



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:54 AM UTC

PDB ID : 5U0A / pdb\_00005u0a  
EMDB ID : EMD-8478  
Title : CRISPR RNA-guided surveillance complex  
Authors : Xiao, Y.; Luo, M.; Hayes, R.P.; Kim, J.; Ng, S.; Ding, F.; Liao, M.; Ke, A.  
Deposited on : 2016-11-23  
Resolution : 3.30 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:

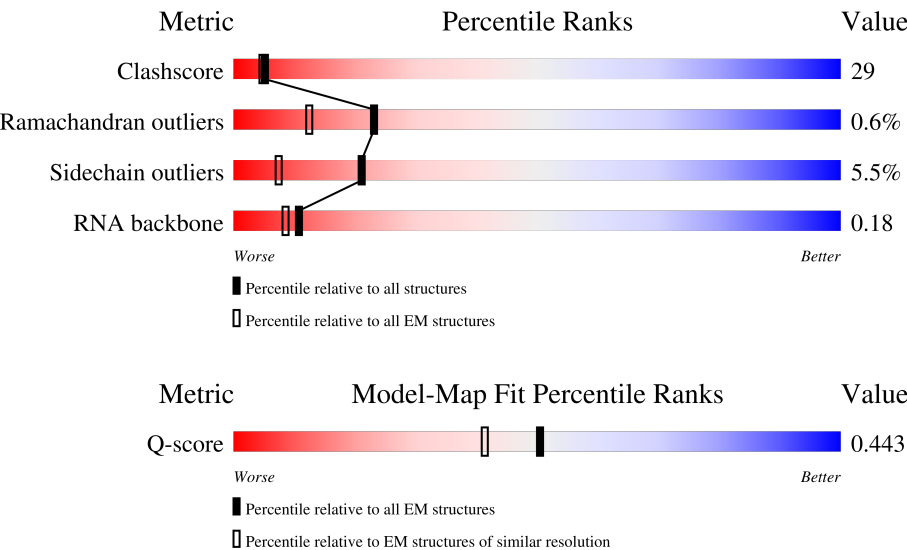
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.30 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                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 15087 ( 2.80 - 3.80 )                                    |

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     | 232    |                  |
| 2   | C     | 549    |                  |
| 3   | D     | 373    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | E     | 373    |                  |
| 3   | F     | 373    |                  |
| 3   | G     | 373    |                  |
| 3   | H     | 373    |                  |
| 3   | I     | 373    |                  |
| 4   | J     | 244    |                  |
| 4   | L     | 244    |                  |
| 5   | K     | 61     |                  |
| 6   | M     | 50     |                  |
| 7   | N     | 254    |                  |
| 8   | O     | 39     |                  |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 28923 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 CRISPR-associated protein, Cse3 family.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1439  | 886 | 290 | 261 | 2 |         |       |

- Molecule 2 is a protein called CRISPR-associated protein, Cse1 family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | C     | 503      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3980  | 2523 | 732 | 716 | 9 |         |       |

- Molecule 3 is a protein called CRISPR-associated protein, Cse4 family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | D     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2017  | 1266 | 356 | 390 | 5 |         |       |
| 3   | E     | 367      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2840  | 1781 | 509 | 545 | 5 |         |       |
| 3   | F     | 367      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2840  | 1781 | 509 | 545 | 5 |         |       |
| 3   | G     | 366      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2829  | 1772 | 508 | 544 | 5 |         |       |
| 3   | H     | 366      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2829  | 1772 | 508 | 544 | 5 |         |       |
| 3   | I     | 329      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2543  | 1596 | 460 | 484 | 3 |         |       |

- Molecule 4 is a protein called Cse2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | J     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1388  | 873 | 278 | 235 | 2 |         |       |
| 4   | L     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1322  | 832 | 264 | 224 | 2 |         |       |

- Molecule 5 is a RNA chain called crRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | K     | 59       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1267  | 565 | 235 | 409 | 58 |         |       |

- Molecule 6 is a DNA chain called Target Strand.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | M     | 50       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1013  | 481 | 179 | 303 | 50 |         |       |

- Molecule 7 is a protein called CRISPR-associated protein, Cas5e family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | N     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1896  | 1204 | 346 | 343 | 3 |         |       |

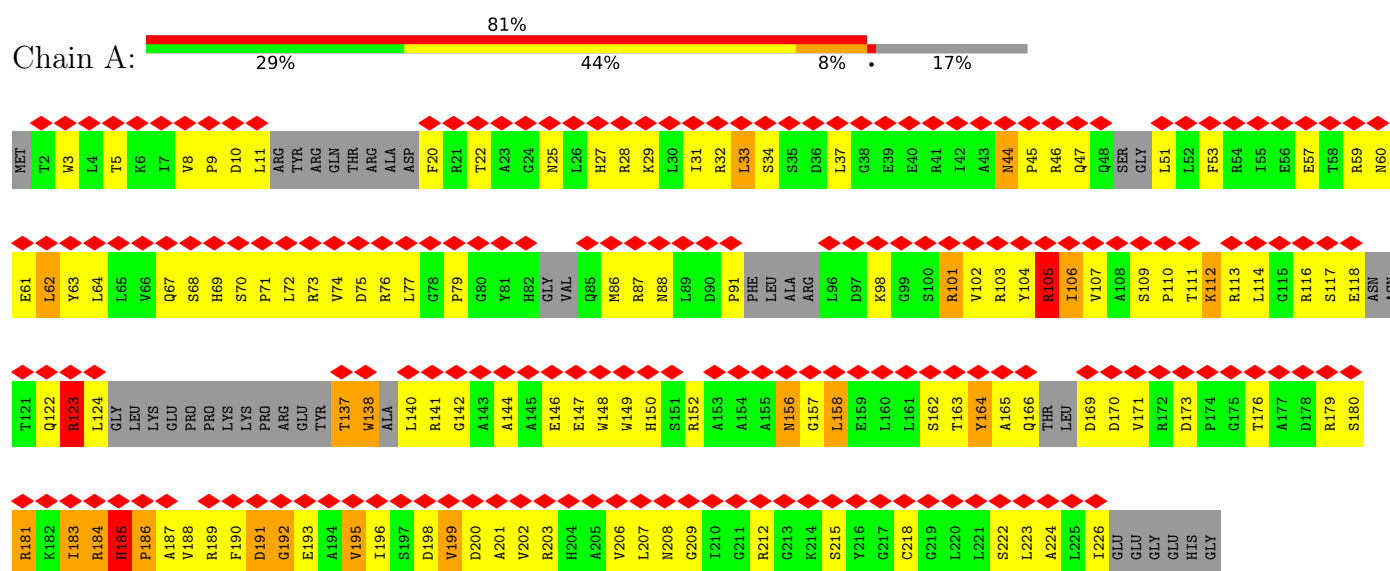
- Molecule 8 is a DNA chain called Nontarget Strand.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | O     | 35       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 720   | 338 | 139 | 208 | 35 |         |       |

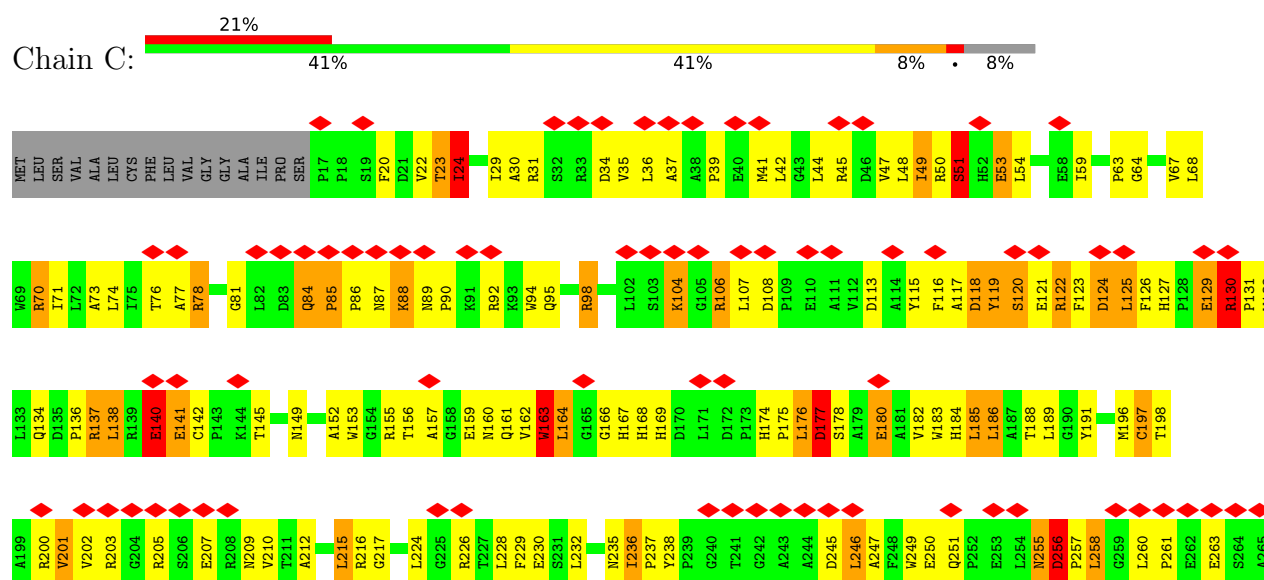
### 3 Residue-property plots

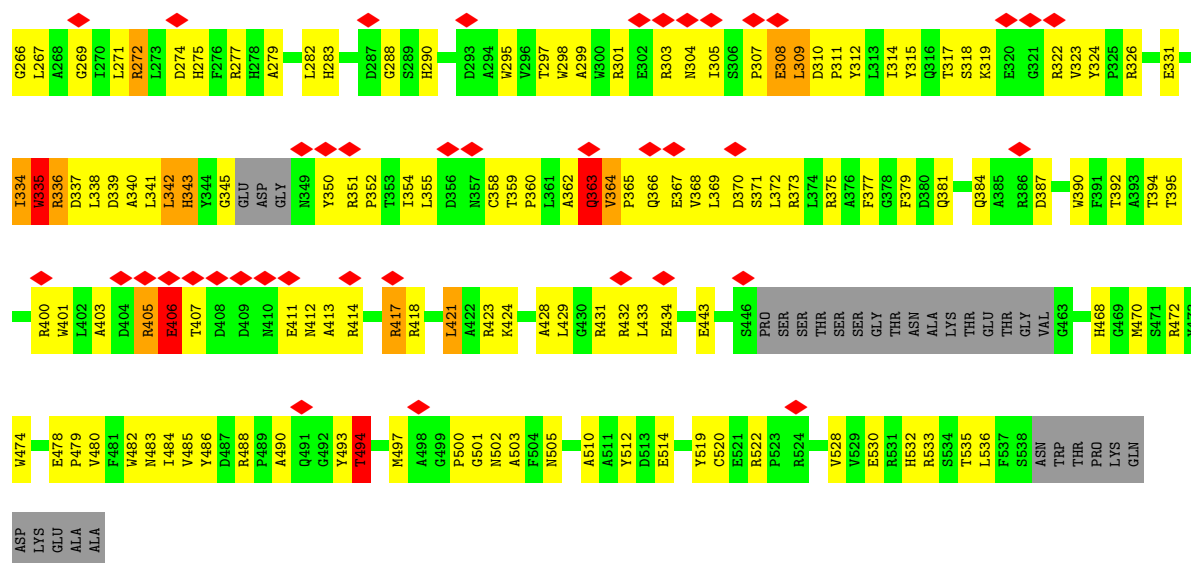
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CRISPR-associated protein, Cse3 family



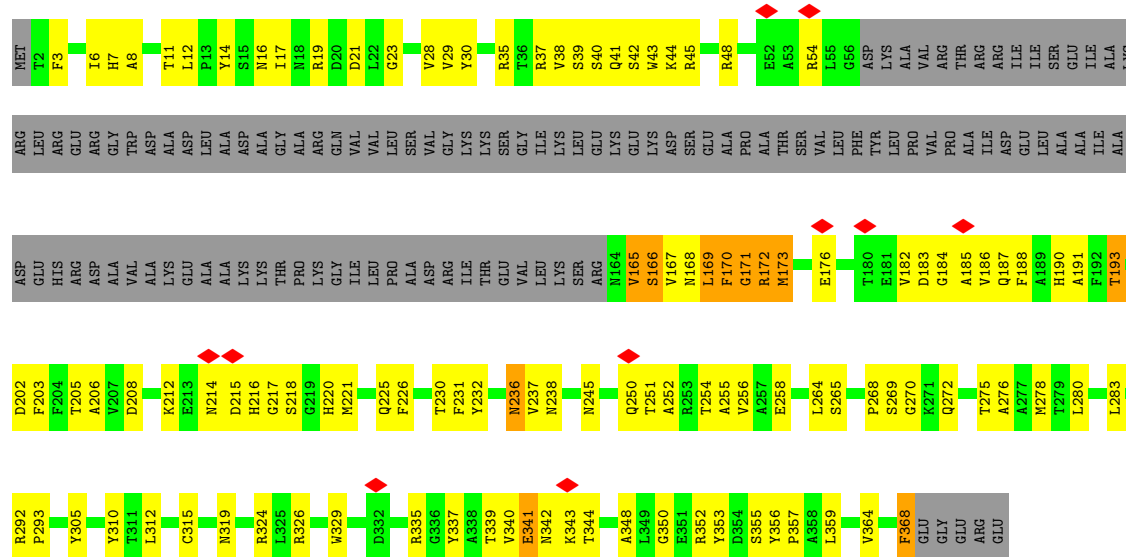
#### • Molecule 2: CRISPR-associated protein, Cse1 family





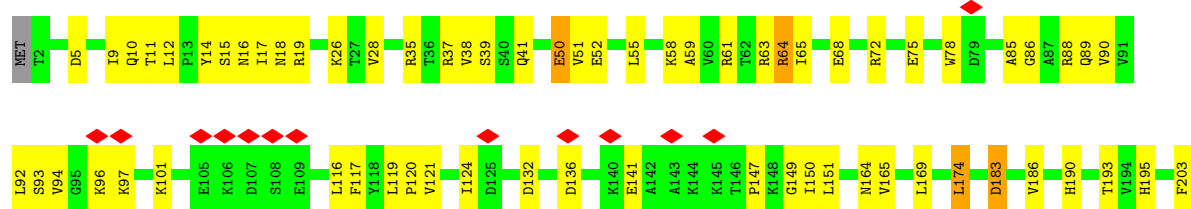
• Molecule 3: CRISPR-associated protein, Cse4 family

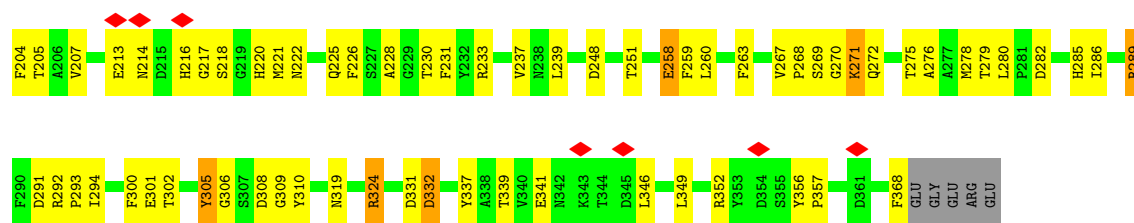
Chain D: 39% 28% 30%



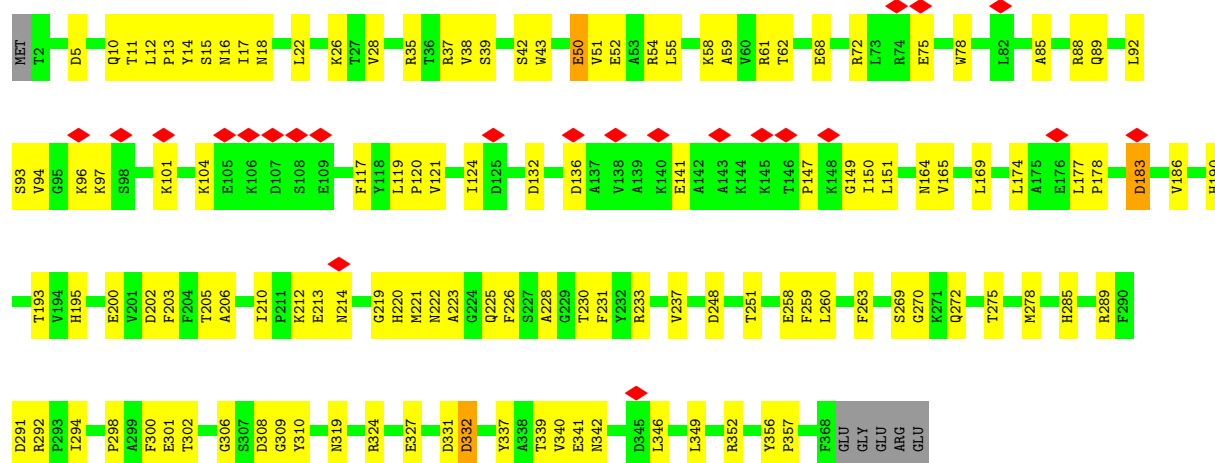
• Molecule 3: CRISPR-associated protein, Cse4 family

Chain E: 5% 63% 32%

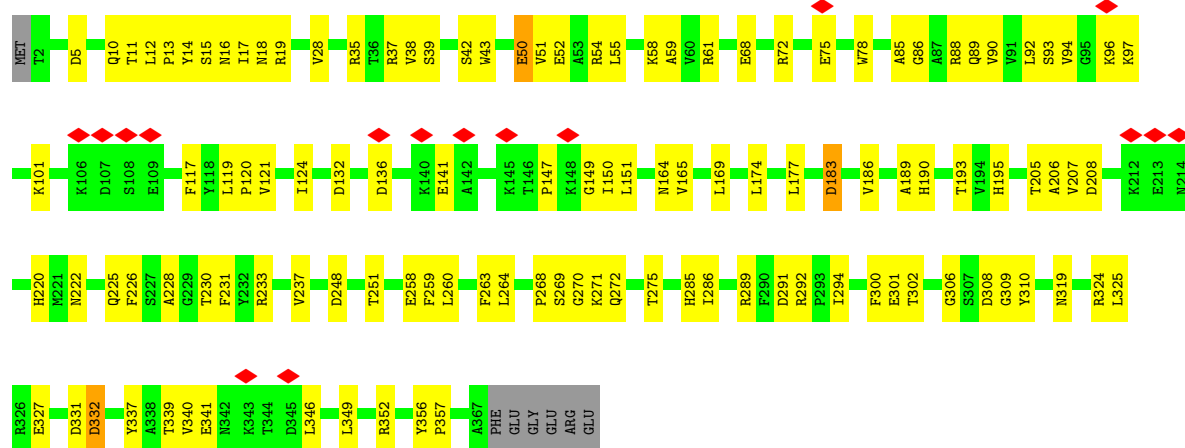




• Molecule 3: CRISPR-associated protein, Cse4 family

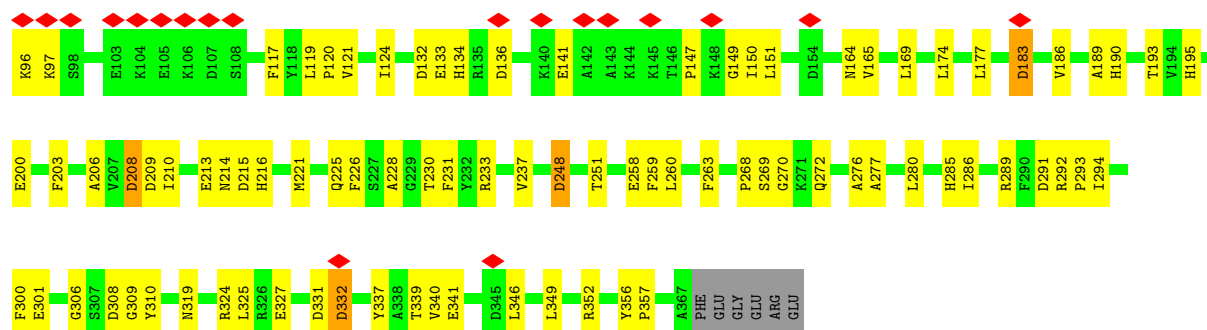


• Molecule 3: CRISPR-associated protein, Cse4 family

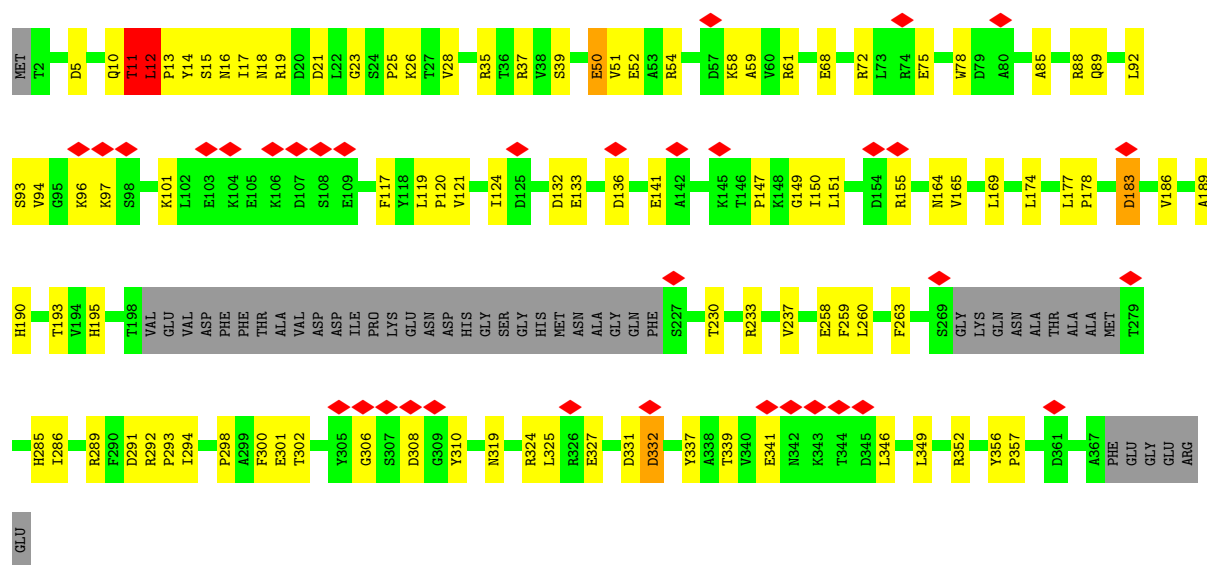


• Molecule 3: CRISPR-associated protein, Cse4 family

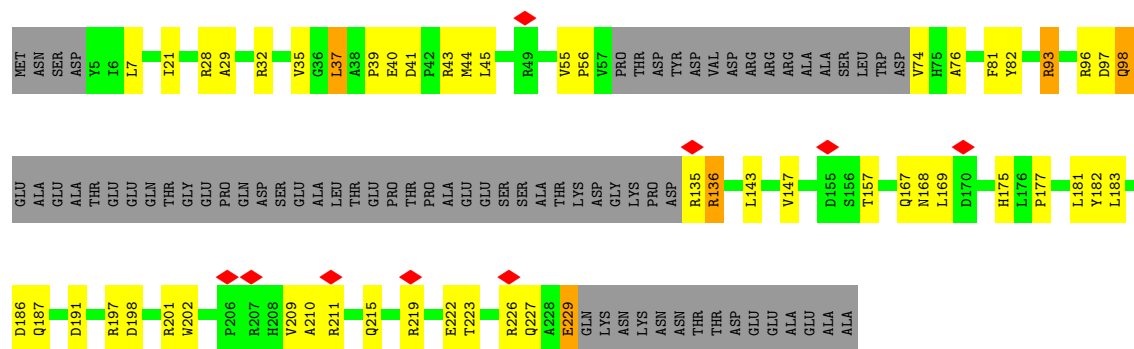




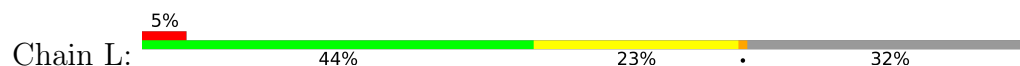
• Molecule 3: CRISPR-associated protein, Cse4 family

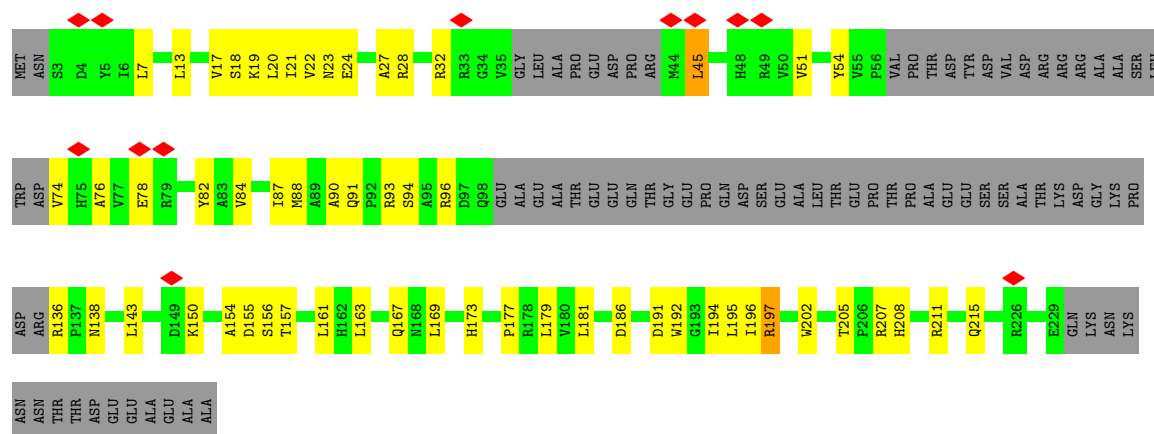


• Molecule 4: Cse2

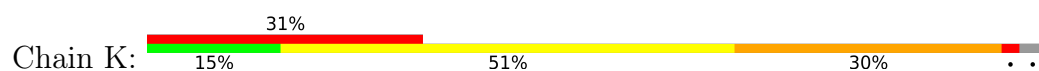


• Molecule 4: Cse2

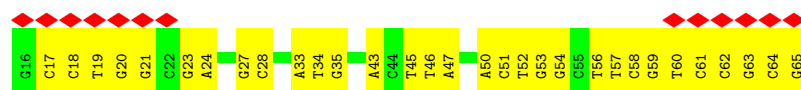




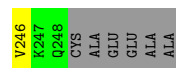
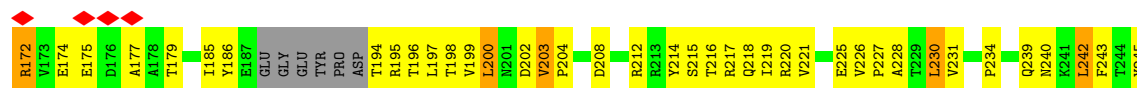
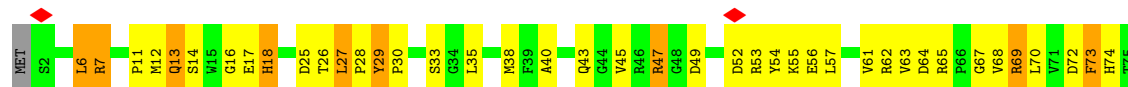
### • Molecule 5: crRNA



### • Molecule 6: Target Strand



### • Molecule 7: CRISPR-associated protein, Cas5e family



### • Molecule 8: Nontarget Strand





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 131292                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 8                                       | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 21000                                   | Depositor |
| Magnification                        | 31000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.479                                   | Depositor |
| Minimum map value                    | -0.298                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.017                                   | Depositor |
| Recommended contour level            | 0.07                                    | Depositor |
| Map size (Å)                         | 314.88, 314.88, 314.88                  | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.23, 1.23, 1.23                        | 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     | 0.47         | 0/1456         | 1.17        | 10/1960 (0.5%)  |
| 2   | C     | 0.57         | 0/4097         | 1.08        | 25/5592 (0.4%)  |
| 3   | D     | 0.67         | 0/2060         | 0.90        | 4/2802 (0.1%)   |
| 3   | E     | 0.59         | 0/2894         | 0.75        | 1/3927 (0.0%)   |
| 3   | F     | 0.57         | 0/2894         | 0.69        | 0/3927          |
| 3   | G     | 0.58         | 0/2882         | 0.71        | 0/3911          |
| 3   | H     | 0.59         | 0/2882         | 0.72        | 3/3911 (0.1%)   |
| 3   | I     | 0.59         | 0/2587         | 0.73        | 3/3509 (0.1%)   |
| 4   | J     | 0.55         | 0/1417         | 0.82        | 0/1924          |
| 4   | L     | 0.51         | 0/1348         | 0.83        | 0/1828          |
| 5   | K     | 0.57         | 1/1417 (0.1%)  | 0.63        | 0/2208          |
| 6   | M     | 0.52         | 0/1132         | 0.55        | 0/1742          |
| 7   | N     | 0.61         | 0/1939         | 0.91        | 4/2638 (0.2%)   |
| 8   | O     | 0.37         | 0/807          | 0.49        | 0/1241          |
| All | All   | 0.57         | 1/29812 (0.0%) | 0.82        | 50/41120 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 5   | K     | 55  | C    | C1'-N1 | 5.79 | 1.57        | 1.48     |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 185 | HIS  | C-N-CD | -12.01 | 75.77       | 125.00   |
| 2   | C     | 166 | GLY  | N-CA-C | -11.99 | 97.58       | 112.68   |
| 2   | C     | 163 | TRP  | N-CA-C | 10.92  | 123.19      | 111.28   |
| 1   | A     | 123 | ARG  | N-CA-C | -9.96  | 96.14       | 110.59   |
| 2   | C     | 236 | ILE  | N-CA-C | 9.13   | 116.98      | 107.76   |
| 3   | D     | 171 | GLY  | N-CA-C | 8.92   | 122.85      | 112.50   |
| 2   | C     | 88  | LYS  | CA-C-N | -8.82  | 113.30      | 122.83   |
| 2   | C     | 88  | LYS  | C-N-CA | -8.82  | 113.30      | 122.83   |
| 2   | C     | 255 | ASN  | N-CA-C | 8.38   | 120.41      | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 67  | GLN  | N-CA-C   | -8.17 | 97.01       | 110.17   |
| 2   | C     | 164 | LEU  | N-CA-C   | 7.59  | 121.85      | 109.85   |
| 2   | C     | 24  | ILE  | N-CA-C   | 7.45  | 118.21      | 111.81   |
| 7   | N     | 73  | PHE  | N-CA-C   | -7.36 | 100.83      | 110.33   |
| 2   | C     | 51  | SER  | N-CA-C   | 6.73  | 118.27      | 111.07   |
| 2   | C     | 235 | ASN  | CA-C-N   | -6.70 | 117.77      | 122.59   |
| 2   | C     | 235 | ASN  | C-N-CA   | -6.70 | 117.77      | 122.59   |
| 2   | C     | 49  | ILE  | N-CA-C   | 6.49  | 117.28      | 110.72   |
| 3   | D     | 170 | PHE  | N-CA-C   | -6.49 | 99.12       | 109.76   |
| 2   | C     | 488 | ARG  | N-CA-C   | -6.29 | 100.89      | 110.01   |
| 2   | C     | 406 | GLU  | N-CA-C   | 6.16  | 118.07      | 111.36   |
| 2   | C     | 177 | ASP  | N-CA-C   | -6.07 | 101.94      | 110.50   |
| 7   | N     | 27  | LEU  | N-CA-C   | -6.07 | 101.39      | 110.24   |
| 3   | I     | 12  | LEU  | CA-C-N   | -5.96 | 114.47      | 120.31   |
| 3   | I     | 12  | LEU  | C-N-CA   | -5.96 | 114.47      | 120.31   |
| 1   | A     | 192 | GLY  | N-CA-C   | 5.92  | 118.02      | 110.20   |
| 3   | H     | 208 | ASP  | N-CA-C   | -5.89 | 101.76      | 110.48   |
| 2   | C     | 494 | THR  | CA-C-N   | -5.85 | 113.73      | 119.76   |
| 2   | C     | 494 | THR  | C-N-CA   | -5.85 | 113.73      | 119.76   |
| 3   | E     | 305 | TYR  | N-CA-C   | 5.81  | 117.41      | 111.14   |
| 2   | C     | 141 | GLU  | N-CA-C   | 5.80  | 120.36      | 113.16   |
| 1   | A     | 191 | ASP  | CA-C-N   | 5.71  | 133.04      | 122.02   |
| 1   | A     | 191 | ASP  | C-N-CA   | 5.71  | 133.04      | 122.02   |
| 2   | C     | 140 | GLU  | N-CA-C   | 5.60  | 117.38      | 111.28   |
| 7   | N     | 27  | LEU  | CA-C-N   | -5.55 | 114.10      | 119.87   |
| 7   | N     | 27  | LEU  | C-N-CA   | -5.55 | 114.10      | 119.87   |
| 2   | C     | 84  | GLN  | CA-C-N   | -5.53 | 114.69      | 120.38   |
| 2   | C     | 84  | GLN  | C-N-CA   | -5.53 | 114.69      | 120.38   |
| 2   | C     | 130 | ARG  | CA-C-N   | -5.50 | 114.30      | 119.85   |
| 2   | C     | 130 | ARG  | C-N-CA   | -5.50 | 114.30      | 119.85   |
| 3   | H     | 16  | ASN  | N-CA-C   | -5.49 | 104.48      | 110.91   |
| 2   | C     | 335 | TRP  | N-CA-C   | -5.46 | 99.62       | 108.41   |
| 1   | A     | 191 | ASP  | N-CA-C   | 5.34  | 117.19      | 108.76   |
| 1   | A     | 158 | LEU  | CA-CB-CG | 5.33  | 134.94      | 116.30   |
| 3   | D     | 251 | THR  | N-CA-C   | -5.29 | 105.51      | 111.28   |
| 1   | A     | 198 | ASP  | N-CA-C   | -5.25 | 99.10       | 108.13   |
| 3   | I     | 11  | THR  | N-CA-C   | -5.21 | 103.15      | 110.50   |
| 3   | D     | 173 | MET  | CA-CB-CG | 5.21  | 124.52      | 114.10   |
| 3   | H     | 213 | GLU  | CA-CB-CG | -5.12 | 103.87      | 114.10   |
| 2   | C     | 98  | ARG  | CB-CG-CD | -5.10 | 99.58       | 111.30   |
| 1   | A     | 164 | TYR  | N-CA-C   | -5.03 | 102.75      | 110.14   |

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     | 1439  | 0        | 1372     | 226     | 0            |
| 2   | C     | 3980  | 0        | 3851     | 423     | 0            |
| 3   | D     | 2017  | 0        | 1937     | 147     | 0            |
| 3   | E     | 2840  | 0        | 2809     | 144     | 0            |
| 3   | F     | 2840  | 0        | 2809     | 111     | 0            |
| 3   | G     | 2829  | 0        | 2800     | 103     | 0            |
| 3   | H     | 2829  | 0        | 2800     | 102     | 0            |
| 3   | I     | 2543  | 0        | 2541     | 107     | 0            |
| 4   | J     | 1388  | 0        | 1409     | 64      | 0            |
| 4   | L     | 1322  | 0        | 1337     | 58      | 0            |
| 5   | K     | 1267  | 0        | 642      | 133     | 0            |
| 6   | M     | 1013  | 0        | 562      | 47      | 0            |
| 7   | N     | 1896  | 0        | 1925     | 153     | 0            |
| 8   | O     | 720   | 0        | 391      | 28      | 0            |
| All | All   | 28923 | 0        | 27185    | 1602    | 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 29.

