# Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 06:07 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 8BHY / pdb_00008bhy |
| EMDB ID | : | EMD-16074 |
| Title | : | DNA-PK Ku80 mediated dimer bound to PAXX and XLF |
| Authors | : | Hardwick, S.W.; Chaplin, A.K. |
| Deposited on | : | 2022-11-01 |
| Resolution | : | 5.33 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

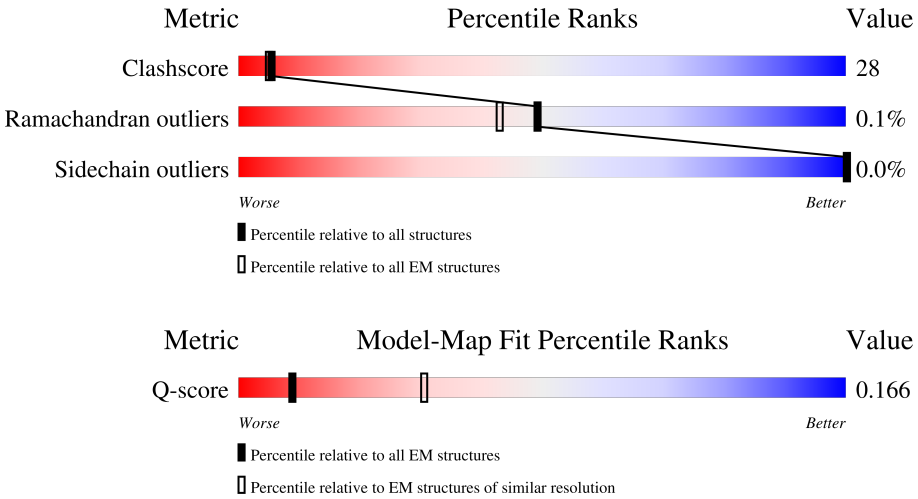
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 5.33 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.







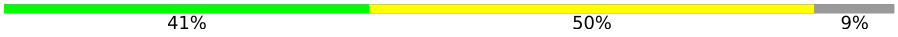
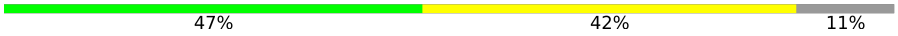
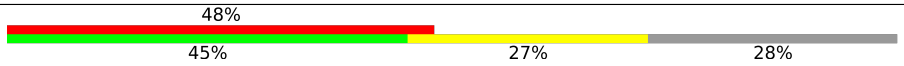
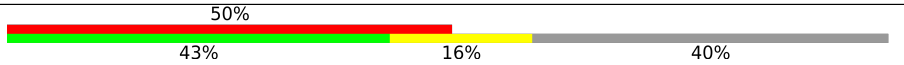
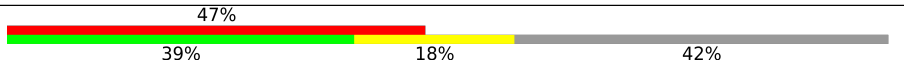
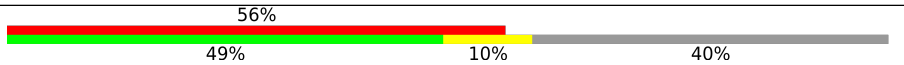
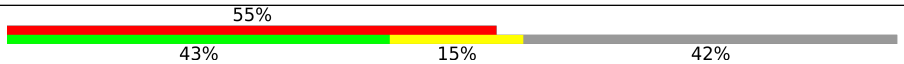
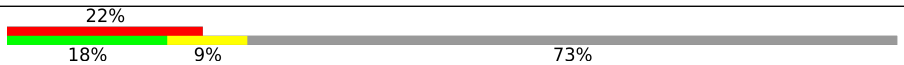
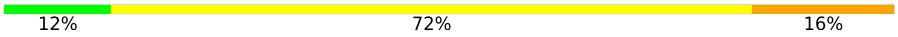
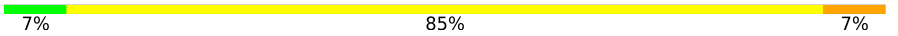
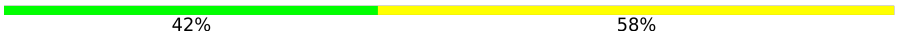
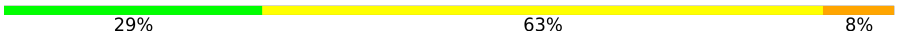
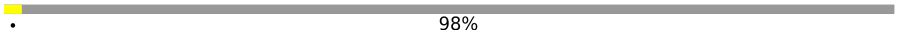
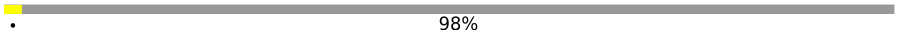
| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 504 ( 4.83 - 5.82 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 4128 | 36% 49% 14% |
| 1 | S | 4128 | 41% 45% 14% |
| 2 | B | 609 | 32% 52% 17% |
| 2 | T | 609 | 39% 43% 18% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | C | 732 |   |
| 3 | L | 732 |   |
| 4 | D | 204 |   |
| 4 | M | 204 |   |
| 5 | G | 336 |   |
| 5 | H | 336 |   |
| 5 | P | 336 |   |
| 5 | Q | 336 |   |
| 6 | I | 911 |   |
| 6 | R | 911 |   |
| 7 | d | 25 |   |
| 8 | e | 27 |   |
| 9 | i | 26 |   |
| 10 | j | 24 |   |
| 11 | f | 299 |   |
| 11 | m | 299 |   |

# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 90193 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 3547 | Total<br>28300 | C<br>18182 | N<br>4780 | O<br>5151 | S<br>187 | 0 | 0 |
| 1 | S | 3538 | Total<br>28342 | C<br>18207 | N<br>4793 | O<br>5154 | S<br>188 | 0 | 0 |

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 507 | Total<br>4085 | C<br>2614 | N<br>693 | O<br>760 | S<br>18 | 0 | 0 |
| 2 | T | 502 | Total<br>4037 | C<br>2587 | N<br>680 | O<br>752 | S<br>18 | 0 | 0 |

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 668 | Total<br>5318 | C<br>3397 | N<br>892 | O<br>1003 | S<br>26 | 0 | 0 |
| 3 | L | 652 | Total<br>5204 | C<br>3324 | N<br>876 | O<br>979 | S<br>25 | 0 | 0 |

- Molecule 4 is a protein called Protein PAXX.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 147 | Total<br>1102 | C<br>702 | N<br>190 | O<br>204 | S<br>6 | 0 | 0 |
| 4 | M | 164 | Total<br>1219 | C<br>767 | N<br>210 | O<br>236 | S<br>6 | 0 | 0 |

- Molecule 5 is a protein called DNA repair protein XRCC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | G | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1628 | 1031 | 278 | 312 | 7 | | |
| 5 | H | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1589 | 1009 | 271 | 302 | 7 | | |
| 5 | P | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1622 | 1028 | 275 | 312 | 7 | | |
| 5 | Q | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1580 | 1003 | 268 | 302 | 7 | | |

- Molecule 6 is a protein called DNA ligase 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | I | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1984 | 1262 | 336 | 373 | 13 | | |
| 6 | R | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1970 | 1252 | 335 | 371 | 12 | | |

- Molecule 7 is a DNA chain called DNA (25-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | d | 25 | Total | C | N | O | P | 0 | 0 |
| | | | 516 | 249 | 87 | 155 | 25 | | |

- Molecule 8 is a DNA chain called DNA (27-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | e | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 554 | 267 | 102 | 158 | 27 | | |

- Molecule 9 is a DNA chain called DNA (26-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | i | 26 | Total | C | N | O | P | 0 | 0 |
| | | | 532 | 257 | 97 | 152 | 26 | | |

- Molecule 10 is a DNA chain called DNA (5'-D(P*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | j | 24 | Total | C | N | O | P | 0 | 0 |
| | | | 497 | 240 | 84 | 149 | 24 | | |

- Molecule 11 is a protein called Non-homologous end-joining factor 1.

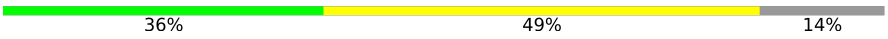
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 11 | f | 7 | Total | C | N | O | 0 | 0 |
| | | | 57 | 37 | 11 | 9 | | |
| 11 | m | 7 | Total | C | N | O | 0 | 0 |
| | | | 57 | 37 | 11 | 9 | | |

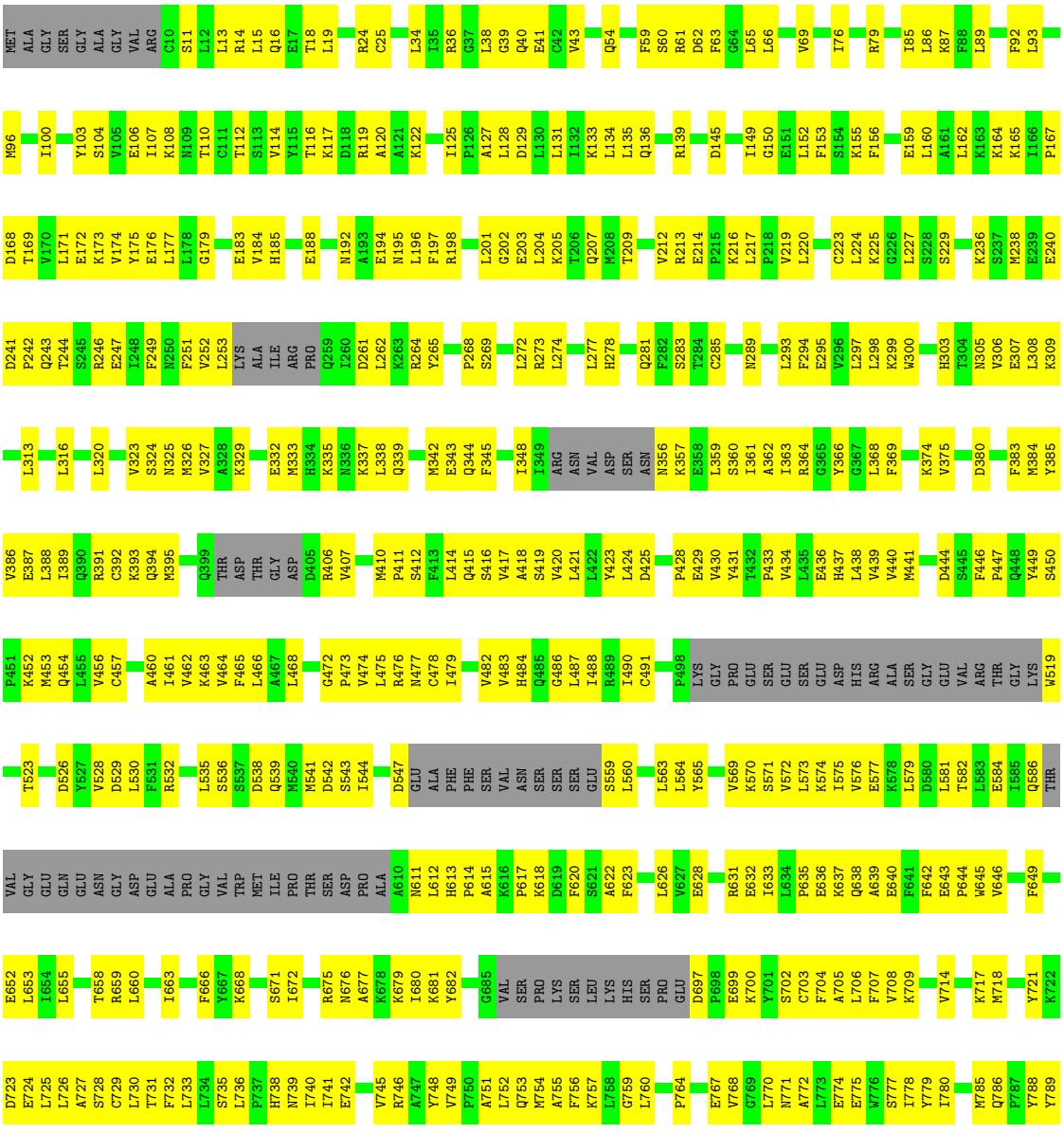
# 3 Residue-property plots (i)

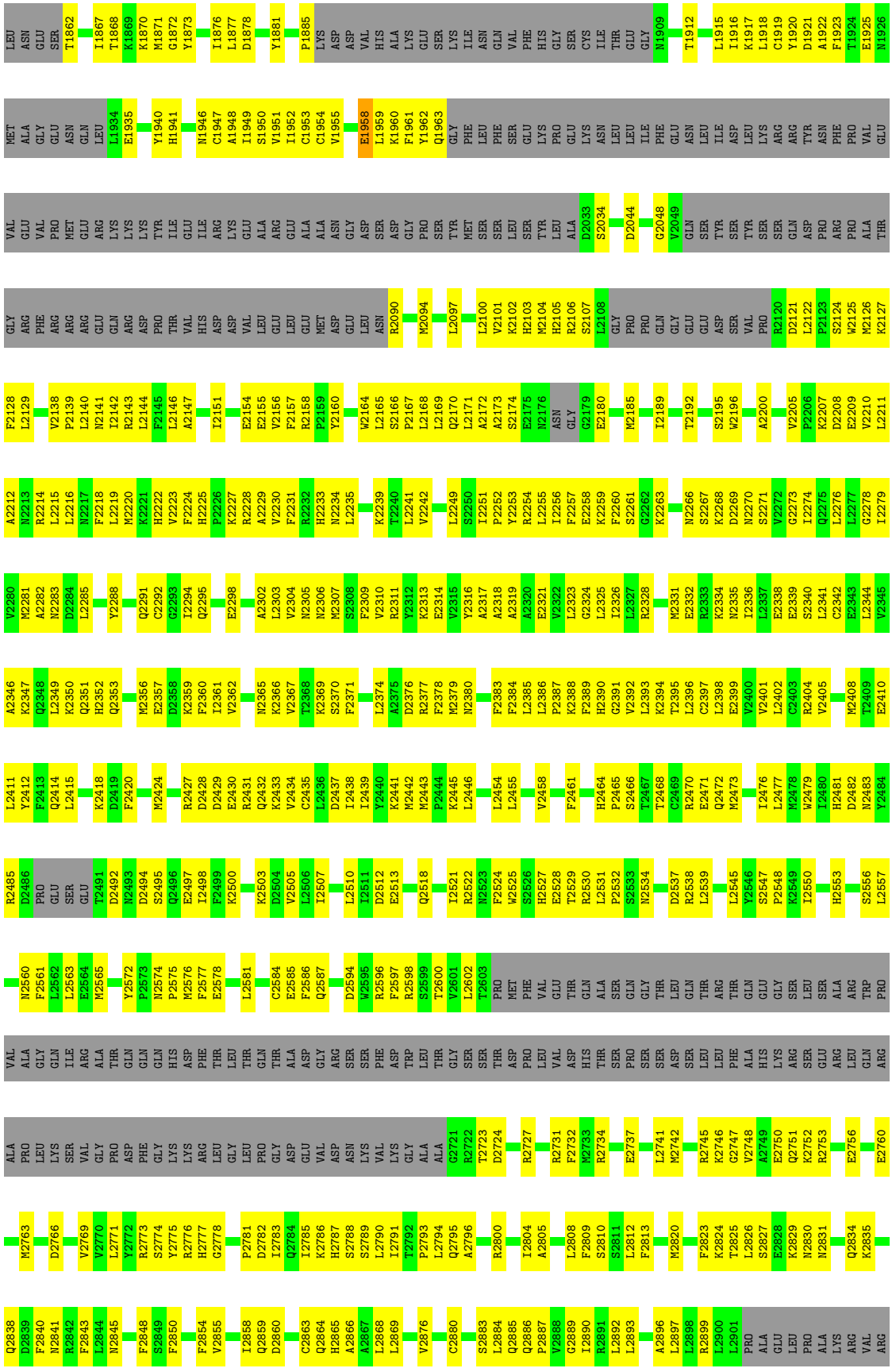
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

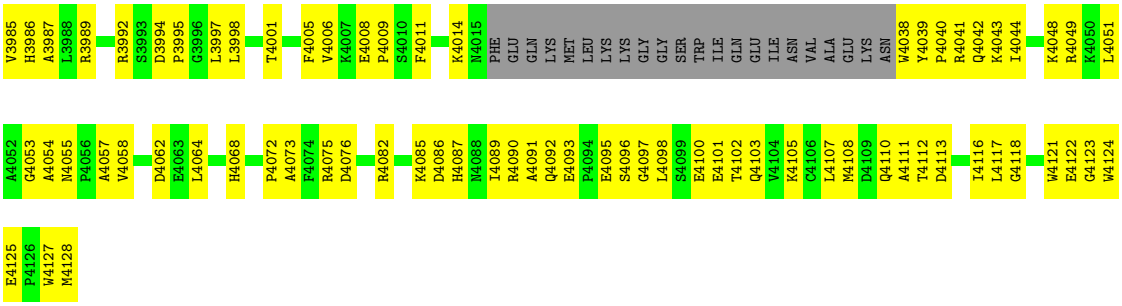
- Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain A:



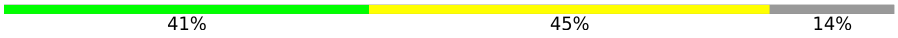



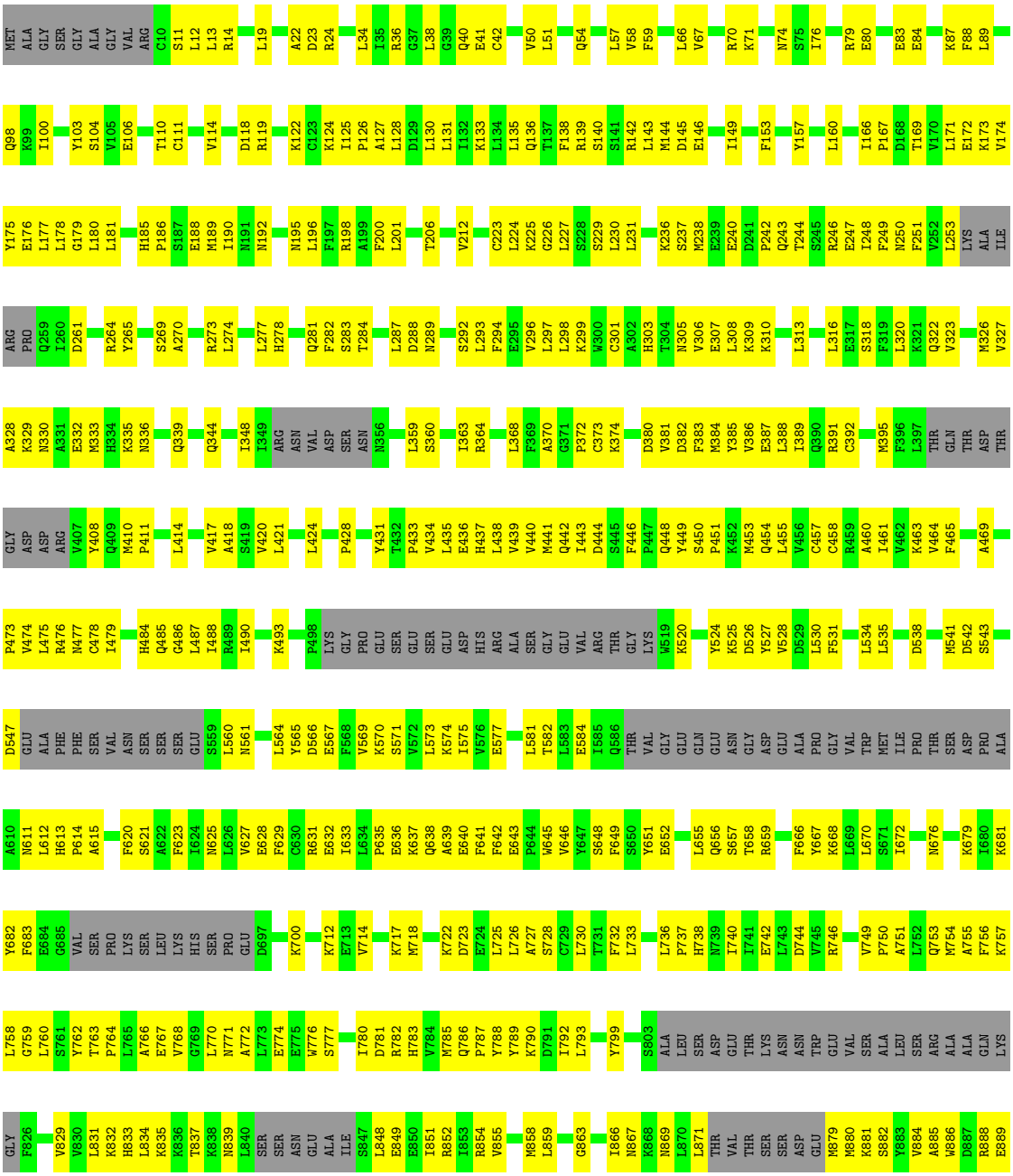


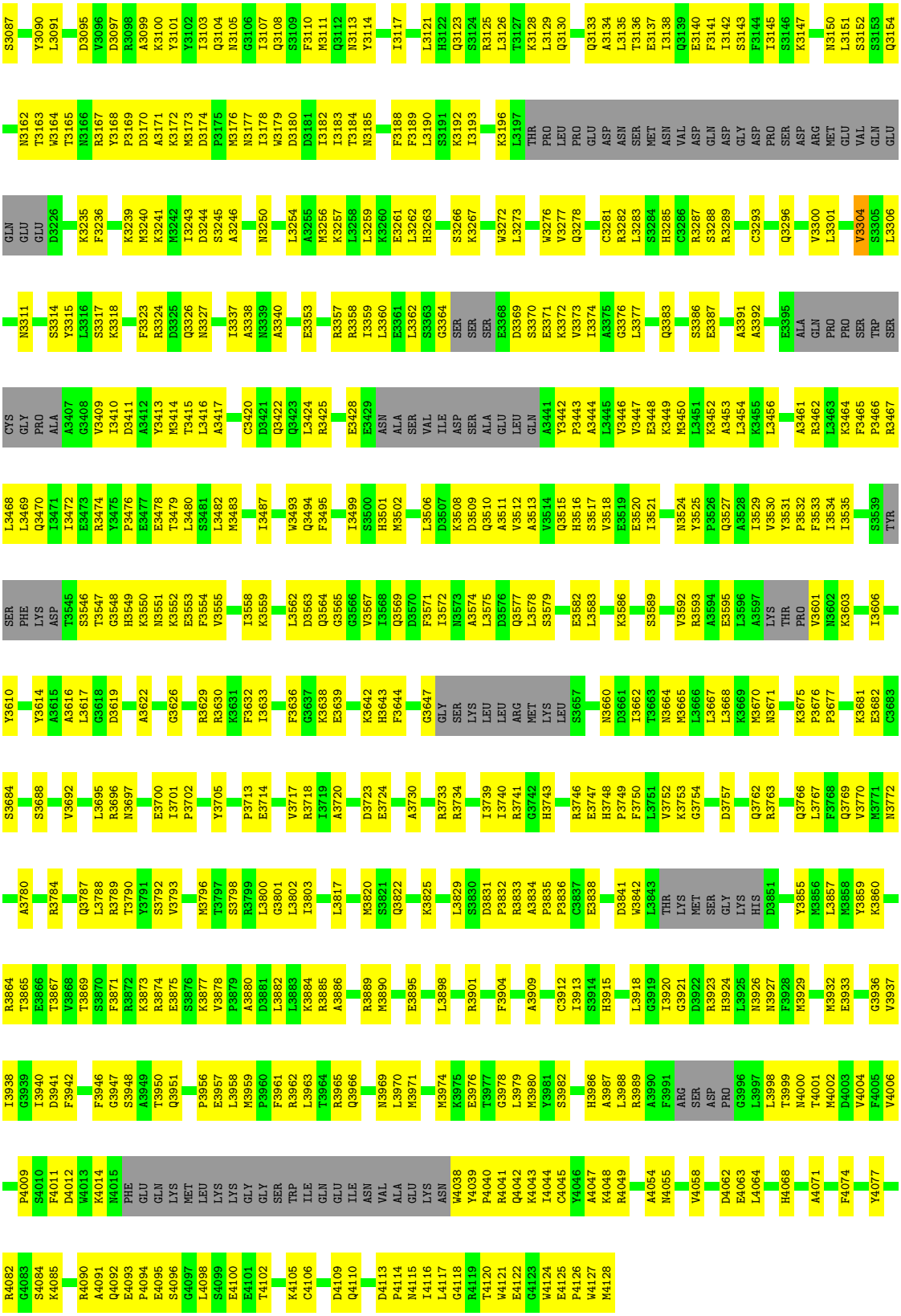


• Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain S:



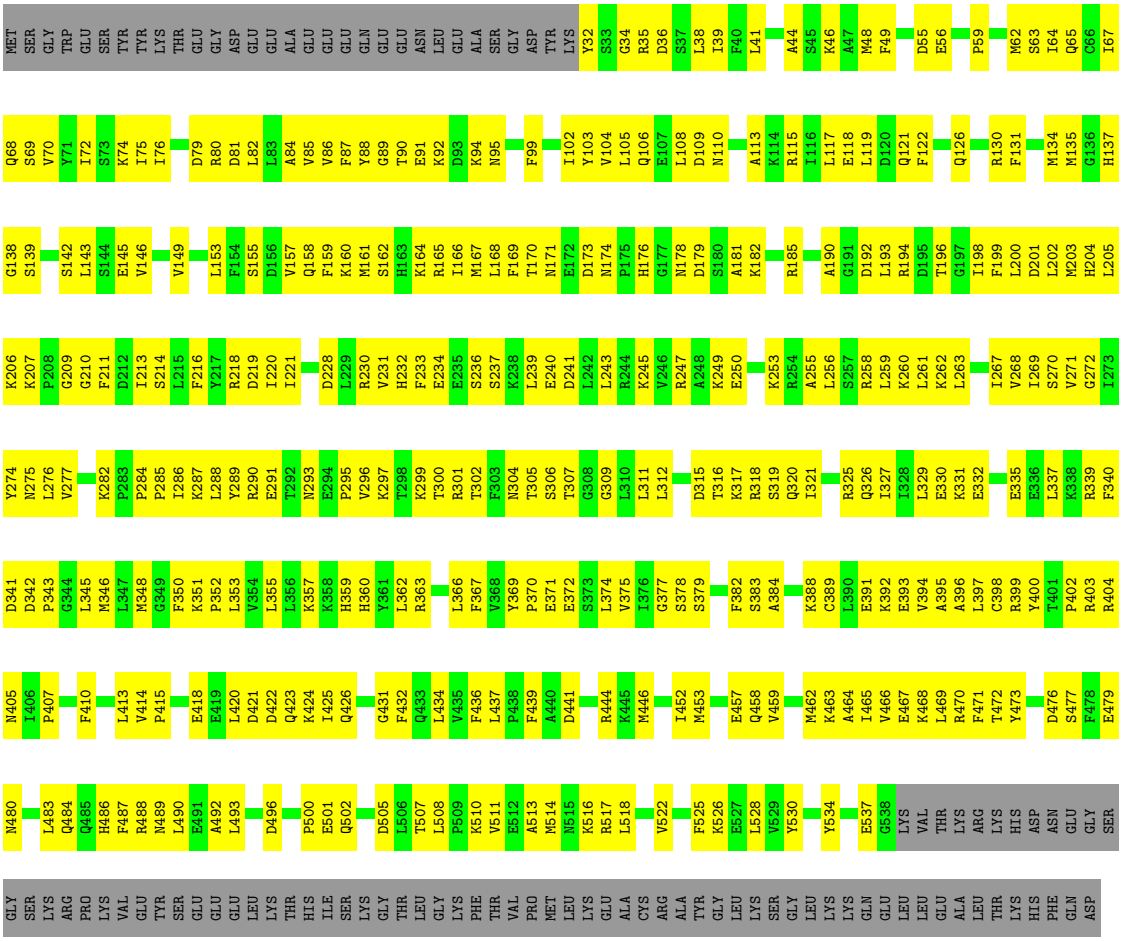





• Molecule 2: X-ray repair cross-complementing protein 6

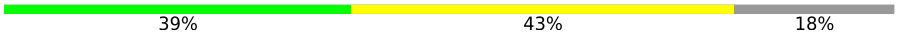
Chain B:

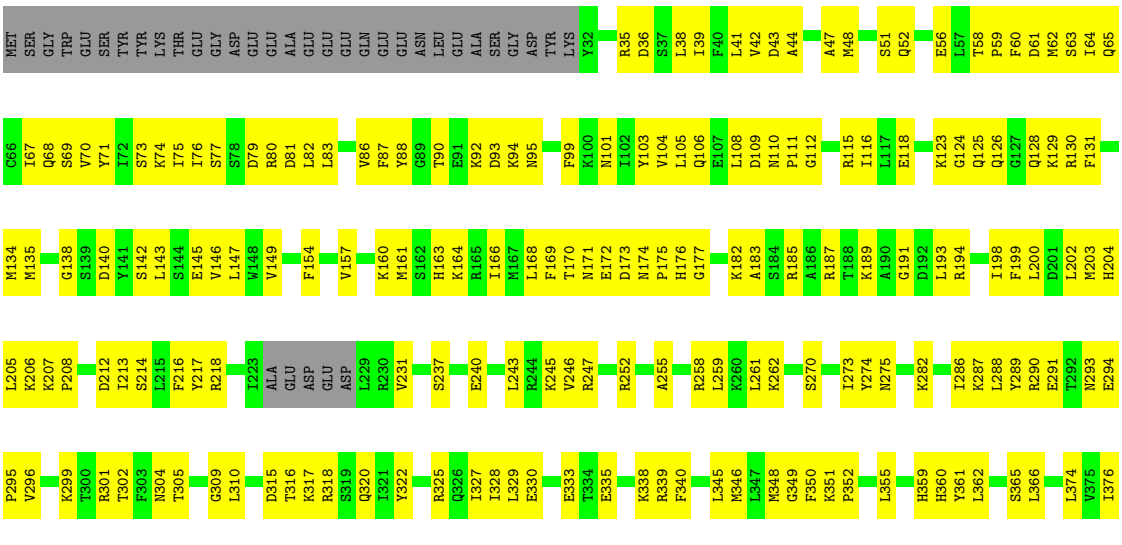


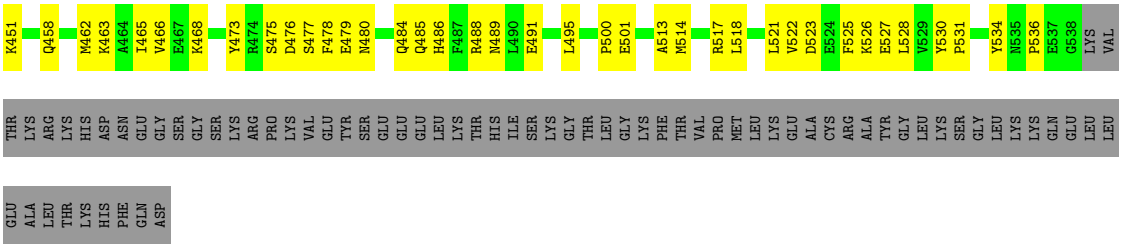


• Molecule 2: X-ray repair cross-complementing protein 6

Chain T:



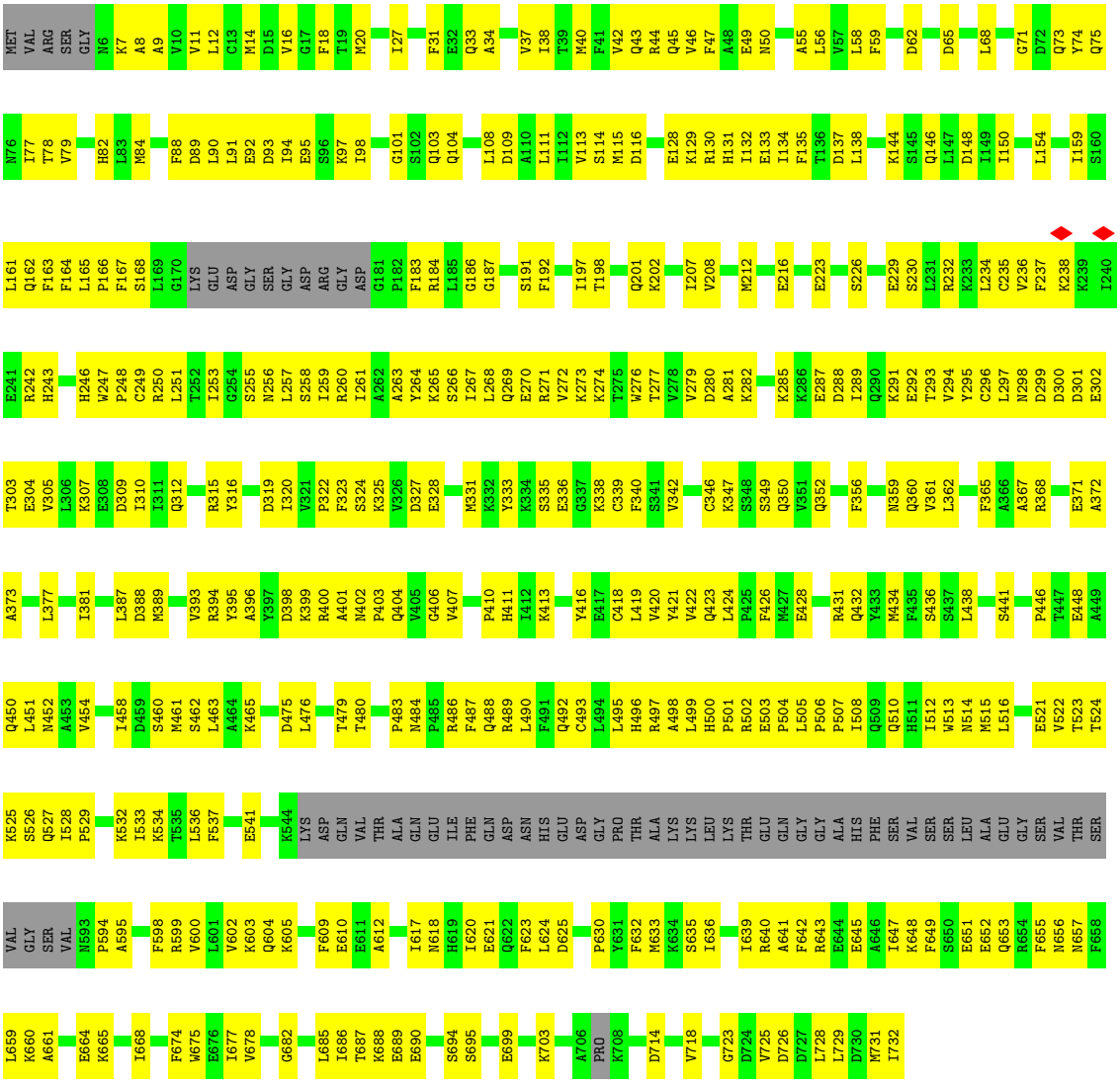





• Molecule 3: X-ray repair cross-complementing protein 5

Chain C:

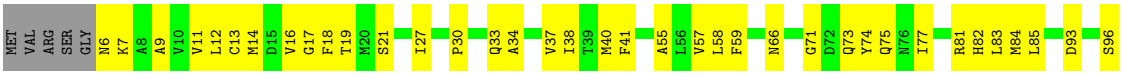


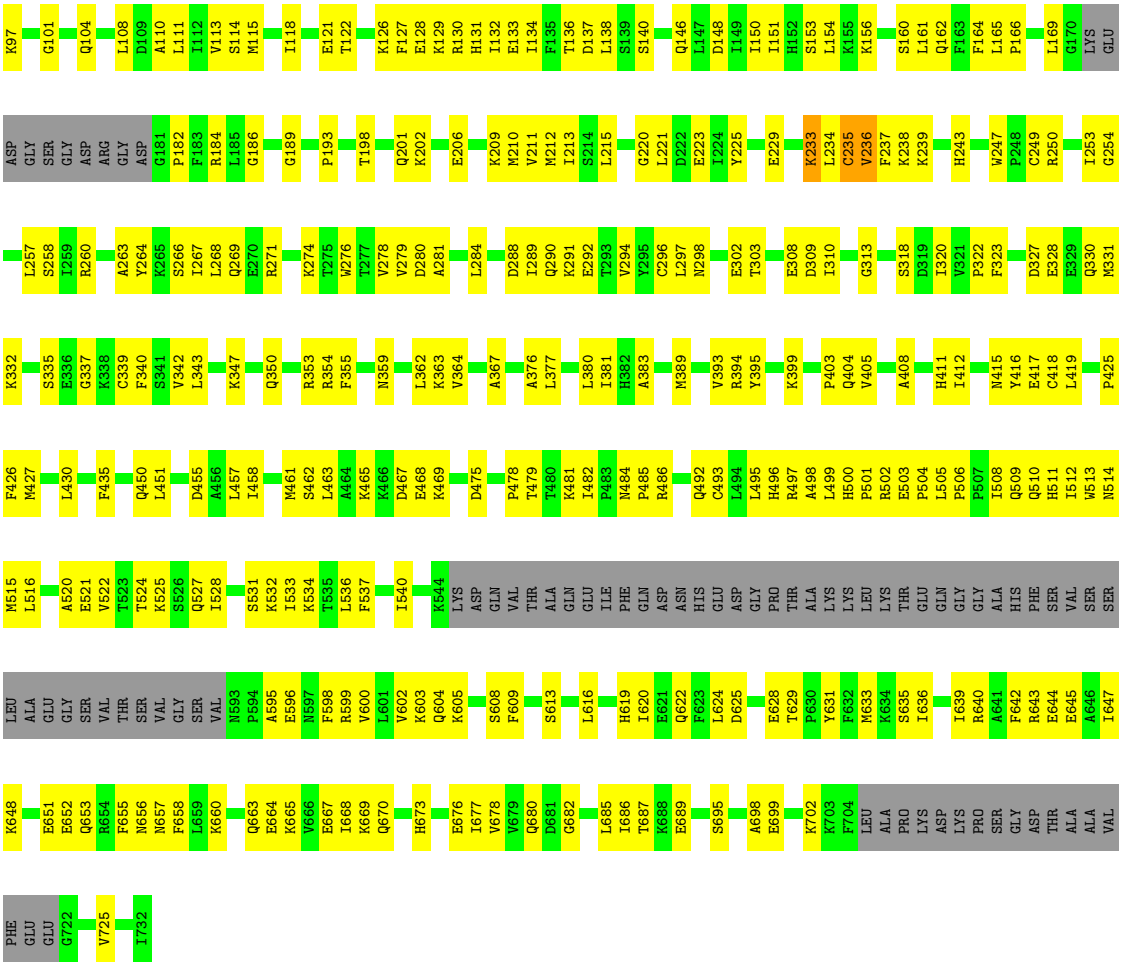



• Molecule 3: X-ray repair cross-complementing protein 5

Chain L:



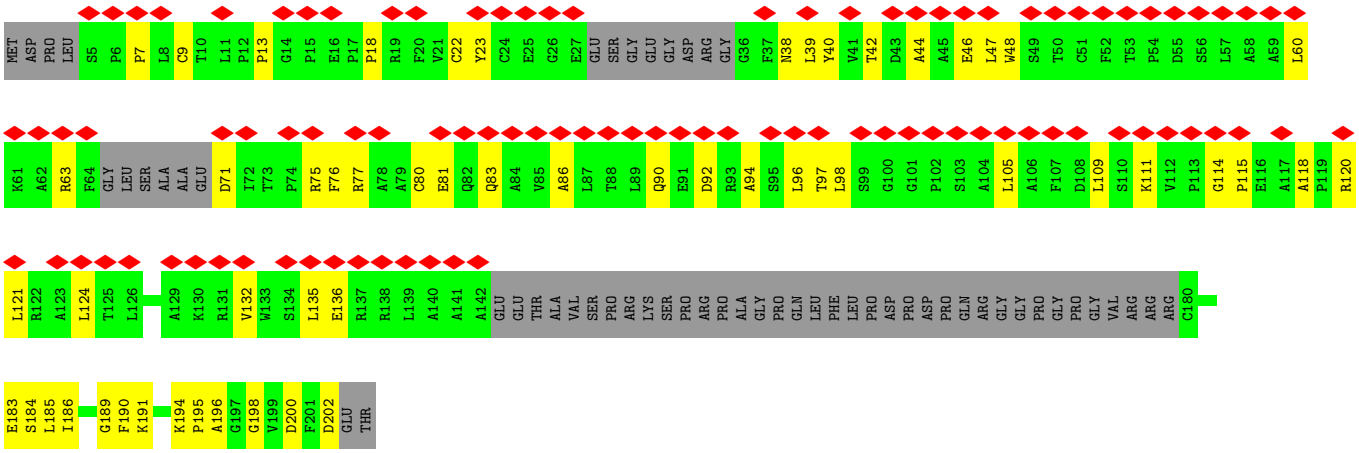





• Molecule 4: Protein PAXX

Chain D:



• Molecule 4: Protein PAXX

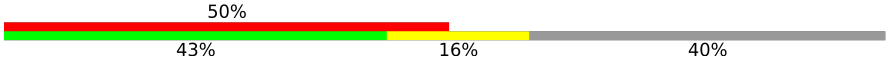
Chain M:

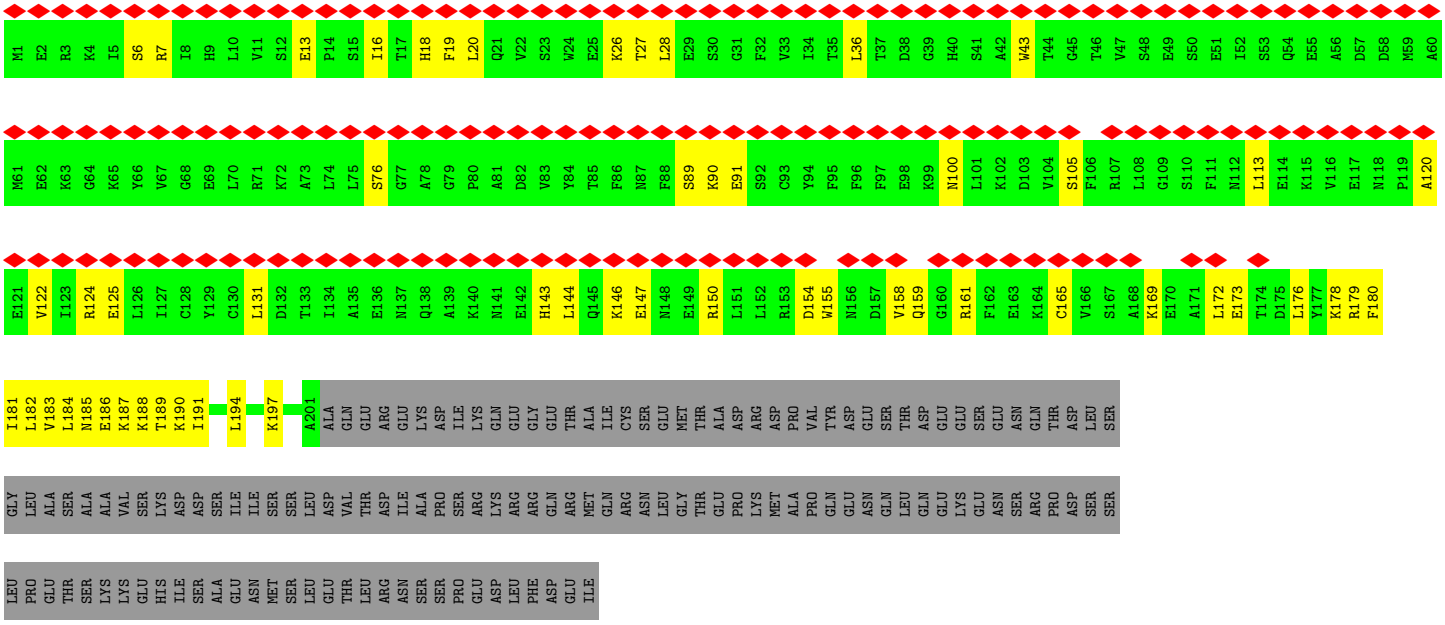





• Molecule 5: DNA repair protein XRCC4

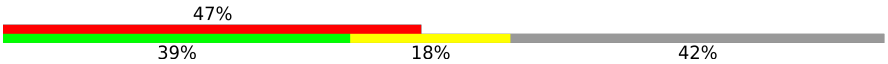
Chain G:

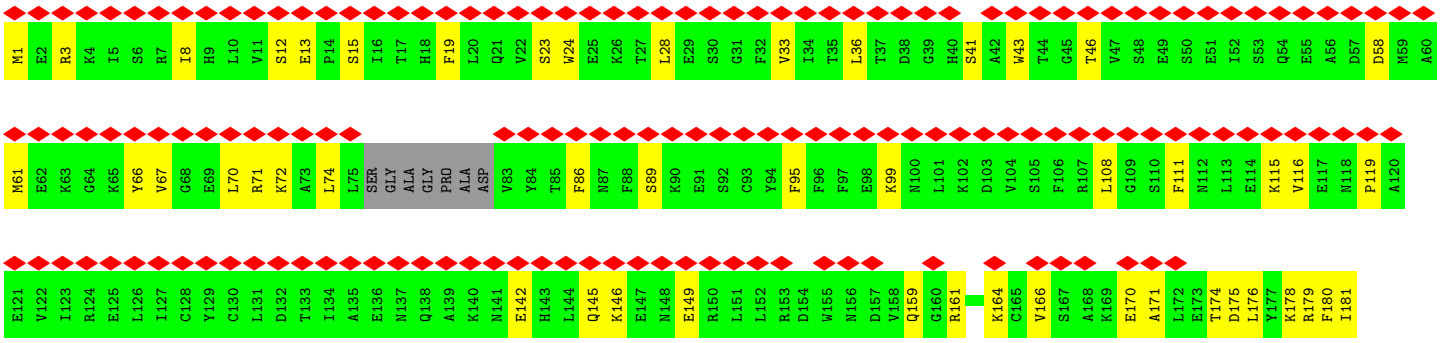


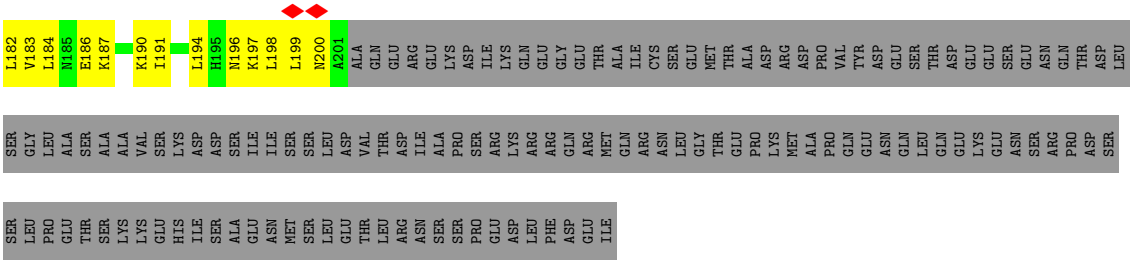




• Molecule 5: DNA repair protein XRCC4

Chain H:

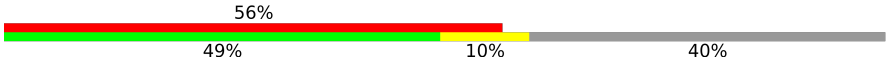


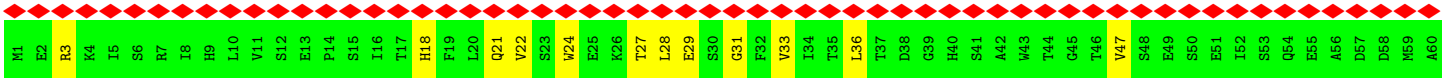



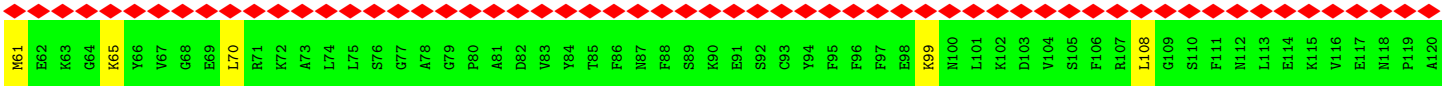


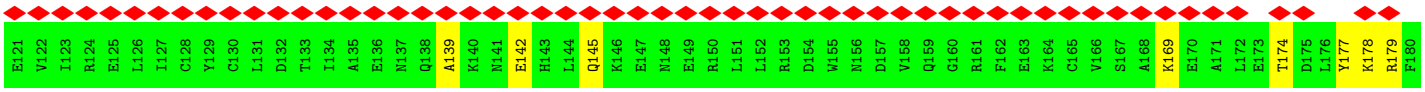

• Molecule 5: DNA repair protein XRCC4

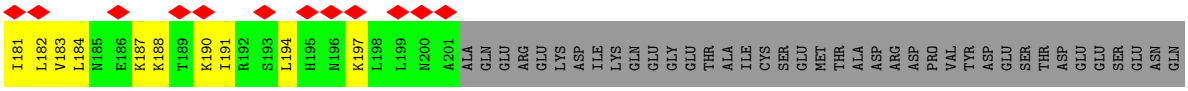
Chain P:



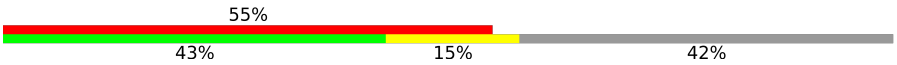



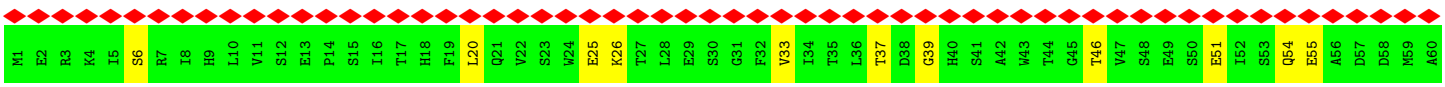



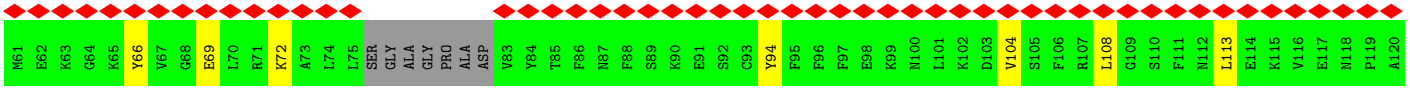



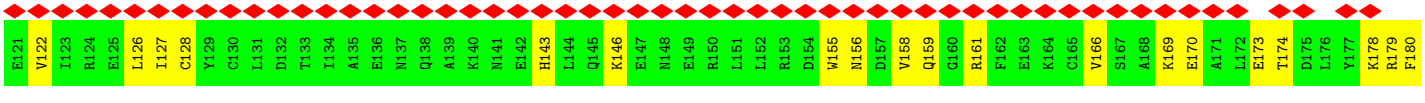

• Molecule 5: DNA repair protein XRCC4

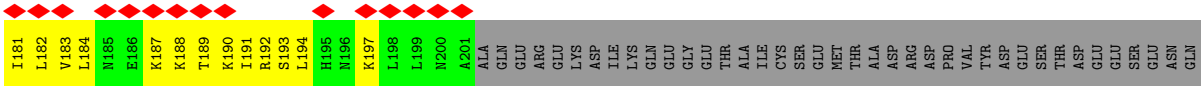
Chain Q:

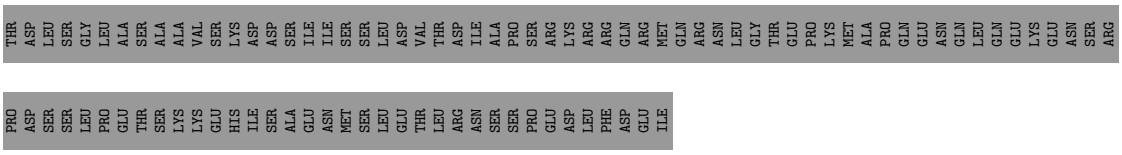


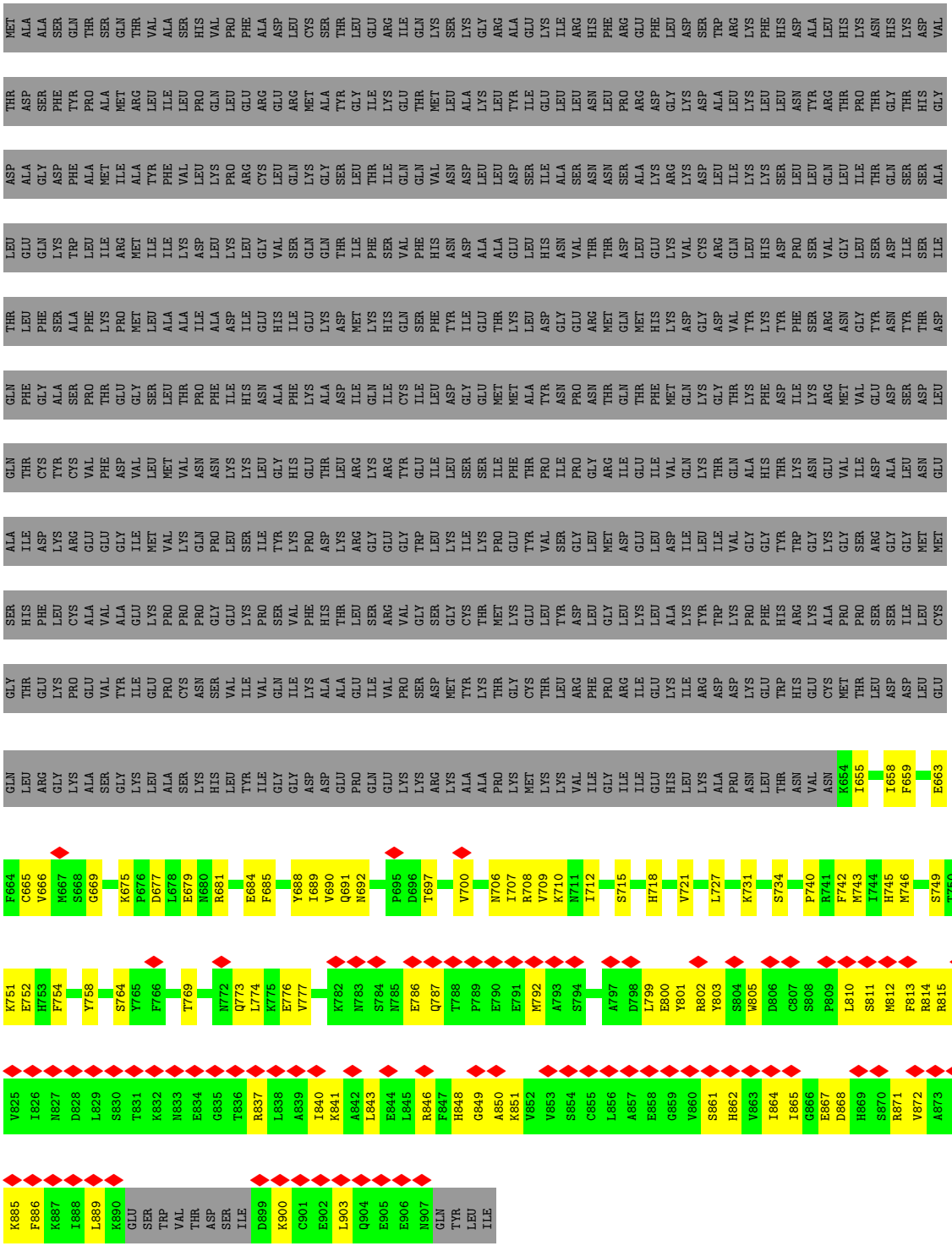






• Molecule 6: DNA ligase 4

Chain I:

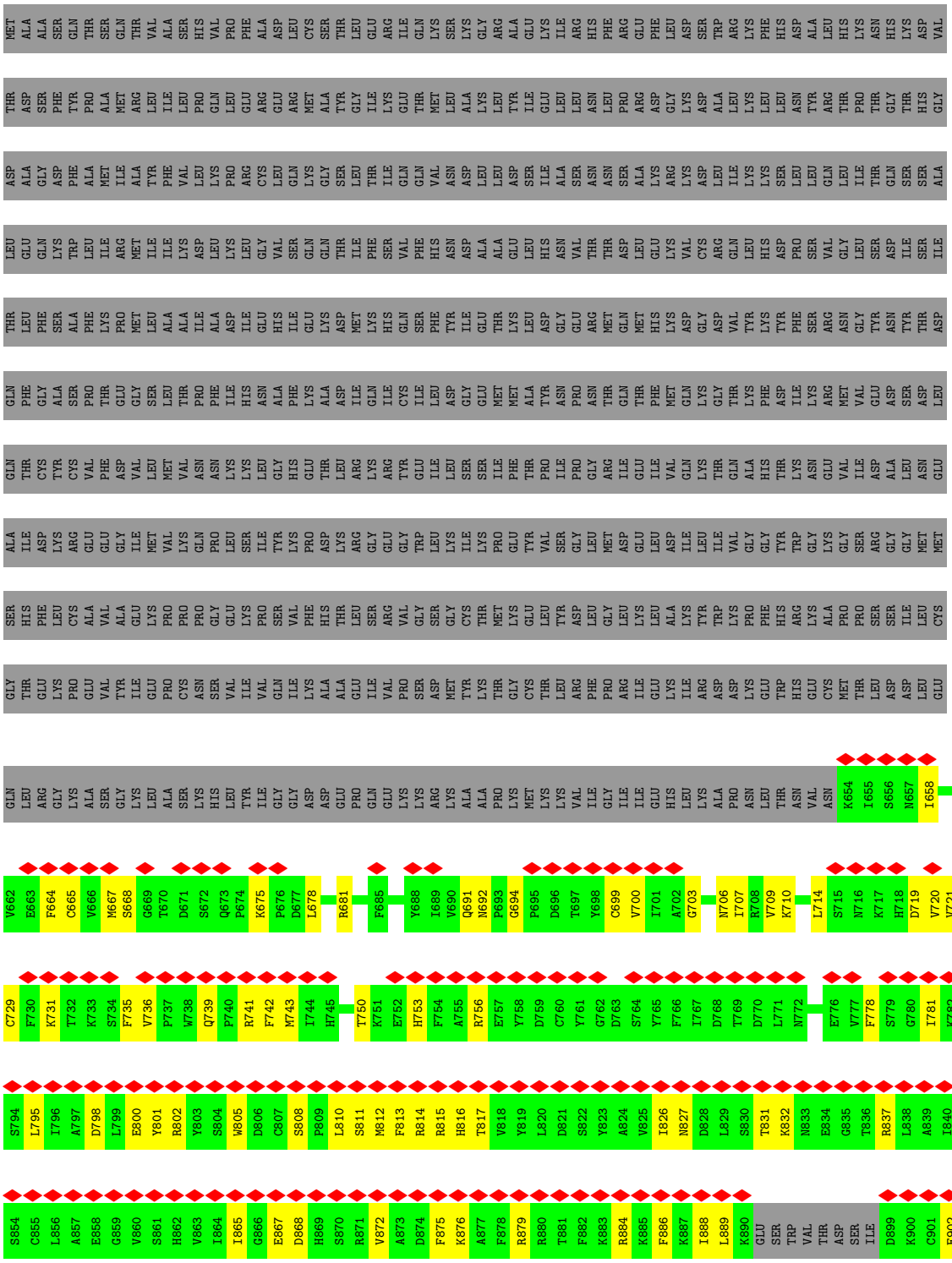


• Molecule 6: DNA ligase 4

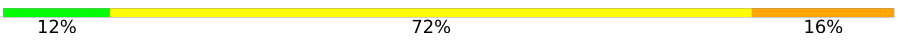
Chain R:




• Molecule 7: DNA (25-MER)

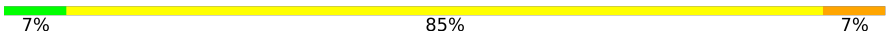
Chain d:






• Molecule 8: DNA (27-MER)

Chain e:

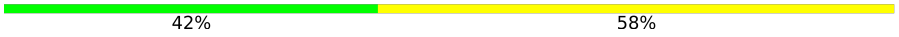


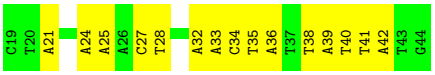




• Molecule 9: DNA (26-MER)

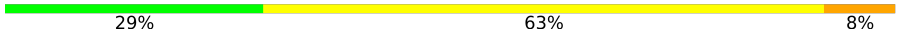
Chain i:




• Molecule 10: DNA (5'-D(P*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*G)-3')

Chain j:

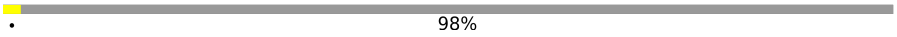






• Molecule 11: Non-homologous end-joining factor 1

Chain f:

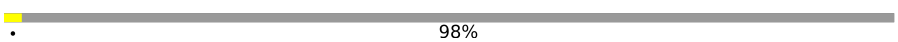


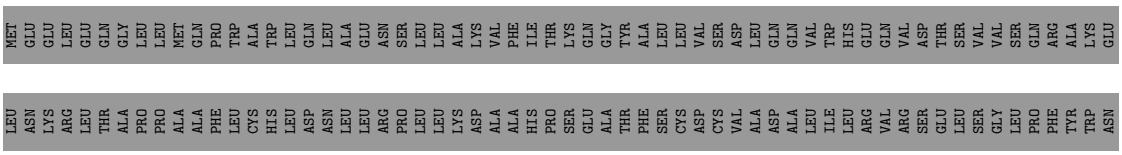


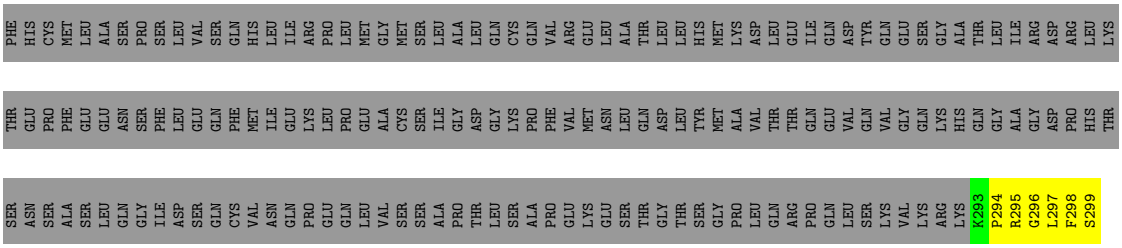


• Molecule 11: Non-homologous end-joining factor 1

Chain m:




PHE HIS CYS MET LEU ALA SER PRO SER LEU VAL SER GLN HIS LEU ILE ARG PRO LEU MET GLY MET SER LEU ALA LEU GLN CYS GLN VAL ARG GLU LEU ALA THR LEU LEU HIS MET LYS ASP LEU GLU ILE GLN ASP TYR GLN GLU SER GLY ALA THR LEU ILE ARG ASP ARG LEU LYS
THR GLU PRO PHE GLU GLU ASN SER PHE LEU GLU GLN GLN PHE MET ILE GLU LYS LEU PRO GLU ALA CYS SER SER ILE GLY ASP GLY LYS PRO PHE VAL MET ASN LEU GLN ASP LEU TYR MET ALA VAL THR THR GLN GLU VAL GLN VAL GLY GLN LYS HIS GLN GLY ALA GLY ASP PRO HIS THR
SER ASN SER ALA SER LEU GLN GLY ILE ASP SER GLN CYS VAL ASN GLN PRO GLU GLN LEU VAL SER SER ALA PRO THR LEU SER ALA PRO GLU LYS GLU SER THR GLY THR SER GLY PRO LEU GLN ARG PRO GLN LEU SER LYS VAL LYS ARG LYS
K293
P294
R295
G296
L297
F298
S299

