



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 10:45 AM UTC

PDB ID : 6PSU / pdb\_00006psu  
EMDB ID : EMD-20464  
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi2)  
with TraR and rpsT P2 promoter  
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2019-07-13  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

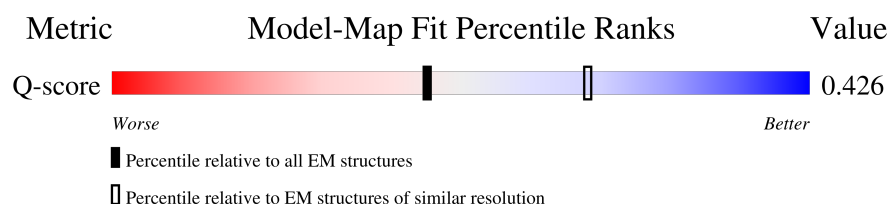
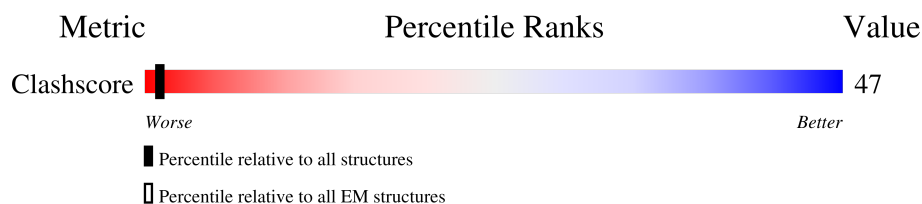
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

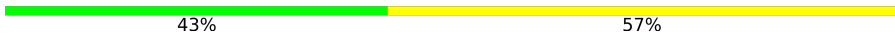
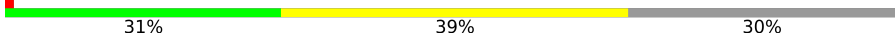
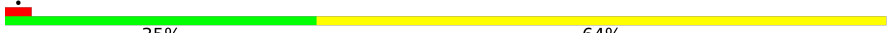
The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric     | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore | 229148                      | 23984                       | -                                                        |
| Q-score    | -                           | 25397                       | 8855 ( 3.40 - 4.40 )                                     |

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   | N     | 72     |  43% 57%        |
| 2   | G     | 329    |  31% 39% 30%    |
| 2   | H     | 329    |  23% 43% 34%    |
| 2   | M     | 329    |  9% 13% 22% 78% |
| 3   | I     | 1342   |  35% 64%        |
| 4   | J     | 1430   |  6% 34% 60% 6%  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 5   | K     | 91     | <div><div><div></div><div></div><div></div></div><div>27%52%21%</div></div>    |
| 6   | L     | 616    | <div><div><div></div><div></div><div></div></div><div>12%25%61%14%</div></div> |
| 7   | O     | 85     | <div><div><div></div><div></div><div></div></div><div>11%46%51%</div></div>    |
| 8   | P     | 85     | <div><div><div></div><div></div><div></div></div><div>13%7%36%56%</div></div>  |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32323 atoms, of which 156 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 Protein TraR.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | N     | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 571   | 353 | 105 | 108 | 5 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | G     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1775  | 1108 | 314 | 347 | 6 |         |       |
| 2   | H     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1043 | 293 | 326 | 6 |         |       |
| 2   | M     | 73       | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 572   | 362  | 100 | 108 | 2 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | I     | 1340     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10567 | 6631 | 1841 | 2052 | 43 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | J     | 1344     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10433 | 6556 | 1856 | 1971 | 50 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 1       | VAL      | -      | expression tag | UNP P0A8T7 |
| J     | 1408    | LEU      | -      | expression tag | UNP P0A8T7 |
| J     | 1409    | GLU      | -      | expression tag | UNP P0A8T7 |
| J     | 1410    | LEU      | -      | expression tag | UNP P0A8T7 |
| J     | 1411    | GLU      | -      | expression tag | UNP P0A8T7 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 1412    | VAL      | -      | expression tag | UNP P0A8T7 |
| J     | 1413    | LEU      | -      | expression tag | UNP P0A8T7 |
| J     | 1414    | PHE      | -      | expression tag | UNP P0A8T7 |
| J     | 1415    | GLN      | -      | expression tag | UNP P0A8T7 |
| J     | 1416    | GLY      | -      | expression tag | UNP P0A8T7 |
| J     | 1417    | PRO      | -      | expression tag | UNP P0A8T7 |
| J     | 1418    | SER      | -      | expression tag | UNP P0A8T7 |
| J     | 1419    | SER      | -      | expression tag | UNP P0A8T7 |
| J     | 1420    | GLY      | -      | expression tag | UNP P0A8T7 |
| J     | 1421    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1422    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1423    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1424    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1425    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1426    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1427    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1428    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1429    | HIS      | -      | expression tag | UNP P0A8T7 |
| J     | 1430    | HIS      | -      | expression tag | UNP P0A8T7 |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | K     | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 577   | 352 | 110 | 114 | 1 |         |       |

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | L     | 529      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4277  | 2677 | 753 | 821 | 26 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | -2      | SER      | -      | expression tag | UNP Q0P6L9 |
| L     | -1      | GLU      | -      | expression tag | UNP Q0P6L9 |
| L     | 0       | PHE      | -      | expression tag | UNP Q0P6L9 |

- Molecule 7 is a DNA chain called DNA (85-MER).



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 10  | L     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 66    | 24 | 39 | 3 |         |

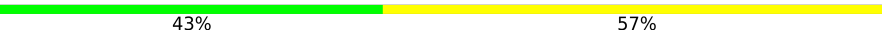
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 11  | J     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

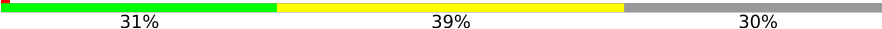
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

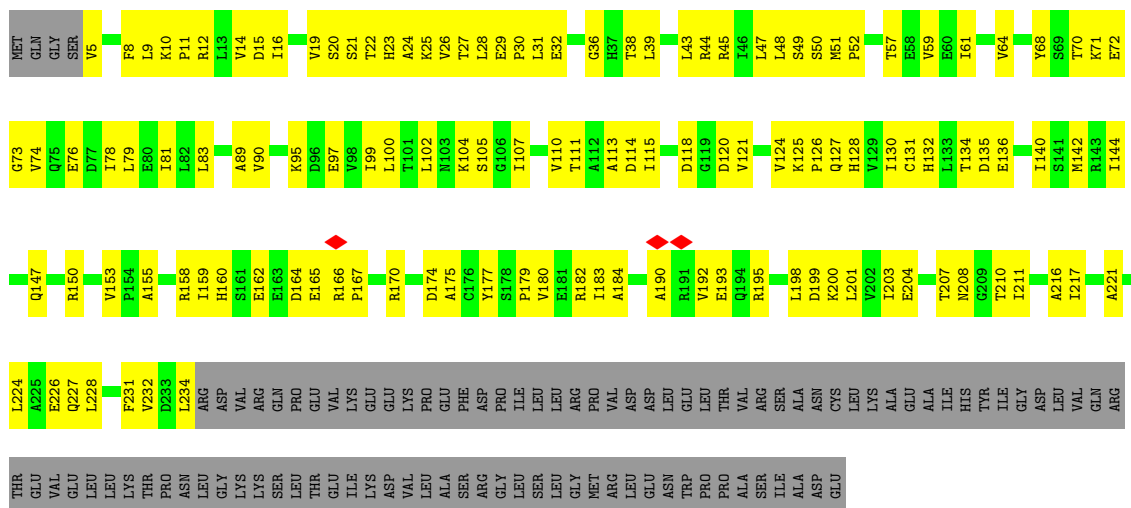
#### • Molecule 1: Protein TraR

Chain N: 

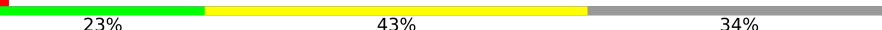


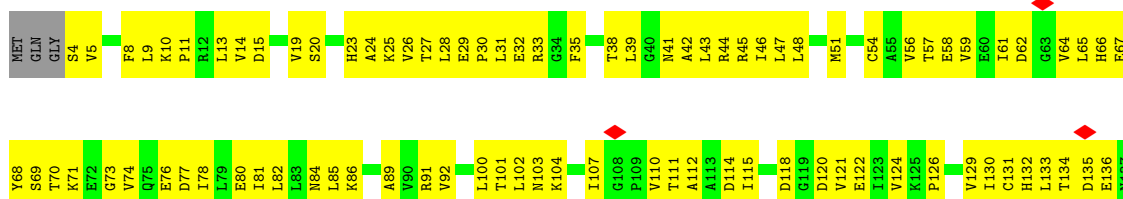
#### • Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain G: 

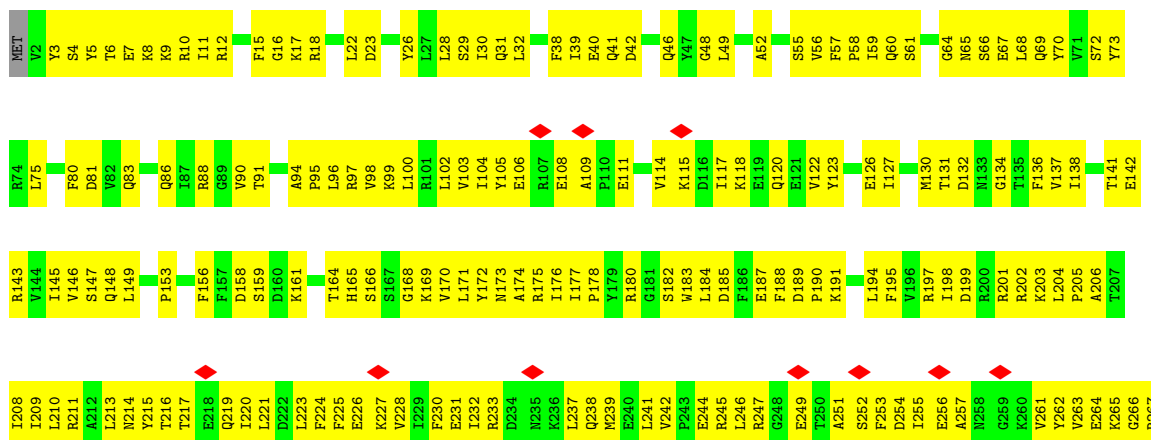
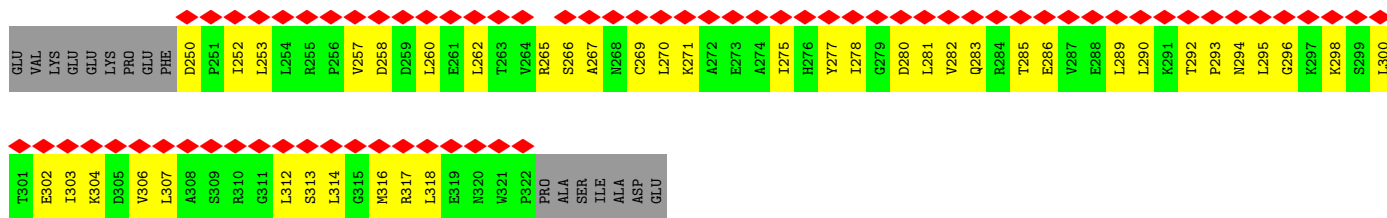


#### • Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain H: 



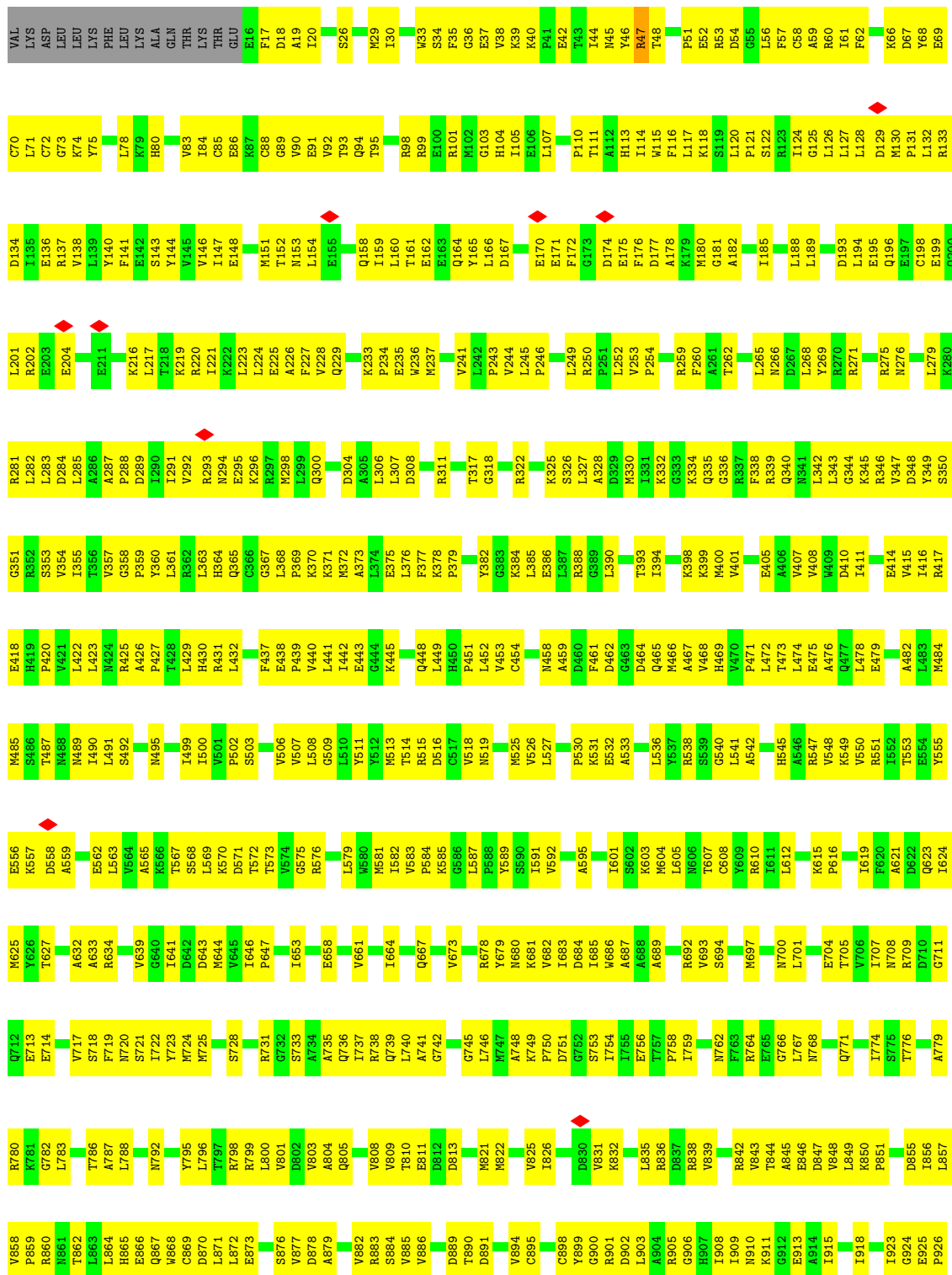




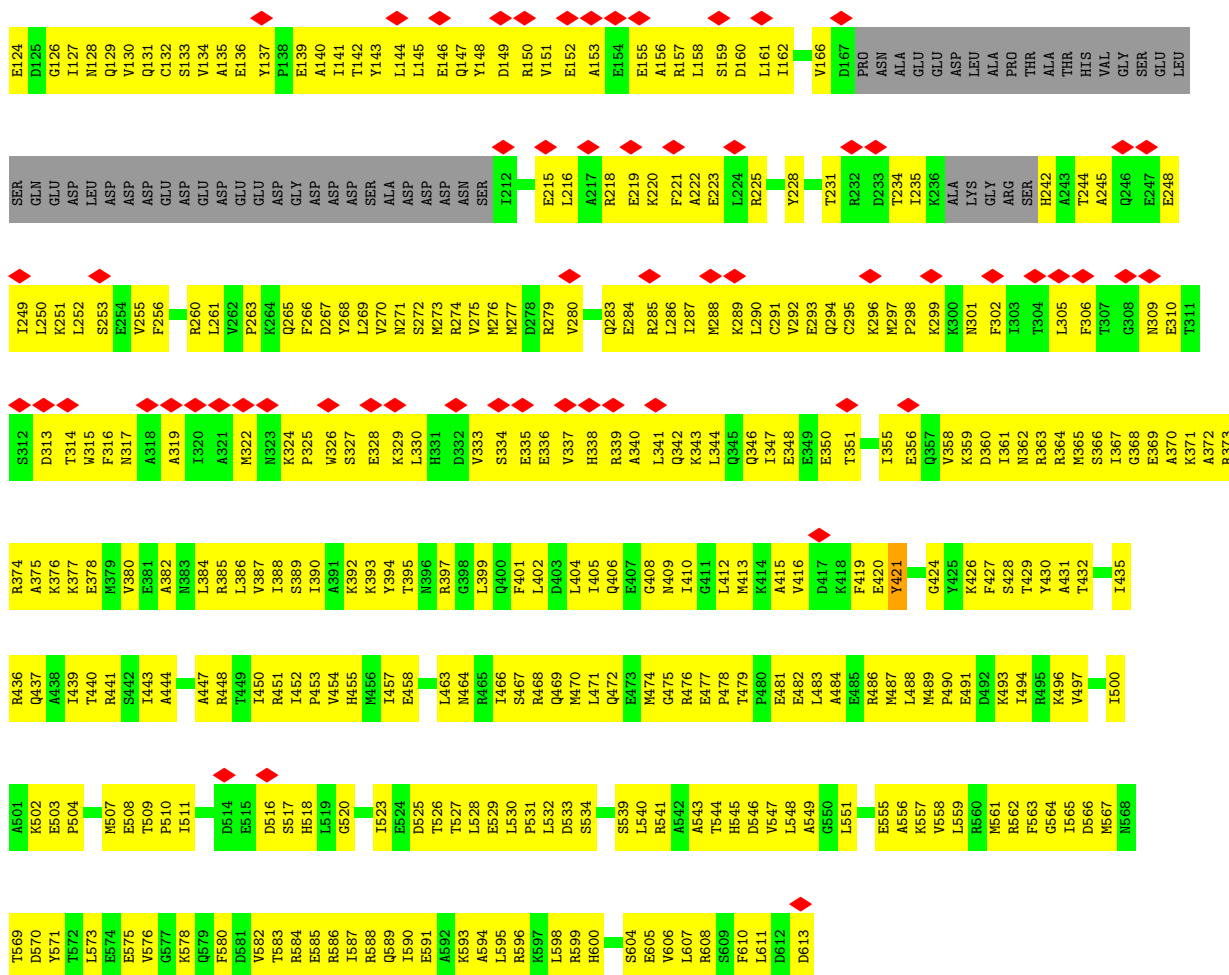




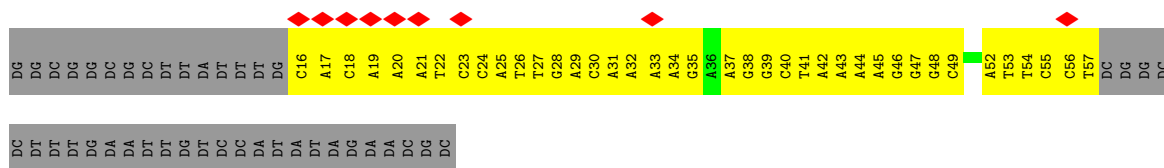
● Molecule 4: DNA-directed RNA polymerase subunit beta'



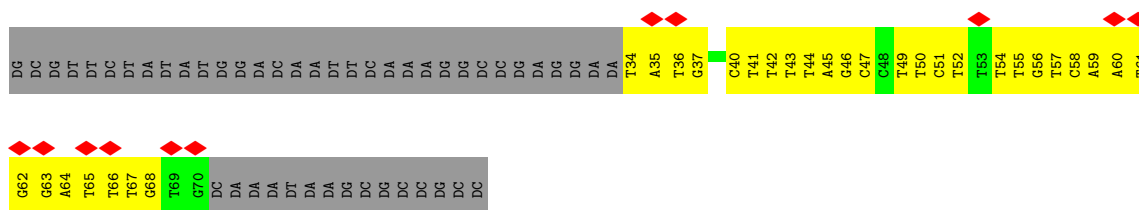




- Molecule 7: DNA (85-MER)



- Molecule 8: DNA (85-MER)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 46553                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 80                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.150                                   | Depositor |
| Minimum map value                    | -0.097                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 332.8, 332.8, 332.8                     | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.3, 1.3, 1.3                           | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, ZN

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   | N     | 0.30         | 0/581   | 0.53        | 0/785          |
| 2   | G     | 0.36         | 0/1797  | 0.54        | 0/2437         |
| 2   | H     | 0.33         | 0/1687  | 0.62        | 1/2287 (0.0%)  |
| 2   | M     | 0.19         | 0/579   | 0.52        | 0/784          |
| 3   | I     | 0.39         | 0/10736 | 0.59        | 5/14487 (0.0%) |
| 4   | J     | 0.37         | 0/10592 | 0.57        | 0/14308        |
| 5   | K     | 0.28         | 0/579   | 0.51        | 0/779          |
| 6   | L     | 0.23         | 0/4329  | 0.51        | 1/5820 (0.0%)  |
| 7   | O     | 0.25         | 0/971   | 0.43        | 0/1495         |
| 8   | P     | 0.25         | 0/837   | 0.47        | 0/1290         |
| All | All   | 0.35         | 0/32688 | 0.56        | 7/44472 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | I     | 0                   | 4                   |
| 4   | J     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | I     | 1167 | GLU  | N-CA-C | 7.51  | 126.79      | 110.80   |
| 2   | H     | 14   | VAL  | N-CA-C | -5.84 | 107.60      | 113.20   |
| 3   | I     | 1166 | ASP  | CA-C-N | 5.74  | 132.50      | 121.54   |
| 3   | I     | 1166 | ASP  | C-N-CA | 5.74  | 132.50      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | I     | 516  | ASP  | N-CA-C | -5.38 | 99.75       | 108.41   |
| 3   | I     | 1156 | ARG  | CA-C-O | -5.24 | 114.18      | 120.10   |
| 6   | L     | 421  | TYR  | N-CA-C | -5.05 | 106.90      | 113.16   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 3   | I     | 1165 | SER  | Peptide |
| 3   | I     | 1166 | ASP  | Peptide |
| 3   | I     | 1240 | ASP  | Peptide |
| 3   | I     | 247  | ARG  | Peptide |
| 4   | J     | 47   | ARG  | Peptide |

## 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   | N     | 571   | 0        | 556      | 52      | 0            |
| 2   | G     | 1775  | 0        | 1803     | 133     | 0            |
| 2   | H     | 1668  | 0        | 1702     | 185     | 0            |
| 2   | M     | 572   | 0        | 602      | 61      | 0            |
| 3   | I     | 10567 | 0        | 10585    | 1051    | 0            |
| 4   | J     | 10433 | 0        | 10625    | 1045    | 0            |
| 5   | K     | 577   | 0        | 588      | 54      | 0            |
| 6   | L     | 4277  | 0        | 4325     | 546     | 0            |
| 7   | O     | 863   | 0        | 471      | 74      | 0            |
| 8   | P     | 752   | 0        | 426      | 74      | 0            |
| 9   | J     | 2     | 0        | 0        | 0       | 0            |
| 9   | N     | 1     | 0        | 0        | 0       | 0            |
| 10  | I     | 27    | 39       | 39       | 7       | 0            |
| 10  | J     | 27    | 39       | 38       | 4       | 0            |
| 10  | L     | 27    | 39       | 37       | 3       | 0            |
| 10  | N     | 27    | 39       | 38       | 4       | 0            |
| 11  | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 32167 | 156      | 31835    | 3030    | 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 47.