All (1602) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 2:C:142:CYS:SG   | 2:C:200:ARG:HB3 | 1.46                     | 1.55              |
| 3:D:169:LEU:HD11 | 3:D:170:PHE:CE2 | 1.54                     | 1.42              |
| 1:A:122:GLN:NE2  | 5:K:44:A:N1     | 1.67                     | 1.40              |
| 2:C:429:LEU:HA   | 2:C:432:ARG:CG  | 1.53                     | 1.35              |
| 3:D:169:LEU:CD1  | 3:D:170:PHE:CE2 | 2.07                     | 1.35              |
| 1:A:122:GLN:OE1  | 5:K:44:A:C5     | 1.82                     | 1.31              |
| 2:C:125:LEU:HD23 | 2:C:126:PHE:N   | 1.43                     | 1.29              |
| 1:A:163:THR:H    | 3:I:19:ARG:NH1  | 1.25                     | 1.28              |
| 2:C:132:TRP:HZ3  | 2:C:249:TRP:CB  | 1.49                     | 1.26              |
| 1:A:185:HIS:HD2  | 1:A:186:PRO:N   | 1.34                     | 1.23              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:142:CYS:SG   | 2:C:200:ARG:CB   | 2.25                     | 1.23              |
| 1:A:164:TYR:CB   | 1:A:188:VAL:HG13 | 1.67                     | 1.22              |
| 2:C:429:LEU:HA   | 2:C:432:ARG:CD   | 1.68                     | 1.22              |
| 1:A:122:GLN:NE2  | 5:K:44:A:C6      | 2.06                     | 1.21              |
| 2:C:429:LEU:HA   | 2:C:432:ARG:HG2  | 1.21                     | 1.18              |
| 2:C:429:LEU:HG   | 2:C:432:ARG:HD3  | 1.26                     | 1.17              |
| 1:A:185:HIS:CD2  | 1:A:186:PRO:N    | 2.11                     | 1.17              |
| 3:D:169:LEU:CD1  | 3:D:170:PHE:CD2  | 2.28                     | 1.17              |
| 1:A:122:GLN:OE1  | 5:K:44:A:C6      | 1.99                     | 1.16              |
| 2:C:73:ALA:O     | 2:C:77:ALA:HB3   | 1.47                     | 1.15              |
| 2:C:343:HIS:NE2  | 2:C:372:LEU:HD11 | 1.60                     | 1.15              |
| 1:A:114:LEU:O    | 1:A:122:GLN:HG2  | 1.46                     | 1.14              |
| 1:A:122:GLN:CD   | 5:K:44:A:C6      | 2.26                     | 1.13              |
| 1:A:183:ILE:CB   | 5:K:45:G:H21     | 1.60                     | 1.13              |
| 1:A:123:ARG:HG2  | 1:A:212:ARG:NH1  | 1.64                     | 1.12              |
| 2:C:23:THR:HG22  | 2:C:45:ARG:HB2   | 1.32                     | 1.11              |
| 3:D:169:LEU:HD11 | 3:D:170:PHE:CD2  | 1.86                     | 1.11              |
| 1:A:164:TYR:HB2  | 1:A:188:VAL:HG13 | 1.17                     | 1.09              |
| 2:C:429:LEU:CG   | 2:C:432:ARG:HD3  | 1.83                     | 1.08              |
| 3:I:101:LYS:CD   | 4:L:93:ARG:HD3   | 1.83                     | 1.08              |
| 2:C:132:TRP:CZ3  | 2:C:249:TRP:CB   | 2.36                     | 1.07              |
| 2:C:429:LEU:HG   | 2:C:432:ARG:CD   | 1.82                     | 1.07              |
| 4:J:98:GLN:O     | 4:J:98:GLN:NE2   | 1.88                     | 1.06              |
| 2:C:334:ILE:HD11 | 7:N:69:ARG:HE    | 1.12                     | 1.05              |
| 3:D:42:SER:HB2   | 5:K:8:G:O2'      | 1.57                     | 1.04              |
| 5:K:8:G:C5       | 5:K:10:C:H5''    | 1.94                     | 1.03              |
| 3:E:302:THR:HG22 | 3:F:309:GLY:HA3  | 1.37                     | 1.02              |
| 3:F:14:TYR:O     | 3:F:275:THR:HG21 | 1.60                     | 1.02              |
| 1:A:103:ARG:O    | 1:A:223:LEU:HA   | 1.60                     | 1.01              |
| 2:C:78:ARG:HD3   | 2:C:115:TYR:HE2  | 1.24                     | 1.01              |
| 3:D:236:ASN:HD22 | 3:D:237:VAL:N    | 1.58                     | 1.01              |
| 2:C:132:TRP:CZ3  | 2:C:249:TRP:CG   | 2.48                     | 1.00              |
| 2:C:336:ARG:HH11 | 7:N:200:LEU:HB3  | 1.20                     | 1.00              |
| 1:A:184:ARG:NH2  | 5:K:46:C:OP1     | 1.93                     | 1.00              |
| 7:N:54:TYR:O     | 7:N:57:LEU:HD23  | 1.62                     | 1.00              |
| 3:D:169:LEU:HD12 | 3:D:170:PHE:CD2  | 1.95                     | 0.99              |
| 2:C:125:LEU:HD23 | 2:C:126:PHE:H    | 0.99                     | 0.99              |
| 1:A:163:THR:N    | 3:I:19:ARG:NH1   | 2.11                     | 0.99              |
| 2:C:132:TRP:HZ3  | 2:C:249:TRP:CG   | 1.80                     | 0.99              |
| 1:A:98:LYS:HE3   | 1:A:199:VAL:HB   | 1.43                     | 0.98              |
| 5:K:1:A:H8       | 5:K:1:A:HO5'     | 0.99                     | 0.98              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:336:ARG:NH1  | 7:N:200:LEU:HB3  | 1.78                     | 0.98              |
| 1:A:138:TRP:N    | 1:A:144:ALA:HB2  | 1.78                     | 0.98              |
| 2:C:429:LEU:CA   | 2:C:432:ARG:CG   | 2.42                     | 0.98              |
| 1:A:163:THR:N    | 3:I:19:ARG:HH12  | 1.61                     | 0.98              |
| 2:C:510:ALA:O    | 2:C:514:GLU:HG2  | 1.63                     | 0.97              |
| 7:N:171:ARG:HB2  | 7:N:171:ARG:HH11 | 1.22                     | 0.97              |
| 2:C:132:TRP:CZ3  | 2:C:249:TRP:HB3  | 1.98                     | 0.97              |
| 3:E:226:PHE:HE1  | 3:E:271:LYS:NZ   | 1.60                     | 0.97              |
| 1:A:138:TRP:H    | 1:A:144:ALA:CB   | 1.77                     | 0.97              |
| 3:D:238:ASN:HB2  | 7:N:135:GLN:HE22 | 1.26                     | 0.97              |
| 2:C:429:LEU:CA   | 2:C:432:ARG:HG2  | 1.96                     | 0.96              |
| 1:A:138:TRP:H    | 1:A:144:ALA:HB3  | 1.31                     | 0.96              |
| 1:A:183:ILE:CB   | 5:K:45:G:N2      | 2.29                     | 0.96              |
| 2:C:180:GLU:HA   | 2:C:183:TRP:CE3  | 2.01                     | 0.95              |
| 7:N:172:ARG:HG3  | 7:N:172:ARG:HH21 | 1.30                     | 0.95              |
| 5:K:8:G:C6       | 5:K:10:C:H5"     | 2.00                     | 0.95              |
| 1:A:183:ILE:C    | 1:A:184:ARG:HD3  | 1.92                     | 0.94              |
| 1:A:87:ARG:NH1   | 1:A:88:ASN:O     | 2.00                     | 0.94              |
| 1:A:169:ASP:O    | 1:A:184:ARG:O    | 1.86                     | 0.94              |
| 2:C:371:SER:HA   | 2:C:400:ARG:HH12 | 1.32                     | 0.94              |
| 3:D:165:VAL:O    | 3:D:169:LEU:HD23 | 1.67                     | 0.94              |
| 3:I:101:LYS:HD3  | 4:L:93:ARG:HD3   | 1.49                     | 0.93              |
| 2:C:406:GLU:OE2  | 2:C:412:ASN:HB2  | 1.69                     | 0.93              |
| 3:D:169:LEU:HD12 | 3:D:170:PHE:CE2  | 2.00                     | 0.93              |
| 3:E:226:PHE:CE1  | 3:E:271:LYS:NZ   | 2.35                     | 0.93              |
| 7:N:7:ARG:HG3    | 7:N:7:ARG:HH11   | 1.34                     | 0.93              |
| 2:C:342:LEU:HA   | 2:C:423:ARG:NH2  | 1.84                     | 0.93              |
| 2:C:51:SER:OG    | 2:C:229:PHE:HB2  | 1.70                     | 0.92              |
| 2:C:334:ILE:HD11 | 7:N:69:ARG:NE    | 1.83                     | 0.92              |
| 1:A:138:TRP:N    | 1:A:144:ALA:CB   | 2.33                     | 0.91              |
| 2:C:429:LEU:CB   | 2:C:432:ARG:HD3  | 2.00                     | 0.91              |
| 2:C:185:LEU:HD11 | 2:C:189:LEU:HD11 | 1.53                     | 0.91              |
| 3:I:13:PRO:HG2   | 3:I:16:ASN:HD22  | 1.35                     | 0.90              |
| 3:D:7:HIS:HD2    | 3:D:232:TYR:OH   | 1.54                     | 0.90              |
| 2:C:168:HIS:CE1  | 2:C:174:HIS:CE1  | 2.60                     | 0.90              |
| 2:C:125:LEU:O    | 2:C:131:PRO:HB3  | 1.73                     | 0.89              |
| 2:C:162:VAL:HG12 | 2:C:167:HIS:HB3  | 1.50                     | 0.89              |
| 3:I:101:LYS:HD2  | 4:L:93:ARG:CD    | 2.03                     | 0.89              |
| 3:E:226:PHE:HE1  | 3:E:271:LYS:HZ3  | 1.12                     | 0.89              |
| 3:F:14:TYR:H     | 3:F:228:ALA:HB2  | 1.38                     | 0.88              |
| 1:A:166:GLN:NE2  | 6:M:23:DG:N7     | 2.22                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:132:TRP:HH2  | 2:C:249:TRP:CD2  | 1.92                     | 0.88              |
| 2:C:162:VAL:CG1  | 2:C:167:HIS:HB3  | 2.04                     | 0.88              |
| 3:G:14:TYR:H     | 3:G:228:ALA:HB2  | 1.39                     | 0.88              |
| 3:D:355:SER:OG   | 3:D:357:PRO:HD2  | 1.74                     | 0.88              |
| 3:I:12:LEU:HD23  | 3:I:13:PRO:HD2   | 1.54                     | 0.88              |
| 2:C:76:THR:HG21  | 2:C:232:LEU:HD23 | 1.55                     | 0.87              |
| 3:E:14:TYR:H     | 3:E:228:ALA:HB2  | 1.39                     | 0.87              |
| 2:C:130:ARG:HD2  | 2:C:130:ARG:N    | 1.87                     | 0.87              |
| 5:K:36:C:O2      | 6:M:27:DG:N2     | 2.07                     | 0.87              |
| 1:A:116:ARG:HA   | 5:K:44:A:N6      | 1.90                     | 0.87              |
| 1:A:164:TYR:HB3  | 1:A:188:VAL:HG13 | 1.57                     | 0.87              |
| 1:A:124:LEU:HG   | 5:K:44:A:H5'     | 1.54                     | 0.87              |
| 3:H:14:TYR:H     | 3:H:228:ALA:HB2  | 1.39                     | 0.87              |
| 3:I:101:LYS:CD   | 4:L:93:ARG:CD    | 2.53                     | 0.86              |
| 7:N:185:ILE:HG12 | 7:N:221:VAL:HG12 | 1.55                     | 0.86              |
| 2:C:106:ARG:HH11 | 2:C:106:ARG:HB3  | 1.40                     | 0.86              |
| 2:C:343:HIS:HE1  | 2:C:359:THR:CB   | 1.88                     | 0.86              |
| 1:A:140:LEU:O    | 1:A:165:ALA:HB1  | 1.75                     | 0.86              |
| 2:C:168:HIS:CE1  | 2:C:174:HIS:HE1  | 1.92                     | 0.86              |
| 2:C:429:LEU:CA   | 2:C:432:ARG:CD   | 2.51                     | 0.86              |
| 4:J:197:ARG:HG2  | 4:J:197:ARG:HH11 | 1.38                     | 0.86              |
| 2:C:405:ARG:CB   | 2:C:405:ARG:HH11 | 1.87                     | 0.86              |
| 2:C:468:HIS:O    | 2:C:472:ARG:HG3  | 1.75                     | 0.86              |
| 2:C:155:ARG:HH12 | 2:C:174:HIS:CE1  | 1.94                     | 0.86              |
| 3:D:3:PHE:CD2    | 3:D:293:PRO:HD3  | 2.11                     | 0.85              |
| 2:C:168:HIS:HE1  | 2:C:174:HIS:CE1  | 1.94                     | 0.85              |
| 2:C:246:LEU:CD1  | 2:C:251:GLN:OE1  | 2.24                     | 0.85              |
| 2:C:180:GLU:HG2  | 2:C:183:TRP:CZ3  | 2.11                     | 0.85              |
| 1:A:27:HIS:HD2   | 1:A:215:SER:HB2  | 1.41                     | 0.85              |
| 2:C:185:LEU:O    | 2:C:185:LEU:HD12 | 1.77                     | 0.85              |
| 1:A:157:GLY:HA2  | 1:A:196:ILE:HA   | 1.59                     | 0.85              |
| 3:F:302:THR:HG22 | 3:G:309:GLY:HA3  | 1.58                     | 0.84              |
| 2:C:106:ARG:HH11 | 2:C:106:ARG:CB   | 1.91                     | 0.84              |
| 7:N:171:ARG:HH11 | 7:N:171:ARG:CB   | 1.89                     | 0.84              |
| 1:A:124:LEU:CG   | 5:K:44:A:H5'     | 2.07                     | 0.84              |
| 2:C:132:TRP:CH2  | 2:C:249:TRP:CD2  | 2.66                     | 0.84              |
| 2:C:257:PRO:HG2  | 2:C:258:LEU:HD13 | 1.60                     | 0.83              |
| 2:C:336:ARG:NH1  | 7:N:200:LEU:HD23 | 1.92                     | 0.83              |
| 1:A:113:ARG:NH2  | 5:K:56:G:H2'     | 1.93                     | 0.83              |
| 7:N:47:ARG:HG3   | 7:N:47:ARG:HH21  | 1.40                     | 0.83              |
| 1:A:141:ARG:HH22 | 3:E:214:ASN:HA   | 1.41                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:510:ALA:O    | 2:C:514:GLU:CG   | 2.27                     | 0.83              |
| 7:N:18:HIS:O     | 7:N:18:HIS:ND1   | 2.12                     | 0.83              |
| 2:C:125:LEU:CD2  | 2:C:126:PHE:H    | 1.88                     | 0.82              |
| 3:D:165:VAL:O    | 3:D:169:LEU:CD2  | 2.27                     | 0.82              |
| 2:C:224:LEU:HB2  | 2:C:373:ARG:O    | 1.78                     | 0.82              |
| 5:K:44:A:H3'     | 5:K:44:A:OP1     | 1.79                     | 0.82              |
| 7:N:93:ARG:HG3   | 7:N:93:ARG:HH11  | 1.43                     | 0.82              |
| 2:C:84:GLN:O     | 2:C:86:PRO:HD3   | 1.78                     | 0.82              |
| 3:D:42:SER:CB    | 5:K:8:G:O2'      | 2.27                     | 0.81              |
| 2:C:132:TRP:HZ3  | 2:C:249:TRP:HB2  | 1.44                     | 0.81              |
| 2:C:125:LEU:HD21 | 2:C:126:PHE:CD1  | 2.16                     | 0.81              |
| 7:N:6:LEU:HD23   | 7:N:149:LEU:O    | 1.80                     | 0.81              |
| 7:N:166:VAL:HG22 | 7:N:245:TYR:CZ   | 2.15                     | 0.81              |
| 5:K:44:A:C4'     | 5:K:45:G:H5''    | 2.11                     | 0.81              |
| 2:C:142:CYS:HG   | 2:C:200:ARG:HB3  | 1.45                     | 0.81              |
| 5:K:49:C:H2'     | 5:K:50:A:H8      | 1.44                     | 0.80              |
| 8:O:43:DC:H2'    | 8:O:43:DC:O2     | 1.81                     | 0.80              |
| 1:A:53:PHE:HB2   | 1:A:64:LEU:HD21  | 1.63                     | 0.80              |
| 2:C:20:PHE:O     | 2:C:124:ASP:HA   | 1.81                     | 0.80              |
| 1:A:33:LEU:HD13  | 1:A:33:LEU:O     | 1.81                     | 0.80              |
| 2:C:23:THR:HB    | 2:C:24:ILE:HD12  | 1.62                     | 0.80              |
| 2:C:125:LEU:CD2  | 2:C:126:PHE:CD1  | 2.64                     | 0.80              |
| 6:M:62:DC:O2     | 8:O:4:DG:N2      | 2.12                     | 0.80              |
| 2:C:303:ARG:NH1  | 2:C:304:ASN:O    | 2.14                     | 0.80              |
| 2:C:210:VAL:HG22 | 2:C:298:TRP:HB3  | 1.63                     | 0.79              |
| 2:C:336:ARG:NH1  | 7:N:200:LEU:CD2  | 2.45                     | 0.79              |
| 2:C:468:HIS:O    | 2:C:472:ARG:CG   | 2.30                     | 0.79              |
| 8:O:11:DG:H2''   | 8:O:12:DC:H5''   | 1.65                     | 0.79              |
| 1:A:180:SER:O    | 1:A:181:ARG:HD3  | 1.83                     | 0.79              |
| 2:C:433:LEU:HD13 | 2:C:536:LEU:HD21 | 1.64                     | 0.79              |
| 2:C:155:ARG:NH1  | 2:C:174:HIS:CE1  | 2.49                     | 0.79              |
| 3:D:193:THR:HG23 | 3:D:231:PHE:CE1  | 2.18                     | 0.79              |
| 3:E:16:ASN:HD22  | 3:E:226:PHE:HD1  | 1.30                     | 0.79              |
| 1:A:122:GLN:OE1  | 5:K:44:A:C4      | 2.36                     | 0.78              |
| 4:J:98:GLN:HG2   | 4:J:187:GLN:OE1  | 1.83                     | 0.78              |
| 1:A:163:THR:H    | 3:I:19:ARG:HH12  | 0.83                     | 0.78              |
| 2:C:237:PRO:HB3  | 2:C:311:PRO:HG3  | 1.65                     | 0.78              |
| 2:C:132:TRP:CH2  | 2:C:249:TRP:CG   | 2.72                     | 0.78              |
| 2:C:177:ASP:HA   | 2:C:290:HIS:ND1  | 1.99                     | 0.78              |
| 1:A:101:ARG:HG2  | 1:A:101:ARG:HH11 | 1.47                     | 0.78              |
| 1:A:124:LEU:HD12 | 5:K:44:A:N3      | 1.98                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:226:ARG:O    | 4:J:229:GLU:HG3  | 1.84                     | 0.78              |
| 3:E:289:ARG:HD3  | 3:E:293:PRO:HA   | 1.64                     | 0.78              |
| 3:F:214:ASN:HA   | 3:I:178:PRO:HG3  | 1.64                     | 0.78              |
| 1:A:114:LEU:O    | 1:A:122:GLN:CG   | 2.31                     | 0.77              |
| 3:D:343:LYS:HD3  | 3:D:344:THR:HG23 | 1.65                     | 0.77              |
| 1:A:164:TYR:HB2  | 1:A:188:VAL:CG1  | 2.06                     | 0.77              |
| 3:D:14:TYR:CE2   | 3:D:226:PHE:HD2  | 2.03                     | 0.77              |
| 1:A:105:ARG:HB2  | 1:A:105:ARG:HH11 | 1.49                     | 0.77              |
| 2:C:180:GLU:HG2  | 2:C:183:TRP:HZ3  | 1.50                     | 0.77              |
| 3:E:275:THR:HG22 | 3:I:190:HIS:CD2  | 2.19                     | 0.77              |
| 1:A:122:GLN:NE2  | 5:K:44:A:C2      | 2.53                     | 0.77              |
| 3:D:165:VAL:HG12 | 3:D:169:LEU:HD23 | 1.65                     | 0.77              |
| 2:C:309:LEU:HB3  | 2:C:315:TYR:CE2  | 2.19                     | 0.77              |
| 2:C:155:ARG:NH2  | 2:C:176:LEU:HD22 | 2.00                     | 0.77              |
| 2:C:73:ALA:O     | 2:C:77:ALA:CB    | 2.31                     | 0.76              |
| 3:D:183:ASP:OD2  | 5:K:1:A:C2       | 2.39                     | 0.76              |
| 7:N:93:ARG:HG3   | 7:N:93:ARG:NH1   | 1.99                     | 0.76              |
| 1:A:123:ARG:HG2  | 1:A:212:ARG:HH12 | 1.47                     | 0.76              |
| 2:C:137:ARG:HH12 | 2:C:256:ASP:HA   | 1.50                     | 0.76              |
| 3:G:121:VAL:O    | 3:G:124:ILE:HG22 | 1.86                     | 0.76              |
| 1:A:27:HIS:CD2   | 1:A:215:SER:HB2  | 2.20                     | 0.76              |
| 3:E:14:TYR:CE2   | 3:E:226:PHE:HB2  | 2.20                     | 0.76              |
| 1:A:101:ARG:HD3  | 1:A:195:VAL:HG23 | 1.67                     | 0.76              |
| 6:M:59:DG:N2     | 8:O:7:DC:O2      | 2.16                     | 0.76              |
| 2:C:163:TRP:CD1  | 7:N:76:ILE:HD13  | 2.20                     | 0.76              |
| 5:K:9:C:H42      | 6:M:54:DG:H1     | 1.34                     | 0.76              |
| 3:E:121:VAL:O    | 3:E:124:ILE:HG22 | 1.86                     | 0.76              |
| 3:G:164:ASN:OD1  | 3:G:165:VAL:N    | 2.19                     | 0.76              |
| 3:I:68:GLU:HG3   | 3:I:72:ARG:HH12  | 1.51                     | 0.76              |
| 4:L:138:ASN:HA   | 4:L:194:ILE:HD13 | 1.67                     | 0.76              |
| 3:F:121:VAL:O    | 3:F:124:ILE:HG22 | 1.86                     | 0.76              |
| 3:G:302:THR:HG22 | 3:H:309:GLY:HA3  | 1.68                     | 0.76              |
| 3:H:68:GLU:HG3   | 3:H:72:ARG:HH12  | 1.51                     | 0.76              |
| 3:F:141:GLU:HG3  | 3:F:150:ILE:HG13 | 1.68                     | 0.76              |
| 3:H:121:VAL:O    | 3:H:124:ILE:HG22 | 1.86                     | 0.76              |
| 1:A:138:TRP:C    | 1:A:144:ALA:CB   | 2.59                     | 0.75              |
| 3:E:68:GLU:HG3   | 3:E:72:ARG:HH12  | 1.51                     | 0.75              |
| 3:F:164:ASN:OD1  | 3:F:165:VAL:N    | 2.19                     | 0.75              |
| 3:H:164:ASN:OD1  | 3:H:165:VAL:N    | 2.19                     | 0.75              |
| 3:I:141:GLU:HG3  | 3:I:150:ILE:HG13 | 1.68                     | 0.75              |
| 3:I:164:ASN:OD1  | 3:I:165:VAL:N    | 2.19                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:78:ARG:HD3   | 2:C:115:TYR:CE2  | 2.15                     | 0.75              |
| 2:C:501:GLY:O    | 2:C:502:ASN:HB2  | 1.85                     | 0.75              |
| 3:I:121:VAL:O    | 3:I:124:ILE:HG22 | 1.85                     | 0.75              |
| 1:A:102:VAL:O    | 1:A:193:GLU:HA   | 1.86                     | 0.75              |
| 2:C:67:VAL:HB    | 2:C:186:LEU:HD23 | 1.68                     | 0.75              |
| 2:C:81:GLY:HA2   | 2:C:94:TRP:HE1   | 1.52                     | 0.75              |
| 2:C:176:LEU:HD12 | 2:C:184:HIS:HD2  | 1.51                     | 0.75              |
| 2:C:379:PHE:HD1  | 2:C:390:TRP:HB3  | 1.52                     | 0.75              |
| 3:D:169:LEU:CD1  | 3:D:170:PHE:CZ   | 2.69                     | 0.75              |
| 4:J:197:ARG:HH12 | 4:J:201:ARG:HH21 | 1.35                     | 0.75              |
| 2:C:191:TYR:CE2  | 2:C:215:LEU:CD1  | 2.70                     | 0.74              |
| 3:G:68:GLU:HG3   | 3:G:72:ARG:HH12  | 1.51                     | 0.74              |
| 3:I:101:LYS:HD2  | 4:L:93:ARG:HD3   | 1.60                     | 0.74              |
| 2:C:45:ARG:HG3   | 2:C:116:PHE:CE2  | 2.23                     | 0.74              |
| 3:I:18:ASN:ND2   | 3:I:26:LYS:HD2   | 2.02                     | 0.74              |
| 4:J:93:ARG:HG2   | 4:J:93:ARG:HH11  | 1.52                     | 0.74              |
| 1:A:124:LEU:CD1  | 5:K:44:A:N3      | 2.50                     | 0.74              |
| 2:C:125:LEU:CD2  | 2:C:126:PHE:N    | 2.38                     | 0.74              |
| 5:K:2:U:OP1      | 7:N:47:ARG:NE    | 2.20                     | 0.74              |
| 3:G:141:GLU:HG3  | 3:G:150:ILE:HG13 | 1.68                     | 0.74              |
| 1:A:141:ARG:HA   | 3:E:216:HIS:HE1  | 1.52                     | 0.74              |
| 2:C:343:HIS:NE2  | 2:C:372:LEU:CD1  | 2.46                     | 0.74              |
| 3:E:164:ASN:OD1  | 3:E:165:VAL:N    | 2.19                     | 0.74              |
| 1:A:124:LEU:HG   | 5:K:44:A:C5'     | 2.16                     | 0.74              |
| 3:F:68:GLU:HG3   | 3:F:72:ARG:HH12  | 1.51                     | 0.74              |
| 1:A:112:LYS:NZ   | 5:K:56:G:OP1     | 2.21                     | 0.73              |
| 3:I:13:PRO:CG    | 3:I:16:ASN:HD22  | 2.02                     | 0.73              |
| 7:N:47:ARG:HG3   | 7:N:47:ARG:NH2   | 1.98                     | 0.73              |
| 3:E:141:GLU:HG3  | 3:E:150:ILE:HG13 | 1.68                     | 0.73              |
| 3:H:141:GLU:HG3  | 3:H:150:ILE:HG13 | 1.68                     | 0.73              |
| 5:K:8:G:C6       | 5:K:10:C:C5'     | 2.70                     | 0.73              |
| 7:N:7:ARG:HD3    | 7:N:148:LEU:O    | 1.88                     | 0.73              |
| 7:N:197:LEU:N    | 7:N:219:ILE:O    | 2.20                     | 0.73              |
| 3:I:183:ASP:N    | 3:I:183:ASP:OD1  | 2.21                     | 0.73              |
| 7:N:83:GLU:O     | 7:N:93:ARG:NH1   | 2.21                     | 0.73              |
| 4:L:194:ILE:HD12 | 4:L:195:LEU:N    | 2.03                     | 0.73              |
| 3:F:183:ASP:OD1  | 3:F:183:ASP:N    | 2.21                     | 0.73              |
| 4:J:136:ARG:NH1  | 4:J:191:ASP:OD2  | 2.21                     | 0.73              |
| 1:A:47:GLN:HG3   | 5:K:59:G:O2'     | 1.89                     | 0.73              |
| 3:E:183:ASP:OD1  | 3:E:183:ASP:N    | 2.21                     | 0.73              |
| 2:C:130:ARG:NH2  | 2:C:130:ARG:HG3  | 2.04                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:197:ARG:HG2  | 4:J:197:ARG:NH1  | 2.00                     | 0.72              |
| 3:D:208:ASP:OD2  | 3:H:64:ARG:NH1   | 2.22                     | 0.72              |
| 3:H:183:ASP:OD1  | 3:H:183:ASP:N    | 2.21                     | 0.72              |
| 2:C:216:ARG:HG3  | 2:C:381:GLN:NE2  | 2.04                     | 0.72              |
| 2:C:343:HIS:CE1  | 2:C:359:THR:CB   | 2.72                     | 0.72              |
| 7:N:172:ARG:HG3  | 7:N:172:ARG:NH2  | 1.95                     | 0.72              |
| 2:C:130:ARG:HG3  | 2:C:130:ARG:HH21 | 1.53                     | 0.72              |
| 4:J:93:ARG:HG2   | 4:J:93:ARG:NH1   | 2.04                     | 0.72              |
| 2:C:202:VAL:HG12 | 2:C:203:ARG:HE   | 1.54                     | 0.72              |
| 2:C:24:ILE:HD12  | 2:C:24:ILE:N     | 2.04                     | 0.72              |
| 1:A:124:LEU:CD1  | 5:K:44:A:C2      | 2.73                     | 0.72              |
| 2:C:152:ALA:HB3  | 2:C:155:ARG:HG3  | 1.71                     | 0.72              |
| 2:C:429:LEU:CD2  | 2:C:505:ASN:HA   | 2.19                     | 0.72              |
| 3:D:172:ARG:HD2  | 3:D:173:MET:O    | 1.89                     | 0.72              |
| 1:A:164:TYR:HB3  | 1:A:188:VAL:HG22 | 1.71                     | 0.71              |
| 2:C:137:ARG:O    | 2:C:140:GLU:HG2  | 1.89                     | 0.71              |
| 1:A:33:LEU:HD11  | 1:A:73:ARG:O     | 1.90                     | 0.71              |
| 3:D:169:LEU:HD11 | 3:D:170:PHE:HE2  | 1.47                     | 0.71              |
| 3:G:183:ASP:N    | 3:G:183:ASP:OD1  | 2.21                     | 0.71              |
| 3:D:341:GLU:O    | 3:D:352:ARG:NH2  | 2.23                     | 0.71              |
| 5:K:43:G:N3      | 5:K:43:G:H5''    | 2.04                     | 0.71              |
| 1:A:113:ARG:HG2  | 1:A:113:ARG:HH11 | 1.56                     | 0.71              |
| 7:N:14:SER:O     | 7:N:139:GLY:HA3  | 1.89                     | 0.71              |
| 2:C:217:GLY:N    | 2:C:381:GLN:HE21 | 1.88                     | 0.71              |
| 7:N:7:ARG:HG3    | 7:N:7:ARG:NH1    | 2.01                     | 0.71              |
| 2:C:185:LEU:CD1  | 2:C:189:LEU:HD11 | 2.20                     | 0.71              |
| 2:C:342:LEU:HD13 | 2:C:342:LEU:O    | 1.91                     | 0.71              |
| 6:M:63:DG:N2     | 8:O:3:DC:O2      | 2.19                     | 0.71              |
| 2:C:142:CYS:SG   | 2:C:200:ARG:HB2  | 2.29                     | 0.71              |
| 3:D:40:SER:CB    | 3:D:190:HIS:CD2  | 2.74                     | 0.71              |
| 2:C:191:TYR:CE2  | 2:C:215:LEU:HD12 | 2.26                     | 0.71              |
| 2:C:336:ARG:HH11 | 7:N:200:LEU:HD23 | 1.55                     | 0.71              |
| 2:C:342:LEU:HA   | 2:C:423:ARG:HH21 | 1.52                     | 0.71              |
| 2:C:45:ARG:HG3   | 2:C:116:PHE:HE2  | 1.57                     | 0.70              |
| 2:C:428:ALA:O    | 2:C:432:ARG:HG2  | 1.90                     | 0.70              |
| 3:D:42:SER:HB2   | 5:K:8:G:HO2'     | 1.54                     | 0.70              |
| 3:E:280:LEU:HD12 | 3:I:325:LEU:HD22 | 1.74                     | 0.70              |
| 7:N:57:LEU:HD13  | 7:N:119:GLY:HA3  | 1.72                     | 0.70              |
| 3:D:40:SER:HB3   | 3:D:190:HIS:CD2  | 2.26                     | 0.70              |
| 1:A:123:ARG:HG2  | 1:A:212:ARG:HH11 | 1.51                     | 0.70              |
| 1:A:124:LEU:CD1  | 5:K:44:A:H5'     | 2.21                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:191:TYR:CZ   | 2:C:215:LEU:CD1  | 2.75                     | 0.70              |
| 1:A:33:LEU:HD12  | 1:A:72:LEU:HG    | 1.73                     | 0.70              |
| 2:C:317:THR:HG22 | 2:C:323:VAL:HG22 | 1.73                     | 0.70              |
| 3:F:14:TYR:CZ    | 3:F:226:PHE:HB2  | 2.26                     | 0.70              |
| 1:A:124:LEU:HD11 | 5:K:44:A:O5'     | 1.91                     | 0.70              |
| 3:D:193:THR:HG23 | 3:D:231:PHE:HE1  | 1.56                     | 0.69              |
| 5:K:44:A:O4'     | 5:K:45:G:H5''    | 1.91                     | 0.69              |
| 3:D:236:ASN:HD22 | 3:D:236:ASN:C    | 2.00                     | 0.69              |
| 4:J:197:ARG:NH1  | 4:J:201:ARG:HH21 | 1.89                     | 0.69              |
| 2:C:494:THR:HG23 | 2:C:497:MET:HB2  | 1.73                     | 0.69              |
| 3:D:169:LEU:HD12 | 3:D:170:PHE:CG   | 2.28                     | 0.69              |
| 2:C:185:LEU:HD12 | 2:C:185:LEU:C    | 2.16                     | 0.69              |
| 1:A:105:ARG:O    | 1:A:106:ILE:CB   | 2.37                     | 0.69              |
| 2:C:176:LEU:HD13 | 2:C:180:GLU:OE1  | 1.93                     | 0.69              |
| 7:N:166:VAL:HG22 | 7:N:245:TYR:CE2  | 2.27                     | 0.69              |
| 2:C:343:HIS:CD2  | 2:C:372:LEU:HD11 | 2.28                     | 0.68              |
| 3:E:289:ARG:NH1  | 3:E:292:ARG:O    | 2.26                     | 0.68              |
| 3:I:12:LEU:HD23  | 3:I:13:PRO:CD    | 2.24                     | 0.68              |
| 3:I:101:LYS:HD3  | 4:L:93:ARG:CD    | 2.21                     | 0.68              |
| 2:C:406:GLU:OE2  | 2:C:412:ASN:CB   | 2.41                     | 0.68              |
| 1:A:33:LEU:HD11  | 1:A:73:ARG:H     | 1.57                     | 0.68              |
| 1:A:113:ARG:CZ   | 5:K:57:U:C6      | 2.76                     | 0.68              |
| 1:A:141:ARG:H    | 1:A:141:ARG:HD2  | 1.57                     | 0.68              |
| 2:C:485:VAL:HG13 | 2:C:486:TYR:HD1  | 1.59                     | 0.68              |
| 3:E:289:ARG:CZ   | 3:E:289:ARG:HB3  | 2.23                     | 0.68              |
| 3:D:171:GLY:HA2  | 3:D:184:GLY:HA2  | 1.75                     | 0.68              |
| 6:M:50:DA:H2'    | 6:M:51:DC:C6     | 2.27                     | 0.68              |
| 1:A:163:THR:H    | 3:I:19:ARG:HH11  | 1.38                     | 0.68              |
| 1:A:173:ASP:N    | 1:A:181:ARG:O    | 2.26                     | 0.68              |
| 2:C:178:SER:O    | 2:C:182:VAL:HG23 | 1.93                     | 0.68              |
| 3:I:18:ASN:HD21  | 3:I:26:LYS:NZ    | 1.91                     | 0.68              |
| 4:L:138:ASN:HA   | 4:L:194:ILE:CD1  | 2.23                     | 0.68              |
| 2:C:251:GLN:OE1  | 2:C:251:GLN:HA   | 1.93                     | 0.68              |
| 3:F:14:TYR:CE1   | 3:F:226:PHE:HB2  | 2.28                     | 0.68              |
| 2:C:23:THR:HG22  | 2:C:116:PHE:CE2  | 2.29                     | 0.68              |
| 2:C:217:GLY:H    | 2:C:381:GLN:HE21 | 1.41                     | 0.68              |
| 3:H:269:SER:HA   | 3:H:272:GLN:CG   | 2.22                     | 0.68              |
| 1:A:98:LYS:HE2   | 1:A:98:LYS:N     | 2.08                     | 0.68              |
| 4:J:40:GLU:HG3   | 4:L:211:ARG:HE   | 1.59                     | 0.67              |
| 3:E:68:GLU:HG3   | 3:E:72:ARG:NH1   | 2.09                     | 0.67              |
| 1:A:141:ARG:NH2  | 3:E:214:ASN:HA   | 2.10                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 5:K:49:C:H2'     | 5:K:50:A:C8     | 2.27                     | 0.67              |
| 7:N:83:GLU:OE1   | 7:N:83:GLU:N    | 2.26                     | 0.67              |
| 3:H:68:GLU:HG3   | 3:H:72:ARG:NH1  | 2.09                     | 0.67              |
| 1:A:116:ARG:HA   | 5:K:44:A:H62    | 1.57                     | 0.67              |
| 3:F:26:LYS:NZ    | 5:K:27:C:OP1    | 2.27                     | 0.67              |
| 3:I:52:GLU:HB3   | 3:I:58:LYS:HG2  | 1.77                     | 0.67              |
| 4:J:93:ARG:HA    | 4:J:96:ARG:HG2  | 1.76                     | 0.67              |
| 2:C:429:LEU:CA   | 2:C:432:ARG:HD3 | 2.20                     | 0.67              |
| 3:F:54:ARG:HD3   | 3:F:258:GLU:OE2 | 1.94                     | 0.67              |
| 3:F:68:GLU:HG3   | 3:F:72:ARG:NH1  | 2.09                     | 0.67              |
| 3:H:52:GLU:HB3   | 3:H:58:LYS:HG2  | 1.77                     | 0.67              |
| 1:A:107:VAL:HG13 | 1:A:218:CYS:HA  | 1.75                     | 0.67              |
| 3:F:52:GLU:HB3   | 3:F:58:LYS:HG2  | 1.77                     | 0.66              |
| 3:I:54:ARG:HD3   | 3:I:258:GLU:OE2 | 1.94                     | 0.66              |
| 2:C:176:LEU:HD12 | 2:C:184:HIS:CD2 | 2.30                     | 0.66              |
| 2:C:255:ASN:O    | 2:C:256:ASP:HB3 | 1.94                     | 0.66              |
| 3:E:17:ILE:HD12  | 3:E:268:PRO:HG2 | 1.76                     | 0.66              |
| 2:C:429:LEU:HG   | 2:C:432:ARG:HD2 | 1.75                     | 0.66              |
| 3:F:17:ILE:O     | 3:F:270:GLY:HA3 | 1.95                     | 0.66              |
| 1:A:124:LEU:CD1  | 5:K:44:A:O5'    | 2.43                     | 0.66              |
| 2:C:141:GLU:HG3  | 2:C:201:VAL:O   | 1.94                     | 0.66              |
| 2:C:138:LEU:CD2  | 2:C:200:ARG:HG3 | 2.26                     | 0.66              |
| 3:G:68:GLU:HG3   | 3:G:72:ARG:NH1  | 2.09                     | 0.66              |
| 3:I:68:GLU:HG3   | 3:I:72:ARG:NH1  | 2.09                     | 0.66              |
| 2:C:379:PHE:CE1  | 2:C:390:TRP:HE3 | 2.14                     | 0.66              |
| 3:E:324:ARG:HH21 | 3:E:324:ARG:HG3 | 1.59                     | 0.66              |
| 3:G:54:ARG:HD3   | 3:G:258:GLU:OE2 | 1.94                     | 0.66              |
| 7:N:171:ARG:HB2  | 7:N:171:ARG:NH1 | 2.05                     | 0.66              |
| 1:A:3:TRP:CZ2    | 1:A:71:PRO:HA   | 2.30                     | 0.66              |
| 1:A:124:LEU:CD1  | 5:K:44:A:C5'    | 2.74                     | 0.66              |
| 2:C:303:ARG:CZ   | 2:C:304:ASN:H   | 2.08                     | 0.66              |
| 3:H:54:ARG:HD3   | 3:H:258:GLU:OE2 | 1.94                     | 0.66              |
| 3:F:18:ASN:ND2   | 3:F:39:SER:OG   | 2.29                     | 0.66              |
| 3:G:52:GLU:HB3   | 3:G:58:LYS:HG2  | 1.77                     | 0.66              |
| 2:C:197:CYS:SG   | 2:C:198:THR:N   | 2.69                     | 0.66              |
| 3:E:14:TYR:HD1   | 3:I:28:VAL:HG13 | 1.60                     | 0.66              |
| 7:N:194:THR:OG1  | 7:N:195:ARG:N   | 2.26                     | 0.65              |
| 1:A:184:ARG:HD2  | 8:O:47:DA:OP1   | 1.96                     | 0.65              |
| 3:F:35:ARG:NH1   | 3:F:300:PHE:O   | 2.21                     | 0.65              |
| 3:G:18:ASN:ND2   | 3:G:39:SER:OG   | 2.29                     | 0.65              |
| 1:A:112:LYS:HE2  | 5:K:43:G:C6     | 2.32                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:122:GLN:NE2  | 5:K:44:A:N6      | 2.44                     | 0.65              |
| 2:C:177:ASP:OD1  | 2:C:177:ASP:N    | 2.29                     | 0.65              |
| 2:C:335:TRP:HE3  | 2:C:474:TRP:CE3  | 2.15                     | 0.65              |
| 3:E:18:ASN:ND2   | 3:E:39:SER:OG    | 2.29                     | 0.65              |
| 3:E:52:GLU:HB3   | 3:E:58:LYS:HG2   | 1.77                     | 0.65              |
| 4:L:87:ILE:HD11  | 4:L:181:LEU:HG   | 1.79                     | 0.65              |
| 2:C:191:TYR:CZ   | 2:C:215:LEU:HD13 | 2.31                     | 0.65              |
| 2:C:246:LEU:HD11 | 2:C:251:GLN:OE1  | 1.96                     | 0.65              |
| 1:A:184:ARG:HD3  | 1:A:184:ARG:N    | 2.12                     | 0.65              |
| 1:A:185:HIS:CD2  | 1:A:186:PRO:CD   | 2.79                     | 0.65              |
| 2:C:127:HIS:O    | 2:C:131:PRO:HG3  | 1.96                     | 0.65              |
| 2:C:345:GLY:O    | 2:C:351:ARG:NH2  | 2.30                     | 0.65              |
| 1:A:98:LYS:CE    | 1:A:199:VAL:HB   | 2.25                     | 0.65              |
| 3:D:292:ARG:NH1  | 7:N:147:PRO:O    | 2.29                     | 0.65              |
| 4:J:136:ARG:NH1  | 4:J:136:ARG:HG2  | 2.11                     | 0.65              |
| 1:A:57:GLU:O     | 1:A:62:LEU:HA    | 1.97                     | 0.64              |
| 1:A:123:ARG:CG   | 1:A:212:ARG:NH1  | 2.51                     | 0.64              |
| 2:C:23:THR:CG2   | 2:C:116:PHE:CE2  | 2.81                     | 0.64              |
| 3:F:101:LYS:HD3  | 4:J:93:ARG:NH1   | 2.11                     | 0.64              |
| 3:D:172:ARG:NH2  | 3:D:176:GLU:O    | 2.31                     | 0.64              |
| 1:A:124:LEU:HD13 | 5:K:44:A:C2      | 2.32                     | 0.64              |
| 1:A:162:SER:CB   | 3:I:23:GLY:HA3   | 2.27                     | 0.64              |
| 2:C:363:GLN:CD   | 2:C:365:PRO:HD2  | 2.23                     | 0.64              |
| 3:D:167:VAL:HG13 | 3:D:172:ARG:HA   | 1.79                     | 0.64              |
| 3:D:236:ASN:OD1  | 3:D:293:PRO:CB   | 2.46                     | 0.64              |
| 7:N:43:GLN:NE2   | 7:N:125:ILE:HG12 | 2.12                     | 0.64              |
| 1:A:105:ARG:HH11 | 1:A:105:ARG:CB   | 2.09                     | 0.64              |
| 1:A:123:ARG:NH1  | 5:K:60:G:O6      | 2.30                     | 0.64              |
| 2:C:123:PHE:HE1  | 2:C:249:TRP:CD1  | 2.15                     | 0.64              |
| 1:A:113:ARG:HA   | 1:A:122:GLN:O    | 1.98                     | 0.64              |
| 1:A:170:ASP:OD1  | 1:A:171:VAL:N    | 2.31                     | 0.64              |
| 2:C:406:GLU:O    | 2:C:407:THR:OG1  | 2.11                     | 0.64              |
| 3:H:18:ASN:ND2   | 3:H:39:SER:OG    | 2.29                     | 0.64              |
| 4:J:56:PRO:HD2   | 4:J:81:PHE:HE2   | 1.61                     | 0.64              |
| 3:E:89:GLN:HE22  | 3:E:147:PRO:HB2  | 1.63                     | 0.64              |
| 1:A:141:ARG:HG3  | 3:E:216:HIS:CE1  | 2.32                     | 0.64              |
| 2:C:95:GLN:HA    | 2:C:98:ARG:HD3   | 1.80                     | 0.64              |
| 3:E:101:LYS:NZ   | 6:M:34:DT:OP1    | 2.26                     | 0.64              |
| 2:C:129:GLU:CG   | 2:C:130:ARG:HD3  | 2.28                     | 0.64              |
| 2:C:334:ILE:CD1  | 7:N:69:ARG:NE    | 2.60                     | 0.64              |
| 3:I:14:TYR:O     | 3:I:17:ILE:HG12  | 1.98                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:64:ASP:HB2   | 7:N:112:VAL:HG13 | 1.80                     | 0.64              |
| 7:N:227:PRO:HG2  | 7:N:230:LEU:HD23 | 1.79                     | 0.64              |
| 1:A:69:HIS:HE1   | 1:A:207:LEU:HD11 | 1.63                     | 0.63              |
| 1:A:112:LYS:HE2  | 5:K:43:G:O6      | 1.98                     | 0.63              |
| 3:D:169:LEU:HD12 | 3:D:170:PHE:CZ   | 2.33                     | 0.63              |
| 3:I:35:ARG:NH1   | 3:I:300:PHE:O    | 2.21                     | 0.63              |
| 3:E:324:ARG:NH1  | 3:F:342:ASN:HB3  | 2.13                     | 0.63              |
| 3:I:89:GLN:HE22  | 3:I:147:PRO:HB2  | 1.63                     | 0.63              |
| 4:L:7:LEU:HD21   | 4:L:136:ARG:HH12 | 1.64                     | 0.63              |
| 1:A:122:GLN:CD   | 5:K:44:A:N1      | 2.44                     | 0.63              |
| 1:A:123:ARG:CG   | 1:A:212:ARG:HH12 | 2.11                     | 0.63              |
| 1:A:185:HIS:HD2  | 1:A:186:PRO:CA   | 2.10                     | 0.63              |
| 2:C:104:LYS:HG2  | 2:C:106:ARG:O    | 1.99                     | 0.63              |
| 1:A:113:ARG:NH1  | 5:K:57:U:O5'     | 2.29                     | 0.63              |
| 3:G:89:GLN:HE22  | 3:G:147:PRO:HB2  | 1.63                     | 0.63              |
| 3:D:3:PHE:HE1    | 3:D:238:ASN:OD1  | 1.81                     | 0.63              |
| 3:D:29:VAL:HG12  | 7:N:70:LEU:HD11  | 1.79                     | 0.63              |
| 1:A:140:LEU:O    | 1:A:165:ALA:CB   | 2.46                     | 0.63              |
| 3:E:276:ALA:HB3  | 3:I:189:ALA:HB2  | 1.80                     | 0.63              |
| 3:H:15:SER:HB2   | 3:H:17:ILE:HG23  | 1.81                     | 0.63              |
| 1:A:162:SER:HA   | 3:I:19:ARG:HH11  | 1.62                     | 0.63              |
| 2:C:98:ARG:HE    | 2:C:363:GLN:CD   | 2.06                     | 0.63              |
| 2:C:118:ASP:HB3  | 2:C:119:TYR:CE1  | 2.34                     | 0.63              |
| 3:H:89:GLN:HE22  | 3:H:147:PRO:HB2  | 1.63                     | 0.63              |
| 4:J:169:LEU:HA   | 4:J:202:TRP:HD1  | 1.64                     | 0.63              |
| 1:A:138:TRP:CE3  | 5:K:43:G:C8      | 2.87                     | 0.63              |
| 2:C:245:ASP:HB2  | 2:C:266:GLY:HA3  | 1.79                     | 0.63              |
| 3:H:35:ARG:NH1   | 3:H:300:PHE:O    | 2.21                     | 0.63              |
| 1:A:101:ARG:HH11 | 1:A:101:ARG:CG   | 2.12                     | 0.62              |
| 2:C:274:ASP:OD1  | 2:C:275:HIS:ND1  | 2.32                     | 0.62              |
| 2:C:362:ALA:O    | 2:C:363:GLN:O    | 2.16                     | 0.62              |
| 3:F:15:SER:HB2   | 3:F:17:ILE:HG23  | 1.81                     | 0.62              |
| 3:F:89:GLN:HE22  | 3:F:147:PRO:HB2  | 1.63                     | 0.62              |
| 3:I:17:ILE:HD12  | 3:I:25:PRO:HB3   | 1.81                     | 0.62              |
| 2:C:130:ARG:HH21 | 2:C:130:ARG:CG   | 2.12                     | 0.62              |
| 3:G:15:SER:HB2   | 3:G:17:ILE:HG23  | 1.81                     | 0.62              |
| 4:J:93:ARG:HH11  | 4:J:93:ARG:CG    | 2.12                     | 0.62              |
| 1:A:109:SER:HB2  | 1:A:185:HIS:NE2  | 2.14                     | 0.62              |
| 2:C:405:ARG:HH11 | 2:C:405:ARG:CG   | 2.13                     | 0.62              |
| 5:K:47:C:H2'     | 5:K:48:C:C6      | 2.34                     | 0.62              |
| 3:H:269:SER:HA   | 3:H:272:GLN:HG2  | 1.80                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:135:ARG:HG3  | 4:J:136:ARG:H    | 1.63                     | 0.62              |
| 1:A:163:THR:OG1  | 3:I:19:ARG:NH2   | 2.28                     | 0.62              |
| 2:C:155:ARG:NH2  | 2:C:176:LEU:CD2  | 2.62                     | 0.62              |
| 2:C:162:VAL:HG12 | 2:C:162:VAL:O    | 2.00                     | 0.62              |
| 2:C:185:LEU:HD11 | 2:C:189:LEU:CD1  | 2.27                     | 0.62              |
| 2:C:247:ALA:HB3  | 2:C:250:GLU:HG3  | 1.81                     | 0.62              |
| 3:I:285:HIS:HD2  | 3:I:349:LEU:HB3  | 1.65                     | 0.62              |
| 5:K:44:A:C1'     | 5:K:45:G:H5''    | 2.29                     | 0.62              |
| 1:A:163:THR:HG1  | 3:I:19:ARG:HH22  | 1.47                     | 0.62              |
| 2:C:130:ARG:HD2  | 2:C:130:ARG:H    | 1.63                     | 0.62              |
| 7:N:40:ALA:HB1   | 7:N:45:VAL:HB    | 1.81                     | 0.62              |
| 3:F:206:ALA:HB3  | 3:F:220:HIS:HB3  | 1.80                     | 0.62              |
| 5:K:47:C:H2'     | 5:K:48:C:H6      | 1.65                     | 0.62              |
| 8:O:32:DA:H2''   | 8:O:33:DT:H71    | 1.80                     | 0.62              |
| 2:C:85:PRO:HB2   | 2:C:90:PRO:HB3   | 1.82                     | 0.62              |
| 2:C:122:ARG:O    | 2:C:122:ARG:HG2  | 1.99                     | 0.62              |
| 3:D:252:ALA:O    | 3:D:256:VAL:HG23 | 2.00                     | 0.62              |
| 4:J:136:ARG:HG2  | 4:J:136:ARG:HH11 | 1.64                     | 0.62              |
| 2:C:23:THR:CG2   | 2:C:45:ARG:HB2   | 2.21                     | 0.62              |
| 2:C:118:ASP:HB3  | 2:C:119:TYR:CD1  | 2.35                     | 0.62              |
| 2:C:263:GLU:HG2  | 2:C:307:PRO:HG3  | 1.81                     | 0.62              |
| 7:N:25:ASP:OD1   | 7:N:69:ARG:NH2   | 2.32                     | 0.62              |
| 3:E:285:HIS:HD2  | 3:E:349:LEU:HB3  | 1.65                     | 0.61              |
| 3:H:285:HIS:HD2  | 3:H:349:LEU:HB3  | 1.65                     | 0.61              |
| 3:H:289:ARG:HH12 | 3:H:294:ILE:CD1  | 2.13                     | 0.61              |
| 4:J:136:ARG:HH11 | 4:J:136:ARG:CG   | 2.12                     | 0.61              |
| 1:A:10:ASP:HB2   | 1:A:77:LEU:HG    | 1.82                     | 0.61              |
| 4:L:74:VAL:HG12  | 4:L:76:ALA:H     | 1.63                     | 0.61              |
| 1:A:138:TRP:C    | 1:A:144:ALA:HB2  | 2.24                     | 0.61              |
| 2:C:373:ARG:HB2  | 2:C:395:THR:HG22 | 1.82                     | 0.61              |
| 3:D:203:PHE:HZ   | 3:D:221:MET:HE3  | 1.65                     | 0.61              |
| 3:F:289:ARG:HH12 | 3:F:294:ILE:CD1  | 2.13                     | 0.61              |
| 4:J:197:ARG:HH12 | 4:J:201:ARG:NH2  | 1.98                     | 0.61              |
| 3:D:7:HIS:CD2    | 3:D:232:TYR:OH   | 2.46                     | 0.61              |
| 3:D:35:ARG:HB2   | 3:D:193:THR:OG1  | 2.01                     | 0.61              |
| 7:N:161:GLU:CD   | 7:N:245:TYR:HH   | 2.09                     | 0.61              |
| 1:A:191:ASP:OD1  | 1:A:192:GLY:N    | 2.34                     | 0.61              |
| 3:G:285:HIS:HD2  | 3:G:349:LEU:HB3  | 1.65                     | 0.61              |
| 3:H:216:HIS:O    | 3:H:216:HIS:ND1  | 2.33                     | 0.61              |
| 3:G:289:ARG:HH12 | 3:G:294:ILE:CD1  | 2.13                     | 0.61              |
| 2:C:175:PRO:HB2  | 2:C:290:HIS:HB3  | 1.83                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:285:HIS:HD2  | 3:F:349:LEU:HB3  | 1.65                     | 0.61              |
| 3:G:289:ARG:NH1  | 3:G:294:ILE:HD12 | 2.16                     | 0.61              |
| 2:C:364:VAL:H    | 2:C:365:PRO:HD2  | 1.65                     | 0.61              |
| 3:F:289:ARG:NH1  | 3:F:294:ILE:HD12 | 2.16                     | 0.61              |
| 2:C:159:GLU:OE1  | 2:C:159:GLU:HA   | 2.00                     | 0.60              |
| 2:C:341:LEU:O    | 2:C:423:ARG:NE   | 2.33                     | 0.60              |
| 3:E:15:SER:HB2   | 3:E:17:ILE:HG23  | 1.81                     | 0.60              |
| 3:F:269:SER:HA   | 3:F:272:GLN:CG   | 2.30                     | 0.60              |
| 7:N:67:GLY:HA3   | 7:N:111:ALA:HB2  | 1.82                     | 0.60              |
| 3:D:305:TYR:O    | 3:D:310:TYR:CE1  | 2.54                     | 0.60              |
| 3:H:289:ARG:NH1  | 3:H:294:ILE:HD12 | 2.16                     | 0.60              |
| 3:H:332:ASP:OD1  | 3:H:332:ASP:N    | 2.33                     | 0.60              |
| 6:M:23:DG:H2''   | 6:M:24:DA:C8     | 2.36                     | 0.60              |
| 1:A:74:VAL:HG21  | 1:A:79:PRO:O     | 2.01                     | 0.60              |
| 2:C:185:LEU:CD1  | 2:C:189:LEU:CD1  | 2.78                     | 0.60              |
| 3:E:19:ARG:HH21  | 5:K:34:G:C5'     | 2.13                     | 0.60              |
| 3:F:14:TYR:H     | 3:F:228:ALA:CB   | 2.12                     | 0.60              |
| 1:A:138:TRP:C    | 1:A:144:ALA:HB1  | 2.26                     | 0.60              |
| 2:C:226:ARG:HD3  | 2:C:371:SER:OG   | 2.00                     | 0.60              |
| 3:F:214:ASN:HA   | 3:I:178:PRO:CG   | 2.30                     | 0.60              |
| 3:I:101:LYS:HB3  | 4:L:93:ARG:NH1   | 2.16                     | 0.60              |
| 4:J:135:ARG:HG3  | 4:J:136:ARG:N    | 2.16                     | 0.60              |
| 3:D:40:SER:HB2   | 3:D:190:HIS:CD2  | 2.37                     | 0.60              |
| 3:E:267:VAL:HG12 | 3:E:268:PRO:HD2  | 1.83                     | 0.60              |
| 3:E:278:MET:HE3  | 3:I:292:ARG:HH11 | 1.66                     | 0.60              |
| 2:C:318:SER:O    | 2:C:319:LYS:C    | 2.44                     | 0.60              |
| 3:D:16:ASN:HB2   | 3:D:226:PHE:CD1  | 2.36                     | 0.60              |
| 3:I:289:ARG:NE   | 3:I:292:ARG:O    | 2.31                     | 0.60              |
| 2:C:152:ALA:CB   | 2:C:155:ARG:HG3  | 2.32                     | 0.60              |
| 3:F:16:ASN:ND2   | 3:F:225:GLN:O    | 2.35                     | 0.60              |
| 2:C:129:GLU:HG3  | 2:C:130:ARG:HD3  | 1.83                     | 0.60              |
| 3:I:332:ASP:N    | 3:I:332:ASP:OD1  | 2.34                     | 0.60              |
| 3:D:169:LEU:O    | 3:D:186:VAL:HG23 | 2.02                     | 0.60              |
| 2:C:414:ARG:O    | 2:C:418:ARG:CG   | 2.49                     | 0.59              |
| 3:E:267:VAL:HG12 | 3:E:268:PRO:CD   | 2.32                     | 0.59              |
| 4:J:219:ARG:O    | 4:J:222:GLU:HG3  | 2.02                     | 0.59              |
| 7:N:13:GLN:HB3   | 7:N:138:LEU:HB3  | 1.82                     | 0.59              |
