



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:52 pm BST

PDB ID : 3SHJ
Title : Proteasome in complex with hydroxyurea derivative HU10
Authors : Gallastegui, N.; Beck, P.; Arciniega, M.; Hillebrand, S.; Huber, R.; Groll, M.
Deposited on : 2011-06-16
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

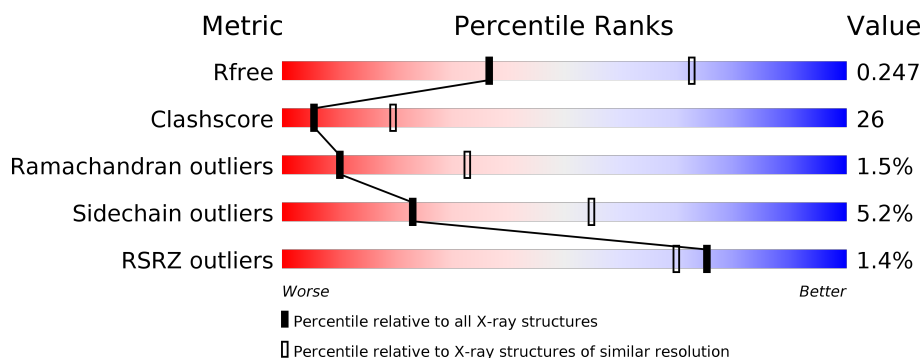
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3140 (2.80-2.80) |
| Clashscore | 141614 | 3569 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RSRZ outliers | 127900 | 3078 (2.80-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 250 | <div> <div>62%</div> <div>36%</div> <div>•</div> </div> |
| 1 | O | 250 | <div>2%</div> <div>64%</div> <div>34%</div> <div>•</div> |
| 2 | B | 244 | <div>2%</div> <div>53%</div> <div>41%</div> <div>6%</div> |
| 2 | P | 244 | <div>2%</div> <div>55%</div> <div>39%</div> <div>6%</div> |
| 3 | C | 241 | <div>2%</div> <div>56%</div> <div>41%</div> <div>•</div> |
| 3 | Q | 241 | <div>7%</div> <div>54%</div> <div>42%</div> <div>•</div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | D | 242 | |
| 4 | R | 242 | |
| 5 | E | 233 | |
| 5 | S | 233 | |
| 6 | F | 244 | |
| 6 | T | 244 | |
| 7 | G | 243 | |
| 7 | U | 243 | |
| 8 | H | 222 | |
| 8 | V | 222 | |
| 9 | I | 204 | |
| 9 | W | 204 | |
| 10 | J | 198 | |
| 10 | X | 198 | |
| 11 | K | 212 | |
| 11 | Y | 212 | |
| 12 | L | 222 | |
| 12 | Z | 222 | |
| 13 | 1 | 233 | |
| 13 | M | 233 | |
| 14 | 2 | 196 | |
| 14 | N | 196 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 15 | MES | K | 1(L) | - | X | - | - |

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |
| 1 | O | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |

- Molecule 2 is a protein called Proteasome component Y13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |
| 2 | P | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |

- Molecule 3 is a protein called Proteasome component PRE6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |
| 3 | Q | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |

- Molecule 4 is a protein called Proteasome component PUP2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |
| 4 | R | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |

- Molecule 5 is a protein called Proteasome component PRE5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |
| 5 | S | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |

- Molecule 6 is a protein called Proteasome component C1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | F | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |
| 6 | T | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |

- Molecule 7 is a protein called Proteasome component C7-alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | G | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |
| 7 | U | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |

- Molecule 8 is a protein called Proteasome component PUP1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8 | H | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1685 | 1061 | 293 | 324 | 7 | | | |
| 8 | V | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1685 | 1061 | 293 | 324 | 7 | | | |

- Molecule 9 is a protein called Proteasome component PUP3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | I | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |
| 9 | W | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |

- Molecule 10 is a protein called Proteasome component C11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | J | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | X | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

- Molecule 11 is a protein called Proteasome component PRE2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 11 | K | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |
| 11 | Y | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |

- Molecule 12 is a protein called Proteasome component C5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12 | L | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |
| 12 | Z | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |

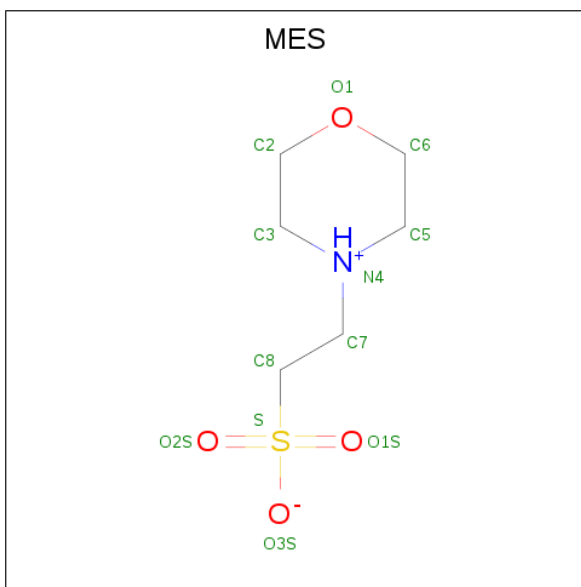
- Molecule 13 is a protein called Proteasome component PRE4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | M | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |
| 13 | 1 | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |

- Molecule 14 is a protein called Proteasome component PRE3.

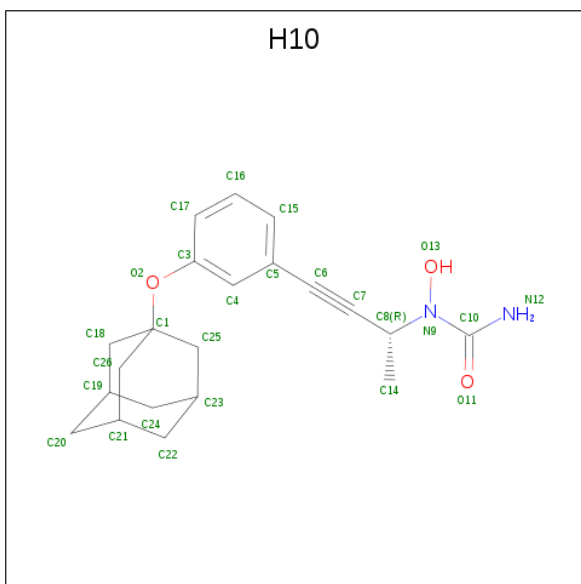
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |
| 14 | 2 | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 15 | K | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 12 | 6 | 1 | 4 | 1 | | |
| 15 | Y | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 12 | 6 | 1 | 4 | 1 | | |

- Molecule 16 is 1-hydroxy-1-[(2R)-4-{3-[(3S,5S,7S)-tricyclo[3.3.1.1^{3,7}]dec-1-yloxy]phenyl}but-3-yn-2-yl]urea (three-letter code: H10) (formula: C₂₁H₂₆N₂O₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 16 | K | 1 | Total | C | N | O | 0 | 0 |
| | | | 26 | 21 | 2 | 3 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 16 | Y | 1 | Total | C | N | O | 0 | 0 |
| | | | 26 | 21 | 2 | 3 | | |

- Molecule 17 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | A | 49 | Total | O | 0 | 0 |
| | | | 49 | 49 | | |
| 17 | B | 36 | Total | O | 0 | 0 |
| | | | 36 | 36 | | |
| 17 | C | 37 | Total | O | 0 | 0 |
| | | | 37 | 37 | | |
| 17 | D | 36 | Total | O | 0 | 0 |
| | | | 36 | 36 | | |
| 17 | E | 23 | Total | O | 0 | 0 |
| | | | 23 | 23 | | |
| 17 | F | 47 | Total | O | 0 | 0 |
| | | | 47 | 47 | | |
| 17 | G | 58 | Total | O | 0 | 0 |
| | | | 58 | 58 | | |
| 17 | H | 46 | Total | O | 0 | 0 |
| | | | 46 | 46 | | |
| 17 | I | 65 | Total | O | 0 | 0 |
| | | | 65 | 65 | | |
| 17 | J | 48 | Total | O | 0 | 0 |
| | | | 48 | 48 | | |
| 17 | K | 49 | Total | O | 0 | 0 |
| | | | 49 | 49 | | |
| 17 | L | 58 | Total | O | 0 | 0 |
| | | | 58 | 58 | | |
| 17 | M | 66 | Total | O | 0 | 0 |
| | | | 66 | 66 | | |
| 17 | N | 56 | Total | O | 0 | 0 |
| | | | 56 | 56 | | |
| 17 | O | 30 | Total | O | 0 | 0 |
| | | | 30 | 30 | | |
| 17 | P | 29 | Total | O | 0 | 0 |
| | | | 29 | 29 | | |
| 17 | Q | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 17 | R | 30 | Total | O | 0 | 0 |
| | | | 30 | 30 | | |

Continued on next page...

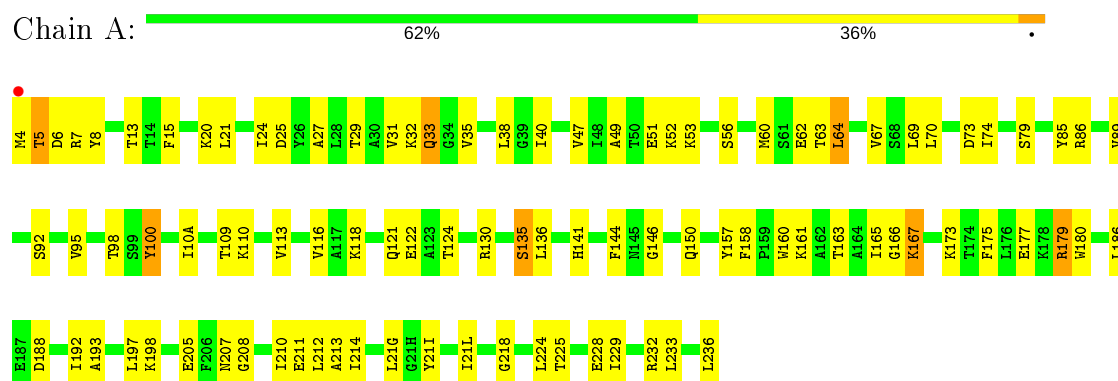
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | S | 19 | Total | O | 0 | 0 |
| | | | 19 | 19 | | |
| 17 | T | 38 | Total | O | 0 | 0 |
| | | | 38 | 38 | | |
| 17 | U | 60 | Total | O | 0 | 0 |
| | | | 60 | 60 | | |
| 17 | V | 42 | Total | O | 0 | 0 |
| | | | 42 | 42 | | |
| 17 | W | 57 | Total | O | 0 | 0 |
| | | | 57 | 57 | | |
| 17 | X | 48 | Total | O | 0 | 0 |
| | | | 48 | 48 | | |
| 17 | Y | 50 | Total | O | 0 | 0 |
| | | | 50 | 50 | | |
| 17 | Z | 50 | Total | O | 0 | 0 |
| | | | 50 | 50 | | |
| 17 | 1 | 69 | Total | O | 0 | 0 |
| | | | 69 | 69 | | |
| 17 | 2 | 61 | Total | O | 0 | 0 |
| | | | 61 | 61 | | |

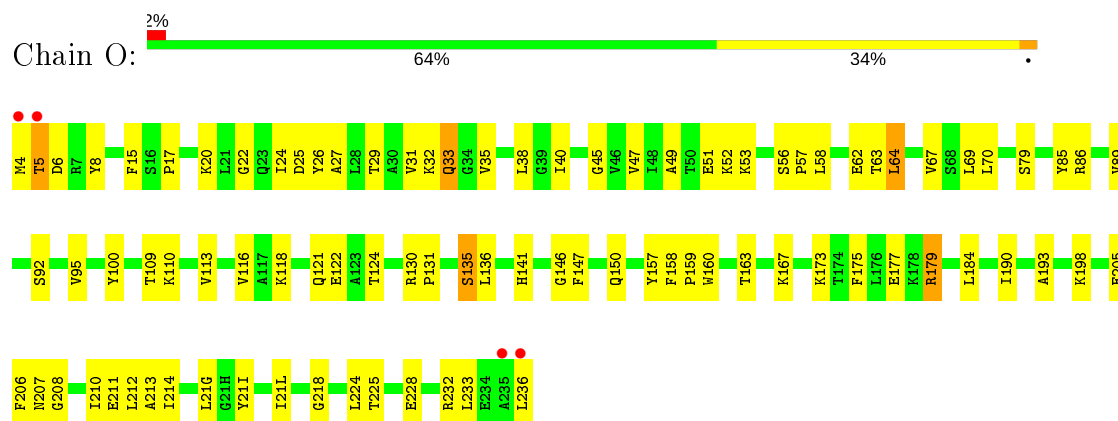
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

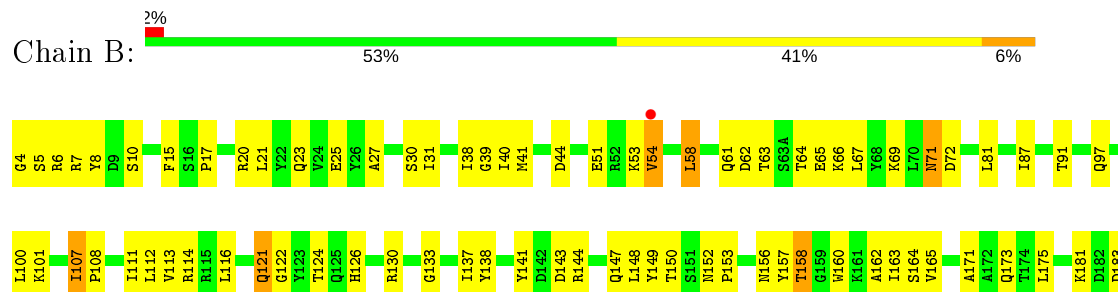
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

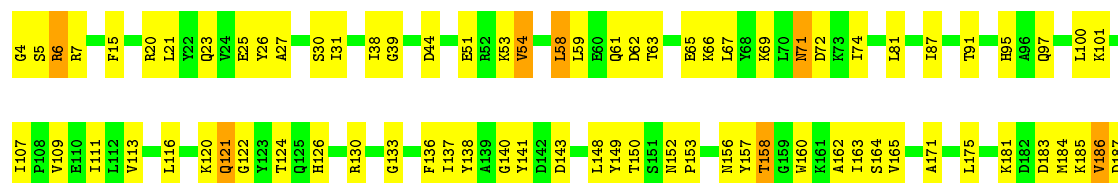


• Molecule 2: Proteasome component Y13

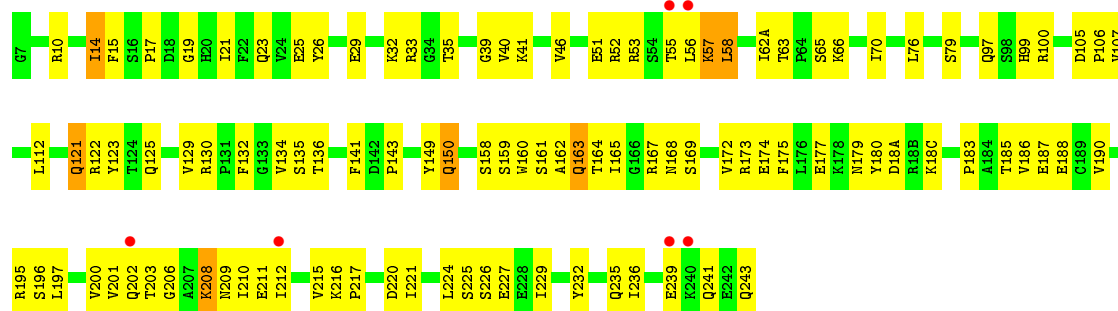




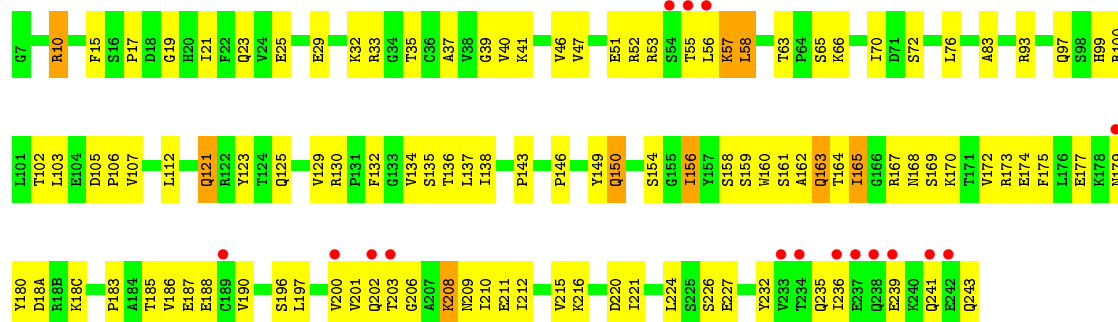
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

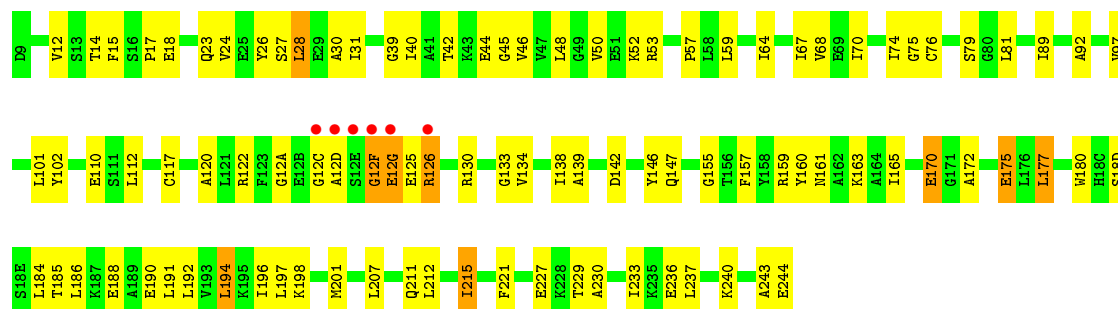


• Molecule 3: Proteasome component PRE6

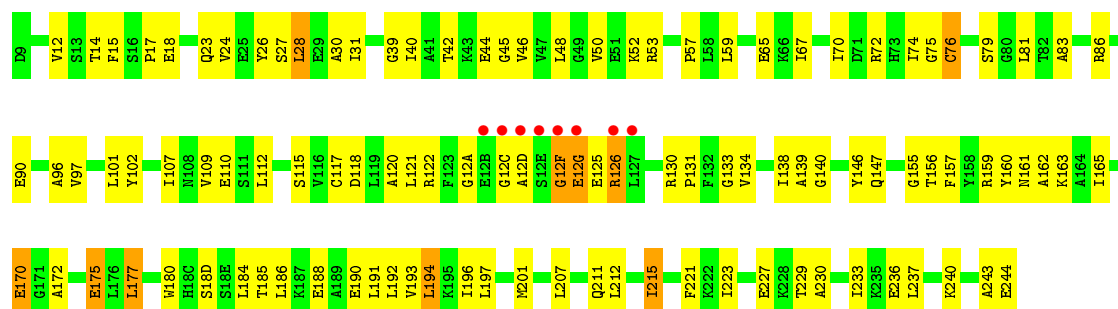


• Molecule 4: Proteasome component PUP2

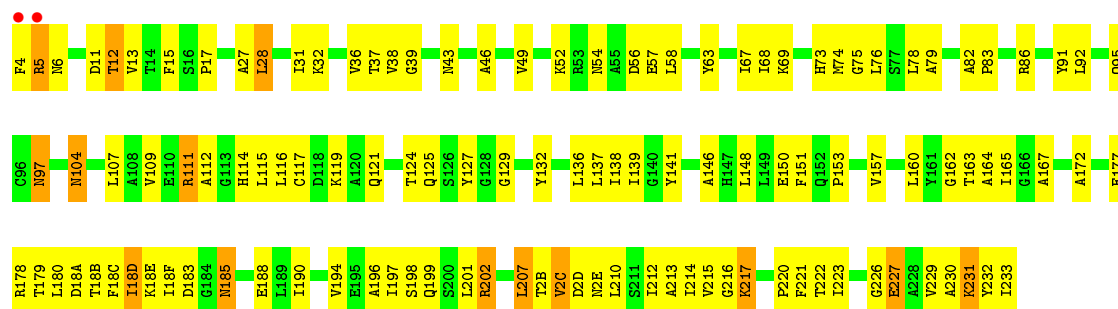




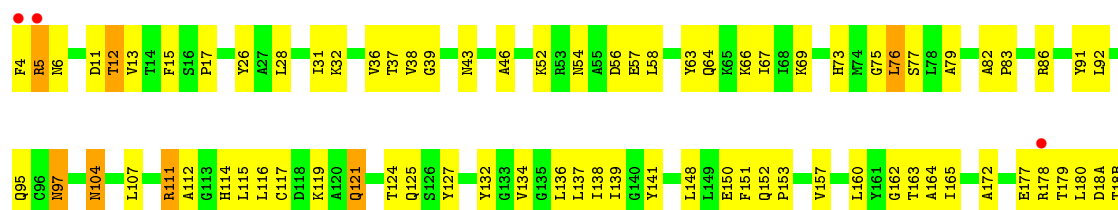
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

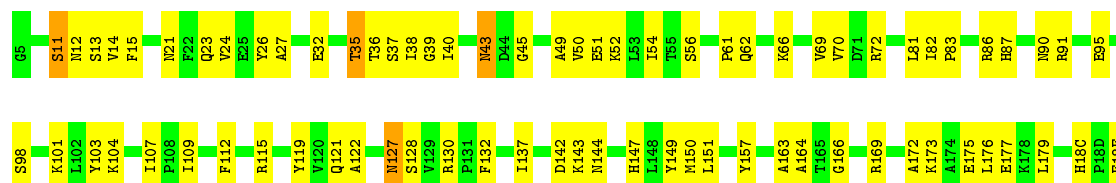


• Molecule 5: Proteasome component PRE5

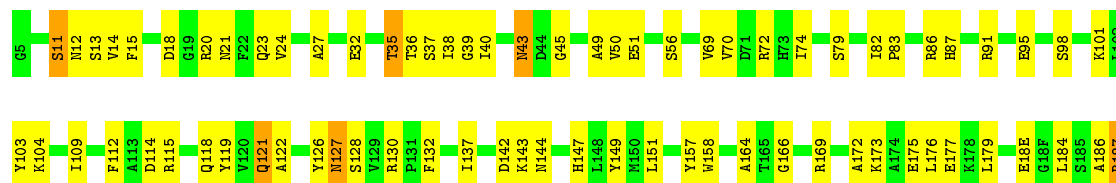




• Molecule 6: Proteasome component C1



• Molecule 6: Proteasome component C1

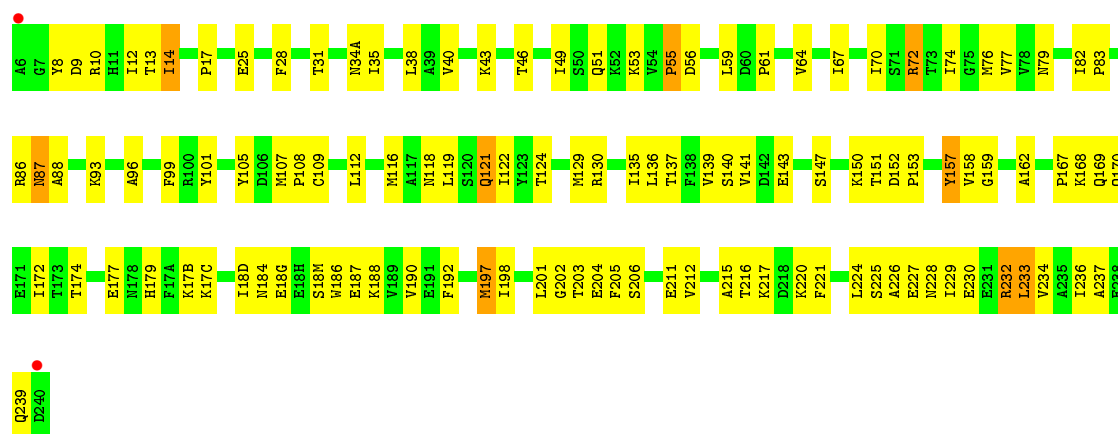


• Molecule 7: Proteasome component C7-alpha

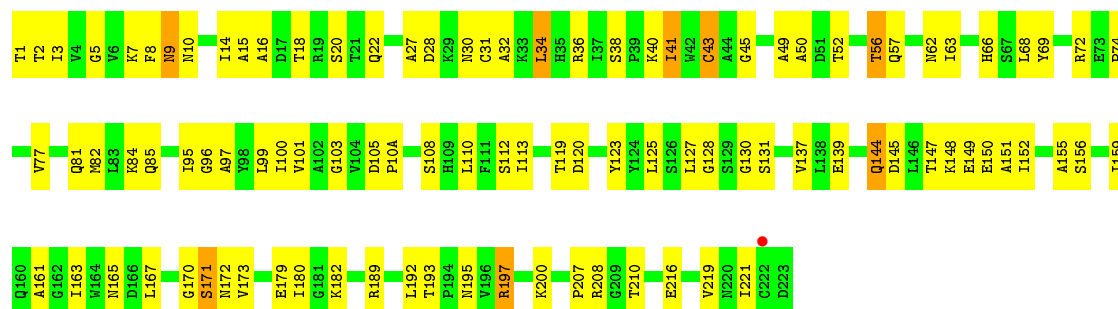


• Molecule 7: Proteasome component C7-alpha

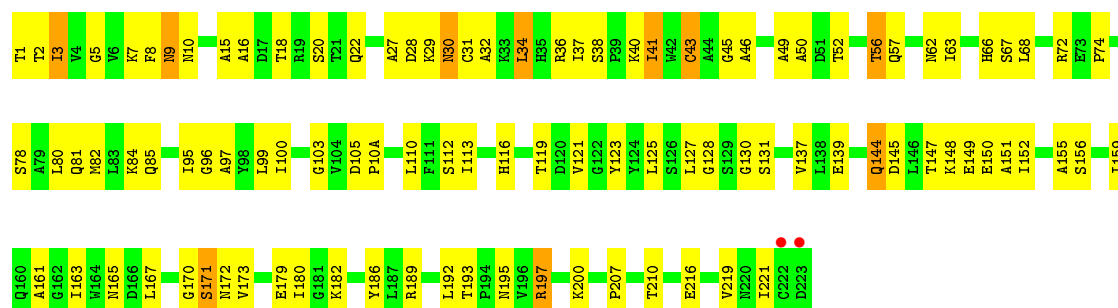




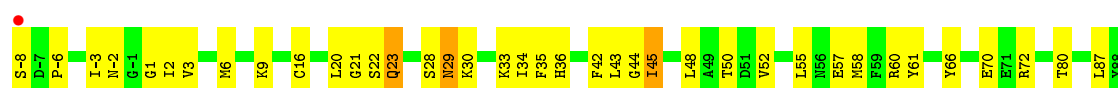
• Molecule 8: Proteasome component PUP1

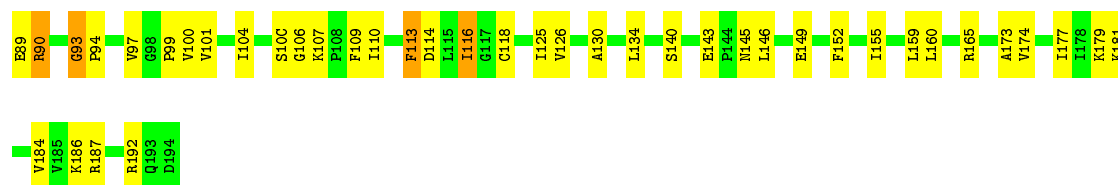


• Molecule 8: Proteasome component PUP1



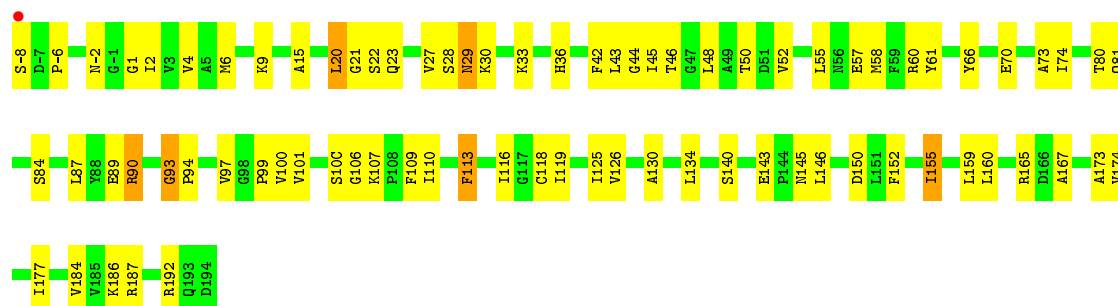
• Molecule 9: Proteasome component PUP3





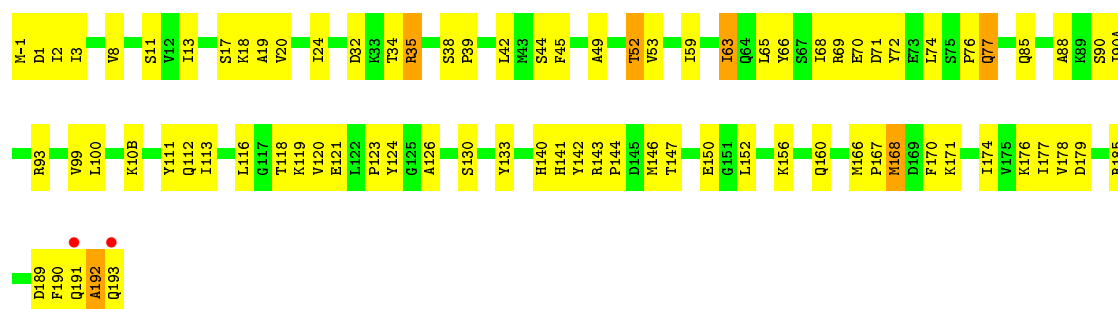
- Molecule 9: Proteasome component PUP3

Chain W: 61% 36%



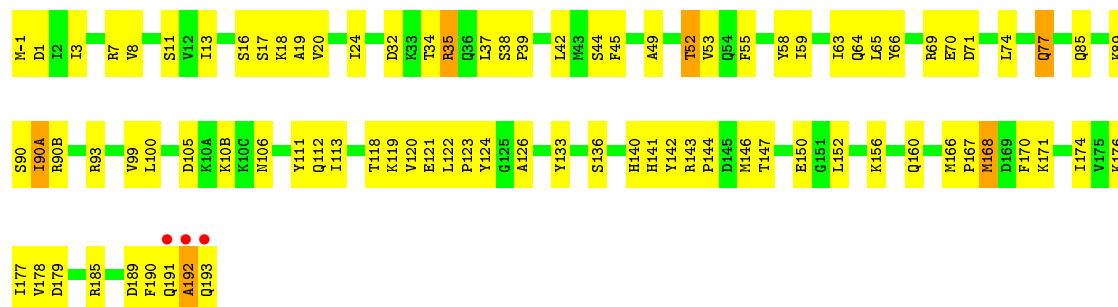
- Molecule 10: Proteasome component C11

Chain J: 58% 39%



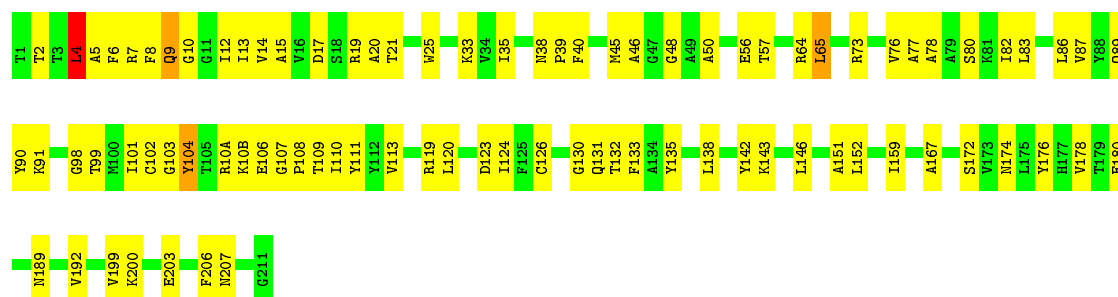
- Molecule 10: Proteasome component C11

Chain X: 56% 41%



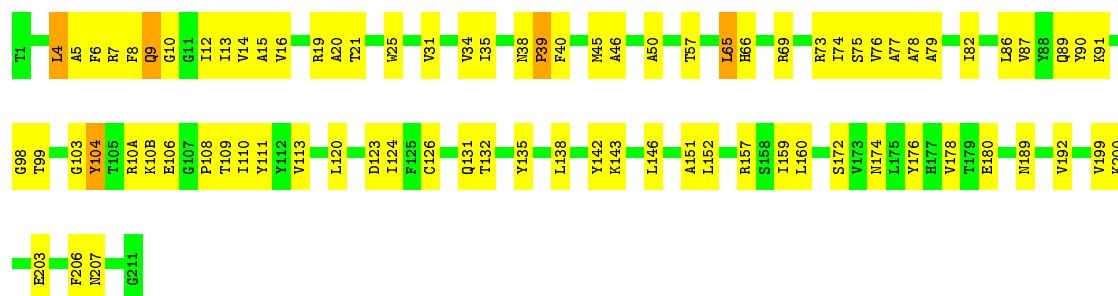
- Molecule 11: Proteasome component PRE2

Chain K: 



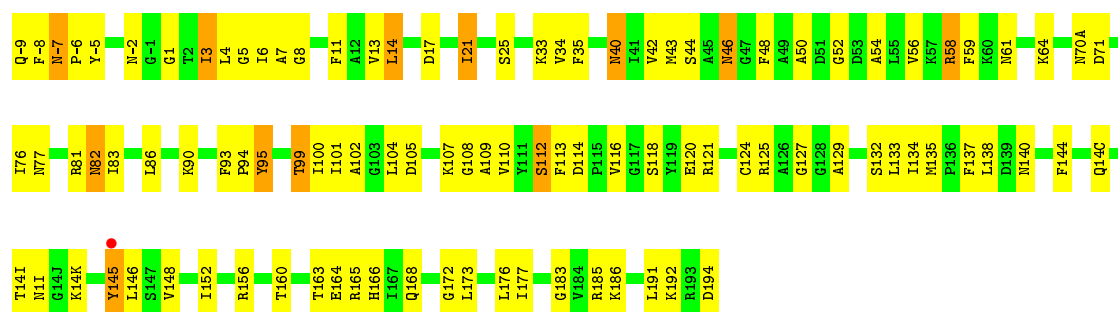
• Molecule 11: Proteasome component PRE2

Chain Y: 



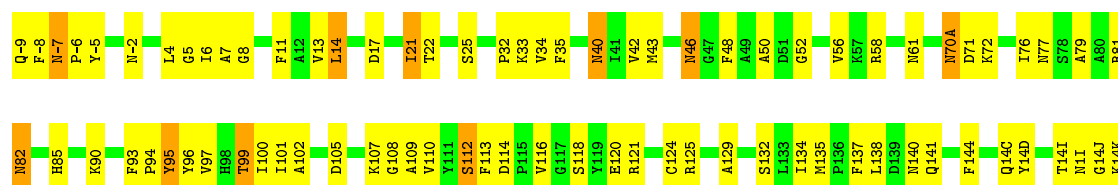
• Molecule 12: Proteasome component C5

Chain L: 



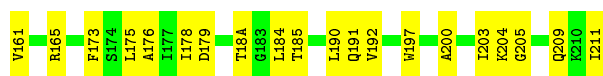
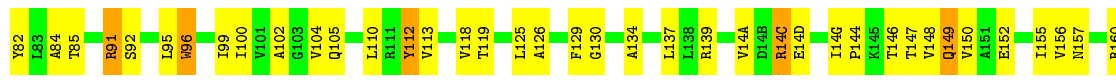
• Molecule 12: Proteasome component C5

Chain Z: 

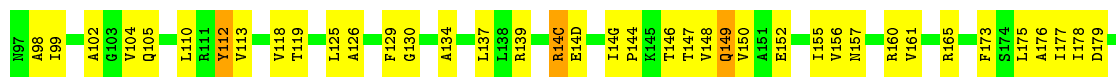
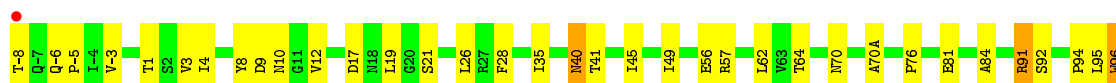




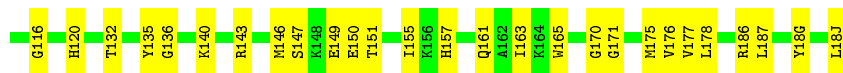
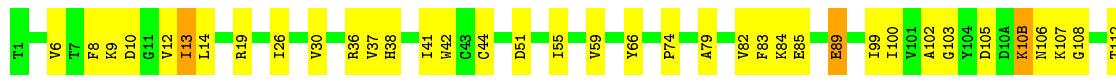
• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4

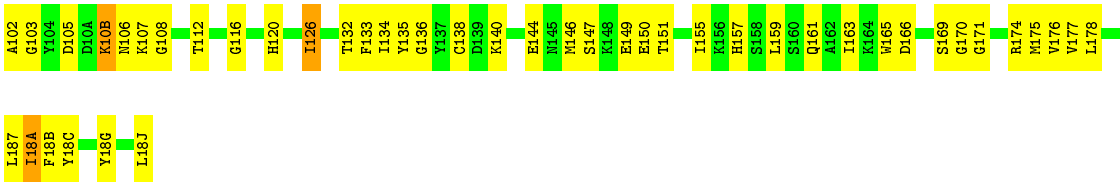


• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 134.12Å 300.56Å 144.06Å 90.00° 112.76° 90.00° | Depositor |
| Resolution (Å) | 49.77 – 2.80 49.77 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 92.3 (49.77-2.80) 92.3 (49.77-2.80) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.49 (at 2.81Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.238 , 0.266 0.222 , 0.247 | Depositor DCC |
| R_{free} test set | 11760 reflections (4.98%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 48.1 | Xtriage |
| Anisotropy | 0.853 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 59.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 50905 | wwPDB-VP |
| Average B, all atoms (Å ²) | 65.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H10, MES

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 | 0.37 | 0/1952 | 0.63 | 0/2642 |
| 1 | O | 0.38 | 0/1952 | 0.64 | 0/2642 |
| 2 | B | 0.37 | 0/1935 | 0.63 | 0/2618 |
| 2 | P | 0.38 | 0/1935 | 0.64 | 0/2618 |
| 3 | C | 0.36 | 0/1920 | 0.62 | 0/2598 |
| 3 | Q | 0.36 | 0/1920 | 0.62 | 0/2598 |
| 4 | D | 0.36 | 0/1887 | 0.64 | 0/2541 |
| 4 | R | 0.36 | 0/1887 | 0.64 | 0/2541 |
| 5 | E | 0.35 | 0/1823 | 0.60 | 0/2463 |
| 5 | S | 0.36 | 0/1823 | 0.61 | 0/2463 |
| 6 | F | 0.37 | 0/1937 | 0.61 | 0/2614 |
| 6 | T | 0.37 | 0/1937 | 0.62 | 0/2614 |
| 7 | G | 0.40 | 0/1959 | 0.63 | 0/2652 |
| 7 | U | 0.40 | 0/1959 | 0.63 | 0/2652 |
| 8 | H | 0.38 | 0/1716 | 0.66 | 0/2326 |
| 8 | V | 0.38 | 0/1716 | 0.66 | 0/2326 |
| 9 | I | 0.38 | 0/1611 | 0.67 | 0/2174 |
| 9 | W | 0.40 | 0/1611 | 0.68 | 0/2174 |
| 10 | J | 0.39 | 0/1613 | 0.66 | 0/2173 |
| 10 | X | 0.40 | 0/1613 | 0.66 | 0/2173 |
| 11 | K | 0.40 | 0/1681 | 0.66 | 1/2274 (0.0%) |
| 11 | Y | 0.40 | 0/1681 | 0.65 | 0/2274 |
| 12 | L | 0.39 | 0/1795 | 0.67 | 1/2420 (0.0%) |
| 12 | Z | 0.38 | 0/1795 | 0.67 | 1/2420 (0.0%) |
| 13 | 1 | 0.39 | 0/1855 | 0.67 | 2/2514 (0.1%) |
| 13 | M | 0.38 | 0/1855 | 0.66 | 1/2514 (0.0%) |
| 14 | 2 | 0.40 | 0/1541 | 0.65 | 0/2087 |
| 14 | N | 0.40 | 0/1541 | 0.66 | 0/2087 |
| All | All | 0.38 | 0/50450 | 0.64 | 6/68192 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 13 | M | 95 | LEU | N-CA-C | -5.85 | 95.22 | 111.00 |
| 13 | 1 | 95 | LEU | N-CA-C | -5.76 | 95.44 | 111.00 |
| 12 | L | 95 | TYR | N-CA-C | -5.49 | 96.17 | 111.00 |
| 12 | Z | 95 | TYR | N-CA-C | -5.22 | 96.90 | 111.00 |
| 11 | K | 4 | LEU | CA-CB-CG | 5.07 | 126.95 | 115.30 |
| 13 | 1 | 98 | ALA | N-CA-C | -5.04 | 97.40 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1915 | 0 | 1926 | 99 | 0 |
| 1 | O | 1915 | 0 | 1926 | 89 | 0 |
| 2 | B | 1905 | 0 | 1901 | 117 | 0 |
| 2 | P | 1905 | 0 | 1901 | 116 | 0 |
| 3 | C | 1891 | 0 | 1900 | 121 | 0 |
| 3 | Q | 1891 | 0 | 1900 | 128 | 0 |
| 4 | D | 1862 | 0 | 1836 | 89 | 0 |
| 4 | R | 1862 | 0 | 1836 | 93 | 0 |
| 5 | E | 1795 | 0 | 1797 | 127 | 0 |
| 5 | S | 1795 | 0 | 1797 | 119 | 0 |
| 6 | F | 1897 | 0 | 1886 | 113 | 0 |
| 6 | T | 1897 | 0 | 1886 | 103 | 0 |
| 7 | G | 1921 | 0 | 1910 | 109 | 0 |
| 7 | U | 1921 | 0 | 1910 | 116 | 0 |
| 8 | H | 1685 | 0 | 1688 | 94 | 0 |
| 8 | V | 1685 | 0 | 1688 | 103 | 0 |
| 9 | I | 1581 | 0 | 1574 | 86 | 0 |
| 9 | W | 1581 | 0 | 1574 | 80 | 0 |
| 10 | J | 1585 | 0 | 1590 | 91 | 0 |
| 10 | X | 1585 | 0 | 1590 | 98 | 0 |
| 11 | K | 1644 | 0 | 1595 | 85 | 0 |
| 11 | Y | 1644 | 0 | 1595 | 92 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | L | 1757 | 0 | 1711 | 105 | 0 |
| 12 | Z | 1757 | 0 | 1711 | 102 | 0 |
| 13 | 1 | 1824 | 0 | 1832 | 81 | 0 |
| 13 | M | 1824 | 0 | 1832 | 87 | 0 |
| 14 | 2 | 1512 | 0 | 1481 | 80 | 0 |
| 14 | N | 1512 | 0 | 1481 | 61 | 0 |
| 15 | K | 12 | 0 | 13 | 0 | 0 |
| 15 | Y | 12 | 0 | 13 | 0 | 0 |
| 16 | K | 26 | 0 | 26 | 4 | 0 |
| 16 | Y | 26 | 0 | 26 | 7 | 0 |
| 17 | 1 | 69 | 0 | 0 | 9 | 0 |
| 17 | 2 | 61 | 0 | 0 | 5 | 0 |
| 17 | A | 49 | 0 | 0 | 3 | 0 |
| 17 | B | 36 | 0 | 0 | 3 | 0 |
| 17 | C | 37 | 0 | 0 | 6 | 0 |
| 17 | D | 36 | 0 | 0 | 4 | 0 |
| 17 | E | 23 | 0 | 0 | 5 | 0 |
| 17 | F | 47 | 0 | 0 | 4 | 0 |
| 17 | G | 58 | 0 | 0 | 5 | 0 |
| 17 | H | 46 | 0 | 0 | 2 | 0 |
| 17 | I | 65 | 0 | 0 | 3 | 0 |
| 17 | J | 48 | 0 | 0 | 4 | 0 |
| 17 | K | 49 | 0 | 0 | 4 | 0 |
| 17 | L | 58 | 0 | 0 | 5 | 0 |
| 17 | M | 66 | 0 | 0 | 5 | 0 |
| 17 | N | 56 | 0 | 0 | 4 | 0 |
| 17 | O | 30 | 0 | 0 | 2 | 0 |
| 17 | P | 29 | 0 | 0 | 4 | 0 |
| 17 | Q | 24 | 0 | 0 | 5 | 0 |
| 17 | R | 30 | 0 | 0 | 4 | 0 |
| 17 | S | 19 | 0 | 0 | 1 | 0 |
| 17 | T | 38 | 0 | 0 | 4 | 0 |
| 17 | U | 60 | 0 | 0 | 7 | 0 |
| 17 | V | 42 | 0 | 0 | 4 | 0 |
| 17 | W | 57 | 0 | 0 | 6 | 0 |
| 17 | X | 48 | 0 | 0 | 8 | 0 |
| 17 | Y | 50 | 0 | 0 | 3 | 0 |
| 17 | Z | 50 | 0 | 0 | 11 | 0 |
| All | All | 50905 | 0 | 49332 | 2529 | 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 26.