All (3030) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:701:1N7:C19  | 10:L:701:1N7:C3   | 1.83                     | 1.57              |
| 10:N:102:1N7:C19  | 10:N:102:1N7:C3   | 1.83                     | 1.51              |
| 10:I:1401:1N7:C3  | 10:I:1401:1N7:C19 | 1.82                     | 1.51              |
| 10:J:1504:1N7:C19 | 10:J:1504:1N7:C3  | 1.83                     | 1.50              |
| 6:L:284:GLU:HA    | 6:L:287:ILE:HB    | 1.36                     | 1.07              |
| 4:J:1167:LYS:HB3  | 4:J:1174:ARG:HD3  | 1.36                     | 1.06              |
| 3:I:1164:PHE:HB3  | 3:I:1165:SER:HB2  | 1.42                     | 1.02              |
| 3:I:1258:PRO:HG2  | 4:J:346:ARG:HB2   | 1.40                     | 1.01              |
| 2:G:61:ILE:HG22   | 2:G:142:MET:HB3   | 1.43                     | 1.01              |
| 4:J:937:ILE:HD11  | 4:J:1134:ILE:HG12 | 1.41                     | 1.01              |
| 6:L:385:ARG:HD2   | 7:O:55:DC:H5'     | 1.39                     | 1.01              |
| 3:I:839:VAL:HA    | 3:I:1049:ILE:HG22 | 1.42                     | 1.01              |
| 6:L:313:ASP:HB3   | 6:L:317:ASN:HB2   | 1.42                     | 1.01              |
| 6:L:567:MET:HG3   | 6:L:569:THR:HB    | 1.42                     | 1.00              |
| 6:L:248:GLU:HA    | 6:L:251:LYS:HE3   | 1.41                     | 1.00              |
| 4:J:937:ILE:O     | 4:J:1133:ASP:OD1  | 1.81                     | 0.99              |
| 3:I:221:LEU:HD23  | 3:I:336:LEU:HD11  | 1.45                     | 0.99              |
| 4:J:964:LYS:HB3   | 4:J:977:SER:HB3   | 1.42                     | 0.99              |
| 4:J:1105:ALA:HA   | 4:J:1124:ILE:HG12 | 1.43                     | 0.98              |
| 6:L:48:ILE:HG23   | 6:L:55:VAL:HG11   | 1.44                     | 0.98              |
| 2:G:45:ARG:HD2    | 2:H:38:THR:HB     | 1.44                     | 0.98              |
| 2:H:28:LEU:HD23   | 2:H:31:LEU:HD21   | 1.45                     | 0.98              |
| 3:I:685:MET:HG3   | 3:I:1235:LEU:HD11 | 1.45                     | 0.98              |
| 4:J:937:ILE:HG12  | 4:J:1134:ILE:O    | 1.61                     | 0.98              |
| 4:J:557:LYS:HB2   | 4:J:563:LEU:HD23  | 1.46                     | 0.97              |
| 3:I:727:VAL:HG23  | 3:I:732:ILE:HG12  | 1.44                     | 0.97              |
| 3:I:998:LEU:HD13  | 3:I:1015:ALA:HA   | 1.47                     | 0.97              |
| 4:J:937:ILE:C     | 4:J:1133:ASP:OD1  | 2.07                     | 0.96              |
| 6:L:126:GLY:HA3   | 6:L:372:ALA:HB2   | 1.47                     | 0.96              |
| 6:L:134:VAL:HG22  | 6:L:273:MET:HE1   | 1.45                     | 0.96              |
| 6:L:161:LEU:HD23  | 6:L:162:ILE:HG23  | 1.48                     | 0.95              |
| 3:I:732:ILE:HD11  | 3:I:769:PRO:HB3   | 1.45                     | 0.95              |
| 3:I:317:LEU:HB2   | 3:I:321:LEU:HB2   | 1.49                     | 0.95              |
| 3:I:750:ILE:HG21  | 3:I:966:ILE:HD12  | 1.49                     | 0.94              |
| 2:H:59:VAL:HG22   | 2:H:144:ILE:HG13  | 1.48                     | 0.94              |
| 4:J:369:PRO:HG2   | 4:J:372:MET:HB2   | 1.46                     | 0.94              |
| 6:L:444:ALA:HB1   | 6:L:457:ILE:HD13  | 1.50                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:937:ILE:HD11  | 4:J:1134:ILE:CG1  | 1.98                     | 0.94              |
| 4:J:51:PRO:HD2    | 4:J:71:LEU:HD21   | 1.50                     | 0.94              |
| 3:I:59:ILE:HG23   | 3:I:476:LYS:HE2   | 1.48                     | 0.93              |
| 4:J:425:ARG:HG2   | 4:J:427:PRO:HD2   | 1.46                     | 0.93              |
| 4:J:1026:PRO:HA   | 4:J:1123:ARG:HA   | 1.48                     | 0.93              |
| 4:J:1060:VAL:HG22 | 4:J:1107:VAL:H    | 1.31                     | 0.93              |
| 4:J:26:SER:HB3    | 4:J:29:MET:HG3    | 1.48                     | 0.93              |
| 3:I:321:LEU:HA    | 3:I:324:LYS:HG2   | 1.50                     | 0.92              |
| 3:I:463:GLN:HG2   | 3:I:505:PHE:HB2   | 1.48                     | 0.92              |
| 4:J:72:CYS:HB3    | 4:J:88:CYS:HB3    | 1.49                     | 0.92              |
| 4:J:1089:LEU:HA   | 4:J:1096:PRO:HA   | 1.52                     | 0.92              |
| 4:J:1179:PRO:HD3  | 4:J:1184:ASP:HB3  | 1.52                     | 0.92              |
| 6:L:336:GLU:HA    | 6:L:339:ARG:HD3   | 1.51                     | 0.91              |
| 4:J:1079:LYS:HD2  | 4:J:1087:ASP:HB3  | 1.52                     | 0.91              |
| 4:J:1314:LEU:HB3  | 4:J:1326:GLN:HE22 | 1.33                     | 0.91              |
| 1:N:46:GLU:HA     | 1:N:49:ARG:HG3    | 1.50                     | 0.91              |
| 6:L:277:MET:HE1   | 6:L:359:LYS:HG2   | 1.54                     | 0.90              |
| 4:J:1144:LEU:HD11 | 4:J:1236:GLU:HG3  | 1.51                     | 0.90              |
| 4:J:975:ILE:HD12  | 4:J:980:THR:HG21  | 1.54                     | 0.90              |
| 4:J:1036:ARG:HG3  | 4:J:1081:VAL:HG21 | 1.54                     | 0.90              |
| 4:J:114:ILE:HD11  | 4:J:311:ARG:HB2   | 1.53                     | 0.89              |
| 6:L:76:ALA:HA     | 6:L:79:ALA:HB3    | 1.54                     | 0.88              |
| 6:L:135:ALA:HA    | 6:L:141:ILE:HD11  | 1.54                     | 0.88              |
| 4:J:519:ASN:HB2   | 4:J:709:ARG:HB2   | 1.56                     | 0.88              |
| 4:J:969:SER:HB2   | 4:J:1119:ASP:HA   | 1.56                     | 0.88              |
| 3:I:1319:MET:HE1  | 4:J:1353:VAL:HG13 | 1.53                     | 0.88              |
| 4:J:1172:LYS:HD3  | 4:J:1189:MET:HB3  | 1.56                     | 0.88              |
| 4:J:1067:ARG:HD3  | 4:J:1072:LYS:HG3  | 1.55                     | 0.88              |
| 3:I:237:LEU:HD11  | 3:I:322:LEU:HD21  | 1.52                     | 0.87              |
| 4:J:950:ILE:HD12  | 4:J:982:LEU:HD22  | 1.56                     | 0.87              |
| 4:J:1026:PRO:HB3  | 4:J:1123:ARG:HG2  | 1.55                     | 0.87              |
| 6:L:151:VAL:HG22  | 6:L:156:ALA:HB3   | 1.54                     | 0.87              |
| 4:J:140:TYR:HB3   | 6:L:100:MET:HE1   | 1.56                     | 0.87              |
| 4:J:1029:THR:HA   | 4:J:1099:TYR:HE2  | 1.39                     | 0.87              |
| 4:J:1050:THR:HA   | 4:J:1057:SER:HA   | 1.57                     | 0.87              |
| 2:H:133:LEU:HD21  | 2:H:138:ALA:HB3   | 1.56                     | 0.87              |
| 4:J:126:LEU:HD11  | 4:J:223:LEU:HD13  | 1.56                     | 0.86              |
| 6:L:112:THR:HG23  | 6:L:115:GLY:HA3   | 1.57                     | 0.86              |
| 4:J:368:LEU:HD23  | 4:J:373:ALA:HB2   | 1.57                     | 0.86              |
| 2:H:19:VAL:HB     | 2:H:23:HIS:HB3    | 1.56                     | 0.86              |
| 2:M:282:VAL:HB    | 2:M:316:MET:HB2   | 1.55                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:13:LEU:HD22  | 2:H:28:LEU:HD12   | 1.56                     | 0.86              |
| 3:I:233:ARG:HD3  | 3:I:238:GLN:HB2   | 1.57                     | 0.86              |
| 3:I:288:PRO:HG2  | 3:I:291:TYR:HB2   | 1.58                     | 0.86              |
| 4:J:1062:LEU:HB3 | 4:J:1066:GLU:HB3  | 1.56                     | 0.86              |
| 2:G:43:LEU:HD13  | 2:G:217:ILE:HD11  | 1.57                     | 0.85              |
| 3:I:689:ALA:HB2  | 3:I:1233:LEU:HD23 | 1.59                     | 0.85              |
| 2:M:270:LEU:HB3  | 2:M:275:ILE:HB    | 1.57                     | 0.85              |
| 3:I:980:VAL:HA   | 3:I:984:VAL:HG23  | 1.59                     | 0.85              |
| 6:L:157:ARG:HB3  | 6:L:160:ASP:HB2   | 1.58                     | 0.85              |
| 6:L:551:LEU:HB2  | 6:L:556:ALA:HB2   | 1.57                     | 0.85              |
| 4:J:322:ARG:HH12 | 6:L:510:PRO:HG3   | 1.42                     | 0.85              |
| 6:L:231:THR:HG21 | 6:L:249:ILE:HG13  | 1.59                     | 0.85              |
| 6:L:149:ASP:OD1  | 6:L:225:ARG:NH2   | 2.10                     | 0.84              |
| 1:N:8:ALA:HB2    | 4:J:786:THR:HG21  | 1.57                     | 0.84              |
| 3:I:1131:MET:HE2 | 3:I:1141:LEU:HD12 | 1.59                     | 0.84              |
| 4:J:153:ASN:HB3  | 4:J:154:LEU:HD12  | 1.60                     | 0.84              |
| 6:L:395:THR:HA   | 6:L:404:LEU:HD11  | 1.59                     | 0.84              |
| 4:J:131:PRO:HG2  | 4:J:134:ASP:HB2   | 1.59                     | 0.84              |
| 4:J:821:MET:HE1  | 4:J:879:ALA:HA    | 1.60                     | 0.84              |
| 4:J:252:LEU:HG   | 4:J:262:THR:HG22  | 1.59                     | 0.84              |
| 4:J:932:MET:HG3  | 4:J:933:ARG:HG2   | 1.59                     | 0.84              |
| 2:H:213:PRO:HA   | 2:H:216:ALA:HB3   | 1.60                     | 0.84              |
| 3:I:257:ALA:HB2  | 3:I:285:ILE:HG22  | 1.58                     | 0.83              |
| 3:I:490:GLN:HE21 | 6:L:472:GLN:HB3   | 1.42                     | 0.83              |
| 4:J:198:CYS:HB3  | 4:J:224:LEU:HD22  | 1.61                     | 0.83              |
| 4:J:573:THR:HG22 | 4:J:575:GLY:H     | 1.42                     | 0.83              |
| 3:I:1120:ALA:HB1 | 3:I:1198:LEU:HB3  | 1.59                     | 0.83              |
| 3:I:560:PRO:HB2  | 4:J:776:THR:HG21  | 1.60                     | 0.82              |
| 2:G:102:LEU:HD22 | 2:G:115:ILE:HG13  | 1.62                     | 0.82              |
| 6:L:479:THR:HG23 | 6:L:482:GLU:H     | 1.44                     | 0.82              |
| 3:I:826:ASP:OD1  | 3:I:829:THR:OG1   | 1.96                     | 0.82              |
| 3:I:558:VAL:HG11 | 3:I:573:ASN:HB3   | 1.62                     | 0.82              |
| 4:J:325:LYS:HD3  | 6:L:508:GLU:HG2   | 1.60                     | 0.82              |
| 6:L:136:GLU:HB3  | 6:L:361:ILE:HG12  | 1.62                     | 0.81              |
| 4:J:355:ILE:HG21 | 4:J:466:MET:HG2   | 1.61                     | 0.81              |
| 4:J:245:LEU:HD21 | 4:J:327:LEU:HD21  | 1.60                     | 0.81              |
| 3:I:811:ASN:HA   | 3:I:815:SER:HB2   | 1.62                     | 0.81              |
| 4:J:474:LEU:HB3  | 5:K:28:ARG:HH12   | 1.44                     | 0.81              |
| 6:L:452:ILE:HG13 | 6:L:457:ILE:HD11  | 1.63                     | 0.81              |
| 8:P:67:DT:H5''   | 2:M:298:LYS:HB2   | 1.62                     | 0.81              |
| 7:O:26:DT:H2''   | 7:O:27:DT:H5'     | 1.60                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:44:DA:H1'     | 7:O:45:DA:H5'     | 1.63                     | 0.81              |
| 6:L:157:ARG:HE    | 6:L:159:SER:HB3   | 1.45                     | 0.81              |
| 3:I:303:ASP:HB3   | 3:I:308:GLU:H     | 1.46                     | 0.80              |
| 4:J:826:ILE:HG12  | 4:J:831:VAL:HA    | 1.62                     | 0.80              |
| 4:J:1047:THR:HG23 | 4:J:1049:GLN:HG3  | 1.63                     | 0.80              |
| 6:L:426:LYS:HB3   | 7:O:52:DA:H5'     | 1.62                     | 0.80              |
| 3:I:1142:ARG:HH21 | 3:I:1165:SER:HB3  | 1.46                     | 0.80              |
| 6:L:118:ASP:HA    | 6:L:121:LYS:HE3   | 1.64                     | 0.80              |
| 6:L:287:ILE:HA    | 6:L:337:VAL:HG13  | 1.63                     | 0.80              |
| 3:I:953:LEU:HD22  | 3:I:1033:ARG:HG3  | 1.63                     | 0.80              |
| 8:P:60:DA:H2'     | 8:P:61:DT:H71     | 1.64                     | 0.80              |
| 3:I:493:ILE:O     | 6:L:472:GLN:NE2   | 2.15                     | 0.80              |
| 4:J:388:ARG:HB3   | 4:J:390:LEU:HD13  | 1.63                     | 0.80              |
| 3:I:5:TYR:HA      | 3:I:8:LYS:HD2     | 1.62                     | 0.79              |
| 6:L:105:MET:HE2   | 6:L:384:LEU:HD12  | 1.63                     | 0.79              |
| 6:L:583:THR:HG22  | 6:L:585:GLU:H     | 1.47                     | 0.79              |
| 8:P:54:DT:H2''    | 8:P:55:DT:H5'     | 1.62                     | 0.79              |
| 4:J:839:VAL:HG12  | 4:J:864:LEU:HD12  | 1.63                     | 0.79              |
| 3:I:1297:ASP:OD2  | 3:I:1300:GLY:N    | 2.13                     | 0.79              |
| 3:I:741:MET:HE3   | 3:I:746:ALA:HB2   | 1.65                     | 0.79              |
| 4:J:1061:VAL:HG21 | 4:J:1101:LEU:HB2  | 1.62                     | 0.79              |
| 3:I:237:LEU:HB2   | 3:I:287:VAL:HG22  | 1.65                     | 0.79              |
| 3:I:992:LEU:HD11  | 3:I:1000:LEU:HD11 | 1.63                     | 0.79              |
| 4:J:1221:LEU:HD12 | 4:J:1229:VAL:HG11 | 1.65                     | 0.79              |
| 4:J:1046:ILE:HD11 | 4:J:1059:LEU:HD13 | 1.65                     | 0.79              |
| 6:L:292:VAL:HA    | 6:L:297:MET:HB3   | 1.65                     | 0.79              |
| 2:G:59:VAL:HG12   | 2:G:144:ILE:HG23  | 1.65                     | 0.78              |
| 2:H:102:LEU:HD21  | 2:H:115:ILE:HG23  | 1.65                     | 0.78              |
| 3:I:1161:LEU:HG   | 3:I:1164:PHE:HD2  | 1.48                     | 0.78              |
| 4:J:925:GLU:HG3   | 4:J:926:PRO:HD3   | 1.63                     | 0.78              |
| 4:J:1275:LEU:HB3  | 4:J:1278:GLU:HB2  | 1.64                     | 0.78              |
| 6:L:406:GLN:HA    | 6:L:409:ASN:HD22  | 1.47                     | 0.78              |
| 6:L:487:MET:HB3   | 6:L:489:MET:HE2   | 1.66                     | 0.78              |
| 2:H:62:ASP:OD1    | 2:H:141:SER:N     | 2.14                     | 0.78              |
| 5:K:38:LEU:HD11   | 5:K:67:ARG:HH22   | 1.48                     | 0.78              |
| 7:O:26:DT:H2'     | 7:O:27:DT:H71     | 1.66                     | 0.78              |
| 3:I:589:THR:OG1   | 3:I:659:GLN:OE1   | 2.02                     | 0.78              |
| 1:N:6:ASP:OD1     | 3:I:678:ARG:NH2   | 2.17                     | 0.77              |
| 2:H:155:ALA:N     | 2:H:174:ASP:OD1   | 2.17                     | 0.77              |
| 3:I:557:ARG:HB3   | 3:I:587:LEU:HD13  | 1.65                     | 0.77              |
| 3:I:1165:SER:OG   | 3:I:1166:ASP:N    | 2.17                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:279:LEU:HD11  | 4:J:296:LYS:HG2   | 1.65                     | 0.77              |
| 3:I:238:GLN:HA    | 3:I:286:GLU:HA    | 1.65                     | 0.77              |
| 3:I:519:ASN:HD21  | 3:I:796:LEU:HD23  | 1.50                     | 0.77              |
| 3:I:1245:ALA:HB1  | 4:J:376:LEU:HD21  | 1.65                     | 0.77              |
| 6:L:595:LEU:O     | 6:L:599:ARG:N     | 2.18                     | 0.77              |
| 4:J:1156:LEU:HD12 | 4:J:1209:VAL:HA   | 1.67                     | 0.77              |
| 5:K:3:ARG:NH2     | 5:K:5:THR:O       | 2.17                     | 0.77              |
| 6:L:392:LYS:HE3   | 7:O:56:DC:H4'     | 1.67                     | 0.77              |
| 3:I:1308:ILE:HG21 | 4:J:379:PRO:HB2   | 1.66                     | 0.77              |
| 6:L:280:VAL:HG21  | 6:L:355:ILE:HG21  | 1.66                     | 0.77              |
| 3:I:216:THR:HG23  | 3:I:219:GLN:HE22  | 1.50                     | 0.77              |
| 3:I:255:ILE:HG22  | 3:I:262:TYR:HB2   | 1.65                     | 0.77              |
| 2:G:14:VAL:HG21   | 2:G:29:GLU:HB2    | 1.67                     | 0.76              |
| 2:G:11:PRO:HA     | 2:G:30:PRO:HD2    | 1.67                     | 0.76              |
| 2:G:71:LYS:HE3    | 2:G:140:ILE:HG22  | 1.65                     | 0.76              |
| 2:M:286:GLU:HG3   | 2:M:300:LEU:HD21  | 1.66                     | 0.76              |
| 8:P:42:DT:H2''    | 8:P:43:DT:H72     | 1.67                     | 0.76              |
| 3:I:120:GLN:NE2   | 3:I:490:GLN:OE1   | 2.19                     | 0.76              |
| 2:G:102:LEU:HB2   | 2:G:142:MET:HG3   | 1.67                     | 0.76              |
| 3:I:560:PRO:O     | 4:J:780:ARG:NH2   | 2.18                     | 0.76              |
| 4:J:74:LYS:NZ     | 4:J:86:GLU:OE1    | 2.18                     | 0.76              |
| 7:O:42:DA:H1'     | 7:O:43:DA:H5'     | 1.67                     | 0.76              |
| 3:I:933:VAL:HG22  | 3:I:1050:VAL:HG12 | 1.67                     | 0.76              |
| 3:I:303:ASP:N     | 3:I:308:GLU:O     | 2.18                     | 0.75              |
| 3:I:569:ILE:HD11  | 4:J:783:LEU:HD22  | 1.66                     | 0.75              |
| 3:I:303:ASP:OD2   | 3:I:306:THR:OG1   | 2.02                     | 0.75              |
| 4:J:679:TYR:OH    | 4:J:754:ILE:O     | 2.01                     | 0.75              |
| 2:H:100:LEU:HB2   | 2:H:144:ILE:HG22  | 1.66                     | 0.75              |
| 6:L:286:LEU:HD23  | 6:L:340:ALA:HB2   | 1.67                     | 0.75              |
| 3:I:848:GLU:HG2   | 3:I:888:THR:HG22  | 1.66                     | 0.75              |
| 3:I:771:VAL:HG11  | 3:I:783:LEU:HD13  | 1.69                     | 0.75              |
| 4:J:950:ILE:HG12  | 4:J:1018:ALA:HB3  | 1.67                     | 0.75              |
| 6:L:132:CYS:O     | 6:L:136:GLU:N     | 2.20                     | 0.74              |
| 4:J:930:LEU:HD23  | 4:J:1244:GLN:HG2  | 1.69                     | 0.74              |
| 4:J:975:ILE:HD13  | 4:J:1003:LEU:HD11 | 1.69                     | 0.74              |
| 6:L:366:SER:HA    | 6:L:369:GLU:HB3   | 1.69                     | 0.74              |
| 3:I:231:GLU:HG2   | 3:I:332:ARG:HA    | 1.69                     | 0.74              |
| 3:I:889:PRO:HA    | 3:I:913:VAL:HA    | 1.69                     | 0.74              |
| 6:L:80:ALA:HA     | 6:L:83:VAL:HG12   | 1.68                     | 0.74              |
| 3:I:120:GLN:HE22  | 3:I:490:GLN:HB2   | 1.52                     | 0.74              |
| 3:I:187:GLU:OE1   | 3:I:197:ARG:NE    | 2.19                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1176:LEU:HD22 | 3:I:1181:PRO:HD3  | 1.69                     | 0.74              |
| 5:K:53:GLU:HG3    | 5:K:59:ILE:HD12   | 1.68                     | 0.74              |
| 3:I:931:VAL:HG22  | 3:I:1052:VAL:HG22 | 1.69                     | 0.74              |
| 4:J:1263:LYS:HE3  | 4:J:1315:ALA:HB1  | 1.68                     | 0.74              |
| 6:L:150:ARG:O     | 6:L:155:GLU:N     | 2.20                     | 0.74              |
| 6:L:478:PRO:HB2   | 6:L:483:LEU:HD11  | 1.69                     | 0.74              |
| 4:J:891:ASP:OD1   | 4:J:1286:LYS:NZ   | 2.21                     | 0.74              |
| 4:J:1346:GLY:O    | 4:J:1350:ASN:ND2  | 2.21                     | 0.74              |
| 4:J:482:ALA:O     | 5:K:16:ARG:NH2    | 2.21                     | 0.73              |
| 4:J:1265:THR:O    | 4:J:1303:SER:N    | 2.20                     | 0.73              |
| 3:I:838:CYS:HB2   | 3:I:918:LEU:HD22  | 1.70                     | 0.73              |
| 4:J:180:MET:SD    | 4:J:293:ARG:NH2   | 2.61                     | 0.73              |
| 4:J:582:ILE:HD13  | 4:J:627:THR:HG21  | 1.71                     | 0.73              |
| 3:I:764:CYS:SG    | 3:I:766:ASN:ND2   | 2.61                     | 0.73              |
| 4:J:516:ASP:HB2   | 4:J:547:ARG:HE    | 1.53                     | 0.73              |
| 8:P:64:DA:H2"     | 8:P:65:DT:H5"     | 1.69                     | 0.73              |
| 4:J:1160:SER:HA   | 4:J:1205:GLU:HA   | 1.70                     | 0.73              |
| 6:L:76:ALA:O      | 6:L:80:ALA:N      | 2.18                     | 0.73              |
| 4:J:111:THR:OG1   | 4:J:300:GLN:OE1   | 2.07                     | 0.73              |
| 2:H:33:ARG:NH1    | 2:H:197:ASP:OD2   | 2.21                     | 0.73              |
| 6:L:555:GLU:HA    | 6:L:558:VAL:HG12  | 1.71                     | 0.73              |
| 2:M:304:LYS:HA    | 2:M:307:LEU:HD12  | 1.71                     | 0.73              |
| 5:K:13:ILE:HD11   | 5:K:19:LEU:HA     | 1.70                     | 0.73              |
| 4:J:291:ILE:HD13  | 6:L:409:ASN:HB3   | 1.69                     | 0.72              |
| 6:L:548:LEU:HA    | 6:L:551:LEU:HG    | 1.71                     | 0.72              |
| 2:H:82:LEU:HG     | 2:H:173:VAL:HG12  | 1.70                     | 0.72              |
| 4:J:661:VAL:HG12  | 4:J:682:VAL:HG23  | 1.69                     | 0.72              |
| 6:L:250:LEU:HD12  | 6:L:253:SER:HB3   | 1.71                     | 0.72              |
| 6:L:470:MET:HE1   | 6:L:486:ARG:HB2   | 1.71                     | 0.72              |
| 3:I:1101:LEU:HD21 | 4:J:508:LEU:HD22  | 1.70                     | 0.72              |
| 4:J:56:LEU:O      | 4:J:250:ARG:NH2   | 2.22                     | 0.72              |
| 3:I:436:ARG:O     | 3:I:436:ARG:NH1   | 2.23                     | 0.72              |
| 4:J:132:LEU:HD23  | 4:J:136:GLU:HG3   | 1.70                     | 0.72              |
| 3:I:12:ARG:NH1    | 3:I:1182:ILE:O    | 2.22                     | 0.72              |
| 3:I:1286:THR:N    | 4:J:479:GLU:OE1   | 2.21                     | 0.72              |
| 3:I:1319:MET:HE3  | 3:I:1320:PRO:HD2  | 1.70                     | 0.72              |
| 4:J:1046:ILE:HD12 | 4:J:1059:LEU:HD22 | 1.72                     | 0.72              |
| 2:G:113:ALA:HB2   | 2:G:126:PRO:HB3   | 1.71                     | 0.72              |
| 3:I:434:ASP:HB2   | 3:I:439:LYS:HE2   | 1.71                     | 0.72              |
| 4:J:364:HIS:HB3   | 4:J:487:THR:HG21  | 1.71                     | 0.72              |
| 1:N:52:PHE:HB2    | 1:N:55:VAL:CG2    | 2.19                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1029:THR:HG22 | 4:J:1119:ASP:H    | 1.55                     | 0.72              |
| 4:J:161:THR:O     | 4:J:165:TYR:N     | 2.19                     | 0.72              |
| 3:I:252:SER:O     | 3:I:265:LYS:NZ    | 2.22                     | 0.72              |
| 4:J:641:ILE:HD12  | 4:J:644:MET:HE3   | 1.71                     | 0.72              |
| 3:I:100:LEU:HD12  | 3:I:493:ILE:HD11  | 1.72                     | 0.71              |
| 3:I:1103:VAL:HG21 | 4:J:639:VAL:HG21  | 1.70                     | 0.71              |
| 3:I:1131:MET:HA   | 3:I:1136:GLN:HG2  | 1.71                     | 0.71              |
| 4:J:1175:LEU:HD11 | 4:J:1200:GLU:HB3  | 1.73                     | 0.71              |
| 4:J:1311:LYS:HD3  | 4:J:1314:LEU:HD21 | 1.71                     | 0.71              |
| 1:N:42:ASN:OD1    | 3:I:267:ARG:NH1   | 2.21                     | 0.71              |
| 4:J:1031:VAL:HG12 | 4:J:1032:SER:H    | 1.56                     | 0.71              |
| 4:J:813:ASP:HA    | 4:J:895:CYS:SG    | 2.31                     | 0.71              |
| 4:J:974:VAL:HA    | 4:J:1003:LEU:HG   | 1.71                     | 0.71              |
| 4:J:1036:ARG:HB2  | 4:J:1081:VAL:HG11 | 1.71                     | 0.71              |
| 4:J:259:ARG:HE    | 6:L:502:LYS:HE3   | 1.54                     | 0.71              |
| 6:L:234:THR:O     | 6:L:242:HIS:N     | 2.24                     | 0.71              |
| 6:L:284:GLU:O     | 6:L:288:MET:N     | 2.21                     | 0.71              |
| 2:H:183:ILE:HD11  | 2:H:203:ILE:HG22  | 1.71                     | 0.71              |
| 4:J:1195:GLN:N    | 4:J:1212:ASP:OD1  | 2.23                     | 0.71              |
| 8:P:43:DT:H1'     | 8:P:44:DT:H5'     | 1.73                     | 0.71              |
| 1:N:64:TYR:HE2    | 3:I:341:LEU:HB2   | 1.56                     | 0.71              |
| 3:I:277:LEU:O     | 3:I:281:ASP:N     | 2.23                     | 0.71              |
| 3:I:561:ILE:HD11  | 3:I:665:ALA:HB1   | 1.73                     | 0.71              |
| 4:J:287:ALA:HB1   | 4:J:288:PRO:HD2   | 1.73                     | 0.71              |
| 6:L:151:VAL:HG12  | 6:L:158:LEU:HD23  | 1.71                     | 0.71              |
| 1:N:48:ARG:NH2    | 1:N:62:GLN:OE1    | 2.24                     | 0.70              |
| 2:G:118:ASP:HB3   | 2:G:121:VAL:HG12  | 1.73                     | 0.70              |
| 3:I:812:PHE:HZ    | 4:J:503:SER:HB2   | 1.56                     | 0.70              |
| 3:I:1164:PHE:HB3  | 3:I:1165:SER:CB   | 2.21                     | 0.70              |
| 4:J:198:CYS:HB3   | 4:J:224:LEU:CD2   | 2.21                     | 0.70              |
| 2:H:47:LEU:HD22   | 2:H:180:VAL:HG11  | 1.73                     | 0.70              |
| 3:I:251:ALA:N     | 3:I:267:ARG:O     | 2.18                     | 0.70              |
| 4:J:44:ILE:HG22   | 4:J:51:PRO:HA     | 1.72                     | 0.70              |
| 3:I:634:VAL:HG11  | 3:I:650:VAL:HG11  | 1.73                     | 0.70              |
| 4:J:201:LEU:HD13  | 4:J:204:GLU:HB2   | 1.73                     | 0.70              |
| 4:J:1064:SER:HA   | 4:J:1067:ARG:HG2  | 1.73                     | 0.70              |
| 4:J:334:LYS:O     | 4:J:340:GLN:HB2   | 1.92                     | 0.70              |
| 4:J:982:LEU:N     | 4:J:995:TYR:O     | 2.24                     | 0.70              |
| 4:J:1089:LEU:CA   | 4:J:1096:PRO:HA   | 2.21                     | 0.70              |
| 2:G:52:PRO:HB3    | 2:H:5:VAL:HG21    | 1.72                     | 0.70              |
| 2:H:61:ILE:HD12   | 2:H:142:MET:HE2   | 1.72                     | 0.70              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:1248:THR:HG21 | 6:L:531:PRO:HG2  | 1.73                     | 0.70              |
| 4:J:417:ARG:NH1   | 5:K:43:ASN:O     | 2.25                     | 0.70              |
| 4:J:748:ALA:HB2   | 4:J:754:ILE:HG12 | 1.73                     | 0.70              |
| 4:J:1164:SER:HA   | 4:J:1200:GLU:HB2 | 1.73                     | 0.70              |
| 4:J:34:SER:OG     | 4:J:36:GLY:O     | 2.06                     | 0.70              |
| 4:J:822:MET:SD    | 4:J:838:ARG:NH2  | 2.64                     | 0.70              |
| 2:G:234:LEU:HD12  | 2:H:218:ARG:HE   | 1.57                     | 0.70              |
| 3:I:42:ASP:OD2    | 3:I:46:GLN:N     | 2.18                     | 0.70              |
| 3:I:148:GLN:NE2   | 3:I:533:LEU:O    | 2.24                     | 0.70              |
| 4:J:984:LEU:HB3   | 4:J:993:GLU:H    | 1.57                     | 0.70              |
| 4:J:984:LEU:N     | 4:J:993:GLU:O    | 2.25                     | 0.70              |
| 3:I:1240:ASP:HB3  | 4:J:445:LYS:HD2  | 1.74                     | 0.69              |
| 2:G:150:ARG:NH1   | 2:H:5:VAL:O      | 2.26                     | 0.69              |
| 3:I:59:ILE:O      | 3:I:68:LEU:N     | 2.23                     | 0.69              |
| 4:J:1029:THR:HG23 | 4:J:1118:GLY:H   | 1.57                     | 0.69              |
| 3:I:1321:GLU:OE2  | 4:J:99:ARG:NE    | 2.22                     | 0.69              |
| 4:J:950:ILE:HD13  | 4:J:997:VAL:HG22 | 1.73                     | 0.69              |
| 5:K:3:ARG:HB2     | 5:K:48:VAL:HG13  | 1.74                     | 0.69              |
| 6:L:114:GLU:HA    | 6:L:117:ILE:HD13 | 1.73                     | 0.69              |
| 6:L:385:ARG:NH1   | 7:O:55:DC:OP2    | 2.25                     | 0.69              |
| 6:L:539:SER:O     | 6:L:543:ALA:N    | 2.20                     | 0.69              |
| 2:H:154:PRO:O     | 2:H:158:ARG:NH1  | 2.25                     | 0.69              |
| 6:L:283:GLN:O     | 6:L:287:ILE:N    | 2.24                     | 0.69              |
| 2:G:104:LYS:NZ    | 2:G:114:ASP:OD2  | 2.19                     | 0.69              |
| 3:I:960:LEU:HD22  | 3:I:1029:LEU:HB2 | 1.73                     | 0.69              |
| 3:I:1243:MET:HE3  | 4:J:445:LYS:HD3  | 1.75                     | 0.69              |
| 4:J:1138:LEU:HB3  | 4:J:1139:PRO:HD3 | 1.74                     | 0.69              |
| 3:I:706:ARG:NH1   | 3:I:791:LEU:O    | 2.24                     | 0.69              |
| 3:I:998:LEU:HB3   | 3:I:1015:ALA:HB2 | 1.75                     | 0.69              |
| 7:O:23:DC:H2'     | 7:O:24:DC:C6     | 2.26                     | 0.69              |
| 3:I:542:ARG:NH1   | 3:I:542:ARG:O    | 2.22                     | 0.69              |
| 3:I:1024:GLU:HA   | 3:I:1027:LYS:HE2 | 1.74                     | 0.69              |
| 4:J:1067:ARG:NE   | 4:J:1072:LYS:HA  | 2.08                     | 0.69              |
| 3:I:12:ARG:NH2    | 3:I:793:GLU:OE2  | 2.24                     | 0.69              |
| 3:I:726:TYR:HA    | 3:I:773:LEU:HD11 | 1.74                     | 0.69              |
| 4:J:701:LEU:HD21  | 4:J:723:TYR:HB2  | 1.75                     | 0.69              |
| 4:J:968:ASN:HA    | 4:J:1118:GLY:HA3 | 1.75                     | 0.69              |
| 2:G:184:ALA:HB2   | 3:I:1091:GLY:HA3 | 1.75                     | 0.69              |
| 3:I:38:PHE:HA     | 3:I:48:GLY:HA2   | 1.75                     | 0.69              |
| 3:I:346:TYR:O     | 3:I:350:THR:OG1  | 2.11                     | 0.69              |
| 6:L:351:THR:HB    | 6:L:358:VAL:HG21 | 1.74                     | 0.69              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:864:LYS:HD2  | 3:I:875:ALA:HB1   | 1.74                     | 0.68              |
| 4:J:478:LEU:HB3  | 5:K:20:VAL:HG13   | 1.74                     | 0.68              |
| 4:J:960:LEU:HB3  | 4:J:963:VAL:HB    | 1.75                     | 0.68              |
| 6:L:494:ILE:O    | 6:L:497:VAL:HG12  | 1.93                     | 0.68              |
| 2:G:208:ASN:OD1  | 2:G:210:THR:OG1   | 2.05                     | 0.68              |
| 3:I:818:VAL:HG22 | 3:I:1096:ILE:HG12 | 1.75                     | 0.68              |
| 6:L:583:THR:HB   | 6:L:586:ARG:HB3   | 1.75                     | 0.68              |
| 3:I:971:LEU:HD13 | 3:I:1018:TYR:HD1  | 1.59                     | 0.68              |
| 2:G:73:GLY:O     | 2:G:134:THR:N     | 2.27                     | 0.68              |
| 3:I:146:VAL:HG23 | 3:I:511:LEU:HD22  | 1.74                     | 0.68              |
| 3:I:994:ARG:HG2  | 3:I:997:TRP:CH2   | 2.29                     | 0.68              |
| 3:I:1121:ALA:HB2 | 3:I:1182:ILE:HD11 | 1.73                     | 0.68              |
| 4:J:1281:GLU:OE1 | 4:J:1283:SER:N    | 2.22                     | 0.68              |
| 6:L:327:SER:HA   | 6:L:330:LEU:HG    | 1.76                     | 0.68              |
| 6:L:333:VAL:HG22 | 6:L:337:VAL:HG23  | 1.74                     | 0.68              |
| 7:O:16:DC:H2''   | 7:O:17:DA:H5'     | 1.74                     | 0.68              |
| 4:J:901:ARG:NH1  | 4:J:906:GLY:O     | 2.26                     | 0.68              |
| 4:J:1029:THR:HA  | 4:J:1099:TYR:CE2  | 2.28                     | 0.68              |
| 6:L:429:THR:HA   | 7:O:53:DT:H71     | 1.74                     | 0.68              |
| 3:I:617:ALA:N    | 3:I:652:TYR:O     | 2.19                     | 0.68              |
| 6:L:263:PRO:HA   | 6:L:266:PHE:HB3   | 1.75                     | 0.68              |
| 3:I:842:ASP:HB3  | 3:I:1047:LEU:HD11 | 1.76                     | 0.68              |
| 4:J:502:PRO:HB3  | 4:J:506:VAL:HG23  | 1.75                     | 0.68              |
| 4:J:984:LEU:HB3  | 4:J:993:GLU:N     | 2.09                     | 0.68              |
| 4:J:1308:GLY:O   | 4:J:1312:ALA:N    | 2.23                     | 0.68              |
| 2:G:14:VAL:HG12  | 2:G:15:ASP:H      | 1.59                     | 0.68              |
| 3:I:404:LYS:NZ   | 3:I:450:ASN:OD1   | 2.25                     | 0.68              |
| 4:J:418:GLU:HG3  | 5:K:48:VAL:HG21   | 1.75                     | 0.68              |
| 6:L:406:GLN:O    | 6:L:410:ILE:HG12  | 1.93                     | 0.68              |
| 6:L:455:HIS:NE2  | 7:O:44:DA:OP2     | 2.18                     | 0.68              |
| 4:J:973:LEU:HB3  | 4:J:1003:LEU:HD12 | 1.75                     | 0.67              |
| 2:M:250:ASP:HB3  | 2:M:253:LEU:HD23  | 1.76                     | 0.67              |
| 2:G:26:VAL:HG22  | 2:G:203:ILE:HB    | 1.75                     | 0.67              |
| 3:I:138:ILE:HG13 | 3:I:143:ARG:HD3   | 1.74                     | 0.67              |
| 4:J:492:SER:OG   | 4:J:495:ASN:O     | 2.11                     | 0.67              |
| 4:J:1077:ALA:HB2 | 4:J:1100:PHE:HA   | 1.77                     | 0.67              |
| 2:G:61:ILE:HG13  | 2:G:64:VAL:HB     | 1.76                     | 0.67              |
| 3:I:233:ARG:O    | 3:I:238:GLN:NE2   | 2.27                     | 0.67              |
| 8:P:57:DT:H2''   | 8:P:58:DC:H5'     | 1.76                     | 0.67              |
| 3:I:406:ASN:ND2  | 3:I:413:GLU:O     | 2.28                     | 0.67              |
| 4:J:1079:LYS:HE3 | 4:J:1081:VAL:HG12 | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:86:LYS:HZ2    | 2:H:174:ASP:HB2   | 1.60                     | 0.67              |
| 4:J:502:PRO:HB3   | 4:J:506:VAL:CG2   | 2.24                     | 0.67              |
| 8:P:43:DT:H2''    | 8:P:44:DT:H5'     | 1.76                     | 0.67              |
| 3:I:256:GLU:HB2   | 3:I:261:VAL:HG22  | 1.77                     | 0.67              |
| 4:J:1105:ALA:HA   | 4:J:1124:ILE:CG1  | 2.23                     | 0.67              |
| 6:L:290:LEU:O     | 6:L:294:GLN:NE2   | 2.27                     | 0.67              |
| 3:I:1142:ARG:HG3  | 3:I:1161:LEU:CD2  | 2.25                     | 0.67              |
| 3:I:494:ASN:HA    | 6:L:472:GLN:HE22  | 1.60                     | 0.67              |
| 6:L:81:ALA:HA     | 6:L:84:LEU:HG     | 1.76                     | 0.67              |
| 3:I:149:LEU:HD13  | 3:I:453:ILE:HG12  | 1.77                     | 0.67              |
| 6:L:269:LEU:O     | 6:L:273:MET:N     | 2.23                     | 0.66              |
| 6:L:305:LEU:HD13  | 6:L:319:ALA:HB2   | 1.76                     | 0.66              |
| 6:L:583:THR:HG22  | 6:L:585:GLU:N     | 2.10                     | 0.66              |
| 3:I:962:GLU:O     | 3:I:966:ILE:HG12  | 1.95                     | 0.66              |
| 8:P:60:DA:H2''    | 8:P:61:DT:H5'     | 1.75                     | 0.66              |
| 2:G:73:GLY:N      | 3:I:728:ASP:OD2   | 2.29                     | 0.66              |
| 3:I:1155:VAL:O    | 3:I:1158:LYS:NZ   | 2.28                     | 0.66              |
| 10:I:1401:1N7:C3  | 10:I:1401:1N7:C2  | 2.69                     | 0.66              |
| 4:J:902:ASP:OD2   | 4:J:1249:ASN:ND2  | 2.28                     | 0.66              |
| 3:I:607:SER:OG    | 3:I:610:GLU:OE1   | 2.11                     | 0.66              |
| 3:I:856:ASN:HA    | 6:L:613:ASP:O     | 1.96                     | 0.66              |
| 6:L:463:LEU:O     | 6:L:467:SER:N     | 2.27                     | 0.66              |
| 2:H:215:GLU:HA    | 2:H:218:ARG:HG2   | 1.76                     | 0.66              |
| 3:I:145:ILE:HG21  | 3:I:456:VAL:HG23  | 1.76                     | 0.66              |
| 3:I:402:ARG:NE    | 3:I:417:SER:O     | 2.28                     | 0.66              |
| 3:I:1109:ILE:HD11 | 4:J:740:LEU:HD11  | 1.77                     | 0.66              |
| 3:I:1157:GLN:O    | 3:I:1158:LYS:NZ   | 2.23                     | 0.66              |
| 4:J:836:ARG:HD2   | 4:J:869:CYS:SG    | 2.36                     | 0.66              |
| 4:J:964:LYS:O     | 4:J:976:THR:OG1   | 2.10                     | 0.66              |
| 3:I:1109:ILE:HG23 | 4:J:644:MET:HE1   | 1.78                     | 0.66              |
| 4:J:1046:ILE:HA   | 4:J:1062:LEU:HD12 | 1.78                     | 0.66              |
| 5:K:36:ASP:HB2    | 5:K:37:PRO:HD2    | 1.78                     | 0.66              |
| 3:I:560:PRO:CB    | 4:J:776:THR:HG21  | 2.25                     | 0.66              |
| 3:I:988:LYS:HA    | 3:I:991:LYS:HG3   | 1.75                     | 0.66              |
| 4:J:20:ILE:HG13   | 4:J:1344:LEU:HD21 | 1.78                     | 0.66              |
| 4:J:835:LEU:HD13  | 4:J:878:ASP:HA    | 1.78                     | 0.66              |
| 4:J:959:LYS:HB3   | 4:J:985:ILE:HD11  | 1.77                     | 0.66              |
| 4:J:1074:LEU:O    | 4:J:1075:ARG:NH1  | 2.27                     | 0.66              |
| 4:J:1152:GLU:OE2  | 4:J:1194:ARG:NE   | 2.29                     | 0.66              |
| 4:J:368:LEU:HG    | 4:J:369:PRO:HD2   | 1.77                     | 0.66              |
| 4:J:1062:LEU:HB3  | 4:J:1066:GLU:CB   | 2.25                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:468:ARG:NH1   | 8:P:35:DA:OP1     | 2.25                     | 0.66              |
| 3:I:1257:GLN:HE22 | 4:J:345:LYS:HE2   | 1.59                     | 0.66              |
| 2:G:180:VAL:HA    | 2:G:207:THR:HG22  | 1.78                     | 0.66              |
| 3:I:65:ASN:O      | 3:I:105:TYR:N     | 2.20                     | 0.66              |
| 1:N:52:PHE:O      | 1:N:55:VAL:HG23   | 1.96                     | 0.65              |
| 3:I:808:ASN:OD1   | 3:I:1216:ARG:NH2  | 2.29                     | 0.65              |
| 3:I:992:LEU:HB2   | 3:I:993:PRO:HD2   | 1.77                     | 0.65              |
| 3:I:998:LEU:HD13  | 3:I:1015:ALA:CA   | 2.24                     | 0.65              |
| 6:L:478:PRO:HB2   | 6:L:483:LEU:CD1   | 2.27                     | 0.65              |
| 3:I:230:PHE:N     | 3:I:333:ILE:O     | 2.29                     | 0.65              |
| 3:I:819:SER:HB2   | 3:I:1085:MET:HG3  | 1.76                     | 0.65              |
| 4:J:926:PRO:HG2   | 4:J:1248:ILE:HD11 | 1.77                     | 0.65              |
| 4:J:952:VAL:N     | 4:J:1015:GLU:O    | 2.27                     | 0.65              |
| 6:L:157:ARG:HG2   | 6:L:160:ASP:H     | 1.59                     | 0.65              |
| 2:H:51:MET:HE1    | 2:H:219:ARG:HG2   | 1.79                     | 0.65              |
| 3:I:254:ASP:HB3   | 3:I:265:LYS:HG3   | 1.78                     | 0.65              |
| 3:I:302:ILE:HG22  | 3:I:309:LEU:HA    | 1.78                     | 0.65              |
| 4:J:253:VAL:HG11  | 6:L:523:ILE:HD13  | 1.79                     | 0.65              |
| 4:J:1024:THR:HB   | 4:J:1123:ARG:HB3  | 1.77                     | 0.65              |
| 4:J:1064:SER:HB3  | 4:J:1072:LYS:HD3  | 1.78                     | 0.65              |
| 6:L:26:GLU:O      | 6:L:30:HIS:N      | 2.29                     | 0.65              |
| 3:I:301:TYR:CE2   | 3:I:333:ILE:HA    | 2.31                     | 0.65              |
| 3:I:906:PHE:CD2   | 6:L:611:LEU:HD11  | 2.30                     | 0.65              |
| 3:I:1005:GLU:HG2  | 3:I:1006:GLU:OE1  | 1.97                     | 0.65              |
| 4:J:884:SER:OG    | 4:J:886:VAL:HG12  | 1.95                     | 0.65              |
| 4:J:1006:GLY:N    | 4:J:1009:GLU:OE2  | 2.26                     | 0.65              |
| 6:L:133:SER:CB    | 6:L:365:MET:HB2   | 2.26                     | 0.65              |
| 6:L:295:CYS:O     | 6:L:326:TRP:HB2   | 1.97                     | 0.65              |
| 3:I:517:GLN:O     | 3:I:517:GLN:HG2   | 1.96                     | 0.65              |
| 2:H:112:ALA:HB3   | 2:H:126:PRO:HA    | 1.77                     | 0.65              |
| 3:I:972:PHE:HD1   | 3:I:975:ILE:HD12  | 1.61                     | 0.65              |
| 4:J:367:GLY:H     | 4:J:448:GLN:HB2   | 1.62                     | 0.65              |
| 4:J:1163:VAL:HG23 | 4:J:1177:ILE:HA   | 1.78                     | 0.65              |
| 6:L:137:TYR:CZ    | 6:L:139:GLU:HB2   | 2.31                     | 0.65              |
| 6:L:162:ILE:HD13  | 6:L:221:PHE:HE2   | 1.62                     | 0.65              |
| 4:J:140:TYR:CB    | 6:L:100:MET:HE1   | 2.26                     | 0.65              |
| 4:J:317:THR:OG1   | 4:J:322:ARG:O     | 2.13                     | 0.65              |
| 4:J:334:LYS:HA    | 4:J:339:ARG:HD3   | 1.79                     | 0.65              |
| 6:L:277:MET:HA    | 6:L:280:VAL:HG12  | 1.78                     | 0.65              |
| 3:I:565:GLU:OE1   | 3:I:684:ASN:ND2   | 2.30                     | 0.65              |
| 4:J:363:LEU:HD23  | 4:J:487:THR:HG22  | 1.79                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:598:LEU:O     | 6:L:604:SER:OG    | 2.14                     | 0.65              |
| 3:I:383:SER:O     | 3:I:387:ASN:ND2   | 2.29                     | 0.65              |
| 3:I:901:LEU:HD22  | 6:L:565:ILE:HD11  | 1.78                     | 0.65              |
| 4:J:20:ILE:HD12   | 4:J:1344:LEU:HD11 | 1.78                     | 0.65              |
| 4:J:978:ARG:NH2   | 4:J:1197:ASN:O    | 2.30                     | 0.65              |
| 3:I:237:LEU:HB2   | 3:I:287:VAL:CG2   | 2.27                     | 0.65              |
| 4:J:423:LEU:HD12  | 4:J:468:VAL:HG12  | 1.79                     | 0.65              |
| 4:J:982:LEU:HB3   | 4:J:995:TYR:HB2   | 1.77                     | 0.65              |
| 4:J:1038:THR:HG21 | 4:J:1079:LYS:HD3  | 1.78                     | 0.65              |
| 5:K:3:ARG:HH21    | 5:K:5:THR:H       | 1.42                     | 0.65              |
| 2:H:158:ARG:HE    | 2:H:172:LEU:HD12  | 1.61                     | 0.64              |
| 3:I:28:LEU:HD13   | 3:I:527:LYS:HD3   | 1.79                     | 0.64              |
| 3:I:202:ARG:HA    | 6:L:29:ASP:OD1    | 1.97                     | 0.64              |
| 3:I:974:ARG:O     | 3:I:978:VAL:HG23  | 1.97                     | 0.64              |
| 4:J:1035:VAL:O    | 4:J:1112:GLY:N    | 2.25                     | 0.64              |
| 8:P:61:DT:H1'     | 8:P:62:DG:H5'     | 1.79                     | 0.64              |
| 2:H:57:THR:O      | 2:H:173:VAL:HG22  | 1.96                     | 0.64              |
| 3:I:242:VAL:HB    | 3:I:245:ARG:HB2   | 1.79                     | 0.64              |
| 3:I:716:ALA:HB3   | 3:I:784:ALA:HB3   | 1.79                     | 0.64              |
| 3:I:798:GLN:HB3   | 3:I:827:ARG:NH2   | 2.12                     | 0.64              |
| 4:J:93:THR:HG22   | 4:J:94:GLN:H      | 1.60                     | 0.64              |
| 2:H:86:LYS:NZ     | 2:H:174:ASP:HB2   | 2.13                     | 0.64              |
| 6:L:593:LYS:HA    | 6:L:596:ARG:HG2   | 1.80                     | 0.64              |
| 2:H:19:VAL:CB     | 2:H:23:HIS:HB3    | 2.27                     | 0.64              |
| 3:I:611:GLU:OE2   | 3:I:637:ARG:NH2   | 2.30                     | 0.64              |
| 3:I:976:ARG:O     | 3:I:980:VAL:HG23  | 1.98                     | 0.64              |
| 3:I:1212:LEU:HD22 | 3:I:1225:VAL:CG2  | 2.27                     | 0.64              |
| 10:I:1401:1N7:C3  | 10:I:1401:1N7:C18 | 2.70                     | 0.64              |
| 6:L:586:ARG:NH1   | 6:L:589:GLN:HB3   | 2.12                     | 0.64              |
| 2:G:50:SER:HB2    | 2:G:150:ARG:HD2   | 1.80                     | 0.64              |
| 6:L:297:MET:HE2   | 6:L:302:PHE:HB2   | 1.79                     | 0.64              |
| 3:I:303:ASP:HB3   | 3:I:308:GLU:N     | 2.11                     | 0.64              |
| 6:L:409:ASN:O     | 6:L:413:MET:HG2   | 1.97                     | 0.64              |
| 7:O:41:DT:H2''    | 7:O:42:DA:N7      | 2.13                     | 0.64              |
| 3:I:387:ASN:HA    | 3:I:391:SER:HB3   | 1.79                     | 0.64              |
| 3:I:772:SER:N     | 3:I:775:GLU:OE1   | 2.20                     | 0.64              |
| 4:J:951:GLN:HA    | 4:J:1016:THR:HA   | 1.80                     | 0.64              |
| 4:J:1061:VAL:HG21 | 4:J:1101:LEU:CB   | 2.28                     | 0.64              |
| 6:L:117:ILE:HG23  | 6:L:421:TYR:CE1   | 2.33                     | 0.64              |
| 6:L:274:ARG:HA    | 6:L:274:ARG:CZ    | 2.28                     | 0.64              |
| 2:G:68:TYR:HB3    | 3:I:756:TYR:CD2   | 2.33                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:591:TYR:OH    | 3:I:637:ARG:NH2   | 2.31                     | 0.64              |
| 3:I:864:LYS:O     | 3:I:871:VAL:HA    | 1.98                     | 0.64              |
| 6:L:487:MET:HB3   | 6:L:489:MET:CE    | 2.27                     | 0.64              |
| 3:I:100:LEU:HD12  | 3:I:493:ILE:CD1   | 2.28                     | 0.64              |
| 3:I:1209:GLN:NE2  | 3:I:1226:THR:OG1  | 2.31                     | 0.64              |
| 4:J:176:PHE:CE2   | 4:J:178:ALA:HB3   | 2.33                     | 0.64              |
| 4:J:1036:ARG:CG   | 4:J:1081:VAL:HG21 | 2.27                     | 0.64              |
| 6:L:166:VAL:HG22  | 6:L:260:ARG:HG3   | 1.79                     | 0.64              |
| 4:J:281:ARG:O     | 4:J:285:LEU:HG    | 1.98                     | 0.64              |
| 2:M:298:LYS:O     | 2:M:302:GLU:HG2   | 1.98                     | 0.64              |
| 1:N:56:THR:O      | 1:N:57:LEU:HD23   | 1.98                     | 0.63              |
| 2:G:9:LEU:HD11    | 2:G:198:LEU:HD13  | 1.80                     | 0.63              |
| 3:I:230:PHE:O     | 3:I:333:ILE:N     | 2.24                     | 0.63              |
| 3:I:1212:LEU:HD22 | 3:I:1225:VAL:HG21 | 1.79                     | 0.63              |
| 4:J:865:HIS:ND1   | 4:J:867:GLN:OE1   | 2.31                     | 0.63              |
| 6:L:287:ILE:HG13  | 6:L:340:ALA:HB1   | 1.78                     | 0.63              |
| 6:L:292:VAL:HG22  | 6:L:297:MET:HG2   | 1.80                     | 0.63              |
| 1:N:9:TYR:OH      | 1:N:13:GLU:OE1    | 2.09                     | 0.63              |
| 3:I:426:ILE:HG22  | 3:I:430:LYS:HD2   | 1.80                     | 0.63              |
| 3:I:681:MET:HB3   | 3:I:685:MET:HE1   | 1.78                     | 0.63              |
| 3:I:1105:SER:HB3  | 4:J:731:ARG:HD3   | 1.80                     | 0.63              |
| 4:J:559:ALA:HB3   | 4:J:562:GLU:HB3   | 1.80                     | 0.63              |
| 4:J:910:ASN:HB3   | 5:K:15:ASN:OD1    | 1.98                     | 0.63              |
| 2:M:269:CYS:HB2   | 2:M:292:THR:HG21  | 1.78                     | 0.63              |
| 2:G:158:ARG:NH1   | 2:G:162:GLU:OE2   | 2.31                     | 0.63              |
| 2:H:58:GLU:HA     | 2:H:172:LEU:HA    | 1.80                     | 0.63              |
| 2:H:100:LEU:HB2   | 2:H:144:ILE:CG2   | 2.28                     | 0.63              |
| 2:H:201:LEU:HG    | 2:H:203:ILE:HG13  | 1.79                     | 0.63              |
| 3:I:58:PRO:HB3    | 3:I:69:GLN:HG2    | 1.80                     | 0.63              |
| 3:I:317:LEU:HD11  | 3:I:322:LEU:HD13  | 1.80                     | 0.63              |
| 4:J:603:LYS:O     | 4:J:607:THR:HG23  | 1.98                     | 0.63              |
| 4:J:1079:LYS:HE3  | 4:J:1081:VAL:CG1  | 2.28                     | 0.63              |
| 4:J:1205:GLU:N    | 4:J:1208:ASP:OD1  | 2.30                     | 0.63              |
| 6:L:306:PHE:HA    | 6:L:315:TRP:HB2   | 1.80                     | 0.63              |
| 3:I:210:LEU:HA    | 3:I:213:LEU:HD12  | 1.80                     | 0.63              |
| 3:I:840:SER:HA    | 3:I:848:GLU:OE1   | 1.98                     | 0.63              |
| 3:I:1073:LYS:HD2  | 4:J:462:ASP:HB2   | 1.80                     | 0.63              |
| 4:J:325:LYS:CD    | 6:L:508:GLU:HG2   | 2.28                     | 0.63              |
| 3:I:590:PRO:HG3   | 3:I:605:TYR:CE1   | 2.32                     | 0.63              |
| 4:J:1314:LEU:HB3  | 4:J:1326:GLN:NE2  | 2.08                     | 0.63              |
| 2:G:22:THR:HB     | 2:G:207:THR:O     | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:130:VAL:HG22 | 6:L:365:MET:HG3   | 1.81                     | 0.63              |
| 4:J:740:LEU:O    | 4:J:762:ASN:HB2   | 1.98                     | 0.63              |
| 3:I:617:ALA:HA   | 3:I:636:CYS:SG    | 2.39                     | 0.63              |
| 3:I:735:LYS:HA   | 3:I:748:ILE:HG22  | 1.80                     | 0.63              |
| 3:I:1086:PRO:O   | 3:I:1094:VAL:HG12 | 1.98                     | 0.63              |
| 4:J:1152:GLU:HB3 | 4:J:1214:PRO:HD2  | 1.80                     | 0.63              |
| 6:L:525:ASP:OD1  | 6:L:526:THR:N     | 2.32                     | 0.63              |
| 6:L:585:GLU:OE1  | 8:P:58:DC:N4      | 2.32                     | 0.63              |
| 2:G:61:ILE:CG2   | 2:G:142:MET:HB3   | 2.25                     | 0.63              |
| 3:I:302:ILE:HA   | 3:I:310:ILE:H     | 1.64                     | 0.63              |
| 6:L:16:GLY:CA    | 6:L:22:LEU:HD11   | 2.28                     | 0.63              |
| 6:L:27:VAL:HG11  | 6:L:45:ILE:HG12   | 1.81                     | 0.63              |
| 6:L:123:ILE:O    | 6:L:127:ILE:HG23  | 1.99                     | 0.63              |
| 7:O:39:DG:H1'    | 7:O:40:DC:C5'     | 2.29                     | 0.63              |
| 4:J:58:CYS:HB3   | 4:J:61:ILE:HB     | 1.80                     | 0.62              |
| 6:L:490:PRO:HD2  | 6:L:493:LYS:HE2   | 1.81                     | 0.62              |
| 8:P:43:DT:C2'    | 8:P:44:DT:H5'     | 2.29                     | 0.62              |
| 8:P:68:DG:OP1    | 2:M:265:ARG:HB3   | 1.99                     | 0.62              |
| 3:I:690:VAL:CG2  | 3:I:1236:ASN:HB3  | 2.29                     | 0.62              |
| 3:I:865:LEU:HD12 | 3:I:869:GLY:C     | 2.24                     | 0.62              |
| 3:I:895:LEU:HD11 | 3:I:900:LYS:HG3   | 1.81                     | 0.62              |
| 4:J:1263:LYS:HA  | 4:J:1281:GLU:HA   | 1.80                     | 0.62              |
| 6:L:23:THR:HB    | 6:L:58:GLU:H      | 1.64                     | 0.62              |
| 6:L:429:THR:HA   | 7:O:53:DT:C7      | 2.29                     | 0.62              |
| 3:I:242:VAL:HB   | 3:I:245:ARG:CB    | 2.28                     | 0.62              |
| 3:I:301:TYR:HB3  | 3:I:325:LEU:HD21  | 1.80                     | 0.62              |
| 3:I:351:LEU:O    | 3:I:354:ASP:HB2   | 1.99                     | 0.62              |
| 3:I:538:LEU:CD2  | 3:I:547:VAL:HG11  | 2.30                     | 0.62              |
| 3:I:623:LEU:HA   | 3:I:630:VAL:HG13  | 1.82                     | 0.62              |
| 3:I:852:ALA:O    | 3:I:854:ILE:HG13  | 2.00                     | 0.62              |
| 6:L:386:LEU:O    | 6:L:390:ILE:HG13  | 1.99                     | 0.62              |
| 2:H:183:ILE:HD12 | 2:H:204:GLU:O     | 2.00                     | 0.62              |
| 3:I:905:ILE:HA   | 6:L:595:LEU:HD12  | 1.81                     | 0.62              |
| 4:J:1025:MET:N   | 4:J:1124:ILE:O    | 2.22                     | 0.62              |
| 4:J:1158:GLU:OE1 | 4:J:1158:GLU:N    | 2.33                     | 0.62              |
| 4:J:279:LEU:O    | 4:J:283:LEU:HG    | 1.98                     | 0.62              |
| 6:L:149:ASP:O    | 6:L:153:ALA:N     | 2.26                     | 0.62              |
| 3:I:66:SER:HB3   | 3:I:104:ILE:HG22  | 1.82                     | 0.62              |
| 3:I:750:ILE:HG21 | 3:I:966:ILE:CD1   | 2.28                     | 0.62              |
| 3:I:1142:ARG:HG3 | 3:I:1161:LEU:HD23 | 1.81                     | 0.62              |
| 4:J:254:PRO:HA   | 4:J:260:PHE:HD2   | 1.65                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:909:ILE:HD11  | 4:J:913:GLU:HB3   | 1.82                     | 0.62              |
| 7:O:39:DG:H1'     | 7:O:40:DC:H5'     | 1.80                     | 0.62              |
| 3:I:149:LEU:HD22  | 3:I:530:ILE:HG21  | 1.82                     | 0.62              |
| 3:I:172:TYR:HB3   | 3:I:432:LEU:HD11  | 1.81                     | 0.62              |
| 3:I:361:SER:HA    | 3:I:364:VAL:HG22  | 1.81                     | 0.62              |
| 4:J:42:GLU:OE2    | 6:L:451:ARG:NH1   | 2.32                     | 0.62              |
| 4:J:1146:GLU:OE1  | 4:J:1308:GLY:HA3  | 2.00                     | 0.62              |
| 6:L:426:LYS:CB    | 7:O:52:DA:H5'     | 2.30                     | 0.62              |
| 3:I:59:ILE:N      | 3:I:68:LEU:O      | 2.21                     | 0.62              |
| 3:I:1083:GLU:OE1  | 3:I:1083:GLU:N    | 2.30                     | 0.62              |
| 4:J:260:PHE:CB    | 6:L:504:PRO:HB3   | 2.29                     | 0.62              |
| 4:J:1155:ILE:O    | 4:J:1156:LEU:HD13 | 2.00                     | 0.62              |
| 4:J:1162:ILE:HD12 | 4:J:1202:GLU:C    | 2.25                     | 0.62              |
| 6:L:145:LEU:HD11  | 6:L:225:ARG:HA    | 1.82                     | 0.62              |
| 6:L:291:CYS:HB3   | 6:L:297:MET:SD    | 2.40                     | 0.62              |
| 6:L:326:TRP:HA    | 6:L:329:LYS:HD2   | 1.81                     | 0.62              |
| 2:M:295:LEU:HD21  | 2:M:300:LEU:HB2   | 1.81                     | 0.62              |
| 2:G:61:ILE:HD12   | 2:G:64:VAL:HG21   | 1.82                     | 0.62              |
| 2:H:74:VAL:HG12   | 2:H:133:LEU:HA    | 1.82                     | 0.62              |
| 3:I:120:GLN:HB3   | 3:I:489:PRO:HD2   | 1.82                     | 0.62              |
| 3:I:289:VAL:HG11  | 3:I:319:LEU:HD12  | 1.81                     | 0.62              |
| 3:I:371:ARG:HB3   | 3:I:374:GLU:OE2   | 1.99                     | 0.62              |
| 4:J:405:GLU:O     | 4:J:408:VAL:HG22  | 2.00                     | 0.62              |
| 10:J:1504:1N7:C3  | 10:J:1504:1N7:C2  | 2.72                     | 0.62              |
| 2:M:313:SER:O     | 2:M:316:MET:HG3   | 2.00                     | 0.62              |
| 4:J:133:ARG:O     | 4:J:137:ARG:HD3   | 2.01                     | 0.61              |
| 4:J:958:ILE:HD11  | 4:J:1011:VAL:HG21 | 1.81                     | 0.61              |
| 3:I:256:GLU:HA    | 3:I:261:VAL:HA    | 1.82                     | 0.61              |
| 3:I:770:CYS:HB3   | 3:I:785:ASP:OD2   | 2.00                     | 0.61              |
| 4:J:555:TYR:CE1   | 4:J:565:ALA:HB2   | 2.35                     | 0.61              |
| 4:J:559:ALA:HB3   | 4:J:562:GLU:CB    | 2.30                     | 0.61              |
| 6:L:292:VAL:HG11  | 6:L:299:LYS:HD2   | 1.82                     | 0.61              |
| 7:O:37:DA:H2''    | 7:O:38:DG:C8      | 2.35                     | 0.61              |
| 2:G:57:THR:HG21   | 2:G:147:GLN:HG2   | 1.83                     | 0.61              |
| 3:I:60:GLN:HG2    | 3:I:61:SER:O      | 2.00                     | 0.61              |
| 4:J:792:ASN:HB2   | 4:J:795:TYR:CD1   | 2.35                     | 0.61              |
| 4:J:1035:VAL:HG21 | 4:J:1113:VAL:HB   | 1.82                     | 0.61              |
| 6:L:426:LYS:N     | 7:O:52:DA:OP2     | 2.33                     | 0.61              |
| 2:G:113:ALA:HB2   | 2:G:126:PRO:CB    | 2.30                     | 0.61              |
| 2:G:226:GLU:HG2   | 2:H:10:LYS:CE     | 2.30                     | 0.61              |
| 2:H:25:LYS:HG2    | 2:H:204:GLU:HG3   | 1.82                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:905:ILE:HG22 | 3:I:906:PHE:CD1   | 2.36                     | 0.61              |
| 4:J:430:HIS:HD2  | 4:J:432:LEU:HB2   | 1.64                     | 0.61              |
| 4:J:553:THR:HB   | 4:J:567:THR:HG22  | 1.82                     | 0.61              |
| 4:J:1268:ASN:HA  | 4:J:1276:GLU:HG3  | 1.83                     | 0.61              |
| 6:L:333:VAL:CG2  | 6:L:337:VAL:HG23  | 2.29                     | 0.61              |
| 3:I:420:LEU:HD13 | 3:I:425:ILE:HD11  | 1.81                     | 0.61              |
| 3:I:685:MET:CG   | 3:I:1235:LEU:HD11 | 2.26                     | 0.61              |
| 3:I:911:SER:OG   | 3:I:912:ASP:N     | 2.33                     | 0.61              |
| 4:J:957:SER:HB3  | 4:J:985:ILE:HB    | 1.83                     | 0.61              |
| 6:L:148:TYR:HA   | 6:L:161:LEU:HD11  | 1.81                     | 0.61              |
| 3:I:1136:GLN:HG3 | 3:I:1140:LYS:HZ1  | 1.64                     | 0.61              |
| 4:J:88:CYS:SG    | 4:J:90:VAL:HG12   | 2.41                     | 0.61              |
| 4:J:961:SER:O    | 4:J:980:THR:HA    | 2.00                     | 0.61              |
| 4:J:1052:GLU:HA  | 4:J:1055:GLY:HA2  | 1.81                     | 0.61              |
| 4:J:1221:LEU:HA  | 4:J:1225:GLY:O    | 2.00                     | 0.61              |
| 6:L:9:LEU:O      | 6:L:13:VAL:HG13   | 2.01                     | 0.61              |
| 6:L:573:LEU:HB3  | 8:P:56:DG:OP2     | 2.00                     | 0.61              |
| 6:L:583:THR:HB   | 6:L:586:ARG:CB    | 2.30                     | 0.61              |
| 1:N:46:GLU:HA    | 1:N:49:ARG:CG     | 2.28                     | 0.61              |
| 2:G:45:ARG:NH2   | 3:I:1215:GLY:O    | 2.29                     | 0.61              |
| 2:G:102:LEU:HB2  | 2:G:142:MET:CG    | 2.31                     | 0.61              |
| 3:I:700:VAL:O    | 3:I:1069:ARG:NH2  | 2.33                     | 0.61              |
| 3:I:745:GLU:HG2  | 3:I:971:LEU:HD11  | 1.82                     | 0.61              |
| 4:J:851:PRO:HD3  | 4:J:877:VAL:HG12  | 1.83                     | 0.61              |
| 4:J:1021:ASP:OD1 | 4:J:1023:HIS:N    | 2.32                     | 0.61              |
| 4:J:1061:VAL:HB  | 4:J:1105:ALA:HB3  | 1.82                     | 0.61              |
| 2:H:211:ILE:HG12 | 2:H:215:GLU:OE1   | 2.01                     | 0.61              |
| 3:I:153:PRO:O    | 3:I:401:GLY:HA2   | 2.00                     | 0.61              |
| 3:I:249:GLU:O    | 3:I:268:ARG:HD3   | 2.00                     | 0.61              |
| 3:I:409:LEU:HD12 | 3:I:427:ASP:HB3   | 1.82                     | 0.61              |
| 4:J:110:PRO:HB2  | 4:J:182:ALA:HB1   | 1.83                     | 0.61              |
| 5:K:56:GLU:OE1   | 5:K:58:LEU:HB2    | 2.00                     | 0.61              |
| 8:P:49:DT:H2'    | 8:P:50:DT:H71     | 1.82                     | 0.61              |
| 2:G:29:GLU:OE1   | 2:G:200:LYS:HG3   | 2.01                     | 0.61              |
| 3:I:358:ASP:OD1  | 3:I:361:SER:HB3   | 2.01                     | 0.61              |
| 3:I:803:ALA:HB2  | 3:I:1094:VAL:HG21 | 1.81                     | 0.61              |
| 3:I:1105:SER:HB2 | 4:J:731:ARG:HG2   | 1.83                     | 0.61              |
| 3:I:1164:PHE:HA  | 3:I:1168:GLU:OE1  | 2.01                     | 0.61              |
| 6:L:586:ARG:NH1  | 6:L:586:ARG:O     | 2.33                     | 0.61              |
| 3:I:434:ASP:HA   | 3:I:437:ASN:HB3   | 1.83                     | 0.61              |
| 3:I:528:ARG:NH2  | 3:I:576:SER:O     | 2.32                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:40:LYS:HB3    | 4:J:42:GLU:OE1    | 2.00                     | 0.61              |
| 4:J:52:GLU:HG3    | 4:J:53:ARG:H      | 1.66                     | 0.61              |
| 4:J:254:PRO:HA    | 4:J:260:PHE:CD2   | 2.36                     | 0.61              |
| 4:J:1163:VAL:HG23 | 4:J:1177:ILE:HG13 | 1.83                     | 0.61              |
| 4:J:1175:LEU:CD1  | 4:J:1200:GLU:HB3  | 2.30                     | 0.61              |
| 3:I:733:VAL:HG23  | 3:I:750:ILE:HG22  | 1.83                     | 0.60              |
| 4:J:968:ASN:HB3   | 4:J:974:VAL:HG22  | 1.82                     | 0.60              |
| 4:J:1042:ASP:OD1  | 4:J:1059:LEU:HD21 | 2.01                     | 0.60              |
| 4:J:1194:ARG:CG   | 4:J:1212:ASP:HB2  | 2.31                     | 0.60              |
| 4:J:1219:ASP:OD1  | 4:J:1222:ARG:NH2  | 2.34                     | 0.60              |
| 6:L:316:PHE:CZ    | 6:L:337:VAL:HB    | 2.36                     | 0.60              |
| 6:L:390:ILE:HD13  | 6:L:432:THR:HG23  | 1.83                     | 0.60              |
| 2:M:266:SER:HA    | 2:M:269:CYS:SG    | 2.41                     | 0.60              |
| 4:J:107:LEU:HA    | 4:J:276:ASN:HD21  | 1.64                     | 0.60              |
| 6:L:270:VAL:O     | 6:L:274:ARG:N     | 2.31                     | 0.60              |
| 4:J:573:THR:HG22  | 4:J:575:GLY:N     | 2.14                     | 0.60              |
| 1:N:14:GLN:O      | 1:N:18:THR:HG23   | 2.00                     | 0.60              |
| 2:H:44:ARG:HH12   | 4:J:538:ARG:HH11  | 1.48                     | 0.60              |
| 3:I:98:VAL:O      | 3:I:122:VAL:N     | 2.33                     | 0.60              |
| 3:I:255:ILE:CG2   | 3:I:262:TYR:HB2   | 2.30                     | 0.60              |
| 3:I:351:LEU:HA    | 3:I:354:ASP:OD1   | 2.02                     | 0.60              |
| 4:J:265:LEU:HD11  | 4:J:330:MET:SD    | 2.40                     | 0.60              |
| 3:I:256:GLU:CB    | 3:I:261:VAL:HG22  | 2.31                     | 0.60              |
| 3:I:317:LEU:HB2   | 3:I:321:LEU:CB    | 2.29                     | 0.60              |
| 4:J:986:ASP:HB2   | 4:J:992:LYS:HG3   | 1.83                     | 0.60              |
| 6:L:13:VAL:O      | 6:L:17:LYS:HE3    | 2.02                     | 0.60              |
| 6:L:16:GLY:HA2    | 6:L:22:LEU:HD11   | 1.83                     | 0.60              |
| 3:I:228:VAL:N     | 3:I:335:THR:O     | 2.30                     | 0.60              |
| 3:I:475:VAL:HG22  | 3:I:492:MET:O     | 2.01                     | 0.60              |
| 3:I:633:LEU:HG    | 3:I:644:LEU:HB3   | 1.82                     | 0.60              |
| 3:I:1125:GLY:HA3  | 3:I:1179:GLY:HA2  | 1.83                     | 0.60              |
| 4:J:423:LEU:CD1   | 4:J:468:VAL:HG12  | 2.31                     | 0.60              |
| 4:J:513:MET:SD    | 4:J:579:LEU:HB2   | 2.42                     | 0.60              |
| 6:L:279:ARG:O     | 6:L:283:GLN:HG2   | 2.02                     | 0.60              |
| 2:H:13:LEU:HD11   | 2:H:15:ASP:O      | 2.02                     | 0.60              |
| 2:H:190:ALA:HB2   | 2:H:200:LYS:HB2   | 1.83                     | 0.60              |
| 3:I:1161:LEU:HG   | 3:I:1164:PHE:CD2  | 2.34                     | 0.60              |
| 4:J:796:LEU:HD12  | 4:J:1142:ALA:HB2  | 1.83                     | 0.60              |
| 4:J:910:ASN:CG    | 5:K:15:ASN:HA     | 2.27                     | 0.60              |
| 6:L:286:LEU:O     | 6:L:337:VAL:HG22  | 2.01                     | 0.60              |
| 6:L:384:LEU:O     | 6:L:387:VAL:HG12  | 2.02                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:474:MET:HE3   | 6:L:482:GLU:OE1   | 2.01                     | 0.60              |
| 6:L:605:GLU:HA    | 6:L:608:ARG:HG2   | 1.82                     | 0.60              |
| 2:G:8:PHE:HA      | 2:G:32:GLU:OE2    | 2.02                     | 0.60              |
| 3:I:519:ASN:O     | 3:I:523:GLU:HG2   | 2.02                     | 0.60              |
| 3:I:801:ARG:HD2   | 3:I:1229:TYR:OH   | 2.01                     | 0.60              |
| 3:I:857:VAL:HG21  | 3:I:862:LEU:HD21  | 1.83                     | 0.60              |
| 3:I:1043:ALA:HB1  | 3:I:1044:PRO:HD2  | 1.83                     | 0.60              |
| 3:I:1131:MET:HE1  | 3:I:1141:LEU:HA   | 1.84                     | 0.60              |
| 4:J:59:ALA:HB2    | 4:J:71:LEU:HD22   | 1.83                     | 0.60              |
| 4:J:839:VAL:CG1   | 4:J:864:LEU:HD12  | 2.31                     | 0.60              |
| 2:M:286:GLU:CG    | 2:M:300:LEU:HD21  | 2.31                     | 0.60              |
| 3:I:870:ILE:HD13  | 3:I:884:VAL:HG13  | 1.83                     | 0.60              |
| 4:J:959:LYS:NZ    | 4:J:961:SER:OG    | 2.34                     | 0.60              |
| 4:J:1039:ASP:OD2  | 4:J:1074:LEU:HB3  | 2.01                     | 0.60              |
| 6:L:12:LEU:HB3    | 6:L:30:HIS:ND1    | 2.16                     | 0.60              |
| 2:H:24:ALA:HB3    | 2:H:213:PRO:HG2   | 1.84                     | 0.60              |
| 3:I:862:LEU:HB3   | 3:I:865:LEU:HD23  | 1.84                     | 0.60              |
| 3:I:1016:GLU:O    | 3:I:1020:GLU:HG2  | 2.01                     | 0.60              |
| 4:J:809:VAL:HG12  | 4:J:911:LYS:HA    | 1.82                     | 0.60              |
| 4:J:813:ASP:OD1   | 4:J:883:ARG:NH2   | 2.35                     | 0.60              |
| 6:L:15:ARG:HA     | 6:L:18:GLU:OE1    | 2.01                     | 0.60              |
| 6:L:375:ALA:HA    | 6:L:378:GLU:OE1   | 2.01                     | 0.60              |
| 6:L:584:ARG:HH22  | 8:P:57:DT:H71     | 1.67                     | 0.60              |
| 3:I:1288:GLN:O    | 3:I:1292:THR:HB   | 2.02                     | 0.59              |
| 4:J:980:THR:HG23  | 4:J:997:VAL:HB    | 1.84                     | 0.59              |
| 4:J:1237:VAL:CG1  | 4:J:1253:ILE:HD13 | 2.32                     | 0.59              |
| 4:J:1318:SER:OG   | 4:J:1319:PHE:N    | 2.31                     | 0.59              |
| 10:N:102:1N7:C3   | 10:N:102:1N7:C18  | 2.71                     | 0.59              |
| 2:H:35:PHE:HA     | 2:H:38:THR:HG22   | 1.83                     | 0.59              |
| 3:I:174:ALA:CB    | 3:I:432:LEU:HD22  | 2.31                     | 0.59              |
| 3:I:203:LYS:O     | 3:I:204:LEU:HD23  | 2.01                     | 0.59              |
| 3:I:469:VAL:O     | 3:I:472:GLU:HG3   | 2.02                     | 0.59              |
| 3:I:521:LEU:HD12  | 3:I:667:LEU:HD12  | 1.83                     | 0.59              |
| 3:I:1024:GLU:HA   | 3:I:1027:LYS:CE   | 2.31                     | 0.59              |
| 3:I:1234:LYS:HZ3  | 3:I:1238:LEU:HD21 | 1.67                     | 0.59              |
| 4:J:20:ILE:CD1    | 4:J:1344:LEU:HD11 | 2.32                     | 0.59              |
| 4:J:117:LEU:HG    | 4:J:118:LYS:HG2   | 1.84                     | 0.59              |
| 6:L:386:LEU:O     | 6:L:389:SER:OG    | 2.11                     | 0.59              |
| 3:I:80:PHE:CE2    | 3:I:88:ARG:HD2    | 2.37                     | 0.59              |
| 3:I:1117:LEU:HD21 | 3:I:1182:ILE:HD12 | 1.85                     | 0.59              |
| 6:L:162:ILE:HD13  | 6:L:221:PHE:CE2   | 2.37                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:360:ASP:HA    | 6:L:363:ARG:HB3   | 1.85                     | 0.59              |
| 6:L:525:ASP:OD1   | 6:L:527:THR:N     | 2.32                     | 0.59              |
| 1:N:36:LEU:HD23   | 1:N:43:PRO:HA     | 1.83                     | 0.59              |
| 3:I:215:TYR:HB3   | 3:I:220:ILE:HD11  | 1.83                     | 0.59              |
| 3:I:965:GLN:O     | 3:I:968:GLU:HG3   | 2.02                     | 0.59              |
| 3:I:1013:GLN:HG2  | 3:I:1017:GLN:NE2  | 2.17                     | 0.59              |
| 6:L:551:LEU:HD21  | 6:L:598:LEU:HD21  | 1.83                     | 0.59              |
| 6:L:595:LEU:HA    | 6:L:598:LEU:HB2   | 1.85                     | 0.59              |
| 2:G:49:SER:OG     | 3:I:1083:GLU:OE2  | 2.20                     | 0.59              |
| 3:I:28:LEU:HD21   | 3:I:524:ILE:HG13  | 1.84                     | 0.59              |
| 3:I:266:GLY:O     | 3:I:267:ARG:NE    | 2.34                     | 0.59              |
| 3:I:670:PHE:HZ    | 3:I:1117:LEU:HD13 | 1.68                     | 0.59              |
| 3:I:798:GLN:HB3   | 3:I:827:ARG:HH22  | 1.68                     | 0.59              |
| 3:I:1064:ASP:O    | 3:I:1076:ILE:HG22 | 2.03                     | 0.59              |
| 4:J:441:LEU:O     | 4:J:442:ILE:HD13  | 2.03                     | 0.59              |
| 7:O:40:DC:C1'     | 7:O:41:DT:H5'     | 2.32                     | 0.59              |
| 2:G:29:GLU:HB3    | 2:G:30:PRO:HD3    | 1.83                     | 0.59              |
| 3:I:1291:LEU:CD2  | 4:J:1351:VAL:HG13 | 2.33                     | 0.59              |
| 4:J:388:ARG:CB    | 4:J:390:LEU:HD13  | 2.32                     | 0.59              |
| 4:J:783:LEU:HA    | 4:J:786:THR:HG22  | 1.85                     | 0.59              |
| 4:J:1049:GLN:NE2  | 4:J:1060:VAL:HB   | 2.18                     | 0.59              |
| 6:L:347:ILE:HA    | 6:L:350:GLU:HB2   | 1.84                     | 0.59              |
| 6:L:368:GLY:O     | 6:L:372:ALA:N     | 2.23                     | 0.59              |