| 2:C:140:GLU:N    | 2:C:140:GLU:OE1  | 2.34                     | 0.59              |
| 2:C:366:GLN:HG2  | 2:C:367:GLU:N    | 2.17                     | 0.59              |
| 3:G:332:ASP:OD1  | 3:G:332:ASP:N    | 2.34                     | 0.59              |
| 1:A:105:ARG:HG3  | 1:A:106:ILE:N    | 2.16                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:HIS:HD2  | 1:A:186:PRO:CD   | 2.11                     | 0.59              |
| 2:C:272:ARG:HH11 | 2:C:272:ARG:CG   | 2.15                     | 0.59              |
| 2:C:303:ARG:NE   | 2:C:304:ASN:H    | 2.01                     | 0.59              |
| 2:C:405:ARG:HH11 | 2:C:405:ARG:HB3  | 1.65                     | 0.59              |
| 3:E:332:ASP:OD1  | 3:E:332:ASP:N    | 2.34                     | 0.59              |
| 3:E:248:ASP:OD2  | 3:E:251:THR:HG23 | 2.02                     | 0.59              |
| 3:F:332:ASP:N    | 3:F:332:ASP:OD1  | 2.34                     | 0.59              |
| 2:C:180:GLU:HA   | 2:C:183:TRP:CZ3  | 2.37                     | 0.59              |
| 2:C:180:GLU:CG   | 2:C:183:TRP:HZ3  | 2.16                     | 0.59              |
| 3:E:324:ARG:HH21 | 3:E:324:ARG:CG   | 2.14                     | 0.59              |
| 3:F:35:ARG:NH2   | 3:F:301:GLU:O    | 2.36                     | 0.59              |
| 3:F:301:GLU:OE2  | 3:G:310:TYR:N    | 2.34                     | 0.59              |
| 2:C:279:ALA:HB2  | 2:C:299:ALA:HB2  | 1.83                     | 0.59              |
| 4:J:44:MET:CE    | 4:J:82:TYR:CD1   | 2.86                     | 0.59              |
| 5:K:1:A:C6       | 7:N:134:TRP:CZ2  | 2.91                     | 0.59              |
| 7:N:47:ARG:HH21  | 7:N:47:ARG:CG    | 2.15                     | 0.59              |
| 1:A:110:PRO:HA   | 1:A:148:TRP:CE2  | 2.38                     | 0.59              |
| 2:C:197:CYS:SG   | 2:C:297:THR:HA   | 2.43                     | 0.59              |
| 4:L:197:ARG:CG   | 4:L:197:ARG:HH11 | 2.15                     | 0.59              |
| 1:A:44:ASN:O     | 5:K:58:G:O2'     | 2.17                     | 0.59              |
| 2:C:202:VAL:HG11 | 2:C:257:PRO:HG3  | 1.83                     | 0.59              |
| 2:C:311:PRO:HB2  | 2:C:354:ILE:HB   | 1.85                     | 0.59              |
| 3:D:193:THR:HG23 | 3:D:231:PHE:CD1  | 2.38                     | 0.59              |
| 3:G:35:ARG:NH2   | 3:G:301:GLU:O    | 2.36                     | 0.59              |
| 3:H:14:TYR:H     | 3:H:228:ALA:CB   | 2.14                     | 0.59              |
| 3:H:35:ARG:NH2   | 3:H:301:GLU:O    | 2.36                     | 0.59              |
| 2:C:137:ARG:NH1  | 2:C:256:ASP:HA   | 2.17                     | 0.58              |
| 3:E:220:HIS:NE2  | 3:E:222:ASN:OD1  | 2.36                     | 0.58              |
| 3:F:269:SER:HA   | 3:F:272:GLN:HG3  | 1.85                     | 0.58              |
| 3:I:35:ARG:NH2   | 3:I:301:GLU:O    | 2.36                     | 0.58              |
| 1:A:147:GLU:HA   | 1:A:150:HIS:NE2  | 2.18                     | 0.58              |
| 1:A:106:ILE:O    | 1:A:189:ARG:HA   | 2.03                     | 0.58              |
| 2:C:267:LEU:O    | 2:C:271:LEU:N    | 2.36                     | 0.58              |
| 6:M:19:DT:H2''   | 6:M:20:DG:C8     | 2.38                     | 0.58              |
| 2:C:98:ARG:NH1   | 2:C:358:CYS:SG   | 2.74                     | 0.58              |
| 2:C:497:MET:HE2  | 2:C:501:GLY:HA2  | 1.84                     | 0.58              |
| 8:O:32:DA:H2''   | 8:O:33:DT:C7     | 2.33                     | 0.58              |
| 1:A:165:ALA:O    | 1:A:166:GLN:NE2  | 2.36                     | 0.58              |
| 1:A:185:HIS:CG   | 5:K:45:G:O6      | 2.57                     | 0.58              |
| 2:C:176:LEU:CD1  | 2:C:184:HIS:CD2  | 2.85                     | 0.58              |
| 3:D:171:GLY:N    | 3:D:184:GLY:HA3  | 2.18                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:246:LEU:HD12 | 2:C:251:GLN:OE1  | 2.03                     | 0.58              |
| 6:M:50:DA:H2'    | 6:M:51:DC:O5'    | 2.02                     | 0.58              |
| 7:N:165:ALA:O    | 7:N:245:TYR:HE2  | 1.87                     | 0.58              |
| 1:A:124:LEU:HD12 | 5:K:44:A:H5'     | 1.84                     | 0.58              |
| 2:C:406:GLU:OE2  | 2:C:412:ASN:CA   | 2.52                     | 0.58              |
| 3:D:250:GLN:O    | 3:D:254:THR:HG23 | 2.03                     | 0.58              |
| 2:C:23:THR:C     | 2:C:24:ILE:HD12  | 2.29                     | 0.58              |
| 2:C:84:GLN:C     | 2:C:86:PRO:HD3   | 2.28                     | 0.58              |
| 2:C:429:LEU:HA   | 2:C:432:ARG:HD3  | 1.69                     | 0.58              |
| 3:G:18:ASN:HD22  | 3:G:39:SER:H     | 1.52                     | 0.58              |
| 4:J:169:LEU:HA   | 4:J:202:TRP:CD1  | 2.39                     | 0.58              |
| 3:G:14:TYR:H     | 3:G:228:ALA:CB   | 2.12                     | 0.58              |
| 2:C:336:ARG:NH1  | 7:N:200:LEU:CB   | 2.61                     | 0.57              |
| 3:D:276:ALA:HB3  | 3:H:189:ALA:HB2  | 1.85                     | 0.57              |
| 3:E:35:ARG:NH2   | 3:E:301:GLU:O    | 2.36                     | 0.57              |
| 3:F:289:ARG:NH1  | 3:F:294:ILE:CD1  | 2.67                     | 0.57              |
| 1:A:116:ARG:NH1  | 5:K:46:C:OP2     | 2.37                     | 0.57              |
| 2:C:334:ILE:HG13 | 7:N:69:ARG:CZ    | 2.33                     | 0.57              |
| 2:C:468:HIS:O    | 2:C:472:ARG:HG2  | 2.04                     | 0.57              |
| 2:C:484:ILE:HD11 | 2:C:503:ALA:HB3  | 1.85                     | 0.57              |
| 3:D:54:ARG:HD2   | 3:D:258:GLU:OE1  | 2.05                     | 0.57              |
| 3:D:215:ASP:HB3  | 3:D:216:HIS:ND1  | 2.18                     | 0.57              |
| 3:H:18:ASN:HD22  | 3:H:39:SER:H     | 1.52                     | 0.57              |
| 7:N:76:ILE:HB    | 7:N:101:ILE:HB   | 1.85                     | 0.57              |
| 2:C:63:PRO:HB3   | 2:C:191:TYR:CD1  | 2.39                     | 0.57              |
| 2:C:180:GLU:CG   | 2:C:183:TRP:CZ3  | 2.86                     | 0.57              |
| 3:D:216:HIS:O    | 3:D:218:SER:N    | 2.37                     | 0.57              |
| 3:E:14:TYR:H     | 3:E:228:ALA:CB   | 2.13                     | 0.57              |
| 3:G:35:ARG:NH1   | 3:G:300:PHE:O    | 2.21                     | 0.57              |
| 3:G:289:ARG:NH1  | 3:G:294:ILE:CD1  | 2.67                     | 0.57              |
| 4:L:197:ARG:NH1  | 4:L:197:ARG:HG2  | 2.20                     | 0.57              |
| 1:A:142:GLY:O    | 1:A:163:THR:HG21 | 2.05                     | 0.57              |
| 3:G:306:GLY:HA2  | 3:G:310:TYR:CE1  | 2.40                     | 0.57              |
| 3:H:289:ARG:NH1  | 3:H:294:ILE:CD1  | 2.67                     | 0.57              |
| 4:J:39:PRO:HA    | 4:J:44:MET:HG2   | 1.87                     | 0.57              |
| 3:F:248:ASP:OD2  | 3:F:251:THR:HG23 | 2.03                     | 0.57              |
| 3:I:19:ARG:HH21  | 5:K:40:C:H2'     | 1.68                     | 0.57              |
| 2:C:134:GLN:HE22 | 2:C:282:LEU:HG   | 1.70                     | 0.57              |
| 3:E:306:GLY:HA2  | 3:E:310:TYR:CE1  | 2.40                     | 0.57              |
| 3:I:18:ASN:HD21  | 3:I:26:LYS:CE    | 2.18                     | 0.57              |
| 4:J:182:TYR:HD1  | 6:M:43:DA:C6     | 2.22                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:44:A:H4'     | 5:K:45:G:OP1     | 2.04                     | 0.57              |
| 3:D:368:PHE:N    | 3:D:368:PHE:CD1  | 2.73                     | 0.57              |
| 3:E:16:ASN:ND2   | 3:E:225:GLN:O    | 2.38                     | 0.57              |
| 3:E:18:ASN:HD22  | 3:E:39:SER:H     | 1.52                     | 0.57              |
| 3:G:17:ILE:HD11  | 3:G:38:VAL:HG21  | 1.87                     | 0.57              |
| 2:C:431:ARG:O    | 2:C:434:GLU:HG3  | 2.04                     | 0.57              |
| 2:C:472:ARG:NH2  | 7:N:70:LEU:CD2   | 2.67                     | 0.57              |
| 5:K:1:A:C2       | 7:N:134:TRP:CE2  | 2.92                     | 0.57              |
| 5:K:1:A:C5       | 7:N:134:TRP:CH2  | 2.93                     | 0.57              |
| 6:M:53:DG:H5'    | 7:N:97:LYS:HE3   | 1.87                     | 0.57              |
| 7:N:196:THR:HG21 | 7:N:218:GLN:OE1  | 2.05                     | 0.57              |
| 2:C:45:ARG:O     | 2:C:49:ILE:HG13  | 2.05                     | 0.57              |
| 2:C:141:GLU:HG2  | 2:C:200:ARG:HB2  | 1.85                     | 0.57              |
| 3:E:324:ARG:HH12 | 3:F:342:ASN:HB3  | 1.69                     | 0.57              |
| 2:C:335:TRP:CZ3  | 2:C:338:LEU:HD13 | 2.40                     | 0.56              |
| 3:E:17:ILE:HD11  | 3:E:38:VAL:HG21  | 1.87                     | 0.56              |
| 3:H:272:GLN:HE22 | 3:H:277:ALA:HB3  | 1.69                     | 0.56              |
| 3:H:306:GLY:HA2  | 3:H:310:TYR:CE1  | 2.40                     | 0.56              |
| 2:C:261:PRO:O    | 2:C:304:ASN:ND2  | 2.38                     | 0.56              |
| 3:F:14:TYR:O     | 3:F:275:THR:CG2  | 2.45                     | 0.56              |
| 3:F:17:ILE:HD11  | 3:F:38:VAL:HG21  | 1.87                     | 0.56              |
| 7:N:13:GLN:HB3   | 7:N:138:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:158:LEU:N    | 1:A:195:VAL:O    | 2.38                     | 0.56              |
| 2:C:70:ARG:O     | 2:C:271:LEU:HD23 | 2.04                     | 0.56              |
| 3:F:18:ASN:HD22  | 3:F:39:SER:H     | 1.52                     | 0.56              |
| 3:F:306:GLY:HA2  | 3:F:310:TYR:CE1  | 2.40                     | 0.56              |
| 3:G:269:SER:HA   | 3:G:272:GLN:CG   | 2.35                     | 0.56              |
| 3:D:337:TYR:HE1  | 3:D:350:GLY:O    | 1.88                     | 0.56              |
| 3:E:35:ARG:NH1   | 3:E:300:PHE:O    | 2.21                     | 0.56              |
| 3:I:306:GLY:HA2  | 3:I:310:TYR:CE1  | 2.40                     | 0.56              |
| 4:J:198:ASP:OD1  | 4:J:201:ARG:NH2  | 2.39                     | 0.56              |
| 1:A:91:PRO:HB2   | 1:A:203:ARG:HE   | 1.71                     | 0.56              |
| 1:A:112:LYS:HG3  | 1:A:112:LYS:O    | 2.05                     | 0.56              |
| 3:D:38:VAL:CG1   | 3:D:43:TRP:CD1   | 2.88                     | 0.56              |
| 4:J:186:ASP:OD1  | 4:J:186:ASP:N    | 2.37                     | 0.56              |
| 1:A:101:ARG:O    | 1:A:226:ILE:HG12 | 2.06                     | 0.56              |
| 1:A:3:TRP:HB2    | 1:A:88:ASN:HA    | 1.87                     | 0.56              |
| 1:A:137:THR:N    | 1:A:138:TRP:HA   | 2.20                     | 0.56              |
| 2:C:89:ASN:HB3   | 2:C:92:ARG:HB3   | 1.87                     | 0.56              |
| 3:D:3:PHE:HD2    | 3:D:293:PRO:HD3  | 1.69                     | 0.56              |
| 3:D:339:THR:HG21 | 3:D:341:GLU:CD   | 2.31                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:275:THR:HG22 | 3:I:190:HIS:HD2  | 1.67                     | 0.56              |
| 3:G:16:ASN:HD22  | 3:G:226:PHE:HD1  | 1.54                     | 0.56              |
| 2:C:106:ARG:HG2  | 2:C:107:LEU:N    | 2.20                     | 0.56              |
| 2:C:216:ARG:NH2  | 2:C:384:GLN:O    | 2.37                     | 0.56              |
| 3:D:214:ASN:HD21 | 6:M:47:DA:H4'    | 1.69                     | 0.56              |
| 3:D:265:SER:O    | 3:H:292:ARG:NE   | 2.39                     | 0.56              |
| 3:H:17:ILE:HD11  | 3:H:38:VAL:HG21  | 1.87                     | 0.56              |
| 3:H:269:SER:HA   | 3:H:272:GLN:HG3  | 1.88                     | 0.56              |
| 1:A:162:SER:CB   | 1:A:190:PHE:HA   | 2.36                     | 0.56              |
| 3:D:215:ASP:HB3  | 3:D:216:HIS:CE1  | 2.41                     | 0.56              |
| 4:J:44:MET:CE    | 4:J:82:TYR:HD1   | 2.19                     | 0.56              |
| 2:C:315:TYR:H    | 2:C:350:TYR:HE2  | 1.54                     | 0.55              |
| 2:C:429:LEU:HA   | 2:C:432:ARG:HD2  | 1.77                     | 0.55              |
| 3:I:19:ARG:NH2   | 5:K:40:C:H2'     | 2.21                     | 0.55              |
| 2:C:125:LEU:HD23 | 2:C:125:LEU:C    | 2.20                     | 0.55              |
| 2:C:176:LEU:CD1  | 2:C:184:HIS:HD2  | 2.19                     | 0.55              |
| 3:F:220:HIS:NE2  | 3:F:222:ASN:OD1  | 2.38                     | 0.55              |
| 4:L:93:ARG:HA    | 4:L:96:ARG:HB2   | 1.87                     | 0.55              |
| 4:L:205:THR:OG1  | 4:L:208:HIS:HD2  | 1.90                     | 0.55              |
| 7:N:137:TYR:HE1  | 7:N:139:GLY:O    | 1.89                     | 0.55              |
| 1:A:101:ARG:HB2  | 1:A:226:ILE:HD13 | 1.89                     | 0.55              |
| 2:C:246:LEU:HB2  | 2:C:250:GLU:HB2  | 1.89                     | 0.55              |
| 2:C:414:ARG:O    | 2:C:418:ARG:HG3  | 2.06                     | 0.55              |
| 3:F:14:TYR:HE1   | 3:F:200:GLU:CD   | 2.15                     | 0.55              |
| 3:I:18:ASN:OD1   | 3:I:19:ARG:N     | 2.39                     | 0.55              |
| 5:K:44:A:H4'     | 5:K:45:G:H5''    | 1.84                     | 0.55              |
| 7:N:43:GLN:HE22  | 7:N:125:ILE:HG12 | 1.72                     | 0.55              |
| 2:C:512:TYR:CE2  | 2:C:533:ARG:HB3  | 2.42                     | 0.55              |
| 3:D:225:GLN:O    | 3:D:226:PHE:HD1  | 1.88                     | 0.55              |
| 3:D:305:TYR:O    | 3:D:310:TYR:HE1  | 1.90                     | 0.55              |
| 3:F:101:LYS:CD   | 4:J:93:ARG:NH1   | 2.69                     | 0.55              |
| 8:O:4:DG:H2''    | 8:O:5:DG:C8      | 2.42                     | 0.55              |
| 2:C:379:PHE:HE1  | 2:C:390:TRP:HE3  | 1.53                     | 0.55              |
| 2:C:384:GLN:NE2  | 8:O:11:DG:C2     | 2.75                     | 0.55              |
| 3:D:21:ASP:HB3   | 7:N:73:PHE:CE1   | 2.42                     | 0.55              |
| 3:I:101:LYS:NZ   | 6:M:28:DC:OP1    | 2.26                     | 0.55              |
| 7:N:16:GLY:HA2   | 7:N:26:THR:HA    | 1.87                     | 0.55              |
| 2:C:42:LEU:CD1   | 2:C:47:VAL:HB    | 2.36                     | 0.55              |
| 2:C:63:PRO:HA    | 2:C:191:TYR:HE1  | 1.72                     | 0.55              |
| 2:C:335:TRP:CD1  | 2:C:478:GLU:OE1  | 2.59                     | 0.55              |
| 2:C:63:PRO:HA    | 2:C:191:TYR:CE1  | 2.41                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:159:GLU:O    | 7:N:88:THR:HG23  | 2.07                     | 0.55              |
| 2:C:429:LEU:O    | 2:C:432:ARG:HG3  | 2.07                     | 0.55              |
| 3:E:204:PHE:CD1  | 3:E:204:PHE:C    | 2.85                     | 0.55              |
| 3:G:248:ASP:OD2  | 3:G:251:THR:HG23 | 2.07                     | 0.55              |
| 3:H:16:ASN:ND2   | 3:H:225:GLN:O    | 2.40                     | 0.55              |
| 2:C:94:TRP:CE3   | 2:C:238:TYR:HD1  | 2.25                     | 0.55              |
| 2:C:230:GLU:OE2  | 2:C:368:VAL:HG13 | 2.06                     | 0.55              |
| 4:J:44:MET:HE3   | 4:J:82:TYR:HD1   | 1.72                     | 0.55              |
| 2:C:22:VAL:HG12  | 2:C:44:LEU:HB2   | 1.89                     | 0.54              |
| 2:C:125:LEU:HD21 | 2:C:126:PHE:CE1  | 2.42                     | 0.54              |
| 2:C:318:SER:HB3  | 2:C:324:TYR:HE1  | 1.71                     | 0.54              |
| 2:C:429:LEU:C    | 2:C:432:ARG:HG2  | 2.31                     | 0.54              |
| 7:N:179:THR:HB   | 7:N:225:GLU:HG2  | 1.87                     | 0.54              |
| 2:C:125:LEU:HA   | 2:C:132:TRP:H    | 1.72                     | 0.54              |
| 3:E:26:LYS:NZ    | 5:K:33:G:OP1     | 2.40                     | 0.54              |
| 4:L:19:LYS:HD2   | 4:L:23:ASN:HD22  | 1.72                     | 0.54              |
| 2:C:45:ARG:CG    | 2:C:116:PHE:HE2  | 2.20                     | 0.54              |
| 2:C:207:GLU:OE1  | 2:C:301:ARG:NH1  | 2.40                     | 0.54              |
| 3:E:267:VAL:CG1  | 3:E:268:PRO:CD   | 2.85                     | 0.54              |
| 3:D:45:ARG:HA    | 3:D:48:ARG:HG2   | 1.89                     | 0.54              |
| 2:C:200:ARG:HD2  | 2:C:297:THR:HG21 | 1.89                     | 0.54              |
| 2:C:314:ILE:HG12 | 2:C:352:PRO:HG3  | 1.90                     | 0.54              |
| 2:C:50:ARG:HA    | 2:C:53:GLU:OE1   | 2.08                     | 0.54              |
| 2:C:371:SER:HA   | 2:C:400:ARG:NH1  | 2.12                     | 0.54              |
| 3:D:171:GLY:CA   | 3:D:184:GLY:CA   | 2.85                     | 0.54              |
| 3:D:278:MET:HG3  | 3:H:293:PRO:HG2  | 1.90                     | 0.54              |
| 3:E:258:GLU:HA   | 3:E:258:GLU:OE2  | 2.08                     | 0.54              |
| 3:F:14:TYR:OH    | 3:F:202:ASP:HB2  | 2.07                     | 0.54              |
| 3:H:120:PRO:HG3  | 3:H:164:ASN:HB2  | 1.90                     | 0.54              |
| 4:J:197:ARG:NH1  | 4:J:201:ARG:NH2  | 2.54                     | 0.54              |
| 2:C:180:GLU:HG2  | 2:C:183:TRP:CE3  | 2.43                     | 0.54              |
| 3:F:22:LEU:HB3   | 4:L:163:LEU:HD12 | 1.89                     | 0.54              |
| 3:G:120:PRO:HG3  | 3:G:164:ASN:HB2  | 1.90                     | 0.54              |
| 4:L:84:VAL:HA    | 4:L:87:ILE:HG22  | 1.89                     | 0.54              |
| 7:N:161:GLU:OE2  | 7:N:245:TYR:OH   | 2.25                     | 0.54              |
| 8:O:7:DC:H2''    | 8:O:8:DG:C8      | 2.43                     | 0.54              |
| 8:O:43:DC:O2     | 8:O:43:DC:C2'    | 2.54                     | 0.54              |
| 1:A:60:ASN:O     | 1:A:61:GLU:C     | 2.50                     | 0.54              |
| 1:A:141:ARG:CG   | 3:E:216:HIS:CE1  | 2.91                     | 0.54              |
| 1:A:180:SER:OG   | 1:A:181:ARG:N    | 2.33                     | 0.54              |
| 2:C:77:ALA:O     | 2:C:81:GLY:N     | 2.28                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:335:TRP:CD1  | 2:C:335:TRP:C    | 2.84                     | 0.54              |
| 3:D:206:ALA:HB2  | 5:K:13:U:H1'     | 1.89                     | 0.54              |
| 3:F:14:TYR:N     | 3:F:228:ALA:HB2  | 2.17                     | 0.54              |
| 3:F:120:PRO:HG3  | 3:F:164:ASN:HB2  | 1.90                     | 0.54              |
| 4:J:167:GLN:O    | 4:J:202:TRP:HZ2  | 1.90                     | 0.54              |
| 6:M:53:DG:H5'    | 7:N:97:LYS:CE    | 2.37                     | 0.54              |
| 7:N:93:ARG:HD3   | 7:N:93:ARG:N     | 2.23                     | 0.54              |
| 7:N:171:ARG:HH11 | 7:N:171:ARG:CG   | 2.21                     | 0.54              |
| 1:A:113:ARG:HG2  | 1:A:113:ARG:NH1  | 2.18                     | 0.53              |
| 2:C:125:LEU:HD23 | 2:C:126:PHE:CD1  | 2.44                     | 0.53              |
| 3:D:171:GLY:HA2  | 3:D:184:GLY:CA   | 2.38                     | 0.53              |
| 3:D:342:ASN:HA   | 3:D:352:ARG:HH22 | 1.73                     | 0.53              |
| 3:H:17:ILE:O     | 3:H:270:GLY:HA3  | 2.08                     | 0.53              |
| 1:A:124:LEU:HD12 | 5:K:44:A:C5'     | 2.37                     | 0.53              |
| 2:C:343:HIS:CD2  | 2:C:372:LEU:CD1  | 2.91                     | 0.53              |
| 2:C:68:LEU:O     | 2:C:71:ILE:HG13  | 2.08                     | 0.53              |
| 7:N:13:GLN:HB3   | 7:N:138:LEU:CB   | 2.38                     | 0.53              |
| 2:C:119:TYR:CD1  | 2:C:119:TYR:N    | 2.76                     | 0.53              |
| 3:H:291:ASP:OD1  | 3:H:291:ASP:N    | 2.41                     | 0.53              |
| 4:J:44:MET:HE3   | 4:J:82:TYR:CD1   | 2.44                     | 0.53              |
| 2:C:42:LEU:HD11  | 2:C:47:VAL:HB    | 1.91                     | 0.53              |
| 2:C:369:LEU:HA   | 2:C:372:LEU:HD23 | 1.90                     | 0.53              |
| 3:D:48:ARG:NH1   | 5:K:7:C:OP1      | 2.42                     | 0.53              |
| 4:L:7:LEU:HD21   | 4:L:136:ARG:NH1  | 2.23                     | 0.53              |
| 1:A:123:ARG:HB3  | 1:A:212:ARG:HH12 | 1.74                     | 0.53              |
| 1:A:164:TYR:H    | 1:A:188:VAL:CG1  | 2.22                     | 0.53              |
| 2:C:48:LEU:O     | 2:C:107:LEU:HD11 | 2.09                     | 0.53              |
| 2:C:122:ARG:NE   | 2:C:249:TRP:O    | 2.42                     | 0.53              |
| 3:E:213:GLU:HG2  | 3:E:214:ASN:OD1  | 2.09                     | 0.53              |
| 5:K:9:C:C4       | 5:K:10:C:N4      | 2.77                     | 0.53              |
| 5:K:13:U:H3      | 6:M:50:DA:H62    | 1.55                     | 0.53              |
| 4:L:17:VAL:O     | 4:L:21:ILE:HG23  | 2.08                     | 0.53              |
| 4:L:88:MET:HE2   | 4:L:192:TRP:CG   | 2.44                     | 0.53              |
| 7:N:179:THR:HA   | 7:N:226:VAL:O    | 2.09                     | 0.53              |
| 1:A:163:THR:OG1  | 3:I:19:ARG:NH1   | 2.39                     | 0.53              |
| 5:K:8:G:O2'      | 5:K:9:C:OP1      | 2.25                     | 0.53              |
| 1:A:103:ARG:HA   | 1:A:192:GLY:O    | 2.09                     | 0.53              |
| 2:C:54:LEU:HB2   | 2:C:228:LEU:HD12 | 1.90                     | 0.53              |
| 2:C:188:THR:HA   | 2:C:191:TYR:O    | 2.09                     | 0.53              |
| 3:E:248:ASP:OD1  | 3:E:251:THR:OG1  | 2.22                     | 0.53              |
| 1:A:123:ARG:NH2  | 5:K:59:G:O6      | 2.42                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:51:SER:HG    | 2:C:229:PHE:HB2  | 1.73                     | 0.53              |
| 2:C:375:ARG:HD3  | 2:C:394:THR:HG22 | 1.90                     | 0.53              |
| 3:G:101:LYS:NZ   | 6:M:46:DT:OP1    | 2.30                     | 0.53              |
| 6:M:60:DT:H2'    | 6:M:61:DC:C6     | 2.44                     | 0.53              |
| 7:N:30:PRO:HB2   | 7:N:35:LEU:HD11  | 1.91                     | 0.52              |
| 7:N:62:ARG:HD3   | 7:N:162:LEU:HB3  | 1.92                     | 0.52              |
| 2:C:279:ALA:HB3  | 2:C:297:THR:O    | 2.09                     | 0.52              |
| 3:I:120:PRO:HG3  | 3:I:164:ASN:HB2  | 1.90                     | 0.52              |
| 4:L:150:LYS:HE2  | 4:L:186:ASP:O    | 2.10                     | 0.52              |
| 7:N:137:TYR:CG   | 7:N:141:ARG:HA   | 2.44                     | 0.52              |
| 1:A:138:TRP:CA   | 1:A:144:ALA:HB2  | 2.39                     | 0.52              |
| 2:C:159:GLU:HB2  | 6:M:57:DT:OP2    | 2.09                     | 0.52              |
| 2:C:384:GLN:NE2  | 8:O:11:DG:N3     | 2.51                     | 0.52              |
| 3:D:236:ASN:ND2  | 3:D:237:VAL:N    | 2.43                     | 0.52              |
| 3:E:324:ARG:NH1  | 3:F:342:ASN:CB   | 2.73                     | 0.52              |
| 1:A:185:HIS:CD2  | 1:A:186:PRO:C    | 2.87                     | 0.52              |
| 2:C:131:PRO:HB2  | 2:C:134:GLN:HB2  | 1.90                     | 0.52              |
| 3:D:8:ALA:HA     | 3:D:283:LEU:O    | 2.09                     | 0.52              |
| 3:E:17:ILE:HD12  | 3:E:268:PRO:CD   | 2.40                     | 0.52              |
| 3:E:120:PRO:HG3  | 3:E:164:ASN:HB2  | 1.90                     | 0.52              |
| 3:F:14:TYR:CZ    | 3:F:226:PHE:CB   | 2.93                     | 0.52              |
| 3:H:133:GLU:HG3  | 3:H:134:HIS:CD2  | 2.43                     | 0.52              |
| 1:A:25:ASN:O     | 1:A:29:LYS:HG2   | 2.09                     | 0.52              |
| 1:A:29:LYS:NZ    | 1:A:32:ARG:HE    | 2.07                     | 0.52              |
| 1:A:141:ARG:HD2  | 1:A:141:ARG:N    | 2.24                     | 0.52              |
| 2:C:73:ALA:C     | 2:C:77:ALA:HB3   | 2.32                     | 0.52              |
| 3:D:42:SER:HB2   | 5:K:9:C:OP1      | 2.10                     | 0.52              |
| 3:E:226:PHE:HE1  | 3:E:271:LYS:HZ1  | 1.53                     | 0.52              |
| 3:E:301:GLU:OE2  | 3:F:310:TYR:N    | 2.43                     | 0.52              |
| 4:L:54:TYR:HD1   | 8:O:43:DC:OP1    | 1.93                     | 0.52              |
| 1:A:141:ARG:CB   | 3:E:216:HIS:CE1  | 2.93                     | 0.52              |
| 2:C:24:ILE:N     | 2:C:24:ILE:CD1   | 2.73                     | 0.52              |
| 2:C:373:ARG:HB2  | 2:C:395:THR:CG2  | 2.40                     | 0.52              |
| 3:D:205:THR:OG1  | 5:K:14:G:N2      | 2.43                     | 0.52              |
| 3:D:212:LYS:C    | 3:D:214:ASN:H    | 2.18                     | 0.52              |
| 3:E:17:ILE:HD12  | 3:E:268:PRO:CG   | 2.38                     | 0.52              |
| 3:E:205:THR:HG22 | 3:E:221:MET:HG2  | 1.90                     | 0.52              |
| 5:K:8:G:C6       | 5:K:10:C:C4'     | 2.93                     | 0.52              |
| 5:K:43:G:N3      | 5:K:43:G:C5'     | 2.73                     | 0.52              |
| 1:A:33:LEU:HD11  | 1:A:73:ARG:N     | 2.25                     | 0.52              |
| 2:C:67:VAL:HB    | 2:C:186:LEU:CD2  | 2.37                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:137:ARG:HG2  | 2:C:138:LEU:N    | 2.24                     | 0.52              |
| 2:C:483:ASN:CB   | 2:C:490:ALA:HB2  | 2.40                     | 0.52              |
| 3:D:44:LYS:HE2   | 5:K:7:C:OP2      | 2.10                     | 0.52              |
| 1:A:176:THR:HB   | 1:A:179:ARG:HD2  | 1.90                     | 0.52              |
| 2:C:191:TYR:CD2  | 2:C:215:LEU:HD12 | 2.44                     | 0.52              |
| 2:C:212:ALA:HB1  | 2:C:216:ARG:HD3  | 1.91                     | 0.52              |
| 2:C:272:ARG:CG   | 2:C:272:ARG:NH1  | 2.73                     | 0.52              |
| 3:E:289:ARG:CZ   | 3:E:289:ARG:CB   | 2.88                     | 0.52              |
| 3:G:207:VAL:HG12 | 5:K:26:G:OP1     | 2.09                     | 0.52              |
| 3:E:272:GLN:HA   | 3:E:275:THR:O    | 2.10                     | 0.52              |
| 3:G:275:THR:O    | 3:G:275:THR:OG1  | 2.28                     | 0.52              |
| 4:J:202:TRP:CZ3  | 4:J:210:ALA:HB2  | 2.44                     | 0.52              |
| 1:A:137:THR:N    | 1:A:138:TRP:CG   | 2.78                     | 0.52              |
| 2:C:113:ASP:O    | 2:C:117:ALA:N    | 2.40                     | 0.52              |
| 2:C:157:ALA:HB3  | 2:C:160:ASN:OD1  | 2.10                     | 0.52              |
| 3:I:12:LEU:CD2   | 3:I:16:ASN:HB2   | 2.40                     | 0.52              |
| 1:A:141:ARG:CA   | 3:E:216:HIS:HE1  | 2.23                     | 0.51              |
| 3:E:207:VAL:HG12 | 5:K:38:G:OP1     | 2.10                     | 0.51              |
| 3:I:289:ARG:HD3  | 3:I:293:PRO:HA   | 1.91                     | 0.51              |
| 4:J:202:TRP:HE3  | 4:J:209:VAL:CG1  | 2.22                     | 0.51              |
| 2:C:76:THR:HG23  | 2:C:77:ALA:N     | 2.24                     | 0.51              |
| 3:F:205:THR:O    | 5:K:32:U:H5"     | 2.09                     | 0.51              |
| 3:F:324:ARG:HG2  | 3:G:340:VAL:O    | 2.10                     | 0.51              |
| 2:C:433:LEU:HD11 | 2:C:512:TYR:HB2  | 1.92                     | 0.51              |
| 3:D:169:LEU:O    | 3:D:184:GLY:O    | 2.29                     | 0.51              |
| 3:E:269:SER:HA   | 3:E:272:GLN:CD   | 2.35                     | 0.51              |
| 4:L:87:ILE:HD13  | 4:L:177:PRO:HB3  | 1.92                     | 0.51              |
| 2:C:260:LEU:HD23 | 2:C:260:LEU:H    | 1.75                     | 0.51              |
| 3:D:182:VAL:HG21 | 5:K:5:A:N3       | 2.26                     | 0.51              |
| 3:F:186:VAL:HG22 | 3:F:237:VAL:HG22 | 1.93                     | 0.51              |
| 4:J:44:MET:HE2   | 4:J:82:TYR:CD1   | 2.46                     | 0.51              |
| 7:N:93:ARG:HH11  | 7:N:93:ARG:CG    | 2.13                     | 0.51              |
| 7:N:202:ASP:HB2  | 7:N:217:ARG:HG2  | 1.91                     | 0.51              |
| 2:C:157:ALA:O    | 7:N:89:ALA:HB3   | 2.10                     | 0.51              |
| 3:D:236:ASN:OD1  | 3:D:293:PRO:HB3  | 2.11                     | 0.51              |
| 3:I:11:THR:HA    | 3:I:230:THR:HA   | 1.92                     | 0.51              |
| 3:I:12:LEU:CD2   | 3:I:13:PRO:HD2   | 2.34                     | 0.51              |
| 3:I:186:VAL:HG22 | 3:I:237:VAL:HG22 | 1.93                     | 0.51              |
| 3:I:331:ASP:OD1  | 3:I:331:ASP:N    | 2.44                     | 0.51              |
| 4:J:168:ASN:C    | 4:J:202:TRP:HE1  | 2.19                     | 0.51              |
| 7:N:33:SER:HB2   | 7:N:202:ASP:O    | 2.11                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:93:ARG:N     | 7:N:93:ARG:CD    | 2.72                     | 0.51              |
| 1:A:137:THR:CB   | 1:A:138:TRP:HA   | 2.40                     | 0.51              |
| 3:D:14:TYR:OH    | 3:D:202:ASP:HB2  | 2.11                     | 0.51              |
| 2:C:335:TRP:HE3  | 2:C:474:TRP:HE3  | 1.58                     | 0.51              |
| 2:C:366:GLN:HG2  | 2:C:367:GLU:H    | 1.76                     | 0.51              |
| 3:F:331:ASP:OD1  | 3:F:331:ASP:N    | 2.44                     | 0.51              |
| 1:A:25:ASN:OD1   | 1:A:29:LYS:HE3   | 2.11                     | 0.51              |
| 1:A:72:LEU:HD22  | 1:A:86:MET:HE1   | 1.93                     | 0.51              |
| 2:C:145:THR:HG22 | 2:C:295:TRP:NE1  | 2.26                     | 0.51              |
| 2:C:258:LEU:N    | 2:C:258:LEU:CD1  | 2.73                     | 0.51              |
| 3:D:19:ARG:HG3   | 5:K:9:C:O2'      | 2.11                     | 0.51              |
| 5:K:28:C:H42     | 6:M:35:DG:H1     | 1.59                     | 0.51              |
| 1:A:124:LEU:CG   | 5:K:44:A:C5'     | 2.81                     | 0.51              |
| 1:A:137:THR:N    | 1:A:138:TRP:CA   | 2.74                     | 0.51              |
| 2:C:81:GLY:HA2   | 2:C:94:TRP:NE1   | 2.24                     | 0.51              |
| 3:G:186:VAL:HG22 | 3:G:237:VAL:HG22 | 1.93                     | 0.51              |
| 7:N:172:ARG:HH21 | 7:N:172:ARG:CG   | 2.11                     | 0.51              |
| 2:C:334:ILE:CG2  | 2:C:474:TRP:HB2  | 2.41                     | 0.51              |
| 3:H:186:VAL:HG22 | 3:H:237:VAL:HG22 | 1.93                     | 0.51              |
| 3:F:35:ARG:HB3   | 3:F:193:THR:OG1  | 2.12                     | 0.50              |
| 5:K:7:C:H1'      | 7:N:76:ILE:HG12  | 1.92                     | 0.50              |
| 5:K:8:G:C4       | 5:K:10:C:H5''    | 2.45                     | 0.50              |
| 4:L:169:LEU:O    | 4:L:173:HIS:HD2  | 1.94                     | 0.50              |
| 6:M:64:DC:H2''   | 6:M:65:DG:C8     | 2.46                     | 0.50              |
| 7:N:175:GLU:OE1  | 7:N:175:GLU:N    | 2.39                     | 0.50              |
| 2:C:153:TRP:HZ3  | 2:C:387:ASP:OD2  | 1.94                     | 0.50              |
| 5:K:5:A:H5''     | 7:N:141:ARG:HB2  | 1.92                     | 0.50              |
| 4:L:191:ASP:O    | 4:L:194:ILE:HG13 | 2.11                     | 0.50              |
| 7:N:93:ARG:HD3   | 7:N:93:ARG:H     | 1.75                     | 0.50              |
| 2:C:201:VAL:HA   | 2:C:205:ARG:O    | 2.11                     | 0.50              |
| 2:C:247:ALA:H    | 2:C:250:GLU:HB2  | 1.77                     | 0.50              |
| 3:I:13:PRO:CG    | 3:I:16:ASN:ND2   | 2.73                     | 0.50              |
| 3:I:72:ARG:O     | 3:I:75:GLU:HG3   | 2.12                     | 0.50              |
| 4:J:98:GLN:HG2   | 4:J:187:GLN:CD   | 2.36                     | 0.50              |
| 1:A:111:THR:HA   | 1:A:124:LEU:O    | 2.11                     | 0.50              |
| 2:C:23:THR:HB    | 2:C:24:ILE:CD1   | 2.36                     | 0.50              |
| 3:E:35:ARG:HB3   | 3:E:193:THR:OG1  | 2.12                     | 0.50              |
| 3:F:72:ARG:O     | 3:F:75:GLU:HG3   | 2.12                     | 0.50              |
| 8:O:5:DG:H2''    | 8:O:6:DA:C8      | 2.45                     | 0.50              |
| 1:A:103:ARG:HB2  | 1:A:224:ALA:HB3  | 1.93                     | 0.50              |
| 1:A:104:TYR:N    | 1:A:192:GLY:O    | 2.36                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:126:PHE:HE2  | 2:C:288:GLY:HA2  | 1.75                     | 0.50              |
| 3:D:216:HIS:HD2  | 5:K:14:G:O6      | 1.94                     | 0.50              |
| 3:G:291:ASP:OD1  | 3:G:291:ASP:N    | 2.41                     | 0.50              |
| 2:C:81:GLY:CA    | 2:C:94:TRP:HE1   | 2.23                     | 0.50              |
| 3:E:64:ARG:NH1   | 3:F:210:ILE:O    | 2.45                     | 0.50              |
| 3:H:16:ASN:HB2   | 3:H:226:PHE:HA   | 1.93                     | 0.50              |
| 7:N:82:LYS:O     | 7:N:82:LYS:HG2   | 2.10                     | 0.50              |
| 1:A:146:GLU:OE2  | 1:A:150:HIS:HD2  | 1.94                     | 0.50              |
| 2:C:334:ILE:CG1  | 7:N:69:ARG:NE    | 2.75                     | 0.50              |
| 2:C:429:LEU:C    | 2:C:432:ARG:CG   | 2.84                     | 0.50              |
| 3:E:225:GLN:N    | 3:E:225:GLN:OE1  | 2.44                     | 0.50              |
| 3:G:189:ALA:HB2  | 3:H:276:ALA:HB3  | 1.92                     | 0.50              |
| 1:A:113:ARG:CZ   | 5:K:57:U:H6      | 2.23                     | 0.50              |
| 2:C:64:GLY:O     | 2:C:68:LEU:HB2   | 2.11                     | 0.50              |
| 2:C:336:ARG:O    | 2:C:337:ASP:CG   | 2.55                     | 0.50              |
| 3:F:291:ASP:OD1  | 3:F:291:ASP:N    | 2.41                     | 0.50              |
| 3:H:14:TYR:CE1   | 3:H:200:GLU:OE1  | 2.65                     | 0.50              |
| 3:I:35:ARG:HB3   | 3:I:193:THR:OG1  | 2.12                     | 0.50              |
| 4:L:197:ARG:CG   | 4:L:197:ARG:NH1  | 2.73                     | 0.50              |
| 3:E:19:ARG:HH21  | 5:K:34:G:H5'     | 1.77                     | 0.50              |
| 3:E:85:ALA:O     | 3:E:89:GLN:HG2   | 2.12                     | 0.50              |
| 3:E:233:ARG:NH2  | 3:E:263:PHE:O    | 2.39                     | 0.50              |
| 3:E:291:ASP:N    | 3:E:291:ASP:OD1  | 2.41                     | 0.50              |
| 3:G:35:ARG:HB3   | 3:G:193:THR:OG1  | 2.12                     | 0.50              |
| 3:H:35:ARG:HB3   | 3:H:193:THR:OG1  | 2.11                     | 0.50              |
| 2:C:45:ARG:CG    | 2:C:116:PHE:CE2  | 2.92                     | 0.49              |
| 3:D:17:ILE:HG21  | 3:D:268:PRO:HG2  | 1.94                     | 0.49              |
| 3:H:72:ARG:O     | 3:H:75:GLU:HG3   | 2.12                     | 0.49              |
| 3:H:225:GLN:HE21 | 4:J:175:HIS:HE1  | 1.58                     | 0.49              |
| 4:J:74:VAL:HG12  | 4:J:76:ALA:H     | 1.77                     | 0.49              |
| 7:N:13:GLN:CB    | 7:N:138:LEU:HB3  | 2.42                     | 0.49              |
| 7:N:164:GLU:HG3  | 7:N:227:PRO:HD2  | 1.93                     | 0.49              |
| 2:C:45:ARG:CB    | 2:C:116:PHE:HE2  | 2.25                     | 0.49              |
| 3:E:14:TYR:CD1   | 3:I:28:VAL:HG13  | 2.45                     | 0.49              |
| 3:E:72:ARG:O     | 3:E:75:GLU:HG3   | 2.12                     | 0.49              |
| 4:L:13:LEU:HA    | 4:L:54:TYR:CD2   | 2.48                     | 0.49              |
| 7:N:6:LEU:CD2    | 7:N:149:LEU:O    | 2.56                     | 0.49              |
| 2:C:132:TRP:HH2  | 2:C:249:TRP:CE2  | 2.29                     | 0.49              |
| 2:C:335:TRP:CE3  | 2:C:338:LEU:HD13 | 2.46                     | 0.49              |
| 2:C:367:GLU:HG2  | 2:C:370:ASP:OD2  | 2.13                     | 0.49              |
| 2:C:484:ILE:HD11 | 2:C:503:ALA:CB   | 2.41                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:186:VAL:HG22 | 3:E:237:VAL:HG22 | 1.93                     | 0.49              |
| 3:G:72:ARG:O     | 3:G:75:GLU:HG3   | 2.12                     | 0.49              |
| 3:I:85:ALA:O     | 3:I:89:GLN:HG2   | 2.12                     | 0.49              |
| 5:K:9:C:N3       | 5:K:10:C:N4      | 2.60                     | 0.49              |
| 2:C:257:PRO:HB2  | 2:C:298:TRP:HZ3  | 1.77                     | 0.49              |
| 3:E:19:ARG:HH21  | 5:K:34:G:H5''    | 1.78                     | 0.49              |
| 3:G:269:SER:HA   | 3:G:272:GLN:HG3  | 1.94                     | 0.49              |
| 3:H:59:ALA:HA    | 3:H:120:PRO:HA   | 1.94                     | 0.49              |
| 6:M:59:DG:C2     | 8:O:8:DG:C2      | 3.00                     | 0.49              |
| 1:A:102:VAL:CG2  | 1:A:223:LEU:HD23 | 2.43                     | 0.49              |
| 2:C:134:GLN:NE2  | 2:C:282:LEU:HG   | 2.27                     | 0.49              |
| 3:G:12:LEU:HD12  | 3:G:231:PHE:CE2  | 2.48                     | 0.49              |
| 3:G:319:ASN:HB2  | 3:G:346:LEU:HD22 | 1.95                     | 0.49              |
| 3:G:331:ASP:OD1  | 3:G:331:ASP:N    | 2.44                     | 0.49              |
| 5:K:5:A:N7       | 5:K:6:C:N4       | 2.61                     | 0.49              |
| 6:M:59:DG:C2     | 8:O:8:DG:N2      | 2.80                     | 0.49              |
| 2:C:405:ARG:CG   | 2:C:405:ARG:NH1  | 2.73                     | 0.49              |
| 3:D:283:LEU:HD12 | 3:D:315:CYS:SG   | 2.52                     | 0.49              |
| 7:N:12:MET:HG3   | 7:N:143:PHE:CD1  | 2.47                     | 0.49              |
| 2:C:31:ARG:NH2   | 2:C:39:PRO:HG3   | 2.28                     | 0.49              |
| 3:D:270:GLY:H    | 3:D:272:GLN:HG2  | 1.78                     | 0.49              |
| 3:F:59:ALA:HA    | 3:F:120:PRO:HA   | 1.94                     | 0.49              |
| 3:H:12:LEU:HD12  | 3:H:231:PHE:CE2  | 2.48                     | 0.49              |
| 7:N:199:VAL:HG22 | 7:N:216:THR:HB   | 1.95                     | 0.49              |
| 3:F:39:SER:HA    | 3:F:190:HIS:ND1  | 2.28                     | 0.49              |
| 3:F:324:ARG:NH1  | 3:F:327:GLU:OE1  | 2.46                     | 0.49              |
| 3:I:133:GLU:OE2  | 3:I:155:ARG:NH2  | 2.46                     | 0.49              |
| 3:I:291:ASP:OD1  | 3:I:291:ASP:N    | 2.41                     | 0.49              |
| 2:C:334:ILE:HG13 | 7:N:69:ARG:NH2   | 2.28                     | 0.49              |
| 3:E:217:GLY:H    | 6:M:23:DG:H21    | 1.60                     | 0.49              |
| 3:E:270:GLY:HA2  | 5:K:35:G:OP1     | 2.13                     | 0.49              |
| 3:F:319:ASN:HB2  | 3:F:346:LEU:HD22 | 1.95                     | 0.49              |
| 3:G:85:ALA:O     | 3:G:89:GLN:HG2   | 2.12                     | 0.49              |
| 3:G:324:ARG:HG2  | 3:H:340:VAL:O    | 2.12                     | 0.49              |
| 3:H:85:ALA:O     | 3:H:89:GLN:HG2   | 2.12                     | 0.49              |
| 5:K:44:A:H3'     | 5:K:44:A:P       | 2.53                     | 0.49              |
| 1:A:113:ARG:NH2  | 5:K:57:U:C6      | 2.81                     | 0.48              |
| 2:C:74:LEU:O     | 2:C:78:ARG:HB3   | 2.12                     | 0.48              |
| 2:C:335:TRP:CE3  | 2:C:474:TRP:CE3  | 2.97                     | 0.48              |
| 3:D:212:LYS:C    | 3:D:214:ASN:N    | 2.71                     | 0.48              |
| 3:E:12:LEU:HD12  | 3:E:231:PHE:CE2  | 2.48                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:17:ILE:HB    | 3:E:268:PRO:HB2  | 1.95                     | 0.48              |
| 3:G:324:ARG:NH1  | 3:G:327:GLU:OE1  | 2.46                     | 0.48              |
| 3:I:50:GLU:HG3   | 3:I:51:VAL:N     | 2.20                     | 0.48              |
| 8:O:35:DT:H2'    | 8:O:36:DG:H5''   | 1.95                     | 0.48              |
| 2:C:274:ASP:OD1  | 2:C:275:HIS:N    | 2.46                     | 0.48              |
| 3:D:48:ARG:NH2   | 3:D:173:MET:HE2  | 2.28                     | 0.48              |
| 3:F:85:ALA:O     | 3:F:89:GLN:HG2   | 2.12                     | 0.48              |
| 3:H:324:ARG:NH1  | 3:H:327:GLU:OE1  | 2.46                     | 0.48              |
| 1:A:3:TRP:HZ2    | 1:A:70:SER:O     | 1.96                     | 0.48              |
| 2:C:30:ALA:HB1   | 2:C:54:LEU:HD13  | 1.95                     | 0.48              |
| 3:F:12:LEU:HD12  | 3:F:231:PHE:CE2  | 2.48                     | 0.48              |
| 3:F:203:PHE:HZ   | 3:F:221:MET:HE3  | 1.77                     | 0.48              |
| 3:H:203:PHE:HZ   | 3:H:221:MET:HE3  | 1.78                     | 0.48              |
| 1:A:9:PRO:HD2    | 1:A:62:LEU:O     | 2.13                     | 0.48              |
| 1:A:51:LEU:HG    | 1:A:68:SER:HB3   | 1.96                     | 0.48              |
| 1:A:72:LEU:HB3   | 1:A:86:MET:HE1   | 1.94                     | 0.48              |
| 2:C:163:TRP:NE1  | 7:N:76:ILE:HD13  | 2.27                     | 0.48              |
| 3:D:324:ARG:NH2  | 7:N:240:ASN:OD1  | 2.47                     | 0.48              |
| 3:H:136:ASP:N    | 3:H:136:ASP:OD1  | 2.46                     | 0.48              |
| 3:E:141:GLU:HG3  | 3:E:150:ILE:CG1  | 2.42                     | 0.48              |
| 3:E:239:LEU:HD22 | 3:E:368:PHE:CZ   | 2.48                     | 0.48              |
| 3:F:269:SER:HA   | 3:F:272:GLN:HG2  | 1.94                     | 0.48              |
| 3:I:59:ALA:HA    | 3:I:120:PRO:HA   | 1.95                     | 0.48              |
| 7:N:28:PRO:HG2   | 7:N:29:TYR:CE2   | 2.49                     | 0.48              |
| 2:C:336:ARG:HH11 | 7:N:200:LEU:CD2  | 2.19                     | 0.48              |
| 2:C:379:PHE:HE2  | 2:C:381:GLN:OE1  | 1.97                     | 0.48              |
| 3:E:59:ALA:HA    | 3:E:120:PRO:HA   | 1.94                     | 0.48              |
| 3:E:141:GLU:O    | 3:E:147:PRO:HB3  | 2.14                     | 0.48              |
| 3:F:141:GLU:O    | 3:F:147:PRO:HB3  | 2.14                     | 0.48              |
| 3:H:11:THR:HA    | 3:H:230:THR:HA   | 1.95                     | 0.48              |
| 3:H:331:ASP:OD1  | 3:H:331:ASP:N    | 2.44                     | 0.48              |
| 3:I:141:GLU:O    | 3:I:147:PRO:HB3  | 2.14                     | 0.48              |
| 3:I:324:ARG:NH1  | 3:I:327:GLU:OE1  | 2.46                     | 0.48              |
| 1:A:44:ASN:HB2   | 1:A:45:PRO:HD3   | 1.96                     | 0.48              |
| 1:A:59:ARG:HD3   | 4:L:45:LEU:HG    | 1.95                     | 0.48              |
| 2:C:63:PRO:HB3   | 2:C:191:TYR:CE1  | 2.49                     | 0.48              |
| 2:C:414:ARG:O    | 2:C:418:ARG:HG2  | 2.13                     | 0.48              |
| 3:F:78:TRP:HZ2   | 3:F:132:ASP:HA   | 1.79                     | 0.48              |
| 3:G:19:ARG:NH1   | 3:G:271:LYS:HZ1  | 2.12                     | 0.48              |
| 3:I:319:ASN:HB2  | 3:I:346:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:34:SER:OG    | 1:A:37:LEU:HD21  | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:196:MET:H    | 2:C:209:ASN:HA   | 1.79                     | 0.48              |
| 4:L:18:SER:O     | 4:L:22:VAL:HG22  | 2.13                     | 0.48              |
| 6:M:56:DT:P      | 7:N:94:ARG:HH21  | 2.36                     | 0.48              |
| 1:A:22:THR:HG23  | 1:A:25:ASN:H     | 1.78                     | 0.48              |
| 1:A:116:ARG:HH21 | 1:A:122:GLN:HB2  | 1.79                     | 0.48              |
| 2:C:116:PHE:O    | 2:C:120:SER:N    | 2.46                     | 0.48              |
| 2:C:432:ARG:NH2  | 2:C:535:THR:O    | 2.47                     | 0.48              |
| 3:F:141:GLU:HG3  | 3:F:150:ILE:CG1  | 2.42                     | 0.48              |
| 2:C:417:ARG:HD2  | 2:C:417:ARG:HA   | 1.59                     | 0.48              |
| 3:D:38:VAL:HG12  | 3:D:43:TRP:CD1   | 2.49                     | 0.48              |
| 3:E:39:SER:HA    | 3:E:190:HIS:ND1  | 2.28                     | 0.48              |
| 3:E:136:ASP:OD1  | 3:E:136:ASP:N    | 2.47                     | 0.48              |
| 3:E:279:THR:HG23 | 3:I:298:PRO:HG2  | 1.96                     | 0.48              |
| 3:E:324:ARG:CG   | 3:E:324:ARG:NH2  | 2.73                     | 0.48              |
| 3:E:331:ASP:N    | 3:E:331:ASP:OD1  | 2.44                     | 0.48              |
| 3:G:59:ALA:HA    | 3:G:120:PRO:HA   | 1.94                     | 0.48              |
| 3:H:141:GLU:O    | 3:H:147:PRO:HB3  | 2.14                     | 0.48              |
| 5:K:9:C:N4       | 6:M:54:DG:H1     | 2.07                     | 0.48              |
| 7:N:174:GLU:HB2  | 7:N:177:ALA:HB2  | 1.96                     | 0.48              |
| 7:N:200:LEU:HD11 | 7:N:217:ARG:HE   | 1.79                     | 0.48              |
| 2:C:113:ASP:O    | 2:C:117:ALA:HB2  | 2.14                     | 0.47              |
| 2:C:207:GLU:CD   | 2:C:301:ARG:HH12 | 2.22                     | 0.47              |
| 2:C:366:GLN:OE1  | 2:C:366:GLN:N    | 2.46                     | 0.47              |
| 3:D:184:GLY:O    | 3:D:185:ALA:HB3  | 2.14                     | 0.47              |
| 3:E:267:VAL:CG1  | 3:E:268:PRO:HD2  | 2.44                     | 0.47              |
| 3:G:11:THR:HA    | 3:G:230:THR:HA   | 1.95                     | 0.47              |
| 3:G:141:GLU:O    | 3:G:147:PRO:HB3  | 2.14                     | 0.47              |
| 3:G:248:ASP:OD1  | 3:G:251:THR:OG1  | 2.27                     | 0.47              |
| 4:J:56:PRO:HD2   | 4:J:81:PHE:CE2   | 2.47                     | 0.47              |
| 4:J:197:ARG:HH11 | 4:J:197:ARG:CG   | 2.15                     | 0.47              |
| 7:N:7:ARG:CD     | 7:N:148:LEU:O    | 2.61                     | 0.47              |
| 7:N:63:VAL:HG23  | 7:N:63:VAL:O     | 2.13                     | 0.47              |
| 2:C:20:PHE:O     | 2:C:124:ASP:CA   | 2.57                     | 0.47              |
| 2:C:122:ARG:NH2  | 2:C:251:GLN:O    | 2.47                     | 0.47              |
| 2:C:336:ARG:NH1  | 7:N:200:LEU:HD22 | 2.26                     | 0.47              |
| 3:D:29:VAL:O     | 7:N:110:ASP:HB2  | 2.14                     | 0.47              |
| 3:G:17:ILE:O     | 3:G:270:GLY:HA3  | 2.14                     | 0.47              |
| 3:H:39:SER:HA    | 3:H:190:HIS:ND1  | 2.28                     | 0.47              |
| 5:K:6:C:H6       | 5:K:6:C:H2'      | 1.53                     | 0.47              |
| 4:L:18:SER:HA    | 4:L:21:ILE:HG12  | 1.96                     | 0.47              |
| 8:O:3:DC:H2''    | 8:O:4:DG:C8      | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:LEU:CD1   | 1:A:73:ARG:H     | 2.24                     | 0.47              |
| 3:D:171:GLY:N    | 3:D:184:GLY:CA   | 2.77                     | 0.47              |
| 3:E:17:ILE:HD12  | 3:E:268:PRO:HD2  | 1.96                     | 0.47              |