All (2529) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:H:15:ALA:HB3 | 8:H:159:ILE:HD11 | 1.25 | 1.17 |
| 2:P:74:ILE:HD11 | 2:P:109:VAL:HG22 | 1.12 | 1.10 |
| 7:U:9:ASP:HA | 7:U:14:ILE:HD11 | 1.25 | 1.10 |
| 2:B:202:THR:HG22 | 2:B:204:SER:H | 1.13 | 1.09 |
| 8:H:50:ALA:HB2 | 9:I:116:ILE:HD13 | 1.33 | 1.09 |
| 8:V:15:ALA:HB3 | 8:V:159:ILE:HD11 | 1.24 | 1.09 |
| 6:T:49:ALA:HB1 | 6:T:197:ILE:HD11 | 1.33 | 1.08 |
| 11:Y:10(B):LYS:H | 11:Y:10(B):LYS:HD2 | 1.20 | 1.06 |
| 2:P:74:ILE:HD13 | 2:P:140:GLY:HA3 | 1.30 | 1.06 |
| 8:H:15:ALA:CB | 8:H:159:ILE:HD11 | 1.86 | 1.06 |
| 4:R:74:ILE:HD11 | 4:R:109:VAL:HG22 | 1.11 | 1.06 |
| 7:G:96:ALA:HA | 7:G:107:MET:HE2 | 1.37 | 1.06 |
| 6:T:49:ALA:CB | 6:T:197:ILE:HD11 | 1.86 | 1.05 |
| 8:V:15:ALA:CB | 8:V:159:ILE:HD11 | 1.84 | 1.05 |
| 2:P:202:THR:HG22 | 2:P:204:SER:H | 1.11 | 1.05 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:HD2 | 1.21 | 1.02 |
| 5:S:38:VAL:HG23 | 5:S:197:ILE:HD13 | 1.38 | 1.02 |
| 7:U:96:ALA:HA | 7:U:107:MET:HE2 | 1.41 | 1.02 |
| 2:B:107:ILE:HD13 | 2:B:108:PRO:O | 1.60 | 1.02 |
| 5:E:49:VAL:HG13 | 5:E:212:ILE:CD1 | 1.89 | 1.01 |
| 7:U:12:ILE:HG13 | 7:U:14:ILE:HD12 | 1.39 | 1.01 |
| 11:Y:7:ARG:HG3 | 11:Y:12:ILE:CD1 | 1.92 | 1.00 |
| 1:A:21:LEU:HB3 | 1:A:24:ILE:HD13 | 1.42 | 0.99 |
| 3:Q:201:VAL:CG2 | 3:Q:210:ILE:HD11 | 1.93 | 0.98 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:CD2 | 1.93 | 0.98 |
| 13:1:40:ASN:HD22 | 13:1:40:ASN:H | 1.10 | 0.98 |
| 5:E:49:VAL:HG13 | 5:E:212:ILE:HD11 | 1.41 | 0.98 |
| 3:Q:201:VAL:HG21 | 3:Q:210:ILE:HD11 | 0.98 | 0.98 |
| 9:I:177:ILE:HD12 | 9:I:187:ARG:HH12 | 1.23 | 0.97 |
| 3:C:70:ILE:HD13 | 3:C:112:LEU:HD11 | 1.45 | 0.96 |
| 8:H:50:ALA:CB | 9:I:116:ILE:HD13 | 1.94 | 0.96 |
| 3:Q:197:LEU:HD13 | 3:Q:210:ILE:HD12 | 1.48 | 0.95 |
| 10:X:37:LEU:HB3 | 10:X:63:ILE:HD13 | 1.49 | 0.95 |
| 11:Y:6:PHE:HB2 | 11:Y:124:ILE:HD13 | 1.49 | 0.95 |
| 4:D:97:VAL:HG21 | 11:K:65:LEU:HD13 | 1.46 | 0.94 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:HH11 | 0.99 | 0.94 |
| 3:Q:201:VAL:HG21 | 3:Q:210:ILE:CD1 | 1.94 | 0.94 |
| 4:R:74:ILE:CD1 | 4:R:109:VAL:HG22 | 1.97 | 0.93 |
| 3:Q:70:ILE:HD13 | 3:Q:112:LEU:HD11 | 1.49 | 0.93 |
| 12:L:3:ILE:HD13 | 12:L:127:GLY:O | 1.67 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:B:107:ILE:HD12 | 2:B:112:LEU:HB2 | 1.47 | 0.93 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:HH11 | 1.04 | 0.92 |
| 8:H:128:GLY:O | 8:H:131:SER:HB2 | 1.70 | 0.92 |
| 6:T:197:ILE:HD13 | 6:T:210:LEU:HD11 | 1.52 | 0.92 |
| 1:O:15:PHE:H | 2:P:23:GLN:HE22 | 1.09 | 0.92 |
| 2:B:15:PHE:H | 3:C:23:GLN:HE22 | 1.13 | 0.91 |
| 13:M:40:ASN:H | 13:M:40:ASN:HD22 | 1.09 | 0.91 |
| 4:R:74:ILE:HD13 | 4:R:140:GLY:HA3 | 1.51 | 0.91 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:HG22 | 1.35 | 0.91 |
| 1:O:130:ARG:HH21 | 7:U:124:THR:HG22 | 1.35 | 0.91 |
| 1:O:124:THR:HG22 | 2:P:130:ARG:HH21 | 1.34 | 0.91 |
| 4:R:97:VAL:HG21 | 11:Y:65:LEU:HD13 | 1.50 | 0.91 |
| 12:L:3:ILE:HD12 | 12:L:46:ASN:HB2 | 1.53 | 0.90 |
| 14:2:17:ASP:HB3 | 14:2:163:ILE:HD11 | 1.54 | 0.90 |
| 14:2:18(A):ILE:HD13 | 14:2:18(B):PHE:N | 1.86 | 0.90 |
| 8:V:128:GLY:O | 8:V:131:SER:HB2 | 1.71 | 0.90 |
| 3:Q:15:PHE:H | 4:R:23:GLN:HE22 | 1.15 | 0.89 |
| 2:P:61:GLN:OE1 | 2:P:208:ASP:HA | 1.74 | 0.88 |
| 8:V:221:ILE:HD11 | 9:W:184:VAL:HB | 1.56 | 0.88 |
| 3:Q:154:SER:OG | 3:Q:156:ILE:HD13 | 1.74 | 0.87 |
| 5:E:221:PHE:CE1 | 5:E:223:ILE:HD11 | 2.10 | 0.87 |
| 13:1:157:ASN:ND2 | 13:1:160:ARG:HH11 | 1.71 | 0.87 |
| 3:C:15:PHE:H | 4:D:23:GLN:HE22 | 1.15 | 0.87 |
| 7:U:70:ILE:HD11 | 7:U:76:MET:HB2 | 1.56 | 0.87 |
| 12:L:83:ILE:HD13 | 12:L:86:LEU:HD12 | 1.57 | 0.86 |
| 1:A:124:THR:HG22 | 2:B:130:ARG:HH21 | 1.40 | 0.86 |
| 9:I:44:GLY:C | 9:I:45:ILE:HD12 | 1.95 | 0.86 |
| 3:Q:163:GLN:HA | 3:Q:163:GLN:HE21 | 1.39 | 0.86 |
| 4:D:28:LEU:HA | 4:D:31:ILE:HD12 | 1.56 | 0.86 |
| 1:A:15:PHE:H | 2:B:23:GLN:HE22 | 1.20 | 0.86 |
| 9:I:152:PHE:HB2 | 9:I:177:ILE:HD11 | 1.58 | 0.85 |
| 11:K:7:ARG:HG2 | 11:K:108:PRO:HB2 | 1.58 | 0.85 |
| 5:S:221:PHE:CE1 | 5:S:223:ILE:HD11 | 2.09 | 0.85 |
| 1:A:179:ARG:HB3 | 1:A:179:ARG:HH11 | 1.40 | 0.85 |
| 3:C:163:GLN:HA | 3:C:163:GLN:HE21 | 1.40 | 0.85 |
| 5:E:28:LEU:HA | 5:E:31:ILE:HD13 | 1.58 | 0.85 |
| 10:J:2:ILE:HD13 | 10:J:130:SER:OG | 1.76 | 0.85 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:ND2 | 1.92 | 0.85 |
| 2:P:194:LEU:HD11 | 2:P:232:ILE:HD13 | 1.59 | 0.85 |
| 11:Y:7:ARG:HG2 | 11:Y:108:PRO:HB2 | 1.57 | 0.85 |
| 6:F:38:ILE:HD12 | 6:F:40:ILE:HD11 | 1.59 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:74:ILE:CD1 | 2:P:109:VAL:HG22 | 2.02 | 0.85 |
| 3:Q:164:THR:HG21 | 3:Q:172:VAL:HG13 | 1.58 | 0.85 |
| 2:P:124:THR:HG22 | 3:Q:130:ARG:HH21 | 1.41 | 0.84 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:HH21 | 1.42 | 0.84 |
| 4:R:28:LEU:HA | 4:R:31:ILE:HD12 | 1.58 | 0.84 |
| 13:M:157:ASN:ND2 | 13:M:160:ARG:HH11 | 1.75 | 0.84 |
| 3:C:164:THR:HG21 | 3:C:172:VAL:HG13 | 1.58 | 0.84 |
| 6:T:49:ALA:HB1 | 6:T:197:ILE:CD1 | 2.07 | 0.84 |
| 10:X:55:PHE:O | 10:X:59:ILE:HD13 | 1.77 | 0.84 |
| 2:B:61:GLN:OE1 | 2:B:208:ASP:HA | 1.77 | 0.84 |
| 8:H:50:ALA:HB2 | 9:I:116:ILE:CD1 | 2.08 | 0.84 |
| 2:B:158:THR:HG22 | 3:C:63:THR:HG23 | 1.59 | 0.83 |
| 7:U:9:ASP:CA | 7:U:14:ILE:HD11 | 2.07 | 0.83 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:HD21 | 1.59 | 0.83 |
| 1:O:179:ARG:HH11 | 1:O:179:ARG:HB3 | 1.42 | 0.83 |
| 3:Q:156:ILE:HD12 | 4:R:83:ALA:HB2 | 1.61 | 0.83 |
| 8:H:221:ILE:HD11 | 9:I:184:VAL:HB | 1.59 | 0.83 |
| 2:B:194:LEU:HD11 | 2:B:232:ILE:HD13 | 1.59 | 0.83 |
| 5:E:207:LEU:HA | 5:E:2(E):ASN:ND2 | 1.92 | 0.83 |
| 11:Y:7:ARG:HG3 | 11:Y:12:ILE:HD11 | 1.58 | 0.83 |
| 2:P:202:THR:HG22 | 2:P:204:SER:N | 1.94 | 0.82 |
| 14:2:163:ILE:HD13 | 14:2:169:SER:HB3 | 1.62 | 0.82 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:NH1 | 1.76 | 0.82 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:NE2 | 1.93 | 0.82 |
| 12:Z:134:ILE:HD12 | 12:Z:158:SER:HB3 | 1.61 | 0.82 |
| 5:E:213:ALA:HB2 | 5:E:223:ILE:HD12 | 1.60 | 0.82 |
| 5:S:15:PHE:H | 6:T:23:GLN:HE22 | 1.26 | 0.82 |
| 9:W:4:VAL:HG13 | 9:W:155:ILE:HD11 | 1.62 | 0.81 |
| 5:E:75:GLY:HA3 | 5:E:221:PHE:CE2 | 2.16 | 0.81 |
| 3:C:163:GLN:NE2 | 3:C:164:THR:H | 1.79 | 0.81 |
| 1:O:130:ARG:HH21 | 7:U:124:THR:CG2 | 1.93 | 0.81 |
| 11:K:102:CYS:SG | 11:K:110:ILE:HD12 | 2.20 | 0.81 |
| 4:R:74:ILE:HD11 | 4:R:109:VAL:CG2 | 2.04 | 0.81 |
| 5:S:75:GLY:HA3 | 5:S:221:PHE:CE2 | 2.16 | 0.81 |
| 12:Z:7:ALA:HB2 | 12:Z:110:VAL:HG23 | 1.61 | 0.81 |
| 5:E:15:PHE:H | 6:F:23:GLN:HE22 | 1.27 | 0.81 |
| 5:S:2(B):THR:H | 5:S:2(E):ASN:HD22 | 1.25 | 0.80 |
| 5:E:97:ASN:HD21 | 12:L:61:ASN:HD21 | 1.29 | 0.80 |
| 5:S:97:ASN:HD21 | 12:Z:61:ASN:HD21 | 1.25 | 0.80 |
| 5:S:213:ALA:HB2 | 5:S:223:ILE:HD12 | 1.62 | 0.80 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:NH1 | 1.80 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 9:W:45:ILE:HB | 9:W:52:VAL:HG13 | 1.62 | 0.80 |
| 13:1:40:ASN:N | 13:1:40:ASN:HD22 | 1.74 | 0.80 |
| 2:P:107:ILE:HD11 | 2:P:111:ILE:HG22 | 1.62 | 0.80 |
| 12:L:7:ALA:HB2 | 12:L:110:VAL:HG23 | 1.64 | 0.79 |
| 12:L:21:ILE:HD12 | 8:V:167:LEU:CD1 | 2.12 | 0.79 |
| 12:L:3:ILE:HD12 | 12:L:46:ASN:CB | 2.11 | 0.79 |
| 1:A:13:THR:HG21 | 1:A:24:ILE:HD11 | 1.63 | 0.79 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:HG3 | 1.63 | 0.79 |
| 2:P:126:HIS:HB3 | 3:Q:129:VAL:HG12 | 1.65 | 0.79 |
| 7:G:121:GLN:O | 7:G:124:THR:HB | 1.83 | 0.79 |
| 3:Q:159:SER:HB2 | 17:Q:1140:HOH:O | 1.83 | 0.79 |
| 14:N:13:ILE:HD13 | 14:N:177:VAL:HG13 | 1.63 | 0.79 |
| 5:E:2(B):THR:H | 5:E:2(E):ASN:HD22 | 1.26 | 0.78 |
| 7:U:67:ILE:HD12 | 7:U:211:GLU:HG2 | 1.64 | 0.78 |
| 6:F:175:GLU:HB3 | 6:F:196:ILE:HD12 | 1.64 | 0.78 |
| 12:L:100:ILE:HG13 | 12:L:112:SER:HB3 | 1.62 | 0.78 |
| 3:Q:55:THR:HG22 | 3:Q:56:LEU:HD22 | 1.65 | 0.78 |
| 7:U:121:GLN:O | 7:U:124:THR:HB | 1.83 | 0.78 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:CD | 1.97 | 0.78 |
| 6:T:175:GLU:HB3 | 6:T:196:ILE:HD12 | 1.63 | 0.78 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:HG3 | 1.65 | 0.78 |
| 3:Q:163:GLN:NE2 | 3:Q:164:THR:H | 1.82 | 0.78 |
| 7:G:198:ILE:HG23 | 7:G:203:THR:O | 1.84 | 0.78 |
| 14:N:161:GLN:NE2 | 14:2:136:GLY:HA2 | 1.98 | 0.78 |
| 1:O:47:VAL:HG21 | 1:O:190:ILE:HD13 | 1.66 | 0.78 |
| 1:A:20:LYS:HE3 | 1:A:25:ASP:OD1 | 1.84 | 0.77 |
| 7:G:67:ILE:HD12 | 7:G:211:GLU:HG2 | 1.64 | 0.77 |
| 11:K:12:ILE:HG21 | 11:K:110:ILE:HD11 | 1.64 | 0.77 |
| 5:S:201:LEU:HD11 | 5:S:207:LEU:HD22 | 1.67 | 0.77 |
| 13:M:40:ASN:HD22 | 13:M:40:ASN:N | 1.75 | 0.77 |
| 7:U:217:LYS:HE3 | 7:U:217:LYS:HA | 1.65 | 0.77 |
| 5:S:190:ILE:HD11 | 5:S:214:ILE:HD12 | 1.67 | 0.77 |
| 8:V:10:ASN:OD1 | 8:V:180:ILE:HD12 | 1.85 | 0.77 |
| 9:W:152:PHE:HD1 | 9:W:177:ILE:HD11 | 1.49 | 0.77 |
| 10:J:90(A):ILE:HD11 | 10:J:116:LEU:HD22 | 1.65 | 0.77 |
| 12:L:59:PHE:CD1 | 12:L:83:ILE:HD11 | 2.19 | 0.77 |
| 5:E:12:THR:HG21 | 5:E:124:THR:HA | 1.66 | 0.77 |
| 14:2:144:GLU:HG2 | 17:2:1115:HOH:O | 1.84 | 0.77 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:CG2 | 1.97 | 0.77 |
| 9:I:45:ILE:HB | 9:I:52:VAL:HG13 | 1.66 | 0.77 |
| 2:B:124:THR:CG2 | 3:C:130:ARG:HH21 | 1.98 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:G:217:LYS:HA | 7:G:217:LYS:HE3 | 1.66 | 0.76 |
| 1:A:179:ARG:HB3 | 1:A:179:ARG:NH1 | 2.00 | 0.76 |
| 6:T:95:GLU:HG2 | 6:T:115:ARG:HB3 | 1.68 | 0.76 |
| 6:T:40:ILE:HD12 | 6:T:193:ALA:HB2 | 1.66 | 0.76 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:HE21 | 1.49 | 0.76 |
| 14:2:13:ILE:HD13 | 14:2:177:VAL:HG13 | 1.67 | 0.76 |
| 3:C:55:THR:HG22 | 3:C:56:LEU:HD22 | 1.66 | 0.76 |
| 2:P:158:THR:HG22 | 3:Q:63:THR:HG23 | 1.66 | 0.76 |
| 5:E:201:LEU:HD11 | 5:E:207:LEU:HD22 | 1.67 | 0.76 |
| 1:O:179:ARG:NH1 | 1:O:179:ARG:HB3 | 2.01 | 0.76 |
| 6:T:237:GLN:O | 6:T:240:ILE:HG22 | 1.86 | 0.76 |
| 3:Q:216:LYS:HB2 | 3:Q:220:ASP:HB3 | 1.69 | 0.75 |
| 4:R:76:CYS:HB2 | 4:R:138:ILE:HD13 | 1.67 | 0.75 |
| 8:V:52:THR:O | 8:V:56:THR:HB | 1.86 | 0.75 |
| 9:W:27:VAL:HG13 | 17:X:622:HOH:O | 1.86 | 0.75 |
| 1:O:20:LYS:HE3 | 1:O:25:ASP:OD1 | 1.86 | 0.75 |
| 3:C:216:LYS:HB2 | 3:C:220:ASP:HB3 | 1.68 | 0.75 |
| 7:U:198:ILE:HG23 | 7:U:203:THR:O | 1.86 | 0.75 |
| 2:B:126:HIS:HB3 | 3:C:129:VAL:HG12 | 1.69 | 0.75 |
| 10:X:156:LYS:O | 10:X:160:GLN:HG3 | 1.85 | 0.75 |
| 14:2:112:THR:HG22 | 14:2:120:HIS:HB2 | 1.69 | 0.75 |
| 11:K:10(B):LYS:N | 11:K:10(B):LYS:HD2 | 2.00 | 0.75 |
| 8:V:80:LEU:HD12 | 8:V:113:ILE:HD11 | 1.68 | 0.74 |
| 1:O:225:THR:OG1 | 1:O:228:GLU:HG3 | 1.87 | 0.74 |
| 8:V:15:ALA:CB | 8:V:159:ILE:CD1 | 2.65 | 0.74 |
| 1:A:100:TYR:N | 1:A:10(A):ILE:HD13 | 2.02 | 0.74 |
| 10:J:152:LEU:HD13 | 10:J:193:GLN:HE22 | 1.53 | 0.74 |
| 11:Y:10(B):LYS:CD | 11:Y:10(B):LYS:H | 1.97 | 0.74 |
| 10:J:156:LYS:O | 10:J:160:GLN:HG3 | 1.88 | 0.74 |
| 3:Q:65:SER:HB2 | 17:Q:303:HOH:O | 1.87 | 0.74 |
| 2:B:107:ILE:CD1 | 2:B:108:PRO:O | 2.33 | 0.74 |
| 1:O:124:THR:CG2 | 2:P:130:ARG:HH21 | 2.00 | 0.74 |
| 5:S:12:THR:HG21 | 5:S:124:THR:HA | 1.68 | 0.74 |
| 13:1:14(C):ARG:HG3 | 13:1:14(C):ARG:HH11 | 1.52 | 0.74 |
| 8:H:15:ALA:CB | 8:H:159:ILE:CD1 | 2.65 | 0.74 |
| 12:L:166:HIS:HD2 | 12:L:168:GLN:H | 1.35 | 0.74 |
| 5:S:38:VAL:HG23 | 5:S:197:ILE:CD1 | 2.15 | 0.74 |
| 11:Y:10(B):LYS:N | 11:Y:10(B):LYS:HD2 | 2.01 | 0.74 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:H | 1.53 | 0.73 |
| 2:B:202:THR:HG22 | 2:B:204:SER:N | 1.96 | 0.73 |
| 6:F:95:GLU:HG2 | 6:F:115:ARG:HB3 | 1.70 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:I:45:ILE:N | 9:I:45:ILE:HD12 | 2.03 | 0.73 |
| 10:X:152:LEU:HD13 | 10:X:193:GLN:HE22 | 1.52 | 0.73 |
| 14:N:161:GLN:HE21 | 14:2:136:GLY:HA2 | 1.53 | 0.73 |
| 5:S:97:ASN:ND2 | 12:Z:61:ASN:HD21 | 1.87 | 0.73 |
| 1:A:124:THR:CG2 | 2:B:130:ARG:HH21 | 2.01 | 0.73 |
| 6:F:109:ILE:HG21 | 6:F:147:HIS:HB2 | 1.69 | 0.73 |
| 9:I:114:ASP:OD2 | 9:I:116:ILE:HD12 | 1.88 | 0.73 |
| 3:Q:41:LYS:HG2 | 3:Q:161:SER:O | 1.89 | 0.73 |
| 5:S:18(C):PHE:HA | 5:S:18(F):ILE:HG12 | 1.71 | 0.73 |
| 9:W:119:ILE:H | 9:W:119:ILE:HD12 | 1.53 | 0.73 |
| 11:Y:7:ARG:HG3 | 11:Y:12:ILE:HD13 | 1.70 | 0.73 |
| 4:R:72:ARG:HG3 | 17:R:1302:HOH:O | 1.88 | 0.72 |
| 7:U:70:ILE:HD11 | 7:U:76:MET:CB | 2.19 | 0.72 |
| 11:K:80:SER:HA | 11:K:101:ILE:HD13 | 1.71 | 0.72 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:HD22 | 1.68 | 0.72 |
| 14:2:126:ILE:H | 14:2:126:ILE:HD13 | 1.53 | 0.72 |
| 12:Z:166:HIS:HD2 | 12:Z:168:GLN:H | 1.36 | 0.72 |
| 3:C:163:GLN:CA | 3:C:163:GLN:HE21 | 2.02 | 0.72 |
| 6:T:109:ILE:HG21 | 6:T:147:HIS:HB2 | 1.69 | 0.72 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:N | 2.04 | 0.72 |
| 14:N:112:THR:HG22 | 14:N:120:HIS:HB2 | 1.72 | 0.72 |
| 6:T:36:THR:HG22 | 6:T:51:GLU:OE2 | 1.89 | 0.72 |
| 5:E:49:VAL:HA | 5:E:212:ILE:HD13 | 1.72 | 0.72 |
| 1:O:47:VAL:CG2 | 1:O:190:ILE:HD13 | 2.20 | 0.72 |
| 5:S:36:VAL:HG13 | 5:S:197:ILE:HD11 | 1.70 | 0.72 |
| 14:N:30:VAL:HG21 | 13:1:203:ILE:HD13 | 1.72 | 0.71 |
| 3:C:185:THR:HG22 | 3:C:187:GLU:H | 1.55 | 0.71 |
| 3:Q:163:GLN:HE21 | 3:Q:163:GLN:CA | 2.02 | 0.71 |
| 5:S:67:ILE:HG21 | 5:S:223:ILE:HD12 | 1.72 | 0.71 |
| 1:A:225:THR:OG1 | 1:A:228:GLU:HG3 | 1.91 | 0.71 |
| 7:G:170:GLN:HE21 | 7:G:174:THR:HG23 | 1.55 | 0.71 |
| 13:M:100:ILE:HD13 | 13:M:112:TYR:HB2 | 1.73 | 0.71 |
| 13:M:152:GLU:O | 13:M:156:VAL:HG23 | 1.90 | 0.71 |
| 2:P:74:ILE:CD1 | 2:P:140:GLY:HA3 | 2.15 | 0.71 |
| 7:U:170:GLN:HE21 | 7:U:174:THR:HG23 | 1.56 | 0.71 |
| 8:V:113:ILE:HG12 | 8:V:119:THR:HG22 | 1.71 | 0.71 |
| 8:V:3:ILE:HD11 | 8:V:127:LEU:HB2 | 1.71 | 0.71 |
| 6:F:237:GLN:O | 6:F:240:ILE:HG22 | 1.90 | 0.71 |
| 13:M:76:PRO:HD2 | 13:M:105:GLN:OE1 | 1.90 | 0.71 |
| 10:X:18:LYS:HD3 | 10:X:174:ILE:HG13 | 1.72 | 0.71 |
| 3:Q:100:ARG:NH1 | 3:Q:106:PRO:HB3 | 2.05 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:C:41:LYS:HG2 | 3:C:161:SER:O | 1.89 | 0.71 |
| 5:E:67:ILE:HG21 | 5:E:223:ILE:HD12 | 1.73 | 0.71 |
| 2:P:15:PHE:H | 3:Q:23:GLN:HE22 | 1.39 | 0.71 |
| 2:P:101:LYS:NZ | 10:X:85:GLN:NE2 | 2.39 | 0.71 |
| 5:S:104:ASN:HB2 | 13:1:81:GLU:HG2 | 1.72 | 0.71 |
| 13:M:8:TYR:CE2 | 13:M:148:VAL:HG22 | 2.26 | 0.71 |
| 4:R:121:LEU:N | 17:R:853:HOH:O | 2.23 | 0.71 |
| 10:X:90(A):ILE:O | 10:X:90(A):ILE:HD13 | 1.91 | 0.71 |
| 1:O:121:GLN:O | 1:O:124:THR:HB | 1.91 | 0.70 |
| 6:T:193:ALA:O | 6:T:197:ILE:HD12 | 1.90 | 0.70 |
| 4:R:76:CYS:CB | 4:R:138:ILE:HD13 | 2.20 | 0.70 |
| 9:W:155:ILE:HD13 | 9:W:155:ILE:O | 1.91 | 0.70 |
| 10:X:55:PHE:CE2 | 10:X:59:ILE:HD11 | 2.26 | 0.70 |
| 2:B:107:ILE:HD11 | 2:B:112:LEU:N | 2.07 | 0.70 |
| 5:E:68:ILE:HD11 | 5:E:78:LEU:HD23 | 1.74 | 0.70 |
| 8:H:52:THR:O | 8:H:56:THR:HB | 1.91 | 0.70 |
| 10:J:90(A):ILE:CD1 | 10:J:116:LEU:HD22 | 2.21 | 0.70 |
| 4:D:70:ILE:HD12 | 4:D:92:ALA:HB3 | 1.73 | 0.70 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:N | 2.06 | 0.70 |
| 12:Z:100:ILE:HG12 | 12:Z:112:SER:HB3 | 1.72 | 0.70 |
| 12:Z:-7:ASN:ND2 | 12:Z:-5:TYR:H | 1.89 | 0.70 |
| 14:2:134:ILE:HD13 | 14:2:138:CYS:SG | 2.31 | 0.70 |
| 9:I:45:ILE:N | 9:I:45:ILE:CD1 | 2.54 | 0.70 |
| 2:P:160:TRP:CE2 | 2:P:163:ILE:HD12 | 2.26 | 0.70 |
| 3:C:100:ARG:NH1 | 3:C:106:PRO:HB3 | 2.07 | 0.70 |
| 7:G:49:ILE:CD1 | 7:G:193:ALA:HB1 | 2.22 | 0.70 |
| 13:M:149:GLN:NE2 | 13:M:149:GLN:H | 1.90 | 0.70 |
| 2:B:160:TRP:CE2 | 2:B:163:ILE:HD12 | 2.27 | 0.70 |
| 8:H:3:ILE:HG13 | 8:H:100:ILE:HD12 | 1.73 | 0.70 |
| 10:J:59:ILE:O | 10:J:63:ILE:HD13 | 1.90 | 0.70 |
| 5:E:97:ASN:HD21 | 12:L:61:ASN:ND2 | 1.90 | 0.70 |
| 6:T:79:SER:HA | 17:T:1238:HOH:O | 1.92 | 0.70 |
| 9:I:177:ILE:CD1 | 9:I:187:ARG:HH12 | 2.01 | 0.70 |
| 9:W:6:MET:HE3 | 9:W:155:ILE:HG12 | 1.73 | 0.70 |
| 6:T:37:SER:HB3 | 6:T:50:VAL:HG23 | 1.72 | 0.69 |
| 7:U:14:ILE:H | 7:U:14:ILE:HD13 | 1.57 | 0.69 |
| 6:F:37:SER:HB3 | 6:F:50:VAL:HG23 | 1.73 | 0.69 |
| 13:1:76:PRO:HD2 | 13:1:105:GLN:OE1 | 1.91 | 0.69 |
| 10:J:24:ILE:HG13 | 10:X:133:TYR:OH | 1.92 | 0.69 |
| 2:P:121:GLN:O | 2:P:124:THR:HB | 1.91 | 0.69 |
| 6:T:175:GLU:CB | 6:T:196:ILE:HD12 | 2.22 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:1:8:TYR:CE2 | 13:1:148:VAL:HG22 | 2.27 | 0.69 |
| 13:M:203:ILE:HD13 | 14:2:30:VAL:HG21 | 1.73 | 0.69 |
| 5:S:97:ASN:HD21 | 12:Z:61:ASN:ND2 | 1.89 | 0.69 |
| 14:2:59:VAL:HG22 | 14:2:82:VAL:HG12 | 1.74 | 0.69 |
| 6:F:175:GLU:CB | 6:F:196:ILE:HD12 | 2.23 | 0.69 |
| 12:L:3:ILE:H | 12:L:3:ILE:HD13 | 1.55 | 0.69 |
| 10:X:37:LEU:HD13 | 10:X:63:ILE:CD1 | 2.22 | 0.69 |
| 5:E:221:PHE:CZ | 5:E:223:ILE:HD11 | 2.28 | 0.69 |
| 9:I:35:PHE:CE1 | 9:I:45:ILE:HD13 | 2.27 | 0.69 |
| 1:O:173:LYS:O | 1:O:177:GLU:HG3 | 1.91 | 0.69 |
| 6:F:36:THR:HG22 | 6:F:51:GLU:OE2 | 1.91 | 0.69 |
| 10:J:18:LYS:HD3 | 10:J:174:ILE:HG13 | 1.75 | 0.69 |
| 5:S:221:PHE:CZ | 5:S:223:ILE:HD11 | 2.28 | 0.69 |
| 1:A:173:LYS:O | 1:A:177:GLU:HG3 | 1.93 | 0.69 |
| 5:E:210:LEU:HD22 | 5:E:233:ILE:HD11 | 1.75 | 0.69 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:HB2 | 1.75 | 0.69 |
| 13:1:149:GLN:H | 13:1:149:GLN:NE2 | 1.91 | 0.69 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:HB2 | 1.75 | 0.69 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:H | 1.58 | 0.69 |
| 13:M:14(C):ARG:HH11 | 13:M:14(C):ARG:HG3 | 1.58 | 0.69 |
| 13:1:152:GLU:O | 13:1:156:VAL:HG23 | 1.92 | 0.68 |
| 2:B:121:GLN:O | 2:B:124:THR:HB | 1.93 | 0.68 |
| 14:N:36:ARG:HG3 | 14:N:42:TRP:CE2 | 2.28 | 0.68 |
| 2:P:137:ILE:HD11 | 2:P:165:VAL:HG22 | 1.74 | 0.68 |
| 3:Q:15:PHE:CD1 | 3:Q:21:ILE:HD11 | 2.28 | 0.68 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:HG13 | 1.75 | 0.68 |
| 5:S:220:PRO:O | 5:S:222:THR:HG23 | 1.94 | 0.68 |
| 14:2:36:ARG:HG3 | 14:2:42:TRP:CE2 | 2.29 | 0.68 |
| 6:F:54:ILE:HD11 | 6:F:209:GLU:HB2 | 1.76 | 0.68 |
| 3:C:185:THR:HB | 3:C:188:GLU:HG2 | 1.75 | 0.68 |
| 6:F:173:LYS:O | 6:F:177:GLU:HG3 | 1.94 | 0.68 |
| 9:I:6:MET:HE3 | 9:I:155:ILE:HG13 | 1.73 | 0.68 |
| 5:E:97:ASN:ND2 | 12:L:61:ASN:HD21 | 1.90 | 0.68 |
| 2:P:74:ILE:HD11 | 2:P:109:VAL:CG2 | 2.07 | 0.68 |
| 12:L:173:LEU:HB2 | 12:L:191:LEU:HD11 | 1.76 | 0.68 |
| 1:O:15:PHE:N | 2:P:23:GLN:HE22 | 1.89 | 0.68 |
| 6:F:49:ALA:HB2 | 6:F:212:ILE:HD12 | 1.74 | 0.68 |
| 8:H:172:ASN:HD22 | 8:H:193:THR:HA | 1.59 | 0.68 |
| 12:L:3:ILE:CD1 | 12:L:127:GLY:O | 2.42 | 0.68 |
| 8:V:41:ILE:HD12 | 8:V:103:GLY:HA3 | 1.75 | 0.68 |
| 14:N:186:ARG:HD3 | 17:N:933:HOH:O | 1.94 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:124:THR:CG2 | 3:Q:130:ARG:HH21 | 2.07 | 0.67 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:HB2 | 1.76 | 0.67 |
| 14:2:112:THR:CG2 | 14:2:120:HIS:HB2 | 2.23 | 0.67 |
| 17:C:247:HOH:O | 10:J:68:ILE:HD13 | 1.93 | 0.67 |
| 12:L:177:ILE:HD13 | 12:L:185:ARG:NH2 | 2.09 | 0.67 |
| 7:G:135:ILE:HD13 | 7:G:152:ASP:HA | 1.75 | 0.67 |
| 1:O:32:LYS:HE2 | 1:O:32:LYS:HA | 1.75 | 0.67 |
| 3:Q:172:VAL:HG23 | 3:Q:196:SER:HB2 | 1.77 | 0.67 |
| 1:A:121:GLN:O | 1:A:124:THR:HB | 1.94 | 0.67 |
| 6:F:184:LEU:HD11 | 6:F:188:GLU:HB3 | 1.76 | 0.67 |
| 9:W:152:PHE:CD1 | 9:W:177:ILE:HD11 | 2.30 | 0.67 |
| 8:V:34:LEU:HB2 | 17:V:578:HOH:O | 1.95 | 0.67 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:H | 1.59 | 0.67 |
| 1:A:32:LYS:HE2 | 1:A:32:LYS:HA | 1.76 | 0.67 |
| 7:G:87:ASN:HD22 | 7:G:87:ASN:C | 1.98 | 0.67 |
| 7:G:8:TYR:O | 7:G:12:ILE:HD13 | 1.94 | 0.67 |
| 8:H:34:LEU:HB2 | 17:H:540:HOH:O | 1.95 | 0.67 |
| 3:Q:185:THR:HB | 3:Q:188:GLU:HG2 | 1.74 | 0.67 |
| 4:R:81:LEU:HD12 | 4:R:133:GLY:HA3 | 1.76 | 0.67 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:HB2 | 1.76 | 0.66 |
| 2:B:137:ILE:HD11 | 2:B:165:VAL:HG22 | 1.77 | 0.66 |
| 7:G:135:ILE:HD13 | 7:G:153:PRO:HD3 | 1.77 | 0.66 |
| 7:G:96:ALA:HA | 7:G:107:MET:CE | 2.22 | 0.66 |
| 5:S:207:LEU:HD23 | 5:S:207:LEU:H | 1.60 | 0.66 |
| 7:U:96:ALA:HA | 7:U:107:MET:CE | 2.21 | 0.66 |
| 12:Z:13:VAL:HG12 | 12:Z:177:ILE:HG13 | 1.76 | 0.66 |
| 5:E:198:SER:HA | 5:E:201:LEU:HG | 1.76 | 0.66 |
| 12:L:21:ILE:HD12 | 8:V:167:LEU:HD11 | 1.76 | 0.66 |
| 13:1:104:VAL:HG23 | 13:1:178:ILE:HG22 | 1.76 | 0.66 |
| 12:Z:100:ILE:HD11 | 12:Z:125:ARG:HG3 | 1.77 | 0.66 |
| 1:A:110:LYS:HG2 | 17:A:285:HOH:O | 1.94 | 0.66 |
| 5:E:111:ARG:HG2 | 5:E:111:ARG:HH11 | 1.60 | 0.66 |
| 14:2:155:ILE:HG22 | 14:2:175:MET:HE2 | 1.77 | 0.66 |
| 2:B:190:ILE:CG2 | 2:B:232:ILE:HD11 | 2.26 | 0.66 |
| 4:R:50:VAL:HG22 | 4:R:67:ILE:HD11 | 1.76 | 0.66 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:HB2 | 1.76 | 0.66 |
| 2:P:190:ILE:CG2 | 2:P:232:ILE:HD11 | 2.26 | 0.66 |
| 7:U:59:LEU:O | 7:U:61:PRO:HD3 | 1.95 | 0.66 |
| 7:U:87:ASN:HD22 | 7:U:87:ASN:C | 1.98 | 0.66 |
| 4:D:50:VAL:HG22 | 4:D:67:ILE:HD11 | 1.77 | 0.66 |
| 5:E:220:PRO:O | 5:E:222:THR:HG23 | 1.95 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:V:172:ASN:HD22 | 8:V:193:THR:HA | 1.61 | 0.66 |
| 4:D:81:LEU:HD12 | 4:D:133:GLY:HA3 | 1.77 | 0.65 |
| 6:F:211:GLU:O | 6:F:212:ILE:HD13 | 1.96 | 0.65 |
| 7:G:77:VAL:HG12 | 7:G:137:THR:HB | 1.79 | 0.65 |
| 5:S:198:SER:HA | 5:S:201:LEU:HG | 1.76 | 0.65 |
| 6:T:82:ILE:HB | 6:T:83:PRO:HD3 | 1.76 | 0.65 |
| 10:X:32:ASP:OD2 | 10:X:34:THR:HG22 | 1.97 | 0.65 |
| 10:X:69:ARG:HD2 | 17:X:553:HOH:O | 1.95 | 0.65 |
| 13:1:35:ILE:CD1 | 13:1:56:GLU:HG3 | 2.26 | 0.65 |
| 4:D:142:ASP:HA | 17:D:1309:HOH:O | 1.95 | 0.65 |
| 9:W:1:GLY:HA3 | 9:W:33:LYS:HE2 | 1.78 | 0.65 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:N | 2.12 | 0.65 |
| 3:Q:37:ALA:HB3 | 3:Q:165:ILE:HD11 | 1.77 | 0.65 |
| 11:K:109:THR:O | 11:K:110:ILE:HD13 | 1.96 | 0.65 |
| 13:M:14(D):GLU:O | 13:M:14(G):ILE:HG12 | 1.96 | 0.65 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:HB2 | 1.77 | 0.65 |
| 4:R:24:VAL:O | 4:R:27:SER:HB3 | 1.97 | 0.65 |
| 5:S:67:ILE:CD1 | 5:S:77:SER:HB3 | 2.26 | 0.65 |
| 1:O:24:ILE:HD11 | 1:O:124:THR:OG1 | 1.95 | 0.65 |
| 6:T:184:LEU:HD11 | 6:T:188:GLU:HB3 | 1.77 | 0.65 |
| 10:J:147:THR:OG1 | 10:J:150:GLU:HG3 | 1.96 | 0.65 |
| 12:L:109:ALA:HB2 | 12:L:121:ARG:NH2 | 2.11 | 0.65 |
| 14:N:112:THR:CG2 | 14:N:120:HIS:HB2 | 2.26 | 0.65 |
| 14:N:59:VAL:HG22 | 14:N:82:VAL:HG12 | 1.77 | 0.65 |
| 4:R:160:TYR:CE2 | 4:R:163:LYS:HD3 | 2.32 | 0.65 |
| 7:U:227:GLU:HG2 | 17:U:1255:HOH:O | 1.94 | 0.65 |
| 8:V:148:LYS:O | 8:V:152:ILE:HG12 | 1.97 | 0.65 |
| 12:Z:14(I):THR:O | 12:Z:14(K):LYS:HB2 | 1.97 | 0.65 |
| 1:A:197:LEU:CD2 | 1:A:210:ILE:HD12 | 2.27 | 0.65 |
| 5:E:177:GLU:OE1 | 6:F:56:SER:HB2 | 1.95 | 0.65 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:H | 1.61 | 0.65 |
| 7:G:49:ILE:HD12 | 7:G:49:ILE:N | 2.12 | 0.65 |
| 13:M:35:ILE:HG12 | 13:M:56:GLU:HG3 | 1.79 | 0.65 |
| 12:L:-9:GLN:HE21 | 13:M:-8:THR:HG21 | 1.61 | 0.65 |
| 4:R:67:ILE:HD12 | 4:R:211:GLN:HE21 | 1.61 | 0.65 |
| 6:T:173:LYS:O | 6:T:177:GLU:HG3 | 1.97 | 0.65 |
| 6:T:45:GLY:HA3 | 6:T:215:CYS:O | 1.97 | 0.64 |
| 6:F:45:GLY:HA3 | 6:F:215:CYS:O | 1.97 | 0.64 |
| 13:M:100:ILE:CD1 | 13:M:112:TYR:HB2 | 2.27 | 0.64 |
| 4:R:156:THR:HG22 | 5:S:83:PRO:HD3 | 1.78 | 0.64 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:HG21 | 1.79 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:C:172:VAL:HG23 | 3:C:196:SER:HB2 | 1.77 | 0.64 |
| 8:H:15:ALA:HB1 | 8:H:159:ILE:CD1 | 2.27 | 0.64 |
| 5:S:132:TYR:O | 5:S:153:PRO:HB3 | 1.96 | 0.64 |
| 8:V:15:ALA:HB1 | 8:V:159:ILE:CD1 | 2.27 | 0.64 |
| 14:N:163:ILE:HG23 | 14:N:170:GLY:HA2 | 1.79 | 0.64 |
| 2:P:101:LYS:HZ2 | 10:X:85:GLN:NE2 | 1.95 | 0.64 |
| 10:X:64:GLN:HA | 17:X:665:HOH:O | 1.97 | 0.64 |
| 14:2:146:MET:HE2 | 14:2:150:GLU:HB3 | 1.78 | 0.64 |
| 5:S:141:TYR:CE2 | 5:S:217:LYS:HA | 2.33 | 0.64 |
| 11:Y:142:TYR:O | 11:Y:143:LYS:HD2 | 1.98 | 0.64 |
| 3:C:15:PHE:N | 4:D:23:GLN:HE22 | 1.93 | 0.64 |
| 7:G:186:TRP:O | 7:G:190:VAL:HG23 | 1.98 | 0.64 |
| 7:U:12:ILE:CG1 | 7:U:14:ILE:HD12 | 2.24 | 0.64 |
| 13:1:35:ILE:HD12 | 13:1:45:ILE:HD12 | 1.80 | 0.64 |
| 14:2:17:ASP:CB | 14:2:163:ILE:HD11 | 2.27 | 0.64 |
| 7:G:59:LEU:O | 7:G:61:PRO:HD3 | 1.97 | 0.64 |
| 12:L:-7:ASN:ND2 | 12:L:-5:TYR:H | 1.95 | 0.64 |
| 13:M:104:VAL:HG23 | 13:M:178:ILE:HG22 | 1.79 | 0.64 |
| 5:S:111:ARG:HH11 | 5:S:111:ARG:HG2 | 1.62 | 0.64 |
| 10:J:168:MET:HE2 | 10:X:168:MET:HE2 | 1.80 | 0.64 |
| 4:D:12(D):ALA:HA | 5:E:129:GLY:HA2 | 1.80 | 0.64 |
| 8:H:41:ILE:HD12 | 8:H:103:GLY:HA3 | 1.80 | 0.64 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:CD1 | 2.27 | 0.64 |
| 13:1:148:VAL:HG23 | 17:1:182:HOH:O | 1.98 | 0.64 |
| 3:C:14:ILE:H | 3:C:14:ILE:HD13 | 1.63 | 0.64 |
| 10:J:38:SER:HB2 | 10:J:39:PRO:HD2 | 1.80 | 0.64 |
| 3:Q:170:LYS:HB2 | 17:Q:833:HOH:O | 1.97 | 0.64 |
| 11:K:10(A):ARG:HG2 | 11:K:10(A):ARG:HH11 | 1.63 | 0.63 |
| 6:T:175:GLU:OE1 | 6:T:199:LEU:HD23 | 1.98 | 0.63 |
| 10:J:168:MET:HG2 | 10:X:168:MET:HE3 | 1.80 | 0.63 |
| 13:M:40:ASN:ND2 | 13:M:40:ASN:N | 2.46 | 0.63 |
| 14:N:155:ILE:HG22 | 14:N:175:MET:HE2 | 1.79 | 0.63 |
| 10:X:147:THR:OG1 | 10:X:150:GLU:HG3 | 1.98 | 0.63 |
| 12:Z:173:LEU:HB2 | 12:Z:191:LEU:HD11 | 1.80 | 0.63 |
| 11:K:142:TYR:O | 11:K:143:LYS:HD2 | 1.97 | 0.63 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:N | 2.13 | 0.63 |
| 4:D:17:PRO:HD2 | 17:D:1171:HOH:O | 1.99 | 0.63 |
| 5:E:104:ASN:HB2 | 13:M:81:GLU:HG2 | 1.79 | 0.63 |
| 10:X:38:SER:HB2 | 10:X:39:PRO:HD2 | 1.80 | 0.63 |
| 11:Y:66:HIS:HA | 17:Y:1210:HOH:O | 1.97 | 0.63 |
| 9:I:1:GLY:HA3 | 9:I:33:LYS:HE2 | 1.79 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:X:133:TYR:CE2 | 10:X:166:MET:HG3 | 2.34 | 0.63 |
| 3:C:33:ARG:CB | 3:C:33:ARG:HH11 | 2.12 | 0.63 |
| 3:C:160:TRP:CE2 | 4:D:59:LEU:HD23 | 2.34 | 0.63 |
| 8:H:3:ILE:HD11 | 8:H:127:LEU:HB2 | 1.80 | 0.63 |
| 10:J:32:ASP:OD2 | 10:J:34:THR:HG22 | 1.99 | 0.63 |
| 4:D:102:TYR:O | 12:L:81:ARG:HG3 | 1.99 | 0.63 |
| 4:D:24:VAL:O | 4:D:27:SER:HB3 | 1.99 | 0.63 |
| 2:P:21:LEU:HD13 | 2:P:124:THR:HG23 | 1.80 | 0.63 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:CB | 2.12 | 0.63 |
| 7:U:186:TRP:O | 7:U:190:VAL:HG23 | 1.98 | 0.63 |
| 2:B:21:LEU:HD13 | 2:B:124:THR:HG23 | 1.79 | 0.63 |
| 8:V:81:GLN:O | 8:V:85:GLN:HG3 | 1.99 | 0.63 |
| 14:2:18(A):ILE:HD12 | 14:2:18(C):TYR:CZ | 2.34 | 0.63 |
| 5:E:18(D):ILE:O | 5:E:18(D):ILE:HD13 | 1.98 | 0.63 |
| 5:E:213:ALA:HB2 | 5:E:223:ILE:CD1 | 2.29 | 0.63 |
| 11:K:143:LYS:HA | 17:K:1394:HOH:O | 1.98 | 0.63 |
| 12:Z:-6:PRO:O | 13:1:91:ARG:NH1 | 2.28 | 0.63 |
| 14:2:163:ILE:CD1 | 14:2:169:SER:HB3 | 2.29 | 0.62 |
| 5:E:141:TYR:CE2 | 5:E:217:LYS:HA | 2.34 | 0.62 |
| 14:N:146:MET:HE2 | 14:N:150:GLU:HB3 | 1.79 | 0.62 |
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:HE | 1.46 | 0.62 |
| 3:Q:168:ASN:HB2 | 3:Q:200:VAL:HG11 | 1.80 | 0.62 |
| 6:T:179:LEU:HD11 | 6:T:192:GLN:HG3 | 1.81 | 0.62 |
| 5:E:213:ALA:CB | 5:E:223:ILE:CD1 | 2.77 | 0.62 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:CB | 2.30 | 0.62 |
| 6:F:179:LEU:HD11 | 6:F:192:GLN:HG3 | 1.81 | 0.62 |
| 6:F:187:ARG:HG3 | 6:F:187:ARG:HH11 | 1.64 | 0.62 |
| 12:L:3:ILE:CD1 | 12:L:46:ASN:HB2 | 2.29 | 0.62 |
| 13:M:74:LEU:HD13 | 13:M:79:ILE:HD11 | 1.81 | 0.62 |
| 5:S:67:ILE:HD13 | 5:S:77:SER:HB3 | 1.81 | 0.62 |
| 14:2:163:ILE:HG23 | 14:2:170:GLY:HA2 | 1.80 | 0.62 |
| 4:D:160:TYR:CE2 | 4:D:163:LYS:HD3 | 2.34 | 0.62 |
| 9:I:33:LYS:O | 9:I:44:GLY:HA2 | 2.00 | 0.62 |
| 3:Q:15:PHE:N | 4:R:23:GLN:HE22 | 1.92 | 0.62 |
| 7:U:236:ILE:HG13 | 7:U:237:ALA:N | 2.14 | 0.62 |
| 9:W:43:LEU:CD2 | 9:W:45:ILE:HD11 | 2.30 | 0.62 |
| 1:O:21(I):TYR:HE2 | 1:O:21(L):ILE:HD13 | 1.64 | 0.62 |
| 5:S:177:GLU:OE1 | 6:T:56:SER:HB2 | 2.00 | 0.62 |
| 12:Z:93:PHE:N | 12:Z:94:PRO:HD3 | 2.14 | 0.62 |
| 1:A:197:LEU:HD23 | 1:A:210:ILE:HD12 | 1.82 | 0.62 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:HE3 | 2.15 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:Q:186:VAL:HG21 | 3:Q:216:LYS:HE2 | 1.81 | 0.62 |
| 11:Y:35:ILE:HD11 | 11:Y:45:MET:CE | 2.29 | 0.62 |
| 12:Z:-9:GLN:HE21 | 13:1:-8:THR:HG21 | 1.63 | 0.62 |
| 9:I:159:LEU:HD21 | 9:I:173:ALA:HB1 | 1.80 | 0.62 |
| 9:I:177:ILE:HD12 | 9:I:187:ARG:NH1 | 2.06 | 0.62 |
| 12:L:14(I):THR:O | 12:L:14(K):LYS:HB2 | 1.99 | 0.62 |
| 12:L:3:ILE:N | 12:L:3:ILE:HD13 | 2.14 | 0.62 |
| 6:T:95:GLU:CG | 6:T:115:ARG:HB3 | 2.30 | 0.62 |
| 3:C:186:VAL:HG21 | 3:C:216:LYS:HE2 | 1.81 | 0.62 |
| 6:F:82:ILE:HB | 6:F:83:PRO:HD3 | 1.80 | 0.62 |
| 9:I:66:TYR:CZ | 9:I:70:GLU:HG3 | 2.35 | 0.62 |
| 3:Q:15:PHE:CE1 | 3:Q:21:ILE:HD11 | 2.35 | 0.62 |
| 11:Y:10(A):ARG:HH11 | 11:Y:10(A):ARG:HG2 | 1.64 | 0.62 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:H | 1.63 | 0.62 |
| 5:E:194:VAL:O | 5:E:197:ILE:HG22 | 2.00 | 0.62 |
| 7:G:77:VAL:CG1 | 7:G:137:THR:HB | 2.30 | 0.62 |
| 9:I:114:ASP:HB2 | 17:I:851:HOH:O | 1.99 | 0.62 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:HD22 | 1.64 | 0.62 |
| 12:Z:109:ALA:HA | 17:Z:375:HOH:O | 2.00 | 0.62 |
| 11:K:172:SER:HA | 11:K:192:VAL:HG23 | 1.82 | 0.62 |
| 3:Q:37:ALA:HB3 | 3:Q:165:ILE:CD1 | 2.29 | 0.62 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:CB | 2.29 | 0.62 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:HE3 | 2.15 | 0.62 |
| 8:H:81:GLN:O | 8:H:85:GLN:HG3 | 2.00 | 0.61 |
| 2:P:190:ILE:HG22 | 2:P:232:ILE:HD11 | 1.82 | 0.61 |
| 11:Y:172:SER:HA | 11:Y:192:VAL:HG23 | 1.82 | 0.61 |
| 4:D:194:LEU:HD22 | 4:D:212:LEU:HD11 | 1.82 | 0.61 |
| 1:O:86:ARG:HE | 7:U:118:ASN:HD21 | 1.48 | 0.61 |
| 6:T:175:GLU:HB3 | 6:T:196:ILE:CD1 | 2.30 | 0.61 |
| 7:U:70:ILE:HD12 | 7:U:74:ILE:HG22 | 1.81 | 0.61 |
| 16:Y:2(I):H10:H22A | 12:Z:125:ARG:NH2 | 2.15 | 0.61 |
| 12:Z:148:VAL:O | 12:Z:152:ILE:HG12 | 1.98 | 0.61 |
| 4:D:67:ILE:HD12 | 4:D:211:GLN:HE21 | 1.65 | 0.61 |
| 7:G:225:SER:O | 7:G:229:ILE:HG12 | 2.00 | 0.61 |
| 16:K:2(I):H10:H22A | 12:L:125:ARG:NH2 | 2.15 | 0.61 |
| 7:U:35:ILE:HD11 | 7:U:53:LYS:HG3 | 1.82 | 0.61 |
| 7:U:77:VAL:HG12 | 7:U:137:THR:HB | 1.82 | 0.61 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:CG2 | 2.30 | 0.61 |
| 2:P:143:ASP:OD2 | 10:X:10(B):LYS:HE2 | 2.01 | 0.61 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:H | 1.65 | 0.61 |
| 9:W:4:VAL:CG1 | 9:W:155:ILE:HD11 | 2.30 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:W:66:TYR:CZ | 9:W:70:GLU:HG3 | 2.34 | 0.61 |
| 5:E:132:TYR:O | 5:E:153:PRO:HB3 | 1.99 | 0.61 |
| 10:J:112:GLN:NE2 | 10:J:126:ALA:H | 1.99 | 0.61 |
| 14:N:30:VAL:CG2 | 13:1:203:ILE:HD13 | 2.31 | 0.61 |
| 9:W:159:LEU:HD21 | 9:W:173:ALA:HB1 | 1.81 | 0.61 |
| 4:R:102:TYR:O | 12:Z:81:ARG:HG3 | 1.99 | 0.61 |
| 12:Z:8:GLY:HA3 | 12:Z:11:PHE:CE2 | 2.35 | 0.61 |
| 14:N:6:VAL:CG2 | 14:N:155:ILE:HD11 | 2.30 | 0.61 |
| 9:W:90:ARG:HH11 | 9:W:90:ARG:HA | 1.65 | 0.61 |
| 11:K:133:PHE:HA | 17:X:203:HOH:O | 2.01 | 0.61 |
| 4:R:12(G):GLU:HG2 | 4:R:125:GLU:H | 1.66 | 0.61 |
| 7:U:35:ILE:CD1 | 7:U:53:LYS:HG3 | 2.29 | 0.61 |
| 1:A:32:LYS:HG2 | 17:A:354:HOH:O | 2.00 | 0.61 |
| 1:A:85:TYR:O | 1:A:89:VAL:HG23 | 2.01 | 0.61 |
| 10:J:133:TYR:CE2 | 10:J:166:MET:HG3 | 2.35 | 0.61 |
| 9:W:33:LYS:O | 9:W:44:GLY:HA2 | 2.01 | 0.61 |
| 11:Y:199:VAL:O | 11:Y:203:GLU:HB3 | 2.00 | 0.61 |
| 1:A:10(A):ILE:HD12 | 1:A:10(A):ILE:N | 2.16 | 0.61 |
| 2:P:184:MET:HE3 | 2:P:188:ASP:HB3 | 1.82 | 0.61 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:CB | 2.31 | 0.61 |
| 8:H:77:VAL:HG22 | 17:H:258:HOH:O | 2.01 | 0.61 |
| 3:Q:186:VAL:O | 3:Q:190:VAL:HG23 | 2.01 | 0.61 |
| 10:J:133:TYR:OH | 10:X:24:ILE:HG12 | 2.00 | 0.61 |
| 11:Y:6:PHE:HB2 | 11:Y:124:ILE:CD1 | 2.25 | 0.61 |
| 1:A:233:LEU:O | 1:A:236:LEU:HB2 | 2.00 | 0.60 |
| 3:C:163:GLN:HE22 | 3:C:173:ARG:HE | 1.47 | 0.60 |
| 9:I:90:ARG:HH11 | 9:I:90:ARG:HA | 1.65 | 0.60 |
| 6:T:187:ARG:HG3 | 6:T:187:ARG:HH11 | 1.65 | 0.60 |
| 13:M:200:ALA:HA | 13:M:203:ILE:HD12 | 1.83 | 0.60 |
| 1:O:233:LEU:O | 1:O:236:LEU:HB2 | 2.00 | 0.60 |
| 5:S:213:ALA:CB | 5:S:223:ILE:CD1 | 2.78 | 0.60 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:CB | 2.31 | 0.60 |
| 8:V:37:ILE:HD11 | 8:V:43:CYS:HB2 | 1.82 | 0.60 |
| 6:T:101:LYS:HE2 | 13:1:57:ARG:HH22 | 1.66 | 0.60 |
| 1:A:21(G):LEU:HD13 | 1:A:218:GLY:HA2 | 1.82 | 0.60 |
| 1:A:69:LEU:HD23 | 1:A:69:LEU:C | 2.22 | 0.60 |
| 3:C:186:VAL:O | 3:C:190:VAL:HG23 | 2.01 | 0.60 |
| 3:C:168:ASN:HB2 | 3:C:200:VAL:HG11 | 1.81 | 0.60 |
| 8:H:148:LYS:O | 8:H:152:ILE:HG12 | 2.01 | 0.60 |
| 3:Q:33:ARG:HB2 | 3:Q:33:ARG:NH1 | 2.16 | 0.60 |
| 3:Q:160:TRP:CE2 | 4:R:59:LEU:HD23 | 2.36 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:S:2(B):THR:N | 5:S:2(E):ASN:HD22 | 1.99 | 0.60 |
| 7:G:96:ALA:CA | 7:G:107:MET:HE2 | 2.23 | 0.60 |
| 7:G:47:VAL:HG12 | 7:G:49:ILE:CD1 | 2.31 | 0.60 |
| 9:W:6:MET:HE1 | 9:W:155:ILE:HA | 1.83 | 0.60 |
| 11:Y:6:PHE:CB | 11:Y:124:ILE:HD13 | 2.28 | 0.60 |
| 12:Z:109:ALA:HB2 | 12:Z:121:ARG:NH2 | 2.15 | 0.60 |
| 6:F:101:LYS:HE2 | 13:M:57:ARG:HH22 | 1.66 | 0.60 |
| 6:F:137:ILE:CD1 | 6:F:150:MET:HB2 | 2.31 | 0.60 |
| 7:G:48:VAL:C | 7:G:49:ILE:HD12 | 2.22 | 0.60 |
| 8:V:15:ALA:HB1 | 8:V:159:ILE:HD11 | 1.78 | 0.60 |
| 10:X:112:GLN:NE2 | 10:X:126:ALA:H | 2.00 | 0.60 |
| 14:N:83:PHE:CE1 | 14:N:99:ILE:HD13 | 2.36 | 0.60 |
| 1:O:21(I):TYR:CE2 | 1:O:21(L):ILE:HD13 | 2.37 | 0.60 |
| 10:X:52:THR:CG2 | 10:X:53:VAL:N | 2.65 | 0.60 |
| 4:D:177:LEU:HD13 | 5:E:58:LEU:HD11 | 1.83 | 0.60 |
| 6:F:175:GLU:OE1 | 6:F:199:LEU:HD23 | 2.01 | 0.60 |
| 9:I:29:ASN:ND2 | 9:I:30:LYS:HG3 | 2.16 | 0.60 |
| 10:J:52:THR:CG2 | 10:J:53:VAL:N | 2.64 | 0.60 |
| 4:R:186:LEU:O | 4:R:190:GLU:HG3 | 2.01 | 0.60 |
| 4:R:194:LEU:HD22 | 4:R:212:LEU:HD11 | 1.83 | 0.60 |
| 8:V:163:ILE:HG23 | 8:V:170:GLY:HA2 | 1.84 | 0.60 |
| 14:2:126:ILE:N | 14:2:126:ILE:HD13 | 2.17 | 0.60 |
| 6:F:101:LYS:HE2 | 13:M:57:ARG:NH2 | 2.17 | 0.60 |
| 6:F:229:LEU:HG | 6:F:233:ILE:HD11 | 1.84 | 0.60 |
| 7:G:35:ILE:HD11 | 7:G:53:LYS:HG3 | 1.83 | 0.60 |
| 9:I:6:MET:CE | 9:I:155:ILE:HA | 2.31 | 0.60 |
| 13:1:41:THR:OG1 | 13:1:76:PRO:HG3 | 2.02 | 0.60 |
| 4:D:12:VAL:CG2 | 4:D:12(A):GLY:HA2 | 2.32 | 0.60 |
| 7:G:35:ILE:CD1 | 7:G:53:LYS:HG3 | 2.32 | 0.60 |
| 4:R:177:LEU:HD13 | 5:S:58:LEU:HD11 | 1.84 | 0.60 |
| 7:U:70:ILE:CD1 | 7:U:76:MET:HB2 | 2.30 | 0.60 |
| 10:X:37:LEU:HB3 | 10:X:63:ILE:CD1 | 2.28 | 0.60 |
| 13:M:203:ILE:HD13 | 14:2:30:VAL:CG2 | 2.31 | 0.59 |
| 3:C:136:THR:O | 3:C:150:GLN:HA | 2.02 | 0.59 |
| 9:I:48:LEU:HG | 9:I:50:THR:HG22 | 1.84 | 0.59 |
| 10:J:168:MET:HE3 | 10:X:168:MET:HG2 | 1.82 | 0.59 |
| 6:F:137:ILE:HD12 | 6:F:163:ALA:HB3 | 1.83 | 0.59 |
| 6:F:137:ILE:HD11 | 6:F:163:ALA:HB1 | 1.84 | 0.59 |
| 3:Q:235:GLN:O | 3:Q:239:GLU:HG2 | 2.02 | 0.59 |
| 7:U:86:ARG:HD2 | 17:U:249:HOH:O | 2.01 | 0.59 |
| 8:V:100:ILE:HD13 | 8:V:112:SER:HB3 | 1.84 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:190:ILE:HG22 | 2:B:232:ILE:HD11 | 1.83 | 0.59 |
| 4:R:81:LEU:HB3 | 17:R:599:HOH:O | 2.02 | 0.59 |
| 5:S:194:VAL:O | 5:S:197:ILE:HG22 | 2.01 | 0.59 |
| 3:C:46:VAL:O | 3:C:215:VAL:HG12 | 2.02 | 0.59 |
| 3:C:33:ARG:HB2 | 3:C:33:ARG:NH1 | 2.17 | 0.59 |
| 5:E:82:ALA:HB3 | 5:E:83:PRO:HD3 | 1.84 | 0.59 |
| 7:G:172:ILE:HD11 | 7:G:201:LEU:HD21 | 1.84 | 0.59 |
| 9:I:3:ILE:HD12 | 9:I:48:LEU:HD13 | 1.85 | 0.59 |
| 9:I:35:PHE:HE1 | 9:I:45:ILE:HD13 | 1.66 | 0.59 |
| 5:S:213:ALA:HB2 | 5:S:223:ILE:CD1 | 2.30 | 0.59 |
| 11:Y:86:LEU:O | 11:Y:89:GLN:HB2 | 2.03 | 0.59 |
| 7:G:43:LYS:HB2 | 7:G:18(G):GLU:O | 2.02 | 0.59 |
| 14:N:13:ILE:CD1 | 14:N:177:VAL:HG13 | 2.32 | 0.59 |
| 3:Q:46:VAL:O | 3:Q:215:VAL:HG12 | 2.02 | 0.59 |
| 4:R:28:LEU:HA | 4:R:31:ILE:CD1 | 2.32 | 0.59 |
| 6:T:101:LYS:HE2 | 13:1:57:ARG:NH2 | 2.17 | 0.59 |
| 9:W:43:LEU:HD21 | 9:W:45:ILE:HD11 | 1.85 | 0.59 |
| 9:W:48:LEU:HG | 9:W:50:THR:HG22 | 1.85 | 0.59 |
| 10:X:90(B):ARG:NH1 | 17:X:266:HOH:O | 2.34 | 0.59 |
| 6:F:69:VAL:HG12 | 17:F:319:HOH:O | 2.01 | 0.59 |
| 3:Q:136:THR:O | 3:Q:150:GLN:HA | 2.03 | 0.59 |
| 8:V:155:ALA:O | 8:V:159:ILE:HD12 | 2.02 | 0.59 |
| 10:X:140:HIS:HD2 | 10:X:141:HIS:CE1 | 2.20 | 0.59 |
| 5:S:82:ALA:HB3 | 5:S:83:PRO:HD3 | 1.84 | 0.59 |
| 7:U:77:VAL:CG1 | 7:U:137:THR:HB | 2.33 | 0.59 |
| 3:C:235:GLN:O | 3:C:239:GLU:HG2 | 2.03 | 0.59 |
| 8:H:113:ILE:HG13 | 8:H:119:THR:HG22 | 1.83 | 0.59 |
| 5:S:46:ALA:HB1 | 5:S:139:ILE:HB | 1.85 | 0.59 |
| 8:V:219:VAL:O | 8:V:221:ILE:HD12 | 2.02 | 0.59 |
| 14:2:161:GLN:HE22 | 14:2:165:TRP:HE1 | 1.50 | 0.59 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:H | 1.51 | 0.59 |
| 3:C:57:LYS:O | 3:C:58:LEU:HB2 | 2.03 | 0.59 |
| 10:J:143:ARG:O | 10:J:146:MET:HG3 | 2.03 | 0.59 |
| 12:L:8:GLY:HA3 | 12:L:11:PHE:CE2 | 2.37 | 0.59 |
| 14:N:42:TRP:HZ2 | 13:1:211:ILE:HD11 | 1.68 | 0.59 |
| 4:R:12(D):ALA:HB3 | 4:R:126:ARG:HD3 | 1.85 | 0.59 |
| 7:U:168:LYS:O | 7:U:172:ILE:HG12 | 2.02 | 0.59 |
| 9:W:2:ILE:HG21 | 9:W:130:ALA:HB3 | 1.85 | 0.59 |
| 6:F:175:GLU:HB3 | 6:F:196:ILE:CD1 | 2.31 | 0.59 |
| 2:P:74:ILE:HD12 | 2:P:109:VAL:HG13 | 1.85 | 0.59 |
| 4:R:53:ARG:HG2 | 4:R:53:ARG:O | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:V:2:THR:OG1 | 8:V:130:GLY:HA3 | 2.03 | 0.59 |
| 11:Y:7:ARG:HD2 | 11:Y:108:PRO:O | 2.01 | 0.59 |
| 2:B:38:ILE:HD12 | 2:B:197:LEU:HG | 1.85 | 0.58 |
| 8:H:173:VAL:HB | 8:H:192:LEU:HB2 | 1.84 | 0.58 |
| 9:I:104:ILE:HD12 | 9:I:181:LYS:N | 2.18 | 0.58 |
| 11:K:76:VAL:N | 11:K:106:GLU:OE2 | 2.36 | 0.58 |
| 6:T:195:LYS:HZ2 | 6:T:196:ILE:HD13 | 1.67 | 0.58 |
| 9:W:6:MET:CE | 9:W:155:ILE:HA | 2.33 | 0.58 |
| 10:X:113:ILE:HG12 | 10:X:119:LYS:HG3 | 1.85 | 0.58 |
| 13:1:175:LEU:HD23 | 13:1:176:ALA:N | 2.18 | 0.58 |
| 4:D:12(F):GLY:HA3 | 17:D:965:HOH:O | 2.03 | 0.58 |
| 4:D:12(G):GLU:HG2 | 4:D:125:GLU:H | 1.66 | 0.58 |
| 12:L:93:PHE:N | 12:L:94:PRO:HD3 | 2.18 | 0.58 |
| 5:S:207:LEU:H | 5:S:207:LEU:CD2 | 2.16 | 0.58 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:HD13 | 1.85 | 0.58 |
| 7:U:43:LYS:HB2 | 7:U:18(G):GLU:O | 2.04 | 0.58 |
| 8:V:221:ILE:HD11 | 9:W:184:VAL:CB | 2.32 | 0.58 |
| 8:V:40:LYS:O | 8:V:41:ILE:HD13 | 2.03 | 0.58 |
| 9:W:29:ASN:ND2 | 9:W:30:LYS:HG3 | 2.18 | 0.58 |
| 11:K:7:ARG:HD2 | 11:K:108:PRO:O | 2.03 | 0.58 |
| 12:L:-6:PRO:O | 13:M:91:ARG:NH1 | 2.34 | 0.58 |
| 10:X:34:THR:HG21 | 10:X:176:LYS:NZ | 2.19 | 0.58 |
| 12:Z:32:PRO:HD2 | 17:Z:1177:HOH:O | 2.04 | 0.58 |
| 5:E:167:ALA:HB3 | 17:E:1131:HOH:O | 2.03 | 0.58 |
| 7:G:8:TYR:C | 7:G:10:ARG:H | 2.06 | 0.58 |
| 2:B:184:MET:HE3 | 2:B:188:ASP:HB3 | 1.85 | 0.58 |
| 4:D:186:LEU:O | 4:D:190:GLU:HG3 | 2.03 | 0.58 |
| 4:R:162:ALA:HB3 | 5:S:58:LEU:HD23 | 1.86 | 0.58 |
| 6:T:197:ILE:HD13 | 6:T:210:LEU:CD1 | 2.29 | 0.58 |
| 7:U:172:ILE:HD11 | 7:U:201:LEU:HD21 | 1.84 | 0.58 |
| 8:V:173:VAL:HB | 8:V:192:LEU:HB2 | 1.85 | 0.58 |
| 9:W:97:VAL:HG23 | 9:W:99:PRO:HD3 | 1.86 | 0.58 |
| 11:Y:146:LEU:HD23 | 11:Y:151:ALA:HA | 1.85 | 0.58 |
| 13:1:205:GLY:HA3 | 13:1:209:GLN:HB3 | 1.85 | 0.58 |
| 2:B:185:LYS:HD3 | 2:B:186:VAL:N | 2.19 | 0.58 |
| 2:B:141:TYR:CD1 | 2:B:21(E):VAL:HG21 | 2.38 | 0.58 |
| 13:M:146:THR:HA | 17:M:1069:HOH:O | 2.04 | 0.58 |
| 14:N:161:GLN:HE22 | 14:N:165:TRP:HE1 | 1.52 | 0.58 |
| 1:O:21(G):LEU:HD13 | 1:O:218:GLY:HA2 | 1.84 | 0.58 |
| 2:P:38:ILE:HD12 | 2:P:197:LEU:HG | 1.86 | 0.58 |
| 2:P:74:ILE:HD13 | 2:P:140:GLY:CA | 2.21 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:P:95:HIS:HB2 | 17:P:249:HOH:O | 2.01 | 0.58 |
| 3:C:122:ARG:NH2 | 17:C:806:HOH:O | 2.36 | 0.58 |
| 8:H:210:THR:HG21 | 12:Z:14(C):GLN:HG2 | 1.86 | 0.58 |
| 13:M:205:GLY:HA3 | 13:M:209:GLN:HB3 | 1.86 | 0.58 |
| 5:S:148:LEU:CD2 | 5:S:162:GLY:HA2 | 2.34 | 0.58 |
| 13:1:19:LEU:HD21 | 13:1:26:LEU:HD22 | 1.86 | 0.58 |
| 5:E:68:ILE:CD1 | 5:E:78:LEU:HD23 | 2.34 | 0.58 |
| 8:H:172:ASN:ND2 | 8:H:193:THR:HG22 | 2.19 | 0.58 |
| 12:Z:105:ASP:OD2 | 12:Z:107:LYS:HB2 | 2.04 | 0.58 |
| 14:2:14:LEU:O | 14:2:175:MET:HA | 2.04 | 0.57 |
| 4:D:12(D):ALA:HB3 | 4:D:126:ARG:HD3 | 1.85 | 0.57 |
| 8:H:219:VAL:O | 8:H:221:ILE:HD12 | 2.04 | 0.57 |
| 7:G:105:TYR:OH | 8:H:66:HIS:HE1 | 1.86 | 0.57 |
| 9:I:2:ILE:HG21 | 9:I:130:ALA:HB3 | 1.84 | 0.57 |
| 9:I:97:VAL:HG23 | 9:I:99:PRO:HD3 | 1.85 | 0.57 |
| 11:K:199:VAL:O | 11:K:203:GLU:HB3 | 2.03 | 0.57 |
| 12:L:105:ASP:OD2 | 12:L:107:LYS:HB2 | 2.04 | 0.57 |
| 6:F:72:ARG:HD2 | 13:M:64:THR:OG1 | 2.02 | 0.57 |
| 1:O:69:LEU:HD23 | 1:O:69:LEU:C | 2.24 | 0.57 |
| 2:P:185:LYS:HD3 | 2:P:186:VAL:N | 2.19 | 0.57 |
| 2:P:141:TYR:CD1 | 2:P:21(E):VAL:HG21 | 2.39 | 0.57 |
| 3:Q:215:VAL:HG23 | 3:Q:221:ILE:HG13 | 1.86 | 0.57 |
| 4:D:70:ILE:CD1 | 4:D:89:ILE:HG23 | 2.34 | 0.57 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:HD2 | 1.69 | 0.57 |
| 6:F:49:ALA:CB | 6:F:212:ILE:HD12 | 2.34 | 0.57 |
| 11:K:99:THR:HG22 | 11:K:113:VAL:O | 2.04 | 0.57 |
| 14:N:14:LEU:O | 14:N:175:MET:HA | 2.03 | 0.57 |
| 13:1:157:ASN:HB3 | 17:1:558:HOH:O | 2.03 | 0.57 |
| 5:E:213:ALA:CB | 5:E:223:ILE:HD12 | 2.34 | 0.57 |
| 6:F:229:LEU:HG | 6:F:233:ILE:CD1 | 2.33 | 0.57 |
| 8:H:147:THR:HG23 | 8:H:150:GLU:OE1 | 2.05 | 0.57 |
| 11:K:25:TRP:CH2 | 12:L:132:SER:HA | 2.40 | 0.57 |
| 8:V:18:THR:HG21 | 8:V:172:ASN:HB2 | 1.86 | 0.57 |
| 13:1:14(D):GLU:O | 13:1:14(G):ILE:HG13 | 2.05 | 0.57 |
| 9:I:28:SER:HB2 | 10:J:120:VAL:HG21 | 1.87 | 0.57 |
| 11:K:146:LEU:HD23 | 11:K:151:ALA:HA | 1.87 | 0.57 |
| 13:M:179:ASP:HB3 | 13:M:18(A):THR:OG1 | 2.05 | 0.57 |
| 1:O:15:PHE:H | 2:P:23:GLN:NE2 | 1.92 | 0.57 |
| 1:O:212:LEU:HD23 | 1:O:213:ALA:N | 2.19 | 0.57 |
| 5:E:46:ALA:HB1 | 5:E:139:ILE:HB | 1.86 | 0.57 |
| 5:E:207:LEU:HA | 5:E:2(E):ASN:HD22 | 1.65 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:207:LEU:CD2 | 5:E:207:LEU:H | 2.17 | 0.57 |
| 6:F:203:GLU:HA | 6:F:203:GLU:OE1 | 2.03 | 0.57 |
| 6:F:95:GLU:CG | 6:F:115:ARG:HB3 | 2.32 | 0.57 |
| 3:Q:15:PHE:H | 4:R:23:GLN:NE2 | 1.95 | 0.57 |
| 7:G:236:ILE:HD12 | 7:G:237:ALA:N | 2.19 | 0.57 |
| 13:M:1:THR:HA | 17:M:849:HOH:O | 2.05 | 0.57 |
| 9:W:74:ILE:HB | 17:W:517:HOH:O | 2.04 | 0.57 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:CG | 2.34 | 0.57 |
| 3:C:206:GLY:HA3 | 3:C:209:ASN:HB2 | 1.86 | 0.57 |
| 6:F:192:GLN:HE21 | 6:F:195:LYS:HE3 | 1.70 | 0.57 |
| 10:J:113:ILE:HG12 | 10:J:119:LYS:HG3 | 1.87 | 0.57 |
| 13:M:12:VAL:HG21 | 13:M:102:ALA:HB1 | 1.86 | 0.57 |
| 13:M:14(G):ILE:N | 13:M:144:PRO:HD2 | 2.20 | 0.57 |
| 1:O:49:ALA:HB2 | 1:O:212:LEU:HG | 1.86 | 0.57 |
| 3:Q:52:ARG:NH2 | 3:Q:211:GLU:HB3 | 2.20 | 0.57 |
| 6:T:186:ALA:O | 6:T:190:VAL:HG23 | 2.04 | 0.57 |
| 7:U:96:ALA:CA | 7:U:107:MET:HE2 | 2.27 | 0.57 |
| 8:V:172:ASN:ND2 | 8:V:193:THR:HG22 | 2.20 | 0.57 |
| 13:1:200:ALA:HA | 13:1:203:ILE:HD12 | 1.86 | 0.57 |
| 13:M:211:ILE:HD11 | 14:2:42:TRP:HZ2 | 1.69 | 0.57 |
| 8:H:155:ALA:O | 8:H:159:ILE:HD12 | 2.04 | 0.57 |
| 9:I:6:MET:HE1 | 9:I:155:ILE:HA | 1.85 | 0.57 |
| 9:I:152:PHE:HB2 | 9:I:177:ILE:CD1 | 2.31 | 0.57 |
| 13:M:100:ILE:HD11 | 13:M:112:TYR:HD1 | 1.70 | 0.57 |
| 1:O:85:TYR:O | 1:O:89:VAL:HG23 | 2.05 | 0.57 |
| 8:V:159:ILE:HD13 | 8:V:173:VAL:HG13 | 1.85 | 0.57 |
| 12:Z:163:THR:HB | 17:Z:200:HOH:O | 2.04 | 0.57 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:HD2 | 1.70 | 0.57 |
| 10:J:185:ARG:HH11 | 10:J:185:ARG:HG2 | 1.69 | 0.57 |
| 12:L:-2:ASN:HA | 12:L:21:ILE:O | 2.05 | 0.57 |
| 2:P:113:VAL:HG22 | 2:P:138:TYR:CD2 | 2.40 | 0.57 |
| 10:X:143:ARG:O | 10:X:146:MET:HG3 | 2.04 | 0.57 |
| 2:B:163:ILE:HG12 | 2:B:164:SER:N | 2.20 | 0.56 |
| 8:H:163:ILE:HG23 | 8:H:170:GLY:HA2 | 1.87 | 0.56 |
| 7:U:158:VAL:HG22 | 7:U:159:GLY:N | 2.20 | 0.56 |
| 14:2:13:ILE:HG13 | 14:2:151:THR:HG21 | 1.86 | 0.56 |
| 6:F:38:ILE:HG12 | 6:F:197:ILE:HD11 | 1.86 | 0.56 |
| 7:G:158:VAL:HG22 | 7:G:159:GLY:N | 2.20 | 0.56 |
| 7:G:56:ASP:HB3 | 7:G:59:LEU:HG | 1.87 | 0.56 |
| 10:J:76:PRO:HD2 | 17:J:296:HOH:O | 2.06 | 0.56 |
| 1:O:86:ARG:HE | 7:U:118:ASN:ND2 | 2.03 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:8:TYR:CD2 | 7:G:12:ILE:HD12 | 2.40 | 0.56 |
| 6:F:87:HIS:HD2 | 6:F:132:PHE:HE2 | 1.53 | 0.56 |
| 10:J:140:HIS:HD2 | 10:J:141:HIS:CE1 | 2.22 | 0.56 |
| 7:U:9:ASP:HA | 7:U:14:ILE:CD1 | 2.18 | 0.56 |
| 1:A:212:LEU:HD23 | 1:A:213:ALA:N | 2.20 | 0.56 |
| 2:B:27:ALA:O | 2:B:31:ILE:HG12 | 2.05 | 0.56 |
| 5:E:28:LEU:CA | 5:E:31:ILE:HD13 | 2.33 | 0.56 |
| 6:F:137:ILE:HD13 | 6:F:150:MET:HB2 | 1.88 | 0.56 |
| 6:F:216:SER:HB3 | 6:F:21(A):GLU:HB2 | 1.87 | 0.56 |
| 2:B:71:ASN:ND2 | 2:B:72:ASP:H | 2.04 | 0.56 |
| 3:C:52:ARG:NH2 | 3:C:211:GLU:HB3 | 2.20 | 0.56 |
| 12:L:4:LEU:HD11 | 12:L:138:LEU:HD21 | 1.85 | 0.56 |
| 13:M:17:ASP:HA | 13:M:173:PHE:CB | 2.35 | 0.56 |
| 3:Q:206:GLY:HA3 | 3:Q:209:ASN:HB2 | 1.88 | 0.56 |
| 12:Z:4:LEU:HD11 | 12:Z:138:LEU:HD21 | 1.88 | 0.56 |
| 12:Z:-7:ASN:C | 12:Z:-7:ASN:HD22 | 2.07 | 0.56 |
| 14:2:163:ILE:HD12 | 14:2:170:GLY:N | 2.20 | 0.56 |
| 4:D:117:CYS:HB3 | 4:D:155:GLY:O | 2.05 | 0.56 |
| 5:E:4:PHE:CE1 | 5:E:17:PRO:HD2 | 2.41 | 0.56 |
| 3:Q:156:ILE:CD1 | 3:Q:156:ILE:N | 2.68 | 0.56 |
| 4:R:12:VAL:CG2 | 4:R:12(A):GLY:HA2 | 2.35 | 0.56 |
| 6:T:121:GLN:NE2 | 17:T:385:HOH:O | 2.38 | 0.56 |
| 7:G:136:LEU:O | 7:G:150:LYS:HA | 2.05 | 0.56 |
| 4:R:117:CYS:HB3 | 4:R:155:GLY:O | 2.05 | 0.56 |
| 4:R:75:GLY:HA3 | 4:R:221:PHE:CD2 | 2.41 | 0.56 |
| 5:S:190:ILE:O | 5:S:194:VAL:HG23 | 2.06 | 0.56 |
| 5:S:207:LEU:N | 5:S:207:LEU:HD23 | 2.20 | 0.56 |
| 11:Y:99:THR:HG22 | 11:Y:113:VAL:O | 2.05 | 0.56 |
| 5:E:49:VAL:HG13 | 5:E:212:ILE:HD13 | 1.83 | 0.56 |
| 7:G:108:PRO:HB3 | 8:H:72:ARG:NH2 | 2.20 | 0.56 |
| 8:H:2:THR:OG1 | 8:H:130:GLY:HA3 | 2.06 | 0.56 |
| 9:I:113:PHE:HA | 9:I:118:CYS:O | 2.06 | 0.56 |
| 12:L:3:ILE:CD1 | 12:L:46:ASN:CB | 2.83 | 0.56 |
| 2:P:107:ILE:HG22 | 17:P:410:HOH:O | 2.06 | 0.56 |
| 5:S:67:ILE:HG21 | 5:S:223:ILE:CD1 | 2.36 | 0.56 |
| 6:T:216:SER:HB3 | 6:T:21(A):GLU:HB2 | 1.88 | 0.56 |
| 5:E:49:VAL:HG22 | 5:E:212:ILE:HD12 | 1.87 | 0.56 |
| 7:G:168:LYS:O | 7:G:172:ILE:HG12 | 2.06 | 0.56 |
| 10:J:52:THR:HG23 | 10:J:53:VAL:N | 2.21 | 0.56 |
| 4:R:39:GLY:O | 4:R:40:ILE:HD13 | 2.06 | 0.56 |
| 2:P:4:GLY:HA3 | 5:S:127:TYR:CE1 | 2.40 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:CD | 2.18 | 0.56 |
| 1:A:21:LEU:CB | 1:A:24:ILE:HD13 | 2.26 | 0.56 |
| 3:C:70:ILE:CD1 | 3:C:112:LEU:HD11 | 2.30 | 0.56 |
| 5:E:2(B):THR:N | 5:E:2(E):ASN:HD22 | 1.99 | 0.56 |
| 7:G:74:ILE:HG21 | 7:G:112:LEU:HD23 | 1.88 | 0.56 |
| 8:H:165:ASN:HD22 | 13:1:139:ARG:HH11 | 1.53 | 0.56 |
| 8:H:200:LYS:HE3 | 9:I:140:SER:O | 2.06 | 0.56 |
| 13:M:41:THR:OG1 | 13:M:76:PRO:HG3 | 2.06 | 0.56 |
| 2:P:163:ILE:HG12 | 2:P:164:SER:N | 2.20 | 0.56 |
| 3:Q:156:ILE:HD12 | 4:R:83:ALA:CB | 2.36 | 0.56 |
| 5:E:58:LEU:HD12 | 5:E:58:LEU:N | 2.21 | 0.56 |
| 6:F:186:ALA:O | 6:F:190:VAL:HG23 | 2.06 | 0.56 |
| 8:V:22:GLN:HG3 | 8:V:27:ALA:HB2 | 1.88 | 0.56 |
| 9:W:87:LEU:HD11 | 9:W:99:PRO:HG2 | 1.88 | 0.56 |
| 4:D:28:LEU:HA | 4:D:31:ILE:CD1 | 2.32 | 0.55 |
| 5:E:190:ILE:O | 5:E:194:VAL:HG23 | 2.05 | 0.55 |
| 10:J:34:THR:HG21 | 10:J:176:LYS:NZ | 2.22 | 0.55 |
| 11:K:12:ILE:CG2 | 11:K:110:ILE:HD11 | 2.34 | 0.55 |
| 12:L:90:LYS:HE3 | 12:L:93:PHE:O | 2.06 | 0.55 |
| 14:N:13:ILE:HG13 | 14:N:151:THR:HG21 | 1.87 | 0.55 |
| 7:U:140:SER:HA | 7:U:215:ALA:HB1 | 1.88 | 0.55 |
| 9:W:113:PHE:HA | 9:W:118:CYS:O | 2.06 | 0.55 |
| 11:Y:12:ILE:HB | 11:Y:178:VAL:HB | 1.89 | 0.55 |
| 3:C:97:GLN:NE2 | 3:C:97:GLN:HA | 2.21 | 0.55 |
| 6:F:210:LEU:HD11 | 6:F:212:ILE:HD11 | 1.88 | 0.55 |
| 8:H:18:THR:HG21 | 8:H:172:ASN:HB2 | 1.88 | 0.55 |
| 10:J:111:TYR:CE1 | 10:J:121:GLU:HG3 | 2.41 | 0.55 |
| 9:W:28:SER:HB2 | 10:X:120:VAL:HG21 | 1.88 | 0.55 |
| 14:2:13:ILE:CD1 | 14:2:177:VAL:HG13 | 2.36 | 0.55 |
| 14:N:51:ASP:O | 14:N:55:ILE:HG12 | 2.07 | 0.55 |
| 11:Y:12:ILE:HD12 | 11:Y:110:ILE:HD11 | 1.89 | 0.55 |
| 12:Z:14:LEU:HD13 | 12:Z:34:VAL:HG13 | 1.87 | 0.55 |
| 14:2:37:VAL:CG2 | 14:2:41:ILE:HG22 | 2.36 | 0.55 |
| 2:B:113:VAL:HG22 | 2:B:138:TYR:CD2 | 2.41 | 0.55 |
| 4:D:75:GLY:HA3 | 4:D:221:PHE:CD2 | 2.41 | 0.55 |
| 7:G:233:LEU:O | 7:G:236:ILE:HG13 | 2.06 | 0.55 |
| 2:P:100:LEU:HG | 9:W:60:ARG:NH2 | 2.22 | 0.55 |
| 12:Z:145:TYR:CD1 | 12:Z:146:LEU:N | 2.75 | 0.55 |
| 8:H:18:THR:HB | 8:H:30:ASN:HD22 | 1.72 | 0.55 |
| 11:K:102:CYS:CB | 11:K:110:ILE:HD12 | 2.37 | 0.55 |
| 2:P:194:LEU:HD11 | 2:P:232:ILE:CD1 | 2.35 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:S:92:LEU:HD11 | 5:S:112:ALA:HB1 | 1.88 | 0.55 |
| 6:T:203:GLU:OE1 | 6:T:203:GLU:HA | 2.05 | 0.55 |
| 7:U:49:ILE:HD13 | 7:U:212:VAL:HG22 | 1.89 | 0.55 |
| 10:X:34:THR:HG21 | 10:X:176:LYS:HZ2 | 1.72 | 0.55 |
| 14:2:13:ILE:HD13 | 14:2:177:VAL:HG22 | 1.88 | 0.55 |
| 7:G:49:ILE:HD13 | 7:G:193:ALA:HB1 | 1.89 | 0.55 |
| 4:R:65:GLU:HA | 17:R:750:HOH:O | 2.06 | 0.55 |
| 12:Z:173:LEU:HG | 12:Z:175:ILE:HD11 | 1.88 | 0.55 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:HD2 | 1.88 | 0.55 |
| 3:C:29:GLU:OE2 | 3:C:32:LYS:HE2 | 2.07 | 0.55 |
| 1:A:86:ARG:HE | 7:G:118:ASN:HD21 | 1.53 | 0.55 |
| 7:G:177:GLU:O | 7:G:17(B):LYS:HG3 | 2.06 | 0.55 |
| 3:Q:125:GLN:NE2 | 17:Q:872:HOH:O | 2.39 | 0.55 |
| 10:X:111:TYR:CE1 | 10:X:121:GLU:HG3 | 2.42 | 0.55 |
| 10:X:52:THR:HG23 | 10:X:53:VAL:N | 2.22 | 0.55 |
| 13:1:12:VAL:HG21 | 13:1:102:ALA:HB1 | 1.88 | 0.55 |
| 10:J:11:SER:HB2 | 10:J:178:VAL:O | 2.07 | 0.55 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:HD22 | 1.55 | 0.55 |
| 6:T:69:VAL:HG12 | 17:1:811:HOH:O | 2.06 | 0.55 |
| 7:U:116:MET:HE3 | 17:U:431:HOH:O | 2.06 | 0.55 |
| 7:U:8:TYR:C | 7:U:10:ARG:H | 2.09 | 0.55 |
| 8:V:18:THR:HB | 8:V:30:ASN:HD22 | 1.72 | 0.55 |
| 13:1:14(G):ILE:N | 13:1:144:PRO:HD2 | 2.21 | 0.55 |
| 13:1:177:ILE:C | 13:1:178:ILE:HD12 | 2.27 | 0.55 |
| 3:C:105:ASP:OD2 | 3:C:106:PRO:HD2 | 2.07 | 0.55 |
| 3:C:33:ARG:HD2 | 17:C:565:HOH:O | 2.07 | 0.55 |
| 7:G:135:ILE:CD1 | 7:G:153:PRO:HD3 | 2.36 | 0.55 |
| 9:I:87:LEU:HD11 | 9:I:99:PRO:HG2 | 1.88 | 0.55 |
| 12:L:59:PHE:CG | 12:L:83:ILE:HD11 | 2.42 | 0.55 |
| 14:N:37:VAL:CG2 | 14:N:41:ILE:HG22 | 2.37 | 0.55 |
| 3:C:35:THR:HB | 3:C:51:GLU:HG3 | 1.89 | 0.55 |
| 4:D:12(F):GLY:O | 4:D:12(G):GLU:HB2 | 2.07 | 0.55 |
| 5:E:125:GLN:HB3 | 17:E:1296:HOH:O | 2.07 | 0.55 |
| 13:M:175:LEU:HD23 | 13:M:176:ALA:N | 2.21 | 0.55 |
| 2:P:224:PHE:N | 2:P:224:PHE:HD2 | 2.05 | 0.55 |
| 3:Q:29:GLU:OE2 | 3:Q:32:LYS:HE2 | 2.07 | 0.55 |
| 1:A:13:THR:HG21 | 1:A:24:ILE:CD1 | 2.35 | 0.54 |
| 2:B:224:PHE:HD2 | 2:B:224:PHE:N | 2.04 | 0.54 |
| 2:B:53:LYS:HG2 | 2:B:54:VAL:HG23 | 1.89 | 0.54 |
| 4:D:59:LEU:HD11 | 4:D:64:ILE:HD11 | 1.88 | 0.54 |
| 5:E:148:LEU:CD2 | 5:E:162:GLY:HA2 | 2.37 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:H:3:ILE:HG22 | 8:H:16:ALA:HB2 | 1.88 | 0.54 |
| 8:H:84:LYS:HG3 | 8:H:85:GLN:N | 2.22 | 0.54 |
| 7:U:136:LEU:O | 7:U:150:LYS:HA | 2.05 | 0.54 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:HD22 | 1.54 | 0.54 |
| 2:B:224:PHE:CD2 | 2:B:224:PHE:N | 2.76 | 0.54 |
| 6:F:12:ASN:HB3 | 6:F:127:ASN:HA | 1.90 | 0.54 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:CB | 2.38 | 0.54 |
| 7:G:230:GLU:O | 7:G:234:VAL:HG23 | 2.07 | 0.54 |
| 2:B:114:ARG:NH1 | 10:J:70:GLU:OE2 | 2.37 | 0.54 |
| 11:K:50:ALA:HB2 | 12:L:116:VAL:HG23 | 1.89 | 0.54 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:CD | 2.19 | 0.54 |
| 6:T:49:ALA:HB3 | 6:T:197:ILE:HD11 | 1.80 | 0.54 |
| 8:V:159:ILE:HG22 | 8:V:163:ILE:CD1 | 2.38 | 0.54 |
| 8:V:200:LYS:HE3 | 9:W:140:SER:O | 2.08 | 0.54 |
| 9:W:15:ALA:HB3 | 9:W:155:ILE:CD1 | 2.37 | 0.54 |
| 14:2:10(B):LYS:C | 14:2:10(B):LYS:HD3 | 2.28 | 0.54 |
| 3:C:216:LYS:HD2 | 3:C:220:ASP:OD1 | 2.07 | 0.54 |
| 8:H:113:ILE:N | 8:H:113:ILE:HD12 | 2.22 | 0.54 |
| 5:S:201:LEU:O | 5:S:202:ARG:HB2 | 2.08 | 0.54 |
| 6:T:87:HIS:HD2 | 6:T:132:PHE:HE2 | 1.54 | 0.54 |
| 7:U:55:PRO:HG2 | 7:U:56:ASP:H | 1.73 | 0.54 |
| 8:V:3:ILE:HG22 | 8:V:16:ALA:HB2 | 1.89 | 0.54 |
| 5:E:111:ARG:NH1 | 5:E:111:ARG:HG2 | 2.23 | 0.54 |
| 12:L:145:TYR:CD1 | 12:L:146:LEU:N | 2.75 | 0.54 |
| 13:M:84:ALA:HA | 13:M:113:VAL:HG21 | 1.90 | 0.54 |
| 7:U:143:GLU:HG2 | 17:U:928:HOH:O | 2.07 | 0.54 |
| 8:V:100:ILE:HD13 | 8:V:112:SER:CB | 2.38 | 0.54 |
| 8:V:84:LYS:HG3 | 8:V:85:GLN:N | 2.23 | 0.54 |
| 12:Z:90:LYS:HE3 | 12:Z:93:PHE:O | 2.07 | 0.54 |
| 5:E:68:ILE:HD12 | 5:E:68:ILE:N | 2.23 | 0.54 |
| 7:G:140:SER:HA | 7:G:215:ALA:HB1 | 1.89 | 0.54 |
| 7:G:87:ASN:ND2 | 7:G:87:ASN:C | 2.61 | 0.54 |
| 9:I:99:PRO:HB2 | 9:I:113:PHE:CD2 | 2.42 | 0.54 |
| 6:T:119:TYR:O | 6:T:122:ALA:HB3 | 2.08 | 0.54 |
| 9:W:9:LYS:HD3 | 9:W:145:ASN:HD22 | 1.71 | 0.54 |
| 10:X:58:TYR:CD2 | 10:X:59:ILE:HD12 | 2.43 | 0.54 |
| 11:Y:12:ILE:HD12 | 11:Y:110:ILE:CG1 | 2.37 | 0.54 |
| 13:1:17:ASP:HA | 13:1:173:PHE:CB | 2.36 | 0.54 |
| 7:G:35:ILE:HG23 | 7:G:51:GLN:HB2 | 1.89 | 0.54 |
| 14:N:10(B):LYS:HD3 | 14:N:10(B):LYS:C | 2.28 | 0.54 |
| 2:P:87:ILE:O | 2:P:91:THR:HG23 | 2.08 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:W:73:ALA:HB1 | 17:W:204:HOH:O | 2.07 | 0.54 |
| 4:D:229:THR:HG22 | 4:D:233:ILE:HD11 | 1.90 | 0.54 |
| 6:F:11:SER:HB3 | 6:F:14:VAL:HG23 | 1.90 | 0.54 |
| 7:G:172:ILE:HD11 | 7:G:201:LEU:CD2 | 2.38 | 0.54 |
| 3:Q:216:LYS:HD2 | 3:Q:220:ASP:OD1 | 2.08 | 0.54 |
| 6:T:127:ASN:HD22 | 6:T:128:SER:N | 2.05 | 0.54 |
| 6:T:72:ARG:HD2 | 13:1:64:THR:OG1 | 2.07 | 0.54 |
| 10:X:185:ARG:HG2 | 10:X:185:ARG:HH11 | 1.73 | 0.54 |
| 3:C:39:GLY:O | 3:C:162:ALA:HA | 2.08 | 0.54 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:N | 2.22 | 0.54 |
| 6:F:238:LYS:HZ2 | 6:F:239:GLU:HG3 | 1.73 | 0.54 |
| 14:N:41:ILE:HD13 | 14:N:79:ALA:HB2 | 1.90 | 0.54 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:CG | 2.37 | 0.54 |
| 4:R:243:ALA:O | 4:R:244:GLU:HB2 | 2.08 | 0.54 |
| 7:U:226:ALA:HA | 7:U:229:ILE:HD12 | 1.90 | 0.54 |
| 9:W:99:PRO:HB2 | 9:W:113:PHE:CD2 | 2.42 | 0.54 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:N | 2.05 | 0.54 |
| 3:C:163:GLN:HA | 3:C:163:GLN:NE2 | 2.18 | 0.54 |
| 7:G:55:PRO:HG2 | 7:G:56:ASP:H | 1.73 | 0.54 |
| 8:H:22:GLN:HG3 | 8:H:27:ALA:HB2 | 1.90 | 0.54 |
| 2:P:27:ALA:O | 2:P:31:ILE:HG12 | 2.07 | 0.54 |
| 3:Q:97:GLN:NE2 | 3:Q:97:GLN:HA | 2.22 | 0.54 |
| 9:W:43:LEU:HG | 9:W:45:ILE:HD11 | 1.90 | 0.54 |
| 12:Z:76:ILE:HG22 | 17:Z:948:HOH:O | 2.08 | 0.54 |
| 1:A:232:ARG:HG3 | 1:A:232:ARG:HH11 | 1.73 | 0.54 |
| 1:A:86:ARG:HE | 7:G:118:ASN:ND2 | 2.06 | 0.54 |
| 12:L:13:VAL:HG12 | 12:L:177:ILE:HG12 | 1.90 | 0.54 |
| 7:U:204:GLU:HG3 | 17:U:1284:HOH:O | 2.07 | 0.54 |
| 7:U:87:ASN:ND2 | 7:U:87:ASN:C | 2.60 | 0.54 |
| 10:X:44:SER:OG | 10:X:100:LEU:HB2 | 2.07 | 0.54 |
| 13:1:150:VAL:HG21 | 17:1:323:HOH:O | 2.08 | 0.53 |
| 1:A:49:ALA:HB2 | 1:A:212:LEU:HG | 1.89 | 0.53 |
| 4:D:161:ASN:HB3 | 4:D:180:TRP:CE2 | 2.43 | 0.53 |
| 5:E:67:ILE:HG21 | 5:E:223:ILE:CD1 | 2.37 | 0.53 |
| 7:G:116:MET:HE3 | 17:G:551:HOH:O | 2.07 | 0.53 |
| 7:G:49:ILE:HD11 | 7:G:193:ALA:CB | 2.39 | 0.53 |
| 11:K:35:ILE:N | 11:K:35:ILE:HD12 | 2.23 | 0.53 |
| 11:K:48:GLY:HA3 | 17:K:406:HOH:O | 2.07 | 0.53 |
| 2:P:235:LYS:C | 2:P:237:GLY:H | 2.11 | 0.53 |
| 3:Q:72:SER:O | 3:Q:221:ILE:HD13 | 2.08 | 0.53 |
| 3:Q:39:GLY:O | 3:Q:162:ALA:HA | 2.08 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:K:10(A):ARG:NH1 | 11:K:10(A):ARG:HG2 | 2.23 | 0.53 |
| 11:K:174:ASN:HD21 | 11:K:189:ASN:HB2 | 1.73 | 0.53 |
| 4:R:207:LEU:C | 4:R:207:LEU:HD23 | 2.29 | 0.53 |
| 4:R:221:PHE:HE1 | 4:R:223:ILE:HD11 | 1.73 | 0.53 |
| 6:T:238:LYS:HZ2 | 6:T:239:GLU:HG3 | 1.74 | 0.53 |
| 7:U:56:ASP:HB3 | 7:U:59:LEU:HG | 1.89 | 0.53 |
| 2:B:15:PHE:N | 3:C:23:GLN:HE22 | 1.96 | 0.53 |
| 5:E:210:LEU:HD22 | 5:E:233:ILE:CD1 | 2.38 | 0.53 |
| 8:H:159:ILE:HD13 | 8:H:173:VAL:HG13 | 1.89 | 0.53 |
| 8:H:40:LYS:O | 8:H:41:ILE:HD13 | 2.09 | 0.53 |
| 13:M:19:LEU:HD21 | 13:M:26:LEU:HD22 | 1.91 | 0.53 |
| 1:O:47:VAL:HG23 | 1:O:212:LEU:HD21 | 1.89 | 0.53 |
| 1:O:35:VAL:HG11 | 1:O:51:GLU:HB3 | 1.89 | 0.53 |
| 3:Q:57:LYS:O | 3:Q:58:LEU:HB2 | 2.07 | 0.53 |
| 7:U:74:ILE:HG21 | 7:U:112:LEU:HD23 | 1.89 | 0.53 |
| 8:V:37:ILE:HD13 | 8:V:41:ILE:HG22 | 1.91 | 0.53 |
| 9:W:100:VAL:HG13 | 9:W:125:ILE:HG21 | 1.89 | 0.53 |
| 5:E:74:MET:HE1 | 5:E:109:VAL:HA | 1.91 | 0.53 |
| 6:F:195:LYS:HZ2 | 6:F:196:ILE:HD13 | 1.73 | 0.53 |
| 8:H:3:ILE:HG22 | 8:H:16:ALA:CB | 2.38 | 0.53 |
| 1:O:118:LYS:HE2 | 1:O:122:GLU:OE1 | 2.08 | 0.53 |
| 3:Q:35:THR:HB | 3:Q:51:GLU:HG3 | 1.90 | 0.53 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:CD1 | 2.39 | 0.53 |
| 6:T:192:GLN:HE21 | 6:T:195:LYS:HE3 | 1.72 | 0.53 |
| 13:1:84:ALA:HA | 13:1:113:VAL:HG21 | 1.90 | 0.53 |
| 7:G:34(A):ASN:HD22 | 7:G:167:PRO:HG2 | 1.73 | 0.53 |
| 10:J:123:PRO:HB2 | 10:J:124:TYR:CD1 | 2.43 | 0.53 |
| 11:Y:25:TRP:CH2 | 12:Z:132:SER:HA | 2.44 | 0.53 |
| 12:Z:-2:ASN:HA | 12:Z:21:ILE:O | 2.08 | 0.53 |
| 13:1:40:ASN:N | 13:1:40:ASN:ND2 | 2.46 | 0.53 |
| 3:C:175:PHE:O | 3:C:179:ASN:HB2 | 2.09 | 0.53 |
| 2:P:224:PHE:CD2 | 2:P:224:PHE:N | 2.76 | 0.53 |
| 2:P:126:HIS:CB | 3:Q:129:VAL:HG12 | 2.37 | 0.53 |
| 4:R:12(F):GLY:O | 4:R:12(G):GLU:HB2 | 2.08 | 0.53 |
| 4:R:161:ASN:HB3 | 4:R:180:TRP:CE2 | 2.43 | 0.53 |
| 5:S:4:PHE:CE1 | 5:S:17:PRO:HD2 | 2.44 | 0.53 |
| 7:U:230:GLU:O | 7:U:234:VAL:HG23 | 2.08 | 0.53 |
| 8:V:40:LYS:C | 8:V:41:ILE:HD13 | 2.29 | 0.53 |
| 10:X:13:ILE:HG12 | 10:X:177:ILE:HD12 | 1.90 | 0.53 |
| 2:B:107:ILE:HD11 | 2:B:112:LEU:H | 1.71 | 0.53 |
| 3:C:21:ILE:HD12 | 3:C:21:ILE:N | 2.24 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:243:ALA:O | 4:D:244:GLU:HB2 | 2.08 | 0.53 |
| 9:I:66:TYR:CE1 | 9:I:70:GLU:HG3 | 2.43 | 0.53 |
| 11:K:35:ILE:HD13 | 11:K:56:GLU:OE1 | 2.09 | 0.53 |
| 11:K:86:LEU:O | 11:K:89:GLN:HB2 | 2.08 | 0.53 |
| 12:L:177:ILE:CD1 | 12:L:185:ARG:NH2 | 2.72 | 0.53 |
| 13:M:42:VAL:HG23 | 13:M:178:ILE:HD11 | 1.89 | 0.53 |
| 2:P:71:ASN:ND2 | 2:P:72:ASP:H | 2.06 | 0.53 |
| 3:Q:100:ARG:HH11 | 3:Q:106:PRO:HB3 | 1.72 | 0.53 |
| 3:Q:70:ILE:CD1 | 3:Q:112:LEU:HD11 | 2.32 | 0.53 |
| 1:A:212:LEU:HD22 | 1:A:224:LEU:HD12 | 1.90 | 0.53 |
| 1:A:144:PHE:CD2 | 9:I:72:ARG:HD2 | 2.43 | 0.53 |
| 10:J:77:GLN:NE2 | 10:J:77:GLN:C | 2.61 | 0.53 |
| 11:K:200:LYS:HE3 | 11:K:206:PHE:O | 2.08 | 0.53 |
| 5:S:15:PHE:H | 6:T:23:GLN:NE2 | 2.03 | 0.53 |
| 4:R:17:PRO:HG3 | 5:S:26:TYR:CE2 | 2.44 | 0.53 |
| 12:Z:175:ILE:HD12 | 12:Z:175:ILE:N | 2.23 | 0.53 |
| 3:C:158:SER:HB2 | 4:D:59:LEU:HD21 | 1.90 | 0.53 |
| 4:D:138:ILE:HD12 | 4:D:138:ILE:N | 2.24 | 0.53 |
| 5:E:15:PHE:H | 6:F:23:GLN:NE2 | 2.04 | 0.53 |
| 8:H:40:LYS:C | 8:H:41:ILE:HD13 | 2.29 | 0.53 |
| 10:J:167:PRO:CB | 10:X:168:MET:HE1 | 2.39 | 0.53 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:HD21 | 1.69 | 0.53 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:HD13 | 1.91 | 0.53 |
| 7:U:35:ILE:HG23 | 7:U:51:GLN:HB2 | 1.89 | 0.53 |
| 8:V:3:ILE:HD11 | 8:V:127:LEU:CB | 2.38 | 0.53 |
| 11:Y:86:LEU:C | 11:Y:86:LEU:HD13 | 2.29 | 0.53 |
| 12:Z:114:ASP:HB2 | 12:Z:118:SER:OG | 2.09 | 0.53 |
| 3:C:14:ILE:HD13 | 3:C:14:ILE:N | 2.24 | 0.53 |
| 4:D:53:ARG:HG2 | 4:D:53:ARG:O | 2.09 | 0.53 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:HE22 | 1.73 | 0.53 |
| 8:H:221:ILE:HD11 | 9:I:184:VAL:CB | 2.34 | 0.53 |
| 9:I:8:SER:O | 9:I:6:PRO:HD3 | 2.09 | 0.53 |
| 1:O:33:GLN:HE21 | 1:O:33:GLN:HA | 1.74 | 0.53 |
| 7:U:49:ILE:CD1 | 7:U:212:VAL:HG22 | 2.39 | 0.53 |
| 8:V:3:ILE:HG22 | 8:V:16:ALA:CB | 2.39 | 0.53 |
| 2:B:235:LYS:C | 2:B:237:GLY:H | 2.12 | 0.52 |
| 3:C:15:PHE:H | 4:D:23:GLN:NE2 | 1.96 | 0.52 |
| 3:C:241:GLN:C | 3:C:243:GLN:H | 2.12 | 0.52 |
| 5:E:201:LEU:O | 5:E:202:ARG:HB2 | 2.09 | 0.52 |
| 8:H:210:THR:CG2 | 12:Z:14(C):GLN:HG2 | 2.39 | 0.52 |
| 1:O:62:GLU:C | 1:O:64:LEU:H | 2.12 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:S:58:LEU:N | 5:S:58:LEU:HD12 | 2.24 | 0.52 |
| 4:D:39:GLY:O | 4:D:40:ILE:HD13 | 2.10 | 0.52 |
| 5:E:214:ILE:O | 5:E:221:PHE:HA | 2.10 | 0.52 |
| 9:I:9:LYS:HD3 | 9:I:145:ASN:HD22 | 1.74 | 0.52 |
| 14:N:9:LYS:O | 14:N:107:LYS:HD3 | 2.09 | 0.52 |
| 14:N:176:VAL:HG12 | 14:N:178:LEU:HD13 | 1.91 | 0.52 |
| 2:P:101:LYS:NZ | 10:X:85:GLN:HE22 | 2.08 | 0.52 |
| 4:R:215:ILE:HD13 | 4:R:215:ILE:C | 2.30 | 0.52 |
| 8:V:216:GLU:HG3 | 9:W:187:ARG:HG2 | 1.91 | 0.52 |
| 9:W:29:ASN:H | 9:W:29:ASN:ND2 | 2.08 | 0.52 |
| 14:2:116:GLY:HA3 | 17:2:192:HOH:O | 2.10 | 0.52 |
| 7:U:101:TYR:OH | 14:2:58:ILE:HD11 | 2.10 | 0.52 |
| 10:J:168:MET:CE | 10:X:168:MET:CE | 2.87 | 0.52 |
| 12:L:114:ASP:HB2 | 12:L:118:SER:OG | 2.09 | 0.52 |
| 6:T:35:THR:HG23 | 6:T:36:THR:N | 2.24 | 0.52 |
| 11:Y:76:VAL:N | 11:Y:106:GLU:OE2 | 2.39 | 0.52 |
| 12:Z:76:ILE:HG23 | 12:Z:77:ASN:N | 2.23 | 0.52 |
| 1:A:33:GLN:HA | 1:A:33:GLN:HE21 | 1.73 | 0.52 |
| 2:B:51:GLU:OE2 | 2:B:202:THR:HG23 | 2.09 | 0.52 |
| 8:H:20:SER:HB3 | 8:H:28:ASP:HB3 | 1.91 | 0.52 |
| 8:H:50:ALA:CB | 9:I:116:ILE:CD1 | 2.76 | 0.52 |
| 9:I:93:GLY:N | 9:I:94:PRO:CD | 2.73 | 0.52 |
| 12:L:14:LEU:HD13 | 12:L:34:VAL:HG13 | 1.91 | 0.52 |
| 3:Q:125:GLN:HG3 | 3:Q:125:GLN:O | 2.09 | 0.52 |
| 3:Q:241:GLN:C | 3:Q:243:GLN:H | 2.13 | 0.52 |
| 3:Q:52:ARG:HD2 | 3:Q:208:LYS:O | 2.10 | 0.52 |
| 11:Y:12:ILE:HD12 | 11:Y:110:ILE:HG13 | 1.91 | 0.52 |
| 12:Z:-8:PHE:HB3 | 13:1:-8:THR:HG23 | 1.92 | 0.52 |
| 3:C:163:GLN:NE2 | 3:C:164:THR:N | 2.55 | 0.52 |
| 5:E:138:ILE:N | 5:E:138:ILE:HD12 | 2.23 | 0.52 |
| 8:H:95:ILE:O | 8:H:97:ALA:N | 2.41 | 0.52 |
| 1:O:110:LYS:HG2 | 17:O:376:HOH:O | 2.10 | 0.52 |
| 3:Q:154:SER:CB | 3:Q:156:ILE:HD13 | 2.38 | 0.52 |
| 3:Q:18(A):ASP:OD1 | 3:Q:18(C):LYS:HB2 | 2.10 | 0.52 |
| 9:W:36:HIS:HB3 | 9:W:42:PHE:CD2 | 2.43 | 0.52 |
| 10:X:52:THR:CG2 | 10:X:53:VAL:H | 2.22 | 0.52 |
| 13:1:91:ARG:HG3 | 13:1:92:SER:N | 2.24 | 0.52 |
| 2:B:143:ASP:OD2 | 10:J:10(B):LYS:HE2 | 2.10 | 0.52 |
| 3:C:40:VAL:HG12 | 3:C:162:ALA:HB1 | 1.92 | 0.52 |
| 10:J:63:ILE:CD1 | 10:J:63:ILE:N | 2.72 | 0.52 |
| 11:K:78:ALA:O | 11:K:82:ILE:HG12 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:O:212:LEU:HD22 | 1:O:224:LEU:HD12 | 1.91 | 0.52 |
| 2:P:53:LYS:HG2 | 2:P:54:VAL:HG23 | 1.92 | 0.52 |
| 1:O:177:GLU:HG2 | 2:P:58:LEU:CD2 | 2.40 | 0.52 |
| 4:R:236:GLU:O | 4:R:240:LYS:HG3 | 2.09 | 0.52 |
| 9:W:101:VAL:O | 9:W:110:ILE:HA | 2.09 | 0.52 |
| 10:X:11:SER:HB2 | 10:X:178:VAL:O | 2.09 | 0.52 |
| 11:Y:35:ILE:HD11 | 11:Y:45:MET:HE3 | 1.91 | 0.52 |
| 2:B:81:LEU:HD23 | 2:B:133:GLY:HA3 | 1.92 | 0.52 |
| 6:F:127:ASN:HD22 | 6:F:128:SER:N | 2.08 | 0.52 |
| 6:F:137:ILE:HD11 | 6:F:150:MET:SD | 2.49 | 0.52 |
| 8:H:101:VAL:HG12 | 8:H:113:ILE:HD11 | 1.91 | 0.52 |
| 9:I:22:SER:O | 9:I:23:GLN:HB2 | 2.10 | 0.52 |
| 12:L:-7:ASN:C | 12:L:-7:ASN:HD22 | 2.12 | 0.52 |
| 14:N:14:LEU:HD11 | 14:N:102:ALA:HB3 | 1.91 | 0.52 |
| 4:R:229:THR:HG22 | 4:R:233:ILE:HD11 | 1.91 | 0.52 |
| 8:V:112:SER:HB3 | 8:V:125:LEU:HD13 | 1.92 | 0.52 |
| 8:V:144:GLN:O | 8:V:145:ASP:HB2 | 2.09 | 0.52 |
| 10:J:13:ILE:N | 10:J:13:ILE:HD12 | 2.25 | 0.52 |
| 5:S:138:ILE:N | 5:S:138:ILE:HD12 | 2.24 | 0.52 |
| 5:S:214:ILE:O | 5:S:221:PHE:HA | 2.09 | 0.52 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:HD2 | 1.91 | 0.52 |
| 13:1:-3:VAL:HG12 | 13:1:49:ILE:HG13 | 1.92 | 0.52 |
| 4:D:198:LYS:HG3 | 17:D:499:HOH:O | 2.10 | 0.52 |
| 6:F:238:LYS:NZ | 6:F:239:GLU:HG3 | 2.25 | 0.52 |
| 3:Q:33:ARG:NH1 | 3:Q:33:ARG:CB | 2.73 | 0.52 |
| 3:Q:17:PRO:HA | 4:R:26:TYR:CD1 | 2.44 | 0.52 |
| 5:S:18(C):PHE:HA | 5:S:18(F):ILE:CG1 | 2.39 | 0.52 |
| 13:1:113:VAL:HA | 13:1:118:VAL:O | 2.10 | 0.52 |
| 14:2:146:MET:CE | 14:2:150:GLU:HB3 | 2.40 | 0.52 |
| 1:A:62:GLU:C | 1:A:64:LEU:H | 2.14 | 0.52 |
| 2:B:87:ILE:O | 2:B:91:THR:HG23 | 2.10 | 0.52 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:HD2 | 1.92 | 0.52 |
| 8:H:144:GLN:O | 8:H:145:ASP:HB2 | 2.09 | 0.52 |
| 13:M:113:VAL:HA | 13:M:118:VAL:O | 2.09 | 0.52 |
| 13:M:110:LEU:HG | 13:M:125:LEU:HD12 | 1.92 | 0.52 |
| 1:O:141:HIS:HA | 1:O:146:GLY:O | 2.10 | 0.52 |
| 2:P:185:LYS:O | 2:P:188:ASP:N | 2.42 | 0.52 |
| 3:Q:52:ARG:HH21 | 3:Q:211:GLU:HB3 | 1.75 | 0.52 |
| 7:U:192:PHE:CD1 | 7:U:192:PHE:C | 2.83 | 0.52 |
| 8:V:20:SER:HB3 | 8:V:28:ASP:HB3 | 1.92 | 0.52 |
| 12:Z:152:ILE:O | 12:Z:156:ARG:HG3 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:1:179:ASP:HB3 | 13:1:18(A):THR:OG1 | 2.10 | 0.51 |
| 14:2:14:LEU:HD11 | 14:2:102:ALA:HB3 | 1.92 | 0.51 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:CD | 2.39 | 0.51 |
| 2:B:173:GLN:HG2 | 3:C:56:LEU:HD12 | 1.92 | 0.51 |
| 4:D:215:ILE:HD13 | 4:D:215:ILE:C | 2.30 | 0.51 |
| 6:F:137:ILE:HD13 | 6:F:150:MET:CB | 2.41 | 0.51 |
| 10:J:133:TYR:HD1 | 17:Y:593:HOH:O | 1.92 | 0.51 |
| 10:J:52:THR:CG2 | 10:J:53:VAL:H | 2.23 | 0.51 |
| 11:K:126:CYS:HB2 | 11:K:135:TYR:CE1 | 2.45 | 0.51 |
| 9:W:80:THR:HG1 | 9:W:109:PHE:HE2 | 1.58 | 0.51 |
| 12:Z:129:ALA:HB1 | 12:Z:166:HIS:CE1 | 2.45 | 0.51 |
| 12:Z:43:MET:HB2 | 12:Z:101:ILE:HG22 | 1.92 | 0.51 |
| 5:E:137:LEU:CD2 | 5:E:150:GLU:HG3 | 2.41 | 0.51 |
| 9:I:104:ILE:HD12 | 9:I:179:LYS:C | 2.30 | 0.51 |
| 11:K:12:ILE:HB | 11:K:178:VAL:HB | 1.91 | 0.51 |
| 12:L:129:ALA:HB1 | 12:L:166:HIS:CE1 | 2.45 | 0.51 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:N | 2.08 | 0.51 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:HD2 | 1.92 | 0.51 |
| 7:U:172:ILE:HD11 | 7:U:201:LEU:CD2 | 2.40 | 0.51 |
| 14:2:146:MET:HE3 | 17:2:774:HOH:O | 2.10 | 0.51 |
| 6:T:12:ASN:HB3 | 6:T:127:ASN:HA | 1.92 | 0.51 |
| 14:2:176:VAL:HG12 | 14:2:178:LEU:HD13 | 1.91 | 0.51 |
| 1:A:21:LEU:HB3 | 1:A:24:ILE:CD1 | 2.28 | 0.51 |
| 10:J:44:SER:OG | 10:J:100:LEU:HB2 | 2.10 | 0.51 |
| 11:K:4:LEU:CD2 | 11:K:15:ALA:HB3 | 2.41 | 0.51 |
| 1:O:232:ARG:HG3 | 1:O:232:ARG:HH11 | 1.76 | 0.51 |
| 5:S:137:LEU:CD2 | 5:S:150:GLU:HG3 | 2.40 | 0.51 |
| 5:S:79:ALA:HB3 | 5:S:165:ILE:HD12 | 1.93 | 0.51 |
| 6:T:115:ARG:HA | 17:T:573:HOH:O | 2.11 | 0.51 |
| 7:U:34(A):ASN:HD22 | 7:U:167:PRO:HG2 | 1.75 | 0.51 |
| 7:U:31:THR:HG21 | 7:U:135:ILE:HG13 | 1.93 | 0.51 |
| 13:1:21:SER:HB2 | 17:1:278:HOH:O | 2.10 | 0.51 |
| 1:A:35:VAL:HG11 | 1:A:51:GLU:HB3 | 1.91 | 0.51 |
| 4:D:207:LEU:HD23 | 4:D:207:LEU:C | 2.31 | 0.51 |
| 13:M:130:GLY:O | 13:M:134:ALA:HB3 | 2.10 | 0.51 |
| 2:P:81:LEU:HD23 | 2:P:133:GLY:HA3 | 1.93 | 0.51 |
| 5:S:46:ALA:O | 5:S:139:ILE:HD12 | 2.11 | 0.51 |
| 6:T:87:HIS:HD2 | 6:T:132:PHE:CE2 | 2.29 | 0.51 |
| 9:W:119:ILE:N | 9:W:119:ILE:HD12 | 2.22 | 0.51 |
| 11:Y:174:ASN:HD21 | 11:Y:189:ASN:HB2 | 1.75 | 0.51 |
| 12:Z:48:PHE:CZ | 12:Z:50:ALA:HB3 | 2.46 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:207:LEU:HA | 5:E:2(E):ASN:HD21 | 1.70 | 0.51 |
| 9:I:36:HIS:HB3 | 9:I:42:PHE:CD2 | 2.46 | 0.51 |
| 10:J:113:ILE:HA | 10:J:118:THR:O | 2.11 | 0.51 |
| 13:M:147:THR:OG1 | 13:M:150:VAL:HG23 | 2.11 | 0.51 |
| 10:X:166:MET:CE | 10:X:168:MET:HB2 | 2.41 | 0.51 |
| 2:B:101:LYS:HG3 | 9:I:57:GLU:HB3 | 1.93 | 0.51 |
| 3:C:195:ARG:HD3 | 17:C:1019:HOH:O | 2.10 | 0.51 |
| 8:H:3:ILE:CG1 | 8:H:100:ILE:HD12 | 2.38 | 0.51 |
| 1:O:206:PHE:CD1 | 1:O:210:ILE:HD11 | 2.44 | 0.51 |
| 2:P:51:GLU:OE2 | 2:P:202:THR:HG23 | 2.10 | 0.51 |
| 3:Q:175:PHE:O | 3:Q:179:ASN:HB2 | 2.10 | 0.51 |
| 3:Q:40:VAL:HG12 | 3:Q:162:ALA:HB1 | 1.93 | 0.51 |
| 6:T:13:SER:HB2 | 7:U:130:ARG:HD3 | 1.93 | 0.51 |
| 6:T:147:HIS:HD2 | 17:T:242:HOH:O | 1.92 | 0.51 |
| 11:K:207:ASN:HD21 | 10:X:144:PRO:HG3 | 1.76 | 0.51 |
| 10:X:16:SER:HB2 | 17:X:1152:HOH:O | 2.10 | 0.51 |
| 1:A:92:SER:OG | 1:A:116:VAL:HG22 | 2.11 | 0.51 |
| 3:C:100:ARG:HH11 | 3:C:106:PRO:HB3 | 1.76 | 0.51 |
| 3:C:18(A):ASP:OD1 | 3:C:18(C):LYS:HB2 | 2.11 | 0.51 |
| 12:L:40:ASN:HD21 | 12:L:183:GLY:HA2 | 1.75 | 0.51 |
| 14:N:18(G):TYR:HA | 14:N:18(J):LEU:HG | 1.93 | 0.51 |
| 1:O:31:VAL:HG11 | 1:O:135:SER:HB2 | 1.91 | 0.51 |
| 3:Q:165:ILE:HD13 | 3:Q:165:ILE:H | 1.75 | 0.51 |
| 3:Q:158:SER:HB2 | 4:R:59:LEU:HD21 | 1.93 | 0.51 |
| 5:S:185:ASN:OD1 | 5:S:188:GLU:HG2 | 2.11 | 0.51 |
| 11:Y:143:LYS:HB2 | 11:Y:146:LEU:CD1 | 2.41 | 0.51 |
| 11:Y:50:ALA:HB2 | 12:Z:116:VAL:HG23 | 1.91 | 0.51 |
| 9:I:165:ARG:NH2 | 12:Z:135:MET:HE3 | 2.26 | 0.51 |
| 3:C:33:ARG:CB | 3:C:33:ARG:NH1 | 2.73 | 0.51 |
| 2:B:4:GLY:HA3 | 5:E:127:TYR:CE1 | 2.46 | 0.51 |
| 12:L:164:GLU:CD | 8:V:197:ARG:HG3 | 2.31 | 0.51 |
| 13:M:70:ASN:ND2 | 13:M:70(A):ALA:HA | 2.26 | 0.51 |
| 1:O:6:ASP:OD2 | 1:O:8:TYR:HB2 | 2.11 | 0.51 |
| 3:Q:165:ILE:HD13 | 3:Q:165:ILE:N | 2.25 | 0.51 |
| 4:R:46:VAL:HG11 | 4:R:139:ALA:HB1 | 1.93 | 0.51 |
| 5:S:31:ILE:HD11 | 5:S:153:PRO:CD | 2.41 | 0.51 |
| 6:T:238:LYS:NZ | 6:T:239:GLU:HG3 | 2.26 | 0.51 |
| 11:Y:200:LYS:HE3 | 11:Y:206:PHE:O | 2.11 | 0.51 |
| 11:Y:4:LEU:CD2 | 11:Y:15:ALA:HB3 | 2.41 | 0.51 |
| 12:Z:177:ILE:HD12 | 12:Z:177:ILE:N | 2.26 | 0.51 |
| 13:1:70:ASN:ND2 | 13:1:70(A):ALA:HA | 2.26 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:98:THR:O | 1:A:10(A):ILE:HD11 | 2.10 | 0.51 |
| 6:F:40:ILE:N | 6:F:40:ILE:HD12 | 2.26 | 0.51 |
| 8:H:108:SER:HB3 | 8:H:180:ILE:HD11 | 1.92 | 0.51 |
| 10:J:3:ILE:HG22 | 10:J:100:LEU:CD1 | 2.41 | 0.51 |
| 12:L:99:THR:C | 12:L:100:ILE:HD12 | 2.30 | 0.51 |
| 14:N:13:ILE:HD13 | 14:N:177:VAL:HG22 | 1.93 | 0.51 |
| 2:P:121:GLN:NE2 | 17:P:462:HOH:O | 2.43 | 0.51 |
| 6:T:32:GLU:HB3 | 6:T:169:ARG:NH2 | 2.26 | 0.51 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:CB | 2.41 | 0.51 |
| 8:V:147:THR:HG23 | 8:V:150:GLU:OE1 | 2.10 | 0.51 |
| 8:V:159:ILE:HD13 | 8:V:173:VAL:CG1 | 2.41 | 0.51 |
| 8:V:32:ALA:HB1 | 17:V:578:HOH:O | 2.11 | 0.51 |
| 12:L:135:MET:CE | 9:W:165:ARG:NH2 | 2.74 | 0.51 |
| 9:W:93:GLY:N | 9:W:94:PRO:CD | 2.73 | 0.51 |
| 11:Y:4:LEU:HD11 | 11:Y:159:ILE:HG12 | 1.93 | 0.51 |
| 12:Z:-7:ASN:ND2 | 12:Z:-7:ASN:C | 2.64 | 0.51 |
| 1:A:6:ASP:OD2 | 1:A:8:TYR:HB2 | 2.11 | 0.50 |
| 5:E:226:GLY:O | 5:E:229:VAL:HG22 | 2.10 | 0.50 |
| 6:F:35:THR:HG23 | 6:F:36:THR:N | 2.26 | 0.50 |
| 10:J:20:VAL:HG11 | 11:K:120:LEU:HD11 | 1.93 | 0.50 |
| 1:O:190:ILE:HD11 | 1:O:214:ILE:CG2 | 2.41 | 0.50 |
| 2:P:101:LYS:HZ1 | 10:X:85:GLN:NE2 | 2.08 | 0.50 |
| 2:P:218:ASN:O | 2:P:21(C):ASP:HB2 | 2.11 | 0.50 |
| 5:S:226:GLY:O | 5:S:229:VAL:HG22 | 2.11 | 0.50 |
| 6:T:11:SER:HB3 | 6:T:14:VAL:HG23 | 1.92 | 0.50 |
| 6:T:43:ASN:HD22 | 6:T:43:ASN:N | 2.10 | 0.50 |
| 9:W:192:ARG:HD2 | 17:W:1258:HOH:O | 2.10 | 0.50 |
| 10:X:35:ARG:O | 10:X:42:LEU:HD12 | 2.11 | 0.50 |
| 13:1:9:ASP:OD1 | 13:1:10:ASN:N | 2.44 | 0.50 |
| 2:B:218:ASN:O | 2:B:21(C):ASP:HB2 | 2.11 | 0.50 |
| 5:E:107:LEU:HD11 | 5:E:111:ARG:HG2 | 1.93 | 0.50 |
| 5:E:185:ASN:OD1 | 5:E:188:GLU:HG2 | 2.10 | 0.50 |
| 11:K:12:ILE:HD13 | 11:K:110:ILE:HD11 | 1.93 | 0.50 |
| 2:P:239:THR:HG22 | 2:P:239:THR:OXT | 2.10 | 0.50 |
| 1:O:130:ARG:NH2 | 7:U:124:THR:HG22 | 2.17 | 0.50 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:CD | 2.41 | 0.50 |
| 10:J:168:MET:HE2 | 10:X:168:MET:CE | 2.41 | 0.50 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:N | 2.09 | 0.50 |
| 5:E:36:VAL:HG22 | 5:E:37:THR:N | 2.26 | 0.50 |
| 6:F:87:HIS:HD2 | 6:F:132:PHE:CE2 | 2.28 | 0.50 |
| 11:K:4:LEU:HD11 | 11:K:159:ILE:HG12 | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:76:ILE:HG23 | 12:L:77:ASN:N | 2.27 | 0.50 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:H | 1.55 | 0.50 |
| 5:S:172:ALA:HB2 | 5:S:196:ALA:O | 2.11 | 0.50 |
| 8:V:50:ALA:HB3 | 9:W:116:ILE:HD12 | 1.93 | 0.50 |
| 8:V:95:ILE:O | 8:V:97:ALA:N | 2.41 | 0.50 |
| 10:X:34:THR:CG2 | 10:X:176:LYS:NZ | 2.75 | 0.50 |
| 12:Z:21:ILE:HB | 12:Z:25:SER:O | 2.11 | 0.50 |
| 1:A:60:MET:HE1 | 17:G:600:HOH:O | 2.12 | 0.50 |
| 3:C:52:ARG:HH21 | 3:C:211:GLU:HB3 | 1.76 | 0.50 |
| 4:D:112:LEU:C | 4:D:112:LEU:HD13 | 2.31 | 0.50 |
| 6:F:119:TYR:O | 6:F:122:ALA:HB3 | 2.11 | 0.50 |
| 9:I:143:GLU:HG3 | 9:I:146:LEU:HD21 | 1.93 | 0.50 |
| 12:L:152:ILE:O | 12:L:156:ARG:HG3 | 2.11 | 0.50 |
| 5:S:36:VAL:HG22 | 5:S:37:THR:N | 2.26 | 0.50 |
| 8:V:172:ASN:ND2 | 8:V:193:THR:HA | 2.25 | 0.50 |
| 13:1:19:LEU:HD12 | 13:1:28:PHE:O | 2.12 | 0.50 |
| 3:C:33:ARG:HB3 | 3:C:33:ARG:HH11 | 1.75 | 0.50 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:CD1 | 2.40 | 0.50 |
| 6:F:70:VAL:HG11 | 6:F:112:PHE:CE1 | 2.45 | 0.50 |
| 7:G:47:VAL:HG12 | 7:G:49:ILE:HD11 | 1.92 | 0.50 |
| 11:K:45:MET:SD | 16:K:2(I):H10:H15 | 2.51 | 0.50 |
| 7:U:107:MET:HE3 | 7:U:112:LEU:HB2 | 1.93 | 0.50 |
| 9:W:66:TYR:CE1 | 9:W:70:GLU:HG3 | 2.46 | 0.50 |
| 10:X:13:ILE:HG12 | 10:X:177:ILE:CD1 | 2.42 | 0.50 |
| 11:Y:4:LEU:HD21 | 11:Y:15:ALA:HB3 | 1.94 | 0.50 |
| 9:I:152:PHE:CB | 9:I:177:ILE:HD11 | 2.38 | 0.50 |
| 10:J:168:MET:CE | 10:X:168:MET:HG2 | 2.42 | 0.50 |
| 2:P:181:LYS:HG3 | 2:P:184:MET:HG3 | 1.94 | 0.50 |
| 4:R:185:THR:OG1 | 4:R:188:GLU:HG3 | 2.12 | 0.50 |
| 9:W:177:ILE:HD12 | 9:W:177:ILE:N | 2.27 | 0.50 |
| 9:W:55:LEU:CD1 | 9:W:97:VAL:HG21 | 2.41 | 0.50 |
| 10:J:166:MET:CE | 10:J:168:MET:HB2 | 2.42 | 0.50 |
| 14:N:13:ILE:HG13 | 14:N:151:THR:CG2 | 2.41 | 0.50 |
| 5:S:73:HIS:HE1 | 5:S:107:LEU:O | 1.94 | 0.50 |
| 7:U:108:PRO:HB3 | 8:V:72:ARG:NH2 | 2.25 | 0.50 |
| 10:X:123:PRO:HB2 | 10:X:124:TYR:CD1 | 2.46 | 0.50 |
| 9:I:165:ARG:NH2 | 12:Z:135:MET:CE | 2.75 | 0.50 |
| 2:B:181:LYS:HD2 | 2:B:183:ASP:OD1 | 2.12 | 0.50 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:CD1 | 2.42 | 0.50 |
| 1:A:86:ARG:HH21 | 7:G:118:ASN:HD22 | 1.60 | 0.50 |
| 9:I:80:THR:HG1 | 9:I:109:PHE:HE2 | 1.60 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:48:PHE:CZ | 12:L:50:ALA:HB3 | 2.47 | 0.50 |
| 13:M:-3:VAL:HG12 | 13:M:49:ILE:HG13 | 1.93 | 0.50 |
| 1:O:67:VAL:HG11 | 1:O:213:ALA:CB | 2.41 | 0.50 |
| 5:S:139:ILE:CD1 | 5:S:215:VAL:HG12 | 2.42 | 0.50 |
| 5:S:38:VAL:HG22 | 5:S:164:ALA:HB2 | 1.92 | 0.50 |
| 17:V:1181:HOH:O | 9:W:150:ASP:HA | 2.11 | 0.50 |
| 1:A:118:LYS:HE2 | 1:A:122:GLU:OE1 | 2.12 | 0.50 |
| 3:C:125:GLN:HG3 | 3:C:125:GLN:O | 2.12 | 0.50 |
| 3:C:35:THR:OG1 | 3:C:66:LYS:NZ | 2.45 | 0.50 |
| 4:D:236:GLU:O | 4:D:240:LYS:HG3 | 2.12 | 0.50 |
| 5:E:73:HIS:HE1 | 5:E:107:LEU:O | 1.95 | 0.50 |
| 5:E:139:ILE:CD1 | 5:E:215:VAL:HG12 | 2.42 | 0.50 |
| 7:G:38:LEU:C | 7:G:38:LEU:HD12 | 2.32 | 0.50 |
| 5:S:111:ARG:NH1 | 5:S:111:ARG:HG2 | 2.25 | 0.50 |
| 7:U:105:TYR:OH | 8:V:66:HIS:HE1 | 1.95 | 0.50 |
| 8:H:197:ARG:HG3 | 12:Z:164:GLU:CD | 2.32 | 0.50 |
| 1:A:141:HIS:HA | 1:A:146:GLY:O | 2.11 | 0.49 |
| 4:D:70:ILE:HD13 | 4:D:89:ILE:HG23 | 1.94 | 0.49 |
| 9:I:94:PRO:HA | 17:I:205:HOH:O | 2.12 | 0.49 |
| 17:E:1080:HOH:O | 12:L:64:LYS:HE3 | 2.11 | 0.49 |
| 14:N:38:HIS:HD2 | 17:N:1366:HOH:O | 1.95 | 0.49 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:CD | 2.42 | 0.49 |
| 12:Z:76:ILE:HD13 | 12:Z:109:ALA:HB3 | 1.93 | 0.49 |
| 3:C:226:SER:HB2 | 3:C:227:GLU:OE1 | 2.12 | 0.49 |
| 11:K:77:ALA:HA | 11:K:111:TYR:CE2 | 2.46 | 0.49 |
| 6:T:35:THR:O | 6:T:166:GLY:HA3 | 2.12 | 0.49 |
| 11:Y:7:ARG:HA | 11:Y:12:ILE:HD13 | 1.94 | 0.49 |
| 12:Z:85:HIS:HE1 | 17:Z:197:HOH:O | 1.96 | 0.49 |
| 12:Z:99:THR:CG2 | 17:Z:231:HOH:O | 2.60 | 0.49 |
| 14:2:175:MET:HB2 | 14:2:187:LEU:HB2 | 1.93 | 0.49 |
| 1:A:47:VAL:HG23 | 1:A:212:LEU:HD21 | 1.94 | 0.49 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:NH2 | 2.21 | 0.49 |
| 5:E:92:LEU:HD11 | 5:E:112:ALA:HB1 | 1.93 | 0.49 |
| 9:I:101:VAL:O | 9:I:110:ILE:HA | 2.11 | 0.49 |
| 9:I:113:PHE:CD2 | 9:I:113:PHE:N | 2.81 | 0.49 |
| 11:K:8:PHE:CE2 | 11:K:13:ILE:HG12 | 2.47 | 0.49 |
| 5:S:107:LEU:HD11 | 5:S:111:ARG:HG2 | 1.93 | 0.49 |
| 7:U:141:VAL:HG21 | 7:U:216:THR:HA | 1.94 | 0.49 |
| 11:Y:74:ILE:HD11 | 11:Y:78:ALA:CB | 2.42 | 0.49 |
| 2:B:107:ILE:HD12 | 2:B:112:LEU:CB | 2.32 | 0.49 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:CD | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:M:9:ASP:OD1 | 13:M:10:ASN:N | 2.46 | 0.49 |
| 1:O:62:GLU:CD | 1:O:62:GLU:H | 2.15 | 0.49 |
| 3:Q:221:ILE:N | 3:Q:221:ILE:HD12 | 2.27 | 0.49 |
| 4:R:172:ALA:HB1 | 4:R:196:ILE:HG21 | 1.94 | 0.49 |
| 11:Y:10(A):ARG:HG2 | 11:Y:10(A):ARG:NH1 | 2.23 | 0.49 |
| 11:Y:200:LYS:HG3 | 11:Y:206:PHE:HB2 | 1.95 | 0.49 |
| 14:2:159:LEU:O | 14:2:163:ILE:HG12 | 2.13 | 0.49 |
| 6:F:109:ILE:CG2 | 6:F:147:HIS:HB2 | 2.41 | 0.49 |
| 13:M:6:MET:HG2 | 13:M:155:ILE:HD11 | 1.95 | 0.49 |
| 14:N:44:CYS:HB2 | 14:N:100:ILE:HB | 1.94 | 0.49 |
| 3:Q:163:GLN:HA | 3:Q:163:GLN:NE2 | 2.18 | 0.49 |
| 5:S:179:THR:HG22 | 5:S:18(B):THR:HB | 1.95 | 0.49 |
| 11:Y:8:PHE:CE2 | 11:Y:13:ILE:HG12 | 2.47 | 0.49 |
| 4:D:27:SER:O | 4:D:31:ILE:HG13 | 2.13 | 0.49 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:CG1 | 2.40 | 0.49 |
| 5:E:54:ASN:ND2 | 5:E:56:ASP:O | 2.45 | 0.49 |
| 7:G:47:VAL:HG12 | 7:G:49:ILE:HD12 | 1.94 | 0.49 |
| 12:L:17:ASP:HA | 12:L:172:GLY:O | 2.12 | 0.49 |
| 2:P:27:ALA:O | 2:P:30:SER:HB3 | 2.13 | 0.49 |
| 7:U:217:LYS:HA | 7:U:217:LYS:CE | 2.41 | 0.49 |
| 7:U:38:LEU:C | 7:U:38:LEU:HD12 | 2.33 | 0.49 |
| 9:W:22:SER:O | 9:W:23:GLN:HB2 | 2.12 | 0.49 |
| 11:K:207:ASN:HD21 | 10:X:144:PRO:CG | 2.25 | 0.49 |
| 14:2:9:LYS:O | 14:2:107:LYS:HD3 | 2.13 | 0.49 |
| 14:2:13:ILE:HG13 | 14:2:151:THR:CG2 | 2.42 | 0.49 |
| 2:B:181:LYS:HG3 | 2:B:184:MET:HG3 | 1.94 | 0.49 |
| 2:B:27:ALA:O | 2:B:30:SER:HB3 | 2.12 | 0.49 |
| 7:G:192:PHE:CD1 | 7:G:192:PHE:C | 2.85 | 0.49 |
| 8:H:8:PHE:HB3 | 8:H:151:ALA:HB2 | 1.95 | 0.49 |
| 10:J:168:MET:HG2 | 10:X:168:MET:CE | 2.41 | 0.49 |
| 10:J:185:ARG:NH1 | 10:J:185:ARG:HG2 | 2.27 | 0.49 |
| 11:K:86:LEU:HD13 | 11:K:86:LEU:C | 2.33 | 0.49 |
| 12:L:5:GLY:O | 12:L:124:CYS:HA | 2.12 | 0.49 |
| 3:Q:105:ASP:OD2 | 3:Q:106:PRO:HD2 | 2.12 | 0.49 |
| 10:X:3:ILE:HG22 | 10:X:100:LEU:CD1 | 2.43 | 0.49 |
| 3:C:41:LYS:HD3 | 3:C:161:SER:HA | 1.95 | 0.49 |
| 4:D:14:THR:HG22 | 4:D:15:PHE:N | 2.27 | 0.49 |
| 10:J:34:THR:HG21 | 10:J:176:LYS:HZ2 | 1.76 | 0.49 |
| 14:N:19:ARG:HG3 | 14:N:26:ILE:HG23 | 1.94 | 0.49 |
| 1:O:92:SER:OG | 1:O:116:VAL:HG22 | 2.12 | 0.49 |
| 3:Q:163:GLN:NE2 | 3:Q:164:THR:N | 2.58 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:V:8:PHE:HB3 | 8:V:151:ALA:HB2 | 1.95 | 0.49 |
| 10:J:167:PRO:HB2 | 10:X:168:MET:HE1 | 1.95 | 0.49 |
| 11:Y:45:MET:SD | 16:Y:2(I):H10:H15 | 2.53 | 0.49 |
| 2:B:107:ILE:HD13 | 2:B:107:ILE:C | 2.33 | 0.49 |
| 5:E:179:THR:HG22 | 5:E:18(B):THR:HB | 1.95 | 0.49 |
| 8:H:172:ASN:ND2 | 8:H:193:THR:HA | 2.25 | 0.49 |
| 8:H:216:GLU:HG3 | 9:I:187:ARG:HG2 | 1.94 | 0.49 |
| 14:N:146:MET:CE | 14:N:150:GLU:HB3 | 2.42 | 0.49 |
| 2:P:181:LYS:HD2 | 2:P:183:ASP:OD1 | 2.13 | 0.49 |
| 13:1:130:GLY:O | 13:1:134:ALA:HB3 | 2.12 | 0.49 |
| 9:I:100:VAL:HG13 | 9:I:125:ILE:HG21 | 1.95 | 0.49 |
| 11:K:4:LEU:HD13 | 11:K:159:ILE:HD11 | 1.94 | 0.49 |
| 12:L:35:PHE:CD2 | 12:L:56:VAL:HG11 | 2.48 | 0.49 |
| 3:Q:137:LEU:HG | 3:Q:165:ILE:HD12 | 1.95 | 0.49 |
| 3:Q:41:LYS:HD3 | 3:Q:161:SER:HA | 1.94 | 0.49 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:HD11 | 1.95 | 0.49 |
| 6:T:158:TRP:CZ3 | 7:U:64:VAL:HA | 2.48 | 0.49 |
| 9:W:143:GLU:HG3 | 9:W:146:LEU:HD21 | 1.94 | 0.49 |
| 7:G:170:GLN:NE2 | 7:G:174:THR:HG23 | 2.27 | 0.48 |
| 12:L:1(I):ASN:HA | 17:L:1110:HOH:O | 2.12 | 0.48 |
| 2:P:196:THR:O | 2:P:200:THR:HG23 | 2.13 | 0.48 |
| 3:Q:55:THR:HG22 | 3:Q:56:LEU:CD2 | 2.40 | 0.48 |
| 3:Q:97:GLN:HA | 3:Q:97:GLN:HE21 | 1.77 | 0.48 |
| 4:R:112:LEU:C | 4:R:112:LEU:HD13 | 2.34 | 0.48 |
| 9:W:113:PHE:CD2 | 9:W:113:PHE:N | 2.81 | 0.48 |
| 10:X:113:ILE:HA | 10:X:118:THR:O | 2.12 | 0.48 |
| 12:Z:99:THR:HG23 | 17:Z:231:HOH:O | 2.13 | 0.48 |
| 2:B:185:LYS:O | 2:B:188:ASP:N | 2.44 | 0.48 |
| 3:C:46:VAL:HB | 3:C:215:VAL:CG1 | 2.43 | 0.48 |
| 4:D:175:GLU:HA | 4:D:175:GLU:OE1 | 2.13 | 0.48 |
| 5:E:210:LEU:CD2 | 5:E:233:ILE:HD11 | 2.41 | 0.48 |
| 7:U:17:PRO:HD3 | 17:U:584:HOH:O | 2.14 | 0.48 |
| 13:1:94:PRO:HA | 17:1:219:HOH:O | 2.12 | 0.48 |
| 2:B:69:LYS:HG3 | 2:B:221:GLN:OE1 | 2.13 | 0.48 |
| 3:C:163:GLN:CA | 3:C:163:GLN:NE2 | 2.75 | 0.48 |
| 4:D:46:VAL:HG11 | 4:D:139:ALA:HB1 | 1.94 | 0.48 |
| 5:E:139:ILE:HG22 | 5:E:148:LEU:HD13 | 1.95 | 0.48 |
| 8:H:112:SER:HB3 | 8:H:125:LEU:HD13 | 1.94 | 0.48 |
| 17:A:242:HOH:O | 8:H:69:TYR:HA | 2.11 | 0.48 |
| 9:I:55:LEU:CD1 | 9:I:97:VAL:HG21 | 2.43 | 0.48 |
| 4:R:175:GLU:OE1 | 4:R:175:GLU:HA | 2.12 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:R:27:SER:O | 4:R:31:ILE:HG13 | 2.13 | 0.48 |
| 5:S:221:PHE:CE1 | 5:S:223:ILE:CD1 | 2.91 | 0.48 |
| 7:U:12:ILE:O | 7:U:14:ILE:HD13 | 2.13 | 0.48 |
| 9:W:89:GLU:O | 9:W:90:ARG:NH1 | 2.47 | 0.48 |
| 11:Y:77:ALA:HA | 11:Y:111:TYR:CE2 | 2.47 | 0.48 |
| 11:Y:20:ALA:HA | 16:Y:2(I):H10:O11 | 2.13 | 0.48 |
| 1:A:67:VAL:HG11 | 1:A:213:ALA:CB | 2.44 | 0.48 |
| 2:B:186:VAL:HG21 | 2:B:216:ARG:HD3 | 1.94 | 0.48 |
| 3:C:52:ARG:HD2 | 3:C:208:LYS:O | 2.13 | 0.48 |
| 9:I:152:PHE:CD1 | 9:I:177:ILE:HD11 | 2.48 | 0.48 |
| 11:K:4:LEU:HD21 | 11:K:15:ALA:HB3 | 1.94 | 0.48 |
| 12:L:43:MET:HB2 | 12:L:101:ILE:HG22 | 1.94 | 0.48 |
| 1:O:27:ALA:O | 1:O:31:VAL:HG23 | 2.13 | 0.48 |
| 11:Y:126:CYS:HB2 | 11:Y:135:TYR:CE1 | 2.48 | 0.48 |
| 12:Z:17:ASP:HA | 12:Z:172:GLY:O | 2.13 | 0.48 |
| 1:A:109:THR:O | 1:A:113:VAL:HG23 | 2.14 | 0.48 |
| 6:F:49:ALA:CB | 6:F:212:ILE:CD1 | 2.91 | 0.48 |
| 11:K:143:LYS:HB2 | 11:K:146:LEU:CD1 | 2.44 | 0.48 |
| 3:Q:173:ARG:O | 3:Q:177:GLU:HG3 | 2.13 | 0.48 |
| 5:S:2(C):VAL:CG1 | 5:S:2(D):ASP:N | 2.76 | 0.48 |
| 5:S:52:LYS:O | 5:S:63:TYR:HD2 | 1.96 | 0.48 |
| 6:T:109:ILE:HG22 | 6:T:149:TYR:CE2 | 2.48 | 0.48 |
| 11:Y:13:ILE:HD12 | 11:Y:152:LEU:HD23 | 1.96 | 0.48 |
| 3:C:17:PRO:HA | 4:D:26:TYR:CD1 | 2.48 | 0.48 |
| 6:F:35:THR:O | 6:F:166:GLY:HA3 | 2.14 | 0.48 |
| 17:G:248:HOH:O | 8:H:82:MET:HA | 2.14 | 0.48 |
| 9:I:29:ASN:H | 9:I:29:ASN:ND2 | 2.11 | 0.48 |
| 10:J:24:ILE:O | 10:J:24:ILE:HG13 | 2.13 | 0.48 |
| 3:Q:52:ARG:HB2 | 3:Q:209:ASN:HA | 1.95 | 0.48 |
| 14:2:174:ARG:HD2 | 17:2:307:HOH:O | 2.14 | 0.48 |
| 1:A:198:LYS:HE3 | 1:A:236:LEU:HD11 | 1.96 | 0.48 |
| 2:B:194:LEU:HD11 | 2:B:232:ILE:CD1 | 2.36 | 0.48 |
| 2:B:237:GLY:O | 2:B:238:ILE:HD13 | 2.14 | 0.48 |
| 5:E:46:ALA:O | 5:E:139:ILE:HD12 | 2.13 | 0.48 |
| 5:E:79:ALA:HB3 | 5:E:165:ILE:HD12 | 1.94 | 0.48 |
| 5:E:67:ILE:HG21 | 5:E:213:ALA:HB2 | 1.95 | 0.48 |
| 2:B:8:TYR:CE2 | 7:G:12:ILE:HD12 | 2.48 | 0.48 |
| 1:A:32:LYS:HE2 | 1:A:32:LYS:CA | 2.43 | 0.48 |
| 1:A:32:LYS:HA | 1:A:32:LYS:CE | 2.43 | 0.48 |
| 3:C:65:SER:HB2 | 17:C:274:HOH:O | 2.13 | 0.48 |
| 12:L:33:LYS:HD2 | 12:L:46:ASN:ND2 | 2.29 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:M:62:LEU:HD13 | 13:M:79:ILE:CD1 | 2.43 | 0.48 |
| 1:O:24:ILE:HD13 | 1:O:131:PRO:CG | 2.44 | 0.48 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:HB3 | 1.77 | 0.48 |
| 4:R:50:VAL:HG22 | 4:R:67:ILE:CD1 | 2.44 | 0.48 |
| 5:S:15:PHE:HB2 | 6:T:23:GLN:HE22 | 1.78 | 0.48 |
| 8:V:84:LYS:HE2 | 8:V:119:THR:HG23 | 1.95 | 0.48 |
| 11:Y:4:LEU:HD13 | 11:Y:159:ILE:HD11 | 1.96 | 0.48 |
| 13:1:112:TYR:O | 13:1:119:THR:HA | 2.14 | 0.48 |
| 2:B:65:GLU:HG3 | 2:B:66:LYS:HG3 | 1.96 | 0.48 |
| 5:E:172:ALA:HB2 | 5:E:196:ALA:O | 2.14 | 0.48 |
| 8:H:32:ALA:HB2 | 8:H:189:ARG:NH1 | 2.27 | 0.48 |
| 12:L:165:ARG:NH2 | 8:V:29:LYS:HE2 | 2.29 | 0.48 |
| 1:O:32:LYS:HA | 1:O:32:LYS:CE | 2.41 | 0.48 |
| 2:P:186:VAL:HG21 | 2:P:216:ARG:HD3 | 1.96 | 0.48 |
| 3:Q:226:SER:HB2 | 3:Q:227:GLU:OE1 | 2.13 | 0.48 |
| 4:R:18:GLU:OE2 | 4:R:18:GLU:N | 2.45 | 0.48 |
| 4:R:227:GLU:OE2 | 4:R:227:GLU:N | 2.45 | 0.48 |
| 13:M:165:ARG:NH1 | 8:V:139:GLU:OE1 | 2.47 | 0.48 |
| 9:W:15:ALA:HB3 | 9:W:155:ILE:HD11 | 1.96 | 0.48 |
| 9:W:43:LEU:CG | 9:W:45:ILE:HD11 | 2.42 | 0.48 |
| 11:Y:66:HIS:CG | 11:Y:74:ILE:HD13 | 2.49 | 0.48 |
| 12:Z:33:LYS:HD2 | 12:Z:46:ASN:ND2 | 2.29 | 0.48 |
| 12:Z:5:GLY:O | 12:Z:124:CYS:HA | 2.13 | 0.48 |
| 13:1:190:LEU:HD12 | 13:1:190:LEU:N | 2.29 | 0.48 |
| 14:2:163:ILE:HD13 | 14:2:169:SER:CB | 2.37 | 0.48 |
| 14:2:40:LYS:C | 14:2:41:ILE:HD12 | 2.34 | 0.48 |
| 3:C:173:ARG:O | 3:C:177:GLU:HG3 | 2.13 | 0.48 |
| 3:C:97:GLN:HA | 3:C:97:GLN:HE21 | 1.77 | 0.48 |
| 1:O:32:LYS:HE2 | 1:O:32:LYS:CA | 2.42 | 0.48 |
| 2:P:65:GLU:HG3 | 2:P:66:LYS:HG3 | 1.96 | 0.48 |
| 3:Q:35:THR:OG1 | 3:Q:66:LYS:NZ | 2.45 | 0.48 |
| 8:V:116:HIS:HB2 | 17:V:1297:HOH:O | 2.12 | 0.48 |
| 8:V:37:ILE:HD11 | 8:V:43:CYS:CB | 2.43 | 0.48 |
| 10:X:11:SER:HB3 | 10:X:179:ASP:HB3 | 1.96 | 0.48 |
| 10:X:37:LEU:HD13 | 10:X:63:ILE:HD13 | 1.93 | 0.48 |
| 10:X:20:VAL:HG11 | 11:Y:120:LEU:HD11 | 1.96 | 0.48 |
| 13:1:14(C):ARG:NH1 | 13:1:14(C):ARG:HG3 | 2.26 | 0.47 |
| 14:2:103:GLY:HA2 | 14:2:178:LEU:HD23 | 1.96 | 0.47 |
| 14:2:18(G):TYR:HA | 14:2:18(J):LEU:HG | 1.95 | 0.47 |
| 1:A:62:GLU:H | 1:A:62:GLU:CD | 2.16 | 0.47 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:HG3 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:70:ILE:HD12 | 7:G:92:ALA:HB3 | 1.96 | 0.47 |
| 11:K:200:LYS:HG3 | 11:K:206:PHE:HB2 | 1.96 | 0.47 |
| 14:N:6:VAL:O | 14:N:12:VAL:HG23 | 2.14 | 0.47 |
| 14:N:132:THR:HA | 14:N:135:TYR:HD2 | 1.79 | 0.47 |
| 13:1:147:THR:OG1 | 13:1:150:VAL:HG23 | 2.14 | 0.47 |
| 2:B:239:THR:OXT | 2:B:239:THR:HG22 | 2.13 | 0.47 |
| 1:A:15:PHE:N | 2:B:23:GLN:HE22 | 2.00 | 0.47 |
| 4:D:70:ILE:HD12 | 4:D:92:ALA:CB | 2.43 | 0.47 |
| 5:E:213:ALA:HB1 | 5:E:223:ILE:CD1 | 2.44 | 0.47 |
| 10:J:34:THR:CG2 | 10:J:176:LYS:NZ | 2.77 | 0.47 |
| 1:O:52:LYS:HG3 | 1:O:211:GLU:HB2 | 1.96 | 0.47 |
| 3:Q:121:GLN:C | 3:Q:121:GLN:NE2 | 2.67 | 0.47 |
| 3:Q:70:ILE:HD11 | 3:Q:76:LEU:HD13 | 1.96 | 0.47 |
| 6:T:127:ASN:HD22 | 6:T:127:ASN:N | 2.11 | 0.47 |
| 1:A:69:LEU:HD23 | 1:A:70:LEU:N | 2.29 | 0.47 |
| 2:B:141:TYR:C | 2:B:141:TYR:CD1 | 2.88 | 0.47 |
| 4:D:172:ALA:HB1 | 4:D:196:ILE:HG21 | 1.96 | 0.47 |
| 5:E:221:PHE:CE1 | 5:E:223:ILE:CD1 | 2.92 | 0.47 |
| 6:F:137:ILE:CD1 | 6:F:163:ALA:CB | 2.92 | 0.47 |
| 6:F:21(B):THR:O | 6:F:21(C):ASN:HB2 | 2.13 | 0.47 |
| 7:G:8:TYR:O | 7:G:12:ILE:CD1 | 2.60 | 0.47 |
| 8:V:207:PRO:HG2 | 8:V:210:THR:OG1 | 2.14 | 0.47 |
| 10:X:77:GLN:C | 10:X:77:GLN:NE2 | 2.68 | 0.47 |
| 6:F:203:GLU:O | 6:F:206:LYS:HD2 | 2.14 | 0.47 |
| 6:F:43:ASN:N | 6:F:43:ASN:HD22 | 2.11 | 0.47 |
| 8:H:5:GLY:HA3 | 8:H:110:LEU:HD11 | 1.96 | 0.47 |
| 9:I:43:LEU:HG | 9:I:45:ILE:HD11 | 1.97 | 0.47 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:N | 2.13 | 0.47 |
| 4:R:230:ALA:HA | 4:R:233:ILE:HD12 | 1.97 | 0.47 |
| 4:R:243:ALA:O | 4:R:244:GLU:CB | 2.62 | 0.47 |
| 8:V:170:GLY:O | 8:V:171:SER:HB2 | 2.15 | 0.47 |
| 8:V:32:ALA:HB2 | 8:V:189:ARG:NH1 | 2.30 | 0.47 |
| 10:X:58:TYR:HD2 | 10:X:59:ILE:HD12 | 1.79 | 0.47 |
| 7:G:197:MET:HG2 | 7:G:205:PHE:CE1 | 2.50 | 0.47 |
| 12:L:1:GLY:HA3 | 12:L:33:LYS:HZ2 | 1.80 | 0.47 |
| 14:N:120:HIS:HA | 17:N:1107:HOH:O | 2.15 | 0.47 |
| 2:P:69:LYS:HG3 | 2:P:221:GLN:OE1 | 2.15 | 0.47 |
| 6:T:203:GLU:O | 6:T:206:LYS:HD2 | 2.13 | 0.47 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:CB | 2.44 | 0.47 |
| 10:X:34:THR:CG2 | 10:X:176:LYS:HZ2 | 2.27 | 0.47 |
| 11:Y:78:ALA:O | 11:Y:82:ILE:HG13 | 2.13 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:2:132:THR:HA | 14:2:135:TYR:HD2 | 1.78 | 0.47 |
| 2:B:196:THR:O | 2:B:200:THR:HG23 | 2.14 | 0.47 |
| 4:D:243:ALA:O | 4:D:244:GLU:CB | 2.62 | 0.47 |
| 5:E:31:ILE:HD12 | 5:E:31:ILE:N | 2.30 | 0.47 |
| 8:H:207:PRO:HG2 | 8:H:210:THR:OG1 | 2.15 | 0.47 |
| 12:L:21:ILE:HD12 | 8:V:167:LEU:HD13 | 1.96 | 0.47 |
| 14:N:85:GLU:O | 14:N:89:GLU:HB2 | 2.14 | 0.47 |
| 6:T:127:ASN:ND2 | 6:T:127:ASN:C | 2.68 | 0.47 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:N | 2.30 | 0.47 |
| 10:J:144:PRO:HG3 | 11:Y:207:ASN:HD21 | 1.80 | 0.47 |
| 14:2:19:ARG:HG3 | 14:2:26:ILE:HG23 | 1.97 | 0.47 |
| 1:A:100:TYR:CA | 1:A:10(A):ILE:HD13 | 2.44 | 0.47 |
| 3:C:15:PHE:CE1 | 3:C:21:ILE:HD11 | 2.50 | 0.47 |
| 9:I:10(C):SER:C | 9:I:107:LYS:H | 2.17 | 0.47 |
| 9:I:43:LEU:HG | 9:I:45:ILE:CD1 | 2.45 | 0.47 |
| 14:N:6:VAL:HG21 | 14:N:155:ILE:HD11 | 1.97 | 0.47 |
| 1:O:150:GLN:O | 1:O:157:TYR:HA | 2.15 | 0.47 |
| 1:O:26:TYR:CD1 | 7:U:17:PRO:HA | 2.50 | 0.47 |
| 1:O:4:MET:CG | 1:O:5:THR:H | 2.26 | 0.47 |
| 5:S:28:LEU:HA | 5:S:31:ILE:HD12 | 1.97 | 0.47 |
| 5:S:54:ASN:ND2 | 5:S:56:ASP:O | 2.48 | 0.47 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:NH1 | 2.30 | 0.47 |
| 9:W:10(C):SER:C | 9:W:107:LYS:H | 2.18 | 0.47 |
| 12:Z:-8:PHE:CB | 13:1:-8:THR:HG23 | 2.45 | 0.47 |
| 1:A:31:VAL:HG11 | 1:A:135:SER:HB2 | 1.97 | 0.47 |
| 2:B:44:ASP:OD1 | 2:B:185:LYS:HE3 | 2.14 | 0.47 |
| 8:H:7:LYS:HG3 | 8:H:123:TYR:HA | 1.96 | 0.47 |
| 12:L:-7:ASN:ND2 | 12:L:-7:ASN:C | 2.67 | 0.47 |
| 3:Q:46:VAL:HB | 3:Q:215:VAL:CG1 | 2.44 | 0.47 |
| 11:Y:16:VAL:HG21 | 11:Y:34:VAL:HG23 | 1.96 | 0.47 |
| 12:Z:35:PHE:CD2 | 12:Z:56:VAL:HG11 | 2.50 | 0.47 |
| 2:B:15:PHE:H | 3:C:23:GLN:NE2 | 1.95 | 0.47 |
| 2:B:229:ILE:O | 2:B:233:LEU:HB2 | 2.15 | 0.47 |
| 6:F:127:ASN:N | 6:F:127:ASN:HD22 | 2.11 | 0.47 |
| 11:Y:12:ILE:HD12 | 11:Y:110:ILE:CD1 | 2.44 | 0.47 |
| 12:Z:21:ILE:HG12 | 12:Z:22:THR:N | 2.30 | 0.47 |
| 3:C:177:GLU:OE2 | 4:D:57:PRO:HD2 | 2.15 | 0.47 |
| 8:H:84:LYS:HE2 | 8:H:119:THR:HG23 | 1.96 | 0.47 |
| 10:J:19:ALA:HB2 | 10:J:171:LYS:HG2 | 1.96 | 0.47 |
| 12:L:-8:PHE:HB3 | 13:M:-8:THR:HG23 | 1.97 | 0.47 |
| 3:Q:55:THR:C | 3:Q:56:LEU:HD22 | 2.36 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:V:100:ILE:HD11 | 8:V:127:LEU:HG | 1.96 | 0.47 |
| 2:B:122:GLY:C | 2:B:124:THR:H | 2.18 | 0.47 |
| 5:E:38:VAL:HG22 | 5:E:164:ALA:HB2 | 1.96 | 0.47 |
| 5:E:2(C):VAL:CG1 | 5:E:2(D):ASP:N | 2.77 | 0.47 |
| 10:J:69:ARG:HD2 | 17:J:514:HOH:O | 2.15 | 0.47 |
| 11:K:20:ALA:HA | 16:K:2(I):H10:O11 | 2.15 | 0.47 |
| 12:L:21:ILE:HB | 12:L:25:SER:O | 2.15 | 0.47 |
| 3:Q:163:GLN:NE2 | 3:Q:163:GLN:CA | 2.74 | 0.47 |
| 3:Q:232:TYR:O | 3:Q:236:ILE:HG13 | 2.14 | 0.47 |
| 5:S:67:ILE:HD13 | 5:S:77:SER:CB | 2.44 | 0.47 |
| 9:W:-8:SER:O | 9:W:-6:PRO:HD3 | 2.15 | 0.47 |
| 12:Z:85:HIS:CE1 | 17:Z:197:HOH:O | 2.68 | 0.47 |
| 13:1:110:LEU:HG | 13:1:125:LEU:HD12 | 1.96 | 0.46 |
| 2:B:21(A):LYS:O | 2:B:21(B):GLY:C | 2.53 | 0.46 |
| 3:C:159:SER:O | 4:D:59:LEU:HD22 | 2.15 | 0.46 |
| 12:L:185:ARG:NH1 | 12:L:185:ARG:HB3 | 2.29 | 0.46 |
| 2:P:21(A):LYS:O | 2:P:21(B):GLY:C | 2.53 | 0.46 |
| 3:Q:134:VAL:HG12 | 3:Q:135:SER:N | 2.31 | 0.46 |
| 6:T:142:ASP:O | 6:T:144:ASN:N | 2.48 | 0.46 |
| 7:U:177:GLU:O | 7:U:17(B):LYS:HG3 | 2.14 | 0.46 |
| 8:V:137:VAL:HG21 | 8:V:161:ALA:HB2 | 1.98 | 0.46 |
| 6:F:192:GLN:O | 6:F:196:ILE:HG12 | 2.15 | 0.46 |
| 7:G:107:MET:HE3 | 7:G:112:LEU:HB2 | 1.98 | 0.46 |
| 7:G:234:VAL:O | 7:G:237:ALA:HB3 | 2.15 | 0.46 |
| 2:P:229:ILE:O | 2:P:233:LEU:HB2 | 2.15 | 0.46 |
| 3:Q:149:TYR:CE1 | 3:Q:159:SER:HB3 | 2.50 | 0.46 |
| 12:Z:8:GLY:HA3 | 12:Z:11:PHE:CZ | 2.51 | 0.46 |
| 12:Z:134:ILE:O | 12:Z:137:PHE:HB3 | 2.15 | 0.46 |
| 13:1:3:VAL:O | 13:1:126:ALA:HA | 2.15 | 0.46 |
| 14:2:8:PHE:CE1 | 14:2:10:ASP:HB2 | 2.51 | 0.46 |
| 1:A:27:ALA:O | 1:A:31:VAL:HG23 | 2.15 | 0.46 |
| 3:C:158:SER:CB | 4:D:59:LEU:HD21 | 2.45 | 0.46 |
| 4:D:227:GLU:OE2 | 4:D:227:GLU:N | 2.46 | 0.46 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:N | 2.30 | 0.46 |
| 7:G:118:ASN:O | 7:G:122:ILE:HD13 | 2.15 | 0.46 |
| 7:G:141:VAL:HG21 | 7:G:216:THR:HA | 1.96 | 0.46 |
| 13:M:3:VAL:O | 13:M:126:ALA:HA | 2.15 | 0.46 |
| 13:M:91:ARG:HG3 | 13:M:92:SER:N | 2.29 | 0.46 |
| 14:N:175:MET:HB2 | 14:N:187:LEU:HB2 | 1.96 | 0.46 |
| 5:S:67:ILE:HG21 | 5:S:213:ALA:HB2 | 1.97 | 0.46 |
| 6:T:127:ASN:HD22 | 6:T:127:ASN:C | 2.19 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:U:225:SER:O | 7:U:229:ILE:HG13 | 2.15 | 0.46 |
| 10:X:45:PHE:HB3 | 10:X:99:VAL:HG12 | 1.96 | 0.46 |
| 12:L:163:THR:HG23 | 17:L:1264:HOH:O | 2.15 | 0.46 |
| 3:Q:57:LYS:HD2 | 3:Q:58:LEU:N | 2.31 | 0.46 |
| 5:S:69:LYS:HB3 | 17:S:528:HOH:O | 2.16 | 0.46 |
| 5:S:15:PHE:N | 6:T:23:GLN:HE22 | 2.04 | 0.46 |
| 7:U:87:ASN:HD22 | 7:U:88:ALA:N | 2.14 | 0.46 |
| 14:2:3:ILE:HD13 | 14:2:3:ILE:N | 2.30 | 0.46 |
| 1:A:24:ILE:H | 1:A:24:ILE:HD12 | 1.81 | 0.46 |
| 3:C:167:ARG:O | 3:C:168:ASN:HB2 | 2.16 | 0.46 |
| 3:C:57:LYS:HD2 | 3:C:58:LEU:N | 2.30 | 0.46 |
| 5:E:52:LYS:O | 5:E:63:TYR:HD2 | 1.98 | 0.46 |
| 7:G:31:THR:HG21 | 7:G:135:ILE:HG12 | 1.96 | 0.46 |
| 11:K:46:ALA:HB3 | 11:K:98:GLY:O | 2.15 | 0.46 |
| 2:P:141:TYR:C | 2:P:141:TYR:CD1 | 2.88 | 0.46 |
| 2:P:5:SER:O | 2:P:7:ARG:N | 2.49 | 0.46 |
| 4:R:101:LEU:CD1 | 11:Y:57:THR:HG22 | 2.45 | 0.46 |
| 4:R:170:GLU:OE1 | 4:R:170:GLU:N | 2.49 | 0.46 |
| 7:U:70:ILE:HD12 | 7:U:74:ILE:CG2 | 2.43 | 0.46 |
| 8:V:7:LYS:HG3 | 8:V:123:TYR:HA | 1.97 | 0.46 |
| 10:X:185:ARG:NH1 | 10:X:185:ARG:HG2 | 2.29 | 0.46 |
| 1:A:13:THR:CG2 | 1:A:24:ILE:CD1 | 2.94 | 0.46 |
| 2:B:41:MET:HE3 | 17:B:240:HOH:O | 2.15 | 0.46 |
| 4:D:170:GLU:N | 4:D:170:GLU:OE1 | 2.49 | 0.46 |
| 4:D:79:SER:HB3 | 4:D:165:ILE:HD12 | 1.96 | 0.46 |
| 5:E:69:LYS:HB3 | 17:E:684:HOH:O | 2.14 | 0.46 |
| 9:I:114:ASP:OD2 | 9:I:116:ILE:CD1 | 2.61 | 0.46 |
| 10:J:11:SER:HB3 | 10:J:179:ASP:HB3 | 1.96 | 0.46 |
| 13:M:184:LEU:HD23 | 13:M:185:THR:N | 2.30 | 0.46 |
| 2:P:122:GLY:C | 2:P:124:THR:H | 2.19 | 0.46 |
| 2:P:190:ILE:HG23 | 2:P:212:PHE:CE2 | 2.50 | 0.46 |
| 4:R:14:THR:HG22 | 4:R:15:PHE:N | 2.30 | 0.46 |
| 4:R:79:SER:HB3 | 4:R:165:ILE:HD12 | 1.96 | 0.46 |
| 5:S:86:ARG:HH11 | 5:S:86:ARG:HG3 | 1.81 | 0.46 |
| 6:T:70:VAL:HG11 | 6:T:112:PHE:CE1 | 2.50 | 0.46 |
| 11:Y:79:ALA:HA | 11:Y:82:ILE:HD12 | 1.98 | 0.46 |
| 12:Z:8:GLY:O | 12:Z:108:GLY:HA3 | 2.15 | 0.46 |
| 5:E:220:PRO:O | 5:E:221:PHE:C | 2.54 | 0.46 |
| 6:F:229:LEU:O | 6:F:233:ILE:HD12 | 2.16 | 0.46 |
| 1:A:130:ARG:NH2 | 7:G:124:THR:HG22 | 2.18 | 0.46 |
| 1:O:198:LYS:HE3 | 1:O:236:LEU:HD11 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:121:GLN:CG | 3:Q:83:ALA:HB1 | 2.46 | 0.46 |
| 4:R:75:GLY:HA3 | 4:R:221:PHE:CE2 | 2.50 | 0.46 |
| 6:T:109:ILE:CG2 | 6:T:147:HIS:HB2 | 2.42 | 0.46 |
| 7:U:25:GLU:O | 7:U:28:PHE:HB2 | 2.16 | 0.46 |
| 1:A:130:ARG:HG3 | 1:A:130:ARG:HH11 | 1.81 | 0.46 |
| 3:C:134:VAL:HG12 | 3:C:135:SER:N | 2.30 | 0.46 |
| 4:D:68:VAL:HG21 | 4:D:89:ILE:HD13 | 1.97 | 0.46 |
| 7:G:49:ILE:CD1 | 7:G:193:ALA:CB | 2.90 | 0.46 |
| 8:H:45:GLY:HA2 | 8:H:99:LEU:HD23 | 1.97 | 0.46 |
| 3:Q:215:VAL:O | 3:Q:215:VAL:HG13 | 2.16 | 0.46 |
| 2:P:121:GLN:HG3 | 3:Q:83:ALA:HB1 | 1.98 | 0.46 |
| 5:S:213:ALA:HB1 | 5:S:223:ILE:CD1 | 2.46 | 0.46 |
| 8:V:45:GLY:HA2 | 8:V:99:LEU:HD23 | 1.98 | 0.46 |
| 8:H:165:ASN:ND2 | 13:I:139:ARG:HH11 | 2.14 | 0.46 |
| 1:A:4:MET:CG | 1:A:5:THR:H | 2.25 | 0.46 |
| 2:B:190:ILE:HG23 | 2:B:212:PHE:CE2 | 2.50 | 0.46 |
| 3:C:212:ILE:HD13 | 3:C:229:ILE:HG23 | 1.98 | 0.46 |
| 5:E:139:ILE:HD12 | 5:E:215:VAL:HG12 | 1.98 | 0.46 |
| 2:B:100:LEU:HG | 9:I:60:ARG:NH2 | 2.31 | 0.46 |
| 11:K:126:CYS:HB2 | 11:K:135:TYR:CZ | 2.51 | 0.46 |
| 14:N:8:PHE:CE1 | 14:N:10:ASP:HB2 | 2.51 | 0.46 |
| 3:Q:159:SER:O | 4:R:59:LEU:HD22 | 2.16 | 0.46 |
| 3:Q:93:ARG:HD2 | 17:Q:314:HOH:O | 2.16 | 0.46 |
| 4:R:160:TYR:CZ | 4:R:163:LYS:HD3 | 2.51 | 0.46 |
| 4:D:185:THR:OG1 | 4:D:188:GLU:HG3 | 2.14 | 0.46 |
| 6:F:137:ILE:CD1 | 6:F:163:ALA:HB3 | 2.45 | 0.46 |
| 8:H:137:VAL:HG21 | 8:H:161:ALA:HB2 | 1.97 | 0.46 |
| 12:L:134:ILE:O | 12:L:137:PHE:HB3 | 2.16 | 0.46 |
| 14:N:147:SER:OG | 14:N:150:GLU:HG3 | 2.16 | 0.46 |
| 4:R:196:ILE:H | 4:R:196:ILE:HD12 | 1.81 | 0.46 |
| 6:T:192:GLN:O | 6:T:196:ILE:HG12 | 2.16 | 0.46 |
| 8:H:159:ILE:HD13 | 8:H:173:VAL:CG1 | 2.47 | 0.45 |
| 12:L:82:ASN:C | 12:L:82:ASN:HD22 | 2.20 | 0.45 |
| 13:M:112:TYR:C | 13:M:112:TYR:CD2 | 2.89 | 0.45 |
| 13:M:147:THR:HB | 13:M:149:GLN:NE2 | 2.31 | 0.45 |
| 13:M:-6:GLN:HG3 | 13:M:-6:GLN:O | 2.15 | 0.45 |
| 5:S:150:GLU:O | 5:S:157:VAL:HA | 2.16 | 0.45 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:CE | 2.79 | 0.45 |
| 7:U:18(M):SER:HB2 | 7:U:187:GLU:OE2 | 2.16 | 0.45 |
| 8:V:5:GLY:HA3 | 8:V:110:LEU:HD11 | 1.98 | 0.45 |
| 10:J:144:PRO:CG | 11:Y:207:ASN:HD21 | 2.29 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:169:SER:HA | 3:C:172:VAL:CG1 | 2.47 | 0.45 |
| 3:C:232:TYR:O | 3:C:236:ILE:HG13 | 2.16 | 0.45 |
| 5:E:43:ASN:HB2 | 5:E:183:ASP:OD1 | 2.16 | 0.45 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:NE2 | 2.31 | 0.45 |
| 7:G:72:ARG:NH1 | 7:G:72:ARG:HB2 | 2.31 | 0.45 |
| 11:K:7:ARG:CG | 11:K:108:PRO:HB2 | 2.40 | 0.45 |
| 11:K:12:ILE:HD13 | 11:K:110:ILE:CD1 | 2.45 | 0.45 |
| 12:L:140:ASN:O | 12:L:144:PHE:HA | 2.16 | 0.45 |
| 8:V:15:ALA:HB1 | 8:V:159:ILE:HD13 | 1.98 | 0.45 |
| 10:X:17:SER:HB2 | 10:X:170:PHE:HB2 | 1.98 | 0.45 |
| 14:2:85:GLU:O | 14:2:89:GLU:HB2 | 2.15 | 0.45 |
| 1:A:179:ARG:CB | 1:A:179:ARG:HH11 | 2.22 | 0.45 |
| 3:C:52:ARG:HB2 | 3:C:209:ASN:HA | 1.98 | 0.45 |
| 1:A:7:ARG:NH1 | 5:E:127:TYR:HD2 | 2.14 | 0.45 |
| 9:I:192:ARG:HD3 | 17:I:1187:HOH:O | 2.15 | 0.45 |
| 9:I:89:GLU:O | 9:I:90:ARG:NH1 | 2.48 | 0.45 |
| 11:K:172:SER:CA | 11:K:192:VAL:HG23 | 2.47 | 0.45 |
| 13:M:29:ASN:N | 17:M:802:HOH:O | 2.50 | 0.45 |
| 1:O:130:ARG:HH11 | 1:O:130:ARG:HG3 | 1.82 | 0.45 |
| 2:P:6:ARG:HG2 | 3:Q:10:ARG:NH2 | 2.32 | 0.45 |
| 5:S:139:ILE:HG22 | 5:S:148:LEU:HD13 | 1.96 | 0.45 |
| 5:S:95:GLN:HG3 | 5:S:115:LEU:HD13 | 1.97 | 0.45 |
| 7:U:70:ILE:HA | 7:U:93:LYS:HG2 | 1.99 | 0.45 |
| 10:X:189:ASP:HA | 10:X:191:GLN:OE1 | 2.16 | 0.45 |
| 10:X:52:THR:HG22 | 10:X:53:VAL:H | 1.81 | 0.45 |
| 1:A:52:LYS:HG3 | 1:A:211:GLU:HB2 | 1.96 | 0.45 |
| 2:B:107:ILE:CD1 | 2:B:112:LEU:H | 2.28 | 0.45 |
| 4:D:12:VAL:HG23 | 4:D:12(A):GLY:HA2 | 1.98 | 0.45 |
| 5:E:15:PHE:N | 6:F:23:GLN:HE22 | 2.05 | 0.45 |
| 10:J:45:PHE:HB3 | 10:J:99:VAL:HG12 | 1.97 | 0.45 |
| 10:J:52:THR:HG22 | 10:J:53:VAL:H | 1.81 | 0.45 |
| 11:K:35:ILE:HD11 | 11:K:45:MET:HB2 | 1.99 | 0.45 |
| 2:P:228:GLU:O | 2:P:232:ILE:HG22 | 2.17 | 0.45 |
| 2:P:235:LYS:C | 2:P:237:GLY:N | 2.69 | 0.45 |
| 3:Q:167:ARG:O | 3:Q:168:ASN:HB2 | 2.16 | 0.45 |
| 3:Q:169:SER:HA | 3:Q:172:VAL:CG1 | 2.46 | 0.45 |
| 5:S:38:VAL:HG12 | 5:S:39:GLY:N | 2.31 | 0.45 |
| 7:U:18(D):ILE:O | 7:U:18(G):GLU:N | 2.49 | 0.45 |
| 7:U:234:VAL:O | 7:U:237:ALA:HB3 | 2.16 | 0.45 |
| 11:Y:6:PHE:HA | 11:Y:123:ASP:O | 2.17 | 0.45 |
| 6:F:32:GLU:HB3 | 6:F:169:ARG:NH2 | 2.31 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:O:31:VAL:HG13 | 1:O:79:SER:O | 2.16 | 0.45 |
| 2:P:138:TYR:HB2 | 2:P:149:TYR:HB2 | 1.98 | 0.45 |
| 2:P:222:LYS:NZ | 2:P:228:GLU:OE2 | 2.46 | 0.45 |
| 3:Q:15:PHE:CD1 | 3:Q:21:ILE:CD1 | 2.99 | 0.45 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:N | 2.28 | 0.45 |
| 7:U:139:VAL:HA | 7:U:147:SER:O | 2.16 | 0.45 |
| 7:U:197:MET:HG2 | 7:U:205:PHE:CE1 | 2.51 | 0.45 |
| 8:H:167:LEU:HB3 | 12:Z:167:ILE:HD13 | 1.99 | 0.45 |
| 12:Z:14(I):THR:O | 12:Z:1(I):ASN:HB3 | 2.16 | 0.45 |
| 12:Z:33:LYS:NZ | 17:Z:754:HOH:O | 2.49 | 0.45 |
| 12:Z:6:ILE:HG12 | 12:Z:124:CYS:CB | 2.47 | 0.45 |
| 13:1:178:ILE:N | 13:1:178:ILE:HD12 | 2.32 | 0.45 |
| 14:2:132:THR:HA | 14:2:135:TYR:CD2 | 2.52 | 0.45 |
| 3:C:79:SER:HB2 | 3:C:165:ILE:HD12 | 1.98 | 0.45 |
| 4:D:75:GLY:HA3 | 4:D:221:PHE:CE2 | 2.51 | 0.45 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:HD13 | 1.99 | 0.45 |
| 8:H:36:ARG:HG3 | 8:H:38:SER:O | 2.17 | 0.45 |
| 8:H:49:ALA:HB1 | 9:I:118:CYS:SG | 2.56 | 0.45 |
| 12:L:11:PHE:CE1 | 12:L:148:VAL:HA | 2.51 | 0.45 |
| 5:S:139:ILE:HD12 | 5:S:215:VAL:HG12 | 1.98 | 0.45 |
| 6:T:24:VAL:O | 6:T:27:ALA:HB3 | 2.17 | 0.45 |
| 7:U:46:THR:HG21 | 7:U:139:VAL:HB | 1.99 | 0.45 |
| 9:W:80:THR:HG23 | 9:W:113:PHE:CE1 | 2.52 | 0.45 |
| 9:W:43:LEU:HG | 9:W:45:ILE:CD1 | 2.47 | 0.45 |
| 11:Y:7:ARG:CG | 11:Y:108:PRO:HB2 | 2.38 | 0.45 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:H | 1.82 | 0.45 |
| 14:2:18(A):ILE:HD12 | 14:2:18(C):TYR:CE2 | 2.52 | 0.45 |
| 1:A:197:LEU:HD21 | 1:A:210:ILE:HD12 | 1.99 | 0.45 |
| 2:B:101:LYS:NZ | 10:J:85:GLN:NE2 | 2.64 | 0.45 |
| 2:B:21:LEU:O | 2:B:25:GLU:HG2 | 2.16 | 0.45 |
| 11:K:6:PHE:HA | 11:K:123:ASP:O | 2.16 | 0.45 |
| 11:K:64:ARG:HD2 | 17:K:959:HOH:O | 2.17 | 0.45 |
| 11:Y:7:ARG:CG | 11:Y:12:ILE:HD11 | 2.39 | 0.45 |
| 12:Z:40:ASN:HD21 | 12:Z:183:GLY:HA2 | 1.81 | 0.45 |
| 13:1:157:ASN:ND2 | 17:1:905:HOH:O | 2.45 | 0.45 |
| 1:A:38:LEU:C | 1:A:38:LEU:HD12 | 2.36 | 0.45 |
| 2:B:171:ALA:O | 2:B:175:LEU:HG | 2.17 | 0.45 |
| 2:B:97:GLN:NE2 | 17:B:246:HOH:O | 2.49 | 0.45 |
| 12:L:14(I):THR:O | 12:L:1(I):ASN:HB3 | 2.16 | 0.45 |
| 1:O:212:LEU:C | 1:O:212:LEU:HD23 | 2.37 | 0.45 |
| 3:Q:190:VAL:HG13 | 3:Q:212:ILE:HG21 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:90:TYR:O | 11:Y:91:LYS:C | 2.55 | 0.45 |
| 14:2:66:TYR:CD2 | 14:2:74:PRO:HB3 | 2.52 | 0.45 |
| 4:D:50:VAL:HG22 | 4:D:67:ILE:CD1 | 2.44 | 0.45 |
| 6:F:142:ASP:O | 6:F:144:ASN:N | 2.50 | 0.45 |
| 6:F:109:ILE:HG22 | 6:F:149:TYR:CE2 | 2.52 | 0.45 |
| 7:G:25:GLU:O | 7:G:28:PHE:HB2 | 2.17 | 0.45 |
| 13:M:19:LEU:HD12 | 13:M:28:PHE:O | 2.17 | 0.45 |
| 14:N:103:GLY:HA2 | 14:N:178:LEU:HD23 | 1.99 | 0.45 |
| 1:O:69:LEU:HD23 | 1:O:70:LEU:N | 2.32 | 0.45 |
| 10:X:185:ARG:NH1 | 17:X:730:HOH:O | 2.50 | 0.45 |
| 2:B:235:LYS:C | 2:B:237:GLY:N | 2.70 | 0.45 |
| 4:D:122:ARG:HG2 | 4:D:122:ARG:HH11 | 1.81 | 0.45 |
| 5:E:38:VAL:HG12 | 5:E:39:GLY:N | 2.32 | 0.45 |
| 5:E:86:ARG:HH11 | 5:E:86:ARG:HG3 | 1.82 | 0.45 |
| 8:H:179:GLU:OE2 | 8:H:182:LYS:HE2 | 2.16 | 0.45 |
| 12:L:90:LYS:HD3 | 12:L:95:TYR:CZ | 2.52 | 0.45 |
| 2:P:224:PHE:H | 2:P:224:PHE:HD2 | 1.65 | 0.45 |
| 4:R:197:LEU:O | 4:R:201:MET:HG3 | 2.17 | 0.45 |
| 4:R:45:GLY:HA2 | 4:R:146:TYR:CE1 | 2.52 | 0.45 |
| 3:Q:177:GLU:OE2 | 4:R:57:PRO:HD2 | 2.17 | 0.45 |
| 6:T:45:GLY:CA | 6:T:215:CYS:O | 2.65 | 0.45 |
| 12:L:192:LYS:HE3 | 8:V:195:ASN:HB3 | 1.99 | 0.45 |
| 2:P:111:ILE:HD11 | 10:X:70:GLU:HG2 | 1.99 | 0.45 |
| 13:1:112:TYR:CD2 | 13:1:112:TYR:C | 2.90 | 0.44 |
| 13:1:147:THR:HB | 13:1:149:GLN:NE2 | 2.31 | 0.44 |
| 1:A:212:LEU:C | 1:A:212:LEU:HD23 | 2.37 | 0.44 |
| 1:A:224:LEU:HB2 | 1:A:229:ILE:HD11 | 1.98 | 0.44 |
| 3:C:215:VAL:HG23 | 3:C:221:ILE:HG12 | 1.99 | 0.44 |
| 3:C:55:THR:HG22 | 3:C:56:LEU:CD2 | 2.42 | 0.44 |
| 5:E:198:SER:HA | 5:E:201:LEU:CG | 2.47 | 0.44 |
| 6:F:18(C):HIS:CE1 | 17:F:1343:HOH:O | 2.70 | 0.44 |
| 6:F:49:ALA:HA | 6:F:211:GLU:O | 2.17 | 0.44 |
| 7:G:18(M):SER:HB2 | 7:G:187:GLU:OE2 | 2.17 | 0.44 |
| 9:I:80:THR:HG23 | 9:I:113:PHE:CE1 | 2.52 | 0.44 |
| 10:J:143:ARG:HB2 | 10:J:146:MET:HG3 | 1.99 | 0.44 |
| 11:K:109:THR:C | 11:K:110:ILE:HD13 | 2.37 | 0.44 |
| 14:N:163:ILE:CG2 | 14:N:170:GLY:HA2 | 2.47 | 0.44 |
| 1:O:40:ILE:HD12 | 1:O:193:ALA:HB2 | 1.98 | 0.44 |
| 1:O:86:ARG:NE | 7:U:118:ASN:HD21 | 2.13 | 0.44 |
| 2:P:44:ASP:OD1 | 2:P:185:LYS:HE3 | 2.16 | 0.44 |
| 3:Q:220:ASP:C | 3:Q:221:ILE:HD12 | 2.37 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:R:117:CYS:SG | 4:R:157:PHE:HB3 | 2.57 | 0.44 |
| 4:R:122:ARG:HG2 | 4:R:122:ARG:HH11 | 1.82 | 0.44 |
| 9:W:29:ASN:C | 9:W:29:ASN:HD22 | 2.21 | 0.44 |
| 11:Y:14:VAL:HB | 11:Y:176:TYR:HB2 | 1.98 | 0.44 |
| 12:Z:140:ASN:O | 12:Z:144:PHE:HA | 2.17 | 0.44 |
| 3:C:121:GLN:C | 3:C:121:GLN:NE2 | 2.71 | 0.44 |
| 5:E:17:PRO:HA | 6:F:26:TYR:CD2 | 2.52 | 0.44 |
| 6:F:45:GLY:CA | 6:F:215:CYS:O | 2.65 | 0.44 |
| 8:H:9:ASN:OD1 | 8:H:10:ASN:N | 2.50 | 0.44 |
| 10:J:189:ASP:HA | 10:J:191:GLN:OE1 | 2.18 | 0.44 |
| 12:L:35:PHE:HA | 17:L:1224:HOH:O | 2.17 | 0.44 |
| 3:Q:125:GLN:HB2 | 4:R:130:ARG:HG2 | 1.99 | 0.44 |
| 8:V:37:ILE:HD12 | 8:V:37:ILE:N | 2.31 | 0.44 |
| 10:X:65:LEU:HD21 | 10:X:69:ARG:HH22 | 1.83 | 0.44 |
| 2:B:181:LYS:O | 2:B:184:MET:HG3 | 2.18 | 0.44 |
| 5:E:91:TYR:CD1 | 5:E:119:LYS:HD2 | 2.52 | 0.44 |
| 6:F:127:ASN:C | 6:F:127:ASN:HD22 | 2.20 | 0.44 |
| 6:F:127:ASN:ND2 | 6:F:127:ASN:C | 2.69 | 0.44 |
| 7:G:8:TYR:C | 7:G:10:ARG:N | 2.70 | 0.44 |
| 9:I:29:ASN:HD22 | 9:I:29:ASN:C | 2.20 | 0.44 |
| 10:J:35:ARG:O | 10:J:42:LEU:HD12 | 2.17 | 0.44 |
| 10:J:66:TYR:CE2 | 10:J:74:LEU:HG | 2.52 | 0.44 |
| 1:O:109:THR:O | 1:O:113:VAL:HG23 | 2.17 | 0.44 |
| 5:S:18(C):PHE:CD1 | 5:S:18(D):ILE:N | 2.85 | 0.44 |
| 7:U:170:GLN:NE2 | 7:U:174:THR:HG23 | 2.27 | 0.44 |
| 8:V:9:ASN:OD1 | 8:V:10:ASN:N | 2.51 | 0.44 |
| 10:X:37:LEU:HD13 | 10:X:63:ILE:HD11 | 1.98 | 0.44 |
| 13:1:-5:PRO:HD3 | 13:1:96:TRP:CE2 | 2.52 | 0.44 |
| 1:A:67:VAL:HG11 | 1:A:213:ALA:HB3 | 1.99 | 0.44 |
| 2:B:63:THR:O | 2:B:63:THR:HG22 | 2.18 | 0.44 |
| 7:G:131:PRO:HB3 | 17:G:243:HOH:O | 2.16 | 0.44 |
| 8:H:34:LEU:HA | 8:H:43:CYS:O | 2.18 | 0.44 |
| 12:L:8:GLY:HA3 | 12:L:11:PHE:CZ | 2.52 | 0.44 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:ND2 | 2.14 | 0.44 |
| 13:M:35:ILE:N | 13:M:35:ILE:HD12 | 2.33 | 0.44 |
| 2:P:63:THR:HG22 | 2:P:63:THR:O | 2.17 | 0.44 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:HG3 | 1.98 | 0.44 |
| 3:Q:197:LEU:O | 3:Q:201:VAL:HG23 | 2.18 | 0.44 |
| 3:Q:99:HIS:CG | 3:Q:107:VAL:HG12 | 2.52 | 0.44 |
| 8:V:36:ARG:HG3 | 8:V:38:SER:O | 2.17 | 0.44 |
| 8:V:3:ILE:CD1 | 8:V:46:ALA:HB2 | 2.48 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:V:63:ILE:CG2 | 8:V:74:PRO:HB3 | 2.46 | 0.44 |
| 8:V:63:ILE:HG23 | 8:V:74:PRO:HB3 | 2.00 | 0.44 |
| 12:Z:113:PHE:N | 12:Z:113:PHE:CD1 | 2.86 | 0.44 |
| 13:1:35:ILE:HD11 | 13:1:56:GLU:HG3 | 1.98 | 0.44 |
| 13:1:45:ILE:HG12 | 13:1:99:ILE:HG12 | 1.98 | 0.44 |
| 6:F:24:VAL:O | 6:F:27:ALA:HB3 | 2.17 | 0.44 |
| 11:K:119:ARG:HG2 | 17:K:1232:HOH:O | 2.18 | 0.44 |
| 13:M:191:GLN:HE21 | 13:M:191:GLN:HB3 | 1.59 | 0.44 |
| 7:U:13:THR:HB | 7:U:124:THR:O | 2.18 | 0.44 |
| 12:Z:11:PHE:CE1 | 12:Z:148:VAL:HA | 2.52 | 0.44 |
| 12:Z:185:ARG:HB3 | 12:Z:185:ARG:NH1 | 2.32 | 0.44 |
| 13:1:147:THR:HB | 13:1:149:GLN:HE22 | 1.83 | 0.44 |
| 14:2:147:SER:OG | 14:2:150:GLU:HG3 | 2.17 | 0.44 |
| 13:M:197:TRP:CH2 | 14:2:171:GLY:HA2 | 2.53 | 0.44 |
| 14:2:37:VAL:HG22 | 14:2:41:ILE:HG22 | 1.99 | 0.44 |
| 2:B:107:ILE:CD1 | 2:B:112:LEU:N | 2.78 | 0.44 |
| 3:C:149:TYR:CE1 | 3:C:159:SER:HB3 | 2.52 | 0.44 |
| 4:D:196:ILE:H | 4:D:196:ILE:HD12 | 1.83 | 0.44 |
| 4:D:45:GLY:HA2 | 4:D:146:TYR:CE1 | 2.52 | 0.44 |
| 5:E:31:ILE:HD12 | 5:E:31:ILE:H | 1.82 | 0.44 |
| 8:H:15:ALA:HB1 | 8:H:159:ILE:HD13 | 1.97 | 0.44 |
| 10:J:35:ARG:HA | 10:J:35:ARG:HD3 | 1.76 | 0.44 |
| 14:N:132:THR:HA | 14:N:135:TYR:CD2 | 2.52 | 0.44 |
| 2:P:171:ALA:O | 2:P:175:LEU:HG | 2.18 | 0.44 |
| 2:P:232:ILE:HG12 | 2:P:232:ILE:O | 2.18 | 0.44 |
| 3:Q:19:GLY:O | 4:R:30:ALA:HB2 | 2.17 | 0.44 |
| 4:R:42:THR:C | 4:R:44:GLU:H | 2.21 | 0.44 |
| 5:S:116:LEU:HA | 5:S:116:LEU:HD23 | 1.86 | 0.44 |
| 5:S:43:ASN:HB2 | 5:S:183:ASP:OD1 | 2.17 | 0.44 |
| 8:V:34:LEU:HA | 8:V:43:CYS:O | 2.17 | 0.44 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:N | 2.33 | 0.44 |
| 12:L:135:MET:HE3 | 9:W:165:ARG:NH2 | 2.32 | 0.44 |
| 13:M:184:LEU:C | 13:M:184:LEU:HD23 | 2.37 | 0.44 |
| 1:O:29:THR:O | 1:O:33:GLN:HG2 | 2.17 | 0.44 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:ND2 | 2.16 | 0.44 |
| 6:T:172:ALA:C | 6:T:176:LEU:HD23 | 2.38 | 0.44 |
| 6:T:18:ASP:OD1 | 6:T:20:ARG:HD3 | 2.17 | 0.44 |
| 10:X:70:GLU:O | 10:X:71:ASP:C | 2.56 | 0.44 |
| 11:Y:5:ALA:HA | 11:Y:13:ILE:O | 2.17 | 0.44 |
| 5:E:160:LEU:HD13 | 5:E:163:THR:HB | 1.99 | 0.44 |
| 9:I:35:PHE:CD1 | 9:I:45:ILE:HD13 | 2.53 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:160:ARG:HB2 | 13:M:192:VAL:HG13 | 2.00 | 0.44 |
| 1:O:190:ILE:HD11 | 1:O:214:ILE:HG22 | 1.99 | 0.44 |
| 1:O:47:VAL:CG2 | 1:O:212:LEU:HD21 | 2.48 | 0.44 |
| 5:S:220:PRO:O | 5:S:221:PHE:C | 2.55 | 0.44 |
| 7:U:35:ILE:HD11 | 7:U:53:LYS:CG | 2.46 | 0.44 |
| 9:W:155:ILE:HD13 | 9:W:155:ILE:C | 2.38 | 0.44 |
| 10:X:19:ALA:HB2 | 10:X:171:LYS:HG2 | 1.98 | 0.44 |
| 11:Y:126:CYS:HB2 | 11:Y:135:TYR:CZ | 2.53 | 0.44 |
| 11:Y:172:SER:CA | 11:Y:192:VAL:HG23 | 2.46 | 0.44 |
| 13:1:184:LEU:C | 13:1:184:LEU:HD23 | 2.38 | 0.44 |
| 14:2:6:VAL:O | 14:2:12:VAL:HG23 | 2.17 | 0.44 |
| 7:G:198:ILE:O | 7:G:202:GLY:N | 2.50 | 0.44 |
| 13:M:74:LEU:HB3 | 13:M:79:ILE:HD11 | 2.00 | 0.44 |
| 14:N:66:TYR:CD2 | 14:N:74:PRO:HB3 | 2.52 | 0.44 |
| 1:O:24:ILE:HD13 | 1:O:131:PRO:HG2 | 1.99 | 0.44 |
| 1:O:33:GLN:HE21 | 1:O:33:GLN:CA | 2.31 | 0.44 |
| 2:P:21:LEU:O | 2:P:25:GLU:HG2 | 2.17 | 0.44 |
| 10:X:93:ARG:CZ | 11:Y:91:LYS:HD3 | 2.48 | 0.44 |
| 1:A:150:GLN:O | 1:A:157:TYR:HA | 2.17 | 0.43 |
| 4:D:160:TYR:CZ | 4:D:163:LYS:HD3 | 2.52 | 0.43 |
| 4:D:18:GLU:OE2 | 4:D:18:GLU:N | 2.50 | 0.43 |
| 8:H:1:THR:CG2 | 8:H:2:THR:N | 2.80 | 0.43 |
| 1:O:17:PRO:HG3 | 2:P:26:TYR:CZ | 2.53 | 0.43 |
| 3:Q:123:TYR:CD1 | 3:Q:132:PHE:HE1 | 2.36 | 0.43 |
| 4:R:70:ILE:HB | 4:R:74:ILE:HG22 | 2.00 | 0.43 |
| 10:X:152:LEU:HD21 | 10:X:177:ILE:HD11 | 2.00 | 0.43 |
| 11:Y:12:ILE:HG23 | 11:Y:110:ILE:HD11 | 2.00 | 0.43 |
| 12:Z:90:LYS:HD3 | 12:Z:95:TYR:CZ | 2.53 | 0.43 |
| 2:B:20:ARG:NH1 | 2:B:20:ARG:HG2 | 2.33 | 0.43 |
| 2:B:5:SER:O | 2:B:7:ARG:N | 2.50 | 0.43 |
| 5:E:4:PHE:O | 5:E:6:ASN:N | 2.51 | 0.43 |
| 10:J:70:GLU:O | 10:J:71:ASP:C | 2.56 | 0.43 |
| 12:L:21:ILE:HD11 | 12:L:168:GLN:NE2 | 2.33 | 0.43 |
| 13:M:13:ILE:HB | 13:M:155:ILE:CD1 | 2.48 | 0.43 |
| 1:O:62:GLU:O | 1:O:64:LEU:N | 2.47 | 0.43 |
| 2:P:39:GLY:O | 2:P:162:ALA:HA | 2.18 | 0.43 |
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:NE | 2.14 | 0.43 |
| 4:R:90:GLU:OE2 | 11:Y:69:ARG:NH1 | 2.51 | 0.43 |
| 6:T:49:ALA:HA | 6:T:211:GLU:O | 2.18 | 0.43 |
| 5:S:114:HIS:HB3 | 6:T:86:ARG:NH2 | 2.33 | 0.43 |
| 9:W:61:TYR:C | 9:W:61:TYR:CD1 | 2.91 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:2:126:ILE:N | 14:2:126:ILE:CD1 | 2.81 | 0.43 |
| 1:A:13:THR:HG22 | 1:A:21:LEU:HD22 | 2.01 | 0.43 |
| 3:C:70:ILE:HD11 | 3:C:76:LEU:HD13 | 1.99 | 0.43 |
| 5:E:95:GLN:HG3 | 5:E:115:LEU:HD13 | 2.00 | 0.43 |
| 5:E:230:ALA:C | 5:E:232:TYR:H | 2.21 | 0.43 |
| 10:J:17:SER:HB2 | 10:J:170:PHE:HB2 | 2.00 | 0.43 |
| 12:L:42:VAL:CG2 | 12:L:102:ALA:HB3 | 2.47 | 0.43 |
| 12:L:113:PHE:CD1 | 12:L:113:PHE:N | 2.86 | 0.43 |
| 13:M:112:TYR:O | 13:M:119:THR:HA | 2.18 | 0.43 |
| 8:V:18:THR:HB | 8:V:30:ASN:HA | 2.00 | 0.43 |
| 14:2:38:HIS:HB3 | 14:2:41:ILE:HB | 2.01 | 0.43 |
| 2:B:231:ASP:O | 2:B:235:LYS:HG2 | 2.19 | 0.43 |
| 4:D:24:VAL:O | 4:D:28:LEU:HD13 | 2.18 | 0.43 |
| 6:F:39:GLY:HA3 | 6:F:137:ILE:HG21 | 2.00 | 0.43 |
| 7:G:70:ILE:HA | 7:G:93:LYS:HG2 | 2.01 | 0.43 |
| 10:J:34:THR:CG2 | 10:J:176:LYS:HZ2 | 2.31 | 0.43 |
| 12:L:8:GLY:O | 12:L:108:GLY:HA3 | 2.17 | 0.43 |
| 1:O:177:GLU:HG2 | 2:P:58:LEU:HD22 | 2.01 | 0.43 |
| 5:S:134:VAL:O | 5:S:153:PRO:HG3 | 2.19 | 0.43 |
| 5:S:216:GLY:O | 5:S:217:LYS:C | 2.57 | 0.43 |
| 8:V:192:LEU:HA | 8:V:192:LEU:HD23 | 1.77 | 0.43 |
| 12:L:135:MET:HE2 | 9:W:165:ARG:NH2 | 2.33 | 0.43 |
| 10:X:166:MET:HA | 10:X:167:PRO:HD3 | 1.72 | 0.43 |
| 2:B:10:SER:HB2 | 17:B:248:HOH:O | 2.18 | 0.43 |
| 2:B:17:PRO:HA | 3:C:26:TYR:CZ | 2.54 | 0.43 |
| 2:B:39:GLY:O | 2:B:162:ALA:HA | 2.19 | 0.43 |
| 4:D:215:ILE:O | 4:D:215:ILE:HD13 | 2.18 | 0.43 |
| 5:E:18(C):PHE:CD1 | 5:E:18(D):ILE:N | 2.86 | 0.43 |
| 6:F:157:TYR:C | 6:F:157:TYR:CD1 | 2.91 | 0.43 |
| 11:K:13:ILE:HD12 | 11:K:152:LEU:HD23 | 2.01 | 0.43 |
| 11:K:14:VAL:HB | 11:K:176:TYR:HB2 | 2.00 | 0.43 |
| 11:K:19:ARG:HG2 | 11:K:21:THR:HG23 | 2.01 | 0.43 |
| 12:L:52:GLY:O | 12:L:56:VAL:HG23 | 2.18 | 0.43 |
| 13:M:190:LEU:HD12 | 13:M:190:LEU:N | 2.33 | 0.43 |
| 1:O:67:VAL:HG11 | 1:O:213:ALA:HB3 | 1.99 | 0.43 |
| 2:P:120:LYS:HZ1 | 2:P:136:PHE:HD1 | 1.67 | 0.43 |
| 2:P:150:THR:O | 2:P:157:TYR:HA | 2.18 | 0.43 |
| 2:P:21(A):LYS:HG3 | 2:P:219:GLU:O | 2.18 | 0.43 |
| 2:P:234:VAL:HA | 2:P:239:THR:HA | 2.00 | 0.43 |
| 2:P:97:GLN:HG2 | 17:P:297:HOH:O | 2.19 | 0.43 |
| 8:V:49:ALA:HB1 | 9:W:118:CYS:SG | 2.58 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:186:LEU:HD21 | 1:A:214:ILE:HD12 | 2.01 | 0.43 |
| 2:B:194:LEU:O | 2:B:198:SER:HB2 | 2.19 | 0.43 |
| 5:E:207:LEU:O | 5:E:233:ILE:HD12 | 2.18 | 0.43 |
| 7:G:139:VAL:HA | 7:G:147:SER:O | 2.18 | 0.43 |
| 7:G:82:ILE:CG2 | 7:G:83:PRO:HD3 | 2.49 | 0.43 |
| 2:P:150:THR:HG22 | 2:P:160:TRP:HE1 | 1.84 | 0.43 |
| 5:S:4:PHE:O | 5:S:6:ASN:N | 2.52 | 0.43 |
| 6:T:21(B):THR:O | 6:T:21(C):ASN:HB2 | 2.18 | 0.43 |
| 8:V:1:THR:CG2 | 8:V:2:THR:N | 2.82 | 0.43 |
| 2:B:149:TYR:OH | 3:C:62(A):ILE:HB | 2.19 | 0.43 |
| 2:B:235:LYS:HD3 | 2:B:235:LYS:N | 2.34 | 0.43 |
| 3:C:123:TYR:CD1 | 3:C:132:PHE:HE1 | 2.37 | 0.43 |
| 5:E:116:LEU:HD23 | 5:E:116:LEU:HA | 1.88 | 0.43 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:CE | 2.81 | 0.43 |
| 7:G:47:VAL:CG1 | 7:G:49:ILE:HD11 | 2.48 | 0.43 |
| 13:M:42:VAL:CG2 | 13:M:178:ILE:HD11 | 2.48 | 0.43 |
| 2:P:20:ARG:NH1 | 2:P:20:ARG:HG2 | 2.33 | 0.43 |
| 4:R:192:LEU:O | 4:R:196:ILE:HD13 | 2.19 | 0.43 |
| 4:R:196:ILE:N | 4:R:196:ILE:HD12 | 2.34 | 0.43 |
| 5:S:67:ILE:HD11 | 5:S:77:SER:HB3 | 1.98 | 0.43 |
| 6:T:21:ASN:OD1 | 6:T:21:ASN:C | 2.57 | 0.43 |
| 11:Y:38:ASN:HB2 | 11:Y:39:PRO:HD2 | 2.00 | 0.43 |
| 11:Y:74:ILE:HG13 | 11:Y:75:SER:N | 2.33 | 0.43 |
| 14:2:8:PHE:HE1 | 14:2:10:ASP:HB2 | 1.84 | 0.43 |
| 1:A:175:PHE:O | 1:A:179:ARG:HG2 | 2.19 | 0.43 |
| 2:B:150:THR:O | 2:B:157:TYR:HA | 2.19 | 0.43 |
| 3:C:99:HIS:CG | 3:C:107:VAL:HG12 | 2.54 | 0.43 |
| 5:E:146:ALA:N | 17:E:1070:HOH:O | 2.51 | 0.43 |
| 7:G:220:LYS:HG2 | 7:G:221:PHE:N | 2.34 | 0.43 |
| 8:H:63:ILE:CG2 | 8:H:74:PRO:HB3 | 2.49 | 0.43 |
| 11:K:207:ASN:ND2 | 10:X:144:PRO:HD3 | 2.34 | 0.43 |
| 10:J:93:ARG:CZ | 11:K:91:LYS:HD3 | 2.49 | 0.43 |
| 12:L:185:ARG:NH1 | 17:L:1161:HOH:O | 2.38 | 0.43 |
| 12:L:3:ILE:CD1 | 12:L:3:ILE:N | 2.80 | 0.43 |
| 13:M:150:VAL:HG21 | 17:M:1069:HOH:O | 2.18 | 0.43 |
| 13:M:17:ASP:HA | 13:M:173:PHE:HB3 | 2.01 | 0.43 |
| 1:O:184:LEU:HB2 | 17:O:486:HOH:O | 2.19 | 0.43 |
| 5:S:136:LEU:HD12 | 5:S:151:PHE:CD2 | 2.54 | 0.43 |
| 5:S:2(C):VAL:HG13 | 5:S:2(D):ASP:N | 2.34 | 0.43 |
| 5:S:83:PRO:O | 5:S:86:ARG:HB3 | 2.18 | 0.43 |
| 7:U:67:ILE:HD12 | 7:U:211:GLU:CG | 2.44 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:V:100:ILE:CD1 | 8:V:112:SER:HB3 | 2.49 | 0.43 |
| 11:Y:46:ALA:HB3 | 11:Y:98:GLY:O | 2.18 | 0.43 |
| 12:Z:137:PHE:CE1 | 12:Z:141:GLN:HG3 | 2.53 | 0.43 |
| 1:A:188:ASP:O | 1:A:192:ILE:HG12 | 2.18 | 0.43 |
| 2:B:228:GLU:O | 2:B:232:ILE:HG22 | 2.19 | 0.43 |
| 2:B:222:LYS:NZ | 2:B:228:GLU:OE2 | 2.47 | 0.43 |
| 3:C:212:ILE:HD12 | 3:C:212:ILE:N | 2.33 | 0.43 |
| 3:C:215:VAL:O | 3:C:215:VAL:HG13 | 2.19 | 0.43 |
| 3:C:55:THR:C | 3:C:56:LEU:HD22 | 2.40 | 0.43 |
| 6:F:91:ARG:O | 6:F:95:GLU:HB2 | 2.19 | 0.43 |
| 10:J:18:LYS:CD | 10:J:174:ILE:HG13 | 2.45 | 0.43 |
| 12:L:148:VAL:O | 12:L:152:ILE:HG13 | 2.19 | 0.43 |
| 1:O:92:SER:O | 1:O:95:VAL:HG12 | 2.18 | 0.43 |
| 3:Q:156:ILE:HD12 | 3:Q:156:ILE:N | 2.33 | 0.43 |
| 7:U:74:ILE:HD12 | 7:U:109:CYS:HA | 2.00 | 0.43 |
| 9:W:174:VAL:HG21 | 9:W:186:LYS:HE3 | 2.01 | 0.43 |
| 14:N:140:LYS:NZ | 14:2:157:HIS:HD2 | 2.17 | 0.43 |
| 1:A:232:ARG:HG3 | 1:A:232:ARG:NH1 | 2.33 | 0.43 |
| 2:B:224:PHE:HD2 | 2:B:224:PHE:H | 1.66 | 0.43 |
| 3:C:160:TRP:NE1 | 4:D:59:LEU:HD23 | 2.34 | 0.43 |
| 6:F:130:ARG:HG2 | 6:F:130:ARG:HH11 | 1.84 | 0.43 |
| 6:F:179:LEU:HD11 | 6:F:192:GLN:CG | 2.49 | 0.43 |
| 9:I:6:MET:HE3 | 9:I:155:ILE:HA | 2.01 | 0.43 |
| 11:K:131:GLN:HG3 | 11:K:132:THR:N | 2.34 | 0.43 |
| 11:K:174:ASN:ND2 | 11:K:189:ASN:HB2 | 2.34 | 0.43 |
| 11:K:40:PHE:CD1 | 11:K:73:ARG:NH1 | 2.87 | 0.43 |
| 11:K:9:GLN:CD | 11:K:10:GLY:N | 2.71 | 0.43 |
| 14:N:14:LEU:N | 14:N:14:LEU:HD12 | 2.33 | 0.43 |
| 6:T:172:ALA:O | 6:T:173:LYS:C | 2.57 | 0.43 |
| 6:T:91:ARG:O | 6:T:95:GLU:HB2 | 2.19 | 0.43 |
| 11:Y:19:ARG:HG2 | 11:Y:21:THR:HG23 | 2.01 | 0.43 |
| 12:Z:134:ILE:HG22 | 12:Z:138:LEU:HD22 | 2.01 | 0.43 |
| 2:B:234:VAL:HA | 2:B:239:THR:HA | 2.00 | 0.42 |
| 3:C:227:GLU:OE1 | 3:C:227:GLU:N | 2.49 | 0.42 |
| 6:F:137:ILE:HD11 | 6:F:163:ALA:CB | 2.47 | 0.42 |
| 6:F:14:VAL:HG12 | 6:F:15:PHE:N | 2.33 | 0.42 |
| 8:H:101:VAL:HG12 | 8:H:113:ILE:CD1 | 2.48 | 0.42 |
| 9:I:3:VAL:HG22 | 9:I:16:CYS:HB3 | 2.01 | 0.42 |
| 11:K:40:PHE:HB3 | 11:K:73:ARG:NH2 | 2.33 | 0.42 |
| 11:K:5:ALA:HA | 11:K:13:ILE:O | 2.19 | 0.42 |
| 12:L:160:THR:O | 12:L:164:GLU:HG2 | 2.18 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:M:147:THR:HB | 13:M:149:GLN:HE22 | 1.84 | 0.42 |
| 2:P:113:VAL:HG22 | 2:P:138:TYR:CG | 2.54 | 0.42 |
| 4:R:23:GLN:HB3 | 4:R:131:PRO:HG2 | 2.01 | 0.42 |
| 6:T:103:TYR:O | 6:T:104:LYS:HB3 | 2.19 | 0.42 |
| 8:V:156:SER:HA | 8:V:159:ILE:HD12 | 2.00 | 0.42 |
| 2:B:147:GLN:HG2 | 3:C:62(A):ILE:HG21 | 2.00 | 0.42 |
| 3:C:190:VAL:HG13 | 3:C:212:ILE:HG21 | 2.01 | 0.42 |
| 3:C:225:SER:O | 3:C:226:SER:C | 2.58 | 0.42 |
| 6:F:52:LYS:HB2 | 6:F:209:GLU:O | 2.19 | 0.42 |
| 8:H:56:THR:HG22 | 8:H:57:GLN:N | 2.33 | 0.42 |
| 10:J:190:PHE:C | 10:J:192:ALA:H | 2.22 | 0.42 |
| 11:K:10(A):ARG:HD3 | 11:K:180:GLU:OE1 | 2.20 | 0.42 |
| 13:M:125:LEU:HA | 17:M:224:HOH:O | 2.19 | 0.42 |
| 4:R:79:SER:O | 4:R:134:VAL:HG23 | 2.18 | 0.42 |
| 11:Y:131:GLN:HG3 | 11:Y:132:THR:N | 2.34 | 0.42 |
| 12:Z:4:LEU:O | 12:Z:14:LEU:HD23 | 2.18 | 0.42 |
| 1:A:33:GLN:HE21 | 1:A:33:GLN:CA | 2.32 | 0.42 |
| 2:B:122:GLY:C | 2:B:124:THR:N | 2.73 | 0.42 |
| 3:C:161:SER:HB3 | 3:C:180:TYR:CE1 | 2.54 | 0.42 |
| 4:D:197:LEU:O | 4:D:201:MET:HG3 | 2.19 | 0.42 |
| 4:D:70:ILE:HB | 4:D:74:ILE:HG22 | 2.00 | 0.42 |
| 5:E:83:PRO:O | 5:E:86:ARG:HB3 | 2.19 | 0.42 |
| 6:F:172:ALA:O | 6:F:173:LYS:C | 2.57 | 0.42 |
| 6:F:66:LYS:HE3 | 6:F:82:ILE:HD12 | 2.01 | 0.42 |
| 7:G:229:ILE:O | 7:G:232:ARG:HB2 | 2.19 | 0.42 |
| 10:J:152:LEU:HD21 | 10:J:177:ILE:HD11 | 2.02 | 0.42 |
| 12:L:42:VAL:HG23 | 12:L:102:ALA:HB3 | 2.01 | 0.42 |
| 14:N:85:GLU:OE2 | 14:N:85:GLU:HA | 2.20 | 0.42 |
| 2:P:121:GLN:NE2 | 2:P:121:GLN:C | 2.73 | 0.42 |
| 4:R:86:ARG:HD3 | 4:R:86:ARG:HA | 1.79 | 0.42 |
| 7:U:152:ASP:HB2 | 7:U:153:PRO:CD | 2.49 | 0.42 |
| 7:U:82:ILE:N | 7:U:83:PRO:HD2 | 2.34 | 0.42 |
| 10:X:136:SER:HA | 17:X:559:HOH:O | 2.20 | 0.42 |
| 12:Z:82:ASN:C | 12:Z:82:ASN:HD22 | 2.20 | 0.42 |
| 12:Z:93:PHE:N | 12:Z:94:PRO:CD | 2.81 | 0.42 |
| 1:A:13:THR:CG2 | 1:A:24:ILE:HD11 | 2.43 | 0.42 |
| 4:D:230:ALA:HA | 4:D:233:ILE:HD12 | 2.00 | 0.42 |
| 4:D:70:ILE:HD11 | 4:D:89:ILE:HG23 | 2.01 | 0.42 |
| 7:G:35:ILE:HD11 | 7:G:53:LYS:CG | 2.47 | 0.42 |
| 7:G:87:ASN:HD22 | 7:G:88:ALA:N | 2.17 | 0.42 |
| 8:H:112:SER:OG | 8:H:120:ASP:HB2 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 9:I:174:VAL:HG21 | 9:I:186:LYS:HE3 | 2.01 | 0.42 |
| 9:I:93:GLY:N | 9:I:94:PRO:HD3 | 2.34 | 0.42 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:C | 2.39 | 0.42 |
| 2:P:194:LEU:HD13 | 2:P:233:LEU:HD12 | 2.01 | 0.42 |
| 5:S:160:LEU:HD13 | 5:S:163:THR:HB | 2.00 | 0.42 |
| 5:S:91:TYR:CD1 | 5:S:119:LYS:HD2 | 2.54 | 0.42 |
| 6:T:130:ARG:HG2 | 6:T:130:ARG:HH11 | 1.84 | 0.42 |
| 6:T:210:LEU:HD12 | 6:T:211:GLU:H | 1.85 | 0.42 |
| 6:T:39:GLY:HA3 | 6:T:137:ILE:HG21 | 2.02 | 0.42 |
| 8:V:179:GLU:OE2 | 8:V:182:LYS:HE2 | 2.19 | 0.42 |
| 1:A:207:ASN:HA | 1:A:233:LEU:CD1 | 2.49 | 0.42 |
| 3:C:197:LEU:O | 3:C:201:VAL:HG23 | 2.19 | 0.42 |
| 5:E:114:HIS:HB3 | 6:F:86:ARG:NH2 | 2.34 | 0.42 |
| 6:F:187:ARG:NH1 | 6:F:187:ARG:HG3 | 2.34 | 0.42 |
| 7:G:168:LYS:HD3 | 17:G:1365:HOH:O | 2.19 | 0.42 |
| 7:G:206:SER:O | 7:G:233:LEU:HD21 | 2.19 | 0.42 |
| 11:K:104:TYR:CE1 | 11:K:180:GLU:HB2 | 2.54 | 0.42 |
| 12:L:59:PHE:CD1 | 12:L:83:ILE:CD1 | 2.98 | 0.42 |
| 13:M:-5:PRO:HD3 | 13:M:96:TRP:CE2 | 2.54 | 0.42 |
| 1:O:160:TRP:CE3 | 1:O:163:THR:HB | 2.55 | 0.42 |
| 3:Q:47:VAL:CG1 | 3:Q:212:ILE:HG23 | 2.50 | 0.42 |
| 4:R:215:ILE:HD13 | 4:R:215:ILE:O | 2.20 | 0.42 |
| 5:S:18(C):PHE:C | 5:S:18(E):LYS:N | 2.73 | 0.42 |
| 6:T:157:TYR:C | 6:T:157:TYR:CD1 | 2.93 | 0.42 |
| 7:U:18(D):ILE:HG22 | 7:U:18(G):GLU:HB2 | 2.01 | 0.42 |
| 7:U:8:TYR:C | 7:U:10:ARG:N | 2.72 | 0.42 |
| 8:V:37:ILE:CD1 | 8:V:43:CYS:HB2 | 2.49 | 0.42 |
| 11:Y:104:TYR:CE1 | 11:Y:180:GLU:HB2 | 2.55 | 0.42 |
| 4:D:117:CYS:SG | 4:D:157:PHE:HB3 | 2.59 | 0.42 |
| 4:D:147:GLN:HG2 | 4:D:159:ARG:CZ | 2.49 | 0.42 |
| 3:C:97:GLN:HG3 | 10:J:65:LEU:HB2 | 2.00 | 0.42 |
| 13:M:100:ILE:HD13 | 13:M:112:TYR:CB | 2.47 | 0.42 |
| 5:S:18(C):PHE:C | 5:S:18(E):LYS:H | 2.23 | 0.42 |
| 5:S:226:GLY:O | 5:S:227:GLU:C | 2.58 | 0.42 |
| 6:T:202:HIS:CG | 6:T:202:HIS:O | 2.73 | 0.42 |
| 12:Z:42:VAL:CG2 | 12:Z:102:ALA:HB3 | 2.50 | 0.42 |
| 14:2:18(A):ILE:HD13 | 14:2:18(B):PHE:H | 1.75 | 0.42 |
| 14:2:48:SER:HB3 | 14:2:51:ASP:HB2 | 2.02 | 0.42 |
| 2:B:107:ILE:HD13 | 2:B:108:PRO:C | 2.36 | 0.42 |
| 2:B:20:ARG:HH11 | 2:B:20:ARG:HG2 | 1.85 | 0.42 |
| 2:B:232:ILE:O | 2:B:232:ILE:HG12 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D:42:THR:C | 4:D:44:GLU:H | 2.22 | 0.42 |
| 5:E:150:GLU:O | 5:E:157:VAL:HA | 2.20 | 0.42 |
| 6:F:54:ILE:HG12 | 6:F:208:PHE:HA | 2.02 | 0.42 |
| 14:N:171:GLY:HA2 | 13:1:197:TRP:CH2 | 2.55 | 0.42 |
| 2:P:215:ILE:N | 2:P:215:ILE:HD12 | 2.34 | 0.42 |
| 2:P:39:GLY:C | 2:P:148:LEU:HD21 | 2.40 | 0.42 |
| 6:T:151:LEU:HD13 | 6:T:157:TYR:HB3 | 2.02 | 0.42 |
| 7:U:118:ASN:O | 7:U:122:ILE:HD13 | 2.19 | 0.42 |
| 7:U:188:LYS:HA | 7:U:188:LYS:HD3 | 1.88 | 0.42 |
| 8:V:3:ILE:HG12 | 8:V:3:ILE:O | 2.19 | 0.42 |
| 11:Y:10(A):ARG:HD3 | 11:Y:180:GLU:OE1 | 2.20 | 0.42 |
| 12:Z:160:THR:O | 12:Z:164:GLU:HG2 | 2.20 | 0.42 |
| 1:A:29:THR:O | 1:A:33:GLN:HG2 | 2.19 | 0.42 |
| 3:C:224:LEU:HD12 | 3:C:224:LEU:N | 2.35 | 0.42 |
| 5:E:194:VAL:CG1 | 5:E:207:LEU:HD11 | 2.50 | 0.42 |
| 9:I:61:TYR:C | 9:I:61:TYR:CD1 | 2.93 | 0.42 |
| 11:K:76:VAL:HG12 | 11:K:111:TYR:HD2 | 1.85 | 0.42 |
| 4:R:147:GLN:HG2 | 4:R:159:ARG:CZ | 2.50 | 0.42 |
| 4:R:96:ALA:HA | 4:R:107:ILE:HG21 | 2.01 | 0.42 |
| 5:S:230:ALA:C | 5:S:232:TYR:H | 2.23 | 0.42 |
| 5:S:64:GLN:NE2 | 5:S:82:ALA:HB2 | 2.35 | 0.42 |
| 8:V:56:THR:HG22 | 8:V:57:GLN:N | 2.34 | 0.42 |
| 10:X:59:ILE:N | 10:X:59:ILE:HD12 | 2.35 | 0.42 |
| 11:Y:40:PHE:CD1 | 11:Y:73:ARG:NH1 | 2.88 | 0.42 |
| 12:Z:167:ILE:C | 12:Z:167:ILE:HD12 | 2.39 | 0.42 |
| 12:Z:76:ILE:CG2 | 12:Z:77:ASN:N | 2.83 | 0.42 |
| 14:2:98:GLY:C | 14:2:99:ILE:HD12 | 2.40 | 0.42 |
| 2:B:17:PRO:HA | 3:C:26:TYR:CE2 | 2.55 | 0.42 |
| 7:G:152:ASP:HB2 | 7:G:153:PRO:CD | 2.50 | 0.42 |
| 7:G:179:HIS:C | 7:G:179:HIS:ND1 | 2.73 | 0.42 |
| 7:G:187:GLU:O | 7:G:191:GLU:HG3 | 2.20 | 0.42 |
| 11:K:38:ASN:HB2 | 11:K:39:PRO:HD2 | 2.00 | 0.42 |
| 2:P:194:LEU:O | 2:P:198:SER:HB2 | 2.19 | 0.42 |
| 2:P:235:LYS:N | 2:P:235:LYS:HD3 | 2.34 | 0.42 |
| 5:S:194:VAL:CG1 | 5:S:207:LEU:HD11 | 2.50 | 0.42 |
| 6:T:14:VAL:HG12 | 6:T:15:PHE:N | 2.35 | 0.42 |
| 6:T:43:ASN:ND2 | 6:T:43:ASN:N | 2.67 | 0.42 |
| 7:U:179:HIS:ND1 | 7:U:179:HIS:C | 2.73 | 0.42 |
| 11:Y:76:VAL:HG22 | 11:Y:103:GLY:HA3 | 2.01 | 0.42 |
| 12:Z:145:TYR:HD1 | 12:Z:146:LEU:N | 2.17 | 0.42 |
| 12:Z:79:ALA:O | 12:Z:82:ASN:HB3 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:1:157:ASN:O | 13:1:161:VAL:HG23 | 2.20 | 0.42 |
| 8:H:139:GLU:OE1 | 13:1:165:ARG:NH1 | 2.53 | 0.42 |
| 14:2:14:LEU:HD12 | 14:2:14:LEU:N | 2.34 | 0.42 |
| 10:J:147:THR:HG23 | 10:J:150:GLU:OE2 | 2.20 | 0.42 |
| 10:J:3:ILE:HG23 | 17:J:195:HOH:O | 2.20 | 0.42 |
| 10:J:65:LEU:HD21 | 10:J:69:ARG:HH22 | 1.84 | 0.42 |
| 12:L:194:ASP:HB2 | 8:V:163:ILE:HG23 | 2.02 | 0.42 |
| 13:M:8:TYR:HB2 | 13:M:146:THR:O | 2.20 | 0.42 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:H | 1.84 | 0.42 |
| 1:O:136:LEU:O | 1:O:150:GLN:HA | 2.20 | 0.42 |
| 1:O:38:LEU:HD12 | 1:O:38:LEU:C | 2.40 | 0.42 |
| 2:P:101:LYS:HG3 | 9:W:57:GLU:HB3 | 2.02 | 0.42 |
| 2:P:184:MET:HE3 | 2:P:188:ASP:CB | 2.48 | 0.42 |
| 6:T:35:THR:CG2 | 6:T:36:THR:N | 2.81 | 0.42 |
| 7:U:206:SER:O | 7:U:233:LEU:HD21 | 2.20 | 0.42 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:HH11 | 1.85 | 0.42 |
| 7:U:82:ILE:CG2 | 7:U:83:PRO:HD3 | 2.50 | 0.42 |
| 9:W:126:VAL:HG11 | 9:W:134:LEU:HB3 | 2.02 | 0.42 |
| 9:W:29:ASN:HD22 | 9:W:30:LYS:HG3 | 1.84 | 0.42 |
| 10:X:85:GLN:O | 10:X:89:LYS:HG3 | 2.20 | 0.42 |
| 11:Y:157:ARG:O | 11:Y:160:LEU:HB3 | 2.20 | 0.42 |
| 13:1:190:LEU:CD1 | 13:1:190:LEU:N | 2.82 | 0.41 |
| 1:A:92:SER:O | 1:A:95:VAL:HG12 | 2.20 | 0.41 |
| 4:D:79:SER:O | 4:D:134:VAL:HG23 | 2.20 | 0.41 |
| 5:E:216:GLY:O | 5:E:217:LYS:C | 2.58 | 0.41 |
| 6:F:35:THR:CG2 | 6:F:36:THR:N | 2.83 | 0.41 |
| 7:G:18(D):ILE:HG22 | 7:G:18(G):GLU:HB2 | 2.02 | 0.41 |
| 7:G:75:GLY:HA3 | 7:G:221:PHE:CE2 | 2.55 | 0.41 |
| 9:I:58:MET:O | 9:I:61:TYR:HB3 | 2.20 | 0.41 |
| 11:K:2:THR:OG1 | 11:K:130:GLY:HA3 | 2.20 | 0.41 |
| 14:N:8:PHE:HE1 | 14:N:10:ASP:HB2 | 1.84 | 0.41 |
| 1:O:175:PHE:O | 1:O:179:ARG:HG2 | 2.19 | 0.41 |
| 1:O:179:ARG:HH11 | 1:O:179:ARG:CB | 2.23 | 0.41 |
| 1:O:207:ASN:HA | 1:O:233:LEU:CD1 | 2.50 | 0.41 |
| 3:Q:97:GLN:CA | 3:Q:97:GLN:HE21 | 2.33 | 0.41 |
| 7:U:17(C):LYS:HE3 | 7:U:17(C):LYS:HB2 | 1.80 | 0.41 |
| 8:V:221:ILE:HD12 | 8:V:221:ILE:N | 2.35 | 0.41 |
| 17:L:199:HOH:O | 9:W:192:ARG:HG3 | 2.19 | 0.41 |
| 11:Y:7:ARG:CG | 11:Y:12:ILE:HD13 | 2.45 | 0.41 |
| 13:1:160:ARG:HB2 | 13:1:192:VAL:HG13 | 2.02 | 0.41 |
| 14:2:97:ALA:HB1 | 14:2:99:ILE:CD1 | 2.49 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:40:ILE:HD12 | 1:A:193:ALA:HB2 | 2.02 | 0.41 |
| 2:B:138:TYR:HB2 | 2:B:149:TYR:HB2 | 2.01 | 0.41 |
| 2:B:230:LYS:O | 2:B:234:VAL:HG23 | 2.21 | 0.41 |
| 4:D:180:TRP:HA | 4:D:184:LEU:HD11 | 2.03 | 0.41 |
| 5:E:18(D):ILE:HG23 | 5:E:18(E):LYS:HG3 | 2.02 | 0.41 |
| 5:E:198:SER:HA | 5:E:201:LEU:CD1 | 2.50 | 0.41 |
| 5:E:67:ILE:HD13 | 5:E:213:ALA:HB2 | 2.02 | 0.41 |
| 6:F:81:LEU:HA | 17:F:313:HOH:O | 2.20 | 0.41 |
| 8:H:18:THR:HB | 8:H:30:ASN:HA | 2.01 | 0.41 |
| 9:I:-2:ASN:HA | 9:I:21:GLY:O | 2.19 | 0.41 |
| 10:J:190:PHE:HA | 10:J:193:GLN:HB2 | 2.03 | 0.41 |
| 10:J:193:GLN:OXT | 10:J:193:GLN:HG2 | 2.20 | 0.41 |
| 12:L:164:GLU:OE1 | 12:L:192:LYS:HD3 | 2.20 | 0.41 |
| 13:M:82:TYR:O | 13:M:85:THR:HB | 2.19 | 0.41 |
| 11:Y:76:VAL:CG2 | 11:Y:103:GLY:HA3 | 2.50 | 0.41 |
| 11:Y:124:ILE:CG2 | 11:Y:138:LEU:HD23 | 2.51 | 0.41 |
| 11:Y:38:ASN:HB2 | 11:Y:39:PRO:CD | 2.50 | 0.41 |
| 3:C:141:PHE:CE1 | 3:C:217:PRO:HG3 | 2.56 | 0.41 |
| 1:A:7:ARG:HH11 | 5:E:127:TYR:HD2 | 1.68 | 0.41 |
| 7:G:158:VAL:HG22 | 7:G:159:GLY:H | 1.85 | 0.41 |
| 8:H:14:ILE:O | 8:H:14:ILE:HG13 | 2.20 | 0.41 |
| 8:H:170:GLY:O | 8:H:171:SER:HB2 | 2.20 | 0.41 |
| 11:K:124:ILE:CG2 | 11:K:138:LEU:HD23 | 2.50 | 0.41 |
| 13:M:5:SER:HB3 | 13:M:14:ILE:HG13 | 2.02 | 0.41 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:N | 2.35 | 0.41 |
| 1:O:232:ARG:HG3 | 1:O:232:ARG:NH1 | 2.35 | 0.41 |
| 1:O:57:PRO:HG2 | 7:U:177:GLU:HG2 | 2.01 | 0.41 |
| 1:O:4:MET:O | 1:O:5:THR:O | 2.39 | 0.41 |
| 5:S:121:GLN:OE1 | 5:S:125:GLN:NE2 | 2.53 | 0.41 |
| 5:S:198:SER:HA | 5:S:201:LEU:CD1 | 2.50 | 0.41 |
| 6:T:109:ILE:HG22 | 6:T:149:TYR:HE2 | 1.85 | 0.41 |
| 10:X:147:THR:HG23 | 10:X:150:GLU:OE2 | 2.20 | 0.41 |
| 10:X:18:LYS:CD | 10:X:174:ILE:HG13 | 2.45 | 0.41 |
| 12:Z:129:ALA:HB1 | 12:Z:166:HIS:NE2 | 2.35 | 0.41 |
| 13:1:14(C):ARG:CG | 13:1:14(C):ARG:HH11 | 2.25 | 0.41 |
| 14:2:44:CYS:HB2 | 14:2:100:ILE:HB | 2.01 | 0.41 |
| 1:A:166:GLY:O | 1:A:167:LYS:C | 2.58 | 0.41 |
| 3:C:14:ILE:HB | 4:D:23:GLN:NE2 | 2.35 | 0.41 |
| 3:C:224:LEU:CD1 | 3:C:224:LEU:N | 2.84 | 0.41 |
| 5:E:2(C):VAL:HG13 | 5:E:2(D):ASP:N | 2.35 | 0.41 |
| 1:A:86:ARG:NE | 7:G:118:ASN:HD21 | 2.18 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:G:18(D):ILE:O | 7:G:18(G):GLU:N | 2.53 | 0.41 |
| 7:G:29:LYS:HD2 | 7:G:29:LYS:HA | 1.77 | 0.41 |
| 9:I:29:ASN:HD22 | 9:I:30:LYS:HG3 | 1.82 | 0.41 |
| 2:P:233:LEU:HA | 2:P:233:LEU:HD12 | 1.91 | 0.41 |
| 1:O:159:PRO:O | 2:P:59:LEU:HD12 | 2.21 | 0.41 |
| 4:R:52:LYS:HE3 | 4:R:211:GLN:HB2 | 2.01 | 0.41 |
| 5:S:190:ILE:CG2 | 5:S:212:ILE:HD13 | 2.50 | 0.41 |
| 12:Z:14(I):THR:HG21 | 12:Z:14(M):VAL:HB | 2.03 | 0.41 |
| 13:1:17:ASP:C | 13:1:17:ASP:OD2 | 2.59 | 0.41 |
| 13:1:184:LEU:HD23 | 13:1:185:THR:N | 2.34 | 0.41 |
| 14:2:105:ASP:HB3 | 14:2:106:ASN:HB2 | 2.02 | 0.41 |
| 14:2:4:MET:CB | 14:2:126:ILE:HG22 | 2.51 | 0.41 |
| 7:G:17(C):LYS:HE3 | 7:G:17(C):LYS:HB2 | 1.81 | 0.41 |
| 7:G:217:LYS:CE | 7:G:217:LYS:HA | 2.43 | 0.41 |
| 7:G:224:LEU:HB3 | 7:G:228:ASN:HB2 | 2.03 | 0.41 |
| 9:I:55:LEU:HD12 | 9:I:97:VAL:HG21 | 2.01 | 0.41 |
| 10:J:88:ALA:O | 10:J:90(A):ILE:HG22 | 2.21 | 0.41 |
| 11:K:104:TYR:HA | 11:K:107:GLY:O | 2.20 | 0.41 |
| 11:K:45:MET:SD | 16:K:2(I):H10:C15 | 3.08 | 0.41 |
| 12:L:4:LEU:O | 12:L:14:LEU:HD23 | 2.21 | 0.41 |
| 1:O:35:VAL:CG1 | 1:O:51:GLU:HB3 | 2.50 | 0.41 |
| 3:Q:55:THR:O | 3:Q:56:LEU:HD22 | 2.21 | 0.41 |
| 5:S:4:PHE:O | 5:S:5:ARG:C | 2.59 | 0.41 |
| 6:T:151:LEU:CD1 | 6:T:157:TYR:HB3 | 2.51 | 0.41 |
| 6:T:184:LEU:CD1 | 6:T:188:GLU:HB3 | 2.48 | 0.41 |
| 7:U:220:LYS:HG2 | 7:U:221:PHE:N | 2.34 | 0.41 |
| 9:W:81:GLN:HG2 | 17:W:949:HOH:O | 2.20 | 0.41 |
| 16:Y:2(I):H10:H22A | 12:Z:125:ARG:HH21 | 1.86 | 0.41 |
| 12:Z:6:ILE:HG12 | 12:Z:124:CYS:HB2 | 2.02 | 0.41 |
| 2:B:186:VAL:O | 2:B:190:ILE:HG13 | 2.20 | 0.41 |
| 3:C:150:GLN:HB3 | 3:C:150:GLN:HE21 | 1.65 | 0.41 |
| 3:C:97:GLN:CA | 3:C:97:GLN:HE21 | 2.32 | 0.41 |
| 4:D:52:LYS:HE3 | 4:D:211:GLN:HB2 | 2.02 | 0.41 |
| 5:E:226:GLY:O | 5:E:227:GLU:C | 2.58 | 0.41 |
| 7:G:188:LYS:HA | 7:G:188:LYS:HD3 | 1.89 | 0.41 |
| 8:H:149:GLU:OE2 | 8:H:149:GLU:N | 2.54 | 0.41 |
| 9:I:80:THR:HG23 | 9:I:113:PHE:CZ | 2.56 | 0.41 |
| 10:J:3:ILE:HG22 | 10:J:100:LEU:HD12 | 2.01 | 0.41 |
| 14:N:105:ASP:HB3 | 14:N:106:ASN:HB2 | 2.02 | 0.41 |
| 3:Q:102:THR:OG1 | 3:Q:103:LEU:HD22 | 2.20 | 0.41 |
| 5:S:15:PHE:HB2 | 6:T:23:GLN:NE2 | 2.36 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:S:2(B):THR:OG1 | 5:S:2(E):ASN:HB3 | 2.21 | 0.41 |
| 8:V:149:GLU:N | 8:V:149:GLU:OE2 | 2.53 | 0.41 |
| 8:V:67:SER:HB2 | 8:V:74:PRO:HG3 | 2.01 | 0.41 |
| 11:K:167:ALA:HB1 | 9:W:167:ALA:O | 2.21 | 0.41 |
| 10:X:105:ASP:O | 10:X:106:ASN:N | 2.53 | 0.41 |
| 11:Y:40:PHE:CD1 | 11:Y:73:ARG:CZ | 3.04 | 0.41 |
| 13:1:4:ILE:HD12 | 13:1:155:ILE:HD12 | 2.03 | 0.41 |
| 1:A:31:VAL:HG13 | 1:A:79:SER:O | 2.21 | 0.41 |
| 4:D:192:LEU:O | 4:D:196:ILE:HD13 | 2.20 | 0.41 |
| 5:E:136:LEU:HB2 | 5:E:151:PHE:HB3 | 2.02 | 0.41 |
| 6:F:184:LEU:CD1 | 6:F:188:GLU:HB3 | 2.47 | 0.41 |
| 6:F:61:PRO:O | 6:F:62:GLN:HB2 | 2.20 | 0.41 |
| 6:F:90:ASN:HA | 6:F:90:ASN:HD22 | 1.64 | 0.41 |
| 2:B:144:ARG:NH1 | 10:J:72:TYR:HB2 | 2.36 | 0.41 |
| 12:L:129:ALA:HB1 | 12:L:166:HIS:NE2 | 2.36 | 0.41 |
| 13:M:137:LEU:HD11 | 13:M:161:VAL:HG21 | 2.03 | 0.41 |
| 13:M:36:PRO:HA | 13:M:42:VAL:HA | 2.03 | 0.41 |
| 3:Q:224:LEU:HD12 | 3:Q:224:LEU:N | 2.36 | 0.41 |
| 4:R:180:TRP:HA | 4:R:184:LEU:HD11 | 2.02 | 0.41 |
| 5:S:76:LEU:HA | 5:S:137:LEU:O | 2.21 | 0.41 |
| 6:T:179:LEU:HD21 | 6:T:192:GLN:HG2 | 2.02 | 0.41 |
| 1:O:58:LEU:HB3 | 7:U:162:ALA:O | 2.21 | 0.41 |
| 8:V:78:SER:O | 8:V:82:MET:HG3 | 2.21 | 0.41 |
| 9:W:93:GLY:N | 9:W:94:PRO:HD3 | 2.35 | 0.41 |
| 9:W:55:LEU:HD12 | 9:W:97:VAL:HG21 | 2.01 | 0.41 |
| 12:Z:14(D):TYR:CG | 12:Z:14(J):GLY:HA2 | 2.56 | 0.41 |
| 8:H:195:ASN:HB3 | 12:Z:192:LYS:HE3 | 2.02 | 0.41 |
| 13:1:125:LEU:HA | 17:1:217:HOH:O | 2.19 | 0.41 |
| 13:1:14(C):ARG:CG | 13:1:14(C):ARG:NH1 | 2.84 | 0.41 |
| 13:1:137:LEU:HD11 | 13:1:161:VAL:HG21 | 2.02 | 0.41 |
| 2:B:113:VAL:HG22 | 2:B:138:TYR:CG | 2.56 | 0.41 |
| 6:F:107:ILE:O | 6:F:107:ILE:HG23 | 2.20 | 0.41 |
| 6:F:179:LEU:HD21 | 6:F:192:GLN:HG2 | 2.02 | 0.41 |
| 7:G:46:THR:HG21 | 7:G:139:VAL:HB | 2.02 | 0.41 |
| 10:J:119:LYS:HE2 | 17:J:408:HOH:O | 2.21 | 0.41 |
| 12:L:6:ILE:HG12 | 12:L:124:CYS:CB | 2.50 | 0.41 |
| 2:P:20:ARG:HH11 | 2:P:20:ARG:HG2 | 1.85 | 0.41 |
| 3:Q:161:SER:HB3 | 3:Q:180:TYR:CE1 | 2.55 | 0.41 |
| 3:Q:46:VAL:HG22 | 3:Q:146:PRO:HB2 | 2.03 | 0.41 |
| 7:U:229:ILE:O | 7:U:232:ARG:HB2 | 2.21 | 0.41 |
| 11:Y:74:ILE:HD11 | 11:Y:78:ALA:HB1 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:1:209:GLN:N | 17:1:367:HOH:O | 2.54 | 0.41 |
| 14:2:134:ILE:C | 14:2:134:ILE:HD12 | 2.41 | 0.41 |
| 14:2:32:ASP:HA | 17:2:307:HOH:O | 2.21 | 0.41 |
| 1:A:124:THR:CG2 | 1:A:124:THR:O | 2.69 | 0.41 |
| 2:B:107:ILE:HD11 | 2:B:111:ILE:HB | 2.03 | 0.41 |
| 2:B:194:LEU:HD13 | 2:B:233:LEU:HD12 | 2.03 | 0.41 |
| 5:E:2(C):VAL:O | 5:E:226:GLY:HA2 | 2.21 | 0.41 |
| 6:F:103:TYR:O | 6:F:104:LYS:HB3 | 2.21 | 0.41 |
| 8:H:221:ILE:N | 8:H:221:ILE:HD12 | 2.35 | 0.41 |
| 11:K:50:ALA:CB | 12:L:116:VAL:HG23 | 2.48 | 0.41 |
| 12:L:145:TYR:HD1 | 12:L:146:LEU:N | 2.18 | 0.41 |
| 13:M:14(A):VAL:O | 13:M:14(A):VAL:HG23 | 2.20 | 0.41 |
| 14:N:37:VAL:HG22 | 14:N:41:ILE:HG22 | 2.01 | 0.41 |
| 1:O:205:GLU:HA | 1:O:205:GLU:OE2 | 2.21 | 0.41 |
| 4:R:12:VAL:HG23 | 4:R:12(A):GLY:HA2 | 2.02 | 0.41 |
| 4:R:160:TYR:HB3 | 4:R:162:ALA:O | 2.21 | 0.41 |
| 7:U:224:LEU:HB3 | 7:U:228:ASN:HB2 | 2.02 | 0.41 |
| 10:X:190:PHE:HA | 10:X:193:GLN:HB2 | 2.03 | 0.41 |
| 10:X:7:ARG:HG2 | 10:X:7:ARG:HH11 | 1.86 | 0.41 |
| 10:X:85:GLN:HG2 | 10:X:89:LYS:HE3 | 2.03 | 0.41 |
| 1:A:160:TRP:CE3 | 1:A:163:THR:HB | 2.56 | 0.41 |
| 1:A:73:ASP:C | 1:A:74:ILE:HG13 | 2.41 | 0.41 |
| 1:A:79:SER:HB2 | 1:A:165:ILE:HD12 | 2.02 | 0.41 |
| 6:F:13:SER:HB2 | 7:G:130:ARG:HD3 | 2.03 | 0.41 |
| 7:G:203:THR:HG22 | 7:G:204:GLU:N | 2.35 | 0.41 |
| 8:H:208:ARG:NH1 | 9:I:149:GLU:HB2 | 2.35 | 0.41 |
| 10:J:63:ILE:HD13 | 10:J:63:ILE:N | 2.36 | 0.41 |
| 11:K:83:LEU:CD2 | 11:K:101:ILE:HD11 | 2.51 | 0.41 |
| 12:L:-8:PHE:CB | 13:M:-8:THR:HG23 | 2.50 | 0.41 |
| 13:M:45:ILE:HG12 | 13:M:99:ILE:HG12 | 2.03 | 0.41 |
| 1:O:21(L):ILE:HD11 | 8:V:186:TYR:CD2 | 2.56 | 0.41 |
| 5:S:4:PHE:CG | 5:S:5:ARG:N | 2.88 | 0.41 |
| 7:U:40:VAL:HB | 7:U:18(D):ILE:HD13 | 2.03 | 0.41 |
| 10:X:66:TYR:CE2 | 10:X:74:LEU:HG | 2.56 | 0.41 |
| 11:Y:9:GLN:CD | 11:Y:10:GLY:N | 2.74 | 0.41 |
| 13:1:-6:GLN:O | 13:1:-6:GLN:HG3 | 2.20 | 0.41 |
| 14:2:51:ASP:O | 14:2:55:ILE:HG13 | 2.22 | 0.41 |
| 1:A:136:LEU:O | 1:A:150:GLN:HA | 2.21 | 0.41 |
| 2:B:21(A):LYS:HG3 | 2:B:219:GLU:O | 2.20 | 0.41 |
| 4:D:196:ILE:N | 4:D:196:ILE:HD12 | 2.35 | 0.41 |
| 5:E:136:LEU:HD12 | 5:E:151:PHE:CD2 | 2.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:2(B):THR:OG1 | 5:E:2(E):ASN:HB3 | 2.21 | 0.41 |
| 6:F:43:ASN:N | 6:F:43:ASN:ND2 | 2.69 | 0.41 |
| 6:F:49:ALA:HB1 | 6:F:212:ILE:CD1 | 2.51 | 0.41 |
| 7:G:49:ILE:CD1 | 7:G:49:ILE:N | 2.80 | 0.41 |
| 8:H:156:SER:HA | 8:H:159:ILE:HD12 | 2.01 | 0.41 |
| 8:H:63:ILE:HG23 | 8:H:74:PRO:HB3 | 2.02 | 0.41 |
| 10:J:-1:MET:CG | 10:J:1:ASP:H | 2.31 | 0.41 |
| 11:K:40:PHE:CD1 | 11:K:73:ARG:CZ | 3.04 | 0.41 |
| 4:D:101:LEU:CD1 | 11:K:57:THR:HG22 | 2.51 | 0.41 |
| 12:L:43:MET:HG2 | 12:L:44:SER:N | 2.36 | 0.41 |
| 13:M:62:LEU:HD13 | 13:M:79:ILE:HD13 | 2.02 | 0.41 |
| 14:N:143:ARG:O | 14:N:146:MET:HG3 | 2.21 | 0.41 |
| 14:N:38:HIS:HB3 | 14:N:41:ILE:HB | 2.02 | 0.41 |
| 2:P:230:LYS:O | 2:P:234:VAL:HG23 | 2.21 | 0.41 |
| 2:P:39:GLY:O | 2:P:148:LEU:HD21 | 2.21 | 0.41 |
| 7:U:79:ASN:HA | 17:U:252:HOH:O | 2.20 | 0.41 |
| 8:V:62:ASN:HB3 | 8:V:82:MET:HE1 | 2.03 | 0.41 |
| 9:W:46:THR:HA | 17:W:608:HOH:O | 2.21 | 0.41 |
| 10:X:35:ARG:HD3 | 10:X:35:ARG:HA | 1.80 | 0.41 |
| 12:Z:52:GLY:O | 12:Z:56:VAL:HG23 | 2.21 | 0.41 |
| 12:Z:-5:TYR:CD2 | 12:Z:96:TYR:HB2 | 2.55 | 0.41 |
| 14:2:161:GLN:NE2 | 14:2:165:TRP:HE1 | 2.18 | 0.40 |
| 8:H:18:THR:OG1 | 8:H:171:SER:HB2 | 2.21 | 0.40 |
| 9:I:126:VAL:HG11 | 9:I:134:LEU:HB3 | 2.03 | 0.40 |
| 10:J:133:TYR:OH | 10:X:24:ILE:CG1 | 2.68 | 0.40 |
| 11:K:90:TYR:O | 11:K:91:LYS:C | 2.59 | 0.40 |
| 12:L:54:ALA:O | 12:L:58:ARG:HB2 | 2.21 | 0.40 |
| 2:P:215:ILE:HG22 | 2:P:215:ILE:O | 2.21 | 0.40 |
| 5:S:31:ILE:HD13 | 5:S:152:GLN:OE1 | 2.21 | 0.40 |
| 9:W:20:LEU:HA | 17:W:240:HOH:O | 2.21 | 0.40 |
| 10:X:190:PHE:C | 10:X:192:ALA:H | 2.22 | 0.40 |
| 11:Y:31:VAL:HG11 | 16:Y:2(I):H10:C15 | 2.51 | 0.40 |
| 11:Y:31:VAL:CG1 | 16:Y:2(I):H10:C15 | 2.99 | 0.40 |
| 12:Z:70(A):ASN:O | 12:Z:72:LYS:N | 2.54 | 0.40 |
| 1:A:24:ILE:N | 1:A:24:ILE:HD12 | 2.36 | 0.40 |
| 3:C:168:ASN:CB | 3:C:200:VAL:HG11 | 2.49 | 0.40 |
| 3:C:19:GLY:O | 4:D:30:ALA:HB2 | 2.21 | 0.40 |
| 5:E:27:ALA:O | 5:E:31:ILE:HD12 | 2.21 | 0.40 |
| 6:F:172:ALA:C | 6:F:176:LEU:HD23 | 2.42 | 0.40 |
| 6:F:21:ASN:C | 6:F:21:ASN:OD1 | 2.59 | 0.40 |
| 6:F:35:THR:HG21 | 6:F:51:GLU:O | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:F:83:PRO:HB2 | 17:F:1240:HOH:O | 2.20 | 0.40 |
| 7:G:13:THR:HB | 7:G:124:THR:O | 2.21 | 0.40 |
| 8:H:62:ASN:HB3 | 8:H:82:MET:HE1 | 2.04 | 0.40 |
| 9:I:16:CYS:SG | 9:I:34:ILE:HG12 | 2.60 | 0.40 |
| 14:N:116:GLY:HA3 | 17:N:194:HOH:O | 2.21 | 0.40 |
| 3:Q:156:ILE:H | 3:Q:156:ILE:CD1 | 2.34 | 0.40 |
| 4:R:40:ILE:HG12 | 4:R:193:VAL:CG2 | 2.51 | 0.40 |
| 5:S:39:GLY:O | 5:S:162:GLY:HA2 | 2.21 | 0.40 |
| 5:S:198:SER:HA | 5:S:201:LEU:CG | 2.46 | 0.40 |
| 7:U:198:ILE:O | 7:U:202:GLY:N | 2.51 | 0.40 |
| 7:U:35:ILE:HD13 | 7:U:53:LYS:HE3 | 2.03 | 0.40 |
| 9:W:58:MET:O | 9:W:61:TYR:HB3 | 2.21 | 0.40 |
| 11:Y:109:THR:HA | 17:Y:595:HOH:O | 2.21 | 0.40 |
| 12:Z:95:TYR:O | 12:Z:97:VAL:N | 2.53 | 0.40 |
| 1:A:205:GLU:OE2 | 1:A:205:GLU:HA | 2.21 | 0.40 |
| 1:A:4:MET:O | 1:A:5:THR:O | 2.39 | 0.40 |
| 2:B:40:ILE:HD12 | 2:B:193:ALA:HB2 | 2.03 | 0.40 |
| 3:C:210:ILE:HG22 | 3:C:212:ILE:CD1 | 2.52 | 0.40 |
| 3:C:79:SER:HA | 17:C:625:HOH:O | 2.22 | 0.40 |
| 4:D:12(G):GLU:HG2 | 4:D:125:GLU:N | 2.34 | 0.40 |
| 1:A:8:TYR:HD2 | 7:G:128:TYR:HB3 | 1.87 | 0.40 |
| 8:H:192:LEU:HD23 | 8:H:192:LEU:HA | 1.79 | 0.40 |
| 11:K:76:VAL:HG22 | 11:K:103:GLY:HA3 | 2.03 | 0.40 |
| 11:K:17:ASP:CG | 11:K:33:LYS:HZ2 | 2.25 | 0.40 |
| 12:L:133:LEU:N | 12:L:133:LEU:HD12 | 2.36 | 0.40 |
| 12:L:176:LEU:HG | 12:L:186:LYS:HG3 | 2.03 | 0.40 |
| 3:Q:227:GLU:N | 3:Q:227:GLU:OE1 | 2.50 | 0.40 |
| 6:T:126:TYR:HE1 | 7:U:129:MET:SD | 2.45 | 0.40 |
| 9:W:84:SER:OG | 9:W:119:ILE:HD11 | 2.21 | 0.40 |
| 10:X:123:PRO:HB3 | 10:X:142:TYR:CE2 | 2.57 | 0.40 |
| 11:Y:38:ASN:OD1 | 11:Y:38:ASN:C | 2.58 | 0.40 |
| 12:Z:32:PRO:CD | 17:Z:1177:HOH:O | 2.65 | 0.40 |
| 12:Z:42:VAL:HG23 | 12:Z:102:ALA:HB3 | 2.03 | 0.40 |
| 13:1:8:TYR:HB2 | 13:1:146:THR:O | 2.21 | 0.40 |
| 14:2:133:PHE:HE2 | 14:2:166:ASP:HB2 | 1.86 | 0.40 |
| 14:N:157:HIS:HD2 | 14:2:140:LYS:NZ | 2.20 | 0.40 |
| 1:A:161:LYS:HD3 | 1:A:180:TRP:CH2 | 2.56 | 0.40 |
| 1:A:21(I):TYR:HE2 | 1:A:21(L):ILE:HD12 | 1.87 | 0.40 |
| 2:B:39:GLY:C | 2:B:148:LEU:HD21 | 2.42 | 0.40 |
| 3:C:125:GLN:HB2 | 4:D:130:ARG:HG2 | 2.03 | 0.40 |
| 4:D:161:ASN:HB3 | 4:D:180:TRP:CZ2 | 2.56 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:151:LEU:HD13 | 6:F:157:TYR:HB3 | 2.03 | 0.40 |
| 8:H:72:ARG:HH11 | 8:H:72:ARG:HG3 | 1.86 | 0.40 |
| 9:I:55:LEU:HD23 | 9:I:55:LEU:HA | 1.84 | 0.40 |
| 9:I:93:GLY:H | 9:I:94:PRO:HD3 | 1.87 | 0.40 |
| 10:J:123:PRO:HB3 | 10:J:142:TYR:CE2 | 2.55 | 0.40 |
| 10:J:133:TYR:CZ | 10:J:166:MET:HG3 | 2.57 | 0.40 |
| 12:L:104:LEU:HA | 12:L:107:LYS:O | 2.22 | 0.40 |
| 2:P:122:GLY:C | 2:P:124:THR:N | 2.74 | 0.40 |
| 4:R:115:SER:O | 4:R:118:ASP:HB2 | 2.22 | 0.40 |
| 7:U:203:THR:HG22 | 7:U:204:GLU:N | 2.36 | 0.40 |
| 11:Y:174:ASN:HA | 11:Y:174:ASN:HD22 | 1.69 | 0.40 |
| 11:Y:45:MET:SD | 16:Y:2(I):H10:C15 | 3.09 | 0.40 |
| 3:C:241:GLN:O | 3:C:243:GLN:N | 2.50 | 0.40 |
| 5:E:4:PHE:O | 5:E:5:ARG:C | 2.58 | 0.40 |
| 7:G:12:ILE:HD13 | 7:G:12:ILE:H | 1.85 | 0.40 |
| 13:M:1:THR:OG1 | 13:M:2:SER:N | 2.55 | 0.40 |
| 1:O:45:GLY:HA2 | 1:O:147:PHE:CE2 | 2.57 | 0.40 |
| 3:Q:76:LEU:HD12 | 3:Q:138:ILE:HG12 | 2.03 | 0.40 |
| 5:S:66:LYS:O | 5:S:77:SER:HA | 2.20 | 0.40 |
| 6:T:114:ASP:O | 6:T:118:GLN:HG2 | 2.21 | 0.40 |
| 6:T:195:LYS:NZ | 6:T:196:ILE:CD1 | 2.85 | 0.40 |
| 6:T:43:ASN:ND2 | 6:T:43:ASN:H | 2.20 | 0.40 |
| 7:U:99:PHE:C | 7:U:99:PHE:CD1 | 2.95 | 0.40 |
| 8:V:100:ILE:HG12 | 8:V:127:LEU:HD12 | 2.03 | 0.40 |
| 9:W:-2:ASN:HA | 9:W:21:GLY:O | 2.22 | 0.40 |
| 10:X:121:GLU:O | 10:X:122:LEU:HD23 | 2.21 | 0.40 |
| 11:Y:76:VAL:HG12 | 11:Y:111:TYR:HD2 | 1.86 | 0.40 |
| 11:Y:50:ALA:CB | 12:Z:116:VAL:HG23 | 2.51 | 0.40 |
| 12:Z:40:ASN:ND2 | 17:Z:799:HOH:O | 2.49 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 248/250 (99%) | 226 (91%) | 15 (6%) | 7 (3%) | 5 | 17 |
| 1 | O | 248/250 (99%) | 226 (91%) | 14 (6%) | 8 (3%) | 4 | 13 |
| 2 | B | 242/244 (99%) | 217 (90%) | 18 (7%) | 7 (3%) | 4 | 15 |
| 2 | P | 242/244 (99%) | 217 (90%) | 19 (8%) | 6 (2%) | 5 | 19 |
| 3 | C | 239/241 (99%) | 219 (92%) | 15 (6%) | 5 (2%) | 7 | 23 |
| 3 | Q | 239/241 (99%) | 217 (91%) | 17 (7%) | 5 (2%) | 7 | 23 |
| 4 | D | 240/242 (99%) | 217 (90%) | 18 (8%) | 5 (2%) | 7 | 23 |
| 4 | R | 240/242 (99%) | 216 (90%) | 19 (8%) | 5 (2%) | 7 | 23 |
| 5 | E | 231/233 (99%) | 201 (87%) | 24 (10%) | 6 (3%) | 5 | 18 |
| 5 | S | 231/233 (99%) | 203 (88%) | 22 (10%) | 6 (3%) | 5 | 18 |
| 6 | F | 242/244 (99%) | 224 (93%) | 17 (7%) | 1 (0%) | 34 | 66 |
| 6 | T | 242/244 (99%) | 223 (92%) | 18 (7%) | 1 (0%) | 34 | 66 |
| 7 | G | 241/243 (99%) | 223 (92%) | 15 (6%) | 3 (1%) | 13 | 39 |
| 7 | U | 241/243 (99%) | 222 (92%) | 16 (7%) | 3 (1%) | 13 | 39 |
| 8 | H | 220/222 (99%) | 207 (94%) | 10 (4%) | 3 (1%) | 11 | 34 |
| 8 | V | 220/222 (99%) | 205 (93%) | 12 (6%) | 3 (1%) | 11 | 34 |
| 9 | I | 202/204 (99%) | 189 (94%) | 10 (5%) | 3 (2%) | 10 | 33 |
| 9 | W | 202/204 (99%) | 189 (94%) | 11 (5%) | 2 (1%) | 15 | 44 |
| 10 | J | 196/198 (99%) | 184 (94%) | 9 (5%) | 3 (2%) | 10 | 33 |
| 10 | X | 196/198 (99%) | 184 (94%) | 9 (5%) | 3 (2%) | 10 | 33 |
| 11 | K | 210/212 (99%) | 197 (94%) | 13 (6%) | 0 | 100 | 100 |
| 11 | Y | 210/212 (99%) | 200 (95%) | 9 (4%) | 1 (0%) | 29 | 61 |
| 12 | L | 220/222 (99%) | 201 (91%) | 18 (8%) | 1 (0%) | 29 | 61 |
| 12 | Z | 220/222 (99%) | 201 (91%) | 18 (8%) | 1 (0%) | 29 | 61 |
| 13 | 1 | 231/233 (99%) | 208 (90%) | 21 (9%) | 2 (1%) | 17 | 46 |
| 13 | M | 231/233 (99%) | 210 (91%) | 19 (8%) | 2 (1%) | 17 | 46 |
| 14 | 2 | 194/196 (99%) | 183 (94%) | 11 (6%) | 0 | 100 | 100 |
| 14 | N | 194/196 (99%) | 180 (93%) | 14 (7%) | 0 | 100 | 100 |
| All | All | 6312/6368 (99%) | 5789 (92%) | 431 (7%) | 92 (2%) | 10 | 33 |

All (92) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | A | 5 | THR |
| 1 | A | 167 | LYS |
| 2 | B | 54 | VAL |
| 3 | C | 58 | LEU |
| 3 | C | 203 | THR |
| 4 | D | 12(G) | GLU |
| 5 | E | 5 | ARG |
| 5 | E | 202 | ARG |
| 6 | F | 143 | LYS |
| 12 | L | 71 | ASP |
| 1 | O | 5 | THR |
| 1 | O | 167 | LYS |
| 2 | P | 54 | VAL |
| 3 | Q | 58 | LEU |
| 3 | Q | 203 | THR |
| 4 | R | 12(G) | GLU |
| 5 | S | 5 | ARG |
| 5 | S | 202 | ARG |
| 6 | T | 143 | LYS |
| 12 | Z | 71 | ASP |
| 1 | A | 53 | LYS |
| 2 | B | 6 | ARG |
| 2 | B | 21(B) | GLY |
| 2 | B | 21(C) | ASP |
| 5 | E | 180 | LEU |
| 5 | E | 217 | LYS |
| 5 | E | 231 | LYS |
| 7 | G | 239 | GLN |
| 8 | H | 9 | ASN |
| 8 | H | 96 | GLY |
| 10 | J | 49 | ALA |
| 10 | J | 192 | ALA |
| 1 | O | 53 | LYS |
| 2 | P | 6 | ARG |
| 2 | P | 21(B) | GLY |
| 2 | P | 21(C) | ASP |
| 5 | S | 180 | LEU |
| 5 | S | 217 | LYS |
| 8 | V | 9 | ASN |
| 8 | V | 96 | GLY |
| 10 | X | 49 | ALA |
| 10 | X | 192 | ALA |
| 13 | 1 | 96 | TRP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | A | 63 | THR |
| 2 | B | 20(A) | SER |
| 4 | D | 12(F) | GLY |
| 5 | E | 18(A) | ASP |
| 13 | M | 96 | TRP |
| 1 | O | 63 | THR |
| 2 | P | 20(A) | SER |
| 4 | R | 120 | ALA |
| 4 | R | 12(F) | GLY |
| 5 | S | 18(A) | ASP |
| 5 | S | 231 | LYS |
| 7 | U | 184 | ASN |
| 7 | U | 239 | GLN |
| 1 | A | 100 | TYR |
| 3 | C | 183 | PRO |
| 3 | C | 202 | GLN |
| 4 | D | 120 | ALA |
| 4 | D | 12(C) | GLY |
| 7 | G | 184 | ASN |
| 3 | Q | 183 | PRO |
| 3 | Q | 202 | GLN |
| 4 | R | 12(C) | GLY |
| 7 | U | 55 | PRO |
| 8 | V | 171 | SER |
| 4 | D | 18(D) | SER |
| 7 | G | 55 | PRO |
| 8 | H | 171 | SER |
| 9 | I | 23 | GLN |
| 9 | I | 93 | GLY |
| 9 | I | 106 | GLY |
| 13 | M | 1 | THR |
| 1 | O | 100 | TYR |
| 3 | Q | 53 | ARG |
| 9 | W | 93 | GLY |
| 9 | W | 106 | GLY |
| 13 | 1 | 1 | THR |
| 1 | A | 208 | GLY |
| 2 | B | 64 | THR |
| 3 | C | 53 | ARG |
| 1 | O | 56 | SER |
| 1 | O | 208 | GLY |
| 4 | R | 18(D) | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 56 | SER |
| 10 | J | 8 | VAL |
| 10 | X | 8 | VAL |
| 1 | O | 22 | GLY |
| 2 | P | 186 | VAL |
| 2 | B | 186 | VAL |
| 11 | Y | 39 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 209/209 (100%) | 204 (98%) | 5 (2%) | 49 | 81 |
| 1 | O | 209/209 (100%) | 204 (98%) | 5 (2%) | 49 | 81 |
| 2 | B | 203/203 (100%) | 188 (93%) | 15 (7%) | 13 | 37 |
| 2 | P | 203/203 (100%) | 188 (93%) | 15 (7%) | 13 | 37 |
| 3 | C | 213/213 (100%) | 204 (96%) | 9 (4%) | 30 | 63 |
| 3 | Q | 213/213 (100%) | 203 (95%) | 10 (5%) | 26 | 59 |
| 4 | D | 198/198 (100%) | 186 (94%) | 12 (6%) | 18 | 48 |
| 4 | R | 198/198 (100%) | 186 (94%) | 12 (6%) | 18 | 48 |
| 5 | E | 192/192 (100%) | 172 (90%) | 20 (10%) | 7 | 21 |
| 5 | S | 192/192 (100%) | 174 (91%) | 18 (9%) | 8 | 26 |
| 6 | F | 201/201 (100%) | 188 (94%) | 13 (6%) | 17 | 44 |
| 6 | T | 201/201 (100%) | 188 (94%) | 13 (6%) | 17 | 44 |
| 7 | G | 207/207 (100%) | 197 (95%) | 10 (5%) | 25 | 58 |
| 7 | U | 207/207 (100%) | 197 (95%) | 10 (5%) | 25 | 58 |
| 8 | H | 181/181 (100%) | 173 (96%) | 8 (4%) | 28 | 61 |
| 8 | V | 181/181 (100%) | 170 (94%) | 11 (6%) | 18 | 48 |
| 9 | I | 172/172 (100%) | 165 (96%) | 7 (4%) | 30 | 64 |
| 9 | W | 172/172 (100%) | 166 (96%) | 6 (4%) | 36 | 70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 10 | J | 175/175 (100%) | 169 (97%) | 6 (3%) | 37 | 71 |
| 10 | X | 175/175 (100%) | 169 (97%) | 6 (3%) | 37 | 71 |
| 11 | K | 169/169 (100%) | 164 (97%) | 5 (3%) | 41 | 75 |
| 11 | Y | 169/169 (100%) | 164 (97%) | 5 (3%) | 41 | 75 |
| 12 | L | 185/185 (100%) | 172 (93%) | 13 (7%) | 15 | 40 |
| 12 | Z | 185/185 (100%) | 173 (94%) | 12 (6%) | 17 | 44 |
| 13 | 1 | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 | 65 |
| 13 | M | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 | 65 |
| 14 | 2 | 162/162 (100%) | 154 (95%) | 8 (5%) | 25 | 57 |
| 14 | N | 162/162 (100%) | 157 (97%) | 5 (3%) | 40 | 74 |
| All | All | 5332/5332 (100%) | 5057 (95%) | 275 (5%) | 23 | 55 |