| 6:L:567:MET:HE3   | 6:L:569:THR:OG1   | 2.02                     | 0.59              |
| 7:O:56:DC:H2''    | 7:O:57:DT:O5'     | 2.02                     | 0.59              |
| 2:M:250:ASP:HB3   | 2:M:253:LEU:CD2   | 2.33                     | 0.59              |
| 3:I:106:GLU:HG2   | 3:I:109:ALA:HB3   | 1.83                     | 0.59              |
| 3:I:1117:LEU:HD12 | 3:I:1195:ILE:HG12 | 1.85                     | 0.59              |
| 3:I:1243:MET:SD   | 4:J:372:MET:HG3   | 2.42                     | 0.59              |
| 4:J:885:VAL:HG13  | 4:J:894:VAL:HG11  | 1.83                     | 0.59              |
| 4:J:1178:THR:HA   | 4:J:1184:ASP:HB3  | 1.83                     | 0.59              |
| 6:L:94:THR:HG22   | 6:L:96:ASP:H      | 1.67                     | 0.59              |
| 6:L:412:LEU:O     | 6:L:416:VAL:HG23  | 2.02                     | 0.59              |
| 8:P:65:DT:H1'     | 8:P:66:DT:H5'     | 1.85                     | 0.59              |
| 3:I:966:ILE:HG23  | 10:I:1401:1N7:H25 | 1.85                     | 0.59              |
| 3:I:1072:ASN:ND2  | 3:I:1111:GLN:OE1  | 2.36                     | 0.59              |
| 4:J:226:ALA:HA    | 4:J:229:GLN:HE21  | 1.67                     | 0.59              |
| 4:J:664:ILE:CG2   | 4:J:678:ARG:HG2   | 2.33                     | 0.59              |
| 6:L:134:VAL:HG22  | 6:L:273:MET:CE    | 2.28                     | 0.59              |
| 6:L:158:LEU:HD22  | 6:L:218:ARG:HD3   | 1.84                     | 0.59              |
| 6:L:361:ILE:HA    | 6:L:364:ARG:NH2   | 2.16                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1128:ILE:HG13 | 3:I:1144:PHE:HE2  | 1.68                     | 0.59              |
| 4:J:289:ASP:HA    | 4:J:292:VAL:HG22  | 1.85                     | 0.59              |
| 4:J:342:LEU:HG    | 4:J:1352:ILE:HD13 | 1.84                     | 0.59              |
| 4:J:515:ARG:O     | 4:J:545:HIS:HB2   | 2.03                     | 0.59              |
| 6:L:130:VAL:HA    | 6:L:365:MET:HG3   | 1.83                     | 0.59              |
| 8:P:59:DA:H2''    | 8:P:60:DA:O5'     | 2.01                     | 0.59              |
| 8:P:67:DT:H5''    | 2:M:298:LYS:CB    | 2.31                     | 0.59              |
| 3:I:588:GLU:HG2   | 3:I:607:SER:N     | 2.17                     | 0.59              |
| 3:I:758:ARG:NH2   | 3:I:762:ASN:OD1   | 2.28                     | 0.59              |
| 3:I:833:ILE:HA    | 3:I:1055:ALA:HA   | 1.84                     | 0.59              |
| 3:I:906:PHE:HD2   | 6:L:611:LEU:HD21  | 1.68                     | 0.59              |
| 3:I:918:LEU:HD12  | 3:I:919:ARG:H     | 1.67                     | 0.59              |
| 3:I:936:ARG:HB3   | 3:I:939:VAL:CG2   | 2.32                     | 0.59              |
| 4:J:1176:VAL:HG12 | 4:J:1184:ASP:HB2  | 1.84                     | 0.59              |
| 6:L:150:ARG:HB3   | 6:L:155:GLU:HB2   | 1.85                     | 0.59              |
| 6:L:231:THR:CG2   | 6:L:249:ILE:HG13  | 2.32                     | 0.59              |
| 6:L:466:ILE:HG23  | 6:L:469:GLN:HE21  | 1.67                     | 0.59              |
| 3:I:1010:GLN:O    | 3:I:1013:GLN:HB3  | 2.03                     | 0.58              |
| 4:J:194:LEU:HB3   | 4:J:228:VAL:HG22  | 1.85                     | 0.58              |
| 4:J:621:ALA:O     | 4:J:624:ILE:HG22  | 2.03                     | 0.58              |
| 4:J:1322:ALA:HA   | 4:J:1325:PHE:HE1  | 1.68                     | 0.58              |
| 6:L:544:THR:HG22  | 6:L:607:LEU:HD21  | 1.85                     | 0.58              |
| 1:N:5:ALA:H       | 3:I:681:MET:HE1   | 1.68                     | 0.58              |
| 2:H:214:GLU:O     | 2:H:218:ARG:NE    | 2.35                     | 0.58              |
| 3:I:177:ILE:HG23  | 3:I:183:TRP:CD1   | 2.38                     | 0.58              |
| 3:I:314:ASN:O     | 3:I:315:MET:HG3   | 2.03                     | 0.58              |
| 3:I:871:VAL:HG13  | 3:I:883:LEU:O     | 2.03                     | 0.58              |
| 3:I:1072:ASN:HD21 | 3:I:1230:MET:HE1  | 1.67                     | 0.58              |
| 6:L:130:VAL:O     | 6:L:134:VAL:HG23  | 2.03                     | 0.58              |
| 7:O:40:DC:H1'     | 7:O:41:DT:H5'     | 1.85                     | 0.58              |
| 2:H:102:LEU:O     | 2:H:141:SER:HA    | 2.03                     | 0.58              |
| 3:I:719:LYS:N     | 3:I:751:TYR:OH    | 2.24                     | 0.58              |
| 4:J:85:CYS:SG     | 4:J:86:GLU:N      | 2.76                     | 0.58              |
| 2:G:44:ARG:O      | 2:G:48:LEU:HG     | 2.03                     | 0.58              |
| 3:I:302:ILE:CG2   | 3:I:309:LEU:HA    | 2.33                     | 0.58              |
| 3:I:914:LYS:HG2   | 3:I:915:ASP:H     | 1.68                     | 0.58              |
| 4:J:384:LYS:HG3   | 4:J:415:VAL:HG12  | 1.86                     | 0.58              |
| 4:J:430:HIS:CD2   | 4:J:432:LEU:HB2   | 2.38                     | 0.58              |
| 4:J:694:SER:O     | 4:J:697:MET:HG3   | 2.04                     | 0.58              |
| 4:J:1281:GLU:OE2  | 4:J:1284:ARG:HG2  | 2.03                     | 0.58              |
| 6:L:315:TRP:CZ3   | 6:L:316:PHE:HB2   | 2.38                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:110:VAL:N     | 2:H:131:CYS:O     | 2.36                     | 0.58              |
| 2:H:192:VAL:HG22  | 2:H:193:GLU:OE1   | 2.04                     | 0.58              |
| 3:I:97:ARG:HH22   | 6:L:475:GLY:HA2   | 1.68                     | 0.58              |
| 3:I:302:ILE:HG22  | 3:I:309:LEU:HD12  | 1.84                     | 0.58              |
| 3:I:565:GLU:OE1   | 3:I:565:GLU:N     | 2.29                     | 0.58              |
| 3:I:753:LEU:HD23  | 3:I:767:GLN:HB2   | 1.86                     | 0.58              |
| 3:I:1103:VAL:HG22 | 3:I:1104:PRO:HD3  | 1.86                     | 0.58              |
| 4:J:442:ILE:HG22  | 4:J:443:GLU:O     | 2.03                     | 0.58              |
| 4:J:527:LEU:HD23  | 4:J:533:ALA:HB2   | 1.84                     | 0.58              |
| 4:J:1156:LEU:CD1  | 4:J:1209:VAL:HA   | 2.33                     | 0.58              |
| 6:L:454:VAL:O     | 6:L:458:GLU:N     | 2.35                     | 0.58              |
| 8:P:42:DT:H2'     | 8:P:43:DT:C7      | 2.34                     | 0.58              |
| 3:I:11:ILE:HG22   | 3:I:1172:LEU:HD11 | 1.86                     | 0.58              |
| 3:I:446:ASP:HB3   | 3:I:546:GLU:O     | 2.03                     | 0.58              |
| 3:I:690:VAL:HG22  | 3:I:1236:ASN:HB3  | 1.85                     | 0.58              |
| 4:J:422:LEU:O     | 4:J:468:VAL:HA    | 2.02                     | 0.58              |
| 4:J:548:VAL:O     | 4:J:572:THR:N     | 2.28                     | 0.58              |
| 6:L:41:ILE:O      | 6:L:45:ILE:HG13   | 2.04                     | 0.58              |
| 6:L:151:VAL:CG2   | 6:L:161:LEU:HD12  | 2.34                     | 0.58              |
| 6:L:157:ARG:HG2   | 6:L:160:ASP:N     | 2.18                     | 0.58              |
| 6:L:271:ASN:O     | 6:L:275:VAL:HG23  | 2.04                     | 0.58              |
| 6:L:385:ARG:HB2   | 7:O:54:DT:H1'     | 1.85                     | 0.58              |
| 6:L:548:LEU:HA    | 6:L:551:LEU:CD1   | 2.34                     | 0.58              |
| 3:I:103:VAL:HA    | 3:I:117:ILE:HG22  | 1.86                     | 0.58              |
| 3:I:569:ILE:CD1   | 4:J:783:LEU:HD22  | 2.33                     | 0.58              |
| 4:J:700:ASN:O     | 4:J:704:GLU:HB2   | 2.03                     | 0.58              |
| 4:J:1322:ALA:HA   | 4:J:1325:PHE:CE1  | 2.39                     | 0.58              |
| 4:J:1356:LEU:HD12 | 4:J:1365:TYR:CG   | 2.39                     | 0.58              |
| 6:L:583:THR:OG1   | 7:O:26:DT:OP2     | 2.20                     | 0.58              |
| 7:O:16:DC:C2'     | 7:O:17:DA:H5'     | 2.34                     | 0.58              |
| 2:G:97:GLU:OE1    | 2:G:99:ILE:HG13   | 2.04                     | 0.58              |
| 3:I:66:SER:HA     | 3:I:104:ILE:HA    | 1.85                     | 0.58              |
| 3:I:66:SER:CB     | 3:I:104:ILE:HG22  | 2.33                     | 0.58              |
| 3:I:98:VAL:HB     | 3:I:122:VAL:CG1   | 2.34                     | 0.58              |
| 4:J:808:VAL:O     | 4:J:810:THR:HG23  | 2.04                     | 0.58              |
| 4:J:984:LEU:O     | 4:J:992:LYS:HB2   | 2.04                     | 0.58              |
| 4:J:1109:LEU:HD12 | 4:J:1109:LEU:H    | 1.69                     | 0.58              |
| 6:L:253:SER:HA    | 6:L:256:PHE:HB3   | 1.85                     | 0.58              |
| 6:L:285:ARG:O     | 6:L:289:LYS:HB3   | 2.04                     | 0.58              |
| 6:L:576:VAL:CG1   | 6:L:587:ILE:HG21  | 2.33                     | 0.58              |
| 2:G:68:TYR:HB3    | 3:I:756:TYR:HD2   | 1.68                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:125:LYS:HG3   | 2:G:127:GLN:OE1   | 2.04                     | 0.58              |
| 3:I:147:SER:HB2   | 3:I:530:ILE:HD13  | 1.86                     | 0.58              |
| 3:I:564:PRO:O     | 3:I:569:ILE:HG12  | 2.03                     | 0.58              |
| 4:J:915:ILE:HA    | 4:J:918:ILE:CG1   | 2.34                     | 0.58              |
| 4:J:1266:ILE:HB   | 4:J:1276:GLU:O    | 2.04                     | 0.58              |
| 4:J:1325:PHE:CE2  | 4:J:1326:GLN:HG3  | 2.38                     | 0.58              |
| 6:L:137:TYR:CD2   | 6:L:276:MET:HE1   | 2.39                     | 0.58              |
| 6:L:151:VAL:HG21  | 6:L:161:LEU:HD12  | 1.85                     | 0.58              |
| 6:L:231:THR:HA    | 6:L:248:GLU:OE1   | 2.03                     | 0.58              |
| 6:L:386:LEU:HB2   | 7:O:54:DT:O2      | 2.03                     | 0.58              |
| 3:I:255:ILE:HB    | 3:I:263:VAL:H     | 1.69                     | 0.58              |
| 3:I:628:HIS:HB3   | 3:I:647:ARG:NH2   | 2.18                     | 0.58              |
| 3:I:1060:ILE:HD11 | 3:I:1066:MET:HE3  | 1.84                     | 0.58              |
| 4:J:378:LYS:HB3   | 4:J:379:PRO:HD3   | 1.85                     | 0.58              |
| 4:J:1061:VAL:CG2  | 4:J:1105:ALA:HB3  | 2.33                     | 0.58              |
| 4:J:1172:LYS:HB3  | 4:J:1190:ILE:C    | 2.28                     | 0.58              |
| 4:J:1175:LEU:O    | 4:J:1187:GLU:HG2  | 2.04                     | 0.58              |
| 4:J:1369:ARG:O    | 4:J:1373:ARG:N    | 2.35                     | 0.58              |
| 6:L:113:ARG:O     | 6:L:117:ILE:HD12  | 2.04                     | 0.58              |
| 6:L:339:ARG:HB3   | 6:L:343:LYS:NZ    | 2.19                     | 0.58              |
| 6:L:370:ALA:O     | 6:L:374:ARG:N     | 2.32                     | 0.58              |
| 6:L:605:GLU:HA    | 6:L:608:ARG:CG    | 2.34                     | 0.58              |
| 1:N:51:ILE:HG13   | 1:N:52:PHE:H      | 1.69                     | 0.57              |
| 2:H:35:PHE:O      | 2:H:38:THR:HG22   | 2.03                     | 0.57              |
| 3:I:5:TYR:HA      | 3:I:8:LYS:CD      | 2.33                     | 0.57              |
| 3:I:519:ASN:ND2   | 3:I:796:LEU:HD23  | 2.18                     | 0.57              |
| 4:J:148:GLU:HB2   | 4:J:177:ASP:HB2   | 1.86                     | 0.57              |
| 4:J:844:THR:HG23  | 4:J:864:LEU:HD21  | 1.86                     | 0.57              |
| 6:L:162:ILE:HG22  | 6:L:261:LEU:CB    | 2.34                     | 0.57              |
| 6:L:440:THR:HG21  | 8:P:37:DG:OP1     | 2.04                     | 0.57              |
| 1:N:39:ALA:HB3    | 1:N:61:CYS:SG     | 2.44                     | 0.57              |
| 3:I:60:GLN:HA     | 3:I:67:GLU:HA     | 1.87                     | 0.57              |
| 3:I:718:ALA:HB3   | 3:I:779:ARG:O     | 2.04                     | 0.57              |
| 3:I:1010:GLN:O    | 3:I:1014:LEU:HG   | 2.04                     | 0.57              |
| 3:I:1192:GLU:O    | 3:I:1196:LYS:HG2  | 2.04                     | 0.57              |
| 4:J:923:ILE:HD11  | 4:J:1253:ILE:HA   | 1.86                     | 0.57              |
| 8:P:61:DT:H1'     | 8:P:62:DG:C5'     | 2.34                     | 0.57              |
| 2:G:26:VAL:CG2    | 2:G:203:ILE:HB    | 2.33                     | 0.57              |
| 3:I:197:ARG:NH2   | 6:L:29:ASP:OD2    | 2.37                     | 0.57              |
| 3:I:823:VAL:HG23  | 3:I:1060:ILE:HG22 | 1.85                     | 0.57              |
| 3:I:866:ASP:HB3   | 3:I:872:TYR:CE1   | 2.39                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1045:THR:CG2  | 4:J:1074:LEU:HD12 | 2.35                     | 0.57              |
| 4:J:1266:ILE:HD13 | 4:J:1278:GLU:HB3  | 1.86                     | 0.57              |
| 6:L:130:VAL:HG22  | 6:L:365:MET:CG    | 2.34                     | 0.57              |
| 6:L:274:ARG:HA    | 6:L:274:ARG:NH1   | 2.19                     | 0.57              |
| 6:L:573:LEU:HA    | 6:L:576:VAL:HG12  | 1.85                     | 0.57              |
| 6:L:585:GLU:O     | 6:L:588:ARG:HG2   | 2.03                     | 0.57              |
| 3:I:15:PHE:CG     | 3:I:1190:ALA:HB2  | 2.40                     | 0.57              |
| 3:I:70:TYR:HA     | 3:I:100:LEU:CD2   | 2.34                     | 0.57              |
| 3:I:141:THR:HB    | 3:I:514:PHE:HE1   | 1.68                     | 0.57              |
| 3:I:1072:ASN:ND2  | 3:I:1230:MET:HE1  | 2.19                     | 0.57              |
| 4:J:694:SER:OG    | 4:J:738:ARG:NE    | 2.18                     | 0.57              |
| 4:J:826:ILE:HD11  | 4:J:831:VAL:HG13  | 1.85                     | 0.57              |
| 6:L:362:ASN:HA    | 6:L:365:MET:HE2   | 1.86                     | 0.57              |
| 2:G:48:LEU:HD21   | 2:G:183:ILE:HG12  | 1.85                     | 0.57              |
| 2:H:134:THR:HG23  | 2:H:136:GLU:H     | 1.67                     | 0.57              |
| 3:I:274:ILE:HA    | 3:I:277:LEU:HD12  | 1.85                     | 0.57              |
| 3:I:636:CYS:HB2   | 3:I:645:PHE:CD2   | 2.39                     | 0.57              |
| 3:I:1245:ALA:HB2  | 4:J:351:GLY:HA3   | 1.87                     | 0.57              |
| 3:I:1307:ASN:HB3  | 3:I:1312:ASN:O    | 2.04                     | 0.57              |
| 5:K:44:ASP:OD1    | 5:K:52:ARG:NH1    | 2.37                     | 0.57              |
| 2:H:41:ASN:ND2    | 3:I:1217:THR:O    | 2.38                     | 0.57              |
| 3:I:230:PHE:CD2   | 3:I:292:ILE:HD12  | 2.40                     | 0.57              |
| 3:I:1144:PHE:O    | 3:I:1147:ARG:HG2  | 2.04                     | 0.57              |
| 4:J:1120:THR:HB   | 4:J:1123:ARG:HH11 | 1.70                     | 0.57              |
| 6:L:51:MET:N      | 6:L:52:GLY:HA2    | 2.19                     | 0.57              |
| 2:G:192:VAL:HG22  | 2:G:193:GLU:H     | 1.70                     | 0.57              |
| 2:H:183:ILE:HD11  | 2:H:203:ILE:CG2   | 2.34                     | 0.57              |
| 3:I:270:THR:O     | 3:I:273:HIS:HB2   | 2.03                     | 0.57              |
| 3:I:397:LEU:N     | 3:I:418:GLY:O     | 2.24                     | 0.57              |
| 3:I:823:VAL:CG2   | 3:I:1060:ILE:HG22 | 2.35                     | 0.57              |
| 4:J:426:ALA:HB3   | 4:J:427:PRO:HD3   | 1.86                     | 0.57              |
| 4:J:454:CYS:O     | 4:J:458:ASN:N     | 2.38                     | 0.57              |
| 4:J:475:GLU:HG3   | 5:K:24:ALA:CB     | 2.35                     | 0.57              |
| 4:J:821:MET:HE1   | 4:J:879:ALA:CA    | 2.34                     | 0.57              |
| 4:J:1087:ASP:O    | 4:J:1096:PRO:HB3  | 2.05                     | 0.57              |
| 4:J:1329:THR:O    | 4:J:1333:THR:HG23 | 2.05                     | 0.57              |
| 3:I:10:ARG:NH2    | 3:I:791:LEU:HB2   | 2.20                     | 0.57              |
| 3:I:1165:SER:HA   | 3:I:1168:GLU:OE1  | 2.05                     | 0.57              |
| 4:J:306:LEU:CD2   | 4:J:307:LEU:HD23  | 2.35                     | 0.57              |
| 4:J:1037:PHE:HE2  | 4:J:1059:LEU:HB2  | 1.69                     | 0.57              |
| 6:L:343:LYS:O     | 6:L:347:ILE:HG13  | 2.05                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:249:GLU:O     | 3:I:268:ARG:HA    | 2.05                     | 0.57              |
| 3:I:1146:GLN:OE1  | 3:I:1160:ASP:HA   | 2.04                     | 0.57              |
| 6:L:124:GLU:O     | 6:L:127:ILE:HG12  | 2.05                     | 0.57              |
| 6:L:374:ARG:HH12  | 6:L:378:GLU:HG3   | 1.70                     | 0.57              |
| 3:I:174:ALA:HB3   | 3:I:432:LEU:HD22  | 1.85                     | 0.57              |
| 4:J:848:VAL:HB    | 4:J:858:VAL:HG22  | 1.86                     | 0.57              |
| 5:K:29:GLN:HE22   | 5:K:64:LEU:HD22   | 1.70                     | 0.57              |
| 6:L:112:THR:HG23  | 6:L:115:GLY:CA    | 2.32                     | 0.57              |
| 6:L:118:ASP:O     | 6:L:121:LYS:HG2   | 2.05                     | 0.57              |
| 6:L:289:LYS:HA    | 6:L:293:GLU:OE1   | 2.05                     | 0.57              |
| 6:L:392:LYS:CE    | 7:O:56:DC:H4'     | 2.35                     | 0.57              |
| 6:L:541:ARG:O     | 6:L:545:HIS:HB2   | 2.05                     | 0.57              |
| 6:L:557:LYS:HB3   | 6:L:580:PHE:HZ    | 1.69                     | 0.57              |
| 6:L:565:ILE:O     | 6:L:567:MET:HG2   | 2.04                     | 0.57              |
| 8:P:36:DT:H2'     | 8:P:37:DG:H5''    | 1.86                     | 0.57              |
| 8:P:43:DT:C1'     | 8:P:44:DT:H5'     | 2.34                     | 0.57              |
| 3:I:15:PHE:CD2    | 3:I:1190:ALA:HB2  | 2.40                     | 0.56              |
| 3:I:404:LYS:NZ    | 3:I:449:GLY:O     | 2.32                     | 0.56              |
| 4:J:384:LYS:HG3   | 4:J:415:VAL:CG1   | 2.35                     | 0.56              |
| 4:J:623:GLN:O     | 4:J:627:THR:HG22  | 2.05                     | 0.56              |
| 4:J:811:GLU:OE2   | 4:J:890:THR:HG23  | 2.05                     | 0.56              |
| 4:J:909:ILE:HD11  | 4:J:913:GLU:CB    | 2.35                     | 0.56              |
| 2:M:283:GLN:HG2   | 2:M:317:ARG:NH2   | 2.20                     | 0.56              |
| 2:H:13:LEU:HD12   | 2:H:29:GLU:OE2    | 2.04                     | 0.56              |
| 3:I:185:ASP:HB2   | 3:I:197:ARG:CG    | 2.35                     | 0.56              |
| 3:I:596:ASP:OD1   | 3:I:596:ASP:N     | 2.36                     | 0.56              |
| 4:J:46:TYR:OH     | 6:L:453:PRO:HG3   | 2.05                     | 0.56              |
| 4:J:514:THR:OG1   | 4:J:595:ALA:O     | 2.23                     | 0.56              |
| 4:J:610:ARG:HD2   | 4:J:866:GLU:HG2   | 1.88                     | 0.56              |
| 4:J:658:GLU:HA    | 4:J:661:VAL:HG22  | 1.86                     | 0.56              |
| 4:J:1060:VAL:HG22 | 4:J:1107:VAL:N    | 2.13                     | 0.56              |
| 4:J:1064:SER:HB3  | 4:J:1072:LYS:CD   | 2.35                     | 0.56              |
| 6:L:148:TYR:HA    | 6:L:161:LEU:CD1   | 2.35                     | 0.56              |
| 2:G:226:GLU:O     | 2:H:10:LYS:HE2    | 2.05                     | 0.56              |
| 3:I:708:VAL:HG11  | 3:I:794:LEU:HD22  | 1.87                     | 0.56              |
| 4:J:37:GLU:HB2    | 4:J:104:HIS:CE1   | 2.40                     | 0.56              |
| 4:J:153:ASN:HB3   | 4:J:154:LEU:CD1   | 2.34                     | 0.56              |
| 4:J:311:ARG:HH21  | 4:J:1329:THR:HG21 | 1.70                     | 0.56              |
| 4:J:367:GLY:N     | 4:J:448:GLN:HB2   | 2.21                     | 0.56              |
| 4:J:900:GLY:O     | 4:J:908:ILE:HD12  | 2.05                     | 0.56              |
| 4:J:1261:LEU:HD13 | 4:J:1304:ARG:HH11 | 1.71                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:K:15:ASN:ND2    | 5:K:17:PHE:HB2    | 2.20                     | 0.56              |
| 6:L:144:LEU:HD21  | 6:L:221:PHE:CD1   | 2.40                     | 0.56              |
| 6:L:280:VAL:HG21  | 6:L:355:ILE:CG2   | 2.35                     | 0.56              |
| 6:L:439:ILE:HG22  | 6:L:443:ILE:CD1   | 2.36                     | 0.56              |
| 6:L:548:LEU:HA    | 6:L:551:LEU:CG    | 2.35                     | 0.56              |
| 2:H:101:THR:O     | 2:H:102:LEU:HD23  | 2.04                     | 0.56              |
| 2:H:192:VAL:HG12  | 2:H:195:ARG:HB2   | 1.87                     | 0.56              |
| 3:I:3:TYR:CE1     | 3:I:11:ILE:HD11   | 2.40                     | 0.56              |
| 3:I:205:PRO:HG2   | 3:I:355:PRO:HD3   | 1.88                     | 0.56              |
| 3:I:514:PHE:CE2   | 3:I:760:ASN:HB3   | 2.41                     | 0.56              |
| 3:I:944:ARG:HA    | 3:I:947:GLU:OE1   | 2.04                     | 0.56              |
| 3:I:1106:ARG:HD2  | 3:I:1106:ARG:H    | 1.70                     | 0.56              |
| 4:J:60:ARG:HG2    | 4:J:89:GLY:O      | 2.05                     | 0.56              |
| 4:J:195:GLU:HA    | 4:J:198:CYS:SG    | 2.44                     | 0.56              |
| 4:J:201:LEU:HA    | 4:J:204:GLU:HB2   | 1.87                     | 0.56              |
| 4:J:235:GLU:OE1   | 4:J:235:GLU:N     | 2.36                     | 0.56              |
| 4:J:1311:LYS:CD   | 4:J:1314:LEU:HD21 | 2.35                     | 0.56              |
| 6:L:593:LYS:HA    | 6:L:596:ARG:HD3   | 1.87                     | 0.56              |
| 2:G:31:LEU:HB3    | 2:G:199:ASP:OD2   | 2.05                     | 0.56              |
| 3:I:683:ALA:O     | 3:I:686:GLN:HB2   | 2.05                     | 0.56              |
| 3:I:1333:LEU:HB2  | 3:I:1335:ILE:HG12 | 1.86                     | 0.56              |
| 4:J:70:CYS:SG     | 4:J:73:GLY:N      | 2.78                     | 0.56              |
| 4:J:128:LEU:HD11  | 4:J:189:LEU:HD21  | 1.88                     | 0.56              |
| 4:J:171:GLU:HG2   | 4:J:172:PHE:CD2   | 2.41                     | 0.56              |
| 4:J:382:TYR:HE1   | 4:J:401:VAL:HG21  | 1.70                     | 0.56              |
| 4:J:502:PRO:HB2   | 4:J:507:VAL:CG1   | 2.36                     | 0.56              |
| 4:J:643:ASP:HB3   | 4:J:720:ASN:OD1   | 2.06                     | 0.56              |
| 6:L:363:ARG:HG2   | 6:L:367:ILE:HD12  | 1.86                     | 0.56              |
| 6:L:390:ILE:HD12  | 6:L:435:ILE:HG21  | 1.87                     | 0.56              |
| 7:O:33:DA:H2'     | 7:O:33:DA:OP2     | 2.04                     | 0.56              |
| 10:N:102:1N7:C3   | 10:N:102:1N7:C2   | 2.73                     | 0.56              |
| 2:G:165:GLU:HG3   | 2:G:170:ARG:NH2   | 2.21                     | 0.56              |
| 4:J:353:SER:OG    | 4:J:354:VAL:N     | 2.38                     | 0.56              |
| 4:J:1267:VAL:HG21 | 4:J:1301:THR:HG22 | 1.86                     | 0.56              |
| 7:O:37:DA:H2''    | 7:O:38:DG:H8      | 1.70                     | 0.56              |
| 3:I:26:TYR:HE2    | 3:I:28:LEU:HB2    | 1.71                     | 0.56              |
| 3:I:105:TYR:CE1   | 3:I:114:VAL:HG12  | 2.41                     | 0.56              |
| 3:I:363:LEU:HD22  | 3:I:382:GLU:OE1   | 2.05                     | 0.56              |
| 3:I:469:VAL:HA    | 3:I:472:GLU:CG    | 2.36                     | 0.56              |
| 4:J:573:THR:HB    | 4:J:576:ARG:HG3   | 1.87                     | 0.56              |
| 4:J:689:ALA:O     | 4:J:693:VAL:HG23  | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:894:VAL:HG21  | 4:J:915:ILE:HD11  | 1.87                     | 0.56              |
| 4:J:1298:VAL:HG22 | 4:J:1299:GLY:O    | 2.06                     | 0.56              |
| 6:L:124:GLU:O     | 6:L:128:ASN:ND2   | 2.39                     | 0.56              |
| 2:H:64:VAL:HA     | 2:H:65:LEU:HB2    | 1.88                     | 0.56              |
| 2:H:82:LEU:HG     | 2:H:173:VAL:CG1   | 2.35                     | 0.56              |
| 3:I:131:THR:HG22  | 3:I:132:ASP:H     | 1.70                     | 0.56              |
| 3:I:350:THR:O     | 3:I:354:ASP:N     | 2.39                     | 0.56              |
| 3:I:724:VAL:HG12  | 3:I:775:GLU:O     | 2.04                     | 0.56              |
| 3:I:877:VAL:HG11  | 3:I:920:VAL:HG21  | 1.87                     | 0.56              |
| 6:L:476:ARG:HD2   | 6:L:477:GLU:N     | 2.21                     | 0.56              |
| 2:M:307:LEU:HA    | 2:M:312:LEU:HB2   | 1.88                     | 0.56              |
| 2:G:164:ASP:OD2   | 2:G:166:ARG:HG3   | 2.06                     | 0.56              |
| 3:I:339:ASN:ND2   | 3:I:341:LEU:HB3   | 2.21                     | 0.56              |
| 3:I:728:ASP:OD1   | 3:I:729:ALA:N     | 2.38                     | 0.56              |
| 4:J:889:ASP:O     | 4:J:1286:LYS:NZ   | 2.27                     | 0.56              |
| 2:M:253:LEU:HA    | 2:M:278:ILE:HB    | 1.87                     | 0.56              |
| 3:I:478:ARG:NE    | 3:I:492:MET:HE1   | 2.20                     | 0.56              |
| 3:I:839:VAL:CA    | 3:I:1049:ILE:HG22 | 2.28                     | 0.56              |
| 4:J:84:ILE:HG22   | 4:J:91:GLU:HG3    | 1.88                     | 0.56              |
| 4:J:306:LEU:HD23  | 4:J:307:LEU:HD23  | 1.86                     | 0.56              |
| 4:J:355:ILE:HG12  | 4:J:464:ASP:O     | 2.05                     | 0.56              |
| 6:L:162:ILE:HG22  | 6:L:261:LEU:HB3   | 1.88                     | 0.56              |
| 2:G:45:ARG:HG3    | 3:I:1083:GLU:HG3  | 1.88                     | 0.55              |
| 3:I:211:ARG:HH22  | 3:I:217:THR:HG22  | 1.70                     | 0.55              |
| 3:I:942:ASP:OD2   | 3:I:943:LYS:N     | 2.39                     | 0.55              |
| 4:J:37:GLU:HB2    | 4:J:104:HIS:NE2   | 2.21                     | 0.55              |
| 4:J:511:TYR:CD2   | 4:J:728:SER:HB3   | 2.40                     | 0.55              |
| 4:J:548:VAL:HG12  | 4:J:550:VAL:HG23  | 1.86                     | 0.55              |
| 4:J:759:ILE:HD11  | 4:J:774:ILE:CG2   | 2.35                     | 0.55              |
| 4:J:1307:LEU:HD23 | 4:J:1311:LYS:HG3  | 1.88                     | 0.55              |
| 5:K:3:ARG:NH1     | 5:K:55:GLU:OE1    | 2.39                     | 0.55              |
| 6:L:143:TYR:HA    | 6:L:146:GLU:HG3   | 1.88                     | 0.55              |
| 3:I:105:TYR:CD1   | 3:I:114:VAL:HA    | 2.41                     | 0.55              |
| 3:I:860:ALA:O     | 3:I:863:SER:HB3   | 2.06                     | 0.55              |
| 3:I:1234:LYS:NZ   | 3:I:1238:LEU:HD21 | 2.21                     | 0.55              |
| 4:J:343:LEU:HD22  | 4:J:1351:VAL:HG12 | 1.88                     | 0.55              |
| 4:J:363:LEU:CD2   | 4:J:487:THR:HG22  | 2.36                     | 0.55              |
| 4:J:502:PRO:HG2   | 4:J:601:ILE:CD1   | 2.37                     | 0.55              |
| 4:J:1164:SER:O    | 4:J:1175:LEU:HG   | 2.06                     | 0.55              |
| 2:H:4:SER:OG      | 2:H:5:VAL:N       | 2.40                     | 0.55              |
| 3:I:146:VAL:HG12  | 3:I:529:ARG:HB3   | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1064:ASP:OD1  | 3:I:1239:VAL:HG12 | 2.07                     | 0.55              |
| 4:J:59:ALA:HB2    | 4:J:71:LEU:CD2    | 2.36                     | 0.55              |
| 4:J:143:SER:CA    | 4:J:180:MET:HE2   | 2.36                     | 0.55              |
| 4:J:701:LEU:CD2   | 4:J:723:TYR:HB2   | 2.35                     | 0.55              |
| 4:J:998:PRO:HG2   | 4:J:1020:TRP:NE1  | 2.21                     | 0.55              |
| 4:J:1048:ARG:CZ   | 4:J:1059:LEU:HG   | 2.37                     | 0.55              |
| 6:L:235:ILE:HD13  | 6:L:245:ALA:CB    | 2.36                     | 0.55              |
| 8:P:36:DT:C2'     | 8:P:37:DG:H3'     | 2.37                     | 0.55              |
| 2:G:192:VAL:HG11  | 2:G:195:ARG:O     | 2.07                     | 0.55              |
| 2:H:211:ILE:CG1   | 2:H:215:GLU:HB3   | 2.37                     | 0.55              |
| 3:I:204:LEU:HD21  | 3:I:369:MET:SD    | 2.46                     | 0.55              |
| 3:I:321:LEU:HA    | 3:I:324:LYS:CG    | 2.29                     | 0.55              |
| 3:I:349:GLU:O     | 3:I:353:VAL:HG23  | 2.06                     | 0.55              |
| 4:J:144:TYR:CD2   | 4:J:180:MET:HE3   | 2.41                     | 0.55              |
| 4:J:259:ARG:HG2   | 10:L:701:1N7:O2   | 2.07                     | 0.55              |
| 4:J:572:THR:HG21  | 4:J:589:TYR:OH    | 2.06                     | 0.55              |
| 4:J:583:VAL:HG13  | 4:J:584:PRO:HD2   | 1.87                     | 0.55              |
| 4:J:857:LEU:HD21  | 4:J:871:LEU:HD22  | 1.88                     | 0.55              |
| 6:L:128:ASN:HA    | 6:L:131:GLN:OE1   | 2.05                     | 0.55              |
| 6:L:351:THR:CB    | 6:L:358:VAL:HG21  | 2.36                     | 0.55              |
| 2:H:130:ILE:HG22  | 2:H:131:CYS:SG    | 2.46                     | 0.55              |
| 2:H:155:ALA:HA    | 2:H:158:ARG:NH2   | 2.22                     | 0.55              |
| 3:I:10:ARG:HD2    | 3:I:1181:PRO:CG   | 2.37                     | 0.55              |
| 3:I:22:LEU:HD22   | 3:I:603:ILE:CD1   | 2.37                     | 0.55              |
| 3:I:161:LYS:HD2   | 3:I:170:VAL:CG2   | 2.35                     | 0.55              |
| 3:I:731:ARG:NH1   | 3:I:752:ASN:OD1   | 2.39                     | 0.55              |
| 3:I:842:ASP:HA    | 3:I:847:PRO:HA    | 1.89                     | 0.55              |
| 4:J:85:CYS:O      | 4:J:89:GLY:HA2    | 2.05                     | 0.55              |
| 4:J:120:LEU:HD12  | 4:J:1330:ARG:HD3  | 1.88                     | 0.55              |
| 4:J:128:LEU:HD11  | 4:J:189:LEU:CD2   | 2.36                     | 0.55              |
| 4:J:527:LEU:HB2   | 4:J:550:VAL:HG22  | 1.88                     | 0.55              |
| 6:L:484:ALA:O     | 6:L:488:LEU:HA    | 2.07                     | 0.55              |
| 3:I:210:LEU:HD12  | 3:I:429:MET:HE1   | 1.89                     | 0.55              |
| 3:I:1013:GLN:HG2  | 3:I:1017:GLN:HE22 | 1.71                     | 0.55              |
| 4:J:518:VAL:HB    | 4:J:707:ILE:HD12  | 1.88                     | 0.55              |
| 4:J:1032:SER:HA   | 4:J:1116:SER:C    | 2.32                     | 0.55              |
| 4:J:1035:VAL:N    | 4:J:1113:VAL:O    | 2.20                     | 0.55              |
| 10:J:1504:1N7:H31 | 10:J:1504:1N7:H5  | 1.88                     | 0.55              |
| 5:K:38:LEU:HD13   | 5:K:58:LEU:HG     | 1.89                     | 0.55              |
| 6:L:322:MET:HB3   | 6:L:324:LYS:CG    | 2.36                     | 0.55              |
| 6:L:347:ILE:HG22  | 6:L:355:ILE:CD1   | 2.37                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:11:PRO:HD3    | 2:H:227:GLN:OE1   | 2.07                     | 0.55              |
| 2:H:61:ILE:HG22   | 2:H:62:ASP:H      | 1.71                     | 0.55              |
| 3:I:771:VAL:HG11  | 3:I:783:LEU:CD1   | 2.36                     | 0.55              |
| 3:I:1117:LEU:CD2  | 3:I:1182:ILE:HD12 | 2.37                     | 0.55              |
| 4:J:474:LEU:HD21  | 5:K:27:ALA:HB1    | 1.87                     | 0.55              |
| 4:J:825:VAL:O     | 4:J:832:LYS:HB2   | 2.07                     | 0.55              |
| 4:J:949:SER:HB3   | 4:J:1016:THR:HG23 | 1.88                     | 0.55              |
| 6:L:13:VAL:HG11   | 6:L:84:LEU:CD2    | 2.36                     | 0.55              |
| 8:P:58:DC:H5'     | 8:P:58:DC:C6      | 2.41                     | 0.55              |
| 3:I:142:GLU:HB3   | 3:I:515:MET:CE    | 2.36                     | 0.55              |
| 3:I:1252:SER:OG   | 3:I:1255:THR:O    | 2.24                     | 0.55              |
| 4:J:847:ASP:HA    | 4:J:858:VAL:O     | 2.06                     | 0.55              |
| 4:J:1160:SER:CA   | 4:J:1205:GLU:HA   | 2.37                     | 0.55              |
| 4:J:1327:GLU:CD   | 4:J:1330:ARG:HB2  | 2.31                     | 0.55              |
| 6:L:405:ILE:O     | 6:L:409:ASN:ND2   | 2.39                     | 0.55              |
| 3:I:1002:LEU:HD22 | 3:I:1007:LYS:HB2  | 1.89                     | 0.55              |
| 3:I:1132:LEU:HD22 | 3:I:1173:ALA:HB1  | 1.88                     | 0.55              |
| 4:J:515:ARG:HH12  | 4:J:717:VAL:HG23  | 1.72                     | 0.55              |
| 4:J:1347:LEU:HG   | 4:J:1357:ILE:CG2  | 2.36                     | 0.55              |
| 6:L:338:HIS:O     | 6:L:342:GLN:HG3   | 2.07                     | 0.55              |
| 1:N:24:ARG:HG3    | 4:J:684:ASP:OD1   | 2.07                     | 0.55              |
| 2:H:54:CYS:SG     | 2:H:92:VAL:HB     | 2.46                     | 0.55              |
| 2:H:73:GLY:O      | 2:H:134:THR:N     | 2.39                     | 0.55              |
| 3:I:663:VAL:HG23  | 3:I:704:MET:HE2   | 1.88                     | 0.55              |
| 3:I:960:LEU:HA    | 3:I:963:GLU:CG    | 2.37                     | 0.55              |
| 3:I:1270:PHE:O    | 4:J:344:GLY:HA2   | 2.07                     | 0.55              |
| 4:J:129:ASP:OD1   | 4:J:220:ARG:NH1   | 2.33                     | 0.55              |
| 4:J:308:ASP:OD2   | 4:J:311:ARG:NH1   | 2.39                     | 0.55              |
| 4:J:349:TYR:CD2   | 4:J:472:LEU:HD11  | 2.42                     | 0.55              |
| 4:J:653:ILE:HG23  | 4:J:692:ARG:NH1   | 2.22                     | 0.55              |
| 4:J:1115:ILE:HB   | 4:J:1119:ASP:OD2  | 2.07                     | 0.55              |
| 4:J:1172:LYS:CD   | 4:J:1189:MET:HB3  | 2.32                     | 0.55              |
| 6:L:252:LEU:HA    | 6:L:255:VAL:HG22  | 1.89                     | 0.55              |
| 6:L:373:ARG:HB3   | 6:L:377:LYS:NZ    | 2.22                     | 0.55              |
| 6:L:471:LEU:HB2   | 6:L:478:PRO:HD3   | 1.88                     | 0.55              |
| 8:P:60:DA:C2'     | 8:P:61:DT:H71     | 2.36                     | 0.55              |
| 2:H:19:VAL:HG12   | 2:H:20:SER:H      | 1.72                     | 0.54              |
| 3:I:122:VAL:HG22  | 3:I:123:TYR:O     | 2.06                     | 0.54              |
| 3:I:217:THR:HB    | 3:I:313:ALA:HB3   | 1.89                     | 0.54              |
| 3:I:349:GLU:N     | 3:I:349:GLU:OE1   | 2.40                     | 0.54              |
| 3:I:387:ASN:CA    | 3:I:391:SER:HB3   | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:563:THR:HG23  | 3:I:564:PRO:HD2   | 1.88                     | 0.54              |
| 3:I:1103:VAL:HG21 | 4:J:639:VAL:HG11  | 1.88                     | 0.54              |
| 4:J:80:HIS:O      | 4:J:83:VAL:HG12   | 2.06                     | 0.54              |
| 4:J:385:LEU:HD13  | 4:J:400:MET:SD    | 2.47                     | 0.54              |
| 4:J:540:GLY:O     | 4:J:541:LEU:HD23  | 2.07                     | 0.54              |
| 4:J:1082:ASP:OD2  | 4:J:1086:ASN:ND2  | 2.39                     | 0.54              |
| 6:L:406:GLN:HA    | 6:L:409:ASN:ND2   | 2.21                     | 0.54              |
| 2:M:257:VAL:HA    | 2:M:260:LEU:HD23  | 1.90                     | 0.54              |
| 3:I:57:PHE:CD2    | 3:I:70:TYR:HB2    | 2.42                     | 0.54              |
| 3:I:765:ILE:HD12  | 3:I:787:PRO:HG3   | 1.89                     | 0.54              |
| 4:J:107:LEU:HA    | 4:J:276:ASN:ND2   | 2.23                     | 0.54              |
| 4:J:1021:ASP:HB3  | 4:J:1024:THR:OG1  | 2.07                     | 0.54              |
| 4:J:1035:VAL:HG12 | 4:J:1037:PHE:HE1  | 1.72                     | 0.54              |
| 4:J:1173:ARG:HH21 | 4:J:1196:LEU:HD23 | 1.72                     | 0.54              |
| 6:L:9:LEU:HA      | 6:L:12:LEU:CD2    | 2.37                     | 0.54              |
| 6:L:464:ASN:O     | 6:L:468:ARG:HG3   | 2.07                     | 0.54              |
| 3:I:56:VAL:CG2    | 3:I:468:LEU:HD12  | 2.37                     | 0.54              |
| 3:I:1281:TYR:OH   | 4:J:431:ARG:O     | 2.18                     | 0.54              |
| 4:J:1060:VAL:HA   | 4:J:1107:VAL:HG23 | 1.89                     | 0.54              |
| 6:L:96:ASP:O      | 6:L:100:MET:HG3   | 2.08                     | 0.54              |
| 6:L:319:ALA:HB1   | 6:L:322:MET:CE    | 2.37                     | 0.54              |
| 6:L:567:MET:O     | 6:L:569:THR:HG22  | 2.07                     | 0.54              |
| 2:G:45:ARG:HD2    | 2:H:38:THR:CB     | 2.29                     | 0.54              |
| 3:I:118:LYS:NZ    | 3:I:488:MET:HG3   | 2.22                     | 0.54              |
| 3:I:549:ASP:OD2   | 4:J:750:PRO:HG2   | 2.07                     | 0.54              |
| 3:I:557:ARG:HB3   | 3:I:587:LEU:CD1   | 2.36                     | 0.54              |
| 3:I:671:LEU:HD23  | 3:I:1186:VAL:HG22 | 1.90                     | 0.54              |
| 3:I:943:LYS:HE3   | 3:I:947:GLU:OE2   | 2.08                     | 0.54              |
| 3:I:1067:ALA:CB   | 3:I:1073:LYS:HA   | 2.38                     | 0.54              |
| 4:J:26:SER:HB2    | 4:J:236:TRP:CZ2   | 2.41                     | 0.54              |
| 4:J:796:LEU:HG    | 4:J:800:LEU:HD23  | 1.89                     | 0.54              |
| 4:J:843:VAL:O     | 4:J:883:ARG:HG2   | 2.07                     | 0.54              |
| 4:J:967:VAL:HG13  | 4:J:971:GLY:C     | 2.32                     | 0.54              |
| 4:J:1267:VAL:HB   | 4:J:1301:THR:C    | 2.32                     | 0.54              |
| 6:L:9:LEU:O       | 6:L:12:LEU:HG     | 2.07                     | 0.54              |
| 6:L:136:GLU:HB3   | 6:L:361:ILE:CG1   | 2.35                     | 0.54              |
| 3:I:1073:LYS:CD   | 4:J:462:ASP:HB2   | 2.38                     | 0.54              |
| 3:I:1121:ALA:HB2  | 3:I:1182:ILE:CD1  | 2.38                     | 0.54              |
| 3:I:1304:MET:HE3  | 3:I:1308:ILE:HG12 | 1.90                     | 0.54              |
| 4:J:114:ILE:HG23  | 4:J:115:TRP:HD1   | 1.72                     | 0.54              |
| 4:J:975:ILE:HG13  | 4:J:997:VAL:HG12  | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1035:VAL:HG21 | 4:J:1109:LEU:HB3  | 1.88                     | 0.54              |
| 4:J:1095:MET:HG2  | 4:J:1096:PRO:O    | 2.08                     | 0.54              |
| 4:J:1179:PRO:HD3  | 4:J:1184:ASP:CB   | 2.31                     | 0.54              |
| 4:J:1265:THR:HG22 | 4:J:1279:GLN:HB3  | 1.89                     | 0.54              |
| 8:P:64:DA:C2'     | 8:P:65:DT:H5''    | 2.36                     | 0.54              |
| 2:G:43:LEU:HD13   | 2:G:217:ILE:CD1   | 2.34                     | 0.54              |
| 2:H:81:ILE:O      | 2:H:85:LEU:HG     | 2.07                     | 0.54              |
| 2:H:102:LEU:HD21  | 2:H:115:ILE:HG12  | 1.88                     | 0.54              |
| 2:H:181:GLU:N     | 2:H:206:GLU:O     | 2.29                     | 0.54              |
| 3:I:490:GLN:NE2   | 6:L:472:GLN:HB3   | 2.19                     | 0.54              |
| 3:I:953:LEU:CD2   | 3:I:1033:ARG:HG3  | 2.35                     | 0.54              |
| 3:I:1291:LEU:HD22 | 4:J:1351:VAL:HG13 | 1.89                     | 0.54              |
| 4:J:166:LEU:O     | 4:J:170:GLU:N     | 2.40                     | 0.54              |
| 4:J:502:PRO:HB2   | 4:J:507:VAL:HG12  | 1.89                     | 0.54              |
| 4:J:1024:THR:HB   | 4:J:1123:ARG:CB   | 2.38                     | 0.54              |
| 4:J:1060:VAL:HG13 | 4:J:1105:ALA:O    | 2.07                     | 0.54              |
| 4:J:1162:ILE:HA   | 4:J:1203:ARG:HA   | 1.89                     | 0.54              |
| 4:J:364:HIS:HB2   | 4:J:485:MET:HE2   | 1.90                     | 0.54              |
| 4:J:418:GLU:CG    | 5:K:48:VAL:HG21   | 2.37                     | 0.54              |
| 4:J:1156:LEU:HD12 | 4:J:1208:ASP:O    | 2.08                     | 0.54              |
| 4:J:1268:ASN:HA   | 4:J:1276:GLU:CG   | 2.37                     | 0.54              |
| 4:J:1332:LEU:O    | 4:J:1336:ALA:N    | 2.41                     | 0.54              |
| 6:L:51:MET:CB     | 6:L:53:ILE:HG13   | 2.38                     | 0.54              |
| 6:L:142:THR:O     | 6:L:146:GLU:HG3   | 2.07                     | 0.54              |
| 6:L:474:MET:HG2   | 6:L:482:GLU:OE2   | 2.08                     | 0.54              |
| 1:N:51:ILE:O      | 1:N:53:PRO:HD3    | 2.08                     | 0.54              |
| 3:I:178:PRO:HG3   | 3:I:395:TYR:CE1   | 2.43                     | 0.54              |
| 3:I:195:PHE:HB3   | 3:I:203:LYS:CG    | 2.38                     | 0.54              |
| 3:I:706:ARG:NH1   | 3:I:793:GLU:HG3   | 2.23                     | 0.54              |
| 3:I:840:SER:OG    | 3:I:850:ILE:HD11  | 2.08                     | 0.54              |
| 3:I:1067:ALA:HB2  | 3:I:1073:LYS:HA   | 1.89                     | 0.54              |
| 3:I:1332:SER:O    | 4:J:243:PRO:HG2   | 2.06                     | 0.54              |
| 4:J:360:TYR:CZ    | 4:J:361:LEU:HD23  | 2.43                     | 0.54              |
| 4:J:418:GLU:HB2   | 5:K:45:LYS:CG     | 2.38                     | 0.54              |
| 4:J:983:LYS:HA    | 4:J:994:SER:HA    | 1.90                     | 0.54              |
| 4:J:1110:GLU:O    | 4:J:1113:VAL:HG23 | 2.07                     | 0.54              |
| 6:L:126:GLY:HA3   | 6:L:372:ALA:CB    | 2.32                     | 0.54              |
| 2:G:16:ILE:HG23   | 2:G:25:LYS:O      | 2.08                     | 0.54              |
| 3:I:839:VAL:HG21  | 3:I:841:ARG:NH1   | 2.23                     | 0.54              |
| 3:I:1272:GLU:OE2  | 3:I:1276:TRP:NE1  | 2.40                     | 0.54              |
| 4:J:122:SER:O     | 4:J:125:GLY:N     | 2.40                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:587:LEU:HD21  | 4:J:608:CYS:HA    | 1.89                     | 0.54              |
| 4:J:1167:LYS:HE3  | 4:J:1170:LYS:HB2  | 1.89                     | 0.54              |
| 6:L:275:VAL:HG12  | 6:L:279:ARG:HD2   | 1.90                     | 0.54              |
| 6:L:582:VAL:O     | 6:L:583:THR:OG1   | 2.25                     | 0.54              |
| 2:G:228:LEU:O     | 2:G:232:VAL:HG12  | 2.07                     | 0.54              |
| 2:H:92:VAL:O      | 2:H:148:ARG:NH2   | 2.39                     | 0.54              |
| 3:I:10:ARG:HD2    | 3:I:1181:PRO:HG2  | 1.90                     | 0.54              |
| 3:I:231:GLU:HA    | 3:I:332:ARG:HA    | 1.90                     | 0.54              |
| 3:I:590:PRO:HB2   | 3:I:655:VAL:CG2   | 2.37                     | 0.54              |
| 3:I:936:ARG:HB3   | 3:I:939:VAL:HG21  | 1.88                     | 0.54              |
| 3:I:1101:LEU:HD23 | 4:J:725:MET:SD    | 2.48                     | 0.54              |
| 4:J:216:LYS:O     | 4:J:219:LYS:HG2   | 2.08                     | 0.54              |
| 4:J:705:THR:OG1   | 4:J:718:SER:HA    | 2.07                     | 0.54              |
| 4:J:901:ARG:O     | 4:J:903:LEU:N     | 2.39                     | 0.54              |
| 4:J:1035:VAL:CG2  | 4:J:1113:VAL:HB   | 2.38                     | 0.54              |
| 4:J:1163:VAL:CG2  | 4:J:1177:ILE:HG13 | 2.37                     | 0.54              |
| 3:I:1085:MET:HE1  | 3:I:1097:VAL:HG23 | 1.89                     | 0.53              |
| 3:I:1101:LEU:O    | 3:I:1104:PRO:HD2  | 2.08                     | 0.53              |
| 3:I:1295:SER:OG   | 4:J:345:LYS:HD3   | 2.08                     | 0.53              |
| 4:J:515:ARG:NH1   | 4:J:717:VAL:HG23  | 2.23                     | 0.53              |
| 10:J:1504:1N7:C3  | 10:J:1504:1N7:C18 | 2.70                     | 0.53              |
| 2:H:77:ASP:OD1    | 2:H:78:ILE:N      | 2.34                     | 0.53              |
| 3:I:617:ALA:HB3   | 3:I:653:MET:HA    | 1.90                     | 0.53              |
| 3:I:622:ASN:HB2   | 3:I:630:VAL:CG2   | 2.37                     | 0.53              |
| 3:I:1319:MET:HE2  | 3:I:1323:PHE:HD2  | 1.73                     | 0.53              |
| 3:I:1331:ARG:HG3  | 4:J:33:TRP:CH2    | 2.43                     | 0.53              |
| 3:I:1340:GLU:HB2  | 4:J:19:ALA:O      | 2.09                     | 0.53              |
| 4:J:279:LEU:CD1   | 4:J:296:LYS:HG2   | 2.35                     | 0.53              |
| 4:J:846:GLU:HG3   | 4:J:847:ASP:O     | 2.08                     | 0.53              |
| 5:K:26:ARG:HG2    | 5:K:59:ILE:HD13   | 1.90                     | 0.53              |
| 6:L:234:THR:C     | 6:L:245:ALA:HB2   | 2.33                     | 0.53              |
| 6:L:310:GLU:OE2   | 6:L:356:GLU:HB2   | 2.08                     | 0.53              |
| 7:O:21:DA:N3      | 2:M:265:ARG:NH1   | 2.42                     | 0.53              |
| 7:O:26:DT:C2'     | 7:O:27:DT:H5'     | 2.35                     | 0.53              |
| 2:G:74:VAL:HG21   | 2:G:81:ILE:HD11   | 1.90                     | 0.53              |
| 2:G:118:ASP:HB3   | 2:G:121:VAL:CG1   | 2.38                     | 0.53              |
| 3:I:59:ILE:CD1    | 3:I:472:GLU:HB2   | 2.39                     | 0.53              |
| 3:I:843:THR:OG1   | 3:I:844:LYS:N     | 2.42                     | 0.53              |
| 3:I:1116:HIS:HE1  | 4:J:641:ILE:H     | 1.57                     | 0.53              |
| 3:I:1127:LYS:O    | 3:I:1131:MET:HG3  | 2.08                     | 0.53              |
| 4:J:553:THR:CB    | 4:J:567:THR:HG22  | 2.38                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:766:GLY:C    | 4:J:767:LEU:HD12  | 2.34                     | 0.53              |
| 4:J:1172:LYS:HB3 | 4:J:1190:ILE:O    | 2.09                     | 0.53              |
| 4:J:1321:SER:HB3 | 4:J:1349:GLU:CD   | 2.32                     | 0.53              |
| 6:L:346:GLN:O    | 6:L:350:GLU:N     | 2.30                     | 0.53              |
| 6:L:371:LYS:HA   | 6:L:374:ARG:HB2   | 1.91                     | 0.53              |
| 6:L:595:LEU:HD23 | 6:L:595:LEU:H     | 1.72                     | 0.53              |
| 2:G:231:PHE:CE1  | 2:H:28:LEU:HD22   | 2.44                     | 0.53              |
| 2:H:65:LEU:HD23  | 2:H:66:HIS:N      | 2.23                     | 0.53              |
| 3:I:56:VAL:HG21  | 3:I:468:LEU:HD12  | 1.91                     | 0.53              |
| 3:I:225:PHE:CE2  | 3:I:347:ILE:HB    | 2.43                     | 0.53              |
| 3:I:1120:ALA:O   | 3:I:1124:ILE:HG12 | 2.08                     | 0.53              |
| 4:J:259:ARG:HH11 | 6:L:502:LYS:HZ1   | 1.56                     | 0.53              |
| 4:J:317:THR:OG1  | 4:J:318:GLY:N     | 2.42                     | 0.53              |
| 6:L:96:ASP:HB2   | 6:L:99:ARG:HG3    | 1.89                     | 0.53              |
| 6:L:351:THR:CG2  | 6:L:358:VAL:HG21  | 2.38                     | 0.53              |
| 6:L:503:GLU:HB2  | 6:L:504:PRO:HD2   | 1.89                     | 0.53              |
| 3:I:298:ALA:HB3  | 3:I:334:GLU:HB3   | 1.91                     | 0.53              |
| 3:I:558:VAL:CG1  | 3:I:573:ASN:HB3   | 2.37                     | 0.53              |
| 3:I:809:GLY:O    | 4:J:359:PRO:HG3   | 2.09                     | 0.53              |
| 4:J:189:LEU:HB3  | 4:J:234:PRO:HB2   | 1.90                     | 0.53              |
| 4:J:799:ARG:NH1  | 4:J:1142:ALA:HB1  | 2.23                     | 0.53              |
| 6:L:394:TYR:O    | 6:L:397:ARG:HG2   | 2.09                     | 0.53              |
| 10:L:701:1N7:C3  | 10:L:701:1N7:C2   | 2.74                     | 0.53              |
| 8:P:50:DT:H2"    | 8:P:51:DC:C5      | 2.42                     | 0.53              |
| 1:N:52:PHE:HB2   | 1:N:55:VAL:HG23   | 1.88                     | 0.53              |
| 2:G:76:GLU:OE1   | 2:G:76:GLU:N      | 2.42                     | 0.53              |
| 3:I:11:ILE:CG2   | 3:I:1172:LEU:HD11 | 2.39                     | 0.53              |
| 3:I:105:TYR:C    | 3:I:115:LYS:HB2   | 2.33                     | 0.53              |
| 3:I:469:VAL:HA   | 3:I:472:GLU:HG3   | 1.91                     | 0.53              |
| 3:I:688:GLN:HB2  | 3:I:1235:LEU:HD22 | 1.91                     | 0.53              |
| 3:I:871:VAL:CG1  | 3:I:883:LEU:HA    | 2.38                     | 0.53              |
| 3:I:975:ILE:HD11 | 3:I:998:LEU:HD11  | 1.90                     | 0.53              |
| 3:I:979:LEU:O    | 3:I:984:VAL:HA    | 2.09                     | 0.53              |
| 4:J:154:LEU:HD11 | 4:J:158:GLN:NE2   | 2.24                     | 0.53              |
| 4:J:306:LEU:O    | 4:J:326:SER:HB2   | 2.08                     | 0.53              |
| 4:J:451:PRO:HA   | 4:J:454:CYS:SG    | 2.49                     | 0.53              |
| 8:P:58:DC:H5'    | 8:P:58:DC:H6      | 1.73                     | 0.53              |
| 3:I:216:THR:OG1  | 3:I:219:GLN:OE1   | 2.14                     | 0.53              |
| 3:I:301:TYR:HB2  | 3:I:311:CYS:SG    | 2.48                     | 0.53              |
| 3:I:657:THR:OG1  | 3:I:1187:PHE:HB2  | 2.09                     | 0.53              |
| 3:I:848:GLU:OE1  | 3:I:886:LYS:HD2   | 2.09                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:959:LYS:HA    | 4:J:1007:ASP:OD1  | 2.08                     | 0.53              |
| 3:I:22:LEU:HD12   | 3:I:23:ASP:H      | 1.74                     | 0.53              |
| 3:I:801:ARG:NH2   | 3:I:1088:ASP:OD2  | 2.40                     | 0.53              |
| 3:I:1284:ALA:N    | 4:J:479:GLU:OE2   | 2.34                     | 0.53              |
| 4:J:233:LYS:O     | 4:J:236:TRP:HB2   | 2.08                     | 0.53              |
| 4:J:490:ILE:HG22  | 4:J:500:ILE:HG21  | 1.89                     | 0.53              |
| 4:J:570:LYS:NZ    | 4:J:589:TYR:HB3   | 2.24                     | 0.53              |
| 4:J:742:GLY:O     | 4:J:762:ASN:HB3   | 2.09                     | 0.53              |
| 4:J:1136:GLY:HA2  | 4:J:1240:VAL:HG13 | 1.91                     | 0.53              |
| 5:K:26:ARG:HD3    | 5:K:64:LEU:HD21   | 1.89                     | 0.53              |
| 6:L:112:THR:CG2   | 6:L:115:GLY:HA3   | 2.36                     | 0.53              |
| 6:L:248:GLU:O     | 6:L:251:LYS:HG2   | 2.09                     | 0.53              |
| 1:N:51:ILE:HG21   | 4:J:667:GLN:OE1   | 2.08                     | 0.53              |
| 3:I:1082:ILE:H    | 3:I:1082:ILE:HD12 | 1.74                     | 0.53              |
| 3:I:1287:LEU:HD21 | 3:I:1291:LEU:HD21 | 1.91                     | 0.53              |
| 4:J:45:ASN:OD1    | 4:J:48:THR:HG22   | 2.09                     | 0.53              |
| 4:J:1023:HIS:HA   | 4:J:1125:PRO:HB3  | 1.91                     | 0.53              |
| 4:J:1027:VAL:HG12 | 4:J:1122:ALA:O    | 2.09                     | 0.53              |
| 6:L:99:ARG:O      | 6:L:103:ARG:HG3   | 2.09                     | 0.53              |
| 6:L:436:ARG:HD2   | 8:P:35:DA:N1      | 2.24                     | 0.53              |
| 3:I:255:ILE:N     | 3:I:263:VAL:O     | 2.41                     | 0.53              |
| 3:I:367:TYR:CD2   | 3:I:381:ALA:HA    | 2.44                     | 0.53              |
| 3:I:623:LEU:CA    | 3:I:630:VAL:HG13  | 2.38                     | 0.53              |
| 3:I:676:ALA:HB3   | 4:J:779:ALA:CB    | 2.38                     | 0.53              |
| 3:I:803:ALA:CB    | 3:I:1094:VAL:HG21 | 2.39                     | 0.53              |
| 3:I:1246:ARG:NH1  | 3:I:1265:PHE:O    | 2.42                     | 0.53              |
| 4:J:117:LEU:O     | 4:J:132:LEU:HD11  | 2.09                     | 0.53              |
| 4:J:308:ASP:OD1   | 4:J:328:ALA:HB3   | 2.09                     | 0.53              |
| 4:J:361:LEU:HB2   | 4:J:365:GLN:HE21  | 1.73                     | 0.53              |
| 4:J:796:LEU:O     | 4:J:800:LEU:HD23  | 2.09                     | 0.53              |
| 6:L:366:SER:HA    | 6:L:369:GLU:CB    | 2.35                     | 0.53              |
| 6:L:395:THR:HA    | 6:L:404:LEU:CD1   | 2.34                     | 0.53              |
| 6:L:497:VAL:O     | 6:L:500:ILE:HB    | 2.09                     | 0.53              |
| 3:I:4:SER:C       | 3:I:8:LYS:HE3     | 2.34                     | 0.52              |
| 3:I:98:VAL:HG12   | 3:I:100:LEU:HG    | 1.91                     | 0.52              |
| 3:I:1089:GLU:HA   | 3:I:1213:TYR:HE1  | 1.73                     | 0.52              |
| 4:J:114:ILE:HD11  | 4:J:311:ARG:CB    | 2.35                     | 0.52              |
| 6:L:123:ILE:HG13  | 6:L:375:ALA:CB    | 2.40                     | 0.52              |
| 6:L:157:ARG:NE    | 6:L:159:SER:HB3   | 2.19                     | 0.52              |
| 2:G:19:VAL:HG12   | 2:G:24:ALA:HA     | 1.91                     | 0.52              |
| 2:G:182:ARG:O     | 2:G:183:ILE:HD13  | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:102:LEU:C    | 2:H:141:SER:HA    | 2.34                     | 0.52              |
| 2:H:183:ILE:HD13 | 2:H:205:MET:CE    | 2.39                     | 0.52              |
| 3:I:4:SER:O      | 3:I:8:LYS:HG3     | 2.10                     | 0.52              |
| 3:I:38:PHE:HE2   | 3:I:127:ILE:HD12  | 1.73                     | 0.52              |
| 3:I:301:TYR:OH   | 3:I:332:ARG:HG3   | 2.10                     | 0.52              |
| 3:I:610:GLU:HB3  | 3:I:614:TYR:HE1   | 1.74                     | 0.52              |
| 3:I:1329:GLU:OE1 | 4:J:330:MET:HE2   | 2.09                     | 0.52              |
| 4:J:153:ASN:C    | 4:J:154:LEU:HD12  | 2.33                     | 0.52              |
| 4:J:937:ILE:HD11 | 4:J:1134:ILE:HG13 | 1.86                     | 0.52              |
| 4:J:1105:ALA:O   | 4:J:1107:VAL:HG23 | 2.09                     | 0.52              |
| 3:I:17:LYS:H     | 3:I:17:LYS:HD2    | 1.74                     | 0.52              |
| 3:I:61:SER:OG    | 3:I:66:SER:HB2    | 2.10                     | 0.52              |
| 3:I:317:LEU:HD13 | 3:I:322:LEU:N     | 2.23                     | 0.52              |
| 3:I:819:SER:CB   | 3:I:1085:MET:HG3  | 2.39                     | 0.52              |
| 3:I:960:LEU:HA   | 3:I:963:GLU:HG3   | 1.90                     | 0.52              |
| 3:I:1211:ARG:NH1 | 3:I:1213:TYR:OH   | 2.42                     | 0.52              |
| 4:J:1367:GLN:O   | 4:J:1370:MET:N    | 2.41                     | 0.52              |
| 6:L:235:ILE:HD13 | 6:L:245:ALA:HB1   | 1.91                     | 0.52              |
| 6:L:309:ASN:ND2  | 6:L:314:THR:HB    | 2.24                     | 0.52              |
| 6:L:455:HIS:HA   | 6:L:458:GLU:HB2   | 1.89                     | 0.52              |
| 1:N:70:LYS:NZ    | 3:I:438:GLY:HA2   | 2.25                     | 0.52              |
| 3:I:39:ILE:CD1   | 3:I:75:LEU:HG     | 2.39                     | 0.52              |
| 3:I:208:ILE:HG23 | 3:I:209:ILE:HD13  | 1.92                     | 0.52              |
| 4:J:260:PHE:HB2  | 6:L:504:PRO:HB3   | 1.91                     | 0.52              |
| 4:J:1003:LEU:HA  | 4:J:1017:VAL:O    | 2.10                     | 0.52              |
| 1:N:8:ALA:HB2    | 4:J:786:THR:CG2   | 2.35                     | 0.52              |
| 3:I:324:LYS:O    | 3:I:327:GLN:HG2   | 2.10                     | 0.52              |
| 3:I:533:LEU:HD21 | 3:I:571:LEU:HD13  | 1.91                     | 0.52              |
| 3:I:551:HIS:CE1  | 3:I:553:THR:HG23  | 2.44                     | 0.52              |
| 3:I:877:VAL:CG1  | 3:I:920:VAL:HG21  | 2.39                     | 0.52              |
| 3:I:1107:MET:CE  | 4:J:739:GLN:HG2   | 2.40                     | 0.52              |
| 3:I:1166:ASP:H   | 3:I:1168:GLU:H    | 1.57                     | 0.52              |
| 3:I:1248:THR:CG2 | 6:L:531:PRO:HG2   | 2.38                     | 0.52              |
| 4:J:925:GLU:CG   | 4:J:926:PRO:HD3   | 2.35                     | 0.52              |
| 6:L:166:VAL:CG2  | 6:L:260:ARG:HG3   | 2.38                     | 0.52              |
| 6:L:253:SER:O    | 6:L:256:PHE:HB3   | 2.09                     | 0.52              |
| 3:I:166:SER:O    | 3:I:166:SER:OG    | 2.23                     | 0.52              |
| 3:I:299:LYS:HB3  | 3:I:334:GLU:OE1   | 2.09                     | 0.52              |
| 3:I:577:VAL:HG23 | 3:I:661:VAL:O     | 2.09                     | 0.52              |
| 4:J:71:LEU:H     | 4:J:90:VAL:HG11   | 1.74                     | 0.52              |
| 4:J:357:VAL:HG13 | 4:J:451:PRO:HG3   | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1176:VAL:HG13 | 4:J:1186:TYR:O    | 2.08                     | 0.52              |
| 2:M:260:LEU:HB3   | 2:M:262:LEU:HG    | 1.91                     | 0.52              |
| 2:M:292:THR:HB    | 2:M:295:LEU:CB    | 2.39                     | 0.52              |
| 1:N:13:GLU:HA     | 1:N:16:THR:HG22   | 1.92                     | 0.52              |
| 1:N:52:PHE:HE2    | 4:J:673:VAL:HG12  | 1.74                     | 0.52              |
| 2:H:182:ARG:NE    | 4:J:581:MET:HE1   | 2.25                     | 0.52              |
| 2:H:192:VAL:HG22  | 2:H:193:GLU:H     | 1.75                     | 0.52              |
| 3:I:158:ASP:OD1   | 3:I:159:SER:N     | 2.42                     | 0.52              |
| 3:I:233:ARG:HB2   | 3:I:238:GLN:HB2   | 1.92                     | 0.52              |
| 3:I:615:VAL:N     | 3:I:651:ASP:OD2   | 2.38                     | 0.52              |
| 3:I:828:PHE:CD2   | 3:I:1066:MET:HE1  | 2.44                     | 0.52              |
| 10:I:1401:1N7:H31 | 10:I:1401:1N7:H5  | 1.92                     | 0.52              |
| 4:J:411:ILE:O     | 4:J:415:VAL:HG13  | 2.09                     | 0.52              |
| 4:J:924:GLY:O     | 4:J:927:GLY:N     | 2.39                     | 0.52              |
| 4:J:1030:GLU:HG2  | 4:J:1031:VAL:HG23 | 1.91                     | 0.52              |
| 4:J:1064:SER:HA   | 4:J:1067:ARG:CG   | 2.40                     | 0.52              |
| 4:J:1064:SER:HB3  | 4:J:1072:LYS:CE   | 2.39                     | 0.52              |
| 4:J:1194:ARG:HG3  | 4:J:1212:ASP:HB2  | 1.91                     | 0.52              |
| 7:O:20:DA:H2"     | 7:O:21:DA:C8      | 2.43                     | 0.52              |
| 3:I:452:ARG:NH1   | 3:I:584:TYR:O     | 2.26                     | 0.52              |
| 3:I:549:ASP:OD1   | 3:I:550:VAL:N     | 2.43                     | 0.52              |
| 3:I:800:MET:HG3   | 3:I:1096:ILE:HD12 | 1.91                     | 0.52              |
| 4:J:58:CYS:H      | 4:J:62:PHE:HD2    | 1.57                     | 0.52              |
| 4:J:164:GLN:HA    | 4:J:167:ASP:CG    | 2.35                     | 0.52              |
| 4:J:1042:ASP:HA   | 4:J:1046:ILE:O    | 2.10                     | 0.52              |
| 4:J:1051:ASP:N    | 4:J:1056:LEU:O    | 2.42                     | 0.52              |
| 4:J:1067:ARG:CD   | 4:J:1072:LYS:HA   | 2.40                     | 0.52              |
| 6:L:98:VAL:O      | 6:L:102:MET:HG2   | 2.09                     | 0.52              |
| 6:L:228:TYR:O     | 6:L:231:THR:N     | 2.40                     | 0.52              |
| 6:L:347:ILE:HG22  | 6:L:355:ILE:HD12  | 1.92                     | 0.52              |
| 6:L:402:LEU:HA    | 6:L:405:ILE:CD1   | 2.39                     | 0.52              |
| 6:L:564:GLY:HA2   | 6:L:569:THR:HG23  | 1.92                     | 0.52              |
| 2:M:282:VAL:CB    | 2:M:316:MET:HB2   | 2.34                     | 0.52              |
| 3:I:28:LEU:CD1    | 3:I:527:LYS:HD3   | 2.39                     | 0.52              |
| 3:I:667:LEU:HD21  | 3:I:705:GLU:HG2   | 1.92                     | 0.52              |
| 3:I:685:MET:HE2   | 3:I:1071:GLY:HA2  | 1.91                     | 0.52              |
| 3:I:994:ARG:HA    | 3:I:997:TRP:CE2   | 2.45                     | 0.52              |
| 4:J:322:ARG:NH1   | 6:L:510:PRO:HG3   | 2.21                     | 0.52              |
| 6:L:81:ALA:HA     | 6:L:84:LEU:CG     | 2.40                     | 0.52              |
| 6:L:393:LYS:HD2   | 8:P:35:DA:N7      | 2.24                     | 0.52              |
| 2:G:9:LEU:HD23    | 2:G:9:LEU:H       | 1.74                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:224:LEU:HD23  | 2:G:228:LEU:HD23  | 1.91                     | 0.52              |
| 3:I:1245:ALA:O    | 4:J:375:GLU:HG2   | 2.09                     | 0.52              |
| 3:I:1247:SER:OG   | 3:I:1248:THR:N    | 2.43                     | 0.52              |
| 4:J:161:THR:CG2   | 4:J:164:GLN:H     | 2.23                     | 0.52              |
| 4:J:612:LEU:HD23  | 4:J:616:PRO:CB    | 2.40                     | 0.52              |
| 4:J:1023:HIS:C    | 4:J:1125:PRO:HA   | 2.35                     | 0.52              |
| 4:J:1056:LEU:HD21 | 4:J:1108:GLN:HE21 | 1.75                     | 0.52              |
| 4:J:1079:LYS:HG3  | 4:J:1098:GLN:HB3  | 1.92                     | 0.52              |
| 6:L:9:LEU:HA      | 6:L:12:LEU:HD23   | 1.91                     | 0.52              |
| 6:L:114:GLU:HA    | 6:L:117:ILE:CD1   | 2.39                     | 0.52              |
| 6:L:540:LEU:HA    | 6:L:610:PHE:HE2   | 1.74                     | 0.52              |
| 2:H:62:ASP:OD2    | 2:H:71:LYS:NZ     | 2.41                     | 0.51              |
| 3:I:7:GLU:O       | 3:I:11:ILE:HB     | 2.10                     | 0.51              |
| 3:I:105:TYR:HA    | 3:I:115:LYS:H     | 1.75                     | 0.51              |
| 3:I:563:THR:CG2   | 3:I:570:GLY:H     | 2.24                     | 0.51              |
| 3:I:685:MET:HG3   | 3:I:1235:LEU:CD1  | 2.28                     | 0.51              |
| 3:I:733:VAL:CG2   | 3:I:748:ILE:HD12  | 2.40                     | 0.51              |
| 4:J:120:LEU:HB2   | 4:J:121:PRO:HD3   | 1.92                     | 0.51              |
| 4:J:128:LEU:O     | 4:J:130:MET:HG3   | 2.09                     | 0.51              |
| 4:J:343:LEU:HD22  | 4:J:1351:VAL:CG1  | 2.39                     | 0.51              |
| 4:J:407:VAL:O     | 4:J:411:ILE:HG12  | 2.11                     | 0.51              |
| 4:J:857:LEU:HD11  | 4:J:871:LEU:HD22  | 1.92                     | 0.51              |
| 6:L:336:GLU:HA    | 6:L:339:ARG:CD    | 2.35                     | 0.51              |
| 6:L:593:LYS:HE2   | 6:L:596:ARG:NH1   | 2.24                     | 0.51              |
| 2:G:73:GLY:O      | 2:G:134:THR:OG1   | 2.19                     | 0.51              |
| 2:H:65:LEU:HB3    | 2:H:69:SER:HB2    | 1.92                     | 0.51              |
| 2:H:180:VAL:HA    | 2:H:207:THR:HA    | 1.92                     | 0.51              |
| 3:I:189:ASP:OD2   | 3:I:191:LYS:HB2   | 2.10                     | 0.51              |
| 3:I:629:PHE:CE2   | 3:I:634:VAL:HG21  | 2.46                     | 0.51              |
| 3:I:1131:MET:HE2  | 3:I:1141:LEU:CD1  | 2.37                     | 0.51              |
| 3:I:1293:VAL:HG21 | 3:I:1304:MET:HB2  | 1.92                     | 0.51              |
| 4:J:281:ARG:HA    | 4:J:284:ASP:OD1   | 2.10                     | 0.51              |
| 4:J:386:GLU:OE2   | 4:J:394:ILE:HG13  | 2.10                     | 0.51              |
| 4:J:1272:SER:OG   | 4:J:1273:ASP:N    | 2.43                     | 0.51              |
| 6:L:127:ILE:HG13  | 6:L:131:GLN:NE2   | 2.24                     | 0.51              |
| 6:L:543:ALA:HB1   | 6:L:606:VAL:CG2   | 2.40                     | 0.51              |
| 7:O:43:DA:H1'     | 7:O:44:DA:H5''    | 1.92                     | 0.51              |
| 8:P:45:DA:H1'     | 8:P:46:DG:C8      | 2.45                     | 0.51              |
| 8:P:62:DG:H2''    | 8:P:63:DG:C8      | 2.44                     | 0.51              |
| 2:M:282:VAL:HG11  | 2:M:312:LEU:HD22  | 1.92                     | 0.51              |
| 1:N:64:TYR:CE2    | 3:I:341:LEU:HB2   | 2.40                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:50:SER:HB2    | 2:H:8:PHE:HZ      | 1.75                     | 0.51              |
| 3:I:31:GLN:NE2    | 3:I:145:ILE:O     | 2.43                     | 0.51              |
| 3:I:49:LEU:HD22   | 3:I:464:PHE:CE2   | 2.46                     | 0.51              |
| 3:I:61:SER:HB2    | 3:I:64:GLY:H      | 1.76                     | 0.51              |
| 3:I:221:LEU:HD11  | 3:I:351:LEU:CD1   | 2.40                     | 0.51              |
| 3:I:594:VAL:HG12  | 3:I:595:THR:O     | 2.10                     | 0.51              |
| 3:I:905:ILE:HA    | 6:L:595:LEU:CD1   | 2.41                     | 0.51              |
| 3:I:975:ILE:HD13  | 3:I:998:LEU:HG    | 1.92                     | 0.51              |
| 3:I:1142:ARG:HG3  | 3:I:1161:LEU:HD22 | 1.92                     | 0.51              |
| 3:I:1246:ARG:HD2  | 3:I:1265:PHE:O    | 2.10                     | 0.51              |
| 4:J:224:LEU:O     | 4:J:228:VAL:HG23  | 2.09                     | 0.51              |
| 4:J:253:VAL:HG21  | 6:L:523:ILE:HG21  | 1.91                     | 0.51              |
| 4:J:482:ALA:HB3   | 5:K:20:VAL:HG22   | 1.91                     | 0.51              |
| 4:J:518:VAL:HG23  | 4:J:707:ILE:HD11  | 1.93                     | 0.51              |
| 4:J:555:TYR:HB2   | 4:J:585:LYS:O     | 2.10                     | 0.51              |
| 4:J:968:ASN:O     | 4:J:971:GLY:N     | 2.40                     | 0.51              |
| 4:J:1163:VAL:HG13 | 4:J:1200:GLU:HA   | 1.93                     | 0.51              |
| 5:K:22:VAL:HG23   | 5:K:25:ARG:HH21   | 1.76                     | 0.51              |
| 6:L:428:SER:HB2   | 7:O:54:DT:O4      | 2.10                     | 0.51              |
| 6:L:463:LEU:HD22  | 6:L:483:LEU:HD23  | 1.91                     | 0.51              |
| 2:H:102:LEU:CD2   | 2:H:115:ILE:HA    | 2.40                     | 0.51              |
| 3:I:130:MET:SD    | 3:I:134:GLY:HA2   | 2.50                     | 0.51              |
| 3:I:435:ILE:HA    | 3:I:439:LYS:O     | 2.11                     | 0.51              |
| 6:L:23:THR:HA     | 6:L:56:MET:O      | 2.10                     | 0.51              |
| 6:L:126:GLY:HA2   | 6:L:129:GLN:OE1   | 2.11                     | 0.51              |
| 6:L:280:VAL:HB    | 6:L:347:ILE:HG21  | 1.93                     | 0.51              |
| 2:G:159:ILE:HA    | 2:G:162:GLU:OE2   | 2.11                     | 0.51              |
| 3:I:16:GLY:O      | 3:I:1156:ARG:HB3  | 2.11                     | 0.51              |
| 3:I:1103:VAL:CG2  | 4:J:639:VAL:HG21  | 2.41                     | 0.51              |
| 4:J:759:ILE:HD11  | 4:J:774:ILE:HG21  | 1.93                     | 0.51              |
| 4:J:1049:GLN:HE22 | 4:J:1060:VAL:HB   | 1.75                     | 0.51              |
| 6:L:421:TYR:O     | 6:L:424:GLY:N     | 2.44                     | 0.51              |
| 8:P:49:DT:C2'     | 8:P:50:DT:H71     | 2.40                     | 0.51              |
| 2:H:41:ASN:O      | 2:H:45:ARG:HG3    | 2.11                     | 0.51              |
| 2:H:118:ASP:HB3   | 2:H:121:VAL:HG23  | 1.92                     | 0.51              |
| 3:I:253:PHE:CD1   | 3:I:288:PRO:HD3   | 2.45                     | 0.51              |
| 3:I:289:VAL:CG1   | 3:I:319:LEU:HD12  | 2.39                     | 0.51              |
| 3:I:1099:ASN:OD1  | 3:I:1100:PRO:HD2  | 2.11                     | 0.51              |
| 4:J:364:HIS:HB2   | 4:J:485:MET:CE    | 2.40                     | 0.51              |
| 4:J:545:HIS:HA    | 4:J:573:THR:CG2   | 2.40                     | 0.51              |
| 6:L:148:TYR:O     | 6:L:152:GLU:HG2   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:L:385:ARG:HD2   | 7:O:55:DC:C5'    | 2.28                     | 0.51              |
| 1:N:72:TYR:HB3    | 3:I:168:GLY:O    | 2.09                     | 0.51              |
