



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:22 PM JST

PDB ID : 7EIZ
EMDB ID : EMD-31146
Title : Coupling of N7-methyltransferase and 3'-5' exoribonuclease with SARS-CoV-2 polymerase reveals mechanisms for capping and proofreading
Authors : Yan, L.; Yang, Y.X.; Li, M.Y.; Zhang, Y.; Zheng, L.T.; Ge, J.; Huang, Y.C.; Liu, Z.Y.; Wang, T.; Gao, S.; Zhang, R.; Huang, Y.Y.; Guddat, L.W.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on : 2021-04-01
Resolution : Not provided

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

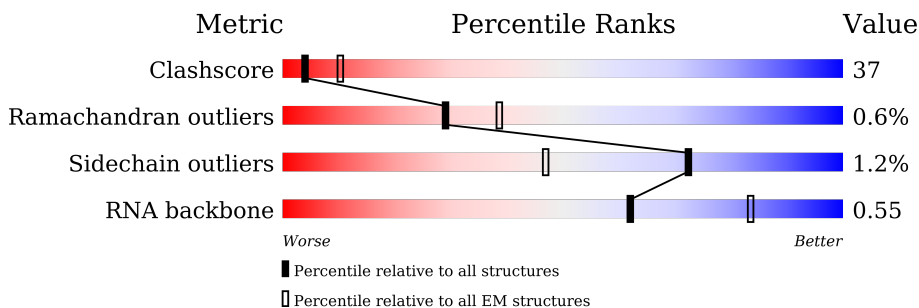
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 929 | 47% 50% . |
| 2 | B | 198 | 46% 47% . 6% |
| 2 | D | 198 | 41% 51% . 6% |
| 3 | C | 83 | 40% 47% 13% |
| 4 | G | 113 | 48% 51% . |
| 5 | H | 139 | 39% 55% 6% |
| 6 | I | 25 | . 56% 40% |
| 7 | J | 27 | 15% 52% 30% . |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 8 | K | 527 | <div><div></div><div>58%</div><div>41%</div><div>..</div></div> |
| 9 | E | 601 | <div><div></div><div>26%</div><div>70%</div><div>..</div></div> |
| 9 | F | 601 | <div><div></div><div>37%</div><div>60%</div><div>..</div></div> |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 926 | Total | C | N | O | S | 0 | 0 |
| | | | 7458 | 4763 | 1251 | 1390 | 54 | | |

- Molecule 2 is a protein called Non-structural protein 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2 | B | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1396 | 872 | 240 | 273 | 11 | | |
| 2 | D | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1414 | 889 | 242 | 272 | 11 | | |

- Molecule 3 is a protein called Non-structural protein 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 3 | C | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 553 | 349 | 91 | 107 | 6 | | |

- Molecule 4 is a protein called Non-structural protein 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | G | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 868 | 549 | 150 | 164 | 5 | | |

- Molecule 5 is a protein called Non-structural protein 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5 | H | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 593 | 160 | 186 | 16 | | |

- Molecule 6 is a RNA chain called primer.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6 | I | 25 | Total | C | N | O | P | 0 | 0 |
| | | | 545 | 242 | 105 | 173 | 25 | | |

- Molecule 7 is a RNA chain called template.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 7 | J | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 565 | 253 | 94 | 191 | 27 | | |

- Molecule 8 is a protein called Proofreading exoribonuclease.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | K | 523 | Total | C | N | O | S | 0 | 0 |
| | | | 4169 | 2674 | 710 | 749 | 36 | | |

- Molecule 9 is a protein called Helicase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | E | 587 | Total | C | N | O | S | 1 | 0 |
| | | | 4544 | 2893 | 765 | 851 | 35 | | |
| 9 | F | 590 | Total | C | N | O | S | 0 | 0 |
| | | | 4602 | 2926 | 781 | 861 | 34 | | |

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 10 | A | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 10 | H | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 10 | K | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 10 | E | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 10 | F | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |

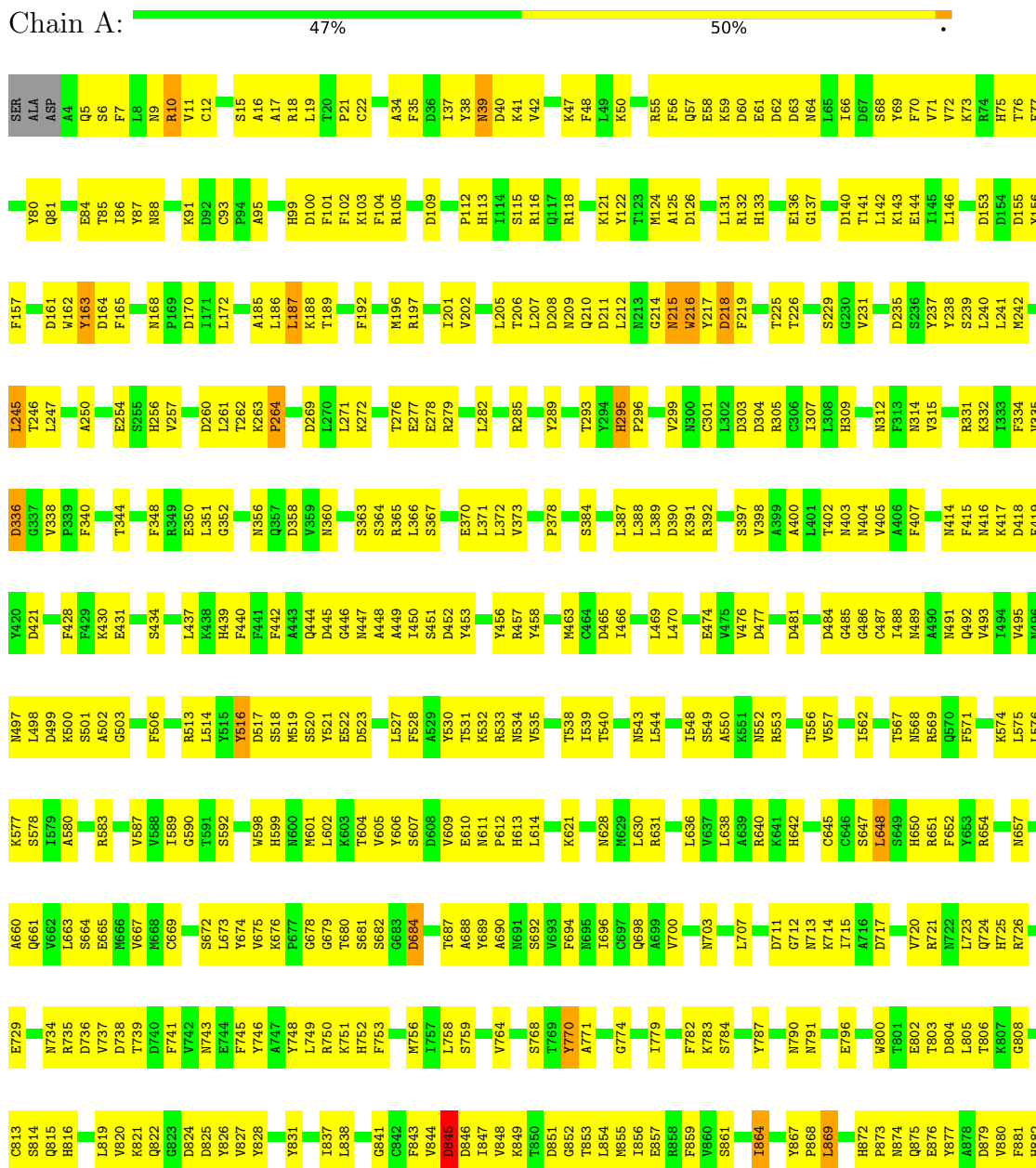
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

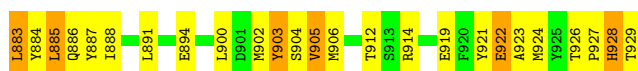
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 11 | K | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

3 Residue-property plots

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

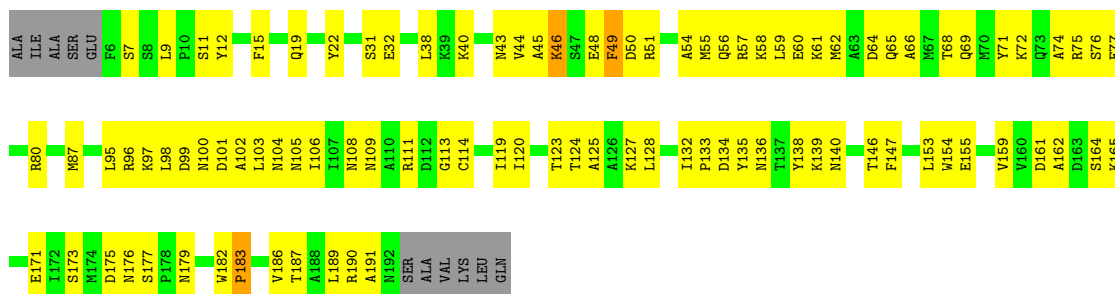
• Molecule 1: RNA-directed RNA polymerase





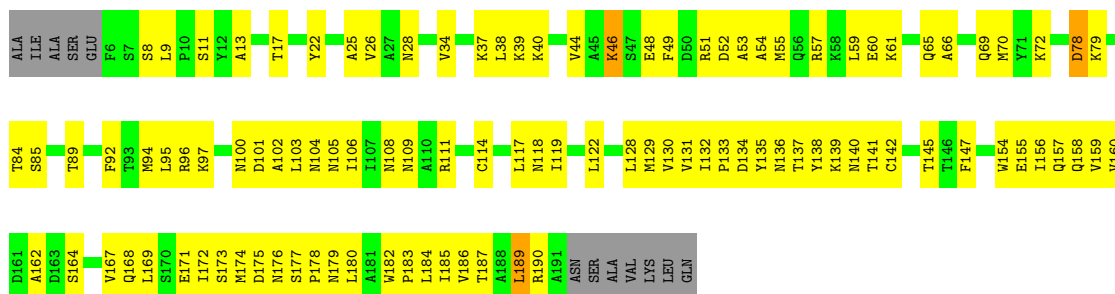
• Molecule 2: Non-structural protein 8

Chain B: 46% 47% 6%



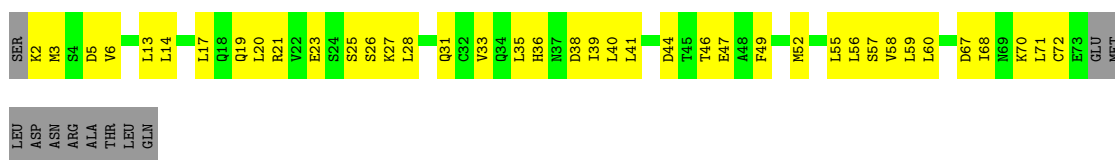
• Molecule 2: Non-structural protein 8

Chain D: 41% 51% 6%



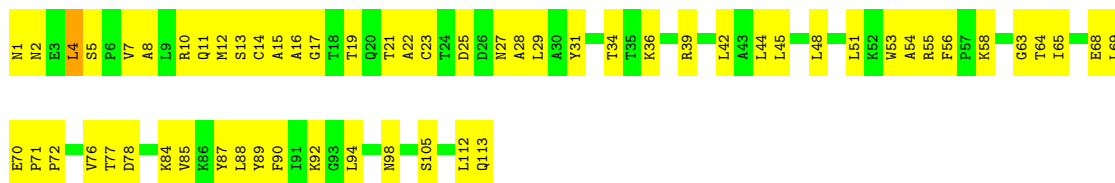
• Molecule 3: Non-structural protein 7

Chain C: 40% 47% 13%



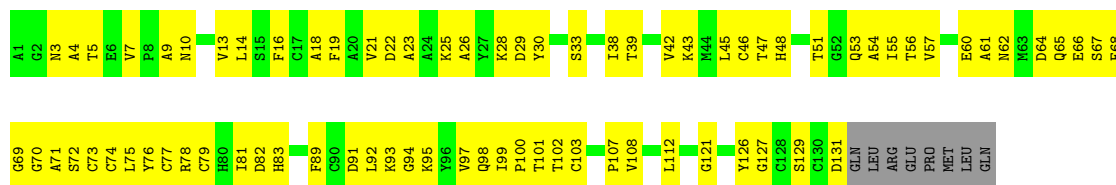
• Molecule 4: Non-structural protein 9

Chain G: 48% 51%



• Molecule 5: Non-structural protein 10

Chain H:  39% 55% 6%




- Molecule 6: primer

Chain I:  56% 40%



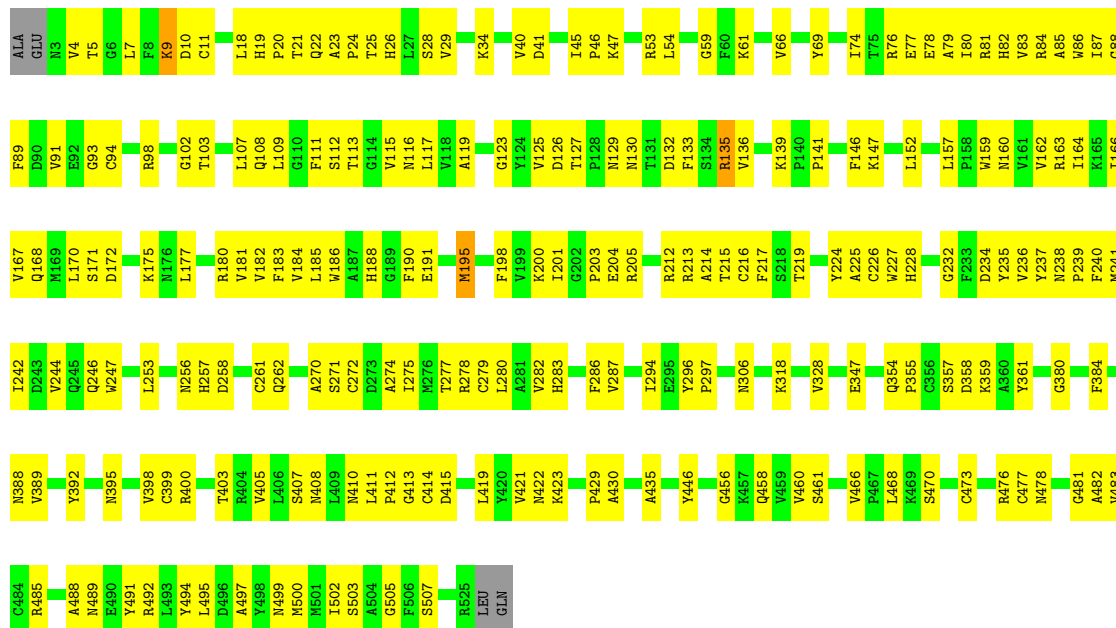
- Molecule 7: template

Chain J:  15% 52% 30%



- Molecule 8: Proofreading exoribonuclease

Chain K:  58% 41%



- Molecule 9: Helicase

Chain E:  26% 70%







4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 80256 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 60 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |

5 Model quality

5.1 Standard geometry

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

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 | 0.98 | 1/7647 (0.0%) | 0.73 | 10/10379 (0.1%) |
| 2 | B | 0.63 | 0/1414 | 0.63 | 0/1922 |
| 2 | D | 0.58 | 0/1433 | 0.64 | 1/1944 (0.1%) |
| 3 | C | 0.79 | 0/556 | 0.76 | 1/749 (0.1%) |
| 4 | G | 0.30 | 0/884 | 0.55 | 1/1200 (0.1%) |
| 5 | H | 0.31 | 0/976 | 0.54 | 0/1327 |
| 6 | I | 1.49 | 5/611 (0.8%) | 1.29 | 1/953 (0.1%) |
| 7 | J | 1.46 | 2/628 (0.3%) | 1.23 | 3/974 (0.3%) |
| 8 | K | 0.29 | 0/4288 | 0.49 | 0/5831 |
| 9 | E | 0.45 | 0/4647 | 0.58 | 0/6329 |
| 9 | F | 0.42 | 0/4706 | 0.56 | 0/6402 |
| All | All | 0.70 | 8/27790 (0.0%) | 0.66 | 17/38010 (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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 2 | B | 0 | 1 |
| 8 | K | 0 | 1 |
| 9 | E | 0 | 1 |
| 9 | F | 0 | 2 |
| All | All | 0 | 7 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | I | 32 | A | N9-C4 | -7.70 | 1.33 | 1.37 |
| 6 | I | 29 | A | N3-C4 | -5.83 | 1.31 | 1.34 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | I | 29 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 6 | I | 31 | C | N1-C6 | -5.60 | 1.33 | 1.37 |
| 7 | J | 26 | A | N9-C4 | -5.43 | 1.34 | 1.37 |
| 1 | A | 216 | TRP | CB-CG | -5.31 | 1.40 | 1.50 |
| 7 | J | 36 | A | N9-C4 | -5.30 | 1.34 | 1.37 |
| 6 | I | 32 | A | N3-C4 | -5.19 | 1.31 | 1.34 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 885 | LEU | CA-CB-CG | -7.54 | 97.97 | 115.30 |
| 7 | J | 34 | C | N1-C2-O2 | -6.39 | 115.06 | 118.90 |
| 1 | A | 187 | LEU | CA-CB-CG | -6.31 | 100.79 | 115.30 |
| 4 | G | 4 | LEU | CA-CB-CG | 5.79 | 128.62 | 115.30 |
| 1 | A | 503 | GLY | C-N-CA | -5.69 | 107.48 | 121.70 |
| 1 | A | 245 | LEU | CB-CG-CD2 | -5.61 | 101.46 | 111.00 |
| 6 | I | 32 | A | C2-N3-C4 | -5.41 | 107.89 | 110.60 |
| 1 | A | 869 | LEU | CA-CB-CG | -5.41 | 102.87 | 115.30 |
| 3 | C | 14 | LEU | CA-CB-CG | -5.37 | 102.95 | 115.30 |
| 7 | J | 34 | C | C2-N1-C1' | -5.35 | 112.92 | 118.80 |
| 1 | A | 845 | ASP | C-N-CA | -5.27 | 108.52 | 121.70 |
| 7 | J | 41 | G | C8-N9-C1' | 5.27 | 133.85 | 127.00 |
| 1 | A | 864 | ILE | CG1-CB-CG2 | -5.22 | 99.92 | 111.40 |
| 2 | D | 189 | LEU | CA-CB-CG | -5.13 | 103.50 | 115.30 |
| 1 | A | 883 | LEU | CA-CB-CG | -5.10 | 103.57 | 115.30 |
| 1 | A | 869 | LEU | CB-CG-CD2 | -5.06 | 102.39 | 111.00 |
| 1 | A | 245 | LEU | CA-CB-CG | -5.04 | 103.70 | 115.30 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 246 | THR | Peptide |
| 1 | A | 848 | VAL | Peptide |
| 2 | B | 182 | TRP | Peptide |
| 9 | E | 406 | PRO | Peptide |
| 9 | F | 442 | ARG | Peptide |
| 9 | F | 45 | VAL | Peptide |
| 8 | K | 195 | MET | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 7458 | 0 | 7191 | 430 | 0 |
| 2 | B | 1396 | 0 | 1365 | 95 | 0 |
| 2 | D | 1414 | 0 | 1416 | 103 | 0 |
| 3 | C | 553 | 0 | 585 | 38 | 0 |
| 4 | G | 868 | 0 | 880 | 59 | 0 |
| 5 | H | 955 | 0 | 911 | 72 | 0 |
| 6 | I | 545 | 0 | 272 | 67 | 0 |
| 7 | J | 565 | 0 | 291 | 64 | 0 |
| 8 | K | 4169 | 0 | 4050 | 196 | 0 |
| 9 | E | 4544 | 0 | 4480 | 524 | 0 |
| 9 | F | 4602 | 0 | 4577 | 390 | 0 |
| 10 | A | 2 | 0 | 0 | 0 | 0 |
| 10 | E | 3 | 0 | 0 | 0 | 0 |
| 10 | F | 3 | 0 | 0 | 0 | 0 |
| 10 | H | 2 | 0 | 0 | 0 | 0 |
| 10 | K | 3 | 0 | 0 | 0 | 0 |
| 11 | K | 1 | 0 | 0 | 0 | 0 |
| All | All | 27083 | 0 | 26018 | 1952 | 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 37.

All (1952) 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) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:55:CYS:SG | 9:F:75:HIS:HE1 | 1.60 | 1.24 |
| 9:E:214:THR:HG1 | 9:E:342:CYS:N | 1.45 | 1.14 |
| 9:E:471:CYS:HA | 9:E:572:ILE:O | 1.49 | 1.11 |
| 9:E:561:PHE:O | 9:E:565:ILE:HB | 1.55 | 1.07 |
| 9:F:8:CYS:SG | 9:F:26:CYS:HB3 | 1.97 | 1.04 |
| 9:E:558:VAL:O | 9:E:562:ASN:HB2 | 1.58 | 1.03 |
| 9:E:55:CYS:SG | 9:E:75:HIS:HE1 | 1.90 | 0.95 |
| 2:D:117:LEU:HD11 | 2:D:131:VAL:HG23 | 1.49 | 0.94 |
| 9:E:576:MET:O | 9:E:579:ARG:NH2 | 2.00 | 0.94 |
| 9:F:284:PRO:HB2 | 9:F:567:ARG:HH22 | 1.33 | 0.92 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:I:19:C:O2 | 7:J:41:G:N2 | 2.01 | 0.92 |
| 1:A:218:ASP:OD2 | 4:G:1:ASN:ND2 | 2.03 | 0.92 |
| 9:E:283:PRO:O | 9:E:288:LYS:NZ | 2.04 | 0.91 |
| 9:F:8:CYS:HB3 | 9:F:29:CYS:SG | 2.11 | 0.91 |
| 2:D:176:ASN:O | 2:D:179:ASN:HB2 | 1.69 | 0.91 |
| 3:C:13:LEU:HD22 | 3:C:55:LEU:HD21 | 1.51 | 0.90 |
| 5:H:3:ASN:H | 8:K:10:ASP:HB3 | 1.34 | 0.90 |
| 9:E:65:LEU:HB3 | 9:E:81:PHE:HB3 | 1.54 | 0.90 |
| 9:E:512:ILE:HD13 | 9:E:544:VAL:HG13 | 1.54 | 0.89 |
| 8:K:257:HIS:CD2 | 8:K:261:CYS:SG | 2.62 | 0.89 |
| 9:F:378:MET:HA | 9:F:406:PRO:HA | 1.54 | 0.88 |
| 9:E:200:PHE:HA | 9:E:211:TYR:HA | 1.54 | 0.88 |
| 8:K:119:ALA:HA | 8:K:157:LEU:H | 1.40 | 0.87 |
| 9:F:453:SER:HB2 | 9:F:459:ASN:HA | 1.57 | 0.87 |
| 9:E:380:THR:HG23 | 9:E:383:ASP:H | 1.37 | 0.86 |
| 8:K:183:PHE:H | 8:K:241:MET:HA | 1.40 | 0.85 |
| 1:A:254:GLU:OE2 | 1:A:285:ARG:NH1 | 2.10 | 0.85 |
| 9:E:370:ILE:HA | 9:E:395:HIS:O | 1.76 | 0.84 |
| 9:E:369:ASP:O | 9:E:395:HIS:N | 2.10 | 0.83 |
| 9:F:332:ARG:NH1 | 9:F:333:ILE:O | 2.11 | 0.83 |
| 9:E:201:GLU:HB2 | 9:E:210:VAL:HB | 1.60 | 0.83 |
| 1:A:336:ASP:HB3 | 1:A:364:SER:HA | 1.60 | 0.83 |
| 9:E:287:GLY:HA3 | 9:E:442:ARG:HH21 | 1.44 | 0.83 |
| 1:A:445:ASP:HB3 | 3:C:33:VAL:HG11 | 1.62 | 0.82 |
| 1:A:305:ARG:NH1 | 1:A:474:GLU:OE2 | 2.13 | 0.82 |
| 1:A:717:ASP:OD2 | 1:A:720:VAL:N | 2.12 | 0.82 |
| 9:E:329:LYS:HB2 | 9:E:354:GLN:HB3 | 1.62 | 0.82 |
| 3:C:21:ARG:NH2 | 3:C:23:GLU:OE2 | 2.12 | 0.81 |
| 9:E:72:CYS:SG | 9:E:73:LYS:N | 2.53 | 0.81 |
| 9:E:512:ILE:HG13 | 9:E:531:GLN:HB3 | 1.61 | 0.81 |
| 9:E:50:CYS:SG | 9:E:72:CYS:HB3 | 2.21 | 0.81 |
| 9:E:457:TYR:HB3 | 9:E:460:LYS:HG2 | 1.61 | 0.81 |
| 9:E:332:ARG:HH11 | 9:E:333:ILE:H | 1.26 | 0.81 |
| 8:K:84:ARG:NH1 | 8:K:297:PRO:O | 2.12 | 0.81 |
| 9:E:152:ALA:HB3 | 9:E:225:PHE:HB2 | 1.62 | 0.81 |
| 9:F:249:ILE:HG12 | 9:F:273:GLY:HA3 | 1.63 | 0.81 |
| 6:I:27:G:N2 | 7:J:34:C:O2 | 2.14 | 0.80 |
| 9:F:50:CYS:SG | 9:F:72:CYS:HB3 | 2.21 | 0.80 |
| 5:H:28:LYS:HE2 | 5:H:112:LEU:HD22 | 1.63 | 0.80 |
| 9:F:329:LYS:HB3 | 9:F:354:GLN:HE21 | 1.46 | 0.80 |
| 9:F:578:ASP:O | 9:F:582:TYR:N | 2.12 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:583:ARG:NH1 | 1:A:590:GLY:O | 2.15 | 0.80 |
| 8:K:135:ARG:NH1 | 8:K:136:VAL:O | 2.15 | 0.80 |
| 6:I:22:G:N1 | 7:J:38:C:N3 | 2.29 | 0.79 |
| 8:K:476:ARG:HE | 8:K:477:CYS:HA | 1.47 | 0.79 |
| 9:E:64:TYR:O | 9:E:71:TYR:N | 2.13 | 0.79 |
| 9:E:441:CYS:HB2 | 9:E:464:HIS:HB2 | 1.64 | 0.79 |
| 9:E:563:VAL:O | 9:E:567:ARG:NH1 | 2.14 | 0.79 |
| 1:A:569:ARG:NH2 | 7:J:28:U:OP2 | 2.16 | 0.79 |
| 9:F:579:ARG:HA | 9:F:582:TYR:HB3 | 1.64 | 0.79 |
| 2:D:154:TRP:HA | 2:D:189:LEU:O | 1.83 | 0.79 |
| 9:F:260:ASP:HA | 9:F:263:SER:HB3 | 1.63 | 0.79 |
| 1:A:725:HIS:NE2 | 1:A:729:GLU:OE2 | 2.16 | 0.79 |
| 1:A:822:GLN:NE2 | 1:A:926:THR:OG1 | 2.16 | 0.79 |
| 8:K:212:ARG:HD2 | 8:K:226:CYS:HB2 | 1.64 | 0.78 |
| 9:E:305:VAL:O | 9:E:371:VAL:HA | 1.83 | 0.78 |
| 9:E:178:ARG:HG3 | 9:E:179:ASN:H | 1.48 | 0.78 |
| 9:E:304:ILE:O | 9:E:355:TYR:HA | 1.84 | 0.78 |
| 9:E:532:THR:HB | 9:E:535:SER:H | 1.48 | 0.78 |
| 2:B:45:ALA:O | 2:B:48:GLU:HG2 | 1.83 | 0.78 |
| 9:F:184:GLY:HA2 | 9:F:225:PHE:HA | 1.66 | 0.78 |
| 1:A:18:ARG:NH1 | 1:A:63:ASP:OD1 | 2.17 | 0.78 |
| 8:K:400:ARG:NH2 | 8:K:430:ALA:O | 2.17 | 0.78 |
| 2:B:51:ARG:NH2 | 6:I:14:A:O2' | 2.18 | 0.77 |
| 1:A:676:LYS:NZ | 1:A:678:GLY:O | 2.17 | 0.77 |
| 9:E:19:CYS:SG | 9:E:39:HIS:HE1 | 2.01 | 0.77 |
| 2:D:134:ASP:OD1 | 2:D:137:THR:N | 2.15 | 0.77 |
| 1:A:277:GLU:OE1 | 1:A:277:GLU:N | 2.17 | 0.77 |
| 9:E:508:LYS:HZ2 | 9:E:543:TYR:HB2 | 1.49 | 0.77 |
| 9:F:199:THR:HG22 | 9:F:212:ARG:HG2 | 1.67 | 0.77 |
| 1:A:549:SER:OG | 1:A:550:ALA:N | 2.14 | 0.77 |
| 7:J:38:C:H2' | 7:J:39:A:C8 | 2.19 | 0.77 |
| 9:F:112:CYS:SG | 9:F:116:ASN:ND2 | 2.57 | 0.77 |
| 9:F:531:GLN:NE2 | 9:F:535:SER:O | 2.18 | 0.77 |
| 9:E:214:THR:OG1 | 9:E:342:CYS:N | 2.17 | 0.77 |
| 1:A:57:GLN:HE22 | 1:A:66:ILE:H | 1.32 | 0.77 |
| 6:I:26:G:H1 | 7:J:34:C:H42 | 1.30 | 0.77 |
| 9:E:330:CYS:O | 9:E:347:LYS:NZ | 2.19 | 0.76 |
| 9:F:542:ASP:HA | 9:F:569:LYS:HB2 | 1.66 | 0.76 |
| 4:G:70:GLU:HB2 | 4:G:90:PHE:H | 1.51 | 0.76 |
| 3:C:17:LEU:HD21 | 3:C:59:LEU:HB2 | 1.68 | 0.76 |
| 9:F:545:ILE:HA | 9:F:573:LEU:HB3 | 1.65 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:51:ASN:HD22 | 9:F:69:SER:HB2 | 1.51 | 0.76 |
| 8:K:183:PHE:HB2 | 8:K:241:MET:HG2 | 1.67 | 0.76 |
| 6:I:18:G:N2 | 7:J:42:C:O2 | 2.19 | 0.76 |
| 9:E:246:TYR:N | 9:E:274:MET:O | 2.18 | 0.76 |
| 9:F:5:CYS:N | 9:F:10:SER:O | 2.18 | 0.76 |
| 5:H:75:LEU:HA | 5:H:78:ARG:HB3 | 1.66 | 0.76 |
| 9:E:284:PRO:HB2 | 9:E:567:ARG:HH22 | 1.50 | 0.75 |
| 9:E:424:SER:HA | 9:E:427:ARG:HB3 | 1.66 | 0.75 |
| 2:D:167:VAL:HG11 | 2:D:180:LEU:HD21 | 1.69 | 0.75 |
| 4:G:84:LYS:NZ | 4:G:85:VAL:O | 2.20 | 0.75 |
| 6:I:20:A:N6 | 7:J:40:U:O4 | 2.19 | 0.75 |
| 1:A:365:ARG:NH1 | 1:A:366:LEU:O | 2.19 | 0.75 |
| 1:A:611:ASN:O | 1:A:768:SER:N | 2.17 | 0.75 |
| 6:I:22:G:N2 | 7:J:38:C:O2 | 2.18 | 0.75 |
| 8:K:278:ARG:NH1 | 8:K:412:PRO:O | 2.20 | 0.75 |
| 2:B:56:GLN:HA | 2:B:59:LEU:HD12 | 1.68 | 0.74 |
| 9:E:318:CYS:HB3 | 9:E:345:LYS:HD3 | 1.67 | 0.74 |
| 1:A:11:VAL:HG21 | 1:A:72:VAL:HG21 | 1.68 | 0.74 |
| 7:J:47:A:H2' | 7:J:48:C:C6 | 2.20 | 0.74 |
| 9:E:309:CYS:N | 9:E:375:GLU:OE2 | 2.20 | 0.74 |
| 1:A:22:CYS:SG | 1:A:55:ARG:NH1 | 2.61 | 0.74 |
| 4:G:11:GLN:NE2 | 4:G:12:MET:O | 2.21 | 0.74 |
| 6:I:17:A:H61 | 7:J:43:U:H3 | 1.34 | 0.74 |
| 9:E:306:TYR:HA | 9:E:372:VAL:HG22 | 1.68 | 0.74 |
| 1:A:370:GLU:OE1 | 1:A:370:GLU:N | 2.18 | 0.74 |
| 9:E:283:PRO:HG2 | 9:E:439:GLY:HA2 | 1.69 | 0.74 |
| 9:E:425:VAL:O | 9:E:429:MET:N | 2.18 | 0.74 |
| 9:E:59:ASP:O | 9:E:62:GLN:NE2 | 2.21 | 0.74 |
| 9:E:386:VAL:HG12 | 9:E:390:ARG:HE | 1.53 | 0.74 |
| 9:F:545:ILE:HG23 | 9:F:573:LEU:HD22 | 1.70 | 0.73 |
| 9:E:309:CYS:O | 9:E:359:THR:OG1 | 2.06 | 0.73 |
| 9:F:116:ASN:HB2 | 9:F:119:ASP:H | 1.52 | 0.73 |
| 1:A:304:ASP:O | 1:A:307:ILE:N | 2.20 | 0.73 |
| 6:I:18:G:N1 | 7:J:42:C:N3 | 2.36 | 0.73 |
| 9:E:480:ILE:HD12 | 9:E:489:ASN:HD22 | 1.52 | 0.73 |
| 9:F:474:MET:HB2 | 9:F:575:ILE:HG22 | 1.69 | 0.73 |
| 9:E:293:ILE:HG21 | 9:E:320:LYS:HB3 | 1.71 | 0.73 |
| 9:F:175:PRO:HB3 | 9:F:485:SER:HB2 | 1.69 | 0.73 |
| 1:A:734:ASN:OD1 | 1:A:735:ARG:N | 2.20 | 0.73 |
| 2:D:162:ALA:HB2 | 2:D:183:PRO:HG2 | 1.71 | 0.73 |
| 8:K:483:VAL:HG12 | 8:K:485:ARG:H | 1.52 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:511:PHE:O | 9:E:519:ASN:ND2 | 2.20 | 0.72 |
| 9:F:124:ASN:O | 9:F:427:ARG:NH2 | 2.21 | 0.72 |
| 2:B:136:ASN:OD1 | 2:B:140:ASN:ND2 | 2.18 | 0.72 |
| 5:H:67:SER:HB2 | 5:H:98:GLN:HG3 | 1.71 | 0.72 |
| 9:E:496:VAL:HG12 | 9:E:575:ILE:HD13 | 1.70 | 0.72 |
| 9:F:455:LEU:HD23 | 9:F:558:VAL:HG13 | 1.72 | 0.72 |
| 2:B:22:TYR:HA | 2:B:38:LEU:HG | 1.71 | 0.72 |
| 9:E:267:ALA:O | 9:E:271:LYS:NZ | 2.21 | 0.72 |
| 1:A:164:ASP:OD1 | 1:A:165:PHE:N | 2.14 | 0.72 |
| 9:E:181:VAL:HG22 | 9:E:199:THR:HG22 | 1.71 | 0.72 |
| 9:E:455:LEU:HG | 9:E:456:VAL:HG13 | 1.72 | 0.72 |
| 9:E:473:LYS:NZ | 9:E:587:PHE:O | 2.22 | 0.72 |
| 2:D:147:PHE:HB3 | 2:D:154:TRP:O | 1.89 | 0.72 |
| 9:E:452:VAL:HG12 | 9:E:585:LEU:HD11 | 1.71 | 0.72 |
| 8:K:184:VAL:HG11 | 8:K:278:ARG:HA | 1.71 | 0.71 |
| 9:E:15:ARG:HD2 | 9:E:22:ARG:HB3 | 1.72 | 0.71 |
| 9:F:300:PRO:O | 9:F:355:TYR:OH | 2.07 | 0.71 |
| 5:H:94:GLY:O | 8:K:47:LYS:NZ | 2.18 | 0.71 |
| 9:E:243:GLN:NE2 | 9:E:277:TYR:O | 2.21 | 0.71 |
| 9:E:248:ARG:NH2 | 9:E:249:ILE:O | 2.23 | 0.71 |
| 9:E:519:ASN:ND2 | 9:E:531:GLN:H | 1.88 | 0.71 |
| 9:F:297:LEU:HD12 | 9:F:300:PRO:HA | 1.72 | 0.71 |
| 2:D:174:MET:O | 2:D:177:SER:OG | 2.07 | 0.71 |
| 5:H:57:VAL:HG22 | 5:H:95:LYS:HE3 | 1.72 | 0.71 |
| 9:E:318:CYS:O | 9:E:345:LYS:NZ | 2.23 | 0.71 |
| 9:F:9:ASN:OD1 | 9:F:129:ARG:NH1 | 2.23 | 0.71 |
| 9:E:546:PHE:O | 9:E:574:CYS:HA | 1.89 | 0.71 |
| 9:F:124:ASN:OD1 | 9:F:381:ASN:ND2 | 2.23 | 0.71 |
| 1:A:12:CYS:SG | 1:A:17:ALA:HA | 2.30 | 0.71 |
| 1:A:854:LEU:O | 2:D:72:LYS:NZ | 2.23 | 0.71 |
| 9:E:301:SER:O | 9:E:303:ARG:NH1 | 2.23 | 0.71 |
| 9:F:6:VAL:HG11 | 9:F:23:PRO:HB2 | 1.71 | 0.71 |
| 1:A:853:THR:HA | 1:A:891:LEU:HD21 | 1.73 | 0.70 |
| 9:E:497:ARG:HD3 | 9:E:526:LEU:HA | 1.73 | 0.70 |
| 2:B:62:MET:O | 2:B:65:GLN:NE2 | 2.24 | 0.70 |
| 1:A:687:THR:O | 1:A:690:ALA:N | 2.25 | 0.70 |
| 1:A:367:SER:N | 1:A:370:GLU:OE2 | 2.22 | 0.70 |
| 7:J:40:U:H2' | 7:J:41:G:H8 | 1.57 | 0.70 |
| 1:A:272:LYS:HA | 2:B:111:ARG:HH22 | 1.56 | 0.69 |
| 9:F:287:GLY:O | 9:F:291:PHE:N | 2.24 | 0.69 |
| 1:A:19:LEU:HD12 | 1:A:56:PHE:HB3 | 1.74 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:293:ILE:HD12 | 9:E:324:TYR:HD2 | 1.57 | 0.69 |
| 1:A:676:LYS:NZ | 1:A:679:GLY:O | 2.25 | 0.69 |
| 3:C:46:THR:HG23 | 3:C:47:GLU:H | 1.57 | 0.69 |
| 8:K:489:ASN:O | 8:K:492:ARG:HB3 | 1.91 | 0.69 |
| 1:A:431:GLU:OE2 | 3:C:2:LYS:N | 2.25 | 0.69 |
| 1:A:520:SER:N | 1:A:523:ASP:OD2 | 2.26 | 0.69 |
| 8:K:253:LEU:HD11 | 8:K:277:THR:HA | 1.74 | 0.69 |
| 9:F:332:ARG:HD2 | 9:F:357:PHE:HB2 | 1.75 | 0.69 |
| 1:A:522:GLU:OE1 | 1:A:522:GLU:N | 2.18 | 0.69 |
| 2:B:134:ASP:OD2 | 2:B:136:ASN:N | 2.19 | 0.69 |
| 2:D:172:ILE:HD12 | 2:D:180:LEU:HD22 | 1.75 | 0.69 |
| 9:E:304:ILE:N | 9:E:354:GLN:O | 2.22 | 0.69 |
| 9:F:11:GLN:HB2 | 9:F:93:TYR:CE2 | 2.28 | 0.69 |
| 9:F:456:VAL:HG13 | 9:F:457:TYR:H | 1.58 | 0.69 |
| 2:B:55:MET:HA | 2:B:58:LYS:HD3 | 1.75 | 0.68 |
| 3:C:71:LEU:HB2 | 2:D:111:ARG:HH21 | 1.58 | 0.68 |
| 1:A:87:TYR:CE1 | 1:A:99:HIS:HB2 | 2.27 | 0.68 |
| 9:F:279:THR:H | 9:F:435:ASP:HB2 | 1.58 | 0.68 |
| 9:E:490:ARG:HB3 | 9:E:491:PRO:HD3 | 1.75 | 0.68 |
| 7:J:41:G:H2' | 7:J:42:C:C6 | 2.28 | 0.68 |
| 9:F:331:SER:HB3 | 9:F:353:GLU:HB2 | 1.75 | 0.68 |
| 9:F:449:VAL:HA | 9:F:452:VAL:HG12 | 1.76 | 0.68 |
| 5:H:93:LYS:NZ | 8:K:127:THR:O | 2.23 | 0.68 |
| 8:K:483:VAL:HA | 8:K:488:ALA:HB2 | 1.76 | 0.68 |
| 9:F:497:ARG:HG2 | 9:F:526:LEU:HB3 | 1.76 | 0.68 |
| 1:A:874:ASN:OD1 | 1:A:875:GLN:N | 2.26 | 0.68 |
| 9:E:580:ASP:O | 9:E:584:LYS:N | 2.25 | 0.68 |
| 2:D:101:ASP:OD1 | 2:D:101:ASP:N | 2.24 | 0.68 |
| 9:E:239:THR:O | 9:E:388:ASN:ND2 | 2.26 | 0.68 |
| 9:E:139:LYS:HB3 | 9:E:232:VAL:HG11 | 1.76 | 0.68 |
| 9:F:305:VAL:HA | 9:F:356:VAL:O | 1.94 | 0.68 |
| 1:A:140:ASP:O | 1:A:143:LYS:N | 2.26 | 0.68 |
| 9:E:271:LYS:HB3 | 9:E:274:MET:HE2 | 1.76 | 0.68 |
| 1:A:904:SER:O | 1:A:906:MET:N | 2.27 | 0.67 |
| 9:F:285:GLY:HA2 | 9:F:288:LYS:HZ3 | 1.59 | 0.67 |
| 2:D:173:SER:N | 2:D:176:ASN:OD1 | 2.26 | 0.67 |
| 9:E:26:CYS:N | 9:E:29:CYS:SG | 2.67 | 0.67 |
| 1:A:335:VAL:HG13 | 1:A:338:VAL:HB | 1.76 | 0.67 |
| 1:A:813:CYS:O | 1:A:815:GLN:NE2 | 2.28 | 0.67 |
| 4:G:72:PRO:HB2 | 4:G:87:TYR:HB3 | 1.76 | 0.67 |
| 9:E:268:ASN:HD22 | 9:E:291:PHE:HE2 | 1.40 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:269:TYR:O | 9:F:272:VAL:HB | 1.94 | 0.67 |
| 1:A:612:PRO:HB2 | 1:A:805:LEU:HD21 | 1.75 | 0.67 |
| 2:B:173:SER:OG | 2:B:176:ASN:N | 2.22 | 0.67 |
| 2:D:51:ARG:HG3 | 6:I:17:A:H4' | 1.76 | 0.67 |
| 9:E:103:VAL:HG12 | 9:E:107:ASN:HD21 | 1.59 | 0.67 |
| 9:F:296:ALA:HB1 | 9:F:304:ILE:HD13 | 1.76 | 0.67 |
| 9:E:55:CYS:SG | 9:E:74:SER:OG | 2.53 | 0.67 |
| 9:F:4:ALA:HA | 9:F:11:GLN:HA | 1.75 | 0.67 |
| 9:F:515:TYR:O | 9:F:519:ASN:ND2 | 2.27 | 0.67 |
| 7:J:40:U:H2' | 7:J:41:G:C8 | 2.29 | 0.67 |
| 1:A:484:ASP:OD1 | 1:A:484:ASP:N | 2.26 | 0.67 |
| 9:F:255:THR:N | 9:F:298:TYR:O | 2.28 | 0.67 |
| 9:F:511:PHE:N | 9:F:529:PRO:O | 2.23 | 0.67 |
| 1:A:336:ASP:N | 1:A:363:SER:O | 2.25 | 0.67 |
| 1:A:715:ILE:O | 1:A:721:ARG:NH2 | 2.26 | 0.67 |
| 7:J:47:A:H2' | 7:J:48:C:H6 | 1.60 | 0.67 |
| 9:E:522:ALA:O | 9:E:526:LEU:N | 2.23 | 0.67 |
| 1:A:647:SER:OG | 1:A:648:LEU:N | 2.27 | 0.66 |
| 2:D:34:VAL:HA | 2:D:37:LYS:HG3 | 1.77 | 0.66 |
| 5:H:30:TYR:HA | 5:H:33:SER:HB3 | 1.77 | 0.66 |
| 9:E:471:CYS:O | 9:E:588:THR:OG1 | 2.13 | 0.66 |
| 9:E:480:ILE:HA | 9:E:489:ASN:HB3 | 1.75 | 0.66 |
| 9:F:182:PHE:HB2 | 9:F:200:PHE:HE2 | 1.59 | 0.66 |
| 9:F:518:GLN:NE2 | 9:F:549:THR:OG1 | 2.28 | 0.66 |
| 9:F:576:MET:HG3 | 9:F:585:LEU:HD21 | 1.77 | 0.66 |
| 2:D:60:GLU:HG3 | 2:D:61:LYS:HD2 | 1.76 | 0.66 |
| 1:A:838:LEU:O | 1:A:841:GLY:N | 2.26 | 0.66 |
| 2:D:11:SER:HB3 | 2:D:49:PHE:HB2 | 1.78 | 0.66 |
| 2:D:100:ASN:HB3 | 2:D:103:LEU:HD23 | 1.77 | 0.66 |
| 9:F:51:ASN:HD21 | 9:F:70:TYR:HD2 | 1.43 | 0.66 |
| 9:F:376:ILE:HG21 | 9:F:398:TYR:HB3 | 1.77 | 0.66 |
| 9:F:396:TYR:HB3 | 9:F:398:TYR:CE2 | 2.30 | 0.66 |
| 6:I:22:G:H2' | 6:I:23:C:C6 | 2.31 | 0.66 |
| 9:E:293:ILE:HD12 | 9:E:324:TYR:CD2 | 2.30 | 0.66 |
| 9:E:548:GLN:HB2 | 9:E:576:MET:HA | 1.77 | 0.66 |
| 1:A:5:GLN:O | 1:A:9:ASN:N | 2.24 | 0.66 |
| 8:K:470:SER:HG | 8:K:473:CYS:HG | 1.43 | 0.66 |
| 9:E:266:VAL:O | 9:E:270:GLN:NE2 | 2.29 | 0.66 |
| 9:E:307:THR:HA | 9:E:358:CYS:O | 1.95 | 0.66 |
| 9:E:327:ILE:HA | 9:E:346:PHE:HE1 | 1.59 | 0.66 |
| 9:E:557:ASN:ND2 | 9:E:559:ASN:OD1 | 2.27 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:441:CYS:O | 9:E:443:ARG:N | 2.28 | 0.66 |
| 9:F:479:VAL:H | 9:F:491:PRO:HG3 | 1.60 | 0.66 |
| 5:H:102:THR:OG1 | 5:H:103:CYS:N | 2.29 | 0.66 |
| 9:E:61:THR:HA | 9:E:84:CYS:HB3 | 1.76 | 0.66 |
| 9:E:152:ALA:N | 9:E:225:PHE:O | 2.29 | 0.66 |
| 9:F:52:ALA:HB3 | 9:F:55:CYS:HB2 | 1.78 | 0.66 |
| 1:A:331:ARG:NH2 | 2:B:114:CYS:SG | 2.69 | 0.66 |
| 1:A:647:SER:OG | 1:A:650:HIS:ND1 | 2.20 | 0.66 |
| 8:K:116:ASN:HD21 | 8:K:271:SER:H | 1.43 | 0.66 |
| 9:F:488:ILE:HG23 | 9:F:518:GLN:HA | 1.78 | 0.66 |
| 1:A:514:LEU:O | 1:A:518:SER:N | 2.24 | 0.65 |
| 2:D:136:ASN:O | 2:D:140:ASN:ND2 | 2.29 | 0.65 |
| 8:K:354:GLN:NE2 | 8:K:355:PRO:O | 2.29 | 0.65 |
| 9:E:38:SER:HA | 9:E:40:LYS:HE2 | 1.78 | 0.65 |
| 9:E:377:SER:OG | 9:E:401:ASP:O | 2.12 | 0.65 |
| 9:F:559:ASN:OD1 | 9:F:562:ASN:ND2 | 2.30 | 0.65 |
| 9:E:52:ALA:HB1 | 9:E:75:HIS:CG | 2.31 | 0.65 |
| 9:E:314:VAL:HA | 9:E:317:LEU:HD12 | 1.76 | 0.65 |
| 9:E:513:SER:HB2 | 9:E:519:ASN:HB2 | 1.78 | 0.65 |
| 9:F:479:VAL:HB | 9:F:491:PRO:HD3 | 1.78 | 0.65 |
| 2:D:136:ASN:HA | 2:D:139:LYS:HD2 | 1.79 | 0.65 |
| 9:F:5:CYS:CB | 9:F:8:CYS:SG | 2.84 | 0.65 |
| 1:A:358:ASP:OD2 | 1:A:533:ARG:NH2 | 2.30 | 0.65 |
| 4:G:48:LEU:HB3 | 4:G:51:LEU:HD11 | 1.78 | 0.65 |
| 9:E:34:VAL:O | 9:E:40:LYS:NZ | 2.25 | 0.65 |
| 9:E:65:LEU:HB2 | 9:E:83:LEU:HD21 | 1.79 | 0.65 |
| 9:E:27:CYS:N | 9:E:97:CYS:SG | 2.69 | 0.65 |
| 2:D:78:ASP:OD1 | 2:D:79:LYS:N | 2.29 | 0.65 |
| 1:A:332:LYS:NZ | 2:B:104:ASN:OD1 | 2.30 | 0.65 |
| 2:D:134:ASP:HA | 2:D:182:TRP:CG | 2.31 | 0.65 |
| 9:E:302:ALA:O | 9:E:354:GLN:NE2 | 2.30 | 0.65 |
| 9:E:381:ASN:HA | 9:E:384:LEU:HB3 | 1.79 | 0.65 |
| 1:A:39:ASN:OD1 | 1:A:41:LYS:N | 2.30 | 0.65 |
| 8:K:219:THR:HG23 | 8:K:235:TYR:HE2 | 1.61 | 0.65 |
| 9:E:88:GLN:NE2 | 9:E:94:LYS:O | 2.28 | 0.65 |
| 2:B:15:PHE:O | 2:B:19:GLN:NE2 | 2.30 | 0.65 |
| 8:K:18:LEU:HB3 | 8:K:22:GLN:HG3 | 1.79 | 0.65 |
| 9:E:279:THR:HA | 9:E:398:TYR:HB2 | 1.79 | 0.65 |
| 9:E:262:PHE:O | 9:E:266:VAL:N | 2.30 | 0.64 |
| 9:F:440:THR:OG1 | 9:F:464:HIS:ND1 | 2.28 | 0.64 |
| 1:A:370:GLU:HA | 1:A:373:VAL:HG22 | 1.79 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:38:TYR:HE1 | 1:A:725:HIS:CE1 | 2.15 | 0.64 |
| 9:E:249:ILE:HG22 | 9:E:252:LEU:HB2 | 1.80 | 0.64 |
| 9:E:510:VAL:HA | 9:E:529:PRO:HD2 | 1.79 | 0.64 |
| 9:F:332:ARG:NH1 | 9:F:357:PHE:O | 2.31 | 0.64 |
| 1:A:816:HIS:HB2 | 1:A:831:TYR:CE1 | 2.32 | 0.64 |
| 9:E:15:ARG:N | 9:E:43:LEU:O | 2.30 | 0.64 |
| 9:F:247:VAL:HG23 | 9:F:248:ARG:HG2 | 1.78 | 0.64 |
| 9:F:308:ALA:HB2 | 9:F:374:ASP:HB3 | 1.79 | 0.64 |
| 9:F:303:ARG:N | 9:F:369:ASP:OD2 | 2.27 | 0.64 |
| 8:K:108:GLN:HA | 8:K:117:LEU:O | 1.98 | 0.64 |
| 9:E:319:GLU:OE2 | 9:E:323:LYS:NZ | 2.25 | 0.64 |
| 9:E:409:ARG:HH22 | 9:E:422:PHE:HA | 1.63 | 0.64 |
| 8:K:183:PHE:O | 8:K:242:ILE:N | 2.25 | 0.64 |
| 9:E:315:ASP:HA | 9:E:343:PHE:HE2 | 1.62 | 0.64 |
| 9:E:44:SER:OG | 9:E:45:VAL:N | 2.27 | 0.64 |
| 9:F:11:GLN:H | 9:F:11:GLN:CD | 1.99 | 0.64 |
| 9:E:532:THR:HG22 | 9:E:534:ASP:H | 1.63 | 0.64 |
| 9:F:331:SER:HB2 | 9:F:347:LYS:HG3 | 1.79 | 0.64 |
| 1:A:845:ASP:N | 1:A:845:ASP:OD1 | 2.28 | 0.64 |
| 4:G:14:CYS:SG | 4:G:15:ALA:N | 2.70 | 0.64 |
| 9:E:236:SER:OG | 9:E:237:ALA:N | 2.30 | 0.64 |
| 9:F:476:TYR:CE2 | 9:F:492:GLN:HA | 2.32 | 0.64 |
| 1:A:42:VAL:HG11 | 1:A:713:ASN:HD21 | 1.62 | 0.63 |
| 9:E:498:GLU:HA | 9:E:501:THR:HG23 | 1.79 | 0.63 |
| 9:F:28:LYS:HD2 | 9:F:99:GLY:H | 1.62 | 0.63 |
| 1:A:849:LYS:C | 1:A:851:ASP:H | 1.99 | 0.63 |
| 5:H:42:VAL:HG23 | 5:H:69:GLY:H | 1.63 | 0.63 |
| 9:F:293:ILE:HD12 | 9:F:325:LEU:HD13 | 1.80 | 0.63 |
| 1:A:202:VAL:HG22 | 1:A:231:VAL:HG22 | 1.80 | 0.63 |
| 9:E:258:ILE:HG23 | 9:E:266:VAL:HG21 | 1.80 | 0.63 |
| 9:F:285:GLY:H | 9:F:288:LYS:HD3 | 1.64 | 0.63 |
| 1:A:711:ASP:OD1 | 1:A:712:GLY:N | 2.29 | 0.63 |
| 9:E:286:THR:HB | 9:E:440:THR:O | 1.98 | 0.63 |
| 9:E:329:LYS:HD2 | 9:E:354:GLN:HG2 | 1.79 | 0.63 |
| 1:A:614:LEU:HB2 | 1:A:802:GLU:HB3 | 1.81 | 0.63 |
| 9:E:420:GLU:HB3 | 9:E:430:LYS:HB2 | 1.79 | 0.63 |
| 8:K:236:VAL:HG12 | 8:K:239:PRO:HG3 | 1.79 | 0.63 |
| 9:E:366:THR:N | 9:E:390:ARG:O | 2.27 | 0.63 |
| 9:F:539:SER:O | 9:F:567:ARG:NE | 2.26 | 0.63 |
| 5:H:48:HIS:NE2 | 5:H:66:GLU:OE1 | 2.20 | 0.63 |
| 8:K:167:VAL:HA | 8:K:170:LEU:HD22 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:15:ARG:HE | 9:F:24:PHE:HE1 | 1.45 | 0.63 |
| 9:F:448:ILE:O | 9:F:451:THR:OG1 | 2.13 | 0.63 |
| 1:A:567:THR:OG1 | 1:A:654:ARG:NH2 | 2.25 | 0.63 |
| 1:A:613:HIS:ND1 | 1:A:803:THR:HA | 2.14 | 0.63 |
| 1:A:140:ASP:OD1 | 1:A:141:THR:N | 2.32 | 0.63 |
| 1:A:861:SER:O | 1:A:864:ILE:HG22 | 1.98 | 0.63 |
| 9:E:322:LEU:HB3 | 9:E:345:LYS:HZ1 | 1.63 | 0.63 |
| 9:E:443:ARG:HH11 | 9:E:567:ARG:HH21 | 1.46 | 0.63 |
| 9:F:195:ILE:O | 9:F:215:THR:OG1 | 2.10 | 0.63 |
| 9:F:265:ASN:HB3 | 9:F:269:TYR:CZ | 2.34 | 0.63 |
| 9:F:493:ILE:HG22 | 9:F:525:ILE:HG21 | 1.81 | 0.63 |
| 1:A:751:LYS:HG3 | 1:A:752:HIS:CD2 | 2.34 | 0.62 |
| 4:G:19:THR:HG23 | 4:G:21:THR:H | 1.63 | 0.62 |
| 9:F:157:VAL:HG13 | 9:F:163:LEU:HD12 | 1.81 | 0.62 |
| 9:F:393:ALA:HB3 | 9:F:396:TYR:HE1 | 1.64 | 0.62 |
| 9:F:465:LYS:HG3 | 9:F:466:ASP:H | 1.64 | 0.62 |
| 9:E:309:CYS:SG | 9:E:310:SER:N | 2.72 | 0.62 |
| 2:B:100:ASN:O | 2:B:104:ASN:ND2 | 2.31 | 0.62 |
| 6:I:22:G:H2' | 6:I:23:C:H6 | 1.65 | 0.62 |
| 9:F:127:THR:O | 9:F:131:LYS:N | 2.31 | 0.62 |
| 2:D:147:PHE:CB | 2:D:154:TRP:O | 2.47 | 0.62 |
| 6:I:25:A:H2' | 6:I:26:G:H8 | 1.64 | 0.62 |
| 9:E:161:ARG:NH2 | 9:E:211:TYR:O | 2.32 | 0.62 |
| 9:F:13:SER:OG | 9:F:13:SER:O | 2.16 | 0.62 |
| 8:K:478:ASN:HA | 8:K:482:ALA:HB2 | 1.80 | 0.62 |
| 9:F:28:LYS:NZ | 9:F:97:CYS:O | 2.29 | 0.62 |
| 2:D:51:ARG:NH2 | 6:I:17:A:H1' | 2.14 | 0.62 |
| 5:H:78:ARG:HD2 | 8:K:24:PRO:HB2 | 1.82 | 0.62 |
| 9:F:381:ASN:OD1 | 9:F:424:SER:N | 2.32 | 0.62 |
| 2:B:56:GLN:HB3 | 2:B:57:ARG:NH1 | 2.14 | 0.62 |
| 3:C:5:ASP:OD1 | 3:C:6:VAL:N | 2.32 | 0.62 |
| 9:E:277:TYR:HB2 | 9:E:398:TYR:HE2 | 1.65 | 0.62 |
| 9:F:135:ALA:HB1 | 9:F:382:TYR:HB2 | 1.81 | 0.62 |
| 1:A:680:THR:OG1 | 1:A:681:SER:N | 2.29 | 0.62 |
| 7:J:43:U:H2' | 7:J:44:A:C8 | 2.35 | 0.62 |
| 9:E:578:ASP:OD1 | 9:E:579:ARG:N | 2.33 | 0.62 |
| 9:F:486:SER:HA | 9:F:515:TYR:HD2 | 1.65 | 0.62 |
| 9:E:304:ILE:HB | 9:E:355:TYR:HD1 | 1.64 | 0.62 |
| 1:A:340:PHE:HE1 | 2:B:95:LEU:HD22 | 1.64 | 0.62 |
| 9:F:288:LYS:HG3 | 9:F:289:SER:H | 1.65 | 0.62 |
| 9:E:332:ARG:NH1 | 9:E:333:ILE:O | 2.33 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:476:TYR:O | 9:F:492:GLN:NE2 | 2.32 | 0.61 |
| 1:A:849:LYS:O | 1:A:851:ASP:N | 2.33 | 0.61 |
| 8:K:380:GLY:O | 8:K:395:ASN:ND2 | 2.33 | 0.61 |
| 1:A:312:ASN:O | 1:A:315:VAL:N | 2.32 | 0.61 |
| 2:D:109:ASN:HB3 | 2:D:114:CYS:SG | 2.39 | 0.61 |
| 4:G:28:ALA:HB1 | 4:G:44:LEU:HD11 | 1.81 | 0.61 |
| 7:J:29:G:N2 | 7:J:30:C:O2 | 2.34 | 0.61 |
| 9:E:255:THR:OG1 | 9:E:298:TYR:O | 2.17 | 0.61 |
| 9:E:476:TYR:HE1 | 9:E:495:VAL:HG21 | 1.65 | 0.61 |
| 1:A:689:TYR:O | 1:A:692:SER:OG | 2.16 | 0.61 |
| 6:I:23:C:H2' | 6:I:24:U:C6 | 2.35 | 0.61 |
| 9:E:304:ILE:HD12 | 9:E:355:TYR:HE1 | 1.65 | 0.61 |
| 9:F:258:ILE:HG23 | 9:F:259:SER:H | 1.65 | 0.61 |
| 9:F:305:VAL:HG22 | 9:F:356:VAL:HB | 1.81 | 0.61 |
| 2:D:173:SER:O | 2:D:177:SER:N | 2.33 | 0.61 |
| 6:I:26:G:H1 | 7:J:34:C:N4 | 1.99 | 0.61 |
| 9:E:327:ILE:HA | 9:E:346:PHE:CE1 | 2.35 | 0.61 |
| 9:F:126:CYS:O | 9:F:131:LYS:NZ | 2.33 | 0.61 |
| 2:B:155:GLU:HG2 | 2:B:191:ALA:HB2 | 1.83 | 0.61 |
| 8:K:283:HIS:HA | 8:K:287:VAL:HG13 | 1.83 | 0.61 |
| 9:E:554:HIS:ND1 | 9:E:554:HIS:O | 2.34 | 0.61 |
| 1:A:34:ALA:HA | 1:A:47:LYS:HA | 1.81 | 0.61 |
| 1:A:60:ASP:OD1 | 1:A:61:GLU:N | 2.34 | 0.61 |
| 1:A:378:PRO:HB3 | 1:A:539:ILE:HD11 | 1.82 | 0.61 |
| 1:A:738:ASP:OD2 | 4:G:36:LYS:NZ | 2.30 | 0.61 |
| 9:E:112:CYS:SG | 9:E:113:ASP:N | 2.73 | 0.61 |
| 9:E:293:ILE:HD13 | 9:E:320:LYS:HB3 | 1.83 | 0.61 |
| 9:F:283:PRO:HB2 | 9:F:286:THR:HG21 | 1.83 | 0.61 |
| 1:A:238:TYR:O | 1:A:241:LEU:N | 2.34 | 0.61 |
| 8:K:258:ASP:O | 8:K:262:GLN:NE2 | 2.34 | 0.61 |
| 9:E:510:VAL:HG22 | 9:E:529:PRO:HG2 | 1.83 | 0.61 |
| 5:H:5:THR:HG23 | 8:K:25:THR:HG21 | 1.81 | 0.60 |
| 2:D:101:ASP:O | 2:D:105:ASN:HB2 | 2.01 | 0.60 |
| 9:F:512:ILE:HG12 | 9:F:531:GLN:HB3 | 1.81 | 0.60 |
| 1:A:389:LEU:HD21 | 1:A:391:LYS:HZ2 | 1.66 | 0.60 |
| 9:E:72:CYS:SG | 9:E:74:SER:OG | 2.56 | 0.60 |
| 3:C:58:VAL:HG22 | 2:D:119:ILE:HG12 | 1.83 | 0.60 |
| 9:E:64:TYR:HE2 | 9:E:73:LYS:HE3 | 1.65 | 0.60 |
| 9:E:332:ARG:HB2 | 9:E:346:PHE:HD2 | 1.66 | 0.60 |
| 9:E:476:TYR:CE2 | 9:E:492:GLN:HG3 | 2.37 | 0.60 |
| 1:A:332:LYS:HA | 1:A:340:PHE:O | 2.02 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:384:SER:O | 1:A:384:SER:OG | 2.18 | 0.60 |
| 2:B:104:ASN:O | 2:B:108:ASN:ND2 | 2.35 | 0.60 |
| 5:H:51:THR:HG23 | 5:H:53:GLN:H | 1.67 | 0.60 |
| 9:F:121:ILE:O | 9:F:125:THR:OG1 | 2.07 | 0.60 |
| 9:F:443:ARG:HB3 | 9:F:540:GLU:HG2 | 1.84 | 0.60 |
| 1:A:902:MET:O | 9:F:96:THR:OG1 | 2.18 | 0.60 |
| 2:B:56:GLN:HB3 | 2:B:57:ARG:HH12 | 1.66 | 0.60 |
| 9:F:486:SER:HB3 | 9:F:517:SER:H | 1.66 | 0.60 |
| 9:F:522:ALA:HA | 9:F:525:ILE:HG12 | 1.84 | 0.60 |
| 9:F:243:GLN:HE22 | 9:F:276:LYS:H | 1.48 | 0.60 |
| 1:A:260:ASP:OD2 | 1:A:263:LYS:NZ | 2.34 | 0.60 |
| 8:K:76:ARG:HA | 8:K:247:TRP:CZ2 | 2.37 | 0.60 |
| 9:E:56:ASP:OD1 | 9:E:56:ASP:N | 2.35 | 0.60 |
| 9:F:266:VAL:HA | 9:F:269:TYR:HB2 | 1.82 | 0.60 |
| 1:A:7:PHE:O | 1:A:10:ARG:N | 2.36 | 0.59 |
| 1:A:88:ASN:O | 1:A:91:LYS:NZ | 2.34 | 0.59 |
| 1:A:855:MET:O | 1:A:857:GLU:N | 2.34 | 0.59 |
| 9:E:287:GLY:HA3 | 9:E:442:ARG:NH2 | 2.14 | 0.59 |
| 5:H:64:ASP:O | 5:H:101:THR:OG1 | 2.20 | 0.59 |
| 9:E:19:CYS:O | 9:E:22:ARG:NH1 | 2.35 | 0.59 |
| 9:E:105:ASP:OD1 | 9:E:106:PHE:N | 2.33 | 0.59 |
| 9:E:197:GLU:N | 9:E:197:GLU:OE2 | 2.34 | 0.59 |
| 1:A:821:LYS:NZ | 1:A:824:ASP:O | 2.34 | 0.59 |
| 4:G:16:ALA:HA | 4:G:54:ALA:HA | 1.85 | 0.59 |
| 9:E:332:ARG:HG3 | 9:E:343:PHE:O | 2.01 | 0.59 |
| 9:F:512:ILE:O | 9:F:546:PHE:HA | 2.02 | 0.59 |
| 9:E:259:SER:HB3 | 9:E:262:PHE:CD2 | 2.38 | 0.59 |
| 9:E:294:GLY:O | 9:E:298:TYR:HB2 | 2.03 | 0.59 |
| 9:E:420:GLU:OE1 | 9:E:427:ARG:NH2 | 2.34 | 0.59 |
| 1:A:388:LEU:HD12 | 1:A:400:ALA:HB2 | 1.82 | 0.59 |
| 2:D:133:PRO:O | 2:D:182:TRP:HB3 | 2.02 | 0.59 |
| 6:I:10:C:O2 | 7:J:50:G:N2 | 2.36 | 0.59 |
| 9:F:26:CYS:SG | 9:F:29:CYS:N | 2.58 | 0.59 |
| 9:F:321:ALA:O | 9:F:325:LEU:N | 2.35 | 0.59 |
| 9:F:566:THR:OG1 | 9:F:567:ARG:NH1 | 2.35 | 0.59 |
| 1:A:667:VAL:O | 1:A:669:CYS:N | 2.32 | 0.59 |
| 4:G:56:PHE:H | 4:G:65:ILE:HG12 | 1.68 | 0.59 |
| 8:K:203:PRO:HB2 | 8:K:205:ARG:HE | 1.66 | 0.59 |
| 9:E:64:TYR:N | 9:E:71:TYR:O | 2.34 | 0.59 |
| 9:E:281:GLN:HE22 | 9:E:402:PRO:HD2 | 1.68 | 0.59 |
| 1:A:804:ASP:OD1 | 1:A:805:LEU:N | 2.36 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:105:ASN:OD1 | 2:B:109:ASN:ND2 | 2.28 | 0.59 |
| 2:B:132:ILE:O | 2:B:183:PRO:HA | 2.03 | 0.59 |
| 2:D:22:TYR:HD1 | 2:D:38:LEU:HB3 | 1.66 | 0.59 |
| 9:E:146:LYS:HA | 9:E:149:TYR:CE1 | 2.36 | 0.59 |
| 9:E:516:ASN:HD21 | 9:E:531:GLN:C | 2.06 | 0.59 |
| 2:B:159:VAL:HG22 | 2:B:186:VAL:HG22 | 1.83 | 0.59 |
| 9:E:50:CYS:SG | 9:E:52:ALA:HB3 | 2.43 | 0.59 |
| 9:E:258:ILE:HD12 | 9:E:266:VAL:HG11 | 1.84 | 0.59 |
| 9:E:498:GLU:HA | 9:E:501:THR:CG2 | 2.33 | 0.59 |
| 9:E:443:ARG:HH11 | 9:E:567:ARG:NH2 | 2.01 | 0.59 |
| 9:F:306:TYR:HB2 | 9:F:357:PHE:CD1 | 2.37 | 0.59 |
| 6:I:11:G:H2' | 6:I:12:G:C8 | 2.38 | 0.59 |
| 9:E:15:ARG:HH11 | 9:E:24:PHE:HE1 | 1.49 | 0.59 |
| 9:E:4:ALA:HA | 9:E:11:GLN:HA | 1.85 | 0.58 |
| 9:E:259:SER:O | 9:E:263:SER:N | 2.36 | 0.58 |
| 9:E:409:ARG:NH2 | 9:E:422:PHE:O | 2.37 | 0.58 |
| 8:K:212:ARG:NH1 | 8:K:226:CYS:SG | 2.76 | 0.58 |
| 9:E:359:THR:OG1 | 9:E:361:ASN:ND2 | 2.35 | 0.58 |
| 9:E:516:ASN:O | 9:E:520:ALA:HB2 | 2.04 | 0.58 |
| 1:A:124:MET:HG3 | 1:A:210:GLN:HG2 | 1.85 | 0.58 |
| 3:C:55:LEU:O | 3:C:58:VAL:N | 2.27 | 0.58 |
| 2:D:52:ASP:OD1 | 2:D:53:ALA:N | 2.36 | 0.58 |
| 9:E:266:VAL:HA | 9:E:269:TYR:CD2 | 2.38 | 0.58 |
| 9:E:347:LYS:NZ | 9:E:353:GLU:OE2 | 2.32 | 0.58 |
| 9:F:203:GLY:HA3 | 9:F:208:ALA:HB3 | 1.86 | 0.58 |
| 1:A:820:VAL:HG22 | 1:A:821:LYS:H | 1.69 | 0.58 |
| 2:D:158:GLN:HE22 | 2:D:160:VAL:HB | 1.66 | 0.58 |
| 5:H:22:ASP:HB3 | 5:H:25:LYS:HE2 | 1.86 | 0.58 |
| 9:E:519:ASN:HD21 | 9:E:531:GLN:H | 1.51 | 0.58 |
| 9:F:21:ARG:NH1 | 9:F:21:ARG:HA | 2.19 | 0.58 |
| 9:F:474:MET:O | 9:F:576:MET:N | 2.35 | 0.58 |
| 1:A:904:SER:OG | 9:F:95:ASN:ND2 | 2.35 | 0.58 |
| 9:E:146:LYS:HD3 | 9:E:149:TYR:CD1 | 2.38 | 0.58 |
| 9:E:161:ARG:HD3 | 9:E:210:VAL:HG13 | 1.84 | 0.58 |
| 9:F:44:SER:OG | 9:F:45:VAL:N | 2.35 | 0.58 |
| 9:F:401:ASP:OD2 | 9:F:404:GLN:NE2 | 2.35 | 0.58 |
| 1:A:304:ASP:OD1 | 1:A:305:ARG:N | 2.36 | 0.58 |
| 2:B:123:THR:O | 2:B:190:ARG:NH2 | 2.31 | 0.58 |
| 8:K:180:ARG:HD3 | 8:K:240:PHE:CD1 | 2.39 | 0.58 |
| 9:E:322:LEU:HD23 | 9:E:345:LYS:HZ1 | 1.69 | 0.58 |
| 9:E:278:SER:HB2 | 9:E:397:VAL:HG23 | 1.86 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:374:ASP:HB2 | 9:E:375:GLU:OE1 | 2.04 | 0.58 |
| 9:E:557:ASN:OD1 | 9:E:560:ARG:N | 2.36 | 0.58 |
| 9:F:159:SER:HB2 | 9:F:162:GLU:H | 1.68 | 0.58 |
| 1:A:497:ASN:O | 1:A:499:ASP:N | 2.36 | 0.58 |
| 1:A:739:THR:O | 1:A:743:ASN:ND2 | 2.37 | 0.58 |
| 3:C:60:LEU:HD12 | 2:D:106:ILE:HD11 | 1.86 | 0.58 |
| 1:A:39:ASN:ND2 | 1:A:42:VAL:HG22 | 2.19 | 0.58 |
| 1:A:682:SER:O | 1:A:682:SER:OG | 2.18 | 0.58 |
| 9:F:382:TYR:O | 9:F:386:VAL:HG23 | 2.04 | 0.58 |
| 9:F:473:LYS:HG3 | 9:F:587:PHE:HB2 | 1.85 | 0.58 |
| 9:F:562:ASN:OD1 | 9:F:563:VAL:N | 2.37 | 0.58 |
| 4:G:29:LEU:HB2 | 4:G:45:LEU:HB3 | 1.86 | 0.57 |
| 9:F:447:GLU:N | 9:F:447:GLU:OE1 | 2.37 | 0.57 |
| 9:E:116:ASN:N | 9:E:119:ASP:OD2 | 2.36 | 0.57 |
| 9:E:243:GLN:HB2 | 9:E:277:TYR:OH | 2.05 | 0.57 |
| 1:A:444:GLN:NE2 | 1:A:553:ARG:O | 2.37 | 0.57 |
| 5:H:7:VAL:HG22 | 5:H:9:ALA:H | 1.70 | 0.57 |
| 5:H:55:ILE:HD13 | 5:H:92:LEU:HD22 | 1.87 | 0.57 |
| 9:E:72:CYS:SG | 9:E:74:SER:N | 2.77 | 0.57 |
| 9:F:409:ARG:O | 9:F:412:LEU:N | 2.37 | 0.57 |
| 1:A:57:GLN:HG2 | 1:A:69:TYR:CE1 | 2.39 | 0.57 |
| 5:H:61:ALA:HB2 | 5:H:98:GLN:HG2 | 1.86 | 0.57 |
| 8:K:83:VAL:HA | 8:K:86:TRP:CD1 | 2.39 | 0.57 |
| 8:K:168:GLN:NE2 | 8:K:232:GLY:H | 2.02 | 0.57 |
| 9:E:283:PRO:C | 9:E:288:LYS:HZ1 | 2.07 | 0.57 |
| 9:F:393:ALA:HB3 | 9:F:396:TYR:CE1 | 2.39 | 0.57 |
| 9:E:163:LEU:O | 9:E:165:LEU:N | 2.37 | 0.57 |
| 9:E:285:GLY:HA3 | 9:E:443:ARG:NH1 | 2.19 | 0.57 |
| 9:E:304:ILE:HB | 9:E:355:TYR:CD1 | 2.39 | 0.57 |
| 9:E:471:CYS:HB3 | 9:E:572:ILE:HG22 | 1.85 | 0.57 |
| 1:A:162:TRP:HA | 1:A:168:ASN:ND2 | 2.19 | 0.57 |
| 9:E:178:ARG:HG3 | 9:E:179:ASN:N | 2.19 | 0.57 |
| 9:F:26:CYS:HB2 | 9:F:97:CYS:HB2 | 1.85 | 0.57 |
| 1:A:356:ASN:HD21 | 1:A:535:VAL:H | 1.50 | 0.57 |
| 6:I:11:G:H2' | 6:I:12:G:H8 | 1.69 | 0.57 |
| 8:K:19:HIS:O | 8:K:21:THR:N | 2.37 | 0.57 |
| 1:A:513:ARG:O | 1:A:517:ASP:CB | 2.53 | 0.57 |
| 2:D:100:ASN:O | 2:D:104:ASN:N | 2.25 | 0.57 |
| 5:H:61:ALA:HA | 5:H:65:GLN:HE21 | 1.70 | 0.57 |
| 7:J:39:A:H2' | 7:J:40:U:C6 | 2.39 | 0.57 |
| 9:E:488:ILE:HG23 | 9:E:521:VAL:HG11 | 1.87 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:ASP:O | 1:A:209:ASN:ND2 | 2.38 | 0.57 |
| 2:B:101:ASP:HA | 2:B:104:ASN:HD22 | 1.69 | 0.57 |
| 9:F:38:SER:O | 9:F:40:LYS:HG2 | 2.05 | 0.57 |
| 9:F:447:GLU:O | 9:F:451:THR:HG23 | 2.05 | 0.57 |
| 1:A:309:HIS:O | 1:A:309:HIS:CG | 2.58 | 0.57 |
| 2:D:147:PHE:HD2 | 2:D:154:TRP:HB2 | 1.70 | 0.57 |
| 5:H:42:VAL:HG12 | 8:K:26:HIS:HA | 1.87 | 0.57 |
| 9:E:397:VAL:HG13 | 9:E:399:ILE:HD11 | 1.87 | 0.57 |
| 9:F:237:ALA:O | 9:F:385:SER:OG | 2.12 | 0.57 |
| 9:E:63:LEU:HB3 | 9:E:83:LEU:HD12 | 1.87 | 0.56 |
| 9:F:269:TYR:HB3 | 9:F:298:TYR:CD2 | 2.40 | 0.56 |
| 1:A:58:GLU:OE1 | 1:A:68:SER:OG | 2.23 | 0.56 |
| 1:A:447:ASN:O | 1:A:451:SER:OG | 2.08 | 0.56 |
| 2:D:51:ARG:N | 2:D:51:ARG:HD2 | 2.20 | 0.56 |
| 5:H:4:ALA:HB1 | 8:K:4:VAL:HB | 1.87 | 0.56 |
| 5:H:74:CYS:SG | 5:H:76:TYR:HB2 | 2.45 | 0.56 |
| 8:K:181:VAL:HG13 | 8:K:239:PRO:HB3 | 1.88 | 0.56 |
| 8:K:405:VAL:HG11 | 8:K:505:GLY:HA2 | 1.87 | 0.56 |
| 9:F:265:ASN:HB3 | 9:F:269:TYR:CE1 | 2.39 | 0.56 |
| 9:F:269:TYR:CE1 | 9:F:295:LEU:HB2 | 2.40 | 0.56 |
| 9:F:332:ARG:HH12 | 9:F:358:CYS:HA | 1.69 | 0.56 |
| 9:F:557:ASN:HB2 | 9:F:560:ARG:HH21 | 1.71 | 0.56 |
| 6:I:18:G:H2' | 6:I:19:C:H6 | 1.70 | 0.56 |
| 9:F:394:LYS:O | 9:F:395:HIS:ND1 | 2.38 | 0.56 |
| 1:A:276:THR:N | 1:A:278:GLU:OE1 | 2.39 | 0.56 |
| 2:B:12:TYR:CD1 | 2:B:49:PHE:HZ | 2.23 | 0.56 |
| 5:H:42:VAL:HG22 | 5:H:72:SER:HB3 | 1.88 | 0.56 |
| 9:E:542:ASP:OD1 | 9:E:542:ASP:N | 2.37 | 0.56 |
| 3:C:67:ASP:OD1 | 3:C:68:ILE:N | 2.38 | 0.56 |
| 9:E:69:SER:HB2 | 9:E:71:TYR:CZ | 2.41 | 0.56 |
| 9:E:584:LYS:O | 9:E:586:GLN:NE2 | 2.37 | 0.56 |
| 2:D:141:THR:OG1 | 2:D:142:CYS:N | 2.39 | 0.56 |
| 4:G:7:VAL:HG21 | 4:G:105:SER:HB2 | 1.88 | 0.56 |
| 8:K:87:ILE:O | 8:K:183:PHE:HA | 2.06 | 0.56 |
| 9:E:255:THR:HG22 | 9:E:257:ASN:H | 1.71 | 0.56 |
| 1:A:921:TYR:O | 1:A:924:MET:N | 2.21 | 0.56 |
| 8:K:18:LEU:HB2 | 8:K:23:ALA:HB2 | 1.87 | 0.56 |
| 9:E:52:ALA:HB2 | 9:E:71:TYR:CD1 | 2.41 | 0.56 |
| 1:A:610:GLU:OE1 | 1:A:610:GLU:N | 2.29 | 0.56 |
| 2:B:77:GLU:O | 2:B:80:ARG:HG2 | 2.06 | 0.56 |
| 2:B:95:LEU:O | 2:B:97:LYS:N | 2.38 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:38:ASP:O | 3:C:41:LEU:N | 2.33 | 0.56 |
| 9:F:540:GLU:O | 9:F:569:LYS:NZ | 2.22 | 0.56 |
| 1:A:365:ARG:HH11 | 1:A:366:LEU:H | 1.54 | 0.56 |
| 2:B:103:LEU:O | 2:B:106:ILE:N | 2.39 | 0.56 |
| 9:E:276:LYS:O | 9:E:395:HIS:HA | 2.06 | 0.56 |
| 9:E:417:LEU:HB3 | 9:E:422:PHE:HE1 | 1.70 | 0.56 |
| 1:A:6:SER:O | 1:A:10:ARG:N | 2.33 | 0.55 |
| 6:I:18:G:H2' | 6:I:19:C:C6 | 2.40 | 0.55 |
| 8:K:466:VAL:H | 8:K:483:VAL:HG21 | 1.72 | 0.55 |
| 9:E:103:VAL:O | 9:E:107:ASN:ND2 | 2.39 | 0.55 |
| 9:E:124:ASN:OD1 | 9:E:381:ASN:ND2 | 2.38 | 0.55 |
| 9:E:387:VAL:HG13 | 9:E:388:ASN:H | 1.70 | 0.55 |
| 9:E:510:VAL:HG13 | 9:E:529:PRO:HB2 | 1.88 | 0.55 |
| 9:E:562:ASN:O | 9:E:565:ILE:HG22 | 2.05 | 0.55 |
| 9:F:167:TRP:CH2 | 9:F:174:PRO:HD2 | 2.41 | 0.55 |
| 9:F:281:GLN:HB2 | 9:F:434:PRO:HG3 | 1.87 | 0.55 |
| 1:A:77:PHE:O | 1:A:80:TYR:HB3 | 2.06 | 0.55 |
| 1:A:388:LEU:HD23 | 1:A:389:LEU:N | 2.21 | 0.55 |
| 1:A:599:HIS:HD2 | 1:A:827:VAL:HA | 1.71 | 0.55 |
| 5:H:99:ILE:HD11 | 5:H:107:PRO:HB3 | 1.88 | 0.55 |
| 8:K:186:TRP:CD2 | 8:K:253:LEU:HD12 | 2.41 | 0.55 |
| 8:K:357:SER:OG | 8:K:358:ASP:N | 2.38 | 0.55 |
| 9:E:175:PRO:HG2 | 9:E:180:TYR:CE1 | 2.41 | 0.55 |
| 9:F:138:LEU:O | 9:F:141:THR:OG1 | 2.23 | 0.55 |
| 9:F:279:THR:OG1 | 9:F:435:ASP:N | 2.40 | 0.55 |
| 1:A:513:ARG:O | 1:A:517:ASP:HB2 | 2.06 | 0.55 |
| 9:E:21:ARG:NH2 | 9:E:136:GLU:OE1 | 2.40 | 0.55 |
| 9:F:73:LYS:HE3 | 9:F:74:SER:HB3 | 1.88 | 0.55 |
| 9:F:104:THR:OG1 | 9:F:105:ASP:N | 2.39 | 0.55 |
| 1:A:161:ASP:O | 1:A:168:ASN:ND2 | 2.35 | 0.55 |
| 1:A:335:VAL:O | 1:A:338:VAL:HB | 2.05 | 0.55 |
| 1:A:397:SER:OG | 1:A:398:VAL:N | 2.37 | 0.55 |
| 1:A:779:ILE:O | 1:A:782:PHE:N | 2.39 | 0.55 |
| 9:E:163:LEU:HD21 | 9:E:219:LEU:HG | 1.88 | 0.55 |
| 9:E:254:PRO:O | 9:E:255:THR:OG1 | 2.25 | 0.55 |
| 9:E:269:TYR:OH | 9:E:291:PHE:O | 2.17 | 0.55 |
| 9:F:326:PRO:HG2 | 9:F:329:LYS:HD2 | 1.87 | 0.55 |
| 9:F:353:GLU:HG3 | 9:F:355:TYR:H | 1.71 | 0.55 |
| 1:A:229:SER:O | 1:A:229:SER:OG | 2.14 | 0.55 |
| 5:H:53:GLN:NE2 | 5:H:121:GLY:HA3 | 2.21 | 0.55 |
| 1:A:856:ILE:O | 1:A:859:PHE:N | 2.39 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:494:GLY:HA2 | 9:E:497:ARG:HB2 | 1.89 | 0.55 |
| 1:A:211:ASP:OD2 | 1:A:215:ASN:ND2 | 2.39 | 0.55 |
| 9:F:420:GLU:HB3 | 9:F:430:LYS:HB2 | 1.88 | 0.55 |
| 8:K:54:LEU:HD11 | 8:K:123:GLY:HA3 | 1.89 | 0.55 |
| 9:E:441:CYS:SG | 9:E:461:LEU:HD22 | 2.47 | 0.55 |
| 1:A:356:ASN:ND2 | 1:A:535:VAL:H | 2.05 | 0.55 |
| 1:A:389:LEU:HD21 | 1:A:391:LYS:NZ | 2.22 | 0.55 |
| 9:E:579:ARG:O | 9:E:583:ASP:N | 2.32 | 0.55 |
| 9:F:90:PHE:HD1 | 9:F:94:LYS:HZ1 | 1.54 | 0.55 |
| 9:F:322:LEU:HD22 | 9:F:343:PHE:HE1 | 1.72 | 0.55 |
| 1:A:651:ARG:O | 1:A:654:ARG:N | 2.39 | 0.54 |
| 1:A:783:LYS:NZ | 1:A:796:GLU:HB2 | 2.22 | 0.54 |
| 2:B:171:GLU:HB3 | 2:B:176:ASN:ND2 | 2.22 | 0.54 |
| 2:D:54:ALA:HA | 2:D:57:ARG:CZ | 2.36 | 0.54 |
| 8:K:499:ASN:O | 8:K:502:ILE:HG12 | 2.07 | 0.54 |
| 9:F:277:TYR:HB2 | 9:F:396:TYR:O | 2.07 | 0.54 |
| 5:H:65:GLN:HB2 | 5:H:99:ILE:O | 2.07 | 0.54 |
| 8:K:83:VAL:HG22 | 8:K:84:ARG:H | 1.72 | 0.54 |
| 9:E:440:THR:O | 9:E:442:ARG:N | 2.34 | 0.54 |
| 1:A:226:THR:HG23 | 1:A:229:SER:HB3 | 1.89 | 0.54 |
| 1:A:278:GLU:CD | 1:A:278:GLU:H | 2.11 | 0.54 |
| 7:J:41:G:H2' | 7:J:42:C:H6 | 1.69 | 0.54 |
| 9:E:7:LEU:HD21 | 9:E:106:PHE:CD1 | 2.43 | 0.54 |
| 9:F:28:LYS:HD2 | 9:F:99:GLY:N | 2.21 | 0.54 |
| 9:F:72:CYS:SG | 9:F:73:LYS:N | 2.80 | 0.54 |
| 1:A:188:LYS:HD2 | 1:A:214:GLY:HA3 | 1.89 | 0.54 |
| 1:A:465:ASP:OD1 | 1:A:466:ILE:N | 2.41 | 0.54 |
| 6:I:21:U:H2' | 6:I:22:G:C8 | 2.42 | 0.54 |
| 9:E:285:GLY:O | 9:E:287:GLY:N | 2.40 | 0.54 |
| 9:E:319:GLU:O | 9:E:322:LEU:HG | 2.08 | 0.54 |
| 9:F:288:LYS:NZ | 9:F:538:GLY:O | 2.40 | 0.54 |
| 1:A:64:ASN:OD1 | 1:A:64:ASN:N | 2.23 | 0.54 |
| 1:A:206:THR:HG21 | 4:G:2:ASN:HD22 | 1.72 | 0.54 |
| 4:G:70:GLU:HG3 | 4:G:90:PHE:HB2 | 1.88 | 0.54 |
| 4:G:71:PRO:HD3 | 4:G:92:LYS:HE2 | 1.90 | 0.54 |
| 9:E:137:THR:O | 9:E:141:THR:HG23 | 2.08 | 0.54 |
| 9:E:487:ALA:HB2 | 9:E:515:TYR:HD2 | 1.73 | 0.54 |
| 9:E:559:ASN:OD1 | 9:E:560:ARG:N | 2.41 | 0.54 |