All (275) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | GLN |
| 1 | A | 64 | LEU |
| 1 | A | 135 | SER |
| 1 | A | 158 | PHE |
| 1 | A | 179 | ARG |
| 2 | B | 58 | LEU |
| 2 | B | 62 | ASP |
| 2 | B | 67 | LEU |
| 2 | B | 71 | ASN |
| 2 | B | 107 | ILE |
| 2 | B | 116 | LEU |
| 2 | B | 121 | GLN |
| 2 | B | 156 | ASN |
| 2 | B | 158 | THR |
| 2 | B | 192 | LEU |
| 2 | B | 198 | SER |
| 2 | B | 212 | PHE |
| 2 | B | 218 | ASN |
| 2 | B | 224 | PHE |
| 2 | B | 232 | ILE |
| 3 | C | 10 | ARG |
| 3 | C | 14 | ILE |
| 3 | C | 25 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 3 | C | 57 | LYS |
| 3 | C | 121 | GLN |
| 3 | C | 150 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 174 | GLU |
| 3 | C | 208 | LYS |
| 4 | D | 28 | LEU |
| 4 | D | 48 | LEU |
| 4 | D | 76 | CYS |
| 4 | D | 110 | GLU |
| 4 | D | 126 | ARG |
| 4 | D | 170 | GLU |
| 4 | D | 175 | GLU |
| 4 | D | 177 | LEU |
| 4 | D | 191 | LEU |
| 4 | D | 194 | LEU |
| 4 | D | 215 | ILE |
| 4 | D | 237 | LEU |
| 5 | E | 11 | ASP |
| 5 | E | 12 | THR |
| 5 | E | 13 | VAL |
| 5 | E | 28 | LEU |
| 5 | E | 32 | LYS |
| 5 | E | 57 | GLU |
| 5 | E | 76 | LEU |
| 5 | E | 97 | ASN |
| 5 | E | 104 | ASN |
| 5 | E | 111 | ARG |
| 5 | E | 117 | CYS |
| 5 | E | 121 | GLN |
| 5 | E | 178 | ARG |
| 5 | E | 18(D) | ILE |
| 5 | E | 185 | ASN |
| 5 | E | 199 | GLN |
| 5 | E | 207 | LEU |
| 5 | E | 2(C) | VAL |
| 5 | E | 227 | GLU |
| 5 | E | 231 | LYS |
| 6 | F | 11 | SER |
| 6 | F | 35 | THR |
| 6 | F | 43 | ASN |
| 6 | F | 98 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |
| 6 | F | 18(E) | GLU |
| 6 | F | 187 | ARG |
| 6 | F | 203 | GLU |
| 6 | F | 204 | ASP |
| 6 | F | 205 | ASN |
| 6 | F | 214 | TRP |
| 6 | F | 21(C) | ASN |
| 7 | G | 12 | ILE |
| 7 | G | 72 | ARG |
| 7 | G | 87 | ASN |
| 7 | G | 119 | LEU |
| 7 | G | 121 | GLN |
| 7 | G | 157 | TYR |
| 7 | G | 169 | GLN |
| 7 | G | 197 | MET |
| 7 | G | 232 | ARG |
| 7 | G | 233 | LEU |
| 8 | H | 31 | CYS |
| 8 | H | 34 | LEU |
| 8 | H | 41 | ILE |
| 8 | H | 43 | CYS |
| 8 | H | 56 | THR |
| 8 | H | 68 | LEU |
| 8 | H | 144 | GLN |
| 8 | H | 197 | ARG |
| 9 | I | 20 | LEU |
| 9 | I | 29 | ASN |
| 9 | I | 45 | ILE |
| 9 | I | 90 | ARG |
| 9 | I | 113 | PHE |
| 9 | I | 116 | ILE |
| 9 | I | 160 | LEU |
| 10 | J | 35 | ARG |
| 10 | J | 52 | THR |
| 10 | J | 63 | ILE |
| 10 | J | 77 | GLN |
| 10 | J | 90 | SER |
| 10 | J | 168 | MET |
| 11 | K | 4 | LEU |
| 11 | K | 9 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 11 | K | 65 | LEU |
| 11 | K | 87 | VAL |
| 11 | K | 104 | TYR |
| 12 | L | -7 | ASN |
| 12 | L | 3 | ILE |
| 12 | L | 14 | LEU |
| 12 | L | 21 | ILE |
| 12 | L | 40 | ASN |
| 12 | L | 46 | ASN |
| 12 | L | 58 | ARG |
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 99 | THR |
| 12 | L | 112 | SER |
| 12 | L | 120 | GLU |
| 12 | L | 145 | TYR |
| 13 | M | 40 | ASN |
| 13 | M | 62 | LEU |
| 13 | M | 91 | ARG |
| 13 | M | 112 | TYR |
| 13 | M | 129 | PHE |
| 13 | M | 14(C) | ARG |
| 13 | M | 149 | GLN |
| 13 | M | 204 | LYS |
| 14 | N | 13 | ILE |
| 14 | N | 84 | LYS |
| 14 | N | 89 | GLU |
| 14 | N | 10(B) | LYS |
| 14 | N | 149 | GLU |
| 1 | O | 33 | GLN |
| 1 | O | 64 | LEU |
| 1 | O | 135 | SER |
| 1 | O | 158 | PHE |
| 1 | O | 179 | ARG |
| 2 | P | 58 | LEU |
| 2 | P | 62 | ASP |
| 2 | P | 67 | LEU |
| 2 | P | 71 | ASN |
| 2 | P | 116 | LEU |
| 2 | P | 121 | GLN |
| 2 | P | 156 | ASN |
| 2 | P | 158 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | P | 187 | ASP |
| 2 | P | 192 | LEU |
| 2 | P | 198 | SER |
| 2 | P | 212 | PHE |
| 2 | P | 218 | ASN |
| 2 | P | 224 | PHE |
| 2 | P | 232 | ILE |
| 3 | Q | 10 | ARG |
| 3 | Q | 25 | GLU |
| 3 | Q | 57 | LYS |
| 3 | Q | 121 | GLN |
| 3 | Q | 150 | GLN |
| 3 | Q | 156 | ILE |
| 3 | Q | 163 | GLN |
| 3 | Q | 165 | ILE |
| 3 | Q | 174 | GLU |
| 3 | Q | 208 | LYS |
| 4 | R | 28 | LEU |
| 4 | R | 48 | LEU |
| 4 | R | 76 | CYS |
| 4 | R | 110 | GLU |
| 4 | R | 126 | ARG |
| 4 | R | 170 | GLU |
| 4 | R | 175 | GLU |
| 4 | R | 177 | LEU |
| 4 | R | 191 | LEU |
| 4 | R | 194 | LEU |
| 4 | R | 215 | ILE |
| 4 | R | 237 | LEU |
| 5 | S | 11 | ASP |
| 5 | S | 12 | THR |
| 5 | S | 13 | VAL |
| 5 | S | 32 | LYS |
| 5 | S | 57 | GLU |
| 5 | S | 76 | LEU |
| 5 | S | 97 | ASN |
| 5 | S | 104 | ASN |
| 5 | S | 111 | ARG |
| 5 | S | 117 | CYS |
| 5 | S | 121 | GLN |
| 5 | S | 178 | ARG |
| 5 | S | 185 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 5 | S | 199 | GLN |
| 5 | S | 207 | LEU |
| 5 | S | 2(C) | VAL |
| 5 | S | 227 | GLU |
| 5 | S | 231 | LYS |
| 6 | T | 11 | SER |
| 6 | T | 35 | THR |
| 6 | T | 43 | ASN |
| 6 | T | 98 | SER |
| 6 | T | 121 | GLN |
| 6 | T | 127 | ASN |
| 6 | T | 18(E) | GLU |
| 6 | T | 187 | ARG |
| 6 | T | 203 | GLU |
| 6 | T | 204 | ASP |
| 6 | T | 205 | ASN |
| 6 | T | 214 | TRP |
| 6 | T | 21(C) | ASN |
| 7 | U | 14 | ILE |
| 7 | U | 72 | ARG |
| 7 | U | 87 | ASN |
| 7 | U | 119 | LEU |
| 7 | U | 121 | GLN |
| 7 | U | 157 | TYR |
| 7 | U | 169 | GLN |
| 7 | U | 197 | MET |
| 7 | U | 232 | ARG |
| 7 | U | 233 | LEU |
| 8 | V | 3 | ILE |
| 8 | V | 30 | ASN |
| 8 | V | 31 | CYS |
| 8 | V | 34 | LEU |
| 8 | V | 41 | ILE |
| 8 | V | 43 | CYS |
| 8 | V | 56 | THR |
| 8 | V | 68 | LEU |
| 8 | V | 121 | VAL |
| 8 | V | 144 | GLN |
| 8 | V | 197 | ARG |
| 9 | W | 20 | LEU |
| 9 | W | 29 | ASN |
| 9 | W | 90 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 9 | W | 113 | PHE |
| 9 | W | 155 | ILE |
| 9 | W | 160 | LEU |
| 10 | X | 35 | ARG |
| 10 | X | 52 | THR |
| 10 | X | 77 | GLN |
| 10 | X | 90 | SER |
| 10 | X | 90(A) | ILE |
| 10 | X | 168 | MET |
| 11 | Y | 4 | LEU |
| 11 | Y | 9 | GLN |
| 11 | Y | 65 | LEU |
| 11 | Y | 87 | VAL |
| 11 | Y | 104 | TYR |
| 12 | Z | -7 | ASN |
| 12 | Z | 14 | LEU |
| 12 | Z | 21 | ILE |
| 12 | Z | 40 | ASN |
| 12 | Z | 46 | ASN |
| 12 | Z | 58 | ARG |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 99 | THR |
| 12 | Z | 112 | SER |
| 12 | Z | 120 | GLU |
| 12 | Z | 145 | TYR |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 62 | LEU |
| 13 | 1 | 91 | ARG |
| 13 | 1 | 112 | TYR |
| 13 | 1 | 129 | PHE |
| 13 | 1 | 14(C) | ARG |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 204 | LYS |
| 14 | 2 | 3 | ILE |
| 14 | 2 | 13 | ILE |
| 14 | 2 | 84 | LYS |
| 14 | 2 | 89 | GLU |
| 14 | 2 | 10(B) | LYS |
| 14 | 2 | 126 | ILE |
| 14 | 2 | 149 | GLU |
| 14 | 2 | 18(A) | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 33 | GLN |
| 1 | A | 97 | HIS |
| 2 | B | 23 | GLN |
| 2 | B | 71 | ASN |
| 2 | B | 97 | GLN |
| 2 | B | 121 | GLN |
| 2 | B | 125 | GLN |
| 2 | B | 156 | ASN |
| 2 | B | 177 | GLN |
| 2 | B | 218 | ASN |
| 3 | C | 23 | GLN |
| 3 | C | 82 | ASN |
| 3 | C | 97 | GLN |
| 3 | C | 121 | GLN |
| 3 | C | 125 | GLN |
| 3 | C | 150 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 209 | ASN |
| 3 | C | 238 | GLN |
| 3 | C | 243 | GLN |
| 4 | D | 23 | GLN |
| 4 | D | 108 | ASN |
| 4 | D | 161 | ASN |
| 4 | D | 211 | GLN |
| 4 | D | 218 | GLN |
| 4 | D | 226 | ASN |
| 5 | E | 7 | ASN |
| 5 | E | 33 | GLN |
| 5 | E | 64 | GLN |
| 5 | E | 73 | HIS |
| 5 | E | 104 | ASN |
| 5 | E | 121 | GLN |
| 5 | E | 123 | ASN |
| 5 | E | 125 | GLN |
| 5 | E | 156 | ASN |
| 5 | E | 185 | ASN |
| 5 | E | 199 | GLN |
| 5 | E | 2(E) | ASN |
| 6 | F | 23 | GLN |
| 6 | F | 43 | ASN |
| 6 | F | 87 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 6 | F | 90 | ASN |
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |
| 6 | F | 192 | GLN |
| 7 | G | 34(A) | ASN |
| 7 | G | 87 | ASN |
| 7 | G | 118 | ASN |
| 7 | G | 121 | GLN |
| 7 | G | 125 | GLN |
| 7 | G | 169 | GLN |
| 7 | G | 170 | GLN |
| 7 | G | 178 | ASN |
| 7 | G | 184 | ASN |
| 8 | H | 22 | GLN |
| 8 | H | 66 | HIS |
| 8 | H | 114 | HIS |
| 8 | H | 144 | GLN |
| 8 | H | 165 | ASN |
| 8 | H | 172 | ASN |
| 9 | I | 29 | ASN |
| 9 | I | 64 | ASN |
| 9 | I | 81 | GLN |
| 9 | I | 145 | ASN |
| 10 | J | 36 | GLN |
| 10 | J | 54 | GLN |
| 10 | J | 77 | GLN |
| 10 | J | 85 | GLN |
| 10 | J | 112 | GLN |
| 10 | J | 140 | HIS |
| 10 | J | 141 | HIS |
| 10 | J | 186 | GLN |
| 10 | J | 193 | GLN |
| 11 | K | 9 | GLN |
| 11 | K | 85 | ASN |
| 11 | K | 131 | GLN |
| 11 | K | 174 | ASN |
| 11 | K | 207 | ASN |
| 12 | L | -9 | GLN |
| 12 | L | -7 | ASN |
| 12 | L | 40 | ASN |
| 12 | L | 46 | ASN |
| 12 | L | 61 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 123 | GLN |
| 12 | L | 14(C) | GLN |
| 12 | L | 1(I) | ASN |
| 12 | L | 166 | HIS |
| 12 | L | 168 | GLN |
| 13 | M | -7 | GLN |
| 13 | M | 10 | ASN |
| 13 | M | 18 | ASN |
| 13 | M | 40 | ASN |
| 13 | M | 89 | GLN |
| 13 | M | 93 | ASN |
| 13 | M | 149 | GLN |
| 13 | M | 157 | ASN |
| 13 | M | 191 | GLN |
| 14 | N | 145 | ASN |
| 14 | N | 157 | HIS |
| 14 | N | 161 | GLN |
| 1 | O | 33 | GLN |
| 1 | O | 97 | HIS |
| 1 | O | 145 | ASN |
| 2 | P | 23 | GLN |
| 2 | P | 71 | ASN |
| 2 | P | 121 | GLN |
| 2 | P | 125 | GLN |
| 2 | P | 156 | ASN |
| 2 | P | 177 | GLN |
| 2 | P | 218 | ASN |
| 3 | Q | 23 | GLN |
| 3 | Q | 82 | ASN |
| 3 | Q | 97 | GLN |
| 3 | Q | 121 | GLN |
| 3 | Q | 125 | GLN |
| 3 | Q | 150 | GLN |
| 3 | Q | 163 | GLN |
| 3 | Q | 209 | ASN |
| 3 | Q | 238 | GLN |
| 3 | Q | 243 | GLN |
| 4 | R | 23 | GLN |
| 4 | R | 108 | ASN |
| 4 | R | 161 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 4 | R | 211 | GLN |
| 4 | R | 218 | GLN |
| 4 | R | 226 | ASN |
| 5 | S | 7 | ASN |
| 5 | S | 33 | GLN |
| 5 | S | 64 | GLN |
| 5 | S | 73 | HIS |
| 5 | S | 104 | ASN |
| 5 | S | 121 | GLN |
| 5 | S | 123 | ASN |
| 5 | S | 125 | GLN |
| 5 | S | 156 | ASN |
| 5 | S | 185 | ASN |
| 5 | S | 199 | GLN |
| 5 | S | 2(E) | ASN |
| 6 | T | 23 | GLN |
| 6 | T | 43 | ASN |
| 6 | T | 87 | HIS |
| 6 | T | 90 | ASN |
| 6 | T | 121 | GLN |
| 6 | T | 127 | ASN |
| 6 | T | 147 | HIS |
| 6 | T | 192 | GLN |
| 7 | U | 34(A) | ASN |
| 7 | U | 87 | ASN |
| 7 | U | 118 | ASN |
| 7 | U | 121 | GLN |
| 7 | U | 125 | GLN |
| 7 | U | 169 | GLN |
| 7 | U | 170 | GLN |
| 7 | U | 178 | ASN |
| 7 | U | 184 | ASN |
| 8 | V | 66 | HIS |
| 8 | V | 144 | GLN |
| 8 | V | 165 | ASN |
| 8 | V | 172 | ASN |
| 9 | W | 29 | ASN |
| 9 | W | 81 | GLN |
| 9 | W | 145 | ASN |
| 10 | X | 36 | GLN |
| 10 | X | 54 | GLN |
| 10 | X | 77 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 10 | X | 85 | GLN |
| 10 | X | 112 | GLN |
| 10 | X | 140 | HIS |
| 10 | X | 141 | HIS |
| 10 | X | 186 | GLN |
| 10 | X | 193 | GLN |
| 11 | Y | 9 | GLN |
| 11 | Y | 85 | ASN |
| 11 | Y | 131 | GLN |
| 11 | Y | 174 | ASN |
| 11 | Y | 207 | ASN |
| 12 | Z | -9 | GLN |
| 12 | Z | -7 | ASN |
| 12 | Z | 40 | ASN |
| 12 | Z | 46 | ASN |
| 12 | Z | 61 | ASN |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 85 | HIS |
| 12 | Z | 123 | GLN |
| 12 | Z | 14(B) | ASN |
| 12 | Z | 1(I) | ASN |
| 12 | Z | 166 | HIS |
| 13 | 1 | -7 | GLN |
| 13 | 1 | 10 | ASN |
| 13 | 1 | 18 | ASN |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 89 | GLN |
| 13 | 1 | 93 | ASN |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 157 | ASN |
| 13 | 1 | 191 | GLN |
| 14 | 2 | 38 | HIS |
| 14 | 2 | 145 | ASN |
| 14 | 2 | 157 | HIS |
| 14 | 2 | 161 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 15 | MES | K | 1(L) | - | 12,12,12 | 2.75 | 8 (66%) | 14,16,16 | 3.19 | 6 (42%) |
| 16 | H10 | Y | 2(I) | - | 27,29,29 | 3.32 | 18 (66%) | 36,43,43 | 1.01 | 2 (5%) |
| 16 | H10 | K | 2(I) | - | 27,29,29 | 3.41 | 18 (66%) | 36,43,43 | 1.05 | 3 (8%) |
| 15 | MES | Y | 1(L) | - | 12,12,12 | 2.74 | 6 (50%) | 14,16,16 | 3.16 | 5 (35%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 15 | MES | K | 1(L) | - | - | 5/6/14/14 | 0/1/1/1 |
| 16 | H10 | Y | 2(I) | - | - | 2/14/45/45 | 0/5/4/4 |
| 16 | H10 | K | 2(I) | - | - | 2/14/45/45 | 0/5/4/4 |
| 15 | MES | Y | 1(L) | - | - | 3/6/14/14 | 0/1/1/1 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 16 | K | 2(I) | H10 | O13-N9 | -11.07 | 1.25 | 1.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 16 | Y | 2(I) | H10 | O13-N9 | -10.31 | 1.26 | 1.40 |
| 16 | Y | 2(I) | H10 | C26-C1 | 5.58 | 1.62 | 1.52 |
| 15 | Y | 1(L) | MES | C8-S | 5.23 | 1.84 | 1.77 |
| 16 | K | 2(I) | H10 | C26-C1 | 5.22 | 1.61 | 1.52 |
| 15 | K | 1(L) | MES | C8-S | 4.98 | 1.84 | 1.77 |
| 16 | K | 2(I) | H10 | C25-C1 | 4.96 | 1.61 | 1.52 |
| 16 | Y | 2(I) | H10 | C25-C1 | 4.95 | 1.61 | 1.52 |
| 16 | K | 2(I) | H10 | C17-C3 | 4.45 | 1.47 | 1.38 |
| 16 | K | 2(I) | H10 | C18-C1 | 4.36 | 1.60 | 1.52 |
| 15 | Y | 1(L) | MES | C7-C8 | -4.34 | 1.40 | 1.52 |
| 16 | Y | 2(I) | H10 | C18-C1 | 4.05 | 1.59 | 1.52 |
| 16 | Y | 2(I) | H10 | C17-C3 | 4.03 | 1.46 | 1.38 |
| 15 | K | 1(L) | MES | C7-C8 | -3.80 | 1.42 | 1.52 |
| 15 | Y | 1(L) | MES | O1-C6 | -3.78 | 1.27 | 1.42 |
| 16 | Y | 2(I) | H10 | C20-C19 | 3.44 | 1.61 | 1.52 |
| 15 | K | 1(L) | MES | O1-C6 | -3.43 | 1.28 | 1.42 |
| 16 | K | 2(I) | H10 | C24-C19 | 3.12 | 1.60 | 1.52 |
| 16 | Y | 2(I) | H10 | C24-C19 | 3.05 | 1.60 | 1.52 |
| 16 | K | 2(I) | H10 | C24-C23 | 3.00 | 1.60 | 1.52 |
| 16 | Y | 2(I) | H10 | C22-C23 | 2.99 | 1.60 | 1.52 |
| 16 | K | 2(I) | H10 | C20-C19 | 2.95 | 1.60 | 1.52 |
| 16 | Y | 2(I) | H10 | C24-C23 | 2.95 | 1.60 | 1.52 |
| 16 | K | 2(I) | H10 | C6-C7 | -2.88 | 1.16 | 1.19 |
| 16 | K | 2(I) | H10 | C22-C21 | 2.87 | 1.60 | 1.52 |
| 16 | Y | 2(I) | H10 | C18-C19 | 2.80 | 1.61 | 1.54 |
| 15 | K | 1(L) | MES | O2S-S | -2.79 | 1.36 | 1.45 |
| 15 | K | 1(L) | MES | C3-N4 | 2.75 | 1.54 | 1.46 |
| 16 | K | 2(I) | H10 | C22-C23 | 2.73 | 1.59 | 1.52 |
| 16 | K | 2(I) | H10 | C18-C19 | 2.73 | 1.61 | 1.54 |
| 16 | Y | 2(I) | H10 | C6-C7 | -2.72 | 1.16 | 1.19 |
| 16 | Y | 2(I) | H10 | C22-C21 | 2.71 | 1.59 | 1.52 |
| 16 | K | 2(I) | H10 | C4-C3 | 2.69 | 1.43 | 1.38 |
| 16 | Y | 2(I) | H10 | C4-C3 | 2.65 | 1.43 | 1.38 |
| 15 | K | 1(L) | MES | O1-C2 | 2.62 | 1.53 | 1.42 |
| 15 | K | 1(L) | MES | O1S-S | 2.61 | 1.52 | 1.45 |
| 15 | Y | 1(L) | MES | C3-N4 | 2.61 | 1.54 | 1.46 |
| 16 | Y | 2(I) | H10 | C20-C21 | 2.46 | 1.59 | 1.52 |
| 16 | K | 2(I) | H10 | C4-C5 | 2.43 | 1.43 | 1.39 |
| 15 | Y | 1(L) | MES | O1-C2 | 2.38 | 1.52 | 1.42 |
| 16 | K | 2(I) | H10 | C16-C17 | 2.33 | 1.43 | 1.38 |
| 16 | Y | 2(I) | H10 | C16-C15 | 2.31 | 1.43 | 1.38 |
| 15 | K | 1(L) | MES | C5-C6 | 2.23 | 1.59 | 1.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | Y | 1(L) | MES | C5-C6 | 2.20 | 1.59 | 1.50 |
| 16 | K | 2(I) | H10 | C20-C21 | 2.13 | 1.58 | 1.52 |
| 16 | Y | 2(I) | H10 | C15-C5 | 2.12 | 1.43 | 1.39 |
| 16 | Y | 2(I) | H10 | C4-C5 | 2.10 | 1.43 | 1.39 |
| 16 | Y | 2(I) | H10 | C16-C17 | 2.07 | 1.43 | 1.38 |
| 16 | K | 2(I) | H10 | C16-C15 | 2.05 | 1.43 | 1.38 |
| 16 | K | 2(I) | H10 | C15-C5 | 2.04 | 1.43 | 1.39 |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | Y | 1(L) | MES | O1S-S-C8 | -9.48 | 95.50 | 106.92 |
| 15 | K | 1(L) | MES | O1S-S-C8 | -9.44 | 95.55 | 106.92 |
| 15 | Y | 1(L) | MES | O2S-S-C8 | 4.18 | 111.95 | 106.92 |
| 15 | Y | 1(L) | MES | O3S-S-O2S | 3.87 | 120.72 | 111.27 |
| 15 | K | 1(L) | MES | O3S-S-O2S | 3.84 | 120.65 | 111.27 |
| 15 | K | 1(L) | MES | O1-C2-C3 | -2.73 | 105.79 | 111.80 |
| 15 | K | 1(L) | MES | C7-N4-C3 | 2.70 | 118.13 | 111.23 |
| 16 | K | 2(I) | H10 | C14-C8-N9 | 2.62 | 114.41 | 110.24 |
| 16 | Y | 2(I) | H10 | C14-C8-N9 | 2.60 | 114.38 | 110.24 |
| 16 | K | 2(I) | H10 | C26-C1-C18 | -2.60 | 106.39 | 109.89 |
| 16 | Y | 2(I) | H10 | O11-C10-N12 | -2.30 | 118.34 | 122.77 |
| 16 | K | 2(I) | H10 | O11-C10-N12 | -2.27 | 118.40 | 122.77 |
| 15 | K | 1(L) | MES | O3S-S-C8 | 2.25 | 109.41 | 105.77 |
| 15 | K | 1(L) | MES | C6-C5-N4 | 2.22 | 113.47 | 110.10 |
| 15 | Y | 1(L) | MES | O1-C2-C3 | -2.07 | 107.24 | 111.80 |
| 15 | Y | 1(L) | MES | C7-N4-C3 | 2.02 | 116.39 | 111.23 |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 15 | K | 1(L) | MES | C7-C8-S-O1S |
| 15 | K | 1(L) | MES | C7-C8-S-O3S |
| 15 | Y | 1(L) | MES | C7-C8-S-O1S |
| 15 | Y | 1(L) | MES | C7-C8-S-O2S |
| 15 | Y | 1(L) | MES | C7-C8-S-O3S |
| 16 | Y | 2(I) | H10 | C5-C6-C7-C8 |
| 16 | K | 2(I) | H10 | C5-C6-C7-C8 |
| 15 | K | 1(L) | MES | C8-C7-N4-C3 |
| 15 | K | 1(L) | MES | C8-C7-N4-C5 |
| 15 | K | 1(L) | MES | C7-C8-S-O2S |

Continued on next page...

Continued from previous page...

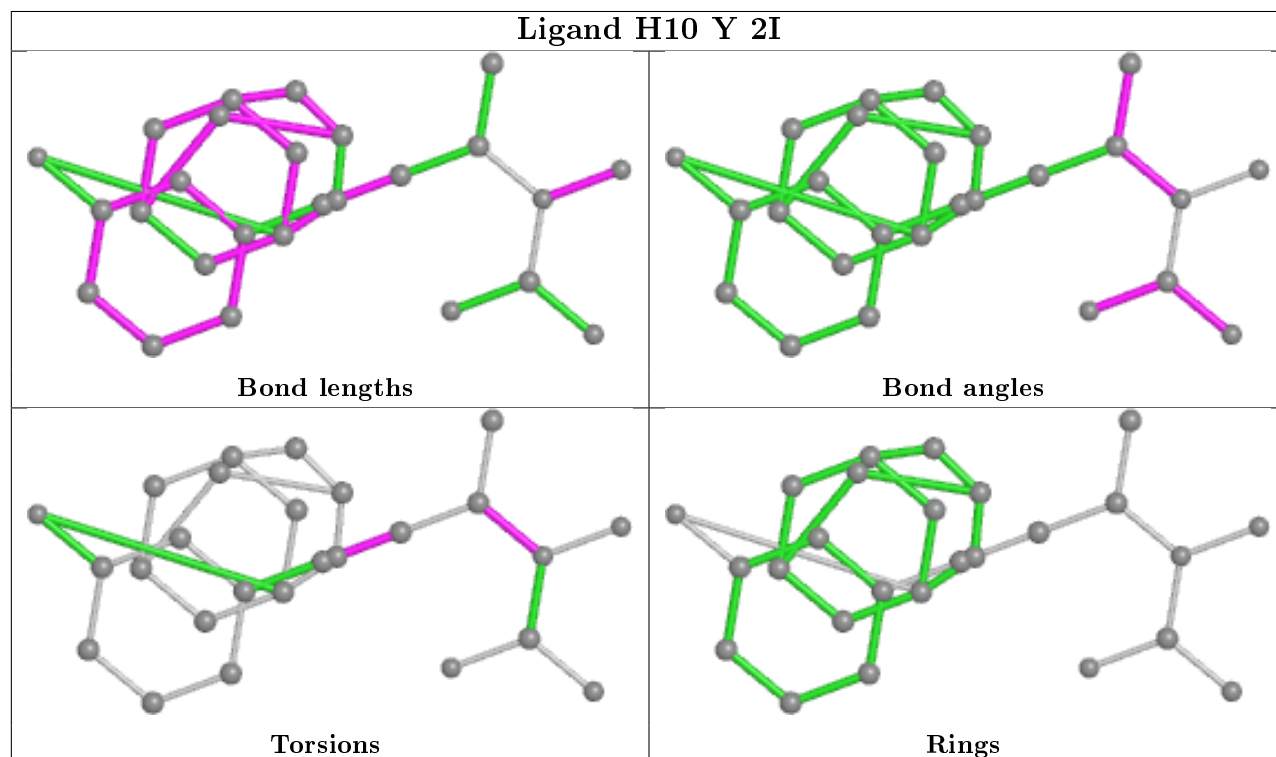
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 16 | Y | 2(I) | H10 | C14-C8-N9-O13 |
| 16 | K | 2(I) | H10 | C14-C8-N9-O13 |