| 2:H:91:ARG:HG3    | 2:H:122:GLU:HB2  | 1.92                     | 0.51              |
| 3:I:813:GLU:HB2   | 4:J:461:PHE:HD1  | 1.76                     | 0.51              |
| 3:I:886:LYS:O     | 3:I:917:SER:OG   | 2.19                     | 0.51              |
| 3:I:933:VAL:HG22  | 3:I:1050:VAL:CG1 | 2.37                     | 0.51              |
| 3:I:956:ALA:O     | 3:I:959:ASP:HB3  | 2.11                     | 0.51              |
| 3:I:994:ARG:HA    | 3:I:997:TRP:CD2  | 2.45                     | 0.51              |
| 7:O:30:DC:H2''    | 7:O:31:DA:C8     | 2.45                     | 0.51              |
| 2:H:19:VAL:CG2    | 2:H:23:HIS:HB3   | 2.41                     | 0.51              |
| 3:I:725:GLN:OE1   | 3:I:735:LYS:HB2  | 2.11                     | 0.51              |
| 3:I:732:ILE:CD1   | 3:I:769:PRO:HB3  | 2.31                     | 0.51              |
| 4:J:161:THR:H     | 4:J:164:GLN:HB2  | 1.76                     | 0.51              |
| 4:J:697:MET:HE3   | 4:J:738:ARG:HA   | 1.93                     | 0.51              |
| 4:J:885:VAL:HG12  | 4:J:1258:ARG:HD2 | 1.92                     | 0.51              |
| 4:J:975:ILE:HG12  | 4:J:1001:ALA:HB3 | 1.92                     | 0.51              |
| 5:K:54:ILE:HD13   | 5:K:59:ILE:O     | 2.10                     | 0.51              |
| 6:L:385:ARG:HB3   | 7:O:54:DT:O3'    | 2.11                     | 0.51              |
| 7:O:44:DA:H5'     | 7:O:44:DA:C8     | 2.46                     | 0.51              |
| 8:P:46:DG:H2''    | 8:P:47:DC:C6     | 2.46                     | 0.51              |
| 2:M:253:LEU:HD22  | 2:M:318:LEU:HD13 | 1.93                     | 0.51              |
| 2:H:33:ARG:HG3    | 2:H:197:ASP:OD2  | 2.11                     | 0.51              |
| 2:H:84:ASN:HD21   | 4:J:551:ARG:HH12 | 1.59                     | 0.51              |
| 3:I:26:TYR:HA     | 3:I:711:ASP:OD1  | 2.10                     | 0.51              |
| 3:I:60:GLN:HA     | 3:I:67:GLU:HG3   | 1.92                     | 0.51              |
| 3:I:188:PHE:HE2   | 3:I:436:ARG:HG2  | 1.76                     | 0.51              |
| 3:I:672:GLU:HG3   | 3:I:673:HIS:CD2  | 2.45                     | 0.51              |
| 3:I:811:ASN:HA    | 3:I:815:SER:CB   | 2.37                     | 0.51              |
| 3:I:858:GLY:N     | 3:I:861:ALA:HB3  | 2.26                     | 0.51              |
| 4:J:949:SER:HA    | 4:J:1020:TRP:CZ3 | 2.46                     | 0.51              |
| 5:K:62:GLN:O      | 5:K:66:VAL:HG12  | 2.11                     | 0.51              |
| 7:O:41:DT:O2      | 8:P:46:DG:N2     | 2.44                     | 0.51              |
| 2:H:42:ALA:O      | 2:H:46:ILE:HG12  | 2.10                     | 0.51              |
| 3:I:30:ILE:HG22   | 3:I:31:GLN:OE1   | 2.10                     | 0.51              |
| 3:I:887:VAL:HG23  | 3:I:913:VAL:HG21 | 1.93                     | 0.51              |
| 3:I:898:GLU:HG3   | 6:L:565:ILE:HG12 | 1.93                     | 0.51              |
| 3:I:1184:THR:HG23 | 3:I:1189:GLY:CA  | 2.41                     | 0.51              |
| 4:J:19:ALA:HA     | 4:J:1343:GLU:HA  | 1.92                     | 0.51              |
| 4:J:518:VAL:HG11  | 4:J:714:GLU:OE2  | 2.10                     | 0.51              |
| 4:J:826:ILE:CG1   | 4:J:831:VAL:HG13 | 2.41                     | 0.51              |
| 4:J:865:HIS:CE1   | 4:J:867:GLN:HB2  | 2.46                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1167:LYS:HG2  | 4:J:1168:GLU:H    | 1.75                     | 0.51              |
| 4:J:1176:VAL:CG1  | 4:J:1184:ASP:HB2  | 2.41                     | 0.51              |
| 6:L:544:THR:O     | 6:L:548:LEU:HB2   | 2.11                     | 0.51              |
| 6:L:565:ILE:HG22  | 6:L:566:ASP:OD2   | 2.11                     | 0.51              |
| 8:P:42:DT:C2'     | 8:P:43:DT:H72     | 2.39                     | 0.51              |
| 2:G:124:VAL:HG11  | 2:G:210:THR:CG2   | 2.41                     | 0.50              |
| 2:H:13:LEU:HB2    | 2:H:29:GLU:HG3    | 1.92                     | 0.50              |
| 2:H:100:LEU:HD23  | 2:H:115:ILE:CG2   | 2.41                     | 0.50              |
| 2:H:211:ILE:HD11  | 2:H:215:GLU:HB3   | 1.93                     | 0.50              |
| 3:I:55:SER:OG     | 3:I:465:ARG:HD2   | 2.11                     | 0.50              |
| 3:I:519:ASN:HB3   | 3:I:522:SER:H     | 1.76                     | 0.50              |
| 3:I:726:TYR:HA    | 3:I:773:LEU:CD1   | 2.41                     | 0.50              |
| 3:I:810:TYR:CZ    | 3:I:1078:LYS:HD2  | 2.46                     | 0.50              |
| 3:I:898:GLU:OE2   | 6:L:565:ILE:HA    | 2.12                     | 0.50              |
| 3:I:898:GLU:CD    | 6:L:565:ILE:HG12  | 2.36                     | 0.50              |
| 3:I:976:ARG:CZ    | 3:I:989:LEU:HB3   | 2.41                     | 0.50              |
| 3:I:1002:LEU:HD23 | 3:I:1003:THR:N    | 2.26                     | 0.50              |
| 4:J:103:GLY:C     | 4:J:244:VAL:HG22  | 2.36                     | 0.50              |
| 4:J:189:LEU:HD13  | 4:J:234:PRO:CB    | 2.41                     | 0.50              |
| 4:J:681:LYS:O     | 4:J:685:ILE:HG12  | 2.12                     | 0.50              |
| 4:J:1052:GLU:HA   | 4:J:1055:GLY:CA   | 2.40                     | 0.50              |
| 4:J:1067:ARG:CZ   | 4:J:1072:LYS:HA   | 2.40                     | 0.50              |
| 4:J:1167:LYS:NZ   | 4:J:1168:GLU:O    | 2.44                     | 0.50              |
| 4:J:1176:VAL:HG11 | 4:J:1184:ASP:O    | 2.10                     | 0.50              |
| 6:L:322:MET:HB3   | 6:L:324:LYS:HG3   | 1.93                     | 0.50              |
| 2:M:267:ALA:O     | 2:M:271:LYS:HG3   | 2.11                     | 0.50              |
| 1:N:37:CYS:O      | 1:N:41:GLY:N      | 2.42                     | 0.50              |
| 3:I:263:VAL:HG12  | 3:I:267:ARG:HG3   | 1.93                     | 0.50              |
| 3:I:1059:ARG:NH1  | 3:I:1059:ARG:HB2  | 2.26                     | 0.50              |
| 5:K:26:ARG:NH1    | 5:K:29:GLN:HB2    | 2.27                     | 0.50              |
| 6:L:277:MET:HA    | 6:L:280:VAL:CG1   | 2.41                     | 0.50              |
| 6:L:593:LYS:O     | 6:L:593:LYS:HD3   | 2.11                     | 0.50              |
| 8:P:36:DT:H2'     | 8:P:37:DG:H3'     | 1.93                     | 0.50              |
| 3:I:448:LEU:HB2   | 3:I:553:THR:OG1   | 2.12                     | 0.50              |
| 3:I:734:ILE:O     | 3:I:734:ILE:HG13  | 2.11                     | 0.50              |
| 3:I:1146:GLN:OE1  | 3:I:1161:LEU:HD13 | 2.11                     | 0.50              |
| 4:J:34:SER:OG     | 4:J:35:PHE:N      | 2.45                     | 0.50              |
| 4:J:67:ASP:OD1    | 4:J:95:THR:HG22   | 2.12                     | 0.50              |
| 4:J:952:VAL:HG22  | 4:J:1015:GLU:HB3  | 1.93                     | 0.50              |
| 4:J:1151:LYS:C    | 4:J:1153:PRO:HD3  | 2.36                     | 0.50              |
| 8:P:54:DT:C2'     | 8:P:55:DT:H5'     | 2.38                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:68:DG:H5"     | 2:M:294:ASN:O     | 2.11                     | 0.50              |
| 1:N:24:ARG:O      | 1:N:27:ILE:HG22   | 2.12                     | 0.50              |
| 2:G:107:ILE:HG13  | 2:G:135:ASP:O     | 2.11                     | 0.50              |
| 2:H:68:TYR:CE1    | 2:H:78:ILE:HB     | 2.46                     | 0.50              |
| 2:H:89:ALA:HB3    | 2:H:124:VAL:HG12  | 1.94                     | 0.50              |
| 3:I:149:LEU:HD22  | 3:I:530:ILE:CG2   | 2.41                     | 0.50              |
| 3:I:1104:PRO:HG2  | 4:J:725:MET:HE3   | 1.91                     | 0.50              |
| 4:J:146:VAL:HA    | 4:J:178:ALA:HB2   | 1.94                     | 0.50              |
| 4:J:475:GLU:HG3   | 5:K:24:ALA:HB1    | 1.93                     | 0.50              |
| 4:J:1031:VAL:HA   | 4:J:1117:SER:OG   | 2.11                     | 0.50              |
| 4:J:1079:LYS:HA   | 4:J:1098:GLN:HA   | 1.93                     | 0.50              |
| 2:H:102:LEU:HB2   | 2:H:142:MET:HG2   | 1.92                     | 0.50              |
| 3:I:226:GLU:HG2   | 3:I:227:LYS:H     | 1.76                     | 0.50              |
| 3:I:300:ASP:HA    | 3:I:312:ALA:HA    | 1.94                     | 0.50              |
| 3:I:435:ILE:HD11  | 3:I:441:GLU:C     | 2.36                     | 0.50              |
| 3:I:898:GLU:HB3   | 6:L:540:LEU:CD2   | 2.41                     | 0.50              |
| 4:J:101:ARG:O     | 4:J:246:PRO:HG3   | 2.12                     | 0.50              |
| 4:J:167:ASP:HA    | 4:J:170:GLU:HB3   | 1.93                     | 0.50              |
| 4:J:545:HIS:HA    | 4:J:573:THR:HG23  | 1.94                     | 0.50              |
| 4:J:801:VAL:O     | 4:J:805:GLN:HB2   | 2.11                     | 0.50              |
| 3:I:108:GLU:HG3   | 3:I:108:GLU:O     | 2.10                     | 0.50              |
| 3:I:219:GLN:O     | 3:I:223:LEU:HG    | 2.11                     | 0.50              |
| 3:I:396:ASP:OD1   | 3:I:418:GLY:HA3   | 2.12                     | 0.50              |
| 3:I:1129:ASN:O    | 3:I:1133:LYS:HG2  | 2.12                     | 0.50              |
| 3:I:1172:LEU:O    | 3:I:1176:LEU:HG   | 2.12                     | 0.50              |
| 4:J:294:ASN:O     | 4:J:298:MET:HG3   | 2.11                     | 0.50              |
| 4:J:509:GLY:HA3   | 4:J:632:ALA:HB2   | 1.93                     | 0.50              |
| 4:J:1040:MET:SD   | 4:J:1077:ALA:N    | 2.85                     | 0.50              |
| 4:J:1318:SER:HB3  | 4:J:1321:SER:OG   | 2.12                     | 0.50              |
| 8:P:66:DT:C6      | 8:P:67:DT:H72     | 2.46                     | 0.50              |
| 3:I:249:GLU:C     | 3:I:268:ARG:HD3   | 2.37                     | 0.50              |
| 3:I:857:VAL:CG2   | 3:I:862:LEU:HD21  | 2.42                     | 0.50              |
| 3:I:1275:VAL:HG13 | 3:I:1287:LEU:HD11 | 1.93                     | 0.50              |
| 6:L:390:ILE:CD1   | 6:L:432:THR:HG23  | 2.41                     | 0.50              |
| 6:L:412:LEU:O     | 6:L:412:LEU:HD12  | 2.12                     | 0.50              |
| 6:L:487:MET:HE2   | 6:L:487:MET:HA    | 1.94                     | 0.50              |
| 6:L:605:GLU:O     | 6:L:608:ARG:HB2   | 2.10                     | 0.50              |
| 2:H:193:GLU:HG2   | 2:H:194:GLN:N     | 2.26                     | 0.50              |
| 3:I:238:GLN:HB3   | 3:I:284:LEU:HD21  | 1.94                     | 0.50              |
| 3:I:670:PHE:CZ    | 3:I:1117:LEU:HD13 | 2.46                     | 0.50              |
| 3:I:794:LEU:HD21  | 3:I:796:LEU:HD11  | 1.93                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1306:LYS:O    | 3:I:1309:VAL:HG22 | 2.12                     | 0.50              |
| 4:J:134:ASP:O     | 4:J:138:VAL:HG23  | 2.12                     | 0.50              |
| 4:J:368:LEU:HD23  | 4:J:373:ALA:CB    | 2.38                     | 0.50              |
| 4:J:788:LEU:O     | 4:J:788:LEU:HD23  | 2.12                     | 0.50              |
| 6:L:40:GLN:O      | 6:L:44:ILE:HG22   | 2.12                     | 0.50              |
| 6:L:287:ILE:HA    | 6:L:337:VAL:CG1   | 2.37                     | 0.50              |
| 6:L:333:VAL:CG2   | 6:L:336:GLU:HB3   | 2.42                     | 0.50              |
| 6:L:551:LEU:CD2   | 6:L:598:LEU:HD21  | 2.42                     | 0.50              |
| 6:L:551:LEU:HD12  | 6:L:556:ALA:HA    | 1.93                     | 0.50              |
| 1:N:48:ARG:HE     | 1:N:55:VAL:HG11   | 1.77                     | 0.50              |
| 2:G:39:LEU:O      | 2:G:43:LEU:HG     | 2.12                     | 0.50              |
| 2:H:13:LEU:HA     | 2:H:29:GLU:CD     | 2.37                     | 0.50              |
| 2:H:100:LEU:HD23  | 2:H:115:ILE:HG21  | 1.93                     | 0.50              |
| 3:I:178:PRO:HA    | 3:I:397:LEU:HG    | 1.94                     | 0.50              |
| 3:I:351:LEU:HD23  | 3:I:354:ASP:OD1   | 2.12                     | 0.50              |
| 3:I:1184:THR:HG23 | 3:I:1189:GLY:HA3  | 1.94                     | 0.50              |
| 4:J:358:GLY:HA3   | 4:J:448:GLN:OE1   | 2.12                     | 0.50              |
| 4:J:697:MET:HE2   | 4:J:741:ALA:HB3   | 1.93                     | 0.50              |
| 4:J:1231:ARG:O    | 4:J:1235:ASN:HB2  | 2.12                     | 0.50              |
| 6:L:385:ARG:CB    | 7:O:54:DT:H1'     | 2.42                     | 0.50              |
| 2:G:12:ARG:H      | 2:G:30:PRO:HD2    | 1.76                     | 0.49              |
| 2:H:104:LYS:N     | 2:H:140:ILE:O     | 2.44                     | 0.49              |
| 3:I:871:VAL:CG2   | 3:I:928:VAL:HG11  | 2.41                     | 0.49              |
| 3:I:921:PRO:HD2   | 3:I:924:VAL:CG2   | 2.42                     | 0.49              |
| 3:I:1132:LEU:HD11 | 3:I:1170:MET:SD   | 2.52                     | 0.49              |
| 3:I:1222:GLU:OE1  | 3:I:1222:GLU:N    | 2.45                     | 0.49              |
| 6:L:298:PRO:HD2   | 6:L:326:TRP:CZ2   | 2.47                     | 0.49              |
| 6:L:401:PHE:O     | 6:L:405:ILE:HG23  | 2.12                     | 0.49              |
| 6:L:540:LEU:O     | 6:L:544:THR:HG23  | 2.12                     | 0.49              |
| 6:L:567:MET:HG3   | 6:L:569:THR:CB    | 2.28                     | 0.49              |
| 6:L:586:ARG:HH21  | 7:O:24:DC:H2'     | 1.77                     | 0.49              |
| 2:G:104:LYS:HD2   | 2:G:105:SER:H     | 1.77                     | 0.49              |
| 3:I:26:TYR:O      | 3:I:29:SER:HB3    | 2.11                     | 0.49              |
| 3:I:254:ASP:N     | 3:I:265:LYS:HG2   | 2.28                     | 0.49              |
| 3:I:453:ILE:HD12  | 3:I:587:LEU:HG    | 1.95                     | 0.49              |
| 3:I:812:PHE:CZ    | 4:J:503:SER:HB2   | 2.44                     | 0.49              |
| 4:J:393:THR:HG21  | 6:L:610:PHE:CE1   | 2.47                     | 0.49              |
| 4:J:955:LYS:HE2   | 4:J:1010:GLN:HE22 | 1.76                     | 0.49              |
| 4:J:1266:ILE:HD12 | 4:J:1278:GLU:O    | 2.12                     | 0.49              |
| 6:L:80:ALA:HA     | 6:L:83:VAL:CG1    | 2.38                     | 0.49              |
| 6:L:81:ALA:HA     | 6:L:84:LEU:CD2    | 2.41                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:394:TYR:HD2  | 6:L:439:ILE:HG21 | 1.78                     | 0.49              |
| 6:L:576:VAL:HG13 | 6:L:587:ILE:HG21 | 1.93                     | 0.49              |
| 1:N:21:ASN:O     | 1:N:25:GLN:HG2   | 2.11                     | 0.49              |
| 1:N:36:LEU:HD23  | 1:N:43:PRO:CA    | 2.42                     | 0.49              |
| 1:N:44:ILE:O     | 1:N:49:ARG:HD3   | 2.13                     | 0.49              |
| 2:H:48:LEU:HD23  | 2:H:183:ILE:HG22 | 1.94                     | 0.49              |
| 3:I:6:THR:O      | 3:I:9:LYS:HB2    | 2.12                     | 0.49              |
| 3:I:361:SER:HA   | 3:I:364:VAL:CG2  | 2.40                     | 0.49              |
| 3:I:593:LYS:HA   | 3:I:652:TYR:CD1  | 2.47                     | 0.49              |
| 3:I:594:VAL:HG13 | 3:I:598:VAL:O    | 2.12                     | 0.49              |
| 3:I:949:GLU:O    | 3:I:953:LEU:HG   | 2.13                     | 0.49              |
| 3:I:1304:MET:HE2 | 4:J:472:LEU:HB3  | 1.94                     | 0.49              |
| 4:J:39:LYS:HB2   | 4:J:54:ASP:OD1   | 2.13                     | 0.49              |
| 4:J:134:ASP:OD1  | 4:J:159:ILE:HD13 | 2.12                     | 0.49              |
| 4:J:143:SER:C    | 4:J:180:MET:HE2  | 2.38                     | 0.49              |
| 4:J:902:ASP:H    | 4:J:1251:LYS:NZ  | 2.11                     | 0.49              |
| 4:J:902:ASP:H    | 4:J:1251:LYS:HZ3 | 1.59                     | 0.49              |
| 6:L:51:MET:HB3   | 6:L:53:ILE:HG13  | 1.94                     | 0.49              |
| 6:L:248:GLU:HG2  | 6:L:251:LYS:NZ   | 2.27                     | 0.49              |
| 2:H:206:GLU:OE1  | 4:J:531:LYS:NZ   | 2.39                     | 0.49              |
| 3:I:963:GLU:HA   | 3:I:966:ILE:HD11 | 1.94                     | 0.49              |
| 3:I:1142:ARG:NH2 | 3:I:1165:SER:HB3 | 2.22                     | 0.49              |
| 3:I:1251:TYR:HB2 | 6:L:528:LEU:CD1  | 2.42                     | 0.49              |
| 4:J:113:HIS:CE1  | 4:J:115:TRP:HB2  | 2.47                     | 0.49              |
| 4:J:865:HIS:HD1  | 4:J:867:GLN:H    | 1.59                     | 0.49              |
| 4:J:968:ASN:HB2  | 4:J:1118:GLY:O   | 2.13                     | 0.49              |
| 4:J:1116:SER:N   | 4:J:1119:ASP:OD2 | 2.20                     | 0.49              |
| 6:L:22:LEU:HB3   | 6:L:26:GLU:OE1   | 2.12                     | 0.49              |
| 6:L:48:ILE:CG2   | 6:L:55:VAL:HG11  | 2.30                     | 0.49              |
| 6:L:470:MET:O    | 6:L:474:MET:HG3  | 2.11                     | 0.49              |
| 6:L:586:ARG:HE   | 7:O:24:DC:C2'    | 2.25                     | 0.49              |
| 8:P:40:DC:C2'    | 8:P:41:DT:H72    | 2.43                     | 0.49              |
| 2:G:221:ALA:HB3  | 2:H:231:PHE:HB3  | 1.95                     | 0.49              |
| 2:H:112:ALA:HB3  | 2:H:126:PRO:C    | 2.38                     | 0.49              |
| 2:H:201:LEU:HG   | 2:H:203:ILE:CG1  | 2.42                     | 0.49              |
| 3:I:57:PHE:HD1   | 3:I:59:ILE:HG13  | 1.78                     | 0.49              |
| 3:I:117:ILE:HG13 | 3:I:117:ILE:O    | 2.13                     | 0.49              |
| 4:J:196:GLN:O    | 4:J:199:GLU:HG3  | 2.12                     | 0.49              |
| 4:J:365:GLN:HB2  | 4:J:438:GLU:O    | 2.12                     | 0.49              |
| 4:J:805:GLN:OE1  | 4:J:1348:LYS:HB2 | 2.12                     | 0.49              |
| 4:J:903:LEU:HB2  | 4:J:905:ARG:O    | 2.11                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1267:VAL:HB   | 4:J:1301:THR:HB   | 1.95                     | 0.49              |
| 6:L:147:GLN:HG3   | 6:L:265:GLN:OE1   | 2.12                     | 0.49              |
| 6:L:158:LEU:HD22  | 6:L:218:ARG:CD    | 2.43                     | 0.49              |
| 6:L:305:LEU:CD1   | 6:L:319:ALA:HB2   | 2.43                     | 0.49              |
| 1:N:14:GLN:HG2    | 10:N:102:1N7:H4   | 1.95                     | 0.49              |
| 2:G:5:VAL:C       | 2:H:150:ARG:HH21  | 2.21                     | 0.49              |
| 2:H:89:ALA:HB3    | 2:H:124:VAL:CG1   | 2.43                     | 0.49              |
| 3:I:619:ALA:HB2   | 3:I:654:ASP:HB2   | 1.94                     | 0.49              |
| 3:I:1004:ASP:OD1  | 3:I:1004:ASP:N    | 2.46                     | 0.49              |
| 3:I:1131:MET:HE3  | 3:I:1140:LYS:HE3  | 1.94                     | 0.49              |
| 4:J:17:PHE:HE2    | 4:J:20:ILE:HG12   | 1.78                     | 0.49              |
| 4:J:355:ILE:HG21  | 4:J:466:MET:CG    | 2.37                     | 0.49              |
| 4:J:367:GLY:CA    | 4:J:448:GLN:HB2   | 2.42                     | 0.49              |
| 4:J:664:ILE:HG22  | 4:J:678:ARG:HG2   | 1.93                     | 0.49              |
| 4:J:960:LEU:CB    | 4:J:963:VAL:HB    | 2.43                     | 0.49              |
| 4:J:976:THR:HA    | 4:J:999:TYR:HE1   | 1.76                     | 0.49              |
| 4:J:1146:GLU:OE2  | 4:J:1310:THR:HG22 | 2.12                     | 0.49              |
| 6:L:322:MET:HG2   | 6:L:324:LYS:NZ    | 2.27                     | 0.49              |
| 1:N:37:CYS:CB     | 1:N:58:CYS:H      | 2.25                     | 0.49              |
| 2:G:90:VAL:HA     | 2:G:124:VAL:HG13  | 1.95                     | 0.49              |
| 2:H:107:ILE:HG13  | 2:H:135:ASP:HA    | 1.95                     | 0.49              |
| 3:I:88:ARG:NH2    | 3:I:1035:LYS:O    | 2.41                     | 0.49              |
| 3:I:420:LEU:CD1   | 3:I:425:ILE:HD11  | 2.43                     | 0.49              |
| 3:I:794:LEU:CD2   | 3:I:796:LEU:HD11  | 2.43                     | 0.49              |
| 3:I:1165:SER:OG   | 3:I:1169:VAL:HG22 | 2.13                     | 0.49              |
| 3:I:1287:LEU:HD13 | 4:J:1357:ILE:HD11 | 1.94                     | 0.49              |
| 4:J:181:GLY:O     | 4:J:185:ILE:HG12  | 2.13                     | 0.49              |
| 4:J:813:ASP:HA    | 4:J:895:CYS:HG    | 1.77                     | 0.49              |
| 4:J:859:PRO:HD2   | 4:J:862:THR:CG2   | 2.43                     | 0.49              |
| 4:J:1162:ILE:HA   | 4:J:1202:GLU:O    | 2.12                     | 0.49              |
| 2:G:124:VAL:HG11  | 2:G:210:THR:HG22  | 1.93                     | 0.49              |
| 3:I:898:GLU:OE2   | 6:L:565:ILE:HG12  | 2.13                     | 0.49              |
| 3:I:1256:GLN:OE1  | 6:L:528:LEU:HD21  | 2.13                     | 0.49              |
| 4:J:71:LEU:N      | 4:J:90:VAL:HG11   | 2.28                     | 0.49              |
| 4:J:129:ASP:HB2   | 4:J:220:ARG:HH22  | 1.78                     | 0.49              |
| 4:J:719:PHE:HD1   | 4:J:724:MET:HE1   | 1.76                     | 0.49              |
| 4:J:949:SER:HB3   | 4:J:1016:THR:CG2  | 2.43                     | 0.49              |
| 4:J:1357:ILE:CG2  | 4:J:1358:PRO:HD2  | 2.43                     | 0.49              |
| 6:L:435:ILE:O     | 6:L:439:ILE:HG12  | 2.12                     | 0.49              |
| 6:L:439:ILE:HG22  | 6:L:443:ILE:HD12  | 1.94                     | 0.49              |
| 6:L:454:VAL:O     | 6:L:458:GLU:HB2   | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:593:LYS:HG2   | 6:L:596:ARG:HH11  | 1.78                     | 0.49              |
| 2:G:89:ALA:O      | 2:G:124:VAL:HG22  | 2.12                     | 0.49              |
| 3:I:103:VAL:HG12  | 3:I:117:ILE:HG22  | 1.95                     | 0.49              |
| 3:I:359:ARG:HD3   | 3:I:360:LEU:HD12  | 1.95                     | 0.49              |
| 3:I:930:ASP:OD1   | 3:I:931:VAL:N     | 2.45                     | 0.49              |
| 3:I:976:ARG:NE    | 3:I:989:LEU:HD23  | 2.28                     | 0.49              |
| 4:J:311:ARG:NH2   | 4:J:1329:THR:HG21 | 2.28                     | 0.49              |
| 4:J:425:ARG:HD2   | 4:J:459:ALA:HB2   | 1.94                     | 0.49              |
| 4:J:926:PRO:CG    | 4:J:1248:ILE:HD11 | 2.42                     | 0.49              |
| 4:J:1047:THR:HG22 | 4:J:1062:LEU:HD21 | 1.94                     | 0.49              |
| 6:L:23:THR:HG21   | 6:L:58:GLU:O      | 2.12                     | 0.49              |
| 6:L:486:ARG:O     | 6:L:487:MET:HE2   | 2.13                     | 0.49              |
| 6:L:575:GLU:OE2   | 6:L:578:LYS:NZ    | 2.26                     | 0.49              |
| 7:O:23:DC:H2''    | 7:O:24:DC:C5'     | 2.43                     | 0.49              |
| 2:G:102:LEU:HD23  | 2:G:144:ILE:HD11  | 1.94                     | 0.49              |
| 2:G:175:ALA:HB1   | 2:G:177:TYR:CZ    | 2.48                     | 0.49              |
| 3:I:221:LEU:HD23  | 3:I:336:LEU:CD1   | 2.29                     | 0.49              |
| 3:I:624:ASP:HB2   | 3:I:630:VAL:HG12  | 1.95                     | 0.49              |
| 4:J:708:ASN:HB2   | 4:J:711:GLY:O     | 2.13                     | 0.49              |
| 4:J:1163:VAL:CG2  | 4:J:1175:LEU:HD21 | 2.43                     | 0.49              |
| 4:J:1278:GLU:HG2  | 4:J:1279:GLN:H    | 1.78                     | 0.49              |
| 6:L:45:ILE:O      | 6:L:48:ILE:HG22   | 2.12                     | 0.49              |
| 2:M:257:VAL:O     | 2:M:260:LEU:HB2   | 2.13                     | 0.49              |
| 3:I:130:MET:CG    | 3:I:134:GLY:HA2   | 2.43                     | 0.48              |
| 3:I:202:ARG:HH12  | 3:I:368:ARG:HH22  | 1.61                     | 0.48              |
| 3:I:214:ASN:ND2   | 3:I:359:ARG:HH21  | 2.10                     | 0.48              |
| 3:I:895:LEU:HD23  | 3:I:895:LEU:H     | 1.78                     | 0.48              |
| 4:J:260:PHE:HB3   | 6:L:504:PRO:HB3   | 1.95                     | 0.48              |
| 4:J:1095:MET:HE3  | 4:J:1096:PRO:O    | 2.13                     | 0.48              |
| 6:L:220:LYS:O     | 6:L:223:GLU:HB3   | 2.12                     | 0.48              |
| 2:M:252:ILE:HG22  | 2:M:312:LEU:HD21  | 1.95                     | 0.48              |
| 2:M:304:LYS:CG    | 2:M:314:LEU:HD11  | 2.43                     | 0.48              |
| 3:I:361:SER:O     | 3:I:365:GLU:HG2   | 2.13                     | 0.48              |
| 3:I:538:LEU:HD21  | 3:I:547:VAL:HG11  | 1.94                     | 0.48              |
| 3:I:1239:VAL:O    | 3:I:1242:LYS:N    | 2.40                     | 0.48              |
| 4:J:164:GLN:HA    | 4:J:167:ASP:OD1   | 2.13                     | 0.48              |
| 4:J:410:ASP:O     | 4:J:414:GLU:HG3   | 2.13                     | 0.48              |
| 4:J:930:LEU:HD11  | 4:J:1241:TYR:CE1  | 2.49                     | 0.48              |
| 4:J:1027:VAL:HG13 | 4:J:1121:LEU:HD22 | 1.95                     | 0.48              |
| 6:L:111:LEU:HD12  | 6:L:382:ALA:HB3   | 1.95                     | 0.48              |
| 6:L:129:GLN:O     | 6:L:133:SER:OG    | 2.27                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:339:ARG:O     | 6:L:342:GLN:N     | 2.47                     | 0.48              |
| 6:L:530:LEU:O     | 6:L:533:ASP:N     | 2.46                     | 0.48              |
| 2:M:289:LEU:O     | 2:M:295:LEU:HD13  | 2.13                     | 0.48              |
| 2:H:58:GLU:HB2    | 2:H:171:LEU:O     | 2.13                     | 0.48              |
| 3:I:122:VAL:HG21  | 3:I:493:ILE:CD1   | 2.43                     | 0.48              |
| 3:I:732:ILE:HD11  | 3:I:769:PRO:CB    | 2.32                     | 0.48              |
| 3:I:754:THR:H     | 3:I:767:GLN:CG    | 2.25                     | 0.48              |
| 3:I:1165:SER:OG   | 3:I:1169:VAL:HG13 | 2.11                     | 0.48              |
| 4:J:1047:THR:HG22 | 4:J:1062:LEU:HD11 | 1.95                     | 0.48              |
| 5:K:60:ASN:OD1    | 5:K:63:ILE:HD13   | 2.13                     | 0.48              |
| 6:L:132:CYS:O     | 6:L:136:GLU:HG2   | 2.13                     | 0.48              |
| 6:L:529:GLU:HG2   | 6:L:534:SER:OG    | 2.13                     | 0.48              |
| 2:G:153:VAL:HB    | 2:G:175:ALA:HB3   | 1.95                     | 0.48              |
| 2:H:104:LYS:HD3   | 2:H:110:VAL:HG22  | 1.95                     | 0.48              |
| 3:I:9:LYS:HD3     | 3:I:791:LEU:HD22  | 1.96                     | 0.48              |
| 3:I:141:THR:O     | 3:I:143:ARG:HG3   | 2.14                     | 0.48              |
| 3:I:738:GLU:HA    | 3:I:741:MET:HB2   | 1.94                     | 0.48              |
| 3:I:802:VAL:HG12  | 3:I:1228:GLY:O    | 2.13                     | 0.48              |
| 3:I:976:ARG:HH12  | 3:I:990:ASP:CB    | 2.27                     | 0.48              |
| 3:I:1136:GLN:HB3  | 3:I:1137:GLU:OE1  | 2.12                     | 0.48              |
| 4:J:342:LEU:O     | 4:J:343:LEU:HD23  | 2.13                     | 0.48              |
| 4:J:859:PRO:HD2   | 4:J:862:THR:HG21  | 1.95                     | 0.48              |
| 4:J:1034:PHE:CE1  | 4:J:1114:GLN:HG3  | 2.48                     | 0.48              |
| 6:L:268:TYR:O     | 6:L:272:SER:N     | 2.40                     | 0.48              |
| 6:L:507:MET:HG2   | 6:L:520:GLY:HA3   | 1.94                     | 0.48              |
| 7:O:21:DA:H5"     | 2:M:294:ASN:ND2   | 2.29                     | 0.48              |
| 1:N:35:TYR:O      | 1:N:43:PRO:HA     | 2.13                     | 0.48              |
| 2:G:57:THR:CG2    | 2:G:147:GLN:HG2   | 2.42                     | 0.48              |
| 3:I:180:ARG:O     | 3:I:395:TYR:HA    | 2.13                     | 0.48              |
| 3:I:714:VAL:HB    | 3:I:786:GLY:HA3   | 1.94                     | 0.48              |
| 3:I:1232:MET:C    | 3:I:1233:LEU:HD12 | 2.39                     | 0.48              |
| 4:J:416:ILE:CG2   | 4:J:439:PRO:HB2   | 2.43                     | 0.48              |
| 4:J:799:ARG:HH12  | 4:J:1142:ALA:HB1  | 1.78                     | 0.48              |
| 4:J:826:ILE:HD13  | 4:J:831:VAL:HG22  | 1.95                     | 0.48              |
| 4:J:998:PRO:HG2   | 4:J:1020:TRP:CE2  | 2.48                     | 0.48              |
| 4:J:1005:LYS:HB3  | 4:J:1009:GLU:OE1  | 2.13                     | 0.48              |
| 4:J:1064:SER:HA   | 4:J:1067:ARG:CD   | 2.43                     | 0.48              |
| 4:J:1289:ASN:ND2  | 4:J:1300:ALA:O    | 2.43                     | 0.48              |
| 6:L:306:PHE:HA    | 6:L:315:TRP:CB    | 2.43                     | 0.48              |
| 6:L:388:ILE:O     | 6:L:392:LYS:HG3   | 2.12                     | 0.48              |
| 6:L:583:THR:O     | 6:L:587:ILE:HG12  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:P:63:DG:H2'    | 8:P:63:DG:OP2     | 2.13                     | 0.48              |
| 2:G:68:TYR:CE1   | 2:G:79:LEU:HD11   | 2.49                     | 0.48              |
| 2:H:47:LEU:CD2   | 2:H:180:VAL:HG11  | 2.42                     | 0.48              |
| 2:H:158:ARG:HE   | 2:H:172:LEU:CD1   | 2.24                     | 0.48              |
| 3:I:57:PHE:HD2   | 3:I:70:TYR:HB2    | 1.77                     | 0.48              |
| 3:I:94:ALA:O     | 3:I:126:GLU:HB2   | 2.14                     | 0.48              |
| 3:I:156:PHE:CE1  | 3:I:177:ILE:HD12  | 2.47                     | 0.48              |
| 3:I:198:ILE:CG2  | 3:I:388:LEU:HD21  | 2.43                     | 0.48              |
| 3:I:296:VAL:O    | 3:I:335:THR:HG23  | 2.14                     | 0.48              |
| 3:I:897:PRO:O    | 3:I:898:GLU:HB2   | 2.14                     | 0.48              |
| 3:I:1107:MET:SD  | 4:J:739:GLN:HG2   | 2.52                     | 0.48              |
| 3:I:1216:ARG:HD3 | 3:I:1216:ARG:H    | 1.79                     | 0.48              |
| 3:I:1279:GLU:OE2 | 4:J:1347:LEU:HB3  | 2.13                     | 0.48              |
| 4:J:152:THR:OG1  | 4:J:153:ASN:N     | 2.46                     | 0.48              |
| 4:J:437:PHE:HZ   | 4:J:453:VAL:HG11  | 1.79                     | 0.48              |
| 4:J:842:ARG:NH2  | 4:J:1254:GLU:OE1  | 2.44                     | 0.48              |
| 4:J:1061:VAL:CB  | 4:J:1105:ALA:HB3  | 2.43                     | 0.48              |
| 4:J:1160:SER:CB  | 4:J:1205:GLU:HA   | 2.43                     | 0.48              |
| 4:J:1239:ASP:HA  | 4:J:1242:ARG:HB2  | 1.96                     | 0.48              |
| 6:L:267:ASP:HA   | 6:L:270:VAL:HB    | 1.96                     | 0.48              |
| 2:G:72:GLU:OE1   | 2:G:72:GLU:N      | 2.47                     | 0.48              |
| 3:I:70:TYR:CZ    | 3:I:72:SER:HA     | 2.49                     | 0.48              |
| 3:I:338:THR:HA   | 3:I:343:HIS:O     | 2.13                     | 0.48              |
| 3:I:628:HIS:HB3  | 3:I:647:ARG:HH21  | 1.77                     | 0.48              |
| 3:I:714:VAL:CG1  | 3:I:787:PRO:HD2   | 2.44                     | 0.48              |
| 4:J:146:VAL:HG21 | 4:J:154:LEU:CD2   | 2.44                     | 0.48              |
| 4:J:342:LEU:C    | 4:J:343:LEU:HD23  | 2.39                     | 0.48              |
| 4:J:926:PRO:HB2  | 4:J:1248:ILE:HD11 | 1.94                     | 0.48              |
| 4:J:988:PHE:HB2  | 4:J:990:ARG:HG2   | 1.96                     | 0.48              |
| 4:J:1036:ARG:HB2 | 4:J:1081:VAL:CG1  | 2.43                     | 0.48              |
| 5:K:37:PRO:HB3   | 5:K:49:ILE:HG21   | 1.96                     | 0.48              |
| 6:L:137:TYR:CE2  | 6:L:276:MET:HE1   | 2.49                     | 0.48              |
| 6:L:150:ARG:HB3  | 6:L:155:GLU:CG    | 2.44                     | 0.48              |
| 3:I:122:VAL:HG21 | 3:I:493:ILE:HG21  | 1.96                     | 0.48              |
| 3:I:588:GLU:HG2  | 3:I:607:SER:CA    | 2.43                     | 0.48              |
| 3:I:828:PHE:O    | 3:I:1234:LYS:HE2  | 2.14                     | 0.48              |
| 3:I:1325:VAL:O   | 3:I:1329:GLU:HG3  | 2.13                     | 0.48              |
| 4:J:526:VAL:HA   | 4:J:549:LYS:O     | 2.13                     | 0.48              |
| 4:J:1147:ALA:HB1 | 4:J:1218:HIS:CD2  | 2.48                     | 0.48              |
| 4:J:1153:PRO:HD2 | 4:J:1194:ARG:HH22 | 1.79                     | 0.48              |
| 6:L:297:MET:HE2  | 6:L:302:PHE:CB    | 2.44                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:600:HIS:NE2   | 2:M:258:ASP:OD2   | 2.46                     | 0.48              |
| 8:P:51:DC:C2'     | 8:P:52:DT:H72     | 2.44                     | 0.48              |
| 2:M:304:LYS:O     | 2:M:304:LYS:HD3   | 2.14                     | 0.48              |
| 2:G:227:GLN:OE1   | 2:G:227:GLN:HA    | 2.14                     | 0.48              |
| 3:I:228:VAL:O     | 3:I:335:THR:N     | 2.47                     | 0.48              |
| 3:I:556:GLY:O     | 3:I:579:ALA:HB2   | 2.14                     | 0.48              |
| 3:I:963:GLU:OE2   | 3:I:964:LEU:HD22  | 2.13                     | 0.48              |
| 3:I:1192:GLU:HG2  | 3:I:1196:LYS:HE3  | 1.96                     | 0.48              |
| 4:J:42:GLU:CB     | 4:J:52:GLU:HG2    | 2.43                     | 0.48              |
| 4:J:161:THR:HG23  | 4:J:164:GLN:H     | 1.78                     | 0.48              |
| 4:J:490:ILE:O     | 4:J:499:ILE:HG22  | 2.13                     | 0.48              |
| 4:J:1026:PRO:HB2  | 4:J:1028:ILE:HG23 | 1.96                     | 0.48              |
| 2:G:155:ALA:HA    | 2:G:158:ARG:HB3   | 1.96                     | 0.48              |
| 2:H:150:ARG:O     | 2:H:177:TYR:HB2   | 2.14                     | 0.48              |
| 3:I:499:SER:HA    | 3:I:502:VAL:HG12  | 1.96                     | 0.48              |
| 3:I:1165:SER:OG   | 3:I:1169:VAL:N    | 2.46                     | 0.48              |
| 4:J:147:ILE:HG13  | 4:J:177:ASP:O     | 2.13                     | 0.48              |
| 4:J:227:PHE:HE1   | 4:J:237:MET:HE3   | 1.79                     | 0.48              |
| 4:J:751:ASP:OD1   | 4:J:753:SER:N     | 2.46                     | 0.48              |
| 4:J:986:ASP:OD2   | 4:J:992:LYS:HD2   | 2.13                     | 0.48              |
| 6:L:297:MET:HE2   | 6:L:302:PHE:CA    | 2.43                     | 0.48              |
| 8:P:57:DT:H2''    | 8:P:58:DC:C5'     | 2.42                     | 0.48              |
| 8:P:68:DG:P       | 2:M:296:GLY:H     | 2.37                     | 0.48              |
| 2:M:282:VAL:CG1   | 2:M:312:LEU:HD22  | 2.44                     | 0.48              |
| 2:H:67:GLU:HA     | 2:H:68:TYR:HA     | 1.58                     | 0.47              |
| 3:I:209:ILE:O     | 3:I:213:LEU:HG    | 2.14                     | 0.47              |
| 3:I:232:ILE:N     | 3:I:331:LYS:O     | 2.42                     | 0.47              |
| 3:I:538:LEU:HD12  | 3:I:538:LEU:O     | 2.14                     | 0.47              |
| 3:I:704:MET:O     | 3:I:704:MET:HE3   | 2.14                     | 0.47              |
| 3:I:840:SER:O     | 3:I:1047:LEU:HB2  | 2.14                     | 0.47              |
| 3:I:1339:LEU:HD23 | 4:J:17:PHE:CG     | 2.48                     | 0.47              |
| 4:J:162:GLU:O     | 4:J:166:LEU:HD23  | 2.14                     | 0.47              |
| 4:J:342:LEU:HD21  | 4:J:1352:ILE:HG23 | 1.96                     | 0.47              |
| 4:J:347:VAL:HG12  | 4:J:348:ASP:O     | 2.14                     | 0.47              |
| 4:J:548:VAL:N     | 4:J:572:THR:O     | 2.47                     | 0.47              |
| 4:J:612:LEU:HD23  | 4:J:616:PRO:HB2   | 1.95                     | 0.47              |
| 4:J:849:LEU:HD13  | 4:J:855:ASP:C     | 2.39                     | 0.47              |
| 4:J:1009:GLU:O    | 4:J:1011:VAL:HG13 | 2.14                     | 0.47              |
| 4:J:1237:VAL:CG1  | 4:J:1253:ILE:HG21 | 2.44                     | 0.47              |
| 5:K:39:VAL:CG2    | 5:K:40:PRO:HD2    | 2.44                     | 0.47              |
| 6:L:98:VAL:HG13   | 6:L:402:LEU:HD11  | 1.95                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:348:GLU:N    | 6:L:355:ILE:HD11  | 2.29                     | 0.47              |
| 6:L:373:ARG:HA   | 6:L:376:LYS:HE2   | 1.96                     | 0.47              |
| 6:L:444:ALA:HB1  | 6:L:457:ILE:CD1   | 2.34                     | 0.47              |
| 6:L:452:ILE:HG13 | 6:L:457:ILE:CD1   | 2.39                     | 0.47              |
| 6:L:486:ARG:HG3  | 6:L:487:MET:HE3   | 1.96                     | 0.47              |
| 6:L:509:THR:HG23 | 6:L:510:PRO:HD2   | 1.96                     | 0.47              |
| 2:M:289:LEU:HD21 | 2:M:303:ILE:HG21  | 1.96                     | 0.47              |
| 2:H:102:LEU:CD2  | 2:H:115:ILE:HG12  | 2.44                     | 0.47              |
| 3:I:120:GLN:NE2  | 3:I:490:GLN:HB2   | 2.26                     | 0.47              |
| 3:I:877:VAL:HG13 | 3:I:881:ASP:HB2   | 1.94                     | 0.47              |
| 3:I:979:LEU:HD12 | 3:I:985:GLU:HG3   | 1.96                     | 0.47              |
| 3:I:1220:GLN:NE2 | 3:I:1221:PHE:O    | 2.47                     | 0.47              |
| 4:J:18:ASP:OD1   | 4:J:19:ALA:N      | 2.47                     | 0.47              |
| 4:J:1282:TYR:HD2 | 4:J:1286:LYS:HB2  | 1.78                     | 0.47              |
| 6:L:432:THR:O    | 6:L:436:ARG:HB2   | 2.14                     | 0.47              |
| 6:L:595:LEU:O    | 6:L:599:ARG:HG3   | 2.14                     | 0.47              |
| 2:H:43:LEU:O     | 2:H:47:LEU:HD12   | 2.14                     | 0.47              |
| 2:H:64:VAL:HA    | 2:H:65:LEU:CB     | 2.44                     | 0.47              |
| 3:I:161:LYS:HD2  | 3:I:170:VAL:HG22  | 1.96                     | 0.47              |
| 3:I:754:THR:H    | 3:I:767:GLN:HG2   | 1.78                     | 0.47              |
| 4:J:83:VAL:O     | 4:J:92:VAL:HG12   | 2.14                     | 0.47              |
| 4:J:745:GLY:C    | 4:J:746:LEU:HD12  | 2.40                     | 0.47              |
| 4:J:1174:ARG:HA  | 4:J:1187:GLU:OE2  | 2.14                     | 0.47              |
| 4:J:1253:ILE:O   | 4:J:1257:VAL:HG23 | 2.15                     | 0.47              |
| 6:L:348:GLU:CG   | 6:L:355:ILE:HG12  | 2.45                     | 0.47              |
| 6:L:593:LYS:CA   | 6:L:596:ARG:HG2   | 2.42                     | 0.47              |
| 3:I:796:LEU:H    | 3:I:796:LEU:HD12  | 1.78                     | 0.47              |
| 4:J:167:ASP:HA   | 4:J:170:GLU:CB    | 2.45                     | 0.47              |
| 4:J:298:MET:HE3  | 6:L:402:LEU:HB2   | 1.96                     | 0.47              |
| 4:J:858:VAL:HB   | 4:J:862:THR:OG1   | 2.15                     | 0.47              |
| 4:J:884:SER:OG   | 4:J:885:VAL:N     | 2.46                     | 0.47              |
| 4:J:975:ILE:CD1  | 4:J:980:THR:HG21  | 2.33                     | 0.47              |
| 6:L:150:ARG:HB3  | 6:L:155:GLU:CB    | 2.44                     | 0.47              |
| 2:G:107:ILE:HD11 | 2:G:136:GLU:HA    | 1.95                     | 0.47              |
| 3:I:103:VAL:CB   | 3:I:117:ILE:HG22  | 2.44                     | 0.47              |
| 4:J:271:ARG:O    | 4:J:275:ARG:HG3   | 2.15                     | 0.47              |
| 4:J:422:LEU:CD1  | 4:J:471:PRO:HG3   | 2.44                     | 0.47              |
| 4:J:1046:ILE:CD1 | 4:J:1059:LEU:HD13 | 2.40                     | 0.47              |
| 4:J:1080:ILE:HB  | 4:J:1097:ALA:HB3  | 1.95                     | 0.47              |
| 4:J:1140:ARG:O   | 4:J:1144:LEU:HB2  | 2.15                     | 0.47              |
| 6:L:128:ASN:HA   | 6:L:131:GLN:CD    | 2.40                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:L:294:GLN:HG3   | 6:L:295:CYS:SG   | 2.54                     | 0.47              |
| 2:G:192:VAL:HG21  | 2:G:198:LEU:HD12 | 1.96                     | 0.47              |
| 2:H:144:ILE:HG12  | 2:H:145:LYS:H    | 1.80                     | 0.47              |
| 3:I:3:TYR:CZ      | 3:I:11:ILE:HD11  | 2.49                     | 0.47              |
| 3:I:122:VAL:HG21  | 3:I:493:ILE:HD12 | 1.97                     | 0.47              |
| 3:I:671:LEU:HD23  | 3:I:1186:VAL:CG2 | 2.45                     | 0.47              |
| 3:I:765:ILE:CD1   | 3:I:787:PRO:HG3  | 2.44                     | 0.47              |
| 3:I:1104:PRO:CG   | 4:J:725:MET:HE3  | 2.45                     | 0.47              |
| 3:I:1213:TYR:CE2  | 3:I:1220:GLN:HG3 | 2.50                     | 0.47              |
| 3:I:1245:ALA:HB1  | 4:J:376:LEU:CD2  | 2.39                     | 0.47              |
| 4:J:38:VAL:HG22   | 4:J:105:ILE:HG12 | 1.96                     | 0.47              |
| 4:J:118:LYS:NZ    | 4:J:136:GLU:OE2  | 2.44                     | 0.47              |
| 4:J:122:SER:OG    | 4:J:132:LEU:HD12 | 2.14                     | 0.47              |
| 6:L:137:TYR:O     | 6:L:140:ALA:HB3  | 2.14                     | 0.47              |
| 6:L:558:VAL:O     | 6:L:561:MET:HB2  | 2.14                     | 0.47              |
| 7:O:28:DG:H2"     | 7:O:29:DA:C8     | 2.50                     | 0.47              |
| 2:M:285:THR:O     | 2:M:289:LEU:HD13 | 2.14                     | 0.47              |
| 2:H:152:TYR:OH    | 4:J:532:GLU:OE2  | 2.32                     | 0.47              |
| 3:I:254:ASP:CB    | 3:I:265:LYS:HG3  | 2.45                     | 0.47              |
| 3:I:724:VAL:HA    | 3:I:734:ILE:HG22 | 1.97                     | 0.47              |
| 3:I:848:GLU:CG    | 3:I:888:THR:HG22 | 2.40                     | 0.47              |
| 3:I:851:THR:OG1   | 3:I:852:ALA:N    | 2.47                     | 0.47              |
| 3:I:980:VAL:O     | 3:I:984:VAL:HB   | 2.15                     | 0.47              |
| 3:I:1286:THR:O    | 3:I:1289:GLU:HG2 | 2.15                     | 0.47              |
| 3:I:1333:LEU:CD2  | 4:J:327:LEU:HD13 | 2.44                     | 0.47              |
| 3:I:1339:LEU:HD23 | 4:J:17:PHE:CD1   | 2.50                     | 0.47              |
| 4:J:279:LEU:HD12  | 4:J:295:GLU:HG3  | 1.95                     | 0.47              |
| 4:J:509:GLY:CA    | 4:J:632:ALA:HB2  | 2.43                     | 0.47              |
| 4:J:826:ILE:CD1   | 4:J:831:VAL:HG13 | 2.45                     | 0.47              |
| 4:J:950:ILE:O     | 4:J:950:ILE:HG13 | 2.15                     | 0.47              |
| 6:L:216:LEU:O     | 6:L:219:GLU:HG2  | 2.14                     | 0.47              |
| 6:L:584:ARG:HH12  | 8:P:57:DT:H72    | 1.79                     | 0.47              |
| 3:I:48:GLY:N      | 3:I:461:GLU:OE2  | 2.48                     | 0.47              |
| 4:J:78:LEU:HD12   | 4:J:78:LEU:O     | 2.15                     | 0.47              |
| 4:J:159:ILE:O     | 4:J:160:LEU:HD23 | 2.15                     | 0.47              |
| 4:J:244:VAL:HA    | 4:J:269:TYR:OH   | 2.14                     | 0.47              |
| 4:J:250:ARG:NH1   | 4:J:266:ASN:OD1  | 2.48                     | 0.47              |
| 4:J:475:GLU:OE1   | 4:J:475:GLU:N    | 2.44                     | 0.47              |
| 4:J:536:LEU:HD23  | 4:J:541:LEU:HB2  | 1.96                     | 0.47              |
| 6:L:141:ILE:O     | 6:L:144:LEU:HB3  | 2.14                     | 0.47              |
| 6:L:234:THR:CG2   | 6:L:244:THR:HB   | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:293:GLU:OE1  | 6:L:293:GLU:N     | 2.48                     | 0.47              |
| 2:H:29:GLU:O     | 2:H:31:LEU:HD22   | 2.15                     | 0.47              |
| 2:H:44:ARG:NH1   | 4:J:538:ARG:HD2   | 2.29                     | 0.47              |
| 2:H:62:ASP:OD2   | 2:H:140:ILE:HA    | 2.15                     | 0.47              |
| 2:H:76:GLU:HA    | 2:H:80:GLU:HG2    | 1.96                     | 0.47              |
| 2:H:201:LEU:HD12 | 2:H:202:VAL:H     | 1.79                     | 0.47              |
| 3:I:40:GLU:HG2   | 3:I:41:GLN:N      | 2.30                     | 0.47              |
| 3:I:246:LEU:HB3  | 3:I:249:GLU:OE2   | 2.15                     | 0.47              |
| 3:I:960:LEU:HD22 | 3:I:1029:LEU:HD12 | 1.95                     | 0.47              |
| 3:I:967:LEU:HD21 | 3:I:1025:PHE:HE2  | 1.79                     | 0.47              |
| 4:J:84:ILE:HG22  | 4:J:91:GLU:HA     | 1.96                     | 0.47              |
| 4:J:514:THR:HB   | 4:J:576:ARG:HG2   | 1.97                     | 0.47              |
| 4:J:733:SER:O    | 4:J:737:ILE:HG12  | 2.14                     | 0.47              |
| 4:J:899:TYR:CE1  | 4:J:1251:LYS:HE2  | 2.49                     | 0.47              |
| 4:J:975:ILE:CD1  | 4:J:1003:LEU:HD11 | 2.43                     | 0.47              |
| 6:L:117:ILE:HG22 | 6:L:121:LYS:CE    | 2.44                     | 0.47              |
| 6:L:402:LEU:HD12 | 6:L:402:LEU:H     | 1.80                     | 0.47              |
| 7:O:44:DA:H5'    | 7:O:44:DA:H8      | 1.79                     | 0.47              |
| 1:N:56:THR:C     | 1:N:57:LEU:HD23   | 2.40                     | 0.47              |
| 2:G:234:LEU:HD13 | 2:H:218:ARG:HH21  | 1.80                     | 0.47              |
| 2:H:56:VAL:HG11  | 2:H:144:ILE:HD11  | 1.97                     | 0.47              |
| 3:I:312:ALA:H    | 3:I:315:MET:CE    | 2.28                     | 0.47              |
| 3:I:521:LEU:HD12 | 3:I:667:LEU:CD1   | 2.44                     | 0.47              |
| 3:I:818:VAL:HB   | 3:I:1076:ILE:HD11 | 1.97                     | 0.47              |
| 3:I:1107:MET:SD  | 4:J:736:GLN:HB3   | 2.55                     | 0.47              |
| 3:I:1122:LYS:HE2 | 3:I:1229:TYR:CE2  | 2.50                     | 0.47              |
| 3:I:1214:ASP:HB3 | 3:I:1217:THR:CG2  | 2.45                     | 0.47              |
| 4:J:556:GLU:HG2  | 4:J:558:ASP:OD2   | 2.15                     | 0.47              |
| 4:J:605:LEU:HD23 | 4:J:605:LEU:HA    | 1.63                     | 0.47              |
| 4:J:1017:VAL:O   | 4:J:1017:VAL:HG12 | 2.15                     | 0.47              |
| 4:J:1029:THR:OG1 | 4:J:1031:VAL:O    | 2.32                     | 0.47              |
| 4:J:1222:ARG:NH1 | 4:J:1223:LEU:HD21 | 2.29                     | 0.47              |
| 5:K:12:LYS:HG3   | 5:K:54:ILE:O      | 2.15                     | 0.47              |
| 6:L:291:CYS:SG   | 6:L:330:LEU:HD22  | 2.55                     | 0.47              |
| 6:L:569:THR:OG1  | 6:L:570:ASP:N     | 2.43                     | 0.47              |
| 1:N:2:SER:OG     | 1:N:3:ASP:N       | 2.47                     | 0.46              |
| 2:G:27:THR:C     | 2:G:28:LEU:HD12   | 2.41                     | 0.46              |
| 2:G:192:VAL:CG2  | 2:G:198:LEU:HD12  | 2.45                     | 0.46              |
| 2:H:61:ILE:HG13  | 2:H:78:ILE:HD12   | 1.97                     | 0.46              |
| 3:I:156:PHE:HE2  | 3:I:450:ASN:HB3   | 1.81                     | 0.46              |
| 3:I:214:ASN:CG   | 3:I:359:ARG:HE    | 2.23                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:242:VAL:HB    | 3:I:245:ARG:HB3   | 1.96                     | 0.46              |
| 3:I:256:GLU:HB3   | 3:I:261:VAL:HG13  | 1.97                     | 0.46              |
| 3:I:324:LYS:HA    | 3:I:327:GLN:CD    | 2.40                     | 0.46              |
| 3:I:358:ASP:OD1   | 3:I:358:ASP:N     | 2.48                     | 0.46              |
| 3:I:895:LEU:HD12  | 3:I:899:GLU:HG3   | 1.97                     | 0.46              |
| 3:I:1204:LEU:HB3  | 3:I:1205:PRO:HD2  | 1.97                     | 0.46              |
| 4:J:616:PRO:O     | 4:J:619:ILE:HG22  | 2.15                     | 0.46              |
| 6:L:123:ILE:HG13  | 6:L:375:ALA:HB3   | 1.97                     | 0.46              |
| 6:L:324:LYS:HB2   | 6:L:327:SER:CB    | 2.45                     | 0.46              |
| 6:L:336:GLU:O     | 6:L:339:ARG:HB2   | 2.15                     | 0.46              |
| 2:M:295:LEU:CD2   | 2:M:300:LEU:HB2   | 2.45                     | 0.46              |
| 2:G:5:VAL:O       | 2:H:150:ARG:NH2   | 2.40                     | 0.46              |
| 2:G:39:LEU:HD21   | 2:H:224:LEU:HD11  | 1.96                     | 0.46              |
| 2:H:59:VAL:O      | 2:H:171:LEU:HD23  | 2.14                     | 0.46              |
| 3:I:636:CYS:O     | 3:I:642:SER:HB2   | 2.14                     | 0.46              |
| 3:I:712:SER:OG    | 3:I:714:VAL:HG22  | 2.15                     | 0.46              |
| 3:I:1103:VAL:CG2  | 3:I:1104:PRO:HD3  | 2.45                     | 0.46              |
| 4:J:84:ILE:O      | 4:J:84:ILE:HG13   | 2.14                     | 0.46              |
| 4:J:735:ALA:O     | 4:J:738:ARG:HB3   | 2.16                     | 0.46              |
| 4:J:915:ILE:HA    | 4:J:918:ILE:HG12  | 1.97                     | 0.46              |
| 4:J:1141:VAL:HG13 | 4:J:1237:VAL:CG2  | 2.45                     | 0.46              |
| 4:J:1172:LYS:HD3  | 4:J:1189:MET:CB   | 2.39                     | 0.46              |
| 4:J:1261:LEU:HD13 | 4:J:1304:ARG:NH1  | 2.30                     | 0.46              |
| 6:L:143:TYR:HB3   | 6:L:269:LEU:HD21  | 1.98                     | 0.46              |
| 6:L:326:TRP:HA    | 6:L:329:LYS:CD    | 2.44                     | 0.46              |
| 6:L:547:VAL:HG23  | 6:L:548:LEU:HD12  | 1.96                     | 0.46              |
| 6:L:593:LYS:HA    | 6:L:596:ARG:CD    | 2.45                     | 0.46              |
| 7:O:28:DG:H2"     | 7:O:29:DA:H8      | 1.79                     | 0.46              |
| 2:G:158:ARG:NH1   | 2:G:158:ARG:O     | 2.39                     | 0.46              |
| 2:H:120:ASP:OD1   | 2:H:120:ASP:N     | 2.47                     | 0.46              |
| 3:I:18:ARG:HG2    | 3:I:1188:ASP:OD1  | 2.15                     | 0.46              |
| 3:I:289:VAL:CG1   | 3:I:322:LEU:HD23  | 2.45                     | 0.46              |
| 3:I:590:PRO:HB2   | 3:I:655:VAL:HG21  | 1.96                     | 0.46              |
| 3:I:633:LEU:HD12  | 3:I:633:LEU:HA    | 1.73                     | 0.46              |
| 4:J:783:LEU:HA    | 4:J:786:THR:CG2   | 2.45                     | 0.46              |
| 4:J:836:ARG:HA    | 4:J:869:CYS:SG    | 2.55                     | 0.46              |
| 4:J:1032:SER:CB   | 4:J:1116:SER:HA   | 2.45                     | 0.46              |
| 4:J:1078:LEU:HD11 | 4:J:1107:VAL:HG11 | 1.97                     | 0.46              |
| 4:J:1089:LEU:CB   | 4:J:1096:PRO:HA   | 2.45                     | 0.46              |
| 4:J:1238:GLN:HG2  | 4:J:1253:ILE:HD12 | 1.97                     | 0.46              |
| 4:J:1314:LEU:HD12 | 4:J:1315:ALA:N    | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:K:26:ARG:HH11  | 5:K:29:GLN:HB2    | 1.80                     | 0.46              |
| 2:G:110:VAL:O    | 2:G:130:ILE:HB    | 2.15                     | 0.46              |
| 3:I:67:GLU:HB3   | 3:I:103:VAL:CG2   | 2.46                     | 0.46              |
| 3:I:178:PRO:HB3  | 3:I:397:LEU:HD11  | 1.98                     | 0.46              |
| 3:I:339:ASN:N    | 3:I:343:HIS:O     | 2.47                     | 0.46              |
| 3:I:388:LEU:HG   | 3:I:389:PHE:CD2   | 2.50                     | 0.46              |
| 3:I:444:ASP:N    | 3:I:444:ASP:OD1   | 2.47                     | 0.46              |
| 3:I:471:VAL:O    | 3:I:475:VAL:HG23  | 2.15                     | 0.46              |
| 3:I:1268:GLN:HG3 | 4:J:467:ALA:HB1   | 1.97                     | 0.46              |
| 3:I:1283:ALA:HB1 | 3:I:1286:THR:HB   | 1.97                     | 0.46              |
| 4:J:174:ASP:CG   | 4:J:175:GLU:HG3   | 2.41                     | 0.46              |
| 4:J:604:MET:HE3  | 4:J:624:ILE:HD12  | 1.98                     | 0.46              |
| 4:J:782:GLY:O    | 4:J:786:THR:HG22  | 2.16                     | 0.46              |
| 4:J:1160:SER:OG  | 4:J:1206:ARG:N    | 2.30                     | 0.46              |
| 3:I:9:LYS:HD3    | 3:I:791:LEU:CD2   | 2.46                     | 0.46              |
| 3:I:230:PHE:HB2  | 3:I:333:ILE:HB    | 1.97                     | 0.46              |
| 3:I:233:ARG:CD   | 3:I:238:GLN:HB2   | 2.37                     | 0.46              |
| 3:I:524:ILE:O    | 3:I:528:ARG:HD3   | 2.16                     | 0.46              |
| 3:I:618:GLN:O    | 3:I:621:SER:OG    | 2.28                     | 0.46              |
| 3:I:1111:GLN:O   | 3:I:1115:THR:HG22 | 2.16                     | 0.46              |
| 3:I:1282:GLY:HA3 | 5:K:17:PHE:CE1    | 2.51                     | 0.46              |
| 4:J:1029:THR:O   | 4:J:1118:GLY:HA2  | 2.15                     | 0.46              |
| 6:L:84:LEU:HD12  | 6:L:84:LEU:O      | 2.15                     | 0.46              |
| 6:L:143:TYR:OH   | 6:L:147:GLN:NE2   | 2.49                     | 0.46              |
| 8:P:34:DT:H73    | 8:P:34:DT:OP1     | 2.14                     | 0.46              |
| 8:P:36:DT:C3'    | 8:P:37:DG:H5''    | 2.45                     | 0.46              |
| 2:H:103:ASN:HA   | 2:H:141:SER:HB2   | 1.97                     | 0.46              |
| 3:I:137:VAL:CG2  | 3:I:142:GLU:HG2   | 2.45                     | 0.46              |
| 3:I:299:LYS:HE2  | 3:I:300:ASP:O     | 2.15                     | 0.46              |
| 3:I:391:SER:OG   | 3:I:394:ARG:HB2   | 2.15                     | 0.46              |
| 3:I:557:ARG:HA   | 3:I:579:ALA:HB2   | 1.97                     | 0.46              |
| 3:I:717:VAL:HG12 | 3:I:782:VAL:HG12  | 1.98                     | 0.46              |
| 3:I:856:ASN:HA   | 6:L:613:ASP:C     | 2.39                     | 0.46              |
| 3:I:976:ARG:HD2  | 3:I:976:ARG:HA    | 1.64                     | 0.46              |
| 3:I:1167:GLU:O   | 3:I:1171:ARG:NH2  | 2.49                     | 0.46              |
| 3:I:1305:TYR:CE1 | 4:J:379:PRO:HG3   | 2.51                     | 0.46              |
| 4:J:176:PHE:CZ   | 4:J:178:ALA:HB3   | 2.51                     | 0.46              |
| 4:J:252:LEU:HG   | 4:J:262:THR:CG2   | 2.40                     | 0.46              |
| 4:J:400:MET:HE3  | 4:J:400:MET:HB2   | 1.82                     | 0.46              |
| 6:L:144:LEU:HD21 | 6:L:221:PHE:CE1   | 2.50                     | 0.46              |
| 6:L:215:GLU:HB3  | 6:L:218:ARG:NH2   | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:468:ARG:HH12  | 8:P:35:DA:P       | 2.38                     | 0.46              |
| 6:L:479:THR:HG22  | 6:L:482:GLU:HB2   | 1.96                     | 0.46              |
| 2:G:11:PRO:O      | 2:G:12:ARG:HG3    | 2.16                     | 0.46              |
| 3:I:498:ILE:H     | 3:I:498:ILE:HD12  | 1.80                     | 0.46              |
| 4:J:30:ILE:HG21   | 4:J:241:VAL:HG12  | 1.97                     | 0.46              |
| 4:J:66:LYS:NZ     | 4:J:69:GLU:OE2    | 2.24                     | 0.46              |
| 4:J:850:LYS:HA    | 4:J:877:VAL:CG1   | 2.45                     | 0.46              |
| 4:J:1319:PHE:HD1  | 4:J:1342:ASP:HB2  | 1.81                     | 0.46              |
| 3:I:1133:LYS:HG3  | 3:I:1134:GLN:N    | 2.31                     | 0.46              |
| 3:I:1325:VAL:HG22 | 4:J:249:LEU:HD22  | 1.98                     | 0.46              |
| 4:J:127:LEU:HD21  | 4:J:234:PRO:HB3   | 1.98                     | 0.46              |
| 4:J:842:ARG:HB3   | 4:J:882:VAL:HG21  | 1.97                     | 0.46              |
| 4:J:1035:VAL:HG23 | 4:J:1113:VAL:O    | 2.15                     | 0.46              |
| 6:L:82:GLN:NE2    | 6:L:85:SER:OG     | 2.49                     | 0.46              |
| 8:P:40:DC:H1'     | 8:P:41:DT:O5'     | 2.15                     | 0.46              |
| 3:I:95:PRO:HA     | 3:I:126:GLU:HB3   | 1.97                     | 0.46              |
| 3:I:161:LYS:HD2   | 3:I:170:VAL:HG21  | 1.97                     | 0.46              |
| 3:I:1088:ASP:OD1  | 3:I:1088:ASP:N    | 2.47                     | 0.46              |
| 3:I:1131:MET:CE   | 3:I:1141:LEU:HD12 | 2.39                     | 0.46              |
| 3:I:1280:ALA:HB1  | 4:J:918:ILE:CG2   | 2.46                     | 0.46              |
| 4:J:399:LYS:HE2   | 4:J:399:LYS:HB3   | 1.65                     | 0.46              |
| 4:J:1002:VAL:O    | 4:J:1018:ALA:HA   | 2.15                     | 0.46              |
| 4:J:1021:ASP:HB3  | 4:J:1024:THR:HG23 | 1.97                     | 0.46              |
| 4:J:1023:HIS:HA   | 4:J:1125:PRO:HA   | 1.97                     | 0.46              |
| 4:J:1026:PRO:CA   | 4:J:1123:ARG:HA   | 2.33                     | 0.46              |
| 4:J:1266:ILE:HA   | 4:J:1302:TYR:HA   | 1.98                     | 0.46              |
| 4:J:1311:LYS:HE2  | 4:J:1314:LEU:HD21 | 1.97                     | 0.46              |
| 6:L:145:LEU:CD1   | 6:L:225:ARG:HA    | 2.46                     | 0.46              |
| 1:N:72:TYR:HB3    | 3:I:170:VAL:HG23  | 1.98                     | 0.46              |
| 3:I:178:PRO:HB3   | 3:I:397:LEU:CD1   | 2.46                     | 0.46              |
| 3:I:344:GLY:HA3   | 3:I:346:TYR:CE2   | 2.50                     | 0.46              |
| 3:I:818:VAL:CG2   | 3:I:1076:ILE:HD12 | 2.46                     | 0.46              |
| 3:I:898:GLU:HA    | 3:I:901:LEU:HB3   | 1.97                     | 0.46              |
| 4:J:38:VAL:CG2    | 4:J:105:ILE:HG12  | 2.46                     | 0.46              |
| 4:J:370:LYS:HG3   | 4:J:441:LEU:HD12  | 1.98                     | 0.46              |
| 4:J:530:PRO:O     | 4:J:533:ALA:HB3   | 2.16                     | 0.46              |
| 4:J:909:ILE:HD12  | 4:J:910:ASN:H     | 1.81                     | 0.46              |
| 4:J:1162:ILE:HD11 | 4:J:1201:GLY:O    | 2.16                     | 0.46              |
| 6:L:27:VAL:O      | 6:L:31:LEU:HG     | 2.16                     | 0.46              |
| 6:L:301:ASN:O     | 6:L:305:LEU:HB2   | 2.16                     | 0.46              |
| 6:L:593:LYS:C     | 6:L:596:ARG:HG2   | 2.40                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:252:ILE:HG22  | 2:M:252:ILE:O     | 2.16                     | 0.46              |
| 2:G:125:LYS:HE3   | 2:G:128:HIS:HB2   | 1.98                     | 0.45              |
| 3:I:194:LEU:C     | 3:I:206:ALA:HB2   | 2.41                     | 0.45              |
| 3:I:404:LYS:HE3   | 3:I:450:ASN:HA    | 1.98                     | 0.45              |
| 3:I:564:PRO:HG2   | 3:I:568:ASN:O     | 2.15                     | 0.45              |
| 3:I:699:LEU:HG    | 3:I:799:ASN:HD22  | 1.81                     | 0.45              |
| 3:I:968:GLU:HB3   | 3:I:1018:TYR:OH   | 2.16                     | 0.45              |
| 3:I:982:GLY:O     | 3:I:1002:LEU:HD11 | 2.16                     | 0.45              |
| 3:I:1191:LYS:N    | 3:I:1194:GLU:OE1  | 2.47                     | 0.45              |
| 4:J:254:PRO:HB3   | 4:J:260:PHE:HE2   | 1.80                     | 0.45              |
| 4:J:478:LEU:HD13  | 5:K:23:ALA:HB3    | 1.99                     | 0.45              |
| 4:J:908:ILE:HG13  | 4:J:909:ILE:O     | 2.16                     | 0.45              |
| 4:J:1144:LEU:HD11 | 4:J:1236:GLU:CG   | 2.34                     | 0.45              |
| 4:J:1165:PHE:HA   | 4:J:1175:LEU:CG   | 2.46                     | 0.45              |
| 4:J:1174:ARG:HG2  | 4:J:1187:GLU:OE1  | 2.16                     | 0.45              |
| 4:J:1178:THR:HA   | 4:J:1184:ASP:CB   | 2.46                     | 0.45              |
| 6:L:151:VAL:CG2   | 6:L:156:ALA:HB3   | 2.36                     | 0.45              |
| 6:L:319:ALA:O     | 6:L:322:MET:HB2   | 2.16                     | 0.45              |
| 6:L:324:LYS:HB2   | 6:L:327:SER:HB3   | 1.98                     | 0.45              |
| 7:O:40:DC:H1'     | 7:O:41:DT:O4'     | 2.15                     | 0.45              |
| 8:P:41:DT:H3'     | 8:P:41:DT:OP1     | 2.17                     | 0.45              |
| 2:M:304:LYS:HG2   | 2:M:314:LEU:HD11  | 1.98                     | 0.45              |
| 3:I:104:ILE:O     | 3:I:115:LYS:N     | 2.49                     | 0.45              |
| 3:I:316:GLU:OE1   | 3:I:316:GLU:N     | 2.40                     | 0.45              |
| 3:I:801:ARG:HD2   | 3:I:1229:TYR:CZ   | 2.52                     | 0.45              |
| 3:I:1119:MET:HG2  | 3:I:1204:LEU:HD13 | 1.99                     | 0.45              |
| 3:I:1129:ASN:OD1  | 3:I:1177:ARG:HG3  | 2.16                     | 0.45              |
| 4:J:151:MET:N     | 4:J:151:MET:SD    | 2.89                     | 0.45              |
| 4:J:582:ILE:HD13  | 4:J:627:THR:CG2   | 2.44                     | 0.45              |
| 4:J:845:ALA:O     | 4:J:860:ARG:HD3   | 2.16                     | 0.45              |
| 4:J:872:LEU:HG    | 4:J:877:VAL:CG2   | 2.46                     | 0.45              |
| 4:J:950:ILE:HD12  | 4:J:982:LEU:CD2   | 2.37                     | 0.45              |
| 4:J:955:LYS:O     | 4:J:984:LEU:HD11  | 2.17                     | 0.45              |
| 4:J:971:GLY:C     | 4:J:972:LYS:HE2   | 2.41                     | 0.45              |
| 4:J:1036:ARG:NH2  | 4:J:1081:VAL:HB   | 2.31                     | 0.45              |
| 4:J:1247:LYS:O    | 4:J:1248:ILE:HG13 | 2.16                     | 0.45              |
| 6:L:315:TRP:CE3   | 6:L:316:PHE:HB2   | 2.51                     | 0.45              |
| 6:L:576:VAL:HG11  | 6:L:587:ILE:HG21  | 1.98                     | 0.45              |
| 2:G:10:LYS:O      | 2:G:30:PRO:HB2    | 2.17                     | 0.45              |
| 2:H:68:TYR:OH     | 2:H:77:ASP:OD1    | 2.35                     | 0.45              |
| 3:I:182:SER:HB3   | 3:I:199:ASP:OD1   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:254:ASP:N    | 3:I:254:ASP:OD1   | 2.47                     | 0.45              |
| 3:I:623:LEU:HD12 | 3:I:627:GLY:HA2   | 1.99                     | 0.45              |
| 3:I:963:GLU:HA   | 3:I:966:ILE:CG1   | 2.46                     | 0.45              |
| 3:I:1281:TYR:CE2 | 4:J:431:ARG:HG3   | 2.52                     | 0.45              |
| 4:J:536:LEU:HD23 | 4:J:536:LEU:O     | 2.15                     | 0.45              |
| 4:J:1152:GLU:HB3 | 4:J:1214:PRO:CD   | 2.45                     | 0.45              |
| 6:L:135:ALA:HB1  | 6:L:253:SER:HB2   | 1.97                     | 0.45              |
| 6:L:399:LEU:HD12 | 6:L:399:LEU:HA    | 1.74                     | 0.45              |
| 6:L:479:THR:CG2  | 6:L:482:GLU:HB2   | 2.47                     | 0.45              |
| 2:H:35:PHE:CA    | 2:H:38:THR:HG22   | 2.45                     | 0.45              |
| 2:H:59:VAL:HG21  | 2:H:85:LEU:HD12   | 1.99                     | 0.45              |
| 3:I:22:LEU:HD22  | 3:I:603:ILE:HD13  | 1.98                     | 0.45              |
| 3:I:566:GLY:HA2  | 4:J:787:ALA:CB    | 2.46                     | 0.45              |
| 3:I:587:LEU:HD23 | 3:I:587:LEU:HA    | 1.86                     | 0.45              |
| 3:I:641:GLU:OE1  | 3:I:641:GLU:N     | 2.49                     | 0.45              |
| 3:I:977:ALA:O    | 3:I:980:VAL:HB    | 2.16                     | 0.45              |
| 3:I:1122:LYS:HG2 | 3:I:1229:TYR:CZ   | 2.52                     | 0.45              |
| 3:I:1258:PRO:HG2 | 4:J:346:ARG:CB    | 2.28                     | 0.45              |
| 4:J:549:LYS:HA   | 4:J:571:ASP:HA    | 1.99                     | 0.45              |
| 4:J:1154:ALA:HB2 | 4:J:1212:ASP:O    | 2.17                     | 0.45              |
| 4:J:1234:VAL:O   | 4:J:1238:GLN:HB2  | 2.16                     | 0.45              |
| 4:J:1267:VAL:CG2 | 4:J:1301:THR:HG22 | 2.47                     | 0.45              |
| 6:L:347:ILE:O    | 6:L:351:THR:N     | 2.38                     | 0.45              |
| 6:L:547:VAL:O    | 6:L:551:LEU:HG    | 2.16                     | 0.45              |
| 7:O:34:DA:H2"    | 7:O:35:DG:C8      | 2.52                     | 0.45              |
| 2:G:71:LYS:CE    | 2:G:140:ILE:HG22  | 2.41                     | 0.45              |
| 3:I:131:THR:HG22 | 3:I:132:ASP:N     | 2.31                     | 0.45              |
| 3:I:239:MET:O    | 3:I:284:LEU:HD12  | 2.17                     | 0.45              |
| 3:I:985:GLU:HB2  | 3:I:989:LEU:HD22  | 1.98                     | 0.45              |
| 3:I:1285:TYR:HE2 | 5:K:21:LEU:HD13   | 1.81                     | 0.45              |
| 4:J:114:ILE:HB   | 4:J:304:ASP:OD1   | 2.16                     | 0.45              |
| 4:J:194:LEU:HB3  | 4:J:228:VAL:CG2   | 2.46                     | 0.45              |
| 4:J:748:ALA:HA   | 4:J:754:ILE:HA    | 1.99                     | 0.45              |
| 4:J:950:ILE:CD1  | 4:J:982:LEU:HD13  | 2.46                     | 0.45              |
| 4:J:1046:ILE:CD1 | 4:J:1059:LEU:HD22 | 2.46                     | 0.45              |
| 4:J:1194:ARG:HG2 | 4:J:1212:ASP:HB2  | 1.97                     | 0.45              |
| 4:J:1327:GLU:OE2 | 4:J:1330:ARG:HB2  | 2.15                     | 0.45              |
| 2:M:290:LEU:HD13 | 2:M:300:LEU:HD13  | 1.97                     | 0.45              |
| 2:G:68:TYR:HE1   | 2:G:79:LEU:HD11   | 1.82                     | 0.45              |
| 2:G:78:ILE:HD13  | 2:G:78:ILE:HA     | 1.83                     | 0.45              |
| 2:H:61:ILE:HG23  | 2:H:140:ILE:HD11  | 1.97                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:68:TYR:CZ     | 2:H:78:ILE:HB    | 2.52                     | 0.45              |
| 3:I:52:ALA:O      | 3:I:55:SER:HB3   | 2.16                     | 0.45              |
| 3:I:75:LEU:HD12   | 3:I:94:ALA:HB3   | 1.98                     | 0.45              |
| 3:I:115:LYS:NZ    | 3:I:485:ASP:OD1  | 2.49                     | 0.45              |
| 3:I:146:VAL:HG23  | 3:I:511:LEU:CD2  | 2.44                     | 0.45              |
| 3:I:224:PHE:CG    | 3:I:347:ILE:HG13 | 2.52                     | 0.45              |
| 3:I:667:LEU:CD2   | 3:I:705:GLU:HG2  | 2.47                     | 0.45              |
| 3:I:1176:LEU:HD22 | 3:I:1181:PRO:CD  | 2.44                     | 0.45              |
| 3:I:1219:GLU:OE2  | 4:J:634:ARG:NH1  | 2.50                     | 0.45              |
| 4:J:74:LYS:HE2    | 4:J:75:TYR:OH    | 2.15                     | 0.45              |
| 4:J:120:LEU:HB2   | 4:J:121:PRO:CD   | 2.47                     | 0.45              |
| 4:J:844:THR:CG2   | 4:J:864:LEU:HD21 | 2.46                     | 0.45              |
| 5:K:9:ALA:HB1     | 5:K:19:LEU:HD13  | 1.98                     | 0.45              |
| 6:L:222:ALA:O     | 6:L:225:ARG:HB3  | 2.17                     | 0.45              |
| 2:G:23:HIS:HE1    | 2:G:204:GLU:HG3  | 1.82                     | 0.45              |
| 2:G:61:ILE:HD11   | 2:G:64:VAL:HG11  | 1.98                     | 0.45              |
| 3:I:195:PHE:HB3   | 3:I:203:LYS:HG3  | 1.98                     | 0.45              |
| 3:I:237:LEU:CD1   | 3:I:322:LEU:HD21 | 2.37                     | 0.45              |
| 3:I:254:ASP:O     | 3:I:256:GLU:HG2  | 2.16                     | 0.45              |
| 3:I:320:ASP:O     | 3:I:324:LYS:HG2  | 2.17                     | 0.45              |
| 3:I:559:CYS:CB    | 3:I:662:SER:HB2  | 2.47                     | 0.45              |
| 3:I:887:VAL:HB    | 3:I:913:VAL:CG2  | 2.46                     | 0.45              |
| 4:J:474:LEU:HD21  | 5:K:27:ALA:CB    | 2.47                     | 0.45              |
| 4:J:1266:ILE:HD13 | 4:J:1275:LEU:O   | 2.17                     | 0.45              |
| 6:L:275:VAL:CG1   | 6:L:279:ARG:HD2  | 2.46                     | 0.45              |
| 6:L:369:GLU:OE1   | 6:L:373:ARG:HD3  | 2.17                     | 0.45              |