| 5:H:33:SER:OG | 8:K:66:VAL:HG22 | 2.08 | 0.54 |
| 9:E:41:LEU:HD12 | 9:E:42:VAL:H | 1.72 | 0.54 |
| 9:E:243:GLN:NE2 | 9:E:275:GLN:OE1 | 2.41 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:494:GLY:HA2 | 9:F:497:ARG:HE | 1.72 | 0.54 |
| 1:A:102:PHE:CE1 | 1:A:113:HIS:HB2 | 2.42 | 0.54 |
| 4:G:94:LEU:HD21 | 4:G:98:ASN:HB2 | 1.90 | 0.54 |
| 5:H:70:GLY:HA2 | 5:H:97:VAL:HG23 | 1.90 | 0.54 |
| 8:K:19:HIS:O | 8:K:22:GLN:HG2 | 2.08 | 0.54 |
| 8:K:164:ILE:HA | 8:K:234:ASP:HB3 | 1.89 | 0.54 |
| 8:K:214:ALA:HB1 | 8:K:224:TYR:HB3 | 1.89 | 0.54 |
| 9:E:73:LYS:HA | 9:E:76:LYS:HG2 | 1.90 | 0.54 |
| 9:F:458:ASP:HB3 | 9:F:460:LYS:HG2 | 1.89 | 0.54 |
| 1:A:879:ASP:O | 1:A:882:HIS:N | 2.41 | 0.54 |
| 4:G:4:LEU:HG | 4:G:5:SER:H | 1.73 | 0.54 |
| 8:K:83:VAL:HG12 | 8:K:296:TYR:CE2 | 2.42 | 0.54 |
| 9:E:8:CYS:SG | 9:E:29:CYS:HB3 | 2.47 | 0.54 |
| 9:E:382:TYR:O | 9:E:386:VAL:HG23 | 2.08 | 0.54 |
| 9:E:404:GLN:HG2 | 9:E:563:VAL:HB | 1.90 | 0.54 |
| 9:F:58:THR:OG1 | 9:F:59:ASP:N | 2.41 | 0.54 |
| 1:A:903:TYR:O | 1:A:905:VAL:N | 2.41 | 0.54 |
| 4:G:23:CYS:HB2 | 4:G:55:ARG:NE | 2.22 | 0.54 |
| 8:K:203:PRO:HB2 | 8:K:205:ARG:NE | 2.22 | 0.54 |
| 9:F:21:ARG:NH2 | 9:F:136:GLU:OE2 | 2.41 | 0.54 |
| 9:F:473:LYS:NZ | 9:F:587:PHE:O | 2.41 | 0.54 |
| 1:A:136:GLU:HB2 | 1:A:163:TYR:CE1 | 2.43 | 0.54 |
| 1:A:303:ASP:OD1 | 1:A:303:ASP:N | 2.36 | 0.54 |
| 2:B:59:LEU:O | 2:B:62:MET:HG3 | 2.08 | 0.54 |
| 9:E:516:ASN:OD1 | 9:E:532:THR:OG1 | 2.09 | 0.54 |
| 9:F:182:PHE:HB2 | 9:F:200:PHE:CE2 | 2.41 | 0.54 |
| 9:F:182:PHE:N | 9:F:198:TYR:O | 2.30 | 0.54 |
| 9:F:252:LEU:HD21 | 9:F:394:LYS:HE2 | 1.90 | 0.54 |
| 9:F:546:PHE:O | 9:F:574:CYS:HA | 2.07 | 0.54 |
| 1:A:303:ASP:O | 1:A:305:ARG:N | 2.41 | 0.53 |
| 2:D:175:ASP:N | 2:D:175:ASP:OD1 | 2.41 | 0.53 |
| 9:E:370:ILE:HD11 | 9:E:397:VAL:HG12 | 1.89 | 0.53 |
| 9:E:372:VAL:HA | 9:E:397:VAL:HG13 | 1.89 | 0.53 |
| 9:F:51:ASN:ND2 | 9:F:70:TYR:H | 2.06 | 0.53 |
| 1:A:533:ARG:O | 1:A:534:ASN:ND2 | 2.42 | 0.53 |
| 2:D:135:TYR:CZ | 2:D:174:MET:HB3 | 2.43 | 0.53 |
| 9:F:425:VAL:HA | 9:F:428:LEU:HD23 | 1.90 | 0.53 |
| 1:A:132:ARG:HB2 | 1:A:133:HIS:ND1 | 2.23 | 0.53 |
| 1:A:242:MET:HB3 | 1:A:463:MET:HE3 | 1.90 | 0.53 |
| 1:A:631:ARG:HG2 | 1:A:663:LEU:HD13 | 1.91 | 0.53 |
| 5:H:19:PHE:HB3 | 8:K:201:ILE:HG23 | 1.90 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:377:SER:HB3 | 9:E:405:LEU:O | 2.08 | 0.53 |
| 9:F:373:PHE:HD1 | 9:F:376:ILE:HG22 | 1.73 | 0.53 |
| 1:A:402:THR:HG22 | 1:A:403:ASN:H | 1.72 | 0.53 |
| 1:A:491:ASN:HB3 | 1:A:521:TYR:CE2 | 2.42 | 0.53 |
| 1:A:568:ASN:OD1 | 1:A:654:ARG:NH2 | 2.42 | 0.53 |
| 1:A:602:LEU:HD12 | 1:A:828:TYR:CD2 | 2.44 | 0.53 |
| 9:E:146:LYS:HD3 | 9:E:149:TYR:CE1 | 2.44 | 0.53 |
| 9:E:278:SER:O | 9:E:398:TYR:N | 2.42 | 0.53 |
| 9:F:5:CYS:SG | 9:F:26:CYS:N | 2.73 | 0.53 |
| 2:B:19:GLN:O | 2:B:22:TYR:N | 2.41 | 0.53 |
| 2:B:56:GLN:O | 2:B:60:GLU:HG2 | 2.08 | 0.53 |
| 2:D:44:VAL:O | 2:D:48:GLU:HG3 | 2.09 | 0.53 |
| 8:K:185:LEU:HD12 | 8:K:188:HIS:HA | 1.91 | 0.53 |
| 9:E:441:CYS:HB2 | 9:E:464:HIS:CB | 2.37 | 0.53 |
| 1:A:726:ARG:HA | 1:A:729:GLU:OE1 | 2.07 | 0.53 |
| 9:F:8:CYS:O | 9:F:10:SER:N | 2.41 | 0.53 |
| 9:F:373:PHE:O | 9:F:399:ILE:HG12 | 2.08 | 0.53 |
| 9:F:559:ASN:HA | 9:F:562:ASN:ND2 | 2.23 | 0.53 |
| 1:A:11:VAL:HG11 | 1:A:56:PHE:HE1 | 1.73 | 0.53 |
| 1:A:295:HIS:CE1 | 1:A:301:CYS:HA | 2.43 | 0.53 |
| 5:H:79:CYS:HB2 | 5:H:81:ILE:HG12 | 1.90 | 0.53 |
| 8:K:491:TYR:HA | 8:K:494:TYR:HB3 | 1.91 | 0.53 |
| 9:E:401:ASP:OD2 | 9:E:403:ALA:HB3 | 2.09 | 0.53 |
| 2:D:22:TYR:O | 2:D:26:VAL:HG22 | 2.09 | 0.53 |
| 7:J:42:C:H2' | 7:J:43:U:H6 | 1.74 | 0.53 |
| 9:E:238:PRO:O | 9:E:388:ASN:ND2 | 2.27 | 0.53 |
| 1:A:642:HIS:CG | 1:A:645:CYS:SG | 2.94 | 0.53 |
| 5:H:33:SER:OG | 5:H:33:SER:O | 2.19 | 0.53 |
| 8:K:470:SER:OG | 8:K:473:CYS:SG | 2.55 | 0.53 |
| 9:E:51:ASN:HD21 | 9:E:70:TYR:H | 1.56 | 0.53 |
| 9:E:186:ARG:HD2 | 9:E:195:ILE:HG12 | 1.91 | 0.53 |
| 9:E:492:GLN:NE2 | 9:E:575:ILE:HG22 | 2.23 | 0.53 |
| 9:E:513:SER:C | 9:E:533:VAL:HG23 | 2.29 | 0.53 |
| 1:A:35:PHE:HZ | 1:A:50:LYS:HB2 | 1.74 | 0.53 |
| 1:A:738:ASP:O | 1:A:741:PHE:N | 2.42 | 0.53 |
| 6:I:20:A:C4 | 7:J:41:G:C2 | 2.97 | 0.53 |
| 8:K:191:GLU:O | 8:K:195:MET:HG3 | 2.08 | 0.53 |
| 8:K:384:PHE:HB2 | 8:K:398:VAL:HG12 | 1.91 | 0.53 |
| 9:E:220:ASN:OD1 | 9:E:221:VAL:N | 2.42 | 0.53 |
| 9:F:287:GLY:HA2 | 9:F:290:HIS:HB3 | 1.90 | 0.53 |
| 1:A:456:TYR:CE2 | 1:A:676:LYS:HG3 | 2.44 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:51:ARG:CZ | 6:I:17:A:HI' | 2.38 | 0.52 |
| 2:D:51:ARG:NH1 | 6:I:17:A:O2' | 2.42 | 0.52 |
| 9:F:372:VAL:HG22 | 9:F:397:VAL:HB | 1.90 | 0.52 |
| 1:A:84:GLU:HG2 | 8:K:98:ARG:HD2 | 1.91 | 0.52 |
| 5:H:43:LYS:HD2 | 5:H:68:PHE:CE1 | 2.44 | 0.52 |
| 9:E:143:GLU:O | 9:E:146:LYS:N | 2.41 | 0.52 |
| 9:E:443:ARG:HA | 9:E:569:LYS:HE3 | 1.90 | 0.52 |
| 9:E:496:VAL:HG11 | 9:E:547:THR:OG1 | 2.10 | 0.52 |
| 9:F:8:CYS:C | 9:F:10:SER:H | 2.13 | 0.52 |
| 9:F:117:ALA:HB2 | 9:F:415:GLY:O | 2.10 | 0.52 |
| 9:F:514:PRO:HD3 | 9:F:546:PHE:CZ | 2.44 | 0.52 |
| 4:G:11:GLN:HE21 | 4:G:12:MET:N | 2.06 | 0.52 |
| 5:H:29:ASP:O | 5:H:33:SER:CB | 2.58 | 0.52 |
| 5:H:42:VAL:HA | 8:K:26:HIS:CD2 | 2.44 | 0.52 |
| 9:F:488:ILE:HD13 | 9:F:521:VAL:HG21 | 1.91 | 0.52 |
| 1:A:903:TYR:N | 1:A:903:TYR:CD1 | 2.76 | 0.52 |
| 4:G:23:CYS:HB2 | 4:G:55:ARG:HE | 1.75 | 0.52 |
| 9:E:330:CYS:HB3 | 9:E:357:PHE:CE2 | 2.44 | 0.52 |
| 9:E:370:ILE:HB | 9:E:395:HIS:HB2 | 1.91 | 0.52 |
| 9:F:15:ARG:O | 9:F:17:GLY:N | 2.43 | 0.52 |
| 9:F:475:PHE:HB2 | 9:F:582:TYR:CZ | 2.44 | 0.52 |
| 1:A:604:THR:O | 1:A:606:TYR:N | 2.42 | 0.52 |
| 2:B:135:TYR:O | 2:B:138:TYR:HB3 | 2.09 | 0.52 |
| 8:K:160:ASN:O | 8:K:164:ILE:HG13 | 2.09 | 0.52 |
| 9:E:245:HIS:NE2 | 9:E:275:GLN:OE1 | 2.42 | 0.52 |
| 9:E:315:ASP:HA | 9:E:343:PHE:CE2 | 2.44 | 0.52 |
| 9:E:423:ASN:O | 9:E:427:ARG:N | 2.29 | 0.52 |
| 9:F:376:ILE:HD11 | 9:F:429:MET:SD | 2.50 | 0.52 |
| 1:A:40:ASP:OD1 | 1:A:41:LYS:N | 2.42 | 0.52 |
| 9:E:489:ASN:O | 9:E:493:ILE:HG12 | 2.10 | 0.52 |
| 9:F:447:GLU:H | 9:F:467:LYS:HG2 | 1.75 | 0.52 |
| 8:K:257:HIS:HE1 | 8:K:279:CYS:HB3 | 1.73 | 0.52 |
| 9:F:3:GLY:HA3 | 9:F:24:PHE:CD2 | 2.45 | 0.52 |
| 9:F:72:CYS:SG | 9:F:74:SER:N | 2.75 | 0.52 |
| 9:F:243:GLN:NE2 | 9:F:276:LYS:H | 2.06 | 0.52 |
| 1:A:256:HIS:HD2 | 1:A:261:LEU:HA | 1.75 | 0.52 |
| 2:B:43:ASN:O | 2:B:46:LYS:HE3 | 2.10 | 0.52 |
| 2:D:13:ALA:O | 2:D:17:THR:HG23 | 2.10 | 0.52 |
| 6:I:32:A:C2 | 7:J:29:G:C2 | 2.98 | 0.52 |
| 9:E:113:ASP:OD1 | 9:E:114:TRP:N | 2.43 | 0.52 |
| 9:F:303:ARG:HG2 | 9:F:368:ALA:HA | 1.91 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:50:ASP:OD2 | 6:I:15:G:H4' | 2.10 | 0.52 |
| 2:B:64:ASP:O | 2:B:68:THR:HG23 | 2.09 | 0.52 |
| 2:D:22:TYR:OH | 2:D:39:LYS:HD3 | 2.10 | 0.52 |
| 5:H:54:ALA:HB1 | 5:H:97:VAL:HA | 1.92 | 0.52 |
| 8:K:407:SER:H | 8:K:410:ASN:ND2 | 2.08 | 0.52 |
| 9:E:101:ASP:O | 9:E:103:VAL:N | 2.41 | 0.52 |
| 9:E:412:LEU:HD11 | 9:E:417:LEU:HB2 | 1.91 | 0.52 |
| 9:F:31:TYR:CE1 | 9:F:87:GLY:HA2 | 2.45 | 0.52 |
| 9:F:109:ILE:HD13 | 9:F:134:ALA:HB2 | 1.91 | 0.52 |
| 1:A:440:PHE:CD1 | 1:A:843:PHE:HE2 | 2.27 | 0.52 |
| 5:H:10:ASN:OD1 | 5:H:39:THR:N | 2.43 | 0.52 |
| 8:K:116:ASN:HD21 | 8:K:270:ALA:H | 1.58 | 0.52 |
| 9:E:37:THR:OG1 | 9:E:38:SER:N | 2.40 | 0.52 |
| 9:E:280:LEU:N | 9:E:398:TYR:O | 2.42 | 0.52 |
| 9:E:366:THR:O | 9:E:391:LEU:HA | 2.09 | 0.52 |
| 9:F:237:ALA:HB2 | 9:F:389:ALA:HB2 | 1.92 | 0.52 |
| 1:A:225:THR:HG22 | 1:A:226:THR:HG22 | 1.92 | 0.51 |
| 1:A:418:ASP:O | 1:A:421:ASP:N | 2.42 | 0.51 |
| 1:A:657:ASN:HB3 | 1:A:661:GLN:HE22 | 1.75 | 0.51 |
| 1:A:867:TYR:CZ | 1:A:922:GLU:HB3 | 2.44 | 0.51 |
| 8:K:216:CYS:HB2 | 8:K:225:ALA:O | 2.10 | 0.51 |
| 9:E:381:ASN:CG | 9:E:424:SER:H | 2.12 | 0.51 |
| 9:E:448:ILE:H | 9:E:448:ILE:HD12 | 1.74 | 0.51 |
| 9:F:46:ASN:HD21 | 9:F:70:TYR:HE2 | 1.58 | 0.51 |
| 1:A:736:ASP:OD1 | 1:A:737:VAL:N | 2.39 | 0.51 |
| 1:A:745:PHE:O | 1:A:748:TYR:N | 2.44 | 0.51 |
| 3:C:55:LEU:HD23 | 3:C:56:LEU:N | 2.25 | 0.51 |
| 1:A:350:GLU:N | 1:A:350:GLU:OE2 | 2.42 | 0.51 |
| 1:A:360:ASN:OD1 | 1:A:360:ASN:N | 2.41 | 0.51 |
| 2:D:134:ASP:O | 2:D:137:THR:OG1 | 2.28 | 0.51 |
| 2:D:147:PHE:CD2 | 2:D:154:TRP:HB2 | 2.45 | 0.51 |
| 4:G:44:LEU:HB3 | 4:G:89:TYR:HB2 | 1.92 | 0.51 |
| 7:J:40:U:O2' | 7:J:41:G:H5' | 2.10 | 0.51 |
| 9:E:266:VAL:HG13 | 9:E:298:TYR:HE2 | 1.75 | 0.51 |
| 9:E:419:PRO:O | 9:E:426:CYS:HB3 | 2.11 | 0.51 |
| 9:F:174:PRO:HB2 | 9:F:180:TYR:CZ | 2.45 | 0.51 |
| 9:F:473:LYS:HZ3 | 9:F:587:PHE:H | 1.57 | 0.51 |
| 1:A:207:LEU:O | 1:A:209:ASN:N | 2.43 | 0.51 |
| 1:A:657:ASN:O | 1:A:661:GLN:NE2 | 2.43 | 0.51 |
| 8:K:19:HIS:HD2 | 8:K:20:PRO:HD2 | 1.75 | 0.51 |
| 9:E:151:ILE:N | 9:E:168:GLU:OE2 | 2.43 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:353:GLU:HG3 | 9:F:355:TYR:N | 2.25 | 0.51 |
| 1:A:131:LEU:HD23 | 1:A:131:LEU:O | 2.10 | 0.51 |
| 2:B:161:ASP:OD2 | 2:B:162:ALA:N | 2.44 | 0.51 |
| 8:K:226:CYS:SG | 8:K:227:TRP:N | 2.83 | 0.51 |
| 9:E:177:ASN:ND2 | 9:E:516:ASN:H | 2.09 | 0.51 |
| 9:E:473:LYS:HG3 | 9:E:589:SER:HA | 1.93 | 0.51 |
| 9:E:526:LEU:HD12 | 9:E:528:LEU:HD12 | 1.93 | 0.51 |
| 1:A:364:SER:OG | 1:A:365:ARG:N | 2.41 | 0.51 |
| 2:B:51:ARG:H | 2:B:51:ARG:HD2 | 1.76 | 0.51 |
| 2:D:22:TYR:HA | 2:D:38:LEU:HD13 | 1.93 | 0.51 |
| 5:H:16:PHE:HE1 | 8:K:69:TYR:CE2 | 2.27 | 0.51 |
| 5:H:126:TYR:N | 5:H:127:GLY:HA2 | 2.26 | 0.51 |
| 8:K:262:GLN:N | 8:K:415:ASP:OD2 | 2.42 | 0.51 |
| 9:E:369:ASP:HA | 9:E:394:LYS:HB2 | 1.92 | 0.51 |
| 9:F:306:TYR:HD2 | 9:F:317:LEU:HD21 | 1.76 | 0.51 |
| 9:F:428:LEU:O | 9:F:432:ILE:N | 2.44 | 0.51 |
| 1:A:260:ASP:OD2 | 1:A:262:THR:OG1 | 2.29 | 0.51 |
| 2:D:158:GLN:O | 2:D:159:VAL:HG23 | 2.10 | 0.51 |
| 5:H:65:GLN:HB3 | 5:H:100:PRO:HA | 1.93 | 0.51 |
| 8:K:76:ARG:HD3 | 8:K:247:TRP:CZ2 | 2.46 | 0.51 |
| 9:F:272:VAL:HG21 | 9:F:295:LEU:HD21 | 1.93 | 0.51 |
| 9:F:278:SER:O | 9:F:397:VAL:HA | 2.11 | 0.51 |
| 1:A:11:VAL:HG11 | 1:A:56:PHE:CE1 | 2.46 | 0.51 |
| 1:A:299:VAL:HA | 1:A:652:PHE:CE2 | 2.46 | 0.51 |
| 1:A:414:ASN:HD21 | 1:A:845:ASP:C | 2.14 | 0.51 |
| 1:A:445:ASP:N | 1:A:445:ASP:OD1 | 2.42 | 0.51 |
| 1:A:446:GLY:O | 1:A:448:ALA:N | 2.43 | 0.51 |
| 1:A:602:LEU:HD12 | 1:A:828:TYR:HD2 | 1.76 | 0.51 |
| 5:H:10:ASN:HD22 | 5:H:13:VAL:HG21 | 1.76 | 0.51 |
| 9:E:446:ALA:HB3 | 9:E:467:LYS:HE2 | 1.93 | 0.51 |
| 1:A:734:ASN:OD1 | 1:A:736:ASP:N | 2.38 | 0.51 |
| 8:K:93:GLY:HA3 | 8:K:190:PHE:CZ | 2.46 | 0.51 |
| 9:E:199:THR:N | 9:E:212:ARG:O | 2.35 | 0.51 |
| 9:E:420:GLU:H | 9:E:430:LYS:HE3 | 1.74 | 0.51 |
| 9:F:19:CYS:HA | 9:F:39:HIS:CE1 | 2.45 | 0.51 |
| 8:K:93:GLY:HA3 | 8:K:190:PHE:HZ | 1.75 | 0.51 |
| 9:E:489:ASN:HD21 | 9:E:518:GLN:NE2 | 2.08 | 0.51 |
| 9:F:441:CYS:O | 9:F:464:HIS:HB2 | 2.11 | 0.51 |
| 9:F:504:PRO:O | 9:F:506:TRP:N | 2.44 | 0.51 |
| 1:A:331:ARG:HB2 | 2:B:113:GLY:O | 2.11 | 0.50 |
| 9:E:283:PRO:HB2 | 9:E:286:THR:HG21 | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:154:VAL:HG23 | 9:F:163:LEU:HD21 | 1.92 | 0.50 |
| 9:F:181:VAL:O | 9:F:227:LEU:HD12 | 2.11 | 0.50 |
| 9:F:499:PHE:HA | 9:F:502:ARG:HG2 | 1.92 | 0.50 |
| 1:A:392:ARG:CZ | 1:A:450:ILE:HG21 | 2.41 | 0.50 |
| 1:A:485:GLY:HA2 | 1:A:574:LYS:HD2 | 1.93 | 0.50 |
| 6:I:21:U:H2' | 6:I:22:G:H8 | 1.76 | 0.50 |
| 9:E:386:VAL:HG12 | 9:E:390:ARG:HH21 | 1.76 | 0.50 |
| 9:E:497:ARG:HD2 | 9:E:526:LEU:HD13 | 1.94 | 0.50 |
| 9:F:5:CYS:O | 9:F:129:ARG:NH1 | 2.40 | 0.50 |
| 9:F:5:CYS:O | 9:F:9:ASN:N | 2.43 | 0.50 |
| 1:A:348:PHE:CD2 | 1:A:351:LEU:HB2 | 2.46 | 0.50 |
| 2:D:122:LEU:HA | 2:D:190:ARG:HH21 | 1.75 | 0.50 |
| 6:I:25:A:H2' | 6:I:26:G:C8 | 2.43 | 0.50 |
| 8:K:237:TYR:C | 8:K:239:PRO:HD3 | 2.31 | 0.50 |
| 9:E:14:LEU:O | 9:E:24:PHE:HA | 2.10 | 0.50 |
| 9:E:173:ARG:N | 9:E:174:PRO:HD3 | 2.27 | 0.50 |
| 9:E:427:ARG:O | 9:E:431:THR:HG23 | 2.11 | 0.50 |
| 9:F:195:ILE:HG13 | 9:F:198:TYR:CE2 | 2.46 | 0.50 |
| 1:A:314:ASN:ND2 | 1:A:350:GLU:O | 2.25 | 0.50 |
| 1:A:476:VAL:HG22 | 1:A:696:ILE:HG22 | 1.94 | 0.50 |
| 1:A:528:PHE:CE2 | 1:A:532:LYS:HE3 | 2.46 | 0.50 |
| 2:D:135:TYR:CE2 | 2:D:174:MET:HB3 | 2.47 | 0.50 |
| 4:G:76:VAL:HG23 | 4:G:113:GLN:HB2 | 1.94 | 0.50 |
| 8:K:84:ARG:O | 8:K:177:LEU:HB3 | 2.12 | 0.50 |
| 8:K:272:CYS:HA | 8:K:275:ILE:HG22 | 1.93 | 0.50 |
| 9:E:164:HIS:CE1 | 9:E:207:ASP:HB3 | 2.47 | 0.50 |
| 9:F:240:LEU:HD11 | 9:F:424:SER:HB2 | 1.93 | 0.50 |
| 9:F:424:SER:O | 9:F:427:ARG:HB3 | 2.12 | 0.50 |
| 1:A:37:ILE:HG21 | 1:A:48:PHE:CE2 | 2.47 | 0.50 |
| 1:A:295:HIS:N | 1:A:295:HIS:CD2 | 2.79 | 0.50 |
| 2:D:168:GLN:HB2 | 2:D:171:GLU:HB2 | 1.94 | 0.50 |
| 2:D:176:ASN:O | 2:D:179:ASN:CB | 2.54 | 0.50 |
| 2:D:182:TRP:O | 2:D:184:LEU:N | 2.38 | 0.50 |
| 9:E:198:TYR:HB2 | 9:E:225:PHE:HE2 | 1.76 | 0.50 |
| 9:E:369:ASP:HA | 9:E:394:LYS:H | 1.75 | 0.50 |
| 9:F:91:GLY:O | 9:F:92:LEU:HD22 | 2.10 | 0.50 |
| 9:F:443:ARG:O | 9:F:569:LYS:HA | 2.12 | 0.50 |
| 9:F:456:VAL:HG13 | 9:F:457:TYR:N | 2.27 | 0.50 |
| 4:G:10:ARG:NH2 | 4:G:34:THR:H | 2.09 | 0.50 |
| 8:K:84:ARG:HH21 | 8:K:421:VAL:HG12 | 1.76 | 0.50 |
| 9:E:124:ASN:HD22 | 9:E:421:TYR:HA | 1.76 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:425:VAL:HG13 | 9:E:426:CYS:H | 1.76 | 0.50 |
| 9:F:557:ASN:OD1 | 9:F:558:VAL:N | 2.45 | 0.50 |
| 1:A:844:VAL:HG21 | 1:A:849:LYS:CB | 2.42 | 0.50 |
| 1:A:875:GLN:O | 1:A:877:TYR:N | 2.45 | 0.50 |
| 9:E:372:VAL:HA | 9:E:397:VAL:CG1 | 2.42 | 0.50 |
| 9:E:420:GLU:O | 9:E:427:ARG:N | 2.45 | 0.50 |
| 9:F:31:TYR:O | 9:F:35:ILE:HG12 | 2.11 | 0.50 |
| 9:F:322:LEU:HD22 | 9:F:343:PHE:CE1 | 2.46 | 0.50 |
| 1:A:806:THR:C | 1:A:808:GLY:H | 2.15 | 0.50 |
| 1:A:853:THR:OG1 | 1:A:894:GLU:OE2 | 2.30 | 0.50 |
| 1:A:903:TYR:C | 1:A:905:VAL:H | 2.15 | 0.50 |
| 8:K:186:TRP:CE3 | 8:K:253:LEU:HD12 | 2.47 | 0.50 |
| 9:F:331:SER:N | 9:F:353:GLU:HG2 | 2.26 | 0.50 |
| 9:F:376:ILE:HG12 | 9:F:400:GLY:HA3 | 1.93 | 0.50 |
| 4:G:19:THR:H | 4:G:22:ALA:HB3 | 1.76 | 0.50 |
| 9:E:552:THR:HG1 | 9:E:554:HIS:CE1 | 2.29 | 0.50 |
| 9:F:124:ASN:HD22 | 9:F:421:TYR:C | 2.14 | 0.50 |
| 9:F:493:ILE:CG2 | 9:F:525:ILE:HG21 | 2.42 | 0.50 |
| 1:A:404:ASN:N | 1:A:404:ASN:OD1 | 2.42 | 0.49 |
| 2:B:76:SER:OG | 2:B:77:GLU:N | 2.45 | 0.49 |
| 2:D:40:LYS:O | 2:D:44:VAL:HG23 | 2.12 | 0.49 |
| 6:I:16:U:H5" | 6:I:17:A:OP2 | 2.11 | 0.49 |
| 7:J:40:U:C2 | 7:J:41:G:C8 | 3.00 | 0.49 |
| 8:K:41:ASP:N | 8:K:41:ASP:OD1 | 2.44 | 0.49 |
| 9:E:114:TRP:CD1 | 9:E:138:LEU:HA | 2.47 | 0.49 |
| 9:E:184:GLY:O | 9:E:195:ILE:N | 2.45 | 0.49 |
| 9:F:105:ASP:HA | 9:F:108:ALA:HB3 | 1.93 | 0.49 |
| 1:A:905:VAL:N | 9:F:95:ASN:HD21 | 2.10 | 0.49 |
| 2:B:127:LYS:NZ | 2:B:187:THR:HB | 2.27 | 0.49 |
| 2:B:153:LEU:C | 2:B:191:ALA:HB3 | 2.32 | 0.49 |
| 4:G:23:CYS:O | 4:G:55:ARG:NH2 | 2.31 | 0.49 |
| 8:K:213:ARG:HH22 | 8:K:238:ASN:HB3 | 1.77 | 0.49 |
| 9:E:177:ASN:HD21 | 9:E:532:THR:HG23 | 1.77 | 0.49 |
| 9:E:220:ASN:N | 9:E:223:ASP:OD2 | 2.45 | 0.49 |
| 9:E:281:GLN:HG2 | 9:E:434:PRO:HB3 | 1.94 | 0.49 |
| 9:E:353:GLU:HB3 | 9:E:356:VAL:HG22 | 1.93 | 0.49 |
| 9:F:261:GLU:O | 9:F:290:HIS:NE2 | 2.32 | 0.49 |
| 1:A:102:PHE:CE1 | 1:A:104:PHE:HB2 | 2.47 | 0.49 |
| 1:A:272:LYS:HA | 2:B:111:ARG:NH2 | 2.23 | 0.49 |
| 6:I:28:G:N2 | 7:J:33:C:C2 | 2.80 | 0.49 |
| 8:K:261:CYS:HB2 | 8:K:414:CYS:SG | 2.52 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:15:ARG:HA | 9:E:23:PRO:O | 2.12 | 0.49 |
| 9:E:305:VAL:HG22 | 9:E:356:VAL:HB | 1.93 | 0.49 |
| 9:E:332:ARG:N | 9:E:346:PHE:HB2 | 2.28 | 0.49 |
| 9:F:186:ARG:HG2 | 9:F:223:ASP:OD1 | 2.11 | 0.49 |
| 9:F:378:MET:O | 9:F:407:ALA:N | 2.45 | 0.49 |
| 3:C:35:LEU:HD23 | 3:C:55:LEU:HB2 | 1.93 | 0.49 |
| 3:C:44:ASP:N | 3:C:44:ASP:OD1 | 2.43 | 0.49 |
| 9:E:322:LEU:HD23 | 9:E:345:LYS:NZ | 2.27 | 0.49 |
| 9:F:5:CYS:HB3 | 9:F:9:ASN:N | 2.27 | 0.49 |
| 9:F:333:ILE:HG23 | 9:F:349:ASN:HA | 1.94 | 0.49 |
| 9:F:334:ILE:HB | 9:F:335:PRO:HD2 | 1.94 | 0.49 |
| 8:K:53:ARG:O | 8:K:126:ASP:N | 2.29 | 0.49 |
| 9:E:77:PRO:HB2 | 9:E:78:PRO:HD2 | 1.95 | 0.49 |
| 9:E:103:VAL:HG12 | 9:E:107:ASN:ND2 | 2.26 | 0.49 |
| 9:E:498:GLU:O | 9:E:501:THR:N | 2.45 | 0.49 |
| 9:F:62:GLN:OE1 | 9:F:62:GLN:N | 2.43 | 0.49 |
| 1:A:205:LEU:HB3 | 1:A:216:TRP:CH2 | 2.48 | 0.49 |
| 1:A:278:GLU:OE1 | 1:A:278:GLU:N | 2.38 | 0.49 |
| 2:B:173:SER:HG | 2:B:176:ASN:H | 1.53 | 0.49 |
| 9:E:19:CYS:SG | 9:E:110:ALA:HB1 | 2.53 | 0.49 |
| 9:E:146:LYS:HD2 | 9:E:227:LEU:HD21 | 1.94 | 0.49 |
| 9:E:162:GLU:HB3 | 9:E:208:ALA:HB1 | 1.93 | 0.49 |
| 9:E:171:LYS:H | 9:E:172:PRO:HD2 | 1.76 | 0.49 |
| 9:E:447:GLU:CD | 9:E:469:ALA:HA | 2.32 | 0.49 |
| 9:F:487:ALA:O | 9:F:518:GLN:HB2 | 2.12 | 0.49 |
| 9:F:542:ASP:N | 9:F:542:ASP:OD1 | 2.46 | 0.49 |
| 1:A:487:CYS:SG | 1:A:532:LYS:NZ | 2.80 | 0.49 |
| 2:B:171:GLU:OE1 | 2:B:171:GLU:N | 2.31 | 0.49 |
| 2:D:155:GLU:OE1 | 2:D:155:GLU:N | 2.45 | 0.49 |
| 8:K:408:ASN:N | 8:K:408:ASN:OD1 | 2.45 | 0.49 |
| 8:K:494:TYR:O | 8:K:497:ALA:HB3 | 2.12 | 0.49 |
| 9:E:5:CYS:O | 9:E:129:ARG:NH2 | 2.46 | 0.49 |
| 1:A:350:GLU:O | 1:A:352:GLY:N | 2.42 | 0.49 |
| 8:K:168:GLN:HE21 | 8:K:232:GLY:H | 1.59 | 0.49 |
| 9:E:320:LYS:O | 9:E:323:LYS:HB2 | 2.12 | 0.49 |
| 9:F:333:ILE:HB | 9:F:358:CYS:HB2 | 1.94 | 0.49 |
| 1:A:428:PHE:C | 1:A:430:LYS:H | 2.15 | 0.49 |
| 1:A:527:LEU:O | 1:A:530:TYR:HB3 | 2.13 | 0.49 |
| 2:D:128:LEU:HD12 | 2:D:129:MET:N | 2.27 | 0.49 |
| 8:K:113:THR:O | 8:K:115:VAL:N | 2.44 | 0.49 |
| 9:E:59:ASP:OD1 | 9:E:60:VAL:N | 2.46 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:576:MET:HB2 | 9:F:582:TYR:HD1 | 1.77 | 0.49 |