| 3:G:78:TRP:HZ2   | 3:G:132:ASP:HA   | 1.79                     | 0.47              |
| 6:M:20:DG:H2''   | 6:M:21:DG:C8     | 2.48                     | 0.47              |
| 2:C:107:LEU:HD12 | 2:C:107:LEU:O    | 2.14                     | 0.47              |
| 2:C:494:THR:HG23 | 2:C:494:THR:O    | 2.13                     | 0.47              |
| 3:E:319:ASN:HB2  | 3:E:346:LEU:HD22 | 1.95                     | 0.47              |
| 3:H:78:TRP:HZ2   | 3:H:132:ASP:HA   | 1.79                     | 0.47              |
| 3:I:39:SER:HA    | 3:I:190:HIS:ND1  | 2.28                     | 0.47              |
| 4:L:143:LEU:HD21 | 4:L:179:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:102:VAL:HA   | 1:A:226:ILE:HG23 | 1.94                     | 0.47              |
| 4:J:182:TYR:CD1  | 6:M:43:DA:C6     | 3.03                     | 0.47              |
| 7:N:208:ASP:O    | 7:N:212:ARG:HG3  | 2.14                     | 0.47              |
| 8:O:6:DA:H2''    | 8:O:7:DC:C6      | 2.49                     | 0.47              |
| 1:A:113:ARG:NH1  | 5:K:57:U:H6      | 2.11                     | 0.47              |
| 3:E:11:THR:HG22  | 3:E:230:THR:HG22 | 1.97                     | 0.47              |
| 3:E:41:GLN:HB2   | 5:K:31:G:H3'     | 1.96                     | 0.47              |
| 3:E:292:ARG:HH11 | 3:F:278:MET:HE3  | 1.78                     | 0.47              |
| 3:G:39:SER:HA    | 3:G:190:HIS:ND1  | 2.28                     | 0.47              |
| 6:M:17:DC:H2''   | 6:M:18:DC:C6     | 2.49                     | 0.47              |
| 7:N:170:HIS:CG   | 7:N:234:PRO:HA   | 2.49                     | 0.47              |
| 8:O:2:DG:H2''    | 8:O:3:DC:C6      | 2.50                     | 0.47              |
| 1:A:200:ASP:OD1  | 1:A:201:ALA:N    | 2.47                     | 0.47              |
| 2:C:45:ARG:HA    | 2:C:116:PHE:HE2  | 1.80                     | 0.47              |
| 3:D:11:THR:HA    | 3:D:230:THR:HA   | 1.96                     | 0.47              |
| 3:D:19:ARG:HD2   | 3:D:23:GLY:HA2   | 1.97                     | 0.47              |
| 3:D:37:ARG:HB2   | 3:D:191:ALA:O    | 2.14                     | 0.47              |
| 3:D:40:SER:HB2   | 3:D:190:HIS:HD2  | 1.79                     | 0.47              |
| 3:D:205:THR:HA   | 3:D:220:HIS:O    | 2.15                     | 0.47              |
| 3:D:280:LEU:HD12 | 3:H:325:LEU:HD22 | 1.96                     | 0.47              |
| 3:E:11:THR:HA    | 3:E:230:THR:HA   | 1.95                     | 0.47              |
| 3:E:28:VAL:CG2   | 3:E:37:ARG:HD3   | 2.45                     | 0.47              |
| 3:E:289:ARG:NH1  | 3:E:289:ARG:CB   | 2.77                     | 0.47              |
| 3:H:14:TYR:N     | 3:H:228:ALA:HB2  | 2.20                     | 0.47              |
| 3:H:233:ARG:NH2  | 3:H:263:PHE:O    | 2.39                     | 0.47              |
| 3:H:319:ASN:HB2  | 3:H:346:LEU:HD22 | 1.95                     | 0.47              |
| 3:I:78:TRP:HZ2   | 3:I:132:ASP:HA   | 1.79                     | 0.47              |
| 2:C:228:LEU:O    | 2:C:232:LEU:HD13 | 2.15                     | 0.47              |
| 3:E:14:TYR:CE2   | 3:E:226:PHE:HD2  | 2.33                     | 0.47              |
| 3:G:28:VAL:CG2   | 3:G:37:ARG:HD3   | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:136:ASP:OD1  | 3:G:136:ASP:N    | 2.46                     | 0.47              |
| 3:H:11:THR:HG22  | 3:H:230:THR:HG22 | 1.97                     | 0.47              |
| 3:I:93:SER:HA    | 3:I:149:GLY:HA3  | 1.96                     | 0.47              |
| 6:M:61:DC:H2'    | 6:M:62:DC:C6     | 2.50                     | 0.47              |
| 7:N:199:VAL:CG2  | 7:N:216:THR:HB   | 2.44                     | 0.47              |
| 2:C:20:PHE:HB3   | 2:C:125:LEU:HD22 | 1.97                     | 0.47              |
| 2:C:23:THR:CB    | 2:C:24:ILE:HD12  | 2.40                     | 0.47              |
| 2:C:339:ASP:O    | 2:C:342:LEU:HB2  | 2.15                     | 0.47              |
| 2:C:363:GLN:CD   | 2:C:365:PRO:CD   | 2.88                     | 0.47              |
| 2:C:480:VAL:HG23 | 2:C:490:ALA:HB1  | 1.96                     | 0.47              |
| 3:D:165:VAL:HG11 | 3:D:255:ALA:HB2  | 1.97                     | 0.47              |
| 3:E:259:PHE:HD2  | 3:E:260:LEU:HD12 | 1.80                     | 0.47              |
| 3:F:11:THR:HA    | 3:F:230:THR:HA   | 1.95                     | 0.47              |
| 3:F:28:VAL:CG2   | 3:F:37:ARG:HD3   | 2.45                     | 0.47              |
| 3:H:206:ALA:HB2  | 5:K:19:G:H1'     | 1.97                     | 0.47              |
| 4:L:78:GLU:OE1   | 4:L:78:GLU:N     | 2.48                     | 0.47              |
| 7:N:204:PRO:HA   | 7:N:214:TYR:CD1  | 2.50                     | 0.47              |
| 7:N:239:GLN:HG2  | 7:N:243:PHE:HE2  | 1.80                     | 0.47              |
| 1:A:101:ARG:CG   | 1:A:101:ARG:NH1  | 2.73                     | 0.47              |
| 1:A:104:TYR:C    | 1:A:222:SER:O    | 2.58                     | 0.47              |
| 2:C:519:TYR:HE1  | 3:D:225:GLN:NE2  | 2.13                     | 0.47              |
| 3:H:28:VAL:CG2   | 3:H:37:ARG:HD3   | 2.45                     | 0.47              |
| 3:H:259:PHE:HD2  | 3:H:260:LEU:HD12 | 1.80                     | 0.47              |
| 4:J:147:VAL:HG22 | 4:J:157:THR:HG21 | 1.96                     | 0.47              |
| 5:K:8:G:HO2'     | 5:K:9:C:P        | 2.36                     | 0.47              |
| 2:C:88:LYS:HG3   | 2:C:88:LYS:O     | 2.15                     | 0.46              |
| 2:C:297:THR:HG22 | 2:C:298:TRP:N    | 2.31                     | 0.46              |
| 2:C:472:ARG:HH21 | 7:N:70:LEU:HD23  | 1.80                     | 0.46              |
| 2:C:485:VAL:HG13 | 2:C:486:TYR:CD1  | 2.45                     | 0.46              |
| 3:E:78:TRP:HZ2   | 3:E:132:ASP:HA   | 1.79                     | 0.46              |
| 3:F:136:ASP:N    | 3:F:136:ASP:OD1  | 2.46                     | 0.46              |
| 3:F:298:PRO:HG3  | 3:G:11:THR:OG1   | 2.14                     | 0.46              |
| 3:G:206:ALA:HB3  | 3:G:220:HIS:HB3  | 1.98                     | 0.46              |
| 2:C:335:TRP:NE1  | 2:C:478:GLU:OE1  | 2.48                     | 0.46              |
| 3:E:268:PRO:O    | 3:E:269:SER:OG   | 2.27                     | 0.46              |
| 3:G:10:GLN:OE1   | 3:G:233:ARG:NH1  | 2.49                     | 0.46              |
| 3:H:93:SER:HA    | 3:H:149:GLY:HA3  | 1.97                     | 0.46              |
| 6:M:33:DA:C2'    | 6:M:34:DT:H5'    | 2.45                     | 0.46              |
| 6:M:62:DC:O2     | 8:O:5:DG:N2      | 2.48                     | 0.46              |
| 3:D:340:VAL:HG12 | 3:D:340:VAL:O    | 2.15                     | 0.46              |
| 3:E:306:GLY:C    | 3:E:308:ASP:H    | 2.24                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:195:HIS:HE1  | 3:I:230:THR:H    | 1.63                     | 0.46              |
| 4:J:55:VAL:HG12  | 4:J:81:PHE:CD2   | 2.50                     | 0.46              |
| 4:L:143:LEU:HD22 | 4:L:161:LEU:HD12 | 1.98                     | 0.46              |
| 3:F:50:GLU:HG3   | 3:F:51:VAL:N     | 2.20                     | 0.46              |
| 3:F:213:GLU:H    | 3:F:213:GLU:CD   | 2.24                     | 0.46              |
| 3:F:289:ARG:HH12 | 3:F:294:ILE:HD11 | 1.80                     | 0.46              |
| 3:G:11:THR:HG22  | 3:G:230:THR:HG22 | 1.97                     | 0.46              |
| 3:G:93:SER:HA    | 3:G:149:GLY:HA3  | 1.97                     | 0.46              |
| 3:G:306:GLY:C    | 3:G:308:ASP:H    | 2.24                     | 0.46              |
| 3:H:195:HIS:HE1  | 3:H:230:THR:H    | 1.63                     | 0.46              |
| 3:I:28:VAL:CG2   | 3:I:37:ARG:HD3   | 2.45                     | 0.46              |
| 4:J:147:VAL:CG2  | 4:J:157:THR:HG21 | 2.45                     | 0.46              |
| 4:J:177:PRO:O    | 4:J:181:LEU:HD13 | 2.15                     | 0.46              |
| 6:M:50:DA:H2'    | 6:M:51:DC:C5     | 2.51                     | 0.46              |
| 1:A:123:ARG:CB   | 1:A:212:ARG:HH12 | 2.28                     | 0.46              |
| 2:C:277:ARG:HD3  | 2:C:303:ARG:CD   | 2.46                     | 0.46              |
| 2:C:483:ASN:HB2  | 2:C:490:ALA:HB2  | 1.98                     | 0.46              |
| 3:D:12:LEU:HD12  | 3:D:231:PHE:CE2  | 2.50                     | 0.46              |
| 3:H:225:GLN:HE21 | 4:J:175:HIS:CE1  | 2.33                     | 0.46              |
| 4:J:21:ILE:HG23  | 4:J:28:ARG:HD3   | 1.97                     | 0.46              |
| 5:K:44:A:H4'     | 5:K:45:G:C5'     | 2.46                     | 0.46              |
| 4:L:197:ARG:HH11 | 4:L:197:ARG:HG2  | 1.77                     | 0.46              |
| 7:N:72:ASP:C     | 7:N:73:PHE:O     | 2.53                     | 0.46              |
| 7:N:88:THR:HG22  | 7:N:89:ALA:H     | 1.79                     | 0.46              |
| 1:A:208:ASN:OD1  | 1:A:209:GLY:N    | 2.49                     | 0.46              |
| 2:C:129:GLU:HG2  | 2:C:130:ARG:HD3  | 1.97                     | 0.46              |
| 2:C:245:ASP:OD2  | 2:C:269:GLY:N    | 2.49                     | 0.46              |
| 3:D:341:GLU:O    | 3:D:341:GLU:HG2  | 2.15                     | 0.46              |
| 3:F:11:THR:HG22  | 3:F:230:THR:HG22 | 1.97                     | 0.46              |
| 3:G:50:GLU:HG3   | 3:G:51:VAL:N     | 2.20                     | 0.46              |
| 5:K:1:A:C4       | 7:N:134:TRP:CE3  | 3.04                     | 0.46              |
| 5:K:43:G:N3      | 5:K:43:G:H3'     | 2.31                     | 0.46              |
| 3:F:195:HIS:HE1  | 3:F:230:THR:H    | 1.63                     | 0.46              |
| 3:G:259:PHE:HD2  | 3:G:260:LEU:HD12 | 1.80                     | 0.46              |
| 3:G:325:LEU:HD22 | 3:H:280:LEU:HD12 | 1.98                     | 0.46              |
| 3:I:259:PHE:HD2  | 3:I:260:LEU:HD12 | 1.80                     | 0.46              |
| 7:N:167:PRO:HB2  | 7:N:242:LEU:HD22 | 1.98                     | 0.46              |
| 2:C:131:PRO:HD3  | 2:C:136:PRO:HB3  | 1.98                     | 0.46              |
| 2:C:478:GLU:HB3  | 2:C:479:PRO:HD3  | 1.98                     | 0.46              |
| 3:D:40:SER:HB3   | 3:D:190:HIS:NE2  | 2.30                     | 0.46              |
| 3:D:275:THR:O    | 3:D:275:THR:OG1  | 2.33                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:93:SER:HA    | 3:E:149:GLY:HA3  | 1.97                     | 0.46              |
| 3:F:93:SER:HA    | 3:F:149:GLY:HA3  | 1.97                     | 0.46              |
| 3:F:306:GLY:C    | 3:F:308:ASP:H    | 2.24                     | 0.46              |
| 3:G:174:LEU:HD23 | 3:G:177:LEU:HB2  | 1.98                     | 0.46              |
| 3:G:195:HIS:HE1  | 3:G:230:THR:H    | 1.63                     | 0.46              |
| 3:G:206:ALA:HB2  | 5:K:25:U:H1'     | 1.97                     | 0.46              |
| 3:H:141:GLU:HG3  | 3:H:150:ILE:CG1  | 2.42                     | 0.46              |
| 3:H:289:ARG:HH12 | 3:H:294:ILE:HD11 | 1.80                     | 0.46              |
| 1:A:20:PHE:CG    | 1:A:20:PHE:O     | 2.69                     | 0.46              |
| 1:A:107:VAL:HA   | 1:A:188:VAL:O    | 2.16                     | 0.46              |
| 1:A:164:TYR:CD1  | 1:A:187:ALA:O    | 2.69                     | 0.46              |
| 2:C:137:ARG:HH12 | 2:C:256:ASP:CA   | 2.25                     | 0.46              |
| 2:C:406:GLU:OE1  | 2:C:411:GLU:HB3  | 2.15                     | 0.46              |
| 2:C:421:LEU:HB3  | 2:C:500:PRO:HD3  | 1.97                     | 0.46              |
| 3:D:17:ILE:HD13  | 3:D:268:PRO:HD2  | 1.98                     | 0.46              |
| 3:D:184:GLY:C    | 3:D:186:VAL:H    | 2.23                     | 0.46              |
| 3:F:259:PHE:HD2  | 3:F:260:LEU:HD12 | 1.80                     | 0.46              |
| 3:G:14:TYR:N     | 3:G:228:ALA:HB2  | 2.18                     | 0.46              |
| 3:G:16:ASN:ND2   | 3:G:225:GLN:O    | 2.49                     | 0.46              |
| 6:M:45:DT:H2''   | 6:M:46:DT:H5'    | 1.97                     | 0.46              |
| 2:C:307:PRO:HB2  | 2:C:308:GLU:OE1  | 2.16                     | 0.46              |
| 3:D:183:ASP:OD2  | 5:K:1:A:N3       | 2.49                     | 0.46              |
| 3:H:306:GLY:C    | 3:H:308:ASP:H    | 2.24                     | 0.46              |
| 4:L:150:LYS:HG3  | 4:L:186:ASP:HB3  | 1.98                     | 0.46              |
| 7:N:30:PRO:HB2   | 7:N:35:LEU:CD1   | 2.45                     | 0.46              |
| 1:A:185:HIS:HD2  | 1:A:186:PRO:C    | 2.23                     | 0.45              |
| 2:C:51:SER:O     | 2:C:228:LEU:HB2  | 2.16                     | 0.45              |
| 3:D:236:ASN:HD22 | 3:D:237:VAL:H    | 1.53                     | 0.45              |
| 3:E:195:HIS:HE1  | 3:E:230:THR:H    | 1.63                     | 0.45              |
| 3:E:324:ARG:HB3  | 3:F:340:VAL:HG13 | 1.98                     | 0.45              |
| 3:I:324:ARG:HD2  | 3:I:324:ARG:HA   | 1.72                     | 0.45              |
| 7:N:13:GLN:HB3   | 7:N:138:LEU:CD2  | 2.46                     | 0.45              |
| 7:N:166:VAL:HG22 | 7:N:245:TYR:OH   | 2.15                     | 0.45              |
| 1:A:72:LEU:HD22  | 1:A:86:MET:CE    | 2.46                     | 0.45              |
| 3:G:61:ARG:O     | 3:H:209:ASP:HB2  | 2.15                     | 0.45              |
| 3:H:174:LEU:HD23 | 3:H:177:LEU:HB2  | 1.98                     | 0.45              |
| 3:I:136:ASP:OD1  | 3:I:136:ASP:N    | 2.47                     | 0.45              |
| 7:N:179:THR:H    | 7:N:228:ALA:H    | 1.64                     | 0.45              |
| 1:A:3:TRP:CB     | 1:A:88:ASN:HA    | 2.46                     | 0.45              |
| 1:A:91:PRO:HG2   | 1:A:203:ARG:HE   | 1.81                     | 0.45              |
| 1:A:137:THR:HB   | 1:A:138:TRP:HA   | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:63:ARG:HB2   | 3:E:116:LEU:HD13 | 1.99                     | 0.45              |
| 3:F:174:LEU:HD23 | 3:F:177:LEU:HB2  | 1.98                     | 0.45              |
| 3:I:96:LYS:HG3   | 3:I:97:LYS:H     | 1.82                     | 0.45              |
| 6:M:58:DC:H2''   | 6:M:59:DG:C8     | 2.52                     | 0.45              |
| 1:A:156:ASN:HB3  | 1:A:202:VAL:HB   | 1.97                     | 0.45              |
| 2:C:532:HIS:O    | 2:C:535:THR:HG22 | 2.16                     | 0.45              |
| 2:C:245:ASP:CB   | 2:C:266:GLY:HA3  | 2.46                     | 0.45              |
| 2:C:283:HIS:HB2  | 2:C:295:TRP:CZ3  | 2.51                     | 0.45              |
| 3:D:166:SER:O    | 3:D:170:PHE:HB2  | 2.16                     | 0.45              |
| 3:F:10:GLN:OE1   | 3:F:233:ARG:NH1  | 2.49                     | 0.45              |
| 3:G:17:ILE:HA    | 3:G:270:GLY:O    | 2.16                     | 0.45              |
| 3:G:292:ARG:NH2  | 3:G:294:ILE:HG12 | 2.32                     | 0.45              |
| 3:H:88:ARG:O     | 3:H:92:LEU:HB2   | 2.17                     | 0.45              |
| 3:H:292:ARG:NH2  | 3:H:294:ILE:HG12 | 2.32                     | 0.45              |
| 3:I:306:GLY:C    | 3:I:308:ASP:H    | 2.24                     | 0.45              |
| 4:J:182:TYR:CE1  | 6:M:43:DA:C5     | 3.05                     | 0.45              |
| 7:N:17:GLU:O     | 7:N:18:HIS:CG    | 2.70                     | 0.45              |
| 1:A:202:VAL:O    | 1:A:206:VAL:HG23 | 2.17                     | 0.45              |
| 2:C:89:ASN:O     | 2:C:90:PRO:C     | 2.60                     | 0.45              |
| 2:C:185:LEU:HD12 | 2:C:189:LEU:CD1  | 2.46                     | 0.45              |
| 2:C:342:LEU:HD22 | 2:C:423:ARG:HH22 | 1.81                     | 0.45              |
| 3:D:225:GLN:O    | 3:D:226:PHE:CD1  | 2.67                     | 0.45              |
| 3:F:101:LYS:CB   | 4:J:93:ARG:HH12  | 2.29                     | 0.45              |
| 3:I:10:GLN:OE1   | 3:I:233:ARG:NH1  | 2.49                     | 0.45              |
| 4:L:211:ARG:HH21 | 4:L:215:GLN:NE2  | 2.15                     | 0.45              |
| 6:M:63:DG:C2     | 8:O:4:DG:C2      | 3.04                     | 0.45              |
| 1:A:8:VAL:CB     | 1:A:63:TYR:CD1   | 2.99                     | 0.45              |
| 2:C:226:ARG:HD3  | 2:C:371:SER:CB   | 2.46                     | 0.45              |
| 2:C:314:ILE:HG21 | 2:C:326:ARG:HH12 | 1.81                     | 0.45              |
| 3:E:16:ASN:ND2   | 3:E:226:PHE:HD1  | 2.07                     | 0.45              |
| 3:F:88:ARG:O     | 3:F:92:LEU:HB2   | 2.17                     | 0.45              |
| 1:A:76:ARG:O     | 1:A:77:LEU:HB3   | 2.17                     | 0.45              |
| 2:C:94:TRP:CZ3   | 2:C:98:ARG:NH2   | 2.85                     | 0.45              |
| 2:C:530:GLU:OE1  | 2:C:533:ARG:HD3  | 2.17                     | 0.45              |
| 3:D:352:ARG:HG3  | 3:D:353:TYR:N    | 2.30                     | 0.45              |
| 3:E:10:GLN:OE1   | 3:E:233:ARG:NH1  | 2.49                     | 0.45              |
| 3:G:96:LYS:HG3   | 3:G:97:LYS:H     | 1.82                     | 0.45              |
| 3:H:337:TYR:OH   | 3:H:352:ARG:HD2  | 2.17                     | 0.45              |
| 3:I:88:ARG:O     | 3:I:92:LEU:HB2   | 2.17                     | 0.45              |
| 4:J:223:THR:O    | 4:J:227:GLN:HG2  | 2.17                     | 0.45              |
| 7:N:171:ARG:NH1  | 7:N:171:ARG:CG   | 2.79                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:O:46:DC:H2''   | 8:O:47:DA:C8     | 2.52                     | 0.45              |
| 1:A:181:ARG:NH2  | 5:K:47:C:H1'     | 2.32                     | 0.45              |
| 3:D:169:LEU:O    | 3:D:186:VAL:CG2  | 2.64                     | 0.45              |
| 3:F:292:ARG:NH2  | 3:F:294:ILE:HG12 | 2.32                     | 0.45              |
| 3:F:324:ARG:HD2  | 3:F:324:ARG:HA   | 1.72                     | 0.45              |
| 5:K:53:C:O2'     | 5:K:55:C:C5      | 2.69                     | 0.45              |
| 4:L:20:LEU:HD11  | 4:L:27:ALA:HB3   | 1.99                     | 0.45              |
| 3:D:319:ASN:OD1  | 3:D:348:ALA:HB3  | 2.17                     | 0.45              |
| 3:G:220:HIS:NE2  | 3:G:222:ASN:OD1  | 2.50                     | 0.45              |
| 3:I:18:ASN:HD21  | 3:I:26:LYS:HD2   | 1.78                     | 0.45              |
| 5:K:44:A:C4'     | 5:K:45:G:C5'     | 2.91                     | 0.45              |
| 7:N:137:TYR:HA   | 7:N:145:PRO:HD3  | 2.00                     | 0.45              |
| 2:C:318:SER:HB2  | 8:O:14:DA:H2''   | 1.99                     | 0.44              |
| 2:C:50:ARG:CA    | 2:C:53:GLU:OE1   | 2.65                     | 0.44              |
| 3:E:292:ARG:NH2  | 3:E:294:ILE:HG12 | 2.32                     | 0.44              |
| 3:F:14:TYR:CE1   | 3:F:200:GLU:CD   | 2.95                     | 0.44              |
| 3:F:96:LYS:HG3   | 3:F:97:LYS:H     | 1.82                     | 0.44              |
| 3:G:141:GLU:HG3  | 3:G:150:ILE:CG1  | 2.42                     | 0.44              |
| 3:G:337:TYR:OH   | 3:G:352:ARG:HD2  | 2.17                     | 0.44              |
| 3:H:10:GLN:OE1   | 3:H:233:ARG:NH1  | 2.49                     | 0.44              |
| 3:I:174:LEU:HD23 | 3:I:177:LEU:HB2  | 1.98                     | 0.44              |
| 4:L:51:VAL:HB    | 4:L:82:TYR:CE1   | 2.52                     | 0.44              |
| 4:L:155:ASP:OD1  | 4:L:156:SER:N    | 2.50                     | 0.44              |
| 7:N:18:HIS:ND1   | 7:N:18:HIS:C     | 2.72                     | 0.44              |
| 2:C:106:ARG:HD3  | 2:C:107:LEU:O    | 2.18                     | 0.44              |
| 3:D:41:GLN:OE1   | 3:D:41:GLN:N     | 2.38                     | 0.44              |
| 3:D:171:GLY:CA   | 3:D:184:GLY:HA2  | 2.44                     | 0.44              |
| 3:E:5:ASP:CG     | 3:E:289:ARG:HD2  | 2.41                     | 0.44              |
| 3:H:324:ARG:HD2  | 3:H:324:ARG:HA   | 1.72                     | 0.44              |
| 3:H:339:THR:CG2  | 3:H:341:GLU:HG2  | 2.48                     | 0.44              |
| 3:I:233:ARG:NH2  | 3:I:263:PHE:O    | 2.39                     | 0.44              |
| 3:I:292:ARG:NH2  | 3:I:294:ILE:HG12 | 2.32                     | 0.44              |
| 5:K:30:U:H5'     | 5:K:31:G:OP1     | 2.17                     | 0.44              |
| 1:A:29:LYS:CE    | 1:A:32:ARG:HE    | 2.29                     | 0.44              |
| 1:A:199:VAL:HG22 | 1:A:203:ARG:HH12 | 1.81                     | 0.44              |
| 3:G:269:SER:HA   | 3:G:272:GLN:HG2  | 1.99                     | 0.44              |
| 5:K:57:U:H2'     | 5:K:58:G:O4'     | 2.17                     | 0.44              |
| 7:N:137:TYR:CE1  | 7:N:139:GLY:O    | 2.69                     | 0.44              |
| 7:N:219:ILE:O    | 7:N:219:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:46:ARG:HA    | 5:K:59:G:H4'     | 2.00                     | 0.44              |
| 2:C:342:LEU:HD13 | 2:C:342:LEU:C    | 2.43                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:429:LEU:CG   | 2:C:432:ARG:CD   | 2.61                     | 0.44              |
| 2:C:519:TYR:CE1  | 3:D:225:GLN:NE2  | 2.85                     | 0.44              |
| 3:D:30:TYR:CD1   | 7:N:11:PRO:HA    | 2.52                     | 0.44              |
| 3:E:5:ASP:OD1    | 3:E:5:ASP:N      | 2.51                     | 0.44              |
| 3:E:14:TYR:N     | 3:E:228:ALA:HB2  | 2.19                     | 0.44              |
| 3:E:96:LYS:HG3   | 3:E:97:LYS:H     | 1.82                     | 0.44              |
| 3:F:337:TYR:OH   | 3:F:352:ARG:HD2  | 2.17                     | 0.44              |
| 7:N:61:VAL:HG22  | 7:N:115:VAL:HB   | 1.99                     | 0.44              |
| 2:C:115:TYR:CD1  | 2:C:115:TYR:C    | 2.95                     | 0.44              |
| 3:G:268:PRO:O    | 3:G:269:SER:OG   | 2.28                     | 0.44              |
| 3:I:5:ASP:OD1    | 3:I:5:ASP:N      | 2.51                     | 0.44              |
| 3:I:337:TYR:OH   | 3:I:352:ARG:HD2  | 2.17                     | 0.44              |
| 4:J:7:LEU:HD21   | 4:J:136:ARG:HH21 | 1.82                     | 0.44              |
| 7:N:18:HIS:O     | 7:N:18:HIS:CG    | 2.70                     | 0.44              |
| 1:A:8:VAL:HA     | 1:A:9:PRO:HD2    | 1.83                     | 0.44              |
| 1:A:28:ARG:HA    | 1:A:31:ILE:HG12  | 2.00                     | 0.44              |
| 1:A:116:ARG:HG2  | 1:A:117:SER:O    | 2.17                     | 0.44              |
| 2:C:45:ARG:HG3   | 2:C:116:PHE:CD2  | 2.52                     | 0.44              |
| 2:C:331:GLU:HG3  | 2:C:470:MET:HB3  | 2.00                     | 0.44              |
| 3:E:16:ASN:HB2   | 3:E:226:PHE:HA   | 2.00                     | 0.44              |
| 3:E:88:ARG:O     | 3:E:92:LEU:HB2   | 2.17                     | 0.44              |
| 6:M:63:DG:H2"    | 6:M:64:DC:C6     | 2.53                     | 0.44              |
| 7:N:63:VAL:HG12  | 7:N:113:PHE:CD1  | 2.52                     | 0.44              |
| 7:N:239:GLN:HG2  | 7:N:243:PHE:CE2  | 2.53                     | 0.44              |
| 1:A:185:HIS:CD2  | 1:A:186:PRO:HD2  | 2.52                     | 0.44              |
| 2:C:145:THR:HG22 | 2:C:295:TRP:CE2  | 2.53                     | 0.44              |
| 3:E:50:GLU:HG3   | 3:E:51:VAL:N     | 2.20                     | 0.44              |
| 3:E:339:THR:CG2  | 3:E:341:GLU:HG2  | 2.48                     | 0.44              |
| 3:G:339:THR:CG2  | 3:G:341:GLU:HG2  | 2.48                     | 0.44              |
| 3:H:96:LYS:HG3   | 3:H:97:LYS:H     | 1.82                     | 0.44              |
| 3:I:141:GLU:HG3  | 3:I:150:ILE:CG1  | 2.42                     | 0.44              |
| 4:L:20:LEU:HD12  | 4:L:24:GLU:OE1   | 2.18                     | 0.44              |
| 1:A:59:ARG:NH1   | 4:L:45:LEU:HD11  | 2.33                     | 0.44              |
| 2:C:89:ASN:O     | 2:C:92:ARG:N     | 2.51                     | 0.44              |
| 2:C:303:ARG:NE   | 2:C:303:ARG:HA   | 2.32                     | 0.44              |
| 2:C:377:PHE:HD1  | 2:C:392:THR:HG22 | 1.83                     | 0.44              |
| 3:G:289:ARG:HH12 | 3:G:294:ILE:HD11 | 1.80                     | 0.44              |
| 1:A:185:HIS:HB2  | 5:K:45:G:N1      | 2.33                     | 0.43              |
| 2:C:44:LEU:O     | 2:C:48:LEU:HG    | 2.18                     | 0.43              |
| 2:C:106:ARG:HH11 | 2:C:106:ARG:CG   | 2.31                     | 0.43              |
| 2:C:272:ARG:HH11 | 2:C:272:ARG:HG3  | 1.82                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:5:ASP:OD1    | 3:G:5:ASP:N      | 2.51                     | 0.43              |
| 3:G:233:ARG:NH2  | 3:G:263:PHE:O    | 2.39                     | 0.43              |
| 5:K:44:A:H1'     | 5:K:45:G:C5'     | 2.48                     | 0.43              |
| 1:A:163:THR:CA   | 3:I:19:ARG:HH12  | 2.30                     | 0.43              |
| 1:A:215:SER:HB3  | 5:K:61:G:OP2     | 2.19                     | 0.43              |
| 2:C:443:GLU:HB3  | 2:C:528:VAL:HG11 | 1.99                     | 0.43              |
| 3:D:41:GLN:HB2   | 5:K:7:C:H2'      | 1.99                     | 0.43              |
| 3:D:187:GLN:HB3  | 3:D:236:ASN:HB3  | 2.00                     | 0.43              |
| 3:E:337:TYR:OH   | 3:E:352:ARG:HD2  | 2.17                     | 0.43              |
| 3:F:101:LYS:HB3  | 4:J:93:ARG:HH12  | 1.83                     | 0.43              |
| 3:G:88:ARG:O     | 3:G:92:LEU:HB2   | 2.17                     | 0.43              |
| 5:K:43:G:H5'     | 5:K:44:A:OP2     | 2.17                     | 0.43              |
| 1:A:11:LEU:C     | 1:A:77:LEU:HD21  | 2.43                     | 0.43              |
| 2:C:132:TRP:O    | 2:C:134:GLN:HG3  | 2.18                     | 0.43              |
| 2:C:191:TYR:CE2  | 2:C:215:LEU:HD13 | 2.45                     | 0.43              |
| 3:H:78:TRP:CZ2   | 3:H:132:ASP:HA   | 2.54                     | 0.43              |
| 3:I:339:THR:CG2  | 3:I:341:GLU:HG2  | 2.48                     | 0.43              |
| 7:N:197:LEU:HB3  | 7:N:219:ILE:HG13 | 2.00                     | 0.43              |
| 1:A:141:ARG:HB3  | 3:E:216:HIS:NE2  | 2.33                     | 0.43              |
| 2:C:149:ASN:HB3  | 2:C:156:THR:O    | 2.18                     | 0.43              |
| 2:C:472:ARG:NH2  | 7:N:70:LEU:HD23  | 2.33                     | 0.43              |
| 3:F:5:ASP:OD1    | 3:F:5:ASP:N      | 2.51                     | 0.43              |
| 3:F:205:THR:HG22 | 3:F:221:MET:HG2  | 2.01                     | 0.43              |
| 3:F:339:THR:CG2  | 3:F:341:GLU:HG2  | 2.48                     | 0.43              |
| 3:I:78:TRP:CZ2   | 3:I:132:ASP:HA   | 2.54                     | 0.43              |
| 7:N:198:THR:HG22 | 7:N:219:ILE:HD11 | 2.00                     | 0.43              |
| 3:D:17:ILE:HG23  | 3:D:268:PRO:HB2  | 2.00                     | 0.43              |
| 3:D:269:SER:HA   | 3:D:272:GLN:HG3  | 2.00                     | 0.43              |
| 3:I:61:ARG:HA    | 3:I:117:PHE:O    | 2.19                     | 0.43              |
| 6:M:59:DG:N1     | 8:O:7:DC:N3      | 2.50                     | 0.43              |
| 1:A:113:ARG:CZ   | 5:K:57:U:C5      | 3.02                     | 0.43              |
| 2:C:403:ALA:HB1  | 2:C:412:ASN:OD1  | 2.19                     | 0.43              |
| 3:D:185:ALA:C    | 7:N:141:ARG:HH21 | 2.26                     | 0.43              |
| 3:D:216:HIS:CD2  | 5:K:16:U:O2'     | 2.72                     | 0.43              |
| 3:D:238:ASN:CB   | 7:N:135:GLN:HE22 | 2.12                     | 0.43              |
| 3:E:61:ARG:HA    | 3:E:117:PHE:O    | 2.19                     | 0.43              |
| 3:F:169:LEU:HD21 | 3:F:259:PHE:HB2  | 2.01                     | 0.43              |
| 3:G:169:LEU:HD21 | 3:G:259:PHE:HB2  | 2.01                     | 0.43              |
| 3:G:301:GLU:OE2  | 3:H:310:TYR:N    | 2.51                     | 0.43              |
| 3:H:248:ASP:OD2  | 3:H:251:THR:HG23 | 2.18                     | 0.43              |
| 2:C:202:VAL:HG11 | 2:C:257:PRO:CG   | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:19:LYS:HB3   | 4:L:19:LYS:HE2   | 1.75                     | 0.43              |
| 3:D:166:SER:HB2  | 3:D:173:MET:HE1  | 2.01                     | 0.43              |
| 3:E:217:GLY:N    | 6:M:23:DG:H21    | 2.16                     | 0.43              |
| 3:F:61:ARG:HA    | 3:F:117:PHE:O    | 2.19                     | 0.43              |
| 6:M:51:DC:H2''   | 6:M:52:DT:H5'    | 2.01                     | 0.43              |
| 1:A:105:ARG:HH11 | 1:A:105:ARG:CG   | 2.31                     | 0.43              |
| 1:A:116:ARG:HB2  | 1:A:122:GLN:HB3  | 2.01                     | 0.43              |
| 7:N:203:VAL:HG12 | 7:N:215:SER:O    | 2.18                     | 0.43              |
| 1:A:109:SER:CB   | 1:A:185:HIS:NE2  | 2.79                     | 0.43              |
| 2:C:129:GLU:HG2  | 2:C:130:ARG:CD   | 2.48                     | 0.43              |
| 3:E:5:ASP:OD2    | 3:E:289:ARG:HD2  | 2.19                     | 0.43              |
| 3:F:233:ARG:NH2  | 3:F:263:PHE:O    | 2.39                     | 0.43              |
| 3:G:61:ARG:HA    | 3:G:117:PHE:O    | 2.19                     | 0.43              |
| 3:H:61:ARG:HA    | 3:H:117:PHE:O    | 2.19                     | 0.43              |
| 3:H:215:ASP:OD1  | 3:H:215:ASP:O    | 2.37                     | 0.43              |
| 4:J:143:LEU:HD23 | 4:J:183:LEU:HD21 | 2.00                     | 0.43              |
| 5:K:44:A:H1'     | 5:K:45:G:H5''    | 2.01                     | 0.43              |
| 1:A:141:ARG:HA   | 3:E:216:HIS:CE1  | 2.42                     | 0.42              |
| 2:C:35:VAL:HG12  | 2:C:37:ALA:HB3   | 2.00                     | 0.42              |
| 3:D:28:VAL:CG2   | 3:D:37:ARG:HD3   | 2.48                     | 0.42              |
| 3:F:13:PRO:O     | 3:F:14:TYR:C     | 2.61                     | 0.42              |
| 3:G:16:ASN:HB2   | 3:G:226:PHE:HA   | 2.01                     | 0.42              |
| 3:G:28:VAL:HG22  | 3:H:14:TYR:CE1   | 2.54                     | 0.42              |
| 3:I:97:LYS:NZ    | 4:L:94:SER:OG    | 2.51                     | 0.42              |
| 6:M:53:DG:H2''   | 6:M:54:DG:O4'    | 2.19                     | 0.42              |
| 1:A:117:SER:O    | 1:A:118:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:183:ILE:O    | 1:A:184:ARG:HD3  | 2.16                     | 0.42              |
| 2:C:132:TRP:HA   | 2:C:132:TRP:CE3  | 2.54                     | 0.42              |
| 3:F:62:THR:HA    | 3:G:208:ASP:OD1  | 2.19                     | 0.42              |
| 3:H:5:ASP:OD1    | 3:H:5:ASP:N      | 2.51                     | 0.42              |
| 4:L:154:ALA:HA   | 4:L:157:THR:HG22 | 2.01                     | 0.42              |
| 7:N:196:THR:HB   | 7:N:218:GLN:HB3  | 2.01                     | 0.42              |
| 2:C:322:ARG:NH2  | 8:O:14:DA:H2'    | 2.34                     | 0.42              |
| 2:C:520:CYS:SG   | 4:J:211:ARG:NH1  | 2.89                     | 0.42              |
| 3:G:356:TYR:HB2  | 3:G:357:PRO:HD3  | 2.02                     | 0.42              |
| 4:J:32:ARG:O     | 4:J:35:VAL:HG23  | 2.20                     | 0.42              |
| 7:N:186:TYR:HB2  | 7:N:220:ARG:HG3  | 2.01                     | 0.42              |
| 3:E:174:LEU:HA   | 3:E:174:LEU:HD22 | 1.78                     | 0.42              |
| 3:E:356:TYR:HB2  | 3:E:357:PRO:HD3  | 2.02                     | 0.42              |
| 3:G:78:TRP:CZ2   | 3:G:132:ASP:HA   | 2.54                     | 0.42              |
| 1:A:74:VAL:HG23  | 1:A:79:PRO:HD2   | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:70:ARG:NH1   | 2:C:310:ASP:OD2  | 2.52                     | 0.42              |
| 2:C:352:PRO:HD2  | 2:C:355:LEU:HD21 | 2.01                     | 0.42              |
| 2:C:482:TRP:HA   | 2:C:485:VAL:HG12 | 2.01                     | 0.42              |
| 3:I:101:LYS:CD   | 4:L:93:ARG:NE    | 2.83                     | 0.42              |
| 5:K:32:U:H2'     | 5:K:33:G:H4'     | 2.02                     | 0.42              |
| 4:L:87:ILE:HD12  | 4:L:87:ILE:HA    | 1.84                     | 0.42              |
| 4:L:167:GLN:O    | 4:L:202:TRP:HZ2  | 2.02                     | 0.42              |
| 7:N:27:LEU:HD21  | 7:N:200:LEU:HD22 | 2.00                     | 0.42              |
| 2:C:29:ILE:HG13  | 2:C:41:MET:HG2   | 2.01                     | 0.42              |
| 2:C:334:ILE:CG1  | 7:N:69:ARG:CZ    | 2.97                     | 0.42              |
| 3:D:355:SER:OG   | 3:D:356:TYR:N    | 2.52                     | 0.42              |
| 3:E:203:PHE:CG   | 3:I:21:ASP:HB2   | 2.55                     | 0.42              |
| 3:H:169:LEU:HD21 | 3:H:259:PHE:HB2  | 2.01                     | 0.42              |
| 2:C:81:GLY:O     | 2:C:94:TRP:NE1   | 2.53                     | 0.42              |
| 3:E:92:LEU:HD12  | 3:E:92:LEU:HA    | 1.86                     | 0.42              |
| 3:G:324:ARG:HA   | 3:G:324:ARG:HD2  | 1.71                     | 0.42              |
| 8:O:10:DA:H2''   | 8:O:11:DG:C8     | 2.55                     | 0.42              |
| 2:C:257:PRO:HA   | 2:C:299:ALA:O    | 2.20                     | 0.42              |
| 2:C:312:TYR:CE1  | 2:C:354:ILE:HD13 | 2.54                     | 0.42              |
| 4:J:41:ASP:CG    | 4:J:43:ARG:HE    | 2.24                     | 0.42              |
| 1:A:185:HIS:HA   | 5:K:45:G:C6      | 2.55                     | 0.42              |
| 2:C:34:ASP:O     | 2:C:36:LEU:N     | 2.41                     | 0.42              |
| 2:C:247:ALA:HB1  | 2:C:249:TRP:CZ3  | 2.55                     | 0.42              |
| 2:C:510:ALA:O    | 2:C:514:GLU:HG3  | 2.16                     | 0.42              |
| 3:D:168:ASN:HD21 | 3:D:245:ASN:HB3  | 1.84                     | 0.42              |
| 3:D:329:TRP:CH2  | 7:N:246:VAL:HG11 | 2.54                     | 0.42              |
| 3:E:78:TRP:CZ2   | 3:E:132:ASP:HA   | 2.54                     | 0.42              |
| 3:F:78:TRP:CZ2   | 3:F:132:ASP:HA   | 2.54                     | 0.42              |
| 3:F:203:PHE:HA   | 3:F:223:ALA:HA   | 2.01                     | 0.42              |
| 4:L:84:VAL:HG11  | 4:L:196:ILE:HG13 | 2.02                     | 0.42              |
| 7:N:52:ASP:O     | 7:N:55:LYS:HB3   | 2.19                     | 0.42              |
| 1:A:32:ARG:NH1   | 1:A:75:ASP:OD2   | 2.53                     | 0.42              |
| 2:C:108:ASP:OD1  | 2:C:108:ASP:N    | 2.53                     | 0.42              |
| 2:C:505:ASN:ND2  | 2:C:536:LEU:O    | 2.53                     | 0.42              |
| 3:E:309:GLY:HA3  | 3:I:302:THR:HG22 | 2.02                     | 0.42              |
| 3:H:260:LEU:HD23 | 3:H:286:ILE:HD13 | 2.02                     | 0.42              |
| 3:I:169:LEU:HD21 | 3:I:259:PHE:HB2  | 2.01                     | 0.42              |
| 3:I:356:TYR:HB2  | 3:I:357:PRO:HD3  | 2.02                     | 0.42              |
| 4:J:98:GLN:NE2   | 4:J:98:GLN:C     | 2.73                     | 0.42              |
| 2:C:63:PRO:CB    | 2:C:191:TYR:CE1  | 3.03                     | 0.41              |
| 2:C:138:LEU:HD21 | 2:C:200:ARG:HG3  | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:318:SER:HB3  | 2:C:324:TYR:CE1  | 2.54                     | 0.41              |
| 7:N:12:MET:O     | 7:N:143:PHE:HB3  | 2.20                     | 0.41              |
| 7:N:168:LEU:HD23 | 7:N:171:ARG:HH22 | 1.85                     | 0.41              |
| 1:A:122:GLN:CD   | 5:K:44:A:N6      | 2.72                     | 0.41              |
| 3:D:45:ARG:NH2   | 7:N:80:LEU:HG    | 2.34                     | 0.41              |
| 3:D:264:LEU:HA   | 3:D:264:LEU:HD23 | 1.80                     | 0.41              |
| 3:D:312:LEU:HD11 | 3:D:344:THR:HG21 | 2.02                     | 0.41              |
| 3:D:315:CYS:SG   | 3:D:341:GLU:OE2  | 2.75                     | 0.41              |
| 4:L:207:ARG:HA   | 4:L:207:ARG:NE   | 2.35                     | 0.41              |
| 7:N:55:LYS:O     | 7:N:56:GLU:HB2   | 2.20                     | 0.41              |
| 2:C:45:ARG:CB    | 2:C:116:PHE:CE2  | 3.03                     | 0.41              |
| 2:C:379:PHE:HE1  | 2:C:390:TRP:CE3  | 2.35                     | 0.41              |
| 7:N:74:HIS:O     | 7:N:103:THR:OG1  | 2.30                     | 0.41              |
| 1:A:8:VAL:CB     | 1:A:63:TYR:HD1   | 2.33                     | 0.41              |
| 2:C:359:THR:N    | 2:C:360:PRO:CD   | 2.83                     | 0.41              |
| 2:C:401:TRP:CH2  | 7:N:195:ARG:HD3  | 2.55                     | 0.41              |
| 3:E:169:LEU:HD21 | 3:E:259:PHE:HB2  | 2.01                     | 0.41              |
| 3:H:55:LEU:HD12  | 3:H:55:LEU:HA    | 1.89                     | 0.41              |
| 3:H:285:HIS:CD2  | 3:H:349:LEU:HB3  | 2.51                     | 0.41              |
| 2:C:48:LEU:HD23  | 2:C:48:LEU:HA    | 1.74                     | 0.41              |
| 3:F:248:ASP:OD1  | 3:F:251:THR:OG1  | 2.35                     | 0.41              |
| 3:I:174:LEU:HD12 | 3:I:174:LEU:HA   | 1.85                     | 0.41              |
| 5:K:3:G:OP2      | 7:N:214:TYR:OH   | 2.27                     | 0.41              |
| 5:K:47:C:C2      | 5:K:48:C:C5      | 3.08                     | 0.41              |
| 4:L:28:ARG:HH22  | 4:L:32:ARG:NH2   | 2.18                     | 0.41              |
| 4:L:191:ASP:HB3  | 4:L:194:ILE:CG1  | 2.50                     | 0.41              |
| 7:N:137:TYR:HB2  | 7:N:143:PHE:O    | 2.20                     | 0.41              |
| 2:C:23:THR:HG21  | 2:C:116:PHE:CD2  | 2.56                     | 0.41              |
| 2:C:106:ARG:HG2  | 2:C:107:LEU:H    | 1.82                     | 0.41              |
| 2:C:413:ALA:O    | 2:C:417:ARG:HB2  | 2.21                     | 0.41              |
| 2:C:530:GLU:OE1  | 4:J:215:GLN:HG2  | 2.20                     | 0.41              |
| 3:D:168:ASN:HD21 | 3:D:245:ASN:CB   | 2.34                     | 0.41              |
| 3:E:260:LEU:HD23 | 3:E:286:ILE:HD13 | 2.02                     | 0.41              |
| 3:G:222:ASN:HD22 | 3:G:222:ASN:HA   | 1.67                     | 0.41              |
| 3:H:50:GLU:HG3   | 3:H:51:VAL:N     | 2.20                     | 0.41              |
| 3:H:96:LYS:HZ2   | 7:N:97:LYS:HZ2   | 1.69                     | 0.41              |
| 3:H:174:LEU:HD12 | 3:H:174:LEU:HA   | 1.85                     | 0.41              |
| 3:I:18:ASN:HD21  | 3:I:26:LYS:CD    | 2.32                     | 0.41              |
| 4:J:37:LEU:HD22  | 4:J:41:ASP:OD2   | 2.21                     | 0.41              |
| 7:N:45:VAL:HG13  | 7:N:49:ASP:HB2   | 2.02                     | 0.41              |
| 3:D:29:VAL:O     | 3:D:29:VAL:HG13  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:223:LEU:N    | 1:A:223:LEU:HD12 | 2.35                     | 0.41              |
| 2:C:155:ARG:NH1  | 2:C:168:HIS:NE2  | 2.63                     | 0.41              |
| 3:D:339:THR:CG2  | 3:D:341:GLU:CD   | 2.94                     | 0.41              |
| 3:D:364:VAL:O    | 3:D:368:PHE:HD1  | 2.04                     | 0.41              |
| 7:N:165:ALA:O    | 7:N:245:TYR:CE2  | 2.71                     | 0.41              |
| 7:N:212:ARG:HH11 | 7:N:212:ARG:HD3  | 1.76                     | 0.41              |
| 1:A:110:PRO:HA   | 1:A:148:TRP:CZ2  | 2.55                     | 0.41              |
| 1:A:138:TRP:CA   | 1:A:144:ALA:CB   | 2.96                     | 0.41              |
| 1:A:149:TRP:O    | 1:A:152:ARG:HB2  | 2.21                     | 0.41              |
| 2:C:205:ARG:HG3  | 2:C:207:GLU:OE1  | 2.21                     | 0.41              |
| 2:C:405:ARG:HH11 | 2:C:405:ARG:HB2  | 1.78                     | 0.41              |
| 2:C:432:ARG:HH21 | 2:C:536:LEU:HA   | 1.85                     | 0.41              |
| 3:E:218:SER:OG   | 6:M:24:DA:N3     | 2.50                     | 0.41              |
| 3:F:356:TYR:HB2  | 3:F:357:PRO:HD3  | 2.02                     | 0.41              |
| 3:G:12:LEU:HD23  | 3:G:12:LEU:HA    | 1.95                     | 0.41              |
| 3:G:42:SER:OG    | 3:G:43:TRP:N     | 2.54                     | 0.41              |
| 3:G:55:LEU:HD23  | 3:G:165:VAL:HG21 | 2.03                     | 0.41              |
| 3:H:356:TYR:HB2  | 3:H:357:PRO:HD3  | 2.02                     | 0.41              |
| 4:J:28:ARG:HG3   | 4:J:29:ALA:N     | 2.35                     | 0.41              |
| 5:K:50:A:N6      | 5:K:58:G:C6      | 2.89                     | 0.41              |
| 4:L:13:LEU:HA    | 4:L:54:TYR:HD2   | 1.85                     | 0.41              |
| 6:M:62:DC:H2"    | 6:M:63:DG:C8     | 2.56                     | 0.41              |
| 2:C:493:TYR:HB2  | 2:C:503:ALA:HB2  | 2.03                     | 0.41              |
| 2:C:519:TYR:HE1  | 3:D:225:GLN:HE22 | 1.67                     | 0.41              |
| 3:D:212:LYS:HE3  | 3:D:212:LYS:HB3  | 1.72                     | 0.41              |
| 3:D:216:HIS:CD2  | 5:K:16:U:HO2'    | 2.38                     | 0.41              |
| 3:F:55:LEU:HD23  | 3:F:165:VAL:HG21 | 2.03                     | 0.41              |
| 3:G:285:HIS:CD2  | 3:G:349:LEU:HB3  | 2.51                     | 0.41              |
| 3:H:96:LYS:NZ    | 7:N:97:LYS:NZ    | 2.69                     | 0.41              |
| 1:A:3:TRP:HZ3    | 1:A:5:THR:HB     | 1.85                     | 0.40              |
| 1:A:101:ARG:HD3  | 1:A:195:VAL:N    | 2.36                     | 0.40              |
| 1:A:164:TYR:N    | 1:A:188:VAL:HG13 | 2.36                     | 0.40              |
| 1:A:166:GLN:CD   | 6:M:23:DG:N7     | 2.78                     | 0.40              |
| 2:C:236:ILE:O    | 2:C:237:PRO:C    | 2.62                     | 0.40              |
| 2:C:257:PRO:HB2  | 2:C:298:TRP:CZ3  | 2.56                     | 0.40              |
| 3:D:326:ARG:CZ   | 3:D:335:ARG:NH2  | 2.84                     | 0.40              |
| 3:D:337:TYR:HA   | 3:D:359:LEU:HD11 | 2.03                     | 0.40              |
| 3:G:259:PHE:CD2  | 3:G:260:LEU:HD12 | 2.56                     | 0.40              |
| 3:G:260:LEU:HD23 | 3:G:286:ILE:HD13 | 2.02                     | 0.40              |
| 4:L:32:ARG:HG3   | 4:L:90:ALA:HB2   | 2.03                     | 0.40              |
| 4:L:91:GLN:HB2   | 4:L:96:ARG:CG    | 2.52                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:38:MET:HE1   | 7:N:149:LEU:HD11 | 2.03                     | 0.40              |
| 2:C:176:LEU:HD11 | 2:C:184:HIS:CD2  | 2.57                     | 0.40              |
| 2:C:277:ARG:HD3  | 2:C:303:ARG:HD3  | 2.02                     | 0.40              |
| 3:F:206:ALA:O    | 3:F:219:GLY:N    | 2.54                     | 0.40              |
| 3:H:42:SER:OG    | 3:H:43:TRP:N     | 2.54                     | 0.40              |
| 3:H:259:PHE:CD2  | 3:H:260:LEU:HD12 | 2.56                     | 0.40              |
| 3:I:59:ALA:HB2   | 3:I:164:ASN:HD22 | 1.87                     | 0.40              |
| 3:I:260:LEU:HD23 | 3:I:286:ILE:HD13 | 2.03                     | 0.40              |
| 6:M:46:DT:H6     | 6:M:46:DT:H2'    | 1.62                     | 0.40              |
| 1:A:137:THR:N    | 1:A:138:TRP:CD1  | 2.89                     | 0.40              |
| 2:C:63:PRO:CB    | 2:C:191:TYR:CD1  | 3.04                     | 0.40              |
| 2:C:303:ARG:HA   | 2:C:303:ARG:HE   | 1.87                     | 0.40              |
| 2:C:340:ALA:C    | 2:C:342:LEU:H    | 2.29                     | 0.40              |
| 2:C:366:GLN:H    | 2:C:366:GLN:CD   | 2.29                     | 0.40              |
| 3:E:289:ARG:NH1  | 3:E:289:ARG:HB2  | 2.35                     | 0.40              |
| 3:G:205:THR:HG23 | 5:K:27:C:H5''    | 2.03                     | 0.40              |
| 3:G:264:LEU:HD23 | 3:G:264:LEU:HA   | 1.83                     | 0.40              |
| 2:C:122:ARG:HG3  | 2:C:122:ARG:NH1  | 2.36                     | 0.40              |
| 2:C:379:PHE:CE2  | 2:C:381:GLN:OE1  | 2.74                     | 0.40              |
| 2:C:433:LEU:HB3  | 2:C:470:MET:HE1  | 2.04                     | 0.40              |
| 3:D:39:SER:HG    | 3:D:41:GLN:CD    | 2.28                     | 0.40              |
| 3:D:225:GLN:C    | 3:D:226:PHE:CD1  | 2.99                     | 0.40              |
| 3:E:14:TYR:CE2   | 3:E:226:PHE:CD2  | 3.09                     | 0.40              |
| 3:F:42:SER:OG    | 3:F:43:TRP:N     | 2.54                     | 0.40              |
| 3:E:9:ILE:O      | 3:E:282:ASP:N    | 2.54                     | 0.40              |
| 3:E:55:LEU:HD23  | 3:E:165:VAL:HG21 | 2.03                     | 0.40              |
| 3:E:86:GLY:O     | 3:E:90:VAL:HG23  | 2.22                     | 0.40              |
| 3:E:278:MET:HE3  | 3:I:292:ARG:NH1  | 2.34                     | 0.40              |
| 3:F:178:PRO:HG3  | 3:H:214:ASN:O    | 2.22                     | 0.40              |
| 3:G:86:GLY:O     | 3:G:90:VAL:HG23  | 2.22                     | 0.40              |
| 3:H:55:LEU:HD23  | 3:H:165:VAL:HG21 | 2.03                     | 0.40              |
| 3:H:268:PRO:O    | 3:H:269:SER:OG   | 2.28                     | 0.40              |
| 5:K:9:C:C2       | 5:K:10:C:C4      | 3.10                     | 0.40              |
| 7:N:43:GLN:HE21  | 7:N:125:ILE:HA   | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 174/232 (75%)   | 152 (87%)  | 13 (8%)  | 9 (5%)   | 1           | 11  |
| 2   | C     | 497/549 (90%)   | 462 (93%)  | 29 (6%)  | 6 (1%)   | 10          | 37  |
| 3   | D     | 256/373 (69%)   | 236 (92%)  | 19 (7%)  | 1 (0%)   | 30          | 60  |
| 3   | E     | 365/373 (98%)   | 352 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 3   | F     | 365/373 (98%)   | 350 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 3   | G     | 364/373 (98%)   | 350 (96%)  | 13 (4%)  | 1 (0%)   | 36          | 65  |
| 3   | H     | 364/373 (98%)   | 349 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 3   | I     | 323/373 (87%)   | 314 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 4   | J     | 167/244 (68%)   | 162 (97%)  | 4 (2%)   | 1 (1%)   | 21          | 52  |
| 4   | L     | 157/244 (64%)   | 152 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 7   | N     | 237/254 (93%)   | 220 (93%)  | 17 (7%)  | 0        | 100         | 100 |
| All | All   | 3269/3761 (87%) | 3099 (95%) | 152 (5%) | 18 (1%)  | 23          | 52  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | ASN  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 106 | ILE  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 186 | PRO  |
| 2   | C     | 363 | GLN  |
| 2   | C     | 364 | VAL  |
| 1   | A     | 105 | ARG  |
| 1   | A     | 181 | ARG  |
| 2   | C     | 85  | PRO  |
| 2   | C     | 124 | ASP  |
| 2   | C     | 308 | GLU  |
| 3   | D     | 217 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 97  | ASP  |
| 1   | A     | 185 | HIS  |
| 2   | C     | 256 | ASP  |
| 1   | A     | 183 | ILE  |
| 3   | G     | 13  | PRO  |

