



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 02:03 PM EST

PDB ID : 6MRC
EMDB ID : EMD-9195
Title : ADP-bound human mitochondrial Hsp60-Hsp10 football complex
Authors : Gomez-Llorente, Y.; Jebara, F.; Patra, M.; Malik, R.; Nissemblat, S.; Azem, A.; Hirsch, J.A.; Ubarretxena-Belandia, I.
Deposited on : 2018-10-12
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

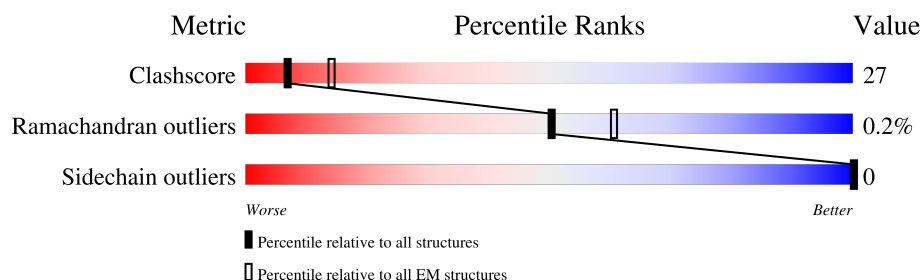
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 528 | <div> <div>18%</div> <div>57%</div> <div>43%</div> </div> |
| 1 | B | 528 | <div> <div>17%</div> <div>56%</div> <div>43%</div> </div> |
| 1 | C | 528 | <div> <div>18%</div> <div>55%</div> <div>45%</div> </div> |
| 1 | D | 528 | <div> <div>17%</div> <div>55%</div> <div>45%</div> </div> |
| 1 | E | 528 | <div> <div>18%</div> <div>56%</div> <div>44%</div> </div> |
| 1 | F | 528 | <div> <div>18%</div> <div>54%</div> <div>45%</div> </div> |
| 1 | G | 528 | <div> <div>19%</div> <div>55%</div> <div>44%</div> </div> |
| 1 | H | 528 | <div> <div>18%</div> <div>57%</div> <div>43%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | I | 528 | <div> <div>18%</div> <div>58%</div> <div>42%</div> </div> |
| 1 | J | 528 | <div> <div>18%</div> <div>55%</div> <div>44%</div> </div> |
| 1 | K | 528 | <div> <div>19%</div> <div>58%</div> <div>42%</div> </div> |
| 1 | L | 528 | <div> <div>17%</div> <div>57%</div> <div>42%</div> </div> |
| 1 | M | 528 | <div> <div>19%</div> <div>54%</div> <div>46%</div> </div> |
| 1 | N | 528 | <div> <div>18%</div> <div>56%</div> <div>44%</div> </div> |
| 2 | 1 | 100 | <div> <div>42%</div> <div>51%</div> <div>49%</div> </div> |
| 2 | 2 | 100 | <div> <div>43%</div> <div>50%</div> <div>49%</div> </div> |
| 2 | O | 100 | <div> <div>42%</div> <div>47%</div> <div>53%</div> </div> |
| 2 | P | 100 | <div> <div>43%</div> <div>47%</div> <div>53%</div> </div> |
| 2 | Q | 100 | <div> <div>41%</div> <div>47%</div> <div>53%</div> </div> |
| 2 | R | 100 | <div> <div>44%</div> <div>48%</div> <div>51%</div> </div> |
| 2 | S | 100 | <div> <div>40%</div> <div>50%</div> <div>50%</div> </div> |
| 2 | T | 100 | <div> <div>42%</div> <div>52%</div> <div>48%</div> </div> |
| 2 | U | 100 | <div> <div>42%</div> <div>52%</div> <div>48%</div> </div> |
| 2 | V | 100 | <div> <div>43%</div> <div>53%</div> <div>46%</div> </div> |
| 2 | W | 100 | <div> <div>43%</div> <div>52%</div> <div>48%</div> </div> |
| 2 | X | 100 | <div> <div>44%</div> <div>52%</div> <div>47%</div> </div> |
| 2 | Y | 100 | <div> <div>42%</div> <div>53%</div> <div>47%</div> </div> |
| 2 | Z | 100 | <div> <div>43%</div> <div>51%</div> <div>48%</div> </div> |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 69132 atoms, of which 2954 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60 kDa heat shock protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|----|---------|-------|
| 1 | H | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | N | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | M | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | L | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | K | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | J | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | I | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | D | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | C | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | B | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | A | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | G | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | F | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |
| 1 | E | 528 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4147 | 2467 | 211 | 672 | 783 | 14 | | |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| H | 1 | GLY | - | expression tag | UNP P10809 |
| H | 2 | SER | - | expression tag | UNP P10809 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| N | 1 | GLY | - | expression tag | UNP P10809 |
| N | 2 | SER | - | expression tag | UNP P10809 |
| M | 1 | GLY | - | expression tag | UNP P10809 |
| M | 2 | SER | - | expression tag | UNP P10809 |
| L | 1 | GLY | - | expression tag | UNP P10809 |
| L | 2 | SER | - | expression tag | UNP P10809 |
| K | 1 | GLY | - | expression tag | UNP P10809 |
| K | 2 | SER | - | expression tag | UNP P10809 |
| J | 1 | GLY | - | expression tag | UNP P10809 |
| J | 2 | SER | - | expression tag | UNP P10809 |
| I | 1 | GLY | - | expression tag | UNP P10809 |
| I | 2 | SER | - | expression tag | UNP P10809 |
| D | 1 | GLY | - | expression tag | UNP P10809 |
| D | 2 | SER | - | expression tag | UNP P10809 |
| C | 1 | GLY | - | expression tag | UNP P10809 |
| C | 2 | SER | - | expression tag | UNP P10809 |
| B | 1 | GLY | - | expression tag | UNP P10809 |
| B | 2 | SER | - | expression tag | UNP P10809 |
| A | 1 | GLY | - | expression tag | UNP P10809 |
| A | 2 | SER | - | expression tag | UNP P10809 |
| G | 1 | GLY | - | expression tag | UNP P10809 |
| G | 2 | SER | - | expression tag | UNP P10809 |
| F | 1 | GLY | - | expression tag | UNP P10809 |
| F | 2 | SER | - | expression tag | UNP P10809 |
| E | 1 | GLY | - | expression tag | UNP P10809 |
| E | 2 | SER | - | expression tag | UNP P10809 |

- Molecule 2 is a protein called 10 kDa heat shock protein, mitochondrial.

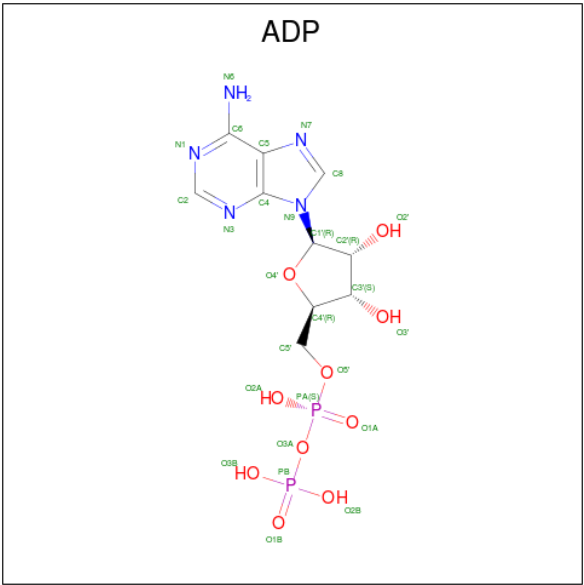
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | V | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | 2 | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | 1 | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | Z | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | Y | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | X | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | W | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | R | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | Q | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | P | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | O | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | U | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | T | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |
| 2 | S | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 486 | 127 | 142 | 1 | | |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3 | H | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | N | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | M | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3 | L | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | K | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | J | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | I | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | C | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | B | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | G | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 3 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 4 | H | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | M | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | L | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | K | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | J | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | I | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4 | C | 1 | Total 1 | Mg 1 | 0 |
| 4 | B | 1 | Total 1 | Mg 1 | 0 |
| 4 | A | 1 | Total 1 | Mg 1 | 0 |
| 4 | G | 1 | Total 1 | Mg 1 | 0 |
| 4 | F | 1 | Total 1 | Mg 1 | 0 |
| 4 | E | 1 | Total 1 | Mg 1 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 5 | H | 7 | Total 7 | O 7 | 0 |
| 5 | N | 7 | Total 7 | O 7 | 0 |
| 5 | M | 7 | Total 7 | O 7 | 0 |
| 5 | L | 7 | Total 7 | O 7 | 0 |
| 5 | K | 7 | Total 7 | O 7 | 0 |
| 5 | J | 7 | Total 7 | O 7 | 0 |
| 5 | I | 7 | Total 7 | O 7 | 0 |
| 5 | D | 7 | Total 7 | O 7 | 0 |
| 5 | C | 7 | Total 7 | O 7 | 0 |
| 5 | B | 7 | Total 7 | O 7 | 0 |
| 5 | A | 7 | Total 7 | O 7 | 0 |
| 5 | G | 7 | Total 7 | O 7 | 0 |
| 5 | F | 7 | Total 7 | O 7 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 5 | E | 7 | Total | O | 0 |
| | | | 7 | 7 | |

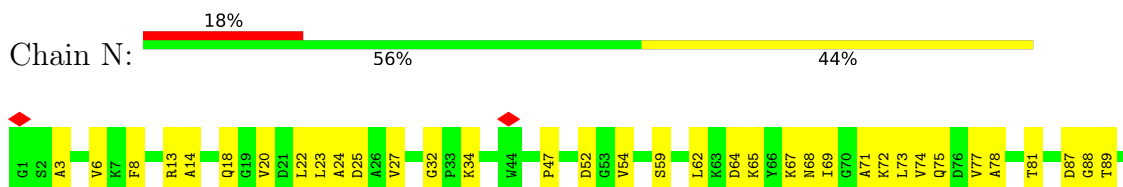
3 Residue-property plots

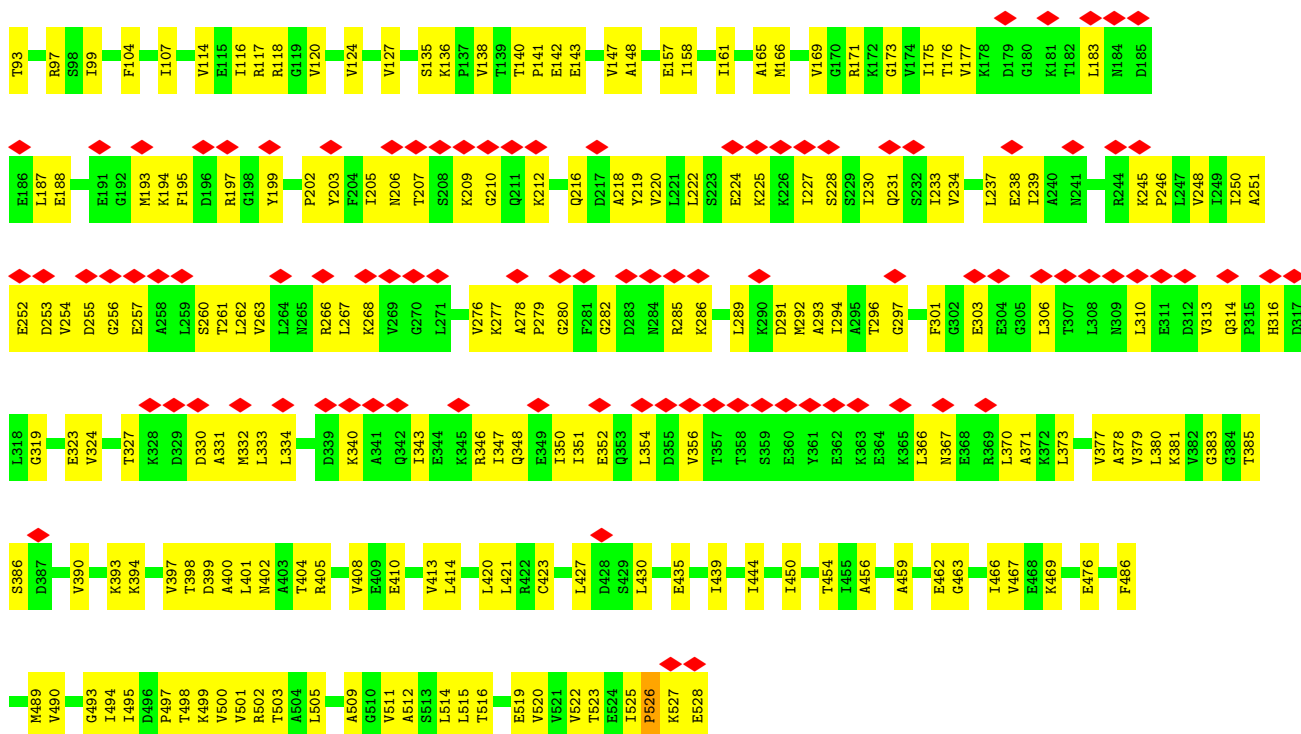
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 60 kDa heat shock protein, mitochondrial

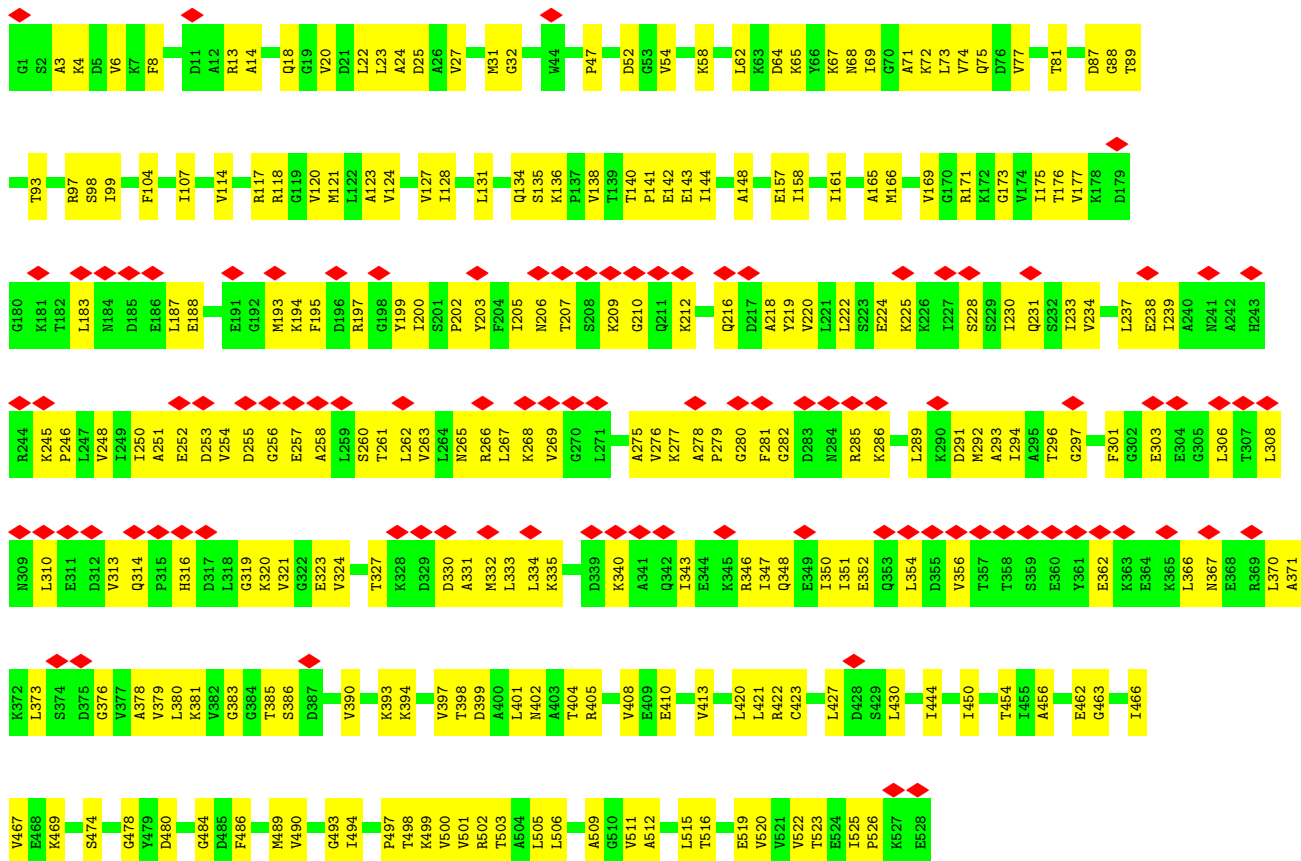


- Molecule 1: 60 kDa heat shock protein, mitochondrial

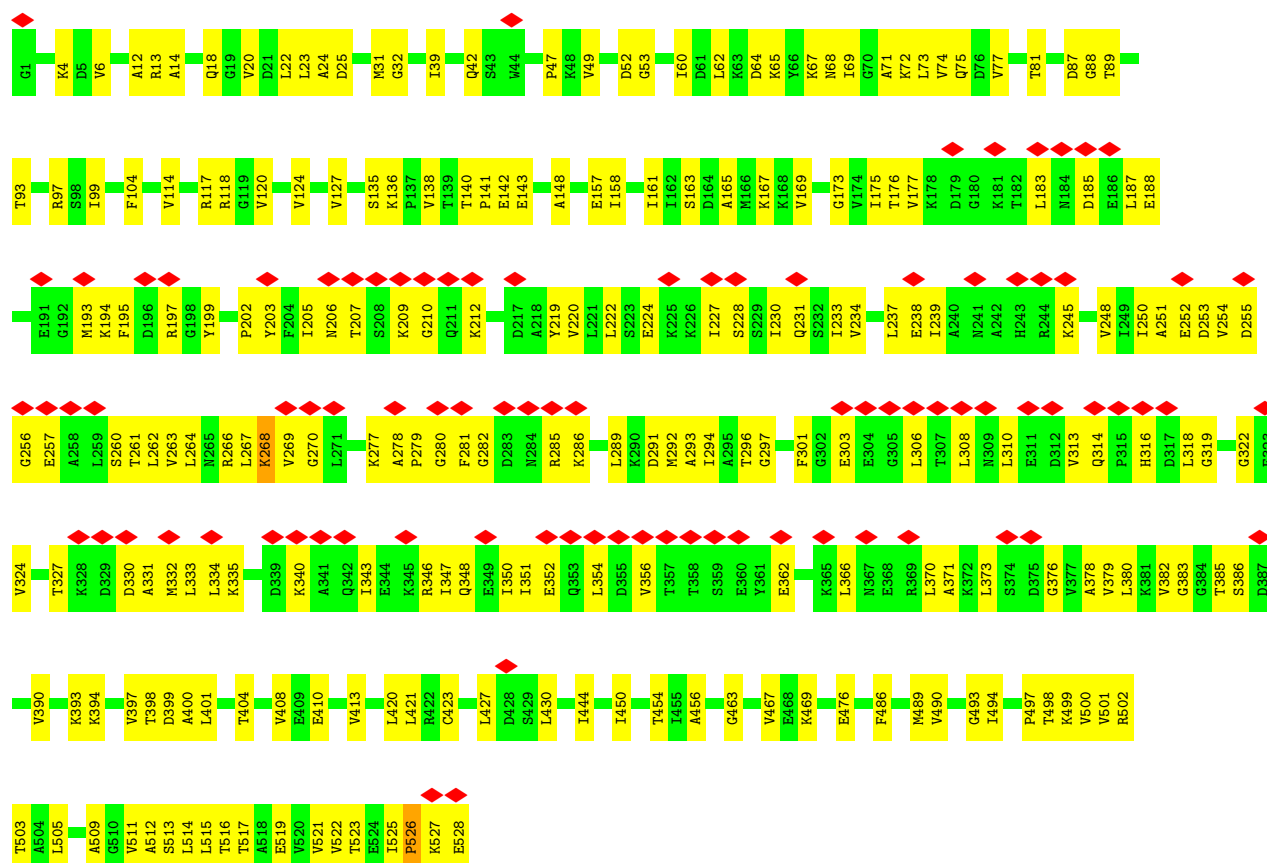




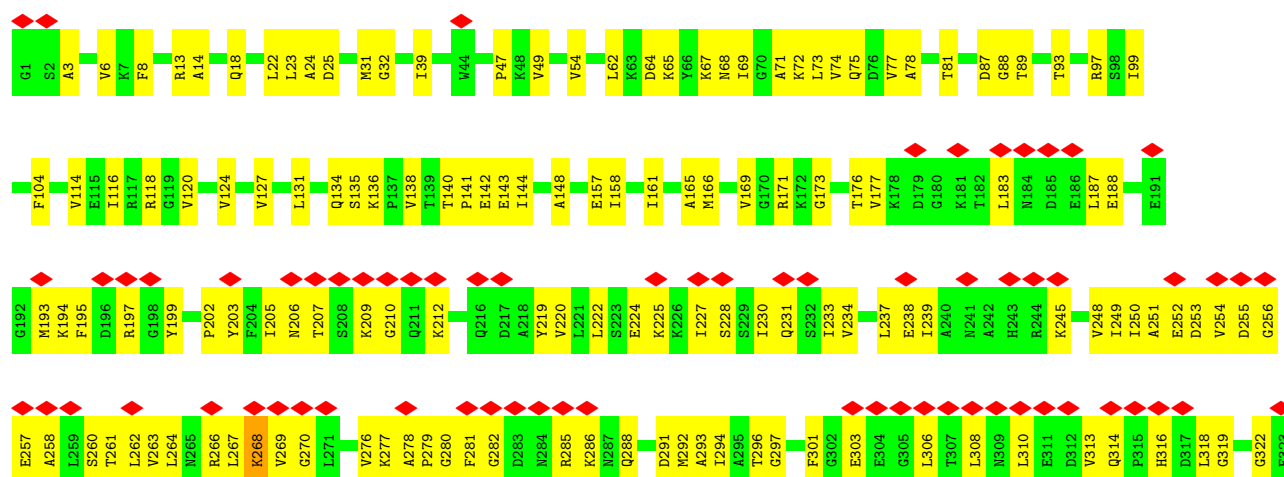
• Molecule 1: 60 kDa heat shock protein, mitochondrial

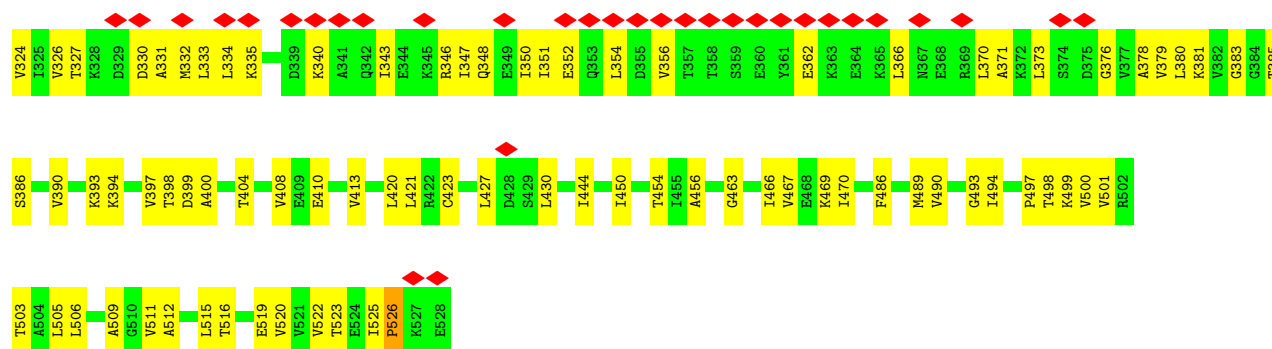


- Molecule 1: 60 kDa heat shock protein, mitochondrial



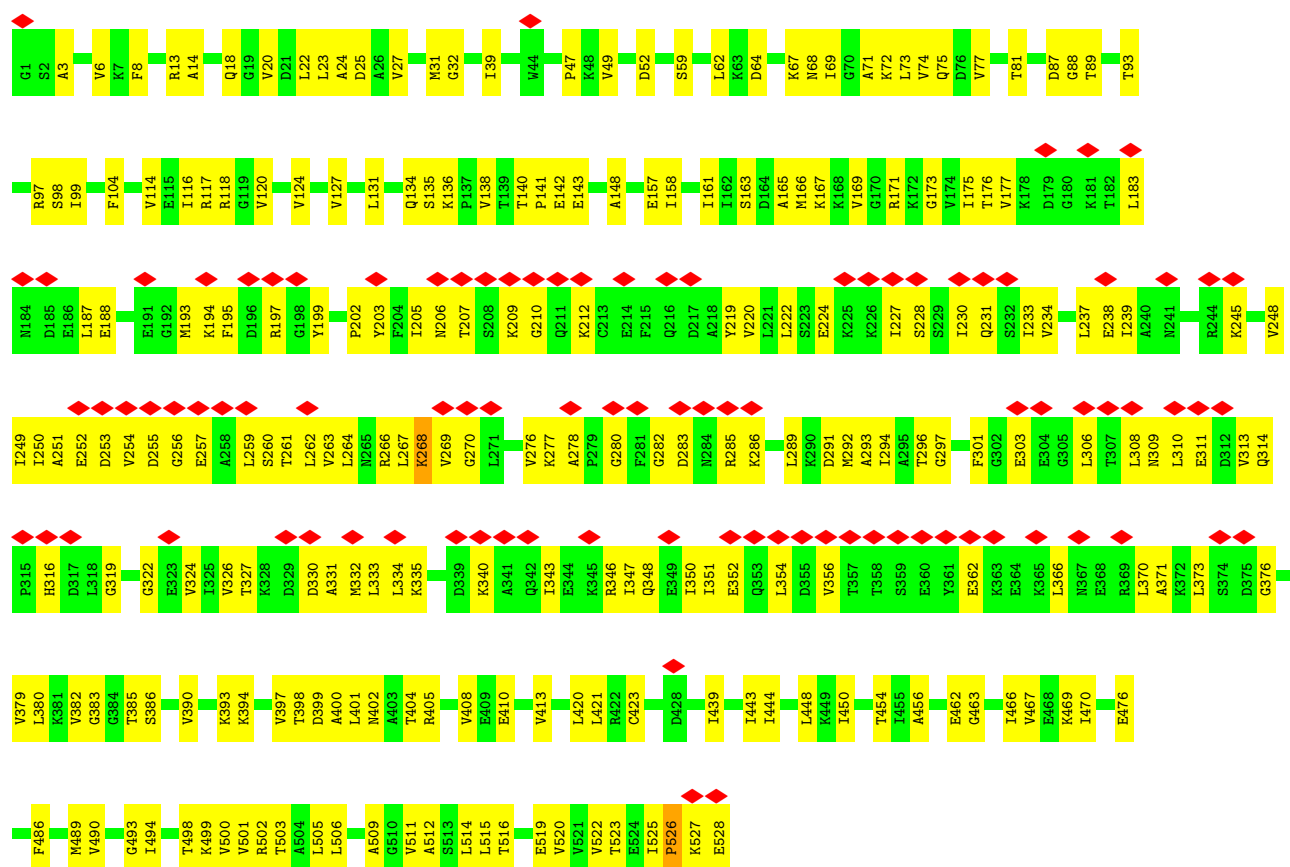
- Molecule 1: 60 kDa heat shock protein, mitochondrial





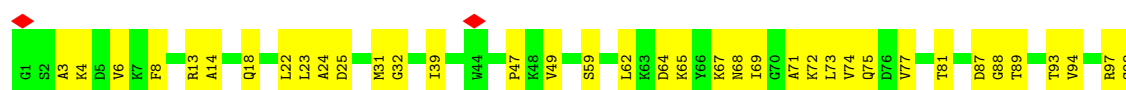
- Molecule 1: 60 kDa heat shock protein, mitochondrial

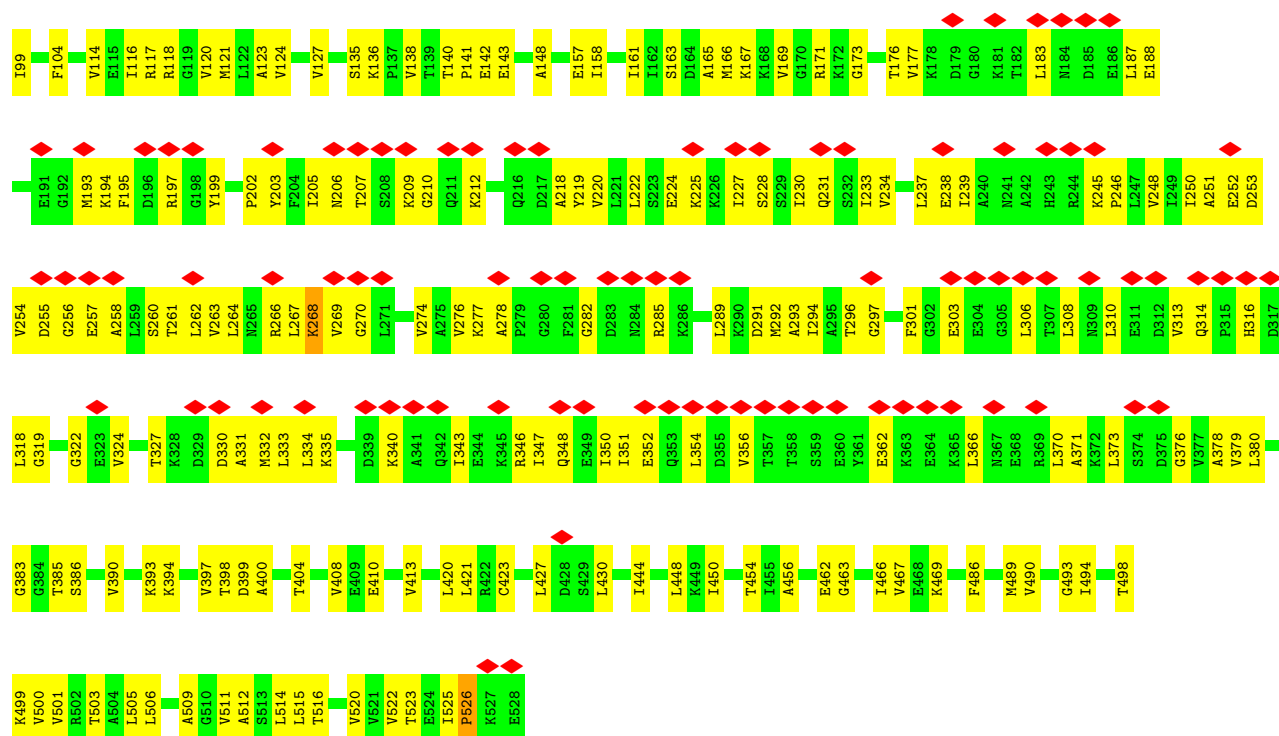
Chain J: 18% 55% 44%



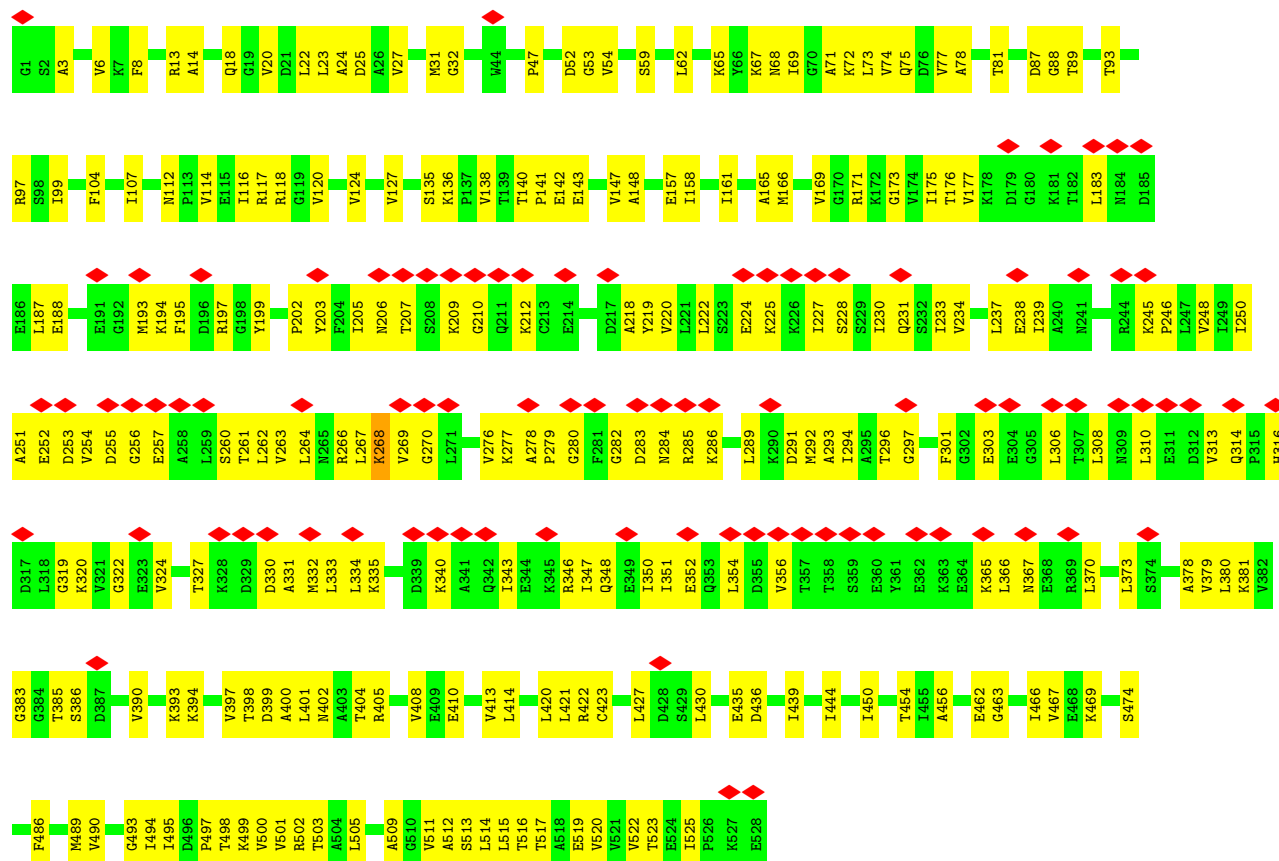
- Molecule 1: 60 kDa heat shock protein, mitochondrial

Chain I: 18% 58% 42%





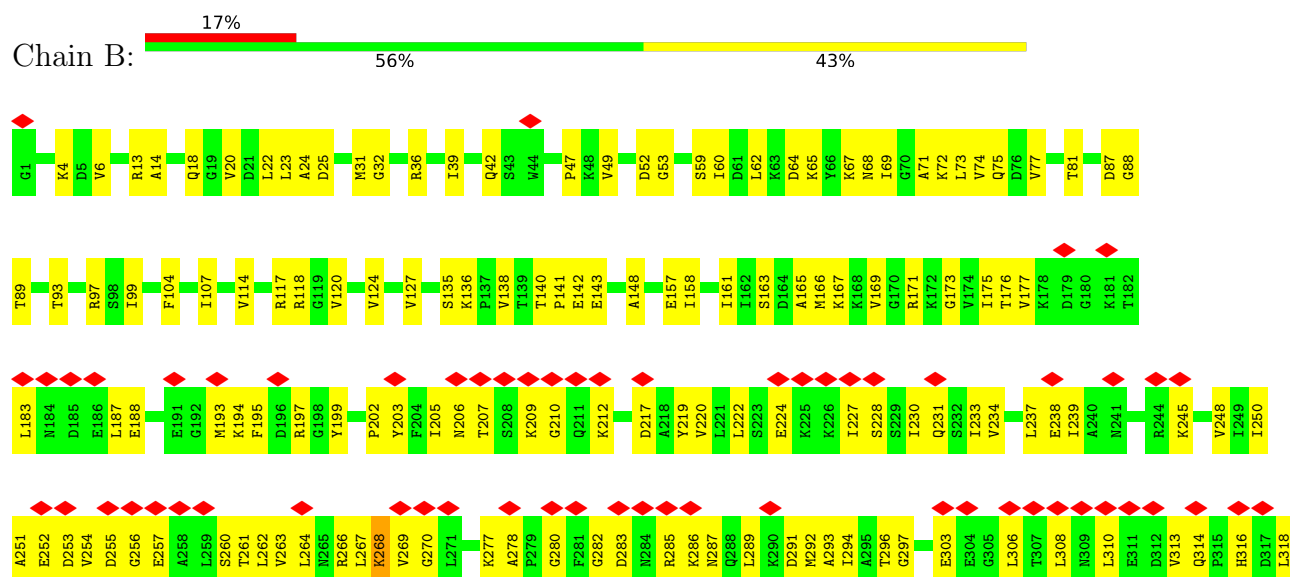
● Molecule 1: 60 kDa heat shock protein, mitochondrial

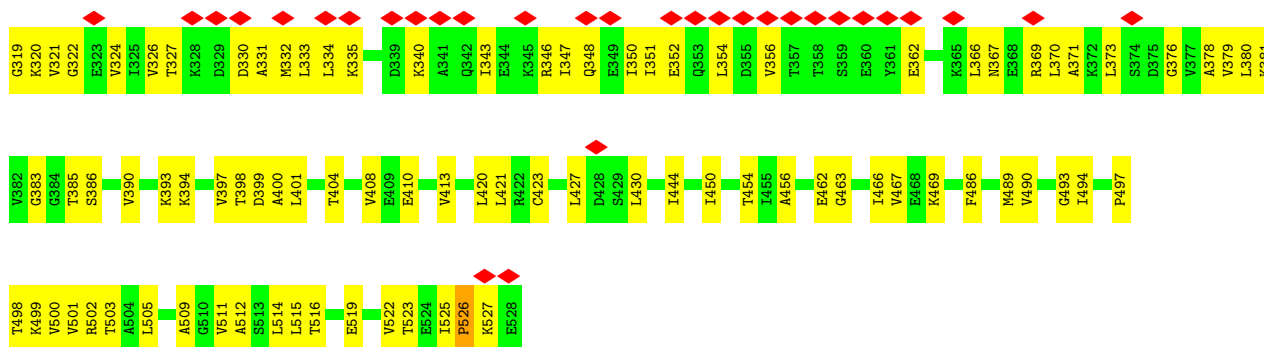


- Molecule 1: 60 kDa heat shock protein, mitochondrial

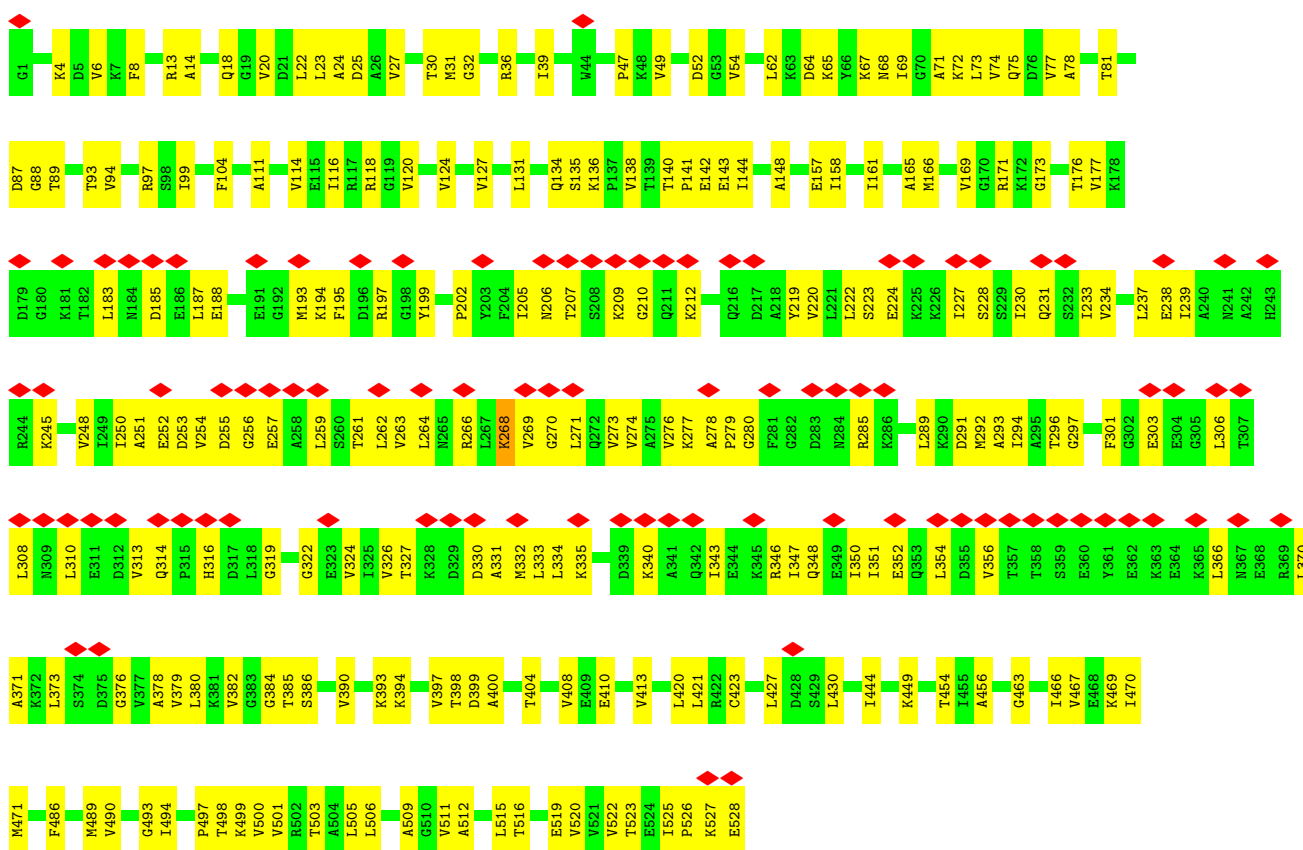


- Molecule 1: 60 kDa heat shock protein, mitochondrial

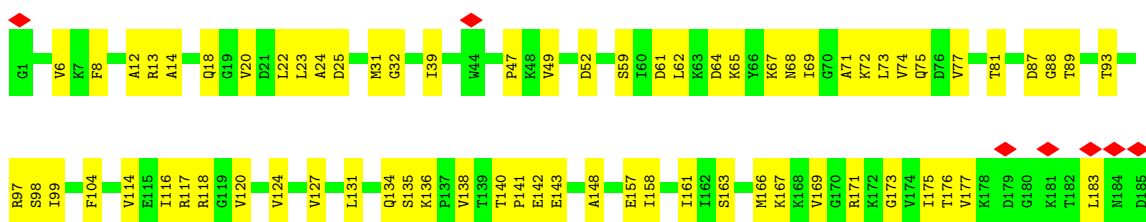


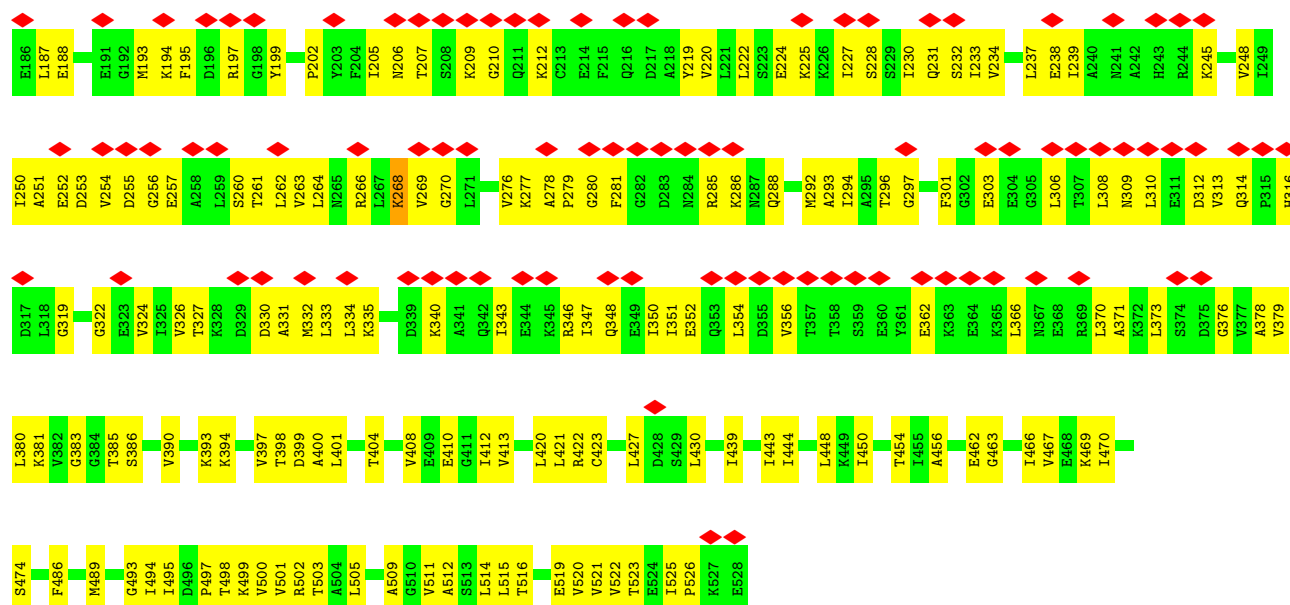


- Molecule 1: 60 kDa heat shock protein, mitochondrial

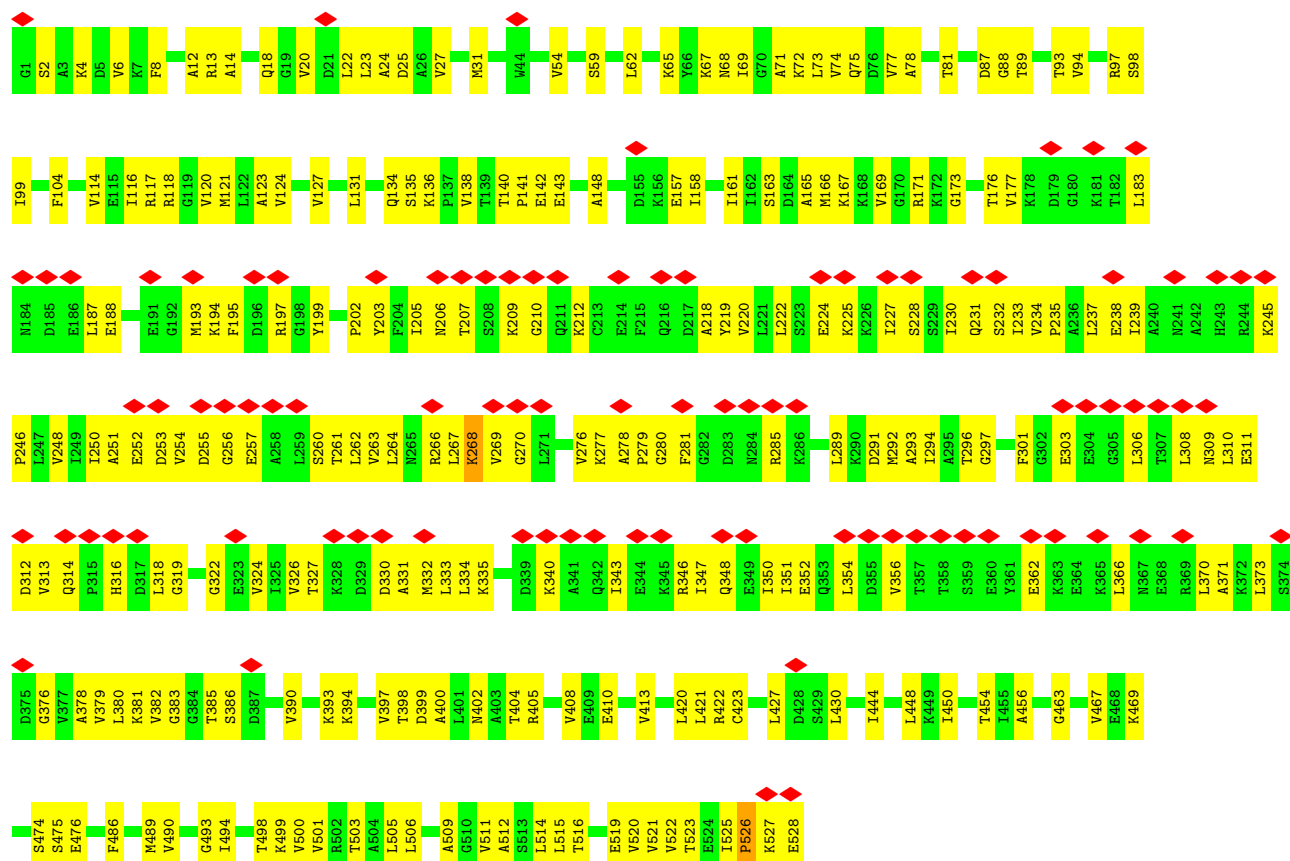


- Molecule 1: 60 kDa heat shock protein, mitochondrial





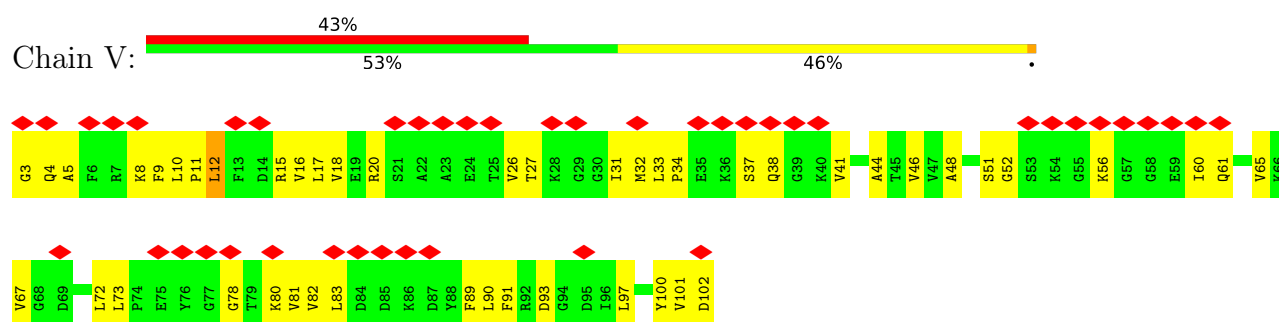
- Molecule 1: 60 kDa heat shock protein, mitochondrial



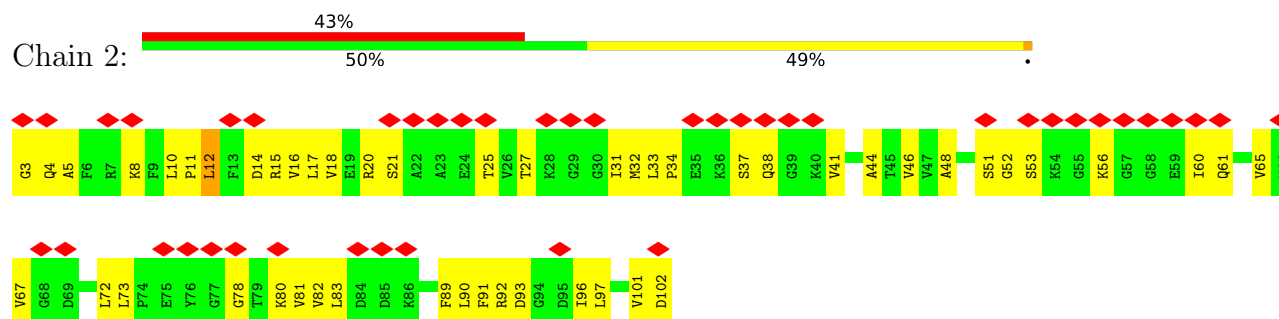
- Molecule 1: 60 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



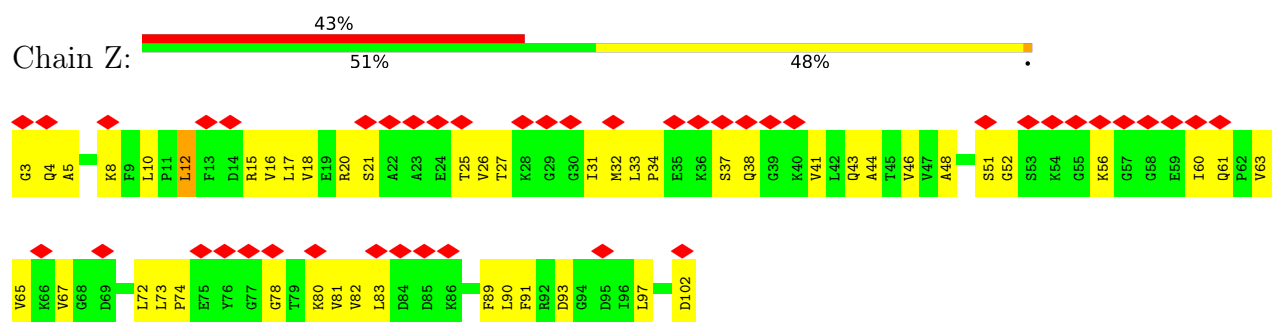
- Molecule 2: 10 kDa heat shock protein, mitochondrial



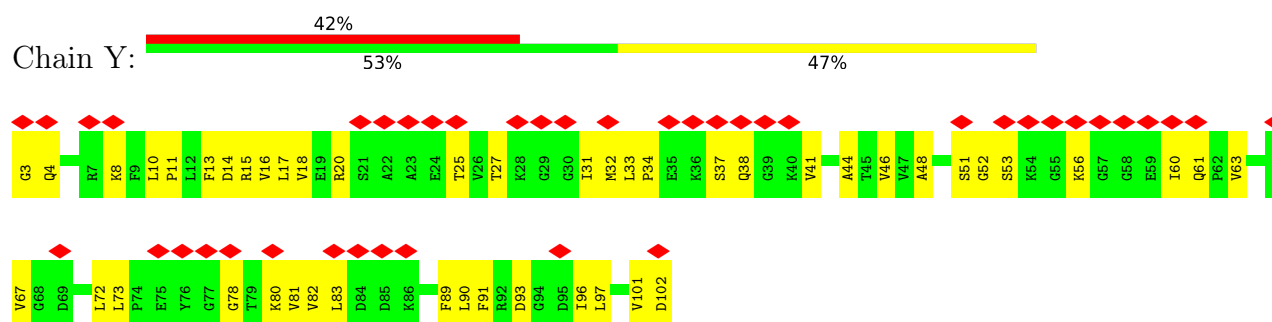
- Molecule 2: 10 kDa heat shock protein, mitochondrial



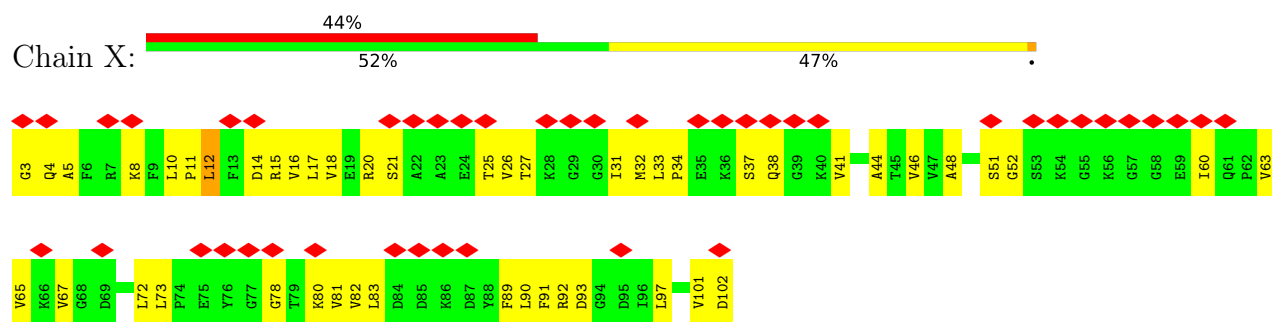
- Molecule 2: 10 kDa heat shock protein, mitochondrial



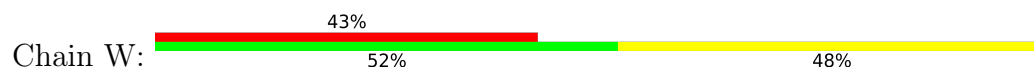
- Molecule 2: 10 kDa heat shock protein, mitochondrial

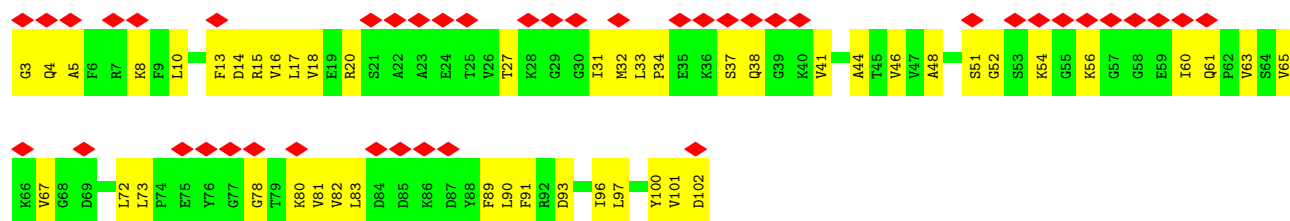


- Molecule 2: 10 kDa heat shock protein, mitochondrial

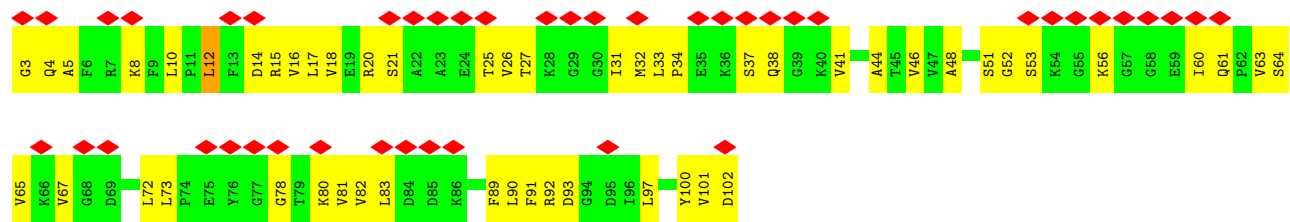
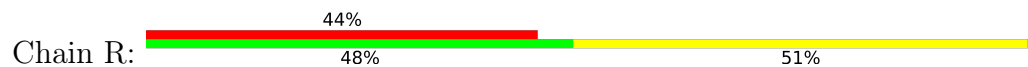


- Molecule 2: 10 kDa heat shock protein, mitochondrial

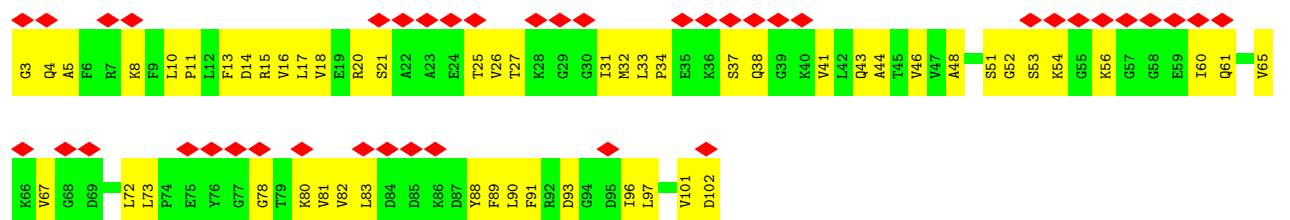
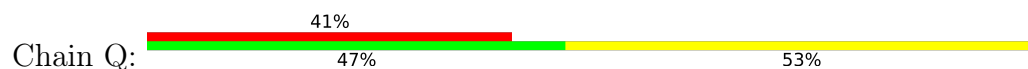




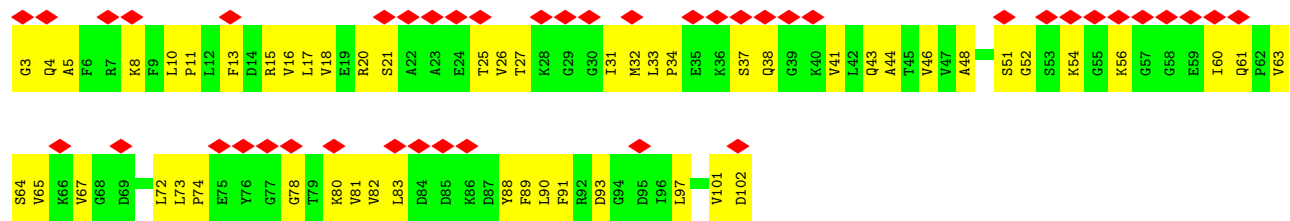
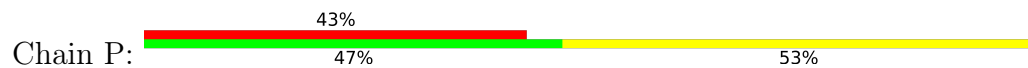
- Molecule 2: 10 kDa heat shock protein, mitochondrial



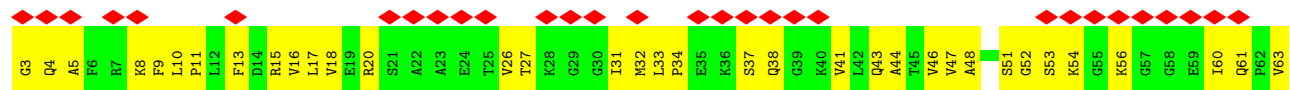
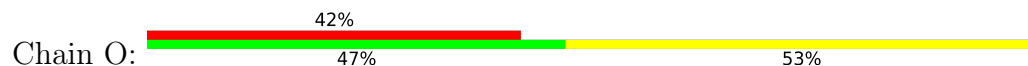
- Molecule 2: 10 kDa heat shock protein, mitochondrial

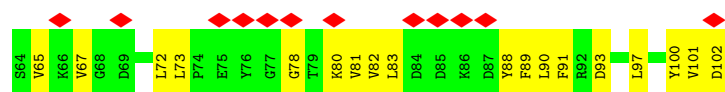


- Molecule 2: 10 kDa heat shock protein, mitochondrial

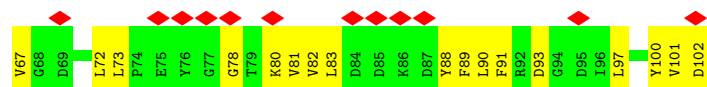
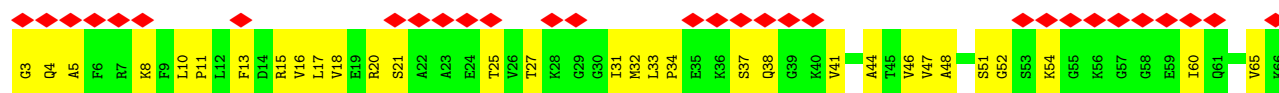
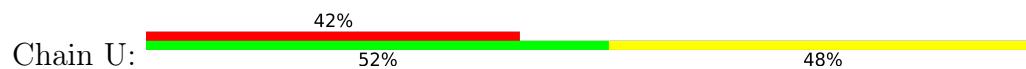


- Molecule 2: 10 kDa heat shock protein, mitochondrial

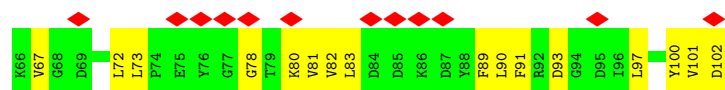
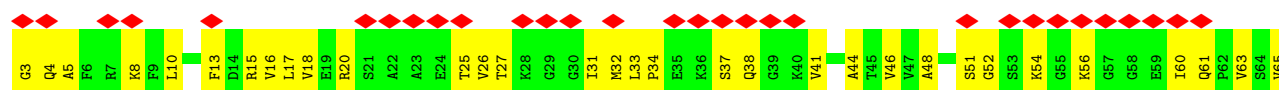
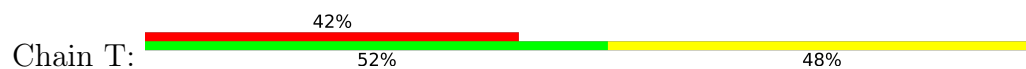




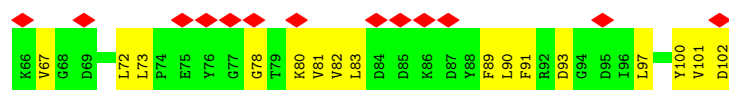
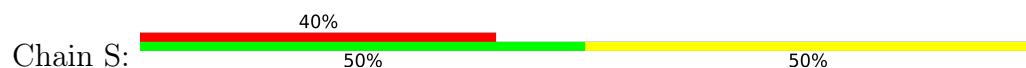
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 66013 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 63 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 3.974 | Depositor |
| Minimum map value | -2.032 | Depositor |
| Average map value | 0.004 | Depositor |
| Map value standard deviation | 0.137 | Depositor |
| Recommended contour level | 0.9 | Depositor |
| Map size (Å) | 376.64, 376.64, 376.64 | wwPDB |
| Map dimensions | 352, 352, 352 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.07, 1.07, 1.07 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.29 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | B | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | C | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | D | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | E | 0.29 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | F | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | G | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | H | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | I | 0.29 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | J | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | K | 0.28 | 0/3968 | 0.49 | 1/5352 (0.0%) |
| 1 | L | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | M | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 1 | N | 0.28 | 0/3968 | 0.48 | 1/5352 (0.0%) |
| 2 | 1 | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | 2 | 0.27 | 0/767 | 0.51 | 0/1030 |
| 2 | O | 0.28 | 0/767 | 0.52 | 0/1030 |
| 2 | P | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | Q | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | R | 0.27 | 0/767 | 0.51 | 0/1030 |
| 2 | S | 0.28 | 0/767 | 0.52 | 0/1030 |
| 2 | T | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | U | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | V | 0.27 | 0/767 | 0.52 | 0/1030 |
| 2 | W | 0.28 | 0/767 | 0.52 | 0/1030 |
| 2 | X | 0.27 | 0/767 | 0.52 | 0/1030 |
| 2 | Y | 0.28 | 0/767 | 0.51 | 0/1030 |
| 2 | Z | 0.27 | 0/767 | 0.51 | 0/1030 |
| All | All | 0.28 | 0/66290 | 0.49 | 14/89348 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 2 |
| 1 | C | 0 | 1 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 2 |
| 1 | F | 0 | 2 |
| 1 | G | 0 | 1 |
| 1 | H | 0 | 1 |
| 1 | I | 0 | 2 |
| 1 | J | 0 | 2 |
| 1 | K | 0 | 2 |
| 1 | L | 0 | 2 |
| 1 | N | 0 | 2 |
| 2 | 2 | 0 | 1 |
| 2 | R | 0 | 1 |
| 2 | V | 0 | 1 |
| 2 | X | 0 | 1 |
| 2 | Z | 0 | 1 |
| All | All | 0 | 26 |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 1 | I | 494 | ILE | CG1-CB-CG2 | 6.65 | 126.03 | 111.40 |
| 1 | B | 494 | ILE | CG1-CB-CG2 | 6.64 | 126.00 | 111.40 |
| 1 | L | 494 | ILE | CG1-CB-CG2 | 6.62 | 125.96 | 111.40 |
| 1 | F | 494 | ILE | CG1-CB-CG2 | 6.58 | 125.89 | 111.40 |
| 1 | H | 494 | ILE | CG1-CB-CG2 | 6.58 | 125.88 | 111.40 |
| 1 | E | 494 | ILE | CG1-CB-CG2 | 6.56 | 125.83 | 111.40 |
| 1 | M | 494 | ILE | CG1-CB-CG2 | 6.55 | 125.80 | 111.40 |
| 1 | J | 494 | ILE | CG1-CB-CG2 | 6.54 | 125.78 | 111.40 |
| 1 | K | 494 | ILE | CG1-CB-CG2 | 6.53 | 125.77 | 111.40 |
| 1 | C | 494 | ILE | CG1-CB-CG2 | 6.53 | 125.76 | 111.40 |
| 1 | A | 494 | ILE | CG1-CB-CG2 | 6.52 | 125.74 | 111.40 |
| 1 | G | 494 | ILE | CG1-CB-CG2 | 6.51 | 125.73 | 111.40 |
| 1 | D | 494 | ILE | CG1-CB-CG2 | 6.40 | 125.47 | 111.40 |
| 1 | N | 494 | ILE | CG1-CB-CG2 | 6.39 | 125.45 | 111.40 |

There are no chirality outliers.

All (26) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | 2 | 12 | LEU | Peptide |
| 1 | A | 268 | LYS | Peptide |
| 1 | B | 268 | LYS | Peptide |
| 1 | B | 526 | PRO | Peptide |
| 1 | C | 268 | LYS | Peptide |
| 1 | D | 268 | LYS | Peptide |
| 1 | E | 268 | LYS | Peptide |
| 1 | E | 526 | PRO | Peptide |
| 1 | F | 268 | LYS | Peptide |
| 1 | F | 526 | PRO | Peptide |
| 1 | G | 268 | LYS | Peptide |
| 1 | H | 268 | LYS | Peptide |
| 1 | I | 268 | LYS | Peptide |
| 1 | I | 526 | PRO | Peptide |
| 1 | J | 268 | LYS | Peptide |
| 1 | J | 526 | PRO | Peptide |
| 1 | K | 268 | LYS | Peptide |
| 1 | K | 526 | PRO | Peptide |
| 1 | L | 268 | LYS | Peptide |
| 1 | L | 526 | PRO | Peptide |
| 1 | N | 306 | LEU | Peptide |
| 1 | N | 526 | PRO | Peptide |
| 2 | R | 12 | LEU | Peptide |
| 2 | V | 12 | LEU | Peptide |
| 2 | X | 12 | LEU | Peptide |
| 2 | Z | 12 | LEU | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3936 | 211 | 4115 | 222 | 0 |
| 1 | B | 3936 | 211 | 4115 | 216 | 0 |
| 1 | C | 3936 | 211 | 4115 | 228 | 0 |
| 1 | D | 3936 | 211 | 4115 | 220 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 3936 | 211 | 4115 | 219 | 0 |
| 1 | F | 3936 | 211 | 4115 | 230 | 0 |
| 1 | G | 3936 | 211 | 4115 | 226 | 0 |
| 1 | H | 3936 | 211 | 4115 | 219 | 0 |
| 1 | I | 3936 | 211 | 4115 | 217 | 0 |
| 1 | J | 3936 | 211 | 4115 | 225 | 0 |
| 1 | K | 3936 | 211 | 4115 | 217 | 0 |
| 1 | L | 3936 | 211 | 4115 | 216 | 0 |
| 1 | M | 3936 | 211 | 4115 | 232 | 0 |
| 1 | N | 3936 | 211 | 4115 | 216 | 0 |
| 2 | 1 | 756 | 0 | 786 | 63 | 0 |
| 2 | 2 | 756 | 0 | 786 | 54 | 0 |
| 2 | O | 756 | 0 | 786 | 66 | 0 |
| 2 | P | 756 | 0 | 786 | 63 | 0 |
| 2 | Q | 756 | 0 | 786 | 64 | 0 |
| 2 | R | 756 | 0 | 786 | 55 | 0 |
| 2 | S | 756 | 0 | 786 | 60 | 0 |
| 2 | T | 756 | 0 | 786 | 60 | 0 |
| 2 | U | 756 | 0 | 786 | 67 | 0 |
| 2 | V | 756 | 0 | 786 | 54 | 0 |
| 2 | W | 756 | 0 | 786 | 58 | 0 |
| 2 | X | 756 | 0 | 786 | 59 | 0 |
| 2 | Y | 756 | 0 | 786 | 54 | 0 |
| 2 | Z | 756 | 0 | 786 | 55 | 0 |
| 3 | A | 27 | 0 | 12 | 2 | 0 |
| 3 | B | 27 | 0 | 12 | 2 | 0 |
| 3 | C | 27 | 0 | 12 | 1 | 0 |
| 3 | D | 27 | 0 | 11 | 2 | 0 |
| 3 | E | 27 | 0 | 12 | 2 | 0 |
| 3 | F | 27 | 0 | 12 | 1 | 0 |
| 3 | G | 27 | 0 | 12 | 2 | 0 |
| 3 | H | 27 | 0 | 12 | 2 | 0 |
| 3 | I | 27 | 0 | 12 | 2 | 0 |
| 3 | J | 27 | 0 | 12 | 2 | 0 |
| 3 | K | 27 | 0 | 11 | 2 | 0 |
| 3 | L | 27 | 0 | 12 | 2 | 0 |
| 3 | M | 27 | 0 | 12 | 2 | 0 |
| 3 | N | 27 | 0 | 12 | 2 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | I | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | K | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 4 | M | 1 | 0 | 0 | 0 | 0 |
| 4 | N | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 7 | 0 | 0 | 3 | 0 |
| 5 | B | 7 | 0 | 0 | 2 | 0 |
| 5 | C | 7 | 0 | 0 | 2 | 0 |
| 5 | D | 7 | 0 | 0 | 3 | 0 |
| 5 | E | 7 | 0 | 0 | 3 | 0 |
| 5 | F | 7 | 0 | 0 | 2 | 0 |
| 5 | G | 7 | 0 | 0 | 3 | 0 |
| 5 | H | 7 | 0 | 0 | 3 | 0 |
| 5 | I | 7 | 0 | 0 | 2 | 0 |
| 5 | J | 7 | 0 | 0 | 3 | 0 |
| 5 | K | 7 | 0 | 0 | 2 | 0 |
| 5 | L | 7 | 0 | 0 | 3 | 0 |
| 5 | M | 7 | 0 | 0 | 3 | 0 |
| 5 | N | 7 | 0 | 0 | 3 | 0 |
| All | All | 66178 | 2954 | 68780 | 3668 | 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 27.

All (3668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:197:ARG:HD3 | 1:C:277:LYS:HB2 | 1.40 | 1.03 |
| 1:H:197:ARG:HD3 | 1:H:277:LYS:HB2 | 1.41 | 1.02 |
| 1:D:197:ARG:HD3 | 1:D:277:LYS:HB2 | 1.41 | 1.02 |
| 1:J:197:ARG:HD3 | 1:J:277:LYS:HB2 | 1.42 | 1.01 |
| 1:E:197:ARG:HD3 | 1:E:277:LYS:HB2 | 1.42 | 1.01 |
| 1:K:197:ARG:HD3 | 1:K:277:LYS:HB2 | 1.43 | 1.01 |
| 1:L:197:ARG:HD3 | 1:L:277:LYS:HB2 | 1.42 | 1.00 |
| 1:G:197:ARG:HD3 | 1:G:277:LYS:HB2 | 1.43 | 1.00 |
| 1:N:197:ARG:HD3 | 1:N:277:LYS:HB2 | 1.40 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:306:LEU:HG | 1:M:308:LEU:HD23 | 1.43 | 0.99 |
| 1:H:306:LEU:HG | 1:H:308:LEU:HD23 | 1.44 | 0.99 |
| 1:B:197:ARG:HD3 | 1:B:277:LYS:HB2 | 1.41 | 0.99 |
| 1:K:306:LEU:HG | 1:K:308:LEU:HD23 | 1.43 | 0.98 |
| 1:I:197:ARG:HD3 | 1:I:277:LYS:HB2 | 1.44 | 0.97 |
| 1:F:197:ARG:HD3 | 1:F:277:LYS:HB2 | 1.43 | 0.97 |
| 1:J:306:LEU:HG | 1:J:308:LEU:HD23 | 1.45 | 0.97 |
| 1:L:306:LEU:HG | 1:L:308:LEU:HD23 | 1.44 | 0.97 |
| 1:M:197:ARG:HD3 | 1:M:277:LYS:HB2 | 1.44 | 0.96 |
| 1:C:306:LEU:HG | 1:C:308:LEU:HD23 | 1.48 | 0.94 |
| 2:Q:17:LEU:HB3 | 2:Q:48:ALA:HB3 | 1.48 | 0.94 |
| 1:B:306:LEU:HG | 1:B:308:LEU:HD23 | 1.48 | 0.94 |
| 1:A:306:LEU:HG | 1:A:308:LEU:HD23 | 1.49 | 0.94 |
| 2:2:17:LEU:HB3 | 2:2:48:ALA:HB3 | 1.51 | 0.93 |
| 1:D:306:LEU:HG | 1:D:308:LEU:HD23 | 1.48 | 0.93 |
| 1:H:264:LEU:HG | 1:H:268:LYS:HE2 | 1.50 | 0.93 |
| 2:S:17:LEU:HB3 | 2:S:48:ALA:HB3 | 1.50 | 0.93 |
| 2:P:17:LEU:HB3 | 2:P:48:ALA:HB3 | 1.51 | 0.93 |
| 2:O:17:LEU:HB3 | 2:O:48:ALA:HB3 | 1.49 | 0.92 |
| 2:1:17:LEU:HB3 | 2:1:48:ALA:HB3 | 1.47 | 0.92 |
| 2:P:15:ARG:HB3 | 2:P:90:LEU:HD11 | 1.52 | 0.92 |
| 2:W:17:LEU:HB3 | 2:W:48:ALA:HB3 | 1.49 | 0.92 |
| 1:E:212:LYS:HG2 | 1:E:327:THR:HG22 | 1.51 | 0.92 |
| 2:T:17:LEU:HB3 | 2:T:48:ALA:HB3 | 1.50 | 0.92 |
| 2:X:90:LEU:HD23 | 2:W:97:LEU:HD12 | 1.53 | 0.91 |
| 2:U:17:LEU:HB3 | 2:U:48:ALA:HB3 | 1.50 | 0.91 |
| 1:A:197:ARG:HD3 | 1:A:277:LYS:HB2 | 1.50 | 0.91 |
| 2:V:17:LEU:HB3 | 2:V:48:ALA:HB3 | 1.50 | 0.91 |
| 1:F:212:LYS:HG2 | 1:F:327:THR:HG22 | 1.53 | 0.90 |
| 2:P:90:LEU:HD23 | 2:O:97:LEU:HD12 | 1.52 | 0.90 |
| 1:A:264:LEU:HG | 1:A:268:LYS:HE2 | 1.53 | 0.90 |
| 1:H:212:LYS:HG2 | 1:H:327:THR:HG22 | 1.52 | 0.90 |
| 1:I:212:LYS:HG2 | 1:I:327:THR:HG22 | 1.51 | 0.90 |
| 2:V:90:LEU:HD23 | 2:2:97:LEU:HD12 | 1.53 | 0.89 |
| 1:M:120:VAL:HG13 | 1:M:444:ILE:HD11 | 1.54 | 0.89 |
| 1:M:212:LYS:HG2 | 1:M:327:THR:HG22 | 1.53 | 0.89 |
| 2:O:15:ARG:HB3 | 2:O:90:LEU:HD11 | 1.54 | 0.88 |
| 1:C:120:VAL:HG13 | 1:C:444:ILE:HD11 | 1.55 | 0.88 |
| 1:F:120:VAL:HG13 | 1:F:444:ILE:HD11 | 1.55 | 0.88 |
| 1:E:281:PHE:HA | 1:E:285:ARG:HH21 | 1.36 | 0.88 |
| 2:S:15:ARG:HB3 | 2:S:90:LEU:HD11 | 1.52 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:212:LYS:HG2 | 1:J:327:THR:HG22 | 1.53 | 0.88 |
| 1:D:6:VAL:HG12 | 1:D:522:VAL:HG22 | 1.54 | 0.88 |
| 1:E:340:LYS:HA | 1:E:343:ILE:HG12 | 1.55 | 0.88 |
| 1:A:212:LYS:HG2 | 1:A:327:THR:HG22 | 1.52 | 0.88 |
| 1:N:340:LYS:HA | 1:N:343:ILE:HG12 | 1.56 | 0.88 |
| 1:D:340:LYS:HA | 1:D:343:ILE:HG12 | 1.56 | 0.88 |
| 1:F:281:PHE:H | 1:F:285:ARG:HD3 | 1.36 | 0.88 |
| 1:B:340:LYS:HA | 1:B:343:ILE:HG12 | 1.56 | 0.88 |
| 1:G:212:LYS:HG2 | 1:G:327:THR:HG22 | 1.52 | 0.88 |
| 2:1:15:ARG:HB3 | 2:1:90:LEU:HD11 | 1.54 | 0.87 |
| 1:N:212:LYS:HG2 | 1:N:327:THR:HG22 | 1.53 | 0.87 |
| 1:C:340:LYS:HA | 1:C:343:ILE:HG12 | 1.56 | 0.87 |
| 1:F:340:LYS:HA | 1:F:343:ILE:HG12 | 1.56 | 0.87 |
| 1:K:212:LYS:HG2 | 1:K:327:THR:HG22 | 1.54 | 0.87 |
| 1:H:120:VAL:HG13 | 1:H:444:ILE:HD11 | 1.57 | 0.87 |
| 1:I:120:VAL:HG13 | 1:I:444:ILE:HD11 | 1.56 | 0.87 |
| 1:F:278:ALA:HB1 | 1:F:289:LEU:HD11 | 1.56 | 0.87 |
| 2:R:17:LEU:HB3 | 2:R:48:ALA:HB3 | 1.55 | 0.87 |
| 1:J:340:LYS:HA | 1:J:343:ILE:HG12 | 1.57 | 0.87 |
| 1:I:340:LYS:HA | 1:I:343:ILE:HG12 | 1.57 | 0.87 |
| 1:A:340:LYS:HA | 1:A:343:ILE:HG12 | 1.57 | 0.87 |
| 1:H:340:LYS:HA | 1:H:343:ILE:HG12 | 1.57 | 0.87 |
| 1:L:212:LYS:HG2 | 1:L:327:THR:HG22 | 1.55 | 0.87 |
| 2:O:90:LEU:HD23 | 2:U:97:LEU:HD12 | 1.57 | 0.86 |
| 1:M:340:LYS:HA | 1:M:343:ILE:HG12 | 1.57 | 0.86 |
| 1:K:340:LYS:HA | 1:K:343:ILE:HG12 | 1.57 | 0.86 |
| 1:L:340:LYS:HA | 1:L:343:ILE:HG12 | 1.58 | 0.86 |
| 1:E:306:LEU:HG | 1:E:308:LEU:HD23 | 1.56 | 0.86 |
| 1:N:6:VAL:HG12 | 1:N:522:VAL:HG22 | 1.57 | 0.86 |
| 1:B:120:VAL:HG13 | 1:B:444:ILE:HD11 | 1.58 | 0.86 |
| 1:C:6:VAL:HG12 | 1:C:522:VAL:HG22 | 1.55 | 0.85 |
| 1:L:120:VAL:HG13 | 1:L:444:ILE:HD11 | 1.58 | 0.85 |
| 2:Y:15:ARG:HB3 | 2:Y:90:LEU:HD11 | 1.58 | 0.85 |
| 1:E:120:VAL:HG13 | 1:E:444:ILE:HD11 | 1.59 | 0.85 |
| 1:A:120:VAL:HG13 | 1:A:444:ILE:HD11 | 1.59 | 0.85 |
| 1:F:278:ALA:HB3 | 1:F:285:ARG:HD2 | 1.59 | 0.85 |
| 2:Z:18:VAL:HG12 | 2:Z:46:VAL:HA | 1.59 | 0.84 |
| 2:R:90:LEU:HD23 | 2:Q:97:LEU:HD12 | 1.60 | 0.84 |
| 1:I:306:LEU:HG | 1:I:308:LEU:HD23 | 1.57 | 0.84 |
| 1:A:6:VAL:HG12 | 1:A:522:VAL:HG22 | 1.59 | 0.84 |
| 1:G:340:LYS:HA | 1:G:343:ILE:HG12 | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:17:LEU:HB3 | 2:Y:48:ALA:HB3 | 1.58 | 0.84 |
| 1:K:6:VAL:HG12 | 1:K:522:VAL:HG22 | 1.56 | 0.84 |
| 1:D:212:LYS:HG2 | 1:D:327:THR:HG22 | 1.58 | 0.84 |
| 2:Z:15:ARG:HB3 | 2:Z:90:LEU:HD11 | 1.58 | 0.84 |
| 2:Z:17:LEU:HB3 | 2:Z:48:ALA:HB3 | 1.58 | 0.83 |
| 1:N:193:MET:HE2 | 1:N:292:MET:HG2 | 1.59 | 0.83 |
| 2:T:52:GLY:HA3 | 2:T:60:ILE:HD12 | 1.57 | 0.83 |
| 1:G:264:LEU:HD11 | 1:G:268:LYS:HE2 | 1.58 | 0.83 |
| 2:W:15:ARG:HB3 | 2:W:90:LEU:HD11 | 1.58 | 0.83 |
| 1:B:278:ALA:HB1 | 1:B:289:LEU:HD11 | 1.59 | 0.83 |
| 2:X:17:LEU:HB3 | 2:X:48:ALA:HB3 | 1.61 | 0.83 |
| 1:E:193:MET:HE2 | 1:E:292:MET:HG2 | 1.59 | 0.83 |
| 1:N:120:VAL:HG13 | 1:N:444:ILE:HD11 | 1.61 | 0.83 |
| 2:Q:15:ARG:HB3 | 2:Q:90:LEU:HD11 | 1.59 | 0.83 |
| 2:Y:18:VAL:HG12 | 2:Y:46:VAL:HA | 1.59 | 0.83 |
| 2:R:15:ARG:HB3 | 2:R:90:LEU:HD11 | 1.61 | 0.83 |
| 1:L:193:MET:HE2 | 1:L:292:MET:HG2 | 1.61 | 0.82 |
| 1:I:264:LEU:HD11 | 1:I:268:LYS:HE2 | 1.61 | 0.82 |
| 1:M:6:VAL:HG12 | 1:M:522:VAL:HG22 | 1.59 | 0.82 |
| 2:T:15:ARG:HB3 | 2:T:90:LEU:HD11 | 1.59 | 0.82 |
| 1:A:278:ALA:HB1 | 1:A:289:LEU:HD11 | 1.59 | 0.81 |
| 2:2:15:ARG:HB3 | 2:2:90:LEU:HD11 | 1.62 | 0.81 |
| 2:R:97:LEU:HD12 | 2:S:90:LEU:HD23 | 1.63 | 0.81 |
| 2:2:90:LEU:HD23 | 2:1:97:LEU:HD12 | 1.60 | 0.81 |
| 1:B:193:MET:HE2 | 1:B:292:MET:HG2 | 1.62 | 0.81 |
| 1:D:120:VAL:HG13 | 1:D:444:ILE:HD11 | 1.63 | 0.81 |
| 1:F:6:VAL:HG12 | 1:F:522:VAL:HG22 | 1.64 | 0.80 |
| 2:V:15:ARG:HB3 | 2:V:90:LEU:HD11 | 1.64 | 0.80 |
| 2:Z:90:LEU:HD23 | 2:Y:97:LEU:HD12 | 1.62 | 0.80 |
| 2:X:18:VAL:HG12 | 2:X:46:VAL:HA | 1.64 | 0.80 |
| 2:W:52:GLY:HA3 | 2:W:60:ILE:HD12 | 1.61 | 0.80 |
| 1:K:354:LEU:HB3 | 1:K:366:LEU:HD12 | 1.63 | 0.80 |
| 1:I:354:LEU:HB3 | 1:I:366:LEU:HD12 | 1.62 | 0.80 |
| 1:D:193:MET:HE2 | 1:D:292:MET:HG2 | 1.60 | 0.80 |
| 1:D:354:LEU:HB3 | 1:D:366:LEU:HD12 | 1.64 | 0.80 |
| 2:U:8:LYS:HG2 | 2:T:102:ASP:HB3 | 1.64 | 0.80 |
| 2:U:15:ARG:HB3 | 2:U:90:LEU:HD11 | 1.63 | 0.80 |
| 2:U:31:ILE:HG21 | 1:G:234:VAL:HG23 | 1.64 | 0.80 |
| 2:U:90:LEU:HD23 | 2:T:97:LEU:HD12 | 1.62 | 0.80 |
| 1:K:120:VAL:HG13 | 1:K:444:ILE:HD11 | 1.63 | 0.80 |
| 1:G:6:VAL:HG12 | 1:G:522:VAL:HG22 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:120:VAL:HG13 | 1:G:444:ILE:HD11 | 1.64 | 0.79 |
| 1:J:24:ALA:HB3 | 1:J:97:ARG:HD3 | 1.65 | 0.79 |
| 1:G:24:ALA:HB3 | 1:G:97:ARG:HD3 | 1.64 | 0.79 |
| 1:I:193:MET:HE2 | 1:I:292:MET:HG2 | 1.65 | 0.79 |
| 1:F:354:LEU:HB3 | 1:F:366:LEU:HD12 | 1.64 | 0.79 |
| 1:L:354:LEU:HB3 | 1:L:366:LEU:HD12 | 1.64 | 0.78 |
| 1:F:207:THR:HG23 | 1:F:209:LYS:H | 1.48 | 0.78 |
| 1:H:354:LEU:HB3 | 1:H:366:LEU:HD12 | 1.64 | 0.78 |
| 1:L:6:VAL:HG12 | 1:L:522:VAL:HG22 | 1.65 | 0.78 |
| 1:J:237:LEU:HD21 | 1:J:262:LEU:HD23 | 1.65 | 0.78 |
| 1:M:421:LEU:HD21 | 1:M:467:VAL:HG13 | 1.63 | 0.78 |
| 1:N:354:LEU:HB3 | 1:N:366:LEU:HD12 | 1.64 | 0.78 |
| 1:E:237:LEU:HD21 | 1:E:262:LEU:HD23 | 1.65 | 0.78 |
| 2:1:90:LEU:HD23 | 2:Z:97:LEU:HD12 | 1.64 | 0.78 |
| 1:M:354:LEU:HB3 | 1:M:366:LEU:HD12 | 1.64 | 0.78 |
| 2:W:27:THR:HG21 | 2:W:31:ILE:HG22 | 1.66 | 0.78 |
| 1:A:354:LEU:HB3 | 1:A:366:LEU:HD12 | 1.65 | 0.77 |
| 2:O:18:VAL:HG12 | 2:O:46:VAL:HA | 1.67 | 0.77 |
| 1:C:421:LEU:HD21 | 1:C:467:VAL:HG13 | 1.65 | 0.77 |
| 1:B:354:LEU:HB3 | 1:B:366:LEU:HD12 | 1.65 | 0.77 |
| 1:K:24:ALA:HB3 | 1:K:97:ARG:HD3 | 1.67 | 0.77 |
| 1:J:207:THR:HG23 | 1:J:209:LYS:H | 1.49 | 0.77 |
| 1:M:222:LEU:HD23 | 1:M:250:ILE:HB | 1.67 | 0.77 |
| 1:F:24:ALA:HB3 | 1:F:97:ARG:HD3 | 1.67 | 0.77 |
| 2:U:27:THR:HG21 | 2:U:31:ILE:HG22 | 1.65 | 0.77 |
| 1:I:278:ALA:HB1 | 1:I:289:LEU:HD11 | 1.65 | 0.77 |
| 1:G:421:LEU:HD21 | 1:G:467:VAL:HG13 | 1.66 | 0.77 |
| 1:I:24:ALA:HB3 | 1:I:97:ARG:HD3 | 1.66 | 0.77 |
| 1:B:303:GLU:HB3 | 1:B:306:LEU:HB3 | 1.67 | 0.77 |
| 1:E:354:LEU:HB3 | 1:E:366:LEU:HD12 | 1.67 | 0.77 |
| 1:J:327:THR:OG1 | 1:J:330:ASP:OD1 | 2.03 | 0.77 |
| 1:A:24:ALA:HB3 | 1:A:97:ARG:HD3 | 1.67 | 0.77 |
| 1:J:354:LEU:HB3 | 1:J:366:LEU:HD12 | 1.64 | 0.76 |
| 1:I:222:LEU:HD23 | 1:I:250:ILE:HB | 1.68 | 0.76 |
| 2:Y:90:LEU:HD23 | 2:X:97:LEU:HD12 | 1.65 | 0.76 |
| 1:N:24:ALA:HB3 | 1:N:97:ARG:HD3 | 1.68 | 0.76 |
| 1:J:222:LEU:HD23 | 1:J:250:ILE:HB | 1.68 | 0.76 |
| 1:B:237:LEU:HD21 | 1:B:262:LEU:HD23 | 1.68 | 0.76 |
| 1:G:354:LEU:HB3 | 1:G:366:LEU:HD12 | 1.65 | 0.76 |
| 1:C:354:LEU:HB3 | 1:C:366:LEU:HD12 | 1.65 | 0.76 |
| 1:E:207:THR:HG23 | 1:E:209:LYS:H | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:207:THR:HG23 | 1:M:209:LYS:H | 1.50 | 0.76 |
| 1:B:24:ALA:HB3 | 1:B:97:ARG:HD3 | 1.67 | 0.76 |
| 1:H:207:THR:HG23 | 1:H:209:LYS:H | 1.49 | 0.76 |
| 1:H:421:LEU:HD21 | 1:H:467:VAL:HG13 | 1.66 | 0.76 |
| 1:B:209:LYS:HG3 | 1:B:210:GLY:H | 1.51 | 0.76 |
| 1:F:237:LEU:HD21 | 1:F:262:LEU:HD23 | 1.68 | 0.76 |
| 1:E:525:ILE:HG23 | 1:E:527:LYS:HG3 | 1.67 | 0.76 |
| 2:T:90:LEU:HD23 | 2:S:97:LEU:HD12 | 1.66 | 0.76 |
| 1:L:24:ALA:HB3 | 1:L:97:ARG:HD3 | 1.68 | 0.76 |
| 1:E:209:LYS:HG3 | 1:E:210:GLY:H | 1.52 | 0.76 |
| 1:D:209:LYS:HG3 | 1:D:210:GLY:H | 1.51 | 0.75 |
| 1:L:209:LYS:HG3 | 1:L:210:GLY:H | 1.51 | 0.75 |
| 1:L:327:THR:OG1 | 1:L:330:ASP:OD1 | 2.04 | 0.75 |
| 1:D:327:THR:OG1 | 1:D:330:ASP:OD1 | 2.05 | 0.75 |
| 1:C:222:LEU:HD23 | 1:C:250:ILE:HB | 1.69 | 0.75 |
| 1:G:327:THR:OG1 | 1:G:330:ASP:OD1 | 2.04 | 0.75 |
| 1:E:6:VAL:HG12 | 1:E:522:VAL:HG22 | 1.69 | 0.75 |
| 1:A:209:LYS:HG3 | 1:A:210:GLY:H | 1.51 | 0.75 |
| 1:K:209:LYS:HG3 | 1:K:210:GLY:H | 1.52 | 0.75 |
| 1:M:327:THR:OG1 | 1:M:330:ASP:OD1 | 2.05 | 0.75 |
| 1:J:6:VAL:HG12 | 1:J:522:VAL:HG22 | 1.66 | 0.75 |
| 1:C:207:THR:HG23 | 1:C:209:LYS:H | 1.51 | 0.75 |
| 2:Y:31:ILE:HG21 | 1:K:234:VAL:HG23 | 1.69 | 0.75 |
| 1:L:237:LEU:HD21 | 1:L:262:LEU:HD23 | 1.68 | 0.75 |
| 1:A:207:THR:HG23 | 1:A:209:LYS:H | 1.51 | 0.75 |
| 1:G:207:THR:HG23 | 1:G:209:LYS:H | 1.50 | 0.75 |
| 1:H:209:LYS:HG3 | 1:H:210:GLY:H | 1.52 | 0.75 |
| 1:K:327:THR:OG1 | 1:K:330:ASP:OD1 | 2.05 | 0.75 |
| 1:F:327:THR:OG1 | 1:F:330:ASP:OD1 | 2.05 | 0.75 |
| 1:H:6:VAL:HG12 | 1:H:522:VAL:HG22 | 1.69 | 0.74 |
| 1:J:209:LYS:HG3 | 1:J:210:GLY:H | 1.52 | 0.74 |
| 1:C:209:LYS:HG3 | 1:C:210:GLY:H | 1.51 | 0.74 |
| 1:M:209:LYS:HG3 | 1:M:210:GLY:H | 1.52 | 0.74 |
| 1:D:207:THR:HG23 | 1:D:209:LYS:H | 1.51 | 0.74 |
| 1:H:24:ALA:HB3 | 1:H:97:ARG:HD3 | 1.69 | 0.74 |
| 1:N:209:LYS:HG3 | 1:N:210:GLY:H | 1.51 | 0.74 |
| 1:E:327:THR:OG1 | 1:E:330:ASP:OD1 | 2.05 | 0.74 |
| 1:F:525:ILE:HG23 | 1:F:527:LYS:HG3 | 1.70 | 0.74 |
| 1:N:207:THR:HG23 | 1:N:209:LYS:H | 1.52 | 0.74 |
| 1:L:207:THR:HG23 | 1:L:209:LYS:H | 1.50 | 0.74 |
| 1:A:327:THR:OG1 | 1:A:330:ASP:OD1 | 2.04 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:207:THR:HG23 | 1:I:209:LYS:H | 1.52 | 0.74 |
| 1:I:327:THR:OG1 | 1:I:330:ASP:OD1 | 2.05 | 0.74 |
| 2:Y:27:THR:HG21 | 2:Y:31:ILE:HG22 | 1.68 | 0.74 |
| 1:N:327:THR:OG1 | 1:N:330:ASP:OD1 | 2.05 | 0.74 |
| 1:F:209:LYS:HG3 | 1:F:210:GLY:H | 1.52 | 0.74 |
| 1:H:327:THR:OG1 | 1:H:330:ASP:OD1 | 2.04 | 0.74 |
| 2:T:27:THR:HG21 | 2:T:31:ILE:HG22 | 1.70 | 0.74 |
| 1:G:209:LYS:HG3 | 1:G:210:GLY:H | 1.52 | 0.74 |
| 2:X:27:THR:HG21 | 2:X:31:ILE:HG22 | 1.69 | 0.74 |
| 2:T:3:GLY:HA3 | 2:T:51:SER:HA | 1.70 | 0.74 |
| 1:D:222:LEU:HD23 | 1:D:250:ILE:HB | 1.70 | 0.74 |
| 1:G:222:LEU:HD23 | 1:G:250:ILE:HB | 1.69 | 0.74 |
| 2:U:34:PRO:HD3 | 1:G:261:THR:HG22 | 1.68 | 0.73 |
| 1:C:327:THR:OG1 | 1:C:330:ASP:OD1 | 2.05 | 0.73 |
| 1:E:283:ASP:HA | 1:E:286:LYS:HD3 | 1.67 | 0.73 |
| 1:N:222:LEU:HD23 | 1:N:250:ILE:HB | 1.71 | 0.73 |
| 2:S:27:THR:HG21 | 2:S:31:ILE:HG22 | 1.69 | 0.73 |
| 1:K:207:THR:HG23 | 1:K:209:LYS:H | 1.53 | 0.73 |
| 1:K:222:LEU:HD23 | 1:K:250:ILE:HB | 1.70 | 0.73 |
| 1:N:237:LEU:HD21 | 1:N:262:LEU:HD23 | 1.71 | 0.73 |
| 1:D:24:ALA:HB3 | 1:D:97:ARG:HD3 | 1.69 | 0.73 |
| 1:E:24:ALA:HB3 | 1:E:97:ARG:HD3 | 1.70 | 0.73 |
| 2:Q:90:LEU:HD23 | 2:P:97:LEU:HD12 | 1.70 | 0.73 |
| 1:I:209:LYS:HG3 | 1:I:210:GLY:H | 1.52 | 0.73 |
| 1:B:327:THR:OG1 | 1:B:330:ASP:OD1 | 2.05 | 0.73 |
| 1:B:207:THR:HG23 | 1:B:209:LYS:H | 1.52 | 0.73 |
| 1:B:25:ASP:OD1 | 1:B:97:ARG:NH1 | 2.22 | 0.73 |
| 1:J:120:VAL:HG13 | 1:J:444:ILE:HD11 | 1.69 | 0.73 |
| 1:G:237:LEU:HD21 | 1:G:262:LEU:HD23 | 1.70 | 0.73 |
| 2:P:20:ARG:NH1 | 2:P:41:VAL:O | 2.22 | 0.72 |
| 2:P:27:THR:HG21 | 2:P:31:ILE:HG22 | 1.69 | 0.72 |
| 2:O:32:MET:HE2 | 1:A:268:LYS:HE3 | 1.71 | 0.72 |
| 2:Z:20:ARG:NH1 | 2:Z:41:VAL:O | 2.22 | 0.72 |
| 2:O:27:THR:HG21 | 2:O:31:ILE:HG22 | 1.69 | 0.72 |
| 2:V:27:THR:HG21 | 2:V:31:ILE:HG22 | 1.70 | 0.72 |
| 1:C:24:ALA:HB3 | 1:C:97:ARG:HD3 | 1.72 | 0.72 |
| 2:P:18:VAL:HG12 | 2:P:46:VAL:HA | 1.71 | 0.72 |
| 1:M:278:ALA:HB1 | 1:M:289:LEU:HD11 | 1.71 | 0.72 |
| 2:X:15:ARG:HB3 | 2:X:90:LEU:HD11 | 1.71 | 0.72 |
| 1:N:278:ALA:HB1 | 1:N:289:LEU:HD11 | 1.70 | 0.72 |
| 1:L:281:PHE:HA | 1:L:285:ARG:HH21 | 1.54 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:264:LEU:HG | 1:D:268:LYS:HE2 | 1.71 | 0.72 |
| 1:A:525:ILE:HG23 | 1:A:527:LYS:HG3 | 1.71 | 0.72 |
| 1:F:25:ASP:OD1 | 1:F:97:ARG:NH1 | 2.22 | 0.72 |
| 2:V:102:ASP:HB3 | 2:W:8:LYS:HG2 | 1.70 | 0.72 |
| 2:Z:27:THR:HG21 | 2:Z:31:ILE:HG22 | 1.71 | 0.72 |
| 1:K:25:ASP:OD1 | 1:K:97:ARG:NH1 | 2.22 | 0.72 |
| 1:G:25:ASP:OD1 | 1:G:97:ARG:NH1 | 2.23 | 0.72 |
| 2:Q:18:VAL:HG12 | 2:Q:46:VAL:HA | 1.71 | 0.72 |
| 1:L:25:ASP:OD1 | 1:L:97:ARG:NH1 | 2.22 | 0.72 |
| 1:E:314:GLN:OE1 | 1:E:316:HIS:NE2 | 2.23 | 0.72 |
| 2:2:27:THR:HG21 | 2:2:31:ILE:HG22 | 1.72 | 0.72 |
| 1:N:314:GLN:OE1 | 1:N:316:HIS:NE2 | 2.23 | 0.72 |
| 1:M:25:ASP:OD1 | 1:M:97:ARG:NH1 | 2.22 | 0.72 |
| 1:I:25:ASP:OD1 | 1:I:97:ARG:NH1 | 2.22 | 0.72 |
| 1:F:222:LEU:HD23 | 1:F:250:ILE:HB | 1.71 | 0.72 |
| 1:H:222:LEU:HD23 | 1:H:250:ILE:HB | 1.72 | 0.71 |
| 1:I:237:LEU:HD21 | 1:I:262:LEU:HD23 | 1.71 | 0.71 |
| 1:D:314:GLN:OE1 | 1:D:316:HIS:NE2 | 2.23 | 0.71 |
| 1:H:237:LEU:HD21 | 1:H:262:LEU:HD23 | 1.71 | 0.71 |
| 2:O:20:ARG:NH1 | 2:O:41:VAL:O | 2.23 | 0.71 |
| 1:L:525:ILE:HG23 | 1:L:527:LYS:HG3 | 1.72 | 0.71 |
| 1:A:25:ASP:OD1 | 1:A:97:ARG:NH1 | 2.22 | 0.71 |
| 3:G:601:ADP:O3B | 5:G:701:HOH:O | 2.08 | 0.71 |
| 1:A:314:GLN:OE1 | 1:A:316:HIS:NE2 | 2.23 | 0.71 |
| 2:S:18:VAL:HG12 | 2:S:46:VAL:HA | 1.70 | 0.71 |
| 1:M:24:ALA:HB3 | 1:M:97:ARG:HD3 | 1.72 | 0.71 |
| 3:M:601:ADP:O1B | 5:M:701:HOH:O | 2.09 | 0.71 |
| 1:G:314:GLN:OE1 | 1:G:316:HIS:NE2 | 2.24 | 0.71 |
| 1:E:421:LEU:HD21 | 1:E:467:VAL:HG13 | 1.69 | 0.71 |
| 1:M:314:GLN:OE1 | 1:M:316:HIS:NE2 | 2.24 | 0.71 |
| 2:1:27:THR:HG21 | 2:1:31:ILE:HG22 | 1.73 | 0.71 |
| 2:Z:5:ALA:HB2 | 2:Z:10:LEU:HD13 | 1.73 | 0.71 |
| 2:Q:20:ARG:NH1 | 2:Q:41:VAL:O | 2.24 | 0.71 |
| 1:L:222:LEU:HD23 | 1:L:250:ILE:HB | 1.71 | 0.71 |
| 1:C:193:MET:HE2 | 1:C:292:MET:HG2 | 1.72 | 0.71 |
| 1:B:314:GLN:OE1 | 1:B:316:HIS:NE2 | 2.23 | 0.71 |
| 1:C:25:ASP:OD1 | 1:C:97:ARG:NH1 | 2.22 | 0.71 |
| 1:A:264:LEU:O | 1:A:268:LYS:HG2 | 1.90 | 0.71 |
| 1:A:303:GLU:HB3 | 1:A:306:LEU:HB3 | 1.73 | 0.71 |
| 2:W:20:ARG:NH1 | 2:W:41:VAL:O | 2.23 | 0.71 |
| 2:R:27:THR:HG21 | 2:R:31:ILE:HG22 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:25:ASP:OD1 | 1:D:97:ARG:NH1 | 2.23 | 0.71 |
| 1:E:25:ASP:OD1 | 1:E:97:ARG:NH1 | 2.24 | 0.71 |
| 1:E:222:LEU:HD23 | 1:E:250:ILE:HB | 1.72 | 0.71 |
| 2:1:20:ARG:NH1 | 2:1:41:VAL:O | 2.24 | 0.71 |
| 2:Y:20:ARG:NH1 | 2:Y:41:VAL:O | 2.23 | 0.71 |
| 1:N:25:ASP:OD1 | 1:N:97:ARG:NH1 | 2.23 | 0.71 |
| 1:D:351:ILE:HG22 | 1:D:370:LEU:HD21 | 1.73 | 0.71 |
| 1:B:525:ILE:HG23 | 1:B:527:LYS:HG3 | 1.73 | 0.71 |
| 2:U:3:GLY:HA3 | 2:U:51:SER:HA | 1.73 | 0.70 |
| 1:L:314:GLN:OE1 | 1:L:316:HIS:NE2 | 2.24 | 0.70 |
| 1:K:158:ILE:HD12 | 1:K:397:VAL:HG22 | 1.73 | 0.70 |
| 1:I:6:VAL:HG12 | 1:I:522:VAL:HG22 | 1.72 | 0.70 |
| 2:W:18:VAL:HG12 | 2:W:46:VAL:HA | 1.73 | 0.70 |
| 1:F:314:GLN:OE1 | 1:F:316:HIS:NE2 | 2.24 | 0.70 |
| 1:H:314:GLN:OE1 | 1:H:316:HIS:NE2 | 2.24 | 0.70 |
| 1:J:25:ASP:OD1 | 1:J:97:ARG:NH1 | 2.23 | 0.70 |
| 3:D:601:ADP:O3B | 5:D:701:HOH:O | 2.07 | 0.70 |
| 1:B:222:LEU:HD23 | 1:B:250:ILE:HB | 1.74 | 0.70 |
| 1:H:25:ASP:OD1 | 1:H:97:ARG:NH1 | 2.23 | 0.70 |
| 2:Y:34:PRO:HD3 | 1:K:261:THR:HG22 | 1.73 | 0.70 |
| 1:I:314:GLN:OE1 | 1:I:316:HIS:NE2 | 2.23 | 0.70 |
| 1:A:237:LEU:HD21 | 1:A:262:LEU:HD23 | 1.72 | 0.70 |
| 2:Q:27:THR:HG21 | 2:Q:31:ILE:HG22 | 1.71 | 0.70 |
| 1:C:303:GLU:HB3 | 1:C:306:LEU:HB3 | 1.73 | 0.70 |
| 1:K:314:GLN:OE1 | 1:K:316:HIS:NE2 | 2.23 | 0.70 |
| 1:C:237:LEU:HD21 | 1:C:262:LEU:HD23 | 1.74 | 0.70 |
| 1:E:264:LEU:HG | 1:E:268:LYS:HE2 | 1.72 | 0.70 |
| 2:U:20:ARG:NH1 | 2:U:41:VAL:O | 2.23 | 0.70 |
| 1:M:281:PHE:HA | 1:M:285:ARG:HH21 | 1.57 | 0.70 |
| 1:M:354:LEU:HB3 | 1:M:366:LEU:CD1 | 2.21 | 0.70 |
| 1:L:354:LEU:HB3 | 1:L:366:LEU:CD1 | 2.21 | 0.70 |
| 1:D:278:ALA:HB1 | 1:D:289:LEU:HD11 | 1.72 | 0.70 |
| 1:D:354:LEU:HB3 | 1:D:366:LEU:CD1 | 2.22 | 0.70 |
| 3:C:601:ADP:O3B | 5:C:701:HOH:O | 2.08 | 0.70 |
| 1:H:354:LEU:HB3 | 1:H:366:LEU:CD1 | 2.21 | 0.70 |
| 1:E:169:VAL:HG12 | 1:E:173:GLY:HA3 | 1.74 | 0.70 |
| 2:1:34:PRO:HD3 | 1:M:261:THR:HG22 | 1.73 | 0.70 |
| 1:M:237:LEU:HD21 | 1:M:262:LEU:HD23 | 1.72 | 0.70 |
| 1:G:354:LEU:HB3 | 1:G:366:LEU:CD1 | 2.21 | 0.70 |
| 2:S:52:GLY:HA3 | 2:S:60:ILE:HD12 | 1.73 | 0.70 |
| 3:I:601:ADP:O1B | 5:I:701:HOH:O | 2.09 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:140:THR:OG1 | 1:C:142:GLU:OE1 | 2.09 | 0.70 |
| 1:C:314:GLN:OE1 | 1:C:316:HIS:NE2 | 2.23 | 0.70 |
| 1:E:354:LEU:HB3 | 1:E:366:LEU:CD1 | 2.22 | 0.70 |
| 1:H:268:LYS:HE3 | 2:V:32:MET:HE3 | 1.73 | 0.69 |
| 3:F:601:ADP:O3B | 5:F:701:HOH:O | 2.09 | 0.69 |
| 1:F:354:LEU:HB3 | 1:F:366:LEU:CD1 | 2.21 | 0.69 |
| 1:H:140:THR:OG1 | 1:H:142:GLU:OE1 | 2.09 | 0.69 |
| 1:E:140:THR:OG1 | 1:E:142:GLU:OE1 | 2.10 | 0.69 |
| 2:P:52:GLY:HA3 | 2:P:60:ILE:HD12 | 1.74 | 0.69 |
| 1:M:158:ILE:HD12 | 1:M:397:VAL:HG22 | 1.73 | 0.69 |
| 1:K:127:VAL:HG23 | 1:K:423:CYS:HB3 | 1.75 | 0.69 |
| 1:K:237:LEU:HD21 | 1:K:262:LEU:HD23 | 1.75 | 0.69 |
| 3:J:601:ADP:O1B | 5:J:701:HOH:O | 2.08 | 0.69 |
| 1:C:158:ILE:HD12 | 1:C:397:VAL:HG22 | 1.74 | 0.69 |
| 1:B:6:VAL:HG12 | 1:B:522:VAL:HG22 | 1.72 | 0.69 |
| 1:G:351:ILE:HG22 | 1:G:370:LEU:HD21 | 1.74 | 0.69 |
| 1:J:354:LEU:HB3 | 1:J:366:LEU:CD1 | 2.21 | 0.69 |
| 1:C:354:LEU:HB3 | 1:C:366:LEU:CD1 | 2.21 | 0.69 |
| 1:B:354:LEU:HB3 | 1:B:366:LEU:CD1 | 2.22 | 0.69 |
| 3:H:601:ADP:O1B | 5:H:701:HOH:O | 2.09 | 0.69 |
| 1:L:421:LEU:HD21 | 1:L:467:VAL:HG13 | 1.74 | 0.69 |
| 1:K:264:LEU:HD11 | 1:K:268:LYS:HE2 | 1.73 | 0.69 |
| 1:I:354:LEU:HB3 | 1:I:366:LEU:CD1 | 2.21 | 0.69 |
| 3:B:601:ADP:O3B | 5:B:701:HOH:O | 2.09 | 0.69 |
| 2:O:3:GLY:HA3 | 2:O:51:SER:HA | 1.75 | 0.69 |
| 1:M:140:THR:OG1 | 1:M:142:GLU:OE1 | 2.09 | 0.69 |
| 1:J:314:GLN:OE1 | 1:J:316:HIS:NE2 | 2.24 | 0.69 |
| 1:A:354:LEU:HB3 | 1:A:366:LEU:CD1 | 2.21 | 0.69 |
| 2:X:20:ARG:NH1 | 2:X:41:VAL:O | 2.24 | 0.69 |
| 2:T:20:ARG:NH1 | 2:T:41:VAL:O | 2.23 | 0.69 |
| 1:K:354:LEU:HB3 | 1:K:366:LEU:CD1 | 2.22 | 0.69 |
| 3:A:601:ADP:O3B | 5:A:701:HOH:O | 2.09 | 0.69 |
| 1:G:140:THR:OG1 | 1:G:142:GLU:OE1 | 2.09 | 0.69 |
| 3:L:601:ADP:O1B | 5:L:701:HOH:O | 2.09 | 0.69 |
| 2:T:73:LEU:HB3 | 2:T:91:PHE:HE2 | 1.58 | 0.69 |
| 1:D:237:LEU:HD21 | 1:D:262:LEU:HD23 | 1.74 | 0.69 |
| 1:B:140:THR:OG1 | 1:B:142:GLU:OE1 | 2.11 | 0.69 |
| 1:A:140:THR:OG1 | 1:A:142:GLU:OE1 | 2.11 | 0.69 |
| 1:D:284:ASN:HD21 | 1:D:365:LYS:HE2 | 1.57 | 0.68 |
| 1:N:354:LEU:HB3 | 1:N:366:LEU:CD1 | 2.22 | 0.68 |
| 1:N:421:LEU:HD21 | 1:N:467:VAL:HG13 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:601:ADP:O1B | 5:N:701:HOH:O | 2.09 | 0.68 |
| 1:E:282:GLY:O | 1:E:285:ARG:HG2 | 1.93 | 0.68 |
| 2:R:5:ALA:HB2 | 2:R:10:LEU:HD13 | 1.75 | 0.68 |
| 1:N:351:ILE:HG22 | 1:N:370:LEU:HD21 | 1.75 | 0.68 |
| 1:L:140:THR:OG1 | 1:L:142:GLU:OE1 | 2.11 | 0.68 |
| 1:A:158:ILE:HD12 | 1:A:397:VAL:HG22 | 1.74 | 0.68 |
| 2:V:20:ARG:NH1 | 2:V:41:VAL:O | 2.23 | 0.68 |
| 2:1:73:LEU:HB3 | 2:1:91:PHE:HE2 | 1.59 | 0.68 |
| 2:S:20:ARG:NH1 | 2:S:41:VAL:O | 2.24 | 0.68 |
| 1:I:140:THR:OG1 | 1:I:142:GLU:OE1 | 2.10 | 0.68 |
| 1:D:140:THR:OG1 | 1:D:142:GLU:OE1 | 2.11 | 0.68 |
| 2:R:18:VAL:HG12 | 2:R:46:VAL:HA | 1.76 | 0.68 |
| 1:J:140:THR:OG1 | 1:J:142:GLU:OE1 | 2.10 | 0.68 |
| 1:B:169:VAL:HG12 | 1:B:173:GLY:HA3 | 1.74 | 0.68 |
| 2:V:27:THR:CG2 | 2:V:31:ILE:HG22 | 2.24 | 0.68 |
| 2:V:97:LEU:HD12 | 2:W:90:LEU:HD23 | 1.76 | 0.68 |
| 2:W:73:LEU:HB3 | 2:W:91:PHE:HE2 | 1.59 | 0.68 |
| 2:V:18:VAL:HG12 | 2:V:46:VAL:HA | 1.76 | 0.67 |
| 1:A:127:VAL:HG23 | 1:A:423:CYS:HB3 | 1.76 | 0.67 |
| 2:Y:73:LEU:HB3 | 2:Y:91:PHE:HE2 | 1.60 | 0.67 |
| 2:U:18:VAL:HG12 | 2:U:46:VAL:HA | 1.76 | 0.67 |
| 3:K:601:ADP:O1B | 5:K:701:HOH:O | 2.10 | 0.67 |
| 2:U:33:LEU:HG | 1:G:230:ILE:HD11 | 1.77 | 0.67 |
| 3:E:601:ADP:O3B | 5:E:701:HOH:O | 2.10 | 0.67 |
| 2:R:20:ARG:NH1 | 2:R:41:VAL:O | 2.24 | 0.67 |
| 2:P:73:LEU:HB3 | 2:P:91:PHE:HE2 | 1.59 | 0.67 |
| 1:D:421:LEU:HD21 | 1:D:467:VAL:HG13 | 1.75 | 0.67 |
| 1:E:158:ILE:HD12 | 1:E:397:VAL:HG22 | 1.76 | 0.67 |
| 2:T:27:THR:CG2 | 2:T:31:ILE:HG22 | 2.24 | 0.67 |
| 1:D:303:GLU:HB3 | 1:D:306:LEU:HB3 | 1.75 | 0.67 |
| 2:2:20:ARG:NH1 | 2:2:41:VAL:O | 2.24 | 0.67 |
| 2:X:27:THR:CG2 | 2:X:31:ILE:HG22 | 2.25 | 0.67 |
| 2:O:52:GLY:HA3 | 2:O:60:ILE:HD12 | 1.76 | 0.67 |
| 1:J:193:MET:HE2 | 1:J:292:MET:HG2 | 1.75 | 0.67 |
| 1:B:135:SER:HB2 | 1:B:498:THR:HG21 | 1.77 | 0.67 |
| 2:1:27:THR:CG2 | 2:1:31:ILE:HG22 | 2.25 | 0.67 |
| 2:T:32:MET:HE3 | 1:F:268:LYS:HE3 | 1.76 | 0.67 |
| 1:J:282:GLY:O | 1:J:285:ARG:HG2 | 1.95 | 0.67 |
| 2:Y:27:THR:CG2 | 2:Y:31:ILE:HG22 | 2.25 | 0.67 |
| 1:A:31:MET:SD | 1:A:454:THR:OG1 | 2.51 | 0.67 |
| 2:2:5:ALA:HB2 | 2:2:10:LEU:HD13 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Z:73:LEU:HB3 | 2:Z:91:PHE:HE2 | 1.60 | 0.66 |
| 2:S:27:THR:CG2 | 2:S:31:ILE:HG22 | 2.24 | 0.66 |
| 2:R:27:THR:CG2 | 2:R:31:ILE:HG22 | 2.25 | 0.66 |
| 2:R:73:LEU:HB3 | 2:R:91:PHE:HE2 | 1.61 | 0.66 |
| 2:U:52:GLY:HA3 | 2:U:60:ILE:HD12 | 1.78 | 0.66 |
| 1:F:421:LEU:HD21 | 1:F:467:VAL:HG13 | 1.76 | 0.66 |
| 2:Z:27:THR:CG2 | 2:Z:31:ILE:HG22 | 2.25 | 0.66 |
| 2:W:27:THR:CG2 | 2:W:31:ILE:HG22 | 2.25 | 0.66 |
| 2:W:34:PRO:HD3 | 1:I:261:THR:HG22 | 1.77 | 0.66 |
| 2:Q:27:THR:CG2 | 2:Q:31:ILE:HG22 | 2.25 | 0.66 |
| 2:Q:73:LEU:HB3 | 2:Q:91:PHE:HE2 | 1.61 | 0.66 |
| 2:U:27:THR:CG2 | 2:U:31:ILE:HG22 | 2.25 | 0.66 |
| 1:J:127:VAL:HG23 | 1:J:423:CYS:HB3 | 1.78 | 0.66 |
| 1:D:282:GLY:O | 1:D:285:ARG:HG2 | 1.96 | 0.66 |
| 2:V:5:ALA:HB2 | 2:V:10:LEU:HD13 | 1.76 | 0.66 |
| 2:2:73:LEU:HB3 | 2:2:91:PHE:HE2 | 1.61 | 0.66 |
| 2:1:18:VAL:HG12 | 2:1:46:VAL:HA | 1.78 | 0.66 |
| 2:R:32:MET:HE3 | 1:D:268:LYS:HE3 | 1.78 | 0.66 |
| 1:F:140:THR:OG1 | 1:F:142:GLU:OE1 | 2.10 | 0.66 |
| 1:H:233:ILE:HG13 | 1:H:237:LEU:HD13 | 1.78 | 0.66 |
| 1:J:135:SER:HB2 | 1:J:498:THR:HG21 | 1.77 | 0.66 |
| 1:C:525:ILE:HG13 | 1:C:526:PRO:HD2 | 1.76 | 0.66 |
| 1:H:268:LYS:O | 1:H:270:GLY:N | 2.29 | 0.66 |
| 2:S:73:LEU:HB3 | 2:S:91:PHE:HE2 | 1.60 | 0.66 |
| 1:N:140:THR:OG1 | 1:N:142:GLU:OE1 | 2.11 | 0.66 |
| 1:I:233:ILE:HG13 | 1:I:237:LEU:HD13 | 1.77 | 0.66 |
| 1:C:31:MET:SD | 1:C:454:THR:OG1 | 2.51 | 0.66 |
| 2:2:27:THR:CG2 | 2:2:31:ILE:HG22 | 2.25 | 0.66 |
| 2:1:31:ILE:HG21 | 1:M:234:VAL:HG23 | 1.77 | 0.66 |
| 1:K:140:THR:OG1 | 1:K:142:GLU:OE1 | 2.11 | 0.66 |
| 1:C:525:ILE:HG23 | 1:C:527:LYS:HG3 | 1.77 | 0.66 |
| 1:E:352:GLU:O | 1:E:356:VAL:HG23 | 1.96 | 0.66 |
| 2:P:27:THR:CG2 | 2:P:31:ILE:HG22 | 2.25 | 0.66 |
| 2:1:32:MET:HE3 | 1:M:268:LYS:HD3 | 1.78 | 0.65 |
| 1:I:352:GLU:O | 1:I:356:VAL:HG23 | 1.97 | 0.65 |
| 2:X:73:LEU:HB3 | 2:X:91:PHE:HE2 | 1.62 | 0.65 |
| 2:O:73:LEU:HB3 | 2:O:91:PHE:HE2 | 1.61 | 0.65 |
| 1:G:193:MET:HE2 | 1:G:292:MET:HG2 | 1.78 | 0.65 |
| 2:T:18:VAL:HG12 | 2:T:46:VAL:HA | 1.78 | 0.65 |
| 2:S:3:GLY:HA3 | 2:S:51:SER:HA | 1.76 | 0.65 |
| 1:F:489:MET:O | 1:F:493:GLY:N | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:203:TYR:HB3 | 1:M:267:LEU:HD11 | 1.79 | 0.65 |
| 1:G:135:SER:HB2 | 1:G:498:THR:HG21 | 1.77 | 0.65 |
| 2:W:3:GLY:HA3 | 2:W:51:SER:HA | 1.78 | 0.65 |
| 2:R:8:LYS:HG2 | 2:Q:102:ASP:HB3 | 1.79 | 0.65 |
| 1:K:148:ALA:HB2 | 1:K:404:THR:HG21 | 1.77 | 0.65 |
| 1:D:352:GLU:O | 1:D:356:VAL:HG23 | 1.97 | 0.65 |
| 1:A:148:ALA:HB2 | 1:A:404:THR:HG21 | 1.78 | 0.65 |
| 1:F:456:ALA:HB3 | 1:F:463:GLY:HA2 | 1.78 | 0.65 |
| 2:V:73:LEU:HB3 | 2:V:91:PHE:HE2 | 1.62 | 0.65 |
| 2:2:18:VAL:HG12 | 2:2:46:VAL:HA | 1.79 | 0.65 |
| 2:P:3:GLY:HA3 | 2:P:51:SER:HA | 1.79 | 0.65 |
| 1:H:193:MET:HE2 | 1:H:292:MET:HG2 | 1.79 | 0.65 |
| 1:N:169:VAL:HG12 | 1:N:173:GLY:HA3 | 1.77 | 0.65 |
| 1:B:280:GLY:O | 1:B:285:ARG:NE | 2.30 | 0.65 |
| 1:J:158:ILE:HD12 | 1:J:397:VAL:HG22 | 1.79 | 0.65 |
| 1:H:158:ILE:HD12 | 1:H:397:VAL:HG22 | 1.77 | 0.64 |
| 2:U:32:MET:CE | 1:G:268:LYS:HE3 | 2.27 | 0.64 |
| 1:L:352:GLU:O | 1:L:356:VAL:HG23 | 1.97 | 0.64 |
| 1:G:158:ILE:HD12 | 1:G:397:VAL:HG22 | 1.78 | 0.64 |
| 1:G:352:GLU:O | 1:G:356:VAL:HG23 | 1.97 | 0.64 |
| 1:F:352:GLU:O | 1:F:356:VAL:HG23 | 1.98 | 0.64 |
| 1:H:456:ALA:HB3 | 1:H:463:GLY:HA2 | 1.78 | 0.64 |
| 1:J:421:LEU:HD21 | 1:J:467:VAL:HG13 | 1.79 | 0.64 |
| 1:A:268:LYS:O | 1:A:270:GLY:N | 2.30 | 0.64 |
| 2:O:8:LYS:HG2 | 2:U:102:ASP:HB3 | 1.78 | 0.64 |
| 1:C:456:ALA:HB3 | 1:C:463:GLY:HA2 | 1.78 | 0.64 |
| 1:H:264:LEU:CG | 1:H:268:LYS:HE2 | 2.26 | 0.64 |
| 1:M:456:ALA:HB3 | 1:M:463:GLY:HA2 | 1.77 | 0.64 |
| 1:E:399:ASP:OD1 | 5:E:702:HOH:O | 2.15 | 0.64 |
| 2:2:37:SER:HB2 | 1:N:257:GLU:OE2 | 1.97 | 0.64 |
| 1:B:31:MET:SD | 1:B:454:THR:OG1 | 2.53 | 0.64 |
| 2:O:27:THR:CG2 | 2:O:31:ILE:HG22 | 2.27 | 0.64 |
| 1:L:282:GLY:O | 1:L:285:ARG:HG2 | 1.98 | 0.64 |
| 2:W:32:MET:CE | 1:I:268:LYS:HE3 | 2.28 | 0.64 |
| 1:L:135:SER:HB2 | 1:L:498:THR:HG21 | 1.79 | 0.64 |
| 1:I:188:GLU:HB3 | 1:I:379:VAL:CG2 | 2.28 | 0.64 |
| 1:I:421:LEU:HD21 | 1:I:467:VAL:HG13 | 1.80 | 0.64 |
| 1:A:222:LEU:HD23 | 1:A:250:ILE:HB | 1.80 | 0.64 |
| 1:H:399:ASP:OD1 | 5:H:702:HOH:O | 2.15 | 0.63 |
| 1:M:233:ILE:HG13 | 1:M:237:LEU:HD13 | 1.81 | 0.63 |
| 1:K:193:MET:HE2 | 1:K:292:MET:HG2 | 1.78 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:188:GLU:HB3 | 1:J:379:VAL:CG2 | 2.29 | 0.63 |
| 1:J:351:ILE:O | 1:J:354:LEU:HG | 1.98 | 0.63 |
| 1:F:188:GLU:HB3 | 1:F:379:VAL:CG2 | 2.28 | 0.63 |
| 2:Z:32:MET:HE3 | 1:L:268:LYS:HE3 | 1.79 | 0.63 |
| 2:P:37:SER:HB2 | 1:B:257:GLU:OE2 | 1.99 | 0.63 |
| 2:S:37:SER:HB2 | 1:E:257:GLU:OE2 | 1.98 | 0.63 |
| 1:J:233:ILE:HG13 | 1:J:237:LEU:HD13 | 1.80 | 0.63 |
| 1:C:264:LEU:HG | 1:C:268:LYS:HE2 | 1.79 | 0.63 |
| 1:E:351:ILE:HG22 | 1:E:370:LEU:HD21 | 1.81 | 0.63 |
| 1:B:351:ILE:O | 1:B:354:LEU:HG | 1.99 | 0.63 |
| 2:2:8:LYS:HG2 | 2:1:102:ASP:HB3 | 1.81 | 0.63 |
| 2:Y:33:LEU:HG | 1:K:230:ILE:HD11 | 1.81 | 0.63 |
| 2:Q:15:ARG:HB3 | 2:Q:90:LEU:CD1 | 2.28 | 0.63 |
| 1:K:169:VAL:HG12 | 1:K:173:GLY:HA3 | 1.81 | 0.63 |
| 2:1:33:LEU:HG | 1:M:230:ILE:HD11 | 1.79 | 0.63 |
| 2:Q:31:ILE:HG21 | 1:C:234:VAL:HG23 | 1.80 | 0.63 |
| 2:P:32:MET:HE3 | 1:B:268:LYS:HE3 | 1.80 | 0.63 |
| 1:I:135:SER:HB2 | 1:I:498:THR:HG21 | 1.81 | 0.63 |
| 1:B:169:VAL:HG21 | 1:B:378:ALA:HB2 | 1.80 | 0.63 |
| 1:E:252:GLU:HG3 | 1:E:285:ARG:NH1 | 2.14 | 0.63 |
| 1:M:297:GLY:O | 1:M:319:GLY:HA2 | 1.99 | 0.63 |
| 1:B:280:GLY:O | 1:B:285:ARG:HB2 | 1.99 | 0.63 |
| 1:D:169:VAL:HG12 | 1:D:173:GLY:HA3 | 1.81 | 0.63 |
| 1:B:351:ILE:HG22 | 1:B:370:LEU:HD21 | 1.80 | 0.63 |
| 1:H:351:ILE:O | 1:H:354:LEU:HG | 1.99 | 0.62 |
| 2:Y:15:ARG:HB3 | 2:Y:90:LEU:CD1 | 2.29 | 0.62 |
| 2:T:37:SER:HB2 | 1:F:257:GLU:OE2 | 1.99 | 0.62 |
| 1:N:127:VAL:HG23 | 1:N:423:CYS:HB3 | 1.81 | 0.62 |
| 1:N:158:ILE:HD12 | 1:N:397:VAL:HG22 | 1.80 | 0.62 |
| 1:J:22:LEU:HD23 | 1:J:62:LEU:HD21 | 1.81 | 0.62 |
| 1:B:352:GLU:O | 1:B:356:VAL:HG23 | 1.99 | 0.62 |
| 1:F:158:ILE:HD12 | 1:F:397:VAL:HG22 | 1.80 | 0.62 |
| 1:H:352:GLU:O | 1:H:356:VAL:HG23 | 1.99 | 0.62 |
| 2:X:5:ALA:HB2 | 2:X:10:LEU:HD13 | 1.81 | 0.62 |
| 1:M:282:GLY:O | 1:M:285:ARG:HG2 | 1.98 | 0.62 |
| 1:K:351:ILE:HG22 | 1:K:370:LEU:HD21 | 1.81 | 0.62 |
| 1:A:188:GLU:HB3 | 1:A:379:VAL:CG2 | 2.29 | 0.62 |
| 2:R:102:ASP:HB3 | 2:S:8:LYS:HG2 | 1.80 | 0.62 |
| 2:S:32:MET:HE3 | 1:E:268:LYS:HE3 | 1.80 | 0.62 |
| 1:N:352:GLU:O | 1:N:356:VAL:HG23 | 1.99 | 0.62 |
| 1:E:281:PHE:HA | 1:E:285:ARG:NH2 | 2.12 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:351:ILE:O | 1:L:354:LEU:HG | 1.98 | 0.62 |
| 1:G:456:ALA:HB3 | 1:G:463:GLY:HA2 | 1.80 | 0.62 |
| 1:E:351:ILE:O | 1:E:354:LEU:HG | 1.99 | 0.62 |
| 1:K:351:ILE:O | 1:K:354:LEU:HG | 2.00 | 0.62 |
| 1:I:22:LEU:HD23 | 1:I:62:LEU:HD21 | 1.82 | 0.62 |
| 1:C:197:ARG:H | 1:C:330:ASP:HA | 1.65 | 0.62 |
| 1:A:351:ILE:HG22 | 1:A:370:LEU:HD21 | 1.80 | 0.62 |
| 2:Y:32:MET:CE | 1:K:268:LYS:HE3 | 2.29 | 0.62 |
| 1:N:351:ILE:O | 1:N:354:LEU:HG | 1.99 | 0.62 |
| 1:L:525:ILE:HG13 | 1:L:526:PRO:HD2 | 1.81 | 0.62 |
| 1:D:351:ILE:O | 1:D:354:LEU:HG | 1.99 | 0.62 |
| 1:B:22:LEU:HD23 | 1:B:62:LEU:HD21 | 1.82 | 0.62 |
| 2:W:33:LEU:HG | 1:I:230:ILE:HD11 | 1.79 | 0.62 |
| 1:M:351:ILE:O | 1:M:354:LEU:HG | 2.00 | 0.62 |
| 1:A:169:VAL:HG12 | 1:A:173:GLY:HA3 | 1.80 | 0.62 |
| 1:L:169:VAL:HG12 | 1:L:173:GLY:HA3 | 1.82 | 0.62 |
| 1:K:264:LEU:CD1 | 1:K:268:LYS:HE2 | 2.30 | 0.62 |
| 1:F:351:ILE:HG22 | 1:F:370:LEU:HD21 | 1.82 | 0.62 |
| 1:F:525:ILE:HG13 | 1:F:526:PRO:HD2 | 1.82 | 0.62 |
| 2:X:34:PRO:HD3 | 1:J:261:THR:HG22 | 1.80 | 0.62 |
| 1:L:297:GLY:O | 1:L:319:GLY:HA2 | 2.00 | 0.62 |
| 1:K:188:GLU:HB3 | 1:K:379:VAL:CG2 | 2.30 | 0.62 |
| 1:I:264:LEU:CD1 | 1:I:268:LYS:HE2 | 2.29 | 0.62 |
| 1:C:352:GLU:O | 1:C:356:VAL:HG23 | 2.00 | 0.62 |
| 1:G:351:ILE:O | 1:G:354:LEU:HG | 1.99 | 0.62 |
| 2:R:37:SER:HB2 | 1:D:257:GLU:OE2 | 2.00 | 0.62 |
| 1:N:297:GLY:O | 1:N:319:GLY:HA2 | 2.00 | 0.62 |
| 1:L:188:GLU:HB3 | 1:L:379:VAL:CG2 | 2.29 | 0.62 |
| 1:I:351:ILE:O | 1:I:354:LEU:HG | 2.00 | 0.62 |
| 1:B:297:GLY:O | 1:B:319:GLY:HA2 | 2.00 | 0.62 |
| 1:B:421:LEU:HD21 | 1:B:467:VAL:HG13 | 1.81 | 0.62 |
| 1:A:351:ILE:O | 1:A:354:LEU:HG | 2.00 | 0.62 |
| 1:I:268:LYS:O | 1:I:270:GLY:N | 2.33 | 0.61 |
| 1:D:268:LYS:O | 1:D:270:GLY:N | 2.33 | 0.61 |
| 1:G:199:TYR:OH | 1:G:205:ILE:HD11 | 2.00 | 0.61 |
| 1:G:233:ILE:HG13 | 1:G:237:LEU:HD13 | 1.82 | 0.61 |
| 1:F:351:ILE:O | 1:F:354:LEU:HG | 2.00 | 0.61 |
| 1:E:525:ILE:HG13 | 1:E:526:PRO:HD2 | 1.82 | 0.61 |
| 1:H:297:GLY:O | 1:H:319:GLY:HA2 | 2.00 | 0.61 |
| 2:T:8:LYS:HG2 | 2:S:102:ASP:HB3 | 1.82 | 0.61 |
| 1:N:282:GLY:O | 1:N:285:ARG:HG2 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:352:GLU:O | 1:M:356:VAL:HG23 | 2.00 | 0.61 |
| 1:L:199:TYR:OH | 1:L:205:ILE:HD11 | 2.00 | 0.61 |
| 1:J:268:LYS:O | 1:J:270:GLY:N | 2.33 | 0.61 |
| 1:E:268:LYS:O | 1:E:270:GLY:N | 2.33 | 0.61 |
| 2:P:15:ARG:NH2 | 2:O:97:LEU:HA | 2.16 | 0.61 |
| 1:M:351:ILE:HG22 | 1:M:370:LEU:HD21 | 1.82 | 0.61 |
| 1:L:351:ILE:HG22 | 1:L:370:LEU:HD21 | 1.82 | 0.61 |
| 1:B:525:ILE:HG13 | 1:B:526:PRO:HD2 | 1.82 | 0.61 |
| 1:A:352:GLU:O | 1:A:356:VAL:HG23 | 2.00 | 0.61 |
| 1:G:22:LEU:HD23 | 1:G:62:LEU:HD21 | 1.82 | 0.61 |
| 1:F:69:ILE:HD11 | 1:F:523:THR:HG22 | 1.82 | 0.61 |
| 1:N:350:ILE:HG23 | 1:N:366:LEU:CD2 | 2.31 | 0.61 |
| 1:K:268:LYS:O | 1:K:270:GLY:N | 2.34 | 0.61 |
| 1:K:352:GLU:O | 1:K:356:VAL:HG23 | 2.00 | 0.61 |
| 1:J:62:LEU:HD13 | 1:J:67:LYS:HB3 | 1.82 | 0.61 |
| 1:D:199:TYR:OH | 1:D:205:ILE:HD11 | 2.01 | 0.61 |
| 1:C:351:ILE:O | 1:C:354:LEU:HG | 2.00 | 0.61 |
| 1:F:193:MET:HE2 | 1:F:292:MET:HG2 | 1.82 | 0.61 |
| 1:H:264:LEU:O | 1:H:268:LYS:HG2 | 2.01 | 0.61 |
| 2:O:31:ILE:HG21 | 1:A:234:VAL:HG23 | 1.82 | 0.61 |
| 2:U:15:ARG:HB3 | 2:U:90:LEU:CD1 | 2.30 | 0.61 |
| 1:M:188:GLU:HB3 | 1:M:379:VAL:CG2 | 2.31 | 0.61 |
| 1:L:127:VAL:HG23 | 1:L:423:CYS:HB3 | 1.83 | 0.61 |
| 1:K:22:LEU:HD23 | 1:K:62:LEU:HD21 | 1.83 | 0.61 |
| 1:K:224:GLU:OE1 | 1:K:303:GLU:HA | 2.01 | 0.61 |
| 1:J:169:VAL:HG12 | 1:J:173:GLY:HA3 | 1.82 | 0.61 |
| 1:B:127:VAL:HG23 | 1:B:423:CYS:HB3 | 1.82 | 0.61 |
| 1:B:350:ILE:HG23 | 1:B:366:LEU:CD2 | 2.31 | 0.61 |
| 1:A:421:LEU:HD21 | 1:A:467:VAL:HG13 | 1.82 | 0.61 |
| 1:A:525:ILE:HG13 | 1:A:526:PRO:HD2 | 1.83 | 0.61 |
| 1:F:268:LYS:O | 1:F:270:GLY:N | 2.33 | 0.61 |
| 1:H:188:GLU:HB3 | 1:H:379:VAL:CG2 | 2.29 | 0.61 |
| 2:2:12:LEU:HD22 | 2:1:96:ILE:O | 2.01 | 0.61 |
| 2:Z:34:PRO:HD3 | 1:L:261:THR:HG22 | 1.83 | 0.61 |
| 2:X:12:LEU:HD22 | 2:W:96:ILE:O | 2.01 | 0.61 |
| 2:O:34:PRO:HD3 | 1:A:261:THR:HG22 | 1.81 | 0.61 |
| 1:K:73:LEU:CD1 | 1:K:515:LEU:HD13 | 2.31 | 0.61 |
| 1:C:268:LYS:O | 1:C:270:GLY:N | 2.34 | 0.61 |
| 1:G:188:GLU:HB3 | 1:G:379:VAL:CG2 | 2.31 | 0.61 |
| 1:F:297:GLY:O | 1:F:319:GLY:HA2 | 2.00 | 0.61 |
| 1:F:399:ASP:OD1 | 5:F:702:HOH:O | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:297:GLY:O | 1:E:319:GLY:HA2 | 2.01 | 0.61 |
| 2:Q:37:SER:HB2 | 1:C:257:GLU:OE2 | 1.99 | 0.61 |
| 1:L:268:LYS:O | 1:L:270:GLY:N | 2.34 | 0.61 |
| 1:D:297:GLY:O | 1:D:319:GLY:HA2 | 1.99 | 0.61 |
| 1:C:188:GLU:HB3 | 1:C:379:VAL:CG2 | 2.31 | 0.61 |
| 1:A:294:ILE:HD11 | 1:A:346:ARG:HG2 | 1.82 | 0.61 |
| 2:P:8:LYS:HG2 | 2:O:102:ASP:HB3 | 1.83 | 0.61 |
| 2:U:16:VAL:HG12 | 2:U:18:VAL:HG13 | 1.83 | 0.61 |
| 1:N:203:TYR:HB3 | 1:N:267:LEU:HD11 | 1.82 | 0.61 |
| 1:M:73:LEU:CD1 | 1:M:515:LEU:HD13 | 2.31 | 0.61 |
| 1:M:216:GLN:HG3 | 1:M:323:GLU:OE1 | 2.00 | 0.61 |
| 1:N:230:ILE:HA | 1:N:233:ILE:HG22 | 1.83 | 0.61 |
| 1:D:13:ARG:NH2 | 1:D:519:GLU:OE1 | 2.34 | 0.61 |
| 1:A:22:LEU:HD23 | 1:A:62:LEU:HD21 | 1.83 | 0.61 |
| 1:H:22:LEU:HD23 | 1:H:62:LEU:HD21 | 1.83 | 0.61 |
| 2:V:12:LEU:HD22 | 2:2:96:ILE:O | 2.00 | 0.61 |
| 2:1:32:MET:CE | 1:M:268:LYS:HD3 | 2.31 | 0.61 |
| 2:Z:37:SER:HB2 | 1:L:257:GLU:OE2 | 2.00 | 0.61 |
| 1:N:199:TYR:OH | 1:N:205:ILE:HD11 | 2.00 | 0.61 |
| 1:N:216:GLN:HG3 | 1:N:323:GLU:OE1 | 2.01 | 0.61 |
| 1:K:233:ILE:HG13 | 1:K:237:LEU:HD13 | 1.81 | 0.61 |
| 1:K:489:MET:O | 1:K:493:GLY:N | 2.32 | 0.61 |
| 1:A:73:LEU:CD1 | 1:A:515:LEU:HD13 | 2.30 | 0.61 |
| 1:G:297:GLY:O | 1:G:319:GLY:HA2 | 2.00 | 0.61 |
| 1:H:234:VAL:HG23 | 2:V:31:ILE:HG21 | 1.83 | 0.60 |
| 2:1:37:SER:HB2 | 1:M:257:GLU:OE2 | 2.00 | 0.60 |
| 1:N:456:ALA:HB3 | 1:N:463:GLY:HA2 | 1.81 | 0.60 |
| 1:J:199:TYR:OH | 1:J:205:ILE:HD11 | 2.01 | 0.60 |
| 1:I:297:GLY:O | 1:I:319:GLY:HA2 | 2.00 | 0.60 |
| 1:D:158:ILE:HD12 | 1:D:397:VAL:HG22 | 1.83 | 0.60 |
| 1:D:350:ILE:HG23 | 1:D:366:LEU:CD2 | 2.31 | 0.60 |
| 1:A:399:ASP:OD1 | 5:A:702:HOH:O | 2.16 | 0.60 |
| 1:H:351:ILE:HG22 | 1:H:370:LEU:HD21 | 1.81 | 0.60 |
| 1:C:297:GLY:O | 1:C:319:GLY:HA2 | 1.99 | 0.60 |
| 1:B:194:LYS:HD2 | 1:B:332:MET:CE | 2.31 | 0.60 |
| 1:H:169:VAL:HG12 | 1:H:173:GLY:HA3 | 1.82 | 0.60 |
| 2:P:33:LEU:HG | 1:B:230:ILE:HD11 | 1.81 | 0.60 |
| 1:C:73:LEU:CD1 | 1:C:515:LEU:HD13 | 2.31 | 0.60 |
| 1:G:268:LYS:O | 1:G:270:GLY:N | 2.34 | 0.60 |
| 1:E:348:GLN:HA | 1:E:351:ILE:HG12 | 1.83 | 0.60 |
| 1:E:350:ILE:HG23 | 1:E:366:LEU:CD2 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:199:TYR:OH | 1:H:205:ILE:HD11 | 2.01 | 0.60 |
| 2:O:37:SER:O | 2:O:38:GLN:HG2 | 2.01 | 0.60 |
| 1:N:207:THR:HG23 | 1:N:209:LYS:N | 2.17 | 0.60 |
| 1:M:199:TYR:OH | 1:M:205:ILE:HD11 | 2.02 | 0.60 |
| 1:L:22:LEU:HD23 | 1:L:62:LEU:HD21 | 1.83 | 0.60 |
| 1:J:264:LEU:CD1 | 1:J:268:LYS:HE2 | 2.32 | 0.60 |
| 1:J:352:GLU:O | 1:J:356:VAL:HG23 | 2.01 | 0.60 |
| 1:D:127:VAL:HG23 | 1:D:423:CYS:HB3 | 1.82 | 0.60 |
| 1:B:268:LYS:O | 1:B:270:GLY:N | 2.33 | 0.60 |
| 1:G:13:ARG:NH2 | 1:G:519:GLU:OE1 | 2.34 | 0.60 |
| 2:Q:32:MET:HE3 | 1:C:268:LYS:HE3 | 1.81 | 0.60 |
| 2:T:33:LEU:HG | 1:F:230:ILE:HD11 | 1.84 | 0.60 |
| 1:M:489:MET:O | 1:M:493:GLY:N | 2.29 | 0.60 |
| 1:K:297:GLY:O | 1:K:319:GLY:HA2 | 2.01 | 0.60 |
| 1:E:127:VAL:HG23 | 1:E:423:CYS:HB3 | 1.84 | 0.60 |
| 2:S:15:ARG:HB3 | 2:S:90:LEU:CD1 | 2.27 | 0.60 |
| 1:N:148:ALA:HB2 | 1:N:404:THR:HG21 | 1.83 | 0.60 |
| 1:L:294:ILE:HD11 | 1:L:346:ARG:HG2 | 1.83 | 0.60 |
| 1:D:69:ILE:HD11 | 1:D:523:THR:HG22 | 1.84 | 0.60 |
| 1:A:350:ILE:HG23 | 1:A:366:LEU:CD2 | 2.32 | 0.60 |
| 1:E:199:TYR:OH | 1:E:205:ILE:HD11 | 2.01 | 0.60 |
| 1:H:230:ILE:HD11 | 2:V:33:LEU:HG | 1.83 | 0.60 |
| 2:P:15:ARG:HB3 | 2:P:90:LEU:CD1 | 2.28 | 0.60 |
| 2:O:15:ARG:HB3 | 2:O:90:LEU:CD1 | 2.30 | 0.60 |
| 2:1:15:ARG:HB3 | 2:1:90:LEU:CD1 | 2.28 | 0.60 |
| 2:Y:37:SER:O | 2:Y:38:GLN:HG2 | 2.02 | 0.60 |
| 1:N:348:GLN:HA | 1:N:351:ILE:HG12 | 1.84 | 0.60 |
| 1:M:22:LEU:HD23 | 1:M:62:LEU:HD21 | 1.84 | 0.60 |
| 1:J:348:GLN:HA | 1:J:351:ILE:HG12 | 1.84 | 0.60 |
| 1:I:351:ILE:HG22 | 1:I:370:LEU:HD21 | 1.83 | 0.60 |
| 1:G:81:THR:HG21 | 1:G:88:GLY:O | 2.02 | 0.60 |
| 1:G:148:ALA:HB2 | 1:G:404:THR:HG21 | 1.84 | 0.60 |
| 1:E:188:GLU:HB3 | 1:E:379:VAL:CG2 | 2.32 | 0.60 |
| 1:E:207:THR:HG23 | 1:E:209:LYS:N | 2.16 | 0.60 |
| 1:H:224:GLU:OE1 | 1:H:303:GLU:HA | 2.02 | 0.60 |
| 1:K:399:ASP:OD1 | 5:K:702:HOH:O | 2.17 | 0.60 |
| 1:A:233:ILE:HG13 | 1:A:237:LEU:HD13 | 1.84 | 0.60 |
| 1:G:73:LEU:CD1 | 1:G:515:LEU:HD13 | 2.32 | 0.60 |
| 2:1:37:SER:O | 2:1:38:GLN:HG2 | 2.02 | 0.60 |
| 2:Q:37:SER:O | 2:Q:38:GLN:HG2 | 2.02 | 0.60 |
| 1:D:188:GLU:HB3 | 1:D:379:VAL:CG2 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:148:ALA:HB2 | 1:B:404:THR:HG21 | 1.84 | 0.60 |
| 2:R:12:LEU:HD22 | 2:Q:96:ILE:O | 2.02 | 0.59 |
| 1:M:127:VAL:HG23 | 1:M:423:CYS:HB3 | 1.84 | 0.59 |
| 1:K:169:VAL:HG21 | 1:K:378:ALA:HB2 | 1.83 | 0.59 |
| 1:D:264:LEU:CG | 1:D:268:LYS:HE2 | 2.32 | 0.59 |
| 1:E:383:GLY:O | 1:E:390:VAL:HG22 | 2.02 | 0.59 |
| 1:H:497:PRO:HB2 | 1:H:500:VAL:HG12 | 1.83 | 0.59 |
| 2:V:8:LYS:HG2 | 2:2:102:ASP:HB3 | 1.83 | 0.59 |
| 2:U:73:LEU:HB3 | 2:U:91:PHE:HE2 | 1.67 | 0.59 |
| 1:I:294:ILE:HD11 | 1:I:346:ARG:HG2 | 1.83 | 0.59 |
| 1:B:199:TYR:OH | 1:B:205:ILE:HD11 | 2.02 | 0.59 |
| 2:X:37:SER:O | 2:X:38:GLN:HG2 | 2.03 | 0.59 |
| 1:K:197:ARG:H | 1:K:330:ASP:HA | 1.67 | 0.59 |
| 1:K:350:ILE:HG23 | 1:K:366:LEU:CD2 | 2.32 | 0.59 |
| 1:J:351:ILE:HG22 | 1:J:370:LEU:HD21 | 1.83 | 0.59 |
| 1:I:199:TYR:OH | 1:I:205:ILE:HD11 | 2.02 | 0.59 |
| 1:D:148:ALA:HB2 | 1:D:404:THR:HG21 | 1.83 | 0.59 |
| 1:D:348:GLN:HA | 1:D:351:ILE:HG12 | 1.84 | 0.59 |
| 1:C:233:ILE:HG13 | 1:C:237:LEU:HD13 | 1.83 | 0.59 |
| 1:C:348:GLN:HA | 1:C:351:ILE:HG12 | 1.84 | 0.59 |
| 1:B:264:LEU:HG | 1:B:268:LYS:HE2 | 1.84 | 0.59 |
| 1:E:22:LEU:HD23 | 1:E:62:LEU:HD21 | 1.84 | 0.59 |
| 1:E:176:THR:CG2 | 1:E:379:VAL:HG12 | 2.32 | 0.59 |
| 1:H:228:SER:HA | 1:H:255:ASP:CB | 2.33 | 0.59 |
| 1:H:489:MET:O | 1:H:493:GLY:N | 2.28 | 0.59 |
| 2:Z:12:LEU:HD22 | 2:Y:96:ILE:O | 2.01 | 0.59 |
| 2:U:37:SER:O | 2:U:38:GLN:HG2 | 2.02 | 0.59 |
| 1:M:294:ILE:HD11 | 1:M:346:ARG:HG2 | 1.84 | 0.59 |
| 1:K:294:ILE:HD11 | 1:K:346:ARG:HG2 | 1.83 | 0.59 |
| 1:D:456:ALA:HB3 | 1:D:463:GLY:HA2 | 1.84 | 0.59 |
| 1:C:148:ALA:HB2 | 1:C:404:THR:HG21 | 1.83 | 0.59 |
| 1:G:197:ARG:H | 1:G:330:ASP:HA | 1.67 | 0.59 |
| 1:G:294:ILE:HD11 | 1:G:346:ARG:HG2 | 1.83 | 0.59 |
| 1:L:350:ILE:HG23 | 1:L:366:LEU:CD2 | 2.32 | 0.59 |
| 1:K:348:GLN:HA | 1:K:351:ILE:HG12 | 1.85 | 0.59 |
| 1:C:194:LYS:HD2 | 1:C:332:MET:CE | 2.33 | 0.59 |
| 1:B:188:GLU:HB3 | 1:B:379:VAL:CG2 | 2.32 | 0.59 |
| 1:B:207:THR:HG23 | 1:B:209:LYS:N | 2.17 | 0.59 |
| 1:A:199:TYR:OH | 1:A:205:ILE:HD11 | 2.02 | 0.59 |
| 1:A:297:GLY:O | 1:A:319:GLY:HA2 | 2.02 | 0.59 |
| 1:F:264:LEU:HG | 1:F:268:LYS:HE2 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:456:ALA:HB3 | 1:E:463:GLY:HA2 | 1.84 | 0.59 |
| 2:2:32:MET:CE | 1:N:268:LYS:HD3 | 2.32 | 0.59 |
| 2:R:97:LEU:HA | 2:S:15:ARG:NH2 | 2.18 | 0.59 |
| 1:L:233:ILE:HG13 | 1:L:237:LEU:HD13 | 1.84 | 0.59 |
| 1:J:176:THR:CG2 | 1:J:379:VAL:HG12 | 2.33 | 0.59 |
| 1:I:73:LEU:CD1 | 1:I:515:LEU:HD13 | 2.31 | 0.59 |
| 1:I:81:THR:HG21 | 1:I:88:GLY:O | 2.02 | 0.59 |
| 1:D:73:LEU:CD1 | 1:D:515:LEU:HD13 | 2.32 | 0.59 |
| 1:C:350:ILE:HG23 | 1:C:366:LEU:CD2 | 2.32 | 0.59 |
| 1:F:73:LEU:CD1 | 1:F:515:LEU:HD13 | 2.32 | 0.59 |
| 2:Y:15:ARG:NH2 | 2:X:97:LEU:HA | 2.17 | 0.59 |
| 2:Q:16:VAL:HG12 | 2:Q:18:VAL:HG13 | 1.83 | 0.59 |
| 1:K:176:THR:CG2 | 1:K:379:VAL:HG12 | 2.33 | 0.59 |
| 1:J:322:GLY:N | 1:J:335:LYS:O | 2.30 | 0.59 |
| 1:I:350:ILE:HG23 | 1:I:366:LEU:CD2 | 2.32 | 0.59 |
| 1:A:228:SER:HA | 1:A:255:ASP:CB | 2.32 | 0.59 |
| 1:F:207:THR:HG23 | 1:F:209:LYS:N | 2.17 | 0.59 |
| 1:H:207:THR:HG23 | 1:H:209:LYS:N | 2.18 | 0.59 |
| 1:H:257:GLU:OE2 | 2:V:37:SER:HB2 | 2.01 | 0.59 |
| 1:H:348:GLN:HA | 1:H:351:ILE:HG12 | 1.85 | 0.59 |
| 2:X:32:MET:CE | 1:J:268:LYS:HE3 | 2.32 | 0.59 |
| 1:J:350:ILE:HG23 | 1:J:366:LEU:CD2 | 2.33 | 0.59 |
| 1:C:22:LEU:HD23 | 1:C:62:LEU:HD21 | 1.84 | 0.59 |
| 1:G:22:LEU:HD11 | 1:F:6:VAL:HG21 | 1.85 | 0.59 |
| 1:G:127:VAL:HG23 | 1:G:423:CYS:HB3 | 1.85 | 0.59 |
| 1:G:383:GLY:O | 1:G:390:VAL:HG22 | 2.02 | 0.59 |
| 2:V:37:SER:O | 2:V:38:GLN:HG2 | 2.03 | 0.59 |
| 1:N:73:LEU:CD1 | 1:N:515:LEU:HD13 | 2.32 | 0.59 |
| 1:M:148:ALA:HB2 | 1:M:404:THR:HG21 | 1.83 | 0.59 |
| 1:L:73:LEU:CD1 | 1:L:515:LEU:HD13 | 2.33 | 0.59 |
| 1:B:348:GLN:HA | 1:B:351:ILE:HG12 | 1.85 | 0.59 |
| 1:B:399:ASP:OD1 | 5:B:702:HOH:O | 2.17 | 0.59 |
| 1:A:348:GLN:HA | 1:A:351:ILE:HG12 | 1.84 | 0.59 |
| 1:F:194:LYS:HD2 | 1:F:332:MET:CE | 2.32 | 0.59 |
| 1:F:350:ILE:HG23 | 1:F:366:LEU:CD2 | 2.33 | 0.59 |
| 2:X:52:GLY:HA3 | 2:X:60:ILE:HD12 | 1.85 | 0.59 |
| 2:W:37:SER:HB2 | 1:I:257:GLU:OE2 | 2.03 | 0.59 |
| 2:P:37:SER:O | 2:P:38:GLN:HG2 | 2.03 | 0.59 |
| 2:T:15:ARG:NH2 | 2:S:97:LEU:HA | 2.18 | 0.59 |
| 1:M:350:ILE:HG23 | 1:M:366:LEU:CD2 | 2.33 | 0.59 |
| 1:L:264:LEU:HG | 1:L:268:LYS:HE2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:456:ALA:HB3 | 1:L:463:GLY:HA2 | 1.85 | 0.59 |
| 1:J:73:LEU:CD1 | 1:J:515:LEU:HD13 | 2.32 | 0.59 |
| 1:J:294:ILE:HD11 | 1:J:346:ARG:HG2 | 1.83 | 0.59 |
| 1:J:456:ALA:HB3 | 1:J:463:GLY:HA2 | 1.82 | 0.59 |
| 1:F:348:GLN:HA | 1:F:351:ILE:HG12 | 1.85 | 0.59 |
| 1:H:197:ARG:H | 1:H:330:ASP:HA | 1.68 | 0.58 |
| 1:H:350:ILE:HG23 | 1:H:366:LEU:CD2 | 2.33 | 0.58 |
| 1:N:294:ILE:HD11 | 1:N:346:ARG:HG2 | 1.84 | 0.58 |
| 1:M:193:MET:HE1 | 1:M:292:MET:HA | 1.83 | 0.58 |
| 1:I:169:VAL:HG12 | 1:I:173:GLY:HA3 | 1.85 | 0.58 |
| 1:I:348:GLN:HA | 1:I:351:ILE:HG12 | 1.85 | 0.58 |
| 1:I:399:ASP:OD1 | 5:I:702:HOH:O | 2.17 | 0.58 |
| 1:I:456:ALA:HB3 | 1:I:463:GLY:HA2 | 1.84 | 0.58 |
| 1:D:62:LEU:HD13 | 1:D:67:LYS:HB3 | 1.85 | 0.58 |
| 1:D:176:THR:CG2 | 1:D:379:VAL:HG12 | 2.33 | 0.58 |
| 1:D:293:ALA:O | 1:D:297:GLY:N | 2.27 | 0.58 |
| 1:G:293:ALA:O | 1:G:297:GLY:N | 2.28 | 0.58 |
| 1:G:350:ILE:HG23 | 1:G:366:LEU:CD2 | 2.33 | 0.58 |
| 2:Z:37:SER:O | 2:Z:38:GLN:HG2 | 2.03 | 0.58 |
| 2:U:46:VAL:HG13 | 2:U:67:VAL:HA | 1.85 | 0.58 |
| 1:M:194:LYS:HD2 | 1:M:332:MET:CE | 2.32 | 0.58 |
| 1:K:62:LEU:HD13 | 1:K:67:LYS:HB3 | 1.85 | 0.58 |
| 1:I:489:MET:O | 1:I:493:GLY:N | 2.30 | 0.58 |
| 1:A:207:THR:HG23 | 1:A:209:LYS:N | 2.19 | 0.58 |
| 1:A:384:GLY:H | 1:A:390:VAL:HG22 | 1.68 | 0.58 |
| 1:F:176:THR:CG2 | 1:F:379:VAL:HG12 | 2.32 | 0.58 |
| 1:F:294:ILE:HD11 | 1:F:346:ARG:HG2 | 1.84 | 0.58 |
| 2:1:15:ARG:NH2 | 2:Z:97:LEU:HA | 2.18 | 0.58 |
| 2:R:37:SER:O | 2:R:38:GLN:HG2 | 2.03 | 0.58 |
| 2:Q:15:ARG:NH2 | 2:P:97:LEU:HA | 2.19 | 0.58 |
| 2:U:8:LYS:HA | 2:T:101:VAL:O | 2.04 | 0.58 |
| 1:L:176:THR:CG2 | 1:L:379:VAL:HG12 | 2.33 | 0.58 |
| 1:J:228:SER:HA | 1:J:255:ASP:CB | 2.34 | 0.58 |
| 1:C:127:VAL:HG23 | 1:C:423:CYS:HB3 | 1.84 | 0.58 |
| 1:C:176:THR:CG2 | 1:C:379:VAL:HG12 | 2.33 | 0.58 |
| 1:B:176:THR:CG2 | 1:B:379:VAL:HG12 | 2.33 | 0.58 |
| 1:B:197:ARG:H | 1:B:330:ASP:HA | 1.66 | 0.58 |
| 1:F:199:TYR:OH | 1:F:205:ILE:HD11 | 2.03 | 0.58 |
| 1:H:73:LEU:CD1 | 1:H:515:LEU:HD13 | 2.33 | 0.58 |
| 2:2:31:ILE:HD12 | 1:N:237:LEU:HB3 | 1.85 | 0.58 |
| 1:M:348:GLN:HA | 1:M:351:ILE:HG12 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:158:ILE:HD12 | 1:B:397:VAL:HG22 | 1.84 | 0.58 |
| 1:F:81:THR:HG21 | 1:F:88:GLY:O | 2.03 | 0.58 |
| 2:W:37:SER:O | 2:W:38:GLN:HG2 | 2.03 | 0.58 |
| 1:D:207:THR:HG23 | 1:D:209:LYS:N | 2.17 | 0.58 |
| 1:E:194:LYS:HD2 | 1:E:332:MET:CE | 2.33 | 0.58 |
| 2:Q:46:VAL:HG13 | 2:Q:67:VAL:HA | 1.85 | 0.58 |
| 2:P:31:ILE:HD12 | 1:B:237:LEU:HB3 | 1.86 | 0.58 |
| 1:M:13:ARG:NH2 | 1:M:519:GLU:OE1 | 2.35 | 0.58 |
| 1:K:421:LEU:HD21 | 1:K:467:VAL:HG13 | 1.86 | 0.58 |
| 1:D:252:GLU:HG3 | 1:D:285:ARG:NH1 | 2.18 | 0.58 |
| 1:D:280:GLY:O | 1:D:285:ARG:NE | 2.36 | 0.58 |
| 1:C:199:TYR:OH | 1:C:205:ILE:HD11 | 2.03 | 0.58 |
| 1:C:351:ILE:HG22 | 1:C:370:LEU:HD21 | 1.84 | 0.58 |
| 1:B:294:ILE:HD11 | 1:B:346:ARG:HG2 | 1.83 | 0.58 |
| 1:E:135:SER:HB2 | 1:E:498:THR:HG21 | 1.84 | 0.58 |
| 1:E:188:GLU:OE1 | 1:E:381:LYS:NZ | 2.37 | 0.58 |
| 1:I:148:ALA:HB2 | 1:I:404:THR:HG21 | 1.85 | 0.58 |
| 1:I:228:SER:HA | 1:I:255:ASP:CB | 2.33 | 0.58 |
| 1:C:294:ILE:HD11 | 1:C:346:ARG:HG2 | 1.85 | 0.58 |
| 1:E:294:ILE:HD11 | 1:E:346:ARG:HG2 | 1.85 | 0.58 |
| 2:X:31:ILE:HG21 | 1:J:234:VAL:HG23 | 1.86 | 0.58 |
| 2:U:31:ILE:HD11 | 1:G:237:LEU:HD22 | 1.86 | 0.58 |
| 2:S:37:SER:O | 2:S:38:GLN:HG2 | 2.03 | 0.58 |
| 1:K:228:SER:HA | 1:K:255:ASP:CB | 2.33 | 0.58 |
| 1:J:194:LYS:HD2 | 1:J:332:MET:CE | 2.33 | 0.58 |
| 1:G:176:THR:CG2 | 1:G:379:VAL:HG12 | 2.33 | 0.58 |
| 1:F:22:LEU:HD23 | 1:F:62:LEU:HD21 | 1.86 | 0.58 |
| 2:T:37:SER:O | 2:T:38:GLN:HG2 | 2.03 | 0.58 |
| 1:N:62:LEU:HD13 | 1:N:67:LYS:HB3 | 1.85 | 0.58 |
| 1:N:81:THR:HG21 | 1:N:88:GLY:O | 2.04 | 0.58 |
| 1:M:231:GLN:O | 1:M:234:VAL:HG12 | 2.04 | 0.58 |
| 1:J:81:THR:HG21 | 1:J:88:GLY:O | 2.03 | 0.58 |
| 1:J:297:GLY:O | 1:J:319:GLY:HA2 | 2.03 | 0.58 |
| 1:D:177:VAL:HG11 | 1:D:398:THR:HG22 | 1.86 | 0.58 |
| 1:D:294:ILE:HD11 | 1:D:346:ARG:HG2 | 1.84 | 0.58 |
| 1:C:383:GLY:O | 1:C:390:VAL:HG22 | 2.04 | 0.58 |
| 1:B:62:LEU:HD13 | 1:B:67:LYS:HB3 | 1.85 | 0.58 |
| 1:B:73:LEU:CD1 | 1:B:515:LEU:HD13 | 2.33 | 0.58 |
| 1:H:176:THR:CG2 | 1:H:379:VAL:HG12 | 2.34 | 0.58 |
| 2:Q:34:PRO:HD3 | 1:C:261:THR:HG22 | 1.85 | 0.58 |
| 2:U:32:MET:HE1 | 1:G:268:LYS:HE3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:22:LEU:HD23 | 1:N:62:LEU:HD21 | 1.86 | 0.58 |
| 1:N:194:LYS:HD2 | 1:N:332:MET:CE | 2.33 | 0.58 |
| 1:L:264:LEU:CD1 | 1:L:268:LYS:HE2 | 2.34 | 0.58 |
| 1:I:224:GLU:OE1 | 1:I:303:GLU:HA | 2.04 | 0.58 |
| 1:B:81:THR:HG21 | 1:B:88:GLY:O | 2.04 | 0.58 |
| 1:A:280:GLY:O | 1:A:285:ARG:HG3 | 2.04 | 0.58 |
| 1:G:231:GLN:O | 1:G:234:VAL:HG12 | 2.04 | 0.58 |
| 1:F:278:ALA:CB | 1:F:285:ARG:HD2 | 2.33 | 0.58 |
| 1:L:348:GLN:HA | 1:L:351:ILE:HG12 | 1.86 | 0.57 |
| 1:B:264:LEU:CD1 | 1:B:268:LYS:HE2 | 2.34 | 0.57 |
| 1:N:177:VAL:HG11 | 1:N:398:THR:HG22 | 1.86 | 0.57 |
| 1:L:81:THR:HG21 | 1:L:88:GLY:O | 2.04 | 0.57 |
| 1:J:264:LEU:HD11 | 1:J:268:LYS:HE2 | 1.85 | 0.57 |
| 1:I:194:LYS:HD2 | 1:I:332:MET:CE | 2.34 | 0.57 |
| 1:D:22:LEU:HD23 | 1:D:62:LEU:HD21 | 1.87 | 0.57 |
| 1:D:194:LYS:HD2 | 1:D:332:MET:CE | 2.34 | 0.57 |
| 1:B:228:SER:HA | 1:B:255:ASP:CB | 2.34 | 0.57 |
| 1:G:348:GLN:HA | 1:G:351:ILE:HG12 | 1.85 | 0.57 |
| 1:F:13:ARG:NH2 | 1:F:519:GLU:OE1 | 2.37 | 0.57 |
| 1:F:233:ILE:HG13 | 1:F:237:LEU:HD13 | 1.85 | 0.57 |
| 2:Z:8:LYS:HG2 | 2:Y:102:ASP:HB3 | 1.86 | 0.57 |
| 2:U:15:ARG:NH2 | 2:T:97:LEU:HA | 2.18 | 0.57 |
| 1:L:69:ILE:HD11 | 1:L:523:THR:HG22 | 1.86 | 0.57 |
| 1:L:148:ALA:HB2 | 1:L:404:THR:HG21 | 1.84 | 0.57 |
| 1:L:194:LYS:HD2 | 1:L:332:MET:CE | 2.33 | 0.57 |
| 1:I:177:VAL:HG11 | 1:I:398:THR:HG22 | 1.86 | 0.57 |
| 1:A:489:MET:O | 1:A:493:GLY:N | 2.31 | 0.57 |
| 1:G:228:SER:HA | 1:G:255:ASP:CB | 2.34 | 0.57 |
| 1:E:73:LEU:CD1 | 1:E:515:LEU:HD13 | 2.33 | 0.57 |
| 1:H:231:GLN:O | 1:H:234:VAL:HG12 | 2.05 | 0.57 |
| 1:N:228:SER:HA | 1:N:255:ASP:CB | 2.34 | 0.57 |
| 1:M:176:THR:CG2 | 1:M:379:VAL:HG12 | 2.33 | 0.57 |
| 1:L:228:SER:HA | 1:L:255:ASP:CB | 2.34 | 0.57 |
| 1:H:81:THR:HG21 | 1:H:88:GLY:O | 2.04 | 0.57 |
| 2:O:15:ARG:NH2 | 2:U:97:LEU:HA | 2.19 | 0.57 |
| 2:T:13:PHE:CD1 | 2:T:54:LYS:HB2 | 2.39 | 0.57 |
| 1:J:383:GLY:O | 1:J:390:VAL:HG22 | 2.04 | 0.57 |
| 1:C:264:LEU:CD1 | 1:C:268:LYS:HE2 | 2.35 | 0.57 |
| 1:H:261:THR:HG22 | 2:V:34:PRO:HD3 | 1.87 | 0.57 |
| 1:N:13:ARG:HD3 | 1:N:104:PHE:HD1 | 1.70 | 0.57 |
| 1:N:135:SER:HB2 | 1:N:498:THR:HG21 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:199:TYR:OH | 1:K:205:ILE:HD11 | 2.04 | 0.57 |
| 1:C:228:SER:HA | 1:C:255:ASP:CB | 2.35 | 0.57 |
| 1:H:194:LYS:HD2 | 1:H:332:MET:CE | 2.34 | 0.57 |
| 2:Z:81:VAL:HG12 | 2:Y:72:LEU:HD21 | 1.86 | 0.57 |
| 2:W:15:ARG:HB3 | 2:W:90:LEU:CD1 | 2.32 | 0.57 |
| 1:C:81:THR:HG21 | 1:C:88:GLY:O | 2.04 | 0.57 |
| 1:N:188:GLU:HB3 | 1:N:379:VAL:CG2 | 2.35 | 0.57 |
| 1:M:81:THR:HG21 | 1:M:88:GLY:O | 2.04 | 0.57 |
| 1:L:158:ILE:HD12 | 1:L:397:VAL:HG22 | 1.86 | 0.57 |
| 1:J:224:GLU:OE1 | 1:J:303:GLU:HA | 2.05 | 0.57 |
| 1:J:231:GLN:O | 1:J:234:VAL:HG12 | 2.04 | 0.57 |
| 1:I:207:THR:HG23 | 1:I:209:LYS:N | 2.19 | 0.57 |
| 2:2:37:SER:O | 2:2:38:GLN:HG2 | 2.04 | 0.57 |
| 2:Y:52:GLY:HA3 | 2:Y:60:ILE:HD12 | 1.87 | 0.57 |
| 1:N:525:ILE:HG23 | 1:N:526:PRO:HD2 | 1.86 | 0.57 |
| 1:A:176:THR:CG2 | 1:A:379:VAL:HG12 | 2.34 | 0.57 |
| 1:G:489:MET:O | 1:G:493:GLY:N | 2.29 | 0.57 |
| 1:H:382:VAL:HG23 | 1:H:390:VAL:HG13 | 1.85 | 0.57 |
| 2:U:16:VAL:HG13 | 2:U:46:VAL:HG23 | 1.86 | 0.57 |
| 1:M:383:GLY:O | 1:M:390:VAL:HG22 | 2.04 | 0.57 |
| 1:I:260:SER:HA | 1:I:263:VAL:HG22 | 1.87 | 0.57 |
| 1:C:231:GLN:O | 1:C:234:VAL:HG12 | 2.05 | 0.57 |
| 1:E:489:MET:O | 1:E:493:GLY:N | 2.32 | 0.57 |
| 2:Y:46:VAL:HG13 | 2:Y:67:VAL:HA | 1.87 | 0.56 |
| 1:N:252:GLU:HG3 | 1:N:285:ARG:NH1 | 2.19 | 0.56 |
| 1:J:13:ARG:NH2 | 1:J:519:GLU:OE1 | 2.38 | 0.56 |
| 1:G:62:LEU:HD13 | 1:G:67:LYS:HB3 | 1.86 | 0.56 |
| 2:V:97:LEU:HA | 2:W:15:ARG:NH2 | 2.19 | 0.56 |
| 1:M:207:THR:HG23 | 1:M:209:LYS:N | 2.20 | 0.56 |
| 1:M:228:SER:HA | 1:M:255:ASP:CB | 2.34 | 0.56 |
| 1:K:293:ALA:O | 1:K:297:GLY:N | 2.27 | 0.56 |
| 1:J:237:LEU:HD21 | 1:J:262:LEU:CD2 | 2.35 | 0.56 |
| 1:I:197:ARG:NE | 1:I:278:ALA:O | 2.38 | 0.56 |
| 1:D:89:THR:O | 1:D:93:THR:HG23 | 2.04 | 0.56 |
| 1:G:177:VAL:HG11 | 1:G:398:THR:HG22 | 1.88 | 0.56 |
| 1:H:294:ILE:HD11 | 1:H:346:ARG:HG2 | 1.86 | 0.56 |
| 2:Y:8:LYS:HG2 | 2:X:102:ASP:HB3 | 1.86 | 0.56 |
| 2:O:37:SER:HB2 | 1:A:257:GLU:OE2 | 2.04 | 0.56 |
| 2:U:15:ARG:HH22 | 2:T:97:LEU:HA | 1.70 | 0.56 |
| 1:N:176:THR:CG2 | 1:N:379:VAL:HG12 | 2.34 | 0.56 |
| 1:C:135:SER:HB2 | 1:C:498:THR:HG21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:169:VAL:HG12 | 1:C:173:GLY:HA3 | 1.87 | 0.56 |
| 1:C:525:ILE:HG23 | 1:C:527:LYS:CG | 2.35 | 0.56 |
| 1:B:383:GLY:O | 1:B:390:VAL:HG22 | 2.05 | 0.56 |
| 1:G:207:THR:HG23 | 1:G:209:LYS:N | 2.19 | 0.56 |
| 1:G:399:ASP:OD1 | 5:G:702:HOH:O | 2.17 | 0.56 |
| 1:F:169:VAL:HG12 | 1:F:173:GLY:HA3 | 1.87 | 0.56 |
| 1:F:177:VAL:HG11 | 1:F:398:THR:HG22 | 1.87 | 0.56 |
| 1:F:230:ILE:HA | 1:F:233:ILE:HG22 | 1.86 | 0.56 |
| 2:T:31:ILE:HD12 | 1:F:237:LEU:HB3 | 1.87 | 0.56 |
| 1:L:197:ARG:H | 1:L:330:ASP:HA | 1.69 | 0.56 |
| 1:L:399:ASP:OD1 | 5:L:702:HOH:O | 2.16 | 0.56 |
| 1:I:176:THR:CG2 | 1:I:379:VAL:HG12 | 2.34 | 0.56 |
| 1:I:525:ILE:HG23 | 1:I:526:PRO:HD2 | 1.88 | 0.56 |
| 1:D:81:THR:HG21 | 1:D:88:GLY:O | 2.04 | 0.56 |
| 1:D:135:SER:HB2 | 1:D:498:THR:HG21 | 1.86 | 0.56 |
| 1:C:283:ASP:HA | 1:C:286:LYS:HD3 | 1.87 | 0.56 |
| 1:A:81:THR:HG21 | 1:A:88:GLY:O | 2.06 | 0.56 |
| 1:G:260:SER:HA | 1:G:263:VAL:HG22 | 1.88 | 0.56 |
| 1:E:293:ALA:O | 1:E:297:GLY:N | 2.28 | 0.56 |
| 1:F:228:SER:HA | 1:F:255:ASP:CB | 2.35 | 0.56 |
| 1:E:228:SER:HA | 1:E:255:ASP:CB | 2.35 | 0.56 |
| 2:U:37:SER:HB2 | 1:G:257:GLU:OE2 | 2.06 | 0.56 |
| 1:M:224:GLU:OE1 | 1:M:303:GLU:HA | 2.06 | 0.56 |
| 1:J:47:PRO:HG3 | 1:I:69:ILE:HG23 | 1.87 | 0.56 |
| 1:D:383:GLY:O | 1:D:390:VAL:HG22 | 2.06 | 0.56 |
| 1:F:264:LEU:CD1 | 1:F:268:LYS:HE2 | 2.34 | 0.56 |
| 2:Y:37:SER:HB2 | 1:K:257:GLU:OE2 | 2.05 | 0.56 |
| 1:M:193:MET:HE2 | 1:M:292:MET:HG2 | 1.87 | 0.56 |
| 1:L:231:GLN:O | 1:L:234:VAL:HG12 | 2.06 | 0.56 |
| 1:K:194:LYS:HD2 | 1:K:332:MET:CE | 2.35 | 0.56 |
| 1:D:228:SER:HA | 1:D:255:ASP:CB | 2.35 | 0.56 |
| 1:C:264:LEU:CG | 1:C:268:LYS:HE2 | 2.36 | 0.56 |
| 1:C:489:MET:O | 1:C:493:GLY:N | 2.29 | 0.56 |
| 1:G:264:LEU:CD1 | 1:G:268:LYS:HE2 | 2.31 | 0.56 |
| 1:F:224:GLU:OE1 | 1:F:303:GLU:HA | 2.06 | 0.56 |
| 1:E:89:THR:O | 1:E:93:THR:HG23 | 2.05 | 0.56 |
| 2:R:15:ARG:NH2 | 2:Q:97:LEU:HA | 2.21 | 0.56 |
| 1:M:13:ARG:HD3 | 1:M:104:PHE:HD1 | 1.70 | 0.56 |
| 1:I:158:ILE:HD12 | 1:I:397:VAL:HG22 | 1.86 | 0.56 |
| 1:D:32:GLY:N | 3:D:601:ADP:O1A | 2.39 | 0.56 |
| 1:C:282:GLY:O | 1:C:285:ARG:HB2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:135:SER:CB | 1:G:498:THR:HG21 | 2.36 | 0.56 |
| 1:G:194:LYS:HD2 | 1:G:332:MET:CE | 2.35 | 0.56 |
| 1:E:237:LEU:HD21 | 1:E:262:LEU:CD2 | 2.34 | 0.56 |
| 1:E:264:LEU:CG | 1:E:268:LYS:HE2 | 2.34 | 0.56 |
| 1:H:89:THR:O | 1:H:93:THR:HG23 | 2.06 | 0.56 |
| 2:2:32:MET:HE3 | 1:N:268:LYS:HD3 | 1.88 | 0.56 |
| 2:Q:32:MET:CE | 1:C:268:LYS:HE3 | 2.36 | 0.56 |
| 2:P:5:ALA:HB2 | 2:P:10:LEU:HD13 | 1.88 | 0.56 |
| 1:A:456:ALA:HB3 | 1:A:463:GLY:HA2 | 1.88 | 0.56 |
| 1:F:237:LEU:HD21 | 1:F:262:LEU:CD2 | 2.36 | 0.56 |
| 1:E:69:ILE:HD11 | 1:E:523:THR:HG22 | 1.87 | 0.56 |
| 1:H:6:VAL:HG21 | 1:I:22:LEU:HD11 | 1.86 | 0.56 |
| 2:Z:52:GLY:HA3 | 2:Z:60:ILE:HD12 | 1.87 | 0.56 |
| 2:W:46:VAL:HG13 | 2:W:67:VAL:HA | 1.88 | 0.56 |
| 1:N:291:ASP:OD1 | 1:N:346:ARG:NE | 2.35 | 0.56 |
| 1:M:219:TYR:CE2 | 1:M:245:LYS:HD2 | 2.41 | 0.56 |
| 1:K:81:THR:HG21 | 1:K:88:GLY:O | 2.06 | 0.56 |
| 1:K:177:VAL:HG11 | 1:K:398:THR:HG22 | 1.88 | 0.56 |
| 1:J:177:VAL:HG11 | 1:J:398:THR:HG22 | 1.88 | 0.56 |
| 1:J:525:ILE:HG23 | 1:J:526:PRO:HD2 | 1.88 | 0.56 |
| 1:I:197:ARG:H | 1:I:330:ASP:HA | 1.70 | 0.56 |
| 1:I:282:GLY:O | 1:I:285:ARG:HG2 | 2.06 | 0.56 |
| 1:D:233:ILE:HG13 | 1:D:237:LEU:HD13 | 1.87 | 0.56 |
| 2:Z:31:ILE:HG21 | 1:L:234:VAL:HG23 | 1.88 | 0.55 |
| 1:M:525:ILE:HG23 | 1:M:526:PRO:HD2 | 1.88 | 0.55 |
| 1:L:260:SER:HA | 1:L:263:VAL:HG22 | 1.88 | 0.55 |
| 1:C:13:ARG:HD3 | 1:C:104:PHE:HD1 | 1.70 | 0.55 |
| 1:B:233:ILE:HG13 | 1:B:237:LEU:HD13 | 1.88 | 0.55 |
| 1:H:127:VAL:HG23 | 1:H:423:CYS:HB3 | 1.88 | 0.55 |
| 2:X:31:ILE:HD12 | 1:J:237:LEU:HB3 | 1.87 | 0.55 |
| 1:L:224:GLU:OE1 | 1:L:303:GLU:HA | 2.06 | 0.55 |
| 1:J:22:LEU:HD11 | 1:I:6:VAL:HG21 | 1.86 | 0.55 |
| 1:F:148:ALA:HB2 | 1:F:404:THR:HG21 | 1.87 | 0.55 |
| 1:E:81:THR:HG21 | 1:E:88:GLY:O | 2.06 | 0.55 |
| 2:X:3:GLY:HA3 | 2:X:51:SER:HA | 1.89 | 0.55 |
| 2:X:8:LYS:HG2 | 2:W:102:ASP:HB3 | 1.88 | 0.55 |
| 2:R:46:VAL:HG13 | 2:R:67:VAL:HA | 1.89 | 0.55 |
| 2:T:46:VAL:HG13 | 2:T:67:VAL:HA | 1.88 | 0.55 |
| 2:1:46:VAL:HG13 | 2:1:67:VAL:HA | 1.89 | 0.55 |
| 2:1:81:VAL:HG12 | 2:Z:72:LEU:HD21 | 1.88 | 0.55 |
| 2:Z:15:ARG:NH2 | 2:Y:97:LEU:HA | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:52:GLY:HA3 | 2:R:60:ILE:HD12 | 1.86 | 0.55 |
| 1:B:22:LEU:HD11 | 1:A:6:VAL:HG21 | 1.88 | 0.55 |
| 2:2:46:VAL:HG13 | 2:2:67:VAL:HA | 1.89 | 0.55 |
| 2:Q:3:GLY:HA3 | 2:Q:51:SER:HA | 1.88 | 0.55 |
| 2:O:26:VAL:HG12 | 2:O:32:MET:CG | 2.35 | 0.55 |
| 1:N:260:SER:HA | 1:N:263:VAL:HG22 | 1.89 | 0.55 |
| 1:J:148:ALA:HB2 | 1:J:404:THR:HG21 | 1.86 | 0.55 |
| 1:A:183:LEU:CD1 | 1:A:385:THR:HG22 | 2.37 | 0.55 |
| 1:H:135:SER:HB2 | 1:H:498:THR:HG21 | 1.88 | 0.55 |
| 2:R:31:ILE:HD12 | 1:D:237:LEU:HB3 | 1.89 | 0.55 |
| 1:M:197:ARG:H | 1:M:330:ASP:HA | 1.72 | 0.55 |
| 1:L:135:SER:CB | 1:L:498:THR:HG21 | 2.37 | 0.55 |
| 1:K:260:SER:HA | 1:K:263:VAL:HG22 | 1.89 | 0.55 |
| 1:K:383:GLY:O | 1:K:390:VAL:HG22 | 2.07 | 0.55 |
| 1:K:525:ILE:HG23 | 1:K:526:PRO:HD2 | 1.88 | 0.55 |
| 1:B:135:SER:CB | 1:B:498:THR:HG21 | 2.36 | 0.55 |
| 1:B:230:ILE:HA | 1:B:233:ILE:HG22 | 1.89 | 0.55 |
| 1:A:194:LYS:HD2 | 1:A:332:MET:CE | 2.36 | 0.55 |
| 2:X:46:VAL:HG13 | 2:X:67:VAL:HA | 1.89 | 0.55 |
| 2:W:31:ILE:HG21 | 1:I:234:VAL:HG23 | 1.87 | 0.55 |
| 2:T:15:ARG:HB3 | 2:T:90:LEU:CD1 | 2.33 | 0.55 |
| 1:N:293:ALA:O | 1:N:297:GLY:N | 2.26 | 0.55 |
| 1:M:169:VAL:HG12 | 1:M:173:GLY:HA3 | 1.87 | 0.55 |
| 1:L:89:THR:O | 1:L:93:THR:HG23 | 2.07 | 0.55 |
| 1:K:177:VAL:HG11 | 1:K:398:THR:CG2 | 2.37 | 0.55 |
| 1:K:207:THR:HG23 | 1:K:209:LYS:N | 2.20 | 0.55 |
| 1:I:231:GLN:O | 1:I:234:VAL:HG12 | 2.06 | 0.55 |
| 1:D:280:GLY:O | 1:D:285:ARG:HB3 | 2.07 | 0.55 |
| 1:C:219:TYR:CE2 | 1:C:245:LYS:HD2 | 2.41 | 0.55 |
| 1:F:89:THR:O | 1:F:93:THR:HG23 | 2.07 | 0.55 |
| 2:P:34:PRO:HD3 | 1:B:261:THR:HG22 | 1.88 | 0.55 |
| 1:M:206:ASN:HB3 | 1:M:266:ARG:HH21 | 1.72 | 0.55 |
| 1:K:231:GLN:O | 1:K:234:VAL:HG12 | 2.06 | 0.55 |
| 1:K:413:VAL:HB | 1:K:498:THR:HG22 | 1.88 | 0.55 |
| 1:D:13:ARG:HD3 | 1:D:104:PHE:HD1 | 1.71 | 0.55 |
| 1:C:226:LYS:HG2 | 1:C:253:ASP:HB3 | 1.89 | 0.55 |
| 1:A:62:LEU:HD13 | 1:A:67:LYS:HB3 | 1.88 | 0.55 |
| 1:A:177:VAL:HG11 | 1:A:398:THR:CG2 | 2.37 | 0.55 |
| 1:A:197:ARG:H | 1:A:330:ASP:HA | 1.72 | 0.55 |
| 1:F:135:SER:HB2 | 1:F:498:THR:HG21 | 1.87 | 0.55 |
| 1:F:420:LEU:HD11 | 1:F:501:VAL:HG13 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:183:LEU:CD1 | 1:H:385:THR:HG22 | 2.36 | 0.55 |
| 2:V:101:VAL:O | 2:W:8:LYS:HA | 2.06 | 0.55 |
| 2:Q:15:ARG:HH22 | 2:P:97:LEU:HA | 1.72 | 0.55 |
| 2:O:33:LEU:HG | 1:A:230:ILE:HD11 | 1.89 | 0.55 |
| 1:L:278:ALA:HB1 | 1:L:289:LEU:HD11 | 1.88 | 0.55 |
| 1:B:224:GLU:OE1 | 1:B:303:GLU:HA | 2.07 | 0.55 |
| 2:Z:33:LEU:HG | 1:L:230:ILE:HD11 | 1.88 | 0.55 |
| 2:O:46:VAL:HG13 | 2:O:67:VAL:HA | 1.89 | 0.55 |
| 2:S:46:VAL:HG13 | 2:S:67:VAL:HA | 1.89 | 0.55 |
| 1:N:99:ILE:HD13 | 1:N:509:ALA:HA | 1.89 | 0.55 |
| 1:J:197:ARG:H | 1:J:330:ASP:HA | 1.71 | 0.55 |
| 1:C:207:THR:HG23 | 1:C:209:LYS:N | 2.19 | 0.55 |
| 1:B:413:VAL:HB | 1:B:498:THR:HG22 | 1.88 | 0.55 |
| 1:G:220:VAL:HG22 | 1:G:248:VAL:CG2 | 2.37 | 0.55 |
| 1:F:383:GLY:O | 1:F:390:VAL:HG22 | 2.06 | 0.55 |
| 2:X:37:SER:HB2 | 1:J:257:GLU:OE2 | 2.06 | 0.54 |
| 2:Q:8:LYS:HG2 | 2:P:102:ASP:HB3 | 1.89 | 0.54 |
| 2:P:46:VAL:HG13 | 2:P:67:VAL:HA | 1.89 | 0.54 |
| 1:N:197:ARG:H | 1:N:330:ASP:HA | 1.72 | 0.54 |
| 1:I:127:VAL:HG23 | 1:I:423:CYS:HB3 | 1.88 | 0.54 |
| 1:D:220:VAL:HG22 | 1:D:248:VAL:CG2 | 2.36 | 0.54 |
| 1:D:228:SER:HA | 1:D:255:ASP:HB2 | 1.88 | 0.54 |
| 1:C:399:ASP:OD1 | 5:C:702:HOH:O | 2.18 | 0.54 |
| 2:V:46:VAL:HG13 | 2:V:67:VAL:HA | 1.89 | 0.54 |
| 1:I:183:LEU:CD1 | 1:I:385:THR:HG22 | 2.38 | 0.54 |
| 1:I:413:VAL:HB | 1:I:498:THR:HG22 | 1.88 | 0.54 |
| 1:C:260:SER:HA | 1:C:263:VAL:HG22 | 1.89 | 0.54 |
| 1:C:420:LEU:HD11 | 1:C:501:VAL:HG13 | 1.88 | 0.54 |
| 1:B:89:THR:O | 1:B:93:THR:HG23 | 2.07 | 0.54 |
| 1:F:195:PHE:CZ | 1:F:331:ALA:HB3 | 2.42 | 0.54 |
| 1:M:420:LEU:HD11 | 1:M:501:VAL:HG13 | 1.88 | 0.54 |
| 1:J:183:LEU:CD1 | 1:J:385:THR:HG22 | 2.37 | 0.54 |
| 1:N:13:ARG:NH2 | 1:N:519:GLU:OE1 | 2.41 | 0.54 |
| 1:J:135:SER:CB | 1:J:498:THR:HG21 | 2.37 | 0.54 |
| 1:D:197:ARG:H | 1:D:330:ASP:HA | 1.71 | 0.54 |
| 1:D:350:ILE:O | 1:D:366:LEU:HD11 | 2.07 | 0.54 |
| 1:C:22:LEU:HD11 | