# Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 10:10 am GMT

| | | |
|---|---|---|
| PDB ID | : | 2JA8 |
| Title | : | CPD lesion containing RNA Polymerase II elongation complex D |
| Authors | : | Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P. |
| Deposited on | : | 2006-11-23 |
| Resolution | : | 3.80 Å(reported) |

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

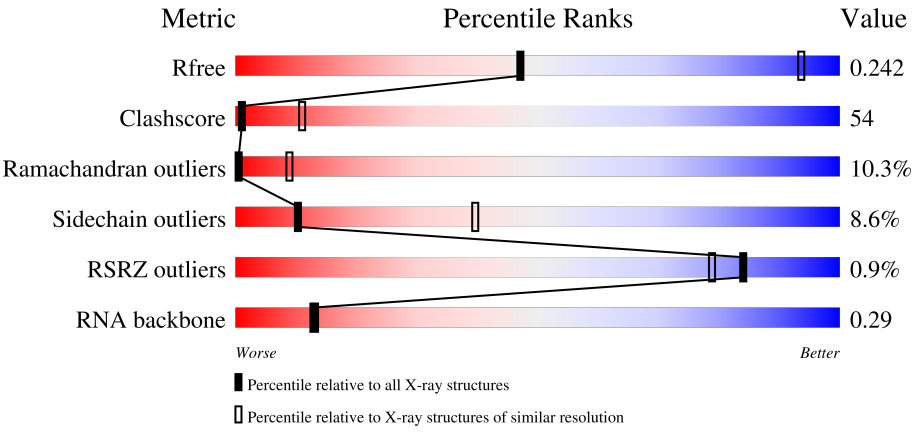
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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.



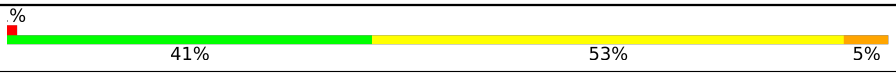
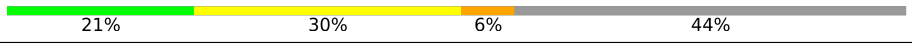
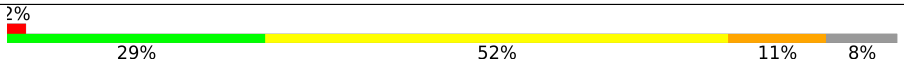
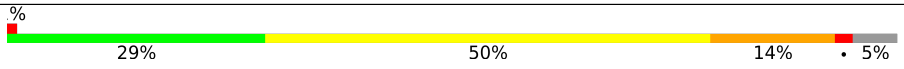
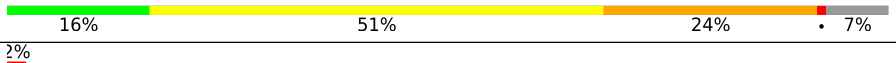
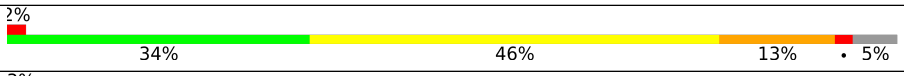
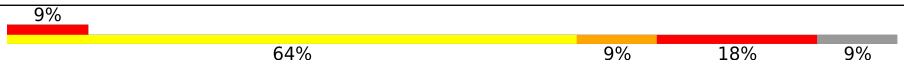

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1212 (4.00-3.60) |
| Clashscore | 141614 | 1288 (4.00-3.60) |
| Ramachandran outliers | 138981 | 1243 (4.00-3.60) |
| Sidechain outliers | 138945 | 1237 (4.00-3.60) |
| RSRZ outliers | 127900 | 1121 (4.00-3.60) |
| RNA backbone | 3102 | 1036 (4.60-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1733 | 25% 46% 10% • 18% |
| 2 | B | 1224 | 28% 52% 11% 9% |
| 3 | C | 318 | 22% 51% 10% • 16% |
| 4 | D | 221 | 27% 40% 12% • 20% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 215 |   |
| 6 | F | 155 |   |
| 7 | G | 171 |   |
| 8 | H | 146 |   |
| 9 | I | 122 |   |
| 10 | J | 70 |   |
| 11 | K | 120 |   |
| 12 | L | 70 |   |
| 13 | N | 14 |   |
| 14 | P | 11 |   |
| 15 | T | 25 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 15 | TT | T | 19 | - | - | X | - |

## 2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1421 | 11186 | 7048 | 1958 | 2118 | 62 | 0 | 0 | 0 |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 1115 | 8866 | 5614 | 1553 | 1644 | 55 | 0 | 0 | 0 |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | C | 267 | 2101 | 1320 | 349 | 419 | 13 | 0 | 0 | 0 |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | D | 177 | 1427 | 882 | 256 | 287 | 2 | 0 | 0 | 0 |

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | E | 214 | 1752 | 1111 | 309 | 321 | 11 | 0 | 0 | 0 |

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 451 | 119 | 132 | 3 | | | |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1340 | 861 | 222 | 249 | 8 | | | |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1084 | 683 | 183 | 214 | 4 | | | |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 944 | 581 | 172 | 181 | 10 | | | |

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 93 | 94 | 6 | | | |

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 919 | 590 | 156 | 171 | 2 | | | |

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 364 | 224 | 72 | 64 | 4 | | | |

- Molecule 13 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | N | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 161 | 79 | 29 | 46 | 7 | | | |

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*AP*UP)-3 '.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | P | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 209 | 95 | 38 | 67 | 9 | | | |

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP* TP*TP*TP*TP*TTP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 15 | T | 19 | Total | Br | C | N | O | P | 0 | 0 | 0 |
| | | | 401 | 1 | 197 | 61 | 124 | 18 | | | |

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 16 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

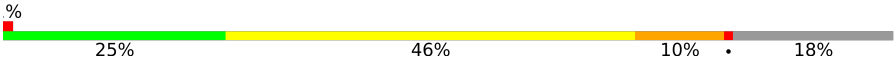
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 17 | A | 8 | Total | Zn | 0 | 0 |
| | | | 8 | 8 | | |

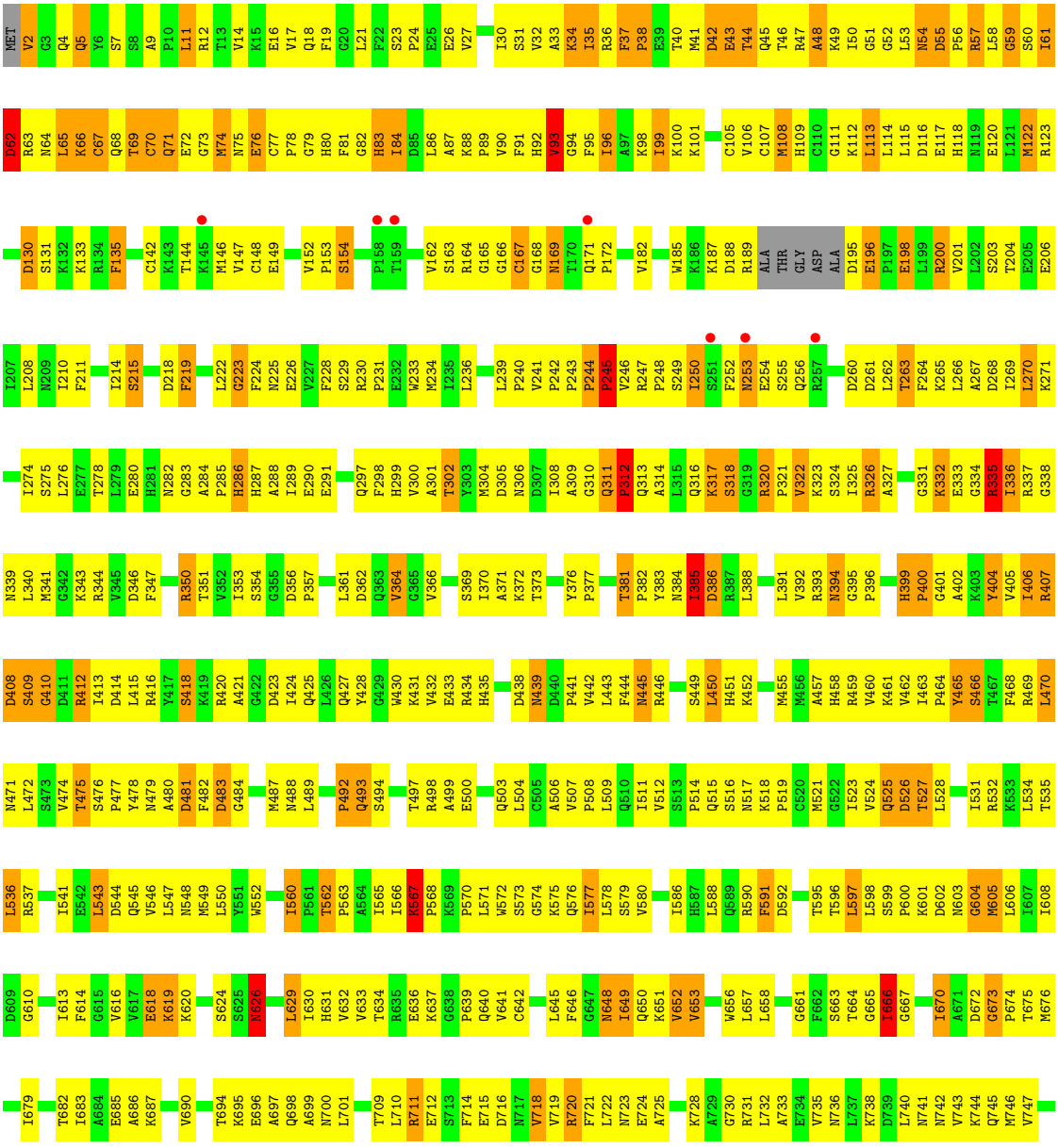
# 3 Residue-property plots (i)

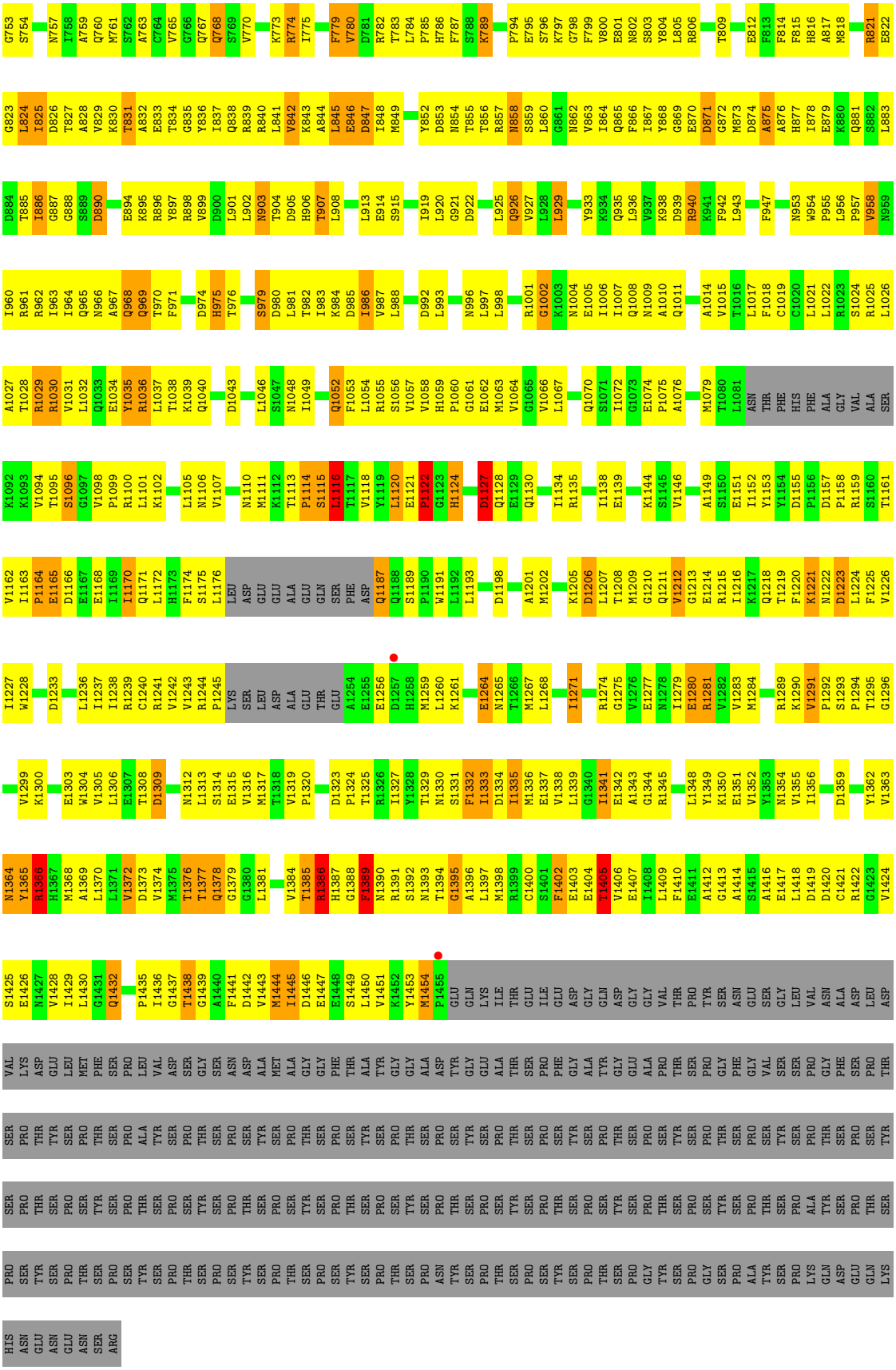
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

Chain A:

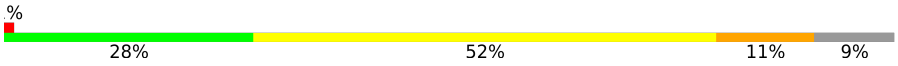


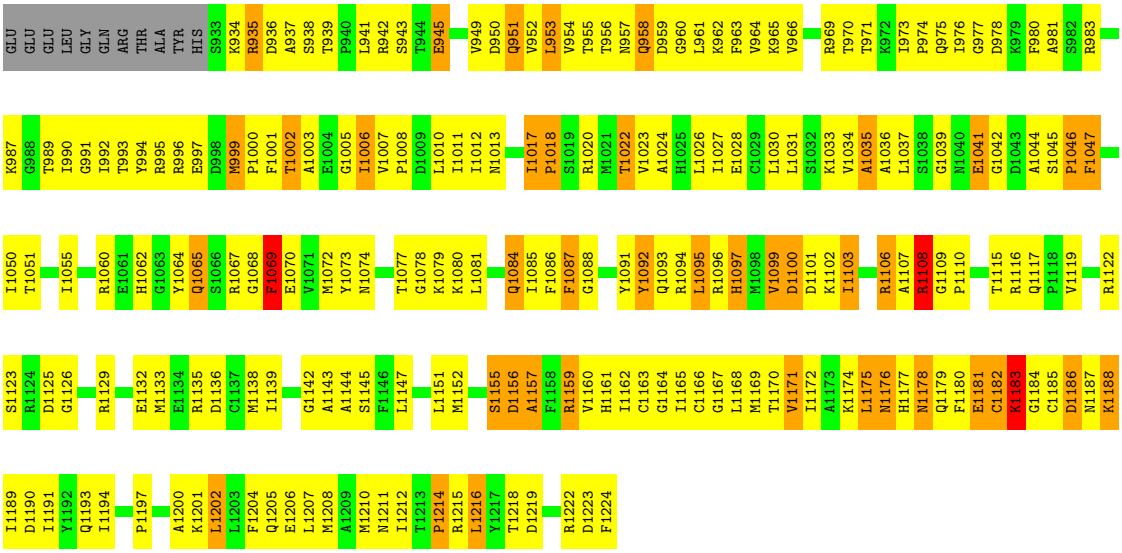





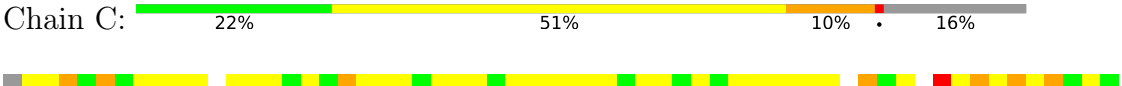
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

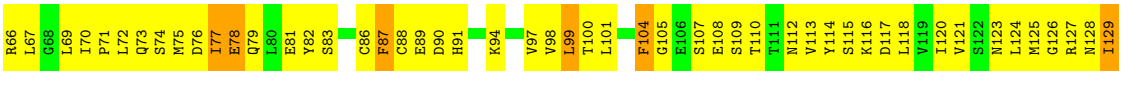
Chain B:

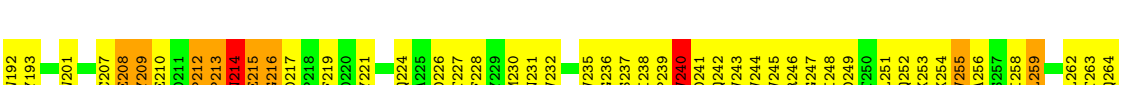


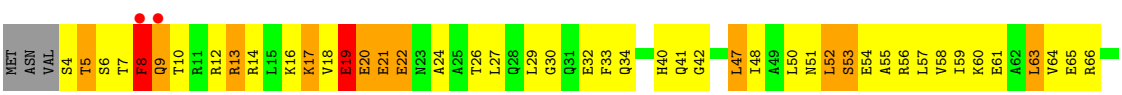


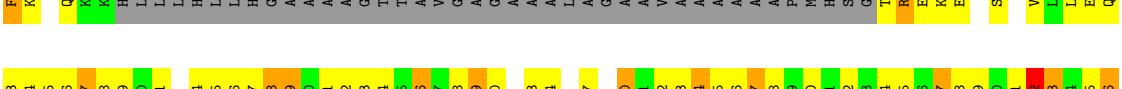








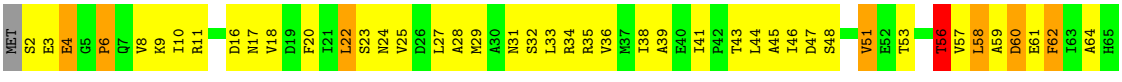


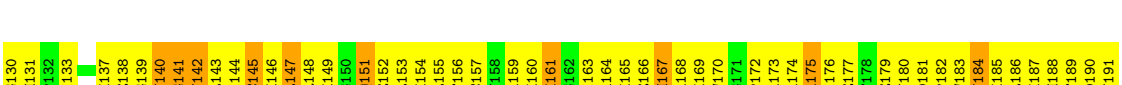


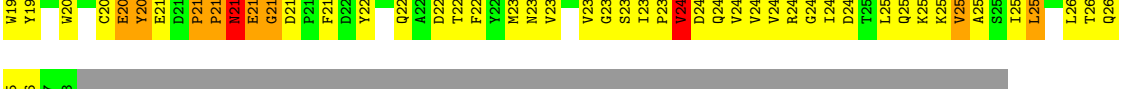
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

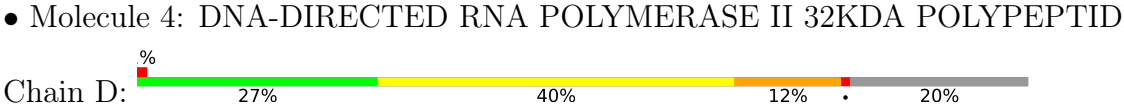
Chain C:

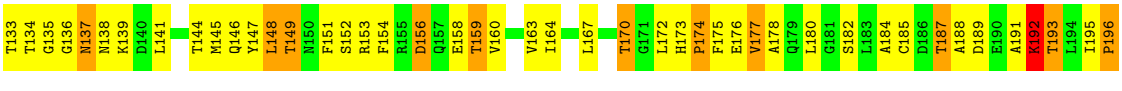








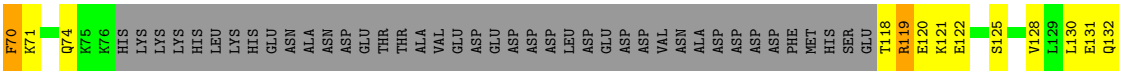


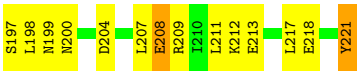
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

Chain D:



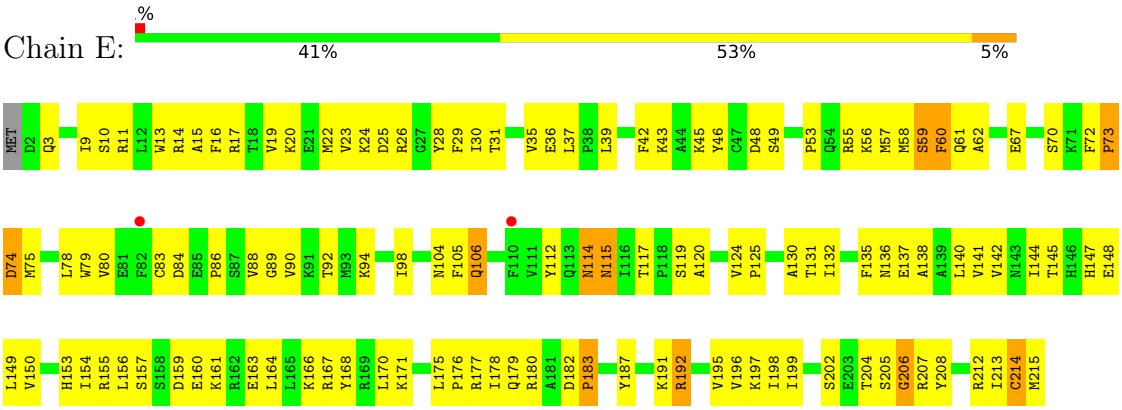




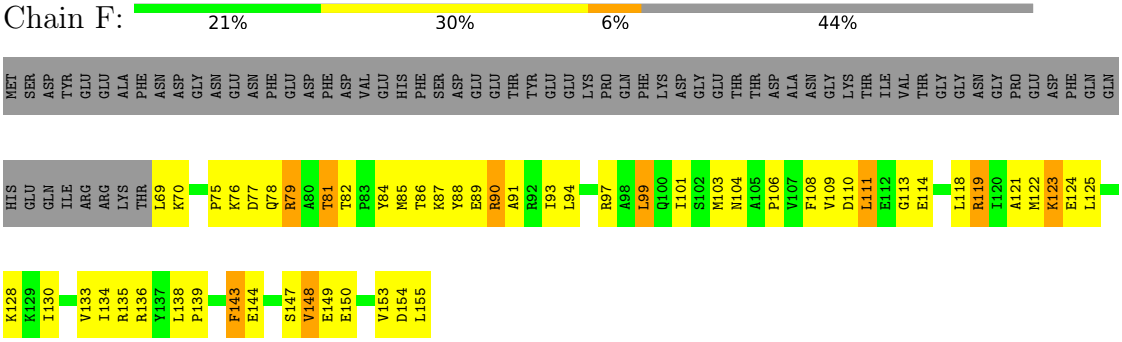

• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

Chain E:



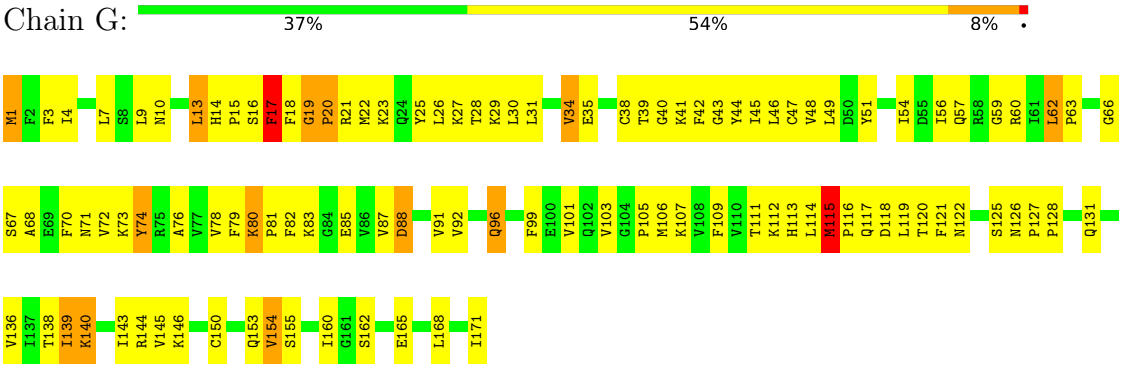

• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain F:



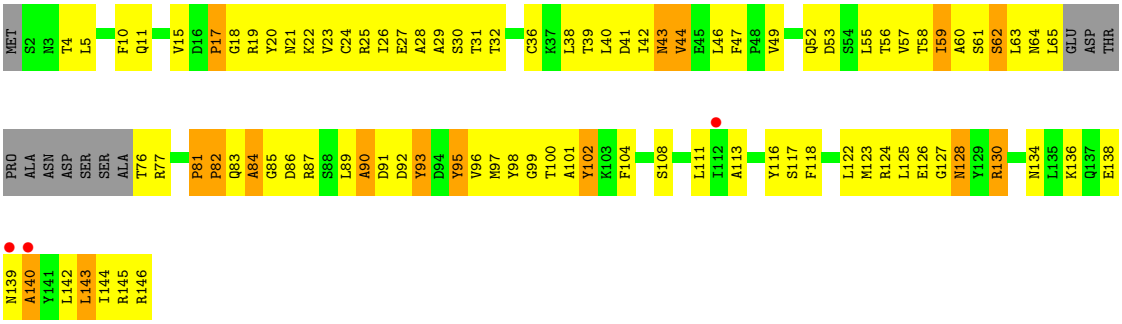

• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

Chain G:



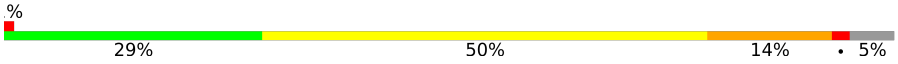

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

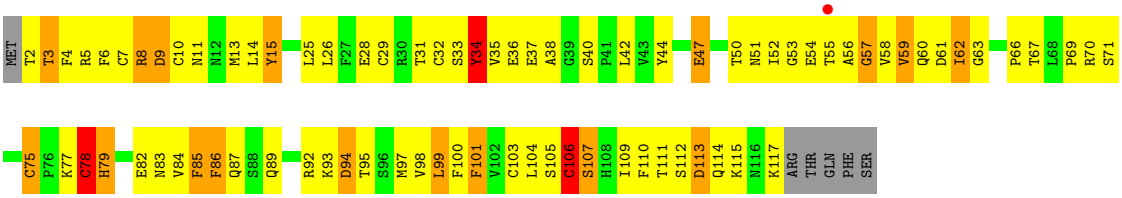
Chain H:



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

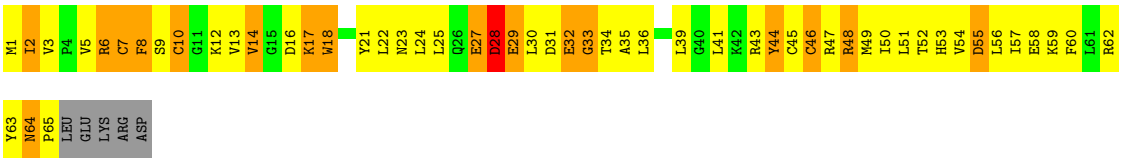
Chain I:



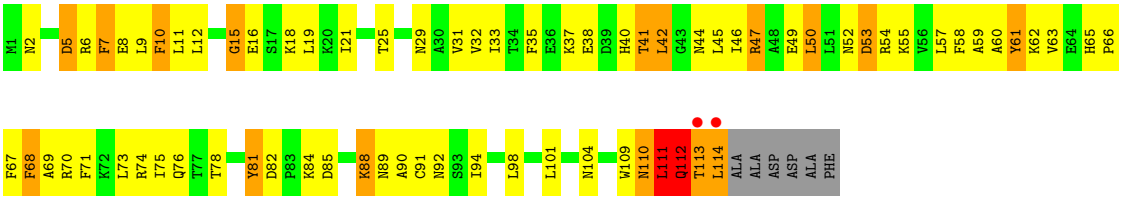
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J:

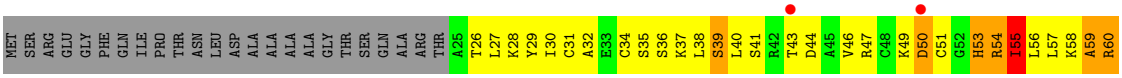
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

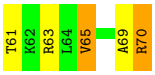
Chain K:

• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

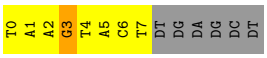
Chain L:



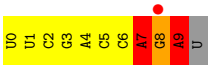

• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain N:


• Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*AP*UP)-3'

Chain P:


• Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TP*TTP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain T:


# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 222.64Å 392.85Å 282.89Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.80<br>48.85 – 3.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.2 (50.00-3.80)<br>99.9 (48.85-3.80) | Depositor<br>EDS |
| $R_{merge}$ | 0.08 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.30 (at 3.77Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.269 , 0.288<br>0.210 , 0.242 | Depositor<br>DCC |
| $R_{free}$ test set | 4685 reflections (1.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 110.0 | Xtriage |
| Anisotropy | 0.478 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.26 , 70.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 32000 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 95.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.46 | 0/11385 | 0.73 | 1/15393 (0.0%) |
| 2 | B | 0.45 | 0/9037 | 0.71 | 2/12181 (0.0%) |
| 3 | C | 0.48 | 0/2138 | 0.71 | 0/2896 |
| 4 | D | 0.42 | 0/1437 | 0.67 | 0/1925 |
| 5 | E | 0.43 | 1/1788 (0.1%) | 0.62 | 0/2406 |
| 6 | F | 0.53 | 0/716 | 0.77 | 0/964 |
| 7 | G | 0.49 | 0/1368 | 0.73 | 0/1844 |
| 8 | H | 0.38 | 0/1102 | 0.65 | 0/1492 |
| 9 | I | 0.39 | 0/962 | 0.68 | 0/1295 |
| 10 | J | 0.48 | 0/541 | 0.80 | 0/727 |
| 11 | K | 0.67 | 3/937 (0.3%) | 0.86 | 4/1265 (0.3%) |
| 12 | L | 0.41 | 0/366 | 0.68 | 0/485 |
| 13 | N | 1.21 | 1/180 (0.6%) | 1.08 | 0/276 |
| 14 | P | 0.85 | 0/233 | 1.41 | 2/361 (0.6%) |
| 15 | T | 1.12 | 2/380 (0.5%) | 1.39 | 3/580 (0.5%) |
| All | All | 0.49 | 7/32570 (0.0%) | 0.74 | 12/44090 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | B | 0 | 1 |
| 15 | T | 0 | 1 |
| All | All | 0 | 2 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | K | 113 | THR | N-CA | 5.90 | 1.58 | 1.46 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | K | 113 | THR | CA-C | 5.73 | 1.67 | 1.52 |
| 15 | T | 12 | DT | N1-C2 | 5.38 | 1.42 | 1.38 |
| 5 | E | 214 | CYS | CB-SG | -5.28 | 1.73 | 1.81 |
| 11 | K | 114 | LEU | N-CA | 5.10 | 1.56 | 1.46 |
| 15 | T | 14 | DC | N1-C2 | 5.10 | 1.45 | 1.40 |
| 13 | N | 3 | DG | N9-C4 | 5.03 | 1.42 | 1.38 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | K | 113 | THR | N-CA-C | 9.56 | 136.81 | 111.00 |
| 15 | T | 24 | DG | O4'-C1'-N9 | 7.22 | 113.06 | 108.00 |
| 15 | T | 21 | DC | O5'-P-OP1 | 7.09 | 119.21 | 110.70 |
| 14 | P | 9 | A | C2'-C3'-O3' | 7.01 | 124.92 | 109.50 |
| 14 | P | 7 | A | N9-C1'-C2' | -6.77 | 104.56 | 112.00 |
| 11 | K | 111 | LEU | N-CA-C | 6.32 | 128.07 | 111.00 |
| 11 | K | 114 | LEU | N-CA-C | 5.93 | 127.00 | 111.00 |
| 2 | B | 111 | ALA | N-CA-C | -5.85 | 95.21 | 111.00 |
| 11 | K | 113 | THR | C-N-CA | 5.83 | 136.26 | 121.70 |
| 15 | T | 10 | DA | OP2-P-O3' | 5.60 | 117.52 | 105.20 |
| 2 | B | 1185 | CYS | N-CA-C | -5.06 | 97.34 | 111.00 |
| 1 | A | 567 | LYS | C-N-CD | 5.02 | 138.93 | 128.40 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 486 | TYR | Sidechain |
| 15 | T | 13 | DA | Sidechain |

## 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 | 11186 | 0 | 11266 | 1310 | 0 |
| 2 | B | 8866 | 0 | 8898 | 1015 | 0 |
| 3 | C | 2101 | 0 | 2055 | 265 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | D | 1427 | 0 | 1451 | 139 | 0 |
| 5 | E | 1752 | 0 | 1776 | 134 | 0 |
| 6 | F | 705 | 0 | 730 | 89 | 0 |
| 7 | G | 1340 | 0 | 1357 | 173 | 0 |
| 8 | H | 1084 | 0 | 1057 | 127 | 0 |
| 9 | I | 944 | 0 | 900 | 110 | 0 |
| 10 | J | 532 | 0 | 542 | 99 | 0 |
| 11 | K | 919 | 0 | 929 | 107 | 0 |
| 12 | L | 364 | 0 | 386 | 47 | 0 |
| 13 | N | 161 | 0 | 93 | 17 | 0 |
| 14 | P | 209 | 0 | 109 | 28 | 0 |
| 15 | T | 401 | 0 | 231 | 64 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 8 | 0 | 0 | 0 | 0 |
| All | All | 32000 | 0 | 31780 | 3425 | 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 54.