| 1:A:131:LEU:HD21 | 1:A:247:LEU:HD22 | 1.95 | 0.49 |
| 1:A:387:LEU:HD12 | 1:A:388:LEU:H | 1.77 | 0.49 |
| 2:B:102:ALA:O | 2:B:105:ASN:HB3 | 2.12 | 0.49 |
| 6:I:10:C:H2' | 7:J:50:G:H22 | 1.76 | 0.49 |
| 9:E:287:GLY:CA | 9:E:290:HIS:HB2 | 2.43 | 0.49 |
| 9:E:409:ARG:HB3 | 9:E:412:LEU:HB3 | 1.94 | 0.49 |
| 7:J:44:A:H2' | 7:J:45:C:C6 | 2.47 | 0.48 |
| 9:E:12:THR:OG1 | 9:E:13:SER:N | 2.44 | 0.48 |
| 9:E:117:ALA:O | 9:E:120:TYR:N | 2.46 | 0.48 |
| 9:F:150:GLY:HA2 | 9:F:171:LYS:HD2 | 1.95 | 0.48 |
| 9:F:420:GLU:HB2 | 9:F:427:ARG:HA | 1.96 | 0.48 |
| 3:C:19:GLN:NE2 | 2:D:84:THR:HG23 | 2.27 | 0.48 |
| 4:G:11:GLN:HE22 | 4:G:29:LEU:C | 2.16 | 0.48 |
| 8:K:132:ASP:OD1 | 8:K:133:PHE:N | 2.46 | 0.48 |
| 9:F:66:GLY:HA3 | 9:F:71:TYR:CD2 | 2.48 | 0.48 |
| 9:F:369:ASP:HB3 | 9:F:394:LYS:HD2 | 1.95 | 0.48 |
| 9:F:401:ASP:OD2 | 9:F:403:ALA:HB3 | 2.13 | 0.48 |
| 9:F:492:GLN:O | 9:F:496:VAL:HG23 | 2.13 | 0.48 |
| 1:A:824:ASP:OD1 | 1:A:825:ASP:N | 2.46 | 0.48 |
| 1:A:864:ILE:HD11 | 1:A:924:MET:HG3 | 1.95 | 0.48 |
| 2:B:135:TYR:CE1 | 2:B:139:LYS:HD3 | 2.49 | 0.48 |
| 2:D:145:THR:O | 2:D:156:ILE:HG13 | 2.13 | 0.48 |
| 6:I:9:G:H2' | 6:I:10:C:C6 | 2.48 | 0.48 |
| 8:K:83:VAL:HG23 | 8:K:86:TRP:CD1 | 2.48 | 0.48 |
| 9:E:561:PHE:HA | 9:E:564:ALA:HB3 | 1.95 | 0.48 |
| 9:F:154:VAL:HG12 | 9:F:223:ASP:O | 2.13 | 0.48 |
| 9:F:384:LEU:HD11 | 9:F:423:ASN:HB2 | 1.95 | 0.48 |
| 5:H:13:VAL:HG22 | 5:H:30:TYR:HE1 | 1.78 | 0.48 |
| 8:K:88:GLY:HA3 | 8:K:274:ALA:HB1 | 1.94 | 0.48 |
| 8:K:91:VAL:HG22 | 8:K:109:LEU:HG | 1.94 | 0.48 |
| 8:K:170:LEU:HD23 | 8:K:227:TRP:CH2 | 2.48 | 0.48 |
| 8:K:413:GLY:HA3 | 8:K:419:LEU:HD13 | 1.95 | 0.48 |
| 9:E:203:GLY:O | 9:E:520:ALA:HB1 | 2.13 | 0.48 |
| 9:E:457:TYR:CG | 9:E:460:LYS:HE3 | 2.49 | 0.48 |
| 9:F:293:ILE:HG13 | 9:F:320:LYS:HG2 | 1.94 | 0.48 |
| 9:F:531:GLN:HG3 | 9:F:535:SER:OG | 2.13 | 0.48 |
| 1:A:577:LYS:O | 1:A:580:ALA:N | 2.46 | 0.48 |
| 1:A:592:SER:HB2 | 7:J:30:C:O3' | 2.13 | 0.48 |
| 2:B:65:GLN:O | 2:B:68:THR:OG1 | 2.26 | 0.48 |
| 8:K:278:ARG:HH22 | 8:K:411:LEU:HB3 | 1.79 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:269:TYR:HE1 | 9:E:291:PHE:CE1 | 2.31 | 0.48 |
| 9:E:425:VAL:HA | 9:E:428:LEU:HG | 1.94 | 0.48 |
| 9:F:283:PRO:CB | 9:F:286:THR:HG21 | 2.43 | 0.48 |
| 1:A:38:TYR:N | 4:G:2:ASN:OD1 | 2.46 | 0.48 |
| 1:A:271:LEU:HD23 | 2:B:119:ILE:HD11 | 1.95 | 0.48 |
| 1:A:571:PHE:HE1 | 1:A:642:HIS:CE1 | 2.31 | 0.48 |
| 1:A:771:ALA:O | 1:A:774:GLY:N | 2.42 | 0.48 |
| 1:A:849:LYS:C | 1:A:851:ASP:N | 2.66 | 0.48 |
| 3:C:3:MET:O | 3:C:6:VAL:HB | 2.14 | 0.48 |
| 6:I:11:G:C5 | 7:J:50:G:C6 | 3.02 | 0.48 |
| 9:E:290:HIS:HA | 9:E:293:ILE:HD11 | 1.94 | 0.48 |
| 9:E:557:ASN:CG | 9:E:560:ARG:H | 2.17 | 0.48 |
| 9:F:417:LEU:HD21 | 9:F:421:TYR:O | 2.13 | 0.48 |
| 1:A:660:ALA:O | 1:A:665:GLU:HB3 | 2.14 | 0.48 |
| 7:J:44:A:H2' | 7:J:45:C:H6 | 1.79 | 0.48 |
| 9:F:12:THR:OG1 | 9:F:25:LEU:O | 2.22 | 0.48 |
| 1:A:38:TYR:HE1 | 1:A:725:HIS:HE1 | 1.56 | 0.48 |
| 1:A:457:ARG:NH1 | 1:A:458:TYR:HE1 | 2.12 | 0.48 |
| 1:A:806:THR:O | 1:A:808:GLY:N | 2.46 | 0.48 |
| 2:D:92:PHE:HB3 | 2:D:96:ARG:NH2 | 2.28 | 0.48 |
| 2:D:157:GLN:O | 2:D:158:GLN:HB2 | 2.14 | 0.48 |
| 4:G:58:LYS:HG2 | 4:G:63:GLY:O | 2.14 | 0.48 |
| 7:J:42:C:H2' | 7:J:43:U:C6 | 2.49 | 0.48 |
| 8:K:79:ALA:HB1 | 8:K:242:ILE:HB | 1.95 | 0.48 |
| 9:F:72:CYS:SG | 9:F:74:SER:OG | 2.62 | 0.48 |
| 9:F:288:LYS:HG3 | 9:F:289:SER:N | 2.28 | 0.48 |
| 9:F:420:GLU:HA | 9:F:426:CYS:HB3 | 1.94 | 0.48 |
| 1:A:35:PHE:CZ | 1:A:50:LYS:HB2 | 2.49 | 0.48 |
| 1:A:501:SER:HB3 | 7:J:26:A:H5' | 1.96 | 0.48 |
| 1:A:758:LEU:HA | 1:A:758:LEU:HD12 | 1.54 | 0.48 |
| 1:A:800:TRP:CD1 | 1:A:800:TRP:N | 2.81 | 0.48 |
| 2:B:177:SER:C | 2:B:179:ASN:H | 2.17 | 0.48 |
| 3:C:19:GLN:HE21 | 2:D:84:THR:HG23 | 1.79 | 0.48 |
| 5:H:16:PHE:CZ | 5:H:26:ALA:HB1 | 2.49 | 0.48 |
| 7:J:39:A:C6 | 7:J:40:U:C4 | 3.02 | 0.48 |
| 9:E:33:HIS:ND1 | 9:E:107:ASN:OD1 | 2.33 | 0.48 |
| 9:E:171:LYS:N | 9:E:172:PRO:HD2 | 2.29 | 0.48 |
| 9:F:57:VAL:HB | 9:F:63:LEU:HD21 | 1.96 | 0.48 |
| 9:F:420:GLU:HB3 | 9:F:430:LYS:CB | 2.44 | 0.48 |
| 1:A:132:ARG:O | 1:A:784:SER:OG | 2.31 | 0.48 |
| 1:A:304:ASP:O | 1:A:307:ILE:HB | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:543:ASN:O | 1:A:556:THR:HA | 2.13 | 0.48 |
| 1:A:543:ASN:ND2 | 1:A:557:VAL:O | 2.44 | 0.48 |
| 1:A:575:LEU:O | 1:A:578:SER:N | 2.46 | 0.48 |
| 1:A:852:GLY:O | 1:A:855:MET:N | 2.28 | 0.48 |
| 1:A:912:THR:O | 1:A:914:ARG:N | 2.47 | 0.48 |
| 3:C:3:MET:O | 3:C:6:VAL:N | 2.46 | 0.48 |
| 8:K:77:GLU:O | 8:K:80:ILE:N | 2.45 | 0.48 |
| 8:K:215:THR:HG23 | 8:K:238:ASN:H | 1.78 | 0.48 |
| 8:K:359:LYS:HA | 8:K:361:TYR:CZ | 2.48 | 0.48 |
| 9:E:24:PHE:O | 9:E:25:LEU:HD23 | 2.13 | 0.48 |
| 9:F:306:TYR:HB2 | 9:F:357:PHE:HD1 | 1.78 | 0.48 |
| 1:A:331:ARG:HG2 | 1:A:344:THR:HG21 | 1.94 | 0.47 |
| 1:A:672:SER:O | 1:A:673:LEU:HD23 | 2.14 | 0.47 |
| 2:D:128:LEU:HD11 | 2:D:130:VAL:CG2 | 2.44 | 0.47 |
| 5:H:14:LEU:O | 5:H:18:ALA:N | 2.47 | 0.47 |
| 9:E:30:CYS:SG | 9:E:89:VAL:HG21 | 2.53 | 0.47 |
| 9:E:37:THR:OG1 | 9:E:39:HIS:N | 2.46 | 0.47 |
| 9:F:155:ARG:HD2 | 9:F:164:HIS:HE1 | 1.79 | 0.47 |
| 9:F:243:GLN:NE2 | 9:F:244:GLU:O | 2.46 | 0.47 |
| 1:A:392:ARG:HG2 | 2:B:133:PRO:HG3 | 1.96 | 0.47 |
| 1:A:851:ASP:HB2 | 2:D:79:LYS:HE3 | 1.96 | 0.47 |
| 1:A:926:THR:HG23 | 1:A:927:PRO:HD2 | 1.95 | 0.47 |
| 2:D:51:ARG:HG3 | 6:I:17:A:C4' | 2.44 | 0.47 |
| 5:H:100:PRO:HG2 | 5:H:126:TYR:HB3 | 1.96 | 0.47 |
| 8:K:261:CYS:HA | 8:K:415:ASP:HB2 | 1.94 | 0.47 |
| 9:E:52:ALA:HB1 | 9:E:75:HIS:ND1 | 2.29 | 0.47 |
| 1:A:539:ILE:O | 1:A:540:THR:OG1 | 2.27 | 0.47 |
| 1:A:610:GLU:O | 1:A:612:PRO:HD3 | 2.14 | 0.47 |
| 2:D:122:LEU:O | 2:D:190:ARG:NE | 2.47 | 0.47 |
| 7:J:39:A:C5 | 7:J:40:U:C4 | 3.02 | 0.47 |
| 9:E:31:TYR:CE1 | 9:E:87:GLY:HA2 | 2.49 | 0.47 |
| 9:E:188:THR:HG22 | 9:E:189:LYS:H | 1.79 | 0.47 |
| 9:E:269:TYR:CE1 | 9:E:295:LEU:HB2 | 2.49 | 0.47 |
| 9:E:513:SER:CB | 9:E:519:ASN:HB2 | 2.45 | 0.47 |
| 9:F:293:ILE:HG23 | 9:F:325:LEU:CD1 | 2.44 | 0.47 |
| 1:A:605:VAL:HG11 | 1:A:756:MET:HE2 | 1.94 | 0.47 |
| 2:B:11:SER:HB3 | 2:B:48:GLU:HG3 | 1.97 | 0.47 |
| 9:E:113:ASP:OD2 | 9:E:115:THR:HB | 2.15 | 0.47 |
| 9:E:295:LEU:HA | 9:E:298:TYR:HB3 | 1.95 | 0.47 |
| 9:E:328:ASP:OD1 | 9:E:329:LYS:N | 2.41 | 0.47 |
| 9:E:329:LYS:HB2 | 9:E:354:GLN:CB | 2.40 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:445:PRO:HG3 | 9:E:468:SER:HB3 | 1.95 | 0.47 |
| 9:E:539:SER:O | 9:E:567:ARG:HD3 | 2.15 | 0.47 |
| 1:A:609:VAL:HG12 | 1:A:751:LYS:O | 2.15 | 0.47 |
| 1:A:872:HIS:ND1 | 1:A:873:PRO:HD2 | 2.28 | 0.47 |
| 1:A:900:LEU:O | 1:A:904:SER:HA | 2.14 | 0.47 |
| 2:B:15:PHE:HD1 | 2:B:45:ALA:CB | 2.27 | 0.47 |
| 2:B:62:MET:HA | 2:B:65:GLN:HG3 | 1.96 | 0.47 |
| 4:G:55:ARG:HA | 4:G:65:ILE:O | 2.14 | 0.47 |
| 8:K:107:LEU:HD21 | 8:K:152:LEU:HB3 | 1.97 | 0.47 |
| 8:K:159:TRP:HB3 | 8:K:163:ARG:NH2 | 2.30 | 0.47 |
| 9:E:218:LYS:NZ | 9:E:220:ASN:HB2 | 2.29 | 0.47 |
| 9:E:381:ASN:ND2 | 9:E:424:SER:H | 2.12 | 0.47 |
| 9:F:456:VAL:HG11 | 9:F:562:ASN:ND2 | 2.29 | 0.47 |
| 1:A:71:VAL:HG12 | 1:A:116:ARG:HH11 | 1.78 | 0.47 |
| 5:H:89:PHE:CD1 | 8:K:129:ASN:HB2 | 2.49 | 0.47 |
| 9:E:185:TYR:HE2 | 9:E:226:VAL:HB | 1.80 | 0.47 |
| 9:E:471:CYS:CB | 9:E:572:ILE:HG22 | 2.44 | 0.47 |
| 9:E:480:ILE:HG13 | 9:E:549:THR:O | 2.15 | 0.47 |
| 9:F:396:TYR:HB3 | 9:F:398:TYR:CZ | 2.50 | 0.47 |
| 1:A:93:CYS:O | 1:A:95:ALA:N | 2.48 | 0.47 |
| 1:A:155:ASP:OD1 | 1:A:156:TYR:N | 2.48 | 0.47 |
| 1:A:269:ASP:OD1 | 1:A:269:ASP:N | 2.47 | 0.47 |
| 1:A:414:ASN:HD21 | 1:A:846:ASP:HA | 1.79 | 0.47 |
| 3:C:60:LEU:HA | 3:C:60:LEU:HD23 | 1.51 | 0.47 |
| 2:D:135:TYR:O | 2:D:138:TYR:HB3 | 2.15 | 0.47 |
| 4:G:15:ALA:HB2 | 4:G:25:ASP:HA | 1.97 | 0.47 |
| 4:G:42:LEU:HD22 | 4:G:98:ASN:HB3 | 1.96 | 0.47 |
| 6:I:20:A:C6 | 7:J:41:G:C6 | 3.03 | 0.47 |
| 8:K:476:ARG:HA | 8:K:477:CYS:C | 2.34 | 0.47 |
| 9:E:33:HIS:HB2 | 9:E:106:PHE:HE2 | 1.78 | 0.47 |
| 9:E:266:VAL:HG13 | 9:E:298:TYR:CE2 | 2.49 | 0.47 |
| 9:E:279:THR:HB | 9:E:429:MET:SD | 2.55 | 0.47 |
| 9:E:283:PRO:HA | 9:E:457:TYR:OH | 2.14 | 0.47 |
| 9:E:409:ARG:HH12 | 9:E:422:PHE:HA | 1.79 | 0.47 |
| 9:F:254:PRO:HB3 | 9:F:299:TYR:CZ | 2.50 | 0.47 |
| 9:F:288:LYS:CG | 9:F:289:SER:H | 2.28 | 0.47 |
| 9:F:473:LYS:HG2 | 9:F:587:PHE:HD2 | 1.79 | 0.47 |
| 9:F:509:ALA:CB | 9:F:545:ILE:HG13 | 2.44 | 0.47 |
| 1:A:39:ASN:OD1 | 1:A:42:VAL:N | 2.44 | 0.47 |
| 1:A:197:ARG:NE | 1:A:289:TYR:OH | 2.43 | 0.47 |
| 1:A:663:LEU:HA | 1:A:663:LEU:HD12 | 1.66 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:177:SER:O | 2:D:180:LEU:N | 2.47 | 0.47 |
| 5:H:29:ASP:OD2 | 8:K:66:VAL:HG21 | 2.14 | 0.47 |
| 8:K:184:VAL:HG21 | 8:K:278:ARG:N | 2.30 | 0.47 |
| 9:E:118:GLY:HA2 | 9:E:121:ILE:HB | 1.97 | 0.47 |
| 9:E:176:LEU:HB3 | 9:E:201:GLU:O | 2.15 | 0.47 |
| 9:E:318:CYS:SG | 9:E:332:ARG:NE | 2.88 | 0.47 |
| 9:F:4:ALA:HB1 | 9:F:9:ASN:O | 2.15 | 0.47 |
| 9:F:10:SER:HB3 | 9:F:97:CYS:HA | 1.95 | 0.47 |
| 9:F:476:TYR:HE2 | 9:F:492:GLN:HA | 1.79 | 0.47 |
| 1:A:312:ASN:O | 1:A:315:VAL:HG12 | 2.15 | 0.47 |
| 1:A:539:ILE:HG22 | 1:A:540:THR:H | 1.78 | 0.47 |
| 1:A:688:ALA:HB1 | 1:A:759:SER:HB3 | 1.97 | 0.47 |
| 1:A:887:TYR:O | 1:A:888:ILE:C | 2.54 | 0.47 |
| 2:D:46:LYS:HE3 | 2:D:46:LYS:HB3 | 1.76 | 0.47 |
| 7:J:47:A:C5 | 7:J:48:C:C4 | 3.03 | 0.47 |
| 9:E:136:GLU:OE2 | 9:E:235:LEU:HD23 | 2.15 | 0.47 |
| 9:E:407:ALA:O | 9:E:409:ARG:N | 2.48 | 0.47 |
| 1:A:439:HIS:HB3 | 1:A:548:ILE:HG12 | 1.97 | 0.47 |
| 1:A:687:THR:OG1 | 1:A:688:ALA:N | 2.48 | 0.47 |
| 3:C:19:GLN:HE22 | 2:D:84:THR:HA | 1.80 | 0.47 |
| 2:D:168:GLN:N | 2:D:171:GLU:OE1 | 2.35 | 0.47 |
| 4:G:58:LYS:NZ | 4:G:65:ILE:HG22 | 2.29 | 0.47 |
| 5:H:13:VAL:HG11 | 5:H:38:ILE:HG12 | 1.97 | 0.47 |
| 5:H:43:LYS:H | 8:K:26:HIS:CD2 | 2.33 | 0.47 |
| 5:H:89:PHE:CE1 | 8:K:129:ASN:HB2 | 2.50 | 0.47 |
| 9:E:21:ARG:HB2 | 9:E:133:PHE:HE1 | 1.79 | 0.47 |
| 9:E:269:TYR:HB3 | 9:E:298:TYR:CD1 | 2.50 | 0.47 |
| 9:F:536:SER:OG | 9:F:537:GLN:N | 2.42 | 0.47 |
| 9:F:554:HIS:HA | 9:F:560:ARG:NH2 | 2.30 | 0.47 |
| 4:G:56:PHE:O | 4:G:65:ILE:HG23 | 2.15 | 0.46 |
| 9:E:171:LYS:O | 9:E:173:ARG:NH2 | 2.46 | 0.46 |
| 9:E:273:GLY:HA2 | 9:E:395:HIS:CE1 | 2.50 | 0.46 |
| 9:E:283:PRO:HB3 | 9:E:461:LEU:HD21 | 1.96 | 0.46 |
| 9:F:562:ASN:HA | 9:F:565:ILE:HG12 | 1.97 | 0.46 |
| 9:F:585:LEU:HD12 | 9:F:587:PHE:HE2 | 1.80 | 0.46 |
| 1:A:122:TYR:OH | 1:A:144:GLU:OE2 | 2.27 | 0.46 |
| 1:A:295:HIS:HE1 | 1:A:301:CYS:HA | 1.79 | 0.46 |
| 1:A:456:TYR:HE2 | 1:A:676:LYS:HG3 | 1.78 | 0.46 |
| 1:A:783:LYS:HZ3 | 1:A:796:GLU:HB2 | 1.81 | 0.46 |
| 8:K:403:THR:HG21 | 8:K:430:ALA:HA | 1.96 | 0.46 |
| 9:E:244:GLU:OE1 | 9:E:244:GLU:N | 2.48 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 9:E:420:GLU:HB2 | 9:E:427:ARG:HA | 1.97 | 0.46 |
| 1:A:124:MET:CG | 1:A:210:GLN:HG2 | 2.45 | 0.46 |
| 1:A:235:ASP:O | 1:A:239:SER:HB3 | 2.16 | 0.46 |
| 1:A:700:VAL:O | 1:A:703:ASN:N | 2.48 | 0.46 |
| 4:G:15:ALA:HB3 | 4:G:55:ARG:O | 2.15 | 0.46 |
| 8:K:407:SER:O | 8:K:410:ASN:ND2 | 2.48 | 0.46 |
| 9:E:561:PHE:HZ | 9:E:572:ILE:HD11 | 1.80 | 0.46 |
| 9:F:132:LEU:HB3 | 9:F:235:LEU:HD11 | 1.97 | 0.46 |
| 9:F:135:ALA:O | 9:F:138:LEU:HB3 | 2.16 | 0.46 |
| 9:F:329:LYS:CB | 9:F:354:GLN:HE21 | 2.22 | 0.46 |
| 1:A:146:LEU:HA | 1:A:146:LEU:HD23 | 1.70 | 0.46 |
| 1:A:261:LEU:HA | 1:A:261:LEU:HD13 | 1.67 | 0.46 |
| 1:A:694:PHE:HE1 | 1:A:698:GLN:HE21 | 1.55 | 0.46 |
| 4:G:17:GLY:N | 4:G:23:CYS:SG | 2.88 | 0.46 |
| 8:K:25:THR:HG23 | 8:K:28:SER:H | 1.79 | 0.46 |
| 8:K:256:ASN:HB3 | 8:K:280:LEU:HD21 | 1.96 | 0.46 |
| 8:K:460:VAL:HA | 8:K:461:SER:HA | 1.63 | 0.46 |
| 9:E:43:LEU:HD23 | 9:E:43:LEU:HA | 1.61 | 0.46 |
| 9:E:109:ILE:C | 9:E:111:THR:H | 2.18 | 0.46 |
| 9:E:262:PHE:O | 9:E:266:VAL:HG23 | 2.15 | 0.46 |
| 9:F:114:TRP:NE1 | 9:F:138:LEU:HA | 2.30 | 0.46 |
| 9:F:576:MET:HE1 | 9:F:581:LEU:HB3 | 1.97 | 0.46 |
| 1:A:470:LEU:HA | 1:A:470:LEU:HD23 | 1.57 | 0.46 |
| 2:D:49:PHE:HA | 2:D:52:ASP:OD2 | 2.16 | 0.46 |
| 6:I:11:G:C2 | 6:I:12:G:C4 | 3.03 | 0.46 |
| 9:E:417:LEU:HB3 | 9:E:422:PHE:CE1 | 2.49 | 0.46 |
| 9:E:474[B]:MET:HE2 | 9:E:575:ILE:HG23 | 1.96 | 0.46 |
| 9:E:531:GLN:HG2 | 9:E:532:THR:O | 2.15 | 0.46 |
| 9:F:285:GLY:O | 9:F:443:ARG:HD2 | 2.14 | 0.46 |
| 9:F:576:MET:HB2 | 9:F:582:TYR:CD1 | 2.50 | 0.46 |
| 1:A:157:PHE:N | 1:A:157:PHE:CD1 | 2.83 | 0.46 |
| 1:A:271:LEU:HD23 | 1:A:271:LEU:HA | 1.73 | 0.46 |
| 3:C:25:SER:OG | 3:C:26:SER:N | 2.48 | 0.46 |
| 3:C:46:THR:HG23 | 3:C:47:GLU:N | 2.28 | 0.46 |
| 4:G:58:LYS:HZ3 | 4:G:65:ILE:HA | 1.81 | 0.46 |
| 8:K:283:HIS:ND1 | 8:K:287:VAL:HG11 | 2.30 | 0.46 |
| 9:F:37:THR:HG23 | 9:F:107:ASN:ND2 | 2.31 | 0.46 |
| 9:F:482:HIS:ND1 | 9:F:487:ALA:HB2 | 2.31 | 0.46 |
| 1:A:495:VAL:HG21 | 1:A:516:TYR:CE2 | 2.51 | 0.46 |
| 1:A:497:ASN:HD22 | 1:A:500:LYS:HE3 | 1.80 | 0.46 |
| 1:A:867:TYR:O | 1:A:869:LEU:N | 2.49 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:28:LYS:NZ | 5:H:112:LEU:HD13 | 2.30 | 0.46 |
| 9:F:65:LEU:HD23 | 9:F:81:PHE:HD2 | 1.81 | 0.46 |
| 9:F:114:TRP:CZ3 | 9:F:123:ALA:HB2 | 2.51 | 0.46 |
| 9:F:118:GLY:HA2 | 9:F:121:ILE:HG12 | 1.97 | 0.46 |
| 9:F:182:PHE:HA | 9:F:226:VAL:O | 2.16 | 0.46 |
| 9:F:373:PHE:N | 9:F:397:VAL:O | 2.39 | 0.46 |
| 9:F:495:VAL:O | 9:F:499:PHE:HB2 | 2.15 | 0.46 |
| 2:B:56:GLN:CD | 2:B:57:ARG:HH22 | 2.19 | 0.46 |
| 2:B:74:ALA:O | 2:B:77:GLU:HG3 | 2.15 | 0.46 |
| 3:C:36:HIS:O | 3:C:38:ASP:N | 2.48 | 0.46 |
| 2:D:85:SER:O | 2:D:89:THR:HG22 | 2.15 | 0.46 |
| 7:J:25:G:N3 | 7:J:25:G:H2' | 2.29 | 0.46 |
| 9:E:139:LYS:HA | 9:E:142:GLU:CD | 2.36 | 0.46 |
| 9:E:444:CYS:SG | 9:E:566:THR:HA | 2.56 | 0.46 |
| 9:E:480:ILE:HD11 | 9:E:492:GLN:OE1 | 2.16 | 0.46 |
| 9:E:514:PRO:HB3 | 9:E:554:HIS:O | 2.14 | 0.46 |
| 9:F:150:GLY:HA3 | 9:F:171:LYS:HB3 | 1.98 | 0.46 |
| 9:F:554:HIS:HA | 9:F:560:ARG:CZ | 2.46 | 0.46 |
| 1:A:84:GLU:HA | 1:A:101:PHE:CZ | 2.50 | 0.46 |
| 1:A:217:TYR:O | 1:A:219:PHE:N | 2.49 | 0.46 |
| 2:B:43:ASN:O | 2:B:46:LYS:HB3 | 2.15 | 0.46 |
| 2:D:172:ILE:HG13 | 2:D:180:LEU:HD13 | 1.98 | 0.46 |
| 5:H:13:VAL:HA | 5:H:30:TYR:CE1 | 2.51 | 0.46 |
| 5:H:21:VAL:HB | 8:K:200:LYS:HB3 | 1.98 | 0.46 |
| 5:H:62:ASN:H | 5:H:65:GLN:HE21 | 1.64 | 0.46 |
| 5:H:75:LEU:HD22 | 5:H:108:VAL:HG11 | 1.97 | 0.46 |
| 6:I:17:A:C4 | 6:I:18:G:C8 | 3.04 | 0.46 |
| 6:I:22:G:O2' | 6:I:23:C:OP1 | 2.30 | 0.46 |
| 7:J:40:U:C2' | 7:J:41:G:H8 | 2.28 | 0.46 |
| 8:K:54:LEU:HA | 8:K:125:VAL:HA | 1.98 | 0.46 |
| 8:K:84:ARG:NH2 | 8:K:421:VAL:HG12 | 2.31 | 0.46 |
| 9:E:279:THR:O | 9:E:435:ASP:HB2 | 2.16 | 0.46 |
| 9:E:283:PRO:HD3 | 9:E:437:PHE:CE1 | 2.51 | 0.46 |
| 9:E:471:CYS:SG | 9:E:572:ILE:HG22 | 2.56 | 0.46 |
| 9:F:353:GLU:HB3 | 9:F:356:VAL:HG22 | 1.98 | 0.46 |
| 1:A:636:LEU:HD23 | 1:A:636:LEU:HA | 1.49 | 0.46 |
| 9:E:334:ILE:HD11 | 9:E:343:PHE:N | 2.31 | 0.46 |
| 9:F:51:ASN:HD22 | 9:F:70:TYR:H | 1.63 | 0.46 |
| 9:F:255:THR:OG1 | 9:F:297:LEU:O | 2.32 | 0.46 |
| 9:F:519:ASN:ND2 | 9:F:532:THR:HA | 2.31 | 0.46 |
| 1:A:491:ASN:HB3 | 1:A:521:TYR:HE2 | 1.80 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:22:TYR:CZ | 2:D:39:LYS:HD3 | 2.52 | 0.45 |
| 2:D:94:MET:O | 2:D:97:LYS:HB3 | 2.17 | 0.45 |
| 8:K:94:CYS:HB2 | 8:K:139:LYS:O | 2.16 | 0.45 |
| 8:K:184:VAL:HA | 8:K:242:ILE:HG23 | 1.98 | 0.45 |
| 8:K:216:CYS:O | 8:K:224:TYR:HA | 2.15 | 0.45 |
| 9:E:284:PRO:HB2 | 9:E:566:THR:HB | 1.97 | 0.45 |
| 9:F:10:SER:OG | 9:F:98:VAL:O | 2.34 | 0.45 |
| 9:F:155:ARG:HD2 | 9:F:164:HIS:CE1 | 2.51 | 0.45 |
| 9:F:470:GLN:HB3 | 9:F:543:TYR:HE1 | 1.81 | 0.45 |
| 1:A:153:ASP:N | 1:A:153:ASP:OD1 | 2.39 | 0.45 |
| 1:A:430:LYS:HE3 | 1:A:430:LYS:HB2 | 1.64 | 0.45 |
| 1:A:814:SER:O | 1:A:814:SER:OG | 2.31 | 0.45 |
| 2:B:95:LEU:HD12 | 2:B:98:LEU:HD21 | 1.98 | 0.45 |
| 2:B:98:LEU:O | 2:B:100:ASN:N | 2.46 | 0.45 |
| 2:B:171:GLU:O | 2:B:176:ASN:HB3 | 2.15 | 0.45 |
| 4:G:48:LEU:HD23 | 4:G:51:LEU:HG | 1.98 | 0.45 |
| 6:I:17:A:H2' | 6:I:18:G:H8 | 1.81 | 0.45 |
| 6:I:21:U:C2 | 6:I:22:G:C8 | 3.04 | 0.45 |
| 9:E:151:ILE:HG12 | 9:E:168:GLU:OE2 | 2.16 | 0.45 |
| 9:F:10:SER:HB2 | 9:F:26:CYS:HB3 | 1.98 | 0.45 |
| 9:F:322:LEU:HD12 | 9:F:327:ILE:CG2 | 2.46 | 0.45 |
| 9:F:576:MET:HB3 | 9:F:582:TYR:HB2 | 1.98 | 0.45 |
| 1:A:469:LEU:HD12 | 1:A:469:LEU:HA | 1.60 | 0.45 |
| 1:A:599:HIS:CD2 | 1:A:827:VAL:HA | 2.50 | 0.45 |
| 1:A:657:ASN:HB3 | 1:A:661:GLN:NE2 | 2.30 | 0.45 |
| 1:A:838:LEU:HA | 1:A:838:LEU:HD23 | 1.65 | 0.45 |
| 1:A:919:GLU:HA | 1:A:922:GLU:OE2 | 2.17 | 0.45 |
| 2:B:136:ASN:HA | 2:B:139:LYS:HZ3 | 1.81 | 0.45 |
| 2:D:114:CYS:HA | 2:D:131:VAL:O | 2.16 | 0.45 |
| 2:D:128:LEU:HD23 | 2:D:154:TRP:CZ3 | 2.52 | 0.45 |
| 6:I:27:G:N1 | 7:J:34:C:N3 | 2.64 | 0.45 |
| 6:I:31:C:H2' | 6:I:32:A:C8 | 2.52 | 0.45 |
| 7:J:39:A:H2' | 7:J:40:U:O4' | 2.17 | 0.45 |
| 9:E:121:ILE:O | 9:E:125:THR:OG1 | 2.16 | 0.45 |
| 9:E:321:ALA:O | 9:E:325:LEU:N | 2.49 | 0.45 |
| 9:F:576:MET:CE | 9:F:577:SER:H | 2.29 | 0.45 |
| 1:A:590:GLY:HA2 | 7:J:29:G:O2' | 2.16 | 0.45 |
| 1:A:753:PHE:CZ | 1:A:764:VAL:HG11 | 2.52 | 0.45 |
| 2:B:134:ASP:OD2 | 2:B:135:TYR:N | 2.50 | 0.45 |
| 3:C:31:GLN:O | 3:C:35:LEU:HD13 | 2.16 | 0.45 |
| 8:K:85:ALA:C | 8:K:182:VAL:HG12 | 2.36 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:K:89:PHE:HA | 8:K:111:PHE:CD1 | 2.51 | 0.45 |
| 8:K:164:ILE:HG22 | 8:K:168:GLN:OE1 | 2.16 | 0.45 |
| 9:E:248:ARG:HH21 | 9:E:251:GLY:N | 2.14 | 0.45 |
| 9:E:291:PHE:HD2 | 9:E:438:LEU:HD21 | 1.82 | 0.45 |
| 9:E:330:CYS:HB2 | 9:E:346:PHE:CD1 | 2.52 | 0.45 |
| 9:F:365:GLU:HA | 9:F:390:ARG:HB3 | 1.99 | 0.45 |
| 9:F:369:ASP:HA | 9:F:394:LYS:HZ2 | 1.82 | 0.45 |
| 1:A:257:VAL:HG21 | 1:A:264:PRO:HD2 | 1.98 | 0.45 |
| 1:A:415:PHE:CE2 | 1:A:417:LYS:HA | 2.52 | 0.45 |
| 1:A:687:THR:O | 1:A:689:TYR:N | 2.48 | 0.45 |
| 2:B:154:TRP:CE3 | 2:B:190:ARG:HA | 2.51 | 0.45 |
| 3:C:28:LEU:HD13 | 3:C:28:LEU:HA | 1.70 | 0.45 |
| 8:K:54:LEU:HD22 | 8:K:103:THR:HG21 | 1.99 | 0.45 |
| 8:K:283:HIS:O | 8:K:287:VAL:HG22 | 2.16 | 0.45 |
| 8:K:476:ARG:NE | 8:K:478:ASN:H | 2.15 | 0.45 |
| 8:K:489:ASN:O | 8:K:492:ARG:CB | 2.62 | 0.45 |
| 9:E:420:GLU:HA | 9:E:426:CYS:O | 2.16 | 0.45 |
| 9:F:64:TYR:CE2 | 9:F:76:LYS:HD2 | 2.51 | 0.45 |
| 9:F:386:VAL:O | 9:F:390:ARG:HG3 | 2.17 | 0.45 |
| 1:A:453:TYR:OH | 1:A:675:VAL:O | 2.35 | 0.45 |
| 2:B:31:SER:OG | 2:B:32:GLU:N | 2.49 | 0.45 |
| 2:B:146:THR:OG1 | 2:B:154:TRP:O | 2.30 | 0.45 |
| 4:G:70:GLU:OE1 | 4:G:71:PRO:HD2 | 2.16 | 0.45 |
| 5:H:56:THR:HG21 | 5:H:60:GLU:H | 1.81 | 0.45 |
| 6:I:32:A:C5 | 6:I:33:G:N7 | 2.85 | 0.45 |
| 8:K:163:ARG:CZ | 8:K:198:PHE:HB3 | 2.47 | 0.45 |
| 8:K:204:GLU:HG3 | 8:K:213:ARG:NH2 | 2.32 | 0.45 |
| 9:E:157:VAL:HG13 | 9:E:163:LEU:HG | 1.99 | 0.45 |
| 9:E:453:SER:HB2 | 9:E:459:ASN:HA | 1.99 | 0.45 |
| 9:E:464:HIS:CD2 | 9:E:465:LYS:HG3 | 2.52 | 0.45 |
| 9:E:492:GLN:O | 9:E:496:VAL:HG13 | 2.17 | 0.45 |
| 9:F:120:TYR:CE2 | 9:F:412:LEU:HB2 | 2.52 | 0.45 |
| 9:F:576:MET:HG3 | 9:F:582:TYR:HA | 1.98 | 0.45 |
| 1:A:136:GLU:N | 1:A:136:GLU:OE1 | 2.50 | 0.45 |
| 1:A:527:LEU:HA | 1:A:527:LEU:HD12 | 1.70 | 0.45 |
| 2:B:171:GLU:O | 2:B:173:SER:N | 2.48 | 0.45 |
| 6:I:20:A:C6 | 6:I:21:U:C4 | 3.05 | 0.45 |
| 6:I:24:U:H2' | 6:I:25:A:C8 | 2.51 | 0.45 |
| 7:J:38:C:H2' | 7:J:39:A:H8 | 1.79 | 0.45 |
| 9:E:239:THR:HG21 | 9:E:381:ASN:HB3 | 1.99 | 0.45 |
| 9:E:489:ASN:C | 9:E:493:ILE:HG12 | 2.37 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:275:GLN:OE1 | 9:F:435:ASP:HB3 | 2.16 | 0.45 |
| 9:F:579:ARG:HG2 | 9:F:582:TYR:HD2 | 1.82 | 0.45 |
| 1:A:165:PHE:HE2 | 1:A:787:TYR:CE2 | 2.35 | 0.45 |
| 8:K:78:GLU:O | 8:K:82:HIS:ND1 | 2.50 | 0.45 |
| 8:K:279:CYS:SG | 8:K:414:CYS:HB2 | 2.57 | 0.45 |
| 9:E:167:TRP:CD2 | 9:E:172:PRO:HB3 | 2.52 | 0.45 |
| 9:E:303:ARG:HB2 | 9:E:368:ALA:HB1 | 1.98 | 0.45 |
| 9:E:314:VAL:HG12 | 9:E:318:CYS:HG | 1.82 | 0.45 |
| 9:E:420:GLU:HB3 | 9:E:430:LYS:CB | 2.46 | 0.45 |
| 9:E:440:THR:HA | 9:E:462:LYS:HE2 | 1.99 | 0.45 |
| 9:F:114:TRP:HB3 | 9:F:120:TYR:HE1 | 1.81 | 0.45 |
| 9:F:384:LEU:HD11 | 9:F:423:ASN:ND2 | 2.31 | 0.45 |
| 2:B:125:ALA:O | 2:B:190:ARG:NH2 | 2.50 | 0.45 |
| 3:C:17:LEU:HD23 | 3:C:17:LEU:HA | 1.68 | 0.45 |
| 7:J:40:U:H2' | 7:J:41:G:O4' | 2.17 | 0.45 |
| 8:K:83:VAL:O | 8:K:84:ARG:HB2 | 2.17 | 0.45 |
| 9:E:93:TYR:O | 9:E:95:ASN:N | 2.50 | 0.45 |
| 9:E:332:ARG:HB2 | 9:E:346:PHE:CD2 | 2.50 | 0.45 |
| 9:E:386:VAL:CG1 | 9:E:390:ARG:HE | 2.27 | 0.45 |
| 9:E:562:ASN:HA | 9:E:565:ILE:HG22 | 1.99 | 0.45 |
| 9:F:295:LEU:O | 9:F:298:TYR:HB3 | 2.17 | 0.45 |
| 9:F:474:MET:HB3 | 9:F:476:TYR:HD1 | 1.82 | 0.45 |
| 1:A:19:LEU:CD1 | 1:A:56:PHE:HB3 | 2.43 | 0.45 |
| 1:A:819:LEU:HD13 | 1:A:828:TYR:CE1 | 2.52 | 0.45 |
| 2:B:177:SER:O | 2:B:179:ASN:N | 2.49 | 0.45 |
| 3:C:70:LYS:HE2 | 3:C:70:LYS:HB2 | 1.68 | 0.45 |
| 2:D:102:ALA:O | 2:D:106:ILE:HG22 | 2.17 | 0.45 |
| 2:D:182:TRP:N | 2:D:183:PRO:HD2 | 2.32 | 0.45 |
| 4:G:112:LEU:HD23 | 4:G:112:LEU:H | 1.82 | 0.45 |
| 7:J:37:G:C6 | 7:J:38:C:C4 | 3.05 | 0.45 |
| 8:K:9:LYS:NZ | 8:K:102:GLY:O | 2.50 | 0.45 |
| 8:K:45:ILE:HD12 | 8:K:46:PRO:HD2 | 1.98 | 0.45 |
| 9:E:9:ASN:H | 9:E:129:ARG:HH22 | 1.64 | 0.45 |
| 9:E:153:THR:HA | 9:E:224:TYR:HA | 1.98 | 0.45 |
| 9:E:365:GLU:OE1 | 9:E:390:ARG:HA | 2.17 | 0.45 |
| 9:E:480:ILE:HA | 9:E:489:ASN:CB | 2.45 | 0.45 |
| 9:F:60:VAL:HA | 9:F:63:LEU:HD12 | 1.98 | 0.45 |
| 1:A:136:GLU:OE1 | 1:A:137:GLY:N | 2.51 | 0.44 |
| 1:A:506:PHE:CE2 | 1:A:562:ILE:HG22 | 2.52 | 0.44 |
| 1:A:847:ILE:HD13 | 1:A:847:ILE:HA | 1.82 | 0.44 |
| 8:K:167:VAL:HG21 | 8:K:235:TYR:N | 2.31 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:K:175:LYS:HE3 | 8:K:228:HIS:HA | 1.99 | 0.44 |
| 9:E:26:CYS:SG | 9:E:97:CYS:HB3 | 2.57 | 0.44 |
| 9:E:149:TYR:C | 9:E:171:LYS:HG3 | 2.37 | 0.44 |
| 9:E:184:GLY:HA2 | 9:E:225:PHE:HA | 1.99 | 0.44 |
| 9:E:248:ARG:HH21 | 9:E:251:GLY:H | 1.64 | 0.44 |
| 9:E:475:PHE:HB2 | 9:E:582:TYR:OH | 2.17 | 0.44 |
| 9:F:30:CYS:O | 9:F:34:VAL:HG13 | 2.17 | 0.44 |
| 9:F:181:VAL:HG12 | 9:F:199:THR:HB | 1.98 | 0.44 |
| 1:A:172:LEU:HA | 1:A:172:LEU:HD23 | 1.73 | 0.44 |
| 1:A:486:GLY:HA2 | 1:A:642:HIS:CD2 | 2.52 | 0.44 |
| 1:A:713:ASN:HB2 | 1:A:714:LYS:NZ | 2.33 | 0.44 |
| 2:D:78:ASP:OD1 | 2:D:78:ASP:C | 2.56 | 0.44 |
| 9:E:220:ASN:HB3 | 9:E:223:ASP:OD1 | 2.17 | 0.44 |
| 9:E:561:PHE:O | 9:E:565:ILE:CB | 2.45 | 0.44 |
| 9:F:21:ARG:O | 9:F:22:ARG:HG2 | 2.16 | 0.44 |
| 1:A:390:ASP:OD1 | 1:A:392:ARG:N | 2.34 | 0.44 |
| 2:B:75:ARG:N | 2:B:75:ARG:HD2 | 2.33 | 0.44 |
| 6:I:14:A:C5 | 7:J:47:A:C6 | 3.05 | 0.44 |
| 7:J:41:G:C2 | 7:J:42:C:C2 | 3.05 | 0.44 |
| 8:K:80:ILE:HD11 | 8:K:247:TRP:HZ3 | 1.82 | 0.44 |
| 9:E:330:CYS:O | 9:E:346:PHE:HB3 | 2.18 | 0.44 |
| 9:E:448:ILE:HG13 | 9:E:587:PHE:CE1 | 2.52 | 0.44 |
| 9:F:372:VAL:HG13 | 9:F:397:VAL:HB | 1.99 | 0.44 |
| 1:A:102:PHE:HE1 | 1:A:104:PHE:HB2 | 1.82 | 0.44 |
| 1:A:272:LYS:HA | 2:B:111:ARG:HH12 | 1.82 | 0.44 |
| 1:A:481:ASP:OD1 | 1:A:481:ASP:N | 2.49 | 0.44 |
| 1:A:577:LYS:NZ | 7:J:29:G:OP1 | 2.45 | 0.44 |
| 1:A:822:GLN:O | 1:A:824:ASP:N | 2.51 | 0.44 |
| 2:B:12:TYR:HA | 2:B:49:PHE:CE1 | 2.53 | 0.44 |
| 4:G:17:GLY:HA3 | 4:G:23:CYS:HA | 1.99 | 0.44 |
| 8:K:88:GLY:H | 8:K:112:SER:CB | 2.30 | 0.44 |
| 8:K:171:SER:O | 8:K:175:LYS:HD2 | 2.17 | 0.44 |
| 9:E:409:ARG:NH2 | 9:E:422:PHE:HA | 2.29 | 0.44 |
| 9:E:479:VAL:HG11 | 9:E:491:PRO:HG2 | 1.99 | 0.44 |
| 9:F:83:LEU:HD22 | 9:F:90:PHE:HB3 | 2.00 | 0.44 |
| 1:A:498:LEU:O | 1:A:513:ARG:HD3 | 2.17 | 0.44 |
| 1:A:687:THR:O | 1:A:688:ALA:C | 2.56 | 0.44 |
| 4:G:53:TRP:HA | 4:G:68:GLU:HA | 1.98 | 0.44 |
| 8:K:81:ARG:NE | 8:K:294:ILE:HD12 | 2.33 | 0.44 |
| 8:K:141:PRO:HB2 | 8:K:146:PHE:CE2 | 2.52 | 0.44 |
| 8:K:399:CYS:HA | 8:K:507:SER:O | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:268:ASN:HA | 9:E:271:LYS:NZ | 2.32 | 0.44 |
| 9:E:268:ASN:HB3 | 9:E:436:MET:HG2 | 1.99 | 0.44 |
| 9:E:492:GLN:HE21 | 9:E:575:ILE:HG22 | 1.83 | 0.44 |
| 9:F:18:ALA:N | 9:F:41:LEU:HB3 | 2.32 | 0.44 |
| 9:F:286:THR:HG22 | 9:F:441:CYS:HA | 1.98 | 0.44 |
| 1:A:15:SER:HB3 | 1:A:118:ARG:HH22 | 1.82 | 0.44 |
| 1:A:532:LYS:HD3 | 1:A:650:HIS:HB3 | 1.99 | 0.44 |
| 1:A:869:LEU:HD22 | 1:A:877:TYR:HB3 | 1.99 | 0.44 |
| 2:D:134:ASP:OD1 | 2:D:134:ASP:C | 2.56 | 0.44 |
| 6:I:30:G:N2 | 6:I:31:C:C2 | 2.85 | 0.44 |
| 8:K:166:ILE:O | 8:K:170:LEU:HD13 | 2.17 | 0.44 |
| 8:K:244:VAL:HG21 | 8:K:277:THR:HG22 | 1.99 | 0.44 |
| 9:E:185:TYR:CE2 | 9:E:226:VAL:HB | 2.52 | 0.44 |
| 9:E:279:THR:C | 9:E:280:LEU:HD12 | 2.38 | 0.44 |
| 9:E:314:VAL:HG12 | 9:E:318:CYS:SG | 2.58 | 0.44 |
| 9:F:279:THR:HG22 | 9:F:398:TYR:HB2 | 2.00 | 0.44 |
| 1:A:211:ASP:OD2 | 1:A:215:ASN:HB2 | 2.17 | 0.44 |
| 2:B:7:SER:O | 2:B:9:LEU:N | 2.43 | 0.44 |
| 3:C:55:LEU:O | 3:C:56:LEU:C | 2.56 | 0.44 |
| 4:G:56:PHE:N | 4:G:65:ILE:HG12 | 2.32 | 0.44 |
| 5:H:46:CYS:SG | 5:H:47:THR:N | 2.91 | 0.44 |
| 6:I:18:G:O6 | 7:J:42:C:N4 | 2.48 | 0.44 |
| 8:K:407:SER:H | 8:K:410:ASN:HD22 | 1.64 | 0.44 |
| 9:E:374:ASP:OD1 | 9:E:399:ILE:HD13 | 2.17 | 0.44 |
| 9:E:381:ASN:HA | 9:E:384:LEU:CB | 2.48 | 0.44 |
| 9:E:386:VAL:HG12 | 9:E:390:ARG:NE | 2.27 | 0.44 |
| 9:F:281:GLN:HG3 | 9:F:434:PRO:HD3 | 1.99 | 0.44 |
| 9:F:487:ALA:HB3 | 9:F:550:THR:HG21 | 1.98 | 0.44 |
| 1:A:450:ILE:HD12 | 1:A:450:ILE:HA | 1.76 | 0.44 |
| 4:G:4:LEU:HG | 4:G:5:SER:N | 2.33 | 0.44 |
| 8:K:5:THR:HB | 8:K:7:LEU:HB3 | 2.00 | 0.44 |
| 9:E:324:TYR:O | 9:E:326:PRO:HD3 | 2.18 | 0.44 |
| 1:A:86:ILE:HA | 1:A:86:ILE:HD13 | 1.75 | 0.44 |
| 1:A:750:ARG:HA | 1:A:750:ARG:HD2 | 1.69 | 0.44 |
| 2:D:59:LEU:HD12 | 2:D:59:LEU:HA | 1.83 | 0.44 |
| 9:E:71:TYR:HD2 | 9:E:77:PRO:HD3 | 1.82 | 0.44 |
| 9:E:126:CYS:HB2 | 9:E:131:LYS:HG3 | 2.00 | 0.44 |
| 9:E:316:ALA:O | 9:E:320:LYS:HD3 | 2.17 | 0.44 |
| 9:E:512:ILE:HA | 9:E:531:GLN:O | 2.17 | 0.44 |
| 9:F:401:ASP:OD2 | 9:F:457:TYR:OH | 2.15 | 0.44 |
| 9:F:425:VAL:HA | 9:F:428:LEU:HB2 | 2.00 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:882:HIS:C | 1:A:886:GLN:HE21 | 2.21 | 0.43 |
| 2:B:96:ARG:HB2 | 2:B:96:ARG:NH1 | 2.32 | 0.43 |
| 5:H:29:ASP:O | 5:H:33:SER:HB2 | 2.17 | 0.43 |
| 6:I:24:U:H3' | 6:I:25:A:H8 | 1.82 | 0.43 |
| 6:I:32:A:H2' | 6:I:33:G:H8 | 1.82 | 0.43 |
| 8:K:116:ASN:ND2 | 8:K:270:ALA:H | 2.16 | 0.43 |
| 9:E:152:ALA:O | 9:E:225:PHE:N | 2.41 | 0.43 |
| 9:E:248:ARG:HG2 | 9:E:249:ILE:H | 1.82 | 0.43 |
| 9:E:489:ASN:ND2 | 9:E:549:THR:HG23 | 2.33 | 0.43 |
| 9:F:66:GLY:HA3 | 9:F:71:TYR:CE2 | 2.52 | 0.43 |
| 9:F:322:LEU:HB2 | 9:F:346:PHE:CZ | 2.53 | 0.43 |
| 9:F:473:LYS:HA | 9:F:574:CYS:O | 2.18 | 0.43 |
| 1:A:418:ASP:O | 1:A:419:PHE:C | 2.57 | 0.43 |
| 6:I:17:A:N6 | 7:J:43:U:H3 | 2.09 | 0.43 |
| 6:I:31:C:N3 | 6:I:32:A:C6 | 2.86 | 0.43 |
| 8:K:19:HIS:O | 8:K:22:GLN:N | 2.47 | 0.43 |
| 8:K:278:ARG:NH2 | 8:K:411:LEU:HB3 | 2.32 | 0.43 |
| 8:K:466:VAL:HG22 | 8:K:483:VAL:HG21 | 2.00 | 0.43 |
| 8:K:468:LEU:HB3 | 8:K:481:GLY:O | 2.18 | 0.43 |
| 8:K:500:MET:O | 8:K:503:SER:OG | 2.32 | 0.43 |
| 9:E:151:ILE:HD12 | 9:E:226:VAL:HA | 2.00 | 0.43 |
| 9:E:384:LEU:HD22 | 9:E:425:VAL:HG12 | 1.99 | 0.43 |
| 9:E:419:PRO:HD2 | 9:E:430:LYS:NZ | 2.33 | 0.43 |
| 9:E:447:GLU:OE1 | 9:E:469:ALA:HA | 2.17 | 0.43 |
| 9:E:474[B]:MET:HE2 | 9:E:474[B]:MET:HB3 | 1.88 | 0.43 |
| 9:F:167:TRP:CD1 | 9:F:173:ARG:HG2 | 2.53 | 0.43 |
| 9:F:304:ILE:HD12 | 9:F:355:TYR:CE1 | 2.53 | 0.43 |
| 9:F:489:ASN:ND2 | 9:F:492:GLN:OE1 | 2.51 | 0.43 |
| 1:A:21:PRO:HB3 | 1:A:56:PHE:CE2 | 2.53 | 0.43 |
| 1:A:69:TYR:CE2 | 1:A:121:LYS:HB2 | 2.54 | 0.43 |
| 1:A:242:MET:O | 1:A:245:LEU:HB2 | 2.18 | 0.43 |
| 1:A:598:TRP:HA | 1:A:601:MET:SD | 2.58 | 0.43 |
| 3:C:20:LEU:HD23 | 3:C:20:LEU:HA | 1.65 | 0.43 |
| 6:I:27:G:C2 | 7:J:34:C:O2 | 2.71 | 0.43 |
| 8:K:59:GLY:HA2 | 8:K:61:LYS:NZ | 2.33 | 0.43 |
| 8:K:76:ARG:HA | 8:K:247:TRP:HZ2 | 1.82 | 0.43 |
| 8:K:422:ASN:HB3 | 8:K:423:LYS:H | 1.62 | 0.43 |
| 8:K:491:TYR:O | 8:K:495:LEU:N | 2.37 | 0.43 |
| 9:E:122:LEU:HA | 9:E:122:LEU:HD13 | 1.65 | 0.43 |
| 9:E:281:GLN:OE1 | 9:E:401:ASP:HA | 2.18 | 0.43 |
| 9:E:387:VAL:HG13 | 9:E:388:ASN:N | 2.32 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:396:TYR:HB2 | 9:E:398:TYR:CE2 | 2.53 | 0.43 |
| 9:F:5:CYS:HA | 9:F:24:PHE:O | 2.17 | 0.43 |
| 9:F:160:ASP:N | 9:F:160:ASP:OD1 | 2.51 | 0.43 |
| 9:F:161:ARG:HH11 | 9:F:210:VAL:HG22 | 1.83 | 0.43 |
| 9:F:184:GLY:CA | 9:F:224:TYR:O | 2.66 | 0.43 |
| 1:A:42:VAL:HG11 | 1:A:713:ASN:ND2 | 2.31 | 0.43 |
| 1:A:456:TYR:N | 1:A:456:TYR:HD1 | 2.17 | 0.43 |
| 1:A:837:ILE:HA | 1:A:837:ILE:HD13 | 1.62 | 0.43 |
| 2:D:128:LEU:HD12 | 2:D:129:MET:C | 2.39 | 0.43 |
| 5:H:67:SER:HA | 5:H:98:GLN:HA | 2.00 | 0.43 |
| 6:I:23:C:H2' | 6:I:24:U:H6 | 1.83 | 0.43 |
| 8:K:80:ILE:HG23 | 8:K:286:PHE:CE2 | 2.54 | 0.43 |
| 8:K:133:PHE:HE1 | 8:K:159:TRP:CD1 | 2.36 | 0.43 |
| 9:E:149:TYR:HA | 9:E:173:ARG:NH2 | 2.34 | 0.43 |
| 9:E:164:HIS:HA | 9:E:207:ASP:O | 2.19 | 0.43 |
| 9:E:167:TRP:CE3 | 9:E:172:PRO:HB3 | 2.53 | 0.43 |
| 9:E:437:PHE:CZ | 9:E:460:LYS:HD2 | 2.52 | 0.43 |
| 9:E:541:TYR:HD2 | 9:E:544:VAL:HG22 | 1.83 | 0.43 |
| 9:F:184:GLY:C | 9:F:195:ILE:HG12 | 2.38 | 0.43 |
| 9:F:243:GLN:OE1 | 9:F:276:LYS:N | 2.51 | 0.43 |
| 9:F:377:SER:HB3 | 9:F:402:PRO:HA | 2.01 | 0.43 |
| 1:A:449:ALA:O | 1:A:452:ASP:N | 2.40 | 0.43 |
| 1:A:707:LEU:HD12 | 1:A:707:LEU:HA | 1.74 | 0.43 |
| 4:G:7:VAL:HG22 | 4:G:8:ALA:H | 1.82 | 0.43 |
| 5:H:102:THR:HG1 | 5:H:103:CYS:N | 2.15 | 0.43 |
| 9:E:510:VAL:HG13 | 9:E:529:PRO:C | 2.38 | 0.43 |
| 9:F:5:CYS:HB3 | 9:F:8:CYS:SG | 2.57 | 0.43 |
| 9:F:182:PHE:CE2 | 9:F:227:LEU:HD13 | 2.53 | 0.43 |
| 9:F:318:CYS:SG | 9:F:357:PHE:HB3 | 2.58 | 0.43 |
| 9:F:447:GLU:OE1 | 9:F:467:LYS:HG2 | 2.19 | 0.43 |
| 9:F:473:LYS:NZ | 9:F:587:PHE:H | 2.17 | 0.43 |
| 9:F:497:ARG:HD3 | 9:F:525:ILE:O | 2.19 | 0.43 |
| 1:A:531:THR:OG1 | 1:A:654:ARG:NH1 | 2.50 | 0.43 |
| 1:A:885:LEU:HD12 | 1:A:885:LEU:HA | 1.53 | 0.43 |
| 2:B:68:THR:OG1 | 2:B:69:GLN:N | 2.51 | 0.43 |
| 8:K:414:CYS:HA | 8:K:415:ASP:HA | 1.54 | 0.43 |
| 9:E:139:LYS:O | 9:E:142:GLU:HG2 | 2.18 | 0.43 |
| 9:E:368:ALA:H | 9:E:393:ALA:HB2 | 1.83 | 0.43 |
| 9:F:293:ILE:HD13 | 9:F:306:TYR:CZ | 2.54 | 0.43 |
| 9:F:368:ALA:N | 9:F:392:ARG:O | 2.46 | 0.43 |
| 9:F:488:ILE:HG12 | 9:F:518:GLN:HA | 1.99 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:562:ASN:O | 9:F:566:THR:HG23 | 2.18 | 0.43 |
| 1:A:821:LYS:HB2 | 1:A:826:TYR:CE1 | 2.54 | 0.43 |
| 2:D:69:GLN:OE1 | 2:D:70:MET:N | 2.52 | 0.43 |
| 2:D:132:ILE:HD13 | 2:D:138:TYR:HA | 2.00 | 0.43 |
| 6:I:25:A:C4 | 6:I:26:G:N7 | 2.86 | 0.43 |
| 9:E:476:TYR:CZ | 9:E:492:GLN:HG3 | 2.52 | 0.43 |
| 9:E:490:ARG:HA | 9:E:490:ARG:HD3 | 1.67 | 0.43 |
| 9:F:182:PHE:HB3 | 9:F:225:PHE:HB3 | 2.00 | 0.43 |
| 9:F:317:LEU:O | 9:F:320:LYS:HB3 | 2.18 | 0.43 |
| 1:A:41:LYS:HG3 | 1:A:42:VAL:HG13 | 2.01 | 0.43 |
| 1:A:95:ALA:O | 1:A:216:TRP:N | 2.52 | 0.43 |
| 1:A:628:ASN:O | 1:A:631:ARG:N | 2.51 | 0.43 |
| 1:A:900:LEU:O | 1:A:900:LEU:HD23 | 2.19 | 0.43 |
| 5:H:77:CYS:SG | 5:H:83:HIS:CE1 | 3.12 | 0.43 |
| 7:J:44:A:C2 | 7:J:45:C:C2 | 3.07 | 0.43 |
| 9:E:65:LEU:HB3 | 9:E:81:PHE:CB | 2.39 | 0.43 |
| 9:E:266:VAL:O | 9:E:269:TYR:N | 2.52 | 0.43 |
| 9:E:285:GLY:H | 9:E:288:LYS:HD2 | 1.83 | 0.43 |
| 9:E:483:ASP:CG | 9:E:484:VAL:H | 2.21 | 0.43 |
| 9:F:14:LEU:HA | 9:F:14:LEU:HD23 | 1.74 | 0.43 |
| 9:F:19:CYS:SG | 9:F:39:HIS:CE1 | 3.11 | 0.43 |
| 9:F:305:VAL:HB | 9:F:371:VAL:HG23 | 2.01 | 0.43 |
| 9:F:519:ASN:HB3 | 9:F:530:THR:OG1 | 2.19 | 0.43 |
| 3:C:67:ASP:HA | 3:C:70:LYS:HE2 | 2.01 | 0.43 |
| 2:D:25:ALA:O | 2:D:28:ASN:N | 2.52 | 0.43 |
| 8:K:59:GLY:HA2 | 8:K:61:LYS:HZ2 | 1.84 | 0.43 |
| 9:E:244:GLU:O | 9:E:244:GLU:HG2 | 2.19 | 0.43 |
| 9:E:262:PHE:N | 9:E:262:PHE:CD1 | 2.85 | 0.43 |
| 9:E:332:ARG:NH1 | 9:E:333:ILE:H | 2.06 | 0.43 |
| 9:E:334:ILE:HB | 9:E:344:ASP:OD2 | 2.19 | 0.43 |
| 9:E:536:SER:OG | 9:E:567:ARG:HG3 | 2.19 | 0.43 |
| 9:F:473:LYS:HB2 | 9:F:589:SER:OG | 2.19 | 0.43 |
| 1:A:37:ILE:HG21 | 1:A:48:PHE:CZ | 2.54 | 0.43 |
| 1:A:105:ARG:HA | 1:A:109:ASP:O | 2.19 | 0.43 |
| 1:A:458:TYR:HE2 | 1:A:621:LYS:HE2 | 1.84 | 0.43 |
| 1:A:575:LEU:O | 1:A:576:LEU:C | 2.57 | 0.43 |
| 2:B:120:ILE:O | 2:B:124:THR:HG22 | 2.18 | 0.43 |
| 3:C:70:LYS:C | 3:C:72:CYS:H | 2.22 | 0.43 |
| 5:H:23:ALA:HA | 5:H:26:ALA:HB3 | 2.01 | 0.43 |
| 5:H:54:ALA:HB1 | 5:H:98:GLN:H | 1.83 | 0.43 |
| 7:J:47:A:C6 | 7:J:48:C:C4 | 3.06 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:266:VAL:HA | 9:E:269:TYR:CG | 2.54 | 0.43 |
| 9:E:296:ALA:HB1 | 9:E:355:TYR:CE1 | 2.54 | 0.43 |
| 9:E:334:ILE:HG12 | 9:E:343:PHE:O | 2.19 | 0.43 |
| 9:E:355:TYR:HB3 | 9:E:357:PHE:CE1 | 2.54 | 0.43 |
| 9:E:489:ASN:N | 9:E:489:ASN:OD1 | 2.51 | 0.43 |
| 9:E:569:LYS:HA | 9:E:569:LYS:HD2 | 1.78 | 0.43 |
| 9:F:83:LEU:HA | 9:F:83:LEU:HD23 | 1.57 | 0.43 |
| 9:F:198:TYR:HA | 9:F:212:ARG:O | 2.18 | 0.43 |
| 9:F:485:SER:O | 9:F:486:SER:OG | 2.27 | 0.43 |
| 1:A:414:ASN:OD1 | 1:A:844:VAL:HG23 | 2.19 | 0.42 |
| 1:A:602:LEU:HA | 1:A:602:LEU:HD23 | 1.70 | 0.42 |
| 1:A:664:SER:O | 1:A:664:SER:OG | 2.32 | 0.42 |
| 1:A:790:ASN:O | 1:A:791:ASN:C | 2.58 | 0.42 |
| 1:A:867:TYR:HA | 1:A:881:PHE:CE1 | 2.54 | 0.42 |
| 2:B:104:ASN:ND2 | 2:B:104:ASN:H | 2.17 | 0.42 |
| 2:B:136:ASN:HA | 2:B:139:LYS:NZ | 2.33 | 0.42 |
| 2:D:8:SER:C | 2:D:9:LEU:HD22 | 2.39 | 0.42 |
| 2:D:177:SER:OG | 2:D:178:PRO:HD3 | 2.19 | 0.42 |
| 8:K:200:LYS:HD3 | 8:K:200:LYS:HA | 1.88 | 0.42 |
| 9:E:64:TYR:CE2 | 9:E:73:LYS:HE3 | 2.51 | 0.42 |
| 9:E:288:LYS:HA | 9:E:438:LEU:CD1 | 2.49 | 0.42 |
| 9:E:505:ALA:C | 9:E:507:ARG:H | 2.21 | 0.42 |
| 9:E:534:ASP:O | 9:E:536:SER:N | 2.52 | 0.42 |
| 9:F:182:PHE:HB3 | 9:F:225:PHE:CB | 2.49 | 0.42 |
| 9:F:335:PRO:O | 9:F:338:ALA:HB2 | 2.19 | 0.42 |
| 1:A:60:ASP:OD2 | 1:A:64:ASN:ND2 | 2.52 | 0.42 |
| 1:A:831:TYR:HB3 | 1:A:868:PRO:HB2 | 2.00 | 0.42 |
| 5:H:91:ASP:OD1 | 5:H:92:LEU:N | 2.52 | 0.42 |
| 8:K:328:VAL:HG23 | 8:K:347:GLU:HB3 | 2.01 | 0.42 |
| 9:E:240:LEU:HD22 | 9:E:428:LEU:HD23 | 2.00 | 0.42 |
| 9:E:366:THR:HG22 | 9:E:367:THR:N | 2.34 | 0.42 |
| 9:F:287:GLY:CA | 9:F:290:HIS:HB3 | 2.49 | 0.42 |
| 1:A:69:TYR:O | 1:A:70:PHE:HD1 | 2.02 | 0.42 |
| 1:A:804:ASP:OD1 | 1:A:806:THR:N | 2.45 | 0.42 |
| 2:B:99:ASP:N | 2:B:99:ASP:OD1 | 2.50 | 0.42 |
| 2:D:108:ASN:O | 2:D:111:ARG:HG2 | 2.20 | 0.42 |
| 2:D:160:VAL:CG2 | 2:D:164:SER:HA | 2.49 | 0.42 |
| 9:E:381:ASN:OD1 | 9:E:384:LEU:HD23 | 2.19 | 0.42 |
| 9:E:516:ASN:HD22 | 9:E:519:ASN:HB3 | 1.84 | 0.42 |
| 1:A:73:LYS:HB2 | 1:A:116:ARG:NH1 | 2.34 | 0.42 |
| 1:A:674:TYR:CD1 | 1:A:674:TYR:N | 2.87 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:928:HIS:HB3 | 1:A:929:THR:H | 1.60 | 0.42 |
| 2:B:46:LYS:HE3 | 2:B:46:LYS:HB3 | 1.88 | 0.42 |
| 2:B:173:SER:OG | 2:B:175:ASP:N | 2.50 | 0.42 |
| 5:H:28:LYS:HZ3 | 5:H:112:LEU:HD13 | 1.83 | 0.42 |
| 6:I:29:A:H2' | 6:I:30:G:H8 | 1.84 | 0.42 |
| 7:J:47:A:C2 | 7:J:48:C:C2 | 3.07 | 0.42 |
| 8:K:283:HIS:CE1 | 8:K:287:VAL:HG21 | 2.54 | 0.42 |
| 8:K:446:TYR:CE1 | 8:K:491:TYR:HB2 | 2.54 | 0.42 |
| 9:E:287:GLY:O | 9:E:291:PHE:N | 2.47 | 0.42 |
| 9:E:345:LYS:HG3 | 9:E:346:PHE:CD2 | 2.55 | 0.42 |
| 9:E:354:GLN:HG3 | 9:E:355:TYR:CE1 | 2.55 | 0.42 |
| 9:F:418:GLU:HB3 | 9:F:419:PRO:HD2 | 2.01 | 0.42 |
| 1:A:81:GLN:O | 1:A:85:THR:HG22 | 2.20 | 0.42 |
| 1:A:187:LEU:HA | 1:A:187:LEU:HD23 | 1.41 | 0.42 |
| 1:A:366:LEU:O | 1:A:366:LEU:HD12 | 2.19 | 0.42 |
| 1:A:416:ASN:O | 1:A:417:LYS:C | 2.56 | 0.42 |
| 2:B:68:THR:O | 2:B:72:LYS:HG2 | 2.19 | 0.42 |
| 8:K:172:ASP:HA | 8:K:175:LYS:HD2 | 2.00 | 0.42 |
| 9:E:128:GLU:OE2 | 9:E:129:ARG:N | 2.53 | 0.42 |
| 9:E:243:GLN:HB2 | 9:E:277:TYR:CZ | 2.54 | 0.42 |
| 9:E:269:TYR:CD1 | 9:E:295:LEU:HD13 | 2.54 | 0.42 |
| 9:E:348:VAL:HG12 | 9:E:349:ASN:ND2 | 2.35 | 0.42 |
| 9:E:540:GLU:HB2 | 9:E:569:LYS:HG2 | 2.01 | 0.42 |
| 9:E:544:VAL:O | 9:E:572:ILE:HA | 2.19 | 0.42 |
| 9:F:185:TYR:HB2 | 9:F:224:TYR:CZ | 2.54 | 0.42 |
| 1:A:48:PHE:N | 1:A:48:PHE:CD1 | 2.87 | 0.42 |
| 1:A:99:HIS:CD2 | 1:A:116:ARG:HG2 | 2.54 | 0.42 |
| 1:A:165:PHE:HE2 | 1:A:787:TYR:CZ | 2.37 | 0.42 |
| 1:A:238:TYR:O | 1:A:240:LEU:N | 2.52 | 0.42 |
| 1:A:371:LEU:HG | 2:B:87:MET:SD | 2.59 | 0.42 |
| 1:A:825:ASP:C | 1:A:826:TYR:HD1 | 2.22 | 0.42 |
| 3:C:40:LEU:O | 3:C:41:LEU:HD12 | 2.19 | 0.42 |
| 6:I:20:A:C2 | 6:I:21:U:C2 | 3.07 | 0.42 |
| 8:K:10:ASP:OD1 | 8:K:11:CYS:N | 2.51 | 0.42 |
| 8:K:182:VAL:HA | 8:K:240:PHE:C | 2.39 | 0.42 |
| 8:K:216:CYS:HB2 | 8:K:225:ALA:H | 1.84 | 0.42 |
| 9:E:334:ILE:HG22 | 9:E:335:PRO:O | 2.19 | 0.42 |
| 9:E:516:ASN:HA | 9:E:519:ASN:HB3 | 2.00 | 0.42 |
| 9:E:576:MET:SD | 9:E:582:TYR:HB2 | 2.60 | 0.42 |
| 9:F:511:PHE:N | 9:F:530:THR:HA | 2.35 | 0.42 |
| 1:A:372:LEU:HD12 | 1:A:372:LEU:HA | 1.70 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:155:GLU:H | 2:D:155:GLU:CD | 2.23 | 0.42 |
| 2:D:186:VAL:HG12 | 2:D:187:THR:N | 2.35 | 0.42 |
| 6:I:26:G:H2' | 6:I:27:G:C8 | 2.55 | 0.42 |
| 7:J:29:G:C2 | 7:J:30:C:C2 | 3.07 | 0.42 |
| 8:K:306:ASN:HD21 | 8:K:423:LYS:NZ | 2.18 | 0.42 |
| 9:E:60:VAL:HA | 9:E:63:LEU:HB2 | 2.02 | 0.42 |
| 9:E:105:ASP:OD1 | 9:E:105:ASP:N | 2.50 | 0.42 |
| 9:E:409:ARG:HH12 | 9:E:417:LEU:HD23 | 1.85 | 0.42 |
| 9:E:457:TYR:HD2 | 9:E:461:LEU:HG | 1.85 | 0.42 |
| 9:F:51:ASN:ND2 | 9:F:70:TYR:HD2 | 2.15 | 0.42 |
| 1:A:34:ALA:HB2 | 1:A:47:LYS:NZ | 2.33 | 0.42 |
| 1:A:75:HIS:CE1 | 1:A:76:THR:HG1 | 2.37 | 0.42 |
| 1:A:390:ASP:OD1 | 1:A:392:ARG:HG3 | 2.19 | 0.42 |
| 1:A:440:PHE:HD1 | 1:A:843:PHE:HE2 | 1.67 | 0.42 |
| 1:A:456:TYR:N | 1:A:456:TYR:CD1 | 2.87 | 0.42 |
| 2:B:71:TYR:O | 2:B:75:ARG:HG2 | 2.19 | 0.42 |
| 2:D:65:GLN:HG3 | 2:D:66:ALA:N | 2.34 | 0.42 |
| 2:D:102:ALA:O | 2:D:105:ASN:HB3 | 2.20 | 0.42 |
| 4:G:55:ARG:HB3 | 4:G:64:THR:OG1 | 2.20 | 0.42 |
| 4:G:70:GLU:OE2 | 4:G:92:LYS:HG2 | 2.19 | 0.42 |
| 5:H:21:VAL:HG21 | 8:K:217:PHE:CE2 | 2.55 | 0.42 |
| 8:K:88:GLY:H | 8:K:112:SER:HB2 | 1.83 | 0.42 |
| 8:K:180:ARG:HD3 | 8:K:240:PHE:CE1 | 2.54 | 0.42 |
| 9:E:557:ASN:ND2 | 9:E:560:ARG:H | 2.17 | 0.42 |
| 9:F:512:ILE:HA | 9:F:531:GLN:O | 2.19 | 0.42 |
| 9:F:532:THR:N | 9:F:535:SER:OG | 2.53 | 0.42 |
| 9:F:557:ASN:HB3 | 9:F:560:ARG:HB2 | 2.02 | 0.42 |
| 1:A:16:ALA:O | 1:A:18:ARG:N | 2.53 | 0.42 |
| 1:A:442:PHE:CD2 | 1:A:552:ASN:HA | 2.54 | 0.42 |
| 1:A:501:SER:OG | 1:A:502:ALA:N | 2.53 | 0.42 |
| 1:A:684:ASP:OD1 | 1:A:684:ASP:N | 2.24 | 0.42 |
| 1:A:844:VAL:HG11 | 1:A:849:LYS:CB | 2.50 | 0.42 |
| 1:A:869:LEU:HA | 1:A:869:LEU:HD23 | 1.77 | 0.42 |
| 2:D:95:LEU:HA | 2:D:95:LEU:HD23 | 1.75 | 0.42 |
| 4:G:34:THR:HA | 4:G:39:ARG:HA | 2.02 | 0.42 |
| 6:I:11:G:N7 | 7:J:50:G:N1 | 2.68 | 0.42 |
| 7:J:43:U:H2' | 7:J:44:A:H8 | 1.80 | 0.42 |
| 9:F:21:ARG:C | 9:F:22:ARG:HG2 | 2.40 | 0.42 |
| 9:F:61:THR:C | 9:F:63:LEU:H | 2.22 | 0.42 |
| 9:F:122:LEU:O | 9:F:126:CYS:N | 2.53 | 0.42 |
| 9:F:493:ILE:HD12 | 9:F:511:PHE:CE1 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:F:526:LEU:HG | 9:F:528:LEU:HB2 | 2.01 | 0.42 |
| 1:A:125:ALA:O | 1:A:126:ASP:C | 2.58 | 0.42 |
| 1:A:278:GLU:O | 1:A:279:ARG:C | 2.59 | 0.42 |
| 1:A:282:LEU:HD23 | 1:A:282:LEU:HA | 1.84 | 0.42 |
| 1:A:303:ASP:O | 1:A:304:ASP:C | 2.57 | 0.42 |
| 1:A:351:LEU:O | 1:A:352:GLY:C | 2.58 | 0.42 |
| 1:A:387:LEU:O | 2:B:128:LEU:HD12 | 2.19 | 0.42 |
| 1:A:405:VAL:HG23 | 1:A:407:PHE:HE1 | 1.85 | 0.42 |
| 1:A:770:TYR:O | 1:A:774:GLY:N | 2.52 | 0.42 |
| 2:B:147:PHE:O | 2:B:153:LEU:HD12 | 2.18 | 0.42 |
| 3:C:35:LEU:O | 3:C:39:ILE:HG12 | 2.20 | 0.42 |
| 5:H:65:GLN:CB | 5:H:100:PRO:HA | 2.50 | 0.42 |
| 5:H:129:SER:O | 5:H:131:ASP:N | 2.53 | 0.42 |
| 6:I:22:G:C6 | 7:J:39:A:C6 | 3.08 | 0.42 |
| 9:E:64:TYR:HD1 | 9:E:81:PHE:O | 2.02 | 0.42 |
| 9:E:149:TYR:HA | 9:E:173:ARG:HH21 | 1.85 | 0.42 |
| 9:E:332:ARG:HG2 | 9:E:345:LYS:HG2 | 2.01 | 0.42 |
| 9:E:443:ARG:O | 9:E:569:LYS:HA | 2.20 | 0.42 |
| 9:E:541:TYR:HB2 | 9:E:544:VAL:CG2 | 2.50 | 0.42 |
| 9:F:235:LEU:HD13 | 9:F:385:SER:OG | 2.20 | 0.42 |
| 9:F:379:ALA:HB1 | 9:F:383:ASP:OD2 | 2.20 | 0.42 |
| 9:F:565:ILE:HG22 | 9:F:572:ILE:HD12 | 2.02 | 0.42 |
| 1:A:142:LEU:HD12 | 1:A:142:LEU:HA | 1.69 | 0.41 |
| 1:A:314:ASN:HB3 | 1:A:350:GLU:HA | 2.01 | 0.41 |
| 1:A:437:LEU:HD23 | 1:A:437:LEU:HA | 1.83 | 0.41 |
| 2:B:189:LEU:HD23 | 2:B:190:ARG:N | 2.35 | 0.41 |
| 8:K:184:VAL:HB | 8:K:244:VAL:HG21 | 2.01 | 0.41 |
| 8:K:186:TRP:CE2 | 8:K:253:LEU:HB2 | 2.55 | 0.41 |
| 9:E:151:ILE:HD12 | 9:E:226:VAL:HG13 | 2.02 | 0.41 |
| 9:E:323:LYS:HB3 | 9:E:324:TYR:CE2 | 2.55 | 0.41 |
| 9:F:280:LEU:HD11 | 9:F:438:LEU:HD23 | 2.01 | 0.41 |
| 9:F:456:VAL:HG11 | 9:F:562:ASN:HD22 | 1.84 | 0.41 |
| 1:A:877:TYR:O | 1:A:880:VAL:HG12 | 2.20 | 0.41 |
| 1:A:921:TYR:O | 1:A:923:ALA:N | 2.53 | 0.41 |
| 2:B:146:THR:OG1 | 2:B:147:PHE:N | 2.53 | 0.41 |
| 2:D:168:GLN:HB3 | 2:D:169:LEU:H | 1.70 | 0.41 |
| 8:K:29:VAL:HG13 | 8:K:34:LYS:HD2 | 2.02 | 0.41 |
| 8:K:318:LYS:HE2 | 8:K:318:LYS:HB2 | 1.88 | 0.41 |
| 9:E:149:TYR:HD2 | 9:E:173:ARG:HB2 | 1.85 | 0.41 |
| 9:E:155:ARG:NE | 9:E:166:SER:OG | 2.53 | 0.41 |
| 9:E:212:ARG:NH1 | 9:E:213:GLY:O | 2.53 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:296:ALA:HB1 | 9:E:355:TYR:CZ | 2.55 | 0.41 |
| 1:A:497:ASN:ND2 | 1:A:500:LYS:HE3 | 2.35 | 0.41 |
| 1:A:513:ARG:HD2 | 1:A:513:ARG:HA | 1.73 | 0.41 |
| 1:A:538:THR:CG2 | 1:A:661:GLN:HG2 | 2.51 | 0.41 |
| 1:A:638:LEU:HD23 | 1:A:638:LEU:HA | 1.77 | 0.41 |
| 1:A:883:LEU:O | 1:A:884:TYR:C | 2.56 | 0.41 |
| 2:B:66:ALA:O | 2:B:69:GLN:HG3 | 2.20 | 0.41 |
| 3:C:27:LYS:HE2 | 3:C:27:LYS:HB3 | 1.87 | 0.41 |
| 8:K:11:CYS:SG | 8:K:103:THR:HB | 2.60 | 0.41 |
| 9:E:263:SER:O | 9:E:266:VAL:HB | 2.20 | 0.41 |
| 9:E:332:ARG:HD2 | 9:E:332:ARG:HA | 1.58 | 0.41 |
| 9:E:414:LYS:HA | 9:E:414:LYS:HD3 | 1.73 | 0.41 |
| 9:F:278:SER:HA | 9:F:435:ASP:OD2 | 2.20 | 0.41 |
| 9:F:473:LYS:O | 9:F:474:MET:HG3 | 2.21 | 0.41 |
| 1:A:519:MET:HE2 | 1:A:519:MET:HB3 | 1.73 | 0.41 |
| 1:A:819:LEU:HB2 | 1:A:828:TYR:CE1 | 2.55 | 0.41 |
| 1:A:856:ILE:O | 1:A:857:GLU:C | 2.59 | 0.41 |
| 4:G:16:ALA:O | 4:G:27:ASN:ND2 | 2.44 | 0.41 |
| 8:K:117:LEU:HD11 | 8:K:162:VAL:HG22 | 2.01 | 0.41 |
| 9:E:146:LYS:HA | 9:E:149:TYR:HE1 | 1.84 | 0.41 |
| 9:E:271:LYS:H | 9:E:271:LYS:HG3 | 1.61 | 0.41 |
| 9:E:370:ILE:HD11 | 9:E:397:VAL:CG1 | 2.51 | 0.41 |
| 9:E:420:GLU:HA | 9:E:426:CYS:C | 2.41 | 0.41 |
| 9:E:579:ARG:O | 9:E:582:TYR:HB3 | 2.19 | 0.41 |
| 9:F:195:ILE:HG13 | 9:F:198:TYR:HE2 | 1.84 | 0.41 |
| 9:F:322:LEU:HD12 | 9:F:327:ILE:HG22 | 2.01 | 0.41 |
| 1:A:419:PHE:HE1 | 1:A:883:LEU:HD21 | 1.85 | 0.41 |
| 1:A:488:ILE:HD11 | 1:A:493:VAL:HG12 | 2.02 | 0.41 |
| 1:A:723:LEU:O | 1:A:724:GLN:C | 2.59 | 0.41 |
| 1:A:805:LEU:N | 1:A:805:LEU:HD12 | 2.36 | 0.41 |
| 2:B:54:ALA:HB1 | 2:B:58:LYS:NZ | 2.35 | 0.41 |
| 4:G:10:ARG:HH22 | 4:G:34:THR:CB | 2.34 | 0.41 |
| 7:J:41:G:N2 | 7:J:42:C:C2 | 2.88 | 0.41 |
| 8:K:119:ALA:CA | 8:K:157:LEU:H | 2.19 | 0.41 |
| 9:E:360:VAL:HG21 | 9:E:383:ASP:OD2 | 2.20 | 0.41 |
| 9:E:453:SER:C | 9:E:459:ASN:H | 2.21 | 0.41 |
| 9:F:14:LEU:O | 9:F:15:ARG:HG3 | 2.21 | 0.41 |
| 9:F:372:VAL:HA | 9:F:397:VAL:HB | 2.03 | 0.41 |
| 9:F:412:LEU:HD11 | 9:F:415:GLY:O | 2.21 | 0.41 |
| 9:F:536:SER:OG | 9:F:567:ARG:HG3 | 2.20 | 0.41 |
| 1:A:39:ASN:HD21 | 1:A:42:VAL:HG22 | 1.85 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:TRP:HA | 1:A:168:ASN:HD22 | 1.84 | 0.41 |
| 1:A:276:THR:O | 1:A:279:ARG:N | 2.54 | 0.41 |
| 1:A:539:ILE:HG23 | 1:A:539:ILE:HD12 | 1.74 | 0.41 |
| 1:A:552:ASN:OD1 | 1:A:552:ASN:N | 2.50 | 0.41 |
| 1:A:768:SER:O | 1:A:771:ALA:N | 2.53 | 0.41 |
| 1:A:770:TYR:HD1 | 1:A:770:TYR:HA | 1.59 | 0.41 |
| 1:A:875:GLN:O | 1:A:876:GLU:C | 2.59 | 0.41 |
| 2:D:160:VAL:HG13 | 2:D:185:ILE:HB | 2.02 | 0.41 |
| 4:G:69:LEU:O | 4:G:92:LYS:HE3 | 2.20 | 0.41 |
| 9:E:201:GLU:OE1 | 9:E:201:GLU:N | 2.54 | 0.41 |
| 9:E:409:ARG:HH22 | 9:E:422:PHE:CA | 2.32 | 0.41 |
| 9:E:453:SER:CB | 9:E:459:ASN:HA | 2.50 | 0.41 |
| 9:E:540:GLU:OE1 | 9:E:569:LYS:HD3 | 2.21 | 0.41 |
| 9:F:258:ILE:HG23 | 9:F:259:SER:N | 2.34 | 0.41 |
| 2:B:153:LEU:HD12 | 2:B:154:TRP:H | 1.85 | 0.41 |
| 3:C:49:PHE:HD1 | 3:C:49:PHE:HA | 1.73 | 0.41 |
| 5:H:45:LEU:HD22 | 8:K:40:VAL:HG22 | 2.02 | 0.41 |
| 8:K:116:ASN:ND2 | 8:K:271:SER:H | 2.13 | 0.41 |
| 9:E:152:ALA:HB2 | 9:E:167:TRP:CH2 | 2.56 | 0.41 |
| 9:E:158:LEU:HB2 | 9:E:162:GLU:O | 2.20 | 0.41 |
| 9:E:363:LEU:HD12 | 9:E:363:LEU:HA | 1.94 | 0.41 |
| 9:F:396:TYR:HB3 | 9:F:398:TYR:HH | 1.85 | 0.41 |
| 9:F:490:ARG:HA | 9:F:490:ARG:HD2 | 1.82 | 0.41 |
| 9:F:577:SER:OG | 9:F:578:ASP:N | 2.52 | 0.41 |
| 1:A:72:VAL:HG22 | 1:A:115:SER:HA | 2.03 | 0.41 |
| 1:A:356:ASN:ND2 | 1:A:534:ASN:HB3 | 2.35 | 0.41 |
| 1:A:630:LEU:HD23 | 1:A:694:PHE:CE1 | 2.55 | 0.41 |
| 2:B:164:SER:O | 2:B:165:LYS:HE2 | 2.21 | 0.41 |
| 4:G:88:LEU:HD12 | 4:G:88:LEU:HA | 1.95 | 0.41 |
| 6:I:11:G:C4 | 6:I:12:G:C8 | 3.08 | 0.41 |
| 6:I:26:G:C2 | 7:J:35:U:N3 | 2.89 | 0.41 |
| 8:K:473:CYS:HB3 | 8:K:491:TYR:CE1 | 2.56 | 0.41 |
| 9:E:42:VAL:O | 9:E:48:TYR:HB2 | 2.21 | 0.41 |
| 9:E:304:ILE:HG23 | 9:E:370:ILE:HG23 | 2.02 | 0.41 |
| 9:E:326:PRO:HB2 | 9:E:328:ASP:OD1 | 2.21 | 0.41 |
| 9:E:334:ILE:HD13 | 9:E:334:ILE:HA | 1.74 | 0.41 |
| 9:F:471:CYS:HA | 9:F:572:ILE:O | 2.20 | 0.41 |
| 1:A:35:PHE:CD2 | 1:A:35:PHE:N | 2.89 | 0.41 |
| 1:A:245:LEU:HD23 | 1:A:245:LEU:HA | 1.61 | 0.41 |
| 1:A:640:ARG:HD3 | 1:A:640:ARG:HA | 1.88 | 0.41 |
| 1:A:847:ILE:C | 1:A:849:LYS:N | 2.72 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:137:THR:HA | 2:D:140:ASN:ND2 | 2.35 | 0.41 |
| 4:G:69:LEU:HB3 | 4:G:89:TYR:HB3 | 2.02 | 0.41 |
| 5:H:56:THR:HG21 | 5:H:60:GLU:N | 2.36 | 0.41 |
| 6:I:12:G:C2 | 7:J:49:C:N3 | 2.89 | 0.41 |
| 8:K:384:PHE:HB3 | 8:K:392:TYR:HE2 | 1.86 | 0.41 |
| 8:K:388:ASN:ND2 | 8:K:429:PRO:HD2 | 2.36 | 0.41 |
| 9:E:18:ALA:HB3 | 9:E:39:HIS:ND1 | 2.36 | 0.41 |
| 9:E:20:ILE:HG23 | 9:E:21:ARG:HG2 | 2.03 | 0.41 |
| 9:E:149:TYR:HB2 | 9:E:227:LEU:CD2 | 2.50 | 0.41 |
| 9:E:168:GLU:OE2 | 9:E:171:LYS:HG2 | 2.21 | 0.41 |
| 9:E:197:GLU:HG2 | 9:E:214:THR:HG22 | 2.03 | 0.41 |
| 9:E:298:TYR:HE1 | 9:E:299:TYR:CZ | 2.38 | 0.41 |
| 9:E:537:GLN:HA | 9:E:567:ARG:HD2 | 2.03 | 0.41 |
| 9:E:541:TYR:HB2 | 9:E:544:VAL:HG23 | 2.03 | 0.41 |
| 9:F:371:VAL:HG11 | 9:F:391:LEU:HD13 | 2.03 | 0.41 |
| 9:F:557:ASN:HB3 | 9:F:560:ARG:HE | 1.86 | 0.41 |
| 1:A:80:TYR:CD1 | 1:A:112:PRO:HB2 | 2.56 | 0.41 |
| 1:A:143:LYS:HA | 1:A:157:PHE:CE2 | 2.56 | 0.41 |
| 1:A:207:LEU:C | 1:A:209:ASN:H | 2.24 | 0.41 |
| 1:A:434:SER:OG | 1:A:876:GLU:OE1 | 2.38 | 0.41 |
| 1:A:587:VAL:HG12 | 1:A:589:ILE:HG13 | 2.02 | 0.41 |
| 1:A:847:ILE:HD12 | 1:A:847:ILE:HG23 | 1.84 | 0.41 |
| 2:D:169:LEU:HD13 | 2:D:169:LEU:HA | 1.96 | 0.41 |
| 4:G:77:THR:OG1 | 4:G:78:ASP:N | 2.54 | 0.41 |
| 9:E:61:THR:H | 9:E:61:THR:HG23 | 1.66 | 0.41 |
| 9:E:278:SER:O | 9:E:398:TYR:HD2 | 2.03 | 0.41 |
| 9:E:557:ASN:ND2 | 9:E:560:ARG:HB2 | 2.35 | 0.41 |
| 9:F:60:VAL:O | 9:F:63:LEU:HB2 | 2.21 | 0.41 |
| 9:F:77:PRO:O | 9:F:79:ILE:N | 2.54 | 0.41 |
| 1:A:489:ASN:HB2 | 1:A:492:GLN:NE2 | 2.36 | 0.40 |
| 1:A:749:LEU:HA | 1:A:749:LEU:HD23 | 1.60 | 0.40 |
| 2:D:118:ASN:O | 2:D:119:ILE:C | 2.59 | 0.40 |
| 4:G:84:LYS:HA | 4:G:84:LYS:HD2 | 1.84 | 0.40 |
| 8:K:392:TYR:HE1 | 8:K:435:ALA:HB1 | 1.86 | 0.40 |
| 9:E:473:LYS:HG3 | 9:E:473:LYS:O | 2.21 | 0.40 |
| 9:E:514:PRO:HA | 9:E:560:ARG:HH22 | 1.86 | 0.40 |
| 9:F:109:ILE:HD12 | 9:F:130:LEU:HD11 | 2.03 | 0.40 |
| 9:F:509:ALA:HB3 | 9:F:545:ILE:HG13 | 2.03 | 0.40 |
| 1:A:185:ALA:O | 1:A:186:LEU:C | 2.58 | 0.40 |
| 1:A:245:LEU:CD2 | 1:A:250:ALA:HB3 | 2.51 | 0.40 |
| 1:A:474:GLU:O | 1:A:477:ASP:HB3 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:55:LEU:O | 3:C:57:SER:N | 2.54 | 0.40 |
| 4:G:11:GLN:HB2 | 4:G:31:TYR:CZ | 2.56 | 0.40 |
| 5:H:53:GLN:HE21 | 5:H:121:GLY:HA3 | 1.83 | 0.40 |
| 7:J:42:C:C2 | 7:J:43:U:C5 | 3.09 | 0.40 |
| 8:K:10:ASP:OD2 | 8:K:53:ARG:HD3 | 2.21 | 0.40 |
| 8:K:359:LYS:HA | 8:K:361:TYR:CE1 | 2.57 | 0.40 |
| 9:E:268:ASN:O | 9:E:272:VAL:HG13 | 2.22 | 0.40 |
| 9:E:283:PRO:HG2 | 9:E:439:GLY:CA | 2.45 | 0.40 |
| 9:E:314:VAL:HA | 9:E:317:LEU:HB2 | 2.03 | 0.40 |
| 9:E:425:VAL:HG13 | 9:E:426:CYS:N | 2.36 | 0.40 |
| 9:F:21:ARG:HA | 9:F:21:ARG:CZ | 2.51 | 0.40 |
| 9:F:182:PHE:O | 9:F:198:TYR:N | 2.50 | 0.40 |
| 9:F:486:SER:CB | 9:F:517:SER:H | 2.32 | 0.40 |
| 9:F:506:TRP:HH2 | 9:F:572:ILE:C | 2.24 | 0.40 |
| 1:A:189:THR:O | 1:A:192:PHE:HB3 | 2.21 | 0.40 |
| 1:A:196:MET:HG2 | 1:A:201:ILE:HB | 2.03 | 0.40 |
| 1:A:746:TYR:CD2 | 1:A:746:TYR:C | 2.95 | 0.40 |
| 2:B:12:TYR:HA | 2:B:49:PHE:CZ | 2.56 | 0.40 |
| 2:B:51:ARG:HH21 | 6:I:14:A:H4' | 1.85 | 0.40 |
| 2:B:106:ILE:HA | 2:B:109:ASN:ND2 | 2.36 | 0.40 |
| 4:G:10:ARG:HH22 | 4:G:34:THR:H | 1.69 | 0.40 |
| 4:G:12:MET:HG2 | 4:G:13:SER:H | 1.86 | 0.40 |
| 6:I:15:G:C6 | 6:I:16:U:C4 | 3.10 | 0.40 |
| 8:K:282:VAL:HG13 | 8:K:419:LEU:HD21 | 2.02 | 0.40 |
| 8:K:328:VAL:HG13 | 8:K:380:GLY:HA3 | 2.04 | 0.40 |
| 9:E:114:TRP:CZ3 | 9:E:123:ALA:HB2 | 2.57 | 0.40 |
| 9:E:332:ARG:HB3 | 9:E:346:PHE:H | 1.86 | 0.40 |
| 9:E:387:VAL:O | 9:E:390:ARG:N | 2.44 | 0.40 |
| 9:E:409:ARG:HB3 | 9:E:412:LEU:CB | 2.52 | 0.40 |
| 9:F:407:ALA:HB3 | 9:F:409:ARG:HG3 | 2.03 | 0.40 |
| 9:F:500:LEU:HD22 | 9:F:526:LEU:HD13 | 2.03 | 0.40 |
| 1:A:18:ARG:O | 1:A:59:LYS:HB2 | 2.22 | 0.40 |
| 1:A:103:LYS:HD2 | 1:A:112:PRO:HA | 2.04 | 0.40 |
| 1:A:334:PHE:HA | 1:A:338:VAL:O | 2.22 | 0.40 |
| 2:B:40:LYS:O | 2:B:44:VAL:HG22 | 2.21 | 0.40 |
| 2:D:52:ASP:O | 2:D:55:MET:HG3 | 2.22 | 0.40 |
| 5:H:71:ALA:O | 5:H:73:CYS:N | 2.46 | 0.40 |
| 8:K:175:LYS:CE | 8:K:228:HIS:HA | 2.51 | 0.40 |
| 8:K:246:GLN:O | 8:K:247:TRP:HD1 | 2.05 | 0.40 |
| 8:K:456:GLY:O | 8:K:458:GLN:N | 2.47 | 0.40 |
| 9:E:6:VAL:HG23 | 9:E:7:LEU:CD2 | 2.51 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:E:425:VAL:O | 9:E:428:LEU:HG | 2.21 | 0.40 |
| 9:F:62:GLN:H | 9:F:62:GLN:CD | 2.22 | 0.40 |
| 9:F:319:GLU:O | 9:F:322:LEU:HB3 | 2.21 | 0.40 |
| 9:F:360:VAL:HA | 9:F:363:LEU:HG | 2.03 | 0.40 |
| 9:F:474:MET:HB3 | 9:F:476:TYR:CD1 | 2.56 | 0.40 |
| 1:A:293:THR:H | 1:A:293:THR:HG23 | 1.61 | 0.40 |
| 1:A:606:TYR:O | 1:A:607:SER:OG | 2.37 | 0.40 |
| 1:A:713:ASN:O | 1:A:714:LYS:HD3 | 2.21 | 0.40 |
| 8:K:127:THR:OG1 | 8:K:130:ASN:O | 2.26 | 0.40 |
| 9:E:139:LYS:HA | 9:E:142:GLU:HG2 | 2.04 | 0.40 |
| 9:E:182:PHE:HB2 | 9:E:225:PHE:HD2 | 1.85 | 0.40 |
| 9:E:375:GLU:HB2 | 9:E:378:MET:HE1 | 2.04 | 0.40 |
| 9:E:510:VAL:HG21 | 9:E:541:TYR:CZ | 2.56 | 0.40 |
| 9:E:580:ASP:O | 9:E:583:ASP:N | 2.55 | 0.40 |
| 9:F:64:TYR:CD2 | 9:F:76:LYS:HD2 | 2.57 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|----------|-------------|-----|
| 1 | A | 924/929 (100%) | 690 (75%) | 226 (24%) | 8 (1%) | 17 | 17 |
| 2 | B | 185/198 (93%) | 163 (88%) | 21 (11%) | 1 (0%) | 29 | 29 |
| 2 | D | 184/198 (93%) | 152 (83%) | 32 (17%) | 0 | 100 | 100 |
| 3 | C | 70/83 (84%) | 48 (69%) | 22 (31%) | 0 | 100 | 100 |
| 4 | G | 111/113 (98%) | 94 (85%) | 17 (15%) | 0 | 100 | 100 |
| 5 | H | 129/139 (93%) | 105 (81%) | 24 (19%) | 0 | 100 | 100 |
| 8 | K | 521/527 (99%) | 424 (81%) | 96 (18%) | 1 (0%) | 47 | 47 |
| 9 | E | 584/601 (97%) | 429 (74%) | 149 (26%) | 6 (1%) | 15 | 15 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 9 | F | 588/601 (98%) | 460 (78%) | 124 (21%) | 4 (1%) | 22 | 22 |
| All | All | 3296/3389 (97%) | 2565 (78%) | 711 (22%) | 20 (1%) | 29 | 25 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 264 | PRO |
| 1 | A | 296 | PRO |
| 1 | A | 905 | VAL |
| 1 | A | 928 | HIS |
| 2 | B | 183 | PRO |
| 9 | E | 171 | LYS |
| 9 | E | 254 | PRO |
| 9 | E | 442 | ARG |
| 9 | E | 169 | VAL |
| 9 | F | 406 | PRO |
| 1 | A | 39 | ASN |
| 1 | A | 218 | ASP |
| 9 | E | 78 | PRO |
| 1 | A | 237 | TYR |
| 1 | A | 336 | ASP |
| 9 | E | 215 | THR |
| 9 | F | 537 | GLN |
| 9 | F | 490 | ARG |
| 8 | K | 389 | VAL |
| 9 | F | 419 | PRO |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 817/820 (100%) | 801 (98%) | 16 (2%) | 55 | 55 |
| 2 | B | 144/167 (86%) | 141 (98%) | 3 (2%) | 53 | 53 |
| 2 | D | 149/167 (89%) | 147 (99%) | 2 (1%) | 69 | 69 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3 | C | 67/77 (87%) | 66 (98%) | 1 (2%) | 65 | 65 |
| 4 | G | 94/94 (100%) | 94 (100%) | 0 | 100 | 100 |
| 5 | H | 105/113 (93%) | 104 (99%) | 1 (1%) | 76 | 76 |
| 8 | K | 458/462 (99%) | 454 (99%) | 4 (1%) | 78 | 78 |
| 9 | E | 503/523 (96%) | 499 (99%) | 4 (1%) | 81 | 81 |
| 9 | F | 513/523 (98%) | 510 (99%) | 3 (1%) | 86 | 86 |
| All | All | 2850/2946 (97%) | 2816 (99%) | 34 (1%) | 72 | 71 |

All (34) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | ARG |
| 1 | A | 62 | ASP |
| 1 | A | 100 | ASP |
| 1 | A | 163 | TYR |
| 1 | A | 170 | ASP |
| 1 | A | 212 | LEU |
| 1 | A | 215 | ASN |
| 1 | A | 295 | HIS |
| 1 | A | 516 | TYR |
| 1 | A | 544 | LEU |
| 1 | A | 648 | LEU |
| 1 | A | 684 | ASP |
| 1 | A | 770 | TYR |
| 1 | A | 845 | ASP |
| 1 | A | 903 | TYR |
| 1 | A | 922 | GLU |
| 2 | B | 46 | LYS |
| 2 | B | 49 | PHE |
| 2 | B | 61 | LYS |
| 3 | C | 52 | MET |
| 2 | D | 46 | LYS |
| 2 | D | 78 | ASP |
| 5 | H | 82 | ASP |
| 8 | K | 9 | LYS |
| 8 | K | 74 | ILE |
| 8 | K | 135 | ARG |
| 8 | K | 147 | LYS |
| 9 | E | 186 | ARG |
| 9 | E | 218 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 9 | E | 474[A] | MET |
| 9 | E | 474[B] | MET |
| 9 | F | 72 | CYS |
| 9 | F | 73 | LYS |
| 9 | F | 579 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | GLN |
| 1 | A | 256 | HIS |
| 1 | A | 292 | GLN |
| 1 | A | 356 | ASN |
| 1 | A | 414 | ASN |
| 1 | A | 534 | ASN |
| 1 | A | 599 | HIS |
| 1 | A | 752 | HIS |
| 1 | A | 822 | GLN |
| 2 | B | 19 | GLN |
| 2 | B | 69 | GLN |
| 2 | B | 108 | ASN |
| 3 | C | 19 | GLN |
| 2 | D | 140 | ASN |
| 4 | G | 1 | ASN |
| 4 | G | 11 | GLN |
| 5 | H | 53 | GLN |
| 5 | H | 65 | GLN |
| 8 | K | 306 | ASN |
| 8 | K | 410 | ASN |
| 9 | E | 62 | GLN |
| 9 | E | 354 | GLN |
| 9 | E | 361 | ASN |
| 9 | E | 464 | HIS |
| 9 | E | 516 | ASN |
| 9 | F | 51 | ASN |
| 9 | F | 75 | HIS |
| 9 | F | 116 | ASN |
| 9 | F | 354 | GLN |
| 9 | F | 489 | ASN |
| 9 | F | 518 | GLN |
| 9 | F | 519 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 6 | I | 24/25 (96%) | 6 (25%) | 1 (4%) |
| 7 | J | 26/27 (96%) | 8 (30%) | 0 |
| All | All | 50/52 (96%) | 14 (28%) | 1 (2%) |

All (14) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | I | 10 | C |
| 6 | I | 11 | G |
| 6 | I | 15 | G |
| 6 | I | 16 | U |
| 6 | I | 23 | C |
| 6 | I | 27 | G |
| 7 | J | 25 | G |
| 7 | J | 28 | U |
| 7 | J | 31 | U |
| 7 | J | 35 | U |
| 7 | J | 39 | A |
| 7 | J | 41 | G |
| 7 | J | 42 | C |
| 7 | J | 49 | C |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | I | 22 | G |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31146. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.