### 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     | 137/193 (71%)   | 127 (93%)  | 10 (7%)  | 13          | 39 |
| 2   | C     | 405/452 (90%)   | 353 (87%)  | 52 (13%) | 4           | 18 |
| 3   | D     | 209/299 (70%)   | 199 (95%)  | 10 (5%)  | 23          | 52 |
| 3   | E     | 294/299 (98%)   | 280 (95%)  | 14 (5%)  | 23          | 52 |
| 3   | F     | 294/299 (98%)   | 286 (97%)  | 8 (3%)   | 39          | 63 |
| 3   | G     | 293/299 (98%)   | 287 (98%)  | 6 (2%)   | 48          | 68 |
| 3   | H     | 293/299 (98%)   | 284 (97%)  | 9 (3%)   | 35          | 60 |
| 3   | I     | 263/299 (88%)   | 254 (97%)  | 9 (3%)   | 32          | 59 |
| 4   | J     | 141/200 (70%)   | 135 (96%)  | 6 (4%)   | 26          | 54 |
| 4   | L     | 134/200 (67%)   | 132 (98%)  | 2 (2%)   | 57          | 72 |
| 7   | N     | 202/211 (96%)   | 182 (90%)  | 20 (10%) | 7           | 27 |
| All | All   | 2665/3050 (87%) | 2519 (94%) | 146 (6%) | 21          | 48 |