All (3425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:53:LEU:HD23 | 1:A:54:ASN:N | 1.61 | 1.13 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:HE | 1.10 | 1.11 |
| 7:G:14:HIS:CD2 | 7:G:16:SER:HB2 | 1.87 | 1.10 |
| 15:T:19:TT:H5R1 | 15:T:19:TT:C1' | 1.83 | 1.09 |
| 1:A:1445:ILE:H | 1:A:1445:ILE:HD12 | 1.16 | 1.09 |
| 15:T:17:DT:H2" | 15:T:18:DT:H5' | 1.32 | 1.08 |
| 2:B:343:ILE:HG23 | 2:B:347:LYS:HB2 | 1.16 | 1.08 |
| 2:B:273:LEU:HB2 | 2:B:276:ILE:HD12 | 1.36 | 1.08 |
| 5:E:22:MET:HE3 | 5:E:26:ARG:HH21 | 1.15 | 1.07 |
| 15:T:19:TT:H5R1 | 15:T:19:TT:H1' | 1.23 | 1.07 |
| 2:B:336:ARG:HG2 | 2:B:348:ARG:HD3 | 1.31 | 1.07 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:H | 1.20 | 1.07 |
| 15:T:17:DT:C2' | 15:T:18:DT:H5' | 1.83 | 1.06 |
| 1:A:34:LYS:HD3 | 1:A:57:ARG:HH22 | 0.92 | 1.04 |
| 4:D:40:HIS:HB3 | 7:G:73:LYS:HZ3 | 1.16 | 1.04 |
| 11:K:47:ARG:HB3 | 11:K:47:ARG:HH11 | 1.17 | 1.03 |
| 1:A:40:THR:HG22 | 1:A:41:MET:HG3 | 1.39 | 1.03 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:H | 1.20 | 1.03 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:H | 1.24 | 1.02 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:58:LEU:HD12 | 1:A:59:GLY:H | 1.23 | 1.01 |
| 1:A:53:LEU:HD23 | 1:A:54:ASN:H | 0.84 | 1.01 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:H | 1.24 | 1.01 |
| 1:A:1402:PHE:CE1 | 1:A:1403:GLU:HG3 | 1.94 | 1.01 |
| 10:J:5:VAL:HG12 | 10:J:6:ARG:HG3 | 1.42 | 1.01 |
| 11:K:111:LEU:C | 11:K:112:GLN:HG2 | 1.76 | 1.01 |
| 1:A:868:TYR:CE1 | 1:A:1064:VAL:HG11 | 1.96 | 1.00 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:HZ | 1.27 | 1.00 |
| 7:G:13:LEU:HD21 | 7:G:17:PHE:HB2 | 1.38 | 1.00 |
| 1:A:34:LYS:HD3 | 1:A:57:ARG:NH2 | 1.77 | 1.00 |
| 1:A:1017:LEU:HB2 | 5:E:206:GLY:H | 1.25 | 0.99 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD2 | 1.91 | 0.98 |
| 1:A:53:LEU:CD2 | 1:A:54:ASN:H | 1.74 | 0.98 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:H | 1.27 | 0.98 |
| 3:C:57:VAL:HG11 | 10:J:60:PHE:HB3 | 1.43 | 0.98 |
| 3:C:43:THR:HG22 | 3:C:44:LEU:H | 1.29 | 0.97 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:HB2 | 1.45 | 0.97 |
| 2:B:214:ALA:HB3 | 2:B:498:THR:HA | 1.46 | 0.97 |
| 2:B:510:LYS:CG | 2:B:511:PRO:HD3 | 1.94 | 0.96 |
| 10:J:1:MET:N | 10:J:57:ILE:H | 1.63 | 0.96 |
| 2:B:1187:ASN:O | 2:B:1188:LYS:HB2 | 1.65 | 0.96 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H | 1.29 | 0.96 |
| 1:A:709:THR:HG23 | 9:I:94:ASP:HA | 1.46 | 0.96 |
| 1:A:590:ARG:HH21 | 1:A:620:LYS:HB3 | 1.31 | 0.96 |
| 1:A:590:ARG:NH2 | 1:A:620:LYS:HB3 | 1.80 | 0.96 |
| 15:T:19:TT:H1' | 15:T:19:TT:C5R | 1.96 | 0.96 |
| 1:A:225:ASN:HD22 | 1:A:228:PHE:H | 1.03 | 0.95 |
| 15:T:18:DT:C2' | 15:T:19:TT:H5'1 | 1.94 | 0.95 |
| 1:A:1394:THR:HG21 | 1:A:1398:MET:SD | 2.06 | 0.95 |
| 2:B:516:ASN:HD22 | 2:B:516:ASN:N | 1.64 | 0.94 |
| 5:E:94:LYS:HE2 | 5:E:98:ILE:HD11 | 1.48 | 0.94 |
| 4:D:144:THR:O | 4:D:148:LEU:HB2 | 1.67 | 0.94 |
| 1:A:567:LYS:HB3 | 8:H:96:VAL:H | 1.33 | 0.94 |
| 2:B:217:ARG:HE | 2:B:405:ARG:HB2 | 1.28 | 0.94 |
| 2:B:502:ILE:H | 2:B:502:ILE:HD12 | 1.31 | 0.94 |
| 9:I:8:ARG:HG3 | 9:I:34:TYR:HE1 | 1.30 | 0.94 |
| 15:T:17:DT:H2" | 15:T:18:DT:C5' | 1.97 | 0.94 |
| 1:A:34:LYS:HE3 | 1:A:57:ARG:HH12 | 1.30 | 0.94 |
| 2:B:168:GLY:H | 2:B:450:ALA:HB1 | 1.32 | 0.94 |
| 11:K:110:ASN:O | 11:K:111:LEU:HD23 | 1.68 | 0.94 |
| 2:B:486:TYR:OH | 2:B:1096:ARG:HB3 | 1.66 | 0.93 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:OE1 | 1.65 | 0.93 |
| 15:T:19:TT:H5M1 | 15:T:21:DC:C5 | 2.03 | 0.93 |
| 1:A:58:LEU:HD21 | 1:A:243:PRO:HA | 1.47 | 0.93 |
| 10:J:1:MET:H1 | 10:J:57:ILE:N | 1.66 | 0.93 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:H | 1.10 | 0.93 |
| 1:A:58:LEU:CD1 | 1:A:59:GLY:H | 1.82 | 0.93 |
| 1:A:34:LYS:CD | 1:A:57:ARG:HH22 | 1.82 | 0.93 |
| 1:A:754:SER:H | 1:A:757:ASN:HD22 | 1.11 | 0.93 |
| 2:B:336:ARG:HH22 | 2:B:345:LYS:HE2 | 1.33 | 0.92 |
| 10:J:48:ARG:HE | 10:J:49:MET:HE2 | 1.31 | 0.92 |
| 15:T:17:DT:C1' | 15:T:18:DT:H5' | 1.99 | 0.92 |
| 2:B:232:SER:HB3 | 2:B:261:ARG:HH21 | 1.32 | 0.92 |
| 3:C:66:ARG:NH1 | 10:J:2:ILE:HG21 | 1.82 | 0.92 |
| 3:C:6:PRO:HB3 | 3:C:25:VAL:HG12 | 1.50 | 0.92 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:H | 1.32 | 0.92 |
| 3:C:6:PRO:HB3 | 3:C:25:VAL:CG1 | 1.99 | 0.92 |
| 1:A:254:GLU:HB2 | 2:B:935:ARG:HH12 | 1.34 | 0.92 |
| 2:B:515:HIS:H | 2:B:518:HIS:HD2 | 1.16 | 0.92 |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:H | 1.35 | 0.91 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CZ2 | 2.05 | 0.91 |
| 14:P:5:C:H2' | 14:P:6:C:O4' | 1.70 | 0.91 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CD1 | 2.04 | 0.91 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:HD3 | 1.51 | 0.91 |
| 8:H:4:THR:HA | 8:H:60:ALA:HB2 | 1.53 | 0.91 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:HG11 | 1.53 | 0.91 |
| 6:F:93:ILE:HD11 | 6:F:134:ILE:HD11 | 1.53 | 0.91 |
| 9:I:85:PHE:H | 9:I:85:PHE:HD2 | 1.18 | 0.91 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H | 1.36 | 0.91 |
| 4:D:40:HIS:HB3 | 7:G:73:LYS:NZ | 1.84 | 0.90 |
| 1:A:1420:ASP:HB3 | 1:A:1422:ARG:HG3 | 1.53 | 0.90 |
| 8:H:100:THR:HG23 | 8:H:138:GLU:HA | 1.49 | 0.90 |
| 1:A:382:PRO:HB3 | 1:A:428:TYR:HE2 | 1.34 | 0.90 |
| 1:A:285:PRO:HG2 | 1:A:288:ALA:HB3 | 1.52 | 0.90 |
| 15:T:22:BRU:H2' | 15:T:23:DG:C8 | 2.07 | 0.90 |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:H | 1.34 | 0.90 |
| 8:H:84:ALA:HA | 8:H:87:ARG:HB2 | 1.53 | 0.90 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:NE | 1.86 | 0.90 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD2 | 2.02 | 0.89 |
| 2:B:549:THR:HG22 | 2:B:550:ASP:H | 1.36 | 0.89 |
| 1:A:836:TYR:CD2 | 1:A:840:ARG:HD2 | 2.08 | 0.89 |
| 15:T:17:DT:H1' | 15:T:18:DT:H5' | 1.53 | 0.89 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:T:19:TT:H2R2 | 15:T:19:TT:H2'1 | 1.55 | 0.89 |
| 1:A:779:PHE:HE1 | 1:A:785:PRO:HD3 | 1.38 | 0.89 |
| 15:T:19:TT:H5R1 | 15:T:19:TT:C2' | 2.02 | 0.88 |
| 15:T:15:DT:H1' | 15:T:16:DT:H5' | 1.53 | 0.88 |
| 2:B:661:LEU:HD11 | 2:B:684:LEU:HD11 | 1.56 | 0.88 |
| 2:B:1072:MET:CE | 2:B:1085:ILE:HB | 2.03 | 0.88 |
| 1:A:901:LEU:H | 1:A:926:GLN:NE2 | 1.71 | 0.88 |
| 2:B:842:ASN:ND2 | 2:B:845:SER:H | 1.72 | 0.88 |
| 1:A:783:THR:HG21 | 1:A:815:PHE:CZ | 2.08 | 0.88 |
| 2:B:824:ILE:HG22 | 2:B:1087:PHE:HE2 | 1.35 | 0.88 |
| 2:B:393:LYS:HA | 2:B:393:LYS:HE3 | 1.56 | 0.88 |
| 1:A:534:LEU:O | 1:A:574:GLY:HA3 | 1.74 | 0.87 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:HA | 1.54 | 0.87 |
| 1:A:58:LEU:HD11 | 1:A:243:PRO:HB3 | 1.56 | 0.87 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HD12 | 1.55 | 0.87 |
| 1:A:93:VAL:HG13 | 1:A:301:ALA:HB1 | 1.55 | 0.86 |
| 2:B:364:ILE:HG12 | 2:B:585:VAL:HG13 | 1.57 | 0.86 |
| 9:I:26:LEU:HD23 | 9:I:37:GLU:HA | 1.56 | 0.86 |
| 1:A:323:LYS:HZ3 | 14:P:1:U:H4' | 1.39 | 0.86 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:HG21 | 1.56 | 0.86 |
| 2:B:942:ARG:HH22 | 15:T:25:DT:P | 1.98 | 0.86 |
| 2:B:510:LYS:HG2 | 2:B:511:PRO:HD3 | 1.58 | 0.86 |
| 3:C:43:THR:HG22 | 3:C:44:LEU:N | 1.89 | 0.86 |
| 1:A:70:CYS:O | 1:A:72:GLU:HG2 | 1.75 | 0.85 |
| 1:A:828:ALA:CB | 2:B:530:GLY:HA2 | 2.06 | 0.85 |
| 1:A:646:PHE:O | 1:A:650:GLN:HG3 | 1.76 | 0.85 |
| 2:B:343:ILE:HG21 | 2:B:348:ARG:HG3 | 1.58 | 0.85 |
| 5:E:19:VAL:O | 5:E:23:VAL:HG23 | 1.76 | 0.85 |
| 9:I:8:ARG:HG3 | 9:I:34:TYR:CE1 | 2.11 | 0.85 |
| 2:B:770:GLN:OE1 | 2:B:983:ARG:HA | 1.76 | 0.85 |
| 6:F:86:THR:OG1 | 6:F:89:GLU:HG3 | 1.77 | 0.85 |
| 8:H:40:LEU:HD13 | 8:H:123:MET:HB2 | 1.59 | 0.85 |
| 9:I:115:LYS:HD3 | 9:I:117:LYS:HE3 | 1.57 | 0.85 |
| 2:B:343:ILE:CG2 | 2:B:348:ARG:HG3 | 2.05 | 0.85 |
| 3:C:47:ASP:HA | 12:L:69:ALA:HB3 | 1.58 | 0.85 |
| 11:K:21:ILE:HG12 | 11:K:33:ILE:HG12 | 1.57 | 0.85 |
| 1:A:320:ARG:HH22 | 14:P:1:U:H1' | 1.40 | 0.85 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:HB3 | 1.59 | 0.85 |
| 1:A:321:PRO:O | 1:A:322:VAL:HB | 1.76 | 0.84 |
| 2:B:46:GLN:HG3 | 2:B:47:GLN:H | 1.41 | 0.84 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:H | 1.94 | 0.84 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:34:VAL:HG12 | 7:G:45:ILE:HG21 | 1.59 | 0.84 |
| 1:A:225:ASN:ND2 | 1:A:228:PHE:H | 1.76 | 0.84 |
| 1:A:855:THR:CG2 | 1:A:857:ARG:HE | 1.90 | 0.84 |
| 2:B:847:ASP:HB3 | 3:C:167:HIS:NE2 | 1.92 | 0.84 |
| 1:A:535:THR:HG21 | 1:A:616:VAL:HA | 1.60 | 0.84 |
| 2:B:343:ILE:HG21 | 2:B:348:ARG:N | 1.92 | 0.84 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:HD2 | 1.59 | 0.84 |
| 14:P:6:C:H2' | 14:P:7:A:C8 | 2.12 | 0.84 |
| 2:B:98:THR:O | 2:B:126:SER:HB2 | 1.78 | 0.84 |
| 6:F:69:LEU:HA | 6:F:70:LYS:N | 1.91 | 0.84 |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:HD11 | 1.60 | 0.83 |
| 3:C:32:SER:O | 3:C:36:VAL:HG23 | 1.78 | 0.83 |
| 1:A:215:SER:HB3 | 1:A:218:ASP:OD2 | 1.77 | 0.83 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:HB | 1.77 | 0.83 |
| 1:A:340:LEU:HD13 | 1:A:1429:ILE:HG23 | 1.59 | 0.83 |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:N | 1.93 | 0.83 |
| 1:A:58:LEU:HD12 | 1:A:59:GLY:N | 1.94 | 0.83 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:N | 1.94 | 0.83 |
| 1:A:1325:THR:O | 5:E:148:GLU:HB2 | 1.79 | 0.83 |
| 1:A:741:ASN:HD22 | 1:A:744:LYS:H | 1.27 | 0.82 |
| 7:G:7:LEU:HB2 | 7:G:74:TYR:CE2 | 2.14 | 0.82 |
| 1:A:709:THR:HG22 | 1:A:711:ARG:H | 1.44 | 0.82 |
| 2:B:642:ASP:HA | 2:B:649:LYS:HA | 1.59 | 0.82 |
| 2:B:363:HIS:O | 2:B:364:ILE:HB | 1.76 | 0.82 |
| 1:A:903:ASN:HD22 | 1:A:904:THR:N | 1.77 | 0.82 |
| 1:A:84:ILE:HD11 | 1:A:270:LEU:HD13 | 1.60 | 0.82 |
| 1:A:590:ARG:HG3 | 1:A:590:ARG:NH1 | 1.94 | 0.82 |
| 8:H:59:ILE:HG22 | 8:H:60:ALA:N | 1.93 | 0.82 |
| 9:I:34:TYR:CD2 | 9:I:35:VAL:N | 2.48 | 0.82 |
| 1:A:472:LEU:O | 1:A:475:THR:HB | 1.79 | 0.82 |
| 2:B:955:THR:HG22 | 2:B:956:THR:H | 1.44 | 0.82 |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:HG2 | 1.44 | 0.81 |
| 9:I:105:SER:O | 9:I:106:CYS:HB3 | 1.77 | 0.81 |
| 1:A:779:PHE:CE1 | 1:A:785:PRO:HD3 | 2.15 | 0.81 |
| 2:B:365:THR:HG23 | 2:B:367:LEU:H | 1.45 | 0.81 |
| 4:D:47:LEU:HD11 | 7:G:3:PHE:CD2 | 2.14 | 0.81 |
| 11:K:47:ARG:HB3 | 11:K:47:ARG:NH1 | 1.96 | 0.81 |
| 2:B:336:ARG:HD3 | 2:B:348:ARG:HH11 | 1.46 | 0.81 |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:HG12 | 1.62 | 0.81 |
| 7:G:80:LYS:HD3 | 7:G:80:LYS:H | 1.45 | 0.81 |
| 7:G:80:LYS:HD3 | 7:G:80:LYS:N | 1.96 | 0.81 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:T:18:DT:C3' | 15:T:19:TT:H4' | 2.11 | 0.81 |
| 1:A:1004:ASN:ND2 | 5:E:167:ARG:HD2 | 1.96 | 0.81 |
| 7:G:128:PRO:O | 7:G:138:THR:HG23 | 1.81 | 0.81 |
| 1:A:49:LYS:HE2 | 1:A:61:ILE:HD12 | 1.62 | 0.81 |
| 1:A:356:ASP:HB2 | 1:A:469:ARG:NH1 | 1.96 | 0.81 |
| 2:B:879:ARG:HH11 | 2:B:883:LEU:HD22 | 1.44 | 0.81 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2 | 1.63 | 0.81 |
| 15:T:18:DT:H2" | 15:T:19:TT:C5' | 2.11 | 0.81 |
| 5:E:16:PHE:CZ | 5:E:20:LYS:HE2 | 2.16 | 0.80 |
| 10:J:7:CYS:HB2 | 10:J:46:CYS:HB3 | 1.63 | 0.80 |
| 15:T:18:DT:H2' | 15:T:19:TT:H5'1 | 1.62 | 0.80 |
| 1:A:427:GLN:HG3 | 1:A:430:TRP:CZ2 | 2.16 | 0.80 |
| 1:A:743:VAL:O | 1:A:747:VAL:HG23 | 1.82 | 0.80 |
| 5:E:192:ARG:HH11 | 5:E:192:ARG:HG3 | 1.45 | 0.80 |
| 3:C:244:VAL:O | 3:C:248:ILE:HG13 | 1.82 | 0.80 |
| 2:B:189:LEU:O | 2:B:192:LEU:N | 2.14 | 0.80 |
| 2:B:467:GLY:H | 2:B:475:SER:HB3 | 1.46 | 0.80 |
| 1:A:1116:LEU:N | 1:A:1308:THR:HG22 | 1.97 | 0.80 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:HD3 | 1.64 | 0.80 |
| 4:D:22:GLU:H | 4:D:22:GLU:CD | 1.85 | 0.80 |
| 9:I:34:TYR:HD2 | 9:I:35:VAL:N | 1.80 | 0.80 |
| 1:A:767:GLN:NE2 | 1:A:774:ARG:HB3 | 1.96 | 0.79 |
| 5:E:22:MET:HE3 | 5:E:26:ARG:NH2 | 1.96 | 0.79 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:CD | 2.12 | 0.79 |
| 15:T:18:DT:H2" | 15:T:19:TT:O5' | 1.82 | 0.79 |
| 10:J:8:PHE:H | 10:J:49:MET:HE1 | 1.46 | 0.79 |
| 1:A:107:CYS:SG | 1:A:171:GLN:HG2 | 2.21 | 0.79 |
| 1:A:821:ARG:HB2 | 1:A:821:ARG:HH11 | 1.45 | 0.79 |
| 1:A:886:ILE:HG22 | 1:A:887:GLY:N | 1.96 | 0.79 |
| 2:B:483:LEU:HD11 | 2:B:491:THR:HG23 | 1.63 | 0.79 |
| 15:T:18:DT:C2' | 15:T:19:TT:C5' | 2.60 | 0.79 |
| 1:A:567:LYS:HE3 | 8:H:46:LEU:HB2 | 1.64 | 0.79 |
| 2:B:171:PRO:HD2 | 2:B:457:LEU:HD13 | 1.62 | 0.79 |
| 2:B:467:GLY:N | 2:B:475:SER:HB3 | 1.98 | 0.79 |
| 1:A:768:GLN:CG | 1:A:816:HIS:HA | 2.12 | 0.79 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:HD2 | 1.65 | 0.79 |
| 1:A:590:ARG:HG3 | 1:A:590:ARG:HH11 | 1.47 | 0.79 |
| 2:B:244:LEU:HD21 | 2:B:366:GLN:NE2 | 1.97 | 0.79 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:HB2 | 1.82 | 0.79 |
| 2:B:112:LEU:HD12 | 2:B:113:TYR:H | 1.48 | 0.79 |
| 2:B:1202:LEU:O | 2:B:1206:GLU:HG3 | 1.82 | 0.79 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:I:34:TYR:HE2 | 9:I:36:GLU:HB3 | 1.48 | 0.79 |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:HB3 | 1.63 | 0.78 |
| 1:A:1030:ARG:HG3 | 1:A:1034:GLU:OE2 | 1.83 | 0.78 |
| 1:A:567:LYS:HB3 | 8:H:95:TYR:HA | 1.64 | 0.78 |
| 1:A:1312:ASN:O | 1:A:1316:VAL:HG23 | 1.83 | 0.78 |
| 1:A:63:ARG:HA | 1:A:74:MET:SD | 2.24 | 0.78 |
| 1:A:1206:ASP:HB3 | 1:A:1274:ARG:HH12 | 1.47 | 0.78 |
| 1:A:93:VAL:HG22 | 1:A:301:ALA:HA | 1.66 | 0.78 |
| 2:B:613:VAL:HG13 | 2:B:627:PHE:O | 1.83 | 0.78 |
| 3:C:147:LEU:HB2 | 3:C:151:GLN:HB2 | 1.65 | 0.78 |
| 2:B:580:VAL:HG22 | 2:B:624:LEU:HB3 | 1.66 | 0.78 |
| 2:B:758:PHE:CE2 | 2:B:1044:ALA:HA | 2.18 | 0.78 |
| 3:C:174:ALA:HB2 | 3:C:235:VAL:HG22 | 1.65 | 0.78 |
| 1:A:34:LYS:CE | 1:A:57:ARG:HH12 | 1.95 | 0.78 |
| 4:D:153:ARG:NH2 | 4:D:184:ALA:HA | 1.99 | 0.78 |
| 8:H:59:ILE:HG22 | 8:H:60:ALA:H | 1.48 | 0.78 |
| 2:B:169:ARG:HB2 | 2:B:454:THR:HG23 | 1.66 | 0.78 |
| 5:E:213:ILE:HG12 | 5:E:214:CYS:H | 1.48 | 0.78 |
| 1:A:346:ASP:HB3 | 2:B:1108:ARG:H | 1.49 | 0.78 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:N | 1.99 | 0.78 |
| 3:C:35:ARG:NH1 | 11:K:41:THR:H | 1.80 | 0.78 |
| 7:G:111:THR:HG22 | 7:G:113:HIS:H | 1.49 | 0.78 |
| 9:I:55:THR:HG21 | 9:I:109:ILE:HD13 | 1.66 | 0.78 |
| 1:A:1028:THR:O | 1:A:1032:LEU:HD12 | 1.84 | 0.78 |
| 2:B:654:ARG:H | 2:B:657:HIS:HD2 | 1.28 | 0.78 |
| 1:A:351:THR:HG22 | 2:B:1103:ILE:HA | 1.64 | 0.77 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:O | 1.84 | 0.77 |
| 8:H:17:PRO:HB3 | 8:H:24:CYS:SG | 2.24 | 0.77 |
| 12:L:53:HIS:HB3 | 12:L:55:ILE:HD11 | 1.66 | 0.77 |
| 1:A:14:VAL:HG21 | 2:B:1216:LEU:HD13 | 1.66 | 0.77 |
| 1:A:528:LEU:O | 1:A:531:ILE:HG22 | 1.84 | 0.77 |
| 1:A:596:THR:O | 1:A:598:LEU:N | 2.18 | 0.77 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:H | 1.48 | 0.77 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:N | 1.97 | 0.77 |
| 2:B:1095:LEU:H | 2:B:1095:LEU:HD12 | 1.49 | 0.77 |
| 2:B:1224:PHE:HE2 | 5:E:171:LYS:HG3 | 1.49 | 0.77 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:H | 1.49 | 0.77 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:HG13 | 2.00 | 0.77 |
| 1:A:794:PRO:HG2 | 1:A:795:GLU:OE2 | 1.85 | 0.77 |
| 1:A:567:LYS:HG3 | 1:A:568:PRO:HD2 | 1.66 | 0.77 |
| 1:A:1036:ARG:HG2 | 1:A:1036:ARG:HH11 | 1.49 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:906:SER:O | 2:B:941:LEU:HD23 | 1.85 | 0.77 |
| 1:A:866:PHE:C | 1:A:867:ILE:HD12 | 2.05 | 0.77 |
| 12:L:32:ALA:HB3 | 12:L:55:ILE:HD12 | 1.67 | 0.77 |
| 1:A:836:TYR:CD1 | 15:T:18:DT:H5" | 2.19 | 0.77 |
| 1:A:903:ASN:ND2 | 1:A:905:ASP:H | 1.83 | 0.77 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:N | 1.99 | 0.77 |
| 13:N:5:DA:H1' | 13:N:6:DC:O5' | 1.85 | 0.77 |
| 1:A:269:ILE:HD13 | 1:A:300:VAL:HG22 | 1.67 | 0.76 |
| 1:A:323:LYS:NZ | 14:P:1:U:H4' | 1.99 | 0.76 |
| 2:B:340:ALA:HB2 | 2:B:343:ILE:HD12 | 1.67 | 0.76 |
| 2:B:737:THR:HG21 | 9:I:66:PRO:HA | 1.67 | 0.76 |
| 4:D:40:HIS:CE1 | 4:D:41:GLN:HG3 | 2.21 | 0.76 |
| 14:P:9:A:N1 | 15:T:19:TT:O4T | 2.17 | 0.76 |
| 1:A:868:TYR:HD2 | 1:A:1058:VAL:HG21 | 1.48 | 0.76 |
| 2:B:778:MET:CE | 2:B:1094:ARG:HD3 | 2.16 | 0.76 |
| 2:B:821:GLN:HE22 | 2:B:851:PHE:HA | 1.50 | 0.76 |
| 4:D:47:LEU:HD13 | 4:D:48:ILE:H | 1.49 | 0.76 |
| 8:H:61:SER:O | 8:H:62:SER:HB3 | 1.85 | 0.76 |
| 1:A:466:SER:O | 2:B:1103:ILE:HD11 | 1.85 | 0.76 |
| 2:B:859:TYR:OH | 2:B:941:LEU:HD12 | 1.85 | 0.76 |
| 1:A:21:LEU:HD11 | 1:A:1414:ALA:HA | 1.68 | 0.76 |
| 1:A:106:VAL:HG13 | 1:A:112:LYS:O | 1.85 | 0.76 |
| 2:B:114:PRO:HG2 | 2:B:115:GLN:H | 1.51 | 0.76 |
| 13:N:3:DG:H1' | 13:N:4:DT:H5' | 1.68 | 0.76 |
| 1:A:1171:GLN:HA | 1:A:1174:PHE:CE1 | 2.21 | 0.76 |
| 1:A:1372:VAL:O | 1:A:1376:THR:HG22 | 1.84 | 0.76 |
| 2:B:44:VAL:HG11 | 2:B:199:MET:HG2 | 1.66 | 0.76 |
| 2:B:217:ARG:NE | 2:B:405:ARG:HB2 | 2.01 | 0.76 |
| 3:C:213:PRO:O | 3:C:214:ASN:HB2 | 1.84 | 0.76 |
| 1:A:1332:PHE:H | 1:A:1332:PHE:HD2 | 1.32 | 0.76 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:N | 1.84 | 0.76 |
| 8:H:36:CYS:HA | 8:H:126:GLU:O | 1.84 | 0.76 |
| 1:A:16:GLU:HB3 | 1:A:1418:LEU:HD11 | 1.66 | 0.75 |
| 1:A:982:THR:HB | 1:A:985:ASP:H | 1.49 | 0.75 |
| 1:A:868:TYR:HE1 | 1:A:1064:VAL:HG11 | 1.48 | 0.75 |
| 2:B:708:GLU:O | 2:B:710:LEU:N | 2.20 | 0.75 |
| 6:F:90:ARG:HD3 | 6:F:155:LEU:HD11 | 1.67 | 0.75 |
| 1:A:986:ILE:HG22 | 1:A:987:VAL:N | 2.00 | 0.75 |
| 2:B:510:LYS:HG3 | 2:B:511:PRO:HD3 | 1.67 | 0.75 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HD13 | 1.68 | 0.75 |
| 1:A:657:LEU:O | 1:A:657:LEU:HD12 | 1.86 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:885:THR:O | 1:A:940:ARG:HD2 | 1.87 | 0.75 |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H | 1.51 | 0.75 |
| 1:A:666:ILE:HD12 | 1:A:667:GLY:H | 1.51 | 0.75 |
| 1:A:230:ARG:H | 1:A:233:TRP:HE3 | 1.35 | 0.75 |
| 1:A:351:THR:HB | 2:B:1103:ILE:HD12 | 1.69 | 0.75 |
| 1:A:385:ILE:HG22 | 1:A:386:ASP:N | 2.01 | 0.75 |
| 1:A:512:VAL:HA | 1:A:519:PRO:HA | 1.68 | 0.75 |
| 1:A:852:TYR:CD2 | 1:A:1060:PRO:HB2 | 2.22 | 0.75 |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:CD1 | 2.16 | 0.75 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:H | 1.31 | 0.75 |
| 2:B:361:LEU:HD21 | 2:B:377:PHE:CD2 | 2.21 | 0.75 |
| 2:B:516:ASN:N | 2:B:516:ASN:ND2 | 2.35 | 0.75 |
| 2:B:637:LEU:HD12 | 2:B:693:ILE:HD12 | 1.69 | 0.75 |
| 11:K:12:LEU:H | 11:K:12:LEU:HD12 | 1.50 | 0.75 |
| 1:A:855:THR:HG23 | 1:A:857:ARG:HG3 | 1.68 | 0.75 |
| 4:D:47:LEU:HD11 | 7:G:3:PHE:HD2 | 1.50 | 0.75 |
| 1:A:87:ALA:CB | 1:A:276:LEU:HD23 | 2.17 | 0.74 |
| 1:A:92:HIS:O | 1:A:94:GLY:N | 2.20 | 0.74 |
| 2:B:701:ILE:HD11 | 2:B:703:ILE:HD11 | 1.67 | 0.74 |
| 1:A:1387:HIS:CE1 | 13:N:4:DT:H4' | 2.21 | 0.74 |
| 7:G:81:PRO:HG3 | 7:G:106:MET:SD | 2.26 | 0.74 |
| 11:K:47:ARG:HH11 | 11:K:47:ARG:CB | 1.98 | 0.74 |
| 7:G:39:THR:HG22 | 7:G:41:LYS:H | 1.52 | 0.74 |
| 1:A:335:ARG:HA | 1:A:339:ASN:HB2 | 1.68 | 0.74 |
| 1:A:754:SER:H | 1:A:757:ASN:ND2 | 1.86 | 0.74 |
| 1:A:1063:MET:SD | 1:A:1436:ILE:HG12 | 2.28 | 0.74 |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:CG | 2.00 | 0.74 |
| 2:B:830:TYR:O | 2:B:832:GLY:N | 2.20 | 0.74 |
| 3:C:212:PRO:HB3 | 3:C:213:PRO:HD2 | 1.69 | 0.74 |
| 7:G:59:GLY:HA3 | 7:G:70:PHE:CD2 | 2.23 | 0.74 |
| 2:B:189:LEU:HA | 2:B:192:LEU:HD12 | 1.68 | 0.74 |
| 2:B:434:ARG:O | 2:B:437:GLU:HB2 | 1.86 | 0.74 |
| 2:B:515:HIS:HD2 | 2:B:517:THR:H | 1.35 | 0.74 |
| 2:B:526:GLU:HG2 | 2:B:538:ASN:HD22 | 1.52 | 0.74 |
| 12:L:30:ILE:O | 12:L:56:LEU:HA | 1.87 | 0.74 |
| 1:A:567:LYS:HD3 | 8:H:95:TYR:CG | 2.23 | 0.74 |
| 2:B:549:THR:H | 2:B:628:THR:HG23 | 1.52 | 0.74 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:H | 2.01 | 0.74 |
| 5:E:157:SER:OG | 5:E:160:GLU:HG3 | 1.87 | 0.74 |
| 1:A:858:ASN:C | 1:A:858:ASN:HD22 | 1.91 | 0.74 |
| 2:B:899:ILE:HD11 | 2:B:911:ILE:HA | 1.70 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1034:VAL:HG12 | 2:B:1035:ALA:N | 2.03 | 0.74 |
| 1:A:798:GLY:HA2 | 1:A:815:PHE:CD1 | 2.22 | 0.73 |
| 7:G:14:HIS:ND1 | 7:G:15:PRO:HD2 | 2.03 | 0.73 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HG3 | 1.69 | 0.73 |
| 1:A:1189:SER:O | 1:A:1241:ARG:HD3 | 1.87 | 0.73 |
| 2:B:1180:PHE:HB3 | 2:B:1191:ILE:HD12 | 1.68 | 0.73 |
| 12:L:38:LEU:O | 12:L:39:SER:HB3 | 1.88 | 0.73 |
| 2:B:332:ASP:O | 2:B:336:ARG:HG3 | 1.86 | 0.73 |
| 4:D:153:ARG:HB3 | 4:D:154:PHE:CE1 | 2.23 | 0.73 |
| 7:G:39:THR:HG22 | 7:G:40:GLY:H | 1.54 | 0.73 |
| 1:A:35:ILE:HG22 | 1:A:35:ILE:O | 1.89 | 0.73 |
| 1:A:63:ARG:HA | 1:A:74:MET:CE | 2.19 | 0.73 |
| 7:G:14:HIS:HD2 | 7:G:16:SER:HB2 | 1.49 | 0.73 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:CZ | 2.18 | 0.73 |
| 1:A:53:LEU:HD22 | 1:A:54:ASN:HD22 | 1.54 | 0.73 |
| 1:A:384:ASN:OD1 | 1:A:388:LEU:HD12 | 1.89 | 0.73 |
| 2:B:1072:MET:HE1 | 2:B:1085:ILE:HB | 1.68 | 0.73 |
| 4:D:66:ARG:HD2 | 4:D:133:THR:HB | 1.71 | 0.73 |
| 1:A:254:GLU:HB2 | 2:B:935:ARG:NH1 | 2.03 | 0.73 |
| 2:B:232:SER:HB3 | 2:B:261:ARG:NH2 | 2.04 | 0.73 |
| 1:A:249:SER:O | 1:A:250:ILE:HG13 | 1.87 | 0.73 |
| 1:A:567:LYS:HB3 | 8:H:96:VAL:N | 2.03 | 0.73 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CD1 | 2.24 | 0.72 |
| 3:C:47:ASP:HA | 12:L:69:ALA:CB | 2.19 | 0.72 |
| 1:A:845:LEU:HB3 | 1:A:848:ILE:HD12 | 1.71 | 0.72 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:N | 2.03 | 0.72 |
| 4:D:130:LEU:O | 4:D:132:GLN:N | 2.21 | 0.72 |
| 3:C:167:HIS:HD2 | 3:C:168:ALA:N | 1.85 | 0.72 |
| 9:I:7:CYS:HB3 | 9:I:14:LEU:HD21 | 1.71 | 0.72 |
| 1:A:67:CYS:O | 1:A:70:CYS:HB3 | 1.89 | 0.72 |
| 1:A:337:ARG:HD3 | 2:B:1132:GLU:OE1 | 1.89 | 0.72 |
| 2:B:778:MET:HE3 | 2:B:1094:ARG:HD3 | 1.71 | 0.72 |
| 3:C:174:ALA:HB2 | 3:C:235:VAL:CG2 | 2.19 | 0.72 |
| 1:A:51:GLY:HA2 | 1:A:56:PRO:HA | 1.70 | 0.72 |
| 2:B:336:ARG:NH2 | 2:B:345:LYS:HG2 | 2.05 | 0.72 |
| 2:B:879:ARG:NH1 | 2:B:883:LEU:HD22 | 2.03 | 0.72 |
| 6:F:103:MET:HE2 | 7:G:66:GLY:H | 1.54 | 0.72 |
| 9:I:111:THR:HG22 | 9:I:112:SER:N | 2.04 | 0.72 |
| 5:E:124:VAL:HG13 | 5:E:132:ILE:HB | 1.71 | 0.72 |
| 1:A:62:ASP:HB3 | 1:A:64:ASN:ND2 | 2.05 | 0.72 |
| 1:A:115:LEU:O | 1:A:122:MET:HE2 | 1.90 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:537:ARG:HD2 | 8:H:20:TYR:HE1 | 1.55 | 0.72 |
| 2:B:343:ILE:CG2 | 2:B:347:LYS:HB2 | 2.07 | 0.72 |
| 2:B:569:TYR:CE1 | 2:B:589:VAL:HG21 | 2.24 | 0.72 |
| 2:B:622:LYS:HE2 | 9:I:59:VAL:HG22 | 1.71 | 0.72 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:CG2 | 2.19 | 0.72 |
| 2:B:1138:MET:HA | 2:B:1138:MET:HE3 | 1.72 | 0.72 |
| 4:D:29:LEU:HD22 | 7:G:82:PHE:CE2 | 2.25 | 0.72 |
| 1:A:58:LEU:HD13 | 1:A:80:HIS:O | 1.90 | 0.72 |
| 2:B:336:ARG:CG | 2:B:348:ARG:HD3 | 2.15 | 0.72 |
| 2:B:999:MET:HG3 | 2:B:1000:PRO:HD2 | 1.71 | 0.72 |
| 2:B:1197:PRO:HG2 | 2:B:1200:ALA:HB2 | 1.72 | 0.72 |
| 15:T:24:DG:H2" | 15:T:25:DT:O5' | 1.89 | 0.72 |
| 2:B:1087:PHE:HD2 | 2:B:1088:GLY:N | 1.86 | 0.72 |
| 1:A:993:LEU:HD22 | 1:A:1046:LEU:HD22 | 1.71 | 0.71 |
| 10:J:1:MET:H1 | 10:J:57:ILE:H | 0.80 | 0.71 |
| 1:A:567:LYS:HD3 | 8:H:95:TYR:CD2 | 2.24 | 0.71 |
| 4:D:134:THR:HG22 | 4:D:136:GLY:H | 1.55 | 0.71 |
| 5:E:180:ARG:HH21 | 5:E:192:ARG:HB2 | 1.54 | 0.71 |
| 1:A:325:ILE:HG21 | 2:B:1210:MET:HG3 | 1.72 | 0.71 |
| 1:A:858:ASN:ND2 | 1:A:860:LEU:H | 1.88 | 0.71 |
| 2:B:516:ASN:HD22 | 2:B:516:ASN:H | 1.37 | 0.71 |
| 14:P:5:C:O2' | 14:P:6:C:H5' | 1.91 | 0.71 |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG | 2.31 | 0.71 |
| 1:A:1171:GLN:HA | 1:A:1174:PHE:CD1 | 2.26 | 0.71 |
| 2:B:815:ARG:HD3 | 2:B:1041:GLU:OE2 | 1.91 | 0.71 |
| 4:D:176:GLU:C | 4:D:178:ALA:H | 1.94 | 0.71 |
| 13:N:6:DC:H2" | 13:N:7:DT:OP2 | 1.89 | 0.71 |
| 15:T:19:TT:H2R2 | 15:T:19:TT:C2' | 2.19 | 0.71 |
| 2:B:310:MET:HE3 | 2:B:387:LEU:HD12 | 1.70 | 0.71 |
| 2:B:336:ARG:HH22 | 2:B:345:LYS:CE | 2.03 | 0.71 |
| 3:C:39:ALA:HA | 3:C:164:ALA:HB3 | 1.72 | 0.71 |
| 2:B:35:SER:HA | 2:B:811:TYR:HE2 | 1.56 | 0.71 |
| 2:B:226:PHE:HA | 2:B:395:GLN:HG3 | 1.73 | 0.71 |
| 2:B:336:ARG:HD3 | 2:B:348:ARG:NH1 | 2.05 | 0.71 |
| 2:B:515:HIS:H | 2:B:518:HIS:CD2 | 2.04 | 0.71 |
| 3:C:208:GLU:O | 3:C:210:GLU:N | 2.24 | 0.71 |
| 8:H:56:THR:HB | 8:H:145:ARG:HG2 | 1.72 | 0.71 |
| 1:A:254:GLU:CB | 2:B:935:ARG:HH12 | 2.04 | 0.71 |
| 1:A:960:ILE:O | 1:A:963:ILE:HG22 | 1.89 | 0.71 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:HD21 | 1.72 | 0.71 |
| 3:C:67:LEU:HD11 | 3:C:155:LEU:CD1 | 2.20 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:807:ARG:HG2 | 2:B:1045:SER:OG | 1.89 | 0.71 |
| 5:E:135:PHE:HD2 | 5:E:140:LEU:HD21 | 1.54 | 0.71 |
| 1:A:382:PRO:HB3 | 1:A:428:TYR:CE2 | 2.23 | 0.71 |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:N | 2.05 | 0.71 |
| 10:J:43:ARG:HG3 | 10:J:45:CYS:SG | 2.30 | 0.71 |
| 10:J:64:ASN:HD22 | 10:J:65:PRO:HD3 | 1.55 | 0.71 |
| 2:B:953:LEU:CD2 | 2:B:965:LYS:HB2 | 2.20 | 0.71 |
| 2:B:955:THR:HG22 | 2:B:956:THR:N | 2.05 | 0.71 |
| 3:C:35:ARG:NH1 | 11:K:41:THR:N | 2.38 | 0.71 |
| 3:C:186:LEU:HD21 | 3:C:224:GLN:O | 1.90 | 0.71 |
| 1:A:69:THR:O | 1:A:71:GLN:N | 2.23 | 0.70 |
| 1:A:326:ARG:HH22 | 1:A:1407:GLU:HG3 | 1.53 | 0.70 |
| 1:A:1348:LEU:HG | 1:A:1372:VAL:CG2 | 2.21 | 0.70 |
| 1:A:1437:GLY:O | 1:A:1439:GLY:N | 2.23 | 0.70 |
| 4:D:134:THR:HG22 | 4:D:135:GLY:N | 2.06 | 0.70 |
| 1:A:541:ILE:HD13 | 1:A:549:MET:CE | 2.21 | 0.70 |
| 2:B:280:ILE:HD13 | 2:B:334:ILE:HG12 | 1.71 | 0.70 |
| 2:B:359:GLU:O | 2:B:362:PRO:HD3 | 1.92 | 0.70 |
| 1:A:546:VAL:O | 1:A:550:LEU:HG | 1.92 | 0.70 |
| 1:A:901:LEU:HG | 1:A:926:GLN:HE21 | 1.55 | 0.70 |
| 4:D:130:LEU:C | 4:D:132:GLN:H | 1.94 | 0.70 |
| 5:E:117:THR:HG22 | 5:E:119:SER:H | 1.56 | 0.70 |
| 9:I:111:THR:HG22 | 9:I:112:SER:H | 1.56 | 0.70 |
| 1:A:567:LYS:CB | 8:H:95:TYR:HA | 2.21 | 0.70 |
| 1:A:741:ASN:HD21 | 1:A:743:VAL:HB | 1.55 | 0.70 |
| 3:C:226:ASP:O | 3:C:227:THR:HB | 1.90 | 0.70 |
| 8:H:40:LEU:CD1 | 8:H:123:MET:HB2 | 2.22 | 0.70 |
| 15:T:18:DT:O3' | 15:T:19:TT:H4' | 1.90 | 0.70 |
| 1:A:18:GLN:HB2 | 2:B:1215:ARG:HB2 | 1.73 | 0.70 |
| 1:A:34:LYS:HB2 | 1:A:36:ARG:HH21 | 1.57 | 0.70 |
| 2:B:1172:ILE:HG22 | 2:B:1172:ILE:O | 1.90 | 0.70 |
| 7:G:39:THR:HG22 | 7:G:40:GLY:N | 2.06 | 0.70 |
| 1:A:55:ASP:N | 1:A:56:PRO:HD3 | 2.04 | 0.70 |
| 1:A:58:LEU:HD11 | 1:A:243:PRO:CB | 2.21 | 0.70 |
| 2:B:615:MET:C | 2:B:616:ILE:HD12 | 2.12 | 0.70 |
| 10:J:7:CYS:CB | 10:J:46:CYS:HB3 | 2.21 | 0.70 |
| 1:A:438:ASP:O | 1:A:439:ASN:HB2 | 1.90 | 0.70 |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:CB | 2.21 | 0.70 |
| 4:D:7:THR:HG21 | 4:D:32:GLU:CD | 2.11 | 0.70 |
| 4:D:8:PHE:CE2 | 4:D:40:HIS:HA | 2.25 | 0.70 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CE1 | 2.25 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1329:THR:HG22 | 1:A:1331:SER:N | 2.06 | 0.70 |
| 1:A:1348:LEU:HG | 1:A:1372:VAL:HG23 | 1.73 | 0.70 |
| 2:B:175:ARG:HG2 | 2:B:175:ARG:HH11 | 1.55 | 0.70 |
| 2:B:336:ARG:HG2 | 2:B:348:ARG:CD | 2.17 | 0.70 |
| 1:A:265:LYS:N | 1:A:265:LYS:HD2 | 2.06 | 0.70 |
| 1:A:1332:PHE:N | 1:A:1332:PHE:CD2 | 2.60 | 0.70 |
| 1:A:34:LYS:H | 1:A:57:ARG:NH2 | 1.90 | 0.70 |
| 8:H:123:MET:HG2 | 8:H:124:ARG:N | 2.07 | 0.70 |
| 1:A:637:LYS:HB3 | 1:A:641:VAL:HG11 | 1.73 | 0.69 |
| 2:B:38:PHE:HD1 | 2:B:811:TYR:CD2 | 2.09 | 0.69 |
| 1:A:996:ASN:O | 1:A:998:LEU:HD12 | 1.91 | 0.69 |
| 1:A:1035:TYR:O | 1:A:1037:LEU:N | 2.25 | 0.69 |
| 1:A:1149:ALA:HB2 | 9:I:47:GLU:HA | 1.74 | 0.69 |
| 2:B:336:ARG:CD | 2:B:348:ARG:HH11 | 2.04 | 0.69 |
| 2:B:824:ILE:CG2 | 2:B:1087:PHE:HE2 | 2.05 | 0.69 |
| 2:B:1069:PHE:H | 2:B:1069:PHE:HD1 | 1.39 | 0.69 |
| 4:D:40:HIS:CB | 7:G:73:LYS:NZ | 2.54 | 0.69 |
| 4:D:34:GLN:O | 4:D:47:LEU:HD23 | 1.92 | 0.69 |
| 6:F:90:ARG:HD3 | 6:F:155:LEU:CD1 | 2.22 | 0.69 |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:N | 2.06 | 0.69 |
| 12:L:53:HIS:HB3 | 12:L:55:ILE:CD1 | 2.22 | 0.69 |
| 1:A:347:PHE:H | 2:B:1107:ALA:HA | 1.57 | 0.69 |
| 1:A:471:ASN:OD1 | 1:A:472:LEU:N | 2.25 | 0.69 |
| 15:T:26:DC:H2" | 15:T:27:DA:H5' | 1.74 | 0.69 |
| 1:A:541:ILE:HG21 | 1:A:549:MET:HE3 | 1.74 | 0.69 |
| 3:C:70:ILE:HG12 | 3:C:142:VAL:HG11 | 1.74 | 0.69 |
| 8:H:100:THR:OG1 | 8:H:138:GLU:HG3 | 1.92 | 0.69 |
| 2:B:847:ASP:HB3 | 3:C:167:HIS:HE2 | 1.54 | 0.69 |
| 2:B:1017:ILE:HB | 2:B:1018:PRO:HD3 | 1.75 | 0.69 |
| 1:A:114:LEU:HD13 | 1:A:171:GLN:HE22 | 1.56 | 0.69 |
| 2:B:745:PRO:O | 2:B:748:ILE:HG12 | 1.93 | 0.69 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:CB | 2.06 | 0.69 |
| 2:B:857:ARG:HD2 | 2:B:945:GLU:OE1 | 1.93 | 0.69 |
| 4:D:213:GLU:O | 4:D:217:LEU:HG | 1.93 | 0.69 |
| 1:A:265:LYS:NZ | 1:A:322:VAL:HG22 | 2.08 | 0.69 |
| 1:A:463:ILE:HB | 1:A:464:PRO:HD2 | 1.74 | 0.69 |
| 1:A:701:LEU:HA | 9:I:115:LYS:HE3 | 1.75 | 0.69 |
| 1:A:836:TYR:HD1 | 15:T:18:DT:H5" | 1.57 | 0.69 |
| 2:B:287:ARG:HG2 | 2:B:292:ILE:HA | 1.73 | 0.69 |
| 2:B:411:PRO:O | 2:B:414:ALA:HB3 | 1.93 | 0.69 |
| 2:B:642:ASP:O | 2:B:644:GLU:N | 2.26 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:975:GLN:HG2 | 2:B:976:ILE:H | 1.58 | 0.69 |
| 2:B:1115:THR:O | 2:B:1116:ARG:HB2 | 1.92 | 0.69 |
| 7:G:23:LYS:HG3 | 7:G:56:ILE:HD11 | 1.75 | 0.69 |
| 10:J:14:VAL:O | 10:J:14:VAL:HG12 | 1.92 | 0.69 |
| 1:A:19:PHE:O | 1:A:1416:ALA:HA | 1.93 | 0.69 |
| 1:A:441:PRO:HD2 | 1:A:498:ARG:NH2 | 2.08 | 0.69 |
| 2:B:1065:GLN:HG3 | 2:B:1067:ARG:H | 1.57 | 0.69 |
| 5:E:198:ILE:CD1 | 5:E:212:ARG:HG3 | 2.23 | 0.69 |
| 8:H:4:THR:HA | 8:H:60:ALA:CB | 2.22 | 0.69 |
| 1:A:382:PRO:HD3 | 1:A:428:TYR:CD2 | 2.28 | 0.69 |
| 1:A:870:GLU:HG2 | 5:E:208:TYR:CG | 2.28 | 0.69 |
| 1:A:901:LEU:HB2 | 1:A:926:GLN:HG2 | 1.74 | 0.69 |
| 1:A:1332:PHE:HD2 | 1:A:1332:PHE:N | 1.90 | 0.69 |
| 7:G:23:LYS:HG3 | 7:G:56:ILE:CD1 | 2.23 | 0.69 |
| 15:T:18:DT:H3' | 15:T:19:TT:H4' | 1.73 | 0.69 |
| 1:A:598:LEU:HA | 8:H:122:LEU:HD13 | 1.75 | 0.68 |
| 2:B:39:ARG:NH2 | 2:B:665:GLU:HG2 | 2.08 | 0.68 |
| 11:K:6:ARG:O | 11:K:9:LEU:HG | 1.93 | 0.68 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:CE1 | 2.28 | 0.68 |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG3 | 1.58 | 0.68 |
| 2:B:180:TYR:HD1 | 2:B:180:TYR:H | 1.41 | 0.68 |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:CE2 | 2.28 | 0.68 |
| 1:A:549:MET:SD | 1:A:577:ILE:HD11 | 2.33 | 0.68 |
| 1:A:856:THR:HB | 1:A:865:GLN:HB2 | 1.75 | 0.68 |
| 2:B:53:GLN:HG2 | 2:B:547:VAL:HG22 | 1.75 | 0.68 |
| 2:B:273:LEU:CB | 2:B:276:ILE:HD12 | 2.19 | 0.68 |
| 11:K:53:ASP:OD1 | 11:K:55:LYS:HB2 | 1.93 | 0.68 |
| 1:A:1445:ILE:HG12 | 7:G:18:PHE:CE2 | 2.28 | 0.68 |
| 2:B:1223:ASP:O | 2:B:1224:PHE:HB2 | 1.92 | 0.68 |
| 4:D:33:PHE:CE1 | 7:G:80:LYS:HE3 | 2.29 | 0.68 |
| 6:F:76:LYS:O | 6:F:79:ARG:HD3 | 1.94 | 0.68 |
| 8:H:102:TYR:OH | 8:H:122:LEU:HD22 | 1.94 | 0.68 |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:H | 1.59 | 0.68 |
| 1:A:1345:ARG:HG3 | 1:A:1376:THR:HG21 | 1.74 | 0.68 |
| 4:D:118:THR:HB | 4:D:121:LYS:HB2 | 1.76 | 0.68 |
| 4:D:189:ASP:O | 4:D:193:THR:HB | 1.92 | 0.68 |
| 5:E:78:LEU:HD21 | 5:E:80:VAL:HG23 | 1.76 | 0.68 |
| 1:A:537:ARG:HD2 | 8:H:20:TYR:CE1 | 2.29 | 0.68 |
| 2:B:121:ASN:HA | 2:B:207:GLY:CA | 2.23 | 0.68 |
| 2:B:863:GLU:OE2 | 2:B:873:THR:HA | 1.94 | 0.68 |
| 2:B:882:THR:HB | 2:B:934:LYS:O | 1.94 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:103:MET:O | 6:F:104:ASN:HB2 | 1.93 | 0.68 |
| 11:K:31:VAL:HG12 | 11:K:32:VAL:N | 2.09 | 0.68 |
| 15:T:19:TT:H2'1 | 15:T:19:TT:C2R | 2.23 | 0.68 |
| 1:A:1436:ILE:O | 1:A:1437:GLY:C | 2.33 | 0.68 |
| 5:E:198:ILE:HD11 | 5:E:212:ARG:HG3 | 1.74 | 0.68 |
| 8:H:84:ALA:CA | 8:H:87:ARG:HB2 | 2.22 | 0.68 |
| 1:A:552:TRP:HE3 | 1:A:651:LYS:HB3 | 1.60 | 0.68 |
| 2:B:232:SER:CB | 2:B:261:ARG:HH21 | 2.06 | 0.68 |
| 2:B:1180:PHE:HB3 | 2:B:1191:ILE:CD1 | 2.24 | 0.68 |
| 5:E:157:SER:C | 5:E:159:ASP:H | 1.97 | 0.68 |
| 1:A:58:LEU:HD21 | 1:A:243:PRO:CA | 2.23 | 0.67 |
| 2:B:1099:VAL:CG1 | 2:B:1100:ASP:N | 2.56 | 0.67 |
| 8:H:130:ARG:H | 8:H:130:ARG:HD2 | 1.59 | 0.67 |
| 1:A:42:ASP:HB3 | 1:A:45:GLN:H | 1.59 | 0.67 |
| 1:A:903:ASN:HD22 | 1:A:903:ASN:C | 1.96 | 0.67 |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HG21 | 1.75 | 0.67 |
| 2:B:351:TYR:O | 2:B:355:ILE:HG13 | 1.95 | 0.67 |
| 2:B:983:ARG:HD2 | 2:B:1091:TYR:HD2 | 1.59 | 0.67 |
| 3:C:35:ARG:HH12 | 11:K:41:THR:H | 1.40 | 0.67 |
| 3:C:232:VAL:HG21 | 3:C:244:VAL:HG22 | 1.77 | 0.67 |
| 6:F:130:ILE:O | 6:F:148:VAL:HG21 | 1.93 | 0.67 |
| 7:G:13:LEU:CD2 | 7:G:17:PHE:HB2 | 2.19 | 0.67 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:CD | 2.25 | 0.67 |
| 1:A:868:TYR:CD2 | 1:A:1058:VAL:HG21 | 2.29 | 0.67 |
| 1:A:901:LEU:H | 1:A:926:GLN:HE21 | 1.40 | 0.67 |
| 1:A:1002:GLY:HA3 | 1:A:1007:ILE:HG21 | 1.75 | 0.67 |
| 1:A:1120:LEU:HD12 | 1:A:1120:LEU:N | 2.09 | 0.67 |
| 2:B:953:LEU:HD23 | 2:B:953:LEU:O | 1.94 | 0.67 |
| 5:E:153:HIS:HB3 | 5:E:196:VAL:CG1 | 2.24 | 0.67 |
| 1:A:34:LYS:HE3 | 1:A:57:ARG:NH1 | 2.08 | 0.67 |
| 10:J:1:MET:H3 | 10:J:56:LEU:N | 1.91 | 0.67 |
| 1:A:68:GLN:C | 1:A:70:CYS:H | 1.97 | 0.67 |
| 1:A:69:THR:C | 1:A:71:GLN:H | 1.96 | 0.67 |
| 2:B:871:THR:HG22 | 2:B:872:GLU:O | 1.94 | 0.67 |
| 2:B:1174:LYS:O | 2:B:1176:ASN:N | 2.28 | 0.67 |
| 3:C:56:THR:HG22 | 3:C:57:VAL:H | 1.60 | 0.67 |
| 5:E:94:LYS:CE | 5:E:98:ILE:HD11 | 2.23 | 0.67 |
| 8:H:143:LEU:HD12 | 8:H:143:LEU:N | 2.08 | 0.67 |
| 15:T:19:TT:H5M1 | 15:T:21:DC:C4 | 2.29 | 0.67 |
| 1:A:253:ASN:HB3 | 2:B:935:ARG:CZ | 2.25 | 0.67 |
| 1:A:384:ASN:O | 1:A:385:ILE:C | 2.33 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1121:GLU:HG2 | 1:A:1122:PRO:HD2 | 1.75 | 0.67 |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.77 | 0.67 |
| 2:B:1159:ARG:HD3 | 2:B:1193:GLN:HG3 | 1.76 | 0.67 |
| 9:I:8:ARG:CG | 9:I:34:TYR:HE1 | 2.06 | 0.67 |
| 1:A:407:ARG:HB3 | 1:A:430:TRP:CE2 | 2.29 | 0.67 |
| 1:A:450:LEU:H | 1:A:450:LEU:HD12 | 1.60 | 0.67 |
| 1:A:527:THR:CG2 | 1:A:650:GLN:HA | 2.25 | 0.67 |
| 5:E:192:ARG:HG3 | 5:E:192:ARG:NH1 | 2.09 | 0.67 |
| 8:H:58:THR:HG22 | 8:H:59:ILE:H | 1.60 | 0.67 |
| 1:A:252:PHE:O | 1:A:253:ASN:HB2 | 1.95 | 0.66 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:HB | 1.75 | 0.66 |
| 3:C:238:ILE:CG2 | 3:C:242:GLN:HB2 | 2.25 | 0.66 |
| 8:H:44:VAL:O | 8:H:44:VAL:HG12 | 1.96 | 0.66 |
| 2:B:516:ASN:ND2 | 2:B:516:ASN:H | 1.92 | 0.66 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:CE1 | 2.31 | 0.66 |
| 1:A:1438:THR:HB | 2:B:1144:ALA:HB3 | 1.78 | 0.66 |
| 1:A:1450:LEU:O | 1:A:1450:LEU:HG | 1.96 | 0.66 |
| 2:B:1085:ILE:N | 2:B:1085:ILE:HD12 | 2.10 | 0.66 |
| 8:H:41:ASP:O | 8:H:42:ILE:HG13 | 1.95 | 0.66 |
| 1:A:881:GLN:NE2 | 1:A:958:VAL:O | 2.28 | 0.66 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:CD2 | 2.24 | 0.66 |
| 2:B:1106:ARG:NH1 | 2:B:1110:PRO:HG2 | 2.11 | 0.66 |
| 2:B:1169:MET:HE1 | 2:B:1201:LYS:HA | 1.77 | 0.66 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:N | 2.58 | 0.66 |
| 3:C:167:HIS:CD2 | 3:C:168:ALA:N | 2.64 | 0.66 |
| 6:F:109:VAL:HG11 | 6:F:123:LYS:HD3 | 1.78 | 0.66 |
| 9:I:75:CYS:SG | 9:I:79:HIS:N | 2.68 | 0.66 |
| 15:T:18:DT:H2" | 15:T:19:TT:H5'1 | 1.72 | 0.66 |
| 1:A:1279:ILE:HG22 | 1:A:1279:ILE:O | 1.96 | 0.66 |
| 2:B:378:LEU:O | 2:B:382:ILE:HG13 | 1.95 | 0.66 |
| 2:B:464:GLY:HA2 | 2:B:479:VAL:O | 1.96 | 0.66 |
| 1:A:1127:ASP:HB3 | 1:A:1130:GLN:HB3 | 1.78 | 0.66 |
| 1:A:1362:TYR:CD1 | 1:A:1363:VAL:N | 2.64 | 0.66 |
| 2:B:18:PHE:N | 2:B:19:GLU:N | 2.44 | 0.66 |
| 2:B:825:VAL:CG1 | 2:B:826:ALA:N | 2.58 | 0.66 |
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:HH21 | 1.93 | 0.66 |
| 1:A:1011:GLN:NE2 | 1:A:1015:VAL:HG21 | 2.11 | 0.66 |
| 2:B:217:ARG:HD2 | 2:B:217:ARG:C | 2.15 | 0.66 |
| 2:B:563:MET:HE3 | 2:B:580:VAL:HB | 1.78 | 0.66 |
| 2:B:794:ASN:O | 2:B:795:ILE:HD12 | 1.95 | 0.66 |
| 2:B:847:ASP:HB3 | 3:C:167:HIS:CD2 | 2.31 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:176:GLU:O | 4:D:178:ALA:N | 2.29 | 0.66 |
| 11:K:46:ILE:O | 11:K:46:ILE:HG22 | 1.96 | 0.66 |
| 2:B:224:GLN:O | 2:B:238:ALA:HA | 1.95 | 0.66 |
| 2:B:840:ILE:HB | 2:B:1011:ILE:HB | 1.77 | 0.66 |
| 1:A:84:ILE:O | 1:A:84:ILE:HG23 | 1.96 | 0.66 |
| 1:A:356:ASP:HB2 | 1:A:469:ARG:HH11 | 1.60 | 0.66 |
| 2:B:842:ASN:ND2 | 2:B:845:SER:OG | 2.29 | 0.66 |
| 10:J:64:ASN:ND2 | 10:J:65:PRO:HD3 | 2.11 | 0.66 |
| 14:P:1:U:O2' | 14:P:2:C:H5' | 1.96 | 0.66 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:CA | 2.26 | 0.65 |
| 2:B:1197:PRO:HG2 | 2:B:1200:ALA:CB | 2.25 | 0.65 |
| 1:A:728:LYS:O | 1:A:732:LEU:HG | 1.97 | 0.65 |
| 1:A:1100:ARG:NH2 | 1:A:1351:GLU:HG2 | 2.11 | 0.65 |
| 2:B:710:LEU:HA | 2:B:733:HIS:HB3 | 1.78 | 0.65 |
| 2:B:824:ILE:HG22 | 2:B:1087:PHE:CE2 | 2.26 | 0.65 |
| 1:A:982:THR:H | 1:A:985:ASP:HB2 | 1.61 | 0.65 |
| 1:A:984:LYS:O | 1:A:988:LEU:HB2 | 1.97 | 0.65 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:NH2 | 2.11 | 0.65 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H | 1.44 | 0.65 |
| 2:B:1069:PHE:HA | 2:B:1085:ILE:O | 1.96 | 0.65 |
| 3:C:66:ARG:NH2 | 10:J:3:VAL:O | 2.29 | 0.65 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N | 2.08 | 0.65 |
| 1:A:164:ARG:HG3 | 1:A:165:GLY:N | 2.11 | 0.65 |
| 1:A:320:ARG:NH2 | 14:P:1:U:O2' | 2.29 | 0.65 |
| 1:A:335:ARG:NH1 | 2:B:1202:LEU:HD13 | 2.11 | 0.65 |
| 1:A:541:ILE:HG22 | 1:A:546:VAL:HG23 | 1.78 | 0.65 |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:N | 2.12 | 0.65 |
| 2:B:557:PHE:C | 2:B:557:PHE:CD2 | 2.70 | 0.65 |
| 11:K:61:TYR:C | 11:K:61:TYR:CD2 | 2.69 | 0.65 |
| 1:A:50:ILE:C | 1:A:52:GLY:H | 2.00 | 0.65 |
| 1:A:899:VAL:HB | 1:A:929:LEU:CD1 | 2.27 | 0.65 |
| 2:B:35:SER:O | 2:B:39:ARG:HG3 | 1.97 | 0.65 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HD13 | 1.79 | 0.65 |
| 3:C:167:HIS:HD2 | 3:C:168:ALA:H | 1.43 | 0.65 |
| 8:H:11:GLN:HA | 8:H:53:ASP:O | 1.96 | 0.65 |
| 1:A:714:PHE:O | 1:A:718:VAL:HG23 | 1.97 | 0.65 |
| 1:A:1005:GLU:O | 1:A:1009:ASN:HB2 | 1.97 | 0.65 |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:N | 2.11 | 0.65 |
| 2:B:1165:ILE:HG22 | 2:B:1166:CYS:N | 2.11 | 0.65 |
| 4:D:71:LYS:HA | 4:D:74:GLN:HB2 | 1.78 | 0.65 |
| 5:E:22:MET:CE | 5:E:26:ARG:HH21 | 2.02 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:152:VAL:CG1 | 1:A:153:PRO:HD2 | 2.26 | 0.65 |
| 1:A:886:ILE:HD11 | 1:A:943:LEU:HB3 | 1.77 | 0.65 |
| 1:A:828:ALA:HB2 | 2:B:530:GLY:HA2 | 1.79 | 0.65 |
| 2:B:308:TRP:HA | 2:B:311:LEU:HD12 | 1.78 | 0.65 |
| 8:H:89:LEU:HB3 | 8:H:91:ASP:OD1 | 1.97 | 0.65 |
| 1:A:69:THR:C | 1:A:71:GLN:N | 2.49 | 0.65 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:HD1 | 1.60 | 0.65 |
| 5:E:114:ASN:O | 5:E:115:ASN:HB3 | 1.97 | 0.65 |
| 1:A:372:LYS:HA | 1:A:435:HIS:ND1 | 2.11 | 0.64 |
| 2:B:770:GLN:HG2 | 2:B:983:ARG:O | 1.97 | 0.64 |
| 2:B:782:LEU:HD12 | 2:B:788:ARG:HH11 | 1.62 | 0.64 |
| 3:C:101:LEU:HD13 | 3:C:118:LEU:HD23 | 1.78 | 0.64 |
| 4:D:47:LEU:HD13 | 4:D:48:ILE:N | 2.11 | 0.64 |
| 4:D:192:LYS:HE3 | 4:D:204:ASP:OD1 | 1.97 | 0.64 |
| 1:A:392:VAL:HG13 | 1:A:415:LEU:HD11 | 1.79 | 0.64 |
| 1:A:450:LEU:HD12 | 1:A:450:LEU:N | 2.13 | 0.64 |
| 1:A:852:TYR:CE2 | 1:A:1060:PRO:HB2 | 2.33 | 0.64 |
| 1:A:1445:ILE:HD12 | 1:A:1445:ILE:N | 1.98 | 0.64 |
| 2:B:589:VAL:CG1 | 2:B:590:HIS:H | 2.07 | 0.64 |
| 5:E:153:HIS:HB3 | 5:E:196:VAL:HG11 | 1.77 | 0.64 |
| 15:T:13:DA:H1' | 15:T:14:DC:H5' | 1.78 | 0.64 |
| 1:A:105:CYS:O | 1:A:114:LEU:HG | 1.97 | 0.64 |
| 1:A:591:PHE:HA | 1:A:595:THR:HG21 | 1.80 | 0.64 |
| 1:A:979:SER:OG | 1:A:980:ASP:N | 2.29 | 0.64 |
| 2:B:185:THR:H | 2:B:188:ASP:HB2 | 1.62 | 0.64 |
| 2:B:467:GLY:H | 2:B:475:SER:CB | 2.10 | 0.64 |
| 2:B:744:HIS:HD2 | 2:B:746:SER:OG | 1.80 | 0.64 |
| 1:A:14:VAL:H | 1:A:1432:GLN:HE22 | 1.45 | 0.64 |
| 1:A:93:VAL:CG2 | 1:A:301:ALA:HA | 2.27 | 0.64 |
| 1:A:265:LYS:HE2 | 1:A:322:VAL:CG1 | 2.27 | 0.64 |
| 1:A:414:ASP:OD1 | 1:A:416:ARG:HG2 | 1.97 | 0.64 |
| 2:B:247:GLY:C | 2:B:249:ARG:H | 1.99 | 0.64 |
| 2:B:776:GLN:HE22 | 14:P:8:G:H5' | 1.62 | 0.64 |
| 2:B:1161:HIS:NE2 | 2:B:1175:LEU:HD21 | 2.11 | 0.64 |
| 3:C:183:TRP:O | 3:C:185:LYS:N | 2.30 | 0.64 |
| 5:E:46:TYR:CD2 | 5:E:58:MET:HG2 | 2.32 | 0.64 |
| 1:A:35:ILE:HA | 1:A:52:GLY:O | 1.97 | 0.64 |
| 1:A:458:HIS:CE1 | 1:A:507:VAL:HG21 | 2.33 | 0.64 |
| 1:A:1006:ILE:HD12 | 5:E:163:GLU:HG3 | 1.78 | 0.64 |
| 2:B:918:ILE:HB | 2:B:935:ARG:HD2 | 1.80 | 0.64 |
| 5:E:9:ILE:HD11 | 5:E:53:PRO:HD3 | 1.78 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:127:PRO:HG2 | 7:G:138:THR:HG21 | 1.79 | 0.64 |
| 1:A:1094:VAL:CG1 | 1:A:1095:THR:H | 2.06 | 0.64 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:HG13 | 1.98 | 0.64 |
| 2:B:745:PRO:O | 2:B:747:MET:N | 2.31 | 0.64 |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:HH11 | 1.62 | 0.64 |
| 4:D:56:ARG:HB2 | 4:D:148:LEU:HD22 | 1.80 | 0.64 |
| 10:J:57:ILE:HA | 10:J:60:PHE:HD2 | 1.61 | 0.64 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:CB | 2.45 | 0.64 |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HG23 | 1.98 | 0.64 |
| 3:C:133:ILE:HD11 | 3:C:237:SER:HA | 1.80 | 0.64 |
| 1:A:254:GLU:O | 1:A:256:GLN:N | 2.30 | 0.64 |
| 1:A:388:LEU:O | 1:A:392:VAL:HG23 | 1.98 | 0.64 |
| 1:A:1063:MET:CG | 1:A:1436:ILE:HG23 | 2.28 | 0.64 |
| 1:A:1444:MET:CG | 7:G:60:ARG:HA | 2.28 | 0.64 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:CD1 | 2.28 | 0.64 |
| 2:B:842:ASN:O | 2:B:846:ILE:HG13 | 1.98 | 0.64 |
| 3:C:36:VAL:HG21 | 3:C:251:LEU:HB2 | 1.79 | 0.64 |
| 6:F:93:ILE:HD11 | 6:F:134:ILE:CD1 | 2.26 | 0.64 |
| 6:F:99:LEU:O | 6:F:103:MET:HG2 | 1.97 | 0.64 |
| 8:H:81:PRO:CB | 8:H:82:PRO:CD | 2.75 | 0.64 |
| 12:L:47:ARG:HH21 | 12:L:54:ARG:HH21 | 1.44 | 0.64 |
| 1:A:34:LYS:CE | 1:A:57:ARG:NH1 | 2.61 | 0.64 |
| 2:B:859:TYR:CZ | 2:B:941:LEU:HD12 | 2.33 | 0.64 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:H | 1.63 | 0.64 |
| 11:K:111:LEU:C | 11:K:112:GLN:CG | 2.59 | 0.64 |
| 2:B:39:ARG:HH21 | 2:B:665:GLU:CD | 2.01 | 0.63 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:N | 2.07 | 0.63 |
| 2:B:1001:PHE:CE1 | 2:B:1073:TYR:HB2 | 2.33 | 0.63 |
| 15:T:22:BRU:C2' | 15:T:23:DG:O4' | 2.46 | 0.63 |
| 1:A:144:THR:O | 1:A:146:MET:HG3 | 1.98 | 0.63 |
| 1:A:567:LYS:CB | 1:A:568:PRO:HD2 | 2.28 | 0.63 |
| 2:B:339:THR:O | 2:B:339:THR:HG22 | 1.98 | 0.63 |
| 2:B:601:ARG:O | 2:B:605:ARG:HG3 | 1.98 | 0.63 |
| 2:B:637:LEU:O | 2:B:690:VAL:HG13 | 1.99 | 0.63 |
| 3:C:133:ILE:CD1 | 3:C:237:SER:HA | 2.28 | 0.63 |
| 1:A:79:GLY:HA3 | 1:A:243:PRO:HG3 | 1.79 | 0.63 |
| 1:A:477:PRO:CG | 1:A:521:MET:HG2 | 2.29 | 0.63 |
| 1:A:675:THR:O | 1:A:679:ILE:HG13 | 1.98 | 0.63 |
| 2:B:211:VAL:O | 2:B:480:SER:HA | 1.99 | 0.63 |
| 2:B:336:ARG:HH21 | 2:B:345:LYS:HG2 | 1.63 | 0.63 |
| 2:B:1084:GLN:N | 2:B:1084:GLN:NE2 | 2.46 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:23:ASN:C | 10:J:25:LEU:H | 1.99 | 0.63 |
| 10:J:28:ASP:O | 10:J:30:LEU:HG | 1.99 | 0.63 |
| 1:A:326:ARG:NH2 | 1:A:1407:GLU:HG3 | 2.13 | 0.63 |
| 1:A:535:THR:HG23 | 1:A:575:LYS:HE2 | 1.81 | 0.63 |
| 2:B:799:PRO:HB3 | 2:B:818:PRO:HG2 | 1.80 | 0.63 |
| 1:A:265:LYS:HD2 | 1:A:265:LYS:H | 1.64 | 0.63 |
| 1:A:518:LYS:HE2 | 1:A:624:SER:O | 1.97 | 0.63 |
| 2:B:23:ALA:HB1 | 2:B:24:PRO:HD2 | 1.80 | 0.63 |
| 2:B:121:ASN:HA | 2:B:207:GLY:HA2 | 1.78 | 0.63 |
| 2:B:125:SER:HA | 2:B:171:PRO:HA | 1.80 | 0.63 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:CD | 2.28 | 0.63 |
| 2:B:957:ASN:O | 2:B:959:ASP:N | 2.31 | 0.63 |
| 3:C:263:THR:C | 3:C:265:MET:H | 2.02 | 0.63 |
| 4:D:52:LEU:O | 4:D:54:GLU:N | 2.32 | 0.63 |
| 7:G:79:PHE:CZ | 7:G:106:MET:HE1 | 2.33 | 0.63 |
| 1:A:598:LEU:HD22 | 8:H:25:ARG:NH1 | 2.14 | 0.63 |
| 6:F:69:LEU:CA | 6:F:70:LYS:N | 2.60 | 0.63 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:H | 1.64 | 0.63 |
| 1:A:588:LEU:O | 1:A:606:LEU:HA | 1.99 | 0.63 |
| 2:B:365:THR:HG23 | 2:B:367:LEU:HG | 1.79 | 0.63 |
| 2:B:975:GLN:O | 2:B:990:ILE:HD12 | 1.99 | 0.63 |
| 3:C:189:THR:HG22 | 3:C:190:ASP:N | 2.14 | 0.63 |
| 7:G:17:PHE:N | 7:G:17:PHE:CD2 | 2.66 | 0.63 |
| 8:H:93:TYR:HB3 | 8:H:144:ILE:O | 1.99 | 0.63 |
| 1:A:321:PRO:O | 1:A:322:VAL:CB | 2.46 | 0.63 |
| 2:B:315:LYS:N | 2:B:316:PRO:HD2 | 2.13 | 0.63 |
| 2:B:916:THR:O | 2:B:935:ARG:HG3 | 1.99 | 0.63 |
| 4:D:7:THR:HB | 7:G:42:PHE:CE2 | 2.34 | 0.63 |
| 6:F:138:LEU:HB3 | 6:F:139:PRO:HD2 | 1.80 | 0.63 |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N | 2.14 | 0.62 |
| 2:B:705:MET:H | 2:B:710:LEU:HD12 | 1.63 | 0.62 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:HG13 | 1.64 | 0.62 |
| 1:A:57:ARG:O | 1:A:68:GLN:HG3 | 1.99 | 0.62 |
| 1:A:87:ALA:HB1 | 1:A:276:LEU:HD23 | 1.80 | 0.62 |
| 9:I:34:TYR:CE2 | 9:I:36:GLU:HB3 | 2.34 | 0.62 |
| 1:A:730:GLY:O | 1:A:732:LEU:N | 2.32 | 0.62 |
| 1:A:979:SER:OG | 1:A:981:LEU:HG | 1.99 | 0.62 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:H | 1.64 | 0.62 |
| 4:D:159:THR:O | 4:D:163:VAL:HG23 | 1.99 | 0.62 |
| 7:G:145:VAL:HG12 | 7:G:146:LYS:N | 2.14 | 0.62 |
| 10:J:12:LYS:O | 10:J:14:VAL:HG23 | 1.99 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:T:15:DT:C1' | 15:T:16:DT:H5' | 2.29 | 0.62 |
| 1:A:335:ARG:HA | 1:A:339:ASN:HD22 | 1.63 | 0.62 |
| 2:B:120:ARG:HG2 | 2:B:955:THR:HG21 | 1.80 | 0.62 |
| 2:B:563:MET:CE | 2:B:580:VAL:HB | 2.29 | 0.62 |
| 2:B:999:MET:HE2 | 2:B:1000:PRO:HD2 | 1.80 | 0.62 |
| 2:B:1034:VAL:O | 2:B:1037:LEU:N | 2.30 | 0.62 |
| 3:C:100:THR:OG1 | 3:C:121:VAL:HG21 | 1.99 | 0.62 |
| 3:C:104:PHE:HD2 | 3:C:105:GLY:H | 1.47 | 0.62 |
| 8:H:81:PRO:CB | 8:H:82:PRO:HD2 | 2.28 | 0.62 |
| 9:I:61:ASP:C | 9:I:63:GLY:H | 2.03 | 0.62 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:HG2 | 1.81 | 0.62 |
| 1:A:567:LYS:CB | 1:A:568:PRO:CD | 2.77 | 0.62 |
| 2:B:616:ILE:HD12 | 2:B:616:ILE:N | 2.14 | 0.62 |
| 3:C:35:ARG:HH11 | 11:K:41:THR:CA | 2.12 | 0.62 |
| 9:I:55:THR:HG22 | 9:I:58:VAL:HG21 | 1.79 | 0.62 |
| 10:J:16:ASP:OD1 | 10:J:17:LYS:HD2 | 1.99 | 0.62 |
| 1:A:741:ASN:ND2 | 1:A:744:LYS:H | 1.98 | 0.62 |
| 1:A:763:ALA:O | 1:A:803:SER:HB3 | 2.00 | 0.62 |
| 1:A:1149:ALA:CB | 9:I:47:GLU:HA | 2.29 | 0.62 |
| 1:A:1209:MET:SD | 1:A:1236:LEU:HD22 | 2.39 | 0.62 |
| 1:A:1412:ALA:HA | 1:A:1417:GLU:OE2 | 1.98 | 0.62 |
| 2:B:842:ASN:HB3 | 2:B:845:SER:OG | 1.99 | 0.62 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N | 1.98 | 0.62 |
| 11:K:10:PHE:N | 11:K:10:PHE:CD2 | 2.68 | 0.62 |
| 11:K:45:LEU:HG | 11:K:94:ILE:HD13 | 1.81 | 0.62 |
| 1:A:58:LEU:CG | 1:A:59:GLY:H | 2.11 | 0.62 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:N | 2.12 | 0.62 |
| 1:A:844:ALA:C | 1:A:845:LEU:HD23 | 2.20 | 0.62 |
| 1:A:1279:ILE:HD11 | 1:A:1316:VAL:HG21 | 1.80 | 0.62 |
| 2:B:465:ASN:HD22 | 2:B:465:ASN:N | 1.98 | 0.62 |
| 3:C:39:ALA:CA | 3:C:164:ALA:HB3 | 2.30 | 0.62 |
| 5:E:39:LEU:O | 5:E:42:PHE:HB3 | 2.00 | 0.62 |
| 5:E:48:ASP:CG | 5:E:49:SER:H | 2.03 | 0.62 |
| 6:F:97:ARG:O | 6:F:101:ILE:HG13 | 1.99 | 0.62 |
| 11:K:67:PHE:C | 11:K:68:PHE:HD2 | 2.03 | 0.62 |
| 2:B:525:ALA:O | 2:B:768:THR:HA | 2.00 | 0.62 |
| 2:B:1007:VAL:CG2 | 2:B:1008:PRO:HD2 | 2.29 | 0.62 |
| 3:C:112:ASN:HB2 | 3:C:114:TYR:CE1 | 2.34 | 0.62 |
| 3:C:253:LYS:O | 3:C:256:ALA:HB3 | 2.00 | 0.62 |
| 4:D:8:PHE:CZ | 4:D:40:HIS:HA | 2.35 | 0.62 |
| 5:E:202:SER:OG | 5:E:204:THR:HG22 | 2.00 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:90:ARG:HG3 | 6:F:91:ALA:N | 2.14 | 0.62 |
| 1:A:53:LEU:CD2 | 1:A:54:ASN:HD22 | 2.13 | 0.62 |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:CE2 | 2.34 | 0.62 |
| 2:B:446:LEU:O | 2:B:447:ALA:HB3 | 1.99 | 0.62 |
| 2:B:797:TYR:HE1 | 2:B:854:LEU:HD23 | 1.65 | 0.62 |
| 2:B:822:ASN:O | 10:J:48:ARG:NH1 | 2.33 | 0.62 |
| 2:B:1182:CYS:O | 2:B:1182:CYS:SG | 2.57 | 0.62 |
| 13:N:5:DA:C2 | 15:T:13:DA:C2 | 2.88 | 0.62 |
| 1:A:567:LYS:CE | 8:H:46:LEU:HB2 | 2.29 | 0.62 |
| 1:A:1244:ARG:HB3 | 1:A:1245:PRO:HD2 | 1.80 | 0.62 |
| 1:A:1441:PHE:CZ | 6:F:89:GLU:HA | 2.34 | 0.62 |
| 2:B:751:VAL:HG13 | 2:B:812:LEU:HD22 | 1.80 | 0.62 |
| 1:A:107:CYS:N | 1:A:114:LEU:HD21 | 2.15 | 0.61 |
| 1:A:849:MET:CE | 1:A:1061:GLY:HA2 | 2.30 | 0.61 |
| 2:B:36:ALA:HA | 2:B:39:ARG:HD2 | 1.81 | 0.61 |
| 2:B:433:GLN:O | 2:B:437:GLU:HG3 | 1.99 | 0.61 |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21 | 1.81 | 0.61 |
| 3:C:44:LEU:HB2 | 3:C:77:ILE:HD11 | 1.82 | 0.61 |
| 1:A:477:PRO:HG2 | 1:A:521:MET:HG2 | 1.82 | 0.61 |
| 1:A:901:LEU:N | 1:A:926:GLN:NE2 | 2.47 | 0.61 |
| 2:B:464:GLY:O | 2:B:477:ALA:HA | 2.00 | 0.61 |
| 10:J:64:ASN:CB | 10:J:65:PRO:HD3 | 2.30 | 0.61 |
| 2:B:336:ARG:NH2 | 2:B:345:LYS:HE2 | 2.10 | 0.61 |
| 2:B:498:THR:HB | 2:B:537:LYS:O | 2.00 | 0.61 |
| 3:C:70:ILE:HD11 | 3:C:144:ILE:HG12 | 1.82 | 0.61 |
| 7:G:34:VAL:CG1 | 7:G:45:ILE:HG21 | 2.29 | 0.61 |
| 10:J:8:PHE:H | 10:J:49:MET:CE | 2.12 | 0.61 |
| 10:J:44:TYR:HA | 10:J:47:ARG:CB | 2.30 | 0.61 |
| 1:A:1066:VAL:O | 1:A:1070:GLN:HG3 | 2.01 | 0.61 |
| 2:B:168:GLY:N | 2:B:450:ALA:HB1 | 2.12 | 0.61 |
| 2:B:616:ILE:CG1 | 2:B:697:GLU:HA | 2.31 | 0.61 |
| 2:B:622:LYS:CE | 9:I:59:VAL:HG22 | 2.30 | 0.61 |
| 3:C:123:ASN:HD22 | 3:C:125:MET:HG2 | 1.66 | 0.61 |
| 1:A:907:THR:CG2 | 1:A:908:LEU:N | 2.63 | 0.61 |
| 1:A:971:PHE:CE2 | 1:A:1040:GLN:HG2 | 2.34 | 0.61 |
| 7:G:143:ILE:HG22 | 7:G:144:ARG:N | 2.15 | 0.61 |
| 3:C:164:ALA:HA | 3:C:167:HIS:O | 2.00 | 0.61 |
| 1:A:450:LEU:HB3 | 1:A:838:GLN:NE2 | 2.15 | 0.61 |
| 2:B:278:GLN:HE22 | 2:B:337:ARG:HH21 | 1.47 | 0.61 |
| 2:B:520:GLY:H | 2:B:748:ILE:HG22 | 1.64 | 0.61 |
| 3:C:69:LEU:N | 3:C:69:LEU:HD12 | 2.16 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:104:PHE:HD2 | 3:C:105:GLY:N | 1.99 | 0.61 |
| 3:C:142:VAL:H | 10:J:16:ASP:HB3 | 1.66 | 0.61 |
| 8:H:24:CYS:HB2 | 8:H:44:VAL:HG21 | 1.82 | 0.61 |
| 8:H:42:ILE:HG23 | 8:H:95:TYR:HE1 | 1.64 | 0.61 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:HE2 | 1.81 | 0.61 |
| 1:A:382:PRO:HD3 | 1:A:428:TYR:HD2 | 1.65 | 0.61 |
| 3:C:34:ARG:O | 3:C:38:ILE:HG13 | 2.01 | 0.61 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:NE1 | 2.16 | 0.61 |
| 2:B:1177:HIS:HB2 | 2:B:1179:GLN:HE21 | 1.65 | 0.61 |
| 3:C:20:PHE:HE1 | 3:C:22:LEU:HD12 | 1.66 | 0.61 |
| 3:C:77:ILE:HG23 | 3:C:161:LYS:HE3 | 1.81 | 0.61 |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2 | 1.83 | 0.61 |
| 5:E:29:PHE:O | 5:E:30:ILE:HG13 | 2.00 | 0.61 |
| 8:H:25:ARG:HA | 8:H:41:ASP:HA | 1.83 | 0.61 |
| 8:H:47:PHE:CD2 | 8:H:95:TYR:HD1 | 2.19 | 0.61 |
| 1:A:427:GLN:HG3 | 1:A:430:TRP:CE2 | 2.34 | 0.60 |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:CG | 2.10 | 0.60 |
| 2:B:811:TYR:N | 2:B:811:TYR:CD1 | 2.68 | 0.60 |
| 2:B:1084:GLN:NE2 | 2:B:1084:GLN:H | 1.99 | 0.60 |
| 6:F:103:MET:CE | 7:G:66:GLY:H | 2.13 | 0.60 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:CB | 2.24 | 0.60 |
| 10:J:48:ARG:HE | 10:J:49:MET:CE | 2.10 | 0.60 |
| 13:N:1:DA:H2" | 13:N:2:DA:OP2 | 2.00 | 0.60 |
| 1:A:320:ARG:NH2 | 14:P:1:U:H1' | 2.15 | 0.60 |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:HE2 | 1.66 | 0.60 |
| 2:B:882:THR:CG2 | 2:B:884:ARG:HB2 | 2.31 | 0.60 |
| 4:D:5:THR:O | 4:D:5:THR:HG23 | 2.01 | 0.60 |
| 11:K:7:PHE:HA | 11:K:10:PHE:CE2 | 2.36 | 0.60 |
| 11:K:114:LEU:HD13 | 11:K:114:LEU:C | 2.20 | 0.60 |
| 1:A:79:GLY:HA3 | 1:A:243:PRO:CG | 2.31 | 0.60 |
| 1:A:899:VAL:HB | 1:A:929:LEU:HD12 | 1.83 | 0.60 |
| 1:A:1095:THR:O | 1:A:1096:SER:HB2 | 1.99 | 0.60 |
| 13:N:0:DT:H2" | 13:N:1:DA:O5' | 2.01 | 0.60 |
| 1:A:886:ILE:CG2 | 1:A:887:GLY:N | 2.64 | 0.60 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:HE1 | 1.66 | 0.60 |
| 2:B:770:GLN:CD | 2:B:983:ARG:HA | 2.21 | 0.60 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:CB | 2.49 | 0.60 |
| 3:C:147:LEU:N | 3:C:147:LEU:HD23 | 2.16 | 0.60 |
| 10:J:1:MET:N | 10:J:56:LEU:N | 2.48 | 0.60 |
| 2:B:112:LEU:HD12 | 2:B:113:TYR:N | 2.15 | 0.60 |
| 2:B:1163:CYS:SG | 2:B:1165:ILE:HB | 2.41 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:65:HIS:HD2 | 11:K:67:PHE:N | 1.92 | 0.60 |
| 1:A:356:ASP:OD2 | 11:K:65:HIS:HE1 | 1.83 | 0.60 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CH2 | 2.36 | 0.60 |
| 1:A:663:SER:OG | 1:A:664:THR:N | 2.33 | 0.60 |
| 1:A:694:THR:O | 1:A:698:GLN:HG3 | 2.00 | 0.60 |
| 1:A:836:TYR:CE2 | 1:A:840:ARG:HD2 | 2.36 | 0.60 |
| 2:B:834:ASN:HB3 | 2:B:840:ILE:HG13 | 1.82 | 0.60 |
| 6:F:79:ARG:HG3 | 6:F:144:GLU:OE1 | 2.02 | 0.60 |
| 6:F:130:ILE:O | 6:F:148:VAL:CG2 | 2.49 | 0.60 |
| 7:G:153:GLN:HG2 | 7:G:154:VAL:HG23 | 1.83 | 0.60 |
| 9:I:86:PHE:CE1 | 9:I:100:PHE:HB2 | 2.36 | 0.60 |
| 11:K:42:LEU:O | 11:K:46:ILE:HG13 | 2.02 | 0.60 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HE3 | 1.82 | 0.60 |
| 1:A:1333:ILE:O | 1:A:1337:GLU:HG3 | 2.02 | 0.60 |
| 3:C:165:LYS:O | 11:K:6:ARG:NH1 | 2.35 | 0.60 |
| 1:A:351:THR:HB | 2:B:1103:ILE:CD1 | 2.32 | 0.60 |
| 1:A:382:PRO:CB | 1:A:428:TYR:HE2 | 2.12 | 0.60 |
| 1:A:783:THR:HG22 | 1:A:784:LEU:HG | 1.84 | 0.60 |
| 1:A:821:ARG:HD2 | 1:A:825:ILE:HD11 | 1.83 | 0.60 |
| 1:A:1289:ARG:HD2 | 1:A:1303:GLU:OE2 | 2.02 | 0.60 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:H | 2.17 | 0.60 |
| 2:B:830:TYR:CE2 | 2:B:1000:PRO:HD3 | 2.37 | 0.60 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:ND1 | 2.17 | 0.60 |
| 1:A:901:LEU:HA | 1:A:907:THR:OG1 | 2.02 | 0.60 |
| 2:B:798:TYR:HE2 | 3:C:62:PHE:CZ | 2.20 | 0.60 |
| 2:B:1001:PHE:CD2 | 3:C:34:ARG:NH2 | 2.70 | 0.60 |
| 3:C:100:THR:HG22 | 3:C:101:LEU:N | 2.16 | 0.60 |
| 4:D:138:ASN:OD1 | 4:D:141:LEU:HB2 | 2.02 | 0.60 |
| 7:G:1:MET:SD | 7:G:79:PHE:CD1 | 2.95 | 0.60 |
| 11:K:68:PHE:N | 11:K:68:PHE:CD2 | 2.67 | 0.60 |
| 15:T:22:BRU:H2' | 15:T:23:DG:O4' | 2.01 | 0.60 |
| 3:C:179:GLU:HG2 | 3:C:180:TYR:N | 2.17 | 0.60 |
| 4:D:4:SER:OG | 4:D:5:THR:N | 2.34 | 0.60 |
| 6:F:77:ASP:C | 6:F:79:ARG:H | 2.06 | 0.60 |
| 7:G:80:LYS:O | 7:G:80:LYS:HG2 | 2.02 | 0.60 |
| 12:L:32:ALA:HB3 | 12:L:55:ILE:CD1 | 2.31 | 0.60 |
| 1:A:12:ARG:HD2 | 2:B:1218:THR:HB | 1.84 | 0.59 |
| 1:A:1017:LEU:HB3 | 5:E:205:SER:HA | 1.83 | 0.59 |
| 2:B:880:THR:O | 2:B:881:ASN:HB2 | 2.01 | 0.59 |
| 3:C:2:SER:N | 3:C:3:GLU:N | 2.50 | 0.59 |
| 3:C:66:ARG:NH2 | 10:J:5:VAL:HG23 | 2.15 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:111:LEU:C | 6:F:113:GLY:H | 2.05 | 0.59 |
| 7:G:119:LEU:HD12 | 7:G:131:GLN:O | 2.01 | 0.59 |
| 1:A:384:ASN:O | 1:A:386:ASP:N | 2.34 | 0.59 |
| 1:A:463:ILE:HD12 | 1:A:469:ARG:HD2 | 1.84 | 0.59 |
| 1:A:1120:LEU:HD13 | 1:A:1304:TRP:O | 2.01 | 0.59 |
| 1:A:1451:VAL:O | 1:A:1454:MET:HG2 | 2.02 | 0.59 |
| 2:B:240:ILE:CG2 | 2:B:254:LEU:HB3 | 2.32 | 0.59 |
| 2:B:603:LEU:HD13 | 2:B:608:ASP:HB2 | 1.83 | 0.59 |
| 2:B:995:ARG:HH12 | 3:C:165:LYS:HG2 | 1.66 | 0.59 |
| 3:C:66:ARG:CZ | 10:J:2:ILE:HG21 | 2.31 | 0.59 |
| 3:C:147:LEU:HD12 | 3:C:151:GLN:O | 2.02 | 0.59 |
| 7:G:49:LEU:HG | 7:G:76:ALA:HA | 1.82 | 0.59 |
| 8:H:127:GLY:O | 8:H:128:ASN:HB2 | 2.02 | 0.59 |
| 15:T:22:BRU:H2' | 15:T:23:DG:H8 | 1.62 | 0.59 |
| 1:A:720:ARG:O | 1:A:724:GLU:HB2 | 2.02 | 0.59 |
| 1:A:1323:ASP:OD1 | 1:A:1325:THR:HB | 2.02 | 0.59 |
| 15:T:17:DT:C2' | 15:T:18:DT:C5' | 2.65 | 0.59 |
| 1:A:590:ARG:O | 1:A:591:PHE:HB2 | 2.01 | 0.59 |
| 1:A:809:THR:H | 1:A:812:GLU:HB2 | 1.66 | 0.59 |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:CG2 | 2.32 | 0.59 |
| 1:A:1063:MET:HG3 | 1:A:1436:ILE:HG23 | 1.83 | 0.59 |
| 2:B:899:ILE:HD13 | 2:B:905:VAL:HG11 | 1.82 | 0.59 |
| 2:B:980:PHE:HD2 | 2:B:1094:ARG:HA | 1.68 | 0.59 |
| 2:B:1079:LYS:HA | 3:C:27:LEU:HD21 | 1.83 | 0.59 |
| 4:D:40:HIS:CB | 7:G:73:LYS:HZ3 | 2.02 | 0.59 |
| 5:E:94:LYS:HE2 | 5:E:98:ILE:CD1 | 2.30 | 0.59 |
| 8:H:40:LEU:HD12 | 8:H:122:LEU:O | 2.03 | 0.59 |
| 1:A:23:SER:HA | 1:A:233:TRP:CD1 | 2.38 | 0.59 |
| 1:A:49:LYS:HZ3 | 1:A:61:ILE:HG13 | 1.67 | 0.59 |
| 1:A:55:ASP:C | 1:A:57:ARG:H | 2.04 | 0.59 |
| 1:A:289:ILE:C | 1:A:291:GLU:H | 2.03 | 0.59 |
| 1:A:405:VAL:HG22 | 1:A:432:VAL:HG13 | 1.85 | 0.59 |
| 1:A:738:LYS:HD2 | 1:A:740:LEU:HD21 | 1.84 | 0.59 |
| 1:A:1261:LYS:O | 1:A:1264:GLU:HB3 | 2.03 | 0.59 |
| 2:B:401:PHE:HD2 | 2:B:521:LEU:HD12 | 1.66 | 0.59 |
| 2:B:579:ARG:HG2 | 2:B:579:ARG:HH11 | 1.66 | 0.59 |
| 2:B:603:LEU:HD12 | 2:B:609:ILE:HG13 | 1.82 | 0.59 |
| 2:B:942:ARG:NH2 | 15:T:25:DT:P | 2.75 | 0.59 |
| 2:B:1103:ILE:O | 2:B:1122:ARG:NH1 | 2.35 | 0.59 |
| 1:A:665:GLY:O | 1:A:667:GLY:N | 2.35 | 0.59 |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:HD2 | 1.84 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:185:THR:H | 2:B:188:ASP:CB | 2.14 | 0.59 |
| 2:B:611:PRO:HB3 | 2:B:685:LEU:HD11 | 1.84 | 0.59 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:N | 2.17 | 0.59 |
| 5:E:177:ARG:C | 5:E:212:ARG:HD3 | 2.22 | 0.59 |
| 10:J:44:TYR:H | 10:J:44:TYR:HD2 | 1.48 | 0.59 |
| 1:A:269:ILE:HD11 | 1:A:300:VAL:HA | 1.83 | 0.59 |
| 1:A:596:THR:C | 1:A:598:LEU:H | 2.05 | 0.59 |
| 1:A:1283:VAL:HG12 | 1:A:1284:MET:N | 2.18 | 0.59 |
| 2:B:616:ILE:HG13 | 2:B:697:GLU:HA | 1.85 | 0.59 |
| 6:F:119:ARG:HH11 | 6:F:119:ARG:HG3 | 1.67 | 0.59 |
| 10:J:36:LEU:HD22 | 10:J:41:LEU:HD12 | 1.83 | 0.59 |
| 1:A:1107:VAL:HG12 | 1:A:1107:VAL:O | 2.02 | 0.59 |
| 1:A:1385:THR:O | 1:A:1387:HIS:N | 2.36 | 0.59 |
| 2:B:1005:GLY:HA2 | 3:C:176:ILE:O | 2.02 | 0.59 |
| 3:C:124:LEU:O | 3:C:127:ARG:HG2 | 2.03 | 0.59 |
| 15:T:26:DC:H2" | 15:T:27:DA:C5' | 2.32 | 0.59 |
| 1:A:765:VAL:HG23 | 1:A:802:ASN:O | 2.03 | 0.59 |
| 1:A:1224:LEU:HD12 | 1:A:1241:ARG:O | 2.02 | 0.59 |
| 4:D:13:ARG:HB2 | 4:D:17:LYS:HZ2 | 1.67 | 0.59 |
| 5:E:15:ALA:O | 5:E:19:VAL:HG23 | 2.03 | 0.59 |
| 8:H:43:ASN:OD1 | 8:H:46:LEU:HG | 2.03 | 0.59 |
| 1:A:75:ASN:O | 1:A:76:GLU:CB | 2.51 | 0.59 |
| 2:B:57:TYR:N | 2:B:57:TYR:HD1 | 2.01 | 0.59 |
| 2:B:229:ALA:HB1 | 2:B:231:PRO:HD2 | 1.85 | 0.59 |
| 2:B:483:LEU:HD11 | 2:B:491:THR:CG2 | 2.33 | 0.59 |
| 2:B:745:PRO:C | 2:B:747:MET:H | 2.06 | 0.59 |
| 2:B:431:TYR:CZ | 2:B:447:ALA:HB2 | 2.38 | 0.58 |
| 2:B:594:ALA:HA | 2:B:617:ARG:NH1 | 2.18 | 0.58 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:HB | 1.84 | 0.58 |
| 8:H:15:VAL:HG22 | 8:H:26:ILE:HG12 | 1.85 | 0.58 |
| 1:A:630:ILE:HD13 | 1:A:646:PHE:CZ | 2.38 | 0.58 |
| 1:A:914:GLU:HB2 | 1:A:979:SER:O | 2.03 | 0.58 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:HD22 | 1.84 | 0.58 |
| 4:D:52:LEU:C | 4:D:54:GLU:H | 2.05 | 0.58 |
| 5:E:157:SER:HG | 5:E:160:GLU:HG3 | 1.68 | 0.58 |
| 7:G:1:MET:SD | 7:G:1:MET:O | 2.61 | 0.58 |
| 10:J:64:ASN:CB | 10:J:65:PRO:CD | 2.81 | 0.58 |
| 1:A:33:ALA:HA | 1:A:57:ARG:NH2 | 2.18 | 0.58 |
| 1:A:528:LEU:C | 1:A:528:LEU:HD12 | 2.23 | 0.58 |
| 1:A:666:ILE:CD1 | 1:A:667:GLY:H | 2.17 | 0.58 |
| 1:A:832:ALA:O | 1:A:833:GLU:C | 2.42 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1116:LEU:HB2 | 1:A:1329:THR:OG1 | 2.03 | 0.58 |
| 1:A:1120:LEU:O | 1:A:1323:ASP:HB2 | 2.03 | 0.58 |
| 8:H:38:LEU:HD12 | 8:H:124:ARG:O | 2.03 | 0.58 |
| 15:T:14:DC:H1' | 15:T:15:DT:H5' | 1.86 | 0.58 |
| 1:A:444:PHE:HB2 | 1:A:458:HIS:HD2 | 1.68 | 0.58 |
| 2:B:225:VAL:HA | 2:B:237:VAL:O | 2.03 | 0.58 |
| 2:B:343:ILE:HG22 | 2:B:345:LYS:H | 1.66 | 0.58 |
| 3:C:174:ALA:O | 3:C:175:ALA:HB2 | 2.04 | 0.58 |
| 4:D:160:VAL:O | 4:D:164:ILE:HG13 | 2.03 | 0.58 |
| 1:A:982:THR:O | 1:A:985:ASP:HB2 | 2.04 | 0.58 |
| 1:A:1118:VAL:CG2 | 1:A:1306:LEU:HB2 | 2.33 | 0.58 |
| 2:B:57:TYR:N | 2:B:57:TYR:CD1 | 2.70 | 0.58 |
| 2:B:309:GLN:OE1 | 9:I:52:ILE:HD11 | 2.04 | 0.58 |
| 2:B:864:LYS:N | 2:B:872:GLU:OE1 | 2.37 | 0.58 |
| 5:E:178:ILE:HG22 | 5:E:213:ILE:O | 2.04 | 0.58 |
| 6:F:111:LEU:H | 6:F:111:LEU:CD1 | 2.13 | 0.58 |
| 1:A:224:PHE:HD2 | 1:A:229:SER:O | 1.86 | 0.58 |
| 1:A:399:HIS:O | 1:A:401:GLY:N | 2.36 | 0.58 |
| 1:A:444:PHE:CB | 1:A:458:HIS:HD2 | 2.15 | 0.58 |
| 2:B:344:LYS:O | 2:B:345:LYS:HB2 | 2.03 | 0.58 |
| 2:B:486:TYR:HH | 2:B:1096:ARG:HB3 | 1.68 | 0.58 |
| 2:B:777:ALA:HA | 2:B:1095:LEU:HA | 1.85 | 0.58 |
| 4:D:53:SER:HB3 | 4:D:153:ARG:H | 1.67 | 0.58 |
| 4:D:66:ARG:O | 4:D:70:PHE:HB2 | 2.04 | 0.58 |
| 7:G:48:VAL:HG13 | 7:G:74:TYR:HD1 | 1.68 | 0.58 |
| 1:A:34:LYS:HB3 | 1:A:36:ARG:HE | 1.69 | 0.58 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:N | 2.01 | 0.58 |
| 1:A:783:THR:HG21 | 1:A:815:PHE:CE2 | 2.39 | 0.58 |
| 1:A:964:ILE:O | 1:A:967:ALA:N | 2.37 | 0.58 |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:CG2 | 2.33 | 0.58 |
| 1:A:1402:PHE:CD1 | 1:A:1403:GLU:HG3 | 2.38 | 0.58 |
| 2:B:990:ILE:HG22 | 2:B:991:GLY:N | 2.19 | 0.58 |
| 2:B:1084:GLN:H | 2:B:1084:GLN:HE21 | 1.50 | 0.58 |
| 2:B:1159:ARG:HE | 2:B:1193:GLN:HE21 | 1.51 | 0.58 |
| 5:E:23:VAL:O | 5:E:28:TYR:HB2 | 2.04 | 0.58 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:CD | 2.34 | 0.58 |
| 1:A:606:LEU:HB3 | 1:A:614:PHE:CE2 | 2.39 | 0.58 |
| 2:B:981:ALA:HB2 | 2:B:987:LYS:HA | 1.86 | 0.58 |
| 4:D:192:LYS:HB3 | 4:D:192:LYS:HZ3 | 1.69 | 0.58 |
| 9:I:25:LEU:HB3 | 9:I:38:ALA:HB2 | 1.84 | 0.58 |
| 1:A:457:ALA:HB3 | 1:A:506:ALA:HA | 1.85 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:475:THR:CG2 | 1:A:476:SER:N | 2.66 | 0.58 |
| 1:A:492:PRO:O | 1:A:493:GLN:NE2 | 2.36 | 0.58 |
| 1:A:648:ASN:O | 1:A:649:ILE:C | 2.41 | 0.58 |
| 1:A:1001:ARG:O | 1:A:1002:GLY:O | 2.22 | 0.58 |
| 2:B:265:SER:O | 2:B:266:ALA:HB3 | 2.04 | 0.58 |
| 2:B:778:MET:CE | 2:B:1094:ARG:CD | 2.82 | 0.58 |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:NH1 | 2.18 | 0.58 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:CG1 | 2.34 | 0.58 |
| 4:D:144:THR:HG21 | 7:G:46:LEU:HD13 | 1.85 | 0.58 |
| 6:F:99:LEU:C | 6:F:99:LEU:HD12 | 2.24 | 0.58 |
| 11:K:111:LEU:O | 11:K:112:GLN:HG2 | 2.03 | 0.58 |
| 15:T:19:TT:H5R1 | 15:T:19:TT:H2'1 | 1.83 | 0.58 |
| 3:C:184:ASN:ND2 | 3:C:187:LYS:HA | 2.19 | 0.58 |
| 4:D:53:SER:HB3 | 4:D:152:SER:CB | 2.33 | 0.58 |
| 6:F:75:PRO:O | 6:F:77:ASP:O | 2.22 | 0.58 |
| 1:A:58:LEU:CG | 1:A:59:GLY:N | 2.66 | 0.57 |
| 1:A:699:ALA:CB | 1:A:701:LEU:HG | 2.34 | 0.57 |
| 1:A:1017:LEU:HB2 | 5:E:206:GLY:N | 2.07 | 0.57 |
| 1:A:1305:VAL:HG12 | 1:A:1306:LEU:N | 2.19 | 0.57 |
| 3:C:214:ASN:HB3 | 3:C:217:ASP:OD2 | 2.03 | 0.57 |
| 4:D:51:ASN:O | 4:D:52:LEU:O | 2.22 | 0.57 |
| 5:E:207:ARG:CB | 5:E:207:ARG:HH11 | 2.16 | 0.57 |
| 1:A:399:HIS:CB | 1:A:400:PRO:HD3 | 2.29 | 0.57 |
| 1:A:1293:SER:OG | 1:A:1294:PRO:HD2 | 2.03 | 0.57 |
| 2:B:229:ALA:CB | 2:B:231:PRO:HD2 | 2.34 | 0.57 |
| 2:B:370:PHE:HD2 | 2:B:373:ARG:HD2 | 1.69 | 0.57 |
| 4:D:134:THR:CG2 | 4:D:135:GLY:N | 2.66 | 0.57 |
| 4:D:167:LEU:HB3 | 4:D:177:VAL:HG13 | 1.85 | 0.57 |
| 7:G:3:PHE:CE1 | 7:G:80:LYS:HE2 | 2.38 | 0.57 |
| 12:L:39:SER:O | 12:L:40:LEU:HG | 2.03 | 0.57 |
| 1:A:471:ASN:O | 1:A:474:VAL:HG12 | 2.04 | 0.57 |
| 1:A:1341:ILE:CG2 | 1:A:1342:GLU:N | 2.67 | 0.57 |
| 2:B:792:MET:HG3 | 2:B:855:PHE:HE1 | 1.69 | 0.57 |
| 2:B:910:VAL:HG12 | 2:B:912:ILE:H | 1.69 | 0.57 |
| 5:E:213:ILE:HG12 | 5:E:214:CYS:N | 2.19 | 0.57 |
| 1:A:699:ALA:HB1 | 1:A:701:LEU:HG | 1.85 | 0.57 |
| 1:A:754:SER:N | 1:A:757:ASN:HD22 | 1.92 | 0.57 |
| 2:B:167:ILE:HG22 | 2:B:453:ILE:HD12 | 1.86 | 0.57 |
| 1:A:37:PHE:N | 1:A:37:PHE:CD1 | 2.72 | 0.57 |
| 1:A:567:LYS:CG | 1:A:568:PRO:CD | 2.76 | 0.57 |
| 1:A:1373:ASP:HA | 1:A:1376:THR:CG2 | 2.34 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:486:TYR:CZ | 2:B:1096:ARG:HB3 | 2.39 | 0.57 |
| 2:B:996:ARG:NH2 | 3:C:175:ALA:HA | 2.20 | 0.57 |
| 4:D:18:VAL:HG13 | 4:D:18:VAL:O | 2.05 | 0.57 |
| 7:G:145:VAL:CG1 | 7:G:146:LYS:N | 2.67 | 0.57 |
| 9:I:103:CYS:HB3 | 9:I:106:CYS:SG | 2.45 | 0.57 |
| 14:P:4:A:O2' | 14:P:5:C:H5' | 2.05 | 0.57 |
| 1:A:42:ASP:HB3 | 1:A:45:GLN:N | 2.19 | 0.57 |
| 1:A:482:PHE:C | 1:A:484:GLY:H | 2.07 | 0.57 |
| 1:A:683:ILE:HD13 | 1:A:801:GLU:HG3 | 1.86 | 0.57 |
| 1:A:709:THR:HG21 | 9:I:93:LYS:O | 2.05 | 0.57 |
| 2:B:521:LEU:HB3 | 2:B:633:VAL:HG11 | 1.86 | 0.57 |
| 2:B:580:VAL:HG22 | 2:B:624:LEU:CB | 2.35 | 0.57 |
| 2:B:1033:LYS:NZ | 2:B:1070:GLU:OE1 | 2.36 | 0.57 |
| 2:B:1159:ARG:HD3 | 2:B:1193:GLN:CG | 2.35 | 0.57 |
| 2:B:1219:ASP:OD1 | 2:B:1219:ASP:O | 2.23 | 0.57 |
| 3:C:46:ILE:HG23 | 3:C:157:CYS:HB3 | 1.86 | 0.57 |
| 5:E:124:VAL:HB | 5:E:125:PRO:HD3 | 1.87 | 0.57 |
| 12:L:58:LYS:O | 12:L:58:LYS:HG2 | 2.03 | 0.57 |
| 1:A:1116:LEU:HB3 | 1:A:1308:THR:HG21 | 1.87 | 0.57 |
| 2:B:195:CYS:SG | 2:B:197:PHE:HB2 | 2.45 | 0.57 |
| 2:B:1023:VAL:O | 2:B:1026:LEU:N | 2.38 | 0.57 |
| 1:A:58:LEU:CD1 | 1:A:243:PRO:HB3 | 2.33 | 0.57 |
| 1:A:699:ALA:O | 1:A:700:ASN:HB3 | 2.04 | 0.57 |
| 1:A:1332:PHE:CE1 | 1:A:1348:LEU:HD13 | 2.39 | 0.57 |
| 2:B:332:ASP:OD1 | 2:B:336:ARG:NE | 2.38 | 0.57 |
| 2:B:340:ALA:CB | 2:B:343:ILE:HD12 | 2.35 | 0.57 |
| 7:G:154:VAL:HG12 | 7:G:155:SER:N | 2.20 | 0.57 |
| 1:A:1226:VAL:HG13 | 1:A:1240:CYS:HB3 | 1.87 | 0.57 |
| 2:B:496:ARG:HB3 | 2:B:496:ARG:HH11 | 1.69 | 0.57 |
| 2:B:744:HIS:HD2 | 2:B:746:SER:CB | 2.16 | 0.57 |
| 2:B:874:PHE:HA | 2:B:913:GLY:O | 2.05 | 0.57 |
| 2:B:1106:ARG:HG3 | 2:B:1107:ALA:N | 2.18 | 0.57 |
| 3:C:46:ILE:HG13 | 3:C:72:LEU:HD11 | 1.87 | 0.57 |
| 4:D:4:SER:O | 4:D:5:THR:HB | 2.03 | 0.57 |
| 1:A:35:ILE:HD12 | 1:A:241:VAL:HG21 | 1.85 | 0.57 |
| 1:A:1095:THR:OG1 | 1:A:1113:THR:HB | 2.05 | 0.57 |
| 1:A:1127:ASP:HB3 | 1:A:1130:GLN:CB | 2.34 | 0.57 |
| 10:J:44:TYR:HA | 10:J:47:ARG:HB3 | 1.87 | 0.57 |
| 1:A:406:ILE:HG13 | 1:A:431:LYS:HB2 | 1.87 | 0.56 |
| 1:A:600:PRO:HG2 | 1:A:601:LYS:H | 1.70 | 0.56 |
| 1:A:709:THR:HB | 1:A:712:GLU:HG3 | 1.87 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:176:SER:O | 2:B:182:SER:HB3 | 2.04 | 0.56 |
| 2:B:386:LEU:O | 2:B:388:CYS:N | 2.37 | 0.56 |
| 3:C:11:ARG:HD3 | 3:C:209:TYR:CE2 | 2.39 | 0.56 |
| 3:C:212:PRO:CB | 3:C:213:PRO:HD2 | 2.35 | 0.56 |
| 5:E:90:VAL:HA | 5:E:120:ALA:HB2 | 1.86 | 0.56 |
| 7:G:88:ASP:OD2 | 7:G:88:ASP:N | 2.37 | 0.56 |
| 9:I:15:TYR:N | 9:I:15:TYR:CD1 | 2.73 | 0.56 |
| 11:K:47:ARG:O | 11:K:47:ARG:HD2 | 2.05 | 0.56 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:N | 2.38 | 0.56 |
| 1:A:982:THR:N | 1:A:985:ASP:HB2 | 2.20 | 0.56 |
| 1:A:1446:ASP:HB3 | 1:A:1449:SER:OG | 2.05 | 0.56 |
| 1:A:1450:LEU:HD21 | 7:G:18:PHE:O | 2.04 | 0.56 |
| 2:B:199:MET:HE2 | 2:B:492:LEU:HD23 | 1.87 | 0.56 |
| 2:B:288:ALA:HA | 2:B:331:LEU:HD12 | 1.87 | 0.56 |
| 2:B:1176:ASN:C | 2:B:1178:ASN:H | 2.08 | 0.56 |
| 3:C:20:PHE:CE1 | 3:C:22:LEU:HD12 | 2.40 | 0.56 |
| 3:C:241:ASP:O | 3:C:245:VAL:HG23 | 2.05 | 0.56 |
| 6:F:81:THR:HG23 | 6:F:144:GLU:OE2 | 2.06 | 0.56 |
| 7:G:51:TYR:C | 7:G:51:TYR:CD2 | 2.79 | 0.56 |
| 9:I:62:ILE:O | 9:I:62:ILE:HG12 | 2.05 | 0.56 |
| 1:A:31:SER:OG | 1:A:82:GLY:HA2 | 2.04 | 0.56 |
| 1:A:222:LEU:O | 1:A:224:PHE:N | 2.38 | 0.56 |
| 1:A:244:PRO:HG2 | 1:A:245:PRO:HD3 | 1.86 | 0.56 |
| 1:A:412:ARG:NH2 | 2:B:1108:ARG:NH1 | 2.54 | 0.56 |
| 1:A:500:GLU:OE1 | 2:B:1143:ALA:C | 2.44 | 0.56 |
| 1:A:525:GLN:HG3 | 2:B:835:GLN:HG2 | 1.86 | 0.56 |
| 1:A:709:THR:HG22 | 1:A:710:LEU:N | 2.20 | 0.56 |
| 1:A:711:ARG:NH2 | 9:I:87:GLN:OE1 | 2.39 | 0.56 |
| 1:A:858:ASN:C | 1:A:858:ASN:ND2 | 2.59 | 0.56 |
| 1:A:866:PHE:O | 1:A:867:ILE:HD12 | 2.06 | 0.56 |
| 1:A:869:GLY:O | 5:E:204:THR:HG21 | 2.04 | 0.56 |
| 1:A:1072:ILE:O | 1:A:1075:PRO:HD2 | 2.05 | 0.56 |
| 1:A:1162:VAL:O | 1:A:1162:VAL:HG12 | 2.06 | 0.56 |
| 1:A:1279:ILE:CD1 | 1:A:1316:VAL:HG21 | 2.35 | 0.56 |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD | 2.45 | 0.56 |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:CD2 | 2.36 | 0.56 |
| 2:B:295:GLY:H | 2:B:298:LEU:HD23 | 1.69 | 0.56 |
| 2:B:1006:ILE:HG22 | 10:J:45:CYS:HB3 | 1.87 | 0.56 |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:N | 2.19 | 0.56 |
| 2:B:1155:SER:OG | 2:B:1156:ASP:N | 2.37 | 0.56 |
| 3:C:98:VAL:C | 3:C:99:LEU:HD23 | 2.26 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:168:TYR:HB2 | 5:E:170:LEU:HG | 1.86 | 0.56 |
| 6:F:89:GLU:OE2 | 6:F:134:ILE:HG21 | 2.05 | 0.56 |
| 7:G:114:LEU:HG | 7:G:162:SER:HB3 | 1.87 | 0.56 |
| 9:I:82:GLU:O | 9:I:104:LEU:HG | 2.05 | 0.56 |
| 1:A:968:GLN:O | 1:A:970:THR:N | 2.38 | 0.56 |
| 2:B:310:MET:HE3 | 2:B:387:LEU:CD1 | 2.34 | 0.56 |
| 2:B:527:THR:OG1 | 2:B:528:PRO:HD2 | 2.04 | 0.56 |
| 2:B:758:PHE:CE1 | 2:B:1027:ILE:HG22 | 2.41 | 0.56 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:HD21 | 1.87 | 0.56 |
| 3:C:58:LEU:HD21 | 10:J:57:ILE:HD12 | 1.88 | 0.56 |
| 3:C:77:ILE:O | 3:C:79:GLN:N | 2.39 | 0.56 |
| 8:H:61:SER:O | 8:H:62:SER:CB | 2.54 | 0.56 |
| 8:H:91:ASP:C | 8:H:93:TYR:H | 2.08 | 0.56 |
| 10:J:44:TYR:CD2 | 10:J:44:TYR:N | 2.73 | 0.56 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:HG21 | 1.88 | 0.56 |
| 1:A:626:ASN:O | 1:A:631:HIS:CD2 | 2.59 | 0.56 |
| 1:A:1124:HIS:HB3 | 1:A:1130:GLN:HG2 | 1.87 | 0.56 |
| 2:B:344:LYS:O | 2:B:345:LYS:CB | 2.53 | 0.56 |
| 2:B:831:SER:HB3 | 2:B:994:TYR:OH | 2.05 | 0.56 |
| 8:H:113:ALA:HB2 | 8:H:126:GLU:HG3 | 1.88 | 0.56 |
| 9:I:55:THR:CG2 | 9:I:58:VAL:HG21 | 2.36 | 0.56 |
| 9:I:92:ARG:HB3 | 9:I:95:THR:OG1 | 2.05 | 0.56 |
| 12:L:58:LYS:O | 12:L:59:ALA:O | 2.24 | 0.56 |
| 1:A:384:ASN:CG | 1:A:388:LEU:HD12 | 2.25 | 0.56 |
| 1:A:730:GLY:C | 1:A:732:LEU:H | 2.09 | 0.56 |
| 1:A:867:ILE:HG22 | 1:A:872:GLY:N | 2.21 | 0.56 |
| 1:A:1436:ILE:HD13 | 2:B:1139:ILE:HG23 | 1.87 | 0.56 |
| 2:B:758:PHE:CE1 | 2:B:1027:ILE:CG2 | 2.88 | 0.56 |
| 2:B:776:GLN:O | 2:B:1095:LEU:HA | 2.06 | 0.56 |
| 6:F:99:LEU:O | 6:F:99:LEU:HD12 | 2.05 | 0.56 |
| 7:G:111:THR:HG22 | 7:G:113:HIS:N | 2.17 | 0.56 |
| 8:H:39:THR:O | 8:H:123:MET:HA | 2.06 | 0.56 |
| 8:H:100:THR:HG22 | 8:H:101:ALA:N | 2.20 | 0.56 |
| 10:J:44:TYR:HD2 | 10:J:44:TYR:N | 2.03 | 0.56 |
| 14:P:3:G:H2' | 14:P:4:A:C8 | 2.41 | 0.56 |
| 1:A:89:PRO:HB2 | 1:A:204:THR:HG22 | 1.87 | 0.56 |
| 1:A:528:LEU:O | 1:A:528:LEU:HD12 | 2.05 | 0.56 |
| 1:A:806:ARG:HH12 | 2:B:729:ILE:CD1 | 2.18 | 0.56 |
| 2:B:521:LEU:HD13 | 2:B:633:VAL:HB | 1.86 | 0.56 |
| 2:B:557:PHE:C | 2:B:557:PHE:HD2 | 2.09 | 0.56 |
| 3:C:176:ILE:HG22 | 3:C:177:GLU:N | 2.21 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:902:LEU:HG | 1:A:926:GLN:HG3 | 1.86 | 0.56 |
| 2:B:343:ILE:HG21 | 2:B:348:ARG:H | 1.70 | 0.56 |
| 2:B:357:GLN:O | 2:B:366:GLN:HA | 2.04 | 0.56 |
| 2:B:635:ARG:NH2 | 2:B:742:GLU:OE2 | 2.37 | 0.56 |
| 2:B:658:ILE:HG22 | 2:B:659:ALA:N | 2.21 | 0.56 |
| 2:B:1002:THR:HG23 | 2:B:1006:ILE:HG13 | 1.88 | 0.56 |
| 8:H:128:ASN:CG | 8:H:128:ASN:O | 2.44 | 0.56 |
| 10:J:36:LEU:O | 10:J:39:LEU:N | 2.37 | 0.56 |
| 14:P:7:A:H2' | 14:P:8:G:C1' | 2.36 | 0.56 |
| 1:A:95:PHE:O | 1:A:96:ILE:C | 2.44 | 0.56 |
| 1:A:442:VAL:HB | 1:A:489:LEU:HD11 | 1.87 | 0.56 |
| 1:A:590:ARG:HB3 | 1:A:605:MET:N | 2.20 | 0.56 |
| 1:A:596:THR:C | 1:A:598:LEU:N | 2.58 | 0.56 |
| 1:A:1387:HIS:NE2 | 13:N:4:DT:H5" | 2.21 | 0.56 |
| 1:A:1410:PHE:HA | 2:B:1212:ILE:CD1 | 2.35 | 0.56 |
| 1:A:1444:MET:HG3 | 7:G:60:ARG:HA | 1.88 | 0.56 |
| 2:B:466:TRP:HA | 2:B:466:TRP:CE3 | 2.41 | 0.56 |
| 2:B:705:MET:H | 2:B:710:LEU:CD1 | 2.19 | 0.56 |
| 2:B:843:GLN:O | 2:B:846:ILE:HB | 2.06 | 0.56 |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA | 1.87 | 0.56 |
| 5:E:105:PHE:O | 5:E:106:GLN:HB2 | 2.06 | 0.56 |
| 8:H:61:SER:HB2 | 8:H:139:ASN:HB3 | 1.87 | 0.56 |
| 11:K:18:LYS:HZ3 | 11:K:38:GLU:HG2 | 1.70 | 0.56 |
| 1:A:98:LYS:O | 1:A:99:ILE:C | 2.44 | 0.56 |
| 1:A:364:VAL:O | 1:A:364:VAL:HG13 | 2.06 | 0.56 |
| 1:A:920:LEU:HD23 | 1:A:921:GLY:N | 2.20 | 0.56 |
| 1:A:929:LEU:HD23 | 1:A:983:ILE:HG21 | 1.88 | 0.56 |
| 1:A:942:PHE:HD2 | 1:A:943:LEU:HD23 | 1.70 | 0.56 |
| 4:D:17:LYS:CA | 4:D:17:LYS:HE3 | 2.35 | 0.56 |
| 11:K:49:GLU:HG3 | 11:K:94:ILE:HG12 | 1.87 | 0.56 |
| 1:A:87:ALA:HB3 | 1:A:276:LEU:HD23 | 1.86 | 0.55 |
| 1:A:108:MET:N | 1:A:108:MET:SD | 2.79 | 0.55 |
| 1:A:239:LEU:HD12 | 1:A:240:PRO:HD2 | 1.87 | 0.55 |
| 1:A:446:ARG:HB2 | 1:A:487:MET:SD | 2.47 | 0.55 |
| 1:A:1397:LEU:HB2 | 1:A:1426:GLU:OE1 | 2.05 | 0.55 |
| 2:B:53:GLN:HG2 | 2:B:547:VAL:CG2 | 2.35 | 0.55 |
| 2:B:1166:CYS:SG | 2:B:1166:CYS:O | 2.63 | 0.55 |
| 3:C:243:VAL:O | 3:C:243:VAL:HG12 | 2.05 | 0.55 |
| 4:D:47:LEU:HD11 | 7:G:3:PHE:CE2 | 2.40 | 0.55 |
| 5:E:78:LEU:HD23 | 5:E:78:LEU:C | 2.26 | 0.55 |
| 1:A:93:VAL:CG1 | 1:A:301:ALA:HB1 | 2.33 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:302:THR:HA | 1:A:305:ASP:O | 2.05 | 0.55 |
| 1:A:449:SER:O | 2:B:1133:MET:HB3 | 2.06 | 0.55 |
| 1:A:883:LEU:HD11 | 1:A:1017:LEU:HD11 | 1.87 | 0.55 |
| 1:A:981:LEU:CD2 | 1:A:1039:LYS:HA | 2.35 | 0.55 |
| 1:A:1377:THR:O | 1:A:1379:GLY:N | 2.39 | 0.55 |
| 2:B:51:PHE:O | 2:B:54:PHE:HB3 | 2.06 | 0.55 |
| 2:B:114:PRO:O | 2:B:116:GLU:N | 2.39 | 0.55 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:CB | 2.36 | 0.55 |
| 3:C:18:VAL:O | 3:C:20:PHE:HD2 | 1.90 | 0.55 |
| 6:F:118:LEU:O | 6:F:122:MET:HG3 | 2.06 | 0.55 |
| 9:I:106:CYS:O | 9:I:107:SER:HB2 | 2.07 | 0.55 |
| 11:K:110:ASN:O | 11:K:111:LEU:CD2 | 2.50 | 0.55 |
| 1:A:42:ASP:HB3 | 1:A:45:GLN:HA | 1.88 | 0.55 |
| 1:A:785:PRO:HG2 | 1:A:786:HIS:HD2 | 1.71 | 0.55 |
| 1:A:898:ARG:HB2 | 1:A:933:TYR:CE1 | 2.41 | 0.55 |
| 3:C:183:TRP:CZ2 | 3:C:207:CYS:HB3 | 2.41 | 0.55 |
| 4:D:52:LEU:HD21 | 4:D:147:TYR:HE2 | 1.71 | 0.55 |
| 4:D:137:ASN:C | 4:D:137:ASN:HD22 | 2.10 | 0.55 |
| 6:F:89:GLU:HB3 | 6:F:134:ILE:CD1 | 2.35 | 0.55 |
| 7:G:83:LYS:HE2 | 7:G:150:CYS:H | 1.72 | 0.55 |
| 8:H:4:THR:CA | 8:H:60:ALA:HB2 | 2.32 | 0.55 |
| 8:H:64:ASN:O | 8:H:65:LEU:HB2 | 2.05 | 0.55 |
| 8:H:83:GLN:C | 8:H:85:GLY:H | 2.09 | 0.55 |
| 8:H:84:ALA:CB | 8:H:87:ARG:HB2 | 2.36 | 0.55 |
| 15:T:10:DA:H2" | 15:T:11:DG:OP2 | 2.06 | 0.55 |
| 1:A:595:THR:O | 1:A:596:THR:HG23 | 2.05 | 0.55 |
| 1:A:852:TYR:CD2 | 1:A:1060:PRO:CB | 2.89 | 0.55 |
| 1:A:1076:ALA:HA | 1:A:1079:MET:CE | 2.36 | 0.55 |
| 3:C:35:ARG:NH1 | 11:K:41:THR:OG1 | 2.40 | 0.55 |
| 4:D:128:VAL:O | 4:D:132:GLN:HG3 | 2.06 | 0.55 |
| 5:E:55:ARG:C | 5:E:57:MET:H | 2.08 | 0.55 |
| 7:G:47:CYS:O | 7:G:76:ALA:HB1 | 2.06 | 0.55 |
| 8:H:40:LEU:HD22 | 8:H:123:MET:HE2 | 1.87 | 0.55 |
| 8:H:82:PRO:C | 8:H:84:ALA:H | 2.09 | 0.55 |
| 9:I:86:PHE:HE1 | 9:I:100:PHE:HB2 | 1.71 | 0.55 |
| 1:A:38:PRO:HA | 1:A:270:LEU:HD23 | 1.88 | 0.55 |
| 1:A:42:ASP:HB3 | 1:A:45:GLN:CA | 2.36 | 0.55 |
| 1:A:61:ILE:O | 1:A:63:ARG:N | 2.40 | 0.55 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CD1 | 2.42 | 0.55 |
| 1:A:670:ILE:HG23 | 1:A:805:LEU:HD21 | 1.86 | 0.55 |
| 1:A:742:ASN:O | 1:A:745:GLN:HB2 | 2.05 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:NH2 | 2.54 | 0.55 |
| 1:A:1114:PRO:O | 1:A:1115:SER:O | 2.24 | 0.55 |
| 2:B:254:LEU:HD23 | 2:B:381:MET:CE | 2.37 | 0.55 |
| 3:C:67:LEU:HD11 | 3:C:155:LEU:HD13 | 1.89 | 0.55 |
| 4:D:7:THR:O | 4:D:9:GLN:N | 2.40 | 0.55 |
| 5:E:157:SER:C | 5:E:159:ASP:N | 2.57 | 0.55 |
| 6:F:69:LEU:N | 6:F:70:LYS:CA | 2.69 | 0.55 |
| 6:F:125:LEU:HG | 6:F:125:LEU:O | 2.07 | 0.55 |
| 8:H:55:LEU:HD22 | 8:H:144:ILE:CG2 | 2.36 | 0.55 |
| 1:A:1191:TRP:CD1 | 1:A:1256:GLU:HB2 | 2.42 | 0.55 |
| 2:B:217:ARG:HD2 | 2:B:217:ARG:O | 2.07 | 0.55 |
| 2:B:466:TRP:O | 2:B:468:GLU:N | 2.39 | 0.55 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:CD1 | 2.30 | 0.55 |
| 3:C:167:HIS:CD2 | 3:C:168:ALA:H | 2.23 | 0.55 |
| 9:I:52:ILE:HG13 | 9:I:52:ILE:O | 2.06 | 0.55 |
| 11:K:69:ALA:O | 11:K:70:ARG:HB3 | 2.06 | 0.55 |
| 1:A:17:VAL:HA | 2:B:1215:ARG:O | 2.06 | 0.55 |
| 1:A:311:GLN:O | 1:A:312:PRO:C | 2.45 | 0.55 |
| 2:B:729:ILE:O | 2:B:729:ILE:HG22 | 2.04 | 0.55 |
| 2:B:792:MET:HA | 2:B:856:PHE:O | 2.06 | 0.55 |
| 2:B:971:THR:OG1 | 3:C:61:GLU:HG3 | 2.06 | 0.55 |
| 2:B:1087:PHE:HD2 | 2:B:1088:GLY:H | 1.50 | 0.55 |
| 7:G:10:ASN:OD1 | 7:G:71:ASN:HA | 2.07 | 0.55 |
| 7:G:20:PRO:HG2 | 7:G:21:ARG:H | 1.70 | 0.55 |
| 15:T:17:DT:H1' | 15:T:18:DT:C5' | 2.33 | 0.55 |
| 1:A:14:VAL:CG2 | 2:B:1216:LEU:HD13 | 2.34 | 0.55 |
| 1:A:68:GLN:O | 1:A:70:CYS:N | 2.39 | 0.55 |
| 1:A:683:ILE:HG21 | 1:A:801:GLU:HG3 | 1.88 | 0.55 |
| 1:A:687:LYS:O | 1:A:690:VAL:HB | 2.06 | 0.55 |
| 1:A:1039:LYS:HE3 | 1:A:1043:ASP:OD2 | 2.07 | 0.55 |
| 1:A:1151:GLU:HA | 9:I:44:TYR:O | 2.07 | 0.55 |
| 1:A:1215:ARG:HA | 1:A:1218:GLN:HG2 | 1.89 | 0.55 |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:CZ | 2.41 | 0.55 |
| 2:B:130:VAL:HB | 2:B:167:ILE:CD1 | 2.36 | 0.55 |
| 2:B:1106:ARG:HD3 | 2:B:1126:GLY:C | 2.27 | 0.55 |
| 3:C:90:ASP:O | 3:C:91:HIS:HB3 | 2.05 | 0.55 |
| 10:J:48:ARG:HD2 | 10:J:49:MET:N | 2.21 | 0.55 |
| 14:P:6:C:H2' | 14:P:7:A:H8 | 1.68 | 0.55 |
| 1:A:115:LEU:HB2 | 1:A:122:MET:HE2 | 1.89 | 0.55 |
| 1:A:341:MET:CE | 2:B:1135:ARG:NH1 | 2.70 | 0.55 |
| 1:A:353:ILE:CD1 | 1:A:487:MET:HE2 | 2.37 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1077:THR:HG22 | 11:K:44:ASN:HD21 | 1.71 | 0.55 |
| 5:E:13:TRP:O | 5:E:16:PHE:HB3 | 2.07 | 0.55 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:CD1 | 2.42 | 0.55 |
| 1:A:47:ARG:HH12 | 1:A:254:GLU:HG2 | 1.72 | 0.55 |
| 1:A:1364:ASN:HD22 | 1:A:1365:TYR:N | 2.05 | 0.55 |
| 2:B:129:PHE:HA | 2:B:165:VAL:O | 2.07 | 0.55 |
| 2:B:343:ILE:CG2 | 2:B:348:ARG:N | 2.66 | 0.55 |
| 2:B:654:ARG:H | 2:B:657:HIS:CD2 | 2.17 | 0.55 |
| 2:B:745:PRO:C | 2:B:747:MET:N | 2.60 | 0.55 |
| 4:D:7:THR:HB | 7:G:42:PHE:HE2 | 1.72 | 0.55 |
| 4:D:176:GLU:C | 4:D:178:ALA:N | 2.60 | 0.55 |
| 1:A:265:LYS:HZ3 | 1:A:322:VAL:HG13 | 1.71 | 0.54 |
| 1:A:548:ASN:HA | 11:K:60:ALA:HB1 | 1.89 | 0.54 |
| 1:A:1120:LEU:N | 1:A:1120:LEU:CD1 | 2.69 | 0.54 |
| 2:B:758:PHE:HE1 | 2:B:1027:ILE:HG22 | 1.72 | 0.54 |
| 2:B:911:ILE:O | 2:B:912:ILE:HG13 | 2.07 | 0.54 |
| 3:C:189:THR:HG22 | 3:C:190:ASP:H | 1.71 | 0.54 |
| 7:G:18:PHE:HA | 7:G:22:MET:CE | 2.36 | 0.54 |
| 1:A:182:VAL:HG22 | 1:A:201:VAL:HA | 1.89 | 0.54 |
| 1:A:265:LYS:HE2 | 1:A:322:VAL:HG11 | 1.89 | 0.54 |
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:N | 2.22 | 0.54 |
| 1:A:1348:LEU:O | 1:A:1352:VAL:HG23 | 2.07 | 0.54 |
| 1:A:1424:VAL:CG1 | 1:A:1436:ILE:HD11 | 2.34 | 0.54 |
| 3:C:97:VAL:HG12 | 3:C:99:LEU:CD2 | 2.37 | 0.54 |
| 4:D:48:ILE:HG21 | 7:G:4:ILE:HB | 1.89 | 0.54 |
| 4:D:63:LEU:HD13 | 4:D:133:THR:OG1 | 2.07 | 0.54 |
| 9:I:50:THR:HG22 | 9:I:52:ILE:H | 1.72 | 0.54 |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N | 2.22 | 0.54 |
| 1:A:1343:ALA:HB2 | 5:E:150:VAL:HG22 | 1.88 | 0.54 |
| 1:A:1445:ILE:HD11 | 7:G:68:ALA:HB1 | 1.90 | 0.54 |
| 2:B:38:PHE:CD1 | 2:B:811:TYR:CD2 | 2.94 | 0.54 |
| 2:B:834:ASN:HA | 2:B:838:SER:O | 2.06 | 0.54 |
| 2:B:1165:ILE:HG12 | 4:D:17:LYS:HD2 | 1.89 | 0.54 |
| 4:D:185:CYS:HB2 | 4:D:211:LEU:HD22 | 1.88 | 0.54 |
| 5:E:35:VAL:C | 5:E:37:LEU:H | 2.10 | 0.54 |
| 1:A:44:THR:O | 1:A:45:GLN:HB2 | 2.07 | 0.54 |
| 1:A:527:THR:HG23 | 1:A:650:GLN:HA | 1.89 | 0.54 |
| 1:A:873:MET:C | 1:A:1058:VAL:HG23 | 2.27 | 0.54 |
| 2:B:129:PHE:HE2 | 2:B:166:PHE:HD1 | 1.56 | 0.54 |
| 2:B:479:VAL:O | 2:B:480:SER:HB3 | 2.07 | 0.54 |
| 2:B:496:ARG:NH1 | 2:B:539:LEU:HB2 | 2.22 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:542:MET:HG2 | 2:B:747:MET:HB3 | 1.89 | 0.54 |
| 2:B:841:MET:O | 2:B:993:THR:HA | 2.08 | 0.54 |
| 2:B:879:ARG:HH11 | 2:B:883:LEU:CD2 | 2.17 | 0.54 |
| 2:B:1187:ASN:O | 2:B:1188:LYS:CB | 2.49 | 0.54 |
| 7:G:143:ILE:CG2 | 7:G:144:ARG:N | 2.71 | 0.54 |
| 8:H:116:TYR:HE2 | 8:H:140:ALA:CB | 2.19 | 0.54 |
| 9:I:101:PHE:N | 9:I:101:PHE:CD1 | 2.76 | 0.54 |
| 1:A:18:GLN:CB | 2:B:1215:ARG:HB2 | 2.38 | 0.54 |
| 1:A:306:ASN:HB2 | 1:A:324:SER:HB3 | 1.90 | 0.54 |
| 2:B:287:ARG:NH1 | 2:B:324:ILE:O | 2.41 | 0.54 |
| 2:B:305:VAL:O | 2:B:305:VAL:HG12 | 2.07 | 0.54 |
| 2:B:865:LYS:NZ | 2:B:869:SER:HA | 2.23 | 0.54 |
| 2:B:872:GLU:CD | 2:B:914:LYS:HE2 | 2.28 | 0.54 |
| 5:E:55:ARG:C | 5:E:57:MET:N | 2.61 | 0.54 |
| 10:J:32:GLU:CD | 10:J:32:GLU:H | 2.10 | 0.54 |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:N | 2.23 | 0.54 |
| 1:A:695:LYS:C | 1:A:697:ALA:H | 2.10 | 0.54 |
| 1:A:814:PHE:O | 1:A:817:ALA:HB3 | 2.08 | 0.54 |
| 2:B:372:SER:O | 2:B:376:PHE:HD1 | 1.90 | 0.54 |
| 3:C:100:THR:HG22 | 3:C:101:LEU:H | 1.71 | 0.54 |
| 14:P:7:A:H2' | 14:P:8:G:O4' | 2.08 | 0.54 |
| 1:A:381:THR:HG21 | 1:A:383:TYR:CD1 | 2.43 | 0.54 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:O | 2.08 | 0.54 |
| 3:C:70:ILE:HD11 | 3:C:144:ILE:CG1 | 2.38 | 0.54 |
| 6:F:69:LEU:N | 6:F:70:LYS:N | 2.56 | 0.54 |
| 7:G:111:THR:HB | 7:G:114:LEU:HB2 | 1.90 | 0.54 |
| 8:H:58:THR:HG22 | 8:H:59:ILE:N | 2.22 | 0.54 |
| 1:A:4:GLN:O | 1:A:5:GLN:HB2 | 2.07 | 0.54 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:CD | 2.29 | 0.54 |
| 2:B:687:GLU:O | 2:B:689:LEU:HG | 2.08 | 0.54 |
| 2:B:705:MET:N | 2:B:710:LEU:HD12 | 2.23 | 0.54 |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:H | 1.72 | 0.54 |
| 2:B:899:ILE:CG2 | 2:B:949:VAL:HG21 | 2.38 | 0.54 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:HB | 1.90 | 0.54 |
| 2:B:1001:PHE:CE2 | 3:C:34:ARG:CZ | 2.90 | 0.54 |
| 2:B:1023:VAL:O | 2:B:1026:LEU:HB2 | 2.08 | 0.54 |
| 3:C:235:VAL:HG13 | 10:J:13:VAL:CG2 | 2.37 | 0.54 |
| 11:K:18:LYS:NZ | 11:K:38:GLU:HG2 | 2.23 | 0.54 |
| 1:A:71:GLN:O | 1:A:73:GLY:N | 2.37 | 0.54 |
| 2:B:63:ILE:O | 2:B:67:SER:HB3 | 2.08 | 0.54 |
| 2:B:942:ARG:NH2 | 15:T:25:DT:OP2 | 2.39 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:969:ARG:HD2 | 3:C:61:GLU:OE2 | 2.08 | 0.54 |
| 9:I:26:LEU:CD2 | 9:I:37:GLU:HA | 2.33 | 0.54 |
| 10:J:57:ILE:HA | 10:J:60:PHE:CD2 | 2.41 | 0.54 |
| 11:K:31:VAL:CG1 | 11:K:32:VAL:N | 2.71 | 0.54 |
| 1:A:164:ARG:HG3 | 1:A:165:GLY:H | 1.72 | 0.54 |
| 1:A:535:THR:CG2 | 1:A:616:VAL:HA | 2.35 | 0.54 |
| 1:A:787:PHE:CE1 | 1:A:796:SER:HA | 2.43 | 0.54 |
| 1:A:821:ARG:HB2 | 1:A:821:ARG:NH1 | 2.18 | 0.54 |
| 1:A:857:ARG:NH1 | 6:F:139:PRO:HB2 | 2.23 | 0.54 |
| 1:A:863:VAL:HG11 | 1:A:866:PHE:CD2 | 2.42 | 0.54 |
| 1:A:1171:GLN:HA | 1:A:1174:PHE:HE1 | 1.71 | 0.54 |
| 2:B:502:ILE:H | 2:B:502:ILE:CD1 | 2.07 | 0.54 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:N | 2.23 | 0.54 |
| 11:K:47:ARG:HD3 | 11:K:59:ALA:O | 2.07 | 0.54 |
| 11:K:55:LYS:HB2 | 11:K:81:TYR:HE1 | 1.73 | 0.54 |
| 1:A:187:LYS:HE3 | 1:A:198:GLU:OE2 | 2.08 | 0.53 |
| 1:A:500:GLU:OE2 | 2:B:1145:SER:HB2 | 2.08 | 0.53 |
| 1:A:1369:ALA:O | 1:A:1372:VAL:HG12 | 2.08 | 0.53 |
| 2:B:549:THR:HG22 | 2:B:550:ASP:N | 2.15 | 0.53 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:HD2 | 1.89 | 0.53 |
| 2:B:952:VAL:HG22 | 2:B:966:VAL:HG13 | 1.90 | 0.53 |
| 2:B:1073:TYR:CE2 | 2:B:1080:LYS:HG2 | 2.43 | 0.53 |
| 1:A:590:ARG:HB2 | 1:A:605:MET:HB3 | 1.90 | 0.53 |
| 1:A:1313:LEU:O | 1:A:1315:GLU:N | 2.41 | 0.53 |
| 2:B:327:ARG:O | 2:B:331:LEU:HD13 | 2.07 | 0.53 |
| 2:B:582:VAL:HG23 | 2:B:626:ILE:HB | 1.90 | 0.53 |
| 2:B:1189:ILE:HG22 | 2:B:1190:ASP:N | 2.22 | 0.53 |
| 3:C:73:GLN:HB3 | 3:C:131:HIS:H | 1.73 | 0.53 |
| 12:L:31:CYS:HB3 | 12:L:34:CYS:C | 2.28 | 0.53 |
| 1:A:886:ILE:HG13 | 1:A:943:LEU:HD12 | 1.89 | 0.53 |
| 2:B:1077:THR:HG22 | 11:K:44:ASN:ND2 | 2.23 | 0.53 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:HG2 | 2.23 | 0.53 |
| 7:G:138:THR:CG2 | 7:G:139:ILE:H | 2.00 | 0.53 |
| 11:K:63:VAL:HG23 | 11:K:63:VAL:O | 2.09 | 0.53 |
| 11:K:109:TRP:O | 11:K:111:LEU:N | 2.39 | 0.53 |
| 12:L:32:ALA:CB | 12:L:55:ILE:HD12 | 2.39 | 0.53 |
| 1:A:42:ASP:C | 1:A:44:THR:H | 2.09 | 0.53 |
| 1:A:761:MET:HA | 1:A:804:TYR:HB2 | 1.89 | 0.53 |
| 1:A:958:VAL:O | 1:A:958:VAL:HG12 | 2.08 | 0.53 |
| 1:A:1102:LYS:O | 1:A:1106:ASN:ND2 | 2.42 | 0.53 |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2 | 2.43 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:830:TYR:O | 2:B:831:SER:C | 2.47 | 0.53 |
| 3:C:177:GLU:HG3 | 3:C:231:ASN:HD22 | 1.73 | 0.53 |
| 11:K:55:LYS:CB | 11:K:81:TYR:HE1 | 2.21 | 0.53 |
| 1:A:1120:LEU:CD1 | 1:A:1120:LEU:H | 2.21 | 0.53 |
| 4:D:198:LEU:O | 4:D:200:ASN:N | 2.42 | 0.53 |
| 5:E:207:ARG:NH1 | 5:E:207:ARG:HB2 | 2.23 | 0.53 |
| 7:G:35:GLU:OE2 | 7:G:48:VAL:HG23 | 2.08 | 0.53 |
| 1:A:53:LEU:CD2 | 1:A:54:ASN:N | 2.51 | 0.53 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:HA | 1.90 | 0.53 |
| 1:A:666:ILE:HD12 | 1:A:666:ILE:N | 2.23 | 0.53 |
| 1:A:816:HIS:CD2 | 2:B:764:SER:HB2 | 2.43 | 0.53 |
| 1:A:982:THR:HB | 1:A:985:ASP:N | 2.23 | 0.53 |
| 2:B:412:LEU:HB3 | 2:B:466:TRP:CZ2 | 2.43 | 0.53 |
| 7:G:91:VAL:HB | 7:G:139:ILE:O | 2.08 | 0.53 |
| 1:A:351:THR:HG21 | 2:B:1103:ILE:HG13 | 1.91 | 0.53 |
| 1:A:446:ARG:CD | 1:A:480:ALA:HB2 | 2.39 | 0.53 |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:H | 1.74 | 0.53 |
| 2:B:408:LEU:HG | 2:B:409:ALA:H | 1.74 | 0.53 |
| 4:D:56:ARG:HD3 | 4:D:149:THR:HA | 1.91 | 0.53 |
| 5:E:163:GLU:O | 5:E:164:LEU:C | 2.47 | 0.53 |
| 1:A:288:ALA:HA | 1:A:291:GLU:OE2 | 2.09 | 0.53 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CZ3 | 2.44 | 0.53 |
| 1:A:478:TYR:O | 1:A:479:ASN:HB3 | 2.08 | 0.53 |
| 2:B:343:ILE:CB | 2:B:348:ARG:HG3 | 2.37 | 0.53 |
| 2:B:1166:CYS:O | 2:B:1168:LEU:N | 2.41 | 0.53 |
| 2:B:1180:PHE:O | 2:B:1181:GLU:O | 2.27 | 0.53 |
| 3:C:239:PRO:HB2 | 3:C:241:ASP:OD1 | 2.08 | 0.53 |
| 4:D:53:SER:HB3 | 4:D:152:SER:HB2 | 1.91 | 0.53 |
| 6:F:124:GLU:HB3 | 6:F:130:ILE:HG12 | 1.90 | 0.53 |
| 2:B:39:ARG:HG2 | 2:B:39:ARG:HH11 | 1.74 | 0.53 |
| 2:B:54:PHE:O | 2:B:58:THR:HB | 2.09 | 0.53 |
| 2:B:899:ILE:CD1 | 2:B:911:ILE:HA | 2.39 | 0.53 |
| 3:C:120:ILE:HD13 | 3:C:124:LEU:HD21 | 1.91 | 0.53 |
| 9:I:111:THR:CG2 | 9:I:112:SER:N | 2.72 | 0.53 |
| 9:I:112:SER:O | 9:I:114:GLN:N | 2.42 | 0.53 |
| 12:L:70:ARG:HG2 | 12:L:70:ARG:HH11 | 1.73 | 0.53 |
| 14:P:1:U:H2' | 14:P:2:C:C6 | 2.43 | 0.53 |
| 15:T:22:BRU:H2" | 15:T:23:DG:O4' | 2.09 | 0.53 |
| 1:A:317:LYS:O | 1:A:318:SER:HB3 | 2.09 | 0.53 |
| 1:A:353:ILE:HD12 | 1:A:470:LEU:HD21 | 1.91 | 0.53 |
| 1:A:608:ILE:C | 1:A:610:GLY:N | 2.63 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:645:LEU:HD11 | 1:A:649:ILE:HD11 | 1.91 | 0.53 |
| 1:A:1153:TYR:CE1 | 9:I:42:LEU:HD13 | 2.44 | 0.53 |
| 1:A:1369:ALA:O | 1:A:1370:LEU:C | 2.46 | 0.53 |
| 1:A:1444:MET:HG2 | 7:G:60:ARG:HA | 1.91 | 0.53 |
| 2:B:683:SER:C | 2:B:685:LEU:N | 2.62 | 0.53 |
| 2:B:756:ILE:O | 2:B:759:PRO:HD3 | 2.08 | 0.53 |
| 2:B:839:MET:CE | 2:B:1010:LEU:HD21 | 2.38 | 0.53 |
| 3:C:263:THR:C | 3:C:265:MET:N | 2.63 | 0.53 |
| 4:D:208:GLU:O | 4:D:212:LYS:HG3 | 2.08 | 0.53 |
| 6:F:86:THR:HG23 | 6:F:89:GLU:OE1 | 2.09 | 0.53 |
| 7:G:44:TYR:CD2 | 7:G:105:PRO:HB2 | 2.44 | 0.53 |
| 13:N:0:DT:H1' | 13:N:1:DA:H5' | 1.90 | 0.53 |
| 1:A:282:ASN:O | 1:A:284:ALA:N | 2.42 | 0.52 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CE2 | 2.42 | 0.52 |
| 1:A:828:ALA:HB1 | 2:B:530:GLY:HA2 | 1.88 | 0.52 |
| 1:A:1214:GLU:O | 1:A:1218:GLN:HG2 | 2.10 | 0.52 |
| 2:B:412:LEU:HB3 | 2:B:466:TRP:HZ2 | 1.74 | 0.52 |
| 2:B:654:ARG:C | 2:B:656:GLY:H | 2.11 | 0.52 |
| 3:C:87:PHE:H | 3:C:87:PHE:HD1 | 1.56 | 0.52 |
| 4:D:19:GLU:O | 4:D:21:GLU:N | 2.42 | 0.52 |
| 9:I:99:LEU:O | 9:I:111:THR:HG23 | 2.09 | 0.52 |
| 9:I:115:LYS:CD | 9:I:117:LYS:HE3 | 2.35 | 0.52 |
| 11:K:60:ALA:O | 11:K:73:LEU:HD12 | 2.09 | 0.52 |
| 14:P:8:G:H8 | 14:P:8:G:OP2 | 1.91 | 0.52 |
| 1:A:19:PHE:HB3 | 1:A:1413:GLY:HA2 | 1.90 | 0.52 |
| 1:A:541:ILE:HD13 | 1:A:549:MET:HE1 | 1.91 | 0.52 |
| 1:A:897:TYR:CD2 | 1:A:936:LEU:HD13 | 2.44 | 0.52 |
| 1:A:903:ASN:ND2 | 1:A:903:ASN:C | 2.63 | 0.52 |
| 1:A:1187:GLN:O | 1:A:1243:VAL:HG13 | 2.09 | 0.52 |
| 2:B:550:ASP:OD1 | 2:B:551:PRO:HD2 | 2.09 | 0.52 |
| 2:B:954:VAL:O | 12:L:55:ILE:O | 2.28 | 0.52 |
| 2:B:1183:LYS:N | 2:B:1183:LYS:CE | 2.72 | 0.52 |
| 3:C:263:THR:O | 3:C:265:MET:N | 2.43 | 0.52 |
| 5:E:168:TYR:CB | 5:E:170:LEU:HG | 2.38 | 0.52 |
| 7:G:1:MET:O | 7:G:3:PHE:CE1 | 2.63 | 0.52 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:HG13 | 1.90 | 0.52 |
| 1:A:54:ASN:HB3 | 1:A:247:ARG:HH22 | 1.74 | 0.52 |
| 1:A:89:PRO:HB2 | 1:A:204:THR:CG2 | 2.39 | 0.52 |
| 1:A:682:THR:HG23 | 1:A:728:LYS:HE3 | 1.91 | 0.52 |
| 1:A:963:ILE:HD13 | 1:A:1049:ILE:HG13 | 1.90 | 0.52 |
| 2:B:95:ILE:HG13 | 2:B:129:PHE:O | 2.08 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:102:VAL:CG2 | 2:B:112:LEU:HD22 | 2.39 | 0.52 |
| 2:B:546:SER:OG | 2:B:631:GLY:N | 2.39 | 0.52 |
| 4:D:29:LEU:HD22 | 7:G:82:PHE:CD2 | 2.44 | 0.52 |
| 5:E:78:LEU:HD23 | 5:E:79:TRP:N | 2.24 | 0.52 |
| 6:F:85:MET:HE1 | 6:F:148:VAL:HG12 | 1.89 | 0.52 |
| 1:A:108:MET:HB3 | 1:A:210:ILE:CD1 | 2.39 | 0.52 |
| 1:A:722:LEU:HD22 | 1:A:799:PHE:CD1 | 2.44 | 0.52 |
| 2:B:223:VAL:HG21 | 2:B:380:TYR:HE2 | 1.75 | 0.52 |
| 2:B:525:ALA:O | 2:B:768:THR:HG23 | 2.09 | 0.52 |
| 2:B:787:VAL:O | 2:B:787:VAL:HG12 | 2.09 | 0.52 |
| 2:B:980:PHE:CD2 | 2:B:1094:ARG:HA | 2.44 | 0.52 |
| 6:F:94:LEU:HD21 | 6:F:122:MET:HA | 1.92 | 0.52 |
| 7:G:51:TYR:O | 7:G:54:ILE:HG13 | 2.10 | 0.52 |
| 7:G:115:MET:HB3 | 7:G:116:PRO:HD2 | 1.91 | 0.52 |
| 1:A:60:SER:C | 1:A:61:ILE:HG13 | 2.29 | 0.52 |
| 1:A:92:HIS:O | 1:A:95:PHE:N | 2.36 | 0.52 |
| 1:A:475:THR:HG23 | 1:A:476:SER:N | 2.25 | 0.52 |
| 1:A:1095:THR:O | 1:A:1096:SER:CB | 2.57 | 0.52 |
| 2:B:274:PRO:O | 2:B:275:TYR:HB2 | 2.09 | 0.52 |
| 2:B:434:ARG:HA | 2:B:437:GLU:CD | 2.29 | 0.52 |
| 2:B:657:HIS:CE1 | 2:B:689:LEU:HD11 | 2.45 | 0.52 |
| 2:B:1201:LYS:O | 2:B:1204:PHE:HB2 | 2.09 | 0.52 |
| 3:C:76:ASP:OD2 | 3:C:128:ASN:N | 2.41 | 0.52 |
| 8:H:102:TYR:N | 8:H:102:TYR:CD2 | 2.77 | 0.52 |
| 13:N:3:DG:C1' | 13:N:4:DT:H5' | 2.38 | 0.52 |
| 1:A:78:PRO:HA | 2:B:1201:LYS:NZ | 2.24 | 0.52 |
| 1:A:115:LEU:HB2 | 1:A:122:MET:CE | 2.39 | 0.52 |
| 1:A:244:PRO:O | 1:A:246:VAL:N | 2.43 | 0.52 |
| 1:A:407:ARG:HD2 | 1:A:413:ILE:HD11 | 1.92 | 0.52 |
| 1:A:567:LYS:HE3 | 8:H:46:LEU:HD12 | 1.91 | 0.52 |
| 1:A:836:TYR:HB2 | 15:T:18:DT:H4' | 1.92 | 0.52 |
| 1:A:838:GLN:O | 1:A:842:VAL:HG23 | 2.09 | 0.52 |
| 1:A:840:ARG:O | 1:A:841:LEU:C | 2.47 | 0.52 |
| 1:A:897:TYR:HD2 | 1:A:936:LEU:HD13 | 1.74 | 0.52 |
| 3:C:66:ARG:NH1 | 3:C:144:ILE:O | 2.43 | 0.52 |
| 4:D:130:LEU:C | 4:D:132:GLN:N | 2.62 | 0.52 |
| 1:A:317:LYS:O | 1:A:318:SER:CB | 2.57 | 0.52 |
| 1:A:341:MET:HE1 | 2:B:1135:ARG:NH1 | 2.24 | 0.52 |
| 1:A:881:GLN:O | 1:A:953:ASN:HA | 2.10 | 0.52 |
| 1:A:1394:THR:CG2 | 1:A:1398:MET:SD | 2.89 | 0.52 |
| 2:B:34:ILE:O | 2:B:37:PHE:N | 2.41 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:953:LEU:HD21 | 2:B:965:LYS:HB2 | 1.91 | 0.52 |
| 2:B:1095:LEU:HD12 | 2:B:1095:LEU:N | 2.21 | 0.52 |
| 7:G:1:MET:HG3 | 7:G:85:GLU:OE2 | 2.10 | 0.52 |
| 8:H:4:THR:O | 8:H:5:LEU:HD23 | 2.09 | 0.52 |
| 10:J:23:ASN:C | 10:J:25:LEU:N | 2.61 | 0.52 |
| 1:A:40:THR:HG22 | 1:A:41:MET:CG | 2.28 | 0.52 |
| 1:A:774:ARG:O | 1:A:775:ILE:C | 2.47 | 0.52 |
| 1:A:956:LEU:HD23 | 1:A:957:PRO:HD2 | 1.92 | 0.52 |
| 1:A:1410:PHE:HA | 2:B:1212:ILE:HD11 | 1.91 | 0.52 |
| 2:B:496:ARG:HH12 | 2:B:539:LEU:HB2 | 1.75 | 0.52 |
| 2:B:654:ARG:N | 2:B:657:HIS:HD2 | 2.04 | 0.52 |
| 2:B:899:ILE:O | 2:B:952:VAL:HG21 | 2.09 | 0.52 |
| 2:B:1022:THR:HG23 | 2:B:1022:THR:O | 2.09 | 0.52 |
| 2:B:1099:VAL:HG12 | 2:B:1100:ASP:N | 2.24 | 0.52 |
| 2:B:1177:HIS:O | 2:B:1179:GLN:N | 2.42 | 0.52 |
| 3:C:167:HIS:CD2 | 3:C:169:LYS:H | 2.27 | 0.52 |
| 3:C:256:ALA:O | 3:C:259:LEU:N | 2.42 | 0.52 |
| 5:E:17:ARG:O | 5:E:20:LYS:HB2 | 2.10 | 0.52 |
| 6:F:125:LEU:N | 6:F:130:ILE:HD11 | 2.23 | 0.52 |
| 7:G:30:LEU:HD22 | 7:G:72:VAL:HG11 | 1.92 | 0.52 |
| 8:H:84:ALA:HA | 8:H:87:ARG:CB | 2.34 | 0.52 |
| 9:I:13:MET:HG3 | 9:I:14:LEU:N | 2.23 | 0.52 |
| 1:A:30:ILE:HD11 | 2:B:1168:LEU:HD13 | 1.92 | 0.52 |
| 1:A:114:LEU:HD13 | 1:A:171:GLN:NE2 | 2.25 | 0.52 |
| 1:A:672:ASP:HB2 | 1:A:736:ASN:OD1 | 2.09 | 0.52 |
| 1:A:886:ILE:HG13 | 1:A:943:LEU:CD1 | 2.40 | 0.52 |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:HD21 | 1.91 | 0.52 |
| 2:B:936:ASP:OD1 | 2:B:938:SER:N | 2.39 | 0.52 |
| 4:D:53:SER:CB | 4:D:153:ARG:H | 2.22 | 0.52 |
| 8:H:62:SER:C | 8:H:64:ASN:H | 2.13 | 0.52 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:CE1 | 2.45 | 0.52 |
| 1:A:58:LEU:CD1 | 1:A:80:HIS:H | 2.23 | 0.52 |
| 1:A:67:CYS:O | 1:A:68:GLN:HB2 | 2.09 | 0.52 |
| 1:A:1441:PHE:HZ | 6:F:89:GLU:HA | 1.74 | 0.52 |
| 2:B:33:VAL:HG21 | 2:B:638:PHE:HZ | 1.75 | 0.52 |
| 2:B:337:ARG:C | 2:B:338:GLY:N | 2.64 | 0.52 |
| 2:B:640:VAL:O | 2:B:641:GLU:C | 2.47 | 0.52 |
| 3:C:33:LEU:O | 3:C:34:ARG:C | 2.48 | 0.52 |
| 5:E:177:ARG:HD3 | 5:E:215:MET:CG | 2.40 | 0.52 |
| 7:G:3:PHE:CD1 | 7:G:80:LYS:NZ | 2.68 | 0.52 |
| 7:G:79:PHE:HZ | 7:G:106:MET:HE1 | 1.71 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:26:ILE:HD13 | 8:H:49:VAL:HG11 | 1.92 | 0.52 |
| 9:I:2:THR:O | 9:I:3:THR:C | 2.47 | 0.52 |
| 9:I:61:ASP:O | 9:I:63:GLY:N | 2.43 | 0.52 |
| 11:K:55:LYS:CB | 11:K:81:TYR:CE1 | 2.93 | 0.52 |
| 1:A:84:ILE:HG22 | 1:A:239:LEU:HB3 | 1.91 | 0.51 |
| 1:A:264:PHE:O | 1:A:267:ALA:HB3 | 2.10 | 0.51 |
| 1:A:350:ARG:HB2 | 1:A:488:ASN:OD1 | 2.09 | 0.51 |
| 1:A:381:THR:CG2 | 1:A:383:TYR:H | 2.23 | 0.51 |
| 1:A:613:ILE:O | 1:A:614:PHE:HB3 | 2.09 | 0.51 |
| 1:A:715:GLU:OE2 | 1:A:774:ARG:NH1 | 2.43 | 0.51 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:HE1 | 1.72 | 0.51 |
| 1:A:965:GLN:O | 1:A:968:GLN:HB2 | 2.10 | 0.51 |
| 1:A:1118:VAL:HG12 | 1:A:1327:ILE:HG13 | 1.92 | 0.51 |
| 2:B:184:ALA:HB1 | 2:B:188:ASP:HB3 | 1.92 | 0.51 |
| 2:B:278:GLN:HG2 | 2:B:279:ASP:H | 1.74 | 0.51 |
| 2:B:376:PHE:CE2 | 2:B:569:TYR:HD2 | 2.27 | 0.51 |
| 2:B:825:VAL:HG13 | 2:B:826:ALA:N | 2.25 | 0.51 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:H | 1.75 | 0.51 |
| 7:G:139:ILE:HG22 | 7:G:140:LYS:N | 2.24 | 0.51 |
| 9:I:14:LEU:HA | 9:I:28:GLU:O | 2.10 | 0.51 |
| 9:I:50:THR:CG2 | 9:I:52:ILE:HG12 | 2.40 | 0.51 |
| 1:A:168:GLY:O | 1:A:169:ASN:C | 2.47 | 0.51 |
| 1:A:822:GLU:HG3 | 2:B:513:GLN:NE2 | 2.26 | 0.51 |
| 1:A:974:ASP:C | 1:A:976:THR:H | 2.13 | 0.51 |
| 2:B:343:ILE:CG2 | 2:B:348:ARG:H | 2.22 | 0.51 |
| 3:C:83:SER:OG | 3:C:160:LYS:HD3 | 2.10 | 0.51 |
| 4:D:17:LYS:HE3 | 4:D:17:LYS:HA | 1.92 | 0.51 |
| 4:D:167:LEU:O | 4:D:170:THR:OG1 | 2.24 | 0.51 |
| 5:E:61:GLN:HG2 | 5:E:62:ALA:N | 2.24 | 0.51 |
| 1:A:107:CYS:H | 1:A:114:LEU:HD21 | 1.74 | 0.51 |
| 1:A:152:VAL:HG13 | 1:A:153:PRO:HD2 | 1.91 | 0.51 |
| 1:A:211:PHE:HA | 1:A:214:ILE:HG13 | 1.92 | 0.51 |
| 1:A:826:ASP:HB2 | 1:A:830:LYS:HD3 | 1.91 | 0.51 |
| 1:A:1376:THR:O | 1:A:1377:THR:C | 2.48 | 0.51 |
| 2:B:278:GLN:NE2 | 2:B:337:ARG:HH21 | 2.08 | 0.51 |
| 2:B:281:PRO:O | 2:B:283:VAL:N | 2.43 | 0.51 |
| 2:B:449:ASN:C | 2:B:451:LYS:H | 2.13 | 0.51 |
| 2:B:693:ILE:HD13 | 2:B:701:ILE:HD13 | 1.93 | 0.51 |
| 3:C:226:ASP:O | 3:C:227:THR:CB | 2.58 | 0.51 |
| 4:D:29:LEU:HD13 | 7:G:82:PHE:CZ | 2.45 | 0.51 |
| 4:D:191:ALA:C | 4:D:193:THR:H | 2.12 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:72:GLU:OE2 | 2:B:1175:LEU:HB2 | 2.11 | 0.51 |
| 1:A:500:GLU:OE2 | 1:A:1438:THR:HG21 | 2.10 | 0.51 |
| 1:A:567:LYS:HB3 | 8:H:95:TYR:CA | 2.38 | 0.51 |
| 1:A:738:LYS:HB2 | 1:A:740:LEU:HG | 1.91 | 0.51 |
| 1:A:1409:LEU:HD13 | 2:B:1207:LEU:HD11 | 1.92 | 0.51 |
| 2:B:37:PHE:HD2 | 2:B:542:MET:SD | 2.33 | 0.51 |
| 2:B:388:CYS:C | 2:B:390:LEU:H | 2.13 | 0.51 |
| 2:B:882:THR:O | 2:B:883:LEU:HB2 | 2.10 | 0.51 |
| 2:B:899:ILE:HG21 | 2:B:949:VAL:HG21 | 1.93 | 0.51 |
| 2:B:902:GLY:O | 12:L:65:VAL:HG11 | 2.11 | 0.51 |
| 2:B:995:ARG:HB3 | 2:B:997:GLU:OE2 | 2.10 | 0.51 |
| 4:D:50:LEU:HD13 | 4:D:55:ALA:HA | 1.93 | 0.51 |
| 13:N:0:DT:H71 | 13:N:1:DA:N6 | 2.24 | 0.51 |
| 1:A:90:VAL:CG1 | 1:A:297:GLN:HA | 2.40 | 0.51 |
| 1:A:982:THR:HG22 | 1:A:984:LYS:H | 1.75 | 0.51 |
| 1:A:1453:TYR:O | 1:A:1454:MET:HB3 | 2.10 | 0.51 |
| 2:B:37:PHE:CD1 | 2:B:41:LYS:HG3 | 2.45 | 0.51 |
| 2:B:483:LEU:CD1 | 2:B:491:THR:HG23 | 2.39 | 0.51 |
| 2:B:852:ARG:NH2 | 12:L:70:ARG:OXT | 2.37 | 0.51 |
| 3:C:56:THR:HG21 | 3:C:145:CYS:SG | 2.51 | 0.51 |
| 7:G:16:SER:HB3 | 7:G:17:PHE:CD2 | 2.46 | 0.51 |
| 1:A:2:VAL:HG21 | 2:B:1157:ALA:C | 2.31 | 0.51 |
| 1:A:55:ASP:CG | 1:A:55:ASP:O | 2.46 | 0.51 |
| 2:B:46:GLN:HG3 | 2:B:47:GLN:N | 2.18 | 0.51 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:CE1 | 2.46 | 0.51 |
| 2:B:606:LYS:HD2 | 2:B:608:ASP:OD2 | 2.11 | 0.51 |
| 3:C:238:ILE:HG22 | 3:C:243:VAL:HG23 | 1.92 | 0.51 |
| 1:A:527:THR:HG21 | 1:A:650:GLN:HA | 1.91 | 0.51 |
| 1:A:626:ASN:O | 1:A:631:HIS:HD2 | 1.93 | 0.51 |
| 1:A:834:THR:O | 1:A:837:ILE:HB | 2.10 | 0.51 |
| 2:B:226:PHE:HA | 2:B:395:GLN:CG | 2.40 | 0.51 |
| 2:B:769:TYR:C | 2:B:771:SER:N | 2.62 | 0.51 |
| 8:H:58:THR:HB | 8:H:143:LEU:HD13 | 1.93 | 0.51 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:N | 2.26 | 0.51 |
| 1:A:730:GLY:C | 1:A:732:LEU:N | 2.62 | 0.51 |
| 1:A:899:VAL:CG2 | 1:A:1029:ARG:HG2 | 2.41 | 0.51 |
| 1:A:1121:GLU:CG | 1:A:1122:PRO:HD2 | 2.41 | 0.51 |
| 2:B:360:PHE:C | 2:B:360:PHE:CD2 | 2.84 | 0.51 |
| 2:B:434:ARG:HA | 2:B:437:GLU:OE2 | 2.10 | 0.51 |
| 2:B:711:GLU:H | 2:B:712:PRO:HD2 | 1.75 | 0.51 |
| 2:B:778:MET:HE2 | 2:B:1094:ARG:HG2 | 1.91 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:825:VAL:HG13 | 2:B:826:ALA:H | 1.76 | 0.51 |
| 3:C:174:ALA:O | 10:J:10:CYS:O | 2.29 | 0.51 |
| 10:J:36:LEU:HA | 10:J:39:LEU:HD12 | 1.91 | 0.51 |
| 1:A:84:ILE:O | 1:A:84:ILE:CG2 | 2.58 | 0.51 |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N | 2.26 | 0.51 |
| 2:B:27:ALA:O | 2:B:29:ASP:N | 2.44 | 0.51 |
| 2:B:310:MET:CE | 2:B:387:LEU:HD12 | 2.37 | 0.51 |
| 2:B:604:ARG:NH1 | 2:B:691:GLU:OE2 | 2.43 | 0.51 |
| 2:B:616:ILE:HG13 | 2:B:697:GLU:HG3 | 1.92 | 0.51 |
| 2:B:896:ASP:OD2 | 12:L:58:LYS:HE3 | 2.11 | 0.51 |
| 3:C:77:ILE:HG22 | 3:C:78:GLU:N | 2.26 | 0.51 |
| 8:H:89:LEU:C | 8:H:91:ASP:H | 2.13 | 0.51 |
| 9:I:5:ARG:HD3 | 9:I:36:GLU:OE2 | 2.11 | 0.51 |
| 1:A:33:ALA:O | 1:A:83:HIS:HD2 | 1.93 | 0.51 |
| 1:A:1362:TYR:HD1 | 1:A:1363:VAL:N | 2.08 | 0.51 |
| 1:A:1420:ASP:O | 1:A:1421:CYS:HB2 | 2.11 | 0.51 |
| 2:B:955:THR:CG2 | 2:B:956:THR:H | 2.19 | 0.51 |
| 4:D:177:VAL:O | 4:D:177:VAL:HG12 | 2.11 | 0.51 |
| 5:E:9:ILE:CD1 | 5:E:53:PRO:HD3 | 2.40 | 0.51 |
| 10:J:44:TYR:HA | 10:J:47:ARG:HB2 | 1.93 | 0.51 |
| 1:A:23:SER:O | 1:A:24:PRO:C | 2.48 | 0.50 |
| 1:A:244:PRO:CB | 1:A:245:PRO:HD3 | 2.41 | 0.50 |
| 1:A:366:VAL:HG21 | 1:A:460:VAL:HG22 | 1.93 | 0.50 |
| 2:B:123:THR:O | 2:B:125:SER:N | 2.44 | 0.50 |
| 2:B:190:TYR:CE1 | 2:B:196:PRO:HG3 | 2.45 | 0.50 |
| 2:B:552:MET:HA | 2:B:555:ILE:HB | 1.93 | 0.50 |
| 7:G:1:MET:SD | 7:G:1:MET:C | 2.89 | 0.50 |
| 7:G:1:MET:O | 7:G:3:PHE:CD1 | 2.65 | 0.50 |
| 11:K:68:PHE:HD2 | 11:K:68:PHE:N | 2.08 | 0.50 |
| 1:A:64:ASN:O | 1:A:65:LEU:C | 2.50 | 0.50 |
| 1:A:284:ALA:O | 1:A:286:HIS:N | 2.36 | 0.50 |
| 1:A:464:PRO:O | 1:A:465:TYR:O | 2.29 | 0.50 |
| 1:A:608:ILE:HD12 | 1:A:613:ILE:CD1 | 2.42 | 0.50 |
| 2:B:43:LEU:HD13 | 2:B:812:LEU:HD23 | 1.93 | 0.50 |
| 2:B:737:THR:CG2 | 9:I:66:PRO:HA | 2.38 | 0.50 |
| 2:B:778:MET:HE2 | 2:B:1094:ARG:CD | 2.41 | 0.50 |
| 4:D:56:ARG:HA | 4:D:148:LEU:HD13 | 1.93 | 0.50 |
| 6:F:77:ASP:O | 6:F:78:GLN:HB2 | 2.11 | 0.50 |
| 7:G:13:LEU:O | 7:G:67:SER:HA | 2.12 | 0.50 |
| 7:G:27:LYS:HE2 | 7:G:54:ILE:HB | 1.93 | 0.50 |
| 8:H:26:ILE:CD1 | 8:H:49:VAL:HG11 | 2.41 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:40:LEU:HD22 | 8:H:123:MET:CE | 2.40 | 0.50 |
| 1:A:316:GLN:O | 1:A:317:LYS:C | 2.49 | 0.50 |
| 1:A:362:ASP:OD2 | 1:A:459:ARG:HD3 | 2.10 | 0.50 |
| 1:A:919:ILE:O | 1:A:920:LEU:C | 2.50 | 0.50 |
| 1:A:1135:ARG:HH21 | 1:A:1284:MET:HG3 | 1.77 | 0.50 |
| 2:B:654:ARG:O | 2:B:656:GLY:N | 2.45 | 0.50 |
| 2:B:955:THR:CG2 | 2:B:956:THR:N | 2.74 | 0.50 |
| 2:B:1099:VAL:O | 2:B:1101:ASP:N | 2.44 | 0.50 |
| 5:E:35:VAL:O | 5:E:37:LEU:N | 2.44 | 0.50 |
| 9:I:111:THR:CG2 | 9:I:112:SER:H | 2.22 | 0.50 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:CD | 2.32 | 0.50 |
| 1:A:244:PRO:O | 1:A:247:ARG:N | 2.43 | 0.50 |
| 1:A:252:PHE:HB2 | 1:A:256:GLN:NE2 | 2.27 | 0.50 |
| 1:A:262:LEU:O | 1:A:264:PHE:N | 2.45 | 0.50 |
| 1:A:710:LEU:N | 1:A:710:LEU:HD12 | 2.27 | 0.50 |
| 1:A:786:HIS:N | 1:A:786:HIS:CD2 | 2.79 | 0.50 |
| 1:A:1283:VAL:HG12 | 1:A:1284:MET:H | 1.76 | 0.50 |
| 1:A:1324:PRO:HB2 | 5:E:142:VAL:HG11 | 1.93 | 0.50 |
| 2:B:515:HIS:N | 2:B:518:HIS:HD2 | 1.98 | 0.50 |
| 2:B:1020:ARG:HB2 | 2:B:1022:THR:HG22 | 1.93 | 0.50 |
| 2:B:1085:ILE:HG22 | 2:B:1086:PHE:N | 2.27 | 0.50 |
| 3:C:89:GLU:O | 3:C:90:ASP:HB3 | 2.11 | 0.50 |
| 3:C:179:GLU:HG2 | 3:C:180:TYR:H | 1.77 | 0.50 |
| 4:D:51:ASN:O | 4:D:54:GLU:HB3 | 2.10 | 0.50 |
| 9:I:61:ASP:C | 9:I:63:GLY:N | 2.63 | 0.50 |
| 11:K:47:ARG:HD2 | 11:K:47:ARG:C | 2.32 | 0.50 |
| 1:A:23:SER:HA | 1:A:233:TRP:NE1 | 2.27 | 0.50 |
| 1:A:54:ASN:HB3 | 1:A:247:ARG:HH12 | 1.76 | 0.50 |
| 1:A:798:GLY:HA2 | 1:A:815:PHE:HD1 | 1.73 | 0.50 |
| 2:B:44:VAL:O | 2:B:45:SER:C | 2.49 | 0.50 |
| 2:B:298:LEU:HD13 | 2:B:314:LEU:HD13 | 1.92 | 0.50 |
| 2:B:653:VAL:CG2 | 2:B:689:LEU:HB3 | 2.40 | 0.50 |
| 2:B:1102:LYS:O | 2:B:1103:ILE:C | 2.49 | 0.50 |
| 3:C:112:ASN:HD22 | 3:C:112:ASN:N | 2.07 | 0.50 |
| 3:C:140:ASN:O | 3:C:141:GLY:O | 2.29 | 0.50 |
| 4:D:27:LEU:HD22 | 4:D:173:HIS:CD2 | 2.46 | 0.50 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:N | 2.23 | 0.50 |
| 6:F:114:GLU:OE2 | 6:F:119:ARG:HG2 | 2.12 | 0.50 |
| 1:A:34:LYS:NZ | 1:A:57:ARG:NH1 | 2.60 | 0.50 |
| 1:A:58:LEU:HD11 | 1:A:80:HIS:H | 1.76 | 0.50 |
| 1:A:310:GLY:O | 1:A:312:PRO:HD2 | 2.12 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:432:VAL:O | 1:A:433:GLU:C | 2.49 | 0.50 |
| 1:A:774:ARG:NH2 | 1:A:797:LYS:HG3 | 2.27 | 0.50 |
| 1:A:809:THR:OG1 | 1:A:812:GLU:HG3 | 2.11 | 0.50 |
| 1:A:960:ILE:O | 1:A:961:ARG:C | 2.50 | 0.50 |
| 2:B:192:LEU:O | 2:B:193:LYS:HB2 | 2.12 | 0.50 |
| 2:B:510:LYS:HG3 | 2:B:511:PRO:CD | 2.38 | 0.50 |
| 3:C:69:LEU:HD12 | 3:C:69:LEU:H | 1.76 | 0.50 |
| 4:D:24:ALA:C | 4:D:26:THR:H | 2.15 | 0.50 |
| 5:E:131:THR:HG21 | 5:E:191:LYS:NZ | 2.26 | 0.50 |
| 7:G:88:ASP:HA | 7:G:144:ARG:HA | 1.92 | 0.50 |
| 7:G:96:GLN:HB3 | 7:G:121:PHE:CE2 | 2.47 | 0.50 |
| 1:A:55:ASP:HA | 1:A:58:LEU:HB3 | 1.94 | 0.50 |
| 1:A:269:ILE:CD1 | 1:A:300:VAL:HA | 2.41 | 0.50 |
| 1:A:350:ARG:HA | 1:A:468:PHE:HE1 | 1.77 | 0.50 |
| 1:A:1341:ILE:CG2 | 1:A:1342:GLU:H | 2.24 | 0.50 |
| 2:B:233:PRO:HG2 | 2:B:234:ILE:CD1 | 2.42 | 0.50 |
| 2:B:329:THR:O | 2:B:332:ASP:HB3 | 2.12 | 0.50 |
| 2:B:497:ARG:NH2 | 2:B:775:LYS:NZ | 2.59 | 0.50 |
| 6:F:69:LEU:N | 6:F:70:LYS:HA | 2.26 | 0.50 |
| 1:A:95:PHE:CZ | 1:A:1414:ALA:HB2 | 2.47 | 0.50 |
| 1:A:130:ASP:O | 1:A:131:SER:C | 2.50 | 0.50 |
| 1:A:195:ASP:O | 1:A:196:GLU:HB3 | 2.12 | 0.50 |
| 1:A:250:ILE:CD1 | 14:P:0:U:H1' | 2.41 | 0.50 |
| 1:A:265:LYS:HZ3 | 1:A:322:VAL:HG22 | 1.75 | 0.50 |
| 1:A:567:LYS:HG3 | 1:A:568:PRO:CD | 2.39 | 0.50 |
| 1:A:1118:VAL:HG23 | 1:A:1118:VAL:O | 2.11 | 0.50 |
| 2:B:213:ILE:HD12 | 2:B:497:ARG:HB3 | 1.94 | 0.50 |
| 2:B:233:PRO:HG2 | 2:B:234:ILE:HD12 | 1.92 | 0.50 |
| 2:B:746:SER:HB2 | 2:B:1046:PRO:HG2 | 1.93 | 0.50 |
| 3:C:22:LEU:HD13 | 3:C:230:MET:CE | 2.42 | 0.50 |
| 4:D:64:VAL:C | 4:D:66:ARG:H | 2.14 | 0.50 |
| 7:G:18:PHE:HA | 7:G:22:MET:HE2 | 1.93 | 0.50 |
| 12:L:55:ILE:O | 12:L:56:LEU:HB2 | 2.11 | 0.50 |
| 1:A:58:LEU:HG | 1:A:59:GLY:N | 2.26 | 0.50 |
| 1:A:853:ASP:OD1 | 1:A:853:ASP:C | 2.50 | 0.50 |
| 2:B:847:ASP:C | 2:B:849:GLY:H | 2.14 | 0.50 |
| 2:B:1033:LYS:NZ | 2:B:1068:GLY:O | 2.45 | 0.50 |
| 15:T:19:TT:C5R | 15:T:19:TT:H2'1 | 2.42 | 0.50 |
| 1:A:37:PHE:HB2 | 1:A:52:GLY:HA3 | 1.94 | 0.49 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:OE1 | 2.11 | 0.49 |
| 1:A:116:ASP:C | 1:A:118:HIS:N | 2.66 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1198:ASP:O | 1:A:1202:MET:HG2 | 2.12 | 0.49 |
| 2:B:122:LEU:O | 2:B:206:ASN:HA | 2.12 | 0.49 |
| 2:B:220:GLY:O | 2:B:222:ILE:HG13 | 2.12 | 0.49 |
| 2:B:365:THR:HG23 | 2:B:367:LEU:N | 2.21 | 0.49 |
| 2:B:549:THR:N | 2:B:628:THR:HG23 | 2.25 | 0.49 |
| 2:B:899:ILE:CG2 | 2:B:903:VAL:HB | 2.42 | 0.49 |
| 4:D:195:ILE:HG22 | 4:D:198:LEU:HG | 1.93 | 0.49 |
| 7:G:59:GLY:CA | 7:G:70:PHE:CD2 | 2.94 | 0.49 |
| 1:A:152:VAL:HG12 | 1:A:153:PRO:HD2 | 1.93 | 0.49 |
| 1:A:541:ILE:HG21 | 1:A:549:MET:CE | 2.39 | 0.49 |
| 1:A:608:ILE:HB | 1:A:613:ILE:HD11 | 1.94 | 0.49 |
| 1:A:867:ILE:CG2 | 1:A:872:GLY:N | 2.75 | 0.49 |
| 1:A:1329:THR:CG2 | 1:A:1331:SER:H | 2.22 | 0.49 |
| 2:B:259:TYR:HB2 | 2:B:268:THR:HG23 | 1.93 | 0.49 |
| 2:B:549:THR:H | 2:B:628:THR:CG2 | 2.22 | 0.49 |
| 3:C:74:SER:HB2 | 3:C:77:ILE:HG12 | 1.93 | 0.49 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CE2 | 2.47 | 0.49 |
| 8:H:116:TYR:HE2 | 8:H:140:ALA:HB1 | 1.76 | 0.49 |
| 9:I:58:VAL:O | 9:I:58:VAL:HG12 | 2.11 | 0.49 |
| 14:P:5:C:C2' | 14:P:6:C:H5' | 2.41 | 0.49 |
| 1:A:244:PRO:HB2 | 1:A:245:PRO:HD3 | 1.93 | 0.49 |
| 1:A:947:PHE:CD2 | 1:A:954:TRP:CE2 | 3.00 | 0.49 |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:CD | 2.42 | 0.49 |
| 2:B:199:MET:CE | 2:B:492:LEU:HD23 | 2.43 | 0.49 |
| 2:B:792:MET:HG3 | 2:B:855:PHE:CE1 | 2.47 | 0.49 |
| 4:D:14:ARG:N | 4:D:17:LYS:HZ3 | 2.10 | 0.49 |
| 4:D:40:HIS:CG | 4:D:41:GLN:N | 2.80 | 0.49 |
| 4:D:57:LEU:O | 4:D:61:GLU:HB2 | 2.12 | 0.49 |
| 6:F:143:PHE:C | 6:F:143:PHE:CD1 | 2.85 | 0.49 |
| 7:G:9:LEU:HD12 | 7:G:10:ASN:H | 1.77 | 0.49 |
| 11:K:21:ILE:HG23 | 11:K:31:VAL:CG1 | 2.42 | 0.49 |
| 15:T:19:TT:H2'1 | 15:T:19:TT:C3R | 2.42 | 0.49 |
| 1:A:767:GLN:HA | 1:A:799:PHE:HA | 1.94 | 0.49 |
| 1:A:1115:SER:OG | 1:A:1116:LEU:N | 2.45 | 0.49 |
| 1:A:1164:PRO:HG2 | 1:A:1165:GLU:H | 1.78 | 0.49 |
| 2:B:797:TYR:HE1 | 2:B:854:LEU:CD2 | 2.24 | 0.49 |
| 2:B:980:PHE:HE2 | 2:B:1094:ARG:HB2 | 1.78 | 0.49 |
| 2:B:1159:ARG:HD2 | 2:B:1159:ARG:C | 2.33 | 0.49 |
| 3:C:123:ASN:HD21 | 3:C:125:MET:HA | 1.78 | 0.49 |
| 3:C:254:LYS:O | 3:C:256:ALA:N | 2.45 | 0.49 |
| 5:E:55:ARG:O | 5:E:57:MET:N | 2.46 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:4:ILE:O | 7:G:4:ILE:HG22 | 2.12 | 0.49 |
| 7:G:26:LEU:O | 7:G:27:LYS:C | 2.50 | 0.49 |
| 10:J:7:CYS:SG | 10:J:8:PHE:N | 2.85 | 0.49 |
| 11:K:12:LEU:HD12 | 11:K:12:LEU:N | 2.22 | 0.49 |
| 12:L:34:CYS:O | 12:L:36:SER:N | 2.46 | 0.49 |
| 1:A:335:ARG:HH11 | 2:B:1202:LEU:HD13 | 1.76 | 0.49 |
| 1:A:601:LYS:HB2 | 1:A:603:ASN:ND2 | 2.27 | 0.49 |
| 1:A:1370:LEU:O | 1:A:1374:VAL:HG23 | 2.11 | 0.49 |
| 2:B:190:TYR:CE2 | 10:J:62:ARG:HB3 | 2.47 | 0.49 |
| 2:B:973:ILE:HG23 | 2:B:974:PRO:HD2 | 1.95 | 0.49 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:N | 2.57 | 0.49 |
| 3:C:241:ASP:OD1 | 3:C:242:GLN:N | 2.39 | 0.49 |
| 4:D:59:ILE:O | 4:D:60:LYS:C | 2.50 | 0.49 |
| 4:D:176:GLU:HB3 | 4:D:198:LEU:HD21 | 1.94 | 0.49 |
| 6:F:119:ARG:HG3 | 6:F:119:ARG:NH1 | 2.26 | 0.49 |
| 7:G:15:PRO:O | 7:G:16:SER:C | 2.50 | 0.49 |
| 8:H:18:GLY:O | 8:H:19:ARG:HB2 | 2.12 | 0.49 |
| 8:H:123:MET:HE3 | 8:H:142:LEU:CD2 | 2.42 | 0.49 |
| 9:I:84:VAL:HG13 | 9:I:84:VAL:O | 2.13 | 0.49 |
| 12:L:38:LEU:O | 12:L:39:SER:CB | 2.60 | 0.49 |
| 1:A:93:VAL:HG21 | 1:A:301:ALA:O | 2.13 | 0.49 |
| 1:A:224:PHE:CZ | 1:A:234:MET:HE2 | 2.47 | 0.49 |
| 1:A:534:LEU:O | 1:A:534:LEU:HG | 2.11 | 0.49 |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG22 | 1.94 | 0.49 |
| 1:A:1017:LEU:CB | 5:E:205:SER:HA | 2.42 | 0.49 |
| 1:A:1139:GLU:O | 1:A:1275:GLY:HA3 | 2.12 | 0.49 |
| 2:B:294:ASP:O | 2:B:296:GLU:N | 2.43 | 0.49 |
| 2:B:309:GLN:HG3 | 9:I:52:ILE:HD11 | 1.94 | 0.49 |
| 3:C:66:ARG:HH12 | 10:J:2:ILE:HG21 | 1.75 | 0.49 |
| 4:D:156:ASP:C | 4:D:158:GLU:H | 2.15 | 0.49 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CG1 | 2.42 | 0.49 |
| 11:K:21:ILE:HG23 | 11:K:31:VAL:HG11 | 1.95 | 0.49 |
| 15:T:17:DT:H2" | 15:T:18:DT:O5' | 2.12 | 0.49 |
| 1:A:147:VAL:O | 1:A:149:GLU:N | 2.46 | 0.49 |
| 1:A:381:THR:HG23 | 1:A:383:TYR:H | 1.78 | 0.49 |
| 1:A:441:PRO:HD2 | 1:A:498:ARG:CZ | 2.43 | 0.49 |
| 1:A:658:LEU:HD13 | 2:B:831:SER:N | 2.27 | 0.49 |
| 1:A:837:ILE:HA | 1:A:840:ARG:HD3 | 1.95 | 0.49 |
| 1:A:1032:LEU:O | 1:A:1036:ARG:HD3 | 2.12 | 0.49 |
| 1:A:1364:ASN:O | 1:A:1365:TYR:C | 2.51 | 0.49 |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CD | 2.15 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:259:TYR:HD1 | 2:B:259:TYR:H | 1.60 | 0.49 |
| 2:B:995:ARG:NH1 | 3:C:165:LYS:HG2 | 2.27 | 0.49 |
| 2:B:1068:GLY:O | 2:B:1069:PHE:O | 2.31 | 0.49 |
| 3:C:175:ALA:HB3 | 10:J:43:ARG:NH2 | 2.28 | 0.49 |
| 4:D:53:SER:HB3 | 4:D:152:SER:CA | 2.42 | 0.49 |
| 1:A:166:GLY:O | 1:A:167:CYS:CB | 2.60 | 0.49 |
| 1:A:966:ASN:O | 1:A:967:ALA:C | 2.51 | 0.49 |
| 1:A:1029:ARG:HG3 | 1:A:1029:ARG:NH1 | 2.24 | 0.49 |
| 1:A:1342:GLU:OE2 | 5:E:212:ARG:NH1 | 2.45 | 0.49 |
| 2:B:46:GLN:CG | 2:B:47:GLN:H | 2.20 | 0.49 |
| 2:B:472:ALA:C | 2:B:474:SER:H | 2.14 | 0.49 |
| 2:B:758:PHE:N | 2:B:759:PRO:CD | 2.76 | 0.49 |
| 2:B:769:TYR:C | 2:B:771:SER:H | 2.16 | 0.49 |
| 2:B:1010:LEU:HD23 | 2:B:1092:TYR:CD1 | 2.47 | 0.49 |
| 2:B:1084:GLN:N | 2:B:1084:GLN:HE21 | 2.10 | 0.49 |
| 3:C:129:ILE:HG23 | 3:C:130:GLY:N | 2.26 | 0.49 |
| 3:C:161:LYS:O | 3:C:170:TRP:NE1 | 2.46 | 0.49 |
| 3:C:254:LYS:C | 3:C:256:ALA:H | 2.16 | 0.49 |
| 1:A:50:ILE:C | 1:A:52:GLY:N | 2.65 | 0.49 |
| 1:A:50:ILE:O | 1:A:52:GLY:N | 2.45 | 0.49 |
| 1:A:401:GLY:C | 1:A:435:HIS:CD2 | 2.86 | 0.49 |
| 1:A:699:ALA:O | 1:A:700:ASN:CB | 2.60 | 0.49 |
| 1:A:894:GLU:HG3 | 1:A:933:TYR:OH | 2.12 | 0.49 |
| 1:A:1334:ASP:O | 1:A:1336:MET:N | 2.46 | 0.49 |
| 1:A:1389:PHE:CD1 | 1:A:1390:ASN:N | 2.81 | 0.49 |
| 1:A:1446:ASP:HB2 | 6:F:133:VAL:CG2 | 2.43 | 0.49 |
| 2:B:23:ALA:H | 2:B:654:ARG:HB3 | 1.78 | 0.49 |
| 2:B:180:TYR:CD1 | 2:B:180:TYR:N | 2.81 | 0.49 |
| 2:B:801:LYS:O | 10:J:52:THR:HG23 | 2.13 | 0.49 |
| 2:B:843:GLN:O | 2:B:844:SER:C | 2.50 | 0.49 |
| 2:B:843:GLN:O | 2:B:846:ILE:N | 2.45 | 0.49 |
| 2:B:910:VAL:HG12 | 2:B:911:ILE:N | 2.28 | 0.49 |
| 3:C:191:TYR:CD2 | 3:C:201:TRP:CD1 | 3.01 | 0.49 |
| 3:C:208:GLU:C | 3:C:210:GLU:H | 2.15 | 0.49 |
| 4:D:135:GLY:C | 4:D:137:ASN:H | 2.15 | 0.49 |
| 10:J:27:GLU:O | 10:J:29:GLU:N | 2.40 | 0.49 |
| 1:A:18:GLN:HB3 | 2:B:1215:ARG:HG3 | 1.94 | 0.49 |
| 1:A:577:ILE:HG13 | 1:A:578:LEU:N | 2.27 | 0.49 |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG21 | 1.95 | 0.49 |
| 1:A:1329:THR:H | 1:A:1335:ILE:HD11 | 1.78 | 0.49 |
| 2:B:222:ILE:O | 2:B:240:ILE:HA | 2.13 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:386:LEU:O | 2:B:387:LEU:C | 2.50 | 0.49 |
| 2:B:1084:GLN:OE1 | 3:C:189:THR:CG2 | 2.61 | 0.49 |
| 2:B:1142:GLY:HA3 | 6:F:88:TYR:HE2 | 1.77 | 0.49 |
| 2:B:1214:PRO:O | 2:B:1214:PRO:HG2 | 2.13 | 0.49 |
| 4:D:173:HIS:ND1 | 4:D:174:PRO:HD2 | 2.28 | 0.49 |
| 5:E:124:VAL:HG13 | 5:E:132:ILE:CB | 2.41 | 0.49 |
| 11:K:52:ASN:O | 11:K:53:ASP:C | 2.51 | 0.49 |
| 1:A:862:ASN:O | 1:A:864:ILE:HG13 | 2.12 | 0.48 |
| 1:A:958:VAL:HG22 | 1:A:1052:GLN:HB3 | 1.95 | 0.48 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:HD13 | 1.95 | 0.48 |
| 2:B:167:ILE:HG22 | 2:B:453:ILE:CD1 | 2.42 | 0.48 |
| 2:B:763:GLN:HG2 | 2:B:765:PRO:HD2 | 1.94 | 0.48 |
| 2:B:863:GLU:O | 2:B:961:LEU:HD22 | 2.12 | 0.48 |
| 3:C:35:ARG:HH11 | 11:K:41:THR:N | 2.10 | 0.48 |
| 3:C:245:VAL:HA | 3:C:248:ILE:HD12 | 1.94 | 0.48 |
| 5:E:136:ASN:OD1 | 5:E:137:GLU:N | 2.46 | 0.48 |
| 9:I:60:GLN:NE2 | 9:I:107:SER:OG | 2.46 | 0.48 |
| 12:L:31:CYS:SG | 12:L:34:CYS:N | 2.84 | 0.48 |
| 1:A:388:LEU:CD2 | 1:A:432:VAL:HB | 2.43 | 0.48 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:H | 1.78 | 0.48 |
| 1:A:961:ARG:HG2 | 1:A:965:GLN:HE21 | 1.78 | 0.48 |
| 1:A:993:LEU:HD23 | 1:A:1022:LEU:HD21 | 1.95 | 0.48 |
| 1:A:1115:SER:HB3 | 1:A:1330:ASN:HD21 | 1.78 | 0.48 |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:CD1 | 2.43 | 0.48 |
| 1:A:1349:TYR:CA | 1:A:1372:VAL:HG21 | 2.43 | 0.48 |
| 2:B:33:VAL:O | 2:B:36:ALA:HB3 | 2.13 | 0.48 |
| 2:B:203:PHE:N | 2:B:203:PHE:CD1 | 2.81 | 0.48 |
| 2:B:344:LYS:O | 2:B:345:LYS:HG3 | 2.13 | 0.48 |
| 2:B:799:PRO:CB | 2:B:818:PRO:HG2 | 2.43 | 0.48 |
| 2:B:978:ASP:O | 2:B:989:THR:HB | 2.12 | 0.48 |
| 2:B:1070:GLU:OE1 | 10:J:44:TYR:OH | 2.30 | 0.48 |
| 2:B:1095:LEU:H | 2:B:1095:LEU:CD1 | 2.16 | 0.48 |
| 2:B:1182:CYS:O | 2:B:1183:LYS:C | 2.51 | 0.48 |
| 3:C:45:ALA:HA | 3:C:72:LEU:HD12 | 1.94 | 0.48 |
| 5:E:10:SER:O | 5:E:14:ARG:HG3 | 2.11 | 0.48 |
| 5:E:124:VAL:HA | 5:E:132:ILE:HD12 | 1.95 | 0.48 |
| 9:I:69:PRO:HB2 | 9:I:85:PHE:CE2 | 2.48 | 0.48 |
| 1:A:35:ILE:CD1 | 1:A:241:VAL:HG11 | 2.42 | 0.48 |
| 1:A:300:VAL:O | 1:A:300:VAL:HG12 | 2.11 | 0.48 |
| 1:A:767:GLN:HE21 | 1:A:774:ARG:HB3 | 1.74 | 0.48 |
| 1:A:947:PHE:CD2 | 1:A:954:TRP:CZ2 | 3.02 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1059:HIS:O | 1:A:1060:PRO:C | 2.52 | 0.48 |
| 2:B:254:LEU:HD23 | 2:B:381:MET:HE3 | 1.94 | 0.48 |
| 2:B:343:ILE:HB | 2:B:348:ARG:HG3 | 1.95 | 0.48 |
| 2:B:1156:ASP:HB3 | 2:B:1197:PRO:HA | 1.95 | 0.48 |
| 8:H:11:GLN:O | 8:H:28:ALA:HB1 | 2.13 | 0.48 |
| 10:J:14:VAL:HG12 | 10:J:50:ILE:HD11 | 1.95 | 0.48 |
| 12:L:47:ARG:HH21 | 12:L:54:ARG:NH2 | 2.11 | 0.48 |
| 13:N:5:DA:H2" | 13:N:6:DC:OP2 | 2.12 | 0.48 |
| 1:A:108:MET:SD | 1:A:210:ILE:HD13 | 2.53 | 0.48 |
| 1:A:701:LEU:HD23 | 9:I:115:LYS:HG3 | 1.95 | 0.48 |
| 1:A:718:VAL:O | 1:A:721:PHE:HB2 | 2.12 | 0.48 |
| 1:A:913:LEU:CD1 | 1:A:914:GLU:N | 2.71 | 0.48 |
| 2:B:363:HIS:O | 2:B:364:ILE:CB | 2.55 | 0.48 |
| 2:B:429:PHE:HA | 2:B:432:MET:HE3 | 1.96 | 0.48 |
| 2:B:603:LEU:HB3 | 2:B:609:ILE:HG13 | 1.93 | 0.48 |
| 2:B:604:ARG:O | 2:B:606:LYS:N | 2.46 | 0.48 |
| 2:B:758:PHE:CE2 | 2:B:1044:ALA:CA | 2.92 | 0.48 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:CD | 2.41 | 0.48 |
| 7:G:80:LYS:N | 7:G:80:LYS:CD | 2.73 | 0.48 |
| 7:G:117:GLN:C | 7:G:119:LEU:H | 2.17 | 0.48 |
| 1:A:43:GLU:O | 1:A:44:THR:CB | 2.61 | 0.48 |
| 1:A:936:LEU:O | 1:A:939:ASP:HB2 | 2.13 | 0.48 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H | 1.78 | 0.48 |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:N | 2.76 | 0.48 |
| 2:B:34:ILE:O | 2:B:35:SER:C | 2.52 | 0.48 |
| 2:B:37:PHE:HE1 | 2:B:41:LYS:CD | 2.26 | 0.48 |
| 2:B:810:GLU:HB3 | 2:B:811:TYR:CE1 | 2.48 | 0.48 |
| 2:B:899:ILE:HD13 | 2:B:905:VAL:CG1 | 2.43 | 0.48 |
| 3:C:209:TYR:H | 3:C:209:TYR:HD1 | 1.58 | 0.48 |
| 7:G:20:PRO:CG | 7:G:21:ARG:H | 2.26 | 0.48 |
| 1:A:399:HIS:CB | 1:A:400:PRO:CD | 2.88 | 0.48 |
| 1:A:420:ARG:O | 1:A:421:ALA:C | 2.50 | 0.48 |
| 1:A:446:ARG:HD2 | 1:A:480:ALA:HB2 | 1.95 | 0.48 |
| 1:A:535:THR:HG22 | 1:A:536:LEU:N | 2.27 | 0.48 |
| 1:A:603:ASN:O | 1:A:604:GLY:C | 2.51 | 0.48 |
| 1:A:1225:PHE:CE2 | 1:A:1227:ILE:HD11 | 2.49 | 0.48 |
| 2:B:128:LEU:HB2 | 2:B:168:GLY:O | 2.13 | 0.48 |
| 2:B:197:PHE:HZ | 2:B:816:GLU:HG2 | 1.78 | 0.48 |
| 2:B:769:TYR:O | 2:B:771:SER:N | 2.47 | 0.48 |
| 9:I:71:SER:OG | 9:I:83:ASN:HB2 | 2.13 | 0.48 |
| 1:A:504:LEU:HD12 | 1:A:504:LEU:N | 2.28 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:868:TYR:CE1 | 1:A:1064:VAL:CG1 | 2.84 | 0.48 |
| 1:A:1030:ARG:NH1 | 1:A:1035:TYR:OH | 2.47 | 0.48 |
| 2:B:39:ARG:HG2 | 2:B:39:ARG:NH1 | 2.29 | 0.48 |
| 2:B:213:ILE:O | 2:B:215:GLN:HG2 | 2.13 | 0.48 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:HE1 | 1.78 | 0.48 |
| 2:B:911:ILE:CG2 | 2:B:966:VAL:HG11 | 2.44 | 0.48 |
| 2:B:1001:PHE:CZ | 2:B:1073:TYR:HB2 | 2.49 | 0.48 |
| 3:C:88:CYS:SG | 3:C:91:HIS:HA | 2.53 | 0.48 |
| 3:C:215:GLU:O | 3:C:216:GLY:C | 2.51 | 0.48 |
| 6:F:85:MET:CE | 6:F:93:ILE:HD12 | 2.44 | 0.48 |
| 7:G:20:PRO:HG2 | 7:G:21:ARG:N | 2.28 | 0.48 |
| 8:H:63:LEU:HD22 | 8:H:90:ALA:HB3 | 1.96 | 0.48 |
| 9:I:85:PHE:CD2 | 9:I:85:PHE:N | 2.68 | 0.48 |
| 1:A:701:LEU:HD23 | 9:I:115:LYS:CG | 2.44 | 0.48 |
| 1:A:844:ALA:O | 1:A:845:LEU:HD23 | 2.13 | 0.48 |
| 1:A:852:TYR:HA | 1:A:1060:PRO:HB3 | 1.96 | 0.48 |
| 1:A:863:VAL:HG11 | 1:A:866:PHE:CE2 | 2.49 | 0.48 |
| 1:A:1076:ALA:HA | 1:A:1079:MET:HE2 | 1.95 | 0.48 |
| 1:A:1259:MET:C | 1:A:1261:LYS:H | 2.16 | 0.48 |
| 2:B:683:SER:C | 2:B:685:LEU:H | 2.15 | 0.48 |
| 1:A:71:GLN:C | 1:A:73:GLY:H | 2.16 | 0.48 |
| 1:A:218:ASP:O | 1:A:219:PHE:O | 2.32 | 0.48 |
| 1:A:353:ILE:HB | 1:A:470:LEU:CD2 | 2.43 | 0.48 |
| 1:A:427:GLN:O | 1:A:428:TYR:C | 2.52 | 0.48 |
| 1:A:618:GLU:O | 1:A:619:LYS:C | 2.52 | 0.48 |
| 1:A:666:ILE:HD12 | 1:A:667:GLY:N | 2.25 | 0.48 |
| 1:A:954:TRP:HB3 | 1:A:955:PRO:HD2 | 1.95 | 0.48 |
| 1:A:1036:ARG:HG2 | 1:A:1036:ARG:NH1 | 2.21 | 0.48 |
| 1:A:1373:ASP:O | 1:A:1376:THR:HG23 | 2.14 | 0.48 |
| 2:B:175:ARG:HG2 | 2:B:175:ARG:NH1 | 2.27 | 0.48 |
| 2:B:575:PRO:HG2 | 2:B:576:ASP:H | 1.79 | 0.48 |
| 2:B:970:THR:HG22 | 2:B:971:THR:N | 2.28 | 0.48 |
| 3:C:82:TYR:O | 3:C:83:SER:C | 2.51 | 0.48 |
| 7:G:122:ASN:ND2 | 7:G:125:SER:HB3 | 2.29 | 0.48 |
| 11:K:110:ASN:C | 11:K:111:LEU:HG | 2.34 | 0.48 |
| 1:A:21:LEU:HG | 1:A:1413:GLY:O | 2.14 | 0.48 |
| 1:A:130:ASP:O | 1:A:133:LYS:N | 2.38 | 0.48 |
| 1:A:1325:THR:O | 1:A:1325:THR:CG2 | 2.61 | 0.48 |
| 1:A:1387:HIS:CE1 | 13:N:4:DT:H5" | 2.48 | 0.48 |
| 1:A:1445:ILE:N | 1:A:1445:ILE:CD1 | 2.68 | 0.48 |
| 1:A:1446:ASP:HB2 | 6:F:133:VAL:HG23 | 1.96 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:236:HIS:CE1 | 2:B:389:ALA:HA | 2.48 | 0.48 |
| 2:B:259:TYR:N | 2:B:259:TYR:CD1 | 2.82 | 0.48 |
| 2:B:446:LEU:O | 2:B:447:ALA:CB | 2.62 | 0.48 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:HG23 | 2.49 | 0.48 |
| 2:B:653:VAL:HG22 | 2:B:689:LEU:HD13 | 1.95 | 0.48 |
| 2:B:899:ILE:HD12 | 2:B:911:ILE:HG23 | 1.95 | 0.48 |
| 2:B:992:ILE:HD11 | 11:K:66:PRO:HB2 | 1.96 | 0.48 |
| 3:C:235:VAL:HG13 | 10:J:13:VAL:HG23 | 1.95 | 0.48 |
| 5:E:161:LYS:HD2 | 5:E:195:VAL:HG23 | 1.95 | 0.48 |
| 5:E:180:ARG:NH2 | 5:E:192:ARG:HB2 | 2.25 | 0.48 |
| 8:H:111:LEU:HD23 | 8:H:127:GLY:O | 2.14 | 0.48 |
| 10:J:23:ASN:O | 10:J:25:LEU:N | 2.47 | 0.48 |
| 1:A:541:ILE:HD13 | 1:A:549:MET:HE3 | 1.93 | 0.47 |
| 1:A:789:LYS:HE3 | 9:I:67:THR:OG1 | 2.14 | 0.47 |
| 1:A:1377:THR:O | 1:A:1378:GLN:C | 2.52 | 0.47 |
| 1:A:1377:THR:HA | 5:E:212:ARG:HH21 | 1.79 | 0.47 |
| 1:A:1397:LEU:O | 1:A:1400:CYS:HB3 | 2.13 | 0.47 |
| 2:B:30:SER:HB3 | 2:B:743:ILE:O | 2.14 | 0.47 |
| 2:B:247:GLY:C | 2:B:249:ARG:N | 2.67 | 0.47 |
| 2:B:310:MET:O | 2:B:313:MET:HB2 | 2.14 | 0.47 |
| 2:B:579:ARG:N | 2:B:589:VAL:HG13 | 2.29 | 0.47 |
| 2:B:1047:PHE:CD1 | 2:B:1047:PHE:N | 2.76 | 0.47 |
| 2:B:1099:VAL:HG12 | 2:B:1100:ASP:H | 1.79 | 0.47 |
| 3:C:29:MET:HE1 | 11:K:98:LEU:HG | 1.95 | 0.47 |
| 3:C:31:ASN:O | 3:C:34:ARG:HB3 | 2.14 | 0.47 |
| 7:G:35:GLU:CG | 7:G:48:VAL:HG23 | 2.44 | 0.47 |
| 11:K:19:LEU:HD22 | 11:K:33:ILE:CG2 | 2.43 | 0.47 |
| 1:A:224:PHE:CE2 | 1:A:231:PRO:HA | 2.49 | 0.47 |
| 1:A:401:GLY:C | 1:A:435:HIS:HD2 | 2.16 | 0.47 |
| 1:A:466:SER:HB2 | 2:B:1099:VAL:HG11 | 1.96 | 0.47 |
| 1:A:600:PRO:C | 1:A:602:ASP:H | 2.16 | 0.47 |
| 2:B:118:ARG:HG2 | 2:B:204:ILE:HD13 | 1.94 | 0.47 |
| 2:B:185:THR:O | 2:B:188:ASP:HB2 | 2.13 | 0.47 |
| 2:B:205:ILE:N | 2:B:205:ILE:HD12 | 2.28 | 0.47 |
| 2:B:459:TYR:C | 2:B:459:TYR:CD2 | 2.88 | 0.47 |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:H | 1.79 | 0.47 |
| 3:C:31:ASN:O | 3:C:32:SER:C | 2.51 | 0.47 |
| 3:C:114:TYR:CD2 | 3:C:140:ASN:HB2 | 2.49 | 0.47 |
| 1:A:381:THR:HG23 | 1:A:382:PRO:HD2 | 1.95 | 0.47 |
| 1:A:399:HIS:CG | 1:A:400:PRO:N | 2.81 | 0.47 |
| 1:A:722:LEU:O | 1:A:725:ALA:HB3 | 2.14 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:100:PRO:HD3 | 2:B:172:ILE:HD12 | 1.96 | 0.47 |
| 2:B:197:PHE:CZ | 2:B:816:GLU:HG2 | 2.49 | 0.47 |
| 2:B:882:THR:CB | 2:B:934:LYS:O | 2.62 | 0.47 |
| 2:B:1031:LEU:HA | 2:B:1055:ILE:HD13 | 1.96 | 0.47 |
| 2:B:1033:LYS:CE | 2:B:1070:GLU:OE1 | 2.62 | 0.47 |
| 2:B:1147:LEU:C | 2:B:1147:LEU:HD23 | 2.35 | 0.47 |
| 3:C:36:VAL:HG11 | 3:C:251:LEU:HB2 | 1.96 | 0.47 |
| 3:C:177:GLU:HB2 | 3:C:231:ASN:HB3 | 1.95 | 0.47 |
| 3:C:242:GLN:C | 3:C:244:VAL:H | 2.16 | 0.47 |
| 7:G:25:TYR:O | 7:G:28:THR:HB | 2.14 | 0.47 |
| 7:G:115:MET:CB | 7:G:116:PRO:HD2 | 2.44 | 0.47 |
| 7:G:154:VAL:HG12 | 7:G:155:SER:H | 1.79 | 0.47 |
| 8:H:26:ILE:CG2 | 8:H:27:GLU:N | 2.77 | 0.47 |
| 8:H:31:THR:O | 8:H:31:THR:HG22 | 2.13 | 0.47 |
| 1:A:325:ILE:O | 1:A:326:ARG:C | 2.52 | 0.47 |
| 1:A:500:GLU:O | 1:A:504:LEU:HD13 | 2.14 | 0.47 |
| 1:A:735:VAL:O | 1:A:735:VAL:HG12 | 2.14 | 0.47 |
| 1:A:770:VAL:HA | 1:A:822:GLU:OE1 | 2.14 | 0.47 |
| 2:B:298:LEU:N | 2:B:298:LEU:CD2 | 2.77 | 0.47 |
| 2:B:696:GLU:O | 2:B:699:GLU:HB2 | 2.14 | 0.47 |
| 2:B:1099:VAL:HG13 | 2:B:1100:ASP:N | 2.27 | 0.47 |
| 2:B:1110:PRO:HB2 | 2:B:1119:VAL:HG21 | 1.96 | 0.47 |
| 2:B:1162:ILE:C | 2:B:1171:VAL:HG21 | 2.34 | 0.47 |
| 3:C:242:GLN:HB3 | 3:C:246:ARG:HG3 | 1.97 | 0.47 |
| 3:C:254:LYS:C | 3:C:256:ALA:N | 2.67 | 0.47 |
| 7:G:34:VAL:HG12 | 7:G:45:ILE:CG2 | 2.39 | 0.47 |
| 11:K:40:HIS:O | 11:K:41:THR:C | 2.53 | 0.47 |
| 1:A:326:ARG:HG2 | 1:A:327:ALA:N | 2.30 | 0.47 |
| 1:A:567:LYS:NZ | 8:H:46:LEU:HB2 | 2.30 | 0.47 |
| 1:A:921:GLY:O | 1:A:922:ASP:C | 2.52 | 0.47 |
| 1:A:1111:MET:HE1 | 1:A:1330:ASN:OD1 | 2.13 | 0.47 |
| 2:B:579:ARG:HG2 | 2:B:579:ARG:NH1 | 2.29 | 0.47 |
| 2:B:841:MET:SD | 2:B:846:ILE:HD11 | 2.54 | 0.47 |
| 14:P:7:A:C2' | 14:P:8:G:O4' | 2.62 | 0.47 |
| 1:A:88:LYS:HE3 | 1:A:280:GLU:OE2 | 2.15 | 0.47 |
| 1:A:331:GLY:O | 1:A:332:LYS:HB3 | 2.15 | 0.47 |
| 1:A:369:SER:HB2 | 11:K:2:ASN:OD1 | 2.15 | 0.47 |
| 1:A:867:ILE:HG22 | 1:A:872:GLY:H | 1.79 | 0.47 |
| 1:A:1166:ASP:OD2 | 1:A:1239:ARG:HD2 | 2.14 | 0.47 |
| 1:A:1356:ILE:HG22 | 1:A:1356:ILE:O | 2.14 | 0.47 |
| 2:B:115:GLN:HG2 | 2:B:193:LYS:HB2 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:386:LEU:O | 2:B:389:ALA:N | 2.47 | 0.47 |
| 2:B:794:ASN:C | 2:B:795:ILE:HD12 | 2.35 | 0.47 |
| 2:B:1064:TYR:O | 2:B:1065:GLN:C | 2.53 | 0.47 |
| 6:F:135:ARG:HD3 | 6:F:143:PHE:CD2 | 2.50 | 0.47 |
| 7:G:3:PHE:CG | 7:G:80:LYS:NZ | 2.73 | 0.47 |
| 8:H:142:LEU:C | 8:H:143:LEU:HD12 | 2.35 | 0.47 |
| 9:I:33:SER:O | 9:I:34:TYR:O | 2.32 | 0.47 |
| 10:J:36:LEU:HD12 | 10:J:47:ARG:NH1 | 2.30 | 0.47 |
| 12:L:30:ILE:HG22 | 12:L:31:CYS:N | 2.29 | 0.47 |
| 12:L:61:THR:HG22 | 12:L:63:ARG:HG2 | 1.96 | 0.47 |
| 1:A:41:MET:HB3 | 1:A:48:ALA:O | 2.15 | 0.47 |
| 1:A:243:PRO:O | 1:A:244:PRO:C | 2.53 | 0.47 |
| 1:A:298:PHE:O | 1:A:301:ALA:HB3 | 2.13 | 0.47 |
| 1:A:339:ASN:O | 1:A:343:LYS:HG2 | 2.14 | 0.47 |
| 1:A:350:ARG:HH11 | 1:A:350:ARG:HG3 | 1.79 | 0.47 |
| 1:A:402:ALA:CB | 1:A:434:ARG:HA | 2.45 | 0.47 |
| 1:A:504:LEU:HD11 | 6:F:91:ALA:HB1 | 1.95 | 0.47 |
| 1:A:565:ILE:O | 1:A:570:PRO:HA | 2.14 | 0.47 |
| 1:A:829:VAL:C | 1:A:831:THR:N | 2.68 | 0.47 |
| 1:A:888:GLY:O | 1:A:940:ARG:NH2 | 2.48 | 0.47 |
| 1:A:899:VAL:HB | 1:A:929:LEU:HD11 | 1.97 | 0.47 |
| 1:A:982:THR:H | 1:A:985:ASP:CB | 2.27 | 0.47 |
| 1:A:1144:LYS:HB2 | 1:A:1268:LEU:O | 2.13 | 0.47 |
| 1:A:1151:GLU:HB3 | 1:A:1153:TYR:HE1 | 1.79 | 0.47 |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:CB | 2.45 | 0.47 |
| 2:B:37:PHE:CD2 | 2:B:542:MET:SD | 3.08 | 0.47 |
| 2:B:168:GLY:HA2 | 2:B:454:THR:OG1 | 2.15 | 0.47 |
| 2:B:653:VAL:HG23 | 2:B:689:LEU:HB3 | 1.97 | 0.47 |
| 2:B:757:PRO:HG3 | 2:B:1028:GLU:OE2 | 2.14 | 0.47 |
| 2:B:839:MET:HB3 | 2:B:1012:ILE:HG22 | 1.96 | 0.47 |
| 2:B:950:ASP:O | 2:B:951:GLN:HB2 | 2.15 | 0.47 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:HB2 | 2.30 | 0.47 |
| 4:D:119:ARG:HG2 | 4:D:120:GLU:N | 2.29 | 0.47 |
| 4:D:134:THR:CG2 | 4:D:135:GLY:H | 2.26 | 0.47 |
| 4:D:191:ALA:O | 4:D:193:THR:N | 2.47 | 0.47 |
| 5:E:31:THR:O | 5:E:35:VAL:HG23 | 2.13 | 0.47 |
| 5:E:84:ASP:O | 5:E:86:PRO:HD3 | 2.15 | 0.47 |
| 6:F:88:TYR:N | 6:F:88:TYR:CD1 | 2.83 | 0.47 |
| 8:H:55:LEU:HD22 | 8:H:144:ILE:HG21 | 1.96 | 0.47 |
| 8:H:93:TYR:CD1 | 8:H:93:TYR:N | 2.82 | 0.47 |
| 8:H:128:ASN:O | 8:H:128:ASN:OD1 | 2.32 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:52:ASN:O | 11:K:54:ARG:N | 2.48 | 0.47 |
| 11:K:89:ASN:O | 11:K:92:ASN:N | 2.48 | 0.47 |
| 1:A:37:PHE:N | 1:A:37:PHE:HD1 | 2.13 | 0.47 |
| 1:A:63:ARG:HA | 1:A:74:MET:HE2 | 1.95 | 0.47 |
| 1:A:534:LEU:HD13 | 1:A:656:TRP:CG | 2.50 | 0.47 |
| 1:A:632:VAL:O | 1:A:633:VAL:C | 2.53 | 0.47 |
| 1:A:774:ARG:H | 1:A:774:ARG:HG2 | 1.42 | 0.47 |
| 1:A:1105:LEU:HD22 | 1:A:1384:VAL:HG21 | 1.97 | 0.47 |
| 1:A:1323:ASP:C | 1:A:1325:THR:H | 2.18 | 0.47 |
| 2:B:361:LEU:HD21 | 2:B:377:PHE:HD2 | 1.72 | 0.47 |
| 2:B:949:VAL:HG12 | 2:B:950:ASP:N | 2.29 | 0.47 |
| 4:D:20:GLU:HA | 4:D:20:GLU:OE2 | 2.14 | 0.47 |
| 5:E:175:LEU:HD23 | 5:E:176:PRO:HD2 | 1.95 | 0.47 |
| 7:G:1:MET:SD | 7:G:79:PHE:CE1 | 3.08 | 0.47 |
| 10:J:7:CYS:SG | 10:J:49:MET:HE3 | 2.54 | 0.47 |
| 11:K:12:LEU:H | 11:K:12:LEU:CD1 | 2.24 | 0.47 |
| 12:L:60:ARG:HG2 | 12:L:61:THR:H | 1.80 | 0.47 |
| 1:A:42:ASP:HA | 1:A:46:THR:O | 2.15 | 0.47 |
| 1:A:853:ASP:O | 1:A:854:ASN:HB2 | 2.15 | 0.47 |
| 1:A:901:LEU:N | 1:A:926:GLN:HE21 | 2.08 | 0.47 |
| 2:B:431:TYR:CE2 | 2:B:447:ALA:HB2 | 2.50 | 0.47 |
| 2:B:582:VAL:HA | 2:B:626:ILE:O | 2.15 | 0.47 |
| 2:B:730:ARG:O | 2:B:731:VAL:O | 2.33 | 0.47 |
| 2:B:758:PHE:HB3 | 2:B:761:HIS:CD2 | 2.50 | 0.47 |
| 2:B:983:ARG:HH11 | 2:B:1091:TYR:HB3 | 1.80 | 0.47 |
| 2:B:1107:ALA:O | 2:B:1108:ARG:HG2 | 2.15 | 0.47 |
| 3:C:168:ALA:O | 3:C:170:TRP:N | 2.48 | 0.47 |
| 7:G:25:TYR:HE2 | 7:G:29:LYS:HD2 | 1.80 | 0.47 |
| 11:K:101:LEU:O | 11:K:101:LEU:HD23 | 2.15 | 0.47 |
| 1:A:43:GLU:O | 1:A:44:THR:HB | 2.15 | 0.47 |
| 1:A:236:LEU:HD11 | 1:A:304:MET:HE1 | 1.96 | 0.47 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:NE1 | 2.30 | 0.47 |
| 1:A:588:LEU:O | 1:A:606:LEU:HD12 | 2.14 | 0.47 |
| 1:A:1280:GLU:O | 1:A:1281:ARG:O | 2.33 | 0.47 |
| 1:A:1410:PHE:HD2 | 2:B:1212:ILE:HD12 | 1.80 | 0.47 |
| 2:B:37:PHE:CE1 | 2:B:41:LYS:HG3 | 2.51 | 0.47 |
| 2:B:388:CYS:C | 2:B:390:LEU:N | 2.67 | 0.47 |
| 2:B:461:LEU:N | 2:B:461:LEU:HD12 | 2.29 | 0.47 |
| 5:E:205:SER:O | 5:E:206:GLY:C | 2.52 | 0.47 |
| 7:G:23:LYS:HG3 | 7:G:56:ILE:HD12 | 1.96 | 0.47 |
| 11:K:111:LEU:O | 11:K:112:GLN:CG | 2.62 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:278:THR:O | 1:A:278:THR:HG22 | 2.15 | 0.46 |
| 1:A:698:GLN:HA | 9:I:97:MET:O | 2.14 | 0.46 |
| 2:B:118:ARG:HH11 | 2:B:204:ILE:HD11 | 1.80 | 0.46 |
| 2:B:640:VAL:O | 2:B:640:VAL:HG12 | 2.16 | 0.46 |