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 30390 | 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 ($e^-/Å^2$) | 48.03 | Depositor |
| Minimum defocus (nm) | 900 | Depositor |
| Maximum defocus (nm) | 2400 | Depositor |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.544 | Depositor |
| Minimum map value | -0.204 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.016 | Depositor |
| Recommended contour level | 0.045 | Depositor |
| Map size (Å) | 678.08, 678.08, 678.08 | wwPDB |
| Map dimensions | 520, 520, 520 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.304, 1.304, 1.304 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.20 | 0/28856 | 0.44 | 0/38971 |
| 1 | S | 0.16 | 0/28899 | 0.40 | 0/39012 |
| 2 | B | 0.17 | 0/4166 | 0.38 | 0/5615 |
| 2 | T | 0.15 | 0/4116 | 0.35 | 0/5547 |
| 3 | C | 0.15 | 0/5419 | 0.36 | 0/7303 |
| 3 | L | 0.15 | 0/5303 | 0.36 | 1/7147 (0.0%) |
| 4 | D | 0.11 | 0/1128 | 0.30 | 0/1533 |
| 4 | M | 0.10 | 0/1247 | 0.27 | 0/1695 |
| 5 | G | 0.10 | 0/1657 | 0.28 | 0/2228 |
| 5 | H | 0.11 | 0/1616 | 0.27 | 0/2170 |
| 5 | P | 0.11 | 0/1651 | 0.30 | 0/2221 |
| 5 | Q | 0.13 | 0/1607 | 0.34 | 0/2159 |
| 6 | I | 0.12 | 0/2028 | 0.37 | 0/2735 |
| 6 | R | 0.19 | 0/2014 | 0.43 | 0/2719 |
| 7 | d | 0.42 | 0/577 | 0.78 | 4/890 (0.4%) |
| 8 | e | 0.33 | 0/622 | 0.53 | 2/957 (0.2%) |
| 9 | i | 0.23 | 0/597 | 0.41 | 0/918 |
| 10 | j | 0.30 | 0/556 | 0.62 | 2/858 (0.2%) |
| 11 | f | 0.30 | 0/58 | 0.80 | 0/74 |
| 11 | m | 0.17 | 0/58 | 0.60 | 0/74 |
| All | All | 0.18 | 0/92175 | 0.40 | 9/124826 (0.0%) |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | j | 27 | DT | P-O3'-C3' | -8.38 | 107.62 | 120.20 |
| 7 | d | 26 | DT | P-O3'-C3' | -7.36 | 109.16 | 120.20 |
| 7 | d | 21 | DA | P-O3'-C3' | -6.97 | 109.74 | 120.20 |
| 8 | e | 31 | DA | P-O3'-C3' | -6.21 | 110.88 | 120.20 |
| 8 | e | 30 | DA | P-O3'-C3' | -5.75 | 111.58 | 120.20 |
| 10 | j | 26 | DT | P-O3'-C3' | -5.73 | 111.60 | 120.20 |
| 7 | d | 27 | DT | P-O3'-C3' | -5.62 | 111.78 | 120.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | d | 20 | DT | P-O3'-C3' | -5.38 | 112.13 | 120.20 |
| 3 | L | 235 | CYS | N-CA-C | -5.20 | 106.04 | 112.38 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 28300 | 0 | 28587 | 1832 | 0 |
| 1 | S | 28342 | 0 | 28717 | 1599 | 0 |
| 2 | B | 4085 | 0 | 4143 | 352 | 0 |
| 2 | T | 4037 | 0 | 4105 | 258 | 0 |
| 3 | C | 5318 | 0 | 5327 | 369 | 0 |
| 3 | L | 5204 | 0 | 5210 | 279 | 0 |
| 4 | D | 1102 | 0 | 1098 | 43 | 0 |
| 4 | M | 1219 | 0 | 1197 | 32 | 0 |
| 5 | G | 1628 | 0 | 1620 | 39 | 0 |
| 5 | H | 1589 | 0 | 1587 | 55 | 0 |
| 5 | P | 1622 | 0 | 1609 | 27 | 0 |
| 5 | Q | 1580 | 0 | 1567 | 43 | 0 |
| 6 | I | 1984 | 0 | 1940 | 84 | 0 |
| 6 | R | 1970 | 0 | 1916 | 66 | 0 |
| 7 | d | 516 | 0 | 288 | 43 | 0 |
| 8 | e | 554 | 0 | 307 | 54 | 0 |
| 9 | i | 532 | 0 | 296 | 23 | 0 |
| 10 | j | 497 | 0 | 277 | 23 | 0 |
| 11 | f | 57 | 0 | 60 | 16 | 0 |
| 11 | m | 57 | 0 | 60 | 15 | 0 |
| All | All | 90193 | 0 | 89911 | 4936 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (4936) 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) |
|---|---|---|---|
| 3:C:461:MET:HE3 | 3:C:526:SER:HB3 | 1.33 | 1.07 |
| 3:L:236:VAL:HA | 11:m:298:PHE:HA | 1.46 | 0.98 |
| 6:I:814:ARG:H | 6:I:850:ALA:H | 1.19 | 0.91 |
| 1:A:1871:MET:HE1 | 1:A:1940:TYR:HA | 1.49 | 0.91 |
| 1:S:2225:HIS:HB2 | 1:S:2231:PHE:HB2 | 1.51 | 0.90 |
| 1:S:2461:PHE:HB3 | 1:S:2464:HIS:HE2 | 1.37 | 0.90 |
| 1:S:2321:GLU:HG2 | 1:S:2366:LYS:HE3 | 1.52 | 0.89 |
| 1:S:1300:SER:HA | 1:S:1304:HIS:HB2 | 1.54 | 0.88 |
| 3:C:731:MET:H | 1:S:1913:LYS:HG2 | 1.36 | 0.88 |
| 1:S:2436:LEU:HD22 | 1:S:2472:GLN:HB3 | 1.55 | 0.88 |
| 1:S:2122:LEU:HB2 | 1:S:2126:MET:HE2 | 1.56 | 0.87 |
| 3:C:295:TYR:H | 3:C:304:GLU:HG3 | 1.39 | 0.86 |
| 3:L:310:ILE:HD13 | 2:T:296:VAL:HB | 1.58 | 0.85 |
| 1:S:1452:VAL:HG22 | 1:S:1517:LEU:HD11 | 1.59 | 0.85 |
| 1:A:939:MET:HE2 | 1:A:2785:ILE:HD12 | 1.58 | 0.84 |
| 3:L:136:THR:HG22 | 3:L:138:LEU:H | 1.41 | 0.84 |
| 6:R:817:THR:H | 6:R:851:LYS:HG2 | 1.41 | 0.84 |
| 3:C:400:ARG:NH2 | 7:d:33:DA:N3 | 2.26 | 0.83 |
| 1:S:2295:GLN:HE21 | 1:S:2298:GLU:HG3 | 1.42 | 0.83 |
| 1:A:1116:ALA:HB2 | 1:A:1180:GLN:HE22 | 1.43 | 0.83 |
| 3:L:500:HIS:HB3 | 3:L:503:GLU:HB2 | 1.58 | 0.83 |
| 2:B:173:ASP:HB2 | 2:B:216:PHE:HB3 | 1.61 | 0.82 |
| 2:B:75:ILE:HA | 2:B:79:ASP:HB3 | 1.63 | 0.80 |
| 1:A:1196:PRO:HG3 | 1:A:1203:SER:HB2 | 1.62 | 0.80 |
| 2:B:230:ARG:HG3 | 2:B:232:HIS:H | 1.46 | 0.80 |
| 1:S:4064:LEU:HB3 | 1:S:4074:PHE:HE1 | 1.46 | 0.80 |
| 1:A:3692:VAL:HG11 | 1:A:3719:ILE:HG12 | 1.64 | 0.80 |
| 1:S:3577:GLN:HE21 | 1:S:3629:ARG:HB3 | 1.47 | 0.80 |
| 1:A:3817:LEU:HA | 1:A:3820:MET:HE2 | 1.64 | 0.80 |
| 1:A:898:PHE:H | 1:A:902:LYS:HE3 | 1.47 | 0.79 |
| 5:G:161:ARG:NH1 | 5:G:165:CYS:SG | 2.56 | 0.79 |
| 1:S:3301:LEU:HB2 | 1:S:3304:VAL:HA | 1.63 | 0.79 |
| 3:C:323:PHE:HE2 | 3:C:328:GLU:HB3 | 1.47 | 0.79 |
| 1:A:2317:ALA:HA | 1:A:2366:LYS:HE3 | 1.63 | 0.79 |
| 1:A:3183:ILE:HG13 | 1:A:3242:MET:HE3 | 1.64 | 0.79 |
| 3:C:238:LYS:HB3 | 11:f:294:PRO:HG3 | 1.66 | 0.78 |
| 3:L:331:MET:SD | 2:T:489:ASN:ND2 | 2.57 | 0.78 |
| 1:A:1300:SER:HA | 1:A:1304:HIS:HB2 | 1.63 | 0.78 |
| 1:A:2310:VAL:HG21 | 1:A:2359:LYS:HE2 | 1.65 | 0.78 |
| 1:A:2415:LEU:HB2 | 1:A:2420:PHE:HB3 | 1.64 | 0.78 |
| 1:A:2273:GLY:HA2 | 1:A:2276:LEU:HD13 | 1.65 | 0.78 |
| 1:S:2750:GLU:HA | 1:S:2753:ARG:HD2 | 1.64 | 0.78 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3874:ARG:HD3 | 1:S:4126:PRO:HB2 | 1.65 | 0.78 |
| 1:A:3574:ALA:HB2 | 1:A:3684:SER:HB2 | 1.64 | 0.78 |
| 1:A:1076:LEU:HB2 | 1:A:1123:THR:HG22 | 1.65 | 0.77 |
| 1:A:3829:LEU:HB3 | 1:A:3833:ARG:HH11 | 1.49 | 0.77 |
| 3:C:20:MET:HB3 | 3:C:31:PHE:HB2 | 1.64 | 0.77 |
| 1:S:225:LYS:HD2 | 1:S:270:ALA:HB1 | 1.66 | 0.77 |
| 1:A:1574:ASN:HD21 | 1:A:1578:ALA:H | 1.32 | 0.77 |
| 1:A:1820:VAL:HA | 1:A:1824:LEU:HD23 | 1.64 | 0.77 |
| 2:B:204:HIS:HB2 | 2:B:236:SER:H | 1.49 | 0.77 |
| 1:A:3717:VAL:HG21 | 1:A:3746:ARG:HB3 | 1.67 | 0.77 |
| 2:B:291:GLU:HA | 6:I:691:GLN:H | 1.49 | 0.77 |
| 1:S:2470:ARG:HA | 1:S:2473:MET:HE2 | 1.66 | 0.77 |
| 1:A:3729:MET:HE1 | 1:A:3737:ARG:HB2 | 1.66 | 0.77 |
| 1:S:139:ARG:HH22 | 1:S:230:LEU:HD11 | 1.49 | 0.76 |
| 1:A:3240:MET:HB2 | 1:A:3272:TRP:HH2 | 1.49 | 0.76 |
| 2:B:261:LEU:HA | 2:B:345:LEU:HB2 | 1.68 | 0.76 |
| 1:A:4055:ASN:HD22 | 1:A:4058:VAL:HG23 | 1.50 | 0.76 |
| 1:A:3186:ARG:HG2 | 1:A:3238:MET:HE3 | 1.66 | 0.76 |
| 6:I:769:THR:HA | 6:I:773:GLN:HE21 | 1.49 | 0.76 |
| 1:S:380:ASP:O | 1:S:383:PHE:HB3 | 1.86 | 0.76 |
| 2:T:75:ILE:HA | 2:T:79:ASP:HB3 | 1.65 | 0.76 |
| 7:d:36:DG:H22 | 8:e:20:DT:H1' | 1.51 | 0.76 |
| 6:R:812:MET:H | 6:R:848:HIS:HB2 | 1.51 | 0.76 |
| 1:S:301:CYS:HA | 1:S:309:LYS:HA | 1.68 | 0.76 |
| 1:S:4090:ARG:HH22 | 1:S:4106:CYS:HA | 1.51 | 0.76 |
| 1:S:2937:ASP:HB2 | 1:S:3979:LEU:HD22 | 1.68 | 0.75 |
| 3:L:605:LYS:HB2 | 3:L:609:PHE:HZ | 1.51 | 0.75 |
| 2:B:318:ARG:HB2 | 2:B:329:LEU:O | 1.87 | 0.75 |
| 4:D:98:LEU:HB3 | 4:D:105:LEU:HB2 | 1.68 | 0.75 |
| 1:A:3069:MET:HA | 1:A:3075:LYS:HD3 | 1.67 | 0.75 |
| 1:A:3446:VAL:HG22 | 1:A:3450:MET:HE2 | 1.66 | 0.75 |
| 1:S:1868:THR:HA | 1:S:1871:MET:HE2 | 1.68 | 0.75 |
| 1:S:582:THR:HG23 | 1:S:615:ALA:HB3 | 1.69 | 0.75 |
| 1:S:639:ALA:HB2 | 1:S:676:ASN:HB3 | 1.69 | 0.75 |
| 1:A:3820:MET:HE1 | 1:A:3829:LEU:HD11 | 1.67 | 0.75 |
| 1:A:4054:ALA:HA | 1:A:4096:SER:HA | 1.69 | 0.75 |
| 1:A:131:LEU:HB3 | 1:A:177:LEU:HD21 | 1.68 | 0.75 |
| 1:A:3680:LEU:HG | 1:A:3688:SER:HA | 1.68 | 0.75 |
| 2:B:258:ARG:NH2 | 8:e:34:DC:OP2 | 2.20 | 0.75 |
| 3:C:293:THR:HG21 | 3:C:307:LYS:HZ1 | 1.52 | 0.75 |
| 1:S:66:LEU:O | 1:S:70:ARG:HB3 | 1.85 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2102:LYS:NZ | 1:S:2155:GLU:OE2 | 2.20 | 0.75 |
| 1:A:1368:LEU:HA | 1:A:1371:VAL:HG22 | 1.67 | 0.74 |
| 1:A:1685:ASP:HB3 | 1:A:1688:LEU:HG | 1.68 | 0.74 |
| 2:T:172:GLU:HG3 | 2:T:175:PRO:HD3 | 1.69 | 0.74 |
| 1:A:134:LEU:HD11 | 1:A:177:LEU:HD22 | 1.70 | 0.74 |
| 1:S:714:VAL:HA | 1:S:717:LYS:HG2 | 1.70 | 0.74 |
| 7:d:29:DG:H2' | 7:d:30:DT:H71 | 1.68 | 0.74 |
| 1:S:1878:ASP:HB3 | 1:S:1947:CYS:HA | 1.69 | 0.74 |
| 2:T:173:ASP:HB2 | 2:T:216:PHE:HB3 | 1.70 | 0.74 |
| 1:A:1354:GLU:HB3 | 1:A:1357:LYS:HD3 | 1.69 | 0.74 |
| 3:L:620:ILE:HD13 | 3:L:635:SER:HB3 | 1.69 | 0.74 |
| 1:S:958:MET:HB3 | 1:S:961:LEU:HB2 | 1.67 | 0.74 |
| 1:A:36:ARG:O | 1:A:40:GLN:NE2 | 2.20 | 0.74 |
| 1:S:1172:LEU:HD11 | 1:S:1187:SER:HB2 | 1.68 | 0.74 |
| 1:A:2893:LEU:HD11 | 1:A:2922:ARG:HB2 | 1.70 | 0.74 |
| 2:B:165:ARG:NH1 | 4:D:185:LEU:O | 2.20 | 0.74 |
| 1:S:3244:ASP:OD1 | 1:S:3282:ARG:NH2 | 2.20 | 0.73 |
| 1:A:2367:VAL:O | 1:A:2371:PHE:N | 2.21 | 0.73 |
| 3:L:602:VAL:HG11 | 3:L:642:PHE:HE1 | 1.53 | 0.73 |
| 1:S:919:LEU:HG | 1:S:920:THR:HG23 | 1.70 | 0.73 |
| 3:L:596:GLU:HA | 3:L:599:ARG:HD2 | 1.70 | 0.73 |
| 6:R:810:LEU:HD21 | 6:R:848:HIS:HD2 | 1.54 | 0.73 |
| 1:A:956:PRO:HA | 1:A:959:TYR:HB2 | 1.71 | 0.73 |
| 1:A:1365:ASN:HD21 | 1:A:1370:ARG:HH22 | 1.36 | 0.73 |
| 2:T:59:PRO:HB3 | 2:T:205:LEU:HD21 | 1.71 | 0.73 |
| 1:A:162:LEU:HB2 | 2:B:301:ARG:HH21 | 1.53 | 0.73 |
| 1:A:1620:THR:HG22 | 1:A:1624:GLN:HE22 | 1.53 | 0.73 |
| 3:C:162:GLN:HG2 | 3:C:223:GLU:HB3 | 1.70 | 0.73 |
| 1:S:318:SER:O | 1:S:322:GLN:NE2 | 2.22 | 0.73 |
| 2:T:458:GLN:HE21 | 2:T:528:LEU:HB3 | 1.52 | 0.73 |
| 1:A:3613:MET:O | 1:A:3617:LEU:N | 2.21 | 0.73 |
| 1:A:2254:ARG:HD3 | 1:A:2294:ILE:HG12 | 1.70 | 0.73 |
| 1:A:2411:LEU:HA | 1:A:2414:GLN:HG2 | 1.70 | 0.73 |
| 1:A:3755:GLY:HA2 | 1:A:3799:ARG:HA | 1.71 | 0.73 |
| 2:T:42:VAL:HA | 2:T:169:PHE:HB2 | 1.70 | 0.73 |
| 2:B:35:ARG:O | 2:B:162:SER:N | 2.22 | 0.73 |
| 1:S:3681:LYS:HG3 | 1:S:3724:GLU:HG2 | 1.70 | 0.73 |
| 2:B:299:LYS:HD2 | 2:B:301:ARG:HH22 | 1.53 | 0.73 |
| 3:L:510:GLN:HA | 3:L:513:TRP:HD1 | 1.54 | 0.73 |
| 3:L:653:GLN:O | 3:L:657:ASN:ND2 | 2.22 | 0.73 |
| 1:S:645:TRP:HB3 | 1:S:649:PHE:HB2 | 1.71 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2441:LYS:O | 1:A:2445:LYS:NZ | 2.22 | 0.72 |
| 3:C:687:THR:HG22 | 3:C:688:LYS:H | 1.54 | 0.72 |
| 1:A:3945:ALA:HB3 | 1:A:3948:SER:HB3 | 1.71 | 0.72 |
| 1:A:4049:ARG:HH21 | 1:A:4058:VAL:HG12 | 1.55 | 0.72 |
| 2:B:496:ASP:OD1 | 6:I:708:ARG:NH2 | 2.21 | 0.72 |
| 1:S:3018:SER:HB2 | 1:S:3031:TRP:HE1 | 1.53 | 0.72 |
| 1:A:3417:ALA:HA | 1:A:3446:VAL:HG23 | 1.69 | 0.72 |
| 2:B:256:LEU:HD13 | 2:B:274:TYR:HA | 1.72 | 0.72 |
| 1:A:2218:PHE:O | 1:A:2222:HIS:ND1 | 2.21 | 0.72 |
| 2:B:389:CYS:HA | 2:B:392:LYS:HB2 | 1.69 | 0.72 |
| 1:S:100:ILE:O | 1:S:104:SER:N | 2.23 | 0.72 |
| 1:A:236:LYS:NZ | 1:A:240:GLU:OE2 | 2.22 | 0.72 |
| 1:A:960:GLN:HA | 1:A:963:LYS:HE2 | 1.71 | 0.71 |
| 1:A:1095:LEU:O | 1:A:1099:PHE:N | 2.23 | 0.71 |
| 1:A:1296:PHE:HA | 1:A:1299:GLU:HG2 | 1.72 | 0.71 |
| 1:A:1649:LEU:HD13 | 1:A:1652:ILE:HD11 | 1.70 | 0.71 |
| 2:B:94:LYS:H | 2:B:103:TYR:HA | 1.54 | 0.71 |
| 2:B:302:THR:HA | 3:C:291:LYS:HA | 1.71 | 0.71 |
| 1:S:2383:PHE:HB3 | 1:S:2418:LYS:HE3 | 1.72 | 0.71 |
| 1:S:2938:VAL:HG23 | 1:S:3979:LEU:HD23 | 1.70 | 0.71 |
| 1:A:392:CYS:HA | 1:A:395:MET:HG3 | 1.72 | 0.71 |
| 2:B:337:LEU:HA | 3:C:489:ARG:HE | 1.52 | 0.71 |
| 1:S:1851:LEU:HG | 1:S:1852:LYS:HE2 | 1.72 | 0.71 |
| 7:d:17:DT:H3 | 8:e:41:DT:H3 | 1.38 | 0.71 |
| 1:A:380:ASP:HB3 | 1:A:384:MET:HE1 | 1.72 | 0.71 |
| 1:A:3114:TYR:HA | 1:A:3117:ILE:HG12 | 1.71 | 0.71 |
| 2:B:403:ARG:HD3 | 8:e:31:DA:H4' | 1.72 | 0.71 |
| 1:A:332:GLU:HB2 | 1:A:335:LYS:HD2 | 1.72 | 0.71 |
| 6:I:811:SER:HB2 | 6:I:850:ALA:HB2 | 1.73 | 0.71 |
| 1:S:2820:MET:HE2 | 1:S:2824:LYS:HG3 | 1.72 | 0.71 |
| 1:A:3686:TRP:HA | 1:A:3690:PHE:HB3 | 1.72 | 0.71 |
| 1:A:3758:LEU:HB2 | 1:A:3795:PRO:HB3 | 1.72 | 0.71 |
| 3:L:253:ILE:HB | 3:L:257:LEU:HB3 | 1.72 | 0.71 |
| 3:L:689:GLU:HA | 3:L:695:SER:HB3 | 1.73 | 0.71 |
| 4:M:75:ARG:NH2 | 4:M:103:SER:O | 2.23 | 0.71 |
| 1:S:1428:ILE:HG13 | 1:S:1431:LEU:HD12 | 1.73 | 0.71 |
| 1:S:1635:LYS:HD3 | 1:S:1683:LYS:HE3 | 1.71 | 0.71 |
| 9:i:21:DA:OP1 | 10:j:36:DG:N2 | 2.24 | 0.71 |
| 1:A:391:ARG:NH1 | 1:A:391:ARG:O | 2.24 | 0.71 |
| 1:A:3588:TRP:HB2 | 1:A:3613:MET:HE3 | 1.73 | 0.71 |
| 1:S:3864:ARG:HE | 1:S:4085:LYS:HA | 1.55 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3142:ILE:O | 1:A:3147:LYS:NZ | 2.23 | 0.71 |
| 5:P:31:GLY:HA2 | 5:P:47:VAL:HB | 1.72 | 0.71 |
| 1:A:3459:ASN:OD1 | 1:A:3708:ARG:NH1 | 2.24 | 0.71 |
| 1:A:3704:GLN:NE2 | 1:A:3804:GLU:OE1 | 2.24 | 0.71 |
| 3:C:236:VAL:HA | 11:f:298:PHE:HA | 1.70 | 0.71 |
| 3:L:380:LEU:HA | 2:T:462:MET:HE1 | 1.73 | 0.71 |
| 1:A:749:VAL:O | 1:A:753:GLN:NE2 | 2.23 | 0.70 |
| 3:C:407:VAL:HB | 3:C:424:LEU:HD11 | 1.72 | 0.70 |
| 3:L:426:PHE:HB3 | 2:T:479:GLU:HA | 1.73 | 0.70 |
| 1:A:628:GLU:O | 1:A:631:ARG:HG3 | 1.91 | 0.70 |
| 2:B:258:ARG:O | 2:B:260:LYS:NZ | 2.24 | 0.70 |
| 2:B:396:ALA:HB3 | 2:B:413:LEU:HB2 | 1.74 | 0.70 |
| 2:T:74:LYS:NZ | 2:T:110:ASN:OD1 | 2.25 | 0.70 |
| 1:A:61:ARG:HB2 | 1:A:103:TYR:HE2 | 1.56 | 0.70 |
| 1:A:2956:ALA:HB2 | 1:A:2971:GLN:HB2 | 1.73 | 0.70 |
| 4:D:42:THR:HG22 | 4:D:44:ALA:H | 1.53 | 0.70 |
| 1:A:2528:GLU:HG3 | 1:A:2532:PRO:HA | 1.71 | 0.70 |
| 1:A:2563:LEU:HD13 | 1:A:2795:GLN:HB3 | 1.73 | 0.70 |
| 1:A:3311:ASN:HB3 | 1:A:3314:SER:HA | 1.72 | 0.70 |
| 1:A:487:LEU:HD11 | 1:A:575:ILE:HG21 | 1.74 | 0.70 |
| 1:A:640:GLU:HA | 1:A:643:GLU:HB2 | 1.73 | 0.70 |
| 2:T:111:PRO:HA | 2:T:115:ARG:HD3 | 1.74 | 0.70 |
| 1:A:38:LEU:HD21 | 1:A:85:ILE:HG13 | 1.73 | 0.70 |
| 5:P:27:THR:HG22 | 5:P:29:GLU:H | 1.57 | 0.70 |
| 1:S:1397:ASP:OD1 | 1:S:1398:VAL:N | 2.23 | 0.70 |
| 1:A:87:LYS:NZ | 1:A:829:VAL:O | 2.24 | 0.70 |
| 1:A:1684:LEU:O | 1:A:1689:LYS:NZ | 2.25 | 0.70 |
| 3:C:327:ASP:O | 3:C:331:MET:HG2 | 1.92 | 0.70 |
| 1:S:1651:LYS:NZ | 1:S:2045:PHE:O | 2.25 | 0.70 |
| 6:I:814:ARG:H | 6:I:850:ALA:N | 1.88 | 0.69 |
| 3:L:247:TRP:HB3 | 3:L:263:ALA:HB3 | 1.74 | 0.69 |
| 1:S:460:ALA:HA | 1:S:463:LYS:HD2 | 1.74 | 0.69 |
| 3:C:115:MET:HE1 | 3:C:132:ILE:HG21 | 1.72 | 0.69 |
| 3:C:657:ASN:HA | 3:C:660:LYS:HD2 | 1.74 | 0.69 |
| 2:T:147:LEU:HD13 | 2:T:189:LYS:HB3 | 1.72 | 0.69 |
| 1:A:1646:LEU:HD11 | 1:A:1692:ALA:HB2 | 1.75 | 0.69 |
| 1:A:3266:SER:HA | 1:A:3272:TRP:HD1 | 1.57 | 0.69 |
| 1:S:939:MET:HE3 | 1:S:2783:ILE:HD13 | 1.74 | 0.69 |
| 1:A:1215:GLU:HG3 | 1:A:1219:PHE:HB2 | 1.75 | 0.69 |
| 1:A:2379:MET:HE1 | 1:A:2404:ARG:HG3 | 1.74 | 0.69 |
| 1:A:3771:MET:HA | 1:A:3774:ILE:HD12 | 1.74 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1419:LEU:HD21 | 1:S:1467:ILE:HB | 1.74 | 0.69 |
| 1:A:3259:LEU:HD11 | 1:A:3283:LEU:HD23 | 1.74 | 0.69 |
| 1:A:3584:LEU:HD22 | 1:A:3799:ARG:HD3 | 1.74 | 0.69 |
| 5:P:99:LYS:HE3 | 5:P:108:LEU:HD11 | 1.73 | 0.69 |
| 3:L:74:TYR:HD1 | 3:L:113:VAL:HG23 | 1.57 | 0.69 |
| 3:L:169:LEU:HD21 | 3:L:225:TYR:HA | 1.75 | 0.69 |
| 5:Q:181:ILE:HG21 | 6:R:795:LEU:HD11 | 1.74 | 0.69 |
| 1:S:2349:LEU:HB3 | 1:S:2360:PHE:HE1 | 1.56 | 0.69 |
| 1:S:3029:LYS:N | 1:S:3074:GLN:OE1 | 2.25 | 0.69 |
| 1:S:3464:LYS:HG3 | 1:S:3468:LEU:HG | 1.74 | 0.69 |
| 1:A:1420:ARG:NH2 | 1:A:1466:ASN:O | 2.23 | 0.69 |
| 1:A:3880:ALA:HB2 | 1:A:3965:ARG:HE | 1.58 | 0.69 |
| 2:B:214:SER:HA | 2:B:218:ARG:HB3 | 1.74 | 0.69 |
| 2:B:480:ASN:HD22 | 2:B:483:LEU:HG | 1.56 | 0.69 |
| 2:B:441:ASP:O | 2:B:444:ARG:NH1 | 2.26 | 0.69 |
| 1:A:2388:LYS:HE2 | 2:B:155:SER:HA | 1.75 | 0.69 |
| 1:S:1070:PRO:HG3 | 1:S:3743:HIS:CD2 | 2.28 | 0.69 |
| 2:B:269:ILE:HG23 | 2:B:378:SER:HB2 | 1.74 | 0.68 |
| 1:A:3716:HIS:O | 1:A:3718:ARG:NH1 | 2.26 | 0.68 |
| 6:I:814:ARG:HB3 | 6:I:849:GLY:HA2 | 1.74 | 0.68 |
| 3:L:496:HIS:O | 3:L:500:HIS:N | 2.27 | 0.68 |
| 1:S:1184:ARG:HE | 1:S:1262:ALA:HB1 | 1.57 | 0.68 |
| 1:S:2461:PHE:HB3 | 1:S:2464:HIS:NE2 | 2.07 | 0.68 |
| 1:S:3126:LEU:O | 1:S:3130:GLN:NE2 | 2.26 | 0.68 |
| 1:S:3720:ALA:HB3 | 1:S:3743:HIS:HA | 1.75 | 0.68 |
| 1:A:155:LYS:NZ | 1:A:159:GLU:OE1 | 2.25 | 0.68 |
| 1:S:1282:LEU:HD12 | 1:S:1359:LEU:HD13 | 1.74 | 0.68 |
| 1:S:2522:ARG:NH2 | 1:S:2795:GLN:OE1 | 2.26 | 0.68 |
| 1:A:391:ARG:NH1 | 1:A:394:GLN:OE1 | 2.24 | 0.68 |
| 1:A:1270:PHE:HB3 | 1:A:1276:VAL:HB | 1.74 | 0.68 |
| 4:M:47:LEU:HD23 | 4:M:112:VAL:HG11 | 1.74 | 0.68 |
| 1:A:188:GLU:O | 1:A:192:ASN:ND2 | 2.26 | 0.68 |
| 1:A:2251:ILE:HD11 | 1:A:2285:LEU:HD13 | 1.76 | 0.68 |
| 1:S:3603:LYS:HG2 | 1:S:3647:GLY:H | 1.59 | 0.68 |
| 1:S:4106:CYS:SG | 1:S:4110:GLN:NE2 | 2.66 | 0.68 |
| 1:A:2140:LEU:HD23 | 1:A:2143:ARG:HD2 | 1.76 | 0.68 |
| 1:S:22:ALA:HA | 1:S:24:ARG:HH11 | 1.57 | 0.68 |
| 1:S:655:LEU:O | 1:S:659:ARG:NH1 | 2.26 | 0.68 |
| 1:A:1403:MET:HA | 1:A:1406:LEU:HD12 | 1.76 | 0.68 |
| 2:B:500:PRO:O | 2:B:502:GLN:NE2 | 2.27 | 0.68 |
| 2:B:537:GLU:OE1 | 3:C:250:ARG:NH1 | 2.27 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1412:LYS:O | 1:S:1416:GLU:N | 2.23 | 0.68 |
| 1:A:3040:TYR:HB3 | 1:A:3044:MET:HE3 | 1.73 | 0.68 |
| 3:C:643:ARG:HE | 3:C:685:LEU:HB3 | 1.59 | 0.68 |
| 1:S:923:ASP:O | 1:S:926:THR:N | 2.25 | 0.68 |
| 1:A:2760:GLU:HA | 1:A:2763:MET:HG3 | 1.75 | 0.68 |
| 1:A:3482:LEU:O | 1:A:3485:LYS:NZ | 2.27 | 0.68 |
| 4:D:60:LEU:HD13 | 4:D:63:ARG:HD3 | 1.74 | 0.68 |
| 5:G:191:ILE:HG13 | 5:H:191:ILE:HD11 | 1.76 | 0.68 |
| 3:L:427:MET:HE3 | 2:T:479:GLU:HB3 | 1.75 | 0.68 |
| 1:S:125:ILE:HA | 1:S:128:LEU:HD12 | 1.76 | 0.68 |
| 1:S:1087:ARG:HG3 | 1:S:1090:ARG:HH21 | 1.59 | 0.68 |
| 1:S:3266:SER:HA | 1:S:3272:TRP:CD1 | 2.28 | 0.68 |
| 1:S:4082:ARG:NH2 | 1:S:4092:GLN:OE1 | 2.27 | 0.68 |
| 2:T:82:LEU:HB3 | 2:T:108:LEU:HB3 | 1.77 | 0.68 |
| 2:T:258:ARG:NH2 | 9:i:35:DT:OP2 | 2.27 | 0.68 |
| 1:A:117:LYS:NZ | 3:C:302:GLU:OE1 | 2.26 | 0.67 |
| 1:A:2102:LYS:HZ3 | 1:A:2155:GLU:HG2 | 1.60 | 0.67 |
| 1:A:2229:ALA:O | 1:A:2731:ARG:NH2 | 2.26 | 0.67 |
| 3:C:362:LEU:HB2 | 3:C:421:TYR:HB3 | 1.76 | 0.67 |
| 4:D:18:PRO:HG3 | 4:M:130:LYS:HB3 | 1.73 | 0.67 |
| 1:S:2442:MET:HG3 | 1:S:2446:LEU:HD11 | 1.77 | 0.67 |
| 1:A:19:LEU:HD22 | 1:A:34:LEU:HA | 1.75 | 0.67 |
| 1:A:958:MET:O | 1:A:962:TYR:N | 2.23 | 0.67 |
| 3:L:11:VAL:HG23 | 3:L:55:ALA:HB3 | 1.76 | 0.67 |
| 3:L:225:TYR:HB2 | 11:m:298:PHE:HE2 | 1.58 | 0.67 |
| 1:S:1066:LEU:HA | 1:S:1069:HIS:CD2 | 2.29 | 0.67 |
| 1:S:4055:ASN:HB2 | 1:S:4095:GLU:HA | 1.75 | 0.67 |
| 1:A:3179:TRP:HE3 | 1:A:3242:MET:HE1 | 1.58 | 0.67 |
| 1:A:149:ILE:O | 1:A:153:PHE:N | 2.24 | 0.67 |
| 1:A:675:ARG:NH2 | 1:A:735:SER:O | 2.26 | 0.67 |
| 1:A:1525:CYS:HB3 | 1:A:1578:ALA:HB2 | 1.76 | 0.67 |
| 1:A:3118:ASP:HB3 | 1:A:3120:LEU:HG | 1.75 | 0.67 |
| 1:A:3717:VAL:HA | 1:A:3743:HIS:HB3 | 1.75 | 0.67 |
| 3:L:82:HIS:HB2 | 3:L:84:MET:HE1 | 1.76 | 0.67 |
| 1:S:1117:ASP:OD1 | 1:S:1118:GLU:N | 2.27 | 0.67 |
| 1:A:777:SER:HA | 1:A:785:MET:HE1 | 1.75 | 0.67 |
| 1:A:3737:ARG:NH2 | 1:A:3807:GLU:OE2 | 2.28 | 0.67 |
| 1:A:3813:LYS:HZ3 | 1:A:3925:LEU:HB3 | 1.58 | 0.67 |
| 1:A:4105:LYS:HA | 1:A:4108:MET:HE3 | 1.77 | 0.67 |
| 1:S:2512:ASP:H | 1:S:2518:GLN:HE21 | 1.42 | 0.67 |
| 1:S:2731:ARG:HA | 1:S:2733:MET:HE1 | 1.75 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3593:ARG:NH2 | 1:S:3664:ASN:OD1 | 2.28 | 0.67 |
| 1:A:708:VAL:HG12 | 1:A:740:ILE:HG23 | 1.77 | 0.67 |
| 1:A:3587:ASP:HB2 | 1:A:3799:ARG:HH21 | 1.60 | 0.67 |
| 1:S:1220:LEU:HB2 | 1:S:1285:GLU:HB2 | 1.75 | 0.67 |
| 2:T:35:ARG:NH1 | 2:T:80:ARG:O | 2.28 | 0.67 |
| 2:T:106:GLN:NE2 | 2:T:118:GLU:OE2 | 2.27 | 0.67 |
| 2:T:514:MET:HE3 | 2:T:518:LEU:HD11 | 1.74 | 0.67 |
| 2:B:469:LEU:HD11 | 2:B:518:LEU:HD11 | 1.74 | 0.67 |
| 3:C:510:GLN:HA | 3:C:513:TRP:HD1 | 1.59 | 0.67 |
| 1:S:584:GLU:N | 1:S:613:HIS:O | 2.28 | 0.67 |
| 1:A:1663:THR:HG22 | 1:A:1664:SER:H | 1.59 | 0.67 |
| 1:A:3833:ARG:HH21 | 1:A:4127:TRP:HE1 | 1.43 | 0.67 |
| 3:C:162:GLN:HE21 | 3:C:223:GLU:HA | 1.60 | 0.67 |
| 3:C:272:VAL:HG22 | 3:C:274:LYS:H | 1.59 | 0.67 |
| 1:S:382:ASP:HA | 1:S:385:TYR:HB3 | 1.76 | 0.67 |
| 1:S:1512:SER:HA | 1:S:1515:LEU:HD12 | 1.77 | 0.67 |
| 1:S:3172:LYS:H | 1:S:3179:TRP:HZ2 | 1.42 | 0.67 |
| 1:A:892:LEU:HG | 1:A:907:LEU:HB2 | 1.77 | 0.67 |
| 2:B:505:ASP:OD2 | 3:C:394:ARG:NH1 | 2.27 | 0.67 |
| 1:S:2335:ASN:HD21 | 1:S:2337:LEU:HD23 | 1.58 | 0.67 |
| 1:A:1923:PHE:HD1 | 1:A:1941:HIS:HB3 | 1.60 | 0.67 |
| 1:A:3462:ARG:HH12 | 1:A:3495:PHE:H | 1.41 | 0.67 |
| 2:B:289:TYR:HE2 | 2:B:291:GLU:HG2 | 1.59 | 0.67 |
| 1:S:2257:PHE:HA | 1:S:2260:PHE:CE2 | 2.30 | 0.67 |
| 1:S:2452:ARG:HB3 | 1:S:2498:ILE:HG13 | 1.76 | 0.67 |
| 1:A:174:VAL:O | 1:A:177:LEU:HB2 | 1.95 | 0.66 |
| 1:A:1047:GLN:O | 1:A:1051:LYS:HB2 | 1.94 | 0.66 |
| 2:B:91:GLU:OE1 | 2:B:137:HIS:N | 2.27 | 0.66 |
| 1:S:1417:THR:O | 1:S:1421:GLU:N | 2.28 | 0.66 |
| 1:A:2820:MET:HE2 | 1:A:2824:LYS:HG3 | 1.77 | 0.66 |
| 1:S:2190:VAL:HA | 1:S:2193:ILE:HD12 | 1.75 | 0.66 |
| 1:A:1456:LYS:HG3 | 1:A:1460:ARG:HE | 1.60 | 0.66 |
| 1:S:2425:ARG:NH1 | 1:S:2457:PRO:O | 2.28 | 0.66 |
| 1:A:3066:ASP:HA | 1:A:3069:MET:HE3 | 1.76 | 0.66 |
| 1:A:3448:GLU:HG2 | 1:A:3482:LEU:HD13 | 1.78 | 0.66 |
| 1:S:1586:SER:HB2 | 1:S:1632:TRP:HH2 | 1.60 | 0.66 |
| 1:A:212:VAL:O | 2:B:404:ARG:NH1 | 2.29 | 0.66 |
| 2:B:289:TYR:CE2 | 2:B:291:GLU:HG2 | 2.31 | 0.66 |
| 3:C:260:ARG:HB3 | 3:C:367:ALA:HB3 | 1.77 | 0.66 |
| 1:S:3029:LYS:N | 1:S:3032:SER:HG | 1.93 | 0.66 |
| 1:A:3259:LEU:O | 1:A:3276:TRP:NE1 | 2.29 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:524:THR:HA | 3:C:527:GLN:HG2 | 1.78 | 0.66 |
| 3:L:647:ILE:HA | 3:L:652:GLU:HG2 | 1.77 | 0.66 |
| 1:S:2094:MET:HA | 1:S:2097:LEU:HD13 | 1.77 | 0.66 |
| 1:S:2348:GLN:HA | 1:S:2351:GLN:HB2 | 1.78 | 0.66 |
| 1:A:3737:ARG:HH12 | 1:A:3749:PRO:HA | 1.60 | 0.66 |
| 1:A:3781:CYS:O | 1:A:3785:ALA:N | 2.28 | 0.66 |
| 2:B:351:LYS:NZ | 3:C:475:ASP:OD1 | 2.29 | 0.66 |
| 3:C:723:GLY:O | 3:C:726:ASP:HB3 | 1.95 | 0.66 |
| 2:T:403:ARG:HD3 | 9:i:32:DA:H4' | 1.78 | 0.66 |
| 1:A:2577:PHE:HD2 | 1:A:2783:ILE:HG21 | 1.61 | 0.66 |
| 1:A:3053:LEU:HD11 | 1:A:3088:LEU:HB3 | 1.77 | 0.66 |
| 1:A:3236:PHE:HB3 | 1:A:3272:TRP:CE2 | 2.30 | 0.66 |
| 1:S:2208:ASP:OD1 | 1:S:2209:GLU:N | 2.29 | 0.66 |
| 1:A:3735:PRO:HB3 | 1:A:3751:LEU:HD21 | 1.78 | 0.66 |
| 1:S:2090:ARG:NH1 | 1:S:2091:HIS:O | 2.29 | 0.66 |
| 1:A:305:ASN:O | 1:A:308:LEU:N | 2.29 | 0.66 |
| 1:A:1961:PHE:HB2 | 1:A:1963:GLN:NE2 | 2.11 | 0.66 |
| 1:A:2920:VAL:O | 1:A:2923:TRP:HB2 | 1.95 | 0.66 |
| 2:B:522:VAL:HG11 | 3:C:256:ASN:HB3 | 1.77 | 0.66 |
| 3:C:216:GLU:OE2 | 11:f:295:ARG:NH2 | 2.29 | 0.66 |
| 1:S:261:ASP:HB3 | 1:S:265:TYR:HD1 | 1.61 | 0.66 |
| 1:S:2402:LEU:HD12 | 1:S:2438:ILE:HG13 | 1.78 | 0.66 |
| 7:d:36:DG:N2 | 7:d:37:DG:O6 | 2.29 | 0.66 |
| 1:A:76:ILE:HA | 1:A:79:ARG:HB3 | 1.78 | 0.65 |
| 1:A:2357:GLU:HA | 1:A:2360:PHE:HB3 | 1.78 | 0.65 |
| 1:A:3823:GLU:OE1 | 1:A:3823:GLU:N | 2.28 | 0.65 |
| 1:S:4039:TYR:HB3 | 1:S:4042:GLN:HG2 | 1.78 | 0.65 |
| 1:A:1322:THR:O | 1:A:1326:GLU:N | 2.29 | 0.65 |
| 2:B:174:ASN:O | 2:B:178:ASN:N | 2.29 | 0.65 |
| 2:B:179:ASP:HB3 | 2:B:182:LYS:HD3 | 1.78 | 0.65 |
| 1:S:527:TYR:O | 1:S:530:LEU:HB3 | 1.95 | 0.65 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:CZ | 2.32 | 0.65 |
| 1:S:895:ALA:HB1 | 1:S:902:LYS:HB3 | 1.78 | 0.65 |
| 1:S:2102:LYS:O | 1:S:2106:ARG:HG2 | 1.96 | 0.65 |
| 1:S:3723:ASP:HB2 | 1:S:3741:ARG:HE | 1.61 | 0.65 |
| 1:S:3740:ILE:O | 1:S:3748:HIS:N | 2.28 | 0.65 |
| 1:A:835:LYS:O | 1:A:839:ASN:ND2 | 2.30 | 0.65 |
| 5:H:43:TRP:HD1 | 5:H:116:VAL:HG12 | 1.61 | 0.65 |
| 1:S:1697:PRO:HA | 1:S:1753:SER:HB3 | 1.77 | 0.65 |
| 1:S:1766:LEU:O | 1:S:1822:ARG:NH1 | 2.29 | 0.65 |
| 1:S:2402:LEU:HD11 | 1:S:2437:ASP:HB2 | 1.76 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:258:ARG:NH1 | 9:i:34:DC:OP2 | 2.30 | 0.65 |
| 1:A:246:ARG:HA | 1:A:249:PHE:CD2 | 2.32 | 0.65 |
| 1:A:3546:SER:O | 1:A:3549:HIS:NE2 | 2.29 | 0.65 |
| 2:B:304:ASN:ND2 | 2:B:307:THR:OG1 | 2.30 | 0.65 |
| 1:S:1910:GLU:O | 1:S:1913:LYS:NZ | 2.26 | 0.65 |
| 8:e:34:DC:H2" | 8:e:35:DT:H5" | 1.77 | 0.65 |
| 1:A:3691:LYS:NZ | 1:A:3692:VAL:O | 2.28 | 0.65 |
| 1:A:3760:GLN:HA | 1:A:3763:ARG:HD3 | 1.78 | 0.65 |
| 1:A:3813:LYS:NZ | 1:A:4125:GLU:OE2 | 2.30 | 0.65 |
| 1:S:1271:ILE:O | 1:S:1274:ARG:NH1 | 2.29 | 0.65 |
| 2:T:61:ASP:OD1 | 2:T:124:GLY:N | 2.27 | 0.65 |
| 1:A:174:VAL:HA | 1:A:177:LEU:HD12 | 1.79 | 0.65 |
| 1:A:570:LYS:HA | 1:A:573:LEU:HD12 | 1.79 | 0.65 |
| 1:A:1606:ARG:HA | 1:A:1608:ARG:HH21 | 1.60 | 0.65 |
| 1:A:1711:ARG:HA | 1:A:1714:LEU:HD12 | 1.78 | 0.65 |
| 1:A:1751:GLU:OE2 | 1:A:1788:ARG:NH1 | 2.30 | 0.65 |
| 3:L:309:ASP:HB3 | 2:T:289:TYR:HE1 | 1.60 | 0.65 |
| 1:S:528:VAL:HB | 1:S:633:ILE:HD11 | 1.77 | 0.65 |
| 1:S:2281:MET:HE1 | 1:S:2326:ILE:HD13 | 1.79 | 0.65 |
| 3:C:37:VAL:HG12 | 11:f:297:LEU:HD23 | 1.78 | 0.65 |
| 5:H:174:THR:HG22 | 6:I:792:MET:SD | 2.37 | 0.65 |
| 3:L:496:HIS:NE2 | 3:L:504:PRO:O | 2.30 | 0.65 |
| 1:S:326:MET:HA | 1:S:329:LYS:HG2 | 1.79 | 0.65 |
| 2:T:404:ARG:HH21 | 9:i:32:DA:H3' | 1.62 | 0.65 |
| 1:A:1690:GLY:HA2 | 1:A:1693:VAL:HG22 | 1.79 | 0.65 |
| 1:A:3353:GLU:OE1 | 1:A:3358:ARG:NH1 | 2.27 | 0.65 |
| 3:C:497:ARG:NH1 | 3:C:500:HIS:O | 2.30 | 0.65 |
| 1:S:658:THR:OG1 | 1:S:659:ARG:NH1 | 2.30 | 0.65 |
| 1:S:2168:LEU:HA | 1:S:2171:LEU:HD12 | 1.79 | 0.65 |
| 1:S:2512:ASP:HB2 | 1:S:2518:GLN:HG2 | 1.78 | 0.65 |
| 1:S:3064:PHE:HA | 1:S:3067:LYS:HE3 | 1.78 | 0.65 |
| 2:B:319:SER:N | 3:C:277:THR:O | 2.30 | 0.65 |
| 2:B:351:LYS:NZ | 3:C:463:LEU:O | 2.30 | 0.65 |
| 3:L:198:THR:HG23 | 3:L:201:GLN:H | 1.62 | 0.65 |
| 3:L:209:LYS:HE2 | 3:L:221:LEU:HD11 | 1.77 | 0.65 |
| 3:L:418:CYS:SG | 3:L:419:LEU:N | 2.71 | 0.65 |
| 1:S:3444:ALA:HB2 | 1:S:3478:GLU:HB3 | 1.78 | 0.65 |
| 1:A:617:PRO:HA | 1:A:620:PHE:HD2 | 1.62 | 0.64 |
| 1:A:1532:LEU:HD22 | 1:A:1560:TYR:HB2 | 1.79 | 0.64 |
| 1:A:1637:SER:O | 1:A:1642:LYS:NZ | 2.30 | 0.64 |
| 1:S:2589:TYR:N | 1:S:2775:TYR:O | 2.30 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:4064:LEU:HB3 | 1:S:4074:PHE:CE1 | 2.32 | 0.64 |
| 1:A:1307:ILE:HG12 | 1:A:1311:LYS:HD2 | 1.79 | 0.64 |
| 2:B:285:PRO:HB3 | 3:C:312:GLN:HE21 | 1.61 | 0.64 |
| 3:C:186:GLY:HA2 | 3:C:232:ARG:HD3 | 1.78 | 0.64 |
| 1:S:1220:LEU:HD11 | 1:S:1287:GLN:HB2 | 1.79 | 0.64 |
| 1:S:1457:GLN:HG2 | 1:S:1460:ARG:HH22 | 1.62 | 0.64 |
| 1:S:2126:MET:O | 1:S:2130:HIS:HB2 | 1.97 | 0.64 |
| 1:S:2211:LEU:HA | 1:S:2214:ARG:HH11 | 1.62 | 0.64 |
| 1:S:2580:PRO:HA | 1:S:2783:ILE:H | 1.61 | 0.64 |
| 1:A:529:ASP:OD1 | 1:A:530:LEU:N | 2.30 | 0.64 |
| 3:C:492:GLN:HE21 | 3:C:506:PRO:HG2 | 1.62 | 0.64 |
| 3:L:331:MET:HE3 | 2:T:500:PRO:HG3 | 1.80 | 0.64 |
| 1:S:770:LEU:HD12 | 1:S:854:ARG:HH21 | 1.61 | 0.64 |
| 2:T:36:ASP:HA | 2:T:163:HIS:HB2 | 1.79 | 0.64 |
| 1:A:793:LEU:HB3 | 1:A:870:LEU:HA | 1.79 | 0.64 |
| 1:A:1512:SER:HA | 1:A:1515:LEU:HD12 | 1.79 | 0.64 |
| 1:A:2281:MET:HG2 | 1:A:2325:LEU:HB3 | 1.78 | 0.64 |
| 3:L:417:GLU:HG3 | 2:T:451:LYS:HE2 | 1.80 | 0.64 |
| 5:Q:189:THR:HG23 | 5:Q:192:ARG:HH21 | 1.61 | 0.64 |
| 1:S:392:CYS:HA | 1:S:395:MET:HB3 | 1.78 | 0.64 |
| 2:T:351:LYS:HB2 | 2:T:355:LEU:HD12 | 1.77 | 0.64 |
| 2:T:468:LYS:HB3 | 2:T:517:ARG:HB3 | 1.79 | 0.64 |
| 1:A:327:VAL:HG13 | 1:A:333:MET:HB2 | 1.80 | 0.64 |
| 1:A:978:GLN:NE2 | 1:A:2594:ASP:OD1 | 2.31 | 0.64 |
| 1:A:2841:ASN:O | 1:A:2845:ASN:ND2 | 2.31 | 0.64 |
| 1:A:3262:LEU:O | 1:A:3266:SER:HB3 | 1.98 | 0.64 |
| 2:B:418:GLU:OE2 | 2:B:426:GLN:NE2 | 2.29 | 0.64 |
| 2:B:477:SER:HB3 | 4:D:198:GLY:H | 1.61 | 0.64 |
| 1:S:571:SER:O | 1:S:575:ILE:HG12 | 1.98 | 0.64 |
| 1:S:4084:SER:H | 1:S:4114:PRO:HB2 | 1.62 | 0.64 |
| 1:A:169:THR:HA | 1:A:172:GLU:HG2 | 1.80 | 0.64 |
| 1:A:897:PRO:HA | 1:A:902:LYS:HG3 | 1.80 | 0.64 |
| 1:A:1673:THR:HA | 1:A:1676:ILE:HD12 | 1.80 | 0.64 |
| 3:L:9:ALA:HB3 | 3:L:130:ARG:HG3 | 1.79 | 0.64 |
| 1:S:953:GLN:HG2 | 1:S:954:GLY:H | 1.61 | 0.64 |
| 1:S:2473:MET:O | 1:S:2477:LEU:HG | 1.96 | 0.64 |
| 1:A:3133:GLN:NE2 | 1:A:3170:ASP:OD2 | 2.31 | 0.64 |
| 1:A:3679:ASN:OD1 | 1:A:3680:LEU:N | 2.28 | 0.64 |
| 1:A:3723:ASP:OD1 | 1:A:3725:ARG:NH2 | 2.28 | 0.64 |
| 1:S:736:LEU:HB3 | 1:S:740:ILE:HD11 | 1.79 | 0.64 |
| 2:B:534:TYR:OH | 3:C:260:ARG:NH2 | 2.31 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1711:ARG:HA | 1:S:1714:LEU:HD12 | 1.78 | 0.64 |
| 1:A:1953:CYS:HB3 | 1:A:2100:LEU:HD12 | 1.80 | 0.64 |
| 1:A:3034:PRO:HD2 | 1:A:3037:GLN:OE1 | 1.98 | 0.64 |
| 1:A:3472:ILE:HA | 1:A:3479:THR:HG21 | 1.80 | 0.64 |
| 3:C:656:ASN:HB3 | 3:C:688:LYS:HA | 1.80 | 0.64 |
| 5:G:26:LYS:HD2 | 5:G:27:THR:HG23 | 1.79 | 0.64 |
| 3:L:455:ASP:HB2 | 2:T:388:LYS:HD2 | 1.79 | 0.64 |
| 1:S:380:ASP:HB3 | 1:S:384:MET:HE1 | 1.79 | 0.64 |
| 1:A:658:THR:OG1 | 1:A:659:ARG:NH1 | 2.31 | 0.64 |
| 1:A:1795:VAL:HG13 | 1:A:1839:PHE:HD1 | 1.62 | 0.64 |
| 1:A:3244:ASP:HB2 | 1:A:3247:ARG:HH21 | 1.62 | 0.64 |
| 1:S:790:LYS:HA | 1:S:869:ASN:HB3 | 1.80 | 0.64 |
| 1:S:1679:LEU:HD22 | 1:S:1693:VAL:HG12 | 1.79 | 0.64 |
| 1:S:2507:ILE:HA | 1:S:2510:LEU:HD12 | 1.80 | 0.64 |
| 1:S:3675:LYS:NZ | 1:S:3676:PRO:O | 2.30 | 0.64 |
| 2:T:329:LEU:HD11 | 2:T:333:GLU:HG3 | 1.79 | 0.64 |
| 1:A:119:ARG:HG3 | 1:A:122:LYS:HD3 | 1.79 | 0.63 |
| 1:A:175:TYR:HB2 | 1:A:223:CYS:HB3 | 1.79 | 0.63 |
| 1:A:2044:ASP:O | 1:A:2048:GLY:N | 2.31 | 0.63 |
| 2:B:288:LEU:HD13 | 2:B:293:ASN:HA | 1.80 | 0.63 |
| 6:I:800:GLU:HA | 6:I:805:TRP:HB2 | 1.80 | 0.63 |
| 3:L:81:ARG:NH2 | 3:L:85:LEU:O | 2.29 | 0.63 |
| 1:S:895:ALA:HA | 1:S:904:VAL:HA | 1.80 | 0.63 |
| 1:S:1071:ASN:HB3 | 1:S:1074:LYS:HD2 | 1.79 | 0.63 |
| 1:A:2227:LYS:O | 1:A:2228:ARG:HD3 | 1.96 | 0.63 |
| 1:A:3348:LEU:HA | 1:A:3351:ILE:HD12 | 1.79 | 0.63 |
| 1:S:863:GLY:HA3 | 1:S:3168:TYR:HB2 | 1.81 | 0.63 |
| 1:A:2863:CYS:HA | 1:A:2869:LEU:HD21 | 1.80 | 0.63 |
| 1:A:3572:ILE:HD12 | 1:A:3796:MET:HE3 | 1.81 | 0.63 |
| 2:B:34:GLY:HA2 | 2:B:160:LYS:HG3 | 1.79 | 0.63 |
| 1:S:976:VAL:HG22 | 1:S:2598:ARG:HH21 | 1.62 | 0.63 |
| 1:S:3150:ASN:HD21 | 1:S:3193:ILE:HG12 | 1.63 | 0.63 |
| 1:A:582:THR:HG23 | 1:A:615:ALA:HB3 | 1.81 | 0.63 |
| 1:A:1139:GLU:HA | 1:A:1197:LEU:HD11 | 1.78 | 0.63 |
| 1:A:2978:LYS:NZ | 1:A:2980:ASP:O | 2.32 | 0.63 |
| 1:A:3657:SER:N | 1:A:3660:ASN:OD1 | 2.32 | 0.63 |
| 1:A:4125:GLU:HG3 | 1:A:4128:MET:HB2 | 1.80 | 0.63 |
| 1:S:1069:HIS:HB2 | 1:S:1074:LYS:HD3 | 1.79 | 0.63 |
| 1:S:1121:LEU:HG | 1:S:1123:THR:H | 1.62 | 0.63 |
| 1:A:960:GLN:O | 1:A:964:ARG:HG2 | 1.97 | 0.63 |
| 1:A:1117:ASP:OD1 | 1:A:1118:GLU:N | 2.27 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2090:ARG:N | 1:A:2180:GLU:OE1 | 2.31 | 0.63 |
| 1:A:2147:ALA:O | 1:A:2151:ILE:HG13 | 1.98 | 0.63 |
| 1:A:2512:ASP:HB2 | 1:A:2518:GLN:HG2 | 1.80 | 0.63 |
| 1:A:2577:PHE:HB2 | 1:A:2783:ILE:HB | 1.80 | 0.63 |
| 2:B:299:LYS:HG3 | 3:C:294:VAL:HB | 1.81 | 0.63 |
| 3:C:497:ARG:HD3 | 3:C:501:PRO:HA | 1.80 | 0.63 |
| 1:S:3948:SER:HA | 1:S:3951:GLN:HB3 | 1.81 | 0.63 |
| 1:A:755:ALA:O | 1:A:759:GLY:N | 2.23 | 0.63 |
| 1:A:3245:SER:HA | 1:A:3248:LYS:HE2 | 1.81 | 0.63 |
| 1:A:3960:PRO:HB3 | 1:A:4107:LEU:HD11 | 1.81 | 0.63 |
| 1:S:1780:SER:HB2 | 1:S:1784:ARG:HH12 | 1.63 | 0.63 |
| 1:A:357:LYS:HA | 1:A:406:ARG:HH22 | 1.63 | 0.63 |
| 2:B:253:LYS:NZ | 3:C:434:MET:O | 2.32 | 0.63 |
| 1:S:229:SER:HA | 1:S:278:HIS:HE1 | 1.64 | 0.63 |
| 1:S:538:ASP:OD1 | 1:S:561:ASN:ND2 | 2.31 | 0.63 |
| 1:S:1624:GLN:O | 1:S:1628:LYS:NZ | 2.27 | 0.63 |
| 2:T:258:ARG:HH22 | 9:i:34:DC:H3' | 1.62 | 0.63 |
| 1:A:655:LEU:O | 1:A:659:ARG:NH1 | 2.32 | 0.63 |
| 1:A:1750:LEU:HD13 | 1:A:1758:LEU:HB2 | 1.80 | 0.63 |
| 5:G:181:ILE:HG13 | 6:I:774:LEU:HD22 | 1.80 | 0.63 |
| 5:P:21:GLN:HB2 | 5:P:33:VAL:HG23 | 1.79 | 0.63 |
| 5:Q:20:LEU:HD21 | 5:Q:37:THR:H | 1.64 | 0.63 |
| 1:S:420:VAL:O | 1:S:424:LEU:N | 2.29 | 0.63 |
| 1:A:652:GLU:HA | 1:A:655:LEU:HD12 | 1.81 | 0.63 |
| 1:S:1231:GLN:HE22 | 1:S:1292:LYS:HB2 | 1.63 | 0.63 |
| 1:S:2723:THR:HA | 1:S:2726:LEU:HD13 | 1.81 | 0.63 |
| 1:S:3324:ARG:HB2 | 1:S:3391:ALA:HB3 | 1.81 | 0.63 |
| 1:A:385:TYR:O | 1:A:389:ILE:HG12 | 1.99 | 0.62 |
| 1:A:672:ILE:O | 1:A:676:ASN:ND2 | 2.31 | 0.62 |
| 1:A:1751:GLU:O | 1:A:1788:ARG:NH1 | 2.29 | 0.62 |
| 1:S:1803:GLU:OE1 | 1:S:1806:ARG:NH2 | 2.32 | 0.62 |
| 1:A:362:ALA:O | 1:A:366:TYR:N | 2.30 | 0.62 |
| 1:A:3126:LEU:O | 1:A:3130:GLN:NE2 | 2.30 | 0.62 |
| 3:C:600:VAL:O | 3:C:604:GLN:HB3 | 1.99 | 0.62 |
| 3:C:602:VAL:HA | 3:C:609:PHE:HD2 | 1.64 | 0.62 |
| 1:S:1514:LEU:HA | 1:S:1517:LEU:HD12 | 1.80 | 0.62 |
| 2:T:485:GLN:NE2 | 2:T:489:ASN:OD1 | 2.31 | 0.62 |
| 1:A:325:ASN:O | 1:A:329:LYS:NZ | 2.29 | 0.62 |
| 1:A:484:HIS:O | 1:A:488:ILE:HG12 | 1.99 | 0.62 |
| 1:A:635:PRO:HB3 | 1:A:672:ILE:HD11 | 1.82 | 0.62 |
| 1:A:1594:SER:O | 1:A:1598:ASN:ND2 | 2.32 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2212:ALA:O | 1:A:2216:LEU:HG | 1.99 | 0.62 |
| 1:A:3631:LYS:HA | 1:A:3634:GLN:HE21 | 1.64 | 0.62 |
| 1:A:4127:TRP:CD1 | 1:A:4128:MET:HG2 | 2.34 | 0.62 |
| 1:S:631:ARG:NH1 | 1:S:632:GLU:HB3 | 2.14 | 0.62 |
| 1:S:2763:MET:HE3 | 1:S:2763:MET:O | 1.99 | 0.62 |
| 1:S:3281:CYS:HB2 | 1:S:3301:LEU:HB3 | 1.79 | 0.62 |
| 1:S:3833:ARG:HA | 1:S:3877:LYS:HE2 | 1.81 | 0.62 |
| 2:T:59:PRO:HD3 | 2:T:206:LYS:HZ2 | 1.63 | 0.62 |
| 1:A:1261:LEU:HD21 | 1:A:1337:VAL:HG22 | 1.80 | 0.62 |
| 1:A:1576:ASP:HB2 | 1:A:1625:HIS:CE1 | 2.35 | 0.62 |
| 6:I:868:ASP:HB2 | 6:I:871:ARG:HD3 | 1.81 | 0.62 |
| 1:S:2218:PHE:HD1 | 1:S:2221:LYS:HZ1 | 1.47 | 0.62 |
| 1:A:1622:ILE:HA | 1:A:1625:HIS:HB2 | 1.81 | 0.62 |
| 1:A:3728:VAL:HG13 | 1:A:3736:LYS:HG2 | 1.81 | 0.62 |
| 1:A:3737:ARG:NH1 | 1:A:3738:ILE:O | 2.31 | 0.62 |
| 3:C:16:VAL:O | 3:C:101:GLY:N | 2.32 | 0.62 |
| 3:C:94:ILE:HA | 3:C:98:ILE:HD13 | 1.81 | 0.62 |
| 3:L:595:ALA:HA | 3:L:598:PHE:CE2 | 2.35 | 0.62 |
| 1:S:621:SER:O | 1:S:625:ASN:ND2 | 2.32 | 0.62 |
| 1:S:2140:LEU:HA | 1:S:2143:ARG:HD3 | 1.82 | 0.62 |
| 1:S:3256:MET:SD | 1:S:3287:ARG:NH1 | 2.73 | 0.62 |
| 1:S:3714:GLU:HB3 | 1:S:3718:ARG:NH1 | 2.15 | 0.62 |
| 7:d:27:DT:H2" | 7:d:28:DA:C8 | 2.35 | 0.62 |
| 1:A:197:PHE:O | 1:A:201:LEU:HG | 1.99 | 0.62 |
| 1:A:2986:PRO:O | 1:A:2991:LYS:NZ | 2.32 | 0.62 |
| 2:B:305:THR:HB | 3:C:288:ASP:HA | 1.80 | 0.62 |
| 3:L:93:ASP:HA | 3:L:97:LYS:HG2 | 1.81 | 0.62 |
| 6:R:872:VAL:HA | 6:R:875:PHE:HD2 | 1.64 | 0.62 |
| 1:S:923:ASP:OD2 | 1:S:2800:ARG:NH1 | 2.33 | 0.62 |
| 1:S:1184:ARG:NH2 | 1:S:1265:GLU:OE1 | 2.32 | 0.62 |
| 1:S:3592:VAL:HG23 | 1:S:3606:ILE:HD12 | 1.80 | 0.62 |
| 7:d:38:DG:N2 | 8:e:20:DT:O4' | 2.21 | 0.62 |
| 1:A:1102:GLU:HA | 1:A:1154:PRO:HB3 | 1.82 | 0.62 |
| 4:M:47:LEU:HD22 | 4:M:120:ARG:HE | 1.63 | 0.62 |
| 1:S:1725:GLN:HG3 | 1:S:1728:GLU:H | 1.65 | 0.62 |
| 1:A:1052:SER:O | 1:A:1055:ASN:ND2 | 2.33 | 0.62 |
| 1:A:1413:ASP:OD1 | 1:A:1414:ILE:N | 2.32 | 0.62 |
| 1:A:1771:GLN:HE22 | 1:A:1774:MET:HA | 1.64 | 0.62 |
| 1:A:3824:GLU:HG2 | 1:A:3828:TYR:HB3 | 1.80 | 0.62 |
| 6:R:722:LYS:HD3 | 6:R:724:ALA:H | 1.65 | 0.62 |
| 1:S:921:ALA:HB3 | 1:S:927:LYS:HB3 | 1.81 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4049:ARG:NH2 | 1:A:4058:VAL:HG12 | 2.15 | 0.62 |
| 2:B:379:SER:HB2 | 3:C:438:LEU:HD22 | 1.82 | 0.62 |
| 3:C:492:GLN:NE2 | 3:C:507:PRO:O | 2.33 | 0.62 |
| 1:A:1766:LEU:O | 1:A:1822:ARG:NH1 | 2.33 | 0.62 |
| 2:B:41:LEU:HB3 | 2:B:88:TYR:HE1 | 1.64 | 0.62 |
| 2:B:315:ASP:OD1 | 3:C:282:LYS:NZ | 2.33 | 0.62 |
| 6:I:712:ILE:HB | 6:I:718:HIS:CE1 | 2.35 | 0.62 |
| 1:S:179:GLY:HA2 | 1:S:231:LEU:HG | 1.81 | 0.62 |
| 1:S:901:MET:HG2 | 1:S:903:PRO:HD3 | 1.80 | 0.62 |
| 1:S:3665:MET:HA | 1:S:3668:LEU:HG | 1.80 | 0.62 |
| 2:T:105:LEU:HG | 2:T:106:GLN:HG3 | 1.81 | 0.62 |
| 1:A:1017:ILE:HG23 | 1:A:1077:GLY:HA3 | 1.82 | 0.61 |
| 1:A:2402:LEU:HD23 | 1:A:2438:ILE:HG13 | 1.82 | 0.61 |
| 1:A:3577:GLN:HG3 | 1:A:3629:ARG:HD3 | 1.82 | 0.61 |
| 3:C:404:GLN:NE2 | 3:C:421:TYR:OH | 2.32 | 0.61 |
| 1:S:1881:TYR:HE2 | 1:S:1953:CYS:HB2 | 1.65 | 0.61 |
| 1:A:135:LEU:HD21 | 1:A:177:LEU:HA | 1.82 | 0.61 |
| 1:A:476:ARG:HH22 | 1:A:1562:LEU:HD23 | 1.64 | 0.61 |
| 1:A:2122:LEU:HG | 1:A:2126:MET:HB2 | 1.81 | 0.61 |
| 2:B:420:LEU:HB3 | 2:B:424:LYS:HA | 1.81 | 0.61 |
| 3:L:522:VAL:HA | 3:L:525:LYS:HE2 | 1.81 | 0.61 |
| 1:S:921:ALA:O | 1:S:927:LYS:NZ | 2.22 | 0.61 |
| 1:S:2965:TYR:HB3 | 1:S:3001:CYS:HB2 | 1.82 | 0.61 |
| 1:A:618:LYS:HD2 | 1:A:2034:SER:HB2 | 1.81 | 0.61 |
| 1:A:1284:THR:HG23 | 1:A:1285:GLU:HG3 | 1.82 | 0.61 |
| 6:R:800:GLU:HA | 6:R:805:TRP:HB2 | 1.81 | 0.61 |
| 1:S:2322:VAL:O | 1:S:2326:ILE:HG12 | 1.99 | 0.61 |
| 1:S:3359:ILE:HD12 | 1:S:3362:LEU:HD12 | 1.81 | 0.61 |
| 2:T:255:ALA:HA | 2:T:274:TYR:HE1 | 1.64 | 0.61 |
| 1:A:348:ILE:HG22 | 1:A:359:LEU:HD23 | 1.82 | 0.61 |
| 1:A:418:ALA:HB2 | 1:A:464:VAL:HG12 | 1.83 | 0.61 |
| 3:L:339:CYS:SG | 3:L:394:ARG:NH1 | 2.73 | 0.61 |
| 1:S:2866:ALA:HB1 | 1:S:2899:ARG:HG3 | 1.83 | 0.61 |
| 1:S:3353:GLU:HA | 1:S:3357:ARG:HD3 | 1.81 | 0.61 |
| 1:A:15:LEU:HD12 | 1:A:41:GLU:HG3 | 1.83 | 0.61 |
| 1:A:384:MET:HA | 1:A:387:GLU:HG2 | 1.83 | 0.61 |
| 2:T:44:ALA:O | 2:T:138:GLY:N | 2.33 | 0.61 |
| 1:A:1017:ILE:HG21 | 1:A:1066:LEU:HD21 | 1.80 | 0.61 |
| 1:A:1444:ASP:O | 1:A:1448:LEU:HG | 2.00 | 0.61 |
| 1:A:3733:ARG:HE | 1:A:3754:GLY:HA3 | 1.66 | 0.61 |
| 1:A:3986:HIS:HA | 1:A:3989:ARG:HE | 1.65 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3995:PRO:HA | 1:A:3998:LEU:HB3 | 1.81 | 0.61 |
| 3:C:595:ALA:HA | 3:C:598:PHE:CE2 | 2.36 | 0.61 |
| 4:D:71:ASP:O | 4:D:75:ARG:NH1 | 2.33 | 0.61 |
| 1:S:1709:GLU:HG2 | 1:S:1710:LEU:HD12 | 1.83 | 0.61 |
| 1:S:2326:ILE:O | 1:S:2330:VAL:N | 2.33 | 0.61 |
| 1:A:953:GLN:H | 1:A:956:PRO:HD3 | 1.66 | 0.61 |
| 1:A:1483:LEU:HA | 1:A:1514:LEU:HD21 | 1.82 | 0.61 |
| 1:A:1686:LEU:HD11 | 1:A:1738:ASN:HB3 | 1.82 | 0.61 |
| 1:A:3462:ARG:NH2 | 1:A:3497:SER:OG | 2.34 | 0.61 |
| 2:B:399:ARG:NH2 | 3:C:516:LEU:O | 2.34 | 0.61 |
| 1:S:855:VAL:O | 1:S:859:LEU:HG | 2.01 | 0.61 |
| 1:S:3575:LEU:HD13 | 1:S:3752:VAL:HG21 | 1.81 | 0.61 |
| 1:A:473:PRO:O | 1:A:477:ASN:ND2 | 2.33 | 0.61 |
| 1:A:775:GLU:HA | 1:A:778:ILE:HD12 | 1.83 | 0.61 |
| 1:A:895:ALA:HA | 1:A:904:VAL:HA | 1.82 | 0.61 |
| 1:A:1354:GLU:HA | 1:A:1357:LYS:HB3 | 1.82 | 0.61 |
| 1:A:2383:PHE:HB3 | 1:A:2418:LYS:HE3 | 1.82 | 0.61 |
| 5:Q:37:THR:HG22 | 5:Q:39:GLY:H | 1.64 | 0.61 |
| 1:S:1663:THR:O | 1:S:1665:HIS:ND1 | 2.34 | 0.61 |
| 1:S:2233:HIS:CE1 | 1:S:2237:ILE:HD11 | 2.36 | 0.61 |
| 2:T:80:ARG:HD3 | 2:T:252:ARG:HE | 1.65 | 0.61 |
| 7:d:25:DT:H2” | 7:d:26:DT:C6 | 2.36 | 0.61 |
| 1:S:1430:GLU:OE1 | 1:S:1430:GLU:N | 2.33 | 0.61 |
| 1:S:1771:GLN:HA | 1:S:1775:GLU:HG3 | 1.83 | 0.61 |
| 1:A:316:LEU:O | 1:A:320:LEU:HG | 2.01 | 0.61 |
| 1:A:4089:ILE:HB | 1:A:4092:GLN:HE22 | 1.66 | 0.61 |
| 2:B:332:GLU:HA | 2:B:335:GLU:HG2 | 1.82 | 0.61 |
| 3:C:269:GLN:HB3 | 3:C:359:ASN:OD1 | 2.00 | 0.61 |
| 5:P:3:ARG:HH21 | 5:P:21:GLN:HG2 | 1.66 | 0.61 |
| 1:S:370:ALA:O | 1:S:374:LYS:N | 2.34 | 0.61 |
| 1:S:935:HIS:HD2 | 1:S:987:LEU:HD21 | 1.65 | 0.61 |
| 1:A:985:GLU:HA | 1:A:988:VAL:HG22 | 1.83 | 0.60 |
| 1:A:1125:GLN:OE1 | 1:A:1125:GLN:N | 2.29 | 0.60 |
| 2:B:288:LEU:HA | 2:B:295:PRO:HA | 1.83 | 0.60 |
| 2:B:345:LEU:HD13 | 2:B:400:TYR:HD1 | 1.66 | 0.60 |
| 6:I:810:LEU:HD12 | 6:I:848:HIS:HA | 1.82 | 0.60 |
| 3:L:250:ARG:NH2 | 3:L:258:SER:O | 2.34 | 0.60 |
| 1:S:2379:MET:HE1 | 1:S:2404:ARG:HG3 | 1.83 | 0.60 |
| 1:S:2785:ILE:HB | 1:S:2790:LEU:HD21 | 1.83 | 0.60 |
| 1:S:3029:LYS:NZ | 1:S:3067:LYS:O | 2.34 | 0.60 |
| 1:A:93:LEU:HD23 | 1:A:136:GLN:HG3 | 1.83 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:168:LEU:HG | 2:B:202:LEU:HD13 | 1.83 | 0.60 |
| 1:S:670:LEU:HB3 | 1:S:732:PHE:HE2 | 1.66 | 0.60 |
| 1:S:2254:ARG:HH22 | 1:S:2292:CYS:HB3 | 1.65 | 0.60 |
| 1:S:2987:THR:HG23 | 1:S:2990:GLU:H | 1.66 | 0.60 |
| 1:S:3152:SER:O | 1:S:3154:GLN:NE2 | 2.33 | 0.60 |
| 1:S:3165:THR:HB | 1:S:3169:PRO:HG3 | 1.83 | 0.60 |
| 1:S:3554:PHE:O | 1:S:3558:ILE:HG12 | 2.01 | 0.60 |
| 1:S:4085:LYS:HG2 | 1:S:4114:PRO:HB3 | 1.82 | 0.60 |
| 1:A:261:ASP:OD1 | 1:A:262:LEU:N | 2.31 | 0.60 |
| 1:A:1877:LEU:HB3 | 1:A:1881:TYR:CZ | 2.36 | 0.60 |
| 1:A:2943:PHE:HA | 1:A:2947:ILE:HB | 1.81 | 0.60 |
| 3:C:699:GLU:O | 3:C:703:LYS:HG2 | 2.00 | 0.60 |
| 3:C:729:LEU:HA | 1:S:1913:LYS:HB3 | 1.83 | 0.60 |
| 3:L:389:MET:HG2 | 2:T:466:VAL:HG11 | 1.83 | 0.60 |
| 1:S:1296:PHE:O | 1:S:1300:SER:N | 2.35 | 0.60 |
| 1:A:2410:GLU:O | 1:A:2414:GLN:NE2 | 2.29 | 0.60 |
| 1:A:2587:GLN:HG2 | 1:A:2777:HIS:HB3 | 1.84 | 0.60 |
| 1:A:3686:TRP:HE1 | 1:A:3696:ARG:HH22 | 1.48 | 0.60 |
| 1:S:3769:GLN:HG3 | 1:S:3790:THR:HG21 | 1.83 | 0.60 |
| 1:A:835:LYS:HA | 1:A:838:LYS:HB2 | 1.82 | 0.60 |
| 1:A:923:ASP:O | 1:A:926:THR:N | 2.33 | 0.60 |
| 1:A:1149:LYS:HB2 | 1:A:1151:ARG:HH11 | 1.67 | 0.60 |
| 1:A:1153:LEU:HD22 | 1:A:1160:SER:HB2 | 1.83 | 0.60 |
| 1:A:1622:ILE:HD12 | 1:A:1625:HIS:HB2 | 1.83 | 0.60 |
| 1:A:1816:ARG:NH2 | 3:C:624:LEU:O | 2.34 | 0.60 |
| 1:A:2274:ILE:HD13 | 1:A:2319:ALA:HB2 | 1.83 | 0.60 |
| 1:A:2399:GLU:HA | 1:A:2402:LEU:HD12 | 1.83 | 0.60 |
| 2:B:34:GLY:HA3 | 2:B:162:SER:HB3 | 1.82 | 0.60 |
| 2:B:145:GLU:OE1 | 2:B:145:GLU:N | 2.35 | 0.60 |
| 3:L:332:LYS:HG3 | 2:T:486:HIS:CE1 | 2.37 | 0.60 |
| 1:S:1909:ASN:OD1 | 1:S:1910:GLU:N | 2.35 | 0.60 |
| 1:A:1296:PHE:O | 1:A:1300:SER:N | 2.34 | 0.60 |
| 1:A:1620:THR:O | 1:A:1624:GLN:NE2 | 2.35 | 0.60 |
| 1:A:1776:GLU:O | 1:A:1779:GLN:NE2 | 2.34 | 0.60 |
| 1:A:3835:PRO:HA | 1:A:3839:TYR:HD2 | 1.67 | 0.60 |
| 1:A:3842:TRP:O | 1:A:3851:ASP:N | 2.34 | 0.60 |
| 1:A:3992:ARG:NH1 | 1:A:4051:LEU:O | 2.35 | 0.60 |
| 1:A:4008:GLU:HG3 | 1:A:4011:PHE:HB2 | 1.82 | 0.60 |
| 2:B:230:ARG:O | 2:B:232:HIS:ND1 | 2.35 | 0.60 |
| 2:B:288:LEU:HD21 | 3:C:322:PRO:HA | 1.83 | 0.60 |
| 2:B:291:GLU:HB3 | 6:I:690:VAL:HG23 | 1.84 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:R:694:GLY:HA2 | 2:T:290:ARG:HD3 | 1.81 | 0.60 |
| 1:S:1153:LEU:HD13 | 1:S:1160:SER:HA | 1.81 | 0.60 |
| 1:S:2510:LEU:O | 1:S:2518:GLN:NE2 | 2.28 | 0.60 |
| 1:A:1915:LEU:HD13 | 1:A:1918:LEU:HD12 | 1.83 | 0.60 |
| 1:A:3564:GLN:HG2 | 1:A:3697:ASN:HB3 | 1.84 | 0.60 |
| 2:B:81:ASP:O | 2:B:110:ASN:ND2 | 2.32 | 0.60 |
| 3:L:450:GLN:NE2 | 3:L:536:LEU:O | 2.30 | 0.60 |
| 4:M:37:PHE:HZ | 4:M:72:ILE:HB | 1.67 | 0.60 |
| 1:S:854:ARG:HG2 | 1:S:858:MET:HE2 | 1.84 | 0.60 |
| 1:S:1369:MET:HG3 | 1:S:1415:LEU:HD13 | 1.82 | 0.60 |
| 1:S:1685:ASP:HB3 | 1:S:1688:LEU:HG | 1.81 | 0.60 |
| 1:S:2271:SER:O | 1:S:2274:ILE:HB | 2.01 | 0.60 |
| 2:T:317:LYS:NZ | 2:T:330:GLU:OE2 | 2.35 | 0.60 |
| 1:A:3497:SER:O | 1:A:3766:GLN:NE2 | 2.34 | 0.60 |
| 1:A:4121:TRP:HD1 | 1:A:4123:GLY:H | 1.49 | 0.60 |
| 3:C:197:ILE:O | 3:C:202:LYS:NZ | 2.35 | 0.60 |
| 3:C:448:GLU:OE2 | 3:C:452:ASN:ND2 | 2.34 | 0.60 |
| 1:S:1784:ARG:HG3 | 1:S:1787:ARG:HH12 | 1.67 | 0.60 |
| 1:S:2851:PHE:HB3 | 1:S:2854:PHE:HB3 | 1.84 | 0.60 |
| 1:S:3762:GLN:HG2 | 1:S:3766:GLN:HE21 | 1.66 | 0.60 |
| 2:T:76:ILE:HG21 | 2:T:247:ARG:HA | 1.83 | 0.60 |
| 1:A:2461:PHE:C | 1:A:2473:MET:HE1 | 2.27 | 0.60 |
| 1:A:2473:MET:HA | 1:A:2476:ILE:HD12 | 1.84 | 0.60 |
| 1:A:3965:ARG:O | 1:A:3969:ASN:N | 2.32 | 0.60 |
| 2:B:464:ALA:O | 2:B:468:LYS:HG2 | 2.01 | 0.60 |
| 2:B:480:ASN:HB3 | 2:B:483:LEU:HB2 | 1.83 | 0.60 |
| 3:C:74:TYR:H | 3:C:109:ASP:HB3 | 1.66 | 0.60 |
| 3:C:133:GLU:OE1 | 11:f:297:LEU:N | 2.30 | 0.60 |
| 3:L:320:ILE:HD13 | 2:T:286:ILE:HG21 | 1.83 | 0.60 |
| 1:S:175:TYR:HA | 1:S:178:LEU:HD12 | 1.83 | 0.60 |
| 1:S:1570:GLU:HA | 1:S:1573:LYS:HE2 | 1.82 | 0.60 |
| 1:S:2460:GLU:OE1 | 1:S:2460:GLU:N | 2.32 | 0.60 |
| 1:S:3880:ALA:HA | 1:S:3966:GLN:HE22 | 1.67 | 0.60 |
| 1:S:3940:ILE:HG13 | 1:S:3941:ASP:H | 1.66 | 0.60 |
| 1:A:2597:PHE:HE2 | 1:A:2766:ASP:H | 1.50 | 0.60 |
| 1:A:2936:TYR:HA | 1:A:2939:LEU:HG | 1.83 | 0.60 |
| 1:A:4086:ASP:HA | 1:A:4089:ILE:HG12 | 1.83 | 0.60 |
| 3:C:678:VAL:O | 3:C:682:GLY:N | 2.35 | 0.60 |
| 3:L:381:ILE:HG13 | 3:L:417:GLU:HB3 | 1.83 | 0.60 |
| 1:S:1691:GLN:N | 1:S:1745:LYS:HZ2 | 1.99 | 0.60 |
| 1:S:1817:GLN:HB3 | 1:S:1868:THR:HB | 1.83 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2928:LYS:HG2 | 1:S:2931:ARG:HH21 | 1.66 | 0.60 |
| 1:S:3483:MET:HE3 | 1:S:3511:ALA:HA | 1.83 | 0.60 |
| 1:S:4055:ASN:ND2 | 1:S:4091:ALA:O | 2.33 | 0.60 |
| 2:T:74:LYS:NZ | 2:T:81:ASP:O | 2.34 | 0.60 |
| 1:A:152:LEU:HA | 1:A:155:LYS:HG2 | 1.83 | 0.59 |
| 1:A:718:MET:HA | 1:A:721:TYR:CD2 | 2.36 | 0.59 |
| 1:A:888:ARG:HB3 | 1:A:3889:ARG:HH12 | 1.67 | 0.59 |
| 1:A:1326:GLU:HG3 | 1:A:1329:ARG:HG2 | 1.84 | 0.59 |
| 1:A:1428:ILE:HA | 1:A:1431:LEU:HB2 | 1.83 | 0.59 |
| 1:A:3118:ASP:H | 1:A:3121:LEU:HD12 | 1.67 | 0.59 |
| 4:D:96:LEU:HD13 | 4:D:109:LEU:HD13 | 1.84 | 0.59 |
| 3:L:19:THR:HG21 | 3:L:140:SER:HA | 1.84 | 0.59 |
| 5:P:183:VAL:HG22 | 5:P:187:LYS:HE2 | 1.84 | 0.59 |
| 1:S:3338:ALA:HB2 | 1:S:3377:LEU:HB2 | 1.84 | 0.59 |
| 2:T:109:ASP:O | 2:T:115:ARG:NH1 | 2.35 | 0.59 |
| 2:T:213:ILE:HD12 | 2:T:218:ARG:HE | 1.66 | 0.59 |
| 2:T:526:LYS:O | 2:T:530:TYR:N | 2.35 | 0.59 |
| 1:A:581:LEU:HB3 | 1:A:660:LEU:HD12 | 1.83 | 0.59 |
| 1:A:1115:HIS:CE1 | 1:A:1182:GLU:H | 2.19 | 0.59 |
| 1:A:2395:THR:OG1 | 1:A:2431:ARG:NH1 | 2.36 | 0.59 |
| 1:A:3258:LEU:O | 1:A:3262:LEU:HG | 2.03 | 0.59 |
| 2:B:426:GLN:H | 3:C:434:MET:HE1 | 1.66 | 0.59 |
| 3:L:236:VAL:HG13 | 11:m:297:LEU:O | 2.02 | 0.59 |
| 3:L:250:ARG:HH21 | 2:T:536:PRO:HB2 | 1.67 | 0.59 |
| 1:S:243:GLN:O | 1:S:246:ARG:HG2 | 2.02 | 0.59 |
| 1:S:681:LYS:NZ | 1:S:683:PHE:O | 2.30 | 0.59 |
| 1:S:2266:ASN:OD1 | 1:S:2267:SER:N | 2.35 | 0.59 |
| 1:A:1787:ARG:HB3 | 1:A:1830:HIS:HE1 | 1.67 | 0.59 |
| 1:A:3410:ILE:HG23 | 1:A:3453:ALA:HB1 | 1.84 | 0.59 |
| 2:B:507:THR:OG1 | 3:C:394:ARG:NH1 | 2.35 | 0.59 |
| 6:I:746:MET:O | 6:I:751:LYS:NZ | 2.35 | 0.59 |
| 3:L:278:VAL:HG13 | 2:T:316:THR:HB | 1.84 | 0.59 |
| 1:S:834:LEU:O | 1:S:837:THR:OG1 | 2.20 | 0.59 |
| 1:S:3714:GLU:HB3 | 1:S:3718:ARG:HH12 | 1.67 | 0.59 |
| 1:A:919:LEU:HD12 | 1:A:968:VAL:HG23 | 1.83 | 0.59 |
| 2:B:348:MET:HB2 | 2:B:397:LEU:HG | 1.83 | 0.59 |
| 3:C:493:CYS:HB3 | 3:C:505:LEU:HD13 | 1.84 | 0.59 |
| 3:L:628:GLU:HB2 | 3:L:631:TYR:HB3 | 1.83 | 0.59 |
| 1:S:1210:ASP:HA | 1:S:1213:LYS:HD2 | 1.83 | 0.59 |
| 1:S:1416:GLU:O | 1:S:1419:LEU:HB3 | 2.02 | 0.59 |
| 1:S:2374:LEU:HB2 | 1:S:2377:ARG:HH22 | 1.67 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2555:LEU:HD13 | 1:S:2806:LYS:HB3 | 1.83 | 0.59 |
| 1:S:2724:ASP:OD1 | 1:S:2725:LEU:N | 2.36 | 0.59 |
| 1:S:3875:GLU:HG3 | 1:S:3965:ARG:HE | 1.66 | 0.59 |
| 1:A:3462:ARG:NH1 | 1:A:3495:PHE:H | 2.01 | 0.59 |
| 1:A:3588:TRP:HD1 | 1:A:3609:MET:HG3 | 1.67 | 0.59 |
| 1:A:4113:ASP:O | 1:A:4117:LEU:HG | 2.02 | 0.59 |
| 2:B:282:LYS:HZ3 | 2:B:483:LEU:HD23 | 1.67 | 0.59 |
| 1:S:732:PHE:CE1 | 1:S:736:LEU:HD21 | 2.38 | 0.59 |
| 1:S:2371:PHE:HD2 | 1:S:2374:LEU:HD23 | 1.67 | 0.59 |
| 1:S:2597:PHE:HA | 1:S:2598:ARG:NH1 | 2.17 | 0.59 |