All (146) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | LEU  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 105 | ARG  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 123 | ARG  |
| 1   | A     | 137 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 138 | TRP  |
| 1   | A     | 184 | ARG  |
| 1   | A     | 195 | VAL  |
| 1   | A     | 199 | VAL  |
| 2   | C     | 23  | THR  |
| 2   | C     | 24  | ILE  |
| 2   | C     | 51  | SER  |
| 2   | C     | 53  | GLU  |
| 2   | C     | 59  | ILE  |
| 2   | C     | 70  | ARG  |
| 2   | C     | 78  | ARG  |
| 2   | C     | 87  | ASN  |
| 2   | C     | 104 | LYS  |
| 2   | C     | 106 | ARG  |
| 2   | C     | 118 | ASP  |
| 2   | C     | 119 | TYR  |
| 2   | C     | 120 | SER  |
| 2   | C     | 121 | GLU  |
| 2   | C     | 122 | ARG  |
| 2   | C     | 125 | LEU  |
| 2   | C     | 129 | GLU  |
| 2   | C     | 130 | ARG  |
| 2   | C     | 137 | ARG  |
| 2   | C     | 138 | LEU  |
| 2   | C     | 140 | GLU  |
| 2   | C     | 161 | GLN  |
| 2   | C     | 163 | TRP  |
| 2   | C     | 164 | LEU  |
| 2   | C     | 169 | HIS  |
| 2   | C     | 176 | LEU  |
| 2   | C     | 177 | ASP  |
| 2   | C     | 180 | GLU  |
| 2   | C     | 185 | LEU  |
| 2   | C     | 186 | LEU  |
| 2   | C     | 197 | CYS  |
| 2   | C     | 201 | VAL  |
| 2   | C     | 215 | LEU  |
| 2   | C     | 246 | LEU  |
| 2   | C     | 256 | ASP  |
| 2   | C     | 258 | LEU  |
| 2   | C     | 272 | ARG  |
| 2   | C     | 305 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 309 | LEU  |
| 2   | C     | 334 | ILE  |
| 2   | C     | 335 | TRP  |
| 2   | C     | 336 | ARG  |
| 2   | C     | 342 | LEU  |
| 2   | C     | 343 | HIS  |
| 2   | C     | 363 | GLN  |
| 2   | C     | 405 | ARG  |
| 2   | C     | 406 | GLU  |
| 2   | C     | 417 | ARG  |
| 2   | C     | 421 | LEU  |
| 2   | C     | 424 | LYS  |
| 2   | C     | 494 | THR  |
| 2   | C     | 522 | ARG  |
| 3   | D     | 6   | ILE  |
| 3   | D     | 165 | VAL  |
| 3   | D     | 166 | SER  |
| 3   | D     | 169 | LEU  |
| 3   | D     | 172 | ARG  |
| 3   | D     | 188 | PHE  |
| 3   | D     | 193 | THR  |
| 3   | D     | 236 | ASN  |
| 3   | D     | 341 | GLU  |
| 3   | D     | 368 | PHE  |
| 3   | E     | 50  | GLU  |
| 3   | E     | 64  | ARG  |
| 3   | E     | 65  | ILE  |
| 3   | E     | 94  | VAL  |
| 3   | E     | 119 | LEU  |
| 3   | E     | 151 | LEU  |
| 3   | E     | 174 | LEU  |
| 3   | E     | 183 | ASP  |
| 3   | E     | 258 | GLU  |
| 3   | E     | 271 | LYS  |
| 3   | E     | 289 | ARG  |
| 3   | E     | 305 | TYR  |
| 3   | E     | 324 | ARG  |
| 3   | E     | 332 | ASP  |
| 3   | F     | 50  | GLU  |
| 3   | F     | 94  | VAL  |
| 3   | F     | 104 | LYS  |
| 3   | F     | 119 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 151 | LEU  |
| 3   | F     | 183 | ASP  |
| 3   | F     | 212 | LYS  |
| 3   | F     | 332 | ASP  |
| 3   | G     | 50  | GLU  |
| 3   | G     | 94  | VAL  |
| 3   | G     | 119 | LEU  |
| 3   | G     | 151 | LEU  |
| 3   | G     | 183 | ASP  |
| 3   | G     | 332 | ASP  |
| 3   | H     | 50  | GLU  |
| 3   | H     | 94  | VAL  |
| 3   | H     | 119 | LEU  |
| 3   | H     | 151 | LEU  |
| 3   | H     | 183 | ASP  |
| 3   | H     | 208 | ASP  |
| 3   | H     | 210 | ILE  |
| 3   | H     | 248 | ASP  |
| 3   | H     | 332 | ASP  |
| 3   | I     | 11  | THR  |
| 3   | I     | 12  | LEU  |
| 3   | I     | 15  | SER  |
| 3   | I     | 50  | GLU  |
| 3   | I     | 94  | VAL  |
| 3   | I     | 119 | LEU  |
| 3   | I     | 151 | LEU  |
| 3   | I     | 183 | ASP  |
| 3   | I     | 332 | ASP  |
| 4   | J     | 37  | LEU  |
| 4   | J     | 45  | LEU  |
| 4   | J     | 93  | ARG  |
| 4   | J     | 98  | GLN  |
| 4   | J     | 136 | ARG  |
| 4   | J     | 229 | GLU  |
| 4   | L     | 45  | LEU  |
| 4   | L     | 197 | ARG  |
| 7   | N     | 6   | LEU  |
| 7   | N     | 7   | ARG  |
| 7   | N     | 13  | GLN  |
| 7   | N     | 18  | HIS  |
| 7   | N     | 29  | TYR  |
| 7   | N     | 47  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | N     | 53  | ARG  |
| 7   | N     | 65  | ARG  |
| 7   | N     | 68  | VAL  |
| 7   | N     | 69  | ARG  |
| 7   | N     | 93  | ARG  |
| 7   | N     | 138 | LEU  |
| 7   | N     | 168 | LEU  |
| 7   | N     | 171 | ARG  |
| 7   | N     | 172 | ARG  |
| 7   | N     | 200 | LEU  |
| 7   | N     | 203 | VAL  |
| 7   | N     | 230 | LEU  |
| 7   | N     | 231 | VAL  |
| 7   | N     | 242 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | HIS  |
| 1   | A     | 69  | HIS  |
| 1   | A     | 150 | HIS  |
| 1   | A     | 166 | GLN  |
| 2   | C     | 161 | GLN  |
| 2   | C     | 168 | HIS  |
| 2   | C     | 174 | HIS  |
| 2   | C     | 184 | HIS  |
| 2   | C     | 316 | GLN  |
| 2   | C     | 343 | HIS  |
| 2   | C     | 381 | GLN  |
| 3   | D     | 7   | HIS  |
| 3   | D     | 190 | HIS  |
| 3   | D     | 236 | ASN  |
| 3   | D     | 273 | ASN  |
| 3   | E     | 16  | ASN  |
| 3   | E     | 18  | ASN  |
| 3   | E     | 89  | GLN  |
| 3   | E     | 195 | HIS  |
| 3   | E     | 216 | HIS  |
| 3   | F     | 18  | ASN  |
| 3   | F     | 89  | GLN  |
| 3   | F     | 195 | HIS  |
| 3   | G     | 16  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 18  | ASN  |
| 3   | G     | 89  | GLN  |
| 3   | G     | 134 | HIS  |
| 3   | G     | 195 | HIS  |
| 3   | G     | 273 | ASN  |
| 3   | H     | 18  | ASN  |
| 3   | H     | 89  | GLN  |
| 3   | H     | 134 | HIS  |
| 3   | H     | 195 | HIS  |
| 3   | H     | 220 | HIS  |
| 3   | H     | 273 | ASN  |
| 3   | I     | 16  | ASN  |
| 3   | I     | 18  | ASN  |
| 3   | I     | 89  | GLN  |
| 3   | I     | 134 | HIS  |
| 3   | I     | 195 | HIS  |
| 4   | J     | 175 | HIS  |
| 4   | J     | 204 | HIS  |
| 4   | L     | 48  | HIS  |
| 4   | L     | 173 | HIS  |
| 4   | L     | 175 | HIS  |
| 4   | L     | 208 | HIS  |
| 4   | L     | 215 | GLN  |
| 4   | L     | 218 | HIS  |
| 7   | N     | 135 | GLN  |
| 7   | N     | 239 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 5   | K     | 57/61 (93%) | 27 (47%)          | 1 (1%)          |