| 2:B:999:MET:HA | 2:B:999:MET:CE | 2.45 | 0.46 |
| 3:C:146:LYS:C | 3:C:147:LEU:HD23 | 2.36 | 0.46 |
| 3:C:256:ALA:C | 3:C:258:ILE:N | 2.68 | 0.46 |
| 4:D:7:THR:HG21 | 4:D:32:GLU:OE2 | 2.15 | 0.46 |
| 4:D:48:ILE:CG2 | 7:G:4:ILE:HB | 2.45 | 0.46 |
| 7:G:39:THR:CG2 | 7:G:40:GLY:H | 2.26 | 0.46 |
| 8:H:42:ILE:O | 8:H:44:VAL:HG23 | 2.15 | 0.46 |
| 1:A:224:PHE:HZ | 1:A:234:MET:CE | 2.27 | 0.46 |
| 1:A:253:ASN:HB3 | 2:B:935:ARG:NH1 | 2.30 | 0.46 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:CG | 2.41 | 0.46 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CE1 | 2.50 | 0.46 |
| 1:A:586:ILE:CD1 | 1:A:633:VAL:HG22 | 2.45 | 0.46 |
| 1:A:1027:ALA:O | 1:A:1031:VAL:HG23 | 2.15 | 0.46 |
| 1:A:1072:ILE:HD11 | 1:A:1368:MET:HA | 1.98 | 0.46 |
| 2:B:212:LEU:HD23 | 2:B:480:SER:HB2 | 1.97 | 0.46 |
| 2:B:823:ALA:O | 2:B:825:VAL:N | 2.48 | 0.46 |
| 2:B:865:LYS:HE2 | 2:B:871:THR:OG1 | 2.15 | 0.46 |
| 2:B:1109:GLY:O | 2:B:1110:PRO:C | 2.54 | 0.46 |
| 2:B:1115:THR:CG2 | 2:B:1117:GLN:HG3 | 2.45 | 0.46 |
| 6:F:123:LYS:O | 6:F:124:GLU:C | 2.54 | 0.46 |
| 8:H:4:THR:HG22 | 8:H:5:LEU:N | 2.29 | 0.46 |
| 10:J:16:ASP:O | 10:J:18:TRP:N | 2.48 | 0.46 |
| 11:K:42:LEU:HD21 | 11:K:46:ILE:HD11 | 1.96 | 0.46 |
| 15:T:11:DG:H2" | 15:T:12:DT:OP2 | 2.15 | 0.46 |
| 1:A:224:PHE:CE2 | 1:A:231:PRO:HG3 | 2.50 | 0.46 |
| 1:A:289:ILE:C | 1:A:291:GLU:N | 2.68 | 0.46 |
| 1:A:343:LYS:NZ | 2:B:1151:LEU:O | 2.40 | 0.46 |
| 1:A:438:ASP:OD1 | 1:A:461:LYS:HA | 2.15 | 0.46 |
| 1:A:634:THR:HG1 | 1:A:642:CYS:HG | 1.63 | 0.46 |
| 1:A:967:ALA:O | 1:A:968:GLN:O | 2.33 | 0.46 |
| 1:A:1175:SER:O | 1:A:1176:LEU:HB2 | 2.15 | 0.46 |
| 1:A:1193:LEU:HD22 | 1:A:1260:LEU:HD11 | 1.97 | 0.46 |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HD11 | 1.96 | 0.46 |
| 1:A:1239:ARG:NH1 | 1:A:1239:ARG:HB3 | 2.30 | 0.46 |
| 2:B:185:THR:N | 2:B:188:ASP:HB2 | 2.27 | 0.46 |
| 2:B:230:ALA:N | 2:B:231:PRO:CD | 2.78 | 0.46 |
| 2:B:467:GLY:N | 2:B:475:SER:CB | 2.71 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:821:GLN:NE2 | 2:B:851:PHE:HA | 2.23 | 0.46 |
| 2:B:861:ASP:OD1 | 2:B:862:GLN:N | 2.48 | 0.46 |
| 3:C:47:ASP:HA | 3:C:169:LYS:NZ | 2.30 | 0.46 |
| 3:C:141:GLY:HA2 | 10:J:16:ASP:HB3 | 1.97 | 0.46 |
| 4:D:54:GLU:O | 4:D:58:VAL:HG23 | 2.14 | 0.46 |
| 4:D:156:ASP:C | 4:D:158:GLU:N | 2.69 | 0.46 |
| 7:G:1:MET:O | 7:G:1:MET:CE | 2.64 | 0.46 |
| 9:I:98:VAL:HG11 | 9:I:113:ASP:OD1 | 2.15 | 0.46 |
| 1:A:42:ASP:C | 1:A:44:THR:N | 2.68 | 0.46 |
| 1:A:261:ASP:O | 1:A:264:PHE:HB2 | 2.15 | 0.46 |
| 1:A:393:ARG:O | 1:A:395:GLY:N | 2.49 | 0.46 |
| 1:A:499:ALA:O | 1:A:503:GLN:HG2 | 2.15 | 0.46 |
| 1:A:871:ASP:OD2 | 1:A:873:MET:HB2 | 2.15 | 0.46 |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HG13 | 1.97 | 0.46 |
| 2:B:39:ARG:CZ | 2:B:665:GLU:HG2 | 2.45 | 0.46 |
| 2:B:383:ASN:O | 2:B:384:ARG:C | 2.53 | 0.46 |
| 2:B:547:VAL:HG12 | 2:B:612:GLU:OE2 | 2.14 | 0.46 |
| 2:B:683:SER:O | 2:B:685:LEU:N | 2.48 | 0.46 |
| 2:B:990:ILE:CG2 | 2:B:991:GLY:N | 2.78 | 0.46 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:SD | 2.89 | 0.46 |
| 4:D:10:THR:HG23 | 4:D:10:THR:O | 2.16 | 0.46 |
| 4:D:151:PHE:CD1 | 4:D:151:PHE:N | 2.83 | 0.46 |
| 5:E:16:PHE:HZ | 5:E:20:LYS:HE2 | 1.77 | 0.46 |
| 5:E:67:GLU:O | 5:E:70:SER:HB3 | 2.15 | 0.46 |
| 9:I:82:GLU:HB3 | 9:I:104:LEU:HD12 | 1.97 | 0.46 |
| 11:K:10:PHE:CD1 | 11:K:11:LEU:CD2 | 2.99 | 0.46 |
| 1:A:34:LYS:HB3 | 1:A:36:ARG:NE | 2.31 | 0.46 |
| 1:A:114:LEU:O | 1:A:115:LEU:HG | 2.14 | 0.46 |
| 1:A:167:CYS:O | 1:A:167:CYS:SG | 2.73 | 0.46 |
| 1:A:224:PHE:CD2 | 1:A:231:PRO:HG3 | 2.50 | 0.46 |
| 1:A:445:ASN:HB2 | 1:A:455:MET:HG2 | 1.98 | 0.46 |
| 1:A:470:LEU:HD22 | 1:A:487:MET:CE | 2.46 | 0.46 |
| 1:A:637:LYS:CB | 1:A:641:VAL:HG11 | 2.45 | 0.46 |
| 1:A:1111:MET:CE | 1:A:1330:ASN:OD1 | 2.64 | 0.46 |
| 1:A:1118:VAL:HG23 | 1:A:1306:LEU:HB2 | 1.96 | 0.46 |
| 2:B:388:CYS:O | 2:B:390:LEU:N | 2.49 | 0.46 |
| 2:B:520:GLY:N | 2:B:748:ILE:HG22 | 2.29 | 0.46 |
| 2:B:604:ARG:C | 2:B:606:LYS:H | 2.18 | 0.46 |
| 3:C:112:ASN:CB | 3:C:114:TYR:CE1 | 2.98 | 0.46 |
| 3:C:152:GLU:OE2 | 3:C:154:LYS:HE3 | 2.15 | 0.46 |
| 8:H:123:MET:HE3 | 8:H:142:LEU:HD22 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:I:51:ASN:O | 9:I:54:GLU:HG3 | 2.16 | 0.46 |
| 1:A:560:ILE:H | 1:A:560:ILE:HG12 | 1.46 | 0.46 |
| 1:A:767:GLN:HB2 | 1:A:799:PHE:HD1 | 1.80 | 0.46 |
| 1:A:1053:PHE:O | 1:A:1055:ARG:N | 2.49 | 0.46 |
| 2:B:39:ARG:NH2 | 2:B:665:GLU:CG | 2.76 | 0.46 |
| 2:B:95:ILE:CG1 | 2:B:130:VAL:HG22 | 2.46 | 0.46 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:HB2 | 1.97 | 0.46 |
| 2:B:763:GLN:C | 2:B:765:PRO:HD2 | 2.36 | 0.46 |
| 2:B:814:PHE:C | 2:B:816:GLU:N | 2.69 | 0.46 |
| 3:C:87:PHE:CD1 | 3:C:87:PHE:N | 2.84 | 0.46 |
| 3:C:99:LEU:HD12 | 3:C:118:LEU:HB3 | 1.96 | 0.46 |
| 3:C:115:SER:HB3 | 3:C:142:VAL:HB | 1.98 | 0.46 |
| 3:C:168:ALA:C | 3:C:170:TRP:N | 2.68 | 0.46 |
| 3:C:175:ALA:HB3 | 10:J:43:ARG:HH22 | 1.81 | 0.46 |
| 4:D:175:PHE:HZ | 7:G:85:GLU:HG3 | 1.79 | 0.46 |
| 5:E:207:ARG:CB | 5:E:207:ARG:NH1 | 2.78 | 0.46 |
| 7:G:138:THR:CG2 | 7:G:139:ILE:N | 2.68 | 0.46 |
| 11:K:85:ASP:O | 11:K:88:LYS:HB2 | 2.15 | 0.46 |
| 1:A:23:SER:CB | 1:A:233:TRP:NE1 | 2.79 | 0.46 |
| 1:A:34:LYS:NZ | 1:A:57:ARG:CZ | 2.79 | 0.46 |
| 1:A:566:ILE:O | 1:A:567:LYS:O | 2.34 | 0.46 |
| 1:A:826:ASP:O | 1:A:827:THR:C | 2.52 | 0.46 |
| 2:B:244:LEU:C | 2:B:246:LYS:N | 2.68 | 0.46 |
| 2:B:360:PHE:O | 2:B:361:LEU:C | 2.54 | 0.46 |
| 2:B:801:LYS:O | 10:J:52:THR:CG2 | 2.64 | 0.46 |
| 2:B:859:TYR:OH | 2:B:941:LEU:CD1 | 2.60 | 0.46 |
| 3:C:114:TYR:HB3 | 3:C:140:ASN:O | 2.16 | 0.46 |
| 9:I:55:THR:HG22 | 9:I:58:VAL:CG2 | 2.45 | 0.46 |
| 9:I:115:LYS:HD3 | 9:I:117:LYS:CE | 2.38 | 0.46 |
| 10:J:27:GLU:C | 10:J:29:GLU:H | 2.17 | 0.46 |
| 1:A:7:SER:C | 1:A:9:ALA:H | 2.19 | 0.46 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:CG1 | 2.74 | 0.46 |
| 1:A:262:LEU:C | 1:A:264:PHE:N | 2.69 | 0.46 |
| 1:A:652:VAL:O | 1:A:653:VAL:C | 2.55 | 0.46 |
| 1:A:835:GLY:HA3 | 15:T:19:TT:O1P | 2.16 | 0.46 |
| 1:A:1152:ILE:HG13 | 9:I:44:TYR:HD2 | 1.81 | 0.46 |
| 1:A:1385:THR:O | 1:A:1388:GLY:N | 2.46 | 0.46 |
| 1:A:1418:LEU:HD12 | 1:A:1419:ASP:N | 2.30 | 0.46 |
| 2:B:900:ALA:HB3 | 12:L:61:THR:OG1 | 2.15 | 0.46 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:CD1 | 2.43 | 0.46 |
| 4:D:29:LEU:HB3 | 7:G:82:PHE:HE2 | 1.81 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:64:VAL:O | 4:D:66:ARG:N | 2.49 | 0.46 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CD2 | 2.50 | 0.46 |
| 7:G:106:MET:CG | 7:G:107:LYS:N | 2.77 | 0.46 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CZ2 | 2.51 | 0.46 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CE2 | 2.51 | 0.46 |
| 1:A:343:LYS:HZ3 | 2:B:1197:PRO:HB3 | 1.81 | 0.46 |
| 1:A:494:SER:O | 1:A:497:THR:N | 2.49 | 0.46 |
| 1:A:883:LEU:CD2 | 1:A:1021:LEU:HB2 | 2.46 | 0.46 |
| 2:B:1110:PRO:HG3 | 2:B:1125:ASP:HB3 | 1.98 | 0.46 |
| 14:P:8:G:H2' | 14:P:9:A:C8 | 2.51 | 0.46 |
| 1:A:18:GLN:O | 2:B:1215:ARG:HG2 | 2.16 | 0.46 |
| 1:A:241:VAL:HG13 | 1:A:266:LEU:HD13 | 1.97 | 0.46 |
| 1:A:332:LYS:NZ | 15:T:19:TT:H7C2 | 2.31 | 0.46 |
| 1:A:474:VAL:C | 1:A:477:PRO:HD2 | 2.36 | 0.46 |
| 1:A:639:PRO:HG2 | 1:A:640:GLN:H | 1.81 | 0.46 |
| 1:A:818:MET:HA | 2:B:514:LEU:HB3 | 1.98 | 0.46 |
| 1:A:857:ARG:HG2 | 1:A:863:VAL:HA | 1.98 | 0.46 |
| 1:A:1222:ASN:O | 1:A:1223:ASP:HB3 | 2.16 | 0.46 |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB2 | 1.97 | 0.46 |
| 1:A:1445:ILE:HD12 | 7:G:59:GLY:O | 2.15 | 0.46 |
| 2:B:210:LYS:HG3 | 2:B:461:LEU:O | 2.16 | 0.46 |
| 2:B:244:LEU:O | 2:B:246:LYS:N | 2.49 | 0.46 |
| 2:B:510:LYS:CG | 2:B:511:PRO:CD | 2.82 | 0.46 |
| 2:B:1045:SER:O | 2:B:1046:PRO:O | 2.34 | 0.46 |
| 3:C:112:ASN:HB2 | 3:C:114:TYR:HE1 | 1.80 | 0.46 |
| 3:C:186:LEU:HB3 | 3:C:188:HIS:CD2 | 2.51 | 0.46 |
| 8:H:38:LEU:HD13 | 8:H:125:LEU:HD13 | 1.98 | 0.46 |
| 12:L:49:LYS:O | 12:L:50:ASP:CB | 2.63 | 0.46 |
| 1:A:244:PRO:HG2 | 1:A:245:PRO:CD | 2.46 | 0.45 |
| 1:A:514:PRO:CB | 1:A:875:ALA:HB3 | 2.47 | 0.45 |
| 1:A:675:THR:OG1 | 1:A:736:ASN:ND2 | 2.49 | 0.45 |
| 1:A:695:LYS:C | 1:A:697:ALA:N | 2.69 | 0.45 |
| 1:A:846:GLU:OE1 | 1:A:1425:SER:OG | 2.33 | 0.45 |
| 1:A:981:LEU:HD21 | 1:A:1038:THR:C | 2.36 | 0.45 |
| 2:B:37:PHE:HE2 | 2:B:542:MET:HA | 1.81 | 0.45 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:N | 2.30 | 0.45 |
| 3:C:41:ILE:HD11 | 3:C:247:GLY:CA | 2.46 | 0.45 |
| 3:C:44:LEU:HD21 | 3:C:159:ALA:CB | 2.46 | 0.45 |
| 3:C:73:GLN:NE2 | 3:C:74:SER:H | 2.14 | 0.45 |
| 12:L:40:LEU:HB3 | 12:L:41:SER:H | 1.68 | 0.45 |
| 12:L:55:ILE:H | 12:L:55:ILE:HG12 | 1.32 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:409:SER:O | 1:A:410:GLY:C | 2.54 | 0.45 |
| 1:A:800:VAL:HA | 1:A:812:GLU:OE2 | 2.16 | 0.45 |
| 1:A:874:ASP:O | 1:A:876:ALA:N | 2.49 | 0.45 |
| 1:A:1004:ASN:O | 1:A:1008:GLN:HB2 | 2.16 | 0.45 |
| 1:A:1445:ILE:HG12 | 7:G:18:PHE:HE2 | 1.78 | 0.45 |
| 2:B:102:VAL:HG12 | 2:B:104:GLU:HG2 | 1.98 | 0.45 |
| 2:B:240:ILE:HG22 | 2:B:254:LEU:HB3 | 1.97 | 0.45 |
| 2:B:798:TYR:CE2 | 3:C:62:PHE:CZ | 3.04 | 0.45 |
| 2:B:1084:GLN:C | 2:B:1085:ILE:HD12 | 2.37 | 0.45 |
| 3:C:167:HIS:ND1 | 12:L:70:ARG:HB3 | 2.31 | 0.45 |
| 4:D:52:LEU:C | 4:D:54:GLU:N | 2.69 | 0.45 |
| 4:D:119:ARG:HD3 | 4:D:221:TYR:CE2 | 2.51 | 0.45 |
| 7:G:22:MET:O | 7:G:23:LYS:C | 2.54 | 0.45 |
| 7:G:39:THR:O | 7:G:43:GLY:HA2 | 2.15 | 0.45 |
| 14:P:2:C:O2' | 14:P:3:G:H5' | 2.16 | 0.45 |
| 1:A:71:GLN:HG3 | 1:A:72:GLU:N | 2.31 | 0.45 |
| 1:A:332:LYS:C | 1:A:334:GLY:H | 2.20 | 0.45 |
| 1:A:500:GLU:OE2 | 2:B:1145:SER:N | 2.49 | 0.45 |
| 1:A:526:ASP:OD1 | 2:B:1013:ASN:ND2 | 2.48 | 0.45 |
| 1:A:730:GLY:O | 1:A:733:ALA:N | 2.49 | 0.45 |
| 1:A:843:LYS:HD3 | 1:A:846:GLU:OE2 | 2.16 | 0.45 |
| 1:A:1319:VAL:HG13 | 1:A:1320:PRO:HD2 | 1.98 | 0.45 |
| 1:A:1381:LEU:HD23 | 1:A:1381:LEU:HA | 1.77 | 0.45 |
| 2:B:758:PHE:HZ | 2:B:1031:LEU:HD22 | 1.82 | 0.45 |
| 1:A:361:LEU:HA | 1:A:471:ASN:ND2 | 2.31 | 0.45 |
| 1:A:370:ILE:O | 1:A:371:ALA:C | 2.52 | 0.45 |
| 1:A:667:GLY:HA3 | 3:C:192:TRP:CH2 | 2.51 | 0.45 |
| 1:A:915:SER:O | 1:A:919:ILE:HG13 | 2.16 | 0.45 |
| 1:A:963:ILE:HD13 | 1:A:1049:ILE:CG1 | 2.47 | 0.45 |
| 1:A:1021:LEU:O | 1:A:1024:SER:HB3 | 2.16 | 0.45 |
| 1:A:1171:GLN:HA | 1:A:1174:PHE:HD1 | 1.80 | 0.45 |
| 1:A:1394:THR:O | 1:A:1395:GLY:O | 2.34 | 0.45 |
| 2:B:96:TYR:HE1 | 2:B:131:ASP:OD2 | 1.99 | 0.45 |
| 2:B:364:ILE:CG1 | 2:B:585:VAL:HG13 | 2.38 | 0.45 |
| 2:B:570:VAL:HG23 | 2:B:573:GLN:HB3 | 1.97 | 0.45 |
| 2:B:825:VAL:HG21 | 2:B:1092:TYR:HE1 | 1.80 | 0.45 |
| 2:B:1065:GLN:HB2 | 3:C:201:TRP:CZ3 | 2.51 | 0.45 |
| 2:B:1184:GLY:C | 2:B:1186:ASP:H | 2.16 | 0.45 |
| 3:C:184:ASN:HD21 | 3:C:187:LYS:HA | 1.80 | 0.45 |
| 9:I:29:CYS:SG | 9:I:31:THR:N | 2.86 | 0.45 |
| 10:J:45:CYS:O | 10:J:48:ARG:HG3 | 2.17 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:N:6:DC:H1' | 13:N:7:DT:H5' | 1.97 | 0.45 |
| 1:A:396:PRO:HG3 | 1:A:416:ARG:HB3 | 1.97 | 0.45 |
| 1:A:885:THR:O | 1:A:885:THR:HG22 | 2.16 | 0.45 |
| 1:A:1111:MET:HE3 | 1:A:1113:THR:O | 2.16 | 0.45 |
| 2:B:833:TYR:CZ | 11:K:66:PRO:HG3 | 2.51 | 0.45 |
| 2:B:1182:CYS:O | 2:B:1183:LYS:O | 2.35 | 0.45 |
| 3:C:22:LEU:HD13 | 3:C:230:MET:HE1 | 1.99 | 0.45 |
| 3:C:113:VAL:CG2 | 3:C:147:LEU:HD21 | 2.47 | 0.45 |
| 3:C:242:GLN:C | 3:C:244:VAL:N | 2.70 | 0.45 |
| 4:D:29:LEU:HB3 | 7:G:82:PHE:CE2 | 2.52 | 0.45 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CB | 2.47 | 0.45 |
| 8:H:40:LEU:HB2 | 8:H:123:MET:HG3 | 1.99 | 0.45 |
| 11:K:11:LEU:HD22 | 11:K:11:LEU:N | 2.32 | 0.45 |
| 11:K:65:HIS:CG | 11:K:66:PRO:HD2 | 2.51 | 0.45 |
| 12:L:27:LEU:HD23 | 12:L:27:LEU:N | 2.32 | 0.45 |
| 1:A:11:LEU:HB2 | 2:B:1193:GLN:OE1 | 2.16 | 0.45 |
| 1:A:32:VAL:HG21 | 1:A:68:GLN:NE2 | 2.32 | 0.45 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CD2 | 2.52 | 0.45 |
| 1:A:381:THR:HG23 | 1:A:382:PRO:CD | 2.47 | 0.45 |
| 1:A:898:ARG:O | 1:A:1029:ARG:NH1 | 2.50 | 0.45 |
| 2:B:502:ILE:CD1 | 2:B:502:ILE:N | 2.78 | 0.45 |
| 2:B:854:LEU:HB3 | 2:B:856:PHE:HE1 | 1.80 | 0.45 |
| 3:C:20:PHE:HE1 | 3:C:22:LEU:CD1 | 2.30 | 0.45 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:CG | 2.79 | 0.45 |
| 3:C:176:ILE:CG2 | 3:C:177:GLU:N | 2.79 | 0.45 |
| 3:C:190:ASP:O | 3:C:191:TYR:C | 2.55 | 0.45 |
| 3:C:191:TYR:HD2 | 3:C:201:TRP:CD1 | 2.34 | 0.45 |
| 5:E:167:ARG:HA | 5:E:167:ARG:HD3 | 1.84 | 0.45 |
| 8:H:99:GLY:HA3 | 8:H:117:SER:O | 2.17 | 0.45 |
| 10:J:43:ARG:O | 10:J:47:ARG:HB2 | 2.17 | 0.45 |
| 1:A:19:PHE:HE1 | 1:A:1396:ALA:HB3 | 1.82 | 0.45 |
| 1:A:23:SER:O | 1:A:26:GLU:N | 2.49 | 0.45 |
| 1:A:1064:VAL:O | 1:A:1064:VAL:HG12 | 2.16 | 0.45 |
| 2:B:58:THR:O | 2:B:62:ILE:HG13 | 2.17 | 0.45 |
| 2:B:282:ILE:HD12 | 2:B:382:ILE:HD13 | 1.99 | 0.45 |
| 2:B:999:MET:HE2 | 2:B:1000:PRO:CD | 2.47 | 0.45 |
| 2:B:1060:ARG:C | 2:B:1062:HIS:H | 2.19 | 0.45 |
| 8:H:4:THR:HG22 | 8:H:5:LEU:H | 1.81 | 0.45 |
| 9:I:69:PRO:HG2 | 9:I:85:PHE:CD2 | 2.52 | 0.45 |
| 11:K:15:GLY:O | 11:K:16:GLU:HG3 | 2.17 | 0.45 |
| 1:A:166:GLY:O | 1:A:167:CYS:SG | 2.74 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:244:PRO:CG | 1:A:245:PRO:HD3 | 2.47 | 0.45 |
| 2:B:223:VAL:HG21 | 2:B:380:TYR:CE2 | 2.51 | 0.45 |
| 2:B:704:ALA:HB2 | 2:B:738:PHE:CD2 | 2.52 | 0.45 |
| 2:B:800:GLN:O | 2:B:801:LYS:C | 2.55 | 0.45 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:CD2 | 2.44 | 0.45 |
| 2:B:860:MET:CG | 2:B:861:ASP:N | 2.80 | 0.45 |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:CZ | 2.51 | 0.45 |
| 2:B:1031:LEU:HD11 | 2:B:1042:GLY:HA3 | 1.99 | 0.45 |
| 3:C:99:LEU:HD23 | 3:C:99:LEU:N | 2.32 | 0.45 |
| 5:E:124:VAL:HB | 5:E:125:PRO:CD | 2.47 | 0.45 |
| 12:L:36:SER:O | 12:L:37:LYS:C | 2.54 | 0.45 |
| 1:A:120:GLU:HA | 1:A:123:ARG:HG3 | 1.99 | 0.45 |
| 1:A:185:TRP:CZ3 | 1:A:200:ARG:HG2 | 2.52 | 0.45 |
| 1:A:482:PHE:O | 1:A:484:GLY:N | 2.49 | 0.45 |
| 1:A:508:PRO:O | 1:A:511:ILE:HG13 | 2.16 | 0.45 |
| 1:A:549:MET:SD | 1:A:577:ILE:CD1 | 3.04 | 0.45 |
| 1:A:666:ILE:CD1 | 1:A:667:GLY:N | 2.80 | 0.45 |
| 1:A:1146:VAL:HG11 | 1:A:1207:LEU:HD12 | 1.99 | 0.45 |
| 1:A:1211:GLN:O | 1:A:1212:VAL:C | 2.55 | 0.45 |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:HE22 | 1.81 | 0.45 |
| 2:B:360:PHE:CD2 | 2:B:361:LEU:HB2 | 2.51 | 0.45 |
| 2:B:582:VAL:HG12 | 2:B:587:HIS:NE2 | 2.32 | 0.45 |
| 2:B:802:PRO:HB3 | 2:B:1091:TYR:CD2 | 2.51 | 0.45 |
| 2:B:911:ILE:O | 2:B:911:ILE:HG22 | 2.17 | 0.45 |
| 2:B:954:VAL:HA | 2:B:964:VAL:HG22 | 1.98 | 0.45 |
| 5:E:60:PHE:CE2 | 5:E:80:VAL:HB | 2.51 | 0.45 |
| 9:I:34:TYR:O | 9:I:35:VAL:HG23 | 2.17 | 0.45 |
| 9:I:70:ARG:HH11 | 9:I:84:VAL:HB | 1.81 | 0.45 |
| 11:K:82:ASP:O | 11:K:85:ASP:HB2 | 2.17 | 0.45 |
| 12:L:28:LYS:HB2 | 12:L:39:SER:HB2 | 1.99 | 0.45 |
| 1:A:313:GLN:O | 1:A:314:ALA:HB3 | 2.17 | 0.45 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CE2 | 2.52 | 0.45 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:CD | 2.38 | 0.45 |
| 1:A:710:LEU:HD13 | 9:I:94:ASP:O | 2.16 | 0.45 |
| 1:A:1220:PHE:O | 1:A:1221:LYS:HB2 | 2.17 | 0.45 |
| 1:A:1333:ILE:HG22 | 1:A:1334:ASP:N | 2.32 | 0.45 |
| 2:B:19:GLU:O | 2:B:20:ASP:C | 2.55 | 0.45 |
| 2:B:405:ARG:HA | 2:B:631:GLY:O | 2.16 | 0.45 |
| 2:B:1164:GLY:HA3 | 2:B:1190:ASP:OD2 | 2.16 | 0.45 |
| 3:C:27:LEU:HD13 | 3:C:228:PHE:HE2 | 1.81 | 0.45 |
| 3:C:215:GLU:O | 3:C:217:ASP:N | 2.50 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:24:LYS:CG | 5:E:25:ASP:N | 2.79 | 0.45 |
| 5:E:29:PHE:C | 5:E:30:ILE:HG13 | 2.37 | 0.45 |
| 7:G:20:PRO:CG | 7:G:21:ARG:N | 2.80 | 0.45 |
| 8:H:10:PHE:CE1 | 8:H:57:VAL:HB | 2.52 | 0.45 |
| 8:H:138:GLU:O | 8:H:139:ASN:C | 2.54 | 0.45 |
| 11:K:31:VAL:O | 11:K:74:ARG:HA | 2.17 | 0.45 |
| 1:A:1206:ASP:O | 1:A:1274:ARG:NH1 | 2.51 | 0.44 |
| 2:B:96:TYR:HB2 | 2:B:129:PHE:HB2 | 1.99 | 0.44 |
| 2:B:118:ARG:CG | 2:B:204:ILE:HD13 | 2.47 | 0.44 |
| 2:B:280:ILE:CD1 | 2:B:334:ILE:HG12 | 2.44 | 0.44 |
| 2:B:295:GLY:O | 2:B:299:GLU:HG3 | 2.18 | 0.44 |
| 2:B:364:ILE:HG12 | 2:B:585:VAL:CG1 | 2.38 | 0.44 |
| 2:B:1138:MET:HA | 2:B:1138:MET:CE | 2.38 | 0.44 |
| 3:C:35:ARG:HH11 | 11:K:41:THR:HA | 1.81 | 0.44 |
| 4:D:33:PHE:CZ | 7:G:80:LYS:HE3 | 2.53 | 0.44 |
| 5:E:112:TYR:CZ | 5:E:136:ASN:HB2 | 2.52 | 0.44 |
| 5:E:163:GLU:O | 5:E:166:LYS:N | 2.50 | 0.44 |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:N | 2.31 | 0.44 |
| 7:G:7:LEU:O | 7:G:73:LYS:HD2 | 2.17 | 0.44 |
| 7:G:9:LEU:HD23 | 7:G:30:LEU:HD12 | 2.00 | 0.44 |
| 7:G:87:VAL:HG23 | 7:G:103:VAL:HG21 | 1.99 | 0.44 |
| 10:J:56:LEU:O | 10:J:59:LYS:N | 2.44 | 0.44 |
| 11:K:35:PHE:CD1 | 11:K:71:PHE:CE1 | 3.05 | 0.44 |
| 15:T:16:DT:H1' | 15:T:17:DT:H5' | 1.98 | 0.44 |
| 1:A:34:LYS:CB | 1:A:36:ARG:HE | 2.28 | 0.44 |
| 1:A:67:CYS:O | 1:A:68:GLN:CB | 2.65 | 0.44 |
| 1:A:75:ASN:O | 1:A:76:GLU:HB2 | 2.17 | 0.44 |
| 1:A:285:PRO:O | 1:A:287:HIS:N | 2.50 | 0.44 |
| 1:A:337:ARG:HH12 | 15:T:18:DT:P | 2.39 | 0.44 |
| 1:A:469:ARG:NH2 | 2:B:991:GLY:O | 2.50 | 0.44 |
| 1:A:567:LYS:HE3 | 8:H:46:LEU:CB | 2.42 | 0.44 |
| 1:A:572:TRP:HA | 1:A:576:GLN:OE1 | 2.17 | 0.44 |
| 1:A:1213:GLY:O | 1:A:1214:GLU:C | 2.56 | 0.44 |
| 1:A:1265:ASN:O | 1:A:1268:LEU:N | 2.47 | 0.44 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:C | 2.37 | 0.44 |
| 2:B:283:VAL:O | 2:B:286:PHE:N | 2.50 | 0.44 |
| 2:B:776:GLN:NE2 | 14:P:8:G:H5' | 2.30 | 0.44 |
| 5:E:30:ILE:HG22 | 5:E:31:THR:N | 2.31 | 0.44 |
| 6:F:90:ARG:CG | 6:F:91:ALA:N | 2.81 | 0.44 |
| 8:H:91:ASP:O | 8:H:93:TYR:N | 2.50 | 0.44 |
| 8:H:143:LEU:N | 8:H:143:LEU:CD1 | 2.79 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:6:ARG:O | 11:K:8:GLU:N | 2.50 | 0.44 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:HE21 | 1.81 | 0.44 |
| 1:A:1265:ASN:C | 1:A:1267:MET:N | 2.69 | 0.44 |
| 2:B:744:HIS:CG | 2:B:745:PRO:HD2 | 2.52 | 0.44 |
| 2:B:847:ASP:C | 2:B:849:GLY:N | 2.71 | 0.44 |
| 2:B:848:ARG:HD2 | 10:J:7:CYS:O | 2.18 | 0.44 |
| 2:B:893:LEU:HD22 | 2:B:897:GLY:C | 2.38 | 0.44 |
| 3:C:45:ALA:HA | 3:C:72:LEU:CD1 | 2.47 | 0.44 |
| 5:E:147:HIS:CD2 | 5:E:149:LEU:H | 2.35 | 0.44 |
| 5:E:180:ARG:HB2 | 5:E:215:MET:OXT | 2.17 | 0.44 |
| 6:F:77:ASP:C | 6:F:79:ARG:N | 2.70 | 0.44 |
| 7:G:1:MET:SD | 7:G:79:PHE:HD1 | 2.40 | 0.44 |
| 7:G:106:MET:HG2 | 7:G:107:LYS:N | 2.31 | 0.44 |
| 7:G:117:GLN:C | 7:G:119:LEU:N | 2.71 | 0.44 |
| 8:H:104:PHE:CZ | 8:H:136:LYS:HA | 2.52 | 0.44 |
| 9:I:55:THR:HG22 | 9:I:55:THR:O | 2.18 | 0.44 |
| 9:I:78:CYS:HB3 | 9:I:106:CYS:SG | 2.58 | 0.44 |
| 10:J:56:LEU:O | 10:J:57:ILE:C | 2.54 | 0.44 |
| 10:J:57:ILE:HA | 10:J:60:PHE:HB2 | 1.98 | 0.44 |
| 15:T:15:DT:H6 | 15:T:15:DT:H2' | 1.61 | 0.44 |
| 1:A:42:ASP:O | 1:A:44:THR:N | 2.38 | 0.44 |
| 1:A:260:ASP:O | 1:A:261:ASP:C | 2.56 | 0.44 |
| 1:A:606:LEU:HB3 | 1:A:614:PHE:CD2 | 2.52 | 0.44 |
| 1:A:825:ILE:O | 1:A:826:ASP:C | 2.55 | 0.44 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:HG13 | 1.99 | 0.44 |
| 1:A:1334:ASP:O | 1:A:1337:GLU:N | 2.50 | 0.44 |
| 1:A:1389:PHE:CD1 | 1:A:1389:PHE:C | 2.90 | 0.44 |
| 2:B:240:ILE:HG23 | 2:B:240:ILE:O | 2.17 | 0.44 |
| 2:B:1223:ASP:HB3 | 2:B:1224:PHE:H | 1.58 | 0.44 |
| 3:C:3:GLU:O | 3:C:4:GLU:HG3 | 2.18 | 0.44 |
| 3:C:239:PRO:O | 3:C:240:VAL:C | 2.55 | 0.44 |
| 4:D:7:THR:O | 4:D:7:THR:HG23 | 2.17 | 0.44 |
| 7:G:91:VAL:HG12 | 7:G:92:VAL:N | 2.32 | 0.44 |
| 9:I:50:THR:HG22 | 9:I:51:ASN:N | 2.32 | 0.44 |
| 1:A:401:GLY:O | 1:A:435:HIS:CD2 | 2.71 | 0.44 |
| 1:A:404:TYR:CE2 | 1:A:414:ASP:HA | 2.53 | 0.44 |
| 1:A:415:LEU:HA | 1:A:415:LEU:HD23 | 1.69 | 0.44 |
| 1:A:452:LYS:HE2 | 1:A:452:LYS:HB3 | 1.71 | 0.44 |
| 1:A:506:ALA:O | 1:A:509:LEU:HB2 | 2.17 | 0.44 |
| 1:A:806:ARG:NH1 | 2:B:729:ILE:HG13 | 2.32 | 0.44 |
| 1:A:829:VAL:C | 1:A:831:THR:H | 2.20 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:929:LEU:CD2 | 1:A:983:ILE:HG21 | 2.48 | 0.44 |
| 1:A:979:SER:HG | 1:A:981:LEU:HG | 1.80 | 0.44 |
| 1:A:996:ASN:C | 1:A:998:LEU:HD12 | 2.36 | 0.44 |
| 1:A:1435:PRO:HA | 1:A:1439:GLY:O | 2.17 | 0.44 |
| 2:B:43:LEU:HD11 | 2:B:811:TYR:O | 2.17 | 0.44 |
| 2:B:210:LYS:HA | 2:B:481:GLN:O | 2.18 | 0.44 |
| 2:B:313:MET:HE2 | 2:B:386:LEU:HD22 | 2.00 | 0.44 |
| 2:B:487:THR:CG2 | 2:B:488:TYR:N | 2.81 | 0.44 |
| 2:B:560:GLU:O | 2:B:561:TRP:CD1 | 2.71 | 0.44 |
| 2:B:1099:VAL:C | 2:B:1101:ASP:H | 2.21 | 0.44 |
| 2:B:1152:MET:HE1 | 2:B:1157:ALA:HA | 1.99 | 0.44 |
| 3:C:18:VAL:O | 3:C:20:PHE:CD2 | 2.70 | 0.44 |
| 3:C:27:LEU:HA | 3:C:228:PHE:CZ | 2.53 | 0.44 |
| 4:D:27:LEU:HG | 4:D:197:SER:HB2 | 1.98 | 0.44 |
| 4:D:146:GLN:O | 4:D:149:THR:HG22 | 2.17 | 0.44 |
| 5:E:23:VAL:HG13 | 5:E:78:LEU:HD13 | 2.00 | 0.44 |
| 5:E:48:ASP:CG | 5:E:49:SER:N | 2.69 | 0.44 |
| 5:E:161:LYS:C | 5:E:163:GLU:N | 2.69 | 0.44 |
| 7:G:73:LYS:HE2 | 7:G:74:TYR:O | 2.18 | 0.44 |
| 11:K:82:ASP:OD1 | 11:K:84:LYS:N | 2.46 | 0.44 |
| 1:A:35:ILE:HD13 | 1:A:241:VAL:HG11 | 1.99 | 0.44 |
| 1:A:56:PRO:O | 1:A:57:ARG:HG3 | 2.18 | 0.44 |
| 1:A:68:GLN:C | 1:A:70:CYS:N | 2.66 | 0.44 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:NE1 | 2.33 | 0.44 |
| 1:A:664:THR:CG2 | 1:A:665:GLY:N | 2.80 | 0.44 |
| 1:A:816:HIS:CD2 | 2:B:764:SER:H | 2.36 | 0.44 |
| 1:A:986:ILE:HD12 | 1:A:1032:LEU:HD11 | 1.98 | 0.44 |
| 1:A:1098:VAL:N | 1:A:1099:PRO:HD2 | 2.32 | 0.44 |
| 1:A:1102:LYS:HG2 | 1:A:1106:ASN:HD21 | 1.82 | 0.44 |
| 2:B:223:VAL:CG1 | 2:B:381:MET:HG2 | 2.48 | 0.44 |
| 2:B:314:LEU:O | 2:B:317:CYS:HB3 | 2.17 | 0.44 |
| 2:B:610:ASN:HA | 2:B:611:PRO:HD3 | 1.89 | 0.44 |
| 2:B:782:LEU:CD1 | 2:B:788:ARG:HH11 | 2.29 | 0.44 |
| 3:C:44:LEU:HD21 | 3:C:159:ALA:HB1 | 1.99 | 0.44 |
| 3:C:77:ILE:C | 3:C:79:GLN:H | 2.21 | 0.44 |
| 7:G:48:VAL:HA | 7:G:76:ALA:HB2 | 1.99 | 0.44 |
| 11:K:18:LYS:NZ | 11:K:37:LYS:O | 2.51 | 0.44 |
| 1:A:71:GLN:C | 1:A:73:GLY:N | 2.71 | 0.44 |
| 1:A:577:ILE:O | 1:A:578:LEU:C | 2.52 | 0.44 |
| 1:A:673:GLY:O | 1:A:676:MET:HB2 | 2.17 | 0.44 |
| 1:A:709:THR:CG2 | 1:A:710:LEU:N | 2.81 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1062:GLU:OE2 | 6:F:88:TYR:OH | 2.35 | 0.44 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:HB3 | 2.00 | 0.44 |
| 2:B:591:ARG:O | 2:B:592:ASN:C | 2.55 | 0.44 |
| 2:B:682:SER:O | 2:B:685:LEU:HB3 | 2.17 | 0.44 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:HB3 | 1.99 | 0.44 |
| 2:B:980:PHE:HE1 | 2:B:990:ILE:HD11 | 1.81 | 0.44 |
| 3:C:238:ILE:HD11 | 3:C:246:ARG:NH1 | 2.33 | 0.44 |
| 3:C:259:LEU:CD1 | 11:K:91:CYS:HB2 | 2.47 | 0.44 |
| 5:E:90:VAL:O | 5:E:90:VAL:HG22 | 2.17 | 0.44 |
| 6:F:89:GLU:HB3 | 6:F:134:ILE:HD13 | 2.00 | 0.44 |
| 7:G:29:LYS:O | 7:G:30:LEU:C | 2.54 | 0.44 |
| 9:I:15:TYR:N | 9:I:15:TYR:HD1 | 2.14 | 0.44 |
| 9:I:32:CYS:SG | 9:I:33:SER:N | 2.90 | 0.44 |
| 9:I:70:ARG:NH1 | 9:I:84:VAL:HB | 2.33 | 0.44 |
| 14:P:4:A:C2' | 14:P:5:C:H5' | 2.47 | 0.44 |
| 15:T:18:DT:C3' | 15:T:19:TT:C5' | 2.96 | 0.44 |
| 1:A:113:LEU:HG | 1:A:218:ASP:OD1 | 2.17 | 0.44 |
| 1:A:548:ASN:OD1 | 11:K:60:ALA:HB1 | 2.18 | 0.44 |
| 1:A:719:VAL:O | 1:A:721:PHE:N | 2.51 | 0.44 |
| 1:A:760:GLN:HG2 | 1:A:765:VAL:O | 2.17 | 0.44 |
| 1:A:1006:ILE:CD1 | 5:E:163:GLU:HG3 | 2.45 | 0.44 |
| 1:A:1094:VAL:CG1 | 1:A:1095:THR:N | 2.63 | 0.44 |
| 2:B:113:TYR:HB3 | 2:B:114:PRO:HD2 | 1.99 | 0.44 |
| 2:B:259:TYR:HD1 | 2:B:259:TYR:N | 2.16 | 0.44 |
| 2:B:1087:PHE:CD2 | 2:B:1088:GLY:N | 2.76 | 0.44 |
| 5:E:197:LYS:HE2 | 5:E:199:ILE:HD11 | 2.00 | 0.44 |
| 7:G:125:SER:OG | 7:G:128:PRO:HA | 2.18 | 0.44 |
| 9:I:110:PHE:H | 9:I:110:PHE:HD2 | 1.66 | 0.44 |
| 13:N:3:DG:H2" | 13:N:4:DT:OP2 | 2.18 | 0.44 |
| 1:A:34:LYS:H | 1:A:57:ARG:HH21 | 1.66 | 0.44 |
| 1:A:34:LYS:HZ1 | 1:A:57:ARG:NH1 | 2.15 | 0.44 |
| 1:A:82:GLY:O | 1:A:241:VAL:N | 2.37 | 0.44 |
| 1:A:388:LEU:HD22 | 1:A:432:VAL:HG21 | 2.00 | 0.44 |
| 1:A:523:ILE:HG22 | 1:A:528:LEU:HB2 | 2.00 | 0.44 |
| 1:A:773:LYS:H | 1:A:773:LYS:HG3 | 1.49 | 0.44 |
| 1:A:1385:THR:C | 1:A:1387:HIS:N | 2.70 | 0.44 |
| 2:B:212:LEU:HD21 | 2:B:466:TRP:CH2 | 2.53 | 0.44 |
| 2:B:343:ILE:HG21 | 2:B:348:ARG:CA | 2.47 | 0.44 |
| 2:B:770:GLN:OE1 | 2:B:983:ARG:CA | 2.58 | 0.44 |
| 2:B:806:THR:CG2 | 2:B:808:ALA:HB3 | 2.48 | 0.44 |
| 2:B:1135:ARG:O | 2:B:1136:ASP:C | 2.56 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1183:LYS:O | 2:B:1183:LYS:HE3 | 2.17 | 0.44 |
| 3:C:36:VAL:HG21 | 3:C:251:LEU:HD22 | 2.00 | 0.44 |
| 3:C:70:ILE:O | 3:C:70:ILE:HG22 | 2.17 | 0.44 |
| 3:C:255:VAL:O | 3:C:255:VAL:HG12 | 2.18 | 0.44 |
| 6:F:128:LYS:HD3 | 6:F:149:GLU:O | 2.18 | 0.44 |
| 7:G:31:LEU:CD2 | 7:G:48:VAL:HG21 | 2.48 | 0.44 |
| 7:G:39:THR:CG2 | 7:G:40:GLY:N | 2.76 | 0.44 |
| 7:G:131:GLN:HG2 | 7:G:136:VAL:HG22 | 1.99 | 0.44 |
| 8:H:40:LEU:HG | 8:H:41:ASP:O | 2.18 | 0.44 |
| 14:P:5:C:C2' | 14:P:6:C:O4' | 2.55 | 0.44 |
| 1:A:37:PHE:HD1 | 1:A:37:PHE:H | 1.65 | 0.43 |
| 1:A:230:ARG:N | 1:A:233:TRP:CE3 | 2.65 | 0.43 |
| 1:A:242:PRO:HA | 1:A:243:PRO:HD2 | 1.75 | 0.43 |
| 1:A:265:LYS:CE | 1:A:322:VAL:HG13 | 2.47 | 0.43 |
| 1:A:783:THR:CG2 | 1:A:815:PHE:CE2 | 3.00 | 0.43 |
| 1:A:935:GLN:O | 1:A:936:LEU:C | 2.56 | 0.43 |
| 2:B:377:PHE:CD2 | 2:B:381:MET:HE2 | 2.53 | 0.43 |
| 2:B:465:ASN:N | 2:B:465:ASN:ND2 | 2.64 | 0.43 |
| 2:B:640:VAL:HB | 2:B:738:PHE:O | 2.19 | 0.43 |
| 2:B:798:TYR:HE2 | 3:C:62:PHE:HZ | 1.63 | 0.43 |
| 2:B:798:TYR:CE2 | 3:C:62:PHE:CE2 | 3.06 | 0.43 |
| 2:B:1183:LYS:N | 2:B:1183:LYS:HE3 | 2.33 | 0.43 |
| 3:C:107:SER:C | 3:C:109:SER:H | 2.21 | 0.43 |
| 4:D:18:VAL:O | 4:D:19:GLU:HB3 | 2.18 | 0.43 |
| 5:E:157:SER:O | 5:E:159:ASP:N | 2.51 | 0.43 |
| 6:F:75:PRO:HG2 | 6:F:78:GLN:HB2 | 2.00 | 0.43 |
| 7:G:18:PHE:HZ | 7:G:68:ALA:HB2 | 1.83 | 0.43 |
| 7:G:80:LYS:O | 7:G:82:PHE:CE1 | 2.71 | 0.43 |
| 1:A:442:VAL:O | 1:A:457:ALA:HA | 2.17 | 0.43 |
| 1:A:474:VAL:HG22 | 1:A:474:VAL:O | 2.19 | 0.43 |
| 1:A:547:LEU:HB3 | 11:K:58:PHE:CE1 | 2.52 | 0.43 |
| 1:A:577:ILE:O | 1:A:580:VAL:HG23 | 2.18 | 0.43 |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N | 2.33 | 0.43 |
| 1:A:935:GLN:O | 1:A:938:LYS:N | 2.50 | 0.43 |
| 1:A:1350:LYS:O | 1:A:1354:ASN:ND2 | 2.47 | 0.43 |
| 2:B:181:LEU:HD22 | 2:B:189:LEU:CD2 | 2.48 | 0.43 |
| 2:B:331:LEU:HD12 | 2:B:331:LEU:N | 2.33 | 0.43 |
| 2:B:449:ASN:O | 2:B:451:LYS:N | 2.51 | 0.43 |
| 2:B:570:VAL:HA | 2:B:571:PRO:HD2 | 1.74 | 0.43 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:HG3 | 2.00 | 0.43 |
| 3:C:249:ASP:O | 3:C:252:GLN:HB3 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:122:GLU:HA | 4:D:125:SER:OG | 2.18 | 0.43 |
| 4:D:141:LEU:HD12 | 4:D:141:LEU:HA | 1.80 | 0.43 |
| 6:F:111:LEU:C | 6:F:113:GLY:N | 2.70 | 0.43 |
| 9:I:7:CYS:HB2 | 9:I:34:TYR:CD1 | 2.53 | 0.43 |
| 12:L:70:ARG:HG2 | 12:L:70:ARG:NH1 | 2.32 | 0.43 |
| 15:T:24:DG:C2' | 15:T:25:DT:O5' | 2.63 | 0.43 |
| 1:A:248:PRO:O | 1:A:260:ASP:HB2 | 2.18 | 0.43 |
| 1:A:699:ALA:HB2 | 9:I:114:GLN:NE2 | 2.32 | 0.43 |
| 1:A:780:VAL:O | 1:A:782:ARG:HG2 | 2.18 | 0.43 |
| 1:A:1243:VAL:HG12 | 1:A:1244:ARG:N | 2.32 | 0.43 |
| 1:A:1290:LYS:O | 1:A:1291:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1341:ILE:O | 1:A:1344:GLY:N | 2.51 | 0.43 |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:HZ | 1.79 | 0.43 |
| 2:B:34:ILE:HD13 | 2:B:747:MET:HE2 | 1.99 | 0.43 |
| 2:B:234:ILE:HD12 | 2:B:234:ILE:N | 2.33 | 0.43 |
| 2:B:616:ILE:N | 2:B:616:ILE:CD1 | 2.81 | 0.43 |
| 2:B:707:PRO:O | 2:B:711:GLU:HG3 | 2.18 | 0.43 |
| 2:B:827:ILE:HD12 | 2:B:1086:PHE:HD2 | 1.84 | 0.43 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:H | 1.83 | 0.43 |
| 4:D:209:ARG:O | 4:D:212:LYS:HB2 | 2.19 | 0.43 |
| 7:G:17:PHE:C | 7:G:19:GLY:H | 2.20 | 0.43 |
| 7:G:99:PHE:CD1 | 7:G:99:PHE:C | 2.91 | 0.43 |
| 8:H:59:ILE:O | 8:H:60:ALA:HB3 | 2.18 | 0.43 |
| 9:I:85:PHE:CD1 | 9:I:99:LEU:HD13 | 2.54 | 0.43 |
| 1:A:347:PHE:CE2 | 1:A:493:GLN:OE1 | 2.72 | 0.43 |
| 1:A:353:ILE:CG2 | 1:A:487:MET:HG3 | 2.45 | 0.43 |
| 1:A:388:LEU:HD22 | 1:A:432:VAL:HB | 1.99 | 0.43 |
| 1:A:546:VAL:O | 1:A:546:VAL:HG12 | 2.18 | 0.43 |
| 1:A:639:PRO:HG2 | 1:A:640:GLN:N | 2.33 | 0.43 |
| 1:A:699:ALA:HB1 | 9:I:114:GLN:HB2 | 2.00 | 0.43 |
| 1:A:802:ASN:ND2 | 1:A:812:GLU:OE1 | 2.42 | 0.43 |
| 1:A:1101:LEU:HB2 | 1:A:1355:VAL:HG11 | 1.99 | 0.43 |
| 1:A:1213:GLY:O | 1:A:1216:ILE:N | 2.52 | 0.43 |
| 1:A:1305:VAL:CG1 | 1:A:1306:LEU:N | 2.81 | 0.43 |
| 2:B:114:PRO:HG2 | 2:B:115:GLN:N | 2.28 | 0.43 |
| 2:B:281:PRO:O | 2:B:282:ILE:C | 2.56 | 0.43 |
| 2:B:291:ILE:HD13 | 2:B:300:HIS:NE2 | 2.34 | 0.43 |
| 2:B:309:GLN:HG3 | 9:I:52:ILE:CD1 | 2.48 | 0.43 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:CG | 2.48 | 0.43 |
| 2:B:661:LEU:C | 2:B:663:ALA:N | 2.70 | 0.43 |
| 2:B:681:TRP:O | 2:B:684:LEU:N | 2.51 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:957:ASN:O | 2:B:960:GLY:N | 2.47 | 0.43 |
| 2:B:997:GLU:H | 2:B:997:GLU:CD | 2.22 | 0.43 |
| 2:B:1123:SER:HB3 | 15:T:24:DG:P | 2.58 | 0.43 |
| 2:B:1156:ASP:O | 2:B:1157:ALA:O | 2.37 | 0.43 |
| 2:B:1181:GLU:O | 2:B:1182:CYS:HB2 | 2.17 | 0.43 |
| 4:D:55:ALA:HB3 | 4:D:148:LEU:HD21 | 1.99 | 0.43 |
| 5:E:88:VAL:HG12 | 5:E:89:GLY:N | 2.33 | 0.43 |
| 7:G:26:LEU:HD23 | 7:G:26:LEU:HA | 1.85 | 0.43 |
| 8:H:23:VAL:HG22 | 8:H:43:ASN:HA | 2.00 | 0.43 |
| 8:H:95:TYR:HB3 | 8:H:144:ILE:HB | 1.99 | 0.43 |
| 15:T:10:DA:H1' | 15:T:11:DG:C8 | 2.54 | 0.43 |
| 1:A:92:HIS:O | 1:A:93:VAL:C | 2.56 | 0.43 |
| 1:A:239:LEU:HA | 1:A:240:PRO:HD2 | 1.89 | 0.43 |
| 1:A:608:ILE:HG13 | 1:A:613:ILE:HD12 | 2.01 | 0.43 |
| 1:A:871:ASP:OD1 | 1:A:1366:ARG:NH2 | 2.52 | 0.43 |
| 1:A:958:VAL:HG12 | 1:A:960:ILE:HG13 | 2.01 | 0.43 |
| 1:A:1209:MET:CE | 1:A:1236:LEU:HB3 | 2.48 | 0.43 |
| 1:A:1226:VAL:HG22 | 1:A:1240:CYS:HB3 | 2.00 | 0.43 |
| 1:A:1316:VAL:O | 1:A:1316:VAL:HG12 | 2.19 | 0.43 |
| 1:A:1404:GLU:O | 1:A:1407:GLU:HB2 | 2.18 | 0.43 |
| 2:B:496:ARG:HB3 | 2:B:496:ARG:NH1 | 2.33 | 0.43 |
| 2:B:765:PRO:O | 2:B:768:THR:N | 2.51 | 0.43 |
| 2:B:1074:ASN:HB2 | 2:B:1081:LEU:HD21 | 2.00 | 0.43 |
| 3:C:86:CYS:O | 3:C:88:CYS:N | 2.52 | 0.43 |
| 3:C:213:PRO:O | 3:C:214:ASN:CB | 2.60 | 0.43 |
| 4:D:51:ASN:C | 4:D:52:LEU:O | 2.56 | 0.43 |
| 5:E:46:TYR:CE2 | 5:E:58:MET:HA | 2.54 | 0.43 |
| 5:E:153:HIS:O | 5:E:154:ILE:CG1 | 2.67 | 0.43 |
| 6:F:118:LEU:O | 6:F:118:LEU:HG | 2.18 | 0.43 |
| 7:G:9:LEU:HD12 | 7:G:10:ASN:N | 2.34 | 0.43 |
| 10:J:34:THR:O | 10:J:35:ALA:C | 2.56 | 0.43 |
| 10:J:53:HIS:NE2 | 10:J:55:ASP:HA | 2.34 | 0.43 |
| 13:N:0:DT:O4 | 15:T:18:DT:O2 | 2.35 | 0.43 |
| 1:A:47:ARG:O | 1:A:48:ALA:HB2 | 2.18 | 0.43 |
| 1:A:335:ARG:N | 1:A:339:ASN:HD22 | 2.17 | 0.43 |
| 1:A:618:GLU:OE2 | 1:A:620:LYS:HB2 | 2.19 | 0.43 |
| 1:A:723:ASN:C | 1:A:725:ALA:N | 2.72 | 0.43 |
| 1:A:795:GLU:CD | 1:A:795:GLU:H | 2.22 | 0.43 |
| 2:B:193:LYS:NZ | 12:L:32:ALA:HB1 | 2.32 | 0.43 |
| 2:B:247:GLY:O | 2:B:249:ARG:N | 2.51 | 0.43 |
| 2:B:628:THR:CG2 | 2:B:628:THR:O | 2.66 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:825:VAL:HG12 | 2:B:826:ALA:N | 2.33 | 0.43 |
| 2:B:857:ARG:HH21 | 2:B:942:ARG:NH1 | 2.16 | 0.43 |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:HG3 | 2.00 | 0.43 |
| 3:C:189:THR:CG2 | 3:C:190:ASP:N | 2.81 | 0.43 |
| 4:D:13:ARG:HB2 | 4:D:17:LYS:NZ | 2.34 | 0.43 |
| 4:D:47:LEU:CD1 | 4:D:48:ILE:N | 2.81 | 0.43 |
| 5:E:124:VAL:CG1 | 5:E:132:ILE:HB | 2.46 | 0.43 |
| 5:E:136:ASN:OD1 | 5:E:138:ALA:N | 2.52 | 0.43 |
| 6:F:121:ALA:O | 6:F:122:MET:C | 2.57 | 0.43 |
| 7:G:99:PHE:CZ | 7:G:143:ILE:HD13 | 2.54 | 0.43 |
| 9:I:33:SER:O | 9:I:35:VAL:HG23 | 2.18 | 0.43 |
| 1:A:265:LYS:HE2 | 1:A:322:VAL:HG13 | 1.98 | 0.43 |
| 1:A:696:GLU:O | 1:A:696:GLU:HG2 | 2.18 | 0.43 |
| 1:A:857:ARG:NH2 | 6:F:139:PRO:HG3 | 2.33 | 0.43 |
| 1:A:877:HIS:O | 1:A:878:ILE:HG12 | 2.19 | 0.43 |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HB | 2.01 | 0.43 |
| 1:A:1362:TYR:HD1 | 1:A:1363:VAL:H | 1.65 | 0.43 |
| 1:A:1385:THR:O | 1:A:1386:ARG:C | 2.57 | 0.43 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:HD11 | 1.99 | 0.43 |
| 2:B:39:ARG:HH21 | 2:B:665:GLU:CG | 2.31 | 0.43 |
| 2:B:189:LEU:O | 2:B:190:TYR:C | 2.55 | 0.43 |
| 2:B:258:LEU:HG | 2:B:258:LEU:O | 2.18 | 0.43 |
| 2:B:410:GLY:O | 2:B:412:LEU:N | 2.52 | 0.43 |
| 2:B:895:ASP:C | 2:B:897:GLY:H | 2.22 | 0.43 |
| 2:B:1184:GLY:C | 2:B:1186:ASP:N | 2.68 | 0.43 |
| 3:C:69:LEU:HB3 | 10:J:6:ARG:HD3 | 1.99 | 0.43 |
| 3:C:262:LEU:HD23 | 3:C:262:LEU:HA | 1.84 | 0.43 |
| 4:D:71:LYS:HA | 4:D:74:GLN:CB | 2.46 | 0.43 |
| 7:G:112:LYS:NZ | 7:G:120:THR:HA | 2.33 | 0.43 |
| 11:K:44:ASN:N | 11:K:61:TYR:CE1 | 2.87 | 0.43 |
| 1:A:35:ILE:HB | 1:A:83:HIS:O | 2.18 | 0.43 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:HD3 | 2.01 | 0.43 |
| 2:B:95:ILE:HG13 | 2:B:130:VAL:HG22 | 1.99 | 0.43 |
| 2:B:515:HIS:O | 2:B:518:HIS:HB2 | 2.19 | 0.43 |
| 2:B:583:ASN:OD1 | 2:B:628:THR:N | 2.50 | 0.43 |
| 7:G:51:TYR:CD2 | 7:G:51:TYR:O | 2.71 | 0.43 |
| 12:L:43:THR:HG22 | 12:L:43:THR:O | 2.19 | 0.43 |
| 1:A:76:GLU:O | 1:A:78:PRO:HD3 | 2.19 | 0.43 |
| 1:A:370:ILE:O | 1:A:373:THR:N | 2.43 | 0.43 |
| 1:A:481:ASP:OD1 | 1:A:483:ASP:OD2 | 2.37 | 0.43 |
| 1:A:506:ALA:C | 1:A:508:PRO:HD2 | 2.39 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:570:PRO:O | 1:A:571:LEU:HD12 | 2.18 | 0.43 |
| 2:B:47:GLN:O | 2:B:173:MET:HE1 | 2.19 | 0.43 |
| 2:B:376:PHE:HE2 | 2:B:569:TYR:HD2 | 1.65 | 0.43 |
| 2:B:642:ASP:CA | 2:B:649:LYS:HA | 2.40 | 0.43 |
| 2:B:797:TYR:HB2 | 2:B:852:ARG:O | 2.19 | 0.43 |
| 2:B:1060:ARG:HA | 2:B:1060:ARG:HD2 | 1.63 | 0.43 |
| 2:B:1064:TYR:O | 2:B:1065:GLN:O | 2.37 | 0.43 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:HG2 | 2.33 | 0.43 |
| 2:B:1147:LEU:CD2 | 2:B:1151:LEU:HD22 | 2.48 | 0.43 |
| 3:C:176:ILE:HG22 | 3:C:177:GLU:O | 2.19 | 0.43 |
| 5:E:195:VAL:HG22 | 5:E:213:ILE:HG13 | 2.01 | 0.43 |
| 8:H:30:SER:CB | 8:H:36:CYS:HB3 | 2.48 | 0.43 |
| 8:H:39:THR:HB | 8:H:124:ARG:HB3 | 2.00 | 0.43 |
| 10:J:2:ILE:HG22 | 10:J:3:VAL:O | 2.18 | 0.43 |
| 11:K:5:ASP:O | 11:K:6:ARG:C | 2.57 | 0.43 |
| 11:K:57:LEU:HB2 | 11:K:76:GLN:HG2 | 2.01 | 0.43 |
| 1:A:49:LYS:CE | 1:A:61:ILE:HD12 | 2.42 | 0.43 |
| 1:A:78:PRO:HB2 | 2:B:1201:LYS:HE3 | 2.01 | 0.43 |
| 1:A:341:MET:HE3 | 2:B:1135:ARG:NH1 | 2.33 | 0.43 |
| 1:A:577:ILE:C | 1:A:579:SER:N | 2.69 | 0.43 |
| 1:A:601:LYS:HB2 | 1:A:603:ASN:HD21 | 1.84 | 0.43 |
| 1:A:672:ASP:O | 1:A:673:GLY:C | 2.58 | 0.43 |
| 1:A:877:HIS:C | 1:A:878:ILE:CG1 | 2.87 | 0.43 |
| 1:A:1127:ASP:O | 1:A:1128:GLN:C | 2.57 | 0.43 |
| 1:A:1130:GLN:O | 1:A:1134:ILE:HG13 | 2.19 | 0.43 |
| 2:B:60:GLN:OE1 | 2:B:95:ILE:HG22 | 2.19 | 0.43 |
| 2:B:251:ILE:O | 2:B:251:ILE:HG22 | 2.19 | 0.43 |
| 2:B:343:ILE:HB | 2:B:348:ARG:HE | 1.84 | 0.43 |
| 2:B:361:LEU:N | 2:B:362:PRO:CD | 2.81 | 0.43 |
| 2:B:785:TYR:CD1 | 2:B:785:TYR:C | 2.91 | 0.43 |
| 2:B:890:TYR:O | 2:B:892:LYS:N | 2.51 | 0.43 |
| 2:B:1202:LEU:HD22 | 2:B:1206:GLU:CD | 2.39 | 0.43 |
| 3:C:3:GLU:O | 3:C:4:GLU:CG | 2.67 | 0.43 |
| 3:C:27:LEU:HD13 | 3:C:228:PHE:CE2 | 2.54 | 0.43 |
| 3:C:38:ILE:HA | 3:C:173:ALA:HB2 | 2.00 | 0.43 |
| 3:C:120:ILE:HD11 | 3:C:130:GLY:O | 2.19 | 0.43 |
| 4:D:51:ASN:ND2 | 4:D:54:GLU:OE2 | 2.52 | 0.43 |
| 4:D:60:LYS:O | 4:D:64:VAL:HG23 | 2.19 | 0.43 |
| 5:E:55:ARG:HD2 | 5:E:83:CYS:O | 2.19 | 0.43 |
| 7:G:34:VAL:HG11 | 7:G:74:TYR:HE1 | 1.84 | 0.43 |
| 11:K:57:LEU:N | 11:K:76:GLN:O | 2.52 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:40:THR:C | 1:A:41:MET:HG3 | 2.39 | 0.42 |
| 1:A:203:SER:OG | 1:A:206:GLU:HB2 | 2.19 | 0.42 |
| 1:A:350:ARG:HG3 | 1:A:350:ARG:NH1 | 2.33 | 0.42 |
| 1:A:925:LEU:O | 1:A:927:VAL:N | 2.52 | 0.42 |
| 1:A:1011:GLN:O | 1:A:1015:VAL:HG23 | 2.19 | 0.42 |
| 1:A:1025:ARG:O | 1:A:1026:LEU:HD23 | 2.19 | 0.42 |
| 2:B:382:ILE:O | 2:B:386:LEU:HG | 2.19 | 0.42 |
| 2:B:764:SER:HB3 | 2:B:765:PRO:CD | 2.49 | 0.42 |
| 3:C:27:LEU:O | 3:C:28:ALA:C | 2.57 | 0.42 |
| 3:C:61:GLU:HA | 3:C:64:ALA:HB3 | 2.00 | 0.42 |
| 4:D:145:MET:O | 4:D:149:THR:HB | 2.19 | 0.42 |
| 6:F:101:ILE:HD11 | 6:F:124:GLU:OE1 | 2.18 | 0.42 |
| 7:G:79:PHE:CE2 | 7:G:105:PRO:HG2 | 2.54 | 0.42 |
| 8:H:139:ASN:O | 8:H:140:ALA:HB2 | 2.19 | 0.42 |
| 9:I:56:ALA:O | 9:I:57:GLY:C | 2.57 | 0.42 |
| 1:A:92:HIS:HD2 | 1:A:304:MET:CE | 2.32 | 0.42 |
| 1:A:335:ARG:O | 1:A:336:ILE:C | 2.55 | 0.42 |
| 1:A:412:ARG:NH2 | 2:B:1108:ARG:HH12 | 2.17 | 0.42 |
| 1:A:674:PRO:C | 1:A:676:MET:N | 2.72 | 0.42 |
| 1:A:1057:VAL:CG1 | 1:A:1058:VAL:N | 2.82 | 0.42 |
| 1:A:1205:LYS:O | 1:A:1206:ASP:C | 2.57 | 0.42 |
| 1:A:1424:VAL:HG22 | 1:A:1436:ILE:HD11 | 2.01 | 0.42 |
| 2:B:654:ARG:C | 2:B:656:GLY:N | 2.72 | 0.42 |
| 2:B:693:ILE:HG22 | 2:B:694:ASP:O | 2.20 | 0.42 |
| 2:B:1197:PRO:O | 2:B:1200:ALA:N | 2.51 | 0.42 |
| 3:C:41:ILE:HD11 | 3:C:247:GLY:HA2 | 2.00 | 0.42 |
| 5:E:160:GLU:O | 5:E:163:GLU:HB3 | 2.19 | 0.42 |
| 6:F:85:MET:HE1 | 6:F:93:ILE:HD12 | 2.01 | 0.42 |
| 7:G:66:GLY:O | 7:G:67:SER:C | 2.55 | 0.42 |
| 8:H:56:THR:HG21 | 8:H:145:ARG:HE | 1.84 | 0.42 |
| 9:I:59:VAL:C | 9:I:61:ASP:H | 2.22 | 0.42 |
| 9:I:101:PHE:HB2 | 9:I:110:PHE:CE2 | 2.55 | 0.42 |
| 1:A:49:LYS:HZ2 | 1:A:60:SER:HA | 1.84 | 0.42 |
| 1:A:299:HIS:C | 1:A:301:ALA:H | 2.23 | 0.42 |
| 1:A:372:LYS:HA | 1:A:435:HIS:HD1 | 1.81 | 0.42 |
| 1:A:870:GLU:HG2 | 5:E:208:TYR:CD1 | 2.54 | 0.42 |
| 1:A:907:THR:HG23 | 1:A:908:LEU:N | 2.33 | 0.42 |
| 1:A:1400:CYS:O | 1:A:1405:THR:HG23 | 2.20 | 0.42 |
| 1:A:1430:LEU:HB2 | 1:A:1432:GLN:HG3 | 2.00 | 0.42 |
| 1:A:1437:GLY:O | 1:A:1438:THR:C | 2.58 | 0.42 |
| 2:B:37:PHE:CE2 | 2:B:542:MET:HA | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:857:ARG:NH2 | 2:B:942:ARG:NH1 | 2.68 | 0.42 |
| 2:B:1162:ILE:O | 2:B:1171:VAL:HG21 | 2.19 | 0.42 |
| 4:D:118:THR:HG22 | 4:D:118:THR:O | 2.19 | 0.42 |
| 5:E:61:GLN:HG2 | 5:E:62:ALA:H | 1.83 | 0.42 |
| 5:E:179:GLN:HB2 | 5:E:182:ASP:HB2 | 2.01 | 0.42 |
| 6:F:79:ARG:HH22 | 6:F:150:GLU:CD | 2.22 | 0.42 |
| 7:G:13:LEU:HD21 | 7:G:17:PHE:CB | 2.28 | 0.42 |
| 1:A:122:MET:O | 1:A:123:ARG:C | 2.58 | 0.42 |
| 1:A:774:ARG:CZ | 1:A:797:LYS:HG3 | 2.48 | 0.42 |
| 1:A:1237:ILE:CG2 | 1:A:1238:ILE:N | 2.83 | 0.42 |
| 1:A:1386:ARG:HE | 1:A:1386:ARG:HB3 | 1.68 | 0.42 |
| 1:A:1387:HIS:CE1 | 13:N:4:DT:C4' | 3.00 | 0.42 |
| 2:B:45:SER:O | 2:B:46:GLN:C | 2.57 | 0.42 |
| 2:B:221:ASN:OD1 | 2:B:242:SER:HA | 2.18 | 0.42 |
| 2:B:364:ILE:HG22 | 2:B:365:THR:N | 2.33 | 0.42 |
| 2:B:467:GLY:CA | 2:B:475:SER:HB3 | 2.49 | 0.42 |
| 3:C:45:ALA:O | 3:C:159:ALA:HA | 2.20 | 0.42 |
| 8:H:95:TYR:CE2 | 8:H:97:MET:CG | 3.02 | 0.42 |
| 9:I:53:GLY:O | 9:I:89:GLN:HB2 | 2.18 | 0.42 |
| 11:K:61:TYR:CD2 | 11:K:61:TYR:O | 2.72 | 0.42 |
| 1:A:208:LEU:O | 1:A:208:LEU:HD23 | 2.20 | 0.42 |
| 1:A:817:ALA:O | 1:A:818:MET:C | 2.56 | 0.42 |
| 1:A:852:TYR:CE1 | 6:F:136:ARG:HG2 | 2.54 | 0.42 |
| 1:A:890:ASP:H | 1:A:1296:GLY:HA3 | 1.83 | 0.42 |
| 1:A:907:THR:HG23 | 1:A:908:LEU:H | 1.85 | 0.42 |
| 1:A:964:ILE:O | 1:A:965:GLN:C | 2.57 | 0.42 |
| 1:A:1198:ASP:HB3 | 1:A:1201:ALA:HB3 | 2.01 | 0.42 |
| 1:A:1315:GLU:C | 1:A:1317:MET:N | 2.72 | 0.42 |
| 1:A:1370:LEU:O | 1:A:1373:ASP:HB2 | 2.20 | 0.42 |
| 1:A:1398:MET:HB2 | 1:A:1426:GLU:OE2 | 2.19 | 0.42 |
| 2:B:45:SER:OG | 2:B:46:GLN:N | 2.49 | 0.42 |
| 2:B:129:PHE:HE2 | 2:B:166:PHE:CD1 | 2.37 | 0.42 |
| 2:B:129:PHE:CE2 | 2:B:166:PHE:HD1 | 2.35 | 0.42 |
| 2:B:405:ARG:NE | 2:B:632:ARG:HG2 | 2.34 | 0.42 |
| 2:B:758:PHE:N | 2:B:759:PRO:HD2 | 2.34 | 0.42 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:CB | 2.49 | 0.42 |
| 2:B:1222:ARG:O | 2:B:1222:ARG:HG2 | 2.19 | 0.42 |
| 3:C:94:LYS:HE3 | 3:C:94:LYS:HB2 | 1.87 | 0.42 |
| 3:C:239:PRO:O | 3:C:241:ASP:N | 2.53 | 0.42 |
| 6:F:86:THR:HG23 | 6:F:89:GLU:CD | 2.39 | 0.42 |
| 7:G:115:MET:CB | 7:G:116:PRO:CD | 2.98 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:10:PHE:HA | 8:H:29:ALA:O | 2.18 | 0.42 |
| 1:A:53:LEU:O | 1:A:54:ASN:C | 2.57 | 0.42 |
| 1:A:477:PRO:HG3 | 1:A:521:MET:HG2 | 2.02 | 0.42 |
| 1:A:543:LEU:HD12 | 1:A:547:LEU:HG | 2.01 | 0.42 |
| 1:A:568:PRO:HB2 | 3:C:221:TYR:CZ | 2.54 | 0.42 |
| 1:A:842:VAL:O | 1:A:844:ALA:N | 2.52 | 0.42 |
| 2:B:597:MET:C | 2:B:599:THR:N | 2.73 | 0.42 |
| 2:B:641:GLU:OE1 | 2:B:641:GLU:HA | 2.20 | 0.42 |
| 2:B:1208:MET:O | 2:B:1211:ASN:N | 2.51 | 0.42 |
| 3:C:47:ASP:CA | 12:L:69:ALA:CB | 2.94 | 0.42 |
| 4:D:7:THR:HB | 7:G:42:PHE:CZ | 2.55 | 0.42 |
| 5:E:180:ARG:NH2 | 5:E:192:ARG:HD2 | 2.34 | 0.42 |
| 8:H:95:TYR:HE2 | 8:H:97:MET:CG | 2.32 | 0.42 |
| 9:I:100:PHE:N | 9:I:100:PHE:CD1 | 2.88 | 0.42 |
| 10:J:32:GLU:O | 10:J:33:GLY:C | 2.57 | 0.42 |
| 12:L:29:TYR:N | 12:L:29:TYR:CD2 | 2.84 | 0.42 |
| 12:L:60:ARG:HG2 | 12:L:61:THR:N | 2.35 | 0.42 |
| 1:A:507:VAL:N | 1:A:508:PRO:CD | 2.82 | 0.42 |
| 1:A:746:MET:CE | 2:B:1018:PRO:HG2 | 2.50 | 0.42 |
| 1:A:846:GLU:HB2 | 1:A:847:ASP:H | 1.68 | 0.42 |
| 1:A:1074:GLU:N | 1:A:1075:PRO:HD2 | 2.35 | 0.42 |
| 1:A:1118:VAL:O | 1:A:1305:VAL:HG13 | 2.20 | 0.42 |
| 1:A:1226:VAL:HG22 | 1:A:1240:CYS:CB | 2.50 | 0.42 |
| 1:A:1315:GLU:C | 1:A:1317:MET:H | 2.22 | 0.42 |
| 1:A:1389:PHE:C | 1:A:1391:ARG:H | 2.22 | 0.42 |
| 2:B:519:TRP:HE1 | 2:B:635:ARG:NH2 | 2.18 | 0.42 |
| 2:B:559:SER:HA | 2:B:563:MET:HB3 | 2.02 | 0.42 |
| 2:B:693:ILE:HD11 | 2:B:740:HIS:CD2 | 2.54 | 0.42 |
| 2:B:781:PHE:O | 2:B:782:LEU:HD23 | 2.19 | 0.42 |
| 3:C:98:VAL:C | 3:C:99:LEU:CD2 | 2.88 | 0.42 |
| 6:F:87:LYS:HG3 | 6:F:88:TYR:CE1 | 2.54 | 0.42 |
| 12:L:28:LYS:HB2 | 12:L:39:SER:HA | 2.02 | 0.42 |
| 1:A:274:ILE:O | 1:A:275:SER:C | 2.57 | 0.42 |
| 1:A:381:THR:O | 1:A:384:ASN:N | 2.50 | 0.42 |
| 1:A:665:GLY:O | 1:A:666:ILE:C | 2.58 | 0.42 |
| 1:A:841:LEU:O | 1:A:845:LEU:HG | 2.20 | 0.42 |
| 1:A:1447:GLU:OE2 | 7:G:23:LYS:HB2 | 2.19 | 0.42 |
| 2:B:102:VAL:HG23 | 2:B:112:LEU:HB2 | 2.02 | 0.42 |
| 2:B:458:LYS:O | 2:B:459:TYR:C | 2.58 | 0.42 |
| 3:C:124:LEU:HD22 | 3:C:129:ILE:HG22 | 2.01 | 0.42 |
| 4:D:170:THR:CG2 | 4:D:172:LEU:HG | 2.50 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:81:THR:HB | 6:F:136:ARG:HH11 | 1.85 | 0.42 |
| 7:G:56:ILE:O | 7:G:57:GLN:HB2 | 2.20 | 0.42 |
| 10:J:1:MET:H3 | 10:J:56:LEU:H | 1.68 | 0.42 |
| 15:T:12:DT:H2" | 15:T:13:DA:OP2 | 2.18 | 0.42 |
| 1:A:162:VAL:HG12 | 1:A:163:SER:N | 2.34 | 0.42 |
| 1:A:270:LEU:O | 1:A:271:LYS:C | 2.57 | 0.42 |
| 1:A:598:LEU:O | 1:A:599:SER:C | 2.58 | 0.42 |
| 1:A:608:ILE:C | 1:A:610:GLY:H | 2.22 | 0.42 |
| 1:A:785:PRO:HG2 | 1:A:786:HIS:CD2 | 2.52 | 0.42 |
| 1:A:1437:GLY:HA3 | 6:F:88:TYR:CD2 | 2.55 | 0.42 |
| 1:A:1438:THR:HB | 2:B:1144:ALA:CB | 2.46 | 0.42 |
| 1:A:1441:PHE:CE2 | 6:F:89:GLU:HG2 | 2.55 | 0.42 |
| 2:B:235:SER:HA | 2:B:261:ARG:NH1 | 2.34 | 0.42 |
| 2:B:597:MET:O | 2:B:599:THR:N | 2.53 | 0.42 |
| 2:B:616:ILE:HG12 | 2:B:697:GLU:HA | 2.01 | 0.42 |
| 2:B:798:TYR:HE2 | 3:C:62:PHE:CE2 | 2.36 | 0.42 |
| 2:B:914:LYS:HD3 | 2:B:937:ALA:CB | 2.50 | 0.42 |
| 2:B:1085:ILE:N | 2:B:1085:ILE:CD1 | 2.79 | 0.42 |
| 3:C:23:SER:O | 3:C:24:ASN:HB3 | 2.19 | 0.42 |
| 3:C:166:GLU:O | 3:C:167:HIS:HB2 | 2.20 | 0.42 |
| 3:C:208:GLU:C | 3:C:210:GLU:N | 2.71 | 0.42 |
| 3:C:213:PRO:HG2 | 3:C:214:ASN:H | 1.84 | 0.42 |
| 4:D:64:VAL:C | 4:D:66:ARG:N | 2.73 | 0.42 |
| 5:E:73:PRO:O | 5:E:75:MET:N | 2.48 | 0.42 |
| 9:I:4:PHE:HE1 | 9:I:6:PHE:CE2 | 2.38 | 0.42 |
| 1:A:7:SER:OG | 2:B:1193:GLN:NE2 | 2.53 | 0.42 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:CE | 2.49 | 0.42 |
| 1:A:382:PRO:CB | 1:A:428:TYR:CE2 | 2.97 | 0.42 |
| 1:A:472:LEU:O | 1:A:475:THR:CB | 2.60 | 0.42 |
| 1:A:856:THR:CB | 1:A:865:GLN:HB2 | 2.47 | 0.42 |
| 1:A:925:LEU:C | 1:A:927:VAL:H | 2.23 | 0.42 |
| 1:A:975:HIS:HA | 1:A:1036:ARG:HG3 | 2.02 | 0.42 |
| 1:A:1215:ARG:HA | 1:A:1215:ARG:HD2 | 1.72 | 0.42 |
| 1:A:1279:ILE:HG23 | 1:A:1308:THR:OG1 | 2.20 | 0.42 |
| 2:B:28:GLU:O | 2:B:28:GLU:HG3 | 2.20 | 0.42 |
| 2:B:763:GLN:O | 2:B:765:PRO:N | 2.53 | 0.42 |
| 2:B:882:THR:HG21 | 2:B:884:ARG:HB2 | 2.02 | 0.42 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:CG2 | 2.49 | 0.42 |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:HE2 | 1.81 | 0.42 |
| 5:E:144:ILE:HD13 | 5:E:183:PRO:HB3 | 2.01 | 0.42 |
| 7:G:38:CYS:HB3 | 7:G:155:SER:HA | 2.02 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:144:ARG:O | 7:G:168:LEU:HD22 | 2.20 | 0.42 |
| 8:H:10:PHE:HE1 | 8:H:57:VAL:HB | 1.85 | 0.42 |
| 8:H:98:TYR:C | 8:H:118:PHE:HD2 | 2.23 | 0.42 |
| 11:K:50:LEU:HD11 | 11:K:75:ILE:CD1 | 2.50 | 0.42 |
| 14:P:1:U:O2' | 14:P:2:C:C5' | 2.67 | 0.42 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:N | 2.32 | 0.41 |
| 1:A:130:ASP:HB3 | 1:A:133:LYS:HB2 | 2.02 | 0.41 |
| 1:A:146:MET:HA | 1:A:171:GLN:HB2 | 2.01 | 0.41 |
| 1:A:786:HIS:O | 1:A:787:PHE:HD2 | 2.03 | 0.41 |
| 2:B:753:ALA:O | 2:B:755:ILE:N | 2.53 | 0.41 |
| 2:B:769:TYR:O | 2:B:772:ALA:N | 2.53 | 0.41 |
| 2:B:953:LEU:HD23 | 2:B:965:LYS:H | 1.85 | 0.41 |
| 2:B:957:ASN:O | 2:B:958:GLN:C | 2.58 | 0.41 |
| 6:F:97:ARG:HA | 6:F:97:ARG:HD2 | 1.83 | 0.41 |
| 7:G:22:MET:O | 7:G:25:TYR:N | 2.53 | 0.41 |
| 7:G:91:VAL:HA | 7:G:101:VAL:HA | 2.02 | 0.41 |
| 11:K:42:LEU:HD21 | 11:K:46:ILE:CD1 | 2.50 | 0.41 |
| 1:A:98:LYS:O | 1:A:101:LYS:N | 2.54 | 0.41 |
| 1:A:108:MET:O | 1:A:109:HIS:HB2 | 2.19 | 0.41 |
| 1:A:469:ARG:HH11 | 1:A:469:ARG:HB3 | 1.85 | 0.41 |
| 1:A:719:VAL:C | 1:A:721:PHE:N | 2.73 | 0.41 |
| 1:A:842:VAL:O | 1:A:843:LYS:C | 2.57 | 0.41 |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:N | 2.35 | 0.41 |
| 2:B:53:GLN:NE2 | 2:B:57:TYR:HB2 | 2.35 | 0.41 |
| 2:B:263:GLY:O | 2:B:264:SER:C | 2.58 | 0.41 |
| 2:B:523:CYS:SG | 2:B:524:PRO:HD2 | 2.60 | 0.41 |
| 2:B:620:ARG:NH2 | 9:I:89:GLN:NE2 | 2.68 | 0.41 |
| 2:B:862:GLN:CG | 2:B:963:PHE:HD1 | 2.33 | 0.41 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:HD22 | 2.01 | 0.41 |
| 3:C:53:THR:O | 3:C:153:LEU:HA | 2.20 | 0.41 |
| 4:D:180:LEU:HD23 | 4:D:180:LEU:HA | 1.88 | 0.41 |
| 5:E:92:THR:HG22 | 5:E:92:THR:O | 2.20 | 0.41 |
| 5:E:157:SER:OG | 5:E:159:ASP:HB2 | 2.21 | 0.41 |
| 5:E:177:ARG:HD3 | 5:E:215:MET:HG2 | 2.02 | 0.41 |
| 8:H:20:TYR:O | 8:H:22:LYS:N | 2.52 | 0.41 |
| 8:H:76:THR:O | 8:H:76:THR:HG22 | 2.19 | 0.41 |
| 9:I:54:GLU:HB3 | 9:I:100:PHE:CE2 | 2.55 | 0.41 |
| 1:A:90:VAL:HG12 | 1:A:91:PHE:N | 2.34 | 0.41 |
| 1:A:117:GLU:H | 1:A:117:GLU:CD | 2.23 | 0.41 |
| 1:A:697:ALA:C | 1:A:699:ALA:H | 2.23 | 0.41 |
| 1:A:722:LEU:HD21 | 1:A:794:PRO:HB3 | 2.03 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:845:LEU:O | 1:A:846:GLU:C | 2.58 | 0.41 |
| 1:A:1329:THR:CG2 | 1:A:1331:SER:HB3 | 2.51 | 0.41 |
| 2:B:95:ILE:HB | 2:B:130:VAL:HG22 | 2.01 | 0.41 |
| 2:B:169:ARG:N | 2:B:454:THR:OG1 | 2.54 | 0.41 |
| 2:B:224:GLN:HA | 2:B:396:ASP:OD2 | 2.19 | 0.41 |
| 2:B:429:PHE:HA | 2:B:432:MET:CE | 2.50 | 0.41 |
| 3:C:29:MET:HE1 | 11:K:98:LEU:CD2 | 2.50 | 0.41 |
| 3:C:236:GLY:O | 3:C:237:SER:C | 2.59 | 0.41 |
| 6:F:143:PHE:C | 6:F:143:PHE:HD1 | 2.23 | 0.41 |
| 8:H:83:GLN:O | 8:H:85:GLY:N | 2.53 | 0.41 |
| 10:J:28:ASP:O | 10:J:29:GLU:C | 2.59 | 0.41 |
| 11:K:91:CYS:O | 11:K:94:ILE:HB | 2.21 | 0.41 |
| 1:A:11:LEU:O | 1:A:11:LEU:HG | 2.16 | 0.41 |
| 1:A:596:THR:O | 1:A:597:LEU:C | 2.59 | 0.41 |
| 1:A:825:ILE:O | 1:A:828:ALA:N | 2.48 | 0.41 |
| 1:A:1157:ASP:C | 1:A:1159:ARG:H | 2.24 | 0.41 |
| 1:A:1444:MET:HG2 | 7:G:59:GLY:O | 2.20 | 0.41 |
| 2:B:48:LEU:O | 2:B:51:PHE:N | 2.51 | 0.41 |
| 2:B:51:PHE:CD2 | 2:B:173:MET:HB3 | 2.56 | 0.41 |
| 2:B:97:VAL:HG12 | 2:B:178:ASN:HD21 | 1.85 | 0.41 |
| 2:B:273:LEU:HD12 | 2:B:280:ILE:HD12 | 2.01 | 0.41 |
| 2:B:336:ARG:NH2 | 2:B:345:LYS:CE | 2.77 | 0.41 |
| 2:B:581:PHE:HA | 2:B:585:VAL:O | 2.20 | 0.41 |
| 2:B:1085:ILE:CG2 | 2:B:1086:PHE:N | 2.82 | 0.41 |
| 2:B:1115:THR:CG2 | 2:B:1117:GLN:CG | 2.98 | 0.41 |
| 4:D:33:PHE:CE2 | 7:G:80:LYS:NZ | 2.82 | 0.41 |
| 4:D:153:ARG:C | 4:D:154:PHE:CD1 | 2.93 | 0.41 |
| 10:J:2:ILE:HG12 | 10:J:57:ILE:HD12 | 2.02 | 0.41 |
| 10:J:22:LEU:O | 10:J:25:LEU:HB2 | 2.20 | 0.41 |
| 1:A:265:LYS:NZ | 1:A:322:VAL:HG13 | 2.36 | 0.41 |
| 1:A:305:ASP:CG | 1:A:326:ARG:HD2 | 2.41 | 0.41 |
| 1:A:335:ARG:HB3 | 1:A:336:ILE:H | 1.68 | 0.41 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:CE | 2.49 | 0.41 |
| 1:A:562:THR:HA | 1:A:563:PRO:HD3 | 1.87 | 0.41 |
| 1:A:818:MET:HG2 | 2:B:514:LEU:HG | 2.03 | 0.41 |
| 1:A:886:ILE:HG22 | 1:A:887:GLY:H | 1.78 | 0.41 |
| 1:A:1010:ALA:O | 1:A:1011:GLN:C | 2.59 | 0.41 |
| 1:A:1018:PHE:O | 1:A:1021:LEU:HB3 | 2.20 | 0.41 |
| 1:A:1445:ILE:H | 1:A:1445:ILE:CD1 | 1.98 | 0.41 |
| 2:B:446:LEU:N | 2:B:446:LEU:HD23 | 2.36 | 0.41 |
| 2:B:705:MET:CE | 2:B:745:PRO:HB3 | 2.51 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:750:GLY:O | 2:B:751:VAL:C | 2.59 | 0.41 |
| 2:B:806:THR:C | 2:B:808:ALA:N | 2.71 | 0.41 |
| 2:B:807:ARG:O | 2:B:811:TYR:HE1 | 2.03 | 0.41 |
| 2:B:980:PHE:HE2 | 2:B:1094:ARG:CB | 2.33 | 0.41 |
| 2:B:1142:GLY:O | 2:B:1144:ALA:N | 2.53 | 0.41 |
| 3:C:70:ILE:HA | 3:C:71:PRO:HD2 | 1.89 | 0.41 |
| 3:C:116:LYS:HD3 | 3:C:140:ASN:HA | 2.02 | 0.41 |
| 4:D:40:HIS:C | 4:D:42:GLY:N | 2.72 | 0.41 |
| 10:J:32:GLU:O | 10:J:35:ALA:N | 2.53 | 0.41 |
| 10:J:53:HIS:CD2 | 10:J:54:VAL:N | 2.88 | 0.41 |
| 1:A:47:ARG:HH12 | 1:A:254:GLU:CG | 2.33 | 0.41 |
| 1:A:62:ASP:HB3 | 1:A:64:ASN:HD21 | 1.83 | 0.41 |
| 1:A:116:ASP:C | 1:A:118:HIS:H | 2.24 | 0.41 |
| 1:A:860:LEU:HD11 | 1:A:1393:ASN:HB2 | 2.02 | 0.41 |
| 1:A:920:LEU:HD23 | 1:A:920:LEU:C | 2.40 | 0.41 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:CD | 2.50 | 0.41 |
| 2:B:400:HIS:O | 2:B:402:GLY:N | 2.53 | 0.41 |
| 2:B:458:LYS:O | 2:B:462:ALA:N | 2.54 | 0.41 |
| 2:B:651:LEU:HD11 | 2:B:707:PRO:CB | 2.51 | 0.41 |
| 2:B:863:GLU:OE1 | 2:B:962:LYS:HB2 | 2.20 | 0.41 |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:HG13 | 2.49 | 0.41 |
| 2:B:1074:ASN:O | 2:B:1078:GLY:N | 2.51 | 0.41 |
| 2:B:1110:PRO:HB2 | 2:B:1119:VAL:CG2 | 2.51 | 0.41 |
| 3:C:76:ASP:O | 3:C:79:GLN:HG2 | 2.21 | 0.41 |
| 5:E:42:PHE:O | 5:E:43:LYS:C | 2.59 | 0.41 |
| 6:F:147:SER:OG | 6:F:150:GLU:HG3 | 2.20 | 0.41 |
| 7:G:62:LEU:HD23 | 7:G:62:LEU:HA | 1.89 | 0.41 |
| 7:G:165:GLU:HB2 | 7:G:168:LEU:HD12 | 2.02 | 0.41 |
| 10:J:21:TYR:CD2 | 10:J:21:TYR:C | 2.94 | 0.41 |
| 12:L:40:LEU:HD22 | 12:L:44:ASP:CB | 2.51 | 0.41 |
| 14:P:6:C:H2' | 14:P:7:A:O4' | 2.20 | 0.41 |
| 1:A:42:ASP:OD1 | 1:A:45:GLN:O | 2.39 | 0.41 |
| 1:A:65:LEU:O | 1:A:66:LYS:C | 2.59 | 0.41 |
| 1:A:89:PRO:HB3 | 1:A:208:LEU:HD12 | 2.03 | 0.41 |
| 1:A:252:PHE:HB2 | 1:A:256:GLN:CD | 2.41 | 0.41 |
| 1:A:526:ASP:O | 1:A:527:THR:C | 2.59 | 0.41 |
| 1:A:629:LEU:O | 1:A:633:VAL:HG23 | 2.21 | 0.41 |
| 1:A:699:ALA:HB2 | 9:I:114:GLN:CD | 2.41 | 0.41 |
| 2:B:324:ILE:CG2 | 2:B:325:GLN:N | 2.83 | 0.41 |
| 2:B:469:GLN:HB2 | 2:B:470:LYS:H | 1.52 | 0.41 |
| 2:B:642:ASP:CA | 2:B:649:LYS:HG3 | 2.50 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1023:VAL:O | 2:B:1024:ALA:C | 2.59 | 0.41 |
| 3:C:59:ALA:O | 3:C:60:ASP:C | 2.58 | 0.41 |
| 5:E:114:ASN:O | 5:E:115:ASN:CB | 2.63 | 0.41 |
| 6:F:97:ARG:NH2 | 6:F:106:PRO:O | 2.54 | 0.41 |
| 10:J:57:ILE:HG23 | 10:J:58:GLU:N | 2.35 | 0.41 |
| 15:T:16:DT:C4 | 15:T:17:DT:C4 | 3.09 | 0.41 |
| 1:A:56:PRO:O | 1:A:57:ARG:NE | 2.47 | 0.41 |
| 1:A:77:CYS:C | 1:A:78:PRO:O | 2.55 | 0.41 |
| 1:A:98:LYS:O | 1:A:100:LYS:N | 2.53 | 0.41 |
| 1:A:135:PHE:HB2 | 1:A:223:GLY:H | 1.85 | 0.41 |
| 1:A:268:ASP:O | 1:A:269:ILE:C | 2.59 | 0.41 |
| 1:A:322:VAL:O | 1:A:322:VAL:HG12 | 2.19 | 0.41 |
| 1:A:715:GLU:O | 1:A:716:ASP:C | 2.59 | 0.41 |
| 1:A:1076:ALA:HA | 1:A:1079:MET:HE3 | 2.01 | 0.41 |
| 1:A:1170:ILE:H | 1:A:1170:ILE:HG13 | 1.55 | 0.41 |
| 1:A:1214:GLU:OE1 | 1:A:1214:GLU:HA | 2.21 | 0.41 |
| 2:B:762:ASN:OD1 | 2:B:1024:ALA:HB3 | 2.21 | 0.41 |
| 2:B:1034:VAL:O | 2:B:1036:ALA:N | 2.54 | 0.41 |
| 3:C:66:ARG:CZ | 10:J:2:ILE:CG2 | 2.98 | 0.41 |
| 3:C:143:LEU:HD21 | 3:C:146:LYS:HE2 | 2.03 | 0.41 |
| 3:C:256:ALA:O | 3:C:258:ILE:N | 2.54 | 0.41 |
| 4:D:187:THR:HG22 | 4:D:188:ALA:H | 1.84 | 0.41 |
| 6:F:89:GLU:O | 6:F:93:ILE:HG13 | 2.20 | 0.41 |
| 6:F:147:SER:O | 6:F:148:VAL:C | 2.58 | 0.41 |
| 7:G:87:VAL:CG2 | 7:G:103:VAL:HG21 | 2.51 | 0.41 |
| 9:I:101:PHE:CE1 | 9:I:112:SER:HB2 | 2.56 | 0.41 |
| 10:J:31:ASP:O | 10:J:32:GLU:C | 2.59 | 0.41 |
| 12:L:60:ARG:HH21 | 12:L:65:VAL:HG21 | 1.86 | 0.41 |
| 1:A:23:SER:HB3 | 1:A:233:TRP:CE2 | 2.56 | 0.41 |
| 1:A:24:PRO:HD2 | 1:A:233:TRP:CD1 | 2.55 | 0.41 |
| 1:A:41:MET:O | 1:A:50:ILE:HG13 | 2.21 | 0.41 |
| 1:A:68:GLN:HE22 | 1:A:80:HIS:CG | 2.39 | 0.41 |
| 1:A:265:LYS:O | 1:A:269:ILE:HG13 | 2.21 | 0.41 |
| 1:A:269:ILE:HG12 | 1:A:299:HIS:HB3 | 2.03 | 0.41 |
| 1:A:335:ARG:CA | 1:A:339:ASN:HD22 | 2.28 | 0.41 |
| 1:A:337:ARG:CZ | 1:A:839:ARG:NH1 | 2.84 | 0.41 |
| 1:A:338:GLY:HA2 | 2:B:1129:ARG:HH22 | 1.86 | 0.41 |
| 1:A:573:SER:OG | 1:A:576:GLN:HB2 | 2.21 | 0.41 |
| 1:A:608:ILE:O | 1:A:610:GLY:N | 2.54 | 0.41 |
| 1:A:722:LEU:HD22 | 1:A:799:PHE:CG | 2.56 | 0.41 |
| 1:A:976:THR:HG23 | 8:H:136:LYS:NZ | 2.36 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N | 2.35 | 0.41 |
| 1:A:1362:TYR:CD1 | 1:A:1362:TYR:C | 2.92 | 0.41 |
| 2:B:24:PRO:O | 2:B:655:LYS:HB2 | 2.21 | 0.41 |
| 2:B:181:LEU:O | 2:B:182:SER:C | 2.59 | 0.41 |
| 2:B:189:LEU:O | 2:B:192:LEU:HB2 | 2.21 | 0.41 |
| 2:B:205:ILE:N | 2:B:205:ILE:CD1 | 2.83 | 0.41 |
| 2:B:583:ASN:HD21 | 2:B:628:THR:HB | 1.86 | 0.41 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:CZ | 2.51 | 0.41 |
| 2:B:597:MET:C | 2:B:599:THR:H | 2.22 | 0.41 |
| 2:B:603:LEU:HD22 | 2:B:603:LEU:HA | 1.95 | 0.41 |
| 2:B:751:VAL:HG13 | 2:B:812:LEU:CD2 | 2.47 | 0.41 |
| 2:B:812:LEU:O | 2:B:813:LYS:C | 2.59 | 0.41 |
| 2:B:909:ASP:OD1 | 2:B:909:ASP:N | 2.51 | 0.41 |
| 2:B:1010:LEU:HD12 | 2:B:1010:LEU:HA | 1.81 | 0.41 |
| 2:B:1107:ALA:O | 2:B:1108:ARG:O | 2.39 | 0.41 |
| 3:C:236:GLY:C | 3:C:238:ILE:N | 2.73 | 0.41 |
| 4:D:56:ARG:NH2 | 4:D:57:LEU:HD21 | 2.35 | 0.41 |
| 4:D:176:GLU:HG2 | 4:D:197:SER:OG | 2.21 | 0.41 |
| 5:E:56:LYS:HE3 | 5:E:84:ASP:HB2 | 2.02 | 0.41 |
| 5:E:58:MET:O | 5:E:59:SER:O | 2.38 | 0.41 |
| 5:E:153:HIS:O | 5:E:154:ILE:HG13 | 2.20 | 0.41 |
| 7:G:27:LYS:O | 7:G:30:LEU:N | 2.54 | 0.41 |
| 8:H:83:GLN:C | 8:H:85:GLY:N | 2.74 | 0.41 |
| 8:H:95:TYR:CE2 | 8:H:97:MET:HG3 | 2.56 | 0.41 |
| 12:L:61:THR:CG2 | 12:L:63:ARG:HG2 | 2.50 | 0.41 |
| 15:T:18:DT:O3' | 15:T:19:TT:C4' | 2.63 | 0.41 |
| 1:A:106:VAL:HA | 1:A:114:LEU:HD21 | 2.04 | 0.41 |
| 1:A:188:ASP:OD1 | 1:A:189:ARG:N | 2.53 | 0.41 |
| 1:A:354:SER:HA | 1:A:482:PHE:CD2 | 2.56 | 0.41 |
| 1:A:532:ARG:O | 1:A:535:THR:HB | 2.21 | 0.41 |
| 1:A:604:GLY:O | 1:A:605:MET:HB2 | 2.21 | 0.41 |
| 1:A:1074:GLU:C | 1:A:1076:ALA:H | 2.25 | 0.41 |
| 1:A:1332:PHE:HE1 | 1:A:1348:LEU:HD13 | 1.85 | 0.41 |
| 2:B:245:GLU:C | 2:B:246:LYS:HG3 | 2.41 | 0.41 |
| 2:B:309:GLN:CD | 9:I:52:ILE:HD11 | 2.41 | 0.41 |
| 2:B:743:ILE:H | 2:B:743:ILE:HG12 | 1.64 | 0.41 |
| 2:B:895:ASP:C | 2:B:897:GLY:N | 2.74 | 0.41 |
| 2:B:953:LEU:HD22 | 2:B:965:LYS:HB2 | 1.98 | 0.41 |
| 3:C:97:VAL:HG12 | 3:C:99:LEU:HD21 | 2.03 | 0.41 |
| 3:C:174:ALA:O | 3:C:175:ALA:CB | 2.67 | 0.41 |
| 5:E:191:LYS:O | 5:E:192:ARG:C | 2.58 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:21:ARG:HD3 | 7:G:21:ARG:HA | 1.81 | 0.41 |
| 7:G:34:VAL:HG11 | 7:G:74:TYR:CE1 | 2.56 | 0.41 |
| 8:H:145:ARG:O | 8:H:146:ARG:HB2 | 2.21 | 0.41 |
| 9:I:77:LYS:O | 9:I:79:HIS:N | 2.54 | 0.41 |
| 10:J:57:ILE:O | 10:J:60:PHE:HB2 | 2.21 | 0.41 |
| 11:K:42:LEU:O | 11:K:42:LEU:HG | 2.22 | 0.41 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:HB2 | 2.56 | 0.41 |
| 1:A:26:GLU:O | 1:A:27:VAL:C | 2.59 | 0.40 |
| 1:A:31:SER:HA | 1:A:81:PHE:O | 2.22 | 0.40 |
| 1:A:219:PHE:O | 1:A:222:LEU:O | 2.38 | 0.40 |
| 1:A:391:LEU:O | 1:A:394:ASN:HB2 | 2.21 | 0.40 |
| 1:A:547:LEU:HD13 | 11:K:58:PHE:CD1 | 2.56 | 0.40 |
| 1:A:606:LEU:CB | 1:A:614:PHE:CE2 | 3.03 | 0.40 |
| 2:B:29:ASP:O | 2:B:30:SER:C | 2.60 | 0.40 |
| 2:B:95:ILE:CB | 2:B:130:VAL:HG22 | 2.51 | 0.40 |
| 2:B:313:MET:CE | 2:B:386:LEU:HD22 | 2.51 | 0.40 |
| 2:B:337:ARG:C | 2:B:338:GLY:CA | 2.90 | 0.40 |
| 2:B:638:PHE:HB3 | 2:B:651:LEU:HD22 | 2.03 | 0.40 |
| 2:B:710:LEU:O | 2:B:711:GLU:OE2 | 2.38 | 0.40 |
| 2:B:744:HIS:CD2 | 2:B:746:SER:HB3 | 2.56 | 0.40 |
| 2:B:834:ASN:CA | 2:B:838:SER:O | 2.69 | 0.40 |
| 2:B:999:MET:HG2 | 2:B:1007:VAL:HG22 | 2.02 | 0.40 |
| 3:C:172:PRO:O | 3:C:235:VAL:HG23 | 2.20 | 0.40 |
| 4:D:192:LYS:HB3 | 4:D:192:LYS:NZ | 2.34 | 0.40 |
| 4:D:195:ILE:N | 4:D:196:PRO:CD | 2.85 | 0.40 |
| 8:H:39:THR:O | 8:H:124:ARG:N | 2.52 | 0.40 |
| 8:H:82:PRO:C | 8:H:84:ALA:N | 2.73 | 0.40 |
| 9:I:34:TYR:O | 9:I:35:VAL:CG2 | 2.69 | 0.40 |
| 10:J:13:VAL:C | 10:J:14:VAL:HG23 | 2.40 | 0.40 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:N | 2.25 | 0.40 |
| 1:A:376:TYR:HA | 1:A:377:PRO:HD2 | 1.93 | 0.40 |
| 1:A:525:GLN:HG3 | 2:B:836:GLU:HG2 | 2.02 | 0.40 |
| 1:A:567:LYS:NZ | 8:H:47:PHE:HB3 | 2.36 | 0.40 |
| 1:A:824:LEU:HD23 | 1:A:824:LEU:HA | 1.85 | 0.40 |
| 1:A:879:GLU:OE1 | 1:A:962:ARG:NH2 | 2.53 | 0.40 |
| 1:A:964:ILE:O | 1:A:966:ASN:N | 2.54 | 0.40 |
| 1:A:1364:ASN:HD22 | 1:A:1364:ASN:C | 2.24 | 0.40 |
| 1:A:1405:THR:HB | 1:A:1406:VAL:H | 1.55 | 0.40 |
| 1:A:1409:LEU:O | 1:A:1412:ALA:HB3 | 2.21 | 0.40 |
| 2:B:175:ARG:NH1 | 2:B:175:ARG:CG | 2.84 | 0.40 |
| 2:B:298:LEU:N | 2:B:298:LEU:HD22 | 2.36 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:448:ILE:O | 2:B:450:ALA:N | 2.55 | 0.40 |
| 2:B:773:MET:HB3 | 2:B:1095:LEU:HD23 | 2.02 | 0.40 |
| 3:C:181:ASP:N | 3:C:182:PRO:CD | 2.84 | 0.40 |
| 4:D:192:LYS:HG2 | 4:D:207:LEU:CD2 | 2.51 | 0.40 |
| 5:E:72:PHE:CE2 | 5:E:155:ARG:NH2 | 2.89 | 0.40 |
| 8:H:59:ILE:CG2 | 8:H:60:ALA:N | 2.65 | 0.40 |
| 9:I:103:CYS:CB | 9:I:106:CYS:SG | 3.09 | 0.40 |
| 11:K:46:ILE:O | 11:K:50:LEU:HB2 | 2.21 | 0.40 |
| 11:K:50:LEU:HD11 | 11:K:75:ILE:HD13 | 2.04 | 0.40 |
| 12:L:46:VAL:HG12 | 12:L:46:VAL:O | 2.22 | 0.40 |
| 12:L:49:LYS:O | 12:L:50:ASP:HB3 | 2.22 | 0.40 |
| 1:A:34:LYS:H | 1:A:57:ARG:HH22 | 1.68 | 0.40 |
| 1:A:58:LEU:HG | 1:A:59:GLY:H | 1.82 | 0.40 |
| 1:A:225:ASN:HD22 | 1:A:228:PHE:N | 1.88 | 0.40 |
| 1:A:230:ARG:N | 1:A:233:TRP:HE3 | 2.11 | 0.40 |
| 1:A:356:ASP:HB2 | 1:A:469:ARG:HH12 | 1.81 | 0.40 |
| 1:A:408:ASP:C | 1:A:410:GLY:H | 2.24 | 0.40 |
| 1:A:481:ASP:OD1 | 1:A:483:ASP:CG | 2.60 | 0.40 |
| 1:A:482:PHE:C | 1:A:484:GLY:N | 2.71 | 0.40 |
| 1:A:834:THR:HG22 | 1:A:835:GLY:N | 2.35 | 0.40 |
| 1:A:869:GLY:O | 1:A:870:GLU:HB2 | 2.21 | 0.40 |
| 1:A:925:LEU:C | 1:A:927:VAL:N | 2.73 | 0.40 |
| 1:A:1031:VAL:O | 1:A:1031:VAL:HG12 | 2.22 | 0.40 |
| 1:A:1053:PHE:O | 1:A:1056:SER:N | 2.51 | 0.40 |
| 1:A:1450:LEU:CD1 | 6:F:108:PHE:CZ | 3.04 | 0.40 |
| 2:B:309:GLN:CG | 9:I:52:ILE:HD11 | 2.51 | 0.40 |
| 2:B:315:LYS:N | 2:B:316:PRO:CD | 2.83 | 0.40 |
| 2:B:658:ILE:O | 2:B:661:LEU:N | 2.42 | 0.40 |
| 2:B:774:GLY:HA2 | 2:B:1093:GLN:HE22 | 1.85 | 0.40 |
| 2:B:824:ILE:CG2 | 2:B:1087:PHE:CE2 | 2.95 | 0.40 |
| 3:C:16:ASP:O | 3:C:17:ASN:CG | 2.59 | 0.40 |
| 7:G:17:PHE:N | 7:G:17:PHE:HD2 | 2.17 | 0.40 |
| 7:G:27:LYS:O | 7:G:30:LEU:HB3 | 2.20 | 0.40 |
| 7:G:109:PHE:O | 7:G:160:ILE:HA | 2.22 | 0.40 |
| 9:I:8:ARG:O | 9:I:10:CYS:N | 2.54 | 0.40 |
| 9:I:56:ALA:O | 9:I:57:GLY:O | 2.39 | 0.40 |
| 1:A:263:THR:O | 1:A:263:THR:HG22 | 2.22 | 0.40 |
| 1:A:332:LYS:O | 1:A:334:GLY:N | 2.55 | 0.40 |
| 1:A:388:LEU:HD22 | 1:A:432:VAL:CB | 2.51 | 0.40 |
| 1:A:466:SER:HB3 | 2:B:1103:ILE:HG12 | 2.02 | 0.40 |
| 1:A:711:ARG:O | 1:A:714:PHE:HB3 | 2.21 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:823:GLY:O | 1:A:825:ILE:N | 2.55 | 0.40 |
| 1:A:852:TYR:CD1 | 6:F:136:ARG:HB3 | 2.56 | 0.40 |
| 1:A:1134:ILE:O | 1:A:1135:ARG:C | 2.59 | 0.40 |
| 2:B:22:SER:HA | 2:B:654:ARG:HG3 | 2.03 | 0.40 |
| 2:B:288:ALA:HA | 2:B:331:LEU:CD1 | 2.49 | 0.40 |
| 2:B:294:ASP:C | 2:B:296:GLU:H | 2.24 | 0.40 |
| 2:B:460:ALA:HB1 | 2:B:466:TRP:CZ3 | 2.57 | 0.40 |
| 2:B:498:THR:CG2 | 2:B:499:ASN:N | 2.84 | 0.40 |
| 2:B:732:SER:HB2 | 2:B:734:HIS:CD2 | 2.57 | 0.40 |
| 2:B:782:LEU:HB3 | 2:B:784:ASN:OD1 | 2.21 | 0.40 |
| 2:B:1030:LEU:HD12 | 2:B:1030:LEU:HA | 1.96 | 0.40 |
| 3:C:10:ILE:HG22 | 3:C:11:ARG:O | 2.21 | 0.40 |
| 3:C:58:LEU:CD2 | 3:C:58:LEU:N | 2.84 | 0.40 |
| 3:C:58:LEU:N | 3:C:58:LEU:HD22 | 2.37 | 0.40 |
| 3:C:187:LYS:HG3 | 3:C:219:PHE:CE1 | 2.56 | 0.40 |
| 7:G:14:HIS:ND1 | 7:G:15:PRO:CD | 2.78 | 0.40 |
| 8:H:38:LEU:HD13 | 8:H:125:LEU:CD1 | 2.51 | 0.40 |
| 1:A:34:LYS:N | 1:A:57:ARG:NH2 | 2.65 | 0.40 |
| 1:A:56:PRO:O | 1:A:57:ARG:CG | 2.70 | 0.40 |
| 1:A:299:HIS:C | 1:A:301:ALA:N | 2.74 | 0.40 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HG13 | 2.51 | 0.40 |
| 1:A:414:ASP:OD1 | 1:A:414:ASP:C | 2.60 | 0.40 |
| 1:A:545:GLN:C | 1:A:547:LEU:N | 2.73 | 0.40 |
| 1:A:682:THR:O | 1:A:682:THR:HG22 | 2.22 | 0.40 |
| 1:A:685:GLU:HG3 | 1:A:686:ALA:N | 2.36 | 0.40 |
| 1:A:939:ASP:O | 1:A:940:ARG:C | 2.59 | 0.40 |
| 1:A:1019:CYS:O | 1:A:1022:LEU:N | 2.54 | 0.40 |
| 1:A:1036:ARG:NH1 | 1:A:1036:ARG:CG | 2.80 | 0.40 |
| 1:A:1168:GLU:O | 1:A:1172:LEU:HG | 2.21 | 0.40 |
| 1:A:1260:LEU:CG | 1:A:1260:LEU:O | 2.70 | 0.40 |
| 2:B:223:VAL:HG11 | 2:B:381:MET:HG2 | 2.03 | 0.40 |
| 2:B:225:VAL:O | 2:B:226:PHE:CD2 | 2.74 | 0.40 |
| 2:B:765:PRO:O | 2:B:766:ARG:C | 2.59 | 0.40 |
| 2:B:766:ARG:HD3 | 2:B:766:ARG:HA | 1.73 | 0.40 |
| 2:B:785:TYR:CD1 | 2:B:786:ASN:N | 2.89 | 0.40 |
| 3:C:137:LYS:HB3 | 3:C:138:GLU:OE1 | 2.21 | 0.40 |
| 4:D:207:LEU:O | 4:D:211:LEU:HG | 2.22 | 0.40 |
| 5:E:11:ARG:HH21 | 5:E:141:VAL:HG21 | 1.87 | 0.40 |
| 5:E:35:VAL:C | 5:E:37:LEU:N | 2.75 | 0.40 |
| 5:E:114:ASN:HD22 | 5:E:114:ASN:HA | 1.68 | 0.40 |
| 6:F:111:LEU:O | 6:F:113:GLY:N | 2.52 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:58:PHE:HB3 | 11:K:76:GLN:HB3 | 2.03 | 0.40 |
| 11:K:62:LYS:O | 11:K:71:PHE:HB2 | 2.21 | 0.40 |
| 11:K:110:ASN:C | 11:K:111:LEU:CG | 2.89 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 1410/1733 (81%) | 962 (68%) | 299 (21%) | 149 (11%) | 0 8 |
| 2 | B | 1096/1224 (90%) | 767 (70%) | 219 (20%) | 110 (10%) | 0 9 |
| 3 | C | 264/318 (83%) | 171 (65%) | 62 (24%) | 31 (12%) | 0 6 |
| 4 | D | 173/221 (78%) | 125 (72%) | 29 (17%) | 19 (11%) | 0 8 |
| 5 | E | 212/215 (99%) | 157 (74%) | 44 (21%) | 11 (5%) | 2 23 |
| 6 | F | 84/155 (54%) | 67 (80%) | 15 (18%) | 2 (2%) | 6 37 |
| 7 | G | 169/171 (99%) | 125 (74%) | 34 (20%) | 10 (6%) | 1 21 |
| 8 | H | 131/146 (90%) | 84 (64%) | 30 (23%) | 17 (13%) | 0 5 |
| 9 | I | 114/122 (93%) | 80 (70%) | 21 (18%) | 13 (11%) | 0 7 |
| 10 | J | 63/70 (90%) | 35 (56%) | 13 (21%) | 15 (24%) | 0 1 |
| 11 | K | 112/120 (93%) | 86 (77%) | 16 (14%) | 10 (9%) | 1 12 |
| 12 | L | 44/70 (63%) | 17 (39%) | 17 (39%) | 10 (23%) | 0 1 |
| All | All | 3872/4565 (85%) | 2676 (69%) | 799 (21%) | 397 (10%) | 0 9 |