| 1:S:3700:GLU:HG2 | 1:S:3718:ARG:HD2 | 1.84 | 0.59 |
| 2:T:41:LEU:HD13 | 2:T:86:VAL:HG13 | 1.85 | 0.59 |
| 1:A:1086:TYR:HA | 1:A:1089:PHE:HB3 | 1.85 | 0.59 |
| 1:A:3110:PHE:CD2 | 1:A:3135:LEU:HD11 | 2.37 | 0.59 |
| 1:A:3833:ARG:HE | 1:A:4127:TRP:NE1 | 2.01 | 0.59 |
| 3:C:529:PRO:HA | 3:C:532:LYS:HG2 | 1.84 | 0.59 |
| 8:e:31:DA:H2" | 8:e:32:DA:C8 | 2.37 | 0.59 |
| 1:A:11:SER:HA | 1:A:14:ARG:HD3 | 1.85 | 0.59 |
| 1:A:2586:PHE:HD1 | 1:A:2778:GLY:HA3 | 1.68 | 0.59 |
| 1:A:3679:ASN:HB2 | 1:A:3725:ARG:HG2 | 1.84 | 0.59 |
| 3:C:287:GLU:OE1 | 3:C:287:GLU:N | 2.35 | 0.59 |
| 6:I:715:SER:O | 6:I:745:HIS:NE2 | 2.35 | 0.59 |
| 1:S:643:GLU:HA | 1:S:646:VAL:HG13 | 1.84 | 0.59 |
| 2:T:247:ARG:NH2 | 2:T:491:GLU:OE1 | 2.36 | 0.59 |
| 2:B:161:MET:O | 2:B:164:LYS:NZ | 2.33 | 0.59 |
| 2:B:350:PHE:HB2 | 3:C:462:SER:HA | 1.83 | 0.59 |
| 6:R:778:PHE:HA | 6:R:781:ILE:HD12 | 1.84 | 0.59 |
| 1:S:1625:HIS:HA | 1:S:1628:LYS:HE2 | 1.84 | 0.59 |
| 1:S:1747:LEU:HD13 | 1:S:1777:LEU:HD22 | 1.85 | 0.59 |
| 1:S:1795:VAL:HG22 | 1:S:1839:PHE:HB2 | 1.84 | 0.59 |
| 1:S:2467:THR:HA | 1:S:2470:ARG:HE | 1.68 | 0.59 |
| 1:S:2804:ILE:HD13 | 1:S:2807:GLN:HE21 | 1.68 | 0.59 |
| 1:S:2923:TRP:HE3 | 1:S:2942:ILE:HG23 | 1.68 | 0.59 |
| 1:A:2428:ASP:HB2 | 1:A:2431:ARG:HD3 | 1.84 | 0.59 |
| 1:A:3778:ASP:HB3 | 1:A:3781:CYS:HB3 | 1.84 | 0.59 |
| 2:B:213:ILE:HG12 | 2:B:231:VAL:HA | 1.85 | 0.59 |
| 3:C:253:ILE:HB | 3:C:257:LEU:HB2 | 1.83 | 0.59 |
| 5:H:166:VAL:HG11 | 6:I:846:ARG:HB3 | 1.85 | 0.59 |
| 1:S:756:PHE:O | 1:S:760:LEU:N | 2.36 | 0.59 |
| 1:A:671:SER:HB3 | 1:A:732:PHE:HA | 1.85 | 0.59 |
| 1:A:775:GLU:HB2 | 1:A:779:TYR:CE2 | 2.37 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2500:LYS:HA | 1:A:2503:LYS:HZ2 | 1.68 | 0.59 |
| 2:B:203:MET:SD | 2:B:237:SER:HB2 | 2.42 | 0.59 |
| 3:C:242:ARG:NH1 | 3:C:243:HIS:O | 2.35 | 0.59 |
| 3:L:486:ARG:HG3 | 2:T:407:PRO:HB3 | 1.85 | 0.59 |
| 6:R:814:ARG:H | 6:R:849:GLY:CA | 2.15 | 0.59 |
| 1:S:714:VAL:HG23 | 1:S:733:LEU:HD21 | 1.84 | 0.59 |
| 1:S:2949:THR:N | 1:S:2990:GLU:OE2 | 2.35 | 0.59 |
| 9:i:21:DA:O4' | 10:j:36:DG:N2 | 2.35 | 0.59 |
| 1:A:281:GLN:OE1 | 1:A:281:GLN:N | 2.35 | 0.58 |
| 1:A:2574:ASN:O | 1:A:2787:HIS:ND1 | 2.36 | 0.58 |
| 1:A:3572:ILE:HG23 | 1:A:3800:LEU:HD23 | 1.85 | 0.58 |
| 1:A:3835:PRO:HA | 1:A:3839:TYR:CD2 | 2.38 | 0.58 |
| 3:C:510:GLN:NE2 | 3:C:514:ASN:OD1 | 2.27 | 0.58 |
| 1:S:240:GLU:HB2 | 1:S:242:PRO:HD2 | 1.84 | 0.58 |
| 1:S:1750:LEU:HD21 | 1:S:1759:LEU:HD23 | 1.84 | 0.58 |
| 1:S:1840:PHE:CD1 | 1:S:1880:MET:HG2 | 2.37 | 0.58 |
| 1:S:2396:LEU:O | 1:S:2400:VAL:HG23 | 2.03 | 0.58 |
| 1:S:3784:ARG:HH21 | 1:S:3986:HIS:HB3 | 1.66 | 0.58 |
| 1:A:736:LEU:HD23 | 1:A:740:ILE:HG21 | 1.85 | 0.58 |
| 1:A:1430:GLU:OE1 | 1:A:1430:GLU:N | 2.34 | 0.58 |
| 1:A:1925:GLU:HB2 | 1:A:1941:HIS:CE1 | 2.39 | 0.58 |
| 1:A:3369:ASP:HB3 | 1:A:3372:LYS:HE2 | 1.84 | 0.58 |
| 1:A:3492:CYS:HB2 | 1:A:3709:GLY:HA2 | 1.85 | 0.58 |
| 3:C:450:GLN:HB3 | 3:C:537:PHE:CZ | 2.38 | 0.58 |
| 1:S:1710:LEU:O | 1:S:1714:LEU:HG | 2.02 | 0.58 |
| 1:S:2209:GLU:HB3 | 1:S:2248:CYS:HB2 | 1.85 | 0.58 |
| 1:S:2225:HIS:HE1 | 1:S:2734:ARG:HH11 | 1.51 | 0.58 |
| 7:d:23:DT:H73 | 8:e:35:DT:C2 | 2.38 | 0.58 |
| 1:A:1112:ALA:HB1 | 1:A:1180:GLN:HG3 | 1.85 | 0.58 |
| 1:A:1862:THR:HA | 3:C:718:VAL:HG21 | 1.85 | 0.58 |
| 1:A:3387:GLU:HA | 1:A:3390:GLN:HG3 | 1.84 | 0.58 |
| 1:A:3414:MET:HE1 | 1:A:3460:GLU:HG3 | 1.85 | 0.58 |
| 3:C:65:ASP:HB3 | 3:C:79:VAL:H | 1.68 | 0.58 |
| 3:C:460:SER:O | 3:C:461:MET:HE2 | 2.03 | 0.58 |
| 3:C:656:ASN:ND2 | 3:C:689:GLU:H | 1.99 | 0.58 |
| 3:L:184:ARG:NH1 | 3:L:514:ASN:O | 2.36 | 0.58 |
| 1:S:1231:GLN:HE21 | 1:S:1235:ILE:HD11 | 1.66 | 0.58 |
| 1:A:1389:VAL:O | 1:A:1392:MET:HG2 | 2.03 | 0.58 |
| 1:A:1416:GLU:HG3 | 1:A:1420:ARG:HH12 | 1.68 | 0.58 |
| 1:A:1574:ASN:ND2 | 1:A:1578:ALA:H | 2.00 | 0.58 |
| 1:A:1954:CYS:SG | 1:A:1955:VAL:N | 2.75 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3971:MET:HE3 | 1:A:3974:MET:HB2 | 1.84 | 0.58 |
| 1:A:4053:GLY:O | 1:A:4097:GLY:N | 2.30 | 0.58 |
| 3:L:463:LEU:HG | 2:T:349:GLY:HA3 | 1.85 | 0.58 |
| 1:S:1062:ARG:NH1 | 1:S:1065:SER:OG | 2.36 | 0.58 |
| 1:A:3805:TRP:HH2 | 1:A:3929:MET:HG3 | 1.68 | 0.58 |
| 1:A:3829:LEU:HD22 | 1:A:3833:ARG:HD2 | 1.86 | 0.58 |
| 3:C:659:LEU:HD22 | 3:C:686:ILE:HA | 1.85 | 0.58 |
| 3:L:415:ASN:HB2 | 2:T:448:PHE:HE1 | 1.67 | 0.58 |
| 1:S:2313:LYS:HA | 1:S:2316:TYR:CZ | 2.39 | 0.58 |
| 1:S:3170:ASP:HB3 | 1:S:3174:ASP:OD2 | 2.03 | 0.58 |
| 1:S:3595:GLU:O | 1:S:3601:VAL:N | 2.36 | 0.58 |
| 1:A:394:GLN:HG3 | 1:A:1737:ASN:HB3 | 1.86 | 0.58 |
| 1:A:1066:LEU:HD23 | 1:A:1078:ALA:HB2 | 1.84 | 0.58 |
| 1:A:2893:LEU:HB3 | 1:A:2926:LEU:HD13 | 1.84 | 0.58 |
| 1:A:3419:PHE:O | 1:A:3422:GLN:HG3 | 2.04 | 0.58 |
| 3:C:501:PRO:HD2 | 3:C:502:ARG:HH11 | 1.68 | 0.58 |
| 5:H:184:LEU:HD21 | 6:I:803:TYR:HE2 | 1.68 | 0.58 |
| 3:L:297:LEU:O | 3:L:302:GLU:HA | 2.03 | 0.58 |
| 1:S:754:MET:HG2 | 1:S:758:LEU:HD23 | 1.85 | 0.58 |
| 1:S:899:ARG:NH2 | 1:S:2533:SER:O | 2.36 | 0.58 |
| 1:S:2847:THR:OG1 | 1:S:2849:SER:O | 2.21 | 0.58 |
| 2:T:60:PHE:O | 2:T:64:ILE:HG12 | 2.04 | 0.58 |
| 1:A:1555:HIS:O | 1:A:1559:PHE:N | 2.28 | 0.58 |
| 1:A:1582:LEU:HD11 | 1:A:1593:VAL:HA | 1.85 | 0.58 |
| 1:A:2388:LYS:NZ | 2:B:157:VAL:O | 2.23 | 0.58 |
| 1:A:3812:LEU:HB2 | 1:A:3925:LEU:HD21 | 1.86 | 0.58 |
| 1:S:1413:ASP:OD1 | 1:S:1414:ILE:N | 2.35 | 0.58 |
| 1:S:2231:PHE:O | 1:S:2235:LEU:HG | 2.03 | 0.58 |
| 2:B:92:LYS:HB2 | 2:B:135:MET:HE1 | 1.86 | 0.58 |
| 5:H:43:TRP:CD1 | 5:H:116:VAL:HG12 | 2.38 | 0.58 |
| 6:R:812:MET:H | 6:R:848:HIS:CB | 2.16 | 0.58 |
| 1:S:754:MET:HA | 1:S:757:LYS:HG2 | 1.84 | 0.58 |
| 1:S:2105:HIS:CG | 1:S:2156:VAL:HG23 | 2.39 | 0.58 |
| 1:A:297:LEU:HD22 | 1:A:316:LEU:HG | 1.85 | 0.58 |
| 1:A:1676:ILE:O | 1:A:1680:ALA:N | 2.35 | 0.58 |
| 1:A:1793:THR:O | 1:A:1797:LEU:HG | 2.04 | 0.58 |
| 1:A:3050:LYS:O | 1:A:3054:GLN:HB2 | 2.03 | 0.58 |
| 1:A:3759:ARG:HG3 | 1:A:3760:GLN:HE21 | 1.67 | 0.58 |
| 2:B:86:VAL:HG22 | 2:B:104:VAL:HG23 | 1.85 | 0.58 |
| 2:B:92:LYS:HE2 | 2:B:135:MET:HA | 1.86 | 0.58 |
| 2:B:346:MET:HB2 | 2:B:399:ARG:HB3 | 1.86 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:484:GLN:NE2 | 2:B:488:ARG:HH22 | 2.01 | 0.58 |
| 3:C:74:TYR:HD1 | 3:C:113:VAL:HG23 | 1.68 | 0.58 |
| 1:S:631:ARG:HB2 | 1:S:672:ILE:HG13 | 1.86 | 0.58 |
| 1:S:898:PHE:HB2 | 1:S:901:MET:O | 2.04 | 0.58 |
| 1:S:2120:ARG:N | 1:S:2159:PRO:O | 2.37 | 0.58 |
| 1:S:2211:LEU:HA | 1:S:2214:ARG:HD3 | 1.86 | 0.58 |
| 1:A:1632:TRP:CD1 | 1:A:1641:THR:HB | 2.38 | 0.58 |
| 1:A:3082:TYR:O | 1:A:3086:LEU:HG | 2.04 | 0.58 |
| 3:C:45:GLN:NE2 | 3:C:50:ASN:OD1 | 2.36 | 0.58 |
| 1:S:941:MET:HB2 | 1:S:958:MET:HE3 | 1.86 | 0.58 |
| 1:S:1915:LEU:HD13 | 1:S:1918:LEU:HD12 | 1.84 | 0.58 |
| 1:A:89:LEU:HB3 | 1:A:133:LYS:HE3 | 1.86 | 0.57 |
| 1:A:2349:LEU:HB3 | 1:A:2360:PHE:HE1 | 1.69 | 0.57 |
| 1:A:3773:GLY:O | 1:A:3777:GLN:NE2 | 2.28 | 0.57 |
| 1:A:3923:ARG:O | 1:A:3962:ARG:NH1 | 2.37 | 0.57 |
| 2:B:282:LYS:HZ1 | 2:B:483:LEU:HA | 1.67 | 0.57 |
| 3:C:347:LYS:HG3 | 3:C:349:SER:H | 1.68 | 0.57 |
| 1:S:1296:PHE:HA | 1:S:1299:GLU:HG2 | 1.85 | 0.57 |
| 1:S:1949:ILE:HG23 | 1:S:2100:LEU:HD22 | 1.85 | 0.57 |
| 1:S:2168:LEU:O | 1:S:2172:ALA:N | 2.26 | 0.57 |
| 1:S:2344:LEU:HA | 1:S:2347:LYS:HZ3 | 1.69 | 0.57 |
| 1:A:901:MET:HE2 | 1:A:2823:PHE:CZ | 2.38 | 0.57 |
| 1:A:1463:LEU:HD12 | 1:A:1466:ASN:HB2 | 1.86 | 0.57 |
| 1:A:2167:PRO:HA | 1:A:2170:GLN:HE21 | 1.69 | 0.57 |
| 1:A:3477:GLU:HG2 | 1:A:3478:GLU:H | 1.69 | 0.57 |
| 6:I:810:LEU:HB2 | 6:I:848:HIS:CG | 2.39 | 0.57 |
| 1:S:1629:CYS:SG | 1:S:1632:TRP:HZ3 | 2.27 | 0.57 |
| 1:S:1727:ARG:NH2 | 1:S:1770:GLN:O | 2.37 | 0.57 |
| 1:S:3575:LEU:HD22 | 1:S:3752:VAL:HG11 | 1.85 | 0.57 |
| 1:A:739:ASN:HA | 1:A:742:GLU:CD | 2.28 | 0.57 |
| 1:A:955:ALA:C | 1:A:957:PRO:HD3 | 2.29 | 0.57 |
| 1:A:981:ARG:O | 1:A:984:TYR:N | 2.36 | 0.57 |
| 1:A:1949:ILE:HG23 | 1:A:2100:LEU:HD13 | 1.86 | 0.57 |
| 1:A:2438:ILE:O | 1:A:2442:MET:HG3 | 2.05 | 0.57 |
| 2:B:275:ASN:OD1 | 3:C:431:ARG:NH1 | 2.37 | 0.57 |
| 3:C:62:ASP:HA | 3:C:103:GLN:HG2 | 1.86 | 0.57 |
| 1:S:1261:LEU:HD22 | 1:S:1336:THR:HG22 | 1.86 | 0.57 |
| 1:S:2538:ARG:HD2 | 1:S:2565:MET:SD | 2.44 | 0.57 |
| 1:S:3702:PRO:O | 1:S:3792:SER:OG | 2.23 | 0.57 |
| 2:T:193:LEU:HB3 | 2:T:198:ILE:HB | 1.85 | 0.57 |
| 7:d:32:DT:H2” | 7:d:33:DA:C8 | 2.40 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:125:ILE:H | 1:A:125:ILE:HD12 | 1.69 | 0.57 |
| 1:A:437:HIS:O | 1:A:441:MET:HG2 | 2.05 | 0.57 |
| 1:A:2869:LEU:HD22 | 1:A:2896:ALA:HB2 | 1.86 | 0.57 |
| 1:A:3531:TYR:CD2 | 1:A:3794:VAL:HB | 2.39 | 0.57 |
| 2:B:200:LEU:HD11 | 2:B:221:ILE:HA | 1.86 | 0.57 |
| 2:B:457:GLU:HG3 | 2:B:528:LEU:HD21 | 1.84 | 0.57 |
| 6:I:769:THR:HA | 6:I:773:GLN:NE2 | 2.19 | 0.57 |
| 3:L:354:ARG:HA | 2:T:365:SER:HB3 | 1.86 | 0.57 |
| 1:S:417:VAL:HA | 1:S:420:VAL:HG22 | 1.87 | 0.57 |
| 1:S:750:PRO:O | 1:S:753:GLN:HB2 | 2.04 | 0.57 |
| 1:S:785:MET:HA | 1:S:788:TYR:CZ | 2.40 | 0.57 |
| 1:S:939:MET:HE1 | 1:S:2781:PRO:HB3 | 1.86 | 0.57 |
| 1:S:1583:MET:HE3 | 1:S:1625:HIS:HB3 | 1.86 | 0.57 |
| 1:S:3946:PHE:HB2 | 1:S:4043:LYS:HD2 | 1.86 | 0.57 |
| 1:A:1168:LEU:HA | 1:A:1171:TRP:HB3 | 1.86 | 0.57 |
| 1:A:1632:TRP:HD1 | 1:A:1641:THR:HB | 1.69 | 0.57 |
| 1:A:3295:GLU:HA | 1:A:3298:LEU:HD12 | 1.87 | 0.57 |
| 1:A:3533:PHE:O | 1:A:3537:SER:OG | 2.20 | 0.57 |
| 1:A:3856:MET:HG3 | 1:A:3860:LYS:NZ | 2.19 | 0.57 |
| 3:C:342:VAL:HA | 3:C:393:VAL:HG12 | 1.86 | 0.57 |
| 3:C:656:ASN:ND2 | 3:C:690:GLU:OE1 | 2.37 | 0.57 |
| 6:I:721:VAL:HG23 | 6:I:742:PHE:CD2 | 2.39 | 0.57 |
| 3:L:220:GLY:O | 3:L:223:GLU:HB3 | 2.04 | 0.57 |
| 3:L:416:TYR:HA | 2:T:451:LYS:HB2 | 1.84 | 0.57 |
| 1:S:612:LEU:HG | 1:S:614:PRO:HD3 | 1.87 | 0.57 |
| 1:S:1614:GLN:HA | 1:S:1617:LYS:HE2 | 1.85 | 0.57 |
| 1:S:1766:LEU:HD13 | 1:S:1778:PHE:CD1 | 2.39 | 0.57 |
| 1:S:3278:GLN:OE1 | 1:S:3326:GLN:NE2 | 2.34 | 0.57 |
| 1:S:3820:MET:HE3 | 1:S:3825:LYS:HA | 1.85 | 0.57 |
| 2:T:71:TYR:OH | 2:T:115:ARG:NH2 | 2.36 | 0.57 |
| 7:d:21:DA:H2' | 7:d:22:DG:C2 | 2.39 | 0.57 |
| 1:A:127:ALA:O | 1:A:131:LEU:HG | 2.05 | 0.57 |
| 1:A:417:VAL:HA | 1:A:420:VAL:HG12 | 1.86 | 0.57 |
| 1:A:3254:LEU:HD13 | 1:A:3283:LEU:HD21 | 1.86 | 0.57 |
| 3:L:458:ILE:HG21 | 2:T:394:VAL:HG21 | 1.87 | 0.57 |
| 1:S:1406:LEU:HA | 1:S:1409:SER:HB3 | 1.86 | 0.57 |
| 1:S:2575:PRO:HA | 1:S:2786:LYS:HA | 1.86 | 0.57 |
| 1:S:3567:VAL:HG12 | 1:S:3696:ARG:HH21 | 1.68 | 0.57 |
| 1:S:3874:ARG:NH2 | 1:S:4117:LEU:O | 2.38 | 0.57 |
| 10:j:16:DA:H2" | 10:j:17:DT:C5 | 2.40 | 0.57 |
| 1:A:238:MET:HE2 | 1:A:283:SER:O | 2.05 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2328:ARG:NH1 | 1:A:2369:LYS:O | 2.37 | 0.57 |
| 1:A:3718:ARG:O | 1:A:3748:HIS:NE2 | 2.36 | 0.57 |
| 3:C:347:LYS:HB3 | 3:C:350:GLN:HG3 | 1.87 | 0.57 |
| 6:I:658:ILE:HD11 | 6:I:734:SER:HA | 1.87 | 0.57 |
| 6:I:879:ARG:HG3 | 6:I:886:PHE:HB2 | 1.86 | 0.57 |
| 1:S:326:MET:O | 1:S:330:ASN:N | 2.37 | 0.57 |
| 1:S:493:LYS:HD3 | 1:S:524:TYR:HB3 | 1.85 | 0.57 |
| 1:S:2261:SER:O | 1:S:2270:ASN:ND2 | 2.34 | 0.57 |
| 1:S:2563:LEU:HD13 | 1:S:2795:GLN:HB2 | 1.85 | 0.57 |
| 1:S:3509:ASP:HB2 | 1:S:3547:THR:HB | 1.86 | 0.57 |
| 2:T:47:ALA:HB1 | 2:T:171:ASN:HD21 | 1.68 | 0.57 |
| 7:d:19:DA:C6 | 8:e:39:DA:N1 | 2.73 | 0.57 |
| 1:A:261:ASP:HB3 | 1:A:265:TYR:CD2 | 2.40 | 0.57 |
| 1:A:395:MET:HE1 | 1:A:410:MET:SD | 2.44 | 0.57 |
| 1:A:1622:ILE:O | 1:A:1626:TRP:N | 2.38 | 0.57 |
| 1:A:3920:ILE:HG21 | 1:A:3942:PHE:HB3 | 1.84 | 0.57 |
| 2:B:286:ILE:HG21 | 3:C:320:ILE:HD13 | 1.86 | 0.57 |
| 3:C:270:GLU:HB2 | 3:C:487:PHE:HZ | 1.70 | 0.57 |
| 5:H:196:ASN:O | 5:H:200:ASN:ND2 | 2.37 | 0.57 |
| 1:S:3113:ASN:O | 1:S:3117:ILE:HG12 | 2.05 | 0.57 |
| 2:T:94:LYS:H | 2:T:103:TYR:HA | 1.69 | 0.57 |
| 2:T:421:ASP:OD1 | 2:T:425:ILE:N | 2.35 | 0.57 |
| 1:A:2365:ASN:ND2 | 1:A:2399:GLU:OE1 | 2.37 | 0.57 |
| 1:A:3009:LYS:HD2 | 1:A:3012:GLU:HB3 | 1.85 | 0.57 |
| 1:A:3622:ALA:HB2 | 1:A:3629:ARG:HH22 | 1.69 | 0.57 |
| 1:A:3762:GLN:NE2 | 1:A:3795:PRO:HD2 | 2.19 | 0.57 |
| 2:B:469:LEU:HD21 | 2:B:518:LEU:HG | 1.87 | 0.57 |
| 3:C:11:VAL:HG12 | 3:C:131:HIS:O | 2.05 | 0.57 |
| 5:G:6:SER:HB3 | 5:G:76:SER:HB2 | 1.87 | 0.57 |
| 3:L:359:ASN:ND2 | 2:T:362:LEU:O | 2.38 | 0.57 |
| 1:S:114:VAL:HG13 | 1:S:119:ARG:HE | 1.70 | 0.57 |
| 1:S:2887:PRO:O | 1:S:2891:ARG:HD3 | 2.05 | 0.57 |
| 1:S:3796:MET:HG2 | 1:S:3801:GLY:HA2 | 1.87 | 0.57 |
| 2:T:247:ARG:HG2 | 2:T:488:ARG:HH12 | 1.70 | 0.57 |
| 2:T:333:GLU:OE1 | 2:T:333:GLU:N | 2.32 | 0.57 |
| 1:A:655:LEU:O | 1:A:659:ARG:HG2 | 2.05 | 0.57 |
| 1:A:2239:LYS:HD3 | 1:A:2279:ILE:HG13 | 1.86 | 0.57 |
| 1:S:2365:ASN:HD22 | 1:S:2396:LEU:HG | 1.68 | 0.57 |
| 1:A:128:LEU:HD21 | 1:A:171:LEU:HD23 | 1.86 | 0.56 |
| 1:A:261:ASP:HB3 | 1:A:265:TYR:HD2 | 1.70 | 0.56 |
| 1:A:264:ARG:HE | 8:e:40:DT:H5' | 1.70 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2323:LEU:HA | 1:A:2326:ILE:HD12 | 1.87 | 0.56 |
| 1:A:2587:GLN:O | 1:A:2777:HIS:N | 2.38 | 0.56 |
| 1:A:3531:TYR:O | 1:A:3535:ILE:HG12 | 2.05 | 0.56 |
| 1:A:3931:ALA:O | 1:A:3935:GLY:N | 2.38 | 0.56 |
| 3:L:450:GLN:HB3 | 3:L:537:PHE:CZ | 2.40 | 0.56 |
| 5:P:187:LYS:HD2 | 5:Q:187:LYS:HG2 | 1.87 | 0.56 |
| 6:R:810:LEU:HD21 | 6:R:848:HIS:CD2 | 2.38 | 0.56 |
| 1:S:2524:PHE:O | 1:S:2530:ARG:NE | 2.35 | 0.56 |
| 1:S:3417:ALA:HA | 1:S:3446:VAL:HB | 1.87 | 0.56 |
| 1:S:3767:LEU:HA | 1:S:3770:VAL:HG22 | 1.87 | 0.56 |
| 1:A:756:PHE:O | 1:A:760:LEU:N | 2.30 | 0.56 |
| 1:A:1253:THR:O | 1:A:1257:LEU:HG | 2.05 | 0.56 |
| 1:A:2791:ILE:HA | 1:A:2794:LEU:HD12 | 1.86 | 0.56 |
| 1:A:3240:MET:HB2 | 1:A:3272:TRP:CH2 | 2.37 | 0.56 |
| 2:B:304:ASN:OD1 | 2:B:306:SER:OG | 2.20 | 0.56 |
| 3:L:636:ILE:O | 3:L:640:ARG:HG2 | 2.05 | 0.56 |
| 1:S:66:LEU:O | 1:S:70:ARG:CB | 2.53 | 0.56 |
| 1:S:144:MET:SD | 1:S:145:ASP:N | 2.79 | 0.56 |
| 1:S:294:PHE:O | 1:S:298:LEU:HG | 2.06 | 0.56 |
| 1:S:336:ASN:HA | 1:S:339:GLN:HB2 | 1.86 | 0.56 |
| 1:S:2133:LEU:HG | 1:S:2171:LEU:HD11 | 1.87 | 0.56 |
| 1:S:2331:MET:O | 1:S:2334:LYS:HG2 | 2.06 | 0.56 |
| 1:S:2414:GLN:OE1 | 1:S:2414:GLN:N | 2.35 | 0.56 |
| 1:S:2824:LYS:O | 1:S:2829:LYS:NZ | 2.33 | 0.56 |
| 2:T:420:LEU:HB3 | 2:T:424:LYS:HA | 1.86 | 0.56 |
| 1:A:309:LYS:O | 1:A:313:LEU:HG | 2.06 | 0.56 |
| 1:A:938:VAL:HA | 1:A:941:MET:HG3 | 1.86 | 0.56 |
| 1:A:1401:ASN:HA | 1:A:1404:LYS:HE2 | 1.87 | 0.56 |
| 1:A:2376:ASP:HB3 | 1:A:2404:ARG:HH22 | 1.70 | 0.56 |
| 1:A:3625:LEU:N | 1:A:3682:GLU:O | 2.38 | 0.56 |
| 2:B:275:ASN:ND2 | 2:B:277:VAL:O | 2.38 | 0.56 |
| 2:B:296:VAL:HA | 3:C:298:ASN:HB3 | 1.87 | 0.56 |
| 2:B:470:ARG:O | 4:D:202:ASP:N | 2.35 | 0.56 |
| 3:C:7:LYS:O | 3:C:128:GLU:N | 2.33 | 0.56 |
| 3:C:234:LEU:HD12 | 3:C:483:PRO:HG3 | 1.86 | 0.56 |
| 5:H:66:TYR:HE1 | 5:H:108:LEU:HD11 | 1.70 | 0.56 |
| 6:I:811:SER:N | 6:I:848:HIS:HB3 | 2.20 | 0.56 |
| 3:L:383:ALA:HB3 | 2:T:462:MET:HE2 | 1.86 | 0.56 |
| 3:L:451:LEU:HB3 | 2:T:388:LYS:HE3 | 1.88 | 0.56 |
| 3:L:457:LEU:O | 3:L:461:MET:N | 2.37 | 0.56 |
| 4:M:75:ARG:HD3 | 4:M:98:LEU:HD23 | 1.86 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:P:190:LYS:HZ1 | 5:Q:191:ILE:HG12 | 1.70 | 0.56 |
| 1:S:910:PHE:CE1 | 1:S:2807:GLN:HG3 | 2.39 | 0.56 |
| 1:S:1064:TYR:HA | 1:S:1106:ILE:HG21 | 1.86 | 0.56 |
| 1:S:1201:ASN:OD1 | 1:S:1202:ARG:N | 2.39 | 0.56 |
| 1:S:1224:PHE:HE1 | 1:S:1266:CYS:HB3 | 1.71 | 0.56 |
| 1:S:1490:GLY:O | 1:S:1502:SER:N | 2.39 | 0.56 |
| 1:S:2164:TRP:O | 1:S:2167:PRO:HD2 | 2.04 | 0.56 |
| 1:S:2514:ASN:HB3 | 1:S:2517:LEU:HB2 | 1.86 | 0.56 |
| 1:S:2535:THR:HA | 1:S:2565:MET:HE1 | 1.88 | 0.56 |
| 1:S:3857:LEU:HA | 1:S:3860:LYS:HE2 | 1.87 | 0.56 |
| 1:S:3882:LEU:HA | 1:S:3885:ARG:HG3 | 1.87 | 0.56 |
| 2:T:288:LEU:HD13 | 2:T:293:ASN:HA | 1.87 | 0.56 |
| 7:d:26:DT:H2' | 7:d:27:DT:H71 | 1.87 | 0.56 |
| 9:i:35:DT:O2 | 10:j:22:DG:N2 | 2.39 | 0.56 |
| 1:A:420:VAL:O | 1:A:424:LEU:N | 2.35 | 0.56 |
| 1:A:1946:ASN:HA | 1:A:1949:ILE:HD12 | 1.86 | 0.56 |
| 1:A:2944:THR:HG21 | 1:A:3977:THR:HG21 | 1.87 | 0.56 |
| 3:C:347:LYS:NZ | 3:C:387:LEU:O | 2.38 | 0.56 |
| 5:H:67:VAL:O | 5:H:71:ARG:HG3 | 2.06 | 0.56 |
| 3:L:279:VAL:HG23 | 2:T:317:LYS:HB2 | 1.86 | 0.56 |
| 3:L:524:THR:HA | 3:L:527:GLN:HG2 | 1.86 | 0.56 |
| 6:R:832:LYS:HE2 | 6:R:842:ALA:HB2 | 1.86 | 0.56 |
| 7:d:30:DT:H2' | 7:d:31:DT:C7 | 2.35 | 0.56 |
| 8:e:42:DA:H1' | 8:e:43:DT:H5' | 1.87 | 0.56 |
| 1:A:721:TYR:HB2 | 1:A:726:LEU:HB3 | 1.88 | 0.56 |
| 1:A:2208:ASP:OD1 | 1:A:2209:GLU:HG3 | 2.06 | 0.56 |
| 1:A:2390:HIS:HA | 1:A:2394:LYS:HE2 | 1.87 | 0.56 |
| 1:A:3603:LYS:HZ2 | 1:A:3647:GLY:H | 1.53 | 0.56 |
| 2:B:367:PHE:HZ | 2:B:369:TYR:HD1 | 1.54 | 0.56 |
| 1:S:124:LYS:HZ2 | 10:j:22:DG:H3' | 1.69 | 0.56 |
| 1:S:465:PHE:HE1 | 1:S:479:ILE:HG21 | 1.71 | 0.56 |
| 1:S:1304:HIS:HD2 | 1:S:1307:ILE:HG23 | 1.69 | 0.56 |
| 1:S:1458:LEU:HD11 | 1:S:1466:ASN:HD21 | 1.70 | 0.56 |
| 1:S:2234:ASN:O | 1:S:2238:ILE:HG12 | 2.06 | 0.56 |
| 1:S:2819:GLU:OE2 | 1:S:2822:LYS:NZ | 2.28 | 0.56 |
| 1:S:3267:LYS:HA | 1:S:3273:LEU:HD12 | 1.86 | 0.56 |
| 1:S:3454:LEU:HD22 | 1:S:3461:ALA:HB1 | 1.87 | 0.56 |
| 1:S:3718:ARG:O | 1:S:3743:HIS:N | 2.35 | 0.56 |
| 1:A:960:GLN:O | 1:A:964:ARG:NH1 | 2.38 | 0.56 |
| 1:A:1201:ASN:HB3 | 1:A:1207:TRP:HB2 | 1.88 | 0.56 |
| 1:A:1794:GLN:O | 1:A:1798:LEU:HG | 2.06 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2584:CYS:SG | 1:A:2585:GLU:N | 2.78 | 0.56 |
| 1:A:3564:GLN:HE22 | 1:A:3699:LEU:HD23 | 1.70 | 0.56 |
| 1:A:3963:LEU:HA | 1:A:3967:PHE:HD2 | 1.69 | 0.56 |
| 3:C:186:GLY:H | 3:C:232:ARG:NH1 | 2.02 | 0.56 |
| 3:C:500:HIS:HB3 | 3:C:503:GLU:HB2 | 1.88 | 0.56 |
| 4:M:198:GLY:H | 2:T:477:SER:HB2 | 1.71 | 0.56 |
| 1:S:50:VAL:O | 1:S:54:GLN:NE2 | 2.28 | 0.56 |
| 1:S:1824:LEU:O | 1:S:1828:LEU:HG | 2.05 | 0.56 |
| 1:S:2281:MET:HE1 | 1:S:2326:ILE:HA | 1.88 | 0.56 |
| 2:T:488:ARG:HG2 | 2:T:501:GLU:HB3 | 1.88 | 0.56 |
| 1:A:306:VAL:HA | 1:A:309:LYS:HG3 | 1.88 | 0.56 |
| 1:A:996:THR:HG23 | 1:A:1043:GLN:HE21 | 1.71 | 0.56 |
| 1:A:3114:TYR:HB2 | 1:A:3128:LYS:HE2 | 1.87 | 0.56 |
| 1:A:3786:LEU:HB3 | 1:A:3910:LEU:HD12 | 1.87 | 0.56 |
| 3:C:131:HIS:NE2 | 11:f:296:GLY:O | 2.26 | 0.56 |
| 3:C:229:GLU:OE1 | 3:C:229:GLU:N | 2.38 | 0.56 |
| 3:C:270:GLU:OE1 | 3:C:270:GLU:N | 2.39 | 0.56 |
| 3:L:308:GLU:O | 2:T:290:ARG:NH2 | 2.39 | 0.56 |
| 1:S:538:ASP:HA | 1:S:541:MET:HG2 | 1.87 | 0.56 |
| 1:S:1783:ARG:HH12 | 1:S:1829:TRP:HB3 | 1.70 | 0.56 |
| 1:S:3747:GLU:HG3 | 1:S:3749:PRO:HD3 | 1.88 | 0.56 |
| 1:A:87:LYS:HG2 | 1:A:831:LEU:HD13 | 1.88 | 0.56 |
| 1:A:535:LEU:HD12 | 1:A:637:LYS:HG3 | 1.88 | 0.56 |
| 1:A:1149:LYS:H | 1:A:1151:ARG:NH1 | 2.04 | 0.56 |
| 1:A:1307:ILE:HG23 | 1:A:1309:ALA:H | 1.70 | 0.56 |
| 1:A:1558:TYR:O | 1:A:1562:LEU:HG | 2.06 | 0.56 |
| 1:A:3138:ILE:O | 1:A:3142:ILE:HG23 | 2.05 | 0.56 |
| 1:A:3923:ARG:HH12 | 1:A:4121:TRP:HB3 | 1.70 | 0.56 |
| 2:B:206:LYS:HD2 | 2:B:234:GLU:HA | 1.88 | 0.56 |
| 5:H:194:LEU:HD23 | 5:H:197:LYS:HD3 | 1.86 | 0.56 |
| 3:L:497:ARG:HD3 | 3:L:501:PRO:HA | 1.87 | 0.56 |
| 6:R:721:VAL:HA | 6:R:742:PHE:HE2 | 1.70 | 0.56 |
| 1:A:438:LEU:O | 1:A:441:MET:HB2 | 2.06 | 0.56 |
| 1:A:772:ALA:HA | 1:A:775:GLU:OE2 | 2.05 | 0.56 |
| 1:A:2737:GLU:O | 1:A:2741:LEU:N | 2.37 | 0.56 |
| 1:A:3530:VAL:HG23 | 1:A:3531:TYR:H | 1.71 | 0.56 |
| 3:C:33:GLN:O | 3:C:37:VAL:HG23 | 2.05 | 0.56 |
| 3:C:432:GLN:NE2 | 4:D:191:LYS:H | 2.03 | 0.56 |
| 3:C:653:GLN:HA | 3:C:656:ASN:ND2 | 2.21 | 0.56 |
| 3:L:17:GLY:HA3 | 3:L:104:GLN:HE22 | 1.70 | 0.56 |
| 1:S:114:VAL:HA | 1:S:119:ARG:HH21 | 1.71 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:437:HIS:O | 1:S:441:MET:HG2 | 2.06 | 0.56 |
| 1:S:1632:TRP:CD1 | 1:S:1645:VAL:HG13 | 2.41 | 0.56 |
| 1:S:3730:ALA:HA | 1:S:3734:ARG:HA | 1.87 | 0.56 |
| 1:S:4071:ALA:HB1 | 1:S:4077:TYR:HE2 | 1.71 | 0.56 |
| 1:A:1058:SER:HA | 1:A:1061:LYS:HE2 | 1.88 | 0.56 |
| 1:A:2507:ILE:HA | 1:A:2510:LEU:HD12 | 1.86 | 0.56 |
| 1:A:2883:SER:O | 1:A:2885:GLN:NE2 | 2.26 | 0.56 |
| 1:A:3749:PRO:HB2 | 1:A:3805:TRP:HD1 | 1.71 | 0.56 |
| 2:B:63:SER:O | 2:B:67:ILE:HG12 | 2.06 | 0.56 |
| 2:B:122:PHE:CG | 2:B:131:PHE:HB2 | 2.41 | 0.56 |
| 2:B:300:THR:HA | 3:C:293:THR:HA | 1.87 | 0.56 |
| 2:B:301:ARG:O | 3:C:292:GLU:N | 2.21 | 0.56 |
| 3:C:411:HIS:N | 3:C:418:CYS:O | 2.23 | 0.56 |
| 5:H:174:THR:O | 5:H:178:LYS:HG2 | 2.06 | 0.56 |
| 6:I:721:VAL:HG23 | 6:I:742:PHE:HD2 | 1.69 | 0.56 |
| 4:M:40:TYR:HB3 | 4:M:47:LEU:HD11 | 1.88 | 0.56 |
| 5:Q:33:VAL:HG22 | 5:Q:46:THR:HB | 1.88 | 0.56 |
| 6:R:865:ILE:HG13 | 6:R:889:LEU:H | 1.69 | 0.56 |
| 1:S:100:ILE:HA | 1:S:103:TYR:HD2 | 1.71 | 0.56 |
| 1:S:195:ASN:O | 1:S:198:ARG:HG2 | 2.05 | 0.56 |
| 1:S:485:GLN:HA | 1:S:488:ILE:HD12 | 1.88 | 0.56 |
| 1:S:1043:GLN:NE2 | 1:S:1044:ILE:HG12 | 2.20 | 0.56 |
| 1:S:2942:ILE:O | 1:S:2945:SER:OG | 2.20 | 0.56 |
| 1:A:450:SER:O | 1:A:454:GLN:HG3 | 2.05 | 0.55 |
| 1:A:1420:ARG:HB2 | 1:A:1424:THR:HG22 | 1.88 | 0.55 |
| 1:A:1444:ASP:OD1 | 1:A:1445:ARG:N | 2.38 | 0.55 |
| 1:A:1671:VAL:O | 1:A:1675:TYR:N | 2.29 | 0.55 |
| 1:A:3698:GLU:HB2 | 1:A:3718:ARG:HD3 | 1.88 | 0.55 |
| 2:B:439:PHE:HB3 | 3:C:483:PRO:HA | 1.86 | 0.55 |
| 3:C:146:GLN:O | 3:C:150:ILE:N | 2.33 | 0.55 |
| 1:S:682:TYR:O | 1:S:700:LYS:NZ | 2.39 | 0.55 |
| 1:S:3487:ILE:HG12 | 1:S:3513:ALA:HB1 | 1.88 | 0.55 |
| 2:T:351:LYS:HD3 | 2:T:355:LEU:HB2 | 1.88 | 0.55 |
| 1:A:19:LEU:HB3 | 1:A:34:LEU:HD23 | 1.88 | 0.55 |
| 1:A:723:ASP:O | 1:A:724:GLU:HG2 | 2.06 | 0.55 |
| 1:A:1672:PHE:O | 1:A:1675:TYR:HB3 | 2.06 | 0.55 |
| 1:A:2391:GLY:O | 1:A:2431:ARG:NH2 | 2.39 | 0.55 |
| 1:A:2482:ASP:HA | 1:A:2485:ARG:HD2 | 1.88 | 0.55 |
| 1:A:3029:LYS:HE3 | 1:A:3074:GLN:HE22 | 1.71 | 0.55 |
| 1:A:3630:ARG:NH1 | 1:A:3630:ARG:O | 2.39 | 0.55 |
| 2:B:99:PHE:CD2 | 2:B:145:GLU:HG3 | 2.42 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:275:ASN:HB3 | 2:B:366:LEU:HD13 | 1.88 | 0.55 |
| 3:C:11:VAL:HG13 | 3:C:132:ILE:HD13 | 1.88 | 0.55 |
| 3:L:30:PRO:HG3 | 3:L:166:PRO:HG3 | 1.87 | 0.55 |
| 1:S:439:VAL:O | 1:S:442:GLN:HG3 | 2.05 | 0.55 |
| 1:S:1776:GLU:O | 1:S:1779:GLN:NE2 | 2.39 | 0.55 |
| 1:S:1844:VAL:HG23 | 1:S:1845:VAL:H | 1.70 | 0.55 |
| 1:S:2305:ASN:O | 1:S:2308:SER:OG | 2.24 | 0.55 |
| 1:S:2571:ASP:O | 1:S:2787:HIS:ND1 | 2.39 | 0.55 |
| 1:A:1867:ILE:O | 1:A:1871:MET:HG2 | 2.07 | 0.55 |
| 1:A:3266:SER:HA | 1:A:3272:TRP:CD1 | 2.37 | 0.55 |
| 1:A:3819:THR:HB | 1:A:3885:ARG:HG2 | 1.88 | 0.55 |
| 1:A:3820:MET:HA | 1:A:3885:ARG:HH21 | 1.71 | 0.55 |
| 3:C:360:GLN:HE21 | 3:C:362:LEU:HD21 | 1.72 | 0.55 |
| 5:G:180:PHE:O | 5:G:184:LEU:HG | 2.06 | 0.55 |
| 3:L:249:CYS:SG | 3:L:250:ARG:N | 2.77 | 0.55 |
| 3:L:600:VAL:O | 3:L:604:GLN:HB3 | 2.05 | 0.55 |
| 1:S:418:ALA:HB2 | 1:S:464:VAL:HG12 | 1.87 | 0.55 |
| 1:S:668:LYS:NZ | 1:S:728:SER:HB3 | 2.21 | 0.55 |
| 1:S:1580:LEU:HD13 | 1:S:1625:HIS:CE1 | 2.41 | 0.55 |
| 1:S:2427:ARG:HH12 | 1:S:2429:ASP:HA | 1.72 | 0.55 |
| 2:T:396:ALA:HB3 | 2:T:413:LEU:HB2 | 1.88 | 0.55 |
| 1:A:941:MET:HE1 | 1:A:962:TYR:CE1 | 2.42 | 0.55 |
| 1:A:1111:LEU:HB3 | 1:A:1186:LYS:HE2 | 1.88 | 0.55 |
| 1:A:1824:LEU:O | 1:A:1827:LEU:HD23 | 2.07 | 0.55 |
| 2:B:170:THR:H | 2:B:202:LEU:HD11 | 1.71 | 0.55 |
| 3:C:163:PHE:HE2 | 3:C:212:MET:HG2 | 1.72 | 0.55 |
| 3:C:688:LYS:NZ | 3:C:694:SER:OG | 2.29 | 0.55 |
| 5:H:67:VAL:HA | 5:H:70:LEU:HD12 | 1.88 | 0.55 |
| 6:I:707:ILE:HA | 6:I:710:LYS:HG2 | 1.88 | 0.55 |
| 3:L:133:GLU:CD | 11:m:297:LEU:H | 2.14 | 0.55 |
| 3:L:253:ILE:HD13 | 3:L:257:LEU:HG | 1.88 | 0.55 |
| 4:M:71:ASP:OD2 | 4:M:73:THR:OG1 | 2.23 | 0.55 |
| 5:P:61:MET:SD | 5:P:65:LYS:NZ | 2.79 | 0.55 |
| 1:S:751:ALA:O | 1:S:755:ALA:N | 2.35 | 0.55 |
| 1:S:832:LYS:HG2 | 1:S:834:LEU:HD22 | 1.89 | 0.55 |
| 2:T:212:ASP:HB2 | 2:T:231:VAL:HG13 | 1.88 | 0.55 |
| 1:A:727:ALA:O | 1:A:731:THR:OG1 | 2.23 | 0.55 |
| 1:A:1357:LYS:HE2 | 1:A:1410:PRO:HG2 | 1.88 | 0.55 |
| 1:A:2748:VAL:HG12 | 1:A:2752:LYS:HE2 | 1.88 | 0.55 |
| 1:A:2887:PRO:HA | 1:A:2890:ILE:HD12 | 1.89 | 0.55 |
| 1:A:3765:GLU:O | 1:A:3769:GLN:NE2 | 2.33 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3856:MET:HE2 | 1:A:4072:PRO:HB2 | 1.88 | 0.55 |
| 2:B:487:PHE:O | 2:B:490:LEU:N | 2.40 | 0.55 |
| 6:R:665:CYS:HB3 | 6:R:700:VAL:HG22 | 1.89 | 0.55 |
| 1:S:992:ILE:HG23 | 1:S:1036:PHE:CD2 | 2.41 | 0.55 |
| 1:S:1368:LEU:H | 1:S:1368:LEU:HD12 | 1.71 | 0.55 |
| 1:S:2196:TRP:CD1 | 1:S:2199:LEU:HB2 | 2.41 | 0.55 |
| 1:S:2365:ASN:OD1 | 1:S:2369:LYS:NZ | 2.36 | 0.55 |
| 1:S:2791:ILE:HA | 1:S:2794:LEU:HD12 | 1.88 | 0.55 |
| 1:S:3616:ALA:O | 1:S:3629:ARG:NH1 | 2.40 | 0.55 |
| 1:S:3677:PRO:HB2 | 1:S:3682:GLU:HB2 | 1.89 | 0.55 |
| 2:T:52:GLN:NE2 | 2:T:56:GLU:OE1 | 2.39 | 0.55 |
| 1:A:202:GLY:HA2 | 1:A:205:LYS:HD2 | 1.89 | 0.55 |
| 1:A:887:ASP:OD1 | 1:A:888:ARG:N | 2.39 | 0.55 |
| 1:A:2863:CYS:HB3 | 1:A:2892:LEU:HB3 | 1.87 | 0.55 |
| 3:C:162:GLN:CD | 11:f:295:ARG:H | 2.14 | 0.55 |
| 5:H:176:LEU:HA | 5:H:179:ARG:HD2 | 1.88 | 0.55 |
| 3:L:363:LYS:HG2 | 2:T:446:MET:SD | 2.47 | 0.55 |
| 3:L:484:ASN:HD21 | 3:L:486:ARG:HB2 | 1.71 | 0.55 |
| 5:Q:166:VAL:HG23 | 5:Q:169:LYS:NZ | 2.21 | 0.55 |
| 1:S:3091:LEU:HG | 1:S:3099:ALA:HB1 | 1.89 | 0.55 |
| 1:S:3256:MET:HA | 1:S:3256:MET:HE3 | 1.89 | 0.55 |
| 1:S:3525:TYR:CZ | 1:S:3705:TYR:HB3 | 2.42 | 0.55 |
| 1:S:4120:THR:HG21 | 1:S:4126:PRO:HB3 | 1.88 | 0.55 |
| 2:T:48:MET:HA | 2:T:59:PRO:HB2 | 1.88 | 0.55 |
| 2:T:183:ALA:HB1 | 2:T:187:ARG:HH21 | 1.71 | 0.55 |
| 1:A:294:PHE:O | 1:A:298:LEU:HG | 2.06 | 0.55 |
| 1:A:584:GLU:HB2 | 1:A:613:HIS:ND1 | 2.21 | 0.55 |
| 1:A:1963:GLN:OE1 | 1:A:2124:SER:HA | 2.06 | 0.55 |
| 1:A:3505:LEU:HD21 | 1:A:3510:GLN:HG2 | 1.88 | 0.55 |
| 1:A:3518:VAL:O | 1:A:3522:THR:HG22 | 2.07 | 0.55 |
| 1:A:3831:ASP:HB3 | 1:A:3832:PRO:HD3 | 1.87 | 0.55 |
| 1:A:3864:ARG:HG3 | 1:A:4085:LYS:HE3 | 1.89 | 0.55 |
| 1:A:3875:GLU:O | 1:A:3965:ARG:NH1 | 2.35 | 0.55 |
| 3:C:508:ILE:HG23 | 3:C:512:ILE:HD12 | 1.89 | 0.55 |
| 4:D:86:ALA:HB3 | 4:D:97:THR:HB | 1.89 | 0.55 |
| 5:Q:94:TYR:HE1 | 5:Q:113:LEU:HD13 | 1.72 | 0.55 |
| 1:S:1437:TYR:HB3 | 1:S:1502:SER:HB2 | 1.89 | 0.55 |
| 1:S:2464:HIS:N | 1:S:2470:ARG:HD3 | 2.22 | 0.55 |
| 1:S:2919:ASP:HA | 1:S:2922:ARG:HH11 | 1.72 | 0.55 |
| 2:T:439:PHE:H | 2:T:442:ASP:HB2 | 1.72 | 0.55 |
| 1:A:702:SER:O | 1:A:706:LEU:HG | 2.06 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2439:ILE:HD12 | 1:A:2454:LEU:HD21 | 1.87 | 0.55 |
| 1:A:3547:THR:HA | 1:A:3550:LYS:HZ3 | 1.71 | 0.55 |
| 1:A:3577:GLN:OE1 | 1:A:3629:ARG:NH1 | 2.39 | 0.55 |
| 1:A:3705:TYR:OH | 1:A:3713:PRO:O | 2.24 | 0.55 |
| 1:A:4055:ASN:HD21 | 1:A:4057:ALA:HB3 | 1.71 | 0.55 |
| 2:B:32:TYR:OH | 2:B:160:LYS:O | 2.24 | 0.55 |
| 2:B:357:LYS:HE2 | 2:B:359:HIS:HE1 | 1.72 | 0.55 |
| 3:C:643:ARG:HD3 | 3:C:655:PHE:CD1 | 2.42 | 0.55 |
| 3:L:280:ASP:HA | 3:L:289:ILE:HD11 | 1.88 | 0.55 |
| 5:P:194:LEU:HG | 5:P:197:LYS:HZ2 | 1.71 | 0.55 |
| 1:S:169:THR:HA | 1:S:172:GLU:HG2 | 1.87 | 0.55 |
| 1:S:1611:GLN:HE21 | 1:S:1614:GLN:HG3 | 1.71 | 0.55 |
| 1:S:3963:LEU:HB3 | 1:S:4124:TRP:HH2 | 1.72 | 0.55 |
| 2:T:82:LEU:HD12 | 2:T:108:LEU:O | 2.06 | 0.55 |
| 1:A:380:ASP:HA | 1:A:383:PHE:HB3 | 1.89 | 0.55 |
| 1:A:430:VAL:HG11 | 1:A:1643:MET:HG3 | 1.88 | 0.55 |
| 1:A:1231:GLN:O | 1:A:1235:ILE:HG13 | 2.07 | 0.55 |
| 1:A:1340:ARG:O | 1:A:1343:GLU:HG2 | 2.07 | 0.55 |
| 1:A:2185:MET:O | 1:A:2189:ILE:HG12 | 2.07 | 0.55 |
| 1:A:3348:LEU:O | 1:A:3352:GLU:N | 2.38 | 0.55 |
| 2:B:121:GLN:O | 2:B:130:ARG:NH1 | 2.40 | 0.55 |
| 2:B:351:LYS:O | 2:B:395:ALA:N | 2.29 | 0.55 |
| 2:B:444:ARG:N | 3:C:266:SER:O | 2.39 | 0.55 |
| 3:L:540:ILE:HD11 | 2:T:376:ILE:HD12 | 1.89 | 0.55 |
| 6:R:675:LYS:HD2 | 6:R:678:LEU:HD12 | 1.88 | 0.55 |
| 6:R:808:SER:OG | 6:R:811:SER:OG | 2.25 | 0.55 |
| 1:S:225:LYS:HG2 | 1:S:274:LEU:HB2 | 1.89 | 0.55 |
| 1:S:652:GLU:O | 1:S:655:LEU:HB3 | 2.07 | 0.55 |
| 1:S:895:ALA:HB2 | 1:S:904:VAL:HG22 | 1.89 | 0.55 |
| 1:S:913:ARG:HG3 | 1:S:2807:GLN:HE22 | 1.72 | 0.55 |
| 1:S:1766:LEU:HD11 | 1:S:1775:GLU:HG2 | 1.88 | 0.55 |
| 1:S:1820:VAL:HA | 1:S:1824:LEU:HD23 | 1.88 | 0.55 |
| 1:S:2986:PRO:O | 1:S:2991:LYS:NZ | 2.39 | 0.55 |
| 1:S:3506:LEU:HD21 | 1:S:3554:PHE:HB2 | 1.88 | 0.55 |
| 1:A:195:ASN:HA | 1:A:198:ARG:HE | 1.71 | 0.55 |
| 1:A:542:ASP:OD1 | 1:A:543:SER:N | 2.40 | 0.55 |
| 1:A:1948:ALA:O | 1:A:1952:ILE:HG12 | 2.06 | 0.55 |
| 1:A:2919:ASP:O | 1:A:2923:TRP:N | 2.35 | 0.55 |
| 1:A:3110:PHE:O | 1:A:3128:LYS:NZ | 2.23 | 0.55 |
| 1:A:3820:MET:O | 1:A:3822:GLN:NE2 | 2.40 | 0.55 |
| 2:B:41:LEU:HB3 | 2:B:88:TYR:CE1 | 2.42 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:39:LEU:HD21 | 4:D:96:LEU:HD22 | 1.88 | 0.55 |
| 1:S:174:VAL:O | 1:S:178:LEU:N | 2.34 | 0.55 |
| 1:S:306:VAL:HA | 1:S:309:LYS:HG3 | 1.88 | 0.55 |
| 1:S:658:THR:HG1 | 1:S:659:ARG:NH1 | 2.05 | 0.55 |
| 1:S:1146:ASN:HB3 | 1:S:1199:PRO:HB3 | 1.89 | 0.55 |
| 1:S:2321:GLU:HA | 1:S:2366:LYS:HG2 | 1.89 | 0.55 |
| 1:S:3532:PRO:HA | 1:S:3535:ILE:HG22 | 1.89 | 0.55 |
| 1:S:3951:GLN:HA | 1:S:4068:HIS:HB2 | 1.89 | 0.55 |
| 2:T:103:TYR:CG | 2:T:135:MET:HE1 | 2.41 | 0.55 |
| 1:A:899:ARG:NH1 | 1:A:2565:MET:O | 2.36 | 0.54 |
| 1:A:1086:TYR:CE1 | 1:A:1133:HIS:HB3 | 2.41 | 0.54 |
| 1:A:1357:LYS:O | 1:A:1360:LYS:HB3 | 2.06 | 0.54 |
| 1:A:3249:GLN:HB2 | 1:A:3251:ASN:OD1 | 2.07 | 0.54 |
| 1:A:3264:LYS:HD3 | 1:A:3267:LYS:HZ1 | 1.73 | 0.54 |
| 1:A:3760:GLN:O | 1:A:3764:VAL:HG23 | 2.06 | 0.54 |
| 2:B:335:GLU:O | 2:B:339:ARG:N | 2.40 | 0.54 |
| 2:B:362:LEU:HD23 | 2:B:436:PHE:HB3 | 1.89 | 0.54 |
| 3:C:645:GLU:HA | 3:C:648:LYS:HE2 | 1.89 | 0.54 |
| 4:D:7:PRO:HD3 | 4:D:77:ARG:HH21 | 1.72 | 0.54 |
| 6:R:739:GLN:HE21 | 6:R:741:ARG:HG2 | 1.71 | 0.54 |
| 1:S:672:ILE:O | 1:S:676:ASN:ND2 | 2.39 | 0.54 |
| 1:S:1665:HIS:H | 1:S:1668:PHE:HB3 | 1.71 | 0.54 |
| 1:S:1750:LEU:HD13 | 1:S:1758:LEU:HB2 | 1.88 | 0.54 |
| 1:S:3090:TYR:O | 1:S:3095:ASP:N | 2.40 | 0.54 |
| 1:S:3262:LEU:O | 1:S:3266:SER:N | 2.39 | 0.54 |
| 1:S:3515:GLN:HA | 1:S:3518:VAL:HG12 | 1.88 | 0.54 |
| 1:A:1128:CYS:HA | 1:A:1131:ILE:HG12 | 1.89 | 0.54 |
| 1:A:1748:ASP:OD1 | 1:A:1749:ALA:N | 2.40 | 0.54 |
| 1:A:2257:PHE:HA | 1:A:2260:PHE:CE2 | 2.41 | 0.54 |
| 1:A:2268:LYS:HB2 | 1:A:2314:GLU:OE2 | 2.07 | 0.54 |
| 1:A:2495:SER:HA | 1:A:2498:ILE:HD12 | 1.88 | 0.54 |
| 1:A:3107:ILE:HD13 | 1:A:3135:LEU:HD13 | 1.89 | 0.54 |
| 1:A:3358:ARG:O | 1:A:3362:LEU:HG | 2.07 | 0.54 |
| 1:A:4093:GLU:N | 1:A:4093:GLU:OE1 | 2.40 | 0.54 |
| 2:B:410:PHE:HB3 | 2:B:437:LEU:HD12 | 1.88 | 0.54 |
| 3:L:298:ASN:ND2 | 2:T:294:GLU:OE2 | 2.38 | 0.54 |
| 1:S:374:LYS:HZ2 | 1:S:424:LEU:HD12 | 1.72 | 0.54 |
| 1:S:449:TYR:HB2 | 1:S:454:GLN:HE21 | 1.72 | 0.54 |
| 1:S:989:MET:HE1 | 1:S:2779:ASP:HA | 1.89 | 0.54 |
| 1:S:2410:GLU:O | 1:S:2414:GLN:NE2 | 2.40 | 0.54 |
| 1:S:2825:THR:HG23 | 1:S:2828:GLU:H | 1.72 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3416:LEU:HG | 1:S:3446:VAL:HG12 | 1.89 | 0.54 |
| 1:S:3448:GLU:HG2 | 1:S:3452:LYS:HE3 | 1.88 | 0.54 |
| 1:A:939:MET:SD | 1:A:2783:ILE:HG23 | 2.47 | 0.54 |
| 1:A:1614:GLN:O | 1:A:1618:LEU:HG | 2.07 | 0.54 |
| 1:A:2424:MET:O | 1:A:2432:GLN:NE2 | 2.37 | 0.54 |
| 1:A:3493:TRP:CZ3 | 1:A:3521:ILE:HA | 2.43 | 0.54 |
| 1:A:3888:VAL:HA | 1:A:3891:SER:HB3 | 1.89 | 0.54 |
| 1:A:4011:PHE:CD1 | 1:A:4014:LYS:HD3 | 2.42 | 0.54 |
| 2:B:35:ARG:NH1 | 2:B:80:ARG:O | 2.41 | 0.54 |
| 2:B:329:LEU:HD13 | 3:C:276:TRP:HH2 | 1.72 | 0.54 |
| 2:B:452:ILE:C | 2:B:453:MET:HE2 | 2.32 | 0.54 |
| 2:B:469:LEU:HD22 | 2:B:514:MET:HG3 | 1.90 | 0.54 |
| 3:C:138:LEU:HD12 | 3:C:167:PHE:HZ | 1.73 | 0.54 |
| 3:L:602:VAL:HG12 | 3:L:609:PHE:HD2 | 1.71 | 0.54 |
| 4:M:23:TYR:CE2 | 4:M:40:TYR:HB2 | 2.43 | 0.54 |
| 1:S:3011:LEU:HB3 | 1:S:3047:SER:OG | 2.08 | 0.54 |
| 1:S:3579:SER:HB2 | 1:S:3583:LEU:HD12 | 1.90 | 0.54 |
| 1:A:575:ILE:O | 1:A:579:LEU:HG | 2.06 | 0.54 |
| 1:A:639:ALA:HB3 | 1:A:680:ILE:HG21 | 1.88 | 0.54 |
| 1:A:1038:LYS:HA | 1:A:1041:ILE:HD12 | 1.88 | 0.54 |
| 1:A:1775:GLU:O | 1:A:1778:PHE:HB3 | 2.07 | 0.54 |
| 1:A:2356:MET:HE1 | 1:A:2359:LYS:H | 1.71 | 0.54 |
| 2:B:44:ALA:O | 2:B:138:GLY:N | 2.40 | 0.54 |
| 3:L:133:GLU:OE2 | 11:m:297:LEU:N | 2.40 | 0.54 |
| 3:L:347:LYS:HB3 | 3:L:350:GLN:HG3 | 1.89 | 0.54 |
| 1:S:111:CYS:SG | 1:S:130:LEU:HG | 2.46 | 0.54 |
| 1:S:264:ARG:HE | 9:i:40:DT:H4' | 1.73 | 0.54 |
| 1:S:1783:ARG:CZ | 1:S:1830:HIS:HB2 | 2.37 | 0.54 |
| 1:S:3574:ALA:HB2 | 1:S:3684:SER:HB3 | 1.89 | 0.54 |
| 2:T:362:LEU:HD13 | 2:T:438:PRO:HB3 | 1.88 | 0.54 |
| 1:A:865:GLN:OE1 | 1:A:3170:ASP:HA | 2.08 | 0.54 |
| 1:A:3504:ALA:HA | 1:A:3536:SER:HB2 | 1.88 | 0.54 |
| 1:A:3822:GLN:HA | 1:A:3825:LYS:HB3 | 1.90 | 0.54 |
| 2:B:267:ILE:HD11 | 3:C:534:LYS:HB3 | 1.88 | 0.54 |
| 2:B:366:LEU:O | 2:B:434:LEU:N | 2.36 | 0.54 |
| 5:H:3:ARG:NH1 | 5:H:23:SER:HB2 | 2.22 | 0.54 |
| 3:L:354:ARG:HH12 | 2:T:428:THR:HG23 | 1.73 | 0.54 |
| 1:S:527:TYR:O | 1:S:531:PHE:N | 2.39 | 0.54 |
| 1:S:777:SER:HA | 1:S:785:MET:HE1 | 1.90 | 0.54 |
| 1:A:462:VAL:O | 1:A:466:LEU:HG | 2.08 | 0.54 |
| 1:A:947:GLN:OE1 | 1:A:948:MET:HG2 | 2.08 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2826:LEU:HA | 1:A:2829:LYS:HE2 | 1.90 | 0.54 |
| 1:A:3422:GLN:N | 1:A:3425:ARG:HH21 | 2.05 | 0.54 |
| 1:A:4049:ARG:HH22 | 1:A:4062:ASP:HB2 | 1.73 | 0.54 |
| 2:B:339:ARG:HA | 2:B:405:ASN:HA | 1.89 | 0.54 |
| 5:H:187:LYS:O | 5:H:190:LYS:HG2 | 2.08 | 0.54 |
| 6:R:845:LEU:HD21 | 6:R:852:VAL:HG13 | 1.89 | 0.54 |
| 1:S:789:TYR:HD1 | 1:S:792:ILE:HD12 | 1.73 | 0.54 |
| 1:S:2203:THR:HB | 1:S:2248:CYS:HB3 | 1.90 | 0.54 |
| 1:S:2319:ALA:O | 1:S:2323:LEU:HG | 2.08 | 0.54 |
| 1:S:3037:GLN:HB3 | 1:S:3044:MET:HE1 | 1.89 | 0.54 |
| 1:S:3921:GLY:HA3 | 1:S:3959:MET:HG2 | 1.89 | 0.54 |
| 9:i:39:DA:N6 | 10:j:19:DA:H61 | 2.06 | 0.54 |
| 9:i:42:DA:H2 | 10:j:15:DA:H5' | 1.73 | 0.54 |
| 1:A:638:GLN:HG3 | 1:A:640:GLU:OE1 | 2.07 | 0.54 |
| 1:A:891:ARG:HH21 | 1:A:961:LEU:HD23 | 1.72 | 0.54 |
| 1:A:1257:LEU:HA | 1:A:1260:LEU:HD12 | 1.89 | 0.54 |
| 1:A:1710:LEU:O | 1:A:1714:LEU:HG | 2.08 | 0.54 |
| 1:A:2125:TRP:O | 1:A:2128:PHE:N | 2.41 | 0.54 |
| 1:A:2362:VAL:HG12 | 1:A:2366:LYS:HZ3 | 1.73 | 0.54 |
| 1:A:3077:ILE:HG23 | 1:A:3081:HIS:HD2 | 1.72 | 0.54 |
| 2:B:109:ASP:HB3 | 2:B:115:ARG:CZ | 2.37 | 0.54 |
| 3:C:247:TRP:CZ2 | 3:C:338:LYS:HG3 | 2.43 | 0.54 |
| 5:G:188:LYS:HA | 5:G:191:ILE:HD12 | 1.89 | 0.54 |
| 3:L:239:LYS:HG3 | 11:m:294:PRO:O | 2.08 | 0.54 |
| 3:L:376:ALA:O | 3:L:380:LEU:HG | 2.08 | 0.54 |
| 1:S:1947:CYS:O | 1:S:1950:SER:OG | 2.20 | 0.54 |
| 2:T:87:PHE:CE2 | 2:T:105:LEU:HB2 | 2.43 | 0.54 |
| 2:T:204:HIS:N | 2:T:237:SER:OG | 2.30 | 0.54 |
| 2:T:348:MET:HB2 | 2:T:397:LEU:HG | 1.90 | 0.54 |
| 9:i:27:DC:H2' | 9:i:28:DT:C6 | 2.43 | 0.54 |
| 1:A:2303:LEU:HB3 | 1:A:2323:LEU:HD21 | 1.88 | 0.54 |
| 1:A:2470:ARG:NH1 | 1:A:2513:GLU:OE2 | 2.40 | 0.54 |
| 1:A:2497:GLU:HA | 1:A:2500:LYS:HE2 | 1.90 | 0.54 |
| 1:A:3287:ARG:O | 1:A:3289:ARG:NH1 | 2.41 | 0.54 |
| 3:L:676:GLU:HG3 | 3:L:677:ILE:H | 1.73 | 0.54 |
| 1:S:316:LEU:O | 1:S:320:LEU:HG | 2.08 | 0.54 |
| 1:S:460:ALA:O | 1:S:464:VAL:HG13 | 2.08 | 0.54 |
| 1:S:584:GLU:O | 1:S:613:HIS:N | 2.40 | 0.54 |
| 1:S:1128:CYS:HA | 1:S:1131:ILE:HG12 | 1.89 | 0.54 |
| 1:S:1583:MET:HG2 | 1:S:1625:HIS:HB3 | 1.90 | 0.54 |
| 1:S:3932:MET:N | 1:S:3932:MET:SD | 2.81 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:75:ILE:HG13 | 2:T:111:PRO:HG2 | 1.89 | 0.54 |
| 2:T:146:VAL:HA | 2:T:149:VAL:HG22 | 1.89 | 0.54 |
| 7:d:34:DT:O2 | 8:e:23:DT:N3 | 2.41 | 0.54 |
| 1:A:461:ILE:O | 1:A:464:VAL:HG22 | 2.07 | 0.54 |
| 1:A:849:GLU:H | 1:A:849:GLU:CD | 2.14 | 0.54 |
| 1:A:1184:ARG:HD3 | 1:A:1266:CYS:SG | 2.47 | 0.54 |
| 1:A:2524:PHE:HA | 1:A:2530:ARG:HH21 | 1.72 | 0.54 |
| 1:A:2776:ARG:NE | 1:A:2782:ASP:OD2 | 2.39 | 0.54 |
| 1:A:3011:LEU:HA | 1:A:3014:CYS:HB3 | 1.89 | 0.54 |
| 1:A:3049:LEU:HA | 1:A:3052:LEU:HB2 | 1.89 | 0.54 |
| 1:A:3148:GLN:OE1 | 1:A:3148:GLN:N | 2.41 | 0.54 |
| 1:A:3260:LYS:O | 1:A:3264:LYS:HG2 | 2.08 | 0.54 |
| 2:B:68:GLN:HE22 | 2:B:119:LEU:HB2 | 1.72 | 0.54 |
| 6:I:812:MET:C | 6:I:850:ALA:HB3 | 2.33 | 0.54 |
| 3:L:655:PHE:HA | 3:L:658:PHE:HB2 | 1.89 | 0.54 |
| 6:R:750:THR:HA | 6:R:753:HIS:HB3 | 1.89 | 0.54 |
| 1:S:542:ASP:OD1 | 1:S:543:SER:N | 2.39 | 0.54 |
| 1:A:2860:ASP:O | 1:A:2864:GLN:HG3 | 2.08 | 0.54 |
| 1:A:2987:THR:HG23 | 1:A:2990:GLU:H | 1.72 | 0.54 |
| 1:A:3169:PRO:HB3 | 1:A:3182:ILE:HG21 | 1.90 | 0.54 |
| 1:A:3236:PHE:HA | 1:A:3239:LYS:HD2 | 1.89 | 0.54 |
| 1:A:3748:HIS:HB3 | 1:A:3750:PHE:CE1 | 2.43 | 0.54 |
| 2:B:353:LEU:HD23 | 2:B:395:ALA:HB2 | 1.90 | 0.54 |
| 2:B:398:CYS:SG | 2:B:399:ARG:N | 2.81 | 0.54 |
| 3:C:18:PHE:N | 3:C:104:GLN:OE1 | 2.41 | 0.54 |
| 3:L:9:ALA:N | 3:L:129:LYS:O | 2.31 | 0.54 |
| 3:L:342:VAL:HA | 3:L:393:VAL:HA | 1.89 | 0.54 |
| 1:S:1632:TRP:HB2 | 1:S:1633:TRP:HD1 | 1.72 | 0.54 |
| 1:S:1795:VAL:HG13 | 1:S:1839:PHE:HD1 | 1.73 | 0.54 |
| 1:S:3162:ASN:OD1 | 1:S:3163:THR:N | 2.40 | 0.54 |
| 1:S:3190:LEU:HB2 | 1:S:3235:LYS:HE3 | 1.89 | 0.54 |
| 1:S:3980:MET:HE2 | 1:S:3980:MET:HA | 1.90 | 0.54 |
| 1:S:4045:CYS:HA | 1:S:4048:LYS:HG2 | 1.88 | 0.54 |
| 1:S:4113:ASP:O | 1:S:4117:LEU:HG | 2.08 | 0.54 |
| 8:e:21:DA:H2" | 8:e:22:DA:C8 | 2.43 | 0.54 |
| 1:A:100:ILE:HG22 | 1:A:103:TYR:HB2 | 1.90 | 0.53 |
| 1:A:359:LEU:O | 1:A:363:ILE:HG13 | 2.07 | 0.53 |
| 1:A:1456:LYS:HE3 | 1:A:1516:GLU:HG3 | 1.89 | 0.53 |
| 1:A:2295:GLN:HG3 | 1:A:2298:GLU:HG3 | 1.90 | 0.53 |
| 1:A:2319:ALA:O | 1:A:2323:LEU:HG | 2.07 | 0.53 |
| 2:B:113:ALA:O | 2:B:117:LEU:HG | 2.08 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1574:ASN:HD21 | 1:S:1577:LEU:HB2 | 1.73 | 0.53 |
| 1:S:2268:LYS:HB3 | 1:S:2315:VAL:HG22 | 1.89 | 0.53 |
| 1:S:2586:PHE:HD2 | 1:S:2776:ARG:HH21 | 1.56 | 0.53 |
| 1:S:3010:SER:HA | 1:S:3013:TYR:CD2 | 2.43 | 0.53 |
| 2:T:64:ILE:HG22 | 2:T:123:LYS:HE3 | 1.89 | 0.53 |
| 1:A:1250:LEU:HB2 | 1:A:1329:ARG:HH22 | 1.72 | 0.53 |
| 1:A:2884:LEU:O | 1:A:2886:GLN:NE2 | 2.40 | 0.53 |
| 1:A:2981:TRP:HD1 | 1:A:2985:GLU:HG2 | 1.72 | 0.53 |
| 1:A:3269:ARG:HE | 1:A:3272:TRP:HB2 | 1.73 | 0.53 |
| 1:A:3380:ARG:O | 1:A:3384:HIS:ND1 | 2.41 | 0.53 |
| 1:A:3881:ASP:OD1 | 1:A:3884:LYS:HB2 | 2.08 | 0.53 |
| 3:C:295:TYR:OH | 3:C:307:LYS:NZ | 2.32 | 0.53 |
| 3:C:487:PHE:HA | 3:C:490:LEU:HD12 | 1.89 | 0.53 |
| 5:H:36:LEU:HG | 5:H:43:TRP:HE3 | 1.73 | 0.53 |
| 4:M:90:GLN:HG3 | 4:M:91:GLU:H | 1.74 | 0.53 |
| 1:S:2462:VAL:HA | 1:S:2473:MET:HE1 | 1.90 | 0.53 |
| 1:S:2751:GLN:O | 1:S:2755:LYS:HG2 | 2.09 | 0.53 |
| 1:S:2803:ILE:HA | 1:S:2806:LYS:HG2 | 1.89 | 0.53 |
| 1:S:3780:ALA:HB1 | 1:S:3784:ARG:HH22 | 1.72 | 0.53 |
| 1:A:476:ARG:HH12 | 1:A:1562:LEU:HD23 | 1.73 | 0.53 |
| 1:A:560:LEU:O | 1:A:564:LEU:HG | 2.09 | 0.53 |
| 1:A:772:ALA:HA | 1:A:775:GLU:CD | 2.33 | 0.53 |
| 1:A:1639:LEU:C | 1:A:1643:MET:HE3 | 2.33 | 0.53 |
| 1:A:2587:GLN:N | 1:A:2777:HIS:O | 2.42 | 0.53 |
| 1:A:2866:ALA:O | 1:A:2899:ARG:NH2 | 2.40 | 0.53 |
| 3:C:71:GLY:C | 3:C:73:GLN:H | 2.15 | 0.53 |
| 3:C:598:PHE:HB2 | 3:C:612:ALA:HB1 | 1.90 | 0.53 |
| 3:L:96:SER:OG | 3:L:97:LYS:NZ | 2.35 | 0.53 |
| 3:L:291:LYS:HB3 | 2:T:302:THR:HG22 | 1.91 | 0.53 |
| 3:L:327:ASP:O | 3:L:330:GLN:NE2 | 2.38 | 0.53 |
| 3:L:342:VAL:HG23 | 3:L:393:VAL:HG22 | 1.91 | 0.53 |
| 5:P:179:ARG:HA | 5:P:182:LEU:CD2 | 2.38 | 0.53 |
| 1:S:348:ILE:HG22 | 1:S:359:LEU:HD23 | 1.90 | 0.53 |
| 1:S:1675:TYR:CE1 | 1:S:1679:LEU:HD21 | 2.42 | 0.53 |
| 1:S:2365:ASN:ND2 | 1:S:2396:LEU:HG | 2.22 | 0.53 |
| 1:S:2512:ASP:N | 1:S:2518:GLN:HE21 | 2.05 | 0.53 |
| 1:S:2880:CYS:HA | 1:S:2885:GLN:HB2 | 1.90 | 0.53 |
| 1:S:3915:HIS:CE1 | 1:S:3921:GLY:HA2 | 2.43 | 0.53 |
| 2:T:174:ASN:O | 2:T:177:GLY:N | 2.42 | 0.53 |
| 1:A:1200:GLY:O | 1:A:1202:ARG:NH1 | 2.42 | 0.53 |
| 1:A:1256:TRP:CE2 | 1:A:1260:LEU:HD11 | 2.44 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2745:ARG:HE | 8:e:44:DG:H2' | 1.72 | 0.53 |
| 1:A:2810:SER:HB2 | 1:A:2864:GLN:HE22 | 1.73 | 0.53 |
| 1:A:3045:ILE:HA | 1:A:3048:LYS:HB2 | 1.90 | 0.53 |
| 1:A:3682:GLU:HA | 1:A:3688:SER:HB3 | 1.89 | 0.53 |
| 2:B:102:ILE:HG13 | 2:B:145:GLU:HB3 | 1.90 | 0.53 |
| 2:B:353:LEU:HD22 | 2:B:414:VAL:HG23 | 1.91 | 0.53 |
| 2:B:421:ASP:OD1 | 2:B:425:ILE:N | 2.34 | 0.53 |
| 2:B:472:THR:N | 4:D:202:ASP:OD2 | 2.40 | 0.53 |
| 3:C:305:VAL:HG13 | 3:C:309:ASP:HB2 | 1.89 | 0.53 |
| 5:H:171:ALA:O | 5:H:174:THR:OG1 | 2.20 | 0.53 |
| 3:L:297:LEU:N | 3:L:303:THR:O | 2.34 | 0.53 |
| 3:L:695:SER:O | 3:L:699:GLU:HG2 | 2.09 | 0.53 |
| 6:R:728:GLU:OE1 | 6:R:741:ARG:NH2 | 2.37 | 0.53 |
| 1:S:1867:ILE:HG22 | 1:S:1871:MET:SD | 2.49 | 0.53 |
| 1:S:2429:ASP:O | 1:S:2433:LYS:HG3 | 2.09 | 0.53 |
| 1:S:3574:ALA:CB | 1:S:3684:SER:HB3 | 2.38 | 0.53 |
| 1:S:4049:ARG:HG2 | 1:S:4054:ALA:HB2 | 1.91 | 0.53 |
| 2:T:142:SER:OG | 2:T:185:ARG:NH1 | 2.40 | 0.53 |
| 1:A:209:THR:O | 1:A:212:VAL:HG22 | 2.08 | 0.53 |
| 1:A:1274:ARG:HH11 | 1:A:1351:THR:HB | 1.74 | 0.53 |
| 1:A:2430:GLU:OE1 | 1:A:2430:GLU:N | 2.41 | 0.53 |
| 1:A:2576:MET:HE3 | 1:A:2790:LEU:HD21 | 1.90 | 0.53 |
| 1:A:2776:ARG:HH21 | 1:A:2782:ASP:HB2 | 1.73 | 0.53 |
| 1:A:3018:SER:HG | 1:A:3031:TRP:CD1 | 2.27 | 0.53 |
| 1:A:3274:VAL:HG11 | 1:A:3311:ASN:HB2 | 1.89 | 0.53 |
| 1:A:3567:VAL:HG21 | 1:A:3696:ARG:HD3 | 1.89 | 0.53 |
| 1:A:3779:SER:O | 1:A:3782:SER:OG | 2.25 | 0.53 |
| 3:C:496:HIS:CG | 3:C:506:PRO:HD3 | 2.43 | 0.53 |
| 6:I:709:VAL:HA | 6:I:712:ILE:HG12 | 1.91 | 0.53 |
| 6:I:812:MET:O | 6:I:850:ALA:HB3 | 2.08 | 0.53 |
| 5:P:184:LEU:O | 5:P:188:LYS:HG2 | 2.08 | 0.53 |
| 1:S:935:HIS:CD2 | 1:S:987:LEU:HD21 | 2.44 | 0.53 |
| 1:S:2477:LEU:HD13 | 1:S:2505:VAL:HG13 | 1.90 | 0.53 |
| 1:S:2574:ASN:O | 1:S:2787:HIS:ND1 | 2.38 | 0.53 |
| 1:A:165:LYS:NZ | 8:e:30:DA:H3' | 2.23 | 0.53 |
| 1:A:192:ASN:O | 1:A:196:LEU:HG | 2.09 | 0.53 |
| 1:A:717:LYS:NZ | 1:A:1120:SER:O | 2.41 | 0.53 |
| 1:A:892:LEU:HA | 1:A:944:LYS:HE2 | 1.89 | 0.53 |
| 1:A:1091:GLU:OE1 | 1:A:1091:GLU:N | 2.42 | 0.53 |
| 1:A:1224:PHE:HE1 | 1:A:1266:CYS:HB2 | 1.74 | 0.53 |
| 1:A:2141:ASN:O | 1:A:2144:LEU:HG | 2.09 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3953:LEU:HB3 | 1:A:3955:VAL:HG12 | 1.89 | 0.53 |
| 2:B:325:ARG:HE | 2:B:327:ILE:HG12 | 1.73 | 0.53 |
| 2:B:493:LEU:HG | 6:I:708:ARG:HD2 | 1.90 | 0.53 |
| 3:L:11:VAL:HG12 | 3:L:131:HIS:O | 2.08 | 0.53 |
| 1:S:2269:ASP:OD1 | 1:S:2270:ASN:N | 2.41 | 0.53 |
| 1:S:2586:PHE:HB2 | 1:S:2776:ARG:HE | 1.72 | 0.53 |
| 1:S:3622:ALA:HB3 | 1:S:3630:ARG:HE | 1.72 | 0.53 |
| 2:T:83:LEU:O | 2:T:109:ASP:N | 2.38 | 0.53 |
| 1:A:108:LYS:NZ | 1:A:145:ASP:O | 2.42 | 0.53 |
| 1:A:447:PRO:HB2 | 1:A:519:TRP:HZ2 | 1.73 | 0.53 |
| 1:A:460:ALA:O | 1:A:464:VAL:HG13 | 2.09 | 0.53 |
| 1:A:677:ALA:O | 1:A:681:LYS:N | 2.42 | 0.53 |
| 1:A:1327:GLY:HA2 | 1:A:1330:TYR:HB3 | 1.91 | 0.53 |
| 1:A:1418:HIS:O | 1:A:1422:LYS:NZ | 2.42 | 0.53 |
| 1:A:1526:GLU:CD | 1:A:1526:GLU:H | 2.16 | 0.53 |
| 1:A:2869:LEU:HB2 | 1:A:2899:ARG:HH21 | 1.74 | 0.53 |
| 2:B:91:GLU:HG3 | 2:B:139:SER:HB3 | 1.91 | 0.53 |
| 2:B:142:SER:HA | 2:B:176:HIS:CD2 | 2.44 | 0.53 |
| 3:C:8:ALA:HA | 3:C:129:LYS:H | 1.73 | 0.53 |
| 3:C:9:ALA:O | 3:C:131:HIS:HB3 | 2.07 | 0.53 |
| 3:C:251:LEU:HD13 | 3:C:340:PHE:CD2 | 2.44 | 0.53 |
| 3:C:297:LEU:HB3 | 3:C:299:ASP:OD1 | 2.08 | 0.53 |
| 3:C:732:ILE:HA | 1:S:1910:GLU:HA | 1.91 | 0.53 |
| 5:G:13:GLU:OE2 | 5:G:90:LYS:NZ | 2.40 | 0.53 |
| 5:H:43:TRP:CD1 | 5:H:115:LYS:HZ3 | 2.26 | 0.53 |
| 6:I:715:SER:OG | 6:I:718:HIS:NE2 | 2.42 | 0.53 |
| 3:L:250:ARG:HG2 | 3:L:260:ARG:HA | 1.91 | 0.53 |
| 3:L:605:LYS:HB2 | 3:L:609:PHE:CZ | 2.40 | 0.53 |
| 6:R:812:MET:SD | 6:R:813:PHE:N | 2.82 | 0.53 |
| 1:S:114:VAL:O | 1:S:119:ARG:HB2 | 2.08 | 0.53 |
| 1:S:852:ARG:NH2 | 1:S:3111:MET:SD | 2.82 | 0.53 |
| 1:S:1784:ARG:HG3 | 1:S:1787:ARG:NH1 | 2.22 | 0.53 |
| 1:S:2572:TYR:HA | 1:S:2787:HIS:HB2 | 1.90 | 0.53 |
| 8:e:28:DT:H2' | 8:e:29:DA:C8 | 2.43 | 0.53 |
| 1:A:247:GLU:HB3 | 1:A:251:PHE:CZ | 2.44 | 0.53 |
| 1:A:345:PHE:O | 1:A:366:TYR:OH | 2.23 | 0.53 |
| 1:A:724:GLU:HB2 | 1:A:2600:THR:HA | 1.90 | 0.53 |
| 1:A:2138:VAL:O | 1:A:2143:ARG:NE | 2.41 | 0.53 |
| 1:A:2380:ASN:ND2 | 2:B:192:ASP:OD1 | 2.42 | 0.53 |
| 1:A:4102:THR:HA | 1:A:4105:LYS:HE3 | 1.90 | 0.53 |
| 3:C:108:LEU:HD11 | 3:C:144:LYS:HA | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:133:GLU:OE2 | 11:f:297:LEU:HB2 | 2.09 | 0.53 |
| 3:C:496:HIS:NE2 | 3:C:504:PRO:O | 2.42 | 0.53 |
| 3:C:656:ASN:CG | 3:C:689:GLU:H | 2.17 | 0.53 |
| 3:L:160:SER:CB | 11:m:295:ARG:HD2 | 2.39 | 0.53 |
| 1:S:273:ARG:O | 1:S:277:LEU:HG | 2.09 | 0.53 |
| 1:S:978:GLN:NE2 | 1:S:2594:ASP:OD1 | 2.42 | 0.53 |
| 1:S:1632:TRP:CD1 | 1:S:1641:THR:HG23 | 2.44 | 0.53 |
| 1:S:1775:GLU:O | 1:S:1778:PHE:HB3 | 2.08 | 0.53 |
| 1:S:2470:ARG:NH2 | 1:S:2513:GLU:OE2 | 2.30 | 0.53 |
| 1:S:3100:LYS:HA | 1:S:3103:ILE:HG22 | 1.90 | 0.53 |
| 2:T:261:LEU:HG | 2:T:345:LEU:HB2 | 1.91 | 0.53 |
| 1:A:131:LEU:HD13 | 1:A:177:LEU:HD11 | 1.89 | 0.53 |
| 1:A:338:LEU:HD12 | 1:A:339:GLN:HG3 | 1.91 | 0.53 |
| 1:A:733:LEU:HA | 1:A:736:LEU:HD13 | 1.90 | 0.53 |
| 1:A:1169:VAL:O | 1:A:1172:LEU:HG | 2.08 | 0.53 |
| 1:A:1229:CYS:HB3 | 1:A:1233:SER:HB3 | 1.91 | 0.53 |
| 1:A:1231:GLN:HB3 | 1:A:1235:ILE:HD11 | 1.90 | 0.53 |
| 1:A:2393:LEU:HA | 1:A:2396:LEU:HB2 | 1.91 | 0.53 |
| 1:A:3137:GLU:O | 1:A:3140:GLU:HG2 | 2.09 | 0.53 |
| 2:B:105:LEU:HG | 2:B:106:GLN:HG3 | 1.90 | 0.53 |
| 2:B:176:HIS:HA | 2:B:182:LYS:HE2 | 1.91 | 0.53 |
| 3:C:267:ILE:HB | 3:C:361:VAL:HB | 1.90 | 0.53 |
| 3:L:531:SER:HA | 3:L:534:LYS:HE3 | 1.91 | 0.53 |
| 3:L:667:GLU:O | 3:L:670:GLN:NE2 | 2.40 | 0.53 |
| 5:Q:25:GLU:HG2 | 5:Q:26:LYS:HD2 | 1.90 | 0.53 |
| 6:R:872:VAL:HG11 | 6:R:888:ILE:HD13 | 1.91 | 0.53 |
| 1:S:287:LEU:HB3 | 1:S:326:MET:SD | 2.49 | 0.53 |
| 1:S:945:ALA:HB2 | 1:S:958:MET:HE1 | 1.91 | 0.53 |
| 1:S:1360:LYS:NZ | 1:S:1409:SER:OG | 2.41 | 0.53 |
| 1:S:1369:MET:HE2 | 1:S:1418:HIS:ND1 | 2.23 | 0.53 |
| 1:S:1568:ASN:HA | 1:S:1600:MET:HE1 | 1.90 | 0.53 |
| 1:S:2162:LYS:HA | 1:S:2200:ALA:HB2 | 1.90 | 0.53 |
| 1:S:3369:ASP:HB3 | 1:S:3372:LYS:HG2 | 1.91 | 0.53 |
| 1:A:391:ARG:NH2 | 1:A:395:MET:HB3 | 2.24 | 0.53 |
| 1:A:628:GLU:O | 1:A:632:GLU:OE1 | 2.27 | 0.53 |
| 1:A:1184:ARG:NH2 | 1:A:1262:ALA:HA | 2.24 | 0.53 |
| 1:A:1935:GLU:OE1 | 1:A:1935:GLU:N | 2.42 | 0.53 |
| 1:A:3572:ILE:HD13 | 1:A:3575:LEU:HD12 | 1.90 | 0.53 |
| 1:A:3596:LEU:HD22 | 1:A:3646:LYS:HE2 | 1.91 | 0.53 |
| 5:H:33:VAL:HG22 | 5:H:46:THR:HG22 | 1.91 | 0.53 |
| 3:L:485:PRO:HG3 | 3:L:515:MET:HE1 | 1.91 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2094:MET:HB2 | 1:S:2149:LEU:HD12 | 1.91 | 0.53 |