All (27) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | K     | 4   | G    |
| 5   | K     | 7   | C    |
| 5   | K     | 8   | G    |
| 5   | K     | 9   | C    |
| 5   | K     | 10  | C    |
| 5   | K     | 11  | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | K     | 15  | A    |
| 5   | K     | 21  | G    |
| 5   | K     | 22  | G    |
| 5   | K     | 27  | C    |
| 5   | K     | 31  | G    |
| 5   | K     | 32  | U    |
| 5   | K     | 33  | G    |
| 5   | K     | 34  | G    |
| 5   | K     | 35  | G    |
| 5   | K     | 36  | C    |
| 5   | K     | 37  | U    |
| 5   | K     | 39  | U    |
| 5   | K     | 40  | C    |
| 5   | K     | 44  | A    |
| 5   | K     | 45  | G    |
| 5   | K     | 46  | C    |
| 5   | K     | 54  | A    |
| 5   | K     | 55  | C    |
| 5   | K     | 56  | G    |
| 5   | K     | 60  | G    |
| 5   | K     | 61  | G    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | K     | 44  | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

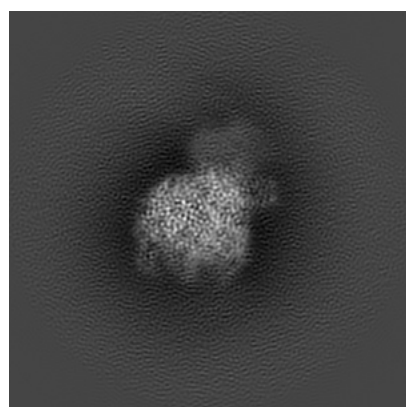
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8478. These allow visual inspection of the internal detail of the map and identification of artifacts.