| 6:L:543:ALA:HB1   | 6:L:606:VAL:HG21 | 1.97                     | 0.45              |
| 1:N:37:CYS:HB2    | 1:N:58:CYS:HB3   | 1.99                     | 0.45              |
| 2:H:35:PHE:HA     | 2:H:38:THR:CG2   | 2.47                     | 0.45              |
| 3:I:26:TYR:CE2    | 3:I:28:LEU:HB2   | 2.50                     | 0.45              |
| 3:I:40:GLU:HG2    | 3:I:41:GLN:H     | 1.81                     | 0.45              |
| 3:I:165:HIS:ND1   | 3:I:165:HIS:O    | 2.50                     | 0.45              |
| 3:I:188:PHE:CE1   | 3:I:194:LEU:HG   | 2.51                     | 0.45              |
| 3:I:194:LEU:CD1   | 3:I:346:TYR:HB3  | 2.46                     | 0.45              |
| 3:I:808:ASN:H     | 4:J:633:ALA:HB2  | 1.82                     | 0.45              |
| 3:I:1289:GLU:OE1  | 4:J:473:THR:OG1  | 2.29                     | 0.45              |
| 4:J:722:ILE:CG2   | 4:J:737:ILE:HD12 | 2.46                     | 0.45              |
| 4:J:809:VAL:CG1   | 4:J:911:LYS:HA   | 2.47                     | 0.45              |
| 4:J:1160:SER:OG   | 4:J:1206:ARG:HG2 | 2.17                     | 0.45              |
| 6:L:297:MET:HE2   | 6:L:302:PHE:N    | 2.32                     | 0.45              |
| 7:O:56:DC:H1'     | 7:O:57:DT:C2     | 2.52                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:202:ARG:NH1   | 3:I:368:ARG:HH22 | 2.14                     | 0.45              |
| 3:I:301:TYR:N     | 3:I:311:CYS:O    | 2.36                     | 0.45              |
| 3:I:466:VAL:O     | 3:I:469:VAL:HG12 | 2.17                     | 0.45              |
| 3:I:854:ILE:HG23  | 3:I:855:PRO:HD2  | 1.98                     | 0.45              |
| 3:I:956:ALA:HB1   | 3:I:1032:LYS:HG2 | 1.99                     | 0.45              |
| 3:I:1151:LEU:HD11 | 3:I:1198:LEU:CD2 | 2.47                     | 0.45              |
| 3:I:1166:ASP:H    | 3:I:1168:GLU:N   | 2.14                     | 0.45              |
| 4:J:525:MET:HG3   | 4:J:527:LEU:CD1  | 2.47                     | 0.45              |
| 4:J:857:LEU:HD21  | 4:J:871:LEU:CD2  | 2.47                     | 0.45              |
| 4:J:862:THR:O     | 4:J:864:LEU:HD23 | 2.15                     | 0.45              |
| 4:J:910:ASN:ND2   | 5:K:15:ASN:HA    | 2.32                     | 0.45              |
| 6:L:426:LYS:HG3   | 6:L:428:SER:H    | 1.82                     | 0.45              |
| 6:L:573:LEU:HD12  | 6:L:573:LEU:O    | 2.17                     | 0.45              |
| 2:G:190:ALA:HB2   | 2:G:199:ASP:C    | 2.42                     | 0.45              |
| 3:I:321:LEU:CA    | 3:I:324:LYS:HG2  | 2.35                     | 0.45              |
| 3:I:377:THR:HG23  | 3:I:380:ALA:HB3  | 1.99                     | 0.45              |
| 3:I:549:ASP:CG    | 4:J:750:PRO:HG2  | 2.42                     | 0.45              |
| 3:I:580:GLN:HG3   | 3:I:581:THR:O    | 2.17                     | 0.45              |
| 4:J:895:CYS:SG    | 4:J:898:CYS:N    | 2.89                     | 0.45              |
| 4:J:913:GLU:OE1   | 4:J:913:GLU:HA   | 2.17                     | 0.45              |
| 4:J:984:LEU:HD23  | 4:J:992:LYS:HB3  | 1.99                     | 0.45              |
| 4:J:1110:GLU:OE2  | 4:J:1110:GLU:N   | 2.49                     | 0.45              |
| 5:K:8:ASP:O       | 5:K:11:GLU:HB3   | 2.16                     | 0.45              |
| 5:K:30:MET:HE1    | 5:K:49:ILE:HG22  | 1.98                     | 0.45              |
| 5:K:38:LEU:HD11   | 5:K:67:ARG:NH2   | 2.25                     | 0.45              |
| 5:K:65:ASP:O      | 5:K:68:GLU:HB2   | 2.17                     | 0.45              |
| 6:L:231:THR:HG21  | 6:L:249:ILE:CG1  | 2.40                     | 0.45              |
| 6:L:448:ARG:HB2   | 6:L:450:ILE:O    | 2.16                     | 0.45              |
| 6:L:481:GLU:HG2   | 6:L:491:GLU:OE2  | 2.17                     | 0.45              |
| 6:L:562:ARG:HD3   | 6:L:591:GLU:HG3  | 1.99                     | 0.45              |
| 2:H:213:PRO:HA    | 2:H:216:ALA:CB   | 2.41                     | 0.44              |
| 3:I:118:LYS:HD3   | 3:I:487:LEU:O    | 2.16                     | 0.44              |
| 3:I:210:LEU:O     | 3:I:215:TYR:HB2  | 2.16                     | 0.44              |
| 3:I:227:LYS:NZ    | 3:I:298:ALA:HB1  | 2.32                     | 0.44              |
| 3:I:887:VAL:HB    | 3:I:913:VAL:HG22 | 1.99                     | 0.44              |
| 3:I:1105:SER:CB   | 4:J:731:ARG:HH11 | 2.30                     | 0.44              |
| 4:J:59:ALA:O      | 4:J:90:VAL:HG23  | 2.17                     | 0.44              |
| 4:J:68:TYR:CE2    | 4:J:78:LEU:HD13  | 2.52                     | 0.44              |
| 4:J:194:LEU:HD23  | 4:J:228:VAL:CG2  | 2.47                     | 0.44              |
| 4:J:418:GLU:HB2   | 5:K:45:LYS:HB2   | 1.99                     | 0.44              |
| 4:J:646:ILE:HD11  | 4:J:762:ASN:ND2  | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1226:VAL:HG13 | 4:J:1227:HIS:CD2  | 2.52                     | 0.44              |
| 4:J:1271:SER:O    | 4:J:1271:SER:OG   | 2.25                     | 0.44              |
| 7:O:48:DG:H2''    | 7:O:49:DC:OP1     | 2.18                     | 0.44              |
| 8:P:40:DC:H2''    | 8:P:41:DT:OP2     | 2.17                     | 0.44              |
| 8:P:51:DC:H2''    | 8:P:52:DT:H72     | 1.98                     | 0.44              |
| 1:N:37:CYS:HB2    | 1:N:58:CYS:H      | 1.82                     | 0.44              |
| 2:H:82:LEU:CG     | 2:H:173:VAL:HG12  | 2.43                     | 0.44              |
| 3:I:221:LEU:HD11  | 3:I:351:LEU:HD11  | 1.99                     | 0.44              |
| 3:I:351:LEU:HA    | 3:I:354:ASP:CG    | 2.42                     | 0.44              |
| 3:I:839:VAL:HG12  | 3:I:1049:ILE:HG21 | 1.99                     | 0.44              |
| 3:I:988:LYS:HA    | 3:I:991:LYS:CG    | 2.45                     | 0.44              |
| 4:J:385:LEU:HD23  | 4:J:385:LEU:HA    | 1.82                     | 0.44              |
| 4:J:473:THR:O     | 4:J:476:ALA:HB3   | 2.17                     | 0.44              |
| 4:J:515:ARG:NH2   | 4:J:718:SER:O     | 2.50                     | 0.44              |
| 4:J:1034:PHE:HB2  | 4:J:1081:VAL:CG2  | 2.47                     | 0.44              |
| 4:J:1153:PRO:O    | 4:J:1194:ARG:NH1  | 2.50                     | 0.44              |
| 4:J:1165:PHE:HA   | 4:J:1175:LEU:HD12 | 1.98                     | 0.44              |
| 4:J:1167:LYS:HG2  | 4:J:1168:GLU:N    | 2.33                     | 0.44              |
| 6:L:120:ALA:HA    | 6:L:123:ILE:HD12  | 1.99                     | 0.44              |
| 2:G:38:THR:OG1    | 2:H:45:ARG:HD3    | 2.16                     | 0.44              |
| 2:H:9:LEU:HD12    | 2:H:32:GLU:OE2    | 2.18                     | 0.44              |
| 3:I:17:LYS:HG3    | 3:I:1153:ALA:O    | 2.17                     | 0.44              |
| 3:I:284:LEU:O     | 3:I:285:ILE:HG23  | 2.17                     | 0.44              |
| 3:I:359:ARG:HD3   | 3:I:360:LEU:CD1   | 2.48                     | 0.44              |
| 3:I:432:LEU:HD12  | 3:I:435:ILE:HG22  | 1.99                     | 0.44              |
| 3:I:494:ASN:HA    | 6:L:472:GLN:NE2   | 2.29                     | 0.44              |
| 3:I:616:ILE:HG22  | 3:I:617:ALA:O     | 2.17                     | 0.44              |
| 3:I:748:ILE:HD11  | 3:I:966:ILE:HB    | 1.99                     | 0.44              |
| 4:J:449:LEU:HA    | 4:J:449:LEU:HD12  | 1.67                     | 0.44              |
| 4:J:800:LEU:O     | 4:J:803:VAL:HG12  | 2.17                     | 0.44              |
| 6:L:14:THR:HG22   | 6:L:18:GLU:OE2    | 2.17                     | 0.44              |
| 7:O:33:DA:H2''    | 7:O:34:DA:OP2     | 2.17                     | 0.44              |
| 8:P:44:DT:H2''    | 8:P:45:DA:N7      | 2.32                     | 0.44              |
| 8:P:63:DG:H1'     | 8:P:64:DA:H5'     | 1.99                     | 0.44              |
| 2:H:13:LEU:HD22   | 2:H:28:LEU:CD1    | 2.39                     | 0.44              |
| 2:H:201:LEU:HD23  | 2:H:203:ILE:HD11  | 2.00                     | 0.44              |
| 3:I:136:PHE:CE2   | 3:I:145:ILE:HD13  | 2.53                     | 0.44              |
| 3:I:136:PHE:O     | 3:I:142:GLU:HA    | 2.17                     | 0.44              |
| 3:I:348:SER:HA    | 3:I:351:LEU:HD12  | 2.00                     | 0.44              |
| 3:I:832:HIS:N     | 3:I:1056:VAL:O    | 2.43                     | 0.44              |
| 3:I:976:ARG:NH2   | 3:I:989:LEU:HB3   | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:1131:MET:CE   | 3:I:1141:LEU:HA  | 2.46                     | 0.44              |
| 3:I:1328:LYS:HD3  | 3:I:1328:LYS:HA  | 1.74                     | 0.44              |
| 4:J:885:VAL:HG23  | 4:J:899:TYR:HA   | 1.99                     | 0.44              |
| 4:J:982:LEU:CD2   | 4:J:995:TYR:HB2  | 2.48                     | 0.44              |
| 7:O:38:DG:H2'     | 7:O:38:DG:OP2    | 2.18                     | 0.44              |
| 2:M:252:ILE:O     | 2:M:278:ILE:HG21 | 2.17                     | 0.44              |
| 2:H:24:ALA:CB     | 2:H:213:PRO:HG2  | 2.46                     | 0.44              |
| 2:H:134:THR:OG1   | 2:H:135:ASP:N    | 2.51                     | 0.44              |
| 3:I:59:ILE:HD11   | 3:I:472:GLU:HB2  | 1.98                     | 0.44              |
| 3:I:60:GLN:CA     | 3:I:67:GLU:HG3   | 2.48                     | 0.44              |
| 3:I:589:THR:HG23  | 3:I:591:TYR:CE2  | 2.52                     | 0.44              |
| 3:I:742:TYR:CD2   | 3:I:743:PRO:HD2  | 2.52                     | 0.44              |
| 3:I:839:VAL:HG21  | 3:I:841:ARG:CZ   | 2.47                     | 0.44              |
| 3:I:871:VAL:HG13  | 3:I:883:LEU:HA   | 1.99                     | 0.44              |
| 3:I:901:LEU:HA    | 6:L:563:PHE:CE1  | 2.53                     | 0.44              |
| 3:I:976:ARG:HH12  | 3:I:990:ASP:HB2  | 1.81                     | 0.44              |
| 4:J:661:VAL:CG1   | 4:J:682:VAL:HG23 | 2.45                     | 0.44              |
| 4:J:923:ILE:HD11  | 4:J:1252:HIS:C   | 2.42                     | 0.44              |
| 4:J:1332:LEU:HD23 | 4:J:1332:LEU:HA  | 1.85                     | 0.44              |
| 4:J:1365:TYR:O    | 4:J:1369:ARG:HG2 | 2.17                     | 0.44              |
| 6:L:10:LYS:O      | 6:L:13:VAL:HG22  | 2.18                     | 0.44              |
| 6:L:13:VAL:HG11   | 6:L:84:LEU:HD22  | 2.00                     | 0.44              |
| 6:L:385:ARG:HH11  | 7:O:55:DC:H5'    | 1.83                     | 0.44              |
| 6:L:451:ARG:HG2   | 6:L:452:ILE:N    | 2.33                     | 0.44              |
| 6:L:470:MET:SD    | 6:L:482:GLU:HG2  | 2.58                     | 0.44              |
| 6:L:590:ILE:O     | 6:L:594:ALA:N    | 2.51                     | 0.44              |
| 6:L:593:LYS:HA    | 6:L:596:ARG:CG   | 2.46                     | 0.44              |
| 8:P:45:DA:H2''    | 8:P:46:DG:OP2    | 2.16                     | 0.44              |
| 2:M:282:VAL:O     | 2:M:316:MET:N    | 2.29                     | 0.44              |
| 2:M:298:LYS:HD2   | 2:M:298:LYS:HA   | 1.79                     | 0.44              |
| 2:H:157:THR:C     | 2:H:158:ARG:HD3  | 2.43                     | 0.44              |
| 3:I:227:LYS:HD3   | 3:I:227:LYS:HA   | 1.77                     | 0.44              |
| 3:I:521:LEU:CD1   | 3:I:667:LEU:HD12 | 2.45                     | 0.44              |
| 3:I:1158:LYS:HA   | 3:I:1158:LYS:HD3 | 1.57                     | 0.44              |
| 4:J:398:LYS:HD3   | 6:L:532:LEU:HD13 | 1.99                     | 0.44              |
| 4:J:601:ILE:HG13  | 4:J:604:MET:HE2  | 2.00                     | 0.44              |
| 4:J:1231:ARG:NH1  | 4:J:1231:ARG:HB3 | 2.33                     | 0.44              |
| 4:J:1282:TYR:CD2  | 4:J:1286:LYS:HB2 | 2.52                     | 0.44              |
| 6:L:146:GLU:O     | 6:L:150:ARG:HG3  | 2.18                     | 0.44              |
| 1:N:24:ARG:HH21   | 4:J:687:ALA:CB   | 2.30                     | 0.44              |
| 2:H:27:THR:HG23   | 2:H:27:THR:O     | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:255:ILE:HB    | 3:I:263:VAL:N     | 2.31                     | 0.44              |
| 3:I:431:LYS:HA    | 3:I:434:ASP:OD1   | 2.17                     | 0.44              |
| 3:I:1167:GLU:O    | 3:I:1168:GLU:HG3  | 2.18                     | 0.44              |
| 3:I:1301:ARG:HG3  | 3:I:1302:THR:N    | 2.33                     | 0.44              |
| 4:J:58:CYS:SG     | 4:J:59:ALA:N      | 2.91                     | 0.44              |
| 4:J:429:LEU:HB3   | 4:J:925:GLU:HB3   | 2.00                     | 0.44              |
| 4:J:502:PRO:HG2   | 4:J:601:ILE:HD13  | 2.00                     | 0.44              |
| 4:J:559:ALA:HB3   | 4:J:562:GLU:HB2   | 2.00                     | 0.44              |
| 4:J:721:SER:O     | 4:J:725:MET:HE2   | 2.17                     | 0.44              |
| 4:J:876:SER:CB    | 4:J:990:ARG:HH21  | 2.31                     | 0.44              |
| 4:J:885:VAL:HG13  | 4:J:894:VAL:CG1   | 2.48                     | 0.44              |
| 4:J:967:VAL:HG13  | 4:J:971:GLY:O     | 2.17                     | 0.44              |
| 4:J:1053:LEU:HD12 | 4:J:1054:THR:N    | 2.32                     | 0.44              |
| 4:J:1152:GLU:O    | 4:J:1214:PRO:HD2  | 2.17                     | 0.44              |
| 4:J:1157:ALA:O    | 4:J:1206:ARG:HA   | 2.17                     | 0.44              |
| 4:J:1176:VAL:HG22 | 4:J:1187:GLU:HB2  | 1.98                     | 0.44              |
| 4:J:1261:LEU:O    | 4:J:1261:LEU:HD12 | 2.17                     | 0.44              |
| 6:L:139:GLU:HA    | 6:L:142:THR:OG1   | 2.17                     | 0.44              |
| 2:M:282:VAL:HB    | 2:M:316:MET:CB    | 2.35                     | 0.44              |
| 3:I:39:ILE:HD11   | 3:I:75:LEU:HG     | 2.00                     | 0.44              |
| 3:I:169:LYS:HD2   | 3:I:169:LYS:HA    | 1.68                     | 0.44              |
| 3:I:590:PRO:HG3   | 3:I:605:TYR:CD1   | 2.53                     | 0.44              |
| 3:I:1160:ASP:C    | 3:I:1161:LEU:HD12 | 2.43                     | 0.44              |
| 4:J:604:MET:HE3   | 4:J:624:ILE:CD1   | 2.48                     | 0.44              |
| 4:J:902:ASP:HB3   | 4:J:1251:LYS:HD3  | 1.99                     | 0.44              |
| 4:J:1075:ARG:HD3  | 4:J:1075:ARG:HA   | 1.75                     | 0.44              |
| 6:L:51:MET:HB2    | 6:L:53:ILE:HG13   | 1.98                     | 0.44              |
| 6:L:117:ILE:HG23  | 6:L:421:TYR:CD1   | 2.53                     | 0.44              |
| 7:O:21:DA:H1'     | 7:O:22:DT:H5'     | 2.00                     | 0.44              |
| 1:N:52:PHE:HB2    | 1:N:55:VAL:HG22   | 1.97                     | 0.44              |
| 2:H:11:PRO:HG3    | 2:H:28:LEU:HD21   | 2.00                     | 0.44              |
| 3:I:176:ILE:O     | 3:I:178:PRO:HD3   | 2.18                     | 0.44              |
| 3:I:566:GLY:HA2   | 4:J:787:ALA:HB1   | 2.00                     | 0.44              |
| 3:I:812:PHE:CE2   | 3:I:813:GLU:HG2   | 2.53                     | 0.44              |
| 3:I:897:PRO:HB2   | 6:L:564:GLY:O     | 2.17                     | 0.44              |
| 3:I:989:LEU:O     | 3:I:992:LEU:HD23  | 2.18                     | 0.44              |
| 3:I:1038:GLN:HG3  | 3:I:1039:GLY:O    | 2.18                     | 0.44              |
| 4:J:615:LYS:HB2   | 4:J:616:PRO:HD3   | 2.00                     | 0.44              |
| 4:J:683:ILE:HD11  | 4:J:756:GLU:HA    | 2.00                     | 0.44              |
| 4:J:783:LEU:HD23  | 4:J:783:LEU:O     | 2.16                     | 0.44              |
| 4:J:986:ASP:HB2   | 4:J:992:LYS:CG    | 2.46                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1106:ILE:O    | 4:J:1122:ALA:HB1  | 2.18                     | 0.44              |
| 6:L:12:LEU:HB3    | 6:L:30:HIS:CG     | 2.51                     | 0.44              |
| 6:L:133:SER:OG    | 6:L:365:MET:HB2   | 2.18                     | 0.44              |
| 7:O:21:DA:H5''    | 2:M:294:ASN:HD21  | 1.82                     | 0.44              |
| 8:P:46:DG:H2''    | 8:P:47:DC:H6      | 1.83                     | 0.44              |
| 1:N:40:CYS:HB3    | 3:I:268:ARG:HB3   | 2.00                     | 0.43              |
| 3:I:99:LYS:O      | 3:I:100:LEU:HD23  | 2.18                     | 0.43              |
| 3:I:976:ARG:HH12  | 3:I:990:ASP:CA    | 2.31                     | 0.43              |
| 3:I:1122:LYS:HG2  | 3:I:1229:TYR:CE1  | 2.53                     | 0.43              |
| 4:J:579:LEU:HD12  | 4:J:582:ILE:HG12  | 2.00                     | 0.43              |
| 4:J:850:LYS:HA    | 4:J:877:VAL:HG11  | 2.00                     | 0.43              |
| 4:J:1049:GLN:O    | 4:J:1058:SER:N    | 2.39                     | 0.43              |
| 4:J:1059:LEU:HD23 | 4:J:1059:LEU:HA   | 1.67                     | 0.43              |
| 4:J:1239:ASP:HA   | 4:J:1242:ARG:CB   | 2.48                     | 0.43              |
| 6:L:348:GLU:HG3   | 6:L:355:ILE:HG12  | 2.00                     | 0.43              |
| 8:P:42:DT:H2''    | 8:P:43:DT:OP2     | 2.18                     | 0.43              |
| 2:G:39:LEU:HA     | 2:G:39:LEU:HD23   | 1.67                     | 0.43              |
| 2:H:57:THR:C      | 2:H:173:VAL:HG22  | 2.43                     | 0.43              |
| 3:I:254:ASP:HB3   | 3:I:265:LYS:N     | 2.33                     | 0.43              |
| 3:I:469:VAL:HA    | 3:I:472:GLU:HG2   | 2.00                     | 0.43              |
| 3:I:637:ARG:O     | 3:I:637:ARG:HG3   | 2.18                     | 0.43              |
| 3:I:838:CYS:O     | 3:I:1049:ILE:HA   | 2.18                     | 0.43              |
| 3:I:903:ARG:HB3   | 3:I:908:GLU:O     | 2.18                     | 0.43              |
| 4:J:115:TRP:CE3   | 4:J:1333:THR:HG22 | 2.54                     | 0.43              |
| 4:J:420:PRO:O     | 4:J:471:PRO:HD2   | 2.18                     | 0.43              |
| 4:J:749:LYS:HD3   | 4:J:753:SER:OG    | 2.18                     | 0.43              |
| 4:J:768:ASN:N     | 4:J:771:GLN:OE1   | 2.50                     | 0.43              |
| 5:K:13:ILE:HD11   | 5:K:19:LEU:CA     | 2.45                     | 0.43              |
| 6:L:280:VAL:HA    | 6:L:347:ILE:CD1   | 2.48                     | 0.43              |
| 6:L:292:VAL:CG1   | 6:L:299:LYS:HD2   | 2.48                     | 0.43              |
| 6:L:555:GLU:HA    | 6:L:558:VAL:CG1   | 2.45                     | 0.43              |
| 8:P:63:DG:H4'     | 8:P:64:DA:OP1     | 2.17                     | 0.43              |
| 2:H:111:THR:HA    | 2:H:129:VAL:HA    | 1.99                     | 0.43              |
| 3:I:921:PRO:HD2   | 3:I:924:VAL:HG23  | 1.99                     | 0.43              |
| 3:I:971:LEU:HD13  | 3:I:1018:TYR:CD1  | 2.46                     | 0.43              |
| 3:I:972:PHE:CD1   | 3:I:975:ILE:HD12  | 2.46                     | 0.43              |
| 3:I:979:LEU:O     | 3:I:984:VAL:HG23  | 2.18                     | 0.43              |
| 3:I:1321:GLU:HG3  | 4:J:99:ARG:HH21   | 1.82                     | 0.43              |
| 4:J:568:SER:OG    | 4:J:569:LEU:N     | 2.51                     | 0.43              |
| 4:J:800:LEU:HD12  | 4:J:1256:ILE:HD12 | 1.99                     | 0.43              |
| 4:J:1275:LEU:CB   | 4:J:1278:GLU:HB2  | 2.42                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:L:261:LEU:CD1   | 6:L:266:PHE:HB2  | 2.47                     | 0.43              |
| 6:L:437:GLN:O     | 6:L:441:ARG:HB3  | 2.18                     | 0.43              |
| 6:L:437:GLN:HB3   | 8:P:37:DG:O6     | 2.18                     | 0.43              |
| 6:L:557:LYS:O     | 6:L:561:MET:HG2  | 2.18                     | 0.43              |
| 8:P:56:DG:C8      | 8:P:57:DT:H72    | 2.52                     | 0.43              |
| 3:I:70:TYR:OH     | 3:I:72:SER:HA    | 2.19                     | 0.43              |
| 3:I:444:ASP:O     | 3:I:447:HIS:HB2  | 2.17                     | 0.43              |
| 3:I:459:MET:SD    | 3:I:511:LEU:HD13 | 2.58                     | 0.43              |
| 3:I:556:GLY:O     | 3:I:576:SER:HB3  | 2.18                     | 0.43              |
| 3:I:633:LEU:CG    | 3:I:644:LEU:HB3  | 2.48                     | 0.43              |
| 3:I:818:VAL:HB    | 3:I:1076:ILE:CD1 | 2.48                     | 0.43              |
| 3:I:842:ASP:OD1   | 3:I:842:ASP:N    | 2.50                     | 0.43              |
| 3:I:898:GLU:O     | 6:L:540:LEU:HD21 | 2.18                     | 0.43              |
| 4:J:129:ASP:CB    | 4:J:220:ARG:HH22 | 2.31                     | 0.43              |
| 4:J:325:LYS:CE    | 6:L:508:GLU:HG2  | 2.48                     | 0.43              |
| 4:J:367:GLY:HA3   | 4:J:448:GLN:HB2  | 1.98                     | 0.43              |
| 6:L:272:SER:O     | 6:L:276:MET:N    | 2.51                     | 0.43              |
| 6:L:347:ILE:C     | 6:L:355:ILE:HD11 | 2.43                     | 0.43              |
| 6:L:584:ARG:HH12  | 8:P:57:DT:C7     | 2.30                     | 0.43              |
| 7:O:55:DC:P       | 7:O:55:DC:H3'    | 2.59                     | 0.43              |
| 1:N:37:CYS:SG     | 1:N:61:CYS:HB2   | 2.58                     | 0.43              |
| 2:G:211:ILE:CG2   | 2:G:216:ALA:HB2  | 2.49                     | 0.43              |
| 2:H:26:VAL:HG13   | 2:H:26:VAL:O     | 2.18                     | 0.43              |
| 3:I:98:VAL:O      | 3:I:122:VAL:HG12 | 2.18                     | 0.43              |
| 3:I:228:VAL:HG13  | 3:I:239:MET:HE3  | 2.00                     | 0.43              |
| 3:I:726:TYR:O     | 3:I:733:VAL:HG12 | 2.19                     | 0.43              |
| 3:I:941:LYS:CB    | 3:I:946:LEU:HD21 | 2.49                     | 0.43              |
| 3:I:1257:GLN:NE2  | 4:J:345:LYS:HE2  | 2.31                     | 0.43              |
| 4:J:132:LEU:HD23  | 4:J:132:LEU:O    | 2.19                     | 0.43              |
| 4:J:252:LEU:O     | 4:J:252:LEU:HD23 | 2.18                     | 0.43              |
| 4:J:300:GLN:O     | 4:J:304:ASP:HB2  | 2.19                     | 0.43              |
| 4:J:452:LEU:HG    | 4:J:625:MET:SD   | 2.58                     | 0.43              |
| 4:J:707:ILE:O     | 4:J:713:GLU:HA   | 2.18                     | 0.43              |
| 4:J:826:ILE:HG12  | 4:J:831:VAL:HG13 | 2.01                     | 0.43              |
| 4:J:1106:ILE:HG12 | 4:J:1125:PRO:HD3 | 2.01                     | 0.43              |
| 4:J:1181:ASP:N    | 4:J:1181:ASP:OD1 | 2.47                     | 0.43              |
| 6:L:97:PRO:HB2    | 6:L:402:LEU:HD22 | 2.00                     | 0.43              |
| 2:G:39:LEU:CD2    | 2:H:228:LEU:HD21 | 2.48                     | 0.43              |
| 2:H:183:ILE:HD13  | 2:H:205:MET:HE3  | 1.99                     | 0.43              |
| 2:H:211:ILE:HD11  | 2:H:215:GLU:CB   | 2.47                     | 0.43              |
| 3:I:142:GLU:CB    | 3:I:515:MET:CE   | 2.96                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:233:ARG:HB2   | 3:I:238:GLN:CG    | 2.49                     | 0.43              |
| 3:I:241:LEU:CD1   | 3:I:285:ILE:HG12  | 2.49                     | 0.43              |
| 3:I:344:GLY:HA3   | 3:I:346:TYR:CZ    | 2.54                     | 0.43              |
| 3:I:1166:ASP:N    | 3:I:1168:GLU:H    | 2.14                     | 0.43              |
| 3:I:1291:LEU:HD21 | 4:J:1351:VAL:HG13 | 2.01                     | 0.43              |
| 4:J:148:GLU:HB2   | 4:J:177:ASP:CB    | 2.49                     | 0.43              |
| 4:J:174:ASP:OD1   | 4:J:175:GLU:HG3   | 2.19                     | 0.43              |
| 4:J:516:ASP:OD1   | 4:J:516:ASP:N     | 2.49                     | 0.43              |
| 4:J:885:VAL:CG2   | 4:J:899:TYR:HA    | 2.49                     | 0.43              |
| 6:L:219:GLU:O     | 6:L:223:GLU:N     | 2.51                     | 0.43              |
| 6:L:365:MET:HE2   | 6:L:365:MET:HB3   | 1.76                     | 0.43              |
| 8:P:43:DT:H1'     | 8:P:44:DT:C5'     | 2.46                     | 0.43              |
| 2:M:277:TYR:O     | 2:M:280:ASP:HB2   | 2.19                     | 0.43              |
| 2:M:293:PRO:O     | 2:M:294:ASN:HB2   | 2.19                     | 0.43              |
| 2:G:100:LEU:HD22  | 2:G:121:VAL:HG11  | 2.01                     | 0.43              |
| 3:I:201:ARG:HD2   | 3:I:370:MET:SD    | 2.58                     | 0.43              |
| 3:I:660:VAL:O     | 3:I:660:VAL:HG22  | 2.19                     | 0.43              |
| 3:I:693:LEU:HD22  | 3:I:829:THR:HB    | 2.01                     | 0.43              |
| 3:I:759:SER:HB3   | 3:I:765:ILE:HG12  | 2.00                     | 0.43              |
| 3:I:842:ASP:CB    | 3:I:847:PRO:HA    | 2.48                     | 0.43              |
| 3:I:866:ASP:OD2   | 3:I:944:ARG:NH1   | 2.52                     | 0.43              |
| 3:I:963:GLU:O     | 3:I:966:ILE:HG13  | 2.19                     | 0.43              |
| 3:I:965:GLN:HA    | 3:I:968:GLU:CG    | 2.48                     | 0.43              |
| 3:I:1079:ILE:HG23 | 3:I:1079:ILE:O    | 2.18                     | 0.43              |
| 3:I:1319:MET:HE2  | 3:I:1323:PHE:CD2  | 2.51                     | 0.43              |
| 3:I:1329:GLU:CD   | 4:J:330:MET:HE2   | 2.44                     | 0.43              |
| 4:J:44:ILE:HD11   | 4:J:252:LEU:HD22  | 2.00                     | 0.43              |
| 4:J:490:ILE:HG13  | 4:J:491:LEU:CD2   | 2.49                     | 0.43              |
| 4:J:949:SER:HA    | 4:J:1020:TRP:CH2  | 2.53                     | 0.43              |
| 4:J:1027:VAL:HG22 | 4:J:1027:VAL:O    | 2.18                     | 0.43              |
| 6:L:11:LEU:HD12   | 6:L:11:LEU:O      | 2.18                     | 0.43              |
| 6:L:315:TRP:CH2   | 6:L:341:LEU:HD11  | 2.54                     | 0.43              |
| 6:L:387:VAL:HG23  | 6:L:435:ILE:HG21  | 2.00                     | 0.43              |
| 6:L:491:GLU:HA    | 6:L:494:ILE:HB    | 2.01                     | 0.43              |
| 7:O:21:DA:H2''    | 7:O:22:DT:C6      | 2.53                     | 0.43              |
| 7:O:34:DA:H4'     | 7:O:35:DG:OP1     | 2.19                     | 0.43              |
| 8:P:36:DT:C2'     | 8:P:37:DG:H5''    | 2.48                     | 0.43              |
| 1:N:5:ALA:HB3     | 3:I:678:ARG:NH2   | 2.34                     | 0.43              |
| 2:G:100:LEU:HD21  | 2:G:121:VAL:HG21  | 2.00                     | 0.43              |
| 2:H:85:LEU:HD21   | 2:H:130:ILE:HG23  | 1.99                     | 0.43              |
| 3:I:97:ARG:HA     | 3:I:97:ARG:HD3    | 1.87                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:173:ASN:HA   | 3:I:187:GLU:HA    | 2.00                     | 0.43              |
| 3:I:499:SER:O    | 3:I:502:VAL:HG12  | 2.18                     | 0.43              |
| 3:I:590:PRO:HB2  | 3:I:655:VAL:HG22  | 2.00                     | 0.43              |
| 3:I:817:LEU:HD11 | 3:I:1080:ASN:ND2  | 2.33                     | 0.43              |
| 3:I:1240:ASP:OD1 | 3:I:1240:ASP:N    | 2.43                     | 0.43              |
| 3:I:1246:ARG:NH2 | 3:I:1249:GLY:H    | 2.16                     | 0.43              |
| 3:I:1290:MET:SD  | 3:I:1294:LYS:NZ   | 2.69                     | 0.43              |
| 4:J:70:CYS:SG    | 4:J:74:LYS:N      | 2.92                     | 0.43              |
| 4:J:103:GLY:CA   | 4:J:244:VAL:HG22  | 2.48                     | 0.43              |
| 4:J:350:SER:HB2  | 4:J:469:HIS:ND1   | 2.34                     | 0.43              |
| 4:J:357:VAL:HG22 | 4:J:461:PHE:CZ    | 2.54                     | 0.43              |
| 4:J:644:MET:O    | 4:J:764:ARG:HD2   | 2.19                     | 0.43              |
| 4:J:1350:ASN:ND2 | 4:J:1358:PRO:HD3  | 2.33                     | 0.43              |
| 6:L:408:GLY:CA   | 6:L:439:ILE:HD11  | 2.48                     | 0.43              |
| 3:I:342:ASP:O    | 3:I:344:GLY:N     | 2.52                     | 0.43              |
| 3:I:387:ASN:CB   | 3:I:391:SER:HB3   | 2.49                     | 0.43              |
| 3:I:714:VAL:HG23 | 3:I:715:THR:H     | 1.83                     | 0.43              |
| 3:I:797:GLY:N    | 3:I:1231:TYR:OH   | 2.52                     | 0.43              |
| 3:I:864:LYS:HD2  | 3:I:875:ALA:CB    | 2.43                     | 0.43              |
| 3:I:887:VAL:CG2  | 3:I:913:VAL:HG21  | 2.48                     | 0.43              |
| 4:J:51:PRO:HB3   | 4:J:57:PHE:O      | 2.19                     | 0.43              |
| 4:J:162:GLU:OE1  | 4:J:162:GLU:HA    | 2.18                     | 0.43              |
| 4:J:371:LYS:HE2  | 4:J:371:LYS:HB2   | 1.80                     | 0.43              |
| 4:J:527:LEU:HD23 | 4:J:533:ALA:CB    | 2.49                     | 0.43              |
| 4:J:647:PRO:HG3  | 4:J:697:MET:HA    | 2.00                     | 0.43              |
| 4:J:759:ILE:HG23 | 4:J:771:GLN:HB3   | 2.00                     | 0.43              |
| 4:J:826:ILE:CD1  | 4:J:831:VAL:HG22  | 2.49                     | 0.43              |
| 4:J:964:LYS:CB   | 4:J:977:SER:HB3   | 2.31                     | 0.43              |
| 4:J:1077:ALA:HB2 | 4:J:1100:PHE:CD1  | 2.53                     | 0.43              |
| 4:J:1256:ILE:O   | 4:J:1260:MET:HG3  | 2.18                     | 0.43              |
| 6:L:147:GLN:NE2  | 6:L:265:GLN:HE22  | 2.17                     | 0.43              |
| 6:L:277:MET:HG2  | 6:L:362:ASN:HD21  | 1.84                     | 0.43              |
| 6:L:335:GLU:O    | 6:L:339:ARG:HG3   | 2.18                     | 0.43              |
| 6:L:339:ARG:O    | 6:L:343:LYS:HD2   | 2.19                     | 0.43              |
| 6:L:588:ARG:HD2  | 8:P:57:DT:H73     | 2.01                     | 0.43              |
| 3:I:137:VAL:HG22 | 3:I:142:GLU:HG2   | 2.00                     | 0.43              |
| 3:I:453:ILE:CD1  | 3:I:587:LEU:HG    | 2.49                     | 0.43              |
| 3:I:1149:TYR:OH  | 3:I:1176:LEU:HD11 | 2.18                     | 0.43              |
| 4:J:536:LEU:HD22 | 4:J:542:ALA:CB    | 2.49                     | 0.43              |
| 4:J:641:ILE:HD12 | 4:J:644:MET:CE    | 2.46                     | 0.43              |
| 4:J:965:SER:OG   | 4:J:975:ILE:HA    | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1005:LYS:HB2  | 4:J:1017:VAL:HG13 | 2.01                     | 0.43              |
| 4:J:1040:MET:HE1  | 4:J:1061:VAL:HG22 | 2.00                     | 0.43              |
| 7:O:29:DA:H2"     | 7:O:30:DC:H5'     | 2.00                     | 0.43              |
| 2:M:281:LEU:HD23  | 2:M:307:LEU:HD21  | 2.01                     | 0.43              |
| 3:I:73:TYR:CD2    | 3:I:96:LEU:HD11   | 2.54                     | 0.42              |
| 3:I:158:ASP:HB3   | 3:I:173:ASN:OD1   | 2.19                     | 0.42              |
| 3:I:714:VAL:HB    | 3:I:787:PRO:HD2   | 2.01                     | 0.42              |
| 3:I:935:THR:HG22  | 3:I:936:ARG:O     | 2.19                     | 0.42              |
| 3:I:964:LEU:HA    | 3:I:967:LEU:HD21  | 2.01                     | 0.42              |
| 4:J:364:HIS:HB3   | 4:J:487:THR:CG2   | 2.44                     | 0.42              |
| 4:J:911:LYS:HE2   | 4:J:911:LYS:HB3   | 1.83                     | 0.42              |
| 4:J:1155:ILE:HD12 | 4:J:1155:ILE:H    | 1.84                     | 0.42              |
| 5:K:12:LYS:HE3    | 5:K:55:GLU:C      | 2.44                     | 0.42              |
| 6:L:583:THR:HG22  | 6:L:586:ARG:H     | 1.83                     | 0.42              |
| 7:O:46:DG:H2"     | 7:O:47:DG:H8      | 1.84                     | 0.42              |
| 2:G:45:ARG:HH22   | 3:I:1216:ARG:HA   | 1.84                     | 0.42              |
| 2:H:13:LEU:HA     | 2:H:29:GLU:OE2    | 2.19                     | 0.42              |
| 3:I:81:ASP:N      | 3:I:81:ASP:OD1    | 2.46                     | 0.42              |
| 3:I:194:LEU:HD11  | 3:I:346:TYR:HB3   | 2.02                     | 0.42              |
| 3:I:1085:MET:HE2  | 3:I:1095:ASP:O    | 2.18                     | 0.42              |
| 4:J:138:VAL:O     | 4:J:181:GLY:HA2   | 2.19                     | 0.42              |
| 4:J:268:LEU:HD23  | 4:J:271:ARG:NH2   | 2.34                     | 0.42              |
| 4:J:842:ARG:CB    | 4:J:882:VAL:HG21  | 2.49                     | 0.42              |
| 6:L:334:SER:O     | 6:L:338:HIS:HB2   | 2.19                     | 0.42              |
| 2:H:222:THR:HA    | 2:H:225:ALA:HB3   | 2.01                     | 0.42              |
| 3:I:11:ILE:HG23   | 3:I:11:ILE:O      | 2.19                     | 0.42              |
| 3:I:111:GLU:H     | 3:I:111:GLU:HG3   | 1.67                     | 0.42              |
| 3:I:164:THR:HB    | 3:I:171:LEU:HD11  | 2.00                     | 0.42              |
| 3:I:210:LEU:HA    | 3:I:213:LEU:HB2   | 2.00                     | 0.42              |
| 3:I:210:LEU:HD23  | 3:I:213:LEU:HD12  | 2.00                     | 0.42              |
| 3:I:432:LEU:O     | 3:I:435:ILE:HG22  | 2.18                     | 0.42              |
| 3:I:1332:SER:OG   | 4:J:327:LEU:HD11  | 2.20                     | 0.42              |
| 4:J:71:LEU:HA     | 4:J:71:LEU:HD12   | 1.74                     | 0.42              |
| 4:J:950:ILE:HG12  | 4:J:1018:ALA:CB   | 2.41                     | 0.42              |
| 6:L:51:MET:HE1    | 6:L:84:LEU:CD2    | 2.50                     | 0.42              |
| 6:L:98:VAL:O      | 6:L:102:MET:HE2   | 2.18                     | 0.42              |
| 6:L:351:THR:HG21  | 6:L:358:VAL:HG21  | 2.01                     | 0.42              |
| 6:L:373:ARG:HB3   | 6:L:377:LYS:HZ3   | 1.83                     | 0.42              |
| 6:L:376:LYS:HE3   | 6:L:376:LYS:HB2   | 1.81                     | 0.42              |
| 6:L:419:PHE:HB2   | 6:L:430:TYR:CD2   | 2.54                     | 0.42              |
| 6:L:496:LYS:O     | 6:L:500:ILE:HG12  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:44:DT:H2''    | 8:P:45:DA:C8      | 2.53                     | 0.42              |
| 2:G:70:THR:OG1    | 3:I:729:ALA:HB3   | 2.19                     | 0.42              |
| 2:H:76:GLU:HG3    | 2:H:80:GLU:HG2    | 2.01                     | 0.42              |
| 2:H:104:LYS:HD2   | 2:H:114:ASP:CG    | 2.44                     | 0.42              |
| 2:H:129:VAL:HG21  | 2:H:132:HIS:CE1   | 2.54                     | 0.42              |
| 2:H:219:ARG:O     | 2:H:223:ILE:HG12  | 2.19                     | 0.42              |
| 3:I:165:HIS:HD2   | 3:I:190:PRO:HG2   | 1.85                     | 0.42              |
| 3:I:289:VAL:HG13  | 3:I:322:LEU:HD23  | 2.00                     | 0.42              |
| 3:I:933:VAL:HA    | 3:I:1050:VAL:HG12 | 2.01                     | 0.42              |
| 4:J:440:VAL:O     | 4:J:442:ILE:HG12  | 2.19                     | 0.42              |
| 4:J:800:LEU:HD12  | 4:J:1256:ILE:CD1  | 2.49                     | 0.42              |
| 4:J:868:TRP:O     | 4:J:872:LEU:HD13  | 2.20                     | 0.42              |
| 4:J:1167:LYS:CE   | 4:J:1170:LYS:HB2  | 2.49                     | 0.42              |
| 8:P:63:DG:H1'     | 8:P:64:DA:C8      | 2.54                     | 0.42              |
| 2:G:131:CYS:SG    | 2:G:140:ILE:HD13  | 2.60                     | 0.42              |
| 2:G:231:PHE:O     | 2:G:234:LEU:HG    | 2.19                     | 0.42              |
| 3:I:22:LEU:HD12   | 3:I:23:ASP:N      | 2.33                     | 0.42              |
| 3:I:198:ILE:HG21  | 3:I:388:LEU:HD21  | 2.02                     | 0.42              |
| 3:I:213:LEU:HD22  | 3:I:422:LYS:HB3   | 2.01                     | 0.42              |
| 3:I:244:GLU:HA    | 3:I:274:ILE:HD13  | 2.00                     | 0.42              |
| 3:I:963:GLU:HA    | 3:I:966:ILE:HG12  | 2.01                     | 0.42              |
| 3:I:1245:ALA:CB   | 4:J:351:GLY:HA3   | 2.48                     | 0.42              |
| 3:I:1293:VAL:CG2  | 3:I:1304:MET:HB2  | 2.50                     | 0.42              |
| 4:J:193:ASP:OD1   | 4:J:195:GLU:N     | 2.52                     | 0.42              |
| 4:J:425:ARG:HH12  | 4:J:464:ASP:HB3   | 1.84                     | 0.42              |
| 4:J:511:TYR:HE2   | 4:J:724:MET:HG3   | 1.84                     | 0.42              |
| 4:J:1291:GLU:O    | 4:J:1294:ALA:HB3  | 2.19                     | 0.42              |
| 6:L:280:VAL:HA    | 6:L:347:ILE:HD13  | 2.01                     | 0.42              |
| 6:L:558:VAL:HB    | 6:L:580:PHE:HE2   | 1.84                     | 0.42              |
| 6:L:571:TYR:HB3   | 6:L:575:GLU:CG    | 2.49                     | 0.42              |
| 1:N:48:ARG:HA     | 1:N:51:ILE:HG12   | 2.01                     | 0.42              |
| 2:H:64:VAL:CA     | 2:H:65:LEU:HB2    | 2.49                     | 0.42              |
| 3:I:103:VAL:HG12  | 3:I:117:ILE:CG2   | 2.48                     | 0.42              |
| 3:I:230:PHE:CE2   | 3:I:292:ILE:HB    | 2.54                     | 0.42              |
| 3:I:254:ASP:H     | 3:I:265:LYS:HG2   | 1.84                     | 0.42              |
| 4:J:72:CYS:SG     | 4:J:74:LYS:HB2    | 2.59                     | 0.42              |
| 4:J:164:GLN:HA    | 4:J:167:ASP:OD2   | 2.20                     | 0.42              |
| 4:J:372:MET:O     | 4:J:376:LEU:HG    | 2.19                     | 0.42              |
| 4:J:986:ASP:HB2   | 4:J:992:LYS:CD    | 2.49                     | 0.42              |
| 4:J:1062:LEU:HD22 | 4:J:1066:GLU:OE2  | 2.20                     | 0.42              |
| 4:J:1120:THR:CB   | 4:J:1123:ARG:HH11 | 2.32                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:1203:ARG:NH2 | 4:J:1205:GLU:OE1 | 2.40                     | 0.42              |
| 4:J:1319:PHE:CD1 | 4:J:1342:ASP:HB2 | 2.55                     | 0.42              |
| 6:L:80:ALA:O     | 6:L:84:LEU:HD23  | 2.19                     | 0.42              |
| 6:L:127:ILE:HG13 | 6:L:131:GLN:HE22 | 1.85                     | 0.42              |
| 6:L:339:ARG:HB3  | 6:L:343:LYS:HZ2  | 1.82                     | 0.42              |
| 6:L:363:ARG:HG2  | 6:L:367:ILE:CD1  | 2.49                     | 0.42              |
| 6:L:415:ALA:O    | 6:L:419:PHE:N    | 2.44                     | 0.42              |
| 6:L:427:PHE:CE2  | 6:L:431:ALA:HB2  | 2.55                     | 0.42              |
| 6:L:586:ARG:HE   | 7:O:24:DC:H2''   | 1.84                     | 0.42              |
| 7:O:56:DC:H6     | 7:O:56:DC:H2'    | 1.66                     | 0.42              |
| 2:G:45:ARG:NH2   | 3:I:1216:ARG:HA  | 2.34                     | 0.42              |
| 2:G:111:THR:O    | 2:G:114:ASP:HB2  | 2.20                     | 0.42              |
| 2:G:179:PRO:HG3  | 2:G:211:ILE:HG13 | 2.00                     | 0.42              |
| 2:H:183:ILE:HD13 | 2:H:205:MET:HE2  | 2.02                     | 0.42              |
| 3:I:387:ASN:HB3  | 3:I:391:SER:HB3  | 2.02                     | 0.42              |
| 3:I:750:ILE:O    | 3:I:750:ILE:HG13 | 2.20                     | 0.42              |
| 3:I:871:VAL:HG21 | 3:I:928:VAL:HG11 | 2.02                     | 0.42              |
| 3:I:1294:LYS:HB3 | 4:J:347:VAL:HG13 | 2.01                     | 0.42              |
| 4:J:58:CYS:SG    | 4:J:60:ARG:N     | 2.93                     | 0.42              |
| 4:J:111:THR:OG1  | 4:J:300:GLN:HA   | 2.20                     | 0.42              |
| 6:L:133:SER:HB3  | 6:L:365:MET:HB2  | 2.00                     | 0.42              |
| 6:L:166:VAL:HG22 | 6:L:260:ARG:CG   | 2.48                     | 0.42              |
| 6:L:325:PRO:O    | 6:L:328:GLU:HB3  | 2.19                     | 0.42              |
| 6:L:426:LYS:HG2  | 7:O:52:DA:H3'    | 2.01                     | 0.42              |
| 2:M:278:ILE:O    | 2:M:282:VAL:HG13 | 2.19                     | 0.42              |
| 2:M:290:LEU:HB2  | 2:M:300:LEU:CD1  | 2.49                     | 0.42              |
| 1:N:44:ILE:O     | 1:N:44:ILE:HG13  | 2.20                     | 0.42              |
| 2:G:76:GLU:OE2   | 2:G:132:HIS:N    | 2.53                     | 0.42              |
| 3:I:59:ILE:CG2   | 3:I:476:LYS:HE2  | 2.33                     | 0.42              |
| 3:I:102:LEU:HD12 | 3:I:103:VAL:H    | 1.84                     | 0.42              |
| 3:I:180:ARG:O    | 3:I:396:ASP:N    | 2.51                     | 0.42              |
| 3:I:992:LEU:HD11 | 3:I:996:ARG:O    | 2.20                     | 0.42              |
| 3:I:1114:GLU:O   | 3:I:1114:GLU:HG2 | 2.16                     | 0.42              |
| 3:I:1120:ALA:CB  | 3:I:1198:LEU:HB3 | 2.39                     | 0.42              |
| 4:J:56:LEU:HD12  | 4:J:56:LEU:N     | 2.35                     | 0.42              |
| 4:J:934:THR:HG23 | 4:J:934:THR:O    | 2.19                     | 0.42              |
| 6:L:277:MET:CG   | 6:L:362:ASN:HD21 | 2.33                     | 0.42              |
| 6:L:361:ILE:HA   | 6:L:364:ARG:HH21 | 1.81                     | 0.42              |
| 6:L:477:GLU:HG2  | 6:L:478:PRO:N    | 2.34                     | 0.42              |
| 1:N:3:ASP:O      | 1:N:6:ASP:N      | 2.51                     | 0.42              |
| 1:N:15:LEU:HD11  | 4:J:750:PRO:O    | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:203:ILE:HG13  | 2:H:203:ILE:H     | 1.54                     | 0.42              |
| 3:I:95:PRO:HA     | 3:I:126:GLU:CB    | 2.50                     | 0.42              |
| 3:I:149:LEU:HD12  | 3:I:452:ARG:O     | 2.20                     | 0.42              |
| 3:I:367:TYR:HD2   | 3:I:381:ALA:HA    | 1.82                     | 0.42              |
| 3:I:971:LEU:O     | 3:I:975:ILE:HG13  | 2.20                     | 0.42              |
| 3:I:975:ILE:HD13  | 3:I:998:LEU:CG    | 2.49                     | 0.42              |
| 3:I:1109:ILE:HD11 | 4:J:740:LEU:CD1   | 2.46                     | 0.42              |
| 3:I:1131:MET:CA   | 3:I:1136:GLN:HG2  | 2.44                     | 0.42              |
| 3:I:1165:SER:HG   | 3:I:1169:VAL:HG13 | 1.84                     | 0.42              |
| 3:I:1172:LEU:O    | 3:I:1172:LEU:HD23 | 2.19                     | 0.42              |
| 4:J:1039:ASP:OD1  | 4:J:1074:LEU:HD13 | 2.19                     | 0.42              |
| 4:J:1222:ARG:C    | 4:J:1223:LEU:HD23 | 2.45                     | 0.42              |
| 4:J:1229:VAL:O    | 4:J:1233:ILE:HG12 | 2.19                     | 0.42              |
| 6:L:12:LEU:CD1    | 6:L:48:ILE:HD12   | 2.49                     | 0.42              |
| 2:H:111:THR:OG1   | 2:H:112:ALA:N     | 2.51                     | 0.42              |
| 3:I:417:SER:OG    | 3:I:418:GLY:N     | 2.52                     | 0.42              |
| 3:I:985:GLU:OE1   | 3:I:989:LEU:HD13  | 2.20                     | 0.42              |
| 3:I:1285:TYR:CE1  | 4:J:1356:LEU:HD11 | 2.55                     | 0.42              |
| 4:J:45:ASN:HB3    | 4:J:48:THR:O      | 2.20                     | 0.42              |
| 4:J:154:LEU:CD2   | 4:J:158:GLN:HB3   | 2.50                     | 0.42              |
| 4:J:571:ASP:OD1   | 4:J:571:ASP:N     | 2.51                     | 0.42              |
| 4:J:1026:PRO:HB2  | 4:J:1028:ILE:CG2  | 2.50                     | 0.42              |
| 4:J:1033:GLY:HA2  | 4:J:1081:VAL:O    | 2.20                     | 0.42              |
| 4:J:1038:THR:HG23 | 4:J:1079:LYS:HB2  | 2.02                     | 0.42              |
| 4:J:1357:ILE:HG23 | 4:J:1358:PRO:HD2  | 2.01                     | 0.42              |
| 6:L:136:GLU:CB    | 6:L:361:ILE:HG12  | 2.42                     | 0.42              |
| 6:L:277:MET:CE    | 6:L:359:LYS:HG2   | 2.38                     | 0.42              |
| 6:L:443:ILE:O     | 6:L:447:ALA:HB3   | 2.20                     | 0.42              |
| 2:M:260:LEU:HD12  | 2:M:306:VAL:HG11  | 2.02                     | 0.42              |
| 2:H:121:VAL:C     | 2:H:122:GLU:HG3   | 2.45                     | 0.41              |
| 3:I:58:PRO:CB     | 3:I:69:GLN:HG2    | 2.48                     | 0.41              |
| 3:I:871:VAL:HG23  | 3:I:928:VAL:HG11  | 2.02                     | 0.41              |
| 3:I:895:LEU:CD1   | 3:I:900:LYS:HG3   | 2.48                     | 0.41              |
| 3:I:905:ILE:HG22  | 3:I:906:PHE:CE1   | 2.54                     | 0.41              |
| 3:I:1132:LEU:HD12 | 3:I:1132:LEU:HA   | 1.73                     | 0.41              |
| 3:I:1287:LEU:HD22 | 4:J:1357:ILE:HD11 | 2.02                     | 0.41              |
| 4:J:35:PHE:CG     | 4:J:101:ARG:HD2   | 2.55                     | 0.41              |
| 4:J:199:GLU:O     | 4:J:202:ARG:HB2   | 2.20                     | 0.41              |
| 4:J:262:THR:HG23  | 6:L:504:PRO:HB2   | 2.02                     | 0.41              |
| 4:J:954:ASN:O     | 4:J:1013:GLY:HA2  | 2.20                     | 0.41              |
| 6:L:31:LEU:HD11   | 6:L:44:ILE:HG21   | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:322:MET:HB3  | 6:L:324:LYS:HG2   | 2.01                     | 0.41              |
| 6:L:344:LEU:HD23 | 6:L:344:LEU:HA    | 1.92                     | 0.41              |
| 6:L:346:GLN:HG2  | 6:L:350:GLU:CD    | 2.44                     | 0.41              |
| 2:H:192:VAL:CG1  | 2:H:195:ARG:HB2   | 2.48                     | 0.41              |
| 3:I:215:TYR:HB3  | 3:I:220:ILE:CD1   | 2.47                     | 0.41              |
| 3:I:699:LEU:HD22 | 3:I:699:LEU:HA    | 1.66                     | 0.41              |
| 3:I:815:SER:HB3  | 3:I:1077:SER:OG   | 2.19                     | 0.41              |
| 4:J:62:PHE:O     | 4:J:98:ARG:HG2    | 2.20                     | 0.41              |
| 4:J:332:LYS:HB3  | 4:J:1328:THR:HB   | 2.02                     | 0.41              |
| 4:J:416:ILE:HD13 | 4:J:416:ILE:HA    | 1.84                     | 0.41              |
| 4:J:641:ILE:HD12 | 4:J:641:ILE:HA    | 1.96                     | 0.41              |
| 4:J:686:TRP:CD2  | 4:J:758:PRO:HG2   | 2.55                     | 0.41              |
| 4:J:847:ASP:HB3  | 4:J:856:ILE:HG13  | 2.01                     | 0.41              |
| 6:L:9:LEU:HD22   | 6:L:31:LEU:CD2    | 2.50                     | 0.41              |
| 6:L:135:ALA:HB1  | 6:L:253:SER:CB    | 2.50                     | 0.41              |
| 6:L:333:VAL:HG23 | 6:L:336:GLU:HB3   | 2.02                     | 0.41              |
| 6:L:420:GLU:OE1  | 6:L:420:GLU:HA    | 2.20                     | 0.41              |
| 6:L:558:VAL:HA   | 6:L:561:MET:HB2   | 2.02                     | 0.41              |
| 7:O:32:DA:H2"    | 7:O:33:DA:C8      | 2.55                     | 0.41              |
| 2:M:292:THR:HB   | 2:M:295:LEU:HB3   | 2.02                     | 0.41              |
| 2:G:20:SER:OG    | 2:G:21:SER:N      | 2.53                     | 0.41              |
| 2:H:82:LEU:HD21  | 2:H:171:LEU:HD12  | 2.03                     | 0.41              |
| 3:I:184:LEU:HD12 | 3:I:185:ASP:N     | 2.35                     | 0.41              |
| 3:I:742:TYR:CG   | 3:I:743:PRO:HD2   | 2.55                     | 0.41              |
| 3:I:1104:PRO:O   | 3:I:1107:MET:HG2  | 2.20                     | 0.41              |
| 3:I:1270:PHE:HZ  | 3:I:1278:LEU:HD12 | 1.85                     | 0.41              |
| 4:J:1030:GLU:CG  | 4:J:1031:VAL:HG23 | 2.49                     | 0.41              |
| 6:L:511:ILE:HG22 | 6:L:517:SER:O     | 2.19                     | 0.41              |
| 2:M:304:LYS:O    | 2:M:307:LEU:HB2   | 2.20                     | 0.41              |
| 2:G:226:GLU:HG2  | 2:H:10:LYS:HE3    | 2.01                     | 0.41              |
| 2:H:44:ARG:NH1   | 4:J:538:ARG:HH11  | 2.14                     | 0.41              |
| 2:H:73:GLY:CA    | 2:H:134:THR:HG22  | 2.50                     | 0.41              |
| 2:H:153:VAL:HB   | 2:H:177:TYR:HE2   | 1.85                     | 0.41              |
| 3:I:10:ARG:HD2   | 3:I:1181:PRO:HG3  | 2.01                     | 0.41              |
| 3:I:94:ALA:C     | 3:I:126:GLU:HB2   | 2.45                     | 0.41              |
| 3:I:755:LYS:CE   | 3:I:755:LYS:HA    | 2.47                     | 0.41              |
| 3:I:779:ARG:HG3  | 3:I:780:GLY:H     | 1.86                     | 0.41              |
| 3:I:811:ASN:OD1  | 3:I:811:ASN:N     | 2.52                     | 0.41              |
| 3:I:871:VAL:HG11 | 3:I:883:LEU:HA    | 2.01                     | 0.41              |
| 3:I:942:ASP:O    | 3:I:946:LEU:HG    | 2.20                     | 0.41              |
| 4:J:154:LEU:HD21 | 4:J:158:GLN:CG    | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:253:VAL:HG21  | 6:L:523:ILE:CG2   | 2.49                     | 0.41              |
| 4:J:1034:PHE:HB2  | 4:J:1081:VAL:HG23 | 2.01                     | 0.41              |
| 4:J:1067:ARG:NH2  | 4:J:1071:GLY:O    | 2.52                     | 0.41              |
| 4:J:1165:PHE:HA   | 4:J:1175:LEU:CB   | 2.50                     | 0.41              |
| 6:L:585:GLU:HG2   | 7:O:27:DT:H73     | 2.01                     | 0.41              |
| 2:G:28:LEU:HD13   | 2:G:201:LEU:HD23  | 2.02                     | 0.41              |
| 2:G:155:ALA:N     | 2:G:174:ASP:OD1   | 2.47                     | 0.41              |
| 3:I:173:ASN:OD1   | 3:I:173:ASN:N     | 2.54                     | 0.41              |
| 3:I:221:LEU:HD11  | 3:I:351:LEU:HD13  | 2.02                     | 0.41              |
| 3:I:351:LEU:HA    | 3:I:354:ASP:HB2   | 2.01                     | 0.41              |
| 3:I:722:GLY:H     | 3:I:777:VAL:HG23  | 1.85                     | 0.41              |
| 3:I:870:ILE:CD1   | 3:I:884:VAL:HG13  | 2.49                     | 0.41              |
| 4:J:429:LEU:HD13  | 4:J:429:LEU:HA    | 1.82                     | 0.41              |
| 4:J:601:ILE:HD11  | 4:J:624:ILE:CD1   | 2.51                     | 0.41              |
| 4:J:851:PRO:HD3   | 4:J:877:VAL:CG1   | 2.49                     | 0.41              |
| 4:J:1034:PHE:H    | 4:J:1081:VAL:HG23 | 1.85                     | 0.41              |
| 4:J:1050:THR:HG23 | 4:J:1050:THR:O    | 2.20                     | 0.41              |
| 4:J:1189:MET:O    | 4:J:1191:PRO:HD3  | 2.20                     | 0.41              |
| 4:J:1226:VAL:HA   | 4:J:1229:VAL:HG12 | 2.02                     | 0.41              |
| 4:J:1265:THR:CG2  | 4:J:1279:GLN:HB3  | 2.50                     | 0.41              |
| 7:O:23:DC:H2''    | 7:O:24:DC:H5'     | 2.01                     | 0.41              |
| 1:N:73:ALA:HB2    | 3:I:168:GLY:C     | 2.46                     | 0.41              |
| 2:G:192:VAL:HG22  | 2:G:193:GLU:N     | 2.35                     | 0.41              |
| 2:H:29:GLU:CB     | 2:H:30:PRO:HD2    | 2.51                     | 0.41              |
| 2:H:103:ASN:HA    | 2:H:141:SER:CB    | 2.50                     | 0.41              |
| 3:I:130:MET:HB2   | 3:I:130:MET:HE3   | 1.83                     | 0.41              |
| 3:I:294:GLY:C     | 3:I:295:LYS:HD3   | 2.46                     | 0.41              |
| 3:I:557:ARG:NH2   | 3:I:611:GLU:OE1   | 2.46                     | 0.41              |
| 3:I:1131:MET:HA   | 3:I:1136:GLN:CG   | 2.46                     | 0.41              |
| 4:J:114:ILE:HD12  | 4:J:304:ASP:OD2   | 2.20                     | 0.41              |
| 4:J:141:PHE:CD1   | 4:J:293:ARG:HG2   | 2.55                     | 0.41              |
| 4:J:246:PRO:HD2   | 4:J:249:LEU:HD12  | 2.02                     | 0.41              |
| 4:J:332:LYS:O     | 4:J:336:GLY:HA3   | 2.20                     | 0.41              |
| 4:J:441:LEU:C     | 4:J:442:ILE:HD13  | 2.45                     | 0.41              |
| 4:J:749:LYS:HB3   | 4:J:750:PRO:CD    | 2.50                     | 0.41              |
| 4:J:1052:GLU:HA   | 4:J:1055:GLY:N    | 2.36                     | 0.41              |
| 4:J:1163:VAL:HG23 | 4:J:1177:ILE:CA   | 2.49                     | 0.41              |
| 6:L:296:LYS:O     | 6:L:298:PRO:HD3   | 2.21                     | 0.41              |
| 7:O:55:DC:H2''    | 7:O:56:DC:N3      | 2.36                     | 0.41              |
| 1:N:40:CYS:CB     | 3:I:268:ARG:HB3   | 2.50                     | 0.41              |
| 2:G:160:HIS:H     | 2:G:162:GLU:HG3   | 1.86                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:5:TYR:HA      | 3:I:8:LYS:CE      | 2.51                     | 0.41              |
| 3:I:230:PHE:CB    | 3:I:333:ILE:HB    | 2.51                     | 0.41              |
| 3:I:839:VAL:HG12  | 3:I:1049:ILE:CG2  | 2.50                     | 0.41              |
| 3:I:896:THR:OG1   | 3:I:899:GLU:HB3   | 2.19                     | 0.41              |
| 3:I:899:GLU:OE2   | 3:I:903:ARG:HG2   | 2.21                     | 0.41              |
| 3:I:1276:TRP:CH2  | 4:J:798:ARG:HA    | 2.55                     | 0.41              |
| 10:I:1401:1N7:C19 | 10:I:1401:1N7:C4  | 2.88                     | 0.41              |
| 4:J:282:LEU:HD21  | 6:L:410:ILE:CD1   | 2.51                     | 0.41              |
| 4:J:353:SER:O     | 4:J:465:GLN:HB3   | 2.21                     | 0.41              |
| 4:J:1075:ARG:HG3  | 4:J:1165:PHE:CZ   | 2.56                     | 0.41              |
| 4:J:1209:VAL:O    | 4:J:1209:VAL:HG23 | 2.21                     | 0.41              |
| 6:L:509:THR:O     | 6:L:518:HIS:HA    | 2.20                     | 0.41              |
| 6:L:546:ASP:O     | 6:L:549:ALA:HB3   | 2.21                     | 0.41              |
| 2:G:79:LEU:O      | 2:G:83:LEU:HD13   | 2.21                     | 0.41              |
| 2:H:70:THR:OG1    | 2:H:71:LYS:N      | 2.53                     | 0.41              |
| 3:I:395:TYR:OH    | 3:I:397:LEU:HD11  | 2.21                     | 0.41              |
| 3:I:519:ASN:OD1   | 3:I:520:PRO:HD2   | 2.20                     | 0.41              |
| 3:I:727:VAL:HG23  | 3:I:732:ILE:CG1   | 2.32                     | 0.41              |
| 3:I:828:PHE:CE2   | 3:I:1066:MET:HE1  | 2.56                     | 0.41              |
| 3:I:1131:MET:O    | 3:I:1136:GLN:HG2  | 2.21                     | 0.41              |
| 4:J:1037:PHE:HD2  | 4:J:1040:MET:HB2  | 1.86                     | 0.41              |
| 4:J:1198:VAL:HG11 | 4:J:1204:VAL:HG11 | 2.03                     | 0.41              |
| 6:L:23:THR:CB     | 6:L:58:GLU:H      | 2.33                     | 0.41              |
| 8:P:41:DT:H2"     | 8:P:42:DT:OP2     | 2.21                     | 0.41              |
| 2:M:270:LEU:HD22  | 2:M:275:ILE:HG13  | 2.03                     | 0.41              |
| 2:G:95:LYS:HE3    | 2:G:120:ASP:OD2   | 2.20                     | 0.41              |
| 2:H:39:LEU:HD23   | 2:H:39:LEU:HA     | 1.81                     | 0.41              |
| 2:H:142:MET:HE2   | 2:H:142:MET:HB3   | 1.78                     | 0.41              |
| 2:H:179:PRO:O     | 2:H:207:THR:HB    | 2.20                     | 0.41              |
| 3:I:175:ARG:HG2   | 3:I:185:ASP:CG    | 2.46                     | 0.41              |
| 3:I:203:LYS:C     | 3:I:204:LEU:HD23  | 2.46                     | 0.41              |
| 3:I:592:ARG:N     | 3:I:653:MET:O     | 2.47                     | 0.41              |
| 3:I:689:ALA:CB    | 3:I:1233:LEU:HD23 | 2.39                     | 0.41              |
| 3:I:932:GLN:O     | 3:I:1050:VAL:HA   | 2.21                     | 0.41              |
| 3:I:975:ILE:CD1   | 3:I:998:LEU:HD11  | 2.50                     | 0.41              |
| 3:I:988:LYS:HA    | 3:I:991:LYS:CD    | 2.51                     | 0.41              |
| 3:I:1223:ARG:HA   | 3:I:1224:PRO:HD2  | 1.90                     | 0.41              |
| 4:J:84:ILE:HG22   | 4:J:91:GLU:CB     | 2.51                     | 0.41              |
| 4:J:116:PHE:O     | 4:J:124:ILE:HG22  | 2.20                     | 0.41              |
| 4:J:162:GLU:HA    | 4:J:165:TYR:HB3   | 2.03                     | 0.41              |
| 4:J:217:LEU:O     | 4:J:221:ILE:HG12  | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:J:225:GLU:O     | 4:J:229:GLN:HG3  | 2.21                     | 0.41              |
| 4:J:377:PHE:CD2   | 4:J:416:ILE:HD11 | 2.56                     | 0.41              |
| 4:J:418:GLU:HB2   | 5:K:45:LYS:HG2   | 2.01                     | 0.41              |
| 4:J:724:MET:HB2   | 4:J:724:MET:HE3  | 1.80                     | 0.41              |
| 4:J:913:GLU:O     | 4:J:915:ILE:HG23 | 2.21                     | 0.41              |
| 4:J:950:ILE:HD12  | 4:J:982:LEU:HD13 | 2.02                     | 0.41              |
| 6:L:234:THR:HG21  | 6:L:244:THR:HB   | 2.01                     | 0.41              |
| 6:L:275:VAL:HG12  | 6:L:279:ARG:CD   | 2.50                     | 0.41              |
| 6:L:319:ALA:HB1   | 6:L:322:MET:HE2  | 2.01                     | 0.41              |
| 6:L:369:GLU:O     | 6:L:373:ARG:HG3  | 2.20                     | 0.41              |
| 6:L:376:LYS:HB3   | 6:L:416:VAL:HG11 | 2.03                     | 0.41              |
| 6:L:586:ARG:HE    | 7:O:24:DC:H2'    | 1.86                     | 0.41              |
| 7:O:42:DA:H1'     | 7:O:43:DA:C5'    | 2.46                     | 0.41              |
| 2:M:262:LEU:HB3   | 2:M:266:SER:OG   | 2.21                     | 0.41              |
| 2:G:50:SER:HB2    | 2:H:8:PHE:CZ     | 2.55                     | 0.41              |
| 2:H:153:VAL:HG12  | 2:H:158:ARG:NH1  | 2.36                     | 0.41              |
| 3:I:90:VAL:HG12   | 3:I:91:THR:N     | 2.36                     | 0.41              |
| 3:I:142:GLU:O     | 3:I:515:MET:HB3  | 2.20                     | 0.41              |
| 3:I:254:ASP:HA    | 3:I:264:GLU:O    | 2.21                     | 0.41              |
| 3:I:515:MET:HG2   | 3:I:517:GLN:HB2  | 2.03                     | 0.41              |
| 3:I:587:LEU:O     | 3:I:607:SER:HA   | 2.21                     | 0.41              |
| 3:I:936:ARG:HB3   | 3:I:939:VAL:HG23 | 2.03                     | 0.41              |
| 4:J:416:ILE:HG21  | 4:J:439:PRO:HB2  | 2.02                     | 0.41              |
| 4:J:1022:PRO:O    | 4:J:1126:GLN:N   | 2.53                     | 0.41              |
| 4:J:1038:THR:CG2  | 4:J:1079:LYS:HD3 | 2.49                     | 0.41              |
| 4:J:1144:LEU:HD22 | 4:J:1237:VAL:HB  | 2.03                     | 0.41              |
| 5:K:53:GLU:CG     | 5:K:59:ILE:HD12  | 2.42                     | 0.41              |
| 7:O:22:DT:H3      | 8:P:64:DA:H61    | 1.69                     | 0.41              |
| 2:M:292:THR:HB    | 2:M:295:LEU:HD13 | 2.03                     | 0.41              |
| 2:M:304:LYS:HD3   | 2:M:304:LYS:C    | 2.46                     | 0.41              |
| 1:N:23:ILE:HG23   | 4:J:680:ASN:ND2  | 2.36                     | 0.40              |
| 2:H:103:ASN:HA    | 2:H:140:ILE:O    | 2.21                     | 0.40              |
| 2:H:118:ASP:H     | 2:H:121:VAL:HB   | 1.85                     | 0.40              |
| 2:H:150:ARG:HD3   | 2:H:150:ARG:HA   | 1.89                     | 0.40              |
| 3:I:368:ARG:O     | 3:I:372:PRO:HA   | 2.20                     | 0.40              |
| 3:I:1007:LYS:O    | 3:I:1011:LEU:HG  | 2.22                     | 0.40              |
| 3:I:1135:GLN:O    | 3:I:1135:GLN:HG3 | 2.21                     | 0.40              |
| 4:J:114:ILE:HG23  | 4:J:115:TRP:CD1  | 2.55                     | 0.40              |
| 4:J:335:GLN:NE2   | 6:L:516:ASP:O    | 2.54                     | 0.40              |
| 4:J:495:ASN:N     | 4:J:495:ASN:OD1  | 2.53                     | 0.40              |
| 4:J:804:ALA:HA    | 4:J:1259:GLN:HG3 | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:274:ARG:HA    | 6:L:274:ARG:NE    | 2.36                     | 0.40              |
| 6:L:559:LEU:HD12  | 6:L:559:LEU:HA    | 1.89                     | 0.40              |
| 7:O:18:DC:H2"     | 7:O:19:DA:C8      | 2.56                     | 0.40              |
| 2:M:262:LEU:HD23  | 2:M:262:LEU:HA    | 1.84                     | 0.40              |
| 2:G:32:GLU:OE1    | 2:H:150:ARG:NH1   | 2.49                     | 0.40              |
| 2:H:112:ALA:HB3   | 2:H:126:PRO:CA    | 2.45                     | 0.40              |
| 3:I:32:LEU:HD23   | 3:I:32:LEU:HA     | 1.79                     | 0.40              |
| 3:I:56:VAL:HG11   | 3:I:468:LEU:HB3   | 2.03                     | 0.40              |
| 3:I:98:VAL:HB     | 3:I:122:VAL:HG12  | 2.02                     | 0.40              |
| 3:I:178:PRO:HG3   | 3:I:395:TYR:HE1   | 1.85                     | 0.40              |
| 3:I:195:PHE:CB    | 3:I:203:LYS:HD2   | 2.52                     | 0.40              |
| 3:I:283:LYS:HE3   | 3:I:283:LYS:HB2   | 1.89                     | 0.40              |
| 3:I:724:VAL:HG11  | 3:I:772:SER:O     | 2.21                     | 0.40              |
| 3:I:805:MET:HE1   | 3:I:1221:PHE:CZ   | 2.57                     | 0.40              |
| 3:I:1079:ILE:HD12 | 3:I:1079:ILE:HA   | 1.94                     | 0.40              |
| 3:I:1326:LEU:HD21 | 4:J:338:PHE:CZ    | 2.56                     | 0.40              |
| 3:I:1333:LEU:HD23 | 4:J:327:LEU:HD13  | 2.02                     | 0.40              |
| 4:J:132:LEU:O     | 4:J:136:GLU:HG3   | 2.21                     | 0.40              |
| 4:J:883:ARG:HG2   | 4:J:883:ARG:H     | 1.69                     | 0.40              |
| 4:J:926:PRO:HG2   | 4:J:1248:ILE:CD1  | 2.48                     | 0.40              |
| 4:J:1034:PHE:HE1  | 4:J:1114:GLN:HG3  | 1.86                     | 0.40              |
| 4:J:1046:ILE:HA   | 4:J:1062:LEU:CD1  | 2.48                     | 0.40              |
| 5:K:30:MET:SD     | 5:K:49:ILE:HB     | 2.61                     | 0.40              |
| 6:L:118:ASP:CA    | 6:L:121:LYS:HE3   | 2.43                     | 0.40              |
| 6:L:470:MET:CE    | 6:L:486:ARG:HB2   | 2.45                     | 0.40              |
| 7:O:46:DG:H2"     | 7:O:47:DG:C8      | 2.56                     | 0.40              |
| 2:G:51:MET:HE1    | 2:G:216:ALA:HA    | 2.02                     | 0.40              |
| 2:H:186:ASN:OD1   | 2:H:186:ASN:N     | 2.51                     | 0.40              |
| 3:I:582:ASN:HB2   | 3:I:586:PHE:O     | 2.21                     | 0.40              |
| 3:I:593:LYS:HB2   | 3:I:604:HIS:CE1   | 2.57                     | 0.40              |
| 3:I:678:ARG:HA    | 3:I:678:ARG:HD3   | 1.62                     | 0.40              |
| 3:I:818:VAL:HG21  | 3:I:1076:ILE:HD12 | 2.03                     | 0.40              |
| 3:I:833:ILE:HG23  | 3:I:1054:LEU:O    | 2.21                     | 0.40              |
| 3:I:965:GLN:HB2   | 10:I:1401:1N7:H24 | 2.02                     | 0.40              |
| 3:I:1168:GLU:O    | 3:I:1172:LEU:N    | 2.40                     | 0.40              |
| 3:I:1252:SER:O    | 3:I:1256:GLN:NE2  | 2.54                     | 0.40              |
| 4:J:45:ASN:O      | 4:J:47:ARG:N      | 2.55                     | 0.40              |
| 4:J:188:LEU:HD23  | 4:J:188:LEU:HA    | 1.95                     | 0.40              |
| 4:J:484:MET:HA    | 4:J:489:ASN:HD21  | 1.86                     | 0.40              |
| 4:J:591:ILE:HG23  | 4:J:592:VAL:HG13  | 2.03                     | 0.40              |
| 4:J:870:ASP:O     | 4:J:873:GLU:HB3   | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:975:ILE:CD1   | 4:J:1003:LEU:HD21 | 2.51                     | 0.40              |
| 6:L:136:GLU:HB2   | 6:L:361:ILE:HG23  | 2.03                     | 0.40              |
| 7:O:25:DA:H2'     | 7:O:26:DT:H5''    | 2.03                     | 0.40              |
| 8:P:50:DT:H6      | 8:P:50:DT:H2'     | 1.72                     | 0.40              |
| 3:I:185:ASP:HB2   | 3:I:197:ARG:HG3   | 2.04                     | 0.40              |
| 3:I:759:SER:HB3   | 3:I:765:ILE:CG1   | 2.51                     | 0.40              |
| 3:I:1021:LEU:O    | 3:I:1024:GLU:HG3  | 2.21                     | 0.40              |
| 3:I:1191:LYS:O    | 3:I:1195:ILE:HG13 | 2.22                     | 0.40              |
| 4:J:20:ILE:HD11   | 4:J:1353:VAL:HG21 | 2.02                     | 0.40              |
| 4:J:1039:ASP:CG   | 4:J:1074:LEU:HB3  | 2.47                     | 0.40              |
| 4:J:1254:GLU:O    | 4:J:1257:VAL:HB   | 2.21                     | 0.40              |
| 5:K:60:ASN:OD1    | 5:K:60:ASN:N      | 2.55                     | 0.40              |
| 6:L:135:ALA:HA    | 6:L:141:ILE:CD1   | 2.38                     | 0.40              |
| 6:L:302:PHE:O     | 6:L:306:PHE:N     | 2.39                     | 0.40              |
| 6:L:573:LEU:HD11  | 6:L:587:ILE:HB    | 2.03                     | 0.40              |
| 2:G:31:LEU:HD23   | 2:G:36:GLY:HA2    | 2.04                     | 0.40              |
| 2:G:47:LEU:O      | 2:G:180:VAL:HG21  | 2.21                     | 0.40              |
| 2:G:81:ILE:HG12   | 2:G:131:CYS:HB3   | 2.04                     | 0.40              |
| 2:G:167:PRO:HG2   | 2:G:170:ARG:NH1   | 2.37                     | 0.40              |
| 3:I:17:LYS:HD2    | 3:I:17:LYS:N      | 2.36                     | 0.40              |
| 3:I:83:GLN:HA     | 3:I:86:GLN:OE1    | 2.21                     | 0.40              |
| 3:I:241:LEU:HD13  | 3:I:285:ILE:HG12  | 2.04                     | 0.40              |
| 3:I:502:VAL:O     | 3:I:506:PHE:HD1   | 2.03                     | 0.40              |
| 3:I:572:ILE:O     | 3:I:572:ILE:HG22  | 2.21                     | 0.40              |
| 3:I:755:LYS:HA    | 3:I:755:LYS:HE3   | 2.04                     | 0.40              |
| 3:I:965:GLN:HA    | 3:I:968:GLU:HG3   | 2.02                     | 0.40              |
| 3:I:1006:GLU:HG2  | 3:I:1007:LYS:N    | 2.35                     | 0.40              |
| 3:I:1017:GLN:HE21 | 3:I:1017:GLN:HB2  | 1.64                     | 0.40              |
| 4:J:384:LYS:HD2   | 4:J:384:LYS:HA    | 1.81                     | 0.40              |
| 4:J:615:LYS:H     | 4:J:615:LYS:HG3   | 1.72                     | 0.40              |
| 4:J:923:ILE:HD11  | 4:J:1253:ILE:CA   | 2.49                     | 0.40              |
| 4:J:1024:THR:OG1  | 4:J:1024:THR:O    | 2.32                     | 0.40              |
| 4:J:1037:PHE:CD2  | 4:J:1040:MET:HG3  | 2.57                     | 0.40              |
| 4:J:1184:ASP:OD1  | 4:J:1184:ASP:N    | 2.53                     | 0.40              |
| 4:J:1251:LYS:HE2  | 4:J:1251:LYS:HB3  | 1.77                     | 0.40              |
| 6:L:51:MET:HB2    | 6:L:53:ILE:CD1    | 2.52                     | 0.40              |
| 6:L:261:LEU:HD11  | 6:L:266:PHE:HB2   | 2.03                     | 0.40              |
| 6:L:380:VAL:HG23  | 6:L:412:LEU:HG    | 2.02                     | 0.40              |
| 6:L:555:GLU:CA    | 6:L:558:VAL:HG12  | 2.46                     | 0.40              |
| 8:P:54:DT:H2'     | 8:P:55:DT:H71     | 2.03                     | 0.40              |
| 2:M:317:ARG:HA    | 2:M:317:ARG:NE    | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 10  | 1N7  | I     | 1401 | -    | 30,30,46     | 4.97 | 15 (50%)    | 47,48,72    | 2.27 | 15 (31%)    |
| 10  | 1N7  | L     | 701  | -    | 30,30,46     | 5.18 | 16 (53%)    | 47,48,72    | 2.17 | 14 (29%)    |
| 10  | 1N7  | N     | 102  | -    | 30,30,46     | 5.11 | 15 (50%)    | 47,48,72    | 2.28 | 16 (34%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | 1N7  | J     | 1504 | -    | 30,30,46     | 5.11 | 15 (50%) | 47,48,72    | 2.12 | 14 (29%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 10  | 1N7  | I     | 1401 | -    | -       | 0/7/72/92 | 0/4/4/4 |
| 10  | 1N7  | L     | 701  | -    | -       | 5/7/72/92 | 0/4/4/4 |
| 10  | 1N7  | N     | 102  | -    | -       | 7/7/72/92 | 0/4/4/4 |
| 10  | 1N7  | J     | 1504 | -    | -       | 1/7/72/92 | 0/4/4/4 |

All (61) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | L     | 701  | 1N7  | C3-C19 | 18.52 | 1.83        | 1.53     |
| 10  | J     | 1504 | 1N7  | C3-C19 | 18.23 | 1.83        | 1.53     |
| 10  | N     | 102  | 1N7  | C3-C19 | 18.12 | 1.83        | 1.53     |
| 10  | I     | 1401 | 1N7  | C3-C19 | 17.68 | 1.82        | 1.53     |
| 10  | N     | 102  | 1N7  | C3-C4  | 12.34 | 1.73        | 1.53     |
| 10  | J     | 1504 | 1N7  | C3-C4  | 12.31 | 1.73        | 1.53     |
| 10  | L     | 701  | 1N7  | C3-C4  | 12.24 | 1.73        | 1.53     |
| 10  | I     | 1401 | 1N7  | C3-C4  | 11.70 | 1.72        | 1.53     |
| 10  | L     | 701  | 1N7  | C5-C4  | -9.45 | 1.40        | 1.54     |
| 10  | N     | 102  | 1N7  | C5-C4  | -9.19 | 1.40        | 1.54     |
| 10  | J     | 1504 | 1N7  | C5-C4  | -8.96 | 1.40        | 1.54     |
| 10  | I     | 1401 | 1N7  | C5-C4  | -8.80 | 1.41        | 1.54     |
| 10  | I     | 1401 | 1N7  | C2-C19 | -7.96 | 1.42        | 1.56     |
| 10  | N     | 102  | 1N7  | C2-C19 | -7.79 | 1.42        | 1.56     |
| 10  | J     | 1504 | 1N7  | C2-C19 | -7.65 | 1.42        | 1.56     |
| 10  | L     | 701  | 1N7  | C2-C19 | -7.56 | 1.42        | 1.56     |
| 10  | I     | 1401 | 1N7  | C8-C7  | 5.98  | 1.70        | 1.54     |
| 10  | L     | 701  | 1N7  | C8-C7  | 5.97  | 1.70        | 1.54     |
| 10  | N     | 102  | 1N7  | C8-C7  | 5.69  | 1.69        | 1.54     |
| 10  | J     | 1504 | 1N7  | C8-C7  | 5.49  | 1.69        | 1.54     |
| 10  | J     | 1504 | 1N7  | C5-C9  | 4.81  | 1.63        | 1.55     |
| 10  | N     | 102  | 1N7  | C5-C9  | 4.37  | 1.62        | 1.55     |
| 10  | L     | 701  | 1N7  | O4-C4  | -4.28 | 1.36        | 1.43     |
| 10  | J     | 1504 | 1N7  | O4-C4  | -4.15 | 1.36        | 1.43     |
| 10  | I     | 1401 | 1N7  | C5-C9  | 4.09  | 1.62        | 1.55     |
| 10  | I     | 1401 | 1N7  | O4-C4  | -4.09 | 1.36        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | L     | 701  | 1N7  | C5-C6   | -4.07 | 1.48        | 1.55     |
| 10  | N     | 102  | 1N7  | C18-C6  | -3.96 | 1.46        | 1.53     |
| 10  | N     | 102  | 1N7  | O4-C4   | -3.89 | 1.37        | 1.43     |
| 10  | L     | 701  | 1N7  | C7-C6   | 3.60  | 1.61        | 1.54     |
| 10  | J     | 1504 | 1N7  | C2-C15  | 3.57  | 1.61        | 1.55     |
| 10  | L     | 701  | 1N7  | C18-C6  | -3.56 | 1.47        | 1.53     |
| 10  | L     | 701  | 1N7  | C2-C15  | 3.55  | 1.60        | 1.55     |
| 10  | L     | 701  | 1N7  | C5-C9   | 3.53  | 1.61        | 1.55     |
| 10  | I     | 1401 | 1N7  | C5-C6   | -3.47 | 1.49        | 1.55     |
| 10  | J     | 1504 | 1N7  | C14-C15 | -3.43 | 1.48        | 1.53     |
| 10  | N     | 102  | 1N7  | C5-C6   | -3.43 | 1.49        | 1.55     |
| 10  | I     | 1401 | 1N7  | C18-C6  | -3.33 | 1.47        | 1.53     |
| 10  | J     | 1504 | 1N7  | C5-C6   | -3.30 | 1.50        | 1.55     |
| 10  | J     | 1504 | 1N7  | C18-C6  | -3.20 | 1.47        | 1.53     |
| 10  | N     | 102  | 1N7  | C7-C6   | 3.17  | 1.60        | 1.54     |
| 10  | I     | 1401 | 1N7  | C14-C15 | -3.17 | 1.48        | 1.53     |
| 10  | N     | 102  | 1N7  | C2-C15  | 2.96  | 1.60        | 1.55     |
| 10  | I     | 1401 | 1N7  | C7-C6   | 2.92  | 1.60        | 1.54     |
| 10  | J     | 1504 | 1N7  | C7-C6   | 2.85  | 1.60        | 1.54     |
| 10  | L     | 701  | 1N7  | C14-C15 | -2.81 | 1.49        | 1.53     |
| 10  | N     | 102  | 1N7  | C10-C5  | 2.74  | 1.58        | 1.54     |
| 10  | I     | 1401 | 1N7  | C2-C15  | 2.71  | 1.59        | 1.55     |
| 10  | N     | 102  | 1N7  | C14-C13 | 2.68  | 1.56        | 1.52     |
| 10  | J     | 1504 | 1N7  | C1-C2   | 2.66  | 1.58        | 1.54     |
| 10  | L     | 701  | 1N7  | C14-C13 | 2.56  | 1.56        | 1.52     |
| 10  | L     | 701  | 1N7  | C16-C15 | 2.50  | 1.57        | 1.53     |
| 10  | L     | 701  | 1N7  | O2-C13  | -2.42 | 1.36        | 1.43     |
| 10  | I     | 1401 | 1N7  | C14-C13 | 2.41  | 1.56        | 1.52     |
| 10  | N     | 102  | 1N7  | O2-C13  | -2.36 | 1.36        | 1.43     |
| 10  | I     | 1401 | 1N7  | C1-C2   | 2.24  | 1.58        | 1.54     |
| 10  | J     | 1504 | 1N7  | O2-C13  | -2.19 | 1.37        | 1.43     |
| 10  | I     | 1401 | 1N7  | O2-C13  | -2.14 | 1.37        | 1.43     |
| 10  | L     | 701  | 1N7  | C10-C5  | 2.13  | 1.57        | 1.54     |
| 10  | N     | 102  | 1N7  | C14-C15 | -2.09 | 1.50        | 1.53     |
| 10  | J     | 1504 | 1N7  | C10-C5  | 2.00  | 1.57        | 1.54     |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 10  | N     | 102  | 1N7  | C7-C6-C18 | -7.38 | 108.23      | 118.36   |
| 10  | I     | 1401 | 1N7  | C7-C6-C18 | -6.22 | 109.83      | 118.36   |
| 10  | J     | 1504 | 1N7  | C7-C6-C18 | -5.97 | 110.17      | 118.36   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | L     | 701  | 1N7  | C9-C5-C4    | -5.58 | 112.65      | 117.67   |
| 10  | L     | 701  | 1N7  | C7-C6-C18   | -5.47 | 110.86      | 118.36   |
| 10  | J     | 1504 | 1N7  | C9-C5-C6    | 5.26  | 105.39      | 100.11   |
| 10  | I     | 1401 | 1N7  | C9-C5-C4    | -5.09 | 113.09      | 117.67   |
| 10  | L     | 701  | 1N7  | C19-C18-C17 | -4.91 | 105.67      | 111.86   |
| 10  | J     | 1504 | 1N7  | C9-C5-C4    | -4.73 | 113.41      | 117.67   |
| 10  | N     | 102  | 1N7  | C9-C5-C4    | -4.70 | 113.44      | 117.67   |
| 10  | N     | 102  | 1N7  | C19-C3-C4   | -4.61 | 108.27      | 114.29   |
| 10  | N     | 102  | 1N7  | C6-C5-C4    | 4.44  | 111.48      | 107.42   |
| 10  | N     | 102  | 1N7  | C5-C6-C18   | 4.13  | 119.95      | 114.72   |
| 10  | I     | 1401 | 1N7  | C21-C20-C22 | -4.02 | 104.12      | 110.34   |
| 10  | I     | 1401 | 1N7  | C19-C3-C4   | -4.00 | 109.07      | 114.29   |
| 10  | L     | 701  | 1N7  | C16-C15-C14 | -3.95 | 106.72      | 111.23   |
| 10  | I     | 1401 | 1N7  | C9-C5-C6    | 3.87  | 104.00      | 100.11   |
| 10  | I     | 1401 | 1N7  | C5-C6-C18   | 3.87  | 119.62      | 114.72   |
| 10  | I     | 1401 | 1N7  | C19-C18-C17 | -3.66 | 107.25      | 111.86   |
| 10  | I     | 1401 | 1N7  | C6-C5-C4    | 3.63  | 110.73      | 107.42   |
| 10  | J     | 1504 | 1N7  | C5-C6-C18   | 3.60  | 119.28      | 114.72   |
| 10  | J     | 1504 | 1N7  | C21-C20-C9  | -3.53 | 107.59      | 112.88   |
| 10  | N     | 102  | 1N7  | C16-C15-C2  | -3.50 | 108.94      | 112.66   |
| 10  | L     | 701  | 1N7  | C21-C20-C9  | -3.48 | 107.67      | 112.88   |
| 10  | N     | 102  | 1N7  | C11-C2-C1   | -3.43 | 102.86      | 108.31   |
| 10  | L     | 701  | 1N7  | C6-C5-C4    | 3.42  | 110.54      | 107.42   |
| 10  | J     | 1504 | 1N7  | C1-C12-C13  | -3.32 | 106.09      | 110.48   |
| 10  | L     | 701  | 1N7  | C1-C12-C13  | -3.30 | 106.11      | 110.48   |
| 10  | I     | 1401 | 1N7  | C1-C12-C13  | -3.25 | 106.17      | 110.48   |
| 10  | L     | 701  | 1N7  | C7-C8-C9    | -3.20 | 98.88       | 105.14   |
| 10  | N     | 102  | 1N7  | C21-C20-C22 | -3.17 | 105.43      | 110.34   |
| 10  | J     | 1504 | 1N7  | C8-C9-C20   | -3.13 | 107.44      | 112.18   |
| 10  | L     | 701  | 1N7  | C21-C20-C22 | -3.12 | 105.51      | 110.34   |
| 10  | L     | 701  | 1N7  | C22-C20-C9  | 3.11  | 116.78      | 110.33   |
| 10  | J     | 1504 | 1N7  | C14-C13-C12 | -3.10 | 106.84      | 110.62   |
| 10  | N     | 102  | 1N7  | C16-C17-C18 | 3.04  | 114.82      | 111.50   |
| 10  | I     | 1401 | 1N7  | C16-C15-C14 | -2.92 | 107.89      | 111.23   |
| 10  | J     | 1504 | 1N7  | C16-C15-C14 | -2.91 | 107.90      | 111.23   |
| 10  | J     | 1504 | 1N7  | C2-C19-C18  | 2.91  | 115.08      | 111.84   |
| 10  | I     | 1401 | 1N7  | C2-C19-C18  | 2.90  | 115.07      | 111.84   |
| 10  | J     | 1504 | 1N7  | C19-C18-C17 | -2.87 | 108.24      | 111.86   |
| 10  | N     | 102  | 1N7  | C19-C18-C17 | -2.81 | 108.32      | 111.86   |
| 10  | I     | 1401 | 1N7  | C8-C7-C6    | -2.62 | 100.02      | 105.14   |
| 10  | L     | 701  | 1N7  | C11-C2-C1   | -2.61 | 104.15      | 108.31   |
| 10  | J     | 1504 | 1N7  | C11-C2-C15  | -2.61 | 106.08      | 110.44   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | J     | 1504 | 1N7  | C3-C19-C18  | -2.54 | 107.14      | 110.89   |
| 10  | I     | 1401 | 1N7  | C8-C9-C20   | -2.47 | 108.44      | 112.18   |
| 10  | N     | 102  | 1N7  | C11-C2-C19  | 2.42  | 114.43      | 111.18   |
| 10  | N     | 102  | 1N7  | C3-C4-C5    | -2.41 | 108.81      | 111.26   |
| 10  | L     | 701  | 1N7  | C16-C17-C18 | -2.41 | 108.87      | 111.50   |
| 10  | I     | 1401 | 1N7  | C10-C5-C9   | -2.40 | 107.44      | 111.20   |
| 10  | L     | 701  | 1N7  | C11-C2-C19  | 2.34  | 114.32      | 111.18   |
| 10  | N     | 102  | 1N7  | C21-C20-C9  | -2.32 | 109.40      | 112.88   |
| 10  | N     | 102  | 1N7  | C10-C5-C4   | -2.27 | 106.78      | 109.06   |
| 10  | I     | 1401 | 1N7  | C3-C19-C18  | -2.19 | 107.66      | 110.89   |
| 10  | N     | 102  | 1N7  | C10-C5-C6   | 2.17  | 114.60      | 111.20   |
| 10  | J     | 1504 | 1N7  | C15-C14-C13 | -2.16 | 109.45      | 112.71   |
| 10  | L     | 701  | 1N7  | O3-C17-C18  | 2.06  | 114.23      | 109.52   |
| 10  | N     | 102  | 1N7  | C22-C20-C9  | 2.01  | 114.49      | 110.33   |