All (397) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 44 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 48 | ALA |
| 1 | A | 57 | ARG |
| 1 | A | 62 | ASP |
| 1 | A | 65 | LEU |
| 1 | A | 74 | MET |
| 1 | A | 93 | VAL |
| 1 | A | 167 | CYS |
| 1 | A | 219 | PHE |
| 1 | A | 223 | GLY |
| 1 | A | 255 | SER |
| 1 | A | 286 | HIS |
| 1 | A | 311 | GLN |
| 1 | A | 312 | PRO |
| 1 | A | 318 | SER |
| 1 | A | 322 | VAL |
| 1 | A | 335 | ARG |
| 1 | A | 385 | ILE |
| 1 | A | 423 | ASP |
| 1 | A | 465 | TYR |
| 1 | A | 536 | LEU |
| 1 | A | 543 | LEU |
| 1 | A | 567 | LYS |
| 1 | A | 597 | LEU |
| 1 | A | 626 | ASN |
| 1 | A | 666 | ILE |
| 1 | A | 753 | GLY |
| 1 | A | 789 | LYS |
| 1 | A | 847 | ASP |
| 1 | A | 875 | ALA |
| 1 | A | 968 | GLN |
| 1 | A | 969 | GLN |
| 1 | A | 986 | ILE |
| 1 | A | 1002 | GLY |
| 1 | A | 1036 | ARG |
| 1 | A | 1096 | SER |
| 1 | A | 1114 | PRO |
| 1 | A | 1115 | SER |
| 1 | A | 1122 | PRO |
| 1 | A | 1212 | VAL |
| 1 | A | 1223 | ASP |
| 1 | A | 1281 | ARG |
| 1 | A | 1314 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1341 | ILE |
| 1 | A | 1365 | TYR |
| 1 | A | 1378 | GLN |
| 1 | A | 1405 | THR |
| 1 | A | 1438 | THR |
| 2 | B | 45 | SER |
| 2 | B | 46 | GLN |
| 2 | B | 108 | VAL |
| 2 | B | 115 | GLN |
| 2 | B | 186 | GLU |
| 2 | B | 258 | LEU |
| 2 | B | 345 | LYS |
| 2 | B | 367 | LEU |
| 2 | B | 467 | GLY |
| 2 | B | 474 | SER |
| 2 | B | 643 | ASP |
| 2 | B | 709 | ASP |
| 2 | B | 727 | LYS |
| 2 | B | 731 | VAL |
| 2 | B | 764 | SER |
| 2 | B | 831 | SER |
| 2 | B | 943 | SER |
| 2 | B | 958 | GLN |
| 2 | B | 1046 | PRO |
| 2 | B | 1069 | PHE |
| 2 | B | 1097 | HIS |
| 2 | B | 1108 | ARG |
| 2 | B | 1156 | ASP |
| 2 | B | 1157 | ALA |
| 2 | B | 1167 | GLY |
| 2 | B | 1175 | LEU |
| 2 | B | 1178 | ASN |
| 2 | B | 1181 | GLU |
| 2 | B | 1182 | CYS |
| 2 | B | 1188 | LYS |
| 3 | C | 4 | GLU |
| 3 | C | 6 | PRO |
| 3 | C | 78 | GLU |
| 3 | C | 87 | PHE |
| 3 | C | 141 | GLY |
| 3 | C | 149 | LYS |
| 3 | C | 156 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 161 | LYS |
| 3 | C | 184 | ASN |
| 3 | C | 209 | TYR |
| 3 | C | 214 | ASN |
| 3 | C | 215 | GLU |
| 4 | D | 5 | THR |
| 4 | D | 8 | PHE |
| 4 | D | 19 | GLU |
| 4 | D | 20 | GLU |
| 4 | D | 52 | LEU |
| 4 | D | 131 | GLU |
| 4 | D | 177 | VAL |
| 4 | D | 199 | ASN |
| 5 | E | 3 | GLN |
| 5 | E | 36 | GLU |
| 5 | E | 59 | SER |
| 5 | E | 73 | PRO |
| 5 | E | 74 | ASP |
| 5 | E | 106 | GLN |
| 5 | E | 130 | ALA |
| 5 | E | 206 | GLY |
| 7 | G | 63 | PRO |
| 7 | G | 139 | ILE |
| 8 | H | 17 | PRO |
| 8 | H | 62 | SER |
| 8 | H | 81 | PRO |
| 8 | H | 82 | PRO |
| 8 | H | 108 | SER |
| 8 | H | 128 | ASN |
| 9 | I | 3 | THR |
| 9 | I | 9 | ASP |
| 9 | I | 79 | HIS |
| 10 | J | 2 | ILE |
| 10 | J | 6 | ARG |
| 10 | J | 32 | GLU |
| 10 | J | 64 | ASN |
| 11 | K | 110 | ASN |
| 12 | L | 35 | SER |
| 12 | L | 50 | ASP |
| 12 | L | 59 | ALA |
| 12 | L | 60 | ARG |
| 1 | A | 42 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 54 | ASN |
| 1 | A | 59 | GLY |
| 1 | A | 61 | ILE |
| 1 | A | 66 | LYS |
| 1 | A | 70 | CYS |
| 1 | A | 76 | GLU |
| 1 | A | 84 | ILE |
| 1 | A | 148 | CYS |
| 1 | A | 154 | SER |
| 1 | A | 250 | ILE |
| 1 | A | 253 | ASN |
| 1 | A | 283 | GLY |
| 1 | A | 386 | ASP |
| 1 | A | 394 | ASN |
| 1 | A | 399 | HIS |
| 1 | A | 439 | ASN |
| 1 | A | 517 | ASN |
| 1 | A | 619 | LYS |
| 1 | A | 661 | GLY |
| 1 | A | 731 | ARG |
| 1 | A | 780 | VAL |
| 1 | A | 979 | SER |
| 1 | A | 1054 | LEU |
| 1 | A | 1116 | LEU |
| 1 | A | 1120 | LEU |
| 1 | A | 1124 | HIS |
| 1 | A | 1127 | ASP |
| 1 | A | 1233 | ASP |
| 1 | A | 1280 | GLU |
| 1 | A | 1377 | THR |
| 1 | A | 1386 | ARG |
| 1 | A | 1395 | GLY |
| 1 | A | 1402 | PHE |
| 2 | B | 28 | GLU |
| 2 | B | 48 | LEU |
| 2 | B | 65 | GLU |
| 2 | B | 260 | GLY |
| 2 | B | 264 | SER |
| 2 | B | 266 | ALA |
| 2 | B | 282 | ILE |
| 2 | B | 387 | LEU |
| 2 | B | 401 | PHE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 450 | ALA |
| 2 | B | 466 | TRP |
| 2 | B | 605 | ARG |
| 2 | B | 613 | VAL |
| 2 | B | 619 | ILE |
| 2 | B | 641 | GLU |
| 2 | B | 655 | LYS |
| 2 | B | 708 | GLU |
| 2 | B | 746 | SER |
| 2 | B | 751 | VAL |
| 2 | B | 792 | MET |
| 2 | B | 869 | SER |
| 2 | B | 881 | ASN |
| 2 | B | 891 | ASP |
| 2 | B | 907 | GLY |
| 2 | B | 945 | GLU |
| 2 | B | 1065 | GLN |
| 2 | B | 1100 | ASP |
| 2 | B | 1155 | SER |
| 2 | B | 1171 | VAL |
| 2 | B | 1183 | LYS |
| 2 | B | 1186 | ASP |
| 3 | C | 81 | GLU |
| 3 | C | 110 | THR |
| 3 | C | 175 | ALA |
| 3 | C | 213 | PRO |
| 3 | C | 216 | GLY |
| 3 | C | 240 | VAL |
| 4 | D | 12 | ARG |
| 4 | D | 21 | GLU |
| 4 | D | 65 | GLU |
| 4 | D | 192 | LYS |
| 5 | E | 45 | LYS |
| 7 | G | 19 | GLY |
| 8 | H | 21 | ASN |
| 8 | H | 32 | THR |
| 8 | H | 59 | ILE |
| 8 | H | 77 | ARG |
| 8 | H | 84 | ALA |
| 8 | H | 140 | ALA |
| 9 | I | 11 | ASN |
| 9 | I | 34 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | I | 57 | GLY |
| 9 | I | 78 | CYS |
| 9 | I | 106 | CYS |
| 10 | J | 14 | VAL |
| 10 | J | 17 | LYS |
| 10 | J | 27 | GLU |
| 10 | J | 28 | ASP |
| 10 | J | 29 | GLU |
| 11 | K | 7 | PHE |
| 11 | K | 15 | GLY |
| 12 | L | 26 | THR |
| 12 | L | 53 | HIS |
| 12 | L | 55 | ILE |
| 1 | A | 263 | THR |
| 1 | A | 336 | ILE |
| 1 | A | 409 | SER |
| 1 | A | 418 | SER |
| 1 | A | 424 | ILE |
| 1 | A | 525 | GLN |
| 1 | A | 526 | ASP |
| 1 | A | 544 | ASP |
| 1 | A | 592 | ASP |
| 1 | A | 648 | ASN |
| 1 | A | 649 | ILE |
| 1 | A | 673 | GLY |
| 1 | A | 759 | ALA |
| 1 | A | 846 | GLU |
| 1 | A | 871 | ASP |
| 1 | A | 1014 | ALA |
| 1 | A | 1165 | GLU |
| 1 | A | 1221 | LYS |
| 1 | A | 1335 | ILE |
| 1 | A | 1392 | SER |
| 2 | B | 94 | LYS |
| 2 | B | 114 | PRO |
| 2 | B | 124 | TYR |
| 2 | B | 259 | TYR |
| 2 | B | 591 | ARG |
| 2 | B | 629 | ASP |
| 2 | B | 711 | GLU |
| 2 | B | 754 | SER |
| 2 | B | 772 | ALA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 818 | PRO |
| 2 | B | 951 | GLN |
| 2 | B | 1041 | GLU |
| 3 | C | 51 | VAL |
| 3 | C | 56 | THR |
| 3 | C | 60 | ASP |
| 3 | C | 148 | ARG |
| 3 | C | 264 | GLN |
| 4 | D | 6 | SER |
| 4 | D | 9 | GLN |
| 4 | D | 30 | GLY |
| 4 | D | 53 | SER |
| 5 | E | 115 | ASN |
| 5 | E | 192 | ARG |
| 6 | F | 81 | THR |
| 7 | G | 140 | LYS |
| 8 | H | 92 | ASP |
| 9 | I | 47 | GLU |
| 9 | I | 62 | ILE |
| 10 | J | 24 | LEU |
| 10 | J | 33 | GLY |
| 10 | J | 55 | ASP |
| 11 | K | 29 | ASN |
| 11 | K | 53 | ASP |
| 11 | K | 88 | LYS |
| 11 | K | 104 | ASN |
| 1 | A | 113 | LEU |
| 1 | A | 169 | ASN |
| 1 | A | 245 | PRO |
| 1 | A | 317 | LYS |
| 1 | A | 332 | LYS |
| 1 | A | 483 | ASP |
| 1 | A | 516 | SER |
| 1 | A | 591 | PHE |
| 1 | A | 605 | MET |
| 1 | A | 636 | GLU |
| 1 | A | 975 | HIS |
| 1 | A | 1277 | GLU |
| 1 | A | 1366 | ARG |
| 1 | A | 1454 | MET |
| 2 | B | 56 | ASP |
| 2 | B | 58 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 229 | ALA |
| 2 | B | 257 | LYS |
| 2 | B | 283 | VAL |
| 2 | B | 322 | PHE |
| 2 | B | 389 | ALA |
| 2 | B | 894 | ASP |
| 2 | B | 1003 | ALA |
| 2 | B | 1017 | ILE |
| 2 | B | 1035 | ALA |
| 3 | C | 117 | ASP |
| 3 | C | 167 | HIS |
| 6 | F | 154 | ASP |
| 7 | G | 17 | PHE |
| 7 | G | 20 | PRO |
| 7 | G | 62 | LEU |
| 7 | G | 154 | VAL |
| 8 | H | 52 | GLN |
| 8 | H | 90 | ALA |
| 9 | I | 107 | SER |
| 9 | I | 113 | ASP |
| 10 | J | 8 | PHE |
| 10 | J | 63 | TYR |
| 11 | K | 90 | ALA |
| 1 | A | 69 | THR |
| 1 | A | 86 | LEU |
| 1 | A | 226 | GLU |
| 1 | A | 244 | PRO |
| 1 | A | 290 | GLU |
| 1 | A | 400 | PRO |
| 1 | A | 604 | GLY |
| 1 | A | 720 | ARG |
| 1 | A | 824 | LEU |
| 1 | A | 895 | LYS |
| 1 | A | 926 | GLN |
| 1 | A | 958 | VAL |
| 1 | A | 1389 | PHE |
| 2 | B | 61 | ASP |
| 2 | B | 231 | PRO |
| 2 | B | 245 | GLU |
| 2 | B | 248 | SER |
| 2 | B | 365 | THR |
| 2 | B | 369 | GLY |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 571 | PRO |
| 2 | B | 728 | ARG |
| 2 | B | 770 | GLN |
| 2 | B | 848 | ARG |
| 2 | B | 880 | THR |
| 2 | B | 1103 | ILE |
| 3 | C | 142 | VAL |
| 3 | C | 208 | GLU |
| 4 | D | 119 | ARG |
| 4 | D | 218 | GLU |
| 7 | G | 115 | MET |
| 8 | H | 43 | ASN |
| 8 | H | 44 | VAL |
| 9 | I | 59 | VAL |
| 10 | J | 18 | TRP |
| 11 | K | 112 | GLN |
| 12 | L | 39 | SER |
| 12 | L | 57 | LEU |
| 1 | A | 43 | GLU |
| 1 | A | 71 | GLN |
| 1 | A | 96 | ILE |
| 1 | A | 111 | GLY |
| 1 | A | 135 | PHE |
| 1 | A | 825 | ILE |
| 2 | B | 100 | PRO |
| 2 | B | 341 | LEU |
| 2 | B | 530 | GLY |
| 2 | B | 752 | ALA |
| 2 | B | 824 | ILE |
| 3 | C | 126 | GLY |
| 4 | D | 196 | PRO |
| 11 | K | 41 | THR |
| 12 | L | 54 | ARG |
| 1 | A | 196 | GLU |
| 2 | B | 1018 | PRO |
| 2 | B | 1214 | PRO |
| 1 | A | 55 | ASP |
| 1 | A | 1158 | PRO |
| 1 | A | 1164 | PRO |
| 2 | B | 364 | ILE |
| 2 | B | 611 | PRO |
| 2 | B | 729 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 901 | PRO |
| 7 | G | 34 | VAL |
| 1 | A | 357 | PRO |
| 1 | A | 364 | VAL |
| 1 | A | 410 | GLY |
| 1 | A | 492 | PRO |
| 1 | A | 718 | VAL |
| 3 | C | 212 | PRO |
| 3 | C | 255 | VAL |
| 1 | A | 35 | ILE |
| 1 | A | 99 | ILE |
| 1 | A | 842 | VAL |
| 2 | B | 758 | PHE |
| 2 | B | 867 | GLY |
| 3 | C | 139 | GLY |
| 1 | A | 652 | VAL |
| 1 | A | 653 | VAL |
| 2 | B | 636 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 1244/1520 (82%) | 1138 (92%) | 106 (8%) | 10 40 |
| 2 | B | 967/1061 (91%) | 890 (92%) | 77 (8%) | 12 42 |
| 3 | C | 235/274 (86%) | 215 (92%) | 20 (8%) | 10 40 |
| 4 | D | 159/200 (80%) | 136 (86%) | 23 (14%) | 3 19 |
| 5 | E | 196/197 (100%) | 191 (97%) | 5 (3%) | 46 69 |
| 6 | F | 77/137 (56%) | 68 (88%) | 9 (12%) | 5 27 |
| 7 | G | 152/152 (100%) | 140 (92%) | 12 (8%) | 12 42 |
| 8 | H | 119/128 (93%) | 112 (94%) | 7 (6%) | 19 51 |
| 9 | I | 110/116 (95%) | 97 (88%) | 13 (12%) | 5 26 |
| 10 | J | 60/65 (92%) | 53 (88%) | 7 (12%) | 5 27 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 11 | K | 99/102 (97%) | 86 (87%) | 13 (13%) | 4 23 |
| 12 | L | 40/57 (70%) | 36 (90%) | 4 (10%) | 7 32 |
| All | All | 3458/4009 (86%) | 3162 (91%) | 296 (9%) | 10 40 |