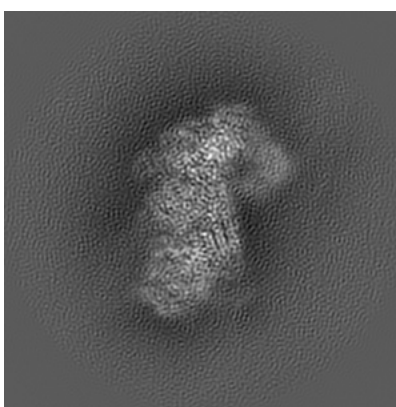
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

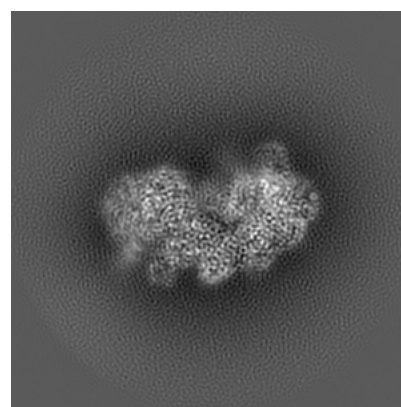
#### 6.1.1 Primary map



X



Y

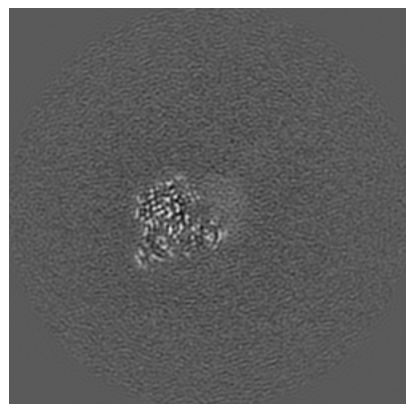


Z

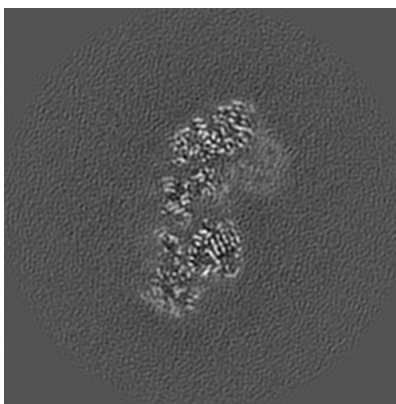
The images above show the map projected in three orthogonal directions.

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

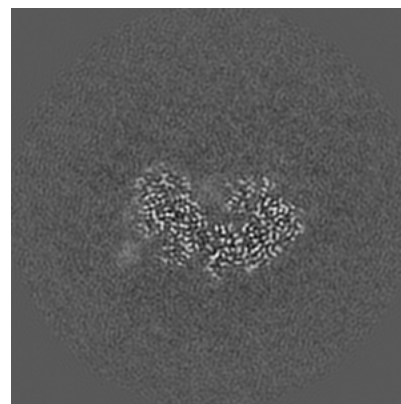
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

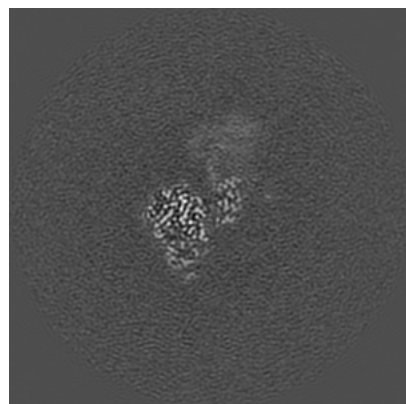


Z Index: 128

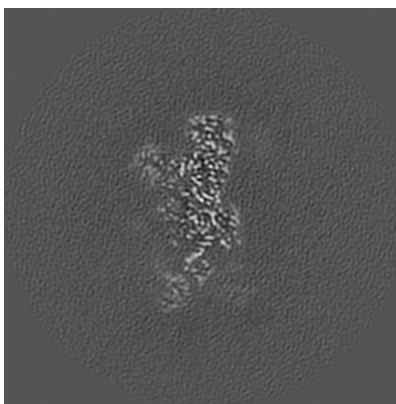
The images above show central slices of the map in three orthogonal directions.

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

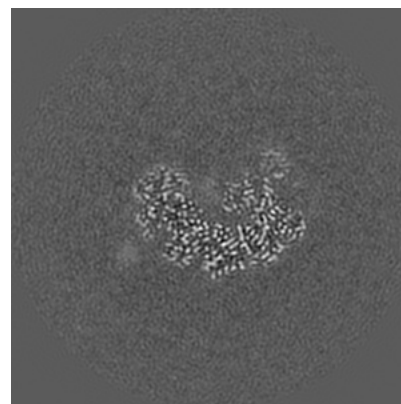
### 6.3.1 Primary map



X Index: 154



Y Index: 112

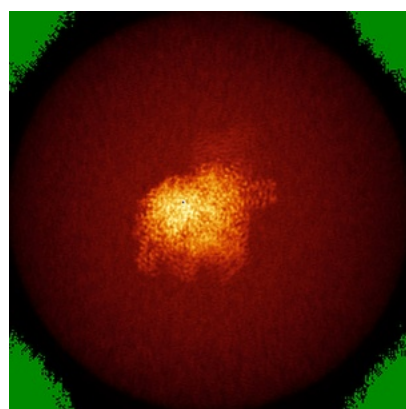


Z Index: 131

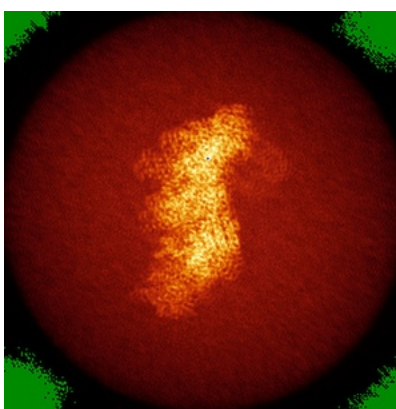
The images above show the largest variance slices of the map in three orthogonal directions.

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

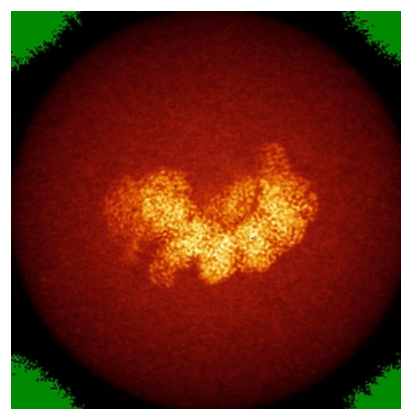
### 6.4.1 Primary map



X



Y

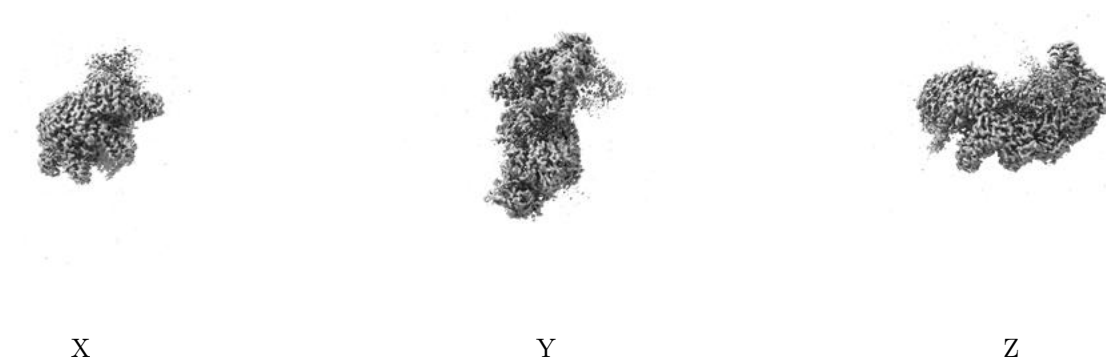


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

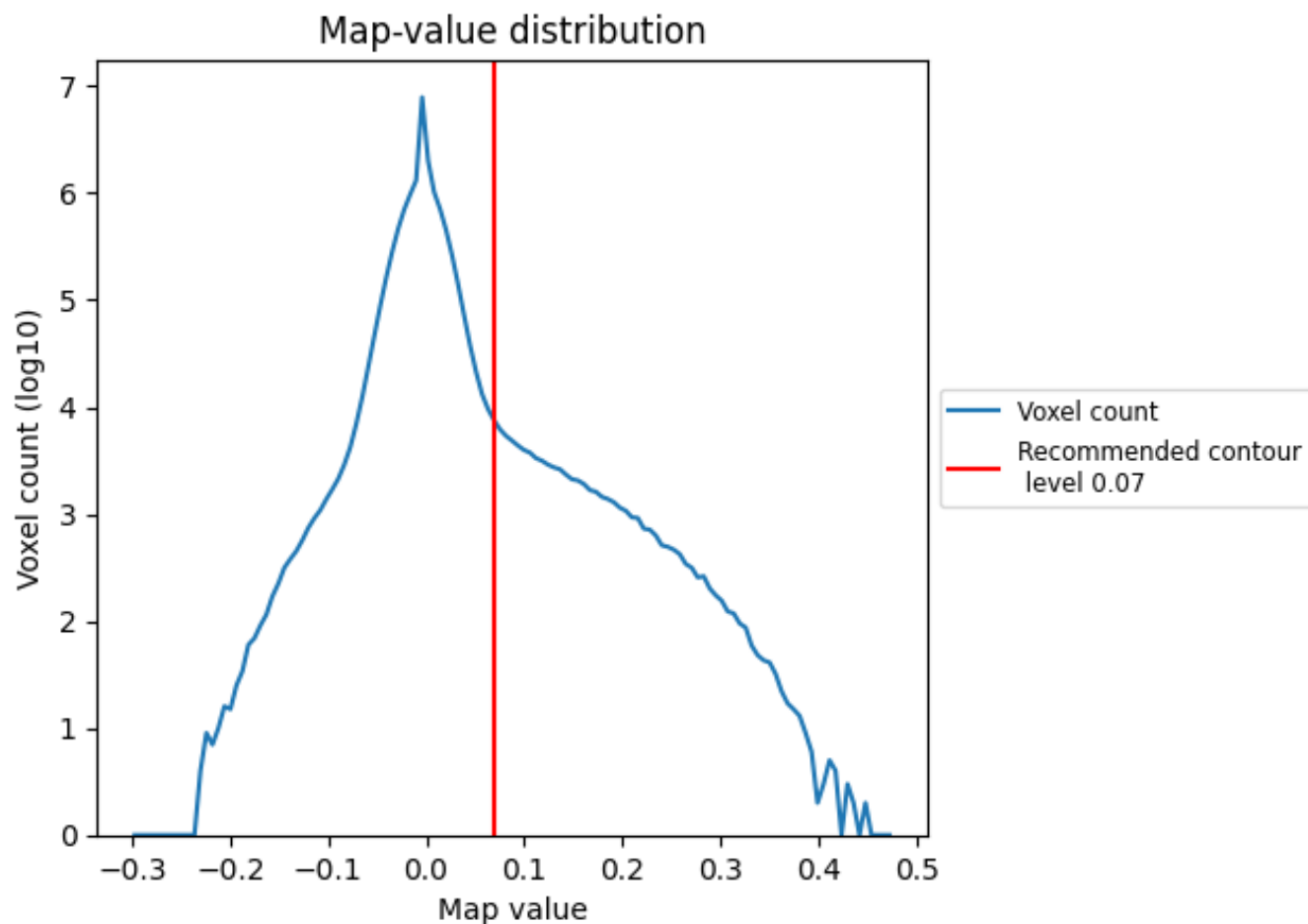
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

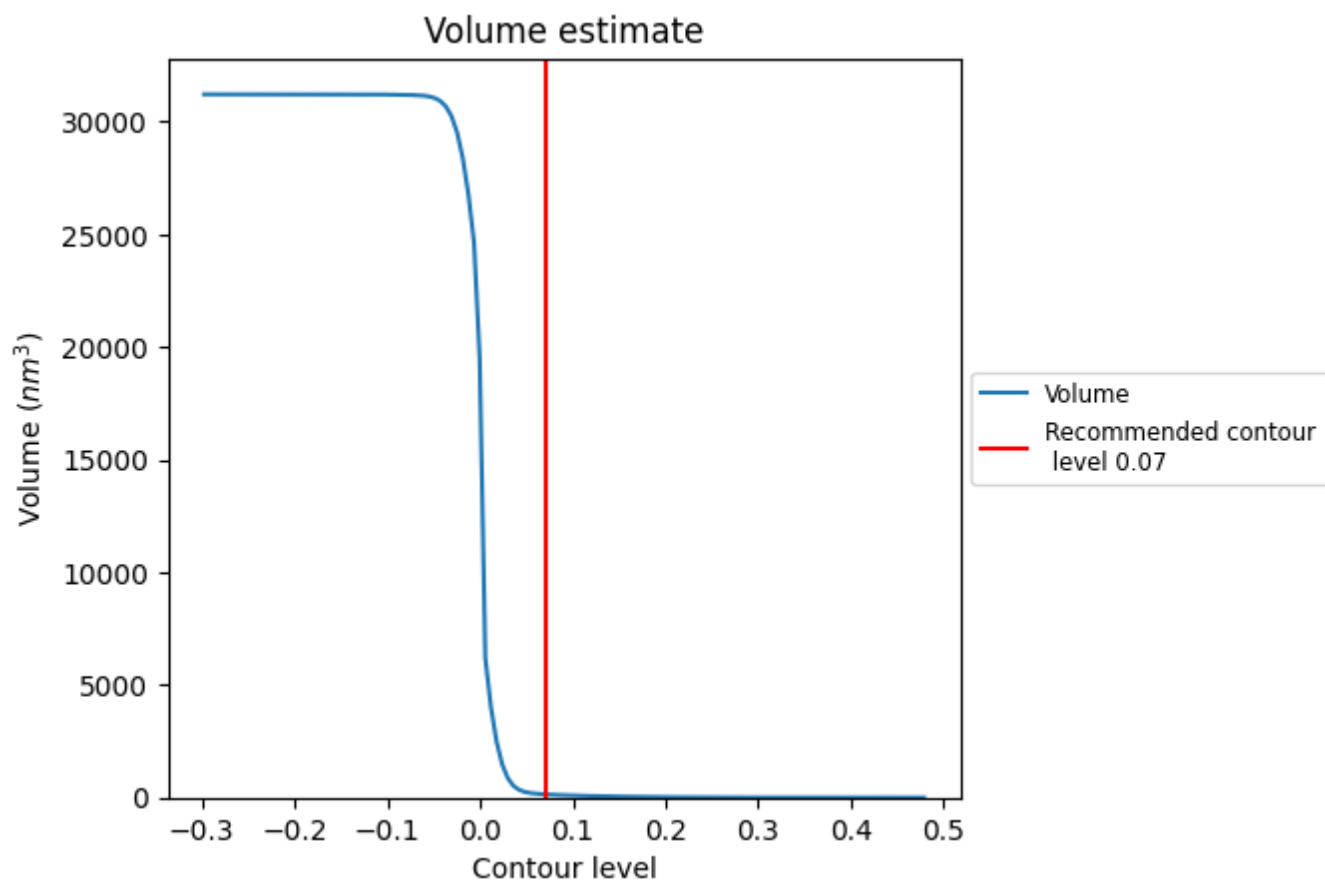
This section contains the results of statistical analysis of the map.

### 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.

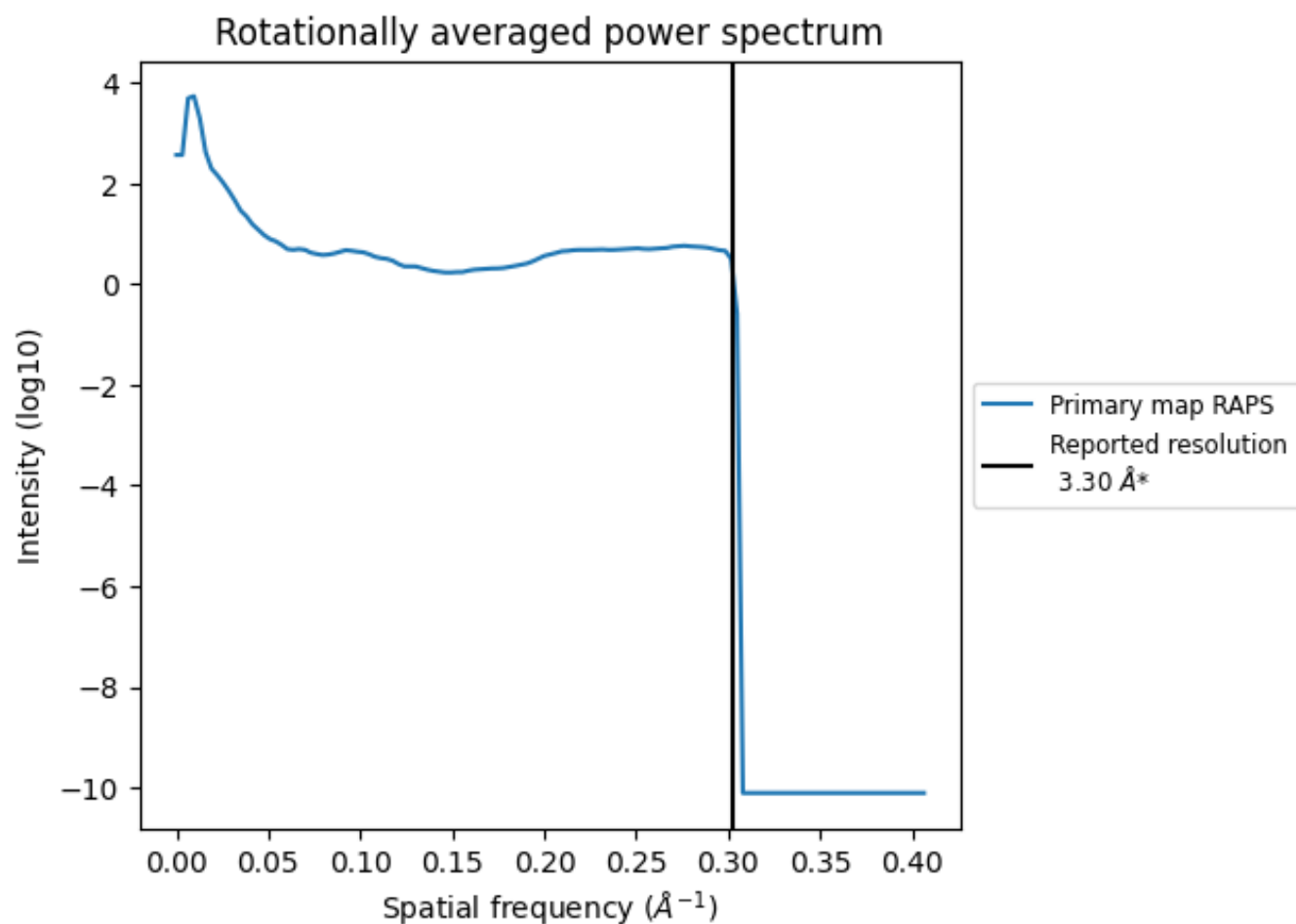
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm<sup>3</sup>; this corresponds to an approximate mass of 128 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 0.303  $\text{\AA}^{-1}$

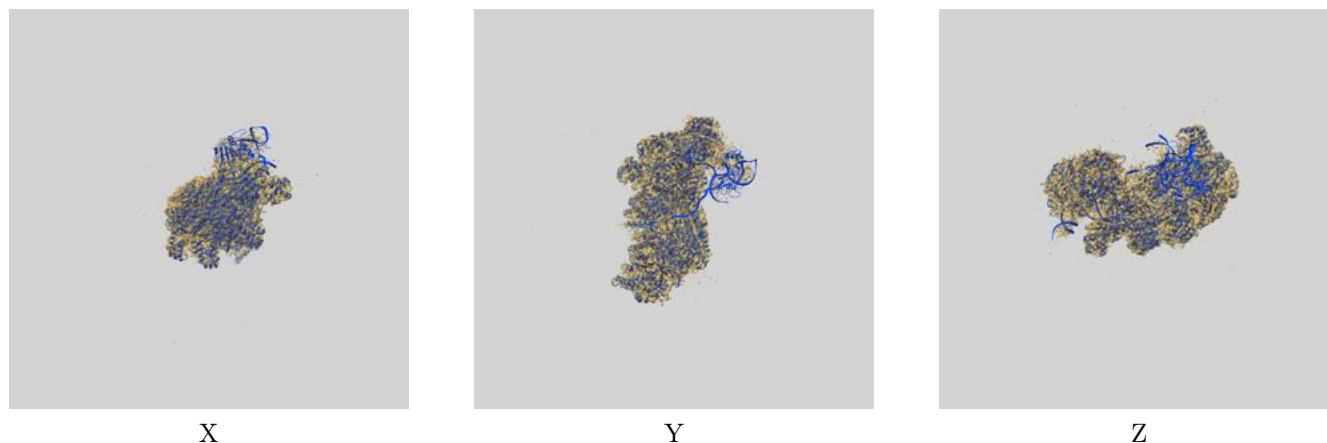
## 8 Fourier-Shell correlation ⓘ

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

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

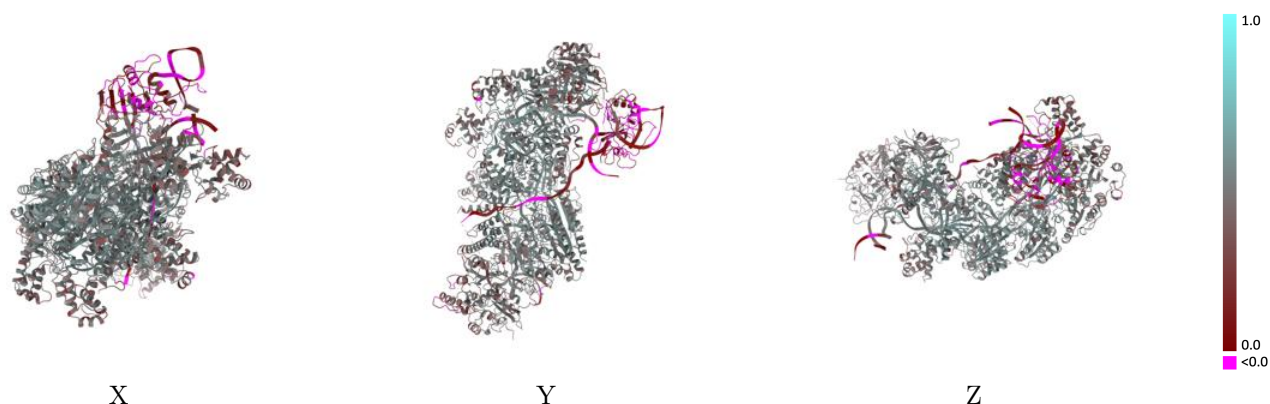
This section contains information regarding the fit between EMDB map EMD-8478 and PDB model 5U0A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



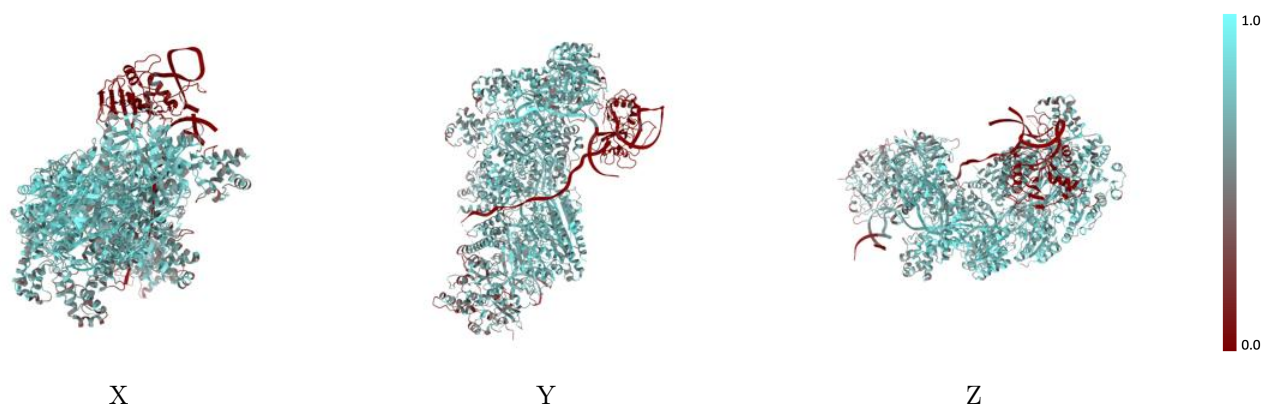
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



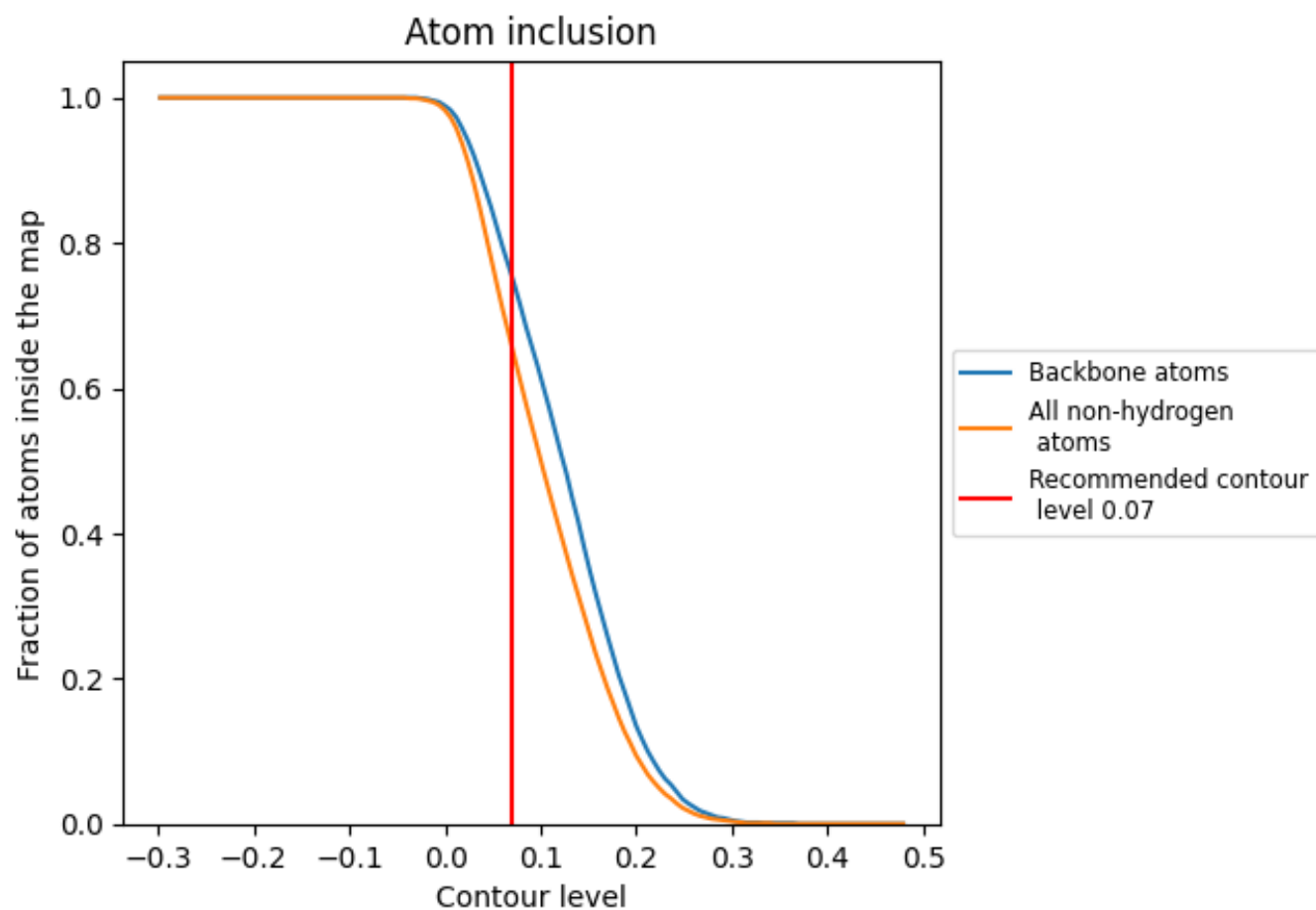
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| All   |  0.6560  |  0.4430  |
| A     |  0.0330  |  0.0730  |
| C     |  0.5750  |  0.4370  |
| D     |  0.7400  |  0.5000  |
| E     |  0.7430  |  0.4850  |
| F     |  0.7370  |  0.4890  |
| G     |  0.7610  |  0.5090  |
| H     |  0.7490  |  0.4860  |
| I     |  0.6810  |  0.4290  |
| J     |  0.7300  |  0.4980  |
| K     |  0.6310  |  0.4000  |
| L     |  0.6820  |  0.4850  |
| M     |  0.6910  |  0.4310  |
| N     |  0.7310  |  0.4870  |
| O     |  0.1900 |  0.1390 |