There are no chirality outliers.

All (13) torsion outliers are listed below:

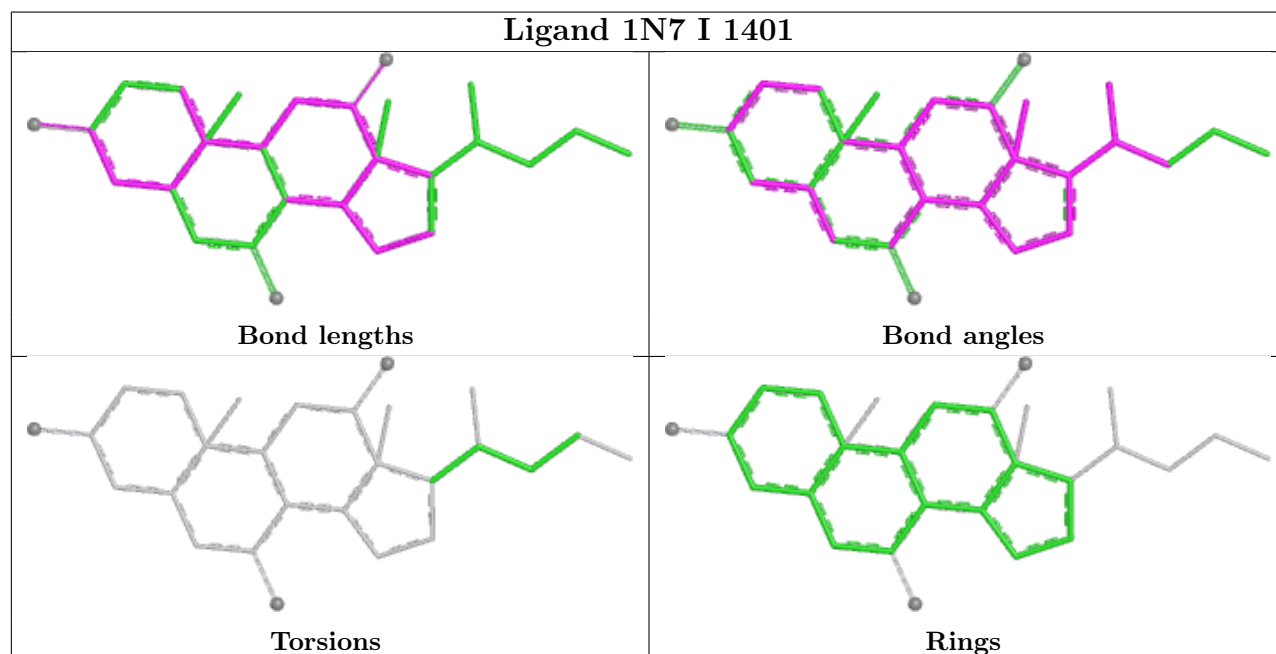
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | N     | 102  | 1N7  | C9-C20-C22-C23  |
| 10  | N     | 102  | 1N7  | C21-C20-C22-C23 |
| 10  | L     | 701  | 1N7  | C22-C20-C9-C5   |
| 10  | L     | 701  | 1N7  | C20-C22-C23-C24 |
| 10  | L     | 701  | 1N7  | C21-C20-C9-C5   |
| 10  | N     | 102  | 1N7  | C21-C20-C9-C5   |
| 10  | N     | 102  | 1N7  | C20-C22-C23-C24 |
| 10  | J     | 1504 | 1N7  | C20-C22-C23-C24 |
| 10  | L     | 701  | 1N7  | C21-C20-C9-C8   |
| 10  | N     | 102  | 1N7  | C21-C20-C9-C8   |
| 10  | L     | 701  | 1N7  | C22-C20-C9-C8   |
| 10  | N     | 102  | 1N7  | C22-C20-C9-C5   |
| 10  | N     | 102  | 1N7  | C22-C20-C9-C8   |

There are no ring outliers.

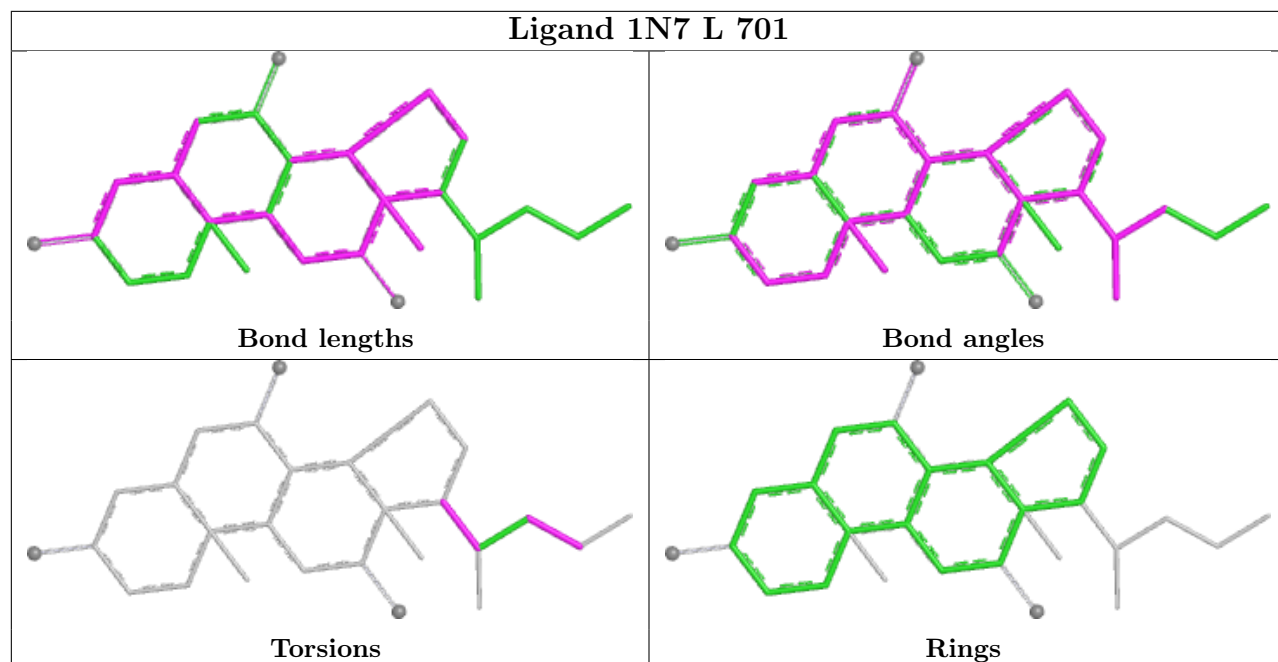
4 monomers are involved in 18 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | I     | 1401 | 1N7  | 7       | 0            |
| 10  | L     | 701  | 1N7  | 3       | 0            |
| 10  | N     | 102  | 1N7  | 4       | 0            |
| 10  | J     | 1504 | 1N7  | 4       | 0            |

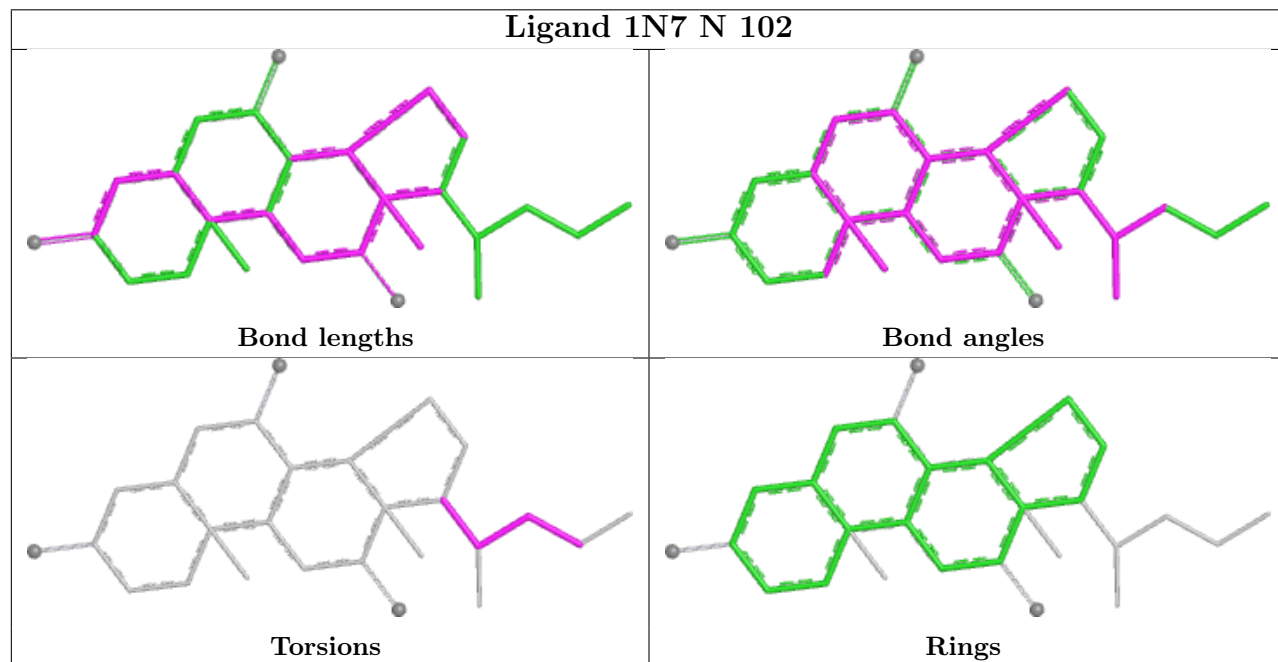
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

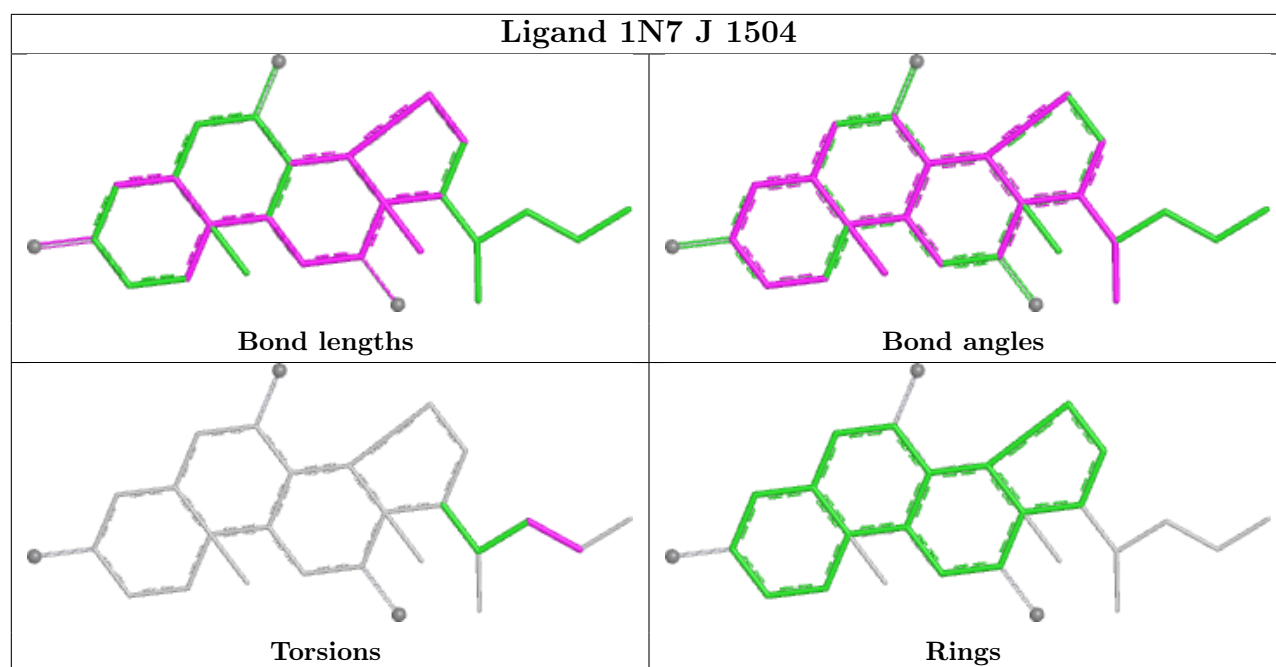


## Ligand 1N7 L 701



## Ligand 1N7 N 102





## 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.

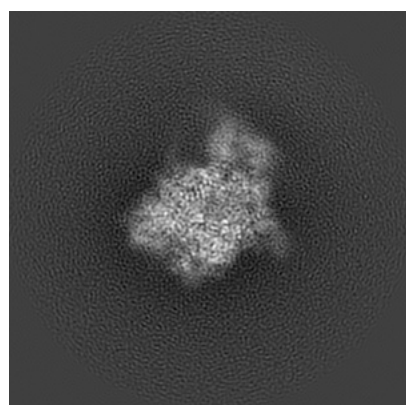
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20464. These allow visual inspection of the internal detail of the map and identification of artifacts.

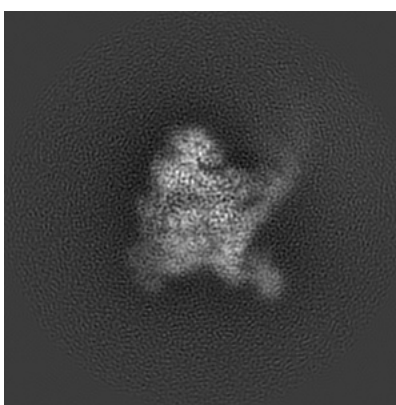
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

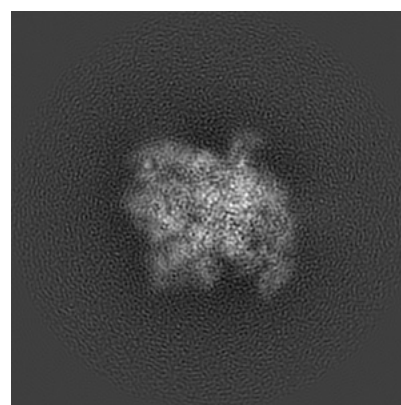
#### 6.1.1 Primary map



X



Y

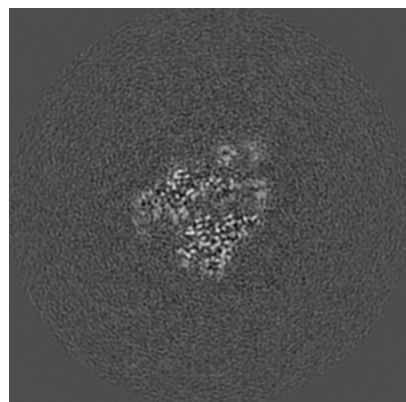


Z

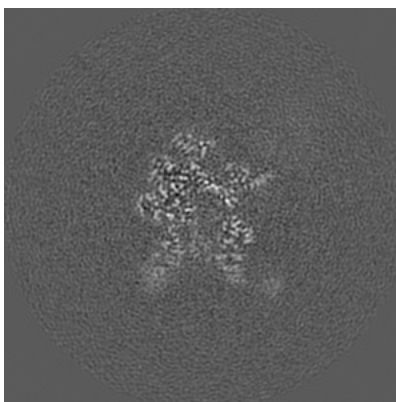
The images above show the map projected in three orthogonal directions.

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

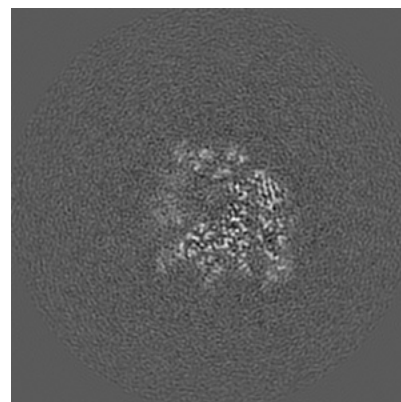
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



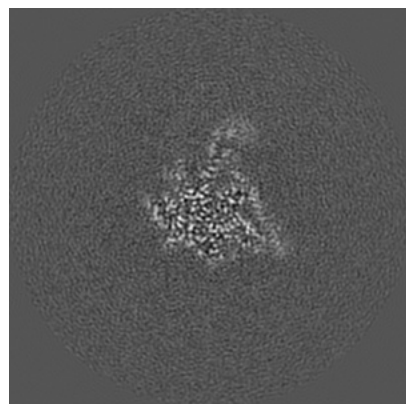
Z Index: 128



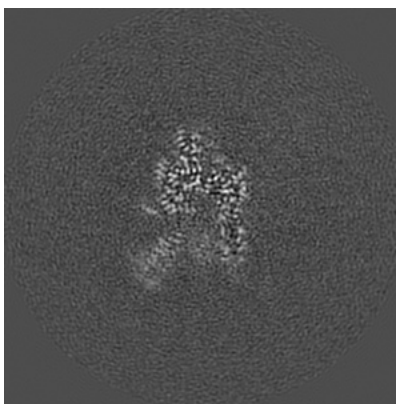
The images above show central slices of the map in three orthogonal directions.

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

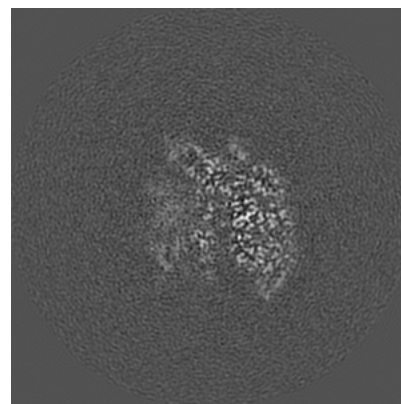
### 6.3.1 Primary map



X Index: 146



Y Index: 123

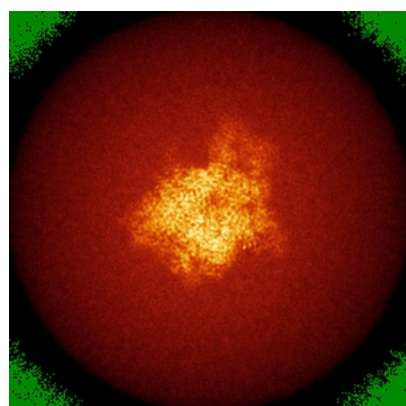


Z Index: 121

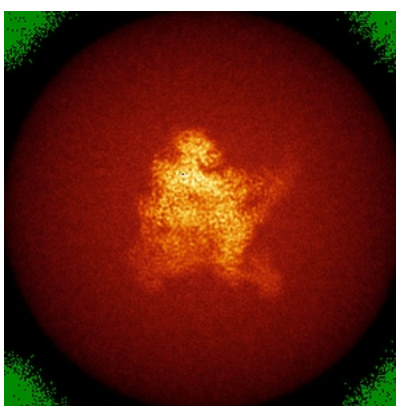
The images above show the largest variance slices of the map in three orthogonal directions.

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

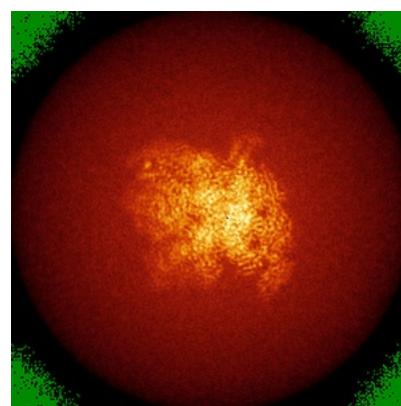
### 6.4.1 Primary map



X



Y



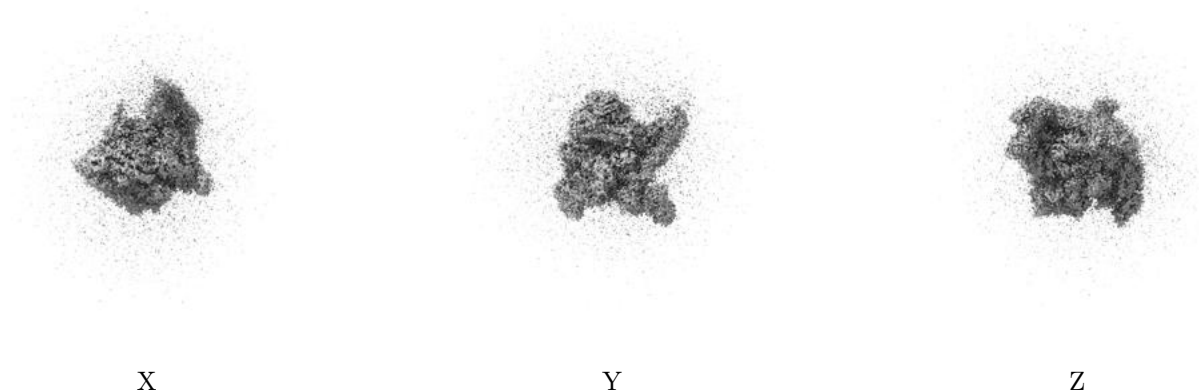
Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

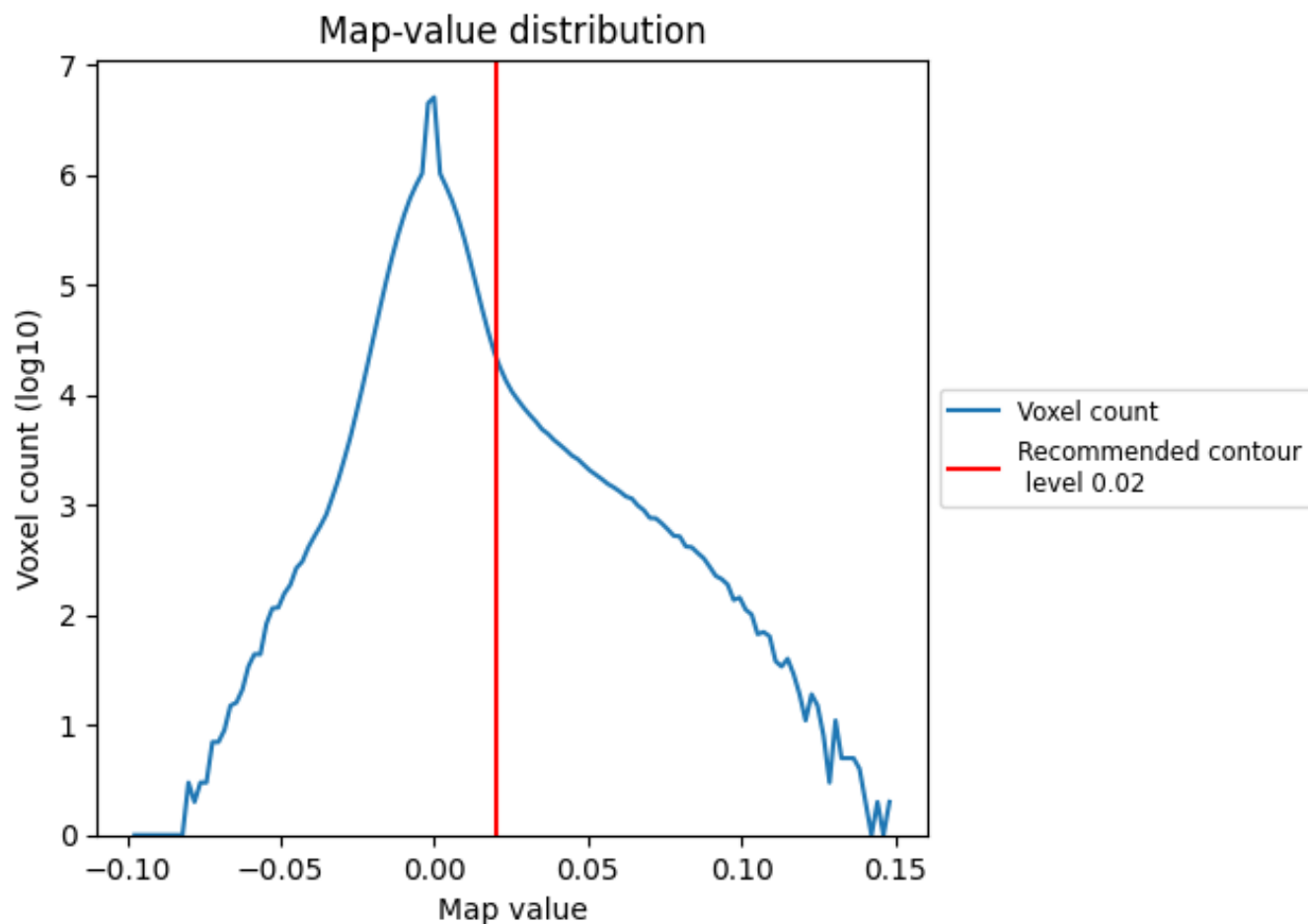
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

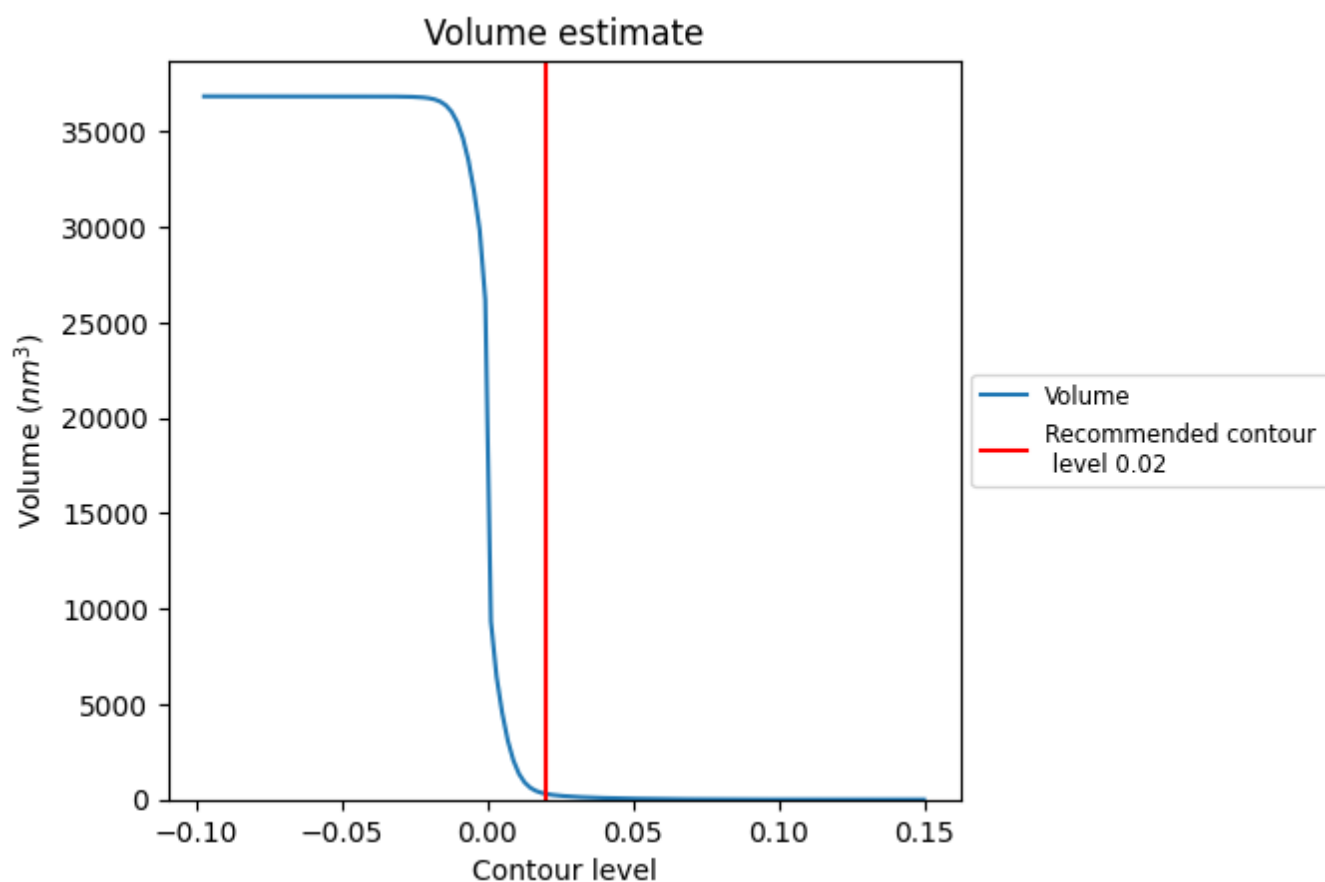
This section contains the results of statistical analysis of the map.

### 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.

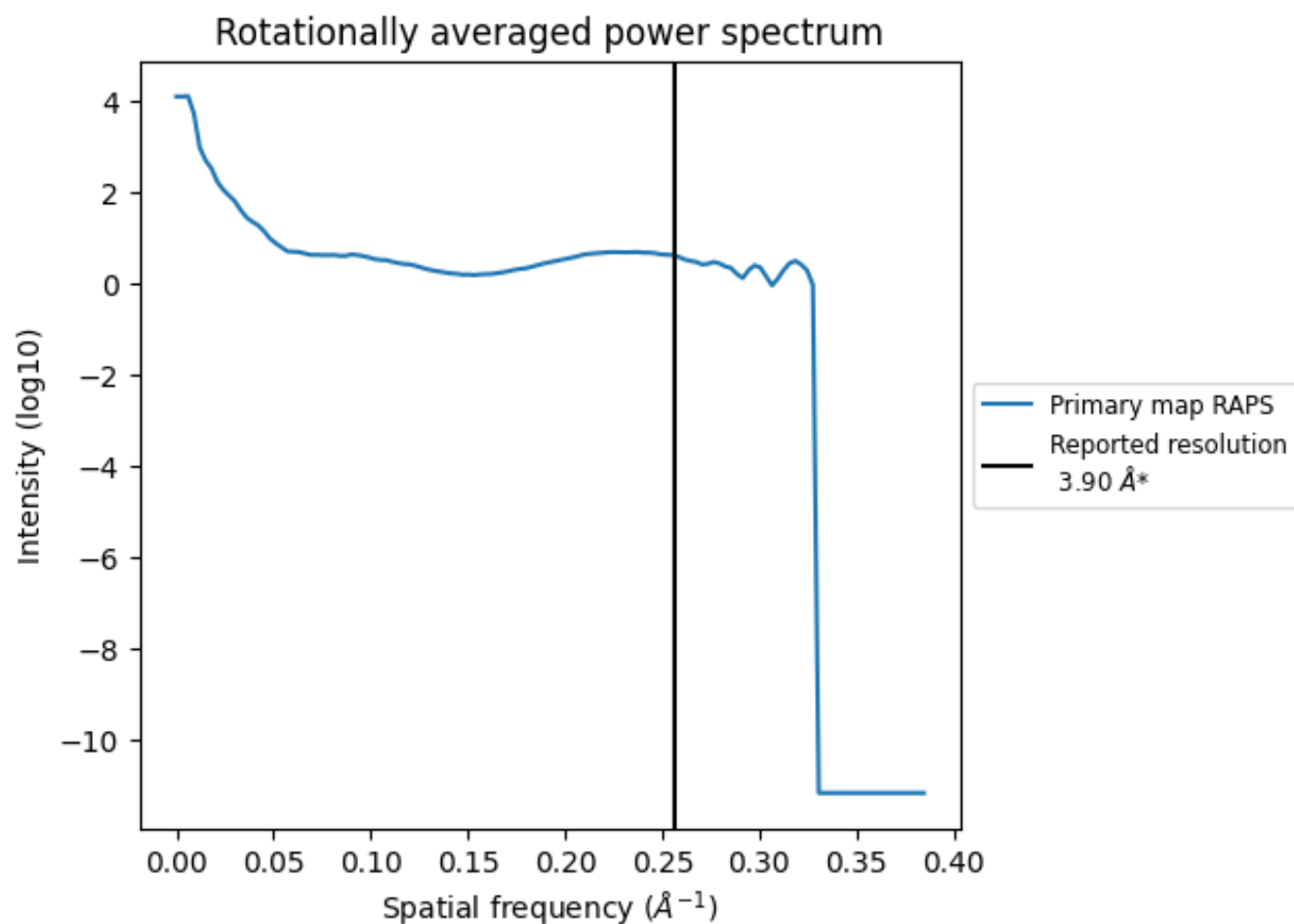
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 302 nm<sup>3</sup>; this corresponds to an approximate mass of 273 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 ⓘ

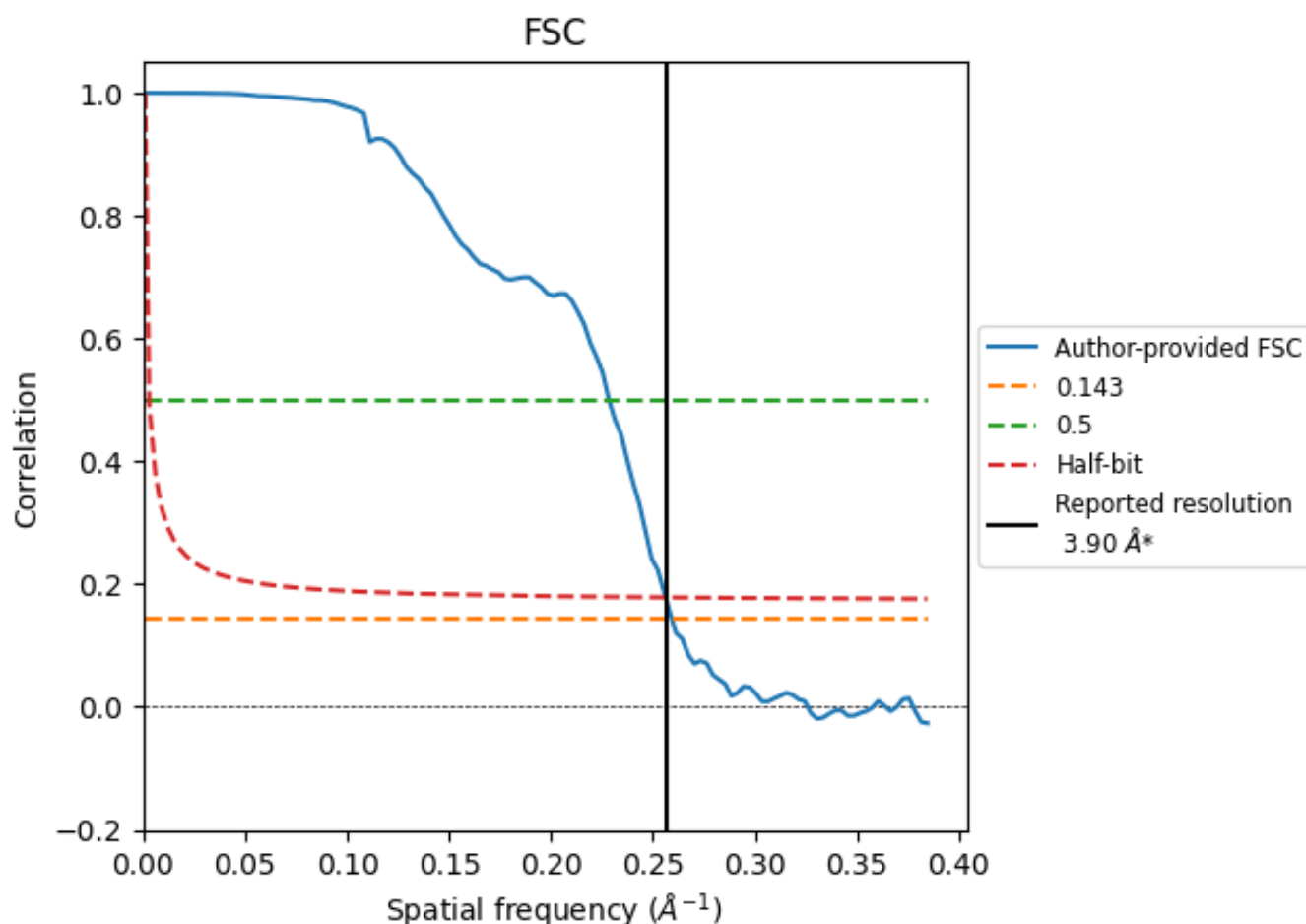


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | 3.86                               | 4.38 | 3.90     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

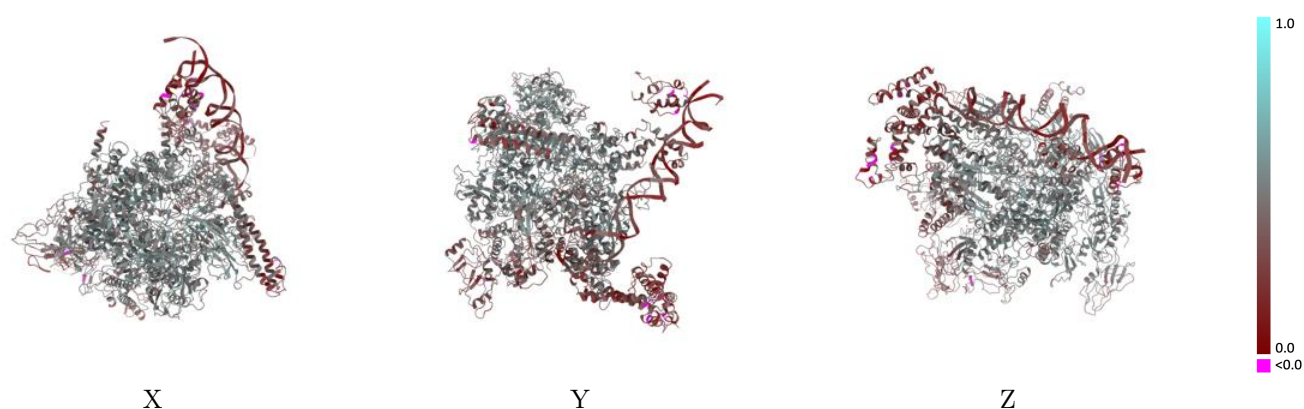
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20464 and PDB model 6PSU. Per-residue inclusion information can be found in section 3 on page 8.

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

This section was not generated.

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



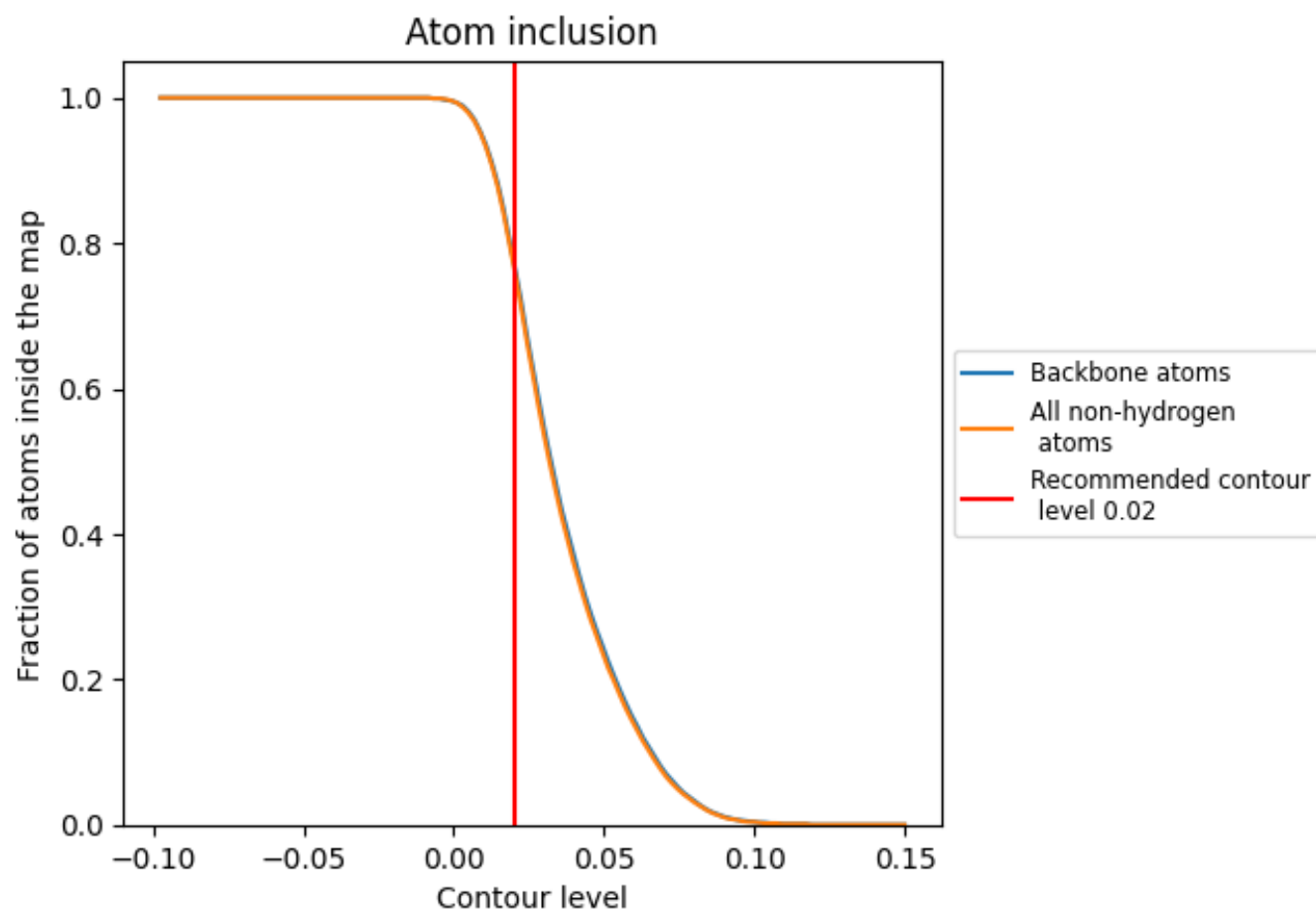
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7690 | <div></div> 0.4260 |
| G     | <div></div> 0.8540 | <div></div> 0.4910 |
| H     | <div></div> 0.8310 | <div></div> 0.4540 |
| I     | <div></div> 0.8310 | <div></div> 0.4600 |
| J     | <div></div> 0.8070 | <div></div> 0.4510 |
| K     | <div></div> 0.6990 | <div></div> 0.4460 |
| L     | <div></div> 0.6740 | <div></div> 0.3370 |
| M     | <div></div> 0.0520 | <div></div> 0.2280 |
| N     | <div></div> 0.8300 | <div></div> 0.4370 |
| O     | <div></div> 0.5680 | <div></div> 0.2450 |
| P     | <div></div> 0.5250 | <div></div> 0.2260 |

1.0

0.0

<0.0