All (296) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | VAL |
| 1 | A | 5 | GLN |
| 1 | A | 11 | LEU |
| 1 | A | 34 | LYS |
| 1 | A | 37 | PHE |
| 1 | A | 38 | PRO |
| 1 | A | 62 | ASP |
| 1 | A | 67 | CYS |
| 1 | A | 83 | HIS |
| 1 | A | 93 | VAL |
| 1 | A | 108 | MET |
| 1 | A | 122 | MET |
| 1 | A | 130 | ASP |
| 1 | A | 142 | CYS |
| 1 | A | 198 | GLU |
| 1 | A | 200 | ARG |
| 1 | A | 215 | SER |
| 1 | A | 245 | PRO |
| 1 | A | 270 | LEU |
| 1 | A | 302 | THR |
| 1 | A | 312 | PRO |
| 1 | A | 320 | ARG |
| 1 | A | 326 | ARG |
| 1 | A | 335 | ARG |
| 1 | A | 344 | ARG |
| 1 | A | 350 | ARG |
| 1 | A | 381 | THR |
| 1 | A | 385 | ILE |
| 1 | A | 404 | TYR |
| 1 | A | 406 | ILE |
| 1 | A | 407 | ARG |
| 1 | A | 408 | ASP |
| 1 | A | 412 | ARG |
| 1 | A | 418 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 425 | GLN |
| 1 | A | 443 | LEU |
| 1 | A | 445 | ASN |
| 1 | A | 450 | LEU |
| 1 | A | 451 | HIS |
| 1 | A | 462 | VAL |
| 1 | A | 466 | SER |
| 1 | A | 470 | LEU |
| 1 | A | 475 | THR |
| 1 | A | 481 | ASP |
| 1 | A | 493 | GLN |
| 1 | A | 515 | GLN |
| 1 | A | 527 | THR |
| 1 | A | 560 | ILE |
| 1 | A | 562 | THR |
| 1 | A | 577 | ILE |
| 1 | A | 618 | GLU |
| 1 | A | 626 | ASN |
| 1 | A | 629 | LEU |
| 1 | A | 666 | ILE |
| 1 | A | 670 | ILE |
| 1 | A | 711 | ARG |
| 1 | A | 768 | GLN |
| 1 | A | 774 | ARG |
| 1 | A | 779 | PHE |
| 1 | A | 821 | ARG |
| 1 | A | 831 | THR |
| 1 | A | 845 | LEU |
| 1 | A | 858 | ASN |
| 1 | A | 859 | SER |
| 1 | A | 886 | ILE |
| 1 | A | 890 | ASP |
| 1 | A | 903 | ASN |
| 1 | A | 906 | HIS |
| 1 | A | 907 | THR |
| 1 | A | 929 | LEU |
| 1 | A | 940 | ARG |
| 1 | A | 969 | GLN |
| 1 | A | 992 | ASP |
| 1 | A | 1029 | ARG |
| 1 | A | 1030 | ARG |
| 1 | A | 1035 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1052 | GLN |
| 1 | A | 1067 | LEU |
| 1 | A | 1110 | ASN |
| 1 | A | 1116 | LEU |
| 1 | A | 1122 | PRO |
| 1 | A | 1127 | ASP |
| 1 | A | 1170 | ILE |
| 1 | A | 1187 | GLN |
| 1 | A | 1206 | ASP |
| 1 | A | 1264 | GLU |
| 1 | A | 1271 | ILE |
| 1 | A | 1291 | VAL |
| 1 | A | 1295 | THR |
| 1 | A | 1309 | ASP |
| 1 | A | 1332 | PHE |
| 1 | A | 1333 | ILE |
| 1 | A | 1359 | ASP |
| 1 | A | 1364 | ASN |
| 1 | A | 1366 | ARG |
| 1 | A | 1372 | VAL |
| 1 | A | 1376 | THR |
| 1 | A | 1385 | THR |
| 1 | A | 1386 | ARG |
| 1 | A | 1389 | PHE |
| 1 | A | 1405 | THR |
| 1 | A | 1432 | GLN |
| 1 | A | 1442 | ASP |
| 1 | A | 1443 | VAL |
| 1 | A | 1444 | MET |
| 1 | A | 1445 | ILE |
| 2 | B | 30 | SER |
| 2 | B | 35 | SER |
| 2 | B | 37 | PHE |
| 2 | B | 57 | TYR |
| 2 | B | 106 | ASP |
| 2 | B | 128 | LEU |
| 2 | B | 175 | ARG |
| 2 | B | 180 | TYR |
| 2 | B | 188 | ASP |
| 2 | B | 194 | GLU |
| 2 | B | 199 | MET |
| 2 | B | 217 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 218 | SER |
| 2 | B | 223 | VAL |
| 2 | B | 268 | THR |
| 2 | B | 298 | LEU |
| 2 | B | 365 | THR |
| 2 | B | 371 | GLU |
| 2 | B | 393 | LYS |
| 2 | B | 396 | ASP |
| 2 | B | 399 | ASP |
| 2 | B | 427 | ASP |
| 2 | B | 429 | PHE |
| 2 | B | 463 | THR |
| 2 | B | 465 | ASN |
| 2 | B | 466 | TRP |
| 2 | B | 485 | ARG |
| 2 | B | 496 | ARG |
| 2 | B | 498 | THR |
| 2 | B | 502 | ILE |
| 2 | B | 513 | GLN |
| 2 | B | 516 | ASN |
| 2 | B | 557 | PHE |
| 2 | B | 582 | VAL |
| 2 | B | 593 | PRO |
| 2 | B | 603 | LEU |
| 2 | B | 615 | MET |
| 2 | B | 635 | ARG |
| 2 | B | 644 | GLU |
| 2 | B | 682 | SER |
| 2 | B | 684 | LEU |
| 2 | B | 724 | ASP |
| 2 | B | 737 | THR |
| 2 | B | 742 | GLU |
| 2 | B | 790 | ASP |
| 2 | B | 811 | TYR |
| 2 | B | 830 | TYR |
| 2 | B | 835 | GLN |
| 2 | B | 837 | ASP |
| 2 | B | 839 | MET |
| 2 | B | 857 | ARG |
| 2 | B | 878 | GLN |
| 2 | B | 901 | PRO |
| 2 | B | 909 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 935 | ARG |
| 2 | B | 939 | THR |
| 2 | B | 953 | LEU |
| 2 | B | 999 | MET |
| 2 | B | 1002 | THR |
| 2 | B | 1006 | ILE |
| 2 | B | 1022 | THR |
| 2 | B | 1047 | PHE |
| 2 | B | 1069 | PHE |
| 2 | B | 1084 | GLN |
| 2 | B | 1087 | PHE |
| 2 | B | 1092 | TYR |
| 2 | B | 1095 | LEU |
| 2 | B | 1099 | VAL |
| 2 | B | 1106 | ARG |
| 2 | B | 1108 | ARG |
| 2 | B | 1159 | ARG |
| 2 | B | 1160 | VAL |
| 2 | B | 1170 | THR |
| 2 | B | 1176 | ASN |
| 2 | B | 1183 | LYS |
| 2 | B | 1202 | LEU |
| 2 | B | 1216 | LEU |
| 3 | C | 22 | LEU |
| 3 | C | 48 | SER |
| 3 | C | 56 | THR |
| 3 | C | 58 | LEU |
| 3 | C | 62 | PHE |
| 3 | C | 77 | ILE |
| 3 | C | 99 | LEU |
| 3 | C | 104 | PHE |
| 3 | C | 108 | GLU |
| 3 | C | 129 | ILE |
| 3 | C | 140 | ASN |
| 3 | C | 145 | CYS |
| 3 | C | 147 | LEU |
| 3 | C | 151 | GLN |
| 3 | C | 163 | ILE |
| 3 | C | 193 | TYR |
| 3 | C | 214 | ASN |
| 3 | C | 240 | VAL |
| 3 | C | 259 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 266 | ASP |
| 4 | D | 8 | PHE |
| 4 | D | 13 | ARG |
| 4 | D | 16 | LYS |
| 4 | D | 17 | LYS |
| 4 | D | 19 | GLU |
| 4 | D | 22 | GLU |
| 4 | D | 47 | LEU |
| 4 | D | 63 | LEU |
| 4 | D | 70 | PHE |
| 4 | D | 137 | ASN |
| 4 | D | 139 | LYS |
| 4 | D | 148 | LEU |
| 4 | D | 149 | THR |
| 4 | D | 156 | ASP |
| 4 | D | 159 | THR |
| 4 | D | 170 | THR |
| 4 | D | 174 | PRO |
| 4 | D | 182 | SER |
| 4 | D | 187 | THR |
| 4 | D | 192 | LYS |
| 4 | D | 193 | THR |
| 4 | D | 208 | GLU |
| 4 | D | 221 | TYR |
| 5 | E | 60 | PHE |
| 5 | E | 74 | ASP |
| 5 | E | 104 | ASN |
| 5 | E | 114 | ASN |
| 5 | E | 183 | PRO |
| 6 | F | 79 | ARG |
| 6 | F | 90 | ARG |
| 6 | F | 99 | LEU |
| 6 | F | 111 | LEU |
| 6 | F | 119 | ARG |
| 6 | F | 123 | LYS |
| 6 | F | 143 | PHE |
| 6 | F | 148 | VAL |
| 6 | F | 153 | VAL |
| 7 | G | 1 | MET |
| 7 | G | 13 | LEU |
| 7 | G | 17 | PHE |
| 7 | G | 74 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | G | 78 | VAL |
| 7 | G | 80 | LYS |
| 7 | G | 88 | ASP |
| 7 | G | 96 | GLN |
| 7 | G | 115 | MET |
| 7 | G | 118 | ASP |
| 7 | G | 126 | ASN |
| 7 | G | 171 | ILE |
| 8 | H | 86 | ASP |
| 8 | H | 93 | TYR |
| 8 | H | 95 | TYR |
| 8 | H | 102 | TYR |
| 8 | H | 130 | ARG |
| 8 | H | 134 | ASN |
| 8 | H | 143 | LEU |
| 9 | I | 8 | ARG |
| 9 | I | 9 | ASP |
| 9 | I | 15 | TYR |
| 9 | I | 34 | TYR |
| 9 | I | 40 | SER |
| 9 | I | 75 | CYS |
| 9 | I | 78 | CYS |
| 9 | I | 85 | PHE |
| 9 | I | 86 | PHE |
| 9 | I | 94 | ASP |
| 9 | I | 99 | LEU |
| 9 | I | 101 | PHE |
| 9 | I | 106 | CYS |
| 10 | J | 7 | CYS |
| 10 | J | 9 | SER |
| 10 | J | 10 | CYS |
| 10 | J | 28 | ASP |
| 10 | J | 44 | TYR |
| 10 | J | 46 | CYS |
| 10 | J | 48 | ARG |
| 11 | K | 5 | ASP |
| 11 | K | 10 | PHE |
| 11 | K | 25 | THR |
| 11 | K | 42 | LEU |
| 11 | K | 47 | ARG |
| 11 | K | 50 | LEU |
| 11 | K | 61 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | K | 68 | PHE |
| 11 | K | 78 | THR |
| 11 | K | 81 | TYR |
| 11 | K | 111 | LEU |
| 11 | K | 112 | GLN |
| 11 | K | 113 | THR |
| 12 | L | 51 | CYS |
| 12 | L | 55 | ILE |
| 12 | L | 65 | VAL |
| 12 | L | 70 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 54 | ASN |
| 1 | A | 64 | ASN |
| 1 | A | 68 | GLN |
| 1 | A | 71 | GLN |
| 1 | A | 83 | HIS |
| 1 | A | 92 | HIS |
| 1 | A | 225 | ASN |
| 1 | A | 339 | ASN |
| 1 | A | 358 | ASN |
| 1 | A | 435 | HIS |
| 1 | A | 479 | ASN |
| 1 | A | 517 | ASN |
| 1 | A | 631 | HIS |
| 1 | A | 654 | ASN |
| 1 | A | 698 | GLN |
| 1 | A | 736 | ASN |
| 1 | A | 741 | ASN |
| 1 | A | 757 | ASN |
| 1 | A | 767 | GLN |
| 1 | A | 768 | GLN |
| 1 | A | 786 | HIS |
| 1 | A | 858 | ASN |
| 1 | A | 903 | ASN |
| 1 | A | 926 | GLN |
| 1 | A | 965 | GLN |
| 1 | A | 1140 | HIS |
| 1 | A | 1218 | GLN |
| 1 | A | 1364 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1432 | GLN |
| 2 | B | 121 | ASN |
| 2 | B | 178 | ASN |
| 2 | B | 215 | GLN |
| 2 | B | 236 | HIS |
| 2 | B | 363 | HIS |
| 2 | B | 366 | GLN |
| 2 | B | 449 | ASN |
| 2 | B | 465 | ASN |
| 2 | B | 513 | GLN |
| 2 | B | 515 | HIS |
| 2 | B | 516 | ASN |
| 2 | B | 518 | HIS |
| 2 | B | 538 | ASN |
| 2 | B | 734 | HIS |
| 2 | B | 744 | HIS |
| 2 | B | 776 | GLN |
| 2 | B | 794 | ASN |
| 2 | B | 821 | GLN |
| 2 | B | 842 | ASN |
| 2 | B | 975 | GLN |
| 2 | B | 1015 | HIS |
| 2 | B | 1025 | HIS |
| 2 | B | 1065 | GLN |
| 2 | B | 1076 | HIS |
| 2 | B | 1084 | GLN |
| 2 | B | 1117 | GLN |
| 2 | B | 1141 | HIS |
| 2 | B | 1179 | GLN |
| 2 | B | 1193 | GLN |
| 3 | C | 73 | GLN |
| 3 | C | 112 | ASN |
| 3 | C | 123 | ASN |
| 3 | C | 167 | HIS |
| 3 | C | 231 | ASN |
| 3 | C | 252 | GLN |
| 4 | D | 39 | ASN |
| 4 | D | 40 | HIS |
| 4 | D | 137 | ASN |
| 5 | E | 8 | ASN |
| 5 | E | 101 | GLN |
| 5 | E | 104 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 114 | ASN |
| 5 | E | 147 | HIS |
| 7 | G | 53 | ASN |
| 7 | G | 97 | HIS |
| 7 | G | 122 | ASN |
| 7 | G | 126 | ASN |
| 9 | I | 12 | ASN |
| 9 | I | 90 | GLN |
| 10 | J | 53 | HIS |
| 10 | J | 64 | ASN |
| 11 | K | 44 | ASN |
| 11 | K | 65 | HIS |
| 11 | K | 76 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 14 | P | 9/11 (81%) | 3 (33%) | 1 (11%) |