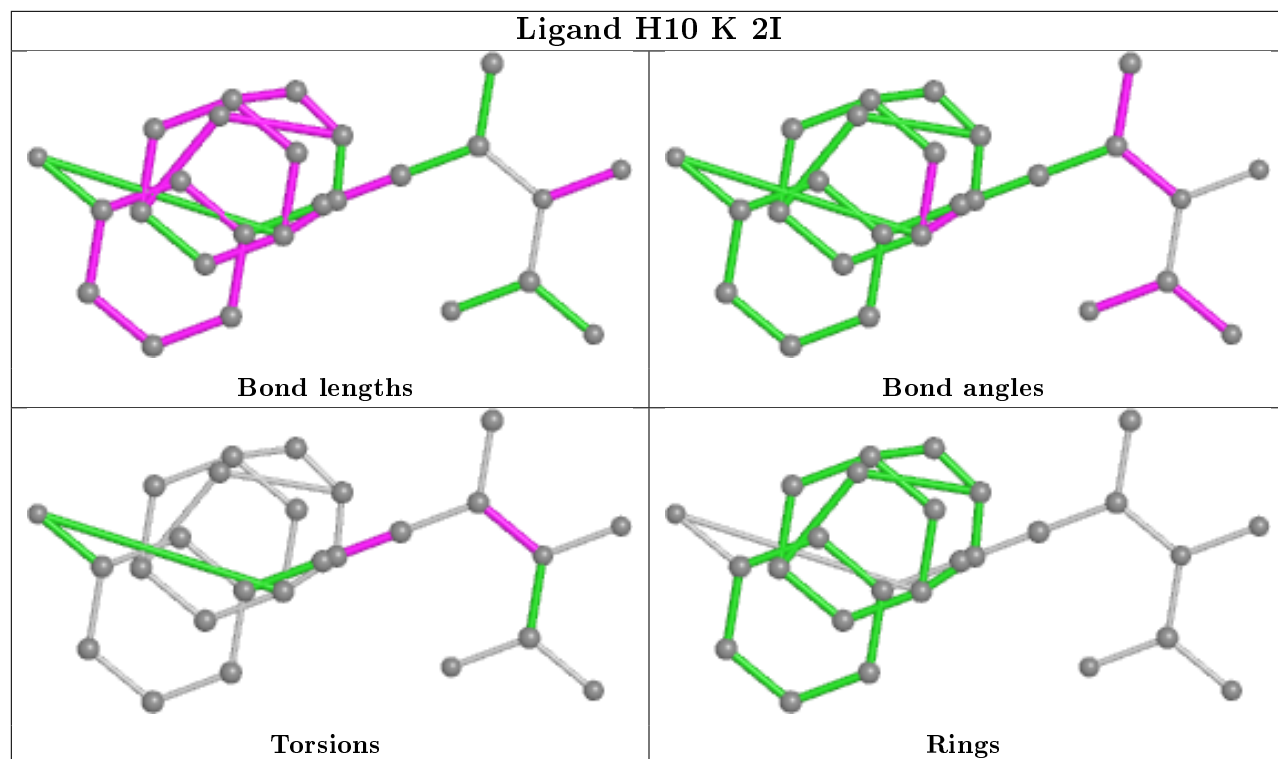
There are no ring outliers.

2 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 16 | Y | 2(I) | H10 | 7 | 0 |
| 16 | K | 2(I) | H10 | 4 | 0 |

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





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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 250/250 (100%) | -0.35 | 1 (0%) 92 91 | 47, 64, 92, 112 | 0 |
| 1 | O | 250/250 (100%) | -0.28 | 4 (1%) 72 66 | 48, 65, 94, 112 | 0 |
| 2 | B | 244/244 (100%) | -0.19 | 5 (2%) 65 56 | 47, 67, 103, 129 | 0 |
| 2 | P | 244/244 (100%) | -0.06 | 6 (2%) 57 47 | 46, 67, 103, 129 | 0 |
| 3 | C | 241/241 (100%) | -0.06 | 6 (2%) 57 47 | 50, 69, 118, 136 | 0 |
| 3 | Q | 241/241 (100%) | 0.06 | 16 (6%) 18 11 | 51, 70, 118, 136 | 0 |
| 4 | D | 242/242 (100%) | -0.12 | 6 (2%) 57 47 | 49, 70, 102, 133 | 0 |
| 4 | R | 242/242 (100%) | -0.13 | 8 (3%) 46 36 | 48, 70, 103, 133 | 0 |
| 5 | E | 233/233 (100%) | -0.21 | 2 (0%) 84 80 | 52, 74, 98, 121 | 0 |
| 5 | S | 233/233 (100%) | 0.02 | 10 (4%) 35 25 | 52, 75, 99, 121 | 0 |
| 6 | F | 244/244 (100%) | -0.24 | 2 (0%) 86 81 | 48, 65, 100, 112 | 0 |
| 6 | T | 244/244 (100%) | -0.24 | 1 (0%) 92 91 | 48, 65, 101, 113 | 0 |
| 7 | G | 243/243 (100%) | -0.37 | 4 (1%) 72 66 | 45, 61, 88, 120 | 0 |
| 7 | U | 243/243 (100%) | -0.32 | 2 (0%) 86 81 | 46, 62, 87, 119 | 0 |
| 8 | H | 222/222 (100%) | -0.39 | 1 (0%) 91 88 | 46, 59, 78, 110 | 0 |
| 8 | V | 222/222 (100%) | -0.41 | 2 (0%) 84 80 | 48, 61, 78, 109 | 0 |
| 9 | I | 204/204 (100%) | -0.36 | 1 (0%) 91 88 | 42, 58, 81, 95 | 0 |
| 9 | W | 204/204 (100%) | -0.21 | 1 (0%) 91 88 | 44, 58, 80, 96 | 0 |
| 10 | J | 198/198 (100%) | -0.46 | 2 (1%) 82 77 | 44, 58, 75, 128 | 0 |
| 10 | X | 198/198 (100%) | -0.43 | 3 (1%) 73 68 | 46, 58, 74, 128 | 0 |
| 11 | K | 212/212 (100%) | -0.43 | 0 100 100 | 42, 57, 73, 84 | 0 |
| 11 | Y | 212/212 (100%) | -0.45 | 0 100 100 | 44, 58, 73, 84 | 0 |
| 12 | L | 222/222 (100%) | -0.37 | 1 (0%) 91 88 | 42, 59, 81, 100 | 0 |
| 12 | Z | 222/222 (100%) | -0.37 | 2 (0%) 84 80 | 42, 60, 81, 99 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 13 | 1 | 233/233 (100%) | -0.53 | 1 (0%) 92 91 | 45, 57, 71, 80 | 0 |
| 13 | M | 233/233 (100%) | -0.47 | 1 (0%) 92 91 | 44, 58, 72, 79 | 0 |
| 14 | 2 | 196/196 (100%) | -0.48 | 0 100 100 | 44, 54, 75, 87 | 0 |
| 14 | N | 196/196 (100%) | -0.56 | 0 100 100 | 42, 53, 74, 88 | 0 |
| All | All | 6368/6368 (100%) | -0.29 | 88 (1%) 75 70 | 42, 62, 95, 136 | 0 |

All (88) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 4 | D | 12(D) | ALA | 8.6 |
| 4 | D | 12(E) | SER | 7.9 |
| 4 | D | 12(F) | GLY | 7.6 |
| 4 | D | 12(C) | GLY | 7.3 |
| 4 | R | 12(F) | GLY | 6.5 |
| 7 | U | 240 | ASP | 5.7 |
| 4 | R | 12(D) | ALA | 5.5 |
| 7 | U | 6 | ALA | 5.4 |
| 2 | P | 218 | ASN | 5.2 |
| 3 | C | 56 | LEU | 5.1 |
| 3 | C | 55 | THR | 5.1 |
| 4 | R | 126 | ARG | 4.6 |
| 2 | B | 218 | ASN | 4.5 |
| 7 | G | 6 | ALA | 4.2 |
| 5 | S | 5 | ARG | 4.1 |
| 4 | R | 12(E) | SER | 4.0 |
| 3 | Q | 56 | LEU | 4.0 |
| 1 | A | 4 | MET | 4.0 |
| 3 | Q | 55 | THR | 3.9 |
| 5 | S | 233 | ILE | 3.9 |
| 8 | V | 223 | ASP | 3.8 |
| 2 | B | 217 | ALA | 3.8 |
| 5 | E | 4 | PHE | 3.8 |
| 4 | D | 126 | ARG | 3.5 |
| 6 | F | 240 | ILE | 3.4 |
| 4 | D | 12(G) | GLU | 3.3 |
| 2 | P | 217 | ALA | 3.3 |
| 10 | J | 193 | GLN | 3.3 |
| 3 | Q | 54 | SER | 3.2 |
| 13 | M | -8 | THR | 3.2 |
| 10 | X | 193 | GLN | 3.2 |
| 3 | Q | 242 | GLU | 3.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 3 | Q | 238 | GLN | 3.1 |
| 3 | Q | 236 | ILE | 3.1 |
| 12 | Z | 145 | TYR | 3.1 |
| 1 | O | 236 | LEU | 3.0 |
| 5 | E | 5 | ARG | 3.0 |
| 5 | S | 197 | ILE | 2.9 |
| 5 | S | 206 | SER | 2.8 |
| 12 | L | 145 | TYR | 2.8 |
| 4 | R | 12(B) | GLU | 2.8 |
| 4 | R | 12(C) | GLY | 2.8 |
| 5 | S | 231 | LYS | 2.8 |
| 5 | S | 232 | TYR | 2.8 |
| 2 | B | 232 | ILE | 2.8 |
| 2 | P | 219 | GLU | 2.7 |
| 6 | F | 204 | ASP | 2.6 |
| 7 | G | 240 | ASP | 2.6 |
| 1 | O | 4 | MET | 2.6 |
| 8 | H | 222 | CYS | 2.6 |
| 4 | R | 12(G) | GLU | 2.6 |
| 7 | G | 237 | ALA | 2.5 |
| 10 | J | 191 | GLN | 2.5 |
| 5 | S | 4 | PHE | 2.5 |
| 10 | X | 191 | GLN | 2.5 |
| 2 | P | 21(C) | ASP | 2.5 |
| 3 | Q | 203 | THR | 2.5 |
| 3 | Q | 202 | GLN | 2.5 |
| 2 | B | 21(B) | GLY | 2.4 |
| 1 | O | 5 | THR | 2.4 |
| 3 | Q | 241 | GLN | 2.4 |
| 1 | O | 235 | ALA | 2.4 |
| 3 | Q | 239 | GLU | 2.4 |
| 13 | 1 | -8 | THR | 2.4 |
| 12 | Z | 14(W) | LYS | 2.3 |
| 3 | C | 239 | GLU | 2.3 |
| 7 | G | 239 | GLN | 2.3 |
| 3 | Q | 200 | VAL | 2.3 |
| 9 | W | -8 | SER | 2.3 |
| 3 | C | 212 | ILE | 2.3 |
| 3 | C | 202 | GLN | 2.3 |
| 3 | Q | 179 | ASN | 2.2 |
| 9 | I | -8 | SER | 2.2 |
| 8 | V | 222 | CYS | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 3 | Q | 233 | VAL | 2.2 |
| 2 | P | 239 | THR | 2.2 |
| 2 | P | 21(B) | GLY | 2.2 |
| 3 | Q | 189 | CYS | 2.2 |
| 5 | S | 178 | ARG | 2.1 |
| 4 | R | 127 | LEU | 2.1 |
| 2 | B | 54 | VAL | 2.1 |
| 3 | Q | 234 | THR | 2.1 |
| 10 | X | 192 | ALA | 2.1 |
| 3 | C | 240 | LYS | 2.1 |
| 5 | S | 223 | ILE | 2.0 |
| 5 | S | 195 | GLU | 2.0 |
| 3 | Q | 237 | GLU | 2.0 |
| 6 | T | 240 | ILE | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

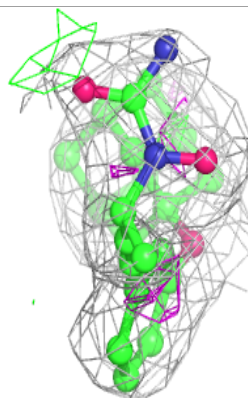
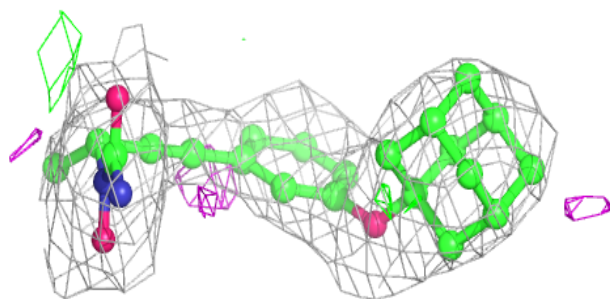
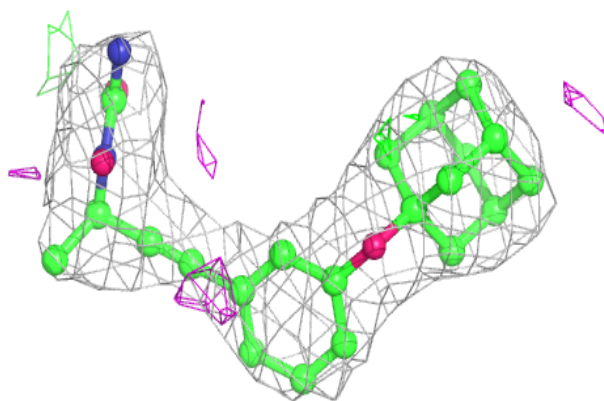
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 16 | H10 | Y | 2(I) | 26/26 | 0.94 | 0.18 | 46,51,60,62 | 0 |
| 16 | H10 | K | 2(I) | 26/26 | 0.96 | 0.20 | 46,50,57,58 | 0 |
| 15 | MES | Y | 1(L) | 12/12 | 0.96 | 0.18 | 63,70,75,76 | 0 |
| 15 | MES | K | 1(L) | 12/12 | 0.97 | 0.16 | 62,70,76,77 | 0 |

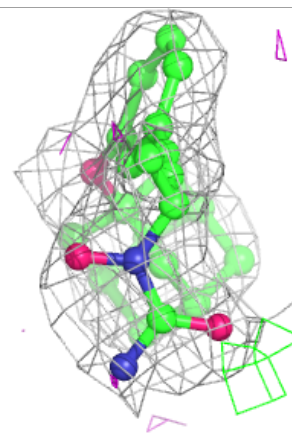
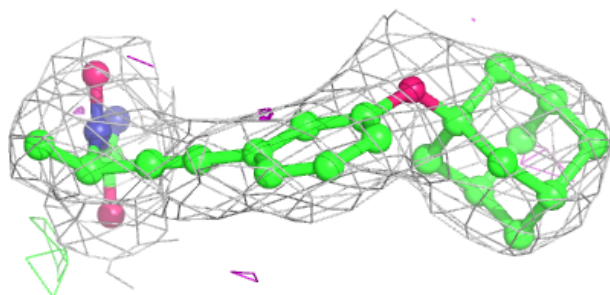
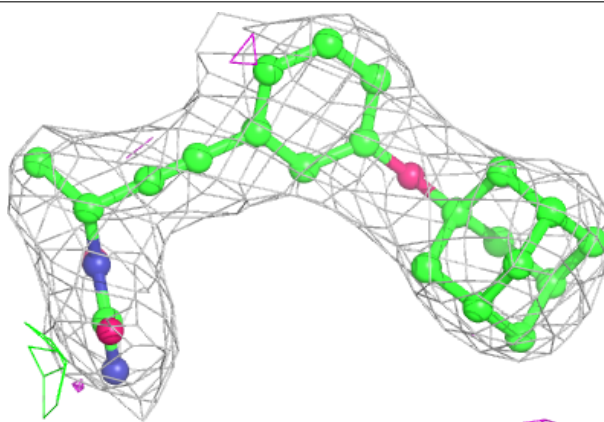
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around H10 Y 2I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around H10 K 2I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.