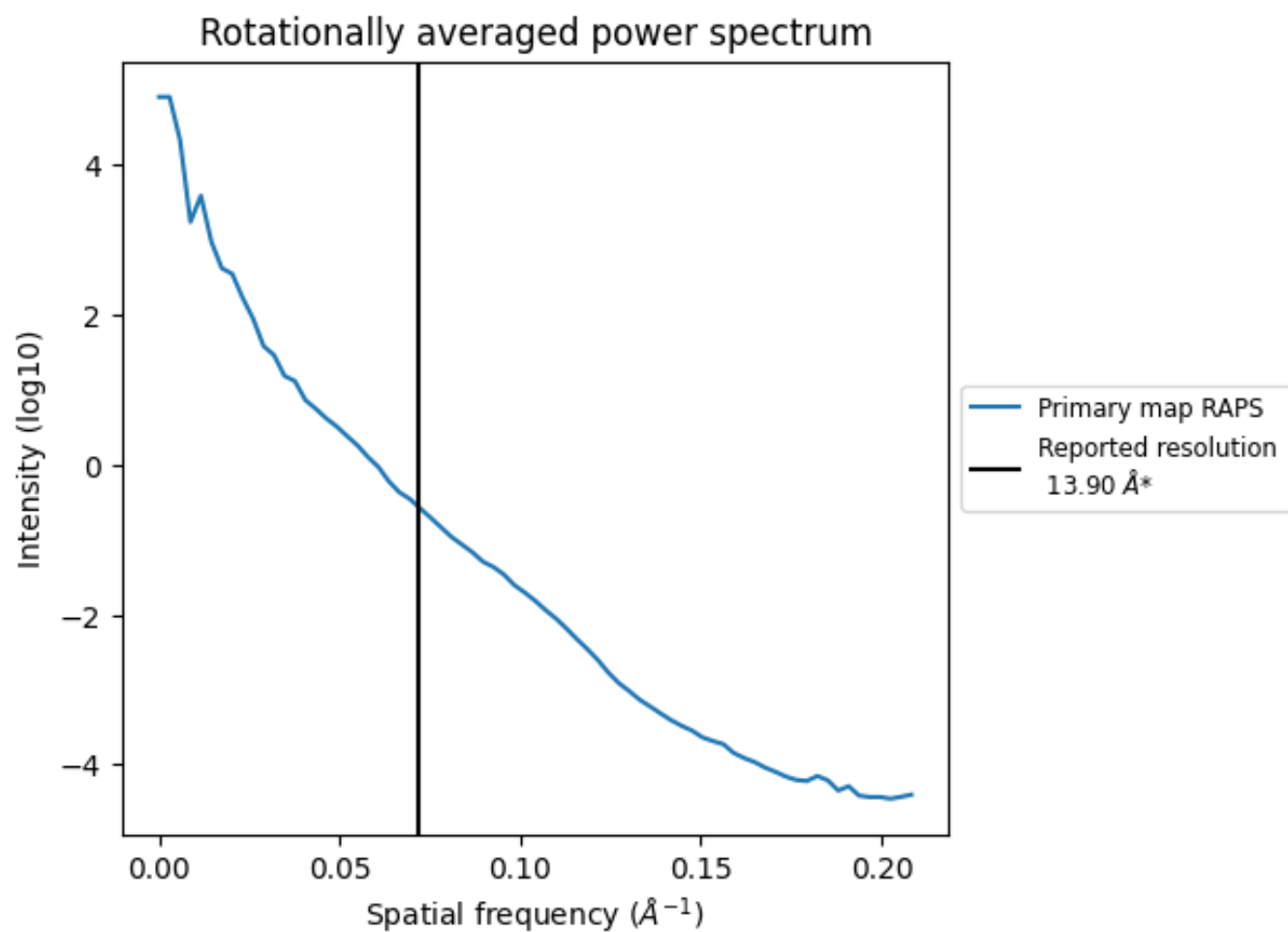
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1235 nm<sup>3</sup>; this corresponds to an approximate mass of 1115 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.072 Å<sup>-1</sup>

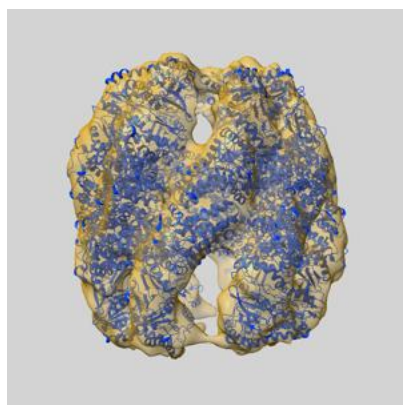
## 8 Fourier-Shell correlation ⓘ

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

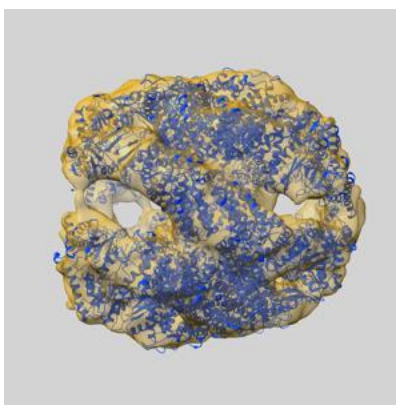
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1962 and PDB model 4A0W. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

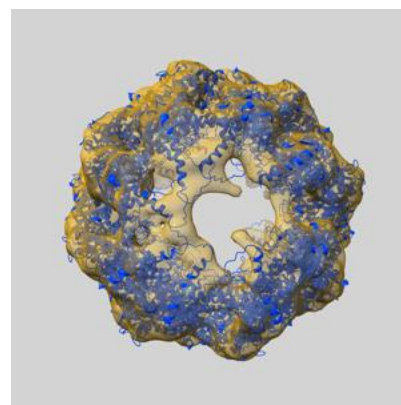
### 9.1 Map-model overlay [i](#)



X



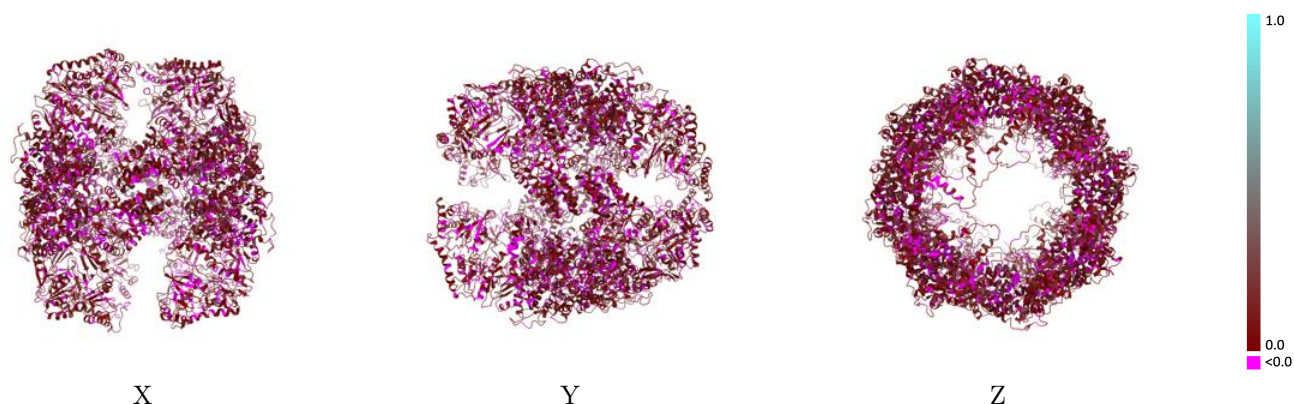
Y



Z

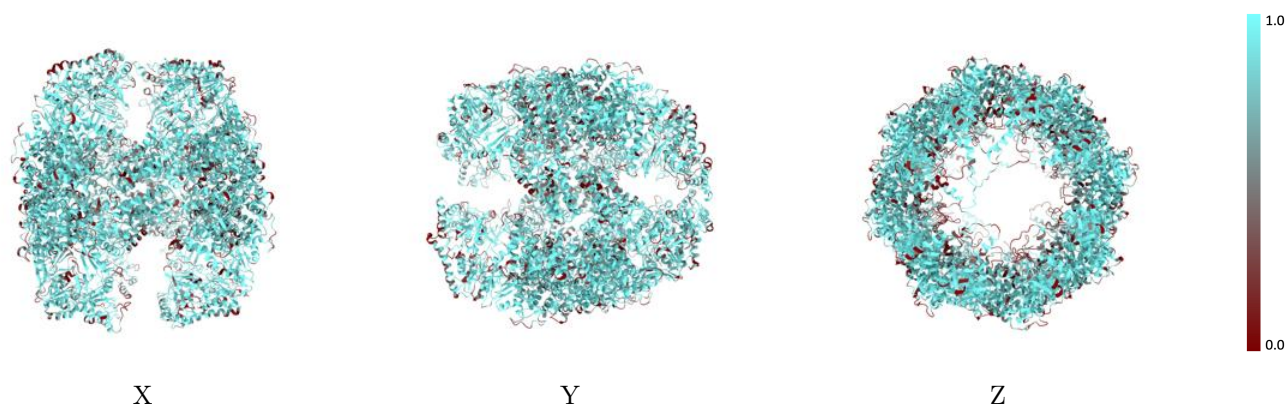
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



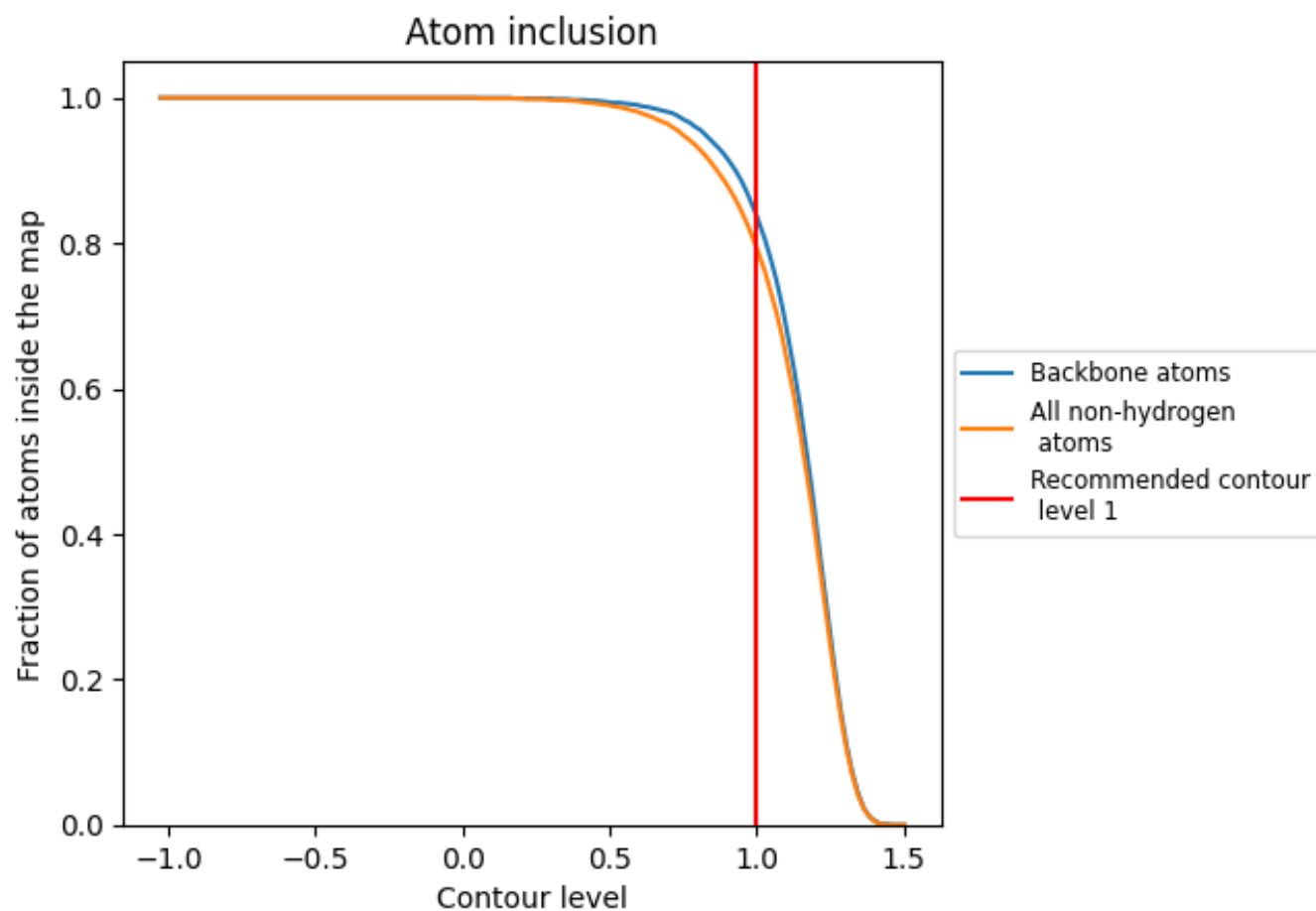
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.7930</div> | <div><div></div>0.0700</div> |
| A     | <div><div></div>0.7890</div> | <div><div></div>0.0710</div> |
| B     | <div><div></div>0.8020</div> | <div><div></div>0.0670</div> |
| C     | <div><div></div>0.8320</div> | <div><div></div>0.0700</div> |
| D     | <div><div></div>0.7680</div> | <div><div></div>0.0750</div> |
| E     | <div><div></div>0.7930</div> | <div><div></div>0.0710</div> |
| F     | <div><div></div>0.7970</div> | <div><div></div>0.0730</div> |
| G     | <div><div></div>0.7920</div> | <div><div></div>0.0650</div> |
| H     | <div><div></div>0.8130</div> | <div><div></div>0.0740</div> |
| I     | <div><div></div>0.7700</div> | <div><div></div>0.0710</div> |
| J     | <div><div></div>0.8060</div> | <div><div></div>0.0720</div> |
| K     | <div><div></div>0.7970</div> | <div><div></div>0.0680</div> |
| L     | <div><div></div>0.7890</div> | <div><div></div>0.0650</div> |
| M     | <div><div></div>0.7790</div> | <div><div></div>0.0660</div> |
| N     | <div><div></div>0.8020</div> | <div><div></div>0.0720</div> |
| O     | <div><div></div>0.7540</div> | <div><div></div>0.0600</div> |
| P     | <div><div></div>0.8010</div> | <div><div></div>0.0740</div> |

1.0

0.0

<0.0