All (3) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | P | 7 | A |
| 14 | P | 8 | G |
| 14 | P | 9 | A |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | P | 7 | A |

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection.

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 15 | BRU | T | 22 | 15,14 | 18,21,22 | 0.44 | 0 | 26,30,33 | 0.99 | 1 (3%) |
| 15 | TT | T | 19 | 15 | 40,43,44 | 4.90 | 12 (30%) | 59,69,72 | 2.36 | 17 (28%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 15 | BRU | T | 22 | 15,14 | - | 0/7/21/22 | 0/2/2/2 |
| 15 | TT | T | 19 | 15 | - | 11/18/105/106 | 0/5/6/6 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | T | 19 | TT | C5-C6 | -21.02 | 1.31 | 1.55 |
| 15 | T | 19 | TT | C5T-C6T | -20.02 | 1.32 | 1.55 |
| 15 | T | 19 | TT | C6-N1 | -5.36 | 1.38 | 1.46 |
| 15 | T | 19 | TT | C1'-N1 | 4.04 | 1.50 | 1.45 |
| 15 | T | 19 | TT | C6T-N1T | -3.72 | 1.40 | 1.46 |
| 15 | T | 19 | TT | O3'-C3' | 2.66 | 1.48 | 1.43 |
| 15 | T | 19 | TT | C2-N1 | 2.58 | 1.41 | 1.36 |
| 15 | T | 19 | TT | C6T-C6 | 2.54 | 1.64 | 1.56 |
| 15 | T | 19 | TT | C1R-N1T | 2.53 | 1.49 | 1.45 |
| 15 | T | 19 | TT | O4-C4 | 2.24 | 1.26 | 1.22 |
| 15 | T | 19 | TT | C4-N3 | 2.07 | 1.40 | 1.37 |
| 15 | T | 19 | TT | O5'-C5' | 2.01 | 1.49 | 1.44 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | T | 19 | TT | C5-C6-N1 | 8.44 | 127.43 | 115.61 |
| 15 | T | 19 | TT | C5T-C6T-N1T | 6.14 | 124.22 | 115.61 |
| 15 | T | 19 | TT | C5T-C5-C6 | 6.02 | 95.86 | 88.38 |
| 15 | T | 19 | TT | C5-C6-C6T | -5.71 | 79.91 | 89.28 |
| 15 | T | 19 | TT | C5-C5T-C6T | -5.45 | 81.59 | 88.38 |
| 15 | T | 19 | TT | O4-C4-C5 | 3.62 | 125.77 | 122.88 |
| 15 | T | 19 | TT | C5'-C4'-C3' | 3.08 | 121.57 | 114.53 |
| 15 | T | 19 | TT | N3T-C2T-N1T | -2.94 | 113.64 | 116.69 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | T | 19 | TT | O4R-C4R-C5R | 2.82 | 118.67 | 109.37 |
| 15 | T | 22 | BRU | C6-C5-C4 | -2.62 | 118.02 | 120.67 |
| 15 | T | 19 | TT | N3-C2-N1 | -2.55 | 114.04 | 116.69 |
| 15 | T | 19 | TT | C6-C6T-N1T | 2.46 | 128.06 | 118.20 |
| 15 | T | 19 | TT | C2R-C1R-N1T | -2.31 | 112.47 | 115.59 |
| 15 | T | 19 | TT | C5A-C5-C6 | -2.30 | 107.08 | 114.16 |
| 15 | T | 19 | TT | C5T-C6T-C6 | 2.26 | 92.99 | 89.28 |
| 15 | T | 19 | TT | O4T-C4T-C5T | 2.14 | 124.58 | 122.88 |
| 15 | T | 19 | TT | C5-C4-N3 | -2.13 | 114.20 | 116.06 |
| 15 | T | 19 | TT | O3R-C3R-C4R | -2.06 | 102.21 | 110.10 |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | T | 19 | TT | C4'-C5'-O5'-P |
| 15 | T | 19 | TT | O3'-C7-O5R-C5R |
| 15 | T | 19 | TT | C2R-C1R-N1T-C6T |
| 15 | T | 19 | TT | C2'-C1'-N1-C6 |
| 15 | T | 19 | TT | C2'-C1'-N1-C2 |
| 15 | T | 19 | TT | O4'-C1'-N1-C2 |
| 15 | T | 19 | TT | O4'-C1'-N1-C6 |
| 15 | T | 19 | TT | O4R-C1R-N1T-C6T |
| 15 | T | 19 | TT | O5R-C7-O3'-C3' |
| 15 | T | 19 | TT | C4R-C5R-O5R-C7 |
| 15 | T | 19 | TT | O4R-C1R-N1T-C2T |