| 1:S:2125:TRP:HB3 | 1:S:2128:PHE:HD2 | 1.74 | 0.53 |
| 1:S:2155:GLU:HA | 1:S:2158:ARG:HD3 | 1.90 | 0.53 |
| 1:A:771:ASN:HA | 1:A:774:GLU:CD | 2.33 | 0.52 |
| 1:A:1511:ALA:O | 1:A:1515:LEU:HG | 2.09 | 0.52 |
| 1:A:1763:THR:O | 1:A:1767:CYS:N | 2.41 | 0.52 |
| 1:A:2121:ASP:HB3 | 1:A:2127:LYS:HG2 | 1.90 | 0.52 |
| 1:A:2139:PRO:O | 1:A:2143:ARG:N | 2.37 | 0.52 |
| 1:A:2556:SER:O | 1:A:2560:ASN:ND2 | 2.42 | 0.52 |
| 1:A:3301:LEU:HD11 | 1:A:3333:THR:HG21 | 1.91 | 0.52 |
| 2:B:94:LYS:HB2 | 2:B:103:TYR:CE2 | 2.44 | 0.52 |
| 4:D:46:GLU:HB3 | 4:D:111:LYS:HE3 | 1.90 | 0.52 |
| 3:L:498:ALA:O | 2:T:325:ARG:NH2 | 2.41 | 0.52 |
| 5:P:177:TYR:O | 5:P:181:ILE:HG12 | 2.09 | 0.52 |
| 1:S:323:VAL:HA | 1:S:326:MET:HG2 | 1.91 | 0.52 |
| 1:S:852:ARG:NH2 | 1:S:3108:GLN:OE1 | 2.40 | 0.52 |
| 1:S:1205:ASN:HB3 | 1:S:1275:THR:HA | 1.91 | 0.52 |
| 1:S:1387:GLY:HA2 | 1:S:1392:MET:HG2 | 1.90 | 0.52 |
| 1:S:2953:THR:HG23 | 1:S:2993:PHE:HE2 | 1.73 | 0.52 |
| 1:S:3753:LYS:O | 1:S:3800:LEU:HD12 | 2.09 | 0.52 |
| 1:A:1155:ARG:HH21 | 1:A:3691:LYS:HB3 | 1.72 | 0.52 |
| 1:A:1824:LEU:HD12 | 1:A:1828:LEU:HD11 | 1.90 | 0.52 |
| 1:A:2470:ARG:HA | 1:A:2473:MET:HE2 | 1.92 | 0.52 |
| 1:A:2850:PHE:HB3 | 1:A:2883:SER:HB2 | 1.91 | 0.52 |
| 1:A:2928:LYS:O | 1:A:2931:ARG:HD3 | 2.08 | 0.52 |
| 1:A:3636:PHE:HA | 1:A:3639:GLU:HG2 | 1.90 | 0.52 |
| 3:C:396:ALA:HB2 | 3:C:403:PRO:HB3 | 1.91 | 0.52 |
| 5:H:184:LEU:HD21 | 6:I:803:TYR:CE2 | 2.43 | 0.52 |
| 3:L:57:VAL:HG21 | 3:L:114:SER:HB2 | 1.89 | 0.52 |
| 3:L:313:GLY:N | 2:T:286:ILE:O | 2.40 | 0.52 |
| 3:L:499:LEU:O | 3:L:502:ARG:NH1 | 2.42 | 0.52 |
| 1:S:13:LEU:HB2 | 1:S:59:PHE:CZ | 2.43 | 0.52 |
| 1:S:486:GLY:O | 1:S:490:ILE:HG12 | 2.09 | 0.52 |
| 1:S:1095:LEU:O | 1:S:1099:PHE:N | 2.31 | 0.52 |
| 1:S:2234:ASN:HA | 1:S:2237:ILE:HD12 | 1.91 | 0.52 |
| 1:S:3632:PHE:HE2 | 1:S:3671:ASN:HB3 | 1.73 | 0.52 |
| 1:A:152:LEU:HB3 | 1:A:156:PHE:CZ | 2.45 | 0.52 |
| 1:A:965:THR:O | 1:A:968:VAL:HG12 | 2.09 | 0.52 |
| 1:A:1297:PHE:HA | 1:A:1301:ILE:HG12 | 1.92 | 0.52 |
| 1:A:2575:PRO:HD3 | 1:A:2786:LYS:HZ2 | 1.75 | 0.52 |
| 1:A:3811:THR:HB | 1:A:3929:MET:HE1 | 1.91 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:297:LYS:HG2 | 3:C:298:ASN:HA | 1.90 | 0.52 |
| 2:B:507:THR:HG1 | 3:C:394:ARG:NH1 | 2.07 | 0.52 |
| 3:C:131:HIS:HE1 | 11:f:296:GLY:N | 2.06 | 0.52 |
| 3:C:144:LYS:HG2 | 3:C:207:ILE:HG13 | 1.90 | 0.52 |
| 3:L:164:PHE:HE2 | 11:m:297:LEU:HD23 | 1.74 | 0.52 |
| 3:L:254:GLY:HA3 | 2:T:514:MET:HG2 | 1.91 | 0.52 |
| 1:S:451:PRO:O | 1:S:455:LEU:HG | 2.09 | 0.52 |
| 1:S:2521:ILE:HG13 | 1:S:2525:TRP:HD1 | 1.74 | 0.52 |
| 1:S:2569:SER:HB3 | 1:S:2572:TYR:HB2 | 1.89 | 0.52 |
| 1:A:538:ASP:HA | 1:A:541:MET:HG3 | 1.91 | 0.52 |
| 1:A:3768:PHE:O | 1:A:3772:ASN:ND2 | 2.42 | 0.52 |
| 2:B:357:LYS:HB2 | 2:B:360:HIS:CE1 | 2.44 | 0.52 |
| 3:C:265:LYS:HD3 | 3:C:268:LEU:HD21 | 1.90 | 0.52 |
| 6:I:814:ARG:N | 6:I:850:ALA:H | 1.99 | 0.52 |
| 3:L:640:ARG:O | 3:L:644:GLU:HG2 | 2.09 | 0.52 |
| 1:S:1072:ALA:HB1 | 1:S:1121:LEU:HD11 | 1.91 | 0.52 |
| 1:S:2166:SER:OG | 1:S:2167:PRO:HD3 | 2.09 | 0.52 |
| 1:S:3692:VAL:HG22 | 1:S:3696:ARG:HD3 | 1.91 | 0.52 |
| 1:S:3970:LEU:HG | 1:S:3971:MET:HG3 | 1.92 | 0.52 |
| 1:A:345:PHE:HB3 | 1:A:366:TYR:CE1 | 2.44 | 0.52 |
| 1:A:1589:ASN:CG | 1:A:1592:MET:HG3 | 2.34 | 0.52 |
| 1:A:1921:ASP:OD1 | 1:A:1921:ASP:N | 2.41 | 0.52 |
| 2:B:476:ASP:OD1 | 2:B:476:ASP:N | 2.40 | 0.52 |
| 3:C:630:PRO:HA | 3:C:633:MET:HE2 | 1.91 | 0.52 |
| 6:R:728:GLU:HA | 6:R:731:LYS:HE2 | 1.90 | 0.52 |
| 1:S:23:ASP:OD2 | 1:S:71:LYS:NZ | 2.27 | 0.52 |
| 1:S:469:ALA:HA | 1:S:475:LEU:HD13 | 1.92 | 0.52 |
| 1:S:524:TYR:HA | 1:S:527:TYR:HE2 | 1.74 | 0.52 |
| 1:S:938:VAL:HA | 1:S:941:MET:HG3 | 1.91 | 0.52 |
| 1:S:1475:LEU:HG | 1:S:1524:LEU:HD22 | 1.90 | 0.52 |
| 1:S:1667:SER:OG | 1:S:1670:GLU:OE1 | 2.26 | 0.52 |
| 1:S:1674:THR:O | 1:S:1678:LEU:HG | 2.09 | 0.52 |
| 1:S:2804:ILE:HD13 | 1:S:2807:GLN:NE2 | 2.24 | 0.52 |
| 1:S:2956:ALA:HB2 | 1:S:2971:GLN:HB2 | 1.90 | 0.52 |
| 1:S:3867:THR:HA | 1:S:4118:GLY:HA2 | 1.91 | 0.52 |
| 1:A:183:GLU:HG2 | 1:A:184:VAL:H | 1.74 | 0.52 |
| 1:A:323:VAL:HA | 1:A:326:MET:HG2 | 1.91 | 0.52 |
| 1:A:1034:ARG:HB2 | 1:A:1085:ILE:HG22 | 1.91 | 0.52 |
| 1:A:1513:GLY:HA2 | 1:A:1516:GLU:OE2 | 2.09 | 0.52 |
| 1:A:1802:TYR:O | 1:A:1806:ARG:NH1 | 2.42 | 0.52 |
| 1:A:2228:ARG:NH2 | 8:e:44:DG:OP1 | 2.37 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2338:GLU:HB3 | 1:A:2341:LEU:HD12 | 1.92 | 0.52 |
| 1:A:2524:PHE:O | 1:A:2530:ARG:NE | 2.41 | 0.52 |
| 1:A:2884:LEU:HD12 | 1:A:2886:GLN:HE22 | 1.75 | 0.52 |
| 1:A:3457:ASN:HB3 | 1:A:3491:PRO:HG2 | 1.92 | 0.52 |
| 1:A:3714:GLU:O | 1:A:3718:ARG:NH2 | 2.39 | 0.52 |
| 2:B:103:TYR:CD2 | 2:B:135:MET:HE1 | 2.44 | 0.52 |
| 1:S:89:LEU:C | 1:S:133:LYS:HZ1 | 2.18 | 0.52 |
| 1:S:770:LEU:HB3 | 1:S:858:MET:HE1 | 1.92 | 0.52 |
| 1:S:2183:HIS:HA | 1:S:2186:VAL:HB | 1.92 | 0.52 |
| 1:S:2464:HIS:H | 1:S:2470:ARG:HD3 | 1.74 | 0.52 |
| 1:S:2553:HIS:O | 1:S:2557:LEU:HG | 2.09 | 0.52 |
| 1:S:4011:PHE:HA | 1:S:4014:LYS:HE2 | 1.92 | 0.52 |
| 1:A:484:HIS:ND1 | 1:A:574:LYS:HE3 | 2.25 | 0.52 |
| 1:A:1593:VAL:O | 1:A:1597:LEU:HG | 2.10 | 0.52 |
| 1:A:1750:LEU:HD21 | 1:A:1759:LEU:HD23 | 1.91 | 0.52 |
| 1:A:2528:GLU:HA | 1:A:2531:LEU:O | 2.10 | 0.52 |
| 1:A:3103:ILE:O | 1:A:3107:ILE:HG12 | 2.10 | 0.52 |
| 1:A:3385:LEU:HD13 | 1:A:3416:LEU:HA | 1.91 | 0.52 |
| 1:A:3665:MET:O | 1:A:3669:LYS:N | 2.33 | 0.52 |
| 2:B:458:GLN:HB3 | 2:B:525:PHE:HE1 | 1.75 | 0.52 |
| 5:P:179:ARG:HA | 5:P:182:LEU:HD23 | 1.91 | 0.52 |
| 1:S:525:LYS:O | 1:S:528:VAL:HG22 | 2.09 | 0.52 |
| 1:S:1484:LEU:HD13 | 1:S:1531:LEU:HD22 | 1.90 | 0.52 |
| 1:S:2121:ASP:HA | 1:S:2127:LYS:HE2 | 1.92 | 0.52 |
| 1:A:1513:GLY:HA2 | 1:A:1516:GLU:CD | 2.35 | 0.52 |
| 1:A:2521:ILE:HG13 | 1:A:2525:TRP:CD1 | 2.45 | 0.52 |
| 1:A:2527:HIS:CD2 | 1:A:2529:THR:H | 2.28 | 0.52 |
| 1:A:3011:LEU:O | 1:A:3015:SER:N | 2.42 | 0.52 |
| 1:A:3263:HIS:HB2 | 1:A:3276:TRP:CE2 | 2.45 | 0.52 |
| 2:B:38:LEU:HD11 | 2:B:167:MET:HB2 | 1.92 | 0.52 |
| 2:B:247:ARG:HG2 | 2:B:488:ARG:HH12 | 1.75 | 0.52 |
| 5:H:115:LYS:NZ | 5:H:116:VAL:O | 2.39 | 0.52 |
| 6:I:665:CYS:HB2 | 6:I:700:VAL:HG12 | 1.91 | 0.52 |
| 3:L:151:ILE:HD11 | 3:L:211:VAL:HG22 | 1.92 | 0.52 |
| 3:L:380:LEU:HA | 2:T:462:MET:CE | 2.39 | 0.52 |
| 6:R:692:ASN:OD1 | 2:T:293:ASN:ND2 | 2.38 | 0.52 |
| 1:S:67:VAL:HG12 | 1:S:71:LYS:HZ3 | 1.75 | 0.52 |
| 1:S:547:ASP:OD1 | 1:S:547:ASP:N | 2.43 | 0.52 |
| 1:S:1196:PRO:HA | 1:S:1202:ARG:HA | 1.90 | 0.52 |
| 1:S:2254:ARG:NH2 | 1:S:2292:CYS:HB3 | 2.24 | 0.52 |
| 1:S:2396:LEU:O | 1:S:2399:GLU:HG3 | 2.10 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3924:HIS:HA | 1:S:3962:ARG:HH21 | 1.75 | 0.52 |
| 2:T:86:VAL:HB | 2:T:104:VAL:HG23 | 1.92 | 0.52 |
| 2:T:207:LYS:HD3 | 2:T:208:PRO:HD2 | 1.91 | 0.52 |
| 1:A:183:GLU:O | 1:A:185:HIS:ND1 | 2.43 | 0.52 |
| 1:A:249:PHE:O | 1:A:252:VAL:HG12 | 2.09 | 0.52 |
| 1:A:668:LYS:NZ | 1:A:728:SER:HB3 | 2.24 | 0.52 |
| 1:A:989:MET:HE2 | 1:A:993:HIS:CE1 | 2.44 | 0.52 |
| 1:A:2267:SER:HA | 1:A:2311:ARG:HH21 | 1.75 | 0.52 |
| 1:A:2347:LYS:O | 1:A:2351:GLN:N | 2.24 | 0.52 |
| 1:A:3586:LYS:NZ | 1:A:3668:LEU:HD22 | 2.25 | 0.52 |
| 3:L:83:LEU:HB2 | 3:L:121:GLU:HB3 | 1.92 | 0.52 |
| 4:M:127:GLY:HA2 | 4:M:130:LYS:HE2 | 1.91 | 0.52 |
| 1:S:178:LEU:HB2 | 1:S:227:LEU:HD12 | 1.91 | 0.52 |
| 1:S:236:LYS:O | 1:S:243:GLN:NE2 | 2.42 | 0.52 |
| 1:S:879:MET:HG3 | 1:S:881:LYS:H | 1.75 | 0.52 |
| 1:S:1651:LYS:HD3 | 1:S:1654:GLN:NE2 | 2.24 | 0.52 |
| 1:A:176:GLU:CD | 1:A:223:CYS:HA | 2.35 | 0.52 |
| 1:A:586:GLN:HB2 | 1:A:613:HIS:CD2 | 2.45 | 0.52 |
| 1:A:1082:PHE:HA | 1:A:1085:ILE:HG12 | 1.92 | 0.52 |
| 1:A:2386:LEU:HD13 | 1:A:2397:CYS:HB2 | 1.91 | 0.52 |
| 1:A:3064:PHE:HA | 1:A:3067:LYS:HD2 | 1.92 | 0.52 |
| 3:C:500:HIS:HA | 3:C:502:ARG:NH1 | 2.25 | 0.52 |
| 3:L:516:LEU:HG | 2:T:399:ARG:HH11 | 1.75 | 0.52 |
| 3:L:678:VAL:O | 3:L:682:GLY:N | 2.37 | 0.52 |
| 1:S:2350:LYS:HG3 | 1:S:2354:ASN:ND2 | 2.25 | 0.52 |
| 1:S:3107:ILE:HG12 | 1:S:3135:LEU:HD11 | 1.91 | 0.52 |
| 1:S:3311:ASN:HB3 | 1:S:3315:TYR:CZ | 2.45 | 0.52 |
| 1:S:3878:VAL:HG11 | 1:S:4127:TRP:HB2 | 1.91 | 0.52 |
| 1:A:932:GLU:OE1 | 1:A:2775:TYR:OH | 2.27 | 0.51 |
| 1:A:1305:ASP:OD1 | 1:A:1334:LYS:NZ | 2.42 | 0.51 |
| 1:A:2158:ARG:NH2 | 1:A:2196:TRP:HB3 | 2.25 | 0.51 |
| 2:B:374:LEU:HB3 | 3:C:541:GLU:HG3 | 1.92 | 0.51 |
| 3:C:495:LEU:O | 3:C:499:LEU:HG | 2.09 | 0.51 |
| 4:D:40:TYR:HB3 | 4:D:47:LEU:HD11 | 1.92 | 0.51 |
| 5:Q:166:VAL:HG23 | 5:Q:169:LYS:HZ1 | 1.75 | 0.51 |
| 1:S:1055:ASN:O | 1:S:1058:SER:OG | 2.27 | 0.51 |
| 1:S:2327:LEU:HD23 | 1:S:2371:PHE:CD2 | 2.45 | 0.51 |
| 2:T:95:ASN:HD21 | 2:T:99:PHE:HB2 | 1.76 | 0.51 |
| 7:d:23:DT:O2 | 7:d:23:DT:H2' | 2.08 | 0.51 |
| 1:A:273:ARG:O | 1:A:277:LEU:HG | 2.10 | 0.51 |
| 1:A:407:VAL:HB | 1:A:410:MET:HE1 | 1.91 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:658:THR:HG1 | 1:A:659:ARG:NH1 | 2.08 | 0.51 |
| 1:A:1365:ASN:ND2 | 1:A:1370:ARG:HH22 | 2.05 | 0.51 |
| 1:A:1368:LEU:HB3 | 1:A:1372:LEU:HD23 | 1.91 | 0.51 |
| 1:A:1912:THR:HA | 1:A:1915:LEU:HD23 | 1.93 | 0.51 |
| 1:A:2379:MET:N | 1:A:2379:MET:SD | 2.83 | 0.51 |
| 1:A:3247:ARG:HG3 | 1:A:3286:CYS:HB2 | 1.93 | 0.51 |
| 1:A:3833:ARG:HA | 1:A:3877:LYS:HD3 | 1.91 | 0.51 |
| 1:A:3985:VAL:HG13 | 1:A:4100:GLU:HG3 | 1.92 | 0.51 |
| 3:L:160:SER:C | 3:L:161:LEU:HD12 | 2.35 | 0.51 |
| 3:L:276:TRP:CE3 | 2:T:320:GLN:HG3 | 2.46 | 0.51 |
| 3:L:318:SER:HB3 | 2:T:110:ASN:HB3 | 1.92 | 0.51 |
| 3:L:653:GLN:HA | 3:L:656:ASN:HB2 | 1.91 | 0.51 |
| 3:L:676:GLU:HG3 | 3:L:677:ILE:N | 2.25 | 0.51 |
| 1:S:978:GLN:O | 1:S:982:GLN:CB | 2.57 | 0.51 |
| 1:S:1139:GLU:HG3 | 1:S:1197:LEU:HD11 | 1.92 | 0.51 |
| 1:S:1687:HIS:O | 1:S:1745:LYS:NZ | 2.43 | 0.51 |
| 1:S:1875:LYS:NZ | 1:S:1943:ALA:HB2 | 2.26 | 0.51 |
| 1:S:2254:ARG:HH21 | 1:S:2291:GLN:NE2 | 2.08 | 0.51 |
| 1:S:2361:ILE:HD11 | 1:S:2393:LEU:HD22 | 1.92 | 0.51 |
| 1:S:3392:ALA:HB1 | 1:S:3409:VAL:HA | 1.93 | 0.51 |
| 2:T:73:SER:HB3 | 2:T:246:VAL:HG22 | 1.92 | 0.51 |
| 1:A:928:VAL:HB | 1:A:2769:VAL:HG11 | 1.92 | 0.51 |
| 1:A:1595:ALA:HA | 1:A:1598:ASN:HD21 | 1.76 | 0.51 |
| 1:A:2263:LYS:NZ | 1:A:2269:ASP:OD2 | 2.43 | 0.51 |
| 1:A:2854:PHE:CE2 | 1:A:2858:ILE:HD11 | 2.44 | 0.51 |
| 1:A:3625:LEU:O | 1:A:3682:GLU:HG3 | 2.09 | 0.51 |
| 2:B:87:PHE:CE2 | 2:B:105:LEU:HB2 | 2.45 | 0.51 |
| 2:B:363:ARG:HB3 | 3:C:359:ASN:HD22 | 1.74 | 0.51 |
| 4:D:183:GLU:OE2 | 4:D:189:GLY:N | 2.43 | 0.51 |
| 6:I:669:GLY:N | 6:I:675:LYS:HD3 | 2.25 | 0.51 |
| 3:L:260:ARG:NE | 2:T:536:PRO:O | 2.38 | 0.51 |
| 6:R:813:PHE:HA | 6:R:850:ALA:HB3 | 1.93 | 0.51 |
| 1:S:528:VAL:HA | 1:S:531:PHE:CD2 | 2.46 | 0.51 |
| 1:S:1675:TYR:O | 1:S:1679:LEU:HG | 2.11 | 0.51 |
| 1:S:3476:PRO:O | 1:S:3480:LEU:HB2 | 2.09 | 0.51 |
| 1:S:3603:LYS:H | 1:S:3606:ILE:HB | 1.74 | 0.51 |
| 2:T:270:SER:HB3 | 2:T:374:LEU:HB2 | 1.92 | 0.51 |
| 1:A:1662:ASN:OD1 | 1:A:1663:THR:N | 2.44 | 0.51 |
| 1:A:1663:THR:O | 1:A:1665:HIS:ND1 | 2.42 | 0.51 |
| 1:A:2398:LEU:HA | 1:A:2401:VAL:HG12 | 1.92 | 0.51 |
| 4:D:184:SER:N | 4:D:190:PHE:O | 2.32 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:408:ALA:HB1 | 3:L:419:LEU:HD21 | 1.91 | 0.51 |
| 1:S:1356:TRP:HD1 | 1:S:1359:LEU:HD11 | 1.75 | 0.51 |
| 1:S:2748:VAL:HG12 | 1:S:2752:LYS:HE2 | 1.91 | 0.51 |
| 7:d:22:DG:H22 | 8:e:35:DT:H3 | 1.59 | 0.51 |
| 1:A:16:GLN:NE2 | 1:A:62:ASP:OD2 | 2.43 | 0.51 |
| 1:A:1603:GLN:HA | 1:A:1606:ARG:HH11 | 1.75 | 0.51 |
| 1:A:1958:GLU:HG2 | 1:A:1959:LEU:HG | 1.92 | 0.51 |
| 1:A:2210:VAL:HG13 | 1:A:2214:ARG:HH12 | 1.76 | 0.51 |
| 1:A:3167:ARG:N | 1:A:3167:ARG:HD2 | 2.25 | 0.51 |
| 1:A:3920:ILE:HG23 | 1:A:3944:HIS:HB2 | 1.93 | 0.51 |
| 3:C:150:ILE:O | 3:C:154:LEU:HB2 | 2.11 | 0.51 |
| 3:C:602:VAL:HG12 | 3:C:609:PHE:HB2 | 1.93 | 0.51 |
| 5:G:43:TRP:HB3 | 5:G:113:LEU:HD21 | 1.92 | 0.51 |
| 3:L:161:LEU:H | 11:m:295:ARG:CZ | 2.24 | 0.51 |
| 1:S:1064:TYR:O | 1:S:1068:LEU:HG | 2.10 | 0.51 |
| 1:S:3550:LYS:O | 1:S:3553:GLU:HG2 | 2.10 | 0.51 |
| 1:S:4055:ASN:HD22 | 1:S:4058:VAL:HG23 | 1.75 | 0.51 |
| 2:T:289:TYR:CE2 | 2:T:291:GLU:HB2 | 2.45 | 0.51 |
| 1:A:240:GLU:HB2 | 1:A:242:PRO:HD2 | 1.93 | 0.51 |
| 1:A:446:PHE:HA | 1:A:449:TYR:CE2 | 2.45 | 0.51 |
| 1:A:1685:ASP:H | 1:A:1688:LEU:HD12 | 1.76 | 0.51 |
| 1:A:1731:PRO:HA | 1:A:1736:PHE:CG | 2.46 | 0.51 |
| 1:A:2324:GLY:HA3 | 1:A:2370:SER:OG | 2.11 | 0.51 |
| 1:A:3235:LYS:HB3 | 1:A:3239:LYS:HZ1 | 1.76 | 0.51 |
| 1:A:3742:GLY:HA2 | 1:A:3748:HIS:HE2 | 1.76 | 0.51 |
| 1:A:3940:ILE:HG22 | 1:A:3941:ASP:N | 2.25 | 0.51 |
| 2:B:325:ARG:CZ | 3:C:498:ALA:HA | 2.41 | 0.51 |
| 3:C:731:MET:HE2 | 1:S:1885:PRO:C | 2.36 | 0.51 |
| 3:L:294:VAL:HB | 2:T:299:LYS:HE3 | 1.92 | 0.51 |
| 5:Q:166:VAL:HG11 | 6:R:846:ARG:HD3 | 1.93 | 0.51 |
| 5:Q:188:LYS:HD3 | 5:Q:191:ILE:HD12 | 1.92 | 0.51 |
| 1:S:986:PRO:HB3 | 1:S:2777:HIS:CE1 | 2.46 | 0.51 |
| 1:S:1425:ALA:HB2 | 1:S:1467:ILE:HG13 | 1.93 | 0.51 |
| 1:S:1816:ARG:HA | 1:S:1819:PHE:CE2 | 2.46 | 0.51 |
| 1:S:2514:ASN:HD22 | 1:S:2517:LEU:HG | 1.76 | 0.51 |
| 1:S:2995:GLU:O | 1:S:2999:LEU:HG | 2.11 | 0.51 |
| 1:S:3667:LEU:HA | 1:S:3670:MET:HE2 | 1.93 | 0.51 |
| 1:S:3962:ARG:NH2 | 1:S:4124:TRP:O | 2.44 | 0.51 |
| 1:A:572:VAL:O | 1:A:576:VAL:HG13 | 2.11 | 0.51 |
| 1:A:1762:MET:HA | 1:A:1765:VAL:HG22 | 1.92 | 0.51 |
| 1:A:1849:ASP:OD1 | 1:A:1850:VAL:N | 2.44 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3512:VAL:HB | 1:A:3516:HIS:HE1 | 1.76 | 0.51 |
| 2:B:106:GLN:HE22 | 2:B:115:ARG:HG2 | 1.76 | 0.51 |
| 3:C:419:LEU:HD23 | 3:C:419:LEU:H | 1.76 | 0.51 |
| 5:H:58:ASP:H | 5:H:61:MET:HE1 | 1.76 | 0.51 |
| 3:L:269:GLN:O | 3:L:271:ARG:NH1 | 2.38 | 0.51 |
| 5:Q:178:LYS:HA | 5:Q:181:ILE:HG22 | 1.93 | 0.51 |
| 6:R:837:ARG:HD3 | 6:R:867:GLU:HB3 | 1.93 | 0.51 |
| 1:S:526:ASP:N | 1:S:526:ASP:OD1 | 2.43 | 0.51 |
| 1:S:958:MET:O | 1:S:962:TYR:N | 2.40 | 0.51 |
| 1:S:1481:THR:HG23 | 1:S:1527:ARG:HH22 | 1.76 | 0.51 |
| 1:S:2501:LEU:O | 1:S:2505:VAL:HG12 | 2.11 | 0.51 |
| 1:S:2577:PHE:HB2 | 1:S:2783:ILE:HG21 | 1.91 | 0.51 |
| 1:S:3254:LEU:HD13 | 1:S:3283:LEU:HD21 | 1.92 | 0.51 |
| 2:T:106:GLN:OE1 | 2:T:115:ARG:NE | 2.35 | 0.51 |
| 1:A:294:PHE:CE2 | 1:A:298:LEU:HD11 | 2.45 | 0.51 |
| 1:A:682:TYR:CZ | 1:A:700:LYS:HG2 | 2.46 | 0.51 |
| 1:A:1470:SER:OG | 1:A:1473:THR:O | 2.23 | 0.51 |
| 1:A:1625:HIS:HA | 1:A:1628:LYS:HD3 | 1.92 | 0.51 |
| 1:A:2233:HIS:CD2 | 1:A:2731:ARG:HG3 | 2.46 | 0.51 |
| 1:A:2746:LYS:O | 1:A:2750:GLU:HG3 | 2.11 | 0.51 |
| 1:A:2824:LYS:O | 1:A:2829:LYS:NZ | 2.40 | 0.51 |
| 1:A:2976:LEU:O | 1:A:2979:GLN:NE2 | 2.44 | 0.51 |
| 1:A:3609:MET:HA | 1:A:3612:ARG:HE | 1.75 | 0.51 |
| 1:A:3904:PHE:CE1 | 1:A:3937:VAL:HB | 2.46 | 0.51 |
| 2:B:59:PRO:HB3 | 2:B:205:LEU:HD23 | 1.93 | 0.51 |
| 2:B:526:LYS:O | 2:B:530:TYR:N | 2.44 | 0.51 |
| 1:S:12:LEU:HA | 1:S:41:GLU:OE2 | 2.11 | 0.51 |
| 1:S:391:ARG:O | 1:S:395:MET:N | 2.43 | 0.51 |
| 1:S:849:GLU:HA | 1:S:852:ARG:HG2 | 1.91 | 0.51 |
| 1:S:924:ARG:HA | 1:S:927:LYS:HG2 | 1.92 | 0.51 |
| 1:S:1722:PHE:HE1 | 1:S:1739:TYR:HB3 | 1.75 | 0.51 |
| 1:S:2438:ILE:O | 1:S:2442:MET:HB2 | 2.11 | 0.51 |
| 1:S:2440:TYR:HA | 1:S:2443:MET:HE1 | 1.93 | 0.51 |
| 1:S:2560:ASN:HD21 | 1:S:2799:GLN:HB3 | 1.76 | 0.51 |
| 1:S:2978:LYS:O | 1:S:2981:TRP:NE1 | 2.38 | 0.51 |
| 1:S:3572:ILE:HG23 | 1:S:3800:LEU:HD23 | 1.92 | 0.51 |
| 2:T:74:LYS:HD3 | 2:T:79:ASP:HA | 1.92 | 0.51 |
| 8:e:26:DA:H1' | 8:e:27:DC:H5' | 1.92 | 0.51 |
| 1:A:1920:TYR:OH | 1:A:1962:TYR:O | 2.29 | 0.51 |
| 1:A:1925:GLU:HB2 | 1:A:1941:HIS:HE1 | 1.75 | 0.51 |
| 1:A:2105:HIS:CG | 1:A:2156:VAL:HG23 | 2.46 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2392:VAL:HA | 1:A:2431:ARG:HH12 | 1.76 | 0.51 |
| 1:A:2995:GLU:O | 1:A:2999:LEU:HG | 2.10 | 0.51 |
| 1:A:3171:ALA:HA | 1:A:3179:TRP:CH2 | 2.46 | 0.51 |
| 1:A:3472:ILE:HG12 | 1:A:3479:THR:HB | 1.92 | 0.51 |
| 1:A:3940:ILE:HG22 | 1:A:3941:ASP:H | 1.74 | 0.51 |
| 2:B:290:ARG:N | 3:C:309:ASP:O | 2.43 | 0.51 |
| 2:B:316:THR:O | 2:B:318:ARG:NH1 | 2.44 | 0.51 |
| 2:B:479:GLU:HA | 3:C:426:PHE:HB3 | 1.93 | 0.51 |
| 6:I:816:HIS:H | 6:I:850:ALA:HA | 1.76 | 0.51 |
| 3:L:377:LEU:O | 3:L:381:ILE:HG12 | 2.11 | 0.51 |
| 6:R:667:MET:HE2 | 6:R:691:GLN:O | 2.10 | 0.51 |
| 1:S:261:ASP:HB3 | 1:S:265:TYR:HA | 1.92 | 0.51 |
| 1:S:627:VAL:O | 1:S:631:ARG:HD2 | 2.11 | 0.51 |
| 1:S:631:ARG:HH11 | 1:S:632:GLU:HB3 | 1.76 | 0.51 |
| 1:S:1019:ASP:O | 1:S:1026:ARG:NH2 | 2.39 | 0.51 |
| 1:S:1948:ALA:HA | 1:S:1951:VAL:HG22 | 1.92 | 0.51 |
| 1:S:2167:PRO:O | 1:S:2170:GLN:HG2 | 2.11 | 0.51 |
| 1:S:2168:LEU:HD12 | 1:S:2169:LEU:N | 2.26 | 0.51 |
| 1:S:2830:ASN:OD1 | 1:S:2834:GLN:NE2 | 2.44 | 0.51 |
| 1:S:2938:VAL:HG13 | 1:S:3974:MET:HB2 | 1.92 | 0.51 |
| 1:S:3546:SER:O | 1:S:3549:HIS:NE2 | 2.44 | 0.51 |
| 2:T:174:ASN:O | 2:T:176:HIS:N | 2.44 | 0.51 |
| 1:A:1919:CYS:O | 1:A:1922:ALA:HB3 | 2.11 | 0.51 |
| 1:A:3117:ILE:HG13 | 1:A:3125:ARG:NE | 2.25 | 0.51 |
| 1:A:3451:LEU:O | 1:A:3455:LYS:N | 2.43 | 0.51 |
| 1:A:3687:MET:HB3 | 1:A:3724:GLU:HG2 | 1.93 | 0.51 |
| 3:C:512:ILE:O | 3:C:516:LEU:HG | 2.10 | 0.51 |
| 5:H:170:GLU:O | 5:H:174:THR:HG23 | 2.10 | 0.51 |
| 3:L:235:CYS:C | 3:L:237:PHE:H | 2.19 | 0.51 |
| 3:L:622:GLN:NE2 | 3:L:628:GLU:OE1 | 2.44 | 0.51 |
| 1:S:389:ILE:HG13 | 1:S:431:TYR:CE2 | 2.46 | 0.51 |
| 1:A:941:MET:HE1 | 1:A:962:TYR:HE1 | 1.75 | 0.50 |
| 1:A:2168:LEU:HA | 1:A:2171:LEU:HD12 | 1.92 | 0.50 |
| 1:A:2362:VAL:HG12 | 1:A:2366:LYS:NZ | 2.26 | 0.50 |
| 1:A:2442:MET:O | 1:A:2446:LEU:HD23 | 2.11 | 0.50 |
| 1:A:3465:PHE:HB3 | 1:A:3466:PRO:HD3 | 1.93 | 0.50 |
| 1:A:3465:PHE:O | 1:A:3469:LEU:HG | 2.11 | 0.50 |
| 1:A:3805:TRP:CD1 | 1:A:3807:GLU:HG3 | 2.46 | 0.50 |
| 1:A:4039:TYR:HD2 | 1:A:4042:GLN:HE22 | 1.60 | 0.50 |
| 2:B:35:ARG:HG2 | 2:B:36:ASP:H | 1.76 | 0.50 |
| 2:B:39:ILE:HG23 | 2:B:84:ALA:HB3 | 1.92 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:65:ASP:H | 3:C:78:THR:HA | 1.77 | 0.50 |
| 3:C:115:MET:SD | 3:C:159:ILE:HD12 | 2.52 | 0.50 |
| 5:G:6:SER:H | 5:G:20:LEU:HB3 | 1.76 | 0.50 |
| 5:G:122:VAL:O | 5:G:125:GLU:HG3 | 2.12 | 0.50 |
| 3:L:233:LYS:NZ | 3:L:482:ILE:HG12 | 2.26 | 0.50 |
| 1:S:960:GLN:O | 1:S:964:ARG:HG2 | 2.11 | 0.50 |
| 1:S:2372:PRO:O | 1:S:2374:LEU:N | 2.39 | 0.50 |
| 1:S:2597:PHE:HA | 1:S:2598:ARG:HH11 | 1.76 | 0.50 |
| 1:S:3150:ASN:O | 1:S:3154:GLN:NE2 | 2.36 | 0.50 |
| 1:S:3695:LEU:HD23 | 1:S:3695:LEU:H | 1.76 | 0.50 |
| 1:S:3986:HIS:HA | 1:S:3989:ARG:HE | 1.76 | 0.50 |
| 2:T:335:GLU:HA | 2:T:338:LYS:HB2 | 1.93 | 0.50 |
| 1:A:324:SER:HB3 | 1:A:368:LEU:HD21 | 1.93 | 0.50 |
| 1:A:1105:VAL:O | 1:A:1109:GLU:OE1 | 2.29 | 0.50 |
| 1:A:1635:LYS:HZ2 | 1:A:1683:LYS:HD3 | 1.76 | 0.50 |
| 1:A:1737:ASN:O | 1:A:1740:VAL:HG22 | 2.12 | 0.50 |
| 1:A:1871:MET:CE | 1:A:1940:TYR:HA | 2.32 | 0.50 |
| 1:A:2155:GLU:HA | 1:A:2158:ARG:HG2 | 1.91 | 0.50 |
| 1:A:2271:SER:O | 1:A:2274:ILE:HB | 2.12 | 0.50 |
| 1:A:2820:MET:HA | 1:A:2823:PHE:CZ | 2.46 | 0.50 |
| 1:A:3811:THR:HG23 | 1:A:3813:LYS:H | 1.76 | 0.50 |
| 1:A:3964:THR:H | 1:A:3967:PHE:HB2 | 1.76 | 0.50 |
| 3:C:327:ASP:OD1 | 3:C:328:GLU:N | 2.42 | 0.50 |
| 6:I:900:LYS:HE2 | 6:I:903:LEU:HA | 1.92 | 0.50 |
| 3:L:148:ASP:HA | 3:L:151:ILE:HD12 | 1.94 | 0.50 |
| 3:L:162:GLN:NE2 | 11:m:294:PRO:HA | 2.26 | 0.50 |
| 3:L:186:GLY:HA3 | 3:L:511:HIS:HB2 | 1.93 | 0.50 |
| 3:L:210:MET:HA | 3:L:213:ILE:HG12 | 1.94 | 0.50 |
| 3:L:243:HIS:HB3 | 2:T:445:LYS:HE3 | 1.92 | 0.50 |
| 1:S:1374:GLN:O | 1:S:1378:GLU:N | 2.36 | 0.50 |
| 1:S:1639:LEU:HA | 1:S:1642:LYS:HD2 | 1.93 | 0.50 |
| 1:S:2133:LEU:HD13 | 1:S:2146:LEU:HD22 | 1.92 | 0.50 |
| 1:S:2257:PHE:O | 1:S:2261:SER:OG | 2.27 | 0.50 |
| 1:S:2826:LEU:HA | 1:S:2829:LYS:HE2 | 1.92 | 0.50 |
| 1:S:3150:ASN:ND2 | 1:S:3196:LYS:HE3 | 2.26 | 0.50 |
| 1:S:3831:ASP:HB3 | 1:S:3832:PRO:HD3 | 1.92 | 0.50 |
| 1:S:3929:MET:SD | 1:S:3938:ILE:HB | 2.52 | 0.50 |
| 2:T:62:MET:HA | 2:T:65:GLN:OE1 | 2.11 | 0.50 |
| 2:T:164:LYS:O | 2:T:199:PHE:HB3 | 2.11 | 0.50 |
| 7:d:22:DG:N2 | 8:e:35:DT:H3 | 2.09 | 0.50 |
| 7:d:30:DT:H2' | 7:d:31:DT:H71 | 1.92 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:356:ASN:OD1 | 1:A:406:ARG:NH1 | 2.44 | 0.50 |
| 1:A:786:GLN:HA | 1:A:789:TYR:CD2 | 2.46 | 0.50 |
| 1:A:963:LYS:HE3 | 1:A:964:ARG:HH12 | 1.77 | 0.50 |
| 1:A:2302:ALA:O | 1:A:2306:ASN:ND2 | 2.44 | 0.50 |
| 1:A:2402:LEU:O | 1:A:2441:LYS:NZ | 2.44 | 0.50 |
| 1:A:2937:ASP:OD2 | 1:A:3979:LEU:HA | 2.12 | 0.50 |
| 1:A:3031:TRP:HA | 1:A:3037:GLN:CD | 2.37 | 0.50 |
| 1:A:3130:GLN:HA | 1:A:3133:GLN:NE2 | 2.27 | 0.50 |
| 1:A:3483:MET:HE2 | 1:A:3513:ALA:HB3 | 1.93 | 0.50 |
| 1:A:3780:ALA:HA | 1:A:3783:GLN:HG3 | 1.94 | 0.50 |
| 2:B:302:THR:HB | 3:C:291:LYS:HD2 | 1.92 | 0.50 |
| 2:B:426:GLN:HB2 | 3:C:434:MET:HE1 | 1.92 | 0.50 |
| 5:H:178:LYS:HA | 5:H:181:ILE:HG12 | 1.93 | 0.50 |
| 1:S:457:CYS:O | 1:S:461:ILE:HG13 | 2.10 | 0.50 |
| 1:S:1782:PHE:HA | 1:S:1785:ILE:HG12 | 1.93 | 0.50 |
| 1:S:2265:PRO:HG3 | 1:S:2269:ASP:OD1 | 2.11 | 0.50 |
| 1:S:2461:PHE:O | 1:S:2464:HIS:CD2 | 2.65 | 0.50 |
| 1:S:2928:LYS:O | 1:S:2932:SER:N | 2.39 | 0.50 |
| 1:S:3793:VAL:HG23 | 1:S:3803:ILE:HG22 | 1.93 | 0.50 |
| 1:A:1624:GLN:O | 1:A:1628:LYS:NZ | 2.32 | 0.50 |
| 1:A:1725:GLN:HG3 | 1:A:1769:GLU:HG2 | 1.92 | 0.50 |
| 1:A:1764:GLU:O | 1:A:1768:ARG:HG3 | 2.12 | 0.50 |
| 1:A:2094:MET:O | 1:A:2097:LEU:HB2 | 2.11 | 0.50 |
| 1:A:2572:TYR:HE1 | 1:A:2791:ILE:HD11 | 1.76 | 0.50 |
| 1:A:3110:PHE:HD2 | 1:A:3135:LEU:HD11 | 1.75 | 0.50 |
| 1:A:3130:GLN:HA | 1:A:3133:GLN:HE21 | 1.77 | 0.50 |
| 1:A:3584:LEU:HB2 | 1:A:3617:LEU:HD11 | 1.93 | 0.50 |
| 2:B:143:LEU:HG | 2:B:176:HIS:CD2 | 2.46 | 0.50 |
| 3:C:295:TYR:HB2 | 3:C:305:VAL:H | 1.76 | 0.50 |
| 3:L:111:LEU:HD21 | 3:L:134:ILE:HG12 | 1.93 | 0.50 |
| 3:L:138:LEU:HB2 | 3:L:201:GLN:HG3 | 1.93 | 0.50 |
| 3:L:290:GLN:NE2 | 2:T:305:THR:HA | 2.26 | 0.50 |
| 1:S:1751:GLU:O | 1:S:1788:ARG:NH1 | 2.44 | 0.50 |
| 1:S:2218:PHE:HA | 1:S:2221:LYS:HE2 | 1.93 | 0.50 |
| 1:S:2363:CYS:O | 1:S:2367:VAL:HG22 | 2.11 | 0.50 |
| 1:A:849:GLU:HG2 | 1:A:850:GLU:H | 1.77 | 0.50 |
| 1:A:889:GLU:HG3 | 1:A:891:ARG:HG3 | 1.93 | 0.50 |
| 1:A:1169:VAL:O | 1:A:1173:LEU:HG | 2.11 | 0.50 |
| 1:A:1516:GLU:HA | 1:A:1519:PHE:CD2 | 2.46 | 0.50 |
| 1:A:1528:LEU:O | 1:A:1532:LEU:HG | 2.11 | 0.50 |
| 1:A:1601:LEU:HD21 | 1:A:1652:ILE:HG22 | 1.92 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1687:HIS:O | 1:A:1745:LYS:NZ | 2.44 | 0.50 |
| 1:A:2166:SER:OG | 1:A:2167:PRO:HD3 | 2.12 | 0.50 |
| 1:A:2167:PRO:O | 1:A:2170:GLN:HG3 | 2.12 | 0.50 |
| 1:A:2827:SER:HA | 1:A:2830:ASN:HD21 | 1.77 | 0.50 |
| 1:A:3077:ILE:HG23 | 1:A:3081:HIS:CD2 | 2.46 | 0.50 |
| 1:A:3921:GLY:O | 1:A:3944:HIS:ND1 | 2.45 | 0.50 |
| 3:C:465:LYS:HB2 | 3:C:476:LEU:HD21 | 1.92 | 0.50 |
| 1:S:269:SER:O | 1:S:273:ARG:HG3 | 2.11 | 0.50 |
| 1:S:994:TRP:CE2 | 1:S:2581:LEU:HD21 | 2.46 | 0.50 |
| 1:S:995:PHE:CE1 | 1:S:1004:GLN:HG3 | 2.46 | 0.50 |
| 1:S:1201:ASN:HB3 | 1:S:1207:TRP:CD1 | 2.47 | 0.50 |
| 1:S:1574:ASN:HD21 | 1:S:1578:ALA:H | 1.58 | 0.50 |
| 1:S:2295:GLN:N | 1:S:2295:GLN:OE1 | 2.44 | 0.50 |
| 1:S:3110:PHE:HB3 | 1:S:3128:LYS:HD2 | 1.94 | 0.50 |
| 1:A:268:PRO:O | 1:A:272:LEU:HG | 2.12 | 0.50 |
| 1:A:412:SER:O | 1:A:415:GLN:HG2 | 2.10 | 0.50 |
| 1:A:967:PRO:C | 1:A:971:ARG:HE | 2.18 | 0.50 |
| 1:A:2773:ARG:HG3 | 1:A:2789:SER:HB2 | 1.93 | 0.50 |
| 1:A:2782:ASP:N | 1:A:2782:ASP:OD1 | 2.43 | 0.50 |
| 1:A:3603:LYS:NZ | 1:A:3645:GLY:O | 2.45 | 0.50 |
| 1:A:3793:VAL:HG23 | 1:A:3803:ILE:HG13 | 1.93 | 0.50 |
| 2:B:369:TYR:OH | 3:C:436:SER:O | 2.30 | 0.50 |
| 3:C:259:ILE:HG23 | 3:C:373:ALA:HB1 | 1.94 | 0.50 |
| 3:C:523:THR:HG22 | 3:C:527:GLN:NE2 | 2.27 | 0.50 |
| 4:D:7:PRO:HG2 | 4:D:76:PHE:HD2 | 1.76 | 0.50 |
| 1:S:1176:CYS:HA | 1:S:1178:ARG:NH1 | 2.27 | 0.50 |
| 1:S:1784:ARG:HA | 1:S:1787:ARG:CZ | 2.41 | 0.50 |
| 1:S:2443:MET:SD | 1:S:2444:PRO:HD3 | 2.52 | 0.50 |
| 1:S:3141:PHE:HB2 | 1:S:3189:PHE:CD2 | 2.47 | 0.50 |
| 1:S:3787:GLN:NE2 | 1:S:3788:LEU:O | 2.45 | 0.50 |
| 2:T:170:THR:C | 2:T:205:LEU:HD23 | 2.36 | 0.50 |
| 1:A:62:ASP:O | 1:A:66:LEU:HB2 | 2.11 | 0.50 |
| 1:A:133:LYS:O | 1:A:136:GLN:HG2 | 2.11 | 0.50 |
| 1:A:134:LEU:HD11 | 1:A:177:LEU:CD2 | 2.41 | 0.50 |
| 1:A:1876:ILE:HG13 | 1:A:1877:LEU:HD22 | 1.92 | 0.50 |
| 1:A:2097:LEU:O | 1:A:2101:VAL:HG23 | 2.11 | 0.50 |
| 1:A:2470:ARG:HA | 1:A:2473:MET:CE | 2.42 | 0.50 |
| 1:A:2578:GLU:OE1 | 1:A:2578:GLU:N | 2.40 | 0.50 |
| 1:A:2830:ASN:O | 1:A:2834:GLN:HG2 | 2.11 | 0.50 |
| 2:B:89:GLY:O | 2:B:139:SER:OG | 2.27 | 0.50 |
| 2:B:479:GLU:OE1 | 2:B:484:GLN:NE2 | 2.45 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:324:SER:OG | 3:C:325:LYS:N | 2.45 | 0.50 |
| 1:S:131:LEU:HB2 | 1:S:173:LYS:HE2 | 1.94 | 0.50 |
| 1:S:200:PHE:HB3 | 1:S:224:LEU:HD13 | 1.93 | 0.50 |
| 1:S:473:PRO:O | 1:S:477:ASN:ND2 | 2.45 | 0.50 |
| 1:S:1181:THR:OG1 | 1:S:1265:GLU:OE1 | 2.26 | 0.50 |
| 1:S:2953:THR:HG23 | 1:S:2993:PHE:CE2 | 2.46 | 0.50 |
| 1:S:3739:ILE:HG23 | 1:S:3747:GLU:HB2 | 1.94 | 0.50 |
| 2:T:154:PHE:O | 2:T:157:VAL:HG12 | 2.12 | 0.50 |
| 1:A:135:LEU:O | 1:A:139:ARG:HD3 | 2.11 | 0.50 |
| 1:A:486:GLY:O | 1:A:490:ILE:HG12 | 2.11 | 0.50 |
| 1:A:767:GLU:OE1 | 1:A:854:ARG:NE | 2.45 | 0.50 |
| 1:A:1178:ARG:HB2 | 1:A:1184:ARG:HB2 | 1.93 | 0.50 |
| 1:A:2104:MET:HE1 | 1:A:2122:LEU:HB3 | 1.94 | 0.50 |
| 1:A:2225:HIS:CD2 | 1:A:2230:VAL:HG23 | 2.46 | 0.50 |
| 1:A:2468:THR:O | 1:A:2472:GLN:HG3 | 2.11 | 0.50 |
| 1:A:3748:HIS:HB3 | 1:A:3750:PHE:HE1 | 1.76 | 0.50 |
| 2:B:94:LYS:HD3 | 2:B:103:TYR:CZ | 2.47 | 0.50 |
| 2:B:444:ARG:HE | 3:C:268:LEU:HD12 | 1.75 | 0.50 |
| 3:C:9:ALA:HB3 | 3:C:130:ARG:HA | 1.94 | 0.50 |
| 3:C:132:ILE:HD12 | 3:C:133:GLU:H | 1.77 | 0.50 |
| 3:C:365:PHE:CZ | 3:C:418:CYS:HB3 | 2.47 | 0.50 |
| 3:L:6:ASN:HB3 | 3:L:128:GLU:HB3 | 1.93 | 0.50 |
| 3:L:677:ILE:HA | 3:L:680:GLN:CD | 2.37 | 0.50 |
| 1:S:320:LEU:HA | 1:S:323:VAL:HG22 | 1.93 | 0.50 |
| 1:S:382:ASP:HB3 | 1:S:424:LEU:HD11 | 1.94 | 0.50 |
| 1:S:1135:CYS:HB2 | 1:S:1194:PHE:HE2 | 1.77 | 0.50 |
| 1:S:1752:LEU:HA | 1:S:1788:ARG:HH12 | 1.77 | 0.50 |
| 1:S:1780:SER:HB2 | 1:S:1784:ARG:NH1 | 2.27 | 0.50 |
| 1:S:2212:ALA:O | 1:S:2216:LEU:HG | 2.10 | 0.50 |
| 1:S:2584:CYS:SG | 1:S:2780:LEU:HD12 | 2.52 | 0.50 |
| 1:S:2946:GLU:O | 1:S:2949:THR:OG1 | 2.30 | 0.50 |
| 1:S:3001:CYS:O | 1:S:3005:LEU:N | 2.39 | 0.50 |
| 1:S:3138:ILE:HA | 1:S:3189:PHE:CZ | 2.46 | 0.50 |
| 1:S:3235:LYS:O | 1:S:3239:LYS:HG2 | 2.12 | 0.50 |
| 1:S:3288:SER:OG | 1:S:3296:GLN:NE2 | 2.44 | 0.50 |
| 1:S:3442:TYR:HB3 | 1:S:3443:PRO:HD3 | 1.94 | 0.50 |
| 1:S:3493:TRP:HE3 | 1:S:3524:ASN:HB2 | 1.76 | 0.50 |
| 1:S:3530:VAL:O | 1:S:3534:ILE:HG12 | 2.12 | 0.50 |
| 2:T:101:ASN:ND2 | 2:T:140:ASP:O | 2.45 | 0.50 |
| 8:e:28:DT:O4 | 8:e:29:DA:N6 | 2.45 | 0.50 |
| 10:j:34:DT:H2” | 10:j:35:DT:C6 | 2.47 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2492:ASP:OD2 | 1:A:2495:SER:N | 2.43 | 0.50 |
| 1:A:3300:VAL:HG11 | 1:A:3360:LEU:HD21 | 1.94 | 0.50 |
| 3:C:725:VAL:HG22 | 1:S:1917:LYS:HE3 | 1.94 | 0.50 |
| 3:L:13:CYS:O | 3:L:134:ILE:HA | 2.11 | 0.50 |
| 1:S:110:THR:O | 1:S:114:VAL:HG23 | 2.12 | 0.50 |
| 1:S:303:HIS:O | 1:S:309:LYS:NZ | 2.33 | 0.50 |
| 1:S:305:ASN:HB3 | 1:S:307:GLU:OE2 | 2.11 | 0.50 |
| 1:S:570:LYS:HA | 1:S:573:LEU:HD12 | 1.94 | 0.50 |
| 1:S:1082:PHE:HA | 1:S:1085:ILE:HG12 | 1.93 | 0.50 |
| 1:S:1115:HIS:CE1 | 1:S:1182:GLU:HB3 | 2.46 | 0.50 |
| 1:S:1453:SER:O | 1:S:1457:GLN:HG3 | 2.12 | 0.50 |
| 1:S:1838:GLU:O | 1:S:1842:THR:OG1 | 2.26 | 0.50 |
| 1:S:1960:LYS:HD2 | 1:S:1960:LYS:O | 2.12 | 0.50 |
| 1:S:2959:ALA:HB1 | 1:S:2967:GLU:HG3 | 1.94 | 0.50 |
| 1:S:3546:SER:O | 1:S:3550:LYS:NZ | 2.44 | 0.50 |
| 1:S:3757:ASP:HB2 | 1:S:3798:SER:HA | 1.93 | 0.50 |
| 1:S:3909:ALA:HB2 | 1:S:3980:MET:SD | 2.52 | 0.50 |
| 2:T:262:LYS:NZ | 2:T:346:MET:SD | 2.75 | 0.50 |
| 1:A:217:LEU:HB2 | 1:A:220:LEU:HB2 | 1.94 | 0.49 |
| 1:A:2165:LEU:HD11 | 1:A:2200:ALA:HB1 | 1.93 | 0.49 |
| 1:A:2278:GLY:O | 1:A:2282:ALA:N | 2.40 | 0.49 |
| 1:A:2344:LEU:HD23 | 1:A:2347:LYS:HZ1 | 1.77 | 0.49 |
| 1:A:2468:THR:O | 1:A:2471:GLU:HG2 | 2.12 | 0.49 |
| 1:A:2473:MET:O | 1:A:2477:LEU:HG | 2.12 | 0.49 |
| 3:C:249:CYS:SG | 3:C:250:ARG:N | 2.84 | 0.49 |
| 3:L:18:PHE:N | 3:L:101:GLY:O | 2.45 | 0.49 |
| 3:L:458:ILE:HG12 | 2:T:350:PHE:CE2 | 2.47 | 0.49 |
| 1:S:1391:VAL:O | 1:S:1395:LEU:HG | 2.11 | 0.49 |
| 1:S:1708:GLU:HG3 | 1:S:1712:ARG:HD3 | 1.94 | 0.49 |
| 1:S:2227:LYS:O | 1:S:2229:ALA:N | 2.44 | 0.49 |
| 1:S:2306:ASN:HA | 1:S:2309:PHE:CD2 | 2.47 | 0.49 |
| 1:S:2864:GLN:HG3 | 1:S:2865:HIS:ND1 | 2.27 | 0.49 |
| 1:S:3467:ARG:HH22 | 1:S:3474:ARG:HD3 | 1.77 | 0.49 |
| 1:S:3950:THR:HG21 | 1:S:3958:LEU:HB3 | 1.94 | 0.49 |
| 2:T:465:ILE:HG13 | 2:T:521:LEU:HD13 | 1.94 | 0.49 |
| 1:A:789:TYR:HD1 | 1:A:792:ILE:HD12 | 1.77 | 0.49 |
| 1:A:1189:GLU:OE1 | 1:A:1193:LYS:NZ | 2.35 | 0.49 |
| 1:A:2168:LEU:O | 1:A:2172:ALA:N | 2.38 | 0.49 |
| 1:A:2786:LYS:O | 1:A:2789:SER:OG | 2.22 | 0.49 |
| 1:A:2920:VAL:HA | 1:A:2923:TRP:HB2 | 1.94 | 0.49 |
| 1:A:3328:ILE:HD12 | 1:A:3415:THR:HG21 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3390:GLN:HA | 1:A:3393:GLU:CD | 2.37 | 0.49 |
| 2:B:64:ILE:O | 2:B:68:GLN:HG2 | 2.12 | 0.49 |
| 3:C:294:VAL:HG13 | 3:C:304:GLU:HB2 | 1.93 | 0.49 |
| 5:Q:155:TRP:HA | 5:Q:158:VAL:HG22 | 1.94 | 0.49 |
| 6:R:707:ILE:HD11 | 2:T:500:PRO:HB3 | 1.94 | 0.49 |
| 1:S:80:GLU:O | 1:S:83:GLU:HG2 | 2.12 | 0.49 |
| 1:S:237:SER:HA | 1:S:281:GLN:HG3 | 1.93 | 0.49 |
| 1:S:939:MET:HE2 | 1:S:2782:ASP:O | 2.12 | 0.49 |
| 1:S:1289:SER:HA | 1:S:1292:LYS:HB3 | 1.94 | 0.49 |
| 1:S:1793:THR:O | 1:S:1797:LEU:HD13 | 2.12 | 0.49 |
| 1:S:1878:ASP:OD1 | 1:S:1879:VAL:N | 2.44 | 0.49 |
| 1:S:2424:MET:HE2 | 1:S:2461:PHE:CZ | 2.47 | 0.49 |
| 1:S:2757:ILE:O | 1:S:2760:GLU:HG3 | 2.12 | 0.49 |
| 1:S:3277:VAL:HG13 | 1:S:3306:LEU:HB3 | 1.94 | 0.49 |
| 1:S:3323:PHE:O | 1:S:3327:ASN:ND2 | 2.45 | 0.49 |
| 1:S:3578:LEU:HD21 | 1:S:3681:LYS:HE3 | 1.94 | 0.49 |
| 9:i:40:DT:H2” | 9:i:41:DT:C5 | 2.47 | 0.49 |
| 1:A:440:VAL:O | 1:A:444:ASP:N | 2.45 | 0.49 |
| 1:A:573:LEU:O | 1:A:576:VAL:HG22 | 2.11 | 0.49 |
| 1:A:1334:LYS:O | 1:A:1338:VAL:HG23 | 2.13 | 0.49 |
| 1:A:1484:LEU:HA | 1:A:1487:VAL:HG12 | 1.94 | 0.49 |
| 1:A:1633:TRP:H | 1:A:1642:LYS:HG2 | 1.76 | 0.49 |
| 1:A:3117:ILE:HG13 | 1:A:3125:ARG:HE | 1.77 | 0.49 |
| 2:B:106:GLN:HB3 | 2:B:115:ARG:HH21 | 1.76 | 0.49 |
| 2:B:213:ILE:HD12 | 2:B:228:ASP:HA | 1.94 | 0.49 |
| 6:R:723:PRO:O | 6:R:727:LEU:HG | 2.12 | 0.49 |
| 1:S:640:GLU:HA | 1:S:643:GLU:CD | 2.37 | 0.49 |
| 1:S:772:ALA:HB1 | 1:S:776:TRP:CZ2 | 2.46 | 0.49 |
| 1:S:886:TRP:CE2 | 1:S:912:PRO:HB3 | 2.48 | 0.49 |
| 1:S:2389:PHE:HB3 | 1:S:2393:LEU:HB2 | 1.95 | 0.49 |
| 1:S:2470:ARG:CA | 1:S:2473:MET:HE2 | 2.40 | 0.49 |
| 1:S:3008:TRP:CD1 | 1:S:3008:TRP:H | 2.30 | 0.49 |
| 1:S:3337:ILE:HD13 | 1:S:3360:LEU:HD12 | 1.94 | 0.49 |
| 1:S:3383:GLN:O | 1:S:3387:GLU:HG3 | 2.12 | 0.49 |
| 1:S:4002:MET:SD | 1:S:4044:ILE:HG22 | 2.51 | 0.49 |
| 10:j:21:DA:H2” | 10:j:22:DG:H8 | 1.76 | 0.49 |
| 1:A:434:VAL:O | 1:A:438:LEU:HG | 2.12 | 0.49 |
| 1:A:724:GLU:OE1 | 1:A:2600:THR:N | 2.43 | 0.49 |
| 1:A:1766:LEU:HD11 | 1:A:1775:GLU:HG2 | 1.93 | 0.49 |
| 1:A:2192:THR:O | 1:A:2195:SER:OG | 2.23 | 0.49 |
| 1:A:3008:TRP:HA | 1:A:3011:LEU:HG | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3499:ILE:O | 1:A:3503:VAL:HG12 | 2.12 | 0.49 |
| 1:A:3874:ARG:O | 1:A:3878:VAL:HG12 | 2.11 | 0.49 |
| 1:A:3980:MET:HE3 | 1:A:3980:MET:H | 1.78 | 0.49 |
| 2:B:240:GLU:HG2 | 2:B:241:ASP:H | 1.77 | 0.49 |
| 3:C:238:LYS:HZ2 | 11:f:294:PRO:HD3 | 1.77 | 0.49 |
| 3:C:728:LEU:HG | 1:S:1916:ILE:HD12 | 1.95 | 0.49 |
| 3:C:731:MET:N | 1:S:1913:LYS:HG2 | 2.16 | 0.49 |
| 5:H:159:GLN:HG3 | 6:I:843:LEU:HD12 | 1.93 | 0.49 |
| 3:L:479:THR:HG21 | 2:T:410:PHE:CG | 2.48 | 0.49 |
| 3:L:635:SER:O | 3:L:639:ILE:HG12 | 2.12 | 0.49 |
| 1:S:584:GLU:C | 1:S:613:HIS:HB3 | 2.37 | 0.49 |
| 1:S:2928:LYS:HA | 1:S:2931:ARG:HG2 | 1.93 | 0.49 |
| 1:S:3047:SER:O | 1:S:3051:LEU:HG | 2.11 | 0.49 |
| 1:S:3311:ASN:HB2 | 1:S:3314:SER:HA | 1.94 | 0.49 |
| 1:A:723:ASP:C | 1:A:725:LEU:H | 2.20 | 0.49 |
| 1:A:1257:LEU:O | 1:A:1261:LEU:HG | 2.12 | 0.49 |
| 1:A:1368:LEU:HD12 | 1:A:1372:LEU:HD23 | 1.94 | 0.49 |
| 1:A:2228:ARG:HA | 1:A:2231:PHE:HB3 | 1.94 | 0.49 |
| 1:A:2346:ALA:HA | 1:A:2349:LEU:HD12 | 1.94 | 0.49 |
| 1:A:2377:ARG:HB2 | 1:A:2378:PHE:CE2 | 2.47 | 0.49 |
| 1:A:3239:LYS:HD3 | 1:A:3262:LEU:HD22 | 1.95 | 0.49 |
| 1:A:3596:LEU:HA | 1:A:3602:ASN:HD21 | 1.77 | 0.49 |
| 1:A:3759:ARG:HH21 | 1:A:4005:PHE:HE2 | 1.61 | 0.49 |
| 1:A:3856:MET:HG3 | 1:A:3860:LYS:HZ3 | 1.77 | 0.49 |
| 2:B:76:ILE:HG21 | 2:B:247:ARG:HA | 1.93 | 0.49 |
| 2:B:299:LYS:HZ3 | 3:C:296:CYS:HB3 | 1.77 | 0.49 |
| 6:I:815:ARG:H | 6:I:850:ALA:N | 2.10 | 0.49 |
| 1:S:172:GLU:HB3 | 1:S:175:TYR:CE2 | 2.47 | 0.49 |
| 1:S:185:HIS:HB3 | 1:S:190:ILE:HD11 | 1.93 | 0.49 |
| 1:S:410:MET:O | 1:S:414:LEU:HG | 2.12 | 0.49 |
| 1:S:976:VAL:O | 1:S:2598:ARG:NH2 | 2.45 | 0.49 |
| 1:S:1476:HIS:HD2 | 1:S:1521:PHE:CD1 | 2.29 | 0.49 |
| 1:S:1589:ASN:HB3 | 1:S:1592:MET:SD | 2.52 | 0.49 |
| 1:S:1696:LEU:HG | 1:S:1697:PRO:HD3 | 1.94 | 0.49 |
| 1:S:1713:VAL:HA | 1:S:1716:GLN:CD | 2.37 | 0.49 |
| 1:S:1713:VAL:HA | 1:S:1716:GLN:HG2 | 1.95 | 0.49 |
| 1:S:2324:GLY:HA3 | 1:S:2367:VAL:HA | 1.93 | 0.49 |
| 1:S:2443:MET:HA | 1:S:2446:LEU:HD13 | 1.95 | 0.49 |
| 1:S:2817:LEU:HD12 | 1:S:2865:HIS:CE1 | 2.48 | 0.49 |
| 1:S:2880:CYS:O | 1:S:2885:GLN:N | 2.46 | 0.49 |
| 1:S:3151:LEU:HD23 | 1:S:3151:LEU:H | 1.77 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:345:LEU:HB3 | 2:T:398:CYS:SG | 2.53 | 0.49 |
| 1:A:300:TRP:HE3 | 1:A:308:LEU:HD21 | 1.78 | 0.49 |
| 1:A:560:LEU:HD13 | 1:A:563:LEU:HD12 | 1.94 | 0.49 |
| 1:A:2211:LEU:HA | 1:A:2214:ARG:HG2 | 1.94 | 0.49 |
| 1:A:2386:LEU:HB3 | 1:A:2387:PRO:HD3 | 1.94 | 0.49 |
| 1:A:3100:LYS:HA | 1:A:3103:ILE:HG22 | 1.95 | 0.49 |
| 1:A:3177:ASN:OD1 | 1:A:3178:ILE:N | 2.46 | 0.49 |
| 1:A:3183:ILE:HG13 | 1:A:3242:MET:CE | 2.38 | 0.49 |
| 1:A:3864:ARG:CZ | 1:A:4085:LYS:HG3 | 2.42 | 0.49 |
| 2:B:343:PRO:HG3 | 2:B:403:ARG:C | 2.38 | 0.49 |
| 2:B:374:LEU:O | 3:C:541:GLU:HA | 2.13 | 0.49 |
| 2:B:423:GLN:HB2 | 2:B:425:ILE:HG12 | 1.94 | 0.49 |
| 3:C:8:ALA:HB2 | 3:C:129:LYS:HE2 | 1.93 | 0.49 |
| 3:C:223:GLU:OE2 | 11:f:293:LYS:HG3 | 2.13 | 0.49 |
| 3:L:291:LYS:HA | 2:T:302:THR:HA | 1.94 | 0.49 |
| 1:S:180:LEU:C | 1:S:185:HIS:HE2 | 2.20 | 0.49 |
| 1:S:560:LEU:O | 1:S:564:LEU:HG | 2.12 | 0.49 |
| 1:S:762:TYR:CD2 | 1:S:764:PRO:HD2 | 2.48 | 0.49 |
| 1:S:1018:VAL:HA | 1:S:1073:PHE:HB3 | 1.94 | 0.49 |
| 1:S:1935:GLU:O | 1:S:1939:LEU:HG | 2.12 | 0.49 |
| 1:S:2184:TYR:HD1 | 1:S:2734:ARG:HH21 | 1.60 | 0.49 |
| 1:S:2347:LYS:O | 1:S:2351:GLN:N | 2.44 | 0.49 |
| 1:S:2796:ALA:O | 1:S:2800:ARG:HG2 | 2.12 | 0.49 |
| 1:S:3314:SER:HB2 | 1:S:3318:LYS:HE3 | 1.94 | 0.49 |
| 1:S:3912:CYS:HA | 1:S:3915:HIS:CD2 | 2.48 | 0.49 |
| 8:e:24:DA:H1' | 8:e:25:DA:H5' | 1.95 | 0.49 |
| 1:A:156:PHE:HA | 1:A:159:GLU:HG2 | 1.93 | 0.49 |
| 1:A:172:GLU:HA | 1:A:174:VAL:HG12 | 1.93 | 0.49 |
| 1:A:253:LEU:HD21 | 1:A:268:PRO:HA | 1.94 | 0.49 |
| 1:A:703:CYS:HB3 | 1:A:707:PHE:CZ | 2.48 | 0.49 |
| 1:A:1868:THR:O | 1:A:1871:MET:HB2 | 2.11 | 0.49 |
| 1:A:2208:ASP:OD1 | 1:A:2209:GLU:N | 2.45 | 0.49 |
| 1:A:2266:ASN:HB2 | 1:A:2311:ARG:HB2 | 1.94 | 0.49 |
| 1:A:2332:GLU:OE1 | 1:A:2334:LYS:NZ | 2.44 | 0.49 |
| 1:A:3180:ASP:OD1 | 1:A:3181:ASP:N | 2.46 | 0.49 |
| 1:A:3190:LEU:HB3 | 1:A:3231:ILE:HD11 | 1.94 | 0.49 |
| 1:A:3254:LEU:HD23 | 1:A:3255:ALA:N | 2.27 | 0.49 |
| 2:B:165:ARG:NH2 | 4:D:186:ILE:O | 2.46 | 0.49 |
| 6:R:720:VAL:N | 6:R:743:MET:HE1 | 2.27 | 0.49 |
| 1:S:384:MET:O | 1:S:387:GLU:HG2 | 2.12 | 0.49 |
| 1:S:2330:VAL:HG12 | 1:S:2333:ARG:HH12 | 1.77 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3450:MET:HG2 | 1:S:3464:LYS:HG2 | 1.95 | 0.49 |
| 1:S:3589:SER:HB3 | 1:S:3593:ARG:CZ | 2.43 | 0.49 |
| 1:S:3762:GLN:HG2 | 1:S:3766:GLN:NE2 | 2.27 | 0.49 |
| 1:S:3988:LEU:HB3 | 1:S:4100:GLU:HB3 | 1.93 | 0.49 |
| 2:T:523:ASP:O | 2:T:527:GLU:HG2 | 2.12 | 0.49 |
| 1:A:89:LEU:O | 1:A:133:LYS:NZ | 2.41 | 0.49 |
| 1:A:861:SER:N | 1:A:3136:THR:HG21 | 2.27 | 0.49 |
| 1:A:1343:GLU:O | 1:A:1346:THR:OG1 | 2.26 | 0.49 |
| 1:A:3008:TRP:HB3 | 1:A:3050:LYS:HE2 | 1.95 | 0.49 |
| 1:A:3512:VAL:HB | 1:A:3516:HIS:CE1 | 2.47 | 0.49 |
| 1:A:3586:LYS:HZ1 | 1:A:3668:LEU:HD22 | 1.78 | 0.49 |
| 1:A:3593:ARG:HG2 | 1:A:3657:SER:HA | 1.95 | 0.49 |
| 1:A:3629:ARG:O | 1:A:3633:ILE:HG12 | 2.12 | 0.49 |
| 1:A:3737:ARG:CZ | 1:A:3739:ILE:HG12 | 2.43 | 0.49 |
| 2:B:59:PRO:HA | 2:B:62:MET:HG2 | 1.94 | 0.49 |
| 3:C:135:PHE:CD1 | 3:C:164:PHE:HB2 | 2.48 | 0.49 |
| 3:C:183:PHE:HB2 | 3:C:192:PHE:HA | 1.94 | 0.49 |
| 3:L:108:LEU:HB3 | 3:L:146:GLN:HB2 | 1.94 | 0.49 |
| 3:L:427:MET:HE1 | 4:M:196:ALA:HB2 | 1.94 | 0.49 |
| 1:S:1690:GLY:HA2 | 1:S:1693:VAL:HG22 | 1.93 | 0.49 |
| 1:S:2138:VAL:HG13 | 1:S:2143:ARG:HG2 | 1.95 | 0.49 |
| 1:S:3133:GLN:O | 1:S:3136:THR:HG22 | 2.13 | 0.49 |
| 2:T:60:PHE:O | 2:T:63:SER:OG | 2.28 | 0.49 |
| 8:e:35:DT:H3' | 8:e:36:DA:C8 | 2.48 | 0.49 |
| 1:A:764:PRO:O | 1:A:768:VAL:HG22 | 2.13 | 0.49 |
| 1:A:941:MET:HE2 | 1:A:958:MET:HE3 | 1.95 | 0.49 |
| 1:A:2353:GLN:HB3 | 1:A:2360:PHE:HB2 | 1.93 | 0.49 |
| 1:A:2596:ARG:O | 1:A:2598:ARG:NH1 | 2.45 | 0.49 |
| 1:A:3312:VAL:O | 1:A:3316:LEU:N | 2.38 | 0.49 |
| 1:A:3608:LYS:O | 1:A:3611:GLU:HG3 | 2.13 | 0.49 |
| 1:A:3740:ILE:HB | 1:A:3748:HIS:HB2 | 1.94 | 0.49 |
| 1:A:3749:PRO:HB2 | 1:A:3805:TRP:CD1 | 2.47 | 0.49 |
| 1:A:3966:GLN:HA | 1:A:3969:ASN:HB2 | 1.94 | 0.49 |
| 2:B:82:LEU:HD12 | 2:B:108:LEU:O | 2.12 | 0.49 |
| 2:B:291:GLU:C | 6:I:691:GLN:HG2 | 2.38 | 0.49 |
| 3:C:191:SER:OG | 3:C:192:PHE:N | 2.46 | 0.49 |
| 3:C:617:ILE:HD13 | 3:C:620:ILE:HD11 | 1.94 | 0.49 |
| 5:G:100:ASN:OD1 | 5:G:105:SER:OG | 2.26 | 0.49 |
| 6:I:740:PRO:HA | 6:I:743:MET:HE2 | 1.95 | 0.49 |
| 1:S:176:GLU:HG3 | 1:S:226:GLY:HA3 | 1.95 | 0.49 |
| 1:S:1295:ALA:HA | 1:S:1298:LEU:HD12 | 1.95 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1873:TYR:O | 1:S:1877:LEU:HD23 | 2.12 | 0.49 |
| 1:S:2953:THR:OG1 | 1:S:2994:TRP:NE1 | 2.43 | 0.49 |
| 1:S:3353:GLU:HG2 | 1:S:3357:ARG:HE | 1.78 | 0.49 |
| 1:S:3639:GLU:OE2 | 1:S:3643:HIS:NE2 | 2.46 | 0.49 |
| 1:A:219:VAL:HG12 | 1:A:223:CYS:SG | 2.53 | 0.49 |
| 1:A:1189:GLU:O | 1:A:1193:LYS:HG2 | 2.13 | 0.49 |
| 1:A:1363:LEU:HD23 | 1:A:1366:THR:HA | 1.95 | 0.49 |
| 1:A:1416:GLU:HA | 1:A:1419:LEU:HD12 | 1.95 | 0.49 |
| 1:A:1469:PRO:O | 1:A:1476:HIS:NE2 | 2.46 | 0.49 |
| 1:A:1878:ASP:HB3 | 1:A:1947:CYS:HA | 1.94 | 0.49 |
| 1:A:2304:VAL:O | 1:A:2307:MET:HB2 | 2.13 | 0.49 |
| 1:A:2402:LEU:HD21 | 1:A:2434:VAL:HB | 1.94 | 0.49 |
| 1:A:2435:CYS:O | 1:A:2439:ILE:HG12 | 2.13 | 0.49 |
| 1:A:2464:HIS:CD2 | 1:A:2465:PRO:HD2 | 2.47 | 0.49 |
| 1:A:3188:PHE:O | 1:A:3192:LYS:HG2 | 2.13 | 0.49 |
| 1:A:3471:ILE:HA | 1:A:3474:ARG:HD3 | 1.95 | 0.49 |
| 1:A:3768:PHE:HB3 | 1:A:3790:THR:HG21 | 1.95 | 0.49 |
| 1:A:3894:PRO:O | 1:A:3898:LEU:HG | 2.13 | 0.49 |
| 2:B:146:VAL:HA | 2:B:149:VAL:HG22 | 1.95 | 0.49 |
| 1:S:23:ASP:N | 1:S:23:ASP:OD1 | 2.45 | 0.49 |
| 1:S:639:ALA:O | 1:S:643:GLU:N | 2.46 | 0.49 |
| 1:S:893:SER:H | 1:S:944:LYS:HZ3 | 1.61 | 0.49 |
| 1:S:1524:LEU:O | 1:S:1528:LEU:HG | 2.12 | 0.49 |
| 1:S:1752:LEU:HA | 1:S:1788:ARG:HH22 | 1.78 | 0.49 |
| 1:S:2300:PHE:HB3 | 1:S:2303:LEU:HD12 | 1.94 | 0.49 |
| 1:S:3048:LYS:HD3 | 1:S:3061:LEU:HB3 | 1.94 | 0.49 |
| 2:T:531:PRO:HD2 | 2:T:534:TYR:HD2 | 1.77 | 0.49 |
| 7:d:30:DT:H2" | 7:d:31:DT:O5' | 2.12 | 0.49 |
| 1:A:1413:ASP:O | 1:A:1416:GLU:HG2 | 2.13 | 0.48 |
| 1:A:1664:SER:HA | 1:A:1668:PHE:CD2 | 2.48 | 0.48 |
| 1:A:1750:LEU:HD11 | 1:A:1755:SER:O | 2.12 | 0.48 |
| 1:A:3247:ARG:HE | 1:A:3282:ARG:NH1 | 2.11 | 0.48 |
| 1:A:3289:ARG:NH1 | 1:A:3295:GLU:OE2 | 2.40 | 0.48 |
| 1:A:3387:GLU:O | 1:A:3390:GLN:NE2 | 2.46 | 0.48 |
| 1:A:4087:HIS:HA | 1:A:4090:ARG:HD2 | 1.95 | 0.48 |
| 2:B:181:ALA:HB1 | 2:B:185:ARG:NH2 | 2.28 | 0.48 |
| 2:B:255:ALA:HA | 2:B:274:TYR:CE2 | 2.48 | 0.48 |
| 2:B:422:ASP:N | 2:B:422:ASP:OD1 | 2.45 | 0.48 |
| 3:C:633:MET:HA | 3:C:636:ILE:HG22 | 1.95 | 0.48 |
| 3:C:688:LYS:HG3 | 3:C:695:SER:HA | 1.94 | 0.48 |
| 3:L:264:TYR:O | 3:L:363:LYS:N | 2.45 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:450:GLN:HG2 | 3:L:536:LEU:HB3 | 1.95 | 0.48 |
| 6:R:681:ARG:HH22 | 6:R:726:LEU:HD11 | 1.77 | 0.48 |
| 1:S:1196:PRO:HD3 | 1:S:1203:SER:HB2 | 1.95 | 0.48 |
| 1:S:1565:GLU:H | 1:S:1565:GLU:CD | 2.20 | 0.48 |
| 1:S:1711:ARG:HB2 | 1:S:1757:MET:HE3 | 1.95 | 0.48 |
| 1:S:1803:GLU:HA | 1:S:1806:ARG:NH2 | 2.27 | 0.48 |
| 1:S:2341:LEU:HD13 | 1:S:2344:LEU:HD12 | 1.94 | 0.48 |
| 1:S:3287:ARG:O | 1:S:3289:ARG:NH2 | 2.39 | 0.48 |
| 2:T:523:ASP:N | 2:T:523:ASP:OD1 | 2.43 | 0.48 |
| 1:A:391:ARG:NH1 | 1:A:394:GLN:HB3 | 2.28 | 0.48 |
| 1:A:472:GLY:O | 1:A:475:LEU:HG | 2.12 | 0.48 |
| 1:A:579:LEU:HD13 | 1:A:623:PHE:HD1 | 1.78 | 0.48 |
| 1:A:1046:PRO:O | 1:A:1050:GLU:HG3 | 2.13 | 0.48 |
| 1:A:1502:SER:OG | 1:A:1503:LEU:N | 2.46 | 0.48 |
| 1:A:1505:LEU:HA | 1:A:1508:LYS:HD2 | 1.95 | 0.48 |
| 1:A:1669:PRO:O | 1:A:1673:THR:N | 2.33 | 0.48 |
| 1:A:1769:GLU:O | 1:A:1772:HIS:ND1 | 2.46 | 0.48 |
| 1:A:2126:MET:HA | 1:A:2129:LEU:HD12 | 1.94 | 0.48 |
| 1:A:2572:TYR:CE1 | 1:A:2791:ILE:HD11 | 2.48 | 0.48 |
| 1:A:3302:LYS:O | 1:A:3303:THR:OG1 | 2.20 | 0.48 |
| 1:A:3551:ASN:O | 1:A:3555:VAL:HG13 | 2.13 | 0.48 |
| 1:A:4041:ARG:O | 1:A:4044:ILE:HG12 | 2.13 | 0.48 |
| 2:B:463:LYS:O | 2:B:467:GLU:HG2 | 2.14 | 0.48 |
| 2:B:505:ASP:OD2 | 2:B:508:LEU:HG | 2.13 | 0.48 |
| 3:C:647:ILE:HA | 3:C:652:GLU:HG2 | 1.95 | 0.48 |
| 3:L:150:ILE:O | 3:L:154:LEU:HG | 2.13 | 0.48 |
| 3:L:665:LYS:O | 3:L:669:LYS:HG2 | 2.13 | 0.48 |
| 6:R:723:PRO:O | 6:R:726:LEU:HG | 2.13 | 0.48 |
| 1:S:149:ILE:O | 1:S:153:PHE:N | 2.36 | 0.48 |
| 1:S:186:PRO:O | 1:S:190:ILE:HG12 | 2.12 | 0.48 |
| 1:S:370:ALA:HB1 | 1:S:381:VAL:HG13 | 1.95 | 0.48 |
| 1:S:786:GLN:HA | 1:S:789:TYR:CD2 | 2.48 | 0.48 |
| 1:S:996:THR:HG21 | 1:S:1039:TRP:HD1 | 1.78 | 0.48 |
| 1:S:2157:PHE:HB2 | 1:S:2160:TYR:HB3 | 1.94 | 0.48 |
| 1:S:2371:PHE:CZ | 1:S:2373:PRO:HG2 | 2.48 | 0.48 |
| 1:S:2724:ASP:HA | 1:S:2727:ARG:NE | 2.27 | 0.48 |
| 1:S:2922:ARG:HA | 1:S:2925:GLU:HB2 | 1.94 | 0.48 |
| 1:S:2978:LYS:NZ | 1:S:2980:ASP:O | 2.46 | 0.48 |
| 1:S:3240:MET:HE3 | 1:S:3272:TRP:CZ3 | 2.48 | 0.48 |
| 1:S:3547:THR:HG23 | 1:S:3550:LYS:HD2 | 1.94 | 0.48 |
| 1:S:3915:HIS:HA | 1:S:3918:LEU:HB3 | 1.95 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1119:LYS:N | 1:A:1119:LYS:HD3 | 2.27 | 0.48 |
| 1:A:1172:LEU:O | 1:A:1176:CYS:N | 2.45 | 0.48 |
| 1:A:1256:TRP:O | 1:A:1260:LEU:HG | 2.13 | 0.48 |
| 1:A:1560:TYR:CE1 | 1:A:1596:VAL:HG12 | 2.48 | 0.48 |
| 1:A:1916:ILE:HG13 | 1:A:1917:LYS:H | 1.78 | 0.48 |
| 1:A:3169:PRO:HG3 | 1:A:3183:ILE:HD11 | 1.94 | 0.48 |
| 1:A:3867:THR:HG23 | 1:A:4118:GLY:CA | 2.43 | 0.48 |
| 3:C:38:ILE:HA | 11:f:297:LEU:HD21 | 1.94 | 0.48 |
| 3:L:468:GLU:O | 3:L:469:LYS:HG3 | 2.11 | 0.48 |
| 4:M:5:SER:HA | 4:M:131:ARG:HH12 | 1.77 | 0.48 |
| 1:S:620:PHE:HB3 | 1:S:2603:THR:HG21 | 1.95 | 0.48 |
| 1:S:939:MET:HE1 | 1:S:2781:PRO:CB | 2.43 | 0.48 |
| 1:S:1419:LEU:HG | 1:S:1467:ILE:HD13 | 1.94 | 0.48 |
| 1:S:2090:ARG:HG3 | 1:S:2092:GLU:OE2 | 2.12 | 0.48 |
| 1:S:2288:TYR:OH | 1:S:2293:GLY:HA3 | 2.14 | 0.48 |
| 1:S:2799:GLN:HE22 | 1:S:2800:ARG:HE | 1.60 | 0.48 |
| 1:S:2834:GLN:HA | 1:S:2837:LEU:HD12 | 1.94 | 0.48 |
| 2:T:340:PHE:HB3 | 2:T:408:PRO:CD | 2.43 | 0.48 |
| 2:T:413:LEU:HD11 | 2:T:434:LEU:HD12 | 1.95 | 0.48 |
| 2:T:413:LEU:HB3 | 2:T:432:PHE:CD2 | 2.48 | 0.48 |
| 1:A:364:ARG:HB2 | 1:A:415:GLN:NE2 | 2.28 | 0.48 |
| 1:A:364:ARG:HB2 | 1:A:415:GLN:HE21 | 1.78 | 0.48 |
| 1:A:725:LEU:O | 1:A:728:SER:OG | 2.27 | 0.48 |
| 1:A:1760:GLU:O | 1:A:1763:THR:N | 2.46 | 0.48 |
| 1:A:2965:TYR:HB3 | 1:A:3001:CYS:HB2 | 1.93 | 0.48 |
| 1:A:2988:GLU:HA | 1:A:2991:LYS:HE2 | 1.94 | 0.48 |
| 1:A:3262:LEU:HB2 | 1:A:3276:TRP:CD1 | 2.47 | 0.48 |
| 1:A:3838:GLU:CD | 1:A:4122:GLU:HB3 | 2.39 | 0.48 |
| 1:A:3867:THR:HG23 | 1:A:4118:GLY:N | 2.28 | 0.48 |
| 2:B:46:LYS:NZ | 2:B:137:HIS:O | 2.41 | 0.48 |
| 2:B:167:MET:CE | 2:B:203:MET:HG2 | 2.43 | 0.48 |
| 2:B:276:LEU:C | 3:C:431:ARG:HG2 | 2.38 | 0.48 |
| 3:C:381:ILE:HD12 | 3:C:410:PRO:HB3 | 1.95 | 0.48 |
| 3:L:309:ASP:HB3 | 2:T:289:TYR:CE1 | 2.46 | 0.48 |
| 5:Q:181:ILE:HD12 | 5:Q:184:LEU:HD12 | 1.94 | 0.48 |
| 1:S:382:ASP:OD1 | 1:S:383:PHE:N | 2.46 | 0.48 |
| 1:S:1027:ASP:O | 1:S:1031:ARG:HG2 | 2.13 | 0.48 |
| 1:S:1307:ILE:HG12 | 1:S:1311:LYS:HD2 | 1.95 | 0.48 |
| 1:S:1583:MET:O | 1:S:1629:CYS:HB2 | 2.13 | 0.48 |
| 1:S:2923:TRP:CE3 | 1:S:2942:ILE:HG23 | 2.48 | 0.48 |
| 2:T:143:LEU:HG | 2:T:176:HIS:CD2 | 2.48 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:476:ARG:NH2 | 1:A:1562:LEU:HD23 | 2.26 | 0.48 |
| 1:A:753:GLN:HA | 1:A:756:PHE:CD2 | 2.49 | 0.48 |
| 1:A:914:VAL:HG13 | 1:A:934:LEU:HD21 | 1.94 | 0.48 |
| 1:A:1157:PHE:HB2 | 1:A:1168:LEU:HD11 | 1.95 | 0.48 |
| 1:A:1780:SER:O | 1:A:1784:ARG:HG3 | 2.14 | 0.48 |
| 1:A:2227:LYS:C | 1:A:2228:ARG:HD3 | 2.39 | 0.48 |
| 1:A:3090:TYR:HB3 | 1:A:3095:ASP:HB2 | 1.96 | 0.48 |
| 1:A:3477:GLU:H | 1:A:3477:GLU:CD | 2.21 | 0.48 |
| 1:A:3578:LEU:O | 1:A:3734:ARG:NH1 | 2.46 | 0.48 |
| 1:A:3913:ILE:HD13 | 1:A:3987:ALA:HB3 | 1.95 | 0.48 |
| 2:B:282:LYS:NZ | 2:B:483:LEU:HD23 | 2.28 | 0.48 |
| 3:C:229:GLU:HG3 | 3:C:232:ARG:NH2 | 2.28 | 0.48 |
| 3:C:301:ASP:OD1 | 3:C:302:GLU:N | 2.36 | 0.48 |
| 3:C:599:ARG:HG2 | 3:C:603:LYS:HZ1 | 1.77 | 0.48 |
| 4:M:37:PHE:HE1 | 4:M:73:THR:HG23 | 1.78 | 0.48 |
| 1:S:23:ASP:HB3 | 1:S:34:LEU:HD11 | 1.95 | 0.48 |
| 1:S:330:ASN:HB3 | 1:S:332:GLU:HG3 | 1.94 | 0.48 |
| 1:S:446:PHE:HA | 1:S:449:TYR:CE2 | 2.49 | 0.48 |
| 1:S:535:LEU:HD12 | 1:S:637:LYS:HZ3 | 1.78 | 0.48 |
| 1:S:581:LEU:HD12 | 1:S:620:PHE:CD1 | 2.49 | 0.48 |
| 1:S:1608:ARG:HB3 | 1:S:1612:LYS:HE3 | 1.94 | 0.48 |
| 1:S:2225:HIS:CG | 1:S:2230:VAL:HG23 | 2.49 | 0.48 |
| 1:S:3413:TYR:CD1 | 1:S:3449:LYS:HB3 | 2.49 | 0.48 |
| 1:S:3495:PHE:HB2 | 1:S:3502:MET:HE1 | 1.95 | 0.48 |
| 1:S:3501:HIS:HE1 | 1:S:4004:VAL:HG21 | 1.79 | 0.48 |
| 1:S:4055:ASN:HB3 | 1:S:4058:VAL:HB | 1.94 | 0.48 |
| 1:A:385:TYR:HE2 | 1:A:428:PRO:HG2 | 1.78 | 0.48 |
| 1:A:1279:LEU:HB3 | 1:A:1356:TRP:HE1 | 1.78 | 0.48 |
| 1:A:2328:ARG:HB2 | 1:A:2370:SER:O | 2.14 | 0.48 |
| 1:A:3156:PRO:HA | 1:A:3159:ARG:NE | 2.29 | 0.48 |
| 1:A:3188:PHE:O | 1:A:3191:SER:OG | 2.26 | 0.48 |
| 2:B:55:ASP:OD1 | 2:B:56:GLU:N | 2.46 | 0.48 |
| 2:B:207:LYS:HG2 | 2:B:209:GLY:H | 1.79 | 0.48 |
| 2:B:384:ALA:HB2 | 3:C:446:PRO:HG3 | 1.96 | 0.48 |
| 3:L:405:VAL:HG22 | 3:L:426:PHE:CE1 | 2.49 | 0.48 |
| 3:L:599:ARG:C | 3:L:603:LYS:HZ2 | 2.22 | 0.48 |
| 1:S:34:LEU:O | 1:S:38:LEU:HG | 2.14 | 0.48 |
| 1:S:296:VAL:HA | 1:S:299:LYS:HG2 | 1.96 | 0.48 |
| 1:S:985:GLU:HA | 1:S:988:VAL:HG22 | 1.95 | 0.48 |
| 1:S:1220:LEU:N | 1:S:1285:GLU:OE1 | 2.47 | 0.48 |
| 1:S:1592:MET:SD | 1:S:1592:MET:N | 2.86 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2507:ILE:HG23 | 1:S:2550:ILE:HD13 | 1.95 | 0.48 |
| 1:S:2983:ASP:OD1 | 1:S:2983:ASP:N | 2.43 | 0.48 |
| 1:S:3369:ASP:O | 1:S:3373:VAL:HG23 | 2.13 | 0.48 |
| 1:S:3946:PHE:HZ | 1:S:4047:ALA:HB2 | 1.78 | 0.48 |
| 1:S:3962:ARG:HH22 | 1:S:4125:GLU:HB3 | 1.78 | 0.48 |
| 2:T:130:ARG:O | 2:T:134:MET:HG3 | 2.14 | 0.48 |
| 7:d:21:DA:C8 | 7:d:22:DG:N1 | 2.81 | 0.48 |
| 8:e:40:DT:H2” | 8:e:41:DT:N1 | 2.28 | 0.48 |
| 1:A:623:PHE:O | 1:A:626:LEU:HG | 2.14 | 0.48 |
| 1:A:916:GLU:O | 1:A:920:THR:N | 2.43 | 0.48 |
| 1:A:1271:ILE:HG13 | 1:A:1272:GLY:N | 2.28 | 0.48 |
| 1:A:2494:ASP:HA | 1:A:2497:GLU:OE1 | 2.14 | 0.48 |
| 1:A:3244:ASP:O | 1:A:3248:LYS:HG3 | 2.13 | 0.48 |
| 1:A:3349:ALA:HA | 1:A:3352:GLU:HB3 | 1.95 | 0.48 |
| 1:A:3733:ARG:NE | 1:A:3755:GLY:H | 2.12 | 0.48 |
| 2:B:131:PHE:O | 2:B:135:MET:N | 2.47 | 0.48 |
| 5:H:142:GLU:O | 5:H:145:GLN:HG3 | 2.14 | 0.48 |
| 3:L:111:LEU:HD21 | 3:L:134:ILE:CG1 | 2.42 | 0.48 |
| 3:L:660:LYS:HE2 | 3:L:687:THR:HB | 1.95 | 0.48 |
| 1:S:192:ASN:O | 1:S:196:LEU:HG | 2.14 | 0.48 |
| 1:S:238:MET:HE2 | 1:S:283:SER:O | 2.13 | 0.48 |
| 1:S:2281:MET:SD | 1:S:2325:LEU:HB3 | 2.54 | 0.48 |
| 1:S:2330:VAL:HG13 | 1:S:2333:ARG:HH22 | 1.78 | 0.48 |
| 1:S:2572:TYR:HE1 | 1:S:2791:ILE:HD11 | 1.79 | 0.48 |
| 1:S:3236:PHE:HB3 | 1:S:3272:TRP:CE3 | 2.48 | 0.48 |
| 9:i:38:DT:H2” | 9:i:39:DA:N7 | 2.28 | 0.48 |
| 1:A:416:SER:O | 1:A:419:SER:OG | 2.29 | 0.48 |
| 1:A:1682:THR:O | 1:A:1689:LYS:NZ | 2.39 | 0.48 |
| 1:A:3173:MET:SD | 1:A:3783:GLN:HG2 | 2.54 | 0.48 |
| 1:A:3464:LYS:O | 1:A:3468:LEU:HG | 2.14 | 0.48 |
| 1:A:4039:TYR:N | 1:A:4042:GLN:OE1 | 2.42 | 0.48 |
| 3:C:131:HIS:CE1 | 11:f:296:GLY:N | 2.81 | 0.48 |
| 5:G:143:HIS:O | 5:G:146:LYS:HG2 | 2.14 | 0.48 |
| 6:I:727:LEU:O | 6:I:731:LYS:HG2 | 2.14 | 0.48 |
| 3:L:643:ARG:HG2 | 3:L:685:LEU:HD13 | 1.95 | 0.48 |
| 6:R:879:ARG:NH2 | 6:R:886:PHE:O | 2.35 | 0.48 |
| 1:S:250:ASN:HA | 1:S:253:LEU:HD13 | 1.94 | 0.48 |
| 1:S:269:SER:OG | 1:S:273:ARG:NH1 | 2.46 | 0.48 |
| 1:S:344:GLN:O | 1:S:348:ILE:HG12 | 2.14 | 0.48 |
| 1:S:668:LYS:O | 1:S:672:ILE:HG12 | 2.14 | 0.48 |
| 1:S:1224:PHE:CE1 | 1:S:1266:CYS:HB3 | 2.47 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1250:LEU:O | 1:S:1254:LEU:HG | 2.14 | 0.48 |
| 1:S:1560:TYR:CE1 | 1:S:1596:VAL:HG12 | 2.49 | 0.48 |
| 1:S:1727:ARG:NH1 | 1:S:1771:GLN:O | 2.47 | 0.48 |
| 1:S:1848:ILE:HG12 | 1:S:1915:LEU:HD11 | 1.95 | 0.48 |
| 1:S:3293:CYS:SG | 1:S:3340:ALA:HB1 | 2.54 | 0.48 |
| 2:T:173:ASP:HB3 | 2:T:217:TYR:CE2 | 2.49 | 0.48 |
| 7:d:29:DG:N2 | 8:e:28:DT:O2 | 2.47 | 0.48 |
| 1:A:194:GLU:O | 1:A:198:ARG:HG3 | 2.14 | 0.48 |
| 1:A:434:VAL:O | 1:A:438:LEU:N | 2.45 | 0.48 |
| 1:A:1740:VAL:HA | 1:A:1743:MET:HG2 | 1.95 | 0.48 |
| 1:A:2492:ASP:CG | 1:A:2495:SER:H | 2.21 | 0.48 |
| 1:A:3864:ARG:NE | 1:A:4085:LYS:HG3 | 2.28 | 0.48 |
| 2:B:466:VAL:HG11 | 3:C:389:MET:HG3 | 1.96 | 0.48 |
| 3:C:523:THR:O | 3:C:527:GLN:NE2 | 2.34 | 0.48 |
| 5:G:155:TRP:O | 5:G:159:GLN:HG2 | 2.14 | 0.48 |
| 3:L:215:LEU:HD23 | 11:m:295:ARG:HH12 | 1.79 | 0.48 |
| 3:L:260:ARG:HB2 | 3:L:367:ALA:HB2 | 1.96 | 0.48 |
| 3:L:644:GLU:O | 3:L:648:LYS:HG3 | 2.14 | 0.48 |
| 1:S:894:PHE:HZ | 1:S:2787:HIS:CD2 | 2.31 | 0.48 |
| 1:S:1708:GLU:OE2 | 1:S:1712:ARG:HB3 | 2.14 | 0.48 |
| 1:S:2187:VAL:HA | 1:S:2190:VAL:HG22 | 1.96 | 0.48 |
| 1:S:2433:LYS:HE3 | 1:S:2468:THR:OG1 | 2.14 | 0.48 |
| 1:S:2522:ARG:O | 1:S:2526:SER:OG | 2.29 | 0.48 |
| 1:S:2859:GLN:NE2 | 1:S:2888:VAL:HG13 | 2.28 | 0.48 |
| 1:S:3052:LEU:HD11 | 1:S:3061:LEU:HD21 | 1.95 | 0.48 |
| 1:S:4054:ALA:HA | 1:S:4096:SER:HA | 1.96 | 0.48 |
| 2:T:62:MET:HA | 2:T:65:GLN:CD | 2.39 | 0.48 |
| 1:A:164:LYS:NZ | 2:B:300:THR:O | 2.46 | 0.48 |
| 1:A:384:MET:O | 1:A:387:GLU:HG2 | 2.14 | 0.48 |
| 1:A:449:TYR:HB3 | 1:A:453:MET:SD | 2.54 | 0.48 |
| 1:A:741:ILE:HA | 1:A:748:TYR:CZ | 2.48 | 0.48 |
| 1:A:947:GLN:HG2 | 1:A:2577:PHE:CE1 | 2.48 | 0.48 |
| 1:A:1008:ALA:O | 1:A:1011:GLU:HG2 | 2.14 | 0.48 |
| 1:A:1645:VAL:O | 1:A:1649:LEU:HD23 | 2.14 | 0.48 |
| 1:A:2389:PHE:O | 1:A:2394:LYS:HE2 | 2.13 | 0.48 |
| 1:A:2527:HIS:O | 1:A:2531:LEU:N | 2.46 | 0.48 |
| 1:A:2919:ASP:O | 1:A:2922:ARG:HG2 | 2.14 | 0.48 |
| 1:A:3241:LYS:HA | 1:A:3244:ASP:OD2 | 2.14 | 0.48 |
| 5:G:197:LYS:HZ3 | 5:H:198:LEU:HD13 | 1.79 | 0.48 |
| 3:L:323:PHE:CZ | 3:L:328:GLU:HB2 | 2.49 | 0.48 |
| 3:L:497:ARG:NH1 | 3:L:503:GLU:O | 2.47 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:608:SER:HA | 3:L:651:GLU:HG2 | 1.96 | 0.48 |
| 6:R:814:ARG:H | 6:R:849:GLY:HA2 | 1.77 | 0.48 |
| 6:R:837:ARG:NH1 | 6:R:867:GLU:OE1 | 2.47 | 0.48 |
| 1:S:139:ARG:NH2 | 1:S:230:LEU:HD11 | 2.26 | 0.48 |
| 1:S:176:GLU:OE1 | 1:S:176:GLU:N | 2.35 | 0.48 |
| 1:S:1039:TRP:NE1 | 1:S:1043:GLN:HG2 | 2.28 | 0.48 |
| 1:S:1167:ASP:HA | 1:S:1170:LYS:NZ | 2.28 | 0.48 |
| 1:S:1258:ASP:HA | 1:S:1261:LEU:HD12 | 1.95 | 0.48 |
| 1:S:1357:LYS:HG3 | 1:S:1361:LYS:HZ3 | 1.77 | 0.48 |
| 1:S:2427:ARG:HH21 | 1:S:2464:HIS:HB3 | 1.79 | 0.48 |
| 1:S:3182:ILE:HG13 | 1:S:3183:ILE:HG12 | 1.96 | 0.48 |
| 1:S:3493:TRP:CD1 | 1:S:3520:GLU:HB3 | 2.49 | 0.48 |
| 1:S:3563:ASP:HB2 | 1:S:3697:ASN:HD22 | 1.78 | 0.48 |
| 1:S:3855:TYR:HB3 | 1:S:3859:TYR:CZ | 2.49 | 0.48 |
| 1:A:532:ARG:O | 1:A:536:SER:N | 2.47 | 0.47 |
| 1:A:2356:MET:SD | 1:A:2357:GLU:N | 2.87 | 0.47 |
| 1:A:2428:ASP:CB | 1:A:2431:ARG:HD3 | 2.44 | 0.47 |
| 1:A:3852:VAL:HA | 1:A:3855:TYR:CZ | 2.49 | 0.47 |
| 2:B:166:ILE:N | 2:B:199:PHE:O | 2.47 | 0.47 |
| 3:C:247:TRP:HB3 | 3:C:263:ALA:HB3 | 1.96 | 0.47 |
| 5:G:197:LYS:HZ3 | 5:H:198:LEU:HD22 | 1.79 | 0.47 |
| 5:H:180:PHE:HE2 | 6:I:799:LEU:HD11 | 1.78 | 0.47 |
| 3:L:430:LEU:HD11 | 2:T:475:SER:HB3 | 1.96 | 0.47 |
| 3:L:508:ILE:HD13 | 2:T:340:PHE:CE1 | 2.49 | 0.47 |
| 1:S:293:LEU:HA | 1:S:296:VAL:HG22 | 1.96 | 0.47 |
| 1:S:1048:GLN:OE1 | 1:S:1051:LYS:NZ | 2.36 | 0.47 |
| 1:S:1191:PHE:O | 1:S:1195:VAL:HG23 | 2.14 | 0.47 |
| 1:S:1642:LYS:O | 1:S:1646:LEU:HG | 2.14 | 0.47 |
| 1:S:1773:VAL:HG12 | 1:S:1773:VAL:O | 2.14 | 0.47 |
| 1:S:3644:PHE:HZ | 1:S:3660:ASN:HA | 1.79 | 0.47 |
| 1:S:3705:TYR:OH | 1:S:3713:PRO:O | 2.28 | 0.47 |
| 1:A:65:LEU:O | 1:A:69:VAL:HG22 | 2.14 | 0.47 |
| 1:A:738:HIS:O | 1:A:742:GLU:N | 2.47 | 0.47 |
| 1:A:850:GLU:HG2 | 1:A:854:ARG:HH22 | 1.77 | 0.47 |
| 1:A:1784:ARG:HA | 1:A:1787:ARG:HH11 | 1.79 | 0.47 |
| 1:A:1962:TYR:HB2 | 3:L:725:VAL:HG21 | 1.95 | 0.47 |
| 1:A:3389:VAL:HG11 | 1:A:3449:LYS:HZ2 | 1.79 | 0.47 |
| 1:A:3529:ILE:O | 1:A:3533:PHE:N | 2.26 | 0.47 |
| 1:A:3750:PHE:CZ | 1:A:3804:GLU:HG2 | 2.50 | 0.47 |
| 1:A:4085:LYS:O | 1:A:4089:ILE:HG23 | 2.14 | 0.47 |
| 2:B:68:GLN:O | 2:B:72:ILE:HG12 | 2.13 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:285:PRO:HB3 | 3:C:312:GLN:HG3 | 1.96 | 0.47 |
| 3:C:349:SER:O | 3:C:352:GLN:NE2 | 2.43 | 0.47 |
| 3:L:16:VAL:HG21 | 3:L:58:LEU:HB3 | 1.96 | 0.47 |
| 3:L:153:SER:HA | 3:L:156:LYS:HG2 | 1.94 | 0.47 |
| 5:Q:179:ARG:O | 5:Q:182:LEU:HG | 2.14 | 0.47 |
| 1:S:246:ARG:HG3 | 1:S:282:PHE:HZ | 1.78 | 0.47 |
| 1:S:309:LYS:O | 1:S:313:LEU:HG | 2.14 | 0.47 |
| 1:S:668:LYS:HZ3 | 1:S:728:SER:HB3 | 1.77 | 0.47 |
| 1:S:1086:TYR:CZ | 1:S:1090:ARG:HD3 | 2.48 | 0.47 |
| 1:S:1118:GLU:HG3 | 1:S:1121:LEU:HB2 | 1.95 | 0.47 |
| 1:S:1322:THR:O | 1:S:1326:GLU:N | 2.48 | 0.47 |
| 1:S:1732:GLY:HA2 | 1:S:1737:ASN:HD21 | 1.79 | 0.47 |
| 1:S:2169:LEU:HD21 | 1:S:2208:ASP:HA | 1.95 | 0.47 |
| 1:S:2304:VAL:HG11 | 1:S:2345:VAL:HG12 | 1.97 | 0.47 |
| 8:e:43:DT:H2" | 8:e:44:DG:N7 | 2.29 | 0.47 |
| 1:A:14:ARG:O | 1:A:18:THR:HG23 | 2.15 | 0.47 |
| 1:A:463:LYS:HZ1 | 1:A:544:ILE:HD13 | 1.78 | 0.47 |
| 1:A:1878:ASP:HA | 1:A:1881:TYR:CD2 | 2.49 | 0.47 |
| 1:A:2805:ALA:HA | 1:A:2808:LEU:HD12 | 1.97 | 0.47 |
| 1:A:3324:ARG:HH11 | 1:A:3412:ALA:HB2 | 1.78 | 0.47 |
| 1:A:3414:MET:CE | 1:A:3460:GLU:HG3 | 2.44 | 0.47 |
| 1:A:3444:ALA:HB1 | 1:A:3482:LEU:HD11 | 1.95 | 0.47 |
| 1:A:3740:ILE:HB | 1:A:3748:HIS:O | 2.14 | 0.47 |
| 3:C:280:ASP:HB2 | 3:C:289:ILE:HD11 | 1.96 | 0.47 |
| 3:L:600:VAL:HA | 3:L:603:LYS:HG2 | 1.97 | 0.47 |
| 6:R:721:VAL:HA | 6:R:742:PHE:CE2 | 2.47 | 0.47 |
| 6:R:728:GLU:CD | 6:R:741:ARG:HH22 | 2.20 | 0.47 |
| 1:S:125:ILE:H | 1:S:125:ILE:HD12 | 1.79 | 0.47 |
| 1:S:448:GLN:HG2 | 1:S:520:LYS:HB2 | 1.95 | 0.47 |
| 1:S:484:HIS:O | 1:S:487:LEU:HG | 2.14 | 0.47 |
| 1:S:996:THR:OG1 | 1:S:1040:SER:HB3 | 2.14 | 0.47 |
| 1:S:2380:ASN:O | 1:S:2384:PHE:N | 2.43 | 0.47 |
| 1:S:3101:TYR:O | 1:S:3104:GLN:HG3 | 2.15 | 0.47 |
| 1:S:3123:GLN:OE1 | 1:S:3123:GLN:N | 2.42 | 0.47 |
| 1:S:3947:GLY:HA3 | 1:S:4063:GLU:CD | 2.39 | 0.47 |
| 1:A:343:GLU:HG2 | 1:A:344:GLN:H | 1.78 | 0.47 |
| 1:A:1111:LEU:HD12 | 1:A:1127:CYS:HB2 | 1.95 | 0.47 |
| 1:A:1201:ASN:CG | 1:A:1207:TRP:HB2 | 2.39 | 0.47 |
| 1:A:1205:ASN:HA | 1:A:1208:LEU:HD13 | 1.96 | 0.47 |
| 1:A:1386:ILE:C | 1:A:1392:MET:HE1 | 2.39 | 0.47 |
| 1:A:1391:VAL:O | 1:A:1395:LEU:HG | 2.15 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1574:ASN:HD21 | 1:A:1577:LEU:HB2 | 1.80 | 0.47 |
| 1:A:3063:THR:O | 1:A:3067:LYS:HG3 | 2.14 | 0.47 |
| 1:A:3588:TRP:CD1 | 1:A:3609:MET:HG3 | 2.49 | 0.47 |
| 1:A:3856:MET:HA | 1:A:3859:TYR:CD2 | 2.49 | 0.47 |
| 1:A:4044:ILE:O | 1:A:4048:LYS:HG3 | 2.13 | 0.47 |
| 2:B:109:ASP:O | 2:B:115:ARG:NH1 | 2.46 | 0.47 |
| 2:B:134:MET:SD | 2:B:135:MET:HB2 | 2.54 | 0.47 |
| 3:C:488:GLN:OE1 | 3:C:488:GLN:N | 2.48 | 0.47 |
| 3:L:416:TYR:HB3 | 2:T:449:THR:O | 2.15 | 0.47 |
| 5:Q:180:PHE:HA | 5:Q:183:VAL:HG12 | 1.95 | 0.47 |
| 6:R:868:ASP:N | 6:R:868:ASP:OD1 | 2.43 | 0.47 |
| 1:S:323:VAL:O | 1:S:327:VAL:HG22 | 2.13 | 0.47 |
| 1:S:639:ALA:HA | 1:S:642:PHE:HB3 | 1.95 | 0.47 |
| 1:S:722:LYS:O | 1:S:726:LEU:N | 2.30 | 0.47 |
| 1:S:1058:SER:HA | 1:S:1061:LYS:HE2 | 1.95 | 0.47 |
| 1:S:1593:VAL:O | 1:S:1597:LEU:HG | 2.15 | 0.47 |
| 1:S:2185:MET:O | 1:S:2189:ILE:HG12 | 2.15 | 0.47 |
| 1:S:3567:VAL:HG11 | 1:S:3696:ARG:HE | 1.80 | 0.47 |
| 2:T:142:SER:HB3 | 2:T:145:GLU:HG3 | 1.95 | 0.47 |
| 7:d:31:DT:H2" | 7:d:32:DT:OP2 | 2.14 | 0.47 |
| 1:A:384:MET:O | 1:A:385:TYR:C | 2.57 | 0.47 |
| 1:A:2211:LEU:HA | 1:A:2214:ARG:HH11 | 1.79 | 0.47 |
| 1:A:2233:HIS:HD2 | 1:A:2731:ARG:HG3 | 1.79 | 0.47 |
| 1:A:2831:ASN:O | 1:A:2835:LYS:HG3 | 2.14 | 0.47 |
| 1:A:3236:PHE:HB3 | 1:A:3272:TRP:CZ2 | 2.49 | 0.47 |
| 2:B:46:LYS:NZ | 2:B:138:GLY:HA3 | 2.30 | 0.47 |
| 6:I:675:LYS:HE3 | 6:I:679:GLU:OE2 | 2.13 | 0.47 |
| 3:L:118:ILE:O | 3:L:122:THR:N | 2.42 | 0.47 |
| 3:L:596:GLU:H | 3:L:596:GLU:CD | 2.23 | 0.47 |
| 1:S:524:TYR:HB2 | 1:S:629:PHE:CZ | 2.49 | 0.47 |
| 1:S:737:PRO:HD2 | 1:S:740:ILE:HD11 | 1.96 | 0.47 |
| 1:S:977:ASP:HB3 | 1:S:980:THR:OG1 | 2.15 | 0.47 |
| 1:S:1626:TRP:CZ2 | 1:S:1674:THR:HG21 | 2.50 | 0.47 |
| 1:S:1787:ARG:HB3 | 1:S:1830:HIS:HE1 | 1.79 | 0.47 |
| 1:S:2090:ARG:HD2 | 1:S:2090:ARG:HA | 1.72 | 0.47 |
| 1:S:2881:LEU:HA | 1:S:2886:GLN:HG2 | 1.97 | 0.47 |
| 1:S:3904:PHE:CE1 | 1:S:3937:VAL:HB | 2.49 | 0.47 |
| 2:T:51:SER:OG | 2:T:206:LYS:NZ | 2.43 | 0.47 |
| 1:A:246:ARG:HA | 1:A:249:PHE:HD2 | 1.80 | 0.47 |
| 1:A:295:GLU:O | 1:A:299:LYS:NZ | 2.46 | 0.47 |
| 1:A:725:LEU:HD21 | 1:A:2602:LEU:HD11 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:745:VAL:HA | 1:A:748:TYR:HD2 | 1.80 | 0.47 |
| 1:A:1071:ASN:HB3 | 1:A:1074:LYS:HD3 | 1.97 | 0.47 |
| 1:A:1264:LEU:O | 1:A:1268:ASN:ND2 | 2.47 | 0.47 |
| 1:A:1370:ARG:O | 1:A:1374:GLN:NE2 | 2.42 | 0.47 |
| 1:A:1948:ALA:HA | 1:A:1951:VAL:HG22 | 1.96 | 0.47 |
| 1:A:2231:PHE:O | 1:A:2235:LEU:HG | 2.15 | 0.47 |
| 1:A:2443:MET:SD | 1:A:2476:ILE:HG23 | 2.54 | 0.47 |
| 1:A:2742:MET:SD | 8:e:44:DG:N1 | 2.69 | 0.47 |
| 1:A:2897:LEU:HD21 | 1:A:2923:TRP:CE2 | 2.49 | 0.47 |
| 1:A:3127:THR:HA | 1:A:3130:GLN:HG2 | 1.97 | 0.47 |
| 1:A:3154:GLN:HE22 | 1:A:3197:LEU:HD21 | 1.78 | 0.47 |
| 1:A:3986:HIS:HB2 | 1:A:3989:ARG:HH21 | 1.79 | 0.47 |
| 5:H:41:SER:HB2 | 5:H:43:TRP:CZ2 | 2.50 | 0.47 |
| 3:L:33:GLN:O | 3:L:37:VAL:HG23 | 2.14 | 0.47 |
| 4:M:48:TRP:NE1 | 4:M:92:ASP:O | 2.48 | 0.47 |
| 5:Q:170:GLU:HG3 | 6:R:847:PHE:HD1 | 1.79 | 0.47 |
| 1:S:1643:MET:HA | 1:S:1646:LEU:HD12 | 1.96 | 0.47 |
| 1:S:1743:MET:O | 1:S:1747:LEU:HG | 2.14 | 0.47 |
| 1:S:1881:TYR:OH | 1:S:1954:CYS:N | 2.40 | 0.47 |
| 1:S:2486:ASP:N | 1:S:2486:ASP:OD1 | 2.47 | 0.47 |
| 1:S:3614:TYR:O | 1:S:3619:ASP:N | 2.37 | 0.47 |
| 2:T:171:ASN:HB3 | 2:T:205:LEU:HG | 1.97 | 0.47 |
| 2:T:191:GLY:HA2 | 2:T:194:ARG:NE | 2.29 | 0.47 |
| 10:j:19:DA:H1' | 10:j:20:DT:H5' | 1.96 | 0.47 |
| 1:A:212:VAL:HG12 | 2:B:335:GLU:OE2 | 2.15 | 0.47 |
| 1:A:741:ILE:HA | 1:A:748:TYR:CE2 | 2.49 | 0.47 |
| 1:A:1087:ARG:HA | 1:A:1090:ARG:NH1 | 2.30 | 0.47 |
| 1:A:1142:HIS:HA | 1:A:1145:LEU:HD13 | 1.96 | 0.47 |
| 1:A:1751:GLU:OE1 | 1:A:1785:ILE:HG13 | 2.14 | 0.47 |
| 1:A:2481:HIS:O | 1:A:2485:ARG:HG3 | 2.15 | 0.47 |
| 1:A:2503:LYS:O | 1:A:2507:ILE:HG12 | 2.15 | 0.47 |
| 1:A:3049:LEU:HD22 | 1:A:3085:GLU:HB2 | 1.97 | 0.47 |
| 1:A:3052:LEU:HD13 | 1:A:3057:ALA:HA | 1.97 | 0.47 |
| 1:A:3090:TYR:CE2 | 1:A:3098:ARG:HB3 | 2.50 | 0.47 |
| 1:A:3587:ASP:HB2 | 1:A:3799:ARG:NH2 | 2.28 | 0.47 |
| 2:B:167:MET:HE3 | 2:B:168:LEU:O | 2.15 | 0.47 |
| 2:B:250:GLU:O | 2:B:250:GLU:HG2 | 2.15 | 0.47 |
| 2:B:339:ARG:NH1 | 2:B:341:ASP:O | 2.48 | 0.47 |
| 2:B:340:PHE:HZ | 3:C:486:ARG:HA | 1.78 | 0.47 |
| 3:C:137:ASP:HA | 3:C:166:PRO:HD3 | 1.97 | 0.47 |
| 3:C:235:CYS:SG | 11:f:294:PRO:HB3 | 2.55 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:297:LEU:HG | 3:C:303:THR:HB | 1.96 | 0.47 |
| 3:C:333:TYR:OH | 3:C:394:ARG:NH2 | 2.45 | 0.47 |
| 3:C:356:PHE:CD2 | 3:C:422:VAL:HG11 | 2.50 | 0.47 |
| 3:C:528:ILE:HG22 | 3:C:532:LYS:NZ | 2.29 | 0.47 |
| 3:C:602:VAL:HA | 3:C:609:PHE:CD2 | 2.47 | 0.47 |
| 5:G:18:HIS:ND1 | 5:G:36:LEU:HD13 | 2.30 | 0.47 |
| 6:I:815:ARG:H | 6:I:849:GLY:C | 2.22 | 0.47 |
| 3:L:235:CYS:C | 3:L:237:PHE:N | 2.70 | 0.47 |
| 3:L:362:LEU:HB3 | 3:L:364:VAL:HG13 | 1.97 | 0.47 |
| 4:M:132:VAL:O | 4:M:136:GLU:HG2 | 2.15 | 0.47 |
| 1:S:289:ASN:O | 1:S:293:LEU:HG | 2.15 | 0.47 |
| 1:S:530:LEU:O | 1:S:534:LEU:HG | 2.14 | 0.47 |
| 1:S:623:PHE:O | 1:S:627:VAL:HG23 | 2.14 | 0.47 |
| 1:S:652:GLU:O | 1:S:656:GLN:N | 2.39 | 0.47 |
| 1:S:978:GLN:O | 1:S:982:GLN:HB3 | 2.15 | 0.47 |
| 1:S:1043:GLN:O | 1:S:1044:ILE:HD13 | 2.15 | 0.47 |
| 1:S:1334:LYS:NZ | 1:S:1382:ILE:O | 2.41 | 0.47 |
| 1:S:1513:GLY:O | 1:S:1517:LEU:HG | 2.15 | 0.47 |
| 1:S:1611:GLN:HG3 | 1:S:1613:HIS:H | 1.79 | 0.47 |
| 1:S:1626:TRP:CD1 | 1:S:1627:LYS:HE3 | 2.49 | 0.47 |
| 1:S:1651:LYS:HD3 | 1:S:1654:GLN:HE21 | 1.79 | 0.47 |
| 1:S:2361:ILE:HG21 | 1:S:2389:PHE:HE2 | 1.80 | 0.47 |
| 1:S:2840:PHE:HB2 | 1:S:2871:LEU:HD11 | 1.97 | 0.47 |
| 1:S:3022:GLU:HB3 | 1:S:3034:PRO:HG3 | 1.97 | 0.47 |
| 1:S:3117:ILE:HG22 | 1:S:3125:ARG:HE | 1.79 | 0.47 |
| 1:S:3143:SER:HA | 1:S:3147:LYS:HG3 | 1.97 | 0.47 |
| 1:S:3176:MET:HA | 1:S:3179:TRP:HB2 | 1.96 | 0.47 |
| 1:S:3606:ILE:O | 1:S:3610:TYR:HB2 | 2.15 | 0.47 |
| 1:S:3682:GLU:HA | 1:S:3688:SER:OG | 2.14 | 0.47 |
| 1:S:3701:ILE:HG23 | 1:S:3750:PHE:HZ | 1.80 | 0.47 |
| 1:A:849:GLU:O | 1:A:853:ILE:HG13 | 2.14 | 0.47 |
| 1:A:1205:ASN:ND2 | 1:A:1275:THR:HA | 2.30 | 0.47 |
| 1:A:1576:ASP:O | 1:A:1580:LEU:N | 2.39 | 0.47 |
| 1:A:1872:GLY:O | 1:A:1876:ILE:HG12 | 2.14 | 0.47 |
| 1:A:1958:GLU:O | 1:A:1959:LEU:HB2 | 2.15 | 0.47 |
| 1:A:3466:PRO:HG2 | 1:A:4001:THR:HG22 | 1.97 | 0.47 |
| 1:A:3620:PRO:HB3 | 1:A:3638:LYS:NZ | 2.29 | 0.47 |
| 2:B:69:SER:HB2 | 2:B:245:LYS:HD2 | 1.97 | 0.47 |
| 2:B:470:ARG:CZ | 3:C:346:CYS:HA | 2.44 | 0.47 |
| 3:C:89:ASP:O | 3:C:92:GLU:HG2 | 2.15 | 0.47 |
| 3:C:315:ARG:NH2 | 3:C:320:ILE:HG13 | 2.30 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:316:TYR:N | 3:C:319:ASP:O | 2.43 | 0.47 |
| 6:I:677:ASP:O | 6:I:681:ARG:HG2 | 2.14 | 0.47 |
| 4:M:11:LEU:HD22 | 4:M:87:LEU:HG | 1.96 | 0.47 |
| 5:P:187:LYS:O | 5:P:191:ILE:HG12 | 2.15 | 0.47 |
| 1:S:139:ARG:HA | 1:S:142:ARG:HH21 | 1.79 | 0.47 |
| 1:S:1219:PHE:O | 1:S:1223:THR:OG1 | 2.32 | 0.47 |
| 1:S:1428:ILE:HA | 1:S:1431:LEU:HG | 1.97 | 0.47 |
| 1:S:1689:LYS:O | 1:S:1693:VAL:HG13 | 2.15 | 0.47 |
| 1:S:1727:ARG:NH2 | 1:S:1769:GLU:OE1 | 2.48 | 0.47 |
| 1:S:2281:MET:CE | 1:S:2326:ILE:HD13 | 2.43 | 0.47 |
| 1:S:2366:LYS:HD2 | 1:S:2369:LYS:HE2 | 1.97 | 0.47 |
| 1:S:3005:LEU:HG | 1:S:3007:GLU:H | 1.79 | 0.47 |
| 1:S:3467:ARG:HD2 | 1:S:4000:ASN:ND2 | 2.30 | 0.47 |
| 2:T:491:GLU:O | 2:T:495:LEU:N | 2.37 | 0.47 |
| 8:e:40:DT:H2” | 8:e:41:DT:C6 | 2.50 | 0.47 |
| 1:A:539:GLN:OE1 | 1:A:539:GLN:N | 2.45 | 0.47 |
| 1:A:771:ASN:HA | 1:A:774:GLU:OE2 | 2.15 | 0.47 |
| 1:A:1416:GLU:HG3 | 1:A:1420:ARG:NH1 | 2.29 | 0.47 |
| 1:A:1632:TRP:C | 1:A:1633:TRP:CD1 | 2.93 | 0.47 |
| 1:A:1648:LEU:HD12 | 1:A:1649:LEU:HD22 | 1.97 | 0.47 |
| 1:A:1916:ILE:HG13 | 1:A:1917:LYS:N | 2.30 | 0.47 |
| 1:A:2859:GLN:HB3 | 1:A:2892:LEU:CD2 | 2.44 | 0.47 |
| 2:B:413:LEU:HD12 | 2:B:432:PHE:HB3 | 1.96 | 0.47 |
| 3:C:602:VAL:HG11 | 3:C:642:PHE:CE1 | 2.50 | 0.47 |
| 4:D:48:TRP:HB3 | 4:D:109:LEU:HB3 | 1.97 | 0.47 |
| 4:D:94:ALA:HB3 | 4:D:109:LEU:HB2 | 1.96 | 0.47 |
| 4:D:136:GLU:CD | 4:M:77:ARG:HH12 | 2.22 | 0.47 |
| 6:I:865:ILE:HD12 | 6:I:875:PHE:CD2 | 2.50 | 0.47 |
| 3:L:493:CYS:HB3 | 3:L:505:LEU:HD22 | 1.97 | 0.47 |
| 1:S:414:LEU:HB2 | 1:S:460:ALA:HB1 | 1.97 | 0.47 |
| 1:S:449:TYR:HB3 | 1:S:454:GLN:HG3 | 1.97 | 0.47 |
| 1:S:1389:VAL:O | 1:S:1392:MET:HG3 | 2.15 | 0.47 |
| 1:S:2120:ARG:HG3 | 1:S:2121:ASP:H | 1.79 | 0.47 |
| 1:S:2831:ASN:O | 1:S:2835:LYS:HG2 | 2.15 | 0.47 |
| 1:S:3263:HIS:HB2 | 1:S:3276:TRP:CZ2 | 2.50 | 0.47 |
| 1:S:3410:ILE:HD11 | 1:S:3456:LEU:HB2 | 1.97 | 0.47 |
| 1:S:3467:ARG:HD2 | 1:S:4000:ASN:HD21 | 1.80 | 0.47 |
| 1:S:3525:TYR:CE1 | 1:S:3705:TYR:HB3 | 2.50 | 0.47 |
| 1:S:3923:ARG:CZ | 1:S:3957:GLU:HG2 | 2.45 | 0.47 |
| 1:A:243:GLN:HA | 1:A:246:ARG:NH1 | 2.29 | 0.47 |
| 1:A:264:ARG:HE | 8:e:40:DT:H3’ | 1.80 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:342:MET:N | 1:A:342:MET:SD | 2.83 | 0.47 |
| 1:A:729:CYS:O | 1:A:733:LEU:HG | 2.15 | 0.47 |
| 1:A:788:TYR:O | 1:A:792:ILE:HG13 | 2.15 | 0.47 |
| 1:A:889:GLU:OE1 | 1:A:3889:ARG:NH2 | 2.47 | 0.47 |
| 1:A:1357:LYS:HG3 | 1:A:1411:TYR:OH | 2.15 | 0.47 |
| 1:A:1576:ASP:HA | 1:A:1579:VAL:HB | 1.96 | 0.47 |
| 1:A:2094:MET:HA | 1:A:2097:LEU:HD13 | 1.96 | 0.47 |
| 1:A:2810:SER:HB2 | 1:A:2864:GLN:NE2 | 2.30 | 0.47 |
| 1:A:3465:PHE:HA | 1:A:3468:LEU:HD12 | 1.96 | 0.47 |
| 1:A:3761:ASP:O | 1:A:3765:GLU:HG2 | 2.15 | 0.47 |
| 1:A:4108:MET:HA | 1:A:4112:THR:OG1 | 2.15 | 0.47 |
| 2:B:86:VAL:HG13 | 2:B:104:VAL:HA | 1.96 | 0.47 |
| 2:B:484:GLN:O | 2:B:488:ARG:HG2 | 2.15 | 0.47 |
| 3:C:163:PHE:CD2 | 3:C:208:VAL:HB | 2.49 | 0.47 |
| 3:L:292:GLU:HG2 | 2:T:301:ARG:HG3 | 1.96 | 0.47 |
| 3:L:309:ASP:HA | 2:T:290:ARG:NE | 2.29 | 0.47 |
| 3:L:624:LEU:HD12 | 3:L:625:ASP:N | 2.29 | 0.47 |
| 6:R:816:HIS:ND1 | 6:R:849:GLY:HA3 | 2.30 | 0.47 |
| 1:S:172:GLU:HA | 1:S:174:VAL:HG22 | 1.96 | 0.47 |
| 1:S:567:GLU:HA | 1:S:570:LYS:HE2 | 1.95 | 0.47 |
| 1:S:1622:ILE:HA | 1:S:1625:HIS:HB2 | 1.96 | 0.47 |
| 1:S:1852:LYS:HE3 | 1:S:1918:LEU:HD22 | 1.96 | 0.47 |
| 1:S:2321:GLU:HA | 1:S:2366:LYS:CG | 2.44 | 0.47 |
| 1:S:2420:PHE:O | 1:S:2424:MET:HG3 | 2.14 | 0.47 |
| 1:S:2940:ARG:NH2 | 1:S:3978:GLY:O | 2.49 | 0.47 |
| 1:S:3031:TRP:O | 1:S:3037:GLN:HB2 | 2.15 | 0.47 |
| 1:S:3041:LEU:HB2 | 1:S:3042:PRO:HD3 | 1.97 | 0.47 |
| 1:S:3971:MET:SD | 1:S:3974:MET:HB3 | 2.55 | 0.47 |
| 1:S:4040:PRO:O | 1:S:4044:ILE:HG23 | 2.14 | 0.47 |
| 2:T:93:ASP:HB3 | 2:T:101:ASN:N | 2.30 | 0.47 |
| 2:T:418:GLU:HB2 | 2:T:430:PRO:HB3 | 1.95 | 0.47 |
| 1:A:414:LEU:HB2 | 1:A:460:ALA:HB1 | 1.96 | 0.46 |
| 1:A:474:VAL:HA | 1:A:477:ASN:HD21 | 1.79 | 0.46 |
| 1:A:2745:ARG:NE | 8:e:44:DG:H2' | 2.30 | 0.46 |
| 1:A:3045:ILE:HD12 | 1:A:3085:GLU:HG3 | 1.97 | 0.46 |
| 1:A:3090:TYR:O | 1:A:3094:ASP:N | 2.48 | 0.46 |
| 1:A:3828:TYR:O | 1:A:3832:PRO:HD2 | 2.14 | 0.46 |
| 1:A:3834:ALA:HB3 | 1:A:3835:PRO:HD3 | 1.96 | 0.46 |
| 1:A:4040:PRO:HA | 1:A:4043:LYS:HD3 | 1.97 | 0.46 |
| 2:B:194:ARG:HH12 | 2:B:220:ILE:C | 2.23 | 0.46 |
| 2:B:413:LEU:HB3 | 2:B:432:PHE:CD2 | 2.50 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:480:ASN:HB3 | 2:B:483:LEU:HD12 | 1.96 | 0.46 |
| 3:C:404:GLN:OE1 | 3:C:423:GLN:HG3 | 2.14 | 0.46 |
| 3:C:632:PHE:CZ | 3:C:677:ILE:HG23 | 2.50 | 0.46 |
| 5:H:175:ASP:OD2 | 5:H:179:ARG:NH2 | 2.48 | 0.46 |
| 3:L:164:PHE:CE2 | 11:m:297:LEU:HD23 | 2.49 | 0.46 |
| 3:L:267:ILE:HD11 | 2:T:360:HIS:HD2 | 1.80 | 0.46 |
| 3:L:310:ILE:HD11 | 2:T:287:LYS:HB3 | 1.97 | 0.46 |
| 1:S:939:MET:O | 1:S:942:LEU:HG | 2.15 | 0.46 |
| 1:S:1415:LEU:HA | 1:S:1418:HIS:HB2 | 1.97 | 0.46 |
| 1:S:2132:LYS:O | 1:S:2135:ASN:ND2 | 2.48 | 0.46 |
| 1:S:2276:LEU:O | 1:S:2280:VAL:HG23 | 2.15 | 0.46 |
| 1:S:2346:ALA:HA | 1:S:2349:LEU:HD12 | 1.97 | 0.46 |
| 1:S:3923:ARG:HG3 | 1:S:4124:TRP:CD1 | 2.50 | 0.46 |
| 9:i:32:DA:H2" | 9:i:33:DA:C8 | 2.50 | 0.46 |
| 1:A:788:TYR:CE2 | 1:A:792:ILE:HD11 | 2.50 | 0.46 |
| 1:A:1407:LYS:HA | 1:A:1412:LYS:HD2 | 1.98 | 0.46 |
| 1:A:1723:PRO:HG3 | 3:C:594:PRO:HD2 | 1.96 | 0.46 |
| 1:A:2227:LYS:O | 1:A:2229:ALA:N | 2.47 | 0.46 |
| 1:A:2351:GLN:O | 1:A:2352:HIS:ND1 | 2.48 | 0.46 |
| 1:A:2384:PHE:HD2 | 1:A:2385:LEU:HD22 | 1.81 | 0.46 |
| 1:A:2937:ASP:OD2 | 1:A:3979:LEU:HD13 | 2.15 | 0.46 |
| 1:A:3516:HIS:O | 1:A:3519:GLU:HB3 | 2.16 | 0.46 |
| 2:B:287:LYS:HB3 | 3:C:310:ILE:HD11 | 1.98 | 0.46 |
| 5:H:13:GLU:OE2 | 5:H:15:SER:OG | 2.30 | 0.46 |
| 5:H:161:ARG:O | 5:H:164:LYS:HG3 | 2.14 | 0.46 |
| 3:L:521:GLU:O | 3:L:525:LYS:HG3 | 2.15 | 0.46 |
| 1:S:1711:ARG:O | 1:S:1714:LEU:HB2 | 2.15 | 0.46 |
| 1:S:1718:ILE:HA | 1:S:1721:HIS:ND1 | 2.29 | 0.46 |
| 1:S:2389:PHE:O | 1:S:2394:LYS:HE2 | 2.16 | 0.46 |
| 1:S:3512:VAL:HG12 | 1:S:3554:PHE:HZ | 1.80 | 0.46 |
| 2:T:182:LYS:HA | 2:T:185:ARG:NE | 2.30 | 0.46 |
| 2:T:468:LYS:HE2 | 2:T:517:ARG:HD3 | 1.97 | 0.46 |
| 7:d:20:DT:H2" | 7:d:21:DA:C5 | 2.51 | 0.46 |
| 7:d:35:DT:H2" | 7:d:36:DG:H8 | 1.81 | 0.46 |
| 8:e:32:DA:H2" | 8:e:33:DA:C8 | 2.50 | 0.46 |
| 10:j:28:DA:C6 | 10:j:29:DG:C6 | 3.03 | 0.46 |
| 1:A:528:VAL:HA | 1:A:633:ILE:HD11 | 1.98 | 0.46 |
| 1:A:575:ILE:HG13 | 1:A:576:VAL:N | 2.30 | 0.46 |
| 1:A:644:PRO:HD2 | 1:A:645:TRP:CZ3 | 2.50 | 0.46 |
| 1:A:936:SER:HB3 | 1:A:2773:ARG:HD2 | 1.97 | 0.46 |
| 1:A:1166:LEU:HA | 1:A:1169:VAL:HB | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2510:LEU:HD21 | 1:A:2525:TRP:CD1 | 2.50 | 0.46 |
| 1:A:2575:PRO:HA | 1:A:2785:ILE:O | 2.16 | 0.46 |
| 1:A:2724:ASP:N | 1:A:2724:ASP:OD1 | 2.48 | 0.46 |
| 1:A:3369:ASP:O | 1:A:3373:VAL:HG23 | 2.16 | 0.46 |
| 1:A:3531:TYR:HD2 | 1:A:3794:VAL:HB | 1.80 | 0.46 |
| 1:A:3686:TRP:NE1 | 1:A:3696:ARG:HH12 | 2.14 | 0.46 |
| 2:B:94:LYS:HE3 | 2:B:104:VAL:O | 2.15 | 0.46 |
| 3:C:40:MET:HG2 | 3:C:44:ARG:NH1 | 2.31 | 0.46 |
| 3:C:111:LEU:HD13 | 3:C:134:ILE:HB | 1.96 | 0.46 |
| 5:G:16:ILE:HG22 | 5:G:36:LEU:HD11 | 1.96 | 0.46 |
| 6:I:666:VAL:HG21 | 6:I:689:ILE:HG23 | 1.97 | 0.46 |
| 3:L:132:ILE:O | 3:L:161:LEU:HA | 2.16 | 0.46 |
| 3:L:184:ARG:HD2 | 3:L:514:ASN:HB3 | 1.96 | 0.46 |
| 3:L:458:ILE:O | 3:L:462:SER:N | 2.48 | 0.46 |
| 3:L:485:PRO:HB2 | 3:L:486:ARG:NH2 | 2.30 | 0.46 |
| 3:L:528:ILE:H | 3:L:528:ILE:HD12 | 1.81 | 0.46 |
| 4:M:201:PHE:HB2 | 2:T:517:ARG:NH1 | 2.30 | 0.46 |
| 1:S:359:LEU:O | 1:S:363:ILE:HG13 | 2.15 | 0.46 |
| 1:S:851:ILE:HD12 | 1:S:854:ARG:HH22 | 1.79 | 0.46 |
| 1:S:1013:ILE:HG13 | 1:S:1014:LEU:N | 2.31 | 0.46 |
| 1:S:2042:GLN:O | 1:S:2045:PHE:HB3 | 2.15 | 0.46 |
| 1:S:2346:ALA:O | 1:S:2349:LEU:HB2 | 2.15 | 0.46 |
| 1:S:3130:GLN:HB3 | 1:S:3178:ILE:HG21 | 1.96 | 0.46 |
| 1:S:3324:ARG:HD2 | 1:S:3392:ALA:HB2 | 1.97 | 0.46 |
| 1:S:3842:TRP:HB3 | 1:S:3855:TYR:CD1 | 2.50 | 0.46 |
| 1:S:3865:THR:O | 1:S:3869:THR:OG1 | 2.27 | 0.46 |
| 2:T:346:MET:HB2 | 2:T:399:ARG:HB3 | 1.98 | 0.46 |
| 1:A:269:SER:O | 1:A:273:ARG:NE | 2.42 | 0.46 |
| 1:A:1611:GLN:HG3 | 1:A:1613:HIS:ND1 | 2.30 | 0.46 |
| 1:A:1670:GLU:O | 1:A:1674:THR:N | 2.35 | 0.46 |
| 1:A:2220:MET:HE1 | 1:A:2255:LEU:HB2 | 1.96 | 0.46 |
| 1:A:2295:GLN:HE21 | 1:A:2298:GLU:CD | 2.23 | 0.46 |
| 1:A:2335:ASN:OD1 | 1:A:2336:ILE:N | 2.48 | 0.46 |
| 1:A:2464:HIS:O | 1:A:2470:ARG:NE | 2.49 | 0.46 |
| 1:A:3114:TYR:HA | 1:A:3117:ILE:CG1 | 2.44 | 0.46 |
| 1:A:3151:LEU:HA | 1:A:3197:LEU:HD22 | 1.97 | 0.46 |
| 1:A:3666:LEU:HA | 1:A:3669:LYS:HG2 | 1.98 | 0.46 |
| 1:A:3789:ARG:H | 1:A:3789:ARG:HD3 | 1.81 | 0.46 |
| 2:B:193:LEU:HB2 | 2:B:198:ILE:HB | 1.97 | 0.46 |
| 2:B:468:LYS:HE3 | 2:B:517:ARG:O | 2.15 | 0.46 |
| 3:C:246:HIS:CD2 | 3:C:248:PRO:HD3 | 2.51 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:144:LEU:O | 5:G:147:GLU:HG2 | 2.15 | 0.46 |
| 5:H:166:VAL:O | 5:H:170:GLU:HG2 | 2.15 | 0.46 |
| 3:L:269:GLN:HA | 2:T:442:ASP:HB3 | 1.97 | 0.46 |
| 1:S:127:ALA:O | 1:S:131:LEU:HG | 2.15 | 0.46 |
| 1:S:384:MET:O | 1:S:388:LEU:HG | 2.15 | 0.46 |
| 1:S:793:LEU:HD21 | 1:S:866:ILE:HG22 | 1.96 | 0.46 |
| 1:S:1215:GLU:O | 1:S:1219:PHE:HB2 | 2.15 | 0.46 |
| 1:S:1358:LEU:HA | 1:S:1361:LYS:HD3 | 1.97 | 0.46 |
| 1:S:2333:ARG:CZ | 1:S:2333:ARG:HA | 2.46 | 0.46 |
| 1:S:2418:LYS:HD3 | 1:S:2418:LYS:HA | 1.75 | 0.46 |
| 1:S:3263:HIS:HB2 | 1:S:3276:TRP:CH2 | 2.50 | 0.46 |
| 2:T:240:GLU:H | 2:T:240:GLU:CD | 2.24 | 0.46 |
| 10:j:19:DA:C5 | 10:j:20:DT:C4 | 3.03 | 0.46 |
| 1:A:153:PHE:HZ | 1:A:192:ASN:HB2 | 1.81 | 0.46 |
| 1:A:559:SER:OG | 1:A:560:LEU:N | 2.32 | 0.46 |
| 1:A:738:HIS:HB2 | 1:A:780:ILE:HD11 | 1.97 | 0.46 |
| 1:A:1072:ALA:HB1 | 1:A:1121:LEU:HD21 | 1.98 | 0.46 |
| 1:A:1081:ALA:O | 1:A:1085:ILE:HG23 | 2.15 | 0.46 |
| 1:A:1143:VAL:C | 1:A:1147:LYS:HZ2 | 2.24 | 0.46 |
| 1:A:1560:TYR:O | 1:A:1564:SER:OG | 2.30 | 0.46 |
| 1:A:1754:GLN:HG2 | 1:A:1785:ILE:HG23 | 1.97 | 0.46 |
| 1:A:2365:ASN:HD21 | 1:A:2399:GLU:HB2 | 1.78 | 0.46 |
| 1:A:3078:LEU:HA | 1:A:3082:TYR:HD2 | 1.80 | 0.46 |
| 1:A:3323:PHE:O | 1:A:3327:ASN:ND2 | 2.48 | 0.46 |
| 1:A:3820:MET:HE3 | 1:A:3825:LYS:HG3 | 1.97 | 0.46 |
| 2:B:62:MET:O | 2:B:65:GLN:NE2 | 2.48 | 0.46 |
| 3:C:14:MET:HE1 | 3:C:34:ALA:HB3 | 1.98 | 0.46 |
| 4:D:80:CYS:O | 4:D:83:GLN:NE2 | 2.48 | 0.46 |
| 5:H:182:LEU:O | 5:H:186:GLU:HG3 | 2.15 | 0.46 |
| 3:L:71:GLY:C | 3:L:73:GLN:H | 2.23 | 0.46 |
| 1:S:265:TYR:HB3 | 1:S:308:LEU:HD21 | 1.97 | 0.46 |
| 1:S:764:PRO:O | 1:S:768:VAL:HG22 | 2.16 | 0.46 |
| 1:S:793:LEU:HD11 | 1:S:867:ASN:HA | 1.98 | 0.46 |
| 1:S:888:ARG:NH1 | 1:S:889:GLU:OE2 | 2.49 | 0.46 |
| 1:S:1560:TYR:CZ | 1:S:1596:VAL:HG12 | 2.50 | 0.46 |
| 1:S:1758:LEU:HA | 1:S:1761:LEU:HD12 | 1.98 | 0.46 |
| 1:S:2223:VAL:HG22 | 1:S:2231:PHE:CE1 | 2.51 | 0.46 |
| 1:S:2891:ARG:HH22 | 1:S:3895:GLU:HA | 1.80 | 0.46 |
| 1:S:3165:THR:HG21 | 1:S:3241:LYS:HD3 | 1.96 | 0.46 |
| 1:S:3424:LEU:O | 1:S:3428:GLU:N | 2.38 | 0.46 |
| 1:S:3638:LYS:O | 1:S:3642:LYS:HG2 | 2.15 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:412:ALA:N | 2:T:435:VAL:O | 2.33 | 0.46 |
| 2:T:514:MET:O | 2:T:518:LEU:HG | 2.15 | 0.46 |
| 1:A:93:LEU:HB3 | 1:A:136:GLN:NE2 | 2.30 | 0.46 |
| 1:A:1018:VAL:HG12 | 1:A:1074:LYS:HG3 | 1.97 | 0.46 |
| 1:A:1220:LEU:HD21 | 1:A:1287:GLN:HB2 | 1.98 | 0.46 |
| 1:A:3994:ASP:O | 1:A:3997:LEU:N | 2.44 | 0.46 |
| 3:C:165:LEU:HD13 | 3:C:167:PHE:CZ | 2.51 | 0.46 |
| 3:C:492:GLN:HE22 | 3:C:507:PRO:C | 2.22 | 0.46 |
| 5:G:155:TRP:HA | 5:G:158:VAL:HG12 | 1.96 | 0.46 |
| 5:P:184:LEU:HD23 | 5:P:187:LYS:HE3 | 1.97 | 0.46 |
| 1:S:1456:LYS:HD2 | 1:S:1516:GLU:HG3 | 1.97 | 0.46 |
| 1:S:1513:GLY:HA2 | 1:S:1516:GLU:CD | 2.40 | 0.46 |
| 1:S:1626:TRP:HZ2 | 1:S:1674:THR:HG21 | 1.81 | 0.46 |
| 1:S:1632:TRP:CD1 | 1:S:1641:THR:CG2 | 2.99 | 0.46 |
| 1:S:1803:GLU:HA | 1:S:1806:ARG:HH21 | 1.80 | 0.46 |
| 1:S:1875:LYS:HZ2 | 1:S:1943:ALA:HB2 | 1.81 | 0.46 |
| 1:S:2161:ALA:HA | 1:S:2164:TRP:HB2 | 1.96 | 0.46 |
| 1:S:2464:HIS:HD2 | 1:S:2470:ARG:HG2 | 1.81 | 0.46 |
| 1:S:2587:GLN:N | 1:S:2777:HIS:O | 2.41 | 0.46 |
| 1:S:3173:MET:HA | 1:S:3173:MET:HE2 | 1.97 | 0.46 |
| 1:S:3185:ASN:OD1 | 1:S:3189:PHE:CZ | 2.68 | 0.46 |
| 1:S:3266:SER:HB2 | 1:S:3273:LEU:HA | 1.98 | 0.46 |
| 1:S:3753:LYS:N | 1:S:3801:GLY:O | 2.32 | 0.46 |
| 1:S:3877:LYS:HE3 | 1:S:4127:TRP:CE2 | 2.51 | 0.46 |
| 2:T:61:ASP:O | 2:T:65:GLN:OE1 | 2.34 | 0.46 |
| 2:T:352:PRO:HA | 2:T:393:GLU:O | 2.16 | 0.46 |
| 1:A:1102:GLU:CD | 1:A:1102:GLU:H | 2.24 | 0.46 |
| 1:A:1323:SER:HA | 1:A:1326:GLU:HA | 1.97 | 0.46 |
| 1:A:1663:THR:HG22 | 1:A:1664:SER:N | 2.29 | 0.46 |
| 1:A:2455:LEU:HD21 | 1:A:2498:ILE:HG23 | 1.97 | 0.46 |
| 1:A:2479:TRP:O | 1:A:2483:ASN:HB2 | 2.16 | 0.46 |
| 1:A:2732:PHE:HE1 | 1:A:2734:ARG:HH11 | 1.64 | 0.46 |
| 1:A:2981:TRP:CD1 | 1:A:2985:GLU:HG2 | 2.51 | 0.46 |
| 1:A:3531:TYR:CZ | 1:A:3796:MET:HG3 | 2.51 | 0.46 |
| 1:A:4044:ILE:C | 1:A:4048:LYS:HZ3 | 2.24 | 0.46 |
| 2:B:49:PHE:HE2 | 2:B:137:HIS:HB2 | 1.81 | 0.46 |
| 2:B:290:ARG:HA | 6:I:692:ASN:OD1 | 2.16 | 0.46 |
| 2:B:418:GLU:HG3 | 2:B:426:GLN:HG2 | 1.98 | 0.46 |
| 3:C:43:GLN:HE21 | 3:C:495:LEU:HB2 | 1.79 | 0.46 |
| 3:C:44:ARG:HB3 | 3:C:237:PHE:CE2 | 2.51 | 0.46 |
| 3:C:91:LEU:O | 3:C:95:GLU:HG3 | 2.16 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:521:GLU:O | 3:C:525:LYS:HG3 | 2.16 | 0.46 |
| 3:L:276:TRP:HB3 | 2:T:318:ARG:HB3 | 1.96 | 0.46 |
| 5:Q:193:SER:O | 5:Q:197:LYS:HG2 | 2.16 | 0.46 |
| 1:S:54:GLN:HA | 1:S:57:LEU:HD12 | 1.98 | 0.46 |
| 1:S:244:THR:O | 1:S:248:ILE:HG12 | 2.16 | 0.46 |
| 1:S:2321:GLU:O | 1:S:2325:LEU:HG | 2.15 | 0.46 |
| 1:S:3364:GLY:HA3 | 1:S:3373:VAL:HA | 1.97 | 0.46 |
| 1:S:3733:ARG:O | 1:S:3754:GLY:N | 2.49 | 0.46 |
| 1:S:3833:ARG:HH21 | 1:S:4125:GLU:HG3 | 1.81 | 0.46 |
| 1:S:4121:TRP:HB3 | 1:S:4124:TRP:HB2 | 1.98 | 0.46 |
| 2:T:39:ILE:HB | 2:T:166:ILE:HA | 1.98 | 0.46 |
| 2:T:304:ASN:ND2 | 2:T:309:GLY:O | 2.42 | 0.46 |
| 2:T:387:ILE:HA | 2:T:390:LEU:HD12 | 1.98 | 0.46 |
| 1:A:103:TYR:HB3 | 1:A:107:ILE:HG23 | 1.98 | 0.46 |
| 1:A:611:ASN:CG | 1:A:612:LEU:H | 2.22 | 0.46 |
| 1:A:751:ALA:O | 1:A:755:ALA:N | 2.29 | 0.46 |
| 1:A:983:LEU:C | 1:A:986:PRO:HD2 | 2.41 | 0.46 |
| 1:A:1208:LEU:HD22 | 1:A:1275:THR:OG1 | 2.16 | 0.46 |
| 1:A:1220:LEU:HD11 | 1:A:1287:GLN:HB2 | 1.98 | 0.46 |
| 1:A:1611:GLN:HE21 | 1:A:1613:HIS:HB2 | 1.80 | 0.46 |
| 1:A:2229:ALA:O | 1:A:2233:HIS:N | 2.44 | 0.46 |
| 1:A:2445:LYS:HD2 | 1:A:2445:LYS:H | 1.80 | 0.46 |
| 1:A:2723:THR:O | 1:A:2727:ARG:HG2 | 2.16 | 0.46 |
| 1:A:2855:VAL:HA | 1:A:2858:ILE:HD12 | 1.98 | 0.46 |
| 1:A:3113:ASN:HB2 | 1:A:3128:LYS:NZ | 2.31 | 0.46 |
| 1:A:3508:LYS:NZ | 1:A:3510:GLN:OE1 | 2.49 | 0.46 |
| 2:B:459:VAL:O | 2:B:463:LYS:HG3 | 2.16 | 0.46 |
| 3:C:111:LEU:O | 3:C:115:MET:HG2 | 2.16 | 0.46 |
| 5:G:185:ASN:HA | 5:G:188:LYS:HZ3 | 1.81 | 0.46 |
| 5:G:188:LYS:NZ | 6:I:769:THR:HG23 | 2.31 | 0.46 |
| 5:H:183:VAL:O | 5:H:187:LYS:HG2 | 2.16 | 0.46 |
| 3:L:528:ILE:O | 3:L:531:SER:OG | 2.24 | 0.46 |
| 1:S:648:SER:O | 1:S:651:TYR:HB3 | 2.16 | 0.46 |
| 1:S:799:TYR:HB3 | 1:S:852:ARG:HB3 | 1.97 | 0.46 |
| 1:S:966:PHE:HB2 | 1:S:1011:GLU:OE1 | 2.16 | 0.46 |
| 1:S:2133:LEU:HD22 | 1:S:2146:LEU:HB3 | 1.98 | 0.46 |
| 1:S:2154:GLU:HA | 1:S:2157:PHE:CZ | 2.51 | 0.46 |
| 1:S:2973:ASP:O | 1:S:2977:ASN:HB2 | 2.15 | 0.46 |
| 7:d:29:DG:N2 | 8:e:28:DT:C2 | 2.84 | 0.46 |
| 1:A:983:LEU:HD12 | 1:A:984:TYR:HD1 | 1.80 | 0.46 |
| 1:A:1133:HIS:O | 1:A:1137:ILE:HG12 | 2.15 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1723:PRO:HB2 | 1:A:1724:MET:SD | 2.56 | 0.46 |
| 1:A:2158:ARG:C | 1:A:2160:TYR:H | 2.24 | 0.46 |
| 1:A:2750:GLU:HA | 1:A:2753:ARG:NE | 2.31 | 0.46 |
| 1:A:2943:PHE:HD1 | 1:A:2947:ILE:HB | 1.81 | 0.46 |
| 1:A:3532:PRO:O | 1:A:3536:SER:HB3 | 2.16 | 0.46 |
| 1:A:3563:ASP:C | 1:A:3564:GLN:HG3 | 2.41 | 0.46 |
| 1:A:3718:ARG:O | 1:A:3742:GLY:HA2 | 2.16 | 0.46 |
| 2:B:276:LEU:HD12 | 3:C:432:GLN:HA | 1.98 | 0.46 |
| 3:C:406:GLY:HA2 | 3:C:424:LEU:HG | 1.98 | 0.46 |
| 3:L:395:TYR:HB3 | 3:L:404:GLN:HG2 | 1.96 | 0.46 |
| 3:L:465:LYS:HZ3 | 3:L:467:ASP:HA | 1.81 | 0.46 |
| 3:L:528:ILE:HG22 | 3:L:532:LYS:HZ2 | 1.81 | 0.46 |
| 5:P:194:LEU:HA | 5:P:197:LYS:HG2 | 1.98 | 0.46 |
| 6:R:816:HIS:H | 6:R:851:LYS:N | 2.13 | 0.46 |
| 1:S:80:GLU:HA | 1:S:83:GLU:CD | 2.41 | 0.46 |
| 1:S:142:ARG:HB2 | 1:S:143:LEU:HD12 | 1.96 | 0.46 |
| 1:S:738:HIS:HB2 | 1:S:780:ILE:HD11 | 1.97 | 0.46 |
| 1:S:767:GLU:HA | 1:S:854:ARG:NH2 | 2.31 | 0.46 |
| 1:S:781:ASP:OD2 | 1:S:783:HIS:ND1 | 2.48 | 0.46 |
| 1:S:1039:TRP:O | 1:S:1043:GLN:HG3 | 2.16 | 0.46 |
| 1:S:1166:LEU:HD13 | 1:S:1198:LEU:HD13 | 1.97 | 0.46 |
| 1:S:2303:LEU:HB3 | 1:S:2323:LEU:HD21 | 1.98 | 0.46 |
| 1:S:2355:THR:OG1 | 1:S:2356:MET:N | 2.49 | 0.46 |
| 1:S:2950:LYS:NZ | 1:S:2983:ASP:OD2 | 2.49 | 0.46 |
| 1:S:3090:TYR:HB2 | 1:S:3099:ALA:HB2 | 1.98 | 0.46 |
| 1:S:3410:ILE:HG23 | 1:S:3453:ALA:HB1 | 1.98 | 0.46 |
| 1:S:3466:PRO:O | 1:S:3470:GLN:HG2 | 2.16 | 0.46 |
| 1:S:3565:GLY:O | 1:S:3569:GLN:HG2 | 2.16 | 0.46 |
| 1:S:3923:ARG:HG3 | 1:S:4124:TRP:HD1 | 1.81 | 0.46 |
| 2:T:94:LYS:HE3 | 2:T:103:TYR:CE1 | 2.51 | 0.46 |
| 7:d:23:DT:N3 | 8:e:33:DA:N1 | 2.64 | 0.46 |
| 1:A:114:VAL:O | 1:A:119:ARG:HB2 | 2.15 | 0.46 |
| 1:A:167:PRO:HA | 1:A:171:LEU:HD12 | 1.98 | 0.46 |
| 1:A:547:ASP:OD1 | 1:A:547:ASP:N | 2.49 | 0.46 |
| 1:A:770:LEU:HD11 | 1:A:858:MET:HG2 | 1.97 | 0.46 |
| 1:A:953:GLN:NE2 | 1:A:1003:SER:O | 2.38 | 0.46 |
| 1:A:1294:VAL:HG13 | 1:A:1367:HIS:NE2 | 2.31 | 0.46 |
| 1:A:1598:ASN:HA | 1:A:1601:LEU:HD12 | 1.97 | 0.46 |
| 1:A:1671:VAL:HA | 1:A:1674:THR:HB | 1.97 | 0.46 |
| 1:A:1885:PRO:HB3 | 1:A:1955:VAL:HG21 | 1.98 | 0.46 |
| 1:A:2169:LEU:O | 1:A:2173:ALA:N | 2.48 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2405:VAL:HA | 1:A:2408:MET:HE2 | 1.98 | 0.46 |
| 1:A:2553:HIS:O | 1:A:2557:LEU:HG | 2.15 | 0.46 |
| 1:A:2756:GLU:O | 1:A:2760:GLU:OE1 | 2.34 | 0.46 |
| 1:A:3166:ASN:OD1 | 1:A:3186:ARG:NH1 | 2.49 | 0.46 |
| 1:A:4082:ARG:HG3 | 1:A:4089:ILE:HG22 | 1.98 | 0.46 |
| 2:B:522:VAL:HG13 | 3:C:257:LEU:HG | 1.96 | 0.46 |
| 3:C:335:SER:OG | 3:C:399:LYS:O | 2.29 | 0.46 |
| 4:D:183:GLU:OE2 | 4:D:190:PHE:N | 2.34 | 0.46 |
| 6:R:710:LYS:O | 6:R:714:LEU:HG | 2.16 | 0.46 |
| 1:S:180:LEU:O | 1:S:185:HIS:NE2 | 2.47 | 0.46 |
| 1:S:200:PHE:CG | 1:S:224:LEU:HD22 | 2.51 | 0.46 |
| 1:S:327:VAL:HB | 1:S:333:MET:SD | 2.56 | 0.46 |
| 1:S:328:ALA:HB2 | 1:S:372:PRO:HG3 | 1.97 | 0.46 |
| 1:S:360:SER:O | 1:S:364:ARG:NE | 2.40 | 0.46 |
| 1:S:374:LYS:NZ | 1:S:424:LEU:HD12 | 2.31 | 0.46 |
| 1:S:524:TYR:CD1 | 1:S:629:PHE:HZ | 2.34 | 0.46 |
| 1:S:749:VAL:O | 1:S:753:GLN:HG2 | 2.16 | 0.46 |
| 1:S:1019:ASP:OD1 | 1:S:1026:ARG:NE | 2.49 | 0.46 |
| 1:S:1418:HIS:HA | 1:S:1421:GLU:HB2 | 1.98 | 0.46 |
| 1:S:1536:ALA:O | 1:S:1555:HIS:ND1 | 2.44 | 0.46 |
| 1:S:3836:PRO:O | 1:S:3873:LYS:HD2 | 2.16 | 0.46 |
| 2:T:191:GLY:HA2 | 2:T:194:ARG:HE | 1.80 | 0.46 |
| 1:A:333:MET:HE2 | 1:A:375:VAL:HG11 | 1.98 | 0.45 |
| 1:A:901:MET:N | 1:A:901:MET:SD | 2.89 | 0.45 |
| 1:A:1173:LEU:HD21 | 1:A:1191:PHE:CG | 2.50 | 0.45 |
| 1:A:1653:LEU:HG | 1:A:1695:LEU:HD11 | 1.97 | 0.45 |
| 1:A:2229:ALA:C | 1:A:2731:ARG:HH21 | 2.21 | 0.45 |
| 1:A:2259:LYS:C | 1:A:2273:GLY:HA3 | 2.41 | 0.45 |
| 1:A:2260:PHE:HE1 | 1:A:2302:ALA:HB3 | 1.81 | 0.45 |
| 1:A:2750:GLU:O | 1:A:2753:ARG:HG2 | 2.16 | 0.45 |
| 1:A:2785:ILE:HG22 | 1:A:2789:SER:OG | 2.16 | 0.45 |
| 1:A:3090:TYR:CB | 1:A:3095:ASP:HB2 | 2.46 | 0.45 |
| 1:A:3176:MET:HE2 | 1:A:3179:TRP:CD1 | 2.51 | 0.45 |
| 1:A:3619:ASP:OD1 | 1:A:3619:ASP:N | 2.49 | 0.45 |
| 1:A:3867:THR:HG21 | 1:A:4085:LYS:NZ | 2.31 | 0.45 |
| 1:A:4009:PRO:HA | 1:A:4038:TRP:HH2 | 1.81 | 0.45 |
| 3:C:297:LEU:N | 3:C:303:THR:O | 2.49 | 0.45 |
| 3:C:689:GLU:HA | 3:C:695:SER:HB3 | 1.98 | 0.45 |
| 5:G:150:ARG:HH21 | 6:I:837:ARG:HD2 | 1.80 | 0.45 |
| 1:S:730:LEU:HB3 | 1:S:754:MET:HE1 | 1.98 | 0.45 |
| 1:S:888:ARG:HG3 | 1:S:889:GLU:OE2 | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1844:VAL:O | 1:S:1848:ILE:HG13 | 2.16 | 0.45 |
| 1:S:2143:ARG:HH22 | 1:S:2175:GLU:CD | 2.22 | 0.45 |
| 1:S:2754:GLU:HA | 1:S:2757:ILE:HD12 | 1.98 | 0.45 |
| 1:S:2806:LYS:HB2 | 1:S:2857:CYS:HB2 | 1.98 | 0.45 |
| 1:S:3508:LYS:HE2 | 1:S:3510:GLN:HE21 | 1.80 | 0.45 |
| 2:T:67:ILE:HA | 2:T:70:VAL:HG22 | 1.98 | 0.45 |
| 1:A:183:GLU:C | 1:A:185:HIS:HD1 | 2.24 | 0.45 |
| 1:A:195:ASN:HA | 1:A:198:ARG:NE | 2.31 | 0.45 |
| 1:A:447:PRO:HB3 | 1:A:523:THR:HG22 | 1.99 | 0.45 |
| 1:A:475:LEU:O | 1:A:479:ILE:HG12 | 2.15 | 0.45 |
| 1:A:697:ASP:CG | 1:A:699:GLU:HG2 | 2.40 | 0.45 |
| 1:A:886:TRP:CZ3 | 1:A:911:LEU:HB2 | 2.51 | 0.45 |
| 1:A:2531:LEU:HB3 | 1:A:2538:ARG:NE | 2.31 | 0.45 |
| 1:A:3534:ILE:O | 1:A:3537:SER:N | 2.48 | 0.45 |
| 1:A:3931:ALA:N | 1:A:3936:GLY:O | 2.39 | 0.45 |
| 2:B:115:ARG:O | 2:B:119:LEU:HG | 2.17 | 0.45 |
| 2:B:201:ASP:OD1 | 2:B:202:LEU:N | 2.49 | 0.45 |
| 2:B:240:GLU:HA | 2:B:243:LEU:HG | 1.97 | 0.45 |
| 2:B:400:TYR:CE2 | 2:B:402:PRO:HG3 | 2.51 | 0.45 |
| 2:B:473:TYR:H | 3:C:350:GLN:HE22 | 1.63 | 0.45 |
| 3:C:599:ARG:HH21 | 3:C:641:ALA:HB3 | 1.79 | 0.45 |
| 4:M:73:THR:OG1 | 4:M:74:PRO:HD3 | 2.16 | 0.45 |
| 1:S:67:VAL:HA | 1:S:71:LYS:HD3 | 1.98 | 0.45 |
| 1:S:3114:TYR:CE2 | 1:S:3125:ARG:HD2 | 2.52 | 0.45 |
| 1:S:3829:LEU:HD13 | 1:S:3833:ARG:HG3 | 1.98 | 0.45 |
| 8:e:35:DT:C4 | 8:e:36:DA:C6 | 3.04 | 0.45 |
| 8:e:39:DA:C5 | 8:e:40:DT:C4 | 3.04 | 0.45 |
| 1:A:264:ARG:HG2 | 1:A:305:ASN:ND2 | 2.31 | 0.45 |
| 1:A:337:LYS:HG2 | 1:A:369:PHE:CZ | 2.51 | 0.45 |
| 1:A:571:SER:O | 1:A:575:ILE:HG12 | 2.17 | 0.45 |
| 1:A:1238:GLN:O | 1:A:1310:GLU:HA | 2.16 | 0.45 |
| 1:A:1303:MET:N | 1:A:1303:MET:SD | 2.90 | 0.45 |
| 1:A:1539:SER:HA | 1:A:1552:HIS:CG | 2.51 | 0.45 |
| 1:A:1696:LEU:HA | 1:A:1699:PHE:HD2 | 1.81 | 0.45 |
| 1:A:2269:ASP:N | 1:A:2269:ASP:OD1 | 2.47 | 0.45 |
| 1:A:2835:LYS:O | 1:A:2838:GLN:HG2 | 2.17 | 0.45 |
| 1:A:2876:VAL:HG11 | 1:A:2892:LEU:HD11 | 1.98 | 0.45 |
| 1:A:3184:THR:HA | 1:A:3187:CYS:SG | 2.57 | 0.45 |
| 1:A:3447:VAL:HA | 1:A:3450:MET:HE3 | 1.99 | 0.45 |
| 1:A:3923:ARG:HH11 | 1:A:4124:TRP:HB2 | 1.81 | 0.45 |
| 2:B:325:ARG:HH22 | 3:C:501:PRO:HB3 | 1.80 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:487:PHE:O | 2:B:488:ARG:C | 2.60 | 0.45 |
| 3:C:184:ARG:NE | 3:C:187:GLY:HA3 | 2.31 | 0.45 |
| 3:C:361:VAL:HG13 | 3:C:420:VAL:HG13 | 1.97 | 0.45 |
| 3:C:400:ARG:NH1 | 7:d:34:DT:O4' | 2.50 | 0.45 |
| 3:C:438:LEU:HA | 3:C:441:SER:HB3 | 1.97 | 0.45 |
| 4:M:180:CYS:HB3 | 4:M:183:GLU:HB2 | 1.97 | 0.45 |
| 1:S:637:LYS:HA | 1:S:637:LYS:HD2 | 1.71 | 0.45 |
| 1:S:1949:ILE:O | 1:S:1952:ILE:HG22 | 2.16 | 0.45 |
| 1:S:2416:LYS:HA | 1:S:2420:PHE:HD1 | 1.80 | 0.45 |
| 1:S:2424:MET:HE1 | 1:S:2457:PRO:HB2 | 1.99 | 0.45 |
| 1:S:2429:ASP:OD1 | 1:S:2430:GLU:N | 2.49 | 0.45 |
| 1:S:2436:LEU:O | 1:S:2436:LEU:HD23 | 2.16 | 0.45 |
| 1:S:2588:GLU:HA | 1:S:2776:ARG:HA | 1.98 | 0.45 |
| 1:S:3632:PHE:CZ | 1:S:3670:MET:HE3 | 2.51 | 0.45 |
| 1:S:3976:GLU:HG2 | 1:S:3980:MET:HG3 | 1.99 | 0.45 |
| 9:i:24:DA:H1' | 9:i:25:DA:H5' | 1.97 | 0.45 |
| 1:A:40:GLN:HA | 1:A:43:VAL:HG22 | 1.98 | 0.45 |
| 1:A:110:THR:O | 1:A:114:VAL:HG23 | 2.17 | 0.45 |
| 1:A:338:LEU:HA | 1:A:342:MET:HE1 | 1.97 | 0.45 |
| 1:A:801:LYS:HE2 | 1:A:3125:ARG:NH2 | 2.31 | 0.45 |
| 1:A:959:TYR:HB3 | 1:A:960:GLN:NE2 | 2.31 | 0.45 |
| 1:A:1039:TRP:HA | 1:A:1042:LYS:HD3 | 1.99 | 0.45 |
| 1:A:1077:GLY:HA2 | 1:A:1080:LEU:HG | 1.98 | 0.45 |
| 1:A:1458:LEU:HG | 1:A:1463:LEU:O | 2.17 | 0.45 |
| 1:A:1639:LEU:O | 1:A:1643:MET:HE3 | 2.16 | 0.45 |
| 1:A:3031:TRP:H | 1:A:3064:PHE:HE2 | 1.63 | 0.45 |
| 1:A:3577:GLN:HE21 | 1:A:3683:CYS:HB3 | 1.81 | 0.45 |
| 1:A:3766:GLN:O | 1:A:3770:VAL:HG23 | 2.16 | 0.45 |
| 2:B:486:HIS:HA | 2:B:489:ASN:HD22 | 1.81 | 0.45 |
| 2:B:488:ARG:HD2 | 2:B:501:GLU:HB3 | 1.98 | 0.45 |
| 3:C:251:LEU:O | 3:C:258:SER:HA | 2.17 | 0.45 |
| 3:C:604:GLN:HE21 | 3:C:605:LYS:NZ | 2.14 | 0.45 |
| 3:C:642:PHE:HD2 | 3:C:655:PHE:CE2 | 2.35 | 0.45 |
| 4:D:77:ARG:O | 4:D:81:GLU:HG2 | 2.16 | 0.45 |
| 6:I:879:ARG:NH2 | 6:I:885:LYS:HB2 | 2.31 | 0.45 |
| 3:L:335:SER:HB3 | 3:L:403:PRO:HD3 | 1.98 | 0.45 |
| 3:L:457:LEU:HD22 | 3:L:533:ILE:HG13 | 1.98 | 0.45 |
| 6:R:692:ASN:HB2 | 2:T:290:ARG:O | 2.16 | 0.45 |
| 6:R:699:CYS:SG | 6:R:719:ASP:HB2 | 2.57 | 0.45 |
| 1:S:240:GLU:HG3 | 1:S:243:GLN:HG2 | 1.98 | 0.45 |
| 1:S:953:GLN:HG2 | 1:S:1003:SER:HB2 | 1.98 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1220:LEU:O | 1:S:1224:PHE:HB2 | 2.16 | 0.45 |
| 1:S:1637:SER:O | 1:S:1642:LYS:HE3 | 2.16 | 0.45 |
| 1:S:1708:GLU:HA | 1:S:1711:ARG:NH1 | 2.31 | 0.45 |
| 1:S:1763:THR:O | 1:S:1767:CYS:N | 2.41 | 0.45 |
| 1:S:2102:LYS:O | 1:S:2106:ARG:NH1 | 2.50 | 0.45 |
| 1:S:3100:LYS:NZ | 1:S:3104:GLN:HB3 | 2.31 | 0.45 |
| 1:S:3113:ASN:O | 1:S:3117:ILE:N | 2.48 | 0.45 |
| 1:S:3257:LYS:HA | 1:S:3257:LYS:HD2 | 1.70 | 0.45 |
| 1:S:3276:TRP:HZ3 | 1:S:3306:LEU:HD22 | 1.81 | 0.45 |
| 1:S:3817:LEU:HG | 1:S:3825:LYS:HE3 | 1.98 | 0.45 |
| 1:S:3915:HIS:HE1 | 1:S:3961:PHE:HA | 1.81 | 0.45 |
| 2:T:90:THR:OG1 | 2:T:135:MET:HE3 | 2.16 | 0.45 |
| 2:T:518:LEU:HB3 | 2:T:522:VAL:HG23 | 1.99 | 0.45 |
| 9:i:35:DT:H2” | 9:i:36:DA:H5’ | 1.99 | 0.45 |
| 1:A:343:GLU:HG2 | 1:A:344:GLN:N | 2.32 | 0.45 |
| 1:A:1430:GLU:H | 1:A:1430:GLU:CD | 2.25 | 0.45 |
| 1:A:1709:GLU:H | 1:A:1709:GLU:CD | 2.24 | 0.45 |
| 1:A:2164:TRP:O | 1:A:2167:PRO:HD2 | 2.16 | 0.45 |
| 1:A:2253:TYR:H | 1:A:2256:ILE:HD12 | 1.81 | 0.45 |
| 1:A:2827:SER:HA | 1:A:2830:ASN:ND2 | 2.32 | 0.45 |
| 1:A:3493:TRP:H | 1:A:3709:GLY:HA2 | 1.81 | 0.45 |
| 3:C:82:HIS:H | 3:C:84:MET:HE1 | 1.80 | 0.45 |
| 3:C:295:TYR:O | 3:C:305:VAL:N | 2.49 | 0.45 |
| 3:C:315:ARG:HA | 3:C:320:ILE:HG12 | 1.97 | 0.45 |
| 3:C:653:GLN:H | 3:C:653:GLN:CD | 2.25 | 0.45 |
| 3:C:656:ASN:CB | 3:C:688:LYS:HA | 2.46 | 0.45 |
| 4:D:132:VAL:HG11 | 4:M:8:LEU:HD21 | 1.99 | 0.45 |
| 3:L:280:ASP:HB2 | 3:L:288:ASP:HB3 | 1.98 | 0.45 |
| 4:M:38:ASN:HB3 | 4:M:40:TYR:CE1 | 2.52 | 0.45 |
| 1:S:962:TYR:HB3 | 1:S:966:PHE:CE2 | 2.51 | 0.45 |
| 1:S:1071:ASN:HB3 | 1:S:1074:LYS:CD | 2.44 | 0.45 |
| 1:S:1634:ALA:C | 1:S:1636:ASP:H | 2.25 | 0.45 |
| 1:S:1798:LEU:HD21 | 1:S:1827:LEU:HB3 | 1.99 | 0.45 |
| 1:S:2328:ARG:HA | 1:S:2333:ARG:HD2 | 1.97 | 0.45 |
| 1:A:194:GLU:N | 1:A:194:GLU:OE1 | 2.49 | 0.45 |
| 1:A:337:LYS:O | 1:A:342:MET:HE1 | 2.16 | 0.45 |
| 1:A:421:LEU:HA | 1:A:424:LEU:HB3 | 1.99 | 0.45 |
| 1:A:934:LEU:HA | 1:A:937:MET:HG2 | 1.98 | 0.45 |
| 1:A:1045:THR:O | 1:A:1049:GLN:HG3 | 2.16 | 0.45 |
| 1:A:1184:ARG:HH21 | 1:A:1262:ALA:HA | 1.82 | 0.45 |
| 1:A:1475:LEU:H | 1:A:1475:LEU:HD12 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1565:GLU:HG2 | 1:A:1566:THR:N | 2.32 | 0.45 |
| 1:A:1645:VAL:HA | 1:A:1648:LEU:HG | 1.97 | 0.45 |
| 1:A:1783:ARG:NH1 | 1:A:1830:HIS:HB2 | 2.31 | 0.45 |
| 1:A:1870:LYS:HA | 1:A:1873:TYR:CD2 | 2.52 | 0.45 |
| 1:A:2339:GLU:HA | 1:A:2342:CYS:SG | 2.56 | 0.45 |
| 1:A:2454:LEU:O | 1:A:2458:VAL:HG23 | 2.17 | 0.45 |
| 1:A:3448:GLU:OE2 | 1:A:3482:LEU:HB3 | 2.16 | 0.45 |
| 1:A:3547:THR:HA | 1:A:3550:LYS:NZ | 2.31 | 0.45 |
| 1:A:3557:ARG:O | 1:A:3561:LYS:HG2 | 2.17 | 0.45 |
| 1:A:3964:THR:O | 1:A:3968:ILE:HG12 | 2.17 | 0.45 |
| 2:B:299:LYS:N | 3:C:294:VAL:O | 2.41 | 0.45 |
| 2:B:352:PRO:HA | 2:B:394:VAL:HA | 1.98 | 0.45 |
| 2:B:366:LEU:HD23 | 2:B:436:PHE:HE2 | 1.82 | 0.45 |
| 2:B:487:PHE:HB2 | 2:B:488:ARG:HH11 | 1.81 | 0.45 |
| 3:C:186:GLY:O | 3:C:515:MET:N | 2.49 | 0.45 |
| 3:C:250:ARG:HG2 | 3:C:260:ARG:HG3 | 1.99 | 0.45 |
| 3:C:271:ARG:O | 3:C:273:LYS:NZ | 2.44 | 0.45 |
| 1:S:133:LYS:O | 1:S:136:GLN:HG2 | 2.17 | 0.45 |
| 1:S:186:PRO:HB2 | 1:S:188:GLU:HG2 | 1.98 | 0.45 |
| 1:S:935:HIS:HE1 | 1:S:2773:ARG:NH2 | 2.15 | 0.45 |
| 1:S:1238:GLN:HB2 | 1:S:1239:PRO:HD3 | 1.99 | 0.45 |
| 1:S:1400:VAL:HA | 1:S:1403:MET:HE3 | 1.98 | 0.45 |
| 1:S:1456:LYS:NZ | 1:S:1516:GLU:O | 2.49 | 0.45 |
| 1:S:2233:HIS:CE1 | 1:S:2728:LEU:HA | 2.52 | 0.45 |
| 1:S:3877:LYS:HE3 | 1:S:4127:TRP:CD2 | 2.52 | 0.45 |
| 1:S:3886:ALA:O | 1:S:3890:MET:HG2 | 2.16 | 0.45 |
| 1:S:4041:ARG:HG3 | 1:S:4044:ILE:HD11 | 1.98 | 0.45 |
| 2:T:58:THR:H | 2:T:125:GLN:NE2 | 2.13 | 0.45 |
| 1:A:384:MET:O | 1:A:388:LEU:HG | 2.17 | 0.45 |
| 1:A:793:LEU:HD21 | 1:A:866:ILE:HG12 | 1.99 | 0.45 |
| 1:A:1185:HIS:HA | 1:A:1188:ILE:HG12 | 1.98 | 0.45 |
| 1:A:1572:LEU:HD11 | 1:A:1603:GLN:HG3 | 1.99 | 0.45 |
| 1:A:1576:ASP:HB2 | 1:A:1625:HIS:HE1 | 1.81 | 0.45 |
| 1:A:3159:ARG:HD3 | 1:A:3159:ARG:N | 2.32 | 0.45 |
| 1:A:3247:ARG:HE | 1:A:3282:ARG:HH12 | 1.63 | 0.45 |
| 1:A:3971:MET:CE | 1:A:3974:MET:HB2 | 2.47 | 0.45 |
| 2:B:211:PHE:CE1 | 2:B:232:HIS:HB2 | 2.52 | 0.45 |
| 2:B:362:LEU:HG | 2:B:363:ARG:H | 1.81 | 0.45 |
| 6:I:663:GLU:HA | 6:I:688:TYR:HB3 | 1.98 | 0.45 |
| 6:I:816:HIS:O | 6:I:851:LYS:N | 2.50 | 0.45 |
| 6:R:729:CYS:SG | 6:R:736:VAL:HG22 | 2.57 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:R:810:LEU:CD2 | 6:R:848:HIS:HD2 | 2.23 | 0.45 |
| 1:S:179:GLY:HA3 | 1:S:230:LEU:HB2 | 1.98 | 0.45 |
| 1:S:440:VAL:HA | 1:S:443:ILE:HD13 | 1.97 | 0.45 |
| 1:S:905:ILE:HD12 | 1:S:2812:LEU:HA | 1.98 | 0.45 |
| 1:S:1936:ARG:HA | 1:S:1939:LEU:HD12 | 1.98 | 0.45 |
| 1:S:2385:LEU:HD13 | 1:S:2389:PHE:CE2 | 2.52 | 0.45 |
| 1:S:2423:VAL:HA | 1:S:2426:HIS:HB3 | 1.99 | 0.45 |
| 1:S:2748:VAL:HA | 1:S:2751:GLN:HG2 | 1.98 | 0.45 |
| 1:S:3263:HIS:HA | 1:S:3266:SER:HB3 | 1.98 | 0.45 |
| 1:S:3480:LEU:HA | 1:S:3483:MET:HB2 | 1.99 | 0.45 |
| 1:S:3999:THR:HA | 1:S:4002:MET:HG3 | 1.99 | 0.45 |
| 2:T:58:THR:H | 2:T:125:GLN:HE22 | 1.62 | 0.45 |
| 1:A:1000:LYS:HA | 1:A:1000:LYS:HE3 | 1.99 | 0.45 |
| 1:A:1538:LEU:O | 1:A:1552:HIS:N | 2.50 | 0.45 |
| 1:A:1756:PRO:O | 1:A:1759:LEU:N | 2.50 | 0.45 |
| 1:A:2507:ILE:HD11 | 1:A:2545:LEU:HD23 | 1.98 | 0.45 |
| 1:A:2522:ARG:HA | 1:A:2561:PHE:CZ | 2.52 | 0.45 |
| 1:A:2924:VAL:O | 1:A:2928:LYS:HG3 | 2.16 | 0.45 |
| 1:A:3164:TRP:HA | 1:A:3168:TYR:CZ | 2.52 | 0.45 |
| 1:A:3189:PHE:O | 1:A:3193:ILE:HG12 | 2.17 | 0.45 |
| 1:A:3871:PHE:CG | 1:A:4117:LEU:HA | 2.52 | 0.45 |
| 5:Q:51:GLU:HA | 5:Q:54:GLN:HE22 | 1.81 | 0.45 |
| 5:Q:187:LYS:O | 5:Q:191:ILE:HG13 | 2.17 | 0.45 |
| 1:S:945:ALA:HB1 | 1:S:957:PRO:HG3 | 1.99 | 0.45 |
| 1:S:1756:PRO:O | 1:S:1760:GLU:HG2 | 2.16 | 0.45 |
| 1:S:2342:CYS:O | 1:S:2345:VAL:HG22 | 2.16 | 0.45 |
| 2:T:147:LEU:HD22 | 2:T:193:LEU:HD12 | 1.99 | 0.45 |
| 2:T:288:LEU:HA | 2:T:295:PRO:HA | 1.99 | 0.45 |
| 7:d:27:DT:H3 | 8:e:29:DA:H61 | 1.64 | 0.45 |
| 11:m:296:GLY:O | 11:m:299:SER:N | 2.49 | 0.45 |
| 1:A:149:ILE:HG13 | 1:A:150:GLY:N | 2.31 | 0.45 |
| 1:A:360:SER:O | 1:A:363:ILE:HB | 2.17 | 0.45 |
| 1:A:1153:LEU:HD13 | 1:A:1160:SER:HA | 1.98 | 0.45 |
| 1:A:1452:VAL:HA | 1:A:1517:LEU:HD11 | 1.99 | 0.45 |
| 1:A:1743:MET:HA | 1:A:1746:PHE:CD2 | 2.52 | 0.45 |
| 1:A:2380:ASN:N | 1:A:2380:ASN:OD1 | 2.50 | 0.45 |
| 1:A:2395:THR:O | 1:A:2399:GLU:HG3 | 2.16 | 0.45 |
| 1:A:2776:ARG:HH22 | 1:A:2785:ILE:HG13 | 1.82 | 0.45 |
| 1:A:2925:GLU:HA | 1:A:2928:LYS:HD2 | 1.98 | 0.45 |
| 1:A:2930:TYR:HB3 | 1:A:2935:GLU:HB3 | 1.98 | 0.45 |
| 1:A:2973:ASP:O | 1:A:2976:LEU:HG | 2.17 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3151:LEU:HD23 | 1:A:3151:LEU:H | 1.81 | 0.45 |
| 1:A:3593:ARG:HD3 | 1:A:3661:ASP:HB2 | 1.99 | 0.45 |
| 1:A:3628:PHE:HE1 | 1:A:3671:ASN:HB3 | 1.81 | 0.45 |
| 2:B:259:LEU:HD11 | 2:B:343:PRO:C | 2.42 | 0.45 |
| 2:B:271:VAL:HG12 | 2:B:370:PRO:HA | 1.99 | 0.45 |
| 4:D:23:TYR:CD2 | 4:D:124:LEU:HD11 | 2.52 | 0.45 |
| 5:H:146:LYS:O | 5:H:149:GLU:HG3 | 2.16 | 0.45 |
| 3:L:297:LEU:HB2 | 3:L:303:THR:HB | 1.98 | 0.45 |
| 5:P:187:LYS:HB3 | 5:Q:187:LYS:NZ | 2.32 | 0.45 |
| 1:S:565:TYR:O | 1:S:569:VAL:HG23 | 2.17 | 0.45 |
| 1:S:667:TYR:HB2 | 1:S:728:SER:HB2 | 1.98 | 0.45 |
| 1:S:1017:ILE:HG23 | 1:S:1077:GLY:HA3 | 1.99 | 0.45 |
| 1:S:1323:SER:N | 1:S:1328:GLU:OE2 | 2.49 | 0.45 |
| 1:S:2825:THR:O | 1:S:2829:LYS:HG3 | 2.17 | 0.45 |
| 1:S:3639:GLU:HG3 | 1:S:3643:HIS:CE1 | 2.52 | 0.45 |
| 1:S:3920:ILE:HG21 | 1:S:3942:PHE:HA | 1.99 | 0.45 |
| 2:T:166:ILE:O | 2:T:200:LEU:HD12 | 2.17 | 0.45 |
| 7:d:16:DA:C6 | 8:e:42:DA:N1 | 2.84 | 0.45 |
| 9:i:32:DA:H2" | 9:i:33:DA:H8 | 1.82 | 0.45 |
| 1:A:179:GLY:HA3 | 1:A:227:LEU:HA | 1.99 | 0.45 |
| 1:A:523:THR:HG23 | 1:A:526:ASP:OD1 | 2.16 | 0.45 |
| 1:A:565:TYR:O | 1:A:569:VAL:HG23 | 2.17 | 0.45 |
| 1:A:745:VAL:HA | 1:A:748:TYR:CD2 | 2.51 | 0.45 |
| 1:A:1452:VAL:HG22 | 1:A:1517:LEU:HD11 | 1.98 | 0.45 |
| 1:A:4073:ALA:HB1 | 1:A:4076:ASP:HB3 | 1.99 | 0.45 |
| 3:C:212:MET:O | 3:C:216:GLU:N | 2.46 | 0.45 |
| 3:C:323:PHE:CE2 | 3:C:328:GLU:HB3 | 2.37 | 0.45 |
| 4:D:120:ARG:O | 4:D:124:LEU:HD23 | 2.16 | 0.45 |
| 5:G:173:GLU:O | 5:G:176:LEU:HG | 2.16 | 0.45 |
| 5:G:178:LYS:O | 5:G:182:LEU:HG | 2.16 | 0.45 |
| 3:L:18:PHE:HA | 3:L:21:SER:HB2 | 1.98 | 0.45 |
| 3:L:137:ASP:OD1 | 3:L:137:ASP:N | 2.49 | 0.45 |
| 5:Q:189:THR:HA | 5:Q:192:ARG:HE | 1.82 | 0.45 |
| 1:S:897:PRO:HA | 1:S:902:LYS:HE3 | 1.98 | 0.45 |
| 1:S:2306:ASN:HA | 1:S:2309:PHE:CE2 | 2.52 | 0.45 |
| 1:S:2448:PRO:O | 1:S:2452:ARG:HG2 | 2.17 | 0.45 |
| 1:S:2597:PHE:CD2 | 1:S:2765:GLN:HG2 | 2.52 | 0.45 |
| 1:S:3420:CYS:CB | 1:S:3446:VAL:HG11 | 2.47 | 0.45 |
| 2:T:90:THR:O | 2:T:101:ASN:HA | 2.17 | 0.45 |
| 1:A:207:GLN:HG3 | 1:A:217:LEU:HD13 | 1.98 | 0.44 |
| 1:A:307:GLU:H | 1:A:307:GLU:CD | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:611:ASN:OD1 | 1:A:612:LEU:N | 2.44 | 0.44 |
| 1:A:933:LEU:HD21 | 1:A:2794:LEU:HD23 | 1.98 | 0.44 |
| 1:A:1118:GLU:HB3 | 1:A:1121:LEU:HB2 | 2.00 | 0.44 |
| 1:A:1328:GLU:H | 1:A:1328:GLU:CD | 2.25 | 0.44 |
| 1:A:1458:LEU:HD11 | 1:A:1463:LEU:HB2 | 1.98 | 0.44 |
| 1:A:1610:ASN:OD1 | 1:A:1610:ASN:N | 2.48 | 0.44 |
| 1:A:1664:SER:HA | 1:A:1668:PHE:HD2 | 1.82 | 0.44 |
| 1:A:2106:ARG:NH1 | 1:A:2107:SER:HB3 | 2.31 | 0.44 |
| 1:A:2418:LYS:HA | 1:A:2418:LYS:HD3 | 1.73 | 0.44 |
| 1:A:3428:GLU:OE1 | 1:A:3474:ARG:NH1 | 2.50 | 0.44 |
| 1:A:3880:ALA:HB2 | 1:A:3965:ARG:NE | 2.27 | 0.44 |
| 2:B:115:ARG:HA | 2:B:118:GLU:OE1 | 2.17 | 0.44 |
| 2:B:366:LEU:HD23 | 2:B:436:PHE:CE2 | 2.52 | 0.44 |
| 2:B:462:MET:HE3 | 2:B:525:PHE:CD1 | 2.51 | 0.44 |
| 2:B:511:VAL:HB | 3:C:255:SER:OG | 2.17 | 0.44 |
| 3:C:674:PHE:HB2 | 3:C:675:TRP:CE3 | 2.52 | 0.44 |
| 3:C:729:LEU:C | 1:S:1913:LYS:HB3 | 2.42 | 0.44 |
| 3:L:11:VAL:HG23 | 3:L:55:ALA:CB | 2.46 | 0.44 |
| 6:R:815:ARG:HA | 6:R:851:LYS:HA | 1.99 | 0.44 |
| 1:S:461:ILE:O | 1:S:464:VAL:HG22 | 2.17 | 0.44 |
| 1:S:524:TYR:HA | 1:S:527:TYR:CE2 | 2.51 | 0.44 |
| 1:S:1034:ARG:HG3 | 1:S:1085:ILE:HA | 1.99 | 0.44 |
| 1:S:1076:LEU:HB3 | 1:S:1123:THR:OG1 | 2.17 | 0.44 |
| 1:S:2925:GLU:HA | 1:S:2928:LYS:HE2 | 2.00 | 0.44 |
| 1:S:3104:GLN:NE2 | 1:S:3105:ASN:OD1 | 2.50 | 0.44 |
| 1:S:3240:MET:HE3 | 1:S:3272:TRP:CH2 | 2.52 | 0.44 |
| 1:S:3324:ARG:HH12 | 1:S:3411:ASP:HB2 | 1.82 | 0.44 |
| 1:S:3383:GLN:O | 1:S:3386:SER:OG | 2.30 | 0.44 |
| 1:S:3448:GLU:O | 1:S:3452:LYS:HG3 | 2.18 | 0.44 |
| 1:S:4006:VAL:HG11 | 1:S:4009:PRO:HG3 | 1.98 | 0.44 |
| 1:S:4093:GLU:HB3 | 1:S:4094:PRO:HD3 | 1.99 | 0.44 |
| 2:T:68:GLN:HE22 | 2:T:116:ILE:HA | 1.82 | 0.44 |
| 1:A:165:LYS:HZ1 | 8:e:30:DA:H3' | 1.81 | 0.44 |
| 1:A:264:ARG:HG3 | 8:e:41:DT:OP2 | 2.17 | 0.44 |
| 1:A:850:GLU:O | 1:A:854:ARG:HG2 | 2.17 | 0.44 |
| 1:A:1365:ASN:HD21 | 1:A:1367:HIS:HB3 | 1.83 | 0.44 |
| 1:A:1389:VAL:HG22 | 1:A:1392:MET:HE3 | 1.98 | 0.44 |
| 1:A:2477:LEU:HD13 | 1:A:2505:VAL:HG13 | 1.98 | 0.44 |
| 1:A:2581:LEU:HB2 | 1:A:2781:PRO:HB2 | 2.00 | 0.44 |
| 1:A:2916:LEU:HD12 | 1:A:2917:PRO:HD2 | 1.99 | 0.44 |
| 1:A:3325:ASP:HA | 1:A:3328:ILE:HB | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3483:MET:HE1 | 1:A:3511:ALA:C | 2.43 | 0.44 |
| 1:A:3679:ASN:O | 1:A:3724:GLU:HG3 | 2.17 | 0.44 |
| 1:A:3743:HIS:C | 1:A:3745:GLU:H | 2.24 | 0.44 |
| 1:A:4085:LYS:HG2 | 1:A:4087:HIS:NE2 | 2.32 | 0.44 |
| 2:B:75:ILE:HG21 | 3:C:316:TYR:CE1 | 2.52 | 0.44 |
| 2:B:413:LEU:HB3 | 2:B:432:PHE:HD2 | 1.83 | 0.44 |
| 2:B:493:LEU:O | 6:I:708:ARG:NH1 | 2.51 | 0.44 |
| 3:C:90:LEU:O | 3:C:94:ILE:HG13 | 2.18 | 0.44 |
| 4:D:98:LEU:HD23 | 4:D:105:LEU:HD13 | 2.00 | 0.44 |
| 5:H:187:LYS:O | 5:H:191:ILE:HG12 | 2.17 | 0.44 |
| 6:I:743:MET:N | 6:I:743:MET:SD | 2.90 | 0.44 |
| 6:I:758:TYR:CD1 | 6:I:764:SER:HB3 | 2.53 | 0.44 |
| 6:I:819:TYR:HB3 | 6:I:862:HIS:HB2 | 2.00 | 0.44 |
| 3:L:427:MET:N | 2:T:478:PHE:O | 2.48 | 0.44 |
| 4:M:58:ALA:HA | 4:M:61:LYS:HE3 | 1.99 | 0.44 |
| 1:S:51:LEU:HD23 | 1:S:51:LEU:H | 1.82 | 0.44 |
| 1:S:229:SER:HA | 1:S:278:HIS:CE1 | 2.50 | 0.44 |
| 1:S:473:PRO:HG3 | 1:S:1558:TYR:CD1 | 2.52 | 0.44 |
| 1:S:571:SER:HA | 1:S:574:LYS:NZ | 2.32 | 0.44 |
| 1:S:1096:VAL:O | 1:S:1100:VAL:HG13 | 2.16 | 0.44 |
| 1:S:1333:SER:O | 1:S:1337:VAL:HG23 | 2.16 | 0.44 |
| 1:S:1423:ILE:HG13 | 1:S:1425:ALA:H | 1.82 | 0.44 |
| 1:S:1513:GLY:HA2 | 1:S:1516:GLU:OE2 | 2.17 | 0.44 |
| 1:S:1725:GLN:OE1 | 1:S:1727:ARG:N | 2.45 | 0.44 |
| 1:S:2215:LEU:HA | 1:S:2218:PHE:CD2 | 2.52 | 0.44 |
| 1:S:2586:PHE:CZ | 1:S:2782:ASP:HB3 | 2.51 | 0.44 |
| 1:S:2735:ASP:OD1 | 1:S:2735:ASP:N | 2.50 | 0.44 |
| 1:S:2979:GLN:HE21 | 1:S:2985:GLU:HB2 | 1.82 | 0.44 |
| 1:S:3617:LEU:HD22 | 1:S:3633:ILE:HG22 | 1.98 | 0.44 |
| 1:S:3718:ARG:H | 1:S:3743:HIS:HB3 | 1.82 | 0.44 |
| 2:T:390:LEU:HD11 | 2:T:417:GLU:CD | 2.42 | 0.44 |
| 1:A:361:ILE:HD12 | 1:A:361:ILE:H | 1.82 | 0.44 |
| 1:A:394:GLN:CG | 1:A:1737:ASN:HB3 | 2.48 | 0.44 |
| 1:A:962:TYR:HB3 | 1:A:966:PHE:CE2 | 2.52 | 0.44 |
| 1:A:1415:LEU:O | 1:A:1419:LEU:HG | 2.17 | 0.44 |
| 1:A:1488:TYR:HA | 1:A:1559:PHE:CE1 | 2.53 | 0.44 |
| 1:A:2430:GLU:HA | 1:A:2433:LYS:HE2 | 1.98 | 0.44 |
| 1:A:2835:LYS:HA | 1:A:2838:GLN:NE2 | 2.33 | 0.44 |
| 1:A:3630:ARG:HA | 1:A:3630:ARG:HD2 | 1.81 | 0.44 |
| 1:A:3868:VAL:O | 1:A:3872:ARG:HD3 | 2.18 | 0.44 |
| 2:B:48:MET:HE3 | 2:B:59:PRO:HB2 | 2.00 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:161:MET:HB2 | 2:B:164:LYS:HE3 | 1.99 | 0.44 |
| 2:B:290:ARG:HG3 | 3:C:309:ASP:C | 2.42 | 0.44 |
| 2:B:480:ASN:CG | 3:C:402:ASN:HD21 | 2.25 | 0.44 |
| 3:C:198:THR:HG23 | 3:C:201:GLN:H | 1.81 | 0.44 |
| 3:L:266:SER:HB3 | 3:L:363:LYS:HB2 | 1.99 | 0.44 |
| 6:R:658:ILE:HD12 | 6:R:735:PHE:H | 1.82 | 0.44 |
| 1:S:22:ALA:HA | 1:S:24:ARG:NH1 | 2.29 | 0.44 |
| 1:S:2264:ASP:HB3 | 1:S:2309:PHE:CZ | 2.52 | 0.44 |
| 1:S:2542:LEU:HA | 1:S:2545:LEU:HD23 | 1.99 | 0.44 |
| 1:S:2571:ASP:HB2 | 1:S:2787:HIS:CE1 | 2.52 | 0.44 |
| 1:S:2854:PHE:CZ | 1:S:2858:ILE:HD11 | 2.52 | 0.44 |
| 1:S:3058:ASP:OD1 | 1:S:3058:ASP:N | 2.50 | 0.44 |
| 1:S:3137:GLU:O | 1:S:3140:GLU:HG2 | 2.18 | 0.44 |
| 1:S:3416:LEU:HD23 | 1:S:3449:LYS:HD2 | 1.99 | 0.44 |
| 2:T:35:ARG:HA | 2:T:252:ARG:HH12 | 1.82 | 0.44 |
| 2:T:275:ASN:HB3 | 2:T:366:LEU:HD13 | 1.99 | 0.44 |
| 1:A:229:SER:HA | 1:A:278:HIS:CE1 | 2.52 | 0.44 |
| 1:A:1101:PHE:O | 1:A:1105:VAL:HG13 | 2.18 | 0.44 |
| 1:A:1206:LEU:HA | 1:A:1209:LYS:HG2 | 1.99 | 0.44 |
| 1:A:1255:CYS:HA | 1:A:1258:ASP:OD2 | 2.18 | 0.44 |
| 1:A:1427:SER:O | 1:A:1431:LEU:HG | 2.18 | 0.44 |
| 1:A:1458:LEU:HA | 1:A:1461:ALA:HB3 | 1.97 | 0.44 |
| 1:A:2295:GLN:NE2 | 1:A:2298:GLU:OE2 | 2.50 | 0.44 |
| 1:A:2428:ASP:O | 1:A:2432:GLN:HG2 | 2.17 | 0.44 |
| 1:A:2925:GLU:O | 1:A:2928:LYS:HB2 | 2.17 | 0.44 |
| 1:A:3714:GLU:OE1 | 1:A:3718:ARG:NH2 | 2.48 | 0.44 |
| 1:A:4064:LEU:O | 1:A:4068:HIS:HB3 | 2.17 | 0.44 |
| 2:B:350:PHE:CZ | 3:C:458:ILE:HG12 | 2.52 | 0.44 |
| 2:B:375:VAL:HG12 | 2:B:378:SER:HB3 | 1.99 | 0.44 |
| 3:C:43:GLN:HG2 | 3:C:47:PHE:CE2 | 2.52 | 0.44 |
| 3:C:636:ILE:O | 3:C:640:ARG:HG2 | 2.18 | 0.44 |
| 3:L:435:PHE:O | 2:T:426:GLN:NE2 | 2.51 | 0.44 |
| 3:L:603:LYS:NZ | 3:L:645:GLU:OE2 | 2.46 | 0.44 |
| 3:L:643:ARG:HB2 | 3:L:655:PHE:CE2 | 2.53 | 0.44 |
| 3:L:673:HIS:ND1 | 3:L:673:HIS:O | 2.49 | 0.44 |
| 6:R:810:LEU:HD23 | 6:R:848:HIS:HB3 | 1.98 | 0.44 |
| 1:S:19:LEU:HD22 | 1:S:34:LEU:HA | 1.99 | 0.44 |
| 1:S:297:LEU:HB3 | 1:S:316:LEU:HD12 | 1.99 | 0.44 |
| 1:S:746:ARG:O | 1:S:750:PRO:HD3 | 2.16 | 0.44 |
| 1:S:1198:LEU:O | 1:S:1202:ARG:NH2 | 2.50 | 0.44 |
| 1:S:2820:MET:O | 1:S:2824:LYS:HG2 | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3358:ARG:O | 1:S:3362:LEU:HG | 2.18 | 0.44 |
| 7:d:38:DG:N1 | 8:e:20:DT:O2 | 2.48 | 0.44 |
| 9:i:40:DT:C4 | 10:j:17:DT:C4 | 3.06 | 0.44 |
| 10:j:26:DT:H2" | 10:j:27:DT:C2 | 2.52 | 0.44 |
| 1:A:204:LEU:HD21 | 1:A:224:LEU:HD21 | 1.98 | 0.44 |
| 1:A:748:TYR:O | 1:A:752:LEU:HD23 | 2.17 | 0.44 |
| 1:A:1049:GLN:O | 1:A:1055:ASN:HB3 | 2.18 | 0.44 |
| 1:A:3584:LEU:O | 1:A:3799:ARG:NH2 | 2.50 | 0.44 |
| 1:A:3723:ASP:HA | 1:A:3741:ARG:HH21 | 1.82 | 0.44 |
| 1:A:3872:ARG:HA | 1:A:3875:GLU:CD | 2.43 | 0.44 |
| 2:B:167:MET:HE1 | 2:B:203:MET:HG2 | 1.99 | 0.44 |
| 2:B:318:ARG:HH21 | 2:B:331:LYS:H | 1.65 | 0.44 |
| 2:B:480:ASN:O | 2:B:484:GLN:HG2 | 2.18 | 0.44 |
| 3:C:620:ILE:HG22 | 3:C:635:SER:HB3 | 2.00 | 0.44 |
| 6:I:743:MET:HE3 | 6:I:754:PHE:CE2 | 2.52 | 0.44 |
| 6:I:758:TYR:HD1 | 6:I:764:SER:HB3 | 1.83 | 0.44 |
| 3:L:496:HIS:CG | 3:L:506:PRO:HD3 | 2.52 | 0.44 |
| 1:S:181:LEU:HA | 1:S:185:HIS:HE1 | 1.82 | 0.44 |
| 1:S:335:LYS:HD2 | 1:S:339:GLN:NE2 | 2.32 | 0.44 |
| 1:S:655:LEU:O | 1:S:659:ARG:HG2 | 2.18 | 0.44 |
| 1:S:2468:THR:O | 1:S:2472:GLN:HG3 | 2.18 | 0.44 |
| 1:S:3796:MET:HG2 | 1:S:3802:LEU:N | 2.32 | 0.44 |
| 1:S:3962:ARG:NH2 | 1:S:4125:GLU:HB3 | 2.32 | 0.44 |
| 1:S:4012:ASP:HB2 | 1:S:4038:TRP:CD2 | 2.52 | 0.44 |
| 1:S:4041:ARG:O | 1:S:4044:ILE:HG12 | 2.17 | 0.44 |
| 1:A:363:ILE:HA | 1:A:366:TYR:HD2 | 1.82 | 0.44 |
| 1:A:392:CYS:HA | 1:A:395:MET:CG | 2.44 | 0.44 |
| 1:A:528:VAL:HG23 | 1:A:532:ARG:HH12 | 1.82 | 0.44 |
| 1:A:921:ALA:HB3 | 1:A:927:LYS:HE2 | 1.99 | 0.44 |
| 1:A:1134:LEU:O | 1:A:1138:ILE:HG12 | 2.18 | 0.44 |
| 1:A:2102:LYS:NZ | 1:A:2155:GLU:HG2 | 2.29 | 0.44 |
| 1:A:2271:SER:HA | 1:A:2274:ILE:HD12 | 1.98 | 0.44 |
| 1:A:2340:SER:O | 1:A:2344:LEU:HG | 2.18 | 0.44 |
| 1:A:2980:ASP:OD1 | 1:A:2980:ASP:N | 2.50 | 0.44 |
| 1:A:3158:LYS:HA | 1:A:3161:LEU:HD21 | 1.99 | 0.44 |
| 1:A:3175:PRO:C | 1:A:3179:TRP:HD1 | 2.25 | 0.44 |
| 1:A:3239:LYS:O | 1:A:3243:ILE:HG12 | 2.18 | 0.44 |
| 1:A:3532:PRO:O | 1:A:3536:SER:CB | 2.66 | 0.44 |
| 1:A:3559:LYS:HA | 1:A:3562:LEU:HD23 | 1.99 | 0.44 |
| 1:A:3571:PHE:CZ | 1:A:3575:LEU:HD11 | 2.53 | 0.44 |
| 2:B:70:VAL:O | 2:B:74:LYS:HG2 | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:190:ALA:O | 2:B:193:LEU:HG | 2.18 | 0.44 |
| 2:B:484:GLN:HE21 | 2:B:488:ARG:HH22 | 1.66 | 0.44 |
| 3:C:454:VAL:O | 3:C:458:ILE:HG13 | 2.18 | 0.44 |
| 3:C:618:ASN:HA | 3:C:621:GLU:CD | 2.43 | 0.44 |
| 3:C:674:PHE:HB2 | 3:C:675:TRP:HE3 | 1.82 | 0.44 |
| 4:D:90:GLN:C | 4:D:92:ASP:H | 2.25 | 0.44 |
| 3:L:34:ALA:O | 3:L:38:ILE:HG12 | 2.18 | 0.44 |
| 3:L:234:LEU:C | 3:L:236:VAL:N | 2.73 | 0.44 |
| 3:L:297:LEU:HD23 | 2:T:296:VAL:HG22 | 1.98 | 0.44 |
| 1:S:41:GLU:OE1 | 1:S:41:GLU:HA | 2.16 | 0.44 |
| 1:S:1226:GLY:HA2 | 1:S:1259:LEU:HG | 1.98 | 0.44 |
| 1:S:1464:LEU:HD12 | 1:S:1521:PHE:HD1 | 1.82 | 0.44 |
| 1:S:1711:ARG:O | 1:S:1715:GLU:OE1 | 2.36 | 0.44 |
| 1:S:2102:LYS:HE2 | 1:S:2102:LYS:HA | 1.99 | 0.44 |
| 1:S:2329:TYR:HA | 1:S:2332:GLU:HA | 2.00 | 0.44 |
| 1:S:2331:MET:HB2 | 1:S:2335:ASN:O | 2.18 | 0.44 |
| 1:S:3008:TRP:O | 1:S:3011:LEU:HB2 | 2.18 | 0.44 |
| 1:S:3134:ALA:HB2 | 1:S:3182:ILE:HG22 | 1.99 | 0.44 |
| 1:S:3493:TRP:CE3 | 1:S:3524:ASN:HB2 | 2.52 | 0.44 |
| 2:T:73:SER:O | 2:T:77:SER:OG | 2.25 | 0.44 |
| 9:i:39:DA:N1 | 10:j:19:DA:C6 | 2.86 | 0.44 |
| 1:A:86:LEU:HB3 | 1:A:129:ASP:CG | 2.43 | 0.44 |
| 1:A:213:ARG:HB3 | 2:B:404:ARG:NH1 | 2.32 | 0.44 |
| 1:A:264:ARG:NE | 8:e:40:DT:H3' | 2.33 | 0.44 |
| 1:A:1299:GLU:O | 1:A:1304:HIS:ND1 | 2.51 | 0.44 |
| 1:A:1630:ASP:HB3 | 1:A:1633:TRP:HE1 | 1.82 | 0.44 |
| 1:A:2361:ILE:HD11 | 1:A:2393:LEU:HD22 | 1.98 | 0.44 |
| 1:A:2371:PHE:CE2 | 1:A:2374:LEU:HB2 | 2.53 | 0.44 |
| 1:A:2532:PRO:HB2 | 1:A:2537:ASP:HB3 | 1.98 | 0.44 |
| 1:A:2574:ASN:N | 1:A:2786:LYS:HD2 | 2.33 | 0.44 |
| 1:A:2889:GLY:O | 1:A:2892:LEU:HG | 2.18 | 0.44 |
| 1:A:3733:ARG:HB3 | 1:A:3754:GLY:CA | 2.48 | 0.44 |
| 2:B:304:ASN:N | 2:B:309:GLY:O | 2.50 | 0.44 |
| 2:B:312:LEU:N | 2:B:315:ASP:OD2 | 2.50 | 0.44 |
| 3:C:45:GLN:O | 3:C:49:GLU:N | 2.50 | 0.44 |
| 3:L:281:ALA:N | 2:T:315:ASP:O | 2.50 | 0.44 |
| 5:P:194:LEU:HD22 | 5:Q:194:LEU:HG | 2.00 | 0.44 |
| 1:S:307:GLU:HA | 1:S:310:LYS:HE2 | 1.99 | 0.44 |
| 1:S:474:VAL:HA | 1:S:477:ASN:HD21 | 1.83 | 0.44 |
| 1:S:1142:HIS:CE1 | 1:S:1146:ASN:HD21 | 2.35 | 0.44 |
| 1:S:1849:ASP:OD1 | 1:S:1850:VAL:N | 2.51 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2295:GLN:HG3 | 1:S:2298:GLU:HG2 | 1.99 | 0.44 |
| 1:S:2368:THR:HA | 1:S:2371:PHE:O | 2.17 | 0.44 |
| 1:S:2461:PHE:O | 1:S:2473:MET:HE1 | 2.17 | 0.44 |
| 1:S:2788:SER:HA | 1:S:2791:ILE:HG12 | 1.99 | 0.44 |
| 1:S:2941:GLY:O | 1:S:2944:THR:OG1 | 2.36 | 0.44 |
| 1:S:3061:LEU:O | 1:S:3065:ILE:HG12 | 2.18 | 0.44 |
| 1:S:4064:LEU:O | 1:S:4068:HIS:HB3 | 2.18 | 0.44 |
| 2:T:317:LYS:HB3 | 2:T:328:ILE:HG23 | 2.00 | 0.44 |
| 1:A:61:ARG:HB2 | 1:A:103:TYR:CE2 | 2.45 | 0.44 |
| 1:A:476:ARG:NH1 | 1:A:1562:LEU:HD23 | 2.33 | 0.44 |
| 1:A:1172:LEU:HA | 1:A:1175:HIS:HB2 | 2.00 | 0.44 |
| 1:A:1779:GLN:HA | 1:A:1782:PHE:HD2 | 1.82 | 0.44 |
| 1:A:1779:GLN:O | 1:A:1783:ARG:HG2 | 2.17 | 0.44 |
| 1:A:2427:ARG:NH2 | 1:A:2428:ASP:HA | 2.32 | 0.44 |
| 1:A:3033:GLU:HB2 | 1:A:3034:PRO:HD3 | 2.00 | 0.44 |
| 1:A:4092:GLN:O | 1:A:4095:GLU:HG2 | 2.18 | 0.44 |
| 1:A:4113:ASP:O | 1:A:4116:ILE:HG22 | 2.18 | 0.44 |
| 2:B:69:SER:OG | 2:B:243:LEU:HA | 2.18 | 0.44 |
| 4:M:196:ALA:HA | 2:T:477:SER:HA | 2.00 | 0.44 |
| 1:S:417:VAL:O | 1:S:421:LEU:HD23 | 2.18 | 0.44 |
| 1:S:435:LEU:HA | 1:S:438:LEU:HD12 | 1.99 | 0.44 |
| 1:S:672:ILE:HG22 | 1:S:676:ASN:HD21 | 1.81 | 0.44 |
| 1:S:831:LEU:HD12 | 1:S:833:HIS:H | 1.83 | 0.44 |
| 1:S:849:GLU:HA | 1:S:852:ARG:HD3 | 1.98 | 0.44 |
| 1:S:1400:VAL:HG12 | 1:S:1404:LYS:HZ2 | 1.82 | 0.44 |
| 1:S:2229:ALA:O | 1:S:2233:HIS:N | 2.45 | 0.44 |
| 1:S:2230:VAL:HA | 1:S:2233:HIS:HB3 | 2.00 | 0.44 |
| 1:S:2284:ASP:N | 1:S:2284:ASP:OD1 | 2.45 | 0.44 |
| 1:S:2331:MET:CE | 1:S:2337:LEU:H | 2.30 | 0.44 |
| 1:S:2340:SER:O | 1:S:2344:LEU:HG | 2.18 | 0.44 |
| 1:S:2840:PHE:HA | 1:S:2843:PHE:CD2 | 2.53 | 0.44 |
| 1:S:2937:ASP:HB3 | 1:S:3978:GLY:C | 2.43 | 0.44 |
| 1:S:3422:GLN:N | 1:S:3425:ARG:HH21 | 2.15 | 0.44 |
| 1:S:4102:THR:O | 1:S:4105:LYS:HG3 | 2.17 | 0.44 |
| 2:T:79:ASP:OD1 | 2:T:79:ASP:N | 2.50 | 0.44 |
| 2:T:345:LEU:HG | 2:T:400:TYR:HD1 | 1.83 | 0.44 |
| 10:j:17:DT:H2" | 10:j:18:DA:C5 | 2.52 | 0.44 |
| 1:A:54:GLN:CD | 1:A:54:GLN:H | 2.26 | 0.44 |
| 1:A:410:MET:N | 1:A:411:PRO:HD2 | 2.33 | 0.44 |
| 1:A:574:LYS:HA | 1:A:577:GLU:OE2 | 2.18 | 0.44 |
| 1:A:655:LEU:O | 1:A:658:THR:OG1 | 2.26 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:745:VAL:O | 1:A:749:VAL:HG23 | 2.17 | 0.44 |
| 1:A:757:LYS:O | 1:A:760:LEU:HB2 | 2.17 | 0.44 |
| 1:A:800:LEU:HB3 | 1:A:3114:TYR:CE2 | 2.52 | 0.44 |
| 1:A:944:LYS:O | 1:A:947:GLN:HG3 | 2.18 | 0.44 |
| 1:A:947:GLN:CD | 1:A:948:MET:HG2 | 2.43 | 0.44 |
| 1:A:1251:GLN:HG2 | 1:A:1252:ALA:N | 2.32 | 0.44 |
| 1:A:1524:LEU:H | 1:A:1524:LEU:HD23 | 1.83 | 0.44 |
| 1:A:1608:ARG:HB3 | 1:A:1612:LYS:CE | 2.48 | 0.44 |
| 1:A:2224:PHE:HA | 1:A:2231:PHE:CD1 | 2.53 | 0.44 |
| 1:A:2393:LEU:O | 1:A:2396:LEU:HB2 | 2.18 | 0.44 |
| 1:A:2437:ASP:O | 1:A:2441:LYS:HG2 | 2.18 | 0.44 |
| 1:A:2948:GLY:HA3 | 1:A:2954:GLN:HE22 | 1.83 | 0.44 |
| 1:A:3177:ASN:OD1 | 1:A:3178:ILE:HG13 | 2.18 | 0.44 |
| 1:A:3531:TYR:CE2 | 1:A:3794:VAL:HB | 2.52 | 0.44 |
| 2:B:299:LYS:NZ | 3:C:296:CYS:HB3 | 2.33 | 0.44 |
| 2:B:446:MET:HE2 | 3:C:264:TYR:HB2 | 2.00 | 0.44 |
| 3:L:521:GLU:O | 3:L:524:THR:OG1 | 2.28 | 0.44 |
| 4:M:120:ARG:HH11 | 4:M:124:LEU:HD13 | 1.82 | 0.44 |
| 1:S:98:GLN:NE2 | 1:S:140:SER:O | 2.45 | 0.44 |
| 1:S:181:LEU:HA | 1:S:185:HIS:CE1 | 2.53 | 0.44 |
| 1:S:475:LEU:O | 1:S:479:ILE:HG12 | 2.18 | 0.44 |
| 1:S:848:LEU:HA | 1:S:851:ILE:HG12 | 2.00 | 0.44 |
| 1:S:1279:LEU:HD23 | 1:S:1279:LEU:H | 1.82 | 0.44 |
| 1:S:1470:SER:HA | 1:S:1476:HIS:HE1 | 1.82 | 0.44 |
| 1:S:1536:ALA:HB3 | 1:S:1555:HIS:HB2 | 1.99 | 0.44 |
| 1:S:2227:LYS:C | 1:S:2229:ALA:H | 2.26 | 0.44 |
| 1:S:2371:PHE:CE2 | 1:S:2373:PRO:HG2 | 2.53 | 0.44 |
| 1:S:2427:ARG:HH12 | 1:S:2429:ASP:CA | 2.29 | 0.44 |
| 1:S:2773:ARG:HE | 1:S:2775:TYR:HE1 | 1.66 | 0.44 |
| 1:A:13:LEU:HB2 | 1:A:59:PHE:CZ | 2.53 | 0.43 |
| 1:A:446:PHE:CZ | 1:A:530:LEU:HD13 | 2.53 | 0.43 |
| 1:A:1481:THR:O | 1:A:1484:LEU:HG | 2.17 | 0.43 |
| 1:A:1580:LEU:O | 1:A:1584:GLN:HG2 | 2.18 | 0.43 |
| 1:A:1751:GLU:CD | 1:A:1784:ARG:HB2 | 2.43 | 0.43 |
| 1:A:2155:GLU:H | 1:A:2155:GLU:CD | 2.22 | 0.43 |
| 1:A:2331:MET:SD | 1:A:2335:ASN:HB3 | 2.58 | 0.43 |
| 1:A:3179:TRP:CE3 | 1:A:3242:MET:HE1 | 2.47 | 0.43 |
| 1:A:3928:PHE:CE2 | 1:A:3962:ARG:HG3 | 2.53 | 0.43 |
| 1:A:4127:TRP:HD1 | 1:A:4128:MET:HG2 | 1.82 | 0.43 |
| 3:C:246:HIS:HB3 | 3:C:264:TYR:CE2 | 2.52 | 0.43 |
| 3:C:610:GLU:CD | 3:C:610:GLU:H | 2.26 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:154:ASP:CG | 6:I:840:ILE:HG13 | 2.43 | 0.43 |
| 5:H:41:SER:HB3 | 5:H:119:PRO:HB3 | 2.00 | 0.43 |
| 6:I:655:ILE:HD12 | 6:I:684:GLU:HB3 | 1.99 | 0.43 |
| 6:I:666:VAL:HB | 6:I:679:GLU:OE2 | 2.18 | 0.43 |
| 3:L:322:PRO:HB2 | 6:R:692:ASN:HD21 | 1.83 | 0.43 |
| 3:L:426:PHE:CE2 | 2:T:480:ASN:HB2 | 2.53 | 0.43 |
| 5:Q:178:LYS:O | 5:Q:181:ILE:HG22 | 2.17 | 0.43 |
| 1:S:408:TYR:HA | 1:S:410:MET:HE1 | 2.00 | 0.43 |
| 1:S:441:MET:O | 1:S:444:ASP:HB3 | 2.18 | 0.43 |
| 1:S:771:ASN:O | 1:S:774:GLU:HG2 | 2.18 | 0.43 |
| 1:S:880:MET:SD | 1:S:882:SER:N | 2.89 | 0.43 |
| 1:S:1140:LYS:HE3 | 1:S:1141:LYS:HZ2 | 1.83 | 0.43 |
| 1:S:1253:THR:O | 1:S:1257:LEU:HG | 2.18 | 0.43 |
| 1:S:1769:GLU:OE1 | 1:S:1772:HIS:HB3 | 2.18 | 0.43 |
| 1:S:1852:LYS:HD3 | 1:S:1852:LYS:HA | 1.74 | 0.43 |
| 1:S:2138:VAL:O | 1:S:2143:ARG:HD2 | 2.17 | 0.43 |
| 1:S:2260:PHE:O | 1:S:2306:ASN:ND2 | 2.51 | 0.43 |
| 1:S:2395:THR:HG23 | 1:S:2434:VAL:HG21 | 2.00 | 0.43 |
| 1:S:2404:ARG:HE | 1:S:2406:GLU:HG3 | 1.83 | 0.43 |
| 1:S:3164:TRP:HE3 | 1:S:3167:ARG:NH1 | 2.16 | 0.43 |
| 1:S:3454:LEU:HD11 | 1:S:3462:ARG:HA | 2.00 | 0.43 |
| 2:T:418:GLU:HA | 2:T:428:THR:O | 2.17 | 0.43 |
| 1:A:60:SER:HA | 1:A:63:PHE:HB2 | 1.99 | 0.43 |
| 1:A:103:TYR:O | 1:A:107:ILE:HG12 | 2.18 | 0.43 |
| 1:A:461:ILE:O | 1:A:465:PHE:CD2 | 2.72 | 0.43 |
| 1:A:966:PHE:HA | 1:A:969:LEU:HD12 | 1.99 | 0.43 |
| 1:A:1195:VAL:HA | 1:A:1198:LEU:HG | 1.99 | 0.43 |
| 1:A:1342:MET:HE1 | 1:A:1398:VAL:HG22 | 1.99 | 0.43 |
| 1:A:2121:ASP:HA | 1:A:2126:MET:HB3 | 2.01 | 0.43 |
| 1:A:2331:MET:O | 1:A:2334:LYS:HG2 | 2.19 | 0.43 |
| 1:A:2376:ASP:HA | 1:A:2379:MET:SD | 2.58 | 0.43 |
| 1:A:2399:GLU:O | 1:A:2402:LEU:HB2 | 2.18 | 0.43 |
| 1:A:3580:ASN:OD1 | 1:A:3674:SER:HB2 | 2.18 | 0.43 |
| 1:A:3718:ARG:H | 1:A:3743:HIS:CB | 2.32 | 0.43 |
| 2:B:317:LYS:O | 3:C:279:VAL:N | 2.50 | 0.43 |
| 2:B:465:ILE:HG12 | 2:B:518:LEU:HD22 | 1.99 | 0.43 |
| 3:C:163:PHE:CE2 | 3:C:212:MET:HE3 | 2.53 | 0.43 |
| 3:L:362:LEU:HD23 | 3:L:362:LEU:HA | 1.93 | 0.43 |
| 4:M:120:ARG:NH1 | 4:M:124:LEU:HD13 | 2.33 | 0.43 |
| 5:Q:166:VAL:HA | 5:Q:169:LYS:HG2 | 2.00 | 0.43 |
| 1:S:38:LEU:HB3 | 1:S:84:GLU:OE1 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1476:HIS:HB2 | 1:S:1521:PHE:CE2 | 2.53 | 0.43 |
| 1:S:1484:LEU:HA | 1:S:1487:VAL:HG12 | 2.00 | 0.43 |
| 1:S:1847:ALA:HA | 1:S:1850:VAL:HG12 | 2.00 | 0.43 |
| 1:S:2105:HIS:HB3 | 1:S:2106:ARG:NH1 | 2.33 | 0.43 |
| 1:S:2799:GLN:HE22 | 1:S:2800:ARG:NE | 2.17 | 0.43 |
| 8:e:36:DA:H2' | 8:e:37:DT:O4' | 2.18 | 0.43 |
| 1:A:614:PRO:HB2 | 1:A:617:PRO:HG3 | 2.00 | 0.43 |
| 1:A:649:PHE:CE2 | 1:A:653:LEU:HD11 | 2.53 | 0.43 |
| 1:A:802:THR:OG1 | 1:A:852:ARG:NH2 | 2.51 | 0.43 |
| 1:A:1219:PHE:HA | 1:A:1222:ASN:HB3 | 2.00 | 0.43 |
| 1:A:1685:ASP:OD1 | 1:A:1686:LEU:N | 2.51 | 0.43 |
| 1:A:2103:HIS:HD1 | 1:A:2106:ARG:NH2 | 2.16 | 0.43 |
| 1:A:2978:LYS:O | 1:A:2981:TRP:NE1 | 2.51 | 0.43 |
| 1:A:3011:LEU:HD13 | 1:A:3046:ARG:HB3 | 1.99 | 0.43 |
| 1:A:3278:GLN:HG2 | 1:A:3329:LEU:HD21 | 2.01 | 0.43 |
| 2:B:85:VAL:HB | 2:B:105:LEU:HD23 | 2.00 | 0.43 |
| 2:B:262:LYS:HA | 2:B:268:VAL:HG22 | 2.00 | 0.43 |
| 2:B:420:LEU:HA | 2:B:425:ILE:O | 2.18 | 0.43 |
| 2:B:510:LYS:H | 2:B:510:LYS:HD2 | 1.83 | 0.43 |
| 3:C:42:VAL:HG11 | 3:C:94:ILE:HD12 | 2.01 | 0.43 |
| 3:C:528:ILE:HG22 | 3:C:532:LYS:HZ1 | 1.82 | 0.43 |
| 3:L:322:PRO:HB3 | 2:T:288:LEU:HD11 | 1.99 | 0.43 |
| 3:L:604:GLN:HG3 | 3:L:605:LYS:HG3 | 2.00 | 0.43 |
| 1:S:247:GLU:HG2 | 1:S:251:PHE:CE1 | 2.53 | 0.43 |
| 1:S:477:ASN:OD1 | 1:S:478:CYS:N | 2.51 | 0.43 |
| 1:S:1392:MET:SD | 1:S:1393:ALA:N | 2.92 | 0.43 |
| 1:S:1414:ILE:O | 1:S:1417:THR:HB | 2.18 | 0.43 |
| 1:S:2548:PRO:HB2 | 1:S:2848:PHE:CE1 | 2.54 | 0.43 |
| 1:S:3113:ASN:HB3 | 1:S:3128:LYS:NZ | 2.34 | 0.43 |
| 1:S:3472:ILE:HG12 | 1:S:3479:THR:HB | 2.01 | 0.43 |
| 1:S:3582:GLU:HB3 | 1:S:3586:LYS:HE2 | 2.00 | 0.43 |
| 1:S:3822:GLN:HA | 1:S:3825:LYS:HG2 | 2.00 | 0.43 |
| 1:S:3884:LYS:NZ | 1:S:3969:ASN:O | 2.51 | 0.43 |
| 2:T:62:MET:HE1 | 2:T:203:MET:HE1 | 2.00 | 0.43 |
| 2:T:112:GLY:O | 2:T:116:ILE:HG12 | 2.19 | 0.43 |
| 1:A:183:GLU:HG2 | 1:A:184:VAL:N | 2.32 | 0.43 |
| 1:A:412:SER:HA | 1:A:415:GLN:NE2 | 2.34 | 0.43 |
| 1:A:992:ILE:HG22 | 1:A:993:HIS:HD2 | 1.83 | 0.43 |
| 1:A:1333:SER:O | 1:A:1337:VAL:HG23 | 2.17 | 0.43 |
| 1:A:2154:GLU:OE1 | 1:A:2154:GLU:N | 2.51 | 0.43 |
| 1:A:2335:ASN:O | 1:A:2336:ILE:HD13 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:207:LYS:NZ | 2:B:210:GLY:O | 2.52 | 0.43 |
| 2:B:263:LEU:HD11 | 2:B:269:ILE:HD12 | 2.01 | 0.43 |
| 2:B:320:GLN:HB3 | 3:C:274:LYS:HZ3 | 1.82 | 0.43 |
| 3:C:271:ARG:NH2 | 7:d:29:DG:OP2 | 2.51 | 0.43 |
| 3:C:377:LEU:O | 3:C:381:ILE:HG12 | 2.19 | 0.43 |
| 3:C:486:ARG:O | 3:C:490:LEU:HG | 2.19 | 0.43 |
| 4:D:90:GLN:O | 4:D:92:ASP:N | 2.50 | 0.43 |
| 3:L:154:LEU:HD13 | 3:L:161:LEU:HD13 | 2.00 | 0.43 |
| 3:L:531:SER:HA | 3:L:534:LYS:HG2 | 2.00 | 0.43 |
| 6:R:798:ASP:O | 6:R:802:ARG:HG2 | 2.18 | 0.43 |
| 1:S:884:VAL:HG21 | 1:S:3933:GLU:HA | 2.01 | 0.43 |
| 1:S:897:PRO:HG3 | 1:S:2787:HIS:HB3 | 1.99 | 0.43 |
| 1:S:1066:LEU:CD1 | 1:S:1078:ALA:HB2 | 2.48 | 0.43 |
| 1:S:1369:MET:HE2 | 1:S:1418:HIS:CE1 | 2.53 | 0.43 |
| 1:S:1867:ILE:HG22 | 1:S:1871:MET:HE1 | 2.00 | 0.43 |
| 1:S:2147:ALA:HA | 1:S:2150:VAL:HG12 | 2.01 | 0.43 |
| 1:S:2191:ALA:HB3 | 1:S:2725:LEU:HD13 | 2.01 | 0.43 |
| 1:S:2358:ASP:OD1 | 1:S:2359:LYS:N | 2.47 | 0.43 |
| 1:S:2782:ASP:OD1 | 1:S:2782:ASP:N | 2.45 | 0.43 |
| 1:S:2821:ASP:HA | 1:S:2829:LYS:HD3 | 1.99 | 0.43 |
| 1:S:3104:GLN:HA | 1:S:3107:ILE:HD12 | 1.99 | 0.43 |
| 1:S:3370:SER:O | 1:S:3374:ILE:HG23 | 2.19 | 0.43 |
| 1:S:3487:ILE:HG13 | 1:S:3516:HIS:HB2 | 2.00 | 0.43 |
| 1:S:3586:LYS:HZ1 | 1:S:3668:LEU:HB3 | 1.82 | 0.43 |
| 2:T:513:ALA:HB1 | 2:T:517:ARG:NH1 | 2.32 | 0.43 |
| 9:i:32:DA:C2 | 9:i:33:DA:C5 | 3.06 | 0.43 |
| 1:A:676:ASN:O | 1:A:679:LYS:HB3 | 2.17 | 0.43 |
| 1:A:700:LYS:HB3 | 1:A:704:PHE:CZ | 2.53 | 0.43 |
| 1:A:771:ASN:O | 1:A:775:GLU:OE1 | 2.36 | 0.43 |
| 1:A:1201:ASN:CB | 1:A:1207:TRP:HB2 | 2.46 | 0.43 |
| 1:A:1386:ILE:HD12 | 1:A:1386:ILE:HA | 1.92 | 0.43 |
| 1:A:2291:GLN:HG2 | 1:A:2292:CYS:N | 2.33 | 0.43 |
| 1:A:3048:LYS:O | 1:A:3052:LEU:HD23 | 2.18 | 0.43 |
| 1:A:3270:ASP:OD1 | 1:A:3271:ASP:N | 2.51 | 0.43 |
| 1:A:3589:SER:HA | 1:A:3592:VAL:HG12 | 2.01 | 0.43 |
| 1:A:4124:TRP:O | 1:A:4125:GLU:HG2 | 2.18 | 0.43 |
| 2:B:168:LEU:HD21 | 2:B:202:LEU:HB2 | 2.01 | 0.43 |
| 3:C:479:THR:HG23 | 3:C:480:THR:HG23 | 2.00 | 0.43 |
| 5:G:176:LEU:HA | 5:G:179:ARG:HG2 | 2.00 | 0.43 |
| 6:I:663:GLU:HB3 | 6:I:697:THR:HA | 2.01 | 0.43 |
| 3:L:458:ILE:HG23 | 2:T:350:PHE:CG | 2.53 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Q:6:SER:O | 5:Q:6:SER:OG | 2.36 | 0.43 |
| 5:Q:122:VAL:O | 5:Q:126:LEU:HG | 2.18 | 0.43 |
| 5:Q:143:HIS:ND1 | 5:Q:146:LYS:HE3 | 2.34 | 0.43 |
| 1:S:885:ALA:HB2 | 1:S:3890:MET:O | 2.19 | 0.43 |
| 1:S:910:PHE:O | 1:S:914:VAL:HG12 | 2.18 | 0.43 |
| 1:S:1046:PRO:O | 1:S:1050:GLU:HG2 | 2.18 | 0.43 |
| 1:S:1086:TYR:CE1 | 1:S:1133:HIS:HB3 | 2.54 | 0.43 |
| 1:S:1184:ARG:HH22 | 1:S:1265:GLU:CD | 2.25 | 0.43 |
| 1:S:1479:VAL:HG21 | 1:S:1518:ALA:HA | 2.00 | 0.43 |
| 1:S:1869:LYS:HB3 | 1:S:1873:TYR:CZ | 2.53 | 0.43 |
| 1:S:3087:SER:OG | 1:S:3099:ALA:O | 2.24 | 0.43 |
| 1:S:3796:MET:HB2 | 1:S:3800:LEU:O | 2.18 | 0.43 |
| 2:T:43:ASP:O | 2:T:48:MET:HG3 | 2.18 | 0.43 |
| 2:T:339:ARG:HB2 | 2:T:405:ASN:HA | 1.99 | 0.43 |
| 10:j:16:DA:H1' | 10:j:17:DT:C2 | 2.54 | 0.43 |
| 1:A:718:MET:SD | 1:A:754:MET:HE2 | 2.59 | 0.43 |
| 1:A:938:VAL:HA | 1:A:941:MET:CG | 2.48 | 0.43 |
| 1:A:1086:TYR:CZ | 1:A:1133:HIS:HB3 | 2.54 | 0.43 |
| 1:A:1188:ILE:HG13 | 1:A:1189:GLU:N | 2.32 | 0.43 |
| 1:A:2205:VAL:HG22 | 1:A:2207:LYS:H | 1.83 | 0.43 |
| 1:A:2547:SER:O | 1:A:2550:ILE:HG12 | 2.18 | 0.43 |
| 1:A:2776:ARG:HH21 | 1:A:2782:ASP:CB | 2.31 | 0.43 |
| 1:A:2788:SER:HA | 1:A:2791:ILE:HG12 | 2.01 | 0.43 |
| 1:A:3414:MET:HE1 | 1:A:3460:GLU:C | 2.44 | 0.43 |
| 1:A:3795:PRO:HA | 1:A:3801:GLY:HA2 | 2.00 | 0.43 |
| 1:A:3818:ASN:O | 1:A:3822:GLN:NE2 | 2.48 | 0.43 |
| 2:B:240:GLU:HG2 | 2:B:241:ASP:N | 2.33 | 0.43 |
| 2:B:290:ARG:HA | 6:I:692:ASN:HB2 | 2.00 | 0.43 |
| 3:C:410:PRO:HA | 3:C:419:LEU:HA | 2.00 | 0.43 |
| 5:G:194:LEU:HB3 | 5:H:194:LEU:HD13 | 2.01 | 0.43 |
| 5:Q:158:VAL:HA | 5:Q:161:ARG:CD | 2.48 | 0.43 |
| 1:S:76:ILE:O | 1:S:80:GLU:HG2 | 2.18 | 0.43 |
| 1:S:176:GLU:CD | 1:S:223:CYS:HA | 2.44 | 0.43 |
| 1:S:297:LEU:HD22 | 1:S:316:LEU:HB2 | 2.00 | 0.43 |
| 1:S:655:LEU:O | 1:S:658:THR:OG1 | 2.28 | 0.43 |
| 1:S:683:PHE:CE1 | 1:S:737:PRO:HG3 | 2.54 | 0.43 |
| 1:S:923:ASP:OD2 | 1:S:926:THR:OG1 | 2.26 | 0.43 |
| 1:S:1672:PHE:CZ | 1:S:1676:ILE:HD11 | 2.54 | 0.43 |
| 1:S:2376:ASP:OD1 | 1:S:2376:ASP:N | 2.51 | 0.43 |
| 1:S:2525:TRP:O | 1:S:2531:LEU:HB2 | 2.19 | 0.43 |
| 1:S:3572:ILE:HG23 | 1:S:3800:LEU:CD2 | 2.48 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:191:GLY:O | 2:T:194:ARG:HG2 | 2.18 | 0.43 |
| 10:j:33:DA:H2" | 10:j:34:DT:C5 | 2.54 | 0.43 |
| 1:A:103:TYR:HA | 1:A:106:GLU:CD | 2.44 | 0.43 |
| 1:A:131:LEU:HD22 | 1:A:177:LEU:HD11 | 2.00 | 0.43 |
| 1:A:363:ILE:O | 1:A:366:TYR:HB2 | 2.19 | 0.43 |
| 1:A:429:GLU:N | 1:A:1640:GLU:OE2 | 2.52 | 0.43 |
| 1:A:571:SER:HA | 1:A:574:LYS:HE2 | 2.00 | 0.43 |
| 1:A:618:LYS:CD | 1:A:2034:SER:HB2 | 2.49 | 0.43 |
| 1:A:638:GLN:OE1 | 1:A:679:LYS:HE3 | 2.19 | 0.43 |
| 1:A:1353:PRO:HD2 | 1:A:1356:TRP:CZ3 | 2.53 | 0.43 |
| 1:A:1392:MET:HA | 1:A:1395:LEU:HG | 2.00 | 0.43 |
| 1:A:1797:LEU:O | 1:A:1801:VAL:HG22 | 2.19 | 0.43 |
| 1:A:1923:PHE:CD1 | 1:A:1941:HIS:HB3 | 2.46 | 0.43 |
| 1:A:2142:ILE:O | 1:A:2146:LEU:HG | 2.19 | 0.43 |
| 1:A:3274:VAL:HG11 | 1:A:3311:ASN:CB | 2.47 | 0.43 |
| 1:A:3779:SER:O | 1:A:3783:GLN:HG3 | 2.18 | 0.43 |
| 2:B:171:ASN:ND2 | 2:B:207:LYS:HB2 | 2.32 | 0.43 |
| 2:B:239:LEU:O | 2:B:243:LEU:N | 2.44 | 0.43 |
| 3:C:68:LEU:HD21 | 3:C:116:ASP:OD2 | 2.18 | 0.43 |
| 4:D:38:ASN:HB2 | 4:D:40:TYR:CZ | 2.54 | 0.43 |
| 5:H:8:ILE:HB | 5:H:86:PHE:CD2 | 2.53 | 0.43 |
| 3:L:75:GLN:O | 3:L:77:ILE:HG13 | 2.19 | 0.43 |
| 3:L:331:MET:HE1 | 2:T:485:GLN:NE2 | 2.34 | 0.43 |
| 3:L:340:PHE:CE2 | 3:L:393:VAL:HG11 | 2.54 | 0.43 |
| 3:L:500:HIS:HA | 3:L:502:ARG:NH1 | 2.33 | 0.43 |
| 6:R:826:ILE:HG22 | 6:R:827:ASN:H | 1.84 | 0.43 |
| 1:S:196:LEU:HB3 | 1:S:200:PHE:CE2 | 2.53 | 0.43 |
| 1:S:465:PHE:CE1 | 1:S:479:ILE:HG21 | 2.52 | 0.43 |
| 1:S:636:GLU:OE2 | 1:S:637:LYS:HG2 | 2.18 | 0.43 |
| 1:S:835:LYS:O | 1:S:839:ASN:N | 2.49 | 0.43 |
| 1:S:2439:ILE:O | 1:S:2442:MET:HB3 | 2.18 | 0.43 |
| 1:S:2796:ALA:HA | 1:S:2799:GLN:HE21 | 1.83 | 0.43 |
| 1:S:3841:ASP:HB2 | 1:S:3873:LYS:HE3 | 2.01 | 0.43 |
| 1:S:3966:GLN:HA | 1:S:3969:ASN:HB2 | 1.99 | 0.43 |
| 1:S:3998:LEU:O | 1:S:4002:MET:HG3 | 2.19 | 0.43 |
| 2:T:259:LEU:HB2 | 2:T:273:ILE:HD11 | 2.01 | 0.43 |
| 1:A:92:PHE:O | 1:A:96:MET:HE2 | 2.19 | 0.43 |
| 1:A:160:LEU:HD21 | 1:A:174:VAL:HG11 | 2.01 | 0.43 |
| 1:A:1525:CYS:O | 1:A:1528:LEU:HG | 2.19 | 0.43 |
| 1:A:2349:LEU:HA | 1:A:2353:GLN:OE1 | 2.19 | 0.43 |
| 1:A:3578:LEU:HB2 | 1:A:3736:LYS:HE2 | 2.01 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3702:PRO:O | 1:A:3792:SER:OG | 2.35 | 0.43 |
| 1:A:3758:LEU:HD13 | 1:A:3795:PRO:HB3 | 2.01 | 0.43 |
| 2:B:67:ILE:HD11 | 2:B:169:PHE:CE2 | 2.54 | 0.43 |
| 2:B:352:PRO:HD2 | 2:B:355:LEU:HD12 | 2.00 | 0.43 |
| 2:B:537:GLU:HB2 | 3:C:250:ARG:HH12 | 1.83 | 0.43 |
| 5:G:7:ARG:HD2 | 5:G:19:PHE:HE1 | 1.83 | 0.43 |
| 4:M:96:LEU:HD23 | 4:M:109:LEU:HD21 | 2.00 | 0.43 |
| 5:P:190:LYS:NZ | 5:Q:191:ILE:HG23 | 2.33 | 0.43 |
| 1:S:188:GLU:HG3 | 1:S:189:MET:H | 1.83 | 0.43 |
| 1:S:789:TYR:CD1 | 1:S:792:ILE:HD12 | 2.53 | 0.43 |
| 1:S:1710:LEU:O | 1:S:1713:VAL:HG22 | 2.19 | 0.43 |
| 1:S:2891:ARG:HH21 | 1:S:3898:LEU:CB | 2.31 | 0.43 |
| 1:S:2920:VAL:HA | 1:S:2923:TRP:HB2 | 2.01 | 0.43 |
| 1:S:2940:ARG:HH21 | 1:S:3982:SER:HB3 | 1.84 | 0.43 |
| 1:S:3074:GLN:HA | 1:S:3077:ILE:HG12 | 2.01 | 0.43 |
| 1:S:3176:MET:HE1 | 1:S:3245:SER:OG | 2.19 | 0.43 |
| 1:S:3192:LYS:O | 1:S:3196:LYS:HG2 | 2.19 | 0.43 |
| 1:S:3723:ASP:HB2 | 1:S:3741:ARG:HB2 | 2.01 | 0.43 |
| 2:T:65:GLN:CG | 2:T:243:LEU:HD11 | 2.49 | 0.43 |
| 7:d:20:DT:H2" | 7:d:21:DA:C6 | 2.54 | 0.43 |
| 1:A:203:GLU:O | 1:A:207:GLN:HG2 | 2.19 | 0.43 |
| 1:A:417:VAL:O | 1:A:421:LEU:HD23 | 2.19 | 0.43 |
| 1:A:436:GLU:O | 1:A:439:VAL:HG22 | 2.19 | 0.43 |
| 1:A:955:ALA:O | 1:A:957:PRO:HD3 | 2.19 | 0.43 |
| 1:A:988:VAL:O | 1:A:991:LEU:HG | 2.19 | 0.43 |
| 1:A:989:MET:HE2 | 1:A:993:HIS:HE1 | 1.81 | 0.43 |
| 1:A:1034:ARG:HH12 | 1:A:1087:ARG:HD2 | 1.84 | 0.43 |
| 1:A:1304:HIS:O | 1:A:1330:TYR:OH | 2.21 | 0.43 |
| 1:A:1373:VAL:HG21 | 1:A:1422:LYS:HE2 | 2.00 | 0.43 |
| 1:A:1632:TRP:CG | 1:A:1645:VAL:HG11 | 2.53 | 0.43 |
| 1:A:2305:ASN:HB3 | 1:A:2309:PHE:CZ | 2.53 | 0.43 |
| 1:A:4049:ARG:NH2 | 1:A:4062:ASP:HB2 | 2.34 | 0.43 |
| 2:B:219:ASP:OD1 | 2:B:219:ASP:N | 2.46 | 0.43 |
| 2:B:388:LYS:HA | 2:B:391:GLU:OE1 | 2.19 | 0.43 |
| 3:C:12:LEU:HB3 | 3:C:56:LEU:HD13 | 2.00 | 0.43 |
| 5:H:99:LYS:HD3 | 5:H:99:LYS:HA | 1.85 | 0.43 |
| 3:L:412:ILE:HG23 | 3:L:417:GLU:HG2 | 2.01 | 0.43 |
| 3:L:664:GLU:O | 3:L:668:ILE:HG23 | 2.19 | 0.43 |
| 3:L:667:GLU:OE2 | 3:L:702:LYS:HD3 | 2.19 | 0.43 |
| 1:S:74:ASN:OD1 | 1:S:118:ASP:HB3 | 2.19 | 0.43 |
| 1:S:284:THR:HA | 1:S:287:LEU:HD23 | 2.01 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:289:ASN:HB3 | 1:S:292:SER:OG | 2.19 | 0.43 |
| 1:S:360:SER:C | 1:S:364:ARG:HE | 2.25 | 0.43 |
| 1:S:442:GLN:NE2 | 1:S:461:ILE:HD11 | 2.34 | 0.43 |
| 1:S:632:GLU:C | 1:S:635:PRO:HD2 | 2.44 | 0.43 |
| 1:S:746:ARG:NH2 | 1:S:788:TYR:HB3 | 2.34 | 0.43 |
| 1:S:998:ASN:HA | 1:S:1001:PHE:CD1 | 2.53 | 0.43 |
| 1:S:1558:TYR:CE2 | 1:S:1562:LEU:HD11 | 2.54 | 0.43 |
| 1:S:1786:ALA:HB2 | 1:S:1827:LEU:HD13 | 2.01 | 0.43 |
| 1:S:2094:MET:O | 1:S:2097:LEU:HB2 | 2.18 | 0.43 |
| 1:S:2422:GLN:O | 1:S:2426:HIS:N | 2.51 | 0.43 |
| 1:S:2840:PHE:O | 1:S:2844:LEU:HG | 2.18 | 0.43 |
| 1:S:3145:ILE:O | 1:S:3150:ASN:HB3 | 2.19 | 0.43 |
| 1:S:3913:ILE:HD13 | 1:S:3987:ALA:HB3 | 2.01 | 0.43 |
| 1:S:3924:HIS:N | 1:S:3927:ASN:OD1 | 2.48 | 0.43 |
| 1:A:389:ILE:HG22 | 1:A:393:LYS:NZ | 2.34 | 0.43 |
| 1:A:933:LEU:HD13 | 1:A:2793:PRO:HG2 | 2.00 | 0.43 |
| 1:A:991:LEU:O | 1:A:995:PHE:N | 2.26 | 0.43 |
| 1:A:1346:THR:O | 1:A:1350:ASN:ND2 | 2.52 | 0.43 |
| 1:A:2254:ARG:HD3 | 1:A:2294:ILE:CG1 | 2.46 | 0.43 |
| 1:A:3008:TRP:H | 1:A:3008:TRP:HE3 | 1.63 | 0.43 |
| 1:A:3132:VAL:HA | 1:A:3135:LEU:HD12 | 2.00 | 0.43 |
| 1:A:3235:LYS:HB3 | 1:A:3239:LYS:NZ | 2.33 | 0.43 |
| 1:A:3586:LYS:HE2 | 1:A:3668:LEU:HD13 | 2.01 | 0.43 |
| 1:A:3629:ARG:NH1 | 1:A:3633:ILE:HD13 | 2.34 | 0.43 |
| 1:A:4008:GLU:HG3 | 1:A:4011:PHE:CB | 2.48 | 0.43 |
| 2:B:35:ARG:HD2 | 2:B:161:MET:HE1 | 2.00 | 0.43 |
| 2:B:159:PHE:HB2 | 2:B:161:MET:HE3 | 2.01 | 0.43 |
| 2:B:320:GLN:HG2 | 3:C:274:LYS:HE2 | 2.01 | 0.43 |
| 2:B:325:ARG:NH2 | 3:C:497:ARG:O | 2.51 | 0.43 |
| 2:B:370:PRO:HB3 | 2:B:382:PHE:CG | 2.54 | 0.43 |
| 3:C:168:SER:HB3 | 3:C:229:GLU:OE2 | 2.19 | 0.43 |
| 3:C:450:GLN:HG2 | 3:C:536:LEU:HB3 | 2.00 | 0.43 |
| 6:I:872:VAL:O | 6:I:876:LYS:HG2 | 2.18 | 0.43 |
| 3:L:278:VAL:HG22 | 2:T:318:ARG:HH21 | 1.83 | 0.43 |
| 3:L:343:LEU:HD21 | 3:L:394:ARG:HB2 | 2.01 | 0.43 |
| 1:S:1092:GLU:OE2 | 1:S:1094:SER:N | 2.43 | 0.43 |
| 1:S:1190:LEU:HA | 1:S:1193:LYS:HG2 | 2.01 | 0.43 |
| 1:S:1254:LEU:HD11 | 1:S:1329:ARG:NH2 | 2.34 | 0.43 |
| 1:S:1474:ASP:N | 1:S:1474:ASP:OD1 | 2.52 | 0.43 |
| 1:S:1506:SER:O | 1:S:1509:GLN:NE2 | 2.52 | 0.43 |
| 1:S:2291:GLN:OE1 | 1:S:2291:GLN:N | 2.52 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3472:ILE:HA | 1:S:3479:THR:HG21 | 2.00 | 0.43 |
| 1:S:3487:ILE:HD11 | 1:S:3517:SER:OG | 2.19 | 0.43 |
| 1:S:3531:TYR:HB2 | 1:S:3532:PRO:HD3 | 2.00 | 0.43 |
| 1:S:3533:PHE:CE2 | 1:S:3559:LYS:HB3 | 2.54 | 0.43 |
| 1:S:3717:VAL:HG21 | 1:S:3746:ARG:HE | 1.84 | 0.43 |
| 1:S:3766:GLN:O | 1:S:3770:VAL:HG13 | 2.19 | 0.43 |
| 1:S:4091:ALA:HA | 1:S:4094:PRO:HD2 | 2.00 | 0.43 |
| 2:T:126:GLN:HA | 2:T:129:LYS:HE2 | 2.01 | 0.43 |
| 7:d:20:DT:C2 | 7:d:21:DA:C2 | 3.07 | 0.43 |
| 8:e:34:DC:C5 | 8:e:35:DT:H72 | 2.53 | 0.43 |
| 1:A:457:CYS:O | 1:A:461:ILE:HG12 | 2.19 | 0.42 |
| 1:A:477:ASN:OD1 | 1:A:478:CYS:N | 2.52 | 0.42 |
| 1:A:849:GLU:OE1 | 1:A:849:GLU:N | 2.34 | 0.42 |
| 1:A:1060:PHE:HB3 | 1:A:1064:TYR:CZ | 2.54 | 0.42 |
| 1:A:1147:LYS:HE3 | 1:A:1147:LYS:HB3 | 1.89 | 0.42 |
| 1:A:1758:LEU:O | 1:A:1762:MET:HG3 | 2.19 | 0.42 |
| 1:A:2252:PRO:C | 1:A:2254:ARG:H | 2.27 | 0.42 |
| 1:A:2318:ALA:O | 1:A:2321:GLU:HG2 | 2.19 | 0.42 |
| 1:A:2747:GLY:O | 1:A:2751:GLN:HG2 | 2.19 | 0.42 |
| 1:A:2785:ILE:HG22 | 1:A:2786:LYS:H | 1.84 | 0.42 |
| 1:A:3364:GLY:HA2 | 1:A:3376:GLY:HA3 | 2.01 | 0.42 |
| 1:A:3380:ARG:HD3 | 1:A:3384:HIS:CE1 | 2.54 | 0.42 |
| 1:A:3423:GLN:O | 1:A:3426:LYS:HG3 | 2.19 | 0.42 |
| 1:A:4107:LEU:HD12 | 1:A:4111:ALA:HB3 | 2.00 | 0.42 |
| 2:B:282:LYS:NZ | 2:B:483:LEU:HA | 2.32 | 0.42 |
| 2:B:291:GLU:OE1 | 6:I:688:TYR:OH | 2.23 | 0.42 |
| 3:C:16:VAL:HB | 3:C:58:LEU:HD22 | 2.01 | 0.42 |
| 3:C:484:ASN:HB3 | 3:C:487:PHE:CE2 | 2.54 | 0.42 |
| 5:H:24:TRP:HA | 5:H:33:VAL:HB | 2.01 | 0.42 |
| 3:L:613:SER:O | 3:L:616:LEU:HG | 2.18 | 0.42 |
| 3:L:689:GLU:HA | 3:L:695:SER:CB | 2.45 | 0.42 |
| 5:P:169:LYS:NZ | 5:Q:173:GLU:HG2 | 2.34 | 0.42 |
| 1:S:782:ARG:HG2 | 1:S:789:TYR:OH | 2.18 | 0.42 |
| 1:S:1748:ASP:OD1 | 1:S:1749:ALA:N | 2.52 | 0.42 |
| 1:S:1916:ILE:H | 1:S:1916:ILE:HG13 | 1.64 | 0.42 |
| 1:S:2158:ARG:C | 1:S:2160:TYR:H | 2.27 | 0.42 |
| 1:S:2205:VAL:O | 1:S:2207:LYS:N | 2.52 | 0.42 |
| 1:S:2436:LEU:HD11 | 1:S:2473:MET:HB3 | 2.00 | 0.42 |
| 1:S:2986:PRO:HG2 | 1:S:2991:LYS:HZ2 | 1.84 | 0.42 |
| 1:S:3121:LEU:O | 1:S:3125:ARG:HG2 | 2.19 | 0.42 |
| 2:T:346:MET:O | 2:T:399:ARG:N | 2.46 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:104:SER:O | 1:A:108:LYS:CB | 2.67 | 0.42 |
| 1:A:112:THR:O | 1:A:116:THR:OG1 | 2.24 | 0.42 |
| 1:A:243:GLN:O | 1:A:247:GLU:HG3 | 2.19 | 0.42 |
| 1:A:895:ALA:HB2 | 1:A:904:VAL:HG22 | 2.01 | 0.42 |
| 1:A:1013:ILE:HD12 | 1:A:1062:ARG:HH21 | 1.83 | 0.42 |
| 1:A:1115:HIS:HE1 | 1:A:1181:THR:N | 2.18 | 0.42 |
| 1:A:1194:PHE:HA | 1:A:1197:LEU:HD23 | 2.01 | 0.42 |
| 1:A:1428:ILE:HD11 | 1:A:1448:LEU:HD23 | 2.02 | 0.42 |
| 1:A:1776:GLU:H | 1:A:1776:GLU:CD | 2.25 | 0.42 |
| 1:A:2270:ASN:OD1 | 1:A:2270:ASN:N | 2.52 | 0.42 |
| 1:A:2369:LYS:HB2 | 1:A:2369:LYS:HE2 | 1.86 | 0.42 |
| 1:A:2962:ARG:NH2 | 1:A:4101:GLU:OE1 | 2.52 | 0.42 |
| 1:A:3493:TRP:HZ3 | 1:A:3521:ILE:HA | 1.83 | 0.42 |
| 1:A:3518:VAL:HA | 1:A:3521:ILE:HB | 2.00 | 0.42 |
| 1:A:3786:LEU:HB3 | 1:A:3910:LEU:CD1 | 2.49 | 0.42 |
| 1:A:3928:PHE:HE2 | 1:A:3962:ARG:HG3 | 1.84 | 0.42 |
| 1:A:3970:LEU:HD23 | 1:A:3971:MET:H | 1.83 | 0.42 |
| 1:A:4089:ILE:O | 1:A:4091:ALA:N | 2.52 | 0.42 |
| 2:B:108:LEU:HG | 2:B:153:LEU:HD21 | 1.99 | 0.42 |
| 2:B:415:PRO:HB3 | 2:B:432:PHE:CZ | 2.54 | 0.42 |
| 3:C:285:LYS:HB3 | 3:C:287:GLU:OE1 | 2.18 | 0.42 |
| 3:C:413:LYS:HD2 | 3:C:416:TYR:CE1 | 2.54 | 0.42 |
| 3:C:502:ARG:H | 3:C:502:ARG:HD3 | 1.83 | 0.42 |
| 3:C:649:PHE:HB2 | 3:C:651:GLU:HG2 | 2.00 | 0.42 |
| 5:G:89:SER:HB3 | 5:G:91:GLU:OE1 | 2.19 | 0.42 |
| 5:H:12:SER:HB3 | 5:H:89:SER:HA | 2.00 | 0.42 |
| 1:S:76:ILE:HA | 1:S:79:ARG:HB3 | 2.01 | 0.42 |
| 1:S:144:MET:HG3 | 1:S:146:GLU:OE1 | 2.19 | 0.42 |
| 1:S:420:VAL:HG23 | 1:S:421:LEU:HD22 | 2.02 | 0.42 |
| 1:S:442:GLN:O | 1:S:446:PHE:N | 2.52 | 0.42 |
| 1:S:476:ARG:HH22 | 1:S:1558:TYR:HE1 | 1.65 | 0.42 |
| 1:S:574:LYS:HA | 1:S:577:GLU:HG3 | 2.00 | 0.42 |
| 1:S:723:ASP:C | 1:S:725:LEU:H | 2.27 | 0.42 |
| 1:S:879:MET:O | 1:S:881:LYS:NZ | 2.47 | 0.42 |
| 1:S:1580:LEU:O | 1:S:1584:GLN:HG2 | 2.19 | 0.42 |
| 1:S:1741:ASP:O | 1:S:1745:LYS:HG3 | 2.18 | 0.42 |
| 1:S:2440:TYR:HA | 1:S:2443:MET:CE | 2.48 | 0.42 |
| 2:T:214:SER:HB3 | 2:T:218:ARG:HD2 | 2.01 | 0.42 |
| 2:T:288:LEU:HD13 | 2:T:293:ASN:HD22 | 1.84 | 0.42 |
| 1:A:117:LYS:HB3 | 3:C:300:ASP:HA | 2.00 | 0.42 |
| 1:A:173:LYS:HA | 1:A:223:CYS:SG | 2.59 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:374:LYS:HD3 | 1:A:423:TYR:HB3 | 2.02 | 0.42 |
| 1:A:1034:ARG:HG3 | 1:A:1088:GLU:HG2 | 2.00 | 0.42 |
| 1:A:1096:VAL:O | 1:A:1100:VAL:HG13 | 2.19 | 0.42 |
| 1:A:1326:GLU:O | 1:A:1329:ARG:HG2 | 2.18 | 0.42 |
| 1:A:1505:LEU:O | 1:A:1508:LYS:N | 2.52 | 0.42 |
| 1:A:1608:ARG:HB3 | 1:A:1612:LYS:HE2 | 2.01 | 0.42 |
| 1:A:1873:TYR:O | 1:A:1877:LEU:HD23 | 2.19 | 0.42 |
| 1:A:2310:VAL:HA | 1:A:2316:TYR:HE1 | 1.84 | 0.42 |
| 1:A:2825:THR:O | 1:A:2829:LYS:HG3 | 2.19 | 0.42 |
| 1:A:3252:PHE:HD1 | 1:A:3287:ARG:HD3 | 1.84 | 0.42 |
| 1:A:3530:VAL:HG23 | 1:A:3531:TYR:N | 2.34 | 0.42 |
| 1:A:3814:ASP:OD1 | 1:A:3814:ASP:N | 2.52 | 0.42 |
| 1:A:3878:VAL:HG13 | 1:A:3965:ARG:HH11 | 1.84 | 0.42 |
| 2:B:513:ALA:O | 2:B:516:LYS:HG3 | 2.19 | 0.42 |
| 3:C:75:GLN:O | 3:C:77:ILE:HG13 | 2.18 | 0.42 |
| 3:C:226:SER:O | 3:C:230:SER:N | 2.48 | 0.42 |
| 3:C:461:MET:HE2 | 3:C:522:VAL:HG12 | 2.01 | 0.42 |
| 3:C:499:LEU:O | 3:C:502:ARG:NH1 | 2.51 | 0.42 |
| 3:C:656:ASN:CG | 3:C:688:LYS:HA | 2.44 | 0.42 |
| 4:D:118:ALA:O | 4:D:121:LEU:HG | 2.20 | 0.42 |
| 3:L:313:GLY:HA2 | 3:L:323:PHE:H | 1.84 | 0.42 |
| 3:L:337:GLY:HA2 | 3:L:399:LYS:N | 2.35 | 0.42 |
| 5:Q:174:THR:HG23 | 6:R:792:MET:SD | 2.59 | 0.42 |
| 6:R:706:ASN:HB2 | 6:R:709:VAL:HG23 | 2.01 | 0.42 |
| 6:R:841:LYS:O | 6:R:845:LEU:HB2 | 2.19 | 0.42 |
| 1:S:138:PHE:HE1 | 1:S:149:ILE:HG21 | 1.84 | 0.42 |
| 1:S:638:GLN:HB2 | 1:S:641:PHE:CE2 | 2.54 | 0.42 |
| 1:S:866:ILE:HG12 | 1:S:3168:TYR:CE2 | 2.53 | 0.42 |
| 1:S:1415:LEU:O | 1:S:1419:LEU:N | 2.37 | 0.42 |
| 1:S:1602:ASP:HB3 | 1:S:1606:ARG:HH12 | 1.83 | 0.42 |
| 1:S:1627:LYS:HG2 | 1:S:1670:GLU:HG3 | 2.01 | 0.42 |
| 1:S:2310:VAL:HG13 | 1:S:2316:TYR:HE2 | 1.85 | 0.42 |
| 1:S:2376:ASP:H | 1:S:2404:ARG:NH1 | 2.17 | 0.42 |
| 1:S:2497:GLU:HA | 1:S:2500:LYS:HE2 | 2.01 | 0.42 |
| 1:S:3410:ILE:O | 1:S:3414:MET:HG2 | 2.19 | 0.42 |
| 1:S:3571:PHE:CZ | 1:S:3575:LEU:HD11 | 2.54 | 0.42 |
| 1:S:3871:PHE:HD1 | 1:S:4117:LEU:HD22 | 1.85 | 0.42 |
| 1:S:4041:ARG:HA | 1:S:4044:ILE:HG12 | 2.02 | 0.42 |
| 2:T:93:ASP:HB3 | 2:T:101:ASN:H | 1.83 | 0.42 |
| 2:T:290:ARG:HG3 | 2:T:291:GLU:HG3 | 2.02 | 0.42 |
| 2:T:322:TYR:HD2 | 2:T:327:ILE:HD12 | 1.83 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:159:GLU:O | 1:A:162:LEU:HB3 | 2.19 | 0.42 |
| 1:A:1236:LEU:HD12 | 1:A:1239:PRO:HG2 | 2.01 | 0.42 |
| 1:A:1267:TYR:HB3 | 1:A:1344:PHE:CE1 | 2.54 | 0.42 |
| 1:A:1611:GLN:NE2 | 1:A:1613:HIS:HB2 | 2.34 | 0.42 |
| 1:A:2215:LEU:HD13 | 1:A:2218:PHE:HD2 | 1.83 | 0.42 |
| 1:A:3462:ARG:HB3 | 1:A:3498:TRP:HH2 | 1.85 | 0.42 |
| 1:A:3480:LEU:HD22 | 1:A:3483:MET:SD | 2.59 | 0.42 |
| 1:A:3527:GLN:C | 1:A:3529:ILE:H | 2.28 | 0.42 |
| 1:A:4073:ALA:H | 1:A:4075:ARG:NH1 | 2.17 | 0.42 |
| 2:B:388:LYS:HE3 | 3:C:451:LEU:HB3 | 2.01 | 0.42 |
| 3:C:368:ARG:NH2 | 3:C:371:GLU:OE2 | 2.49 | 0.42 |
| 5:G:194:LEU:HD23 | 5:G:197:LYS:HE2 | 2.02 | 0.42 |
| 6:I:861:SER:O | 6:I:861:SER:OG | 2.35 | 0.42 |
| 3:L:399:LYS:NZ | 10:j:34:DT:O5' | 2.39 | 0.42 |
| 5:P:142:GLU:O | 5:P:145:GLN:HG3 | 2.19 | 0.42 |
| 1:S:581:LEU:HD12 | 1:S:620:PHE:CE1 | 2.54 | 0.42 |
| 1:S:1221:ILE:HA | 1:S:1224:PHE:O | 2.19 | 0.42 |
| 1:S:1729:PHE:HD1 | 1:S:1735:ARG:HE | 1.66 | 0.42 |
| 1:S:1783:ARG:NH1 | 1:S:1830:HIS:HB2 | 2.34 | 0.42 |
| 1:S:2331:MET:HE3 | 1:S:2337:LEU:HG | 2.02 | 0.42 |
| 1:S:2451:LEU:HD23 | 1:S:2498:ILE:HD13 | 2.00 | 0.42 |
| 1:S:3465:PHE:O | 1:S:3469:LEU:HG | 2.19 | 0.42 |
| 1:S:3509:ASP:OD1 | 1:S:3509:ASP:N | 2.51 | 0.42 |
| 1:S:3834:ALA:HB3 | 1:S:3835:PRO:HD3 | 2.01 | 0.42 |
| 1:A:39:GLY:O | 1:A:43:VAL:HG13 | 2.19 | 0.42 |
| 1:A:313:LEU:HA | 1:A:316:LEU:HD12 | 2.01 | 0.42 |
| 1:A:487:LEU:HD13 | 1:A:575:ILE:HD13 | 2.02 | 0.42 |
| 1:A:1070:PRO:CG | 1:A:3744:ASP:HA | 2.49 | 0.42 |
| 1:A:1136:ARG:HA | 1:A:1139:GLU:CD | 2.45 | 0.42 |
| 1:A:1425:ALA:O | 1:A:1428:ILE:HG22 | 2.19 | 0.42 |
| 1:A:1565:GLU:OE1 | 1:A:1565:GLU:N | 2.30 | 0.42 |
| 1:A:1580:LEU:HD13 | 1:A:1625:HIS:CD2 | 2.54 | 0.42 |
| 1:A:1961:PHE:HB2 | 1:A:1963:GLN:HE22 | 1.82 | 0.42 |
| 1:A:2223:VAL:HG23 | 1:A:2234:ASN:HB2 | 2.02 | 0.42 |
| 1:A:2260:PHE:HA | 1:A:2270:ASN:O | 2.20 | 0.42 |
| 1:A:2391:GLY:C | 1:A:2431:ARG:HH22 | 2.28 | 0.42 |
| 1:A:2534:ASN:HB3 | 1:A:2537:ASP:HB2 | 2.01 | 0.42 |
| 1:A:3050:LYS:O | 1:A:3054:GLN:CB | 2.68 | 0.42 |
| 1:A:3123:GLN:OE1 | 1:A:3123:GLN:N | 2.39 | 0.42 |
| 1:A:3295:GLU:O | 1:A:3299:THR:HG22 | 2.18 | 0.42 |
| 1:A:3301:LEU:O | 1:A:3306:LEU:HD22 | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3462:ARG:NH1 | 1:A:3494:GLN:HB2 | 2.35 | 0.42 |
| 1:A:3490:VAL:HA | 1:A:3495:PHE:CE2 | 2.54 | 0.42 |
| 1:A:3753:LYS:O | 1:A:3800:LEU:HD12 | 2.20 | 0.42 |
| 2:B:339:ARG:HH22 | 2:B:342:ASP:HA | 1.84 | 0.42 |
| 3:C:248:PRO:HA | 3:C:261:ILE:O | 2.18 | 0.42 |
| 3:C:265:LYS:NZ | 8:e:23:DT:OP1 | 2.51 | 0.42 |
| 3:C:398:ASP:OD1 | 3:C:401:ALA:N | 2.53 | 0.42 |
| 3:C:522:VAL:HA | 3:C:525:LYS:HE2 | 2.01 | 0.42 |
| 3:L:296:CYS:C | 2:T:296:VAL:HG13 | 2.45 | 0.42 |
| 3:L:383:ALA:HB1 | 2:T:463:LYS:HG3 | 2.00 | 0.42 |
| 3:L:509:GLN:HB2 | 3:L:512:ILE:HG13 | 2.01 | 0.42 |
| 5:Q:104:VAL:O | 5:Q:104:VAL:HG13 | 2.20 | 0.42 |
| 6:R:668:SER:O | 6:R:703:GLY:N | 2.52 | 0.42 |
| 1:S:135:LEU:HB2 | 1:S:177:LEU:HD21 | 2.01 | 0.42 |
| 1:S:450:SER:OG | 1:S:453:MET:HG3 | 2.20 | 0.42 |
| 1:S:458:CYS:HA | 1:S:461:ILE:HD12 | 2.01 | 0.42 |
| 1:S:788:TYR:O | 1:S:792:ILE:HG13 | 2.19 | 0.42 |
| 1:S:1400:VAL:HG12 | 1:S:1404:LYS:NZ | 2.34 | 0.42 |
| 1:S:1565:GLU:HG2 | 1:S:1566:THR:H | 1.85 | 0.42 |
| 1:S:1844:VAL:HG23 | 1:S:1845:VAL:N | 2.33 | 0.42 |
| 1:S:2595:TRP:CE3 | 1:S:2765:GLN:HB3 | 2.54 | 0.42 |
| 1:S:3314:SER:O | 1:S:3317:SER:OG | 2.26 | 0.42 |
| 2:T:458:GLN:HB3 | 2:T:525:PHE:CE2 | 2.54 | 0.42 |
| 7:d:21:DA:C2 | 8:e:36:DA:N1 | 2.87 | 0.42 |
| 1:A:156:PHE:HA | 1:A:159:GLU:CD | 2.44 | 0.42 |
| 1:A:300:TRP:CE3 | 1:A:308:LEU:HD21 | 2.54 | 0.42 |
| 1:A:344:GLN:O | 1:A:348:ILE:HG12 | 2.20 | 0.42 |
| 1:A:571:SER:O | 1:A:574:LYS:HG2 | 2.19 | 0.42 |
| 1:A:705:ALA:O | 1:A:709:LYS:HD3 | 2.19 | 0.42 |
| 1:A:786:GLN:O | 1:A:788:TYR:N | 2.52 | 0.42 |
| 1:A:910:PHE:O | 1:A:914:VAL:HG12 | 2.20 | 0.42 |
| 1:A:945:ALA:HB2 | 1:A:958:MET:HE1 | 2.00 | 0.42 |
| 1:A:978:GLN:HG2 | 1:A:979:VAL:N | 2.33 | 0.42 |
| 1:A:1015:ASP:OD1 | 1:A:1015:ASP:N | 2.49 | 0.42 |
| 1:A:1208:LEU:HA | 1:A:1211:VAL:HG12 | 2.00 | 0.42 |
| 1:A:1597:LEU:O | 1:A:1601:LEU:HG | 2.20 | 0.42 |
| 1:A:1675:TYR:HA | 1:A:1678:LEU:HD12 | 2.00 | 0.42 |
| 1:A:1726:SER:OG | 1:A:1772:HIS:O | 2.36 | 0.42 |
| 1:A:1803:GLU:HA | 1:A:1806:ARG:NH1 | 2.34 | 0.42 |
| 1:A:2241:LEU:HD12 | 1:A:2242:VAL:N | 2.35 | 0.42 |
| 1:A:2412:TYR:O | 1:A:2415:LEU:HG | 2.20 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3448:GLU:OE1 | 1:A:3485:LYS:HD2 | 2.20 | 0.42 |
| 1:A:3574:ALA:CB | 1:A:3684:SER:HB2 | 2.42 | 0.42 |
| 1:A:3959:MET:SD | 1:A:4124:TRP:NE1 | 2.92 | 0.42 |
| 2:B:92:LYS:HB2 | 2:B:135:MET:CE | 2.49 | 0.42 |
| 2:B:260:LYS:HB2 | 2:B:262:LYS:HZ1 | 1.84 | 0.42 |
| 3:C:93:ASP:HA | 3:C:97:LYS:HG2 | 2.00 | 0.42 |
| 3:C:114:SER:OG | 3:C:132:ILE:HD13 | 2.19 | 0.42 |
| 3:C:461:MET:CE | 3:C:522:VAL:HG12 | 2.49 | 0.42 |
| 3:C:623:PHE:CE1 | 3:C:632:PHE:HB2 | 2.55 | 0.42 |
| 3:L:12:LEU:HB3 | 3:L:14:MET:HE3 | 2.02 | 0.42 |
| 3:L:66:ASN:HD21 | 3:L:74:TYR:HB3 | 1.84 | 0.42 |
| 3:L:229:GLU:O | 3:L:233:LYS:HG3 | 2.19 | 0.42 |
| 3:L:599:ARG:O | 3:L:603:LYS:NZ | 2.46 | 0.42 |
| 5:P:22:VAL:HG22 | 5:P:24:TRP:HE3 | 1.85 | 0.42 |
| 1:S:738:HIS:O | 1:S:742:GLU:HG3 | 2.20 | 0.42 |
| 1:S:1597:LEU:O | 1:S:1601:LEU:HG | 2.19 | 0.42 |
| 1:S:1755:SER:HB2 | 1:S:1758:LEU:HD12 | 2.01 | 0.42 |
| 1:S:1950:SER:OG | 1:S:1951:VAL:N | 2.52 | 0.42 |
| 1:S:2580:PRO:HG2 | 1:S:2583:GLU:HB2 | 2.02 | 0.42 |
| 1:S:3527:GLN:C | 1:S:3529:ILE:H | 2.28 | 0.42 |
| 1:S:3563:ASP:C | 1:S:3564:GLN:HG3 | 2.45 | 0.42 |
| 1:S:3898:LEU:HA | 1:S:3901:ARG:NH2 | 2.34 | 0.42 |
| 2:T:93:ASP:HA | 2:T:103:TYR:HB2 | 2.02 | 0.42 |
| 7:d:21:DA:C8 | 7:d:22:DG:C6 | 3.06 | 0.42 |
| 7:d:22:DG:H1' | 7:d:23:DT:H5' | 2.02 | 0.42 |
| 1:A:225:LYS:HG2 | 1:A:274:LEU:HB2 | 2.01 | 0.42 |
| 1:A:461:ILE:HA | 1:A:464:VAL:HG22 | 2.01 | 0.42 |
| 1:A:1556:GLY:HA2 | 1:A:1559:PHE:CD2 | 2.54 | 0.42 |
| 1:A:1756:PRO:O | 1:A:1759:LEU:HB2 | 2.20 | 0.42 |
| 1:A:2258:GLU:HA | 1:A:2261:SER:OG | 2.20 | 0.42 |
| 1:A:2464:HIS:CE1 | 1:A:2466:SER:H | 2.38 | 0.42 |
| 1:A:2539:LEU:HD11 | 1:A:2813:PHE:HD1 | 1.84 | 0.42 |
| 1:A:3359:ILE:HD12 | 1:A:3362:LEU:HD12 | 2.02 | 0.42 |
| 1:A:3549:HIS:HA | 1:A:3552:LYS:HG2 | 2.02 | 0.42 |
| 1:A:3568:ILE:O | 1:A:3572:ILE:HG12 | 2.20 | 0.42 |
| 2:B:41:LEU:HD12 | 2:B:88:TYR:HD1 | 1.85 | 0.42 |
| 2:B:382:PHE:CE1 | 2:B:431:GLY:HA2 | 2.55 | 0.42 |
| 2:B:486:HIS:HA | 2:B:489:ASN:ND2 | 2.35 | 0.42 |
| 2:B:511:VAL:HA | 2:B:514:MET:HE2 | 2.01 | 0.42 |
| 3:C:20:MET:CB | 3:C:31:PHE:HB2 | 2.44 | 0.42 |
| 5:G:169:LYS:O | 5:G:172:LEU:HG | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:H:28:LEU:HD12 | 5:H:71:ARG:HA | 2.01 | 0.42 |
| 5:H:196:ASN:O | 5:H:199:LEU:HG | 2.20 | 0.42 |
| 6:I:900:LYS:HE2 | 6:I:903:LEU:HD23 | 2.02 | 0.42 |
| 3:L:7:LYS:HB2 | 3:L:126:LYS:O | 2.19 | 0.42 |
| 3:L:182:PRO:HG2 | 3:L:520:ALA:H | 1.84 | 0.42 |
| 3:L:212:MET:HG2 | 3:L:223:GLU:HG2 | 2.01 | 0.42 |
| 3:L:279:VAL:HB | 3:L:284:LEU:C | 2.44 | 0.42 |
| 4:M:191:LYS:HB2 | 4:M:191:LYS:HE2 | 1.82 | 0.42 |
| 5:P:28:LEU:HG | 5:P:70:LEU:HD23 | 2.02 | 0.42 |
| 5:P:139:ALA:O | 5:P:142:GLU:HG3 | 2.20 | 0.42 |
| 5:Q:127:ILE:HG13 | 5:Q:128:CYS:N | 2.35 | 0.42 |
| 5:Q:156:ASN:O | 5:Q:159:GLN:HG2 | 2.19 | 0.42 |
| 6:R:876:LYS:HA | 6:R:876:LYS:HD3 | 1.88 | 0.42 |
| 6:R:902:GLU:HG2 | 6:R:903:LEU:N | 2.35 | 0.42 |
| 1:S:118:ASP:O | 1:S:122:LYS:HG2 | 2.20 | 0.42 |
| 1:S:225:LYS:HA | 1:S:274:LEU:HD22 | 2.02 | 0.42 |
| 1:S:898:PHE:H | 1:S:902:LYS:HE3 | 1.84 | 0.42 |
| 1:S:939:MET:HE3 | 1:S:2783:ILE:CD1 | 2.46 | 0.42 |
| 1:S:1512:SER:O | 1:S:1516:GLU:OE1 | 2.37 | 0.42 |
| 1:S:1653:LEU:HB3 | 1:S:1698:PHE:CE2 | 2.55 | 0.42 |
| 1:S:2120:ARG:HG3 | 1:S:2121:ASP:N | 2.34 | 0.42 |
| 1:S:2219:LEU:O | 1:S:2223:VAL:N | 2.53 | 0.42 |
| 1:S:2918:PRO:O | 1:S:2921:LEU:HB3 | 2.19 | 0.42 |
| 1:S:3337:ILE:HG21 | 1:S:3360:LEU:HG | 2.02 | 0.42 |
| 1:S:3447:VAL:HG23 | 1:S:3482:LEU:HD12 | 2.01 | 0.42 |
| 1:S:4071:ALA:HB1 | 1:S:4077:TYR:CE2 | 2.53 | 0.42 |
| 2:T:282:LYS:HE3 | 2:T:486:HIS:HB3 | 2.02 | 0.42 |
| 2:T:484:GLN:O | 2:T:488:ARG:NH1 | 2.52 | 0.42 |
| 1:A:582:THR:H | 1:A:620:PHE:HZ | 1.67 | 0.42 |
| 1:A:1057:LYS:HG3 | 1:A:1061:LYS:HZ1 | 1.85 | 0.42 |
| 1:A:1360:LYS:HD2 | 1:A:1411:TYR:CE2 | 2.54 | 0.42 |
| 1:A:1784:ARG:HA | 1:A:1787:ARG:HG2 | 2.00 | 0.42 |
| 1:A:2494:ASP:O | 1:A:2498:ILE:HG13 | 2.19 | 0.42 |
| 1:A:2967:GLU:O | 1:A:2971:GLN:HG2 | 2.19 | 0.42 |
| 1:A:3173:MET:HG3 | 1:A:3174:ASP:N | 2.35 | 0.42 |
| 1:A:3486:GLU:HA | 1:A:3489:SER:OG | 2.19 | 0.42 |
| 1:A:3588:TRP:CZ3 | 1:A:3592:VAL:HG11 | 2.55 | 0.42 |
| 1:A:3723:ASP:HB2 | 1:A:3741:ARG:HB2 | 2.02 | 0.42 |
| 1:A:3909:ALA:O | 1:A:3913:ILE:HG22 | 2.20 | 0.42 |
| 1:A:3912:CYS:HA | 1:A:3915:HIS:CD2 | 2.55 | 0.42 |
| 1:A:3980:MET:N | 1:A:3980:MET:SD | 2.92 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:468:LYS:O | 2:B:517:ARG:NH1 | 2.52 | 0.42 |
| 3:C:138:LEU:HB2 | 3:C:201:GLN:HA | 2.02 | 0.42 |
| 3:C:246:HIS:HB3 | 3:C:264:TYR:CZ | 2.54 | 0.42 |
| 3:C:347:LYS:NZ | 3:C:388:ASP:HB3 | 2.35 | 0.42 |
| 3:C:635:SER:O | 3:C:639:ILE:HG12 | 2.19 | 0.42 |
| 5:G:120:ALA:O | 5:G:124:ARG:HD3 | 2.19 | 0.42 |
| 5:G:183:VAL:HG21 | 5:H:180:PHE:HZ | 1.85 | 0.42 |
| 5:H:28:LEU:HD13 | 5:H:74:LEU:HD12 | 2.02 | 0.42 |
| 5:H:86:PHE:HE1 | 5:H:95:PHE:HE1 | 1.68 | 0.42 |
| 6:I:708:ARG:O | 6:I:712:ILE:HG23 | 2.19 | 0.42 |
| 3:L:268:LEU:HG | 3:L:271:ARG:HH12 | 1.85 | 0.42 |
| 5:Q:108:LEU:H | 5:Q:108:LEU:HD23 | 1.83 | 0.42 |
| 1:S:58:VAL:HG13 | 1:S:59:PHE:CD1 | 2.55 | 0.42 |
| 1:S:438:LEU:O | 1:S:441:MET:HB2 | 2.19 | 0.42 |
| 1:S:528:VAL:HA | 1:S:531:PHE:HB2 | 2.02 | 0.42 |
| 1:S:712:LYS:HE2 | 1:S:744:ASP:HB3 | 2.02 | 0.42 |
| 1:S:1102:GLU:CD | 1:S:1102:GLU:H | 2.28 | 0.42 |
| 1:S:1142:HIS:O | 1:S:1146:ASN:N | 2.48 | 0.42 |
| 1:S:1741:ASP:O | 1:S:1744:LYS:HG2 | 2.19 | 0.42 |
| 1:S:1769:GLU:H | 1:S:1772:HIS:CE1 | 2.37 | 0.42 |
| 1:S:2552:VAL:HG13 | 1:S:2851:PHE:CE1 | 2.54 | 0.42 |
| 1:S:2597:PHE:HD2 | 1:S:2765:GLN:HG2 | 1.83 | 0.42 |
| 1:S:3004:HIS:CD2 | 1:S:3177:ASN:HD21 | 2.38 | 0.42 |
| 1:S:3097:ASP:OD1 | 1:S:3097:ASP:N | 2.53 | 0.42 |
| 1:S:3171:ALA:HA | 1:S:3179:TRP:CZ2 | 2.55 | 0.42 |
| 1:S:3300:VAL:HB | 1:S:3337:ILE:HD11 | 2.02 | 0.42 |
| 1:S:4091:ALA:HB2 | 1:S:4110:GLN:HG2 | 2.02 | 0.42 |
| 2:T:83:LEU:HB2 | 2:T:115:ARG:HH12 | 1.85 | 0.42 |
| 2:T:86:VAL:HA | 2:T:104:VAL:HA | 2.00 | 0.42 |
| 8:e:34:DC:H1' | 8:e:35:DT:O4' | 2.20 | 0.42 |
| 1:A:152:LEU:O | 1:A:156:PHE:CD2 | 2.73 | 0.42 |
| 1:A:289:ASN:O | 1:A:293:LEU:HG | 2.20 | 0.42 |
| 1:A:394:GLN:CD | 1:A:1737:ASN:HB3 | 2.45 | 0.42 |
| 1:A:633:ILE:O | 1:A:636:GLU:HG2 | 2.19 | 0.42 |
| 1:A:643:GLU:O | 1:A:646:VAL:HB | 2.18 | 0.42 |
| 1:A:660:LEU:HD23 | 1:A:660:LEU:HA | 1.82 | 0.42 |
| 1:A:989:MET:SD | 1:A:990:GLN:HG3 | 2.60 | 0.42 |
| 1:A:1343:GLU:O | 1:A:1347:THR:HG23 | 2.20 | 0.42 |
| 1:A:1801:VAL:HG23 | 1:A:1824:LEU:HD11 | 2.02 | 0.42 |
| 1:A:2510:LEU:HD21 | 1:A:2525:TRP:HD1 | 1.85 | 0.42 |
| 1:A:3043:TYR:HA | 1:A:3046:ARG:HB2 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3334:TYR:CD2 | 1:A:3380:ARG:HB3 | 2.55 | 0.42 |
| 1:A:4041:ARG:HD2 | 1:A:4044:ILE:HD11 | 2.01 | 0.42 |
| 1:A:4075:ARG:HG2 | 1:A:4076:ASP:N | 2.34 | 0.42 |
| 2:B:126:GLN:O | 2:B:130:ARG:HG3 | 2.20 | 0.42 |
| 2:B:196:THR:OG1 | 2:B:198:ILE:HG12 | 2.20 | 0.42 |
| 2:B:352:PRO:HB2 | 2:B:355:LEU:HG | 2.02 | 0.42 |
| 3:C:20:MET:HB3 | 3:C:31:PHE:CB | 2.44 | 0.42 |
| 3:C:342:VAL:HG23 | 3:C:393:VAL:HG12 | 2.01 | 0.42 |
| 3:C:423:GLN:HG2 | 3:C:424:LEU:N | 2.33 | 0.42 |
| 3:C:661:ALA:O | 3:C:664:GLU:HG3 | 2.20 | 0.42 |
| 3:C:665:LYS:O | 3:C:668:ILE:HG12 | 2.20 | 0.42 |
| 4:D:9:CYS:SG | 4:D:22:CYS:HB3 | 2.60 | 0.42 |
| 5:G:28:LEU:HD12 | 5:G:28:LEU:HA | 1.92 | 0.42 |
| 5:G:186:GLU:O | 5:G:190:LYS:HG3 | 2.19 | 0.42 |
| 1:S:243:GLN:O | 1:S:282:PHE:HE1 | 2.02 | 0.42 |
| 1:S:446:PHE:HB3 | 1:S:527:TYR:CE1 | 2.54 | 0.42 |
| 1:S:849:GLU:OE1 | 1:S:849:GLU:N | 2.46 | 0.42 |
| 1:S:910:PHE:CZ | 1:S:2808:LEU:HD23 | 2.55 | 0.42 |
| 1:S:1709:GLU:H | 1:S:1709:GLU:CD | 2.25 | 0.42 |
| 1:S:1776:GLU:H | 1:S:1776:GLU:CD | 2.24 | 0.42 |
| 1:S:2371:PHE:CD2 | 1:S:2374:LEU:HD23 | 2.51 | 0.42 |
| 1:S:2814:SER:C | 1:S:2818:LYS:HZ2 | 2.28 | 0.42 |
| 1:S:2970:LYS:NZ | 1:S:2974:GLU:HB2 | 2.35 | 0.42 |
| 1:S:3371:GLU:HB2 | 1:S:3372:LYS:HZ2 | 1.85 | 0.42 |
| 1:A:174:VAL:HA | 1:A:177:LEU:CD1 | 2.48 | 0.42 |
| 1:A:1675:TYR:O | 1:A:1678:LEU:HB2 | 2.20 | 0.42 |
| 1:A:2223:VAL:O | 1:A:2223:VAL:HG13 | 2.19 | 0.42 |
| 1:A:2774:SER:OG | 1:A:2785:ILE:HG23 | 2.20 | 0.42 |
| 1:A:2865:HIS:HB2 | 1:A:2868:LEU:HG | 2.01 | 0.42 |
| 1:A:2880:CYS:HB2 | 1:A:2885:GLN:O | 2.20 | 0.42 |
| 1:A:3263:HIS:HB2 | 1:A:3276:TRP:CZ2 | 2.55 | 0.42 |
| 1:A:3459:ASN:HA | 1:A:3462:ARG:HB2 | 2.01 | 0.42 |
| 1:A:3515:GLN:HA | 1:A:3518:VAL:HG22 | 2.00 | 0.42 |
| 1:A:4082:ARG:HD2 | 1:A:4092:GLN:NE2 | 2.34 | 0.42 |
| 2:B:48:MET:HE3 | 2:B:59:PRO:CB | 2.50 | 0.42 |
| 2:B:240:GLU:H | 2:B:240:GLU:CD | 2.25 | 0.42 |
| 2:B:325:ARG:HB3 | 3:C:88:PHE:CZ | 2.55 | 0.42 |
| 3:C:365:PHE:HZ | 3:C:416:TYR:CD2 | 2.38 | 0.42 |
| 3:C:714:ASP:OD1 | 3:C:714:ASP:N | 2.53 | 0.42 |
| 6:I:731:LYS:HA | 6:I:731:LYS:HD3 | 1.87 | 0.42 |
| 3:L:625:ASP:OD1 | 1:S:1816:ARG:NH2 | 2.46 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Q:187:LYS:HE2 | 5:Q:190:LYS:HE3 | 2.01 | 0.42 |
| 6:R:664:PHE:CD1 | 6:R:699:CYS:HB2 | 2.55 | 0.42 |
| 1:S:1006:THR:O | 1:S:1009:LEU:HG | 2.20 | 0.42 |
| 1:S:1086:TYR:CD1 | 1:S:1133:HIS:HB3 | 2.55 | 0.42 |
| 1:S:1708:GLU:HA | 1:S:1711:ARG:HH11 | 1.85 | 0.42 |
| 1:S:1802:TYR:O | 1:S:1805:PHE:HB3 | 2.20 | 0.42 |
| 1:S:1862:THR:OG1 | 1:S:1863:PHE:N | 2.52 | 0.42 |
| 1:S:2803:ILE:O | 1:S:2807:GLN:HG2 | 2.19 | 0.42 |
| 1:S:2938:VAL:O | 1:S:2942:ILE:HG12 | 2.19 | 0.42 |
| 1:S:3048:LYS:HB3 | 1:S:3061:LEU:HD13 | 2.00 | 0.42 |
| 1:S:3789:ARG:HH11 | 1:S:3936:GLY:HA3 | 1.85 | 0.42 |
| 2:T:413:LEU:HD12 | 2:T:432:PHE:HB3 | 2.01 | 0.42 |
| 1:A:214:GLU:C | 1:A:216:LYS:H | 2.28 | 0.41 |
| 1:A:851:ILE:HD13 | 1:A:854:ARG:HH21 | 1.85 | 0.41 |
| 1:A:912:PRO:O | 1:A:915:THR:HB | 2.20 | 0.41 |
| 1:A:1365:ASN:HD21 | 1:A:1370:ARG:NH2 | 2.12 | 0.41 |
| 1:A:1574:ASN:OD1 | 1:A:1575:LEU:N | 2.52 | 0.41 |
| 1:A:1661:PHE:HE2 | 1:A:1667:SER:H | 1.68 | 0.41 |
| 1:A:1878:ASP:N | 1:A:1878:ASP:OD1 | 2.52 | 0.41 |
| 1:A:3758:LEU:HD13 | 1:A:3801:GLY:HA3 | 2.02 | 0.41 |
| 2:B:158:GLN:OE1 | 2:B:158:GLN:N | 2.29 | 0.41 |
| 2:B:339:ARG:HH11 | 2:B:405:ASN:H | 1.66 | 0.41 |
| 2:B:530:TYR:CD1 | 3:C:372:ALA:HB1 | 2.56 | 0.41 |
| 3:C:74:TYR:C | 3:C:77:ILE:HD12 | 2.45 | 0.41 |
| 3:C:280:ASP:OD1 | 3:C:281:ALA:N | 2.53 | 0.41 |
| 4:D:39:LEU:HD23 | 4:D:109:LEU:HD11 | 2.02 | 0.41 |
| 6:I:801:TYR:HB3 | 6:I:802:ARG:HH21 | 1.85 | 0.41 |
| 3:L:40:MET:SD | 3:L:41:PHE:N | 2.93 | 0.41 |
| 3:L:502:ARG:H | 3:L:502:ARG:HD3 | 1.85 | 0.41 |
| 1:S:988:VAL:O | 1:S:992:ILE:HG13 | 2.20 | 0.41 |
| 1:S:1418:HIS:HA | 1:S:1421:GLU:CD | 2.45 | 0.41 |
| 1:S:2173:ALA:HB1 | 1:S:2214:ARG:HH22 | 1.84 | 0.41 |
| 1:S:2212:ALA:O | 1:S:2215:LEU:HG | 2.20 | 0.41 |
| 1:S:2500:LYS:HA | 1:S:2503:LYS:NZ | 2.35 | 0.41 |
| 1:S:2507:ILE:O | 1:S:2510:LEU:HB2 | 2.20 | 0.41 |
| 1:S:3180:ASP:O | 1:S:3184:THR:HG22 | 2.20 | 0.41 |
| 1:S:3371:GLU:HB2 | 1:S:3372:LYS:NZ | 2.35 | 0.41 |
| 1:S:3838:GLU:HG2 | 1:S:4122:GLU:HB2 | 2.02 | 0.41 |
| 1:S:4049:ARG:NH2 | 1:S:4055:ASN:H | 2.18 | 0.41 |
| 1:A:479:ILE:O | 1:A:483:VAL:HG22 | 2.21 | 0.41 |
| 1:A:849:GLU:HG2 | 1:A:850:GLU:N | 2.34 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:855:VAL:O | 1:A:859:LEU:HG | 2.20 | 0.41 |
| 1:A:1459:HIS:ND1 | 1:A:1464:LEU:HD21 | 2.35 | 0.41 |
| 1:A:1619:ALA:HA | 1:A:1622:ILE:HG22 | 2.01 | 0.41 |
| 1:A:2804:ILE:O | 1:A:2808:LEU:HG | 2.20 | 0.41 |
| 1:A:3257:LYS:HD2 | 1:A:3257:LYS:HA | 1.88 | 0.41 |
| 1:A:3373:VAL:O | 1:A:3377:LEU:HG | 2.20 | 0.41 |
| 2:B:261:LEU:HD12 | 2:B:345:LEU:HB3 | 2.02 | 0.41 |
| 2:B:272:GLY:N | 2:B:369:TYR:O | 2.50 | 0.41 |
| 2:B:318:ARG:HH21 | 2:B:330:GLU:CA | 2.33 | 0.41 |
| 3:C:132:ILE:HG23 | 3:C:161:LEU:HB2 | 2.00 | 0.41 |
| 3:C:281:ALA:HB3 | 3:C:282:LYS:NZ | 2.35 | 0.41 |
| 3:C:620:ILE:HD13 | 3:C:639:ILE:HD11 | 2.02 | 0.41 |
| 3:C:665:LYS:HD2 | 3:C:668:ILE:HD11 | 2.02 | 0.41 |
| 6:I:786:GLU:H | 6:I:787:GLN:NE2 | 2.19 | 0.41 |
| 3:L:238:LYS:H | 11:m:299:SER:HA | 1.86 | 0.41 |
| 3:L:660:LYS:NZ | 3:L:698:ALA:HB1 | 2.35 | 0.41 |
| 1:S:103:TYR:HA | 1:S:106:GLU:HG2 | 2.02 | 0.41 |
| 1:S:386:VAL:HG13 | 1:S:431:TYR:OH | 2.20 | 0.41 |
| 1:S:1066:LEU:HD11 | 1:S:1078:ALA:HB2 | 2.01 | 0.41 |
| 1:S:1075:ARG:HH21 | 1:S:1113:LEU:HD21 | 1.84 | 0.41 |
| 1:S:1195:VAL:HB | 1:S:1203:SER:HB2 | 2.02 | 0.41 |
| 1:S:1275:THR:HG23 | 1:S:1276:VAL:HG23 | 2.02 | 0.41 |
| 1:S:1418:HIS:O | 1:S:1422:LYS:HG2 | 2.21 | 0.41 |
| 1:S:2138:VAL:HG13 | 1:S:2143:ARG:CG | 2.51 | 0.41 |
| 1:S:2345:VAL:O | 1:S:2349:LEU:HG | 2.21 | 0.41 |
| 1:S:2835:LYS:HA | 1:S:2835:LYS:HD3 | 1.79 | 0.41 |
| 1:S:3114:TYR:HD2 | 1:S:3128:LYS:HG2 | 1.86 | 0.41 |
| 1:S:3257:LYS:O | 1:S:3261:GLU:HG2 | 2.20 | 0.41 |
| 1:S:3767:LEU:HD21 | 1:S:4001:THR:OG1 | 2.20 | 0.41 |
| 2:T:41:LEU:HD11 | 2:T:88:TYR:CD2 | 2.55 | 0.41 |
| 2:T:64:ILE:O | 2:T:68:GLN:HG2 | 2.20 | 0.41 |
| 2:T:168:LEU:HD21 | 2:T:202:LEU:HA | 2.01 | 0.41 |
| 2:T:275:ASN:HB3 | 2:T:366:LEU:CD1 | 2.50 | 0.41 |
| 1:A:168:ASP:H | 1:A:171:LEU:HD12 | 1.84 | 0.41 |
| 1:A:172:GLU:C | 1:A:174:VAL:N | 2.78 | 0.41 |
| 1:A:283:SER:C | 1:A:285:CYS:H | 2.28 | 0.41 |
| 1:A:1571:LEU:HG | 1:A:1600:MET:HE2 | 2.02 | 0.41 |
| 1:A:1718:ILE:HA | 1:A:1721:HIS:ND1 | 2.34 | 0.41 |
| 1:A:1801:VAL:O | 1:A:1804:MET:HG3 | 2.20 | 0.41 |
| 1:A:2225:HIS:HB2 | 1:A:2231:PHE:HB2 | 2.01 | 0.41 |
| 1:A:2405:VAL:O | 1:A:2408:MET:HG2 | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2481:HIS:CD2 | 1:A:2524:PHE:HZ | 2.37 | 0.41 |
| 1:A:2531:LEU:HD23 | 1:A:2531:LEU:HA | 1.89 | 0.41 |
| 1:A:2897:LEU:HD21 | 1:A:2923:TRP:CD2 | 2.55 | 0.41 |
| 1:A:3135:LEU:O | 1:A:3138:ILE:HG12 | 2.20 | 0.41 |
| 1:A:3384:HIS:HA | 1:A:3387:GLU:HG2 | 2.02 | 0.41 |
| 1:A:3483:MET:SD | 1:A:3511:ALA:HB3 | 2.60 | 0.41 |
| 1:A:3608:LYS:NZ | 1:A:3611:GLU:OE2 | 2.41 | 0.41 |
| 1:A:3829:LEU:O | 1:A:3833:ARG:HB3 | 2.20 | 0.41 |
| 1:A:3980:MET:SD | 1:A:3981:TYR:N | 2.93 | 0.41 |
| 2:B:95:ASN:HD21 | 2:B:99:PHE:H | 1.67 | 0.41 |
| 2:B:372:GLU:CD | 2:B:377:GLY:H | 2.28 | 0.41 |
| 3:C:27:ILE:HG12 | 3:C:183:PHE:CD2 | 2.55 | 0.41 |
| 3:C:497:ARG:NH2 | 3:C:503:GLU:O | 2.53 | 0.41 |
| 6:I:749:SER:O | 6:I:752:GLU:HG3 | 2.20 | 0.41 |
| 3:L:115:MET:SD | 3:L:153:SER:HB3 | 2.61 | 0.41 |
| 3:L:619:HIS:CD2 | 3:L:635:SER:HA | 2.55 | 0.41 |
| 3:L:629:THR:O | 3:L:633:MET:HG2 | 2.20 | 0.41 |
| 6:R:753:HIS:HA | 6:R:756:ARG:NE | 2.35 | 0.41 |
| 1:S:643:GLU:O | 1:S:646:VAL:HG22 | 2.19 | 0.41 |
| 1:S:786:GLN:N | 1:S:787:PRO:HD2 | 2.35 | 0.41 |
| 1:S:955:ALA:N | 1:S:1003:SER:OG | 2.53 | 0.41 |
| 1:S:976:VAL:HG22 | 1:S:2598:ARG:NH2 | 2.34 | 0.41 |
| 1:S:2158:ARG:HA | 1:S:2158:ARG:HD2 | 1.90 | 0.41 |
| 1:S:2318:ALA:O | 1:S:2321:GLU:HB2 | 2.19 | 0.41 |
| 1:S:2339:GLU:O | 1:S:2343:GLU:HG2 | 2.20 | 0.41 |
| 1:S:3548:GLY:O | 1:S:3552:LYS:HG2 | 2.19 | 0.41 |
| 1:S:3946:PHE:CD1 | 1:S:4043:LYS:HB3 | 2.55 | 0.41 |
| 2:T:62:MET:HA | 2:T:65:GLN:NE2 | 2.35 | 0.41 |
| 2:T:109:ASP:OD2 | 2:T:115:ARG:HD2 | 2.20 | 0.41 |
| 2:T:142:SER:HA | 2:T:182:LYS:HD2 | 2.02 | 0.41 |
| 10:j:19:DA:OP2 | 10:j:19:DA:H8 | 2.03 | 0.41 |
| 1:A:217:LEU:HG | 1:A:217:LEU:O | 2.20 | 0.41 |
| 1:A:241:ASP:O | 1:A:244:THR:N | 2.54 | 0.41 |
| 1:A:386:VAL:HG13 | 1:A:431:TYR:OH | 2.19 | 0.41 |
| 1:A:425:ASP:OD1 | 1:A:425:ASP:N | 2.53 | 0.41 |
| 1:A:491:CYS:HB2 | 1:A:622:ALA:HB1 | 2.02 | 0.41 |
| 1:A:888:ARG:HH21 | 1:A:3889:ARG:HB3 | 1.85 | 0.41 |
| 1:A:959:TYR:O | 1:A:962:TYR:HB2 | 2.20 | 0.41 |
| 1:A:1121:LEU:HG | 1:A:1123:THR:H | 1.84 | 0.41 |
| 1:A:1781:SER:HA | 1:A:1784:ARG:CZ | 2.50 | 0.41 |
| 1:A:1816:ARG:HD3 | 1:A:1819:PHE:CE2 | 2.55 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2174:SER:O | 1:A:2174:SER:OG | 2.30 | 0.41 |
| 1:A:2276:LEU:HA | 1:A:2279:ILE:HD13 | 2.01 | 0.41 |
| 1:A:2356:MET:SD | 1:A:2359:LYS:HG2 | 2.60 | 0.41 |
| 1:A:2771:LEU:HD23 | 1:A:2771:LEU:H | 1.85 | 0.41 |
| 1:A:2840:PHE:HA | 1:A:2843:PHE:CD2 | 2.55 | 0.41 |
| 1:A:3003:ASN:HD22 | 1:A:3011:LEU:HD22 | 1.86 | 0.41 |
| 1:A:3589:SER:C | 1:A:3593:ARG:HE | 2.28 | 0.41 |
| 1:A:3680:LEU:HD12 | 1:A:3724:GLU:HB3 | 2.02 | 0.41 |
| 1:A:3813:LYS:HG2 | 1:A:3925:LEU:HD23 | 2.02 | 0.41 |
| 2:B:249:LYS:C | 2:B:250:GLU:OE1 | 2.63 | 0.41 |
| 2:B:295:PRO:C | 3:C:298:ASN:HD22 | 2.28 | 0.41 |
| 2:B:325:ARG:HD3 | 3:C:88:PHE:CE2 | 2.55 | 0.41 |
| 3:C:59:PHE:HB3 | 3:C:77:ILE:HG12 | 2.02 | 0.41 |
| 5:H:115:LYS:HD2 | 5:H:115:LYS:HA | 1.79 | 0.41 |
| 6:I:773:GLN:HA | 6:I:776:GLU:HG3 | 2.01 | 0.41 |
| 3:L:239:LYS:H | 11:m:299:SER:HB2 | 1.85 | 0.41 |
| 3:L:663:GLN:CG | 3:L:702:LYS:HG2 | 2.50 | 0.41 |
| 5:P:174:THR:O | 5:P:178:LYS:HG2 | 2.20 | 0.41 |
| 5:Q:184:LEU:O | 5:Q:188:LYS:HG2 | 2.19 | 0.41 |
| 1:S:74:ASN:HA | 1:S:122:LYS:HD3 | 2.01 | 0.41 |
| 1:S:87:LYS:NZ | 1:S:829:VAL:O | 2.54 | 0.41 |
| 1:S:418:ALA:HB2 | 1:S:464:VAL:CG1 | 2.50 | 0.41 |
| 1:S:525:LYS:HE2 | 1:S:525:LYS:HB2 | 1.79 | 0.41 |
| 1:S:879:MET:HG3 | 1:S:881:LYS:N | 2.35 | 0.41 |
| 1:S:1443:VAL:O | 1:S:1447:ARG:HG2 | 2.20 | 0.41 |
| 1:S:2587:GLN:HG3 | 1:S:2777:HIS:O | 2.20 | 0.41 |
| 1:S:2916:LEU:HA | 1:S:2917:PRO:HD3 | 1.93 | 0.41 |
| 1:S:3077:ILE:HG13 | 1:S:3078:LEU:N | 2.35 | 0.41 |
| 1:S:3090:TYR:HB3 | 1:S:3095:ASP:HB2 | 2.02 | 0.41 |
| 1:S:3188:PHE:CZ | 1:S:3192:LYS:HE3 | 2.55 | 0.41 |
| 1:S:3243:ILE:HG23 | 1:S:3283:LEU:HD22 | 2.02 | 0.41 |
| 1:S:3420:CYS:SG | 1:S:3446:VAL:HG21 | 2.60 | 0.41 |
| 1:S:3626:GLY:H | 1:S:3630:ARG:HH22 | 1.67 | 0.41 |
| 1:S:3886:ALA:HA | 1:S:3889:ARG:HG2 | 2.02 | 0.41 |
| 8:e:38:DT:H2" | 8:e:39:DA:C5 | 2.56 | 0.41 |
| 9:i:34:DC:H6 | 9:i:34:DC:H2' | 1.71 | 0.41 |
| 1:A:313:LEU:O | 1:A:316:LEU:HB2 | 2.21 | 0.41 |
| 1:A:348:ILE:HG21 | 1:A:362:ALA:HB2 | 2.02 | 0.41 |
| 1:A:414:LEU:HA | 1:A:417:VAL:HG22 | 2.03 | 0.41 |
| 1:A:789:TYR:HA | 1:A:792:ILE:HD12 | 2.02 | 0.41 |
| 1:A:917:LEU:CD1 | 1:A:2804:ILE:HD11 | 2.50 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1011:GLU:HA | 1:A:1014:LEU:HG | 2.03 | 0.41 |
| 1:A:1264:LEU:HD23 | 1:A:1340:ARG:HB3 | 2.02 | 0.41 |
| 1:A:1358:LEU:O | 1:A:1361:LYS:HB3 | 2.21 | 0.41 |
| 1:A:1605:PHE:HB2 | 1:A:1655:ILE:HD11 | 2.02 | 0.41 |
| 1:A:1674:THR:O | 1:A:1678:LEU:HG | 2.19 | 0.41 |
| 1:A:1713:VAL:HA | 1:A:1716:GLN:OE1 | 2.19 | 0.41 |
| 1:A:2346:ALA:O | 1:A:2350:LYS:HG2 | 2.20 | 0.41 |
| 1:A:2928:LYS:HA | 1:A:2931:ARG:NE | 2.36 | 0.41 |
| 1:A:2959:ALA:HB1 | 1:A:2964:ASP:HB3 | 2.01 | 0.41 |
| 1:A:3049:LEU:HD21 | 1:A:3088:LEU:HB2 | 2.03 | 0.41 |
| 1:A:3161:LEU:HB2 | 1:A:3186:ARG:HH12 | 1.86 | 0.41 |
| 1:A:3507:ASP:OD1 | 1:A:3539:SER:HB2 | 2.20 | 0.41 |
| 1:A:3923:ARG:NH1 | 1:A:4124:TRP:HB2 | 2.36 | 0.41 |
| 2:B:41:LEU:O | 2:B:169:PHE:N | 2.54 | 0.41 |
| 2:B:106:GLN:OE1 | 2:B:115:ARG:HB3 | 2.20 | 0.41 |
| 2:B:270:SER:C | 2:B:371:GLU:HG2 | 2.46 | 0.41 |
| 2:B:284:PRO:O | 2:B:286:ILE:HD12 | 2.21 | 0.41 |
| 2:B:353:LEU:HD12 | 2:B:393:GLU:HG2 | 2.02 | 0.41 |
| 2:B:362:LEU:HD12 | 2:B:362:LEU:HA | 1.92 | 0.41 |
| 2:B:480:ASN:H | 3:C:428:GLU:CD | 2.28 | 0.41 |
| 3:C:234:LEU:HD11 | 3:C:488:GLN:HE22 | 1.85 | 0.41 |
| 6:I:813:PHE:HA | 6:I:850:ALA:C | 2.46 | 0.41 |
| 3:L:57:VAL:CG2 | 3:L:114:SER:HB2 | 2.51 | 0.41 |
| 3:L:182:PRO:O | 3:L:189:GLY:HA3 | 2.20 | 0.41 |
| 5:Q:51:GLU:HA | 5:Q:54:GLN:NE2 | 2.36 | 0.41 |
| 1:S:87:LYS:HD3 | 1:S:831:LEU:HB2 | 2.01 | 0.41 |
| 1:S:98:GLN:HE22 | 1:S:140:SER:C | 2.28 | 0.41 |
| 1:S:244:THR:HA | 1:S:247:GLU:HB2 | 2.01 | 0.41 |
| 1:S:428:PRO:HG2 | 1:S:431:TYR:CE2 | 2.55 | 0.41 |
| 1:S:435:LEU:HD12 | 1:S:436:GLU:N | 2.35 | 0.41 |
| 1:S:535:LEU:HB3 | 1:S:637:LYS:NZ | 2.35 | 0.41 |
| 1:S:611:ASN:OD1 | 1:S:612:LEU:N | 2.54 | 0.41 |
| 1:S:786:GLN:O | 1:S:786:GLN:NE2 | 2.54 | 0.41 |
| 1:S:1649:LEU:HA | 1:S:1652:ILE:HD12 | 2.03 | 0.41 |
| 1:S:1736:PHE:O | 1:S:1740:VAL:HG13 | 2.20 | 0.41 |
| 1:S:1737:ASN:O | 1:S:1740:VAL:HG22 | 2.20 | 0.41 |
| 1:S:1750:LEU:HA | 1:S:1753:SER:OG | 2.20 | 0.41 |
| 1:S:1959:LEU:HD23 | 1:S:1959:LEU:H | 1.85 | 0.41 |
| 1:S:2044:ASP:O | 1:S:2048:GLY:N | 2.54 | 0.41 |
| 1:S:2206:PRO:O | 1:S:2210:VAL:HG23 | 2.19 | 0.41 |
| 10:j:32:DT:H6 | 10:j:32:DT:H2' | 1.60 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:300:TRP:HA | 1:A:303:HIS:ND1 | 2.36 | 0.41 |
| 1:A:306:VAL:HG12 | 1:A:309:LYS:HZ3 | 1.84 | 0.41 |
| 1:A:1003:SER:H | 1:A:1006:THR:HG23 | 1.86 | 0.41 |
| 1:A:1008:ALA:HA | 1:A:1011:GLU:OE2 | 2.20 | 0.41 |
| 1:A:1093:GLU:OE1 | 1:A:1093:GLU:N | 2.50 | 0.41 |
| 1:A:1323:SER:N | 1:A:1328:GLU:OE2 | 2.53 | 0.41 |
| 1:A:2279:ILE:O | 1:A:2283:ASN:ND2 | 2.54 | 0.41 |
| 1:A:2281:MET:HE3 | 1:A:2325:LEU:C | 2.46 | 0.41 |
| 1:A:3631:LYS:HA | 1:A:3634:GLN:NE2 | 2.32 | 0.41 |
| 1:A:4102:THR:HA | 1:A:4105:LYS:CE | 2.50 | 0.41 |
| 2:B:207:LYS:O | 2:B:233:PHE:HB2 | 2.21 | 0.41 |
| 2:B:366:LEU:N | 2:B:434:LEU:O | 2.44 | 0.41 |
| 3:C:42:VAL:O | 3:C:46:VAL:HG23 | 2.21 | 0.41 |
| 4:D:135:LEU:HD22 | 4:M:132:VAL:HG23 | 2.02 | 0.41 |
| 3:L:475:ASP:O | 3:L:478:PRO:HD3 | 2.20 | 0.41 |
| 1:S:83:GLU:OE1 | 1:S:126:PRO:HD3 | 2.21 | 0.41 |
| 1:S:1480:GLY:HA3 | 1:S:1527:ARG:NH1 | 2.35 | 0.41 |
| 1:S:1506:SER:HA | 1:S:1509:GLN:HE21 | 1.85 | 0.41 |
| 1:S:1779:GLN:O | 1:S:1783:ARG:HG2 | 2.20 | 0.41 |
| 1:S:1959:LEU:HD12 | 1:S:2123:PRO:HG2 | 2.02 | 0.41 |
| 1:S:2101:VAL:O | 1:S:2104:MET:HG3 | 2.20 | 0.41 |
| 1:S:3246:ALA:O | 1:S:3250:ASN:N | 2.54 | 0.41 |
| 2:T:38:LEU:HB2 | 2:T:83:LEU:HD22 | 2.02 | 0.41 |
| 2:T:103:TYR:CD2 | 2:T:135:MET:HE1 | 2.55 | 0.41 |
| 7:d:18:DA:C8 | 8:e:39:DA:N1 | 2.87 | 0.41 |
| 1:A:264:ARG:HH21 | 8:e:40:DT:C2' | 2.33 | 0.41 |
| 1:A:1695:LEU:HD12 | 1:A:1698:PHE:CD1 | 2.54 | 0.41 |
| 1:A:1751:GLU:HG2 | 1:A:1784:ARG:HE | 1.84 | 0.41 |
| 1:A:1754:GLN:OE1 | 1:A:1788:ARG:HB2 | 2.20 | 0.41 |
| 1:A:1769:GLU:HB2 | 1:A:1772:HIS:CG | 2.56 | 0.41 |
| 1:A:2140:LEU:HA | 1:A:2143:ARG:HB2 | 2.03 | 0.41 |
| 1:A:2154:GLU:HA | 1:A:2157:PHE:CZ | 2.55 | 0.41 |
| 1:A:2253:TYR:CE1 | 1:A:2288:TYR:HA | 2.56 | 0.41 |
| 1:A:3041:LEU:N | 1:A:3042:PRO:HD2 | 2.36 | 0.41 |
| 1:A:3589:SER:OG | 1:A:3593:ARG:NH2 | 2.53 | 0.41 |
| 1:A:3730:ALA:HA | 1:A:3734:ARG:HA | 2.01 | 0.41 |
| 1:A:3742:GLY:HA2 | 1:A:3748:HIS:NE2 | 2.34 | 0.41 |
| 1:A:3901:ARG:HD2 | 1:A:3970:LEU:O | 2.21 | 0.41 |
| 2:B:363:ARG:HB3 | 3:C:359:ASN:ND2 | 2.35 | 0.41 |
| 2:B:471:PHE:HD1 | 4:D:200:ASP:OD1 | 2.04 | 0.41 |
| 6:I:883:LYS:HE2 | 6:I:883:LYS:HB2 | 1.86 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:411:HIS:CD2 | 2:T:359:HIS:HB3 | 2.56 | 0.41 |
| 4:M:79:ALA:O | 4:M:83:GLN:N | 2.54 | 0.41 |
| 6:R:831:THR:O | 6:R:831:THR:HG23 | 2.21 | 0.41 |
| 1:S:128:LEU:HD23 | 1:S:171:LEU:HD23 | 2.03 | 0.41 |
| 1:S:206:THR:HG22 | 1:S:212:VAL:HG11 | 2.03 | 0.41 |
| 1:S:1296:PHE:O | 1:S:1300:SER:OG | 2.38 | 0.41 |
| 1:S:1468:LEU:HD11 | 1:S:1471:GLN:HE21 | 1.86 | 0.41 |
| 1:S:1633:TRP:CE3 | 1:S:1674:THR:HG23 | 2.55 | 0.41 |
| 1:S:1714:LEU:O | 1:S:1718:ILE:HG12 | 2.21 | 0.41 |
| 1:S:1816:ARG:HD3 | 1:S:1819:PHE:CE2 | 2.56 | 0.41 |
| 1:S:1837:ARG:HH21 | 1:S:1880:MET:HE3 | 1.85 | 0.41 |
| 1:S:2786:LYS:O | 1:S:2790:LEU:HG | 2.20 | 0.41 |
| 1:S:2926:LEU:O | 1:S:2930:TYR:N | 2.42 | 0.41 |
| 1:S:3125:ARG:O | 1:S:3129:LEU:HG | 2.20 | 0.41 |
| 1:S:3239:LYS:O | 1:S:3243:ILE:HG13 | 2.21 | 0.41 |
| 1:S:3411:ASP:O | 1:S:3415:THR:HG23 | 2.21 | 0.41 |
| 1:S:4095:GLU:O | 1:S:4098:LEU:HB3 | 2.20 | 0.41 |
| 2:T:365:SER:HA | 2:T:436:PHE:HE1 | 1.85 | 0.41 |
| 1:A:104:SER:O | 1:A:108:LYS:HB3 | 2.21 | 0.41 |
| 1:A:204:LEU:HD21 | 1:A:224:LEU:CD2 | 2.50 | 0.41 |
| 1:A:333:MET:O | 1:A:337:LYS:HB2 | 2.20 | 0.41 |
| 1:A:663:ILE:HB | 1:A:666:PHE:CD2 | 2.54 | 0.41 |
| 1:A:697:ASP:HB3 | 1:A:700:LYS:HG3 | 2.02 | 0.41 |
| 1:A:746:ARG:O | 1:A:749:VAL:HB | 2.21 | 0.41 |
| 1:A:950:GLU:O | 1:A:956:PRO:HD2 | 2.21 | 0.41 |
| 1:A:963:LYS:HG2 | 1:A:1007:VAL:HG13 | 2.02 | 0.41 |
| 1:A:2295:GLN:OE1 | 1:A:2295:GLN:N | 2.54 | 0.41 |
| 1:A:2392:VAL:HA | 1:A:2431:ARG:HH22 | 1.86 | 0.41 |
| 1:A:2398:LEU:O | 1:A:2402:LEU:N | 2.48 | 0.41 |
| 1:A:2986:PRO:HG3 | 1:A:2994:TRP:CH2 | 2.56 | 0.41 |
| 1:A:3247:ARG:HH12 | 1:A:3248:LYS:HG2 | 1.86 | 0.41 |
| 1:A:3677:PRO:HB2 | 1:A:3682:GLU:HG2 | 2.02 | 0.41 |
| 1:A:3692:VAL:HB | 1:A:3721:GLY:H | 1.86 | 0.41 |
| 1:A:3749:PRO:HG2 | 1:A:3805:TRP:C | 2.46 | 0.41 |
| 1:A:3821:SER:OG | 1:A:3824:GLU:HB3 | 2.20 | 0.41 |
| 1:A:4039:TYR:HB2 | 1:A:4042:GLN:HE22 | 1.85 | 0.41 |
| 3:C:533:ILE:HG23 | 3:C:537:PHE:CD2 | 2.56 | 0.41 |
| 3:C:642:PHE:HD2 | 3:C:655:PHE:HE2 | 1.67 | 0.41 |
| 5:G:187:LYS:HD2 | 5:G:190:LYS:HE2 | 2.02 | 0.41 |
| 3:L:59:PHE:HB3 | 3:L:110:ALA:HB2 | 2.02 | 0.41 |
| 6:R:884:ARG:HD3 | 6:R:884:ARG:HA | 1.95 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:410:MET:N | 1:S:411:PRO:HD2 | 2.36 | 0.41 |
| 1:S:718:MET:HE2 | 1:S:726:LEU:HD11 | 2.01 | 0.41 |
| 1:S:1096:VAL:HG21 | 1:S:1141:LYS:HE3 | 2.03 | 0.41 |
| 1:S:1184:ARG:NH2 | 1:S:1265:GLU:HB3 | 2.35 | 0.41 |
| 1:S:1762:MET:HA | 1:S:1765:VAL:HG12 | 2.02 | 0.41 |
| 1:S:1783:ARG:HA | 1:S:1783:ARG:HD2 | 1.87 | 0.41 |
| 1:S:2574:ASN:HA | 1:S:2575:PRO:HD3 | 1.96 | 0.41 |
| 1:S:3034:PRO:O | 1:S:3038:GLU:HG3 | 2.20 | 0.41 |
| 2:T:259:LEU:HD13 | 2:T:273:ILE:HD13 | 2.03 | 0.41 |
| 1:A:152:LEU:O | 1:A:155:LYS:HG2 | 2.20 | 0.41 |
| 1:A:411:PRO:HB2 | 1:A:456:VAL:HG12 | 2.03 | 0.41 |
| 1:A:479:ILE:HA | 1:A:482:VAL:HG22 | 2.03 | 0.41 |
| 1:A:730:LEU:HA | 1:A:733:LEU:HB2 | 2.02 | 0.41 |
| 1:A:767:GLU:OE2 | 1:A:771:ASN:ND2 | 2.39 | 0.41 |
| 1:A:1183:CYS:O | 1:A:1186:LYS:HG2 | 2.20 | 0.41 |
| 1:A:1400:VAL:HA | 1:A:1403:MET:HE2 | 2.03 | 0.41 |
| 1:A:1570:GLU:HA | 1:A:1573:LYS:HE2 | 2.02 | 0.41 |
| 1:A:2225:HIS:N | 1:A:2231:PHE:HB2 | 2.36 | 0.41 |
| 1:A:2399:GLU:HA | 1:A:2402:LEU:CD1 | 2.49 | 0.41 |
| 1:A:2796:ALA:O | 1:A:2800:ARG:HG2 | 2.20 | 0.41 |
| 1:A:2886:GLN:O | 1:A:2890:ILE:HG13 | 2.21 | 0.41 |
| 1:A:3326:GLN:O | 1:A:3329:LEU:HG | 2.21 | 0.41 |
| 1:A:3692:VAL:HA | 1:A:3696:ARG:HH22 | 1.86 | 0.41 |
| 1:A:4095:GLU:O | 1:A:4098:LEU:HB3 | 2.20 | 0.41 |
| 2:B:90:THR:OG1 | 2:B:135:MET:HE3 | 2.20 | 0.41 |
| 2:B:106:GLN:NE2 | 2:B:118:GLU:OE1 | 2.54 | 0.41 |
| 2:B:299:LYS:O | 3:C:294:VAL:N | 2.44 | 0.41 |
| 2:B:325:ARG:NE | 3:C:498:ALA:HA | 2.36 | 0.41 |
| 2:B:383:SER:HB3 | 3:C:438:LEU:HD11 | 2.02 | 0.41 |
| 2:B:477:SER:HB3 | 4:D:198:GLY:N | 2.30 | 0.41 |
| 2:B:477:SER:HA | 4:D:196:ALA:HA | 2.02 | 0.41 |
| 2:B:492:ALA:O | 2:B:496:ASP:N | 2.54 | 0.41 |
| 3:C:12:LEU:N | 3:C:55:ALA:O | 2.52 | 0.41 |
| 3:C:247:TRP:CE2 | 3:C:338:LYS:HE3 | 2.56 | 0.41 |
| 3:C:340:PHE:HD1 | 3:C:395:TYR:HA | 1.86 | 0.41 |
| 4:D:114:GLY:N | 4:D:115:PRO:HD2 | 2.36 | 0.41 |
| 5:G:131:LEU:HD11 | 5:H:19:PHE:CE1 | 2.56 | 0.41 |
| 5:G:186:GLU:O | 5:G:189:THR:OG1 | 2.36 | 0.41 |
| 3:L:202:LYS:O | 3:L:206:GLU:HG2 | 2.20 | 0.41 |
| 3:L:291:LYS:HB3 | 3:L:291:LYS:HE3 | 1.93 | 0.41 |
| 3:L:353:ARG:NH2 | 2:T:361:TYR:HB2 | 2.36 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:492:GLN:O | 3:L:495:LEU:HG | 2.21 | 0.41 |
| 3:L:599:ARG:O | 3:L:603:LYS:HG2 | 2.21 | 0.41 |
| 5:Q:69:GLU:HA | 5:Q:72:LYS:HG2 | 2.03 | 0.41 |
| 1:S:36:ARG:HE | 1:S:40:GLN:HG2 | 1.86 | 0.41 |
| 1:S:166:ILE:N | 1:S:167:PRO:HD3 | 2.35 | 0.41 |
| 1:S:484:HIS:O | 1:S:488:ILE:HG13 | 2.21 | 0.41 |
| 1:S:625:ASN:HA | 1:S:628:GLU:HG2 | 2.03 | 0.41 |
| 1:S:727:ALA:O | 1:S:730:LEU:HG | 2.21 | 0.41 |
| 1:S:901:MET:C | 1:S:902:LYS:HD2 | 2.46 | 0.41 |
| 1:S:1020:PRO:HA | 1:S:1073:PHE:CZ | 2.55 | 0.41 |
| 1:S:1137:ILE:HA | 1:S:1140:LYS:HE2 | 2.03 | 0.41 |
| 1:S:1630:ASP:HA | 1:S:1633:TRP:HE1 | 1.85 | 0.41 |
| 1:S:1630:ASP:HA | 1:S:1633:TRP:NE1 | 2.35 | 0.41 |
| 1:S:1682:THR:HA | 1:S:1689:LYS:NZ | 2.36 | 0.41 |
| 1:S:1751:GLU:HG3 | 1:S:1785:ILE:HG23 | 2.03 | 0.41 |
| 1:S:1935:GLU:OE1 | 1:S:1935:GLU:N | 2.54 | 0.41 |
| 1:S:2246:LYS:HD3 | 1:S:2285:LEU:HD21 | 2.03 | 0.41 |
| 1:S:2376:ASP:HA | 1:S:2379:MET:HE2 | 2.03 | 0.41 |
| 1:S:2531:LEU:HD23 | 1:S:2531:LEU:HA | 1.92 | 0.41 |
| 1:S:2563:LEU:HD22 | 1:S:2795:GLN:CD | 2.46 | 0.41 |
| 1:S:2931:ARG:HH22 | 1:S:2996:LEU:HD13 | 1.86 | 0.41 |
| 1:S:2943:PHE:CE2 | 1:S:2947:ILE:HG22 | 2.55 | 0.41 |
| 1:S:3012:GLU:O | 1:S:3016:THR:HG23 | 2.21 | 0.41 |
| 1:S:3013:TYR:HA | 1:S:3016:THR:HG23 | 2.03 | 0.41 |
| 1:S:3091:LEU:HD21 | 1:S:3142:ILE:HG12 | 2.03 | 0.41 |
| 1:S:3259:LEU:HD21 | 1:S:3283:LEU:HD23 | 2.03 | 0.41 |
| 1:S:3266:SER:CB | 1:S:3273:LEU:HA | 2.50 | 0.41 |
| 1:S:3371:GLU:O | 1:S:3374:ILE:HG12 | 2.21 | 0.41 |
| 1:S:3462:ARG:NE | 1:S:3494:GLN:HB2 | 2.36 | 0.41 |
| 1:S:3551:ASN:O | 1:S:3555:VAL:HG22 | 2.21 | 0.41 |
| 1:S:3741:ARG:CZ | 1:S:3747:GLU:HB3 | 2.51 | 0.41 |
| 1:S:3772:ASN:HB3 | 1:S:3787:GLN:HE22 | 1.86 | 0.41 |
| 1:S:4055:ASN:ND2 | 1:S:4058:VAL:HG23 | 2.36 | 0.41 |
| 1:S:4062:ASP:OD1 | 1:S:4063:GLU:N | 2.53 | 0.41 |
| 1:S:4109:ASP:O | 1:S:4114:PRO:HD3 | 2.20 | 0.41 |
| 2:T:69:SER:HB2 | 2:T:245:LYS:HD2 | 2.03 | 0.41 |
| 2:T:92:LYS:HD2 | 2:T:135:MET:HA | 2.01 | 0.41 |
| 2:T:160:LYS:HD2 | 2:T:161:MET:H | 1.86 | 0.41 |
| 7:d:18:DA:C6 | 7:d:19:DA:N6 | 2.87 | 0.41 |
| 1:A:24:ARG:NH1 | 1:A:25:CYS:HB3 | 2.36 | 0.41 |
| 1:A:85:ILE:O | 1:A:89:LEU:HG | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:194:GLU:HA | 1:A:197:PHE:CD2 | 2.55 | 0.41 |
| 1:A:452:LYS:O | 1:A:456:VAL:HG23 | 2.20 | 0.41 |
| 1:A:699:GLU:O | 1:A:702:SER:OG | 2.30 | 0.41 |
| 1:A:943:GLY:HA3 | 1:A:2783:ILE:HD13 | 2.03 | 0.41 |
| 1:A:1465:HIS:HA | 1:A:1468:LEU:O | 2.20 | 0.41 |
| 1:A:1482:GLU:H | 1:A:1482:GLU:CD | 2.26 | 0.41 |
| 1:A:1563:PHE:HB3 | 1:A:1566:THR:OG1 | 2.21 | 0.41 |
| 1:A:1766:LEU:O | 1:A:1772:HIS:HE1 | 2.04 | 0.41 |
| 1:A:1829:TRP:CE3 | 1:A:1829:TRP:HA | 2.55 | 0.41 |
| 1:A:2809:PHE:HA | 1:A:2812:LEU:HG | 2.03 | 0.41 |
| 1:A:3040:TYR:C | 1:A:3044:MET:HG2 | 2.45 | 0.41 |
| 1:A:3466:PRO:O | 1:A:3470:GLN:HG2 | 2.21 | 0.41 |
| 1:A:3502:MET:HA | 1:A:3505:LEU:HB2 | 2.02 | 0.41 |
| 1:A:3962:ARG:HE | 1:A:3962:ARG:HB3 | 1.63 | 0.41 |
| 1:A:4082:ARG:O | 1:A:4110:GLN:HB2 | 2.21 | 0.41 |
| 2:B:318:ARG:HD3 | 2:B:318:ARG:N | 2.36 | 0.41 |
| 2:B:426:GLN:HB2 | 3:C:434:MET:CE | 2.51 | 0.41 |
| 2:B:480:ASN:ND2 | 3:C:402:ASN:HD21 | 2.18 | 0.41 |
| 6:I:700:VAL:O | 6:I:721:VAL:HG12 | 2.21 | 0.41 |
| 1:S:42:CYS:HA | 1:S:88:PHE:CE1 | 2.56 | 0.41 |
| 1:S:566:ASP:O | 1:S:570:LYS:HG3 | 2.20 | 0.41 |
| 1:S:657:SER:HA | 1:S:666:PHE:CD2 | 2.56 | 0.41 |
| 1:S:759:GLY:HA3 | 1:S:766:ALA:HB2 | 2.02 | 0.41 |
| 1:S:1057:LYS:HG2 | 1:S:1099:PHE:CE2 | 2.56 | 0.41 |
| 1:S:1921:ASP:OD1 | 1:S:1922:ALA:N | 2.53 | 0.41 |
| 1:S:2436:LEU:CD2 | 1:S:2472:GLN:HB3 | 2.39 | 0.41 |
| 1:S:3240:MET:HG2 | 1:S:3272:TRP:HZ3 | 1.85 | 0.41 |
| 1:S:3364:GLY:HA2 | 1:S:3376:GLY:HA3 | 2.02 | 0.41 |
| 1:S:3530:VAL:HG12 | 1:S:3562:LEU:HB3 | 2.03 | 0.41 |
| 1:S:3662:ILE:HA | 1:S:3665:MET:HE2 | 2.01 | 0.41 |
| 1:S:3923:ARG:O | 1:S:3962:ARG:NE | 2.54 | 0.41 |
| 1:S:3956:PRO:HD2 | 1:S:4121:TRP:CE3 | 2.56 | 0.41 |
| 1:S:4098:LEU:HD23 | 1:S:4098:LEU:H | 1.86 | 0.41 |
| 9:i:36:DA:N6 | 10:j:22:DG:C6 | 2.90 | 0.41 |
| 1:A:117:LYS:O | 1:A:120:ALA:N | 2.38 | 0.40 |
| 1:A:475:LEU:HD12 | 1:A:476:ARG:N | 2.35 | 0.40 |
| 1:A:714:VAL:HG23 | 1:A:733:LEU:HD11 | 2.04 | 0.40 |
| 1:A:1416:GLU:HG3 | 1:A:1420:ARG:HH22 | 1.84 | 0.40 |
| 1:A:1538:LEU:HB3 | 1:A:1553:PHE:CE2 | 2.56 | 0.40 |
| 1:A:1769:GLU:O | 1:A:1822:ARG:NH1 | 2.50 | 0.40 |
| 1:A:3141:PHE:HA | 1:A:3144:PHE:CZ | 2.56 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3353:GLU:CD | 1:A:3358:ARG:HH12 | 2.25 | 0.40 |
| 1:A:3582:GLU:HG2 | 1:A:3668:LEU:HD12 | 2.03 | 0.40 |
| 1:A:3583:LEU:HB3 | 1:A:3733:ARG:CZ | 2.51 | 0.40 |
| 1:A:3733:ARG:HB3 | 1:A:3754:GLY:HA3 | 2.01 | 0.40 |
| 1:A:3736:LYS:O | 1:A:3751:LEU:HA | 2.21 | 0.40 |
| 1:A:3812:LEU:CB | 1:A:3925:LEU:HD21 | 2.49 | 0.40 |
| 1:A:3870:SER:HA | 1:A:3873:LYS:HE2 | 2.03 | 0.40 |
| 1:A:4040:PRO:O | 1:A:4044:ILE:HG23 | 2.21 | 0.40 |
| 2:B:118:GLU:O | 2:B:121:GLN:HG2 | 2.21 | 0.40 |
| 3:C:236:VAL:CA | 11:f:298:PHE:HA | 2.46 | 0.40 |
| 3:C:336:GLU:HB2 | 3:C:339:CYS:SG | 2.61 | 0.40 |
| 4:D:194:LYS:HE3 | 4:D:195:PRO:O | 2.21 | 0.40 |
| 5:H:197:LYS:HA | 5:H:200:ASN:HD21 | 1.86 | 0.40 |
| 5:Q:55:GLU:OE1 | 5:Q:66:TYR:OH | 2.23 | 0.40 |
| 6:R:801:TYR:HB2 | 6:R:802:ARG:HH11 | 1.87 | 0.40 |
| 1:S:434:VAL:O | 1:S:438:LEU:N | 2.49 | 0.40 |
| 1:S:943:GLY:O | 1:S:947:GLN:HB2 | 2.21 | 0.40 |
| 1:S:1923:PHE:HD1 | 1:S:1941:HIS:HB3 | 1.86 | 0.40 |
| 1:S:2404:ARG:HB3 | 1:S:2407:GLY:HA3 | 2.02 | 0.40 |
| 1:S:2928:LYS:HA | 1:S:2931:ARG:HE | 1.85 | 0.40 |
| 1:S:3107:ILE:CG1 | 1:S:3135:LEU:HD11 | 2.51 | 0.40 |
| 1:S:3644:PHE:CZ | 1:S:3660:ASN:HA | 2.56 | 0.40 |
| 1:S:3763:ARG:O | 1:S:3767:LEU:HG | 2.21 | 0.40 |
| 1:S:3946:PHE:CZ | 1:S:4047:ALA:HB2 | 2.56 | 0.40 |
| 1:S:4127:TRP:CD1 | 1:S:4128:MET:H | 2.40 | 0.40 |
| 1:A:1412:LYS:NZ | 1:A:1416:GLU:OE1 | 2.53 | 0.40 |
| 1:A:1819:PHE:HZ | 3:C:625:ASP:HB3 | 1.86 | 0.40 |
| 1:A:1881:TYR:HB2 | 1:A:1950:SER:HB2 | 2.03 | 0.40 |
| 1:A:2376:ASP:HB3 | 1:A:2404:ARG:NH2 | 2.35 | 0.40 |
| 1:A:3483:MET:HE1 | 1:A:3511:ALA:O | 2.22 | 0.40 |
| 1:A:3492:CYS:HB2 | 1:A:3709:GLY:CA | 2.49 | 0.40 |
| 1:A:3967:PHE:O | 1:A:3970:LEU:HD22 | 2.22 | 0.40 |
| 1:A:4006:VAL:HB | 1:A:4009:PRO:HD3 | 2.03 | 0.40 |
| 1:A:4055:ASN:ND2 | 1:A:4057:ALA:HB3 | 2.36 | 0.40 |
| 2:B:304:ASN:N | 2:B:311:LEU:HG | 2.36 | 0.40 |
| 2:B:346:MET:O | 2:B:399:ARG:N | 2.32 | 0.40 |
| 2:B:363:ARG:HA | 3:C:359:ASN:HA | 2.03 | 0.40 |
| 3:C:88:PHE:HA | 3:C:91:LEU:HD12 | 2.03 | 0.40 |
| 3:C:510:GLN:NE2 | 3:C:513:TRP:HB2 | 2.36 | 0.40 |
| 5:H:1:MET:HE3 | 5:H:3:ARG:NH1 | 2.37 | 0.40 |
| 5:H:72:LYS:HD3 | 5:H:72:LYS:HA | 1.79 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:I:864:ILE:HA | 6:I:889:LEU:HD13 | 2.03 | 0.40 |
| 3:L:122:THR:HA | 3:L:127:PHE:CE2 | 2.56 | 0.40 |
| 3:L:274:LYS:O | 2:T:320:GLN:NE2 | 2.55 | 0.40 |
| 3:L:383:ALA:HB3 | 2:T:462:MET:CE | 2.51 | 0.40 |
| 1:S:201:LEU:HD22 | 1:S:249:PHE:CE2 | 2.56 | 0.40 |
| 1:S:288:ASP:OD1 | 1:S:288:ASP:N | 2.49 | 0.40 |
| 1:S:370:ALA:HA | 1:S:373:CYS:HB3 | 2.03 | 0.40 |
| 1:S:433:PRO:O | 1:S:436:GLU:HB3 | 2.21 | 0.40 |
| 1:S:614:PRO:HB3 | 1:S:620:PHE:CE1 | 2.56 | 0.40 |
| 1:S:763:THR:OG1 | 1:S:764:PRO:HD3 | 2.20 | 0.40 |
| 1:S:936:SER:HB3 | 1:S:2773:ARG:HD2 | 2.02 | 0.40 |
| 1:S:1092:GLU:HG3 | 1:S:1095:LEU:H | 1.86 | 0.40 |
| 1:S:1279:LEU:HB3 | 1:S:1356:TRP:HE1 | 1.87 | 0.40 |
| 1:S:1341:ILE:O | 1:S:1345:THR:HG23 | 2.20 | 0.40 |
| 1:S:1372:LEU:O | 1:S:1375:THR:HB | 2.21 | 0.40 |
| 1:S:1448:LEU:O | 1:S:1452:VAL:HG23 | 2.21 | 0.40 |
| 1:S:1744:LYS:HE2 | 1:S:1744:LYS:HB3 | 1.88 | 0.40 |
| 1:S:2595:TRP:HE3 | 1:S:2765:GLN:HB3 | 1.86 | 0.40 |
| 1:S:2830:ASN:CG | 1:S:2834:GLN:HE22 | 2.29 | 0.40 |
| 1:S:3285:HIS:HB2 | 1:S:3301:LEU:HD23 | 2.03 | 0.40 |
| 1:S:3924:HIS:CD2 | 1:S:3926:ASN:HB2 | 2.56 | 0.40 |
| 1:S:4115:ASN:OD1 | 1:S:4116:ILE:N | 2.53 | 0.40 |
| 2:T:329:LEU:HG | 2:T:330:GLU:H | 1.86 | 0.40 |
| 2:T:458:GLN:HG3 | 2:T:528:LEU:HD13 | 2.03 | 0.40 |
| 2:T:484:GLN:HB3 | 2:T:488:ARG:CZ | 2.51 | 0.40 |
| 7:d:23:DT:H72 | 8:e:34:DC:C2 | 2.56 | 0.40 |
| 1:A:637:LYS:HA | 1:A:637:LYS:HD2 | 1.80 | 0.40 |
| 1:A:935:HIS:HD2 | 1:A:2773:ARG:HE | 1.68 | 0.40 |
| 1:A:1002:GLU:C | 1:A:1004:GLN:H | 2.30 | 0.40 |
| 1:A:1092:GLU:OE2 | 1:A:1094:SER:OG | 2.39 | 0.40 |
| 1:A:1256:TRP:HE1 | 1:A:1260:LEU:HD21 | 1.87 | 0.40 |
| 1:A:1474:ASP:OD1 | 1:A:1474:ASP:N | 2.52 | 0.40 |
| 1:A:1665:HIS:O | 1:A:1668:PHE:HB3 | 2.22 | 0.40 |
| 1:A:1833:LEU:O | 1:A:1836:LEU:HB3 | 2.21 | 0.40 |
| 1:A:2219:LEU:HA | 1:A:2222:HIS:HB2 | 2.03 | 0.40 |
| 1:A:2227:LYS:C | 1:A:2229:ALA:H | 2.28 | 0.40 |
| 1:A:2745:ARG:HG3 | 8:e:44:DG:C2 | 2.55 | 0.40 |
| 1:A:3327:ASN:HB2 | 1:A:3388:ALA:HB2 | 2.03 | 0.40 |
| 1:A:4044:ILE:HG13 | 1:A:4048:LYS:NZ | 2.35 | 0.40 |
| 2:B:321:ILE:HA | 2:B:326:GLN:HA | 2.03 | 0.40 |
| 2:B:389:CYS:O | 2:B:393:GLU:N | 2.53 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:407:PRO:HG2 | 3:C:486:ARG:NE | 2.36 | 0.40 |
| 2:B:459:VAL:HG12 | 2:B:463:LYS:HE3 | 2.03 | 0.40 |
| 4:D:13:PRO:HG3 | 4:D:83:GLN:HB3 | 2.03 | 0.40 |
| 6:I:659:PHE:HB2 | 6:I:685:PHE:O | 2.22 | 0.40 |
| 6:I:706:ASN:H | 6:I:709:VAL:CG2 | 2.34 | 0.40 |
| 6:I:774:LEU:HA | 6:I:777:VAL:HG12 | 2.03 | 0.40 |
| 3:L:350:GLN:OE1 | 2:T:473:TYR:N | 2.55 | 0.40 |
| 3:L:481:LYS:C | 2:T:440:ALA:HB2 | 2.47 | 0.40 |
| 3:L:686:ILE:HD12 | 3:L:702:LYS:HG3 | 2.04 | 0.40 |
| 5:P:18:HIS:CE1 | 5:P:36:LEU:HD22 | 2.57 | 0.40 |
| 1:S:157:TYR:O | 1:S:160:LEU:HG | 2.21 | 0.40 |
| 1:S:320:LEU:HB3 | 1:S:368:LEU:HD11 | 2.03 | 0.40 |
| 1:S:446:PHE:HB3 | 1:S:527:TYR:HE1 | 1.86 | 0.40 |
| 1:S:871:LEU:HD21 | 1:S:3125:ARG:HG3 | 2.02 | 0.40 |
| 1:S:934:LEU:O | 1:S:938:VAL:HG22 | 2.22 | 0.40 |
| 1:S:1057:LYS:HG2 | 1:S:1099:PHE:HE2 | 1.87 | 0.40 |
| 1:S:1331:ASN:C | 1:S:1331:ASN:HD22 | 2.29 | 0.40 |
| 1:S:1582:LEU:HD11 | 1:S:1593:VAL:HA | 2.02 | 0.40 |
| 1:S:2220:MET:HE1 | 1:S:2238:ILE:HG13 | 2.03 | 0.40 |
| 1:S:2291:GLN:CD | 1:S:2292:CYS:H | 2.29 | 0.40 |
| 1:S:2742:MET:HE1 | 1:S:2745:ARG:HH11 | 1.86 | 0.40 |
| 1:S:2750:GLU:O | 1:S:2754:GLU:HG3 | 2.21 | 0.40 |
| 1:S:3177:ASN:HA | 1:S:3180:ASP:OD2 | 2.21 | 0.40 |
| 1:S:3285:HIS:HA | 1:S:3296:GLN:HE22 | 1.87 | 0.40 |
| 1:S:3636:PHE:CG | 1:S:3670:MET:HE1 | 2.56 | 0.40 |
| 1:S:3924:HIS:HD2 | 1:S:3926:ASN:N | 2.20 | 0.40 |
| 7:d:34:DT:H2' | 7:d:35:DT:N3 | 2.37 | 0.40 |
| 10:j:35:DT:N3 | 10:j:36:DG:O6 | 2.54 | 0.40 |
| 1:A:565:TYR:OH | 1:A:642:PHE:HB2 | 2.22 | 0.40 |
| 1:A:935:HIS:CE1 | 1:A:987:LEU:HD22 | 2.56 | 0.40 |
| 1:A:1750:LEU:HD13 | 1:A:1758:LEU:HD12 | 2.03 | 0.40 |
| 1:A:1840:PHE:O | 1:A:1844:VAL:HG23 | 2.21 | 0.40 |
| 1:A:2429:ASP:OD1 | 1:A:2430:GLU:N | 2.52 | 0.40 |
| 1:A:2548:PRO:HB2 | 1:A:2848:PHE:CD1 | 2.56 | 0.40 |
| 1:A:2935:GLU:HG3 | 1:A:2938:VAL:HG22 | 2.03 | 0.40 |
| 1:A:3519:GLU:OE2 | 1:A:3561:LYS:NZ | 2.42 | 0.40 |
| 1:A:3929:MET:HB2 | 1:A:3938:ILE:HD11 | 2.03 | 0.40 |
| 1:A:4098:LEU:HD11 | 1:A:4103:GLN:HA | 2.02 | 0.40 |
| 2:B:290:ARG:O | 6:I:691:GLN:HB2 | 2.22 | 0.40 |
| 2:B:318:ARG:HH21 | 2:B:330:GLU:HA | 1.86 | 0.40 |
| 3:C:639:ILE:HD13 | 3:C:639:ILE:HA | 1.88 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:27:ILE:HG12 | 3:L:193:PRO:HD3 | 2.04 | 0.40 |
| 3:L:165:LEU:HD23 | 3:L:201:GLN:HE21 | 1.86 | 0.40 |
| 3:L:280:ASP:OD1 | 3:L:281:ALA:N | 2.54 | 0.40 |
| 1:S:670:LEU:CB | 1:S:732:PHE:HE2 | 2.33 | 0.40 |
| 1:S:2428:ASP:O | 1:S:2432:GLN:HG2 | 2.22 | 0.40 |
| 1:S:3300:VAL:O | 1:S:3300:VAL:HG13 | 2.21 | 0.40 |
| 1:S:3499:ILE:HD13 | 1:S:3521:ILE:HG21 | 2.04 | 0.40 |
| 1:S:3869:THR:HG22 | 1:S:3873:LYS:NZ | 2.36 | 0.40 |
| 2:T:212:ASP:OD1 | 2:T:213:ILE:N | 2.55 | 0.40 |
| 2:T:476:ASP:OD1 | 2:T:476:ASP:N | 2.54 | 0.40 |
| 8:e:31:DA:H2" | 8:e:32:DA:H8 | 1.83 | 0.40 |
| 1:A:421:LEU:HD13 | 1:A:424:LEU:HD23 | 2.02 | 0.40 |
| 1:A:433:PRO:O | 1:A:436:GLU:HG3 | 2.21 | 0.40 |
| 1:A:465:PHE:HA | 1:A:468:LEU:HG | 2.03 | 0.40 |
| 1:A:893:SER:H | 1:A:944:LYS:NZ | 2.19 | 0.40 |
| 1:A:1191:PHE:HA | 1:A:1194:PHE:CD2 | 2.57 | 0.40 |
| 1:A:1222:ASN:C | 1:A:1222:ASN:HD22 | 2.28 | 0.40 |
| 1:A:1389:VAL:HG23 | 1:A:1391:VAL:HG12 | 2.03 | 0.40 |
| 1:A:1952:ILE:HD12 | 1:A:1961:PHE:CE1 | 2.56 | 0.40 |
| 1:A:2216:LEU:HD11 | 1:A:2249:LEU:HD22 | 2.04 | 0.40 |
| 1:A:2597:PHE:HE2 | 1:A:2766:ASP:N | 2.17 | 0.40 |
| 1:A:3149:GLY:O | 1:A:3153:SER:HB2 | 2.21 | 0.40 |
| 1:A:3252:PHE:HA | 1:A:3287:ARG:CZ | 2.51 | 0.40 |
| 1:A:3818:ASN:OD1 | 1:A:3819:THR:N | 2.55 | 0.40 |
| 3:C:148:ASP:N | 3:C:148:ASP:OD1 | 2.54 | 0.40 |
| 3:C:223:GLU:OE1 | 11:f:295:ARG:HB2 | 2.20 | 0.40 |
| 3:C:406:GLY:HA3 | 3:C:421:TYR:CZ | 2.56 | 0.40 |
| 5:H:95:PHE:HE2 | 5:H:111:PHE:HD2 | 1.69 | 0.40 |
| 6:I:841:LYS:HZ1 | 6:I:867:GLU:N | 2.19 | 0.40 |
| 3:L:134:ILE:HG22 | 3:L:136:THR:OG1 | 2.21 | 0.40 |
| 3:L:355:PHE:O | 3:L:425:PRO:HD3 | 2.22 | 0.40 |
| 1:S:11:SER:HA | 1:S:14:ARG:HG3 | 2.04 | 0.40 |
| 1:S:174:VAL:HA | 1:S:177:LEU:HD12 | 2.03 | 0.40 |
| 1:S:637:LYS:O | 1:S:679:LYS:NZ | 2.54 | 0.40 |
| 1:S:888:ARG:NE | 1:S:3890:MET:HE1 | 2.37 | 0.40 |
| 1:S:913:ARG:NH1 | 1:S:2801:ASP:OD2 | 2.47 | 0.40 |
| 1:S:994:TRP:NE1 | 1:S:2581:LEU:HD21 | 2.37 | 0.40 |
| 1:S:1207:TRP:O | 1:S:1211:VAL:HG23 | 2.21 | 0.40 |
| 1:S:1301:ILE:HG21 | 1:S:1371:VAL:HG21 | 2.03 | 0.40 |
| 1:S:1457:GLN:HA | 1:S:1460:ARG:CZ | 2.51 | 0.40 |
| 1:S:2344:LEU:CA | 1:S:2347:LYS:HZ3 | 2.33 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2569:SER:OG | 1:S:2571:ASP:OD1 | 2.40 | 0.40 |
| 1:S:2571:ASP:OD1 | 1:S:2571:ASP:N | 2.51 | 0.40 |
| 1:S:2816:ILE:HD12 | 1:S:2816:ILE:HA | 1.96 | 0.40 |
| 1:S:2938:VAL:HG23 | 1:S:3979:LEU:CD2 | 2.47 | 0.40 |
| 1:S:2950:LYS:HB3 | 1:S:2952:ILE:HG22 | 2.03 | 0.40 |
| 1:S:2975:ALA:HA | 1:S:2981:TRP:CZ2 | 2.56 | 0.40 |
| 1:S:3410:ILE:HD11 | 1:S:3456:LEU:HD13 | 2.03 | 0.40 |
| 1:S:3502:MET:O | 1:S:3506:LEU:N | 2.54 | 0.40 |
| 1:S:4048:LYS:HB3 | 1:S:4048:LYS:HE3 | 1.95 | 0.40 |
| 2:T:125:GLN:OE1 | 2:T:128:GLN:NE2 | 2.55 | 0.40 |
| 2:T:131:PHE:O | 2:T:135:MET:N | 2.54 | 0.40 |
| 2:T:301:ARG:HB2 | 2:T:310:LEU:HD11 | 2.03 | 0.40 |
| 2:T:416:GLN:O | 2:T:431:GLY:N | 2.54 | 0.40 |
| 7:d:16:DA:N1 | 8:e:42:DA:C6 | 2.90 | 0.40 |
| 7:d:16:DA:N6 | 8:e:42:DA:N1 | 2.70 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 3473/4128 (84%) | 3140 (90%) | 330 (10%) | 3 (0%) | 48 | 82 |
| 1 | S | 3462/4128 (84%) | 3180 (92%) | 280 (8%) | 2 (0%) | 48 | 82 |
| 2 | B | 505/609 (83%) | 468 (93%) | 37 (7%) | 0 | 100 | 100 |
| 2 | T | 498/609 (82%) | 468 (94%) | 30 (6%) | 0 | 100 | 100 |
| 3 | C | 660/732 (90%) | 619 (94%) | 41 (6%) | 0 | 100 | 100 |
| 3 | L | 644/732 (88%) | 608 (94%) | 35 (5%) | 1 (0%) | 43 | 77 |
| 4 | D | 139/204 (68%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 4 | M | 160/204 (78%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 5 | G | 199/336 (59%) | 195 (98%) | 4 (2%) | 0 | 100 | 100 |
| 5 | H | 190/336 (56%) | 188 (99%) | 2 (1%) | 0 | 100 | 100 |
| 5 | P | 199/336 (59%) | 196 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | Q | 190/336 (56%) | 184 (97%) | 6 (3%) | 0 | 100 | 100 |
| 6 | I | 242/911 (27%) | 213 (88%) | 29 (12%) | 0 | 100 | 100 |
| 6 | R | 242/911 (27%) | 215 (89%) | 27 (11%) | 0 | 100 | 100 |
| 11 | f | 5/299 (2%) | 3 (60%) | 2 (40%) | 0 | 100 | 100 |
| 11 | m | 5/299 (2%) | 4 (80%) | 1 (20%) | 0 | 100 | 100 |
| All | All | 10813/15110 (72%) | 9969 (92%) | 838 (8%) | 6 (0%) | 49 | 82 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3304 | VAL |
| 1 | S | 3304 | VAL |
| 1 | A | 1960 | LYS |
| 3 | L | 236 | VAL |
| 1 | S | 956 | PRO |
| 1 | A | 956 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 3123/3671 (85%) | 3121 (100%) | 2 (0%) | 88 | 88 |
| 1 | S | 3142/3671 (86%) | 3142 (100%) | 0 | 100 | 100 |
| 2 | B | 455/548 (83%) | 455 (100%) | 0 | 100 | 100 |
| 2 | T | 452/548 (82%) | 452 (100%) | 0 | 100 | 100 |
| 3 | C | 589/649 (91%) | 589 (100%) | 0 | 100 | 100 |
| 3 | L | 576/649 (89%) | 575 (100%) | 1 (0%) | 87 | 85 |
| 4 | D | 116/160 (72%) | 116 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | M | 127/160 (79%) | 127 (100%) | 0 | 100 | 100 |
| 5 | G | 180/303 (59%) | 180 (100%) | 0 | 100 | 100 |
| 5 | H | 177/303 (58%) | 177 (100%) | 0 | 100 | 100 |
| 5 | P | 179/303 (59%) | 179 (100%) | 0 | 100 | 100 |
| 5 | Q | 175/303 (58%) | 175 (100%) | 0 | 100 | 100 |
| 6 | I | 220/808 (27%) | 220 (100%) | 0 | 100 | 100 |
| 6 | R | 217/808 (27%) | 217 (100%) | 0 | 100 | 100 |
| 11 | f | 6/262 (2%) | 6 (100%) | 0 | 100 | 100 |
| 11 | m | 6/262 (2%) | 6 (100%) | 0 | 100 | 100 |
| All | All | 9740/13408 (73%) | 9737 (100%) | 3 (0%) | 100 | 100 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1958 | GLU |
| 1 | A | 3161 | LEU |
| 3 | L | 233 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 16 | GLN |
| 1 | A | 40 | GLN |
| 1 | A | 192 | ASN |
| 1 | A | 195 | ASN |
| 1 | A | 305 | ASN |
| 1 | A | 339 | GLN |
| 1 | A | 415 | GLN |
| 1 | A | 442 | GLN |
| 1 | A | 448 | GLN |
| 1 | A | 638 | GLN |
| 1 | A | 676 | ASN |
| 1 | A | 839 | ASN |
| 1 | A | 867 | ASN |
| 1 | A | 990 | GLN |
| 1 | A | 1115 | HIS |
| 1 | A | 1133 | HIS |
| 1 | A | 1205 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1222 | ASN |
| 1 | A | 1598 | ASN |
| 1 | A | 1611 | GLN |
| 1 | A | 1624 | GLN |
| 1 | A | 1946 | ASN |
| 1 | A | 2105 | HIS |
| 1 | A | 2213 | ASN |
| 1 | A | 2225 | HIS |
| 1 | A | 2306 | ASN |
| 1 | A | 2365 | ASN |
| 1 | A | 2456 | ASN |
| 1 | A | 2553 | HIS |
| 1 | A | 2831 | ASN |
| 1 | A | 2838 | GLN |
| 1 | A | 2864 | GLN |
| 1 | A | 3081 | HIS |
| 1 | A | 3105 | ASN |
| 1 | A | 3133 | GLN |
| 1 | A | 3185 | ASN |
| 1 | A | 3327 | ASN |
| 1 | A | 3564 | GLN |
| 1 | A | 3766 | GLN |
| 1 | A | 4055 | ASN |
| 1 | A | 4088 | ASN |
| 1 | A | 4092 | GLN |
| 1 | A | 4110 | GLN |
| 2 | B | 106 | GLN |
| 2 | B | 132 | GLN |
| 2 | B | 304 | ASN |
| 2 | B | 359 | HIS |
| 2 | B | 484 | GLN |
| 2 | B | 485 | GLN |
| 2 | B | 489 | ASN |
| 2 | B | 502 | GLN |
| 3 | C | 43 | GLN |
| 3 | C | 162 | GLN |
| 3 | C | 312 | GLN |
| 3 | C | 402 | ASN |
| 3 | C | 432 | GLN |
| 3 | C | 492 | GLN |
| 3 | C | 604 | GLN |
| 3 | C | 663 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 83 | GLN |
| 5 | G | 137 | ASN |
| 5 | G | 145 | GLN |
| 5 | H | 141 | ASN |
| 5 | H | 200 | ASN |
| 6 | I | 673 | GLN |
| 6 | I | 773 | GLN |
| 3 | L | 146 | GLN |
| 3 | L | 162 | GLN |
| 3 | L | 201 | GLN |
| 3 | L | 423 | GLN |
| 3 | L | 484 | ASN |
| 3 | L | 514 | ASN |
| 3 | L | 517 | ASN |
| 3 | L | 653 | GLN |
| 3 | L | 657 | ASN |
| 3 | L | 663 | GLN |
| 5 | P | 159 | GLN |
| 5 | Q | 21 | GLN |
| 6 | R | 716 | ASN |
| 6 | R | 833 | ASN |
| 6 | R | 848 | HIS |
| 1 | S | 192 | ASN |
| 1 | S | 195 | ASN |
| 1 | S | 322 | GLN |
| 1 | S | 415 | GLN |
| 1 | S | 442 | GLN |
| 1 | S | 454 | GLN |
| 1 | S | 656 | GLN |
| 1 | S | 676 | ASN |
| 1 | S | 720 | GLN |
| 1 | S | 739 | ASN |
| 1 | S | 753 | GLN |
| 1 | S | 935 | HIS |
| 1 | S | 953 | GLN |
| 1 | S | 997 | ASN |
| 1 | S | 1043 | GLN |
| 1 | S | 1098 | GLN |
| 1 | S | 1115 | HIS |
| 1 | S | 1126 | GLN |
| 1 | S | 1146 | ASN |
| 1 | S | 1442 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 1465 | HIS |
| 1 | S | 1476 | HIS |
| 1 | S | 1509 | GLN |
| 1 | S | 1574 | ASN |
| 1 | S | 1611 | GLN |
| 1 | S | 1613 | HIS |
| 1 | S | 1625 | HIS |
| 1 | S | 1654 | GLN |
| 1 | S | 1830 | HIS |
| 1 | S | 1963 | GLN |
| 1 | S | 2225 | HIS |
| 1 | S | 2233 | HIS |
| 1 | S | 2234 | ASN |
| 1 | S | 2306 | ASN |
| 1 | S | 2335 | ASN |
| 1 | S | 2390 | HIS |
| 1 | S | 2493 | ASN |
| 1 | S | 2518 | GLN |
| 1 | S | 2560 | ASN |
| 1 | S | 2765 | GLN |
| 1 | S | 2799 | GLN |
| 1 | S | 2807 | GLN |
| 1 | S | 2865 | HIS |
| 1 | S | 2951 | GLN |
| 1 | S | 2971 | GLN |
| 1 | S | 2979 | GLN |
| 1 | S | 3004 | HIS |
| 1 | S | 3059 | GLN |
| 1 | S | 3093 | GLN |
| 1 | S | 3150 | ASN |
| 1 | S | 3249 | GLN |
| 1 | S | 3379 | GLN |
| 1 | S | 3459 | ASN |
| 1 | S | 3510 | GLN |
| 1 | S | 3573 | ASN |
| 1 | S | 3577 | GLN |
| 1 | S | 3660 | ASN |
| 1 | S | 3822 | GLN |
| 1 | S | 3924 | HIS |
| 1 | S | 3926 | ASN |
| 1 | S | 4087 | HIS |
| 1 | S | 4110 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | T | 95 | ASN |
| 2 | T | 125 | GLN |
| 2 | T | 128 | GLN |
| 2 | T | 137 | HIS |
| 2 | T | 174 | ASN |
| 2 | T | 176 | HIS |
| 2 | T | 293 | ASN |
| 2 | T | 326 | GLN |
| 2 | T | 359 | HIS |
| 2 | T | 360 | HIS |
| 2 | T | 426 | GLN |
| 2 | T | 480 | ASN |
| 2 | T | 484 | GLN |
| 2 | T | 485 | GLN |
| 2 | T | 489 | ASN |
| 2 | T | 515 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains

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

### 5.5 Carbohydrates

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

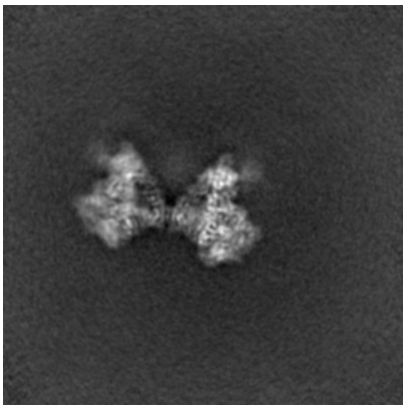
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16074. These allow visual inspection of the internal detail of the map and identification of artifacts.

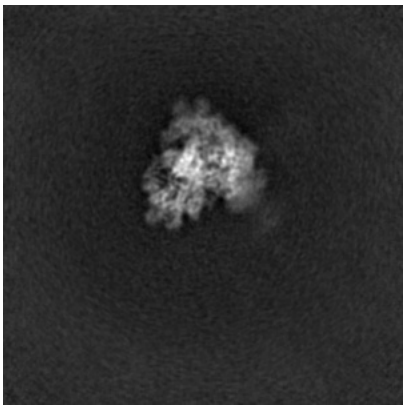
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

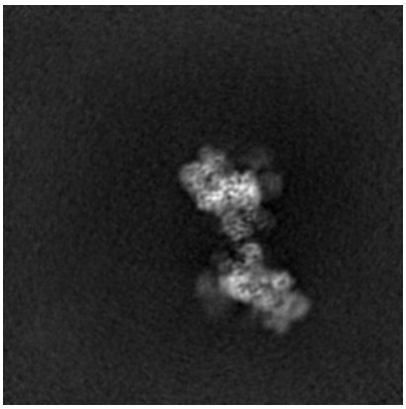
### 6.1.1 Primary map



X

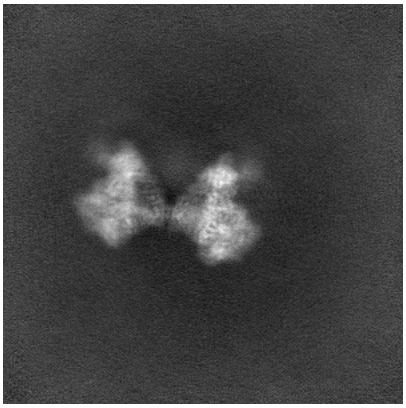


Y

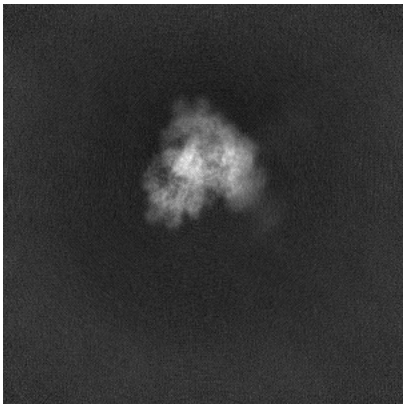


Z

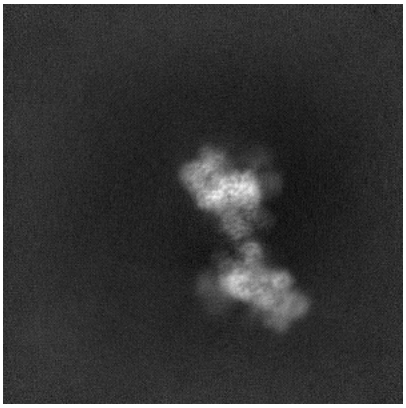
### 6.1.2 Raw map



X



Y

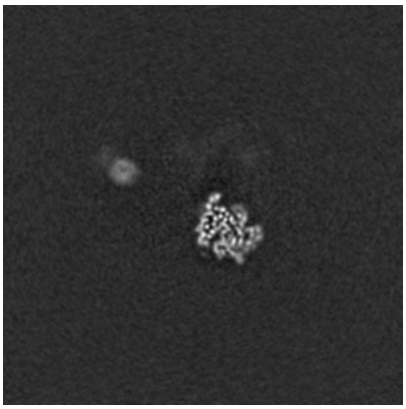


Z

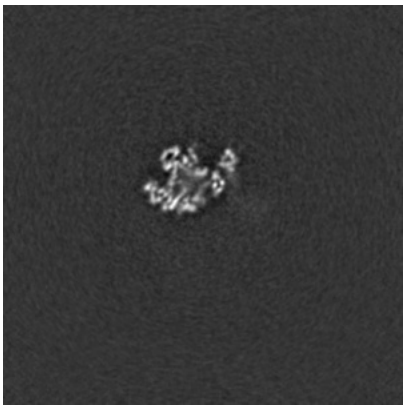
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

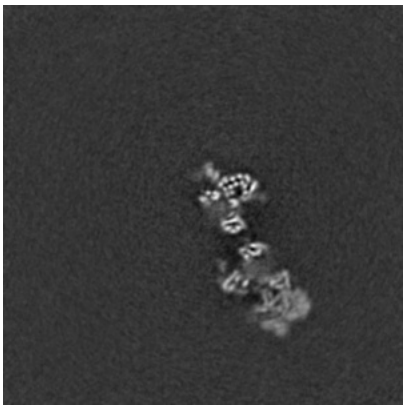
### 6.2.1 Primary map



X Index: 260

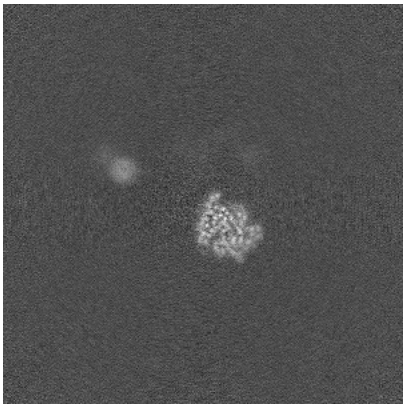


Y Index: 260

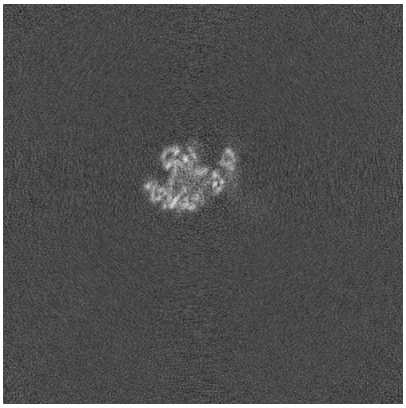


Z Index: 260

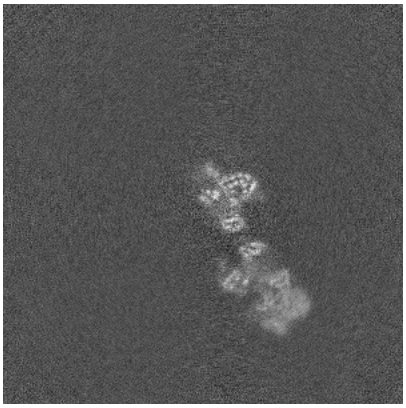
### 6.2.2 Raw map



X Index: 260



Y Index: 260

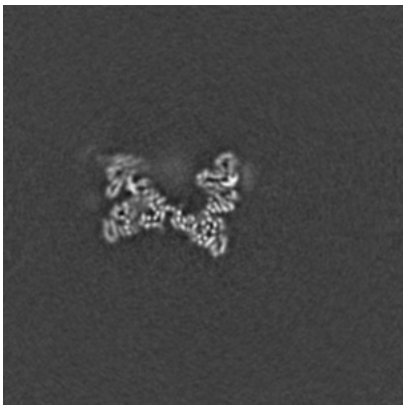


Z Index: 260

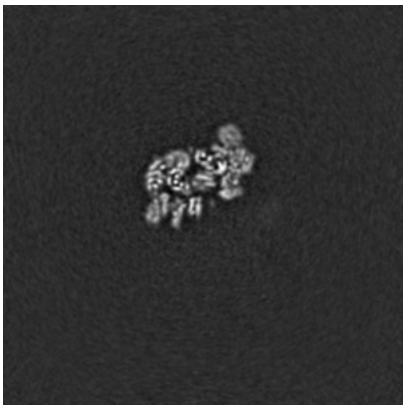
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

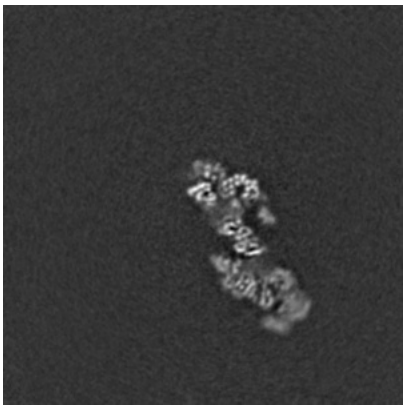
### 6.3.1 Primary map



X Index: 316

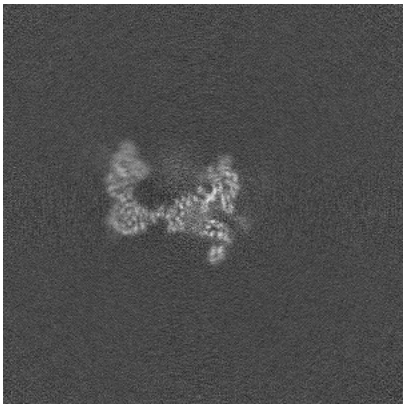


Y Index: 283

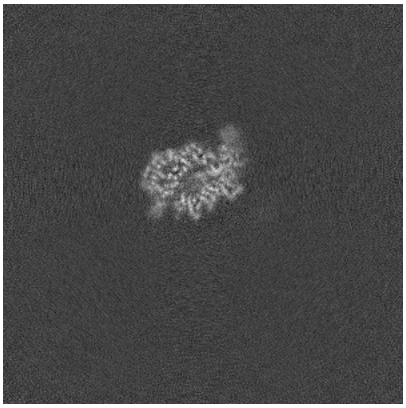


Z Index: 253

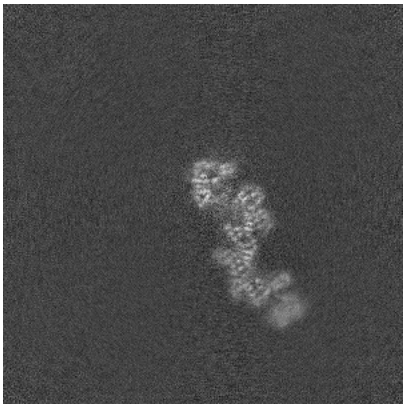
### 6.3.2 Raw map



X Index: 302



Y Index: 275

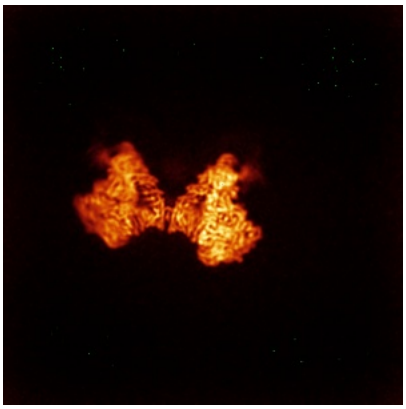


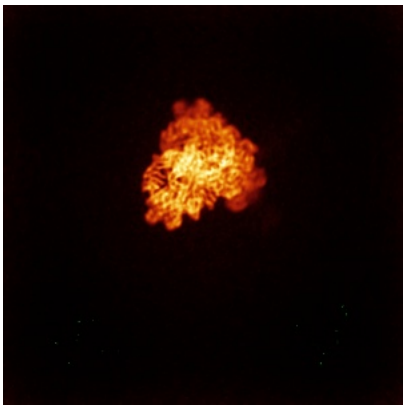
Z Index: 242

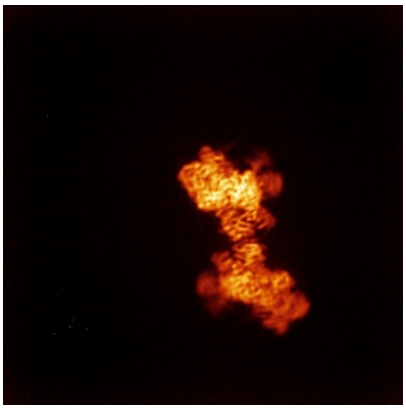
The images above show the largest variance slices of the map in three orthogonal directions.

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

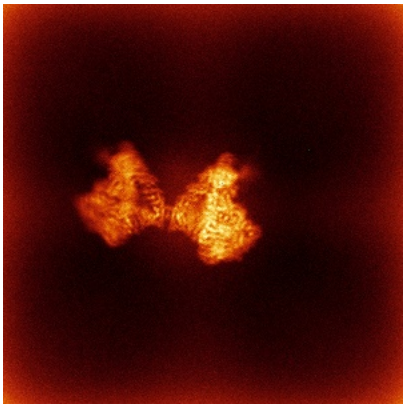
### 6.4.1 Primary map

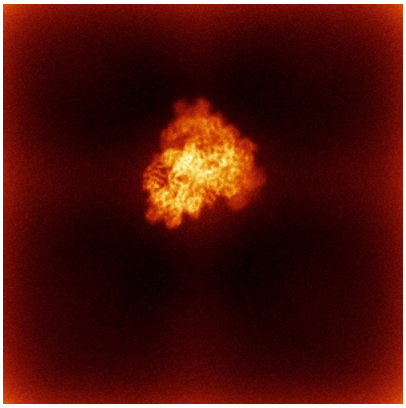

X

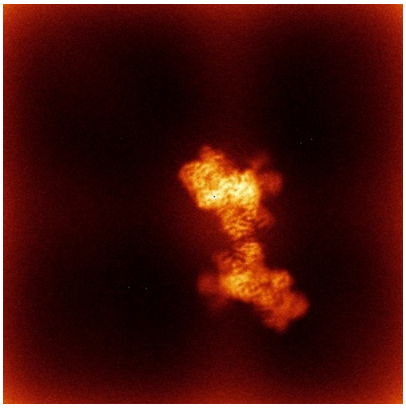

Y


Z

### 6.4.2 Raw map


X


Y


Z

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

## 6.5 Orthogonal surface views (i)

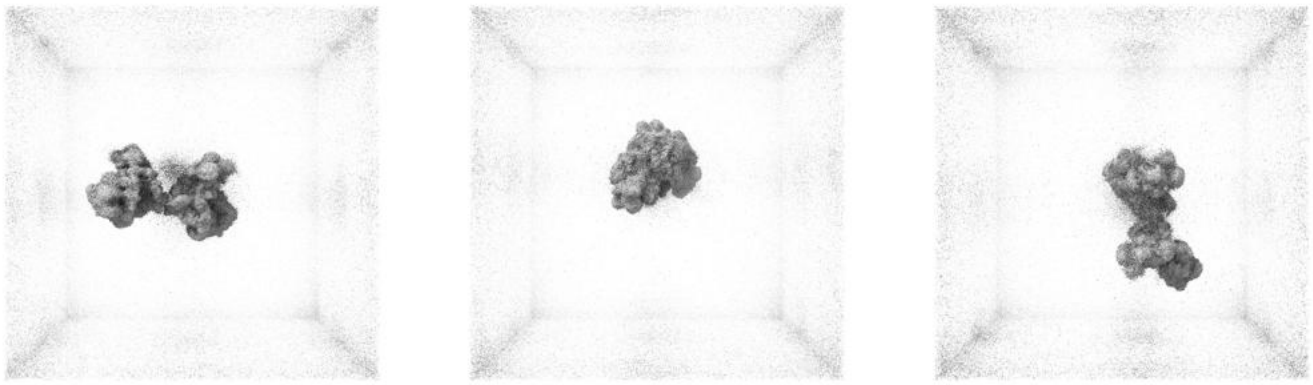
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

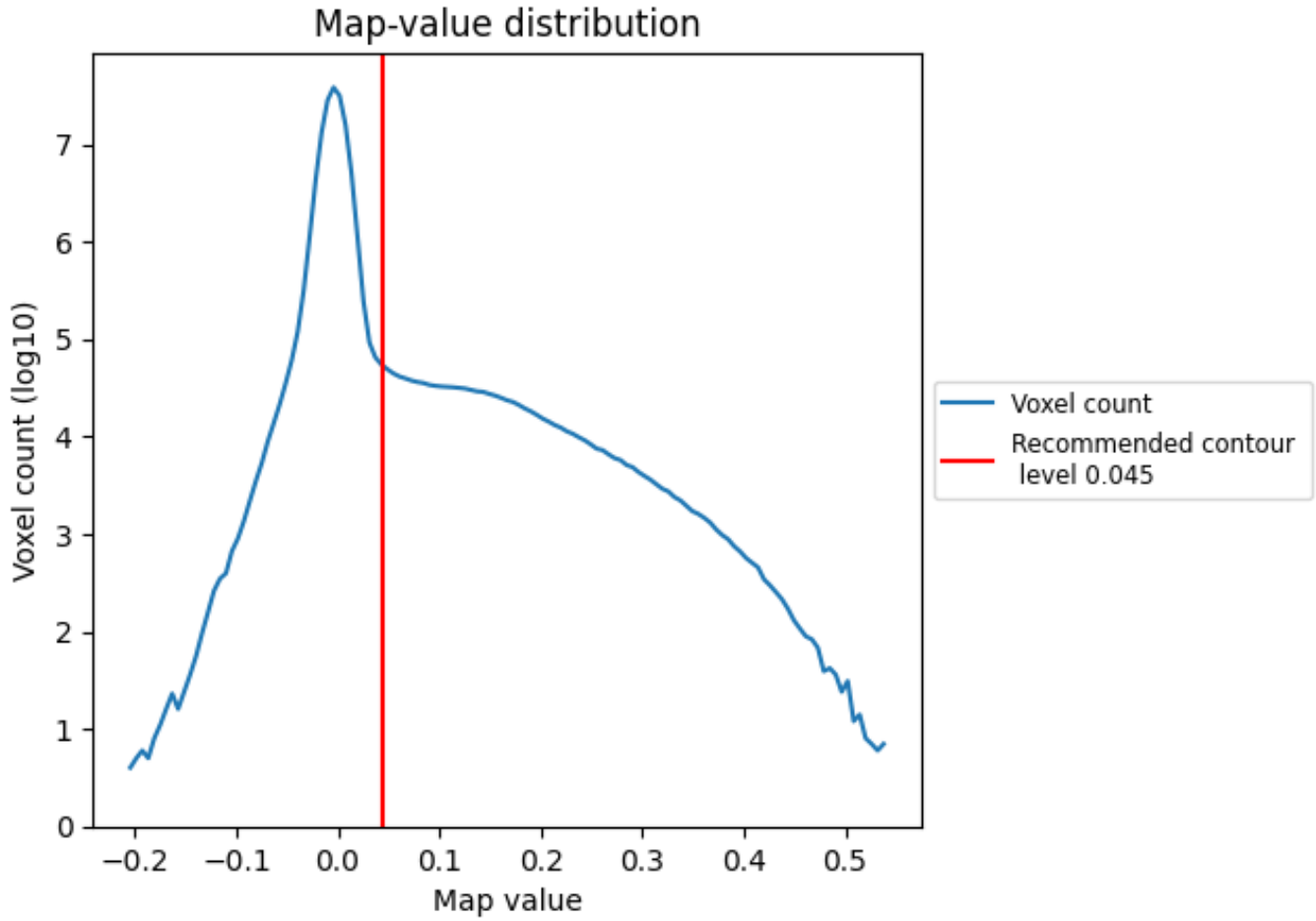
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

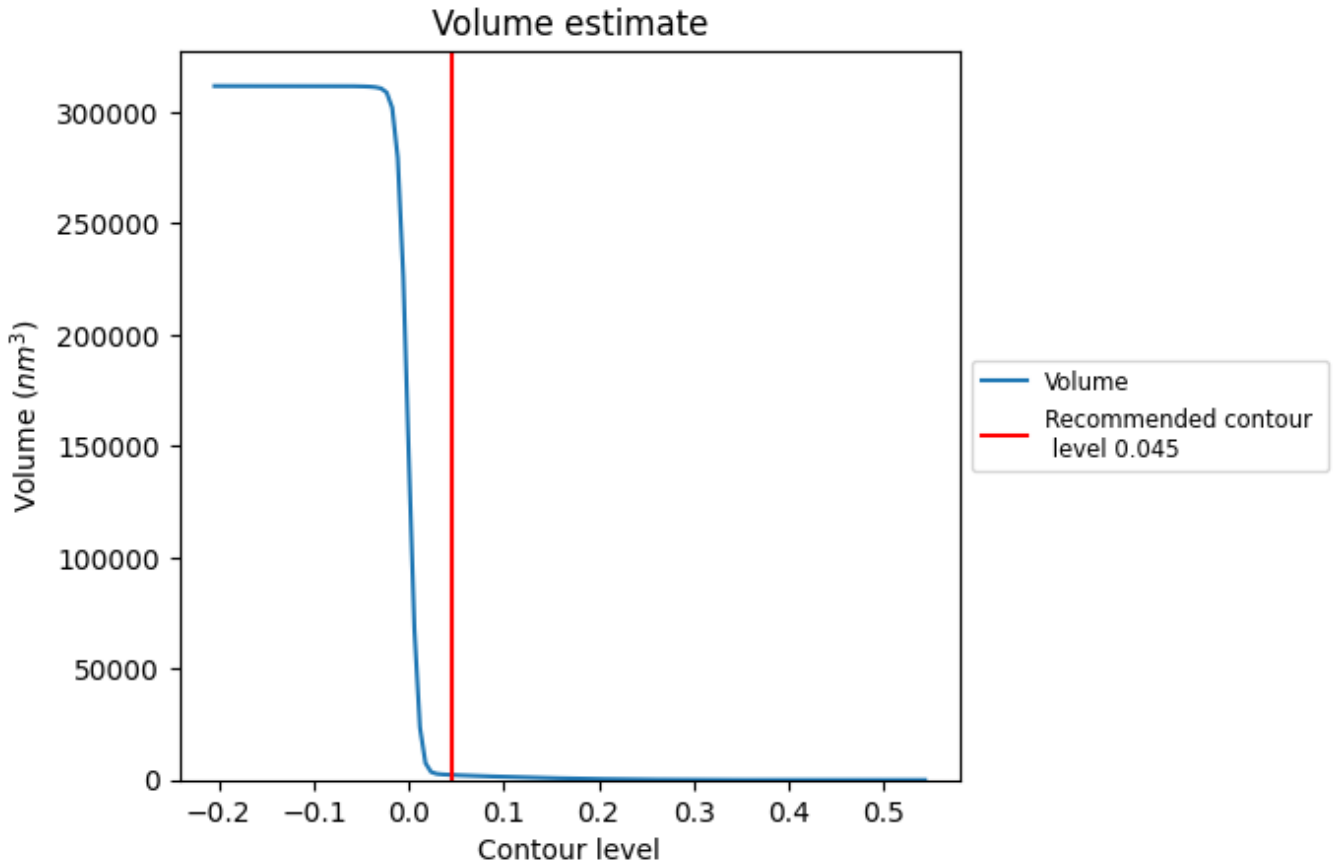
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

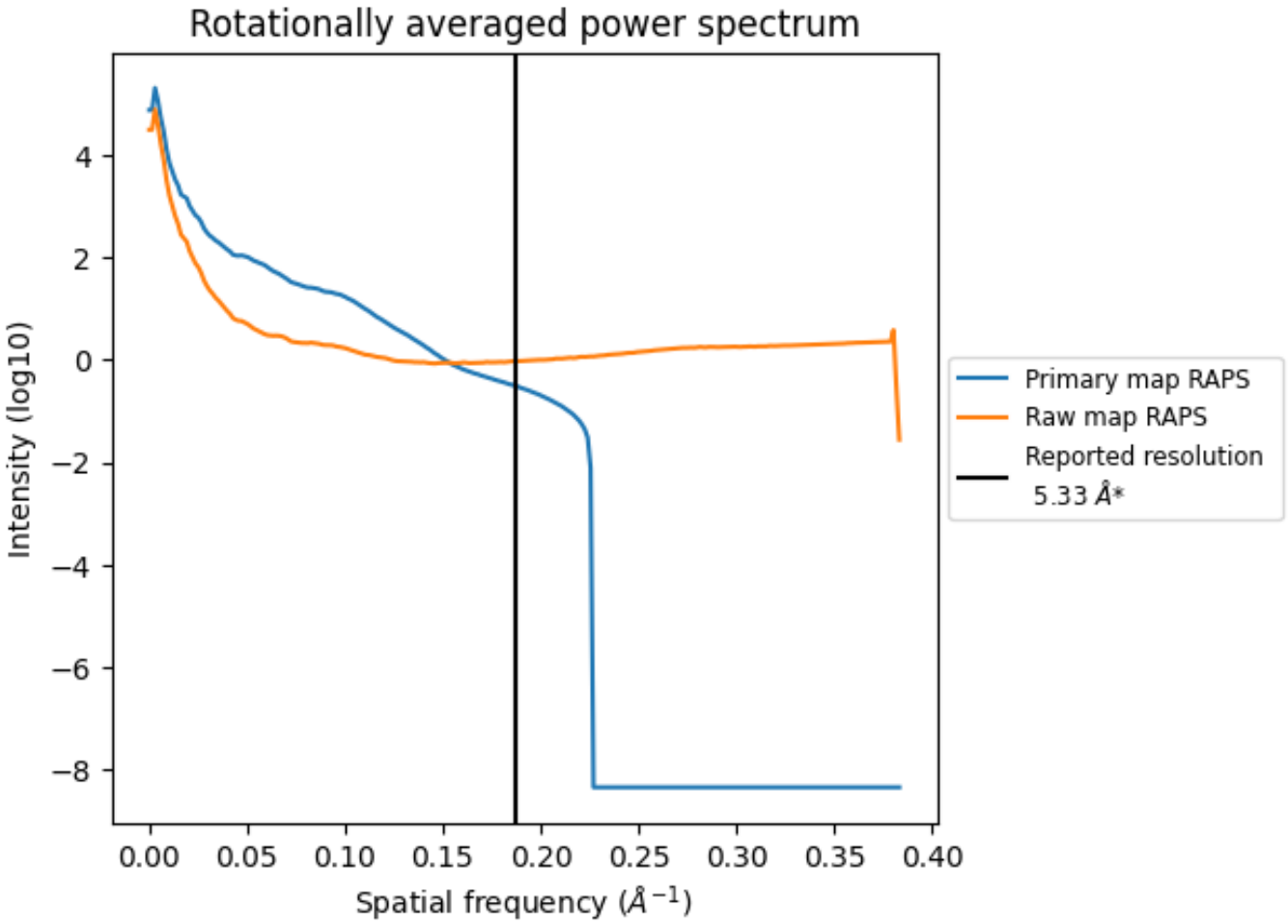
## 7.2 Volume estimate




The volume at the recommended contour level is 2267 $nm^3$; this corresponds to an approximate mass of 2048 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

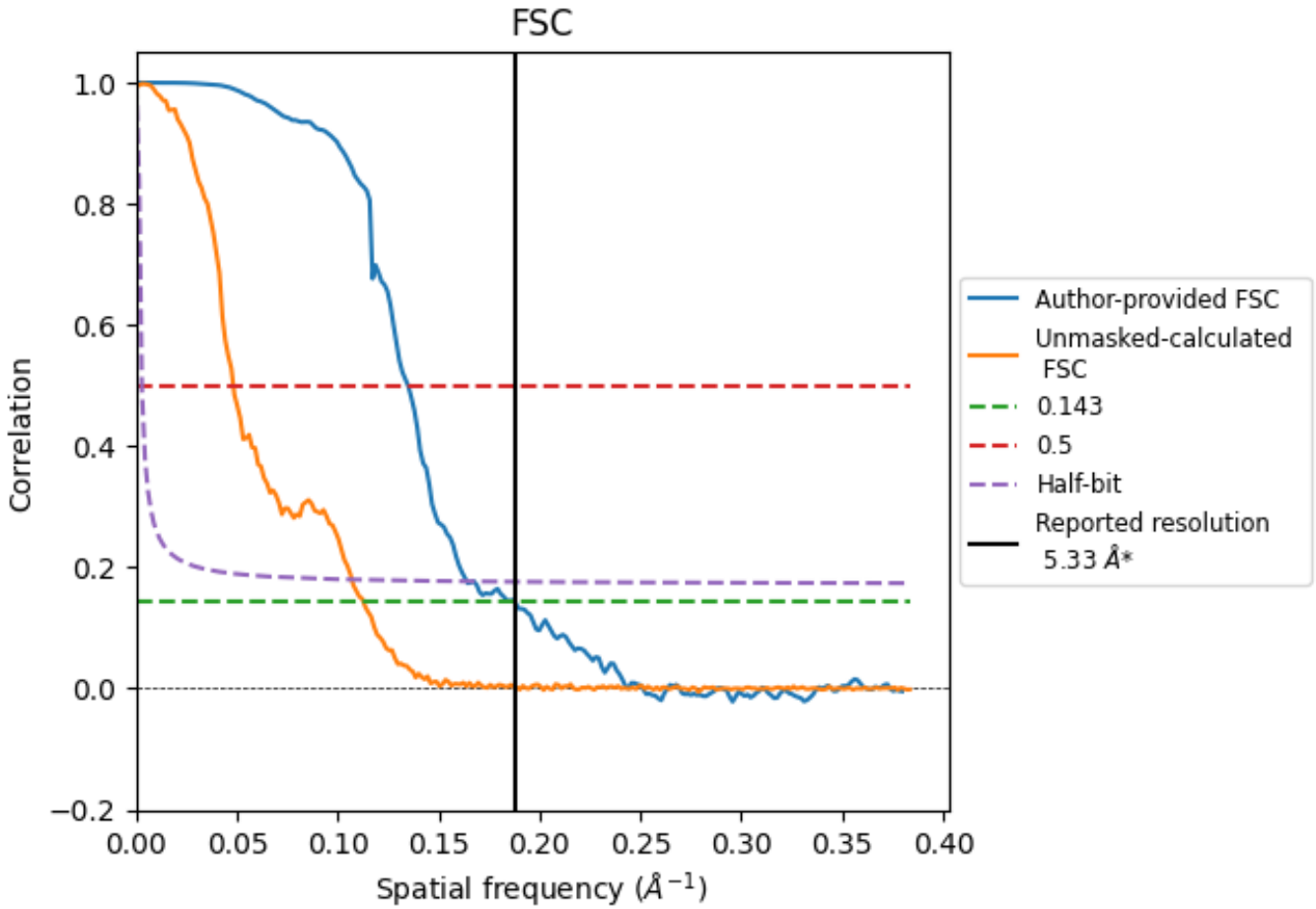



*Reported resolution corresponds to spatial frequency of 0.188 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.188 Å$^{-1}$

## 8.2 Resolution estimates (i)

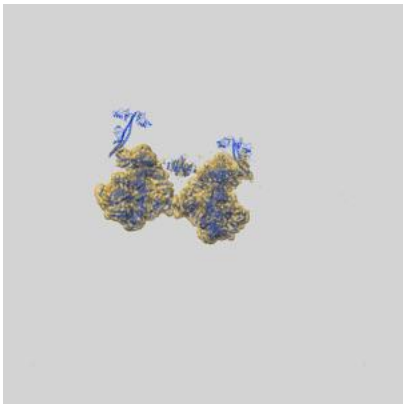
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 5.33 | - | - |
| Author-provided FSC curve | 5.33 | 7.42 | 6.10 |
| Unmasked-calculated* | 8.88 | 20.79 | 9.35 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.88 differs from the reported value 5.33 by more than 10 %

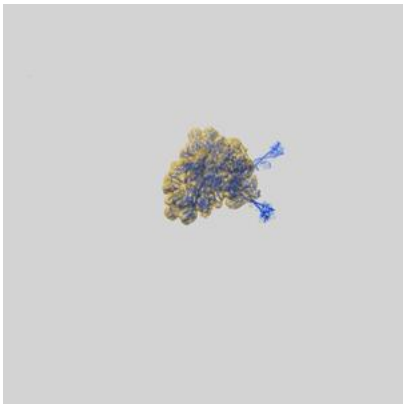
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16074 and PDB model 8BHY. Per-residue inclusion information can be found in section 3 on page 7.

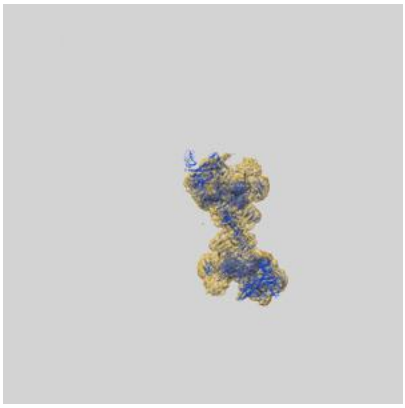
## 9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

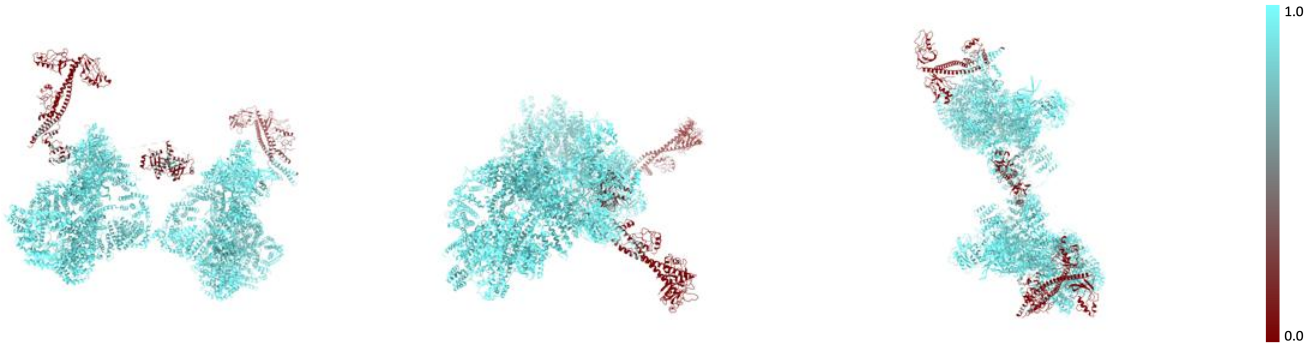
## 9.2 Q-score mapped to coordinate model




X Y Z

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

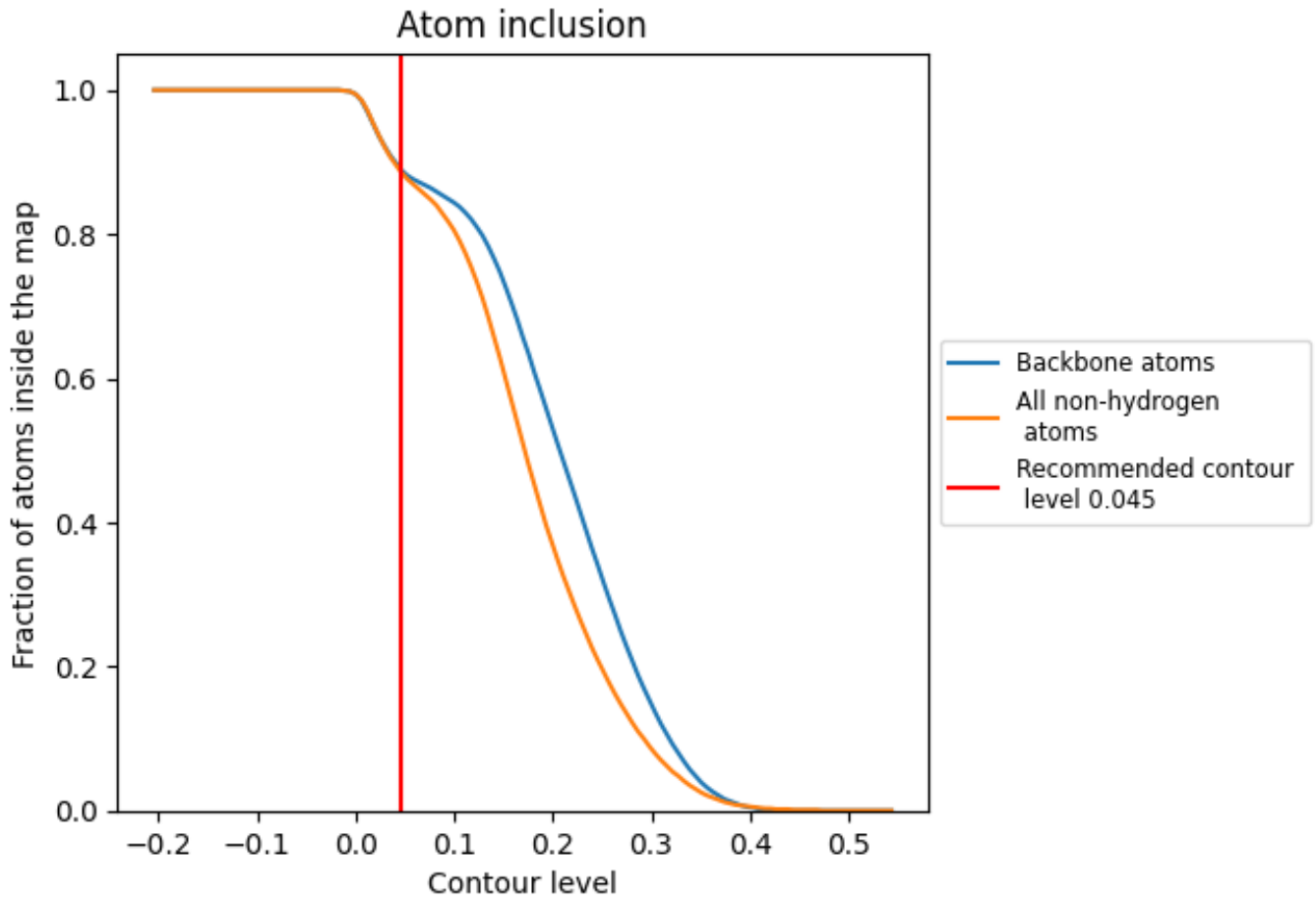
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

## 9.4 Atom inclusion (i)




At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8880 | 0.1660 |
| A | 0.9940 | 0.1980 |
| B | 0.9970 | 0.2050 |
| C | 0.9930 | 0.1680 |
| D | 0.3220 | 0.0840 |
| G | 0.1640 | 0.0630 |
| H | 0.1830 | 0.0900 |
| I | 0.5710 | 0.1120 |
| L | 0.9970 | 0.1310 |
| M | 0.3140 | 0.0980 |
| P | 0.0650 | 0.0810 |
| Q | 0.0430 | 0.0600 |
| R | 0.1750 | 0.0790 |
| S | 0.9950 | 0.1680 |
| T | 0.9970 | 0.1550 |
| d | 1.0000 | 0.2620 |
| e | 1.0000 | 0.2710 |
| f | 0.9820 | 0.0580 |
| i | 1.0000 | 0.2200 |
| j | 1.0000 | 0.2340 |
| m | 1.0000 | 0.0260 |