There are no ring outliers.

2 monomers are involved in 31 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 15 | T | 22 | BRU | 5 | 0 |
| 15 | T | 19 | TT | 26 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 2 | B | 2 |
| 3 | C | 1 |
| 6 | F | 1 |
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 2:SER | C | 3:GLU | N | 4.15 |
| 1 | B | 18:PHE | C | 19:GLU | N | 3.85 |
| 1 | F | 69:LEU | C | 70:LYS | N | 3.50 |
| 1 | A | 1175:SER | C | 1176:LEU | N | 3.39 |
| 1 | B | 337:ARG | C | 338:GLY | N | 2.64 |

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 1421/1733 (81%) | -0.37 | 9 (0%) 89 85 | 17, 78, 152, 199 | 0 |
| 2 | B | 1115/1224 (91%) | -0.28 | 12 (1%) 80 74 | 20, 91, 167, 200 | 0 |
| 3 | C | 267/318 (83%) | -0.41 | 0 100 100 | 39, 77, 139, 165 | 0 |
| 4 | D | 177/221 (80%) | -0.17 | 2 (1%) 80 74 | 61, 111, 160, 175 | 0 |
| 5 | E | 214/215 (99%) | -0.28 | 2 (0%) 84 79 | 50, 133, 184, 188 | 0 |
| 6 | F | 87/155 (56%) | -0.52 | 0 100 100 | 27, 56, 100, 138 | 0 |
| 7 | G | 171/171 (100%) | -0.28 | 0 100 100 | 57, 80, 126, 137 | 0 |
| 8 | H | 135/146 (92%) | 0.24 | 3 (2%) 62 54 | 95, 138, 173, 183 | 0 |
| 9 | I | 116/122 (95%) | -0.12 | 1 (0%) 84 79 | 75, 134, 166, 186 | 0 |
| 10 | J | 65/70 (92%) | -0.61 | 0 100 100 | 42, 73, 117, 125 | 0 |
| 11 | K | 114/120 (95%) | -0.33 | 2 (1%) 68 61 | 38, 83, 112, 167 | 0 |
| 12 | L | 46/70 (65%) | 0.16 | 2 (4%) 35 30 | 78, 156, 175, 181 | 0 |
| 13 | N | 8/14 (57%) | 0.51 | 0 100 100 | 129, 140, 153, 155 | 0 |
| 14 | P | 10/11 (90%) | 0.12 | 1 (10%) 7 6 | 115, 126, 152, 158 | 0 |
| 15 | T | 17/25 (68%) | 0.37 | 0 100 100 | 125, 138, 151, 153 | 0 |
| All | All | 3963/4615 (85%) | -0.29 | 34 (0%) 84 79 | 17, 89, 165, 200 | 0 |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | K | 114 | LEU | 7.5 |
| 2 | B | 471 | LYS | 6.3 |
| 11 | K | 113 | THR | 5.0 |
| 2 | B | 882 | THR | 4.0 |
| 2 | B | 883 | LEU | 3.4 |
| 1 | A | 1257 | ASP | 3.2 |
| 2 | B | 334 | ILE | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | B | 472 | ALA | 3.0 |
| 5 | E | 110 | PHE | 2.8 |
| 8 | H | 139 | ASN | 2.6 |
| 2 | B | 734 | HIS | 2.6 |
| 1 | A | 257 | ARG | 2.5 |
| 2 | B | 341 | LEU | 2.5 |
| 2 | B | 709 | ASP | 2.5 |
| 1 | A | 253 | ASN | 2.4 |
| 2 | B | 340 | ALA | 2.4 |
| 1 | A | 159 | THR | 2.4 |
| 1 | A | 1455 | PRO | 2.3 |
| 5 | E | 82 | PHE | 2.3 |
| 1 | A | 171 | GLN | 2.3 |
| 12 | L | 50 | ASP | 2.2 |
| 9 | I | 55 | THR | 2.2 |
| 12 | L | 43 | THR | 2.2 |
| 14 | P | 8 | G | 2.2 |
| 1 | A | 251 | SER | 2.2 |
| 2 | B | 113 | TYR | 2.2 |
| 8 | H | 112 | ILE | 2.1 |
| 4 | D | 9 | GLN | 2.1 |
| 8 | H | 140 | ALA | 2.1 |
| 1 | A | 158 | PRO | 2.1 |
| 2 | B | 133 | LYS | 2.1 |
| 2 | B | 884 | ARG | 2.1 |
| 1 | A | 145 | LYS | 2.0 |
| 4 | D | 8 | PHE | 2.1 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 15 | BRU | T | 22 | 20/21 | 0.78 | 0.24 | 112,118,124,128 | 0 |
| 15 | TT | T | 19 | 38/39 | 0.84 | 0.27 | 130,144,163,166 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 17 | ZN | A | 2461 | 1/1 | 0.95 | 0.12 | 200,200,200,200 | 0 |
| 17 | ZN | A | 2459 | 1/1 | 0.98 | 0.03 | 125,125,125,125 | 0 |
| 17 | ZN | A | 2464 | 1/1 | 0.98 | 0.07 | 87,87,87,87 | 0 |
| 17 | ZN | A | 2460 | 1/1 | 0.99 | 0.14 | 88,88,88,88 | 0 |
| 17 | ZN | A | 2458 | 1/1 | 0.99 | 0.16 | 57,57,57,57 | 0 |
| 17 | ZN | A | 2462 | 1/1 | 0.99 | 0.07 | 39,39,39,39 | 0 |
| 17 | ZN | A | 2463 | 1/1 | 0.99 | 0.14 | 47,47,47,47 | 0 |
| 16 | MG | A | 2457 | 1/1 | 0.99 | 0.16 | 35,35,35,35 | 0 |
| 17 | ZN | A | 2465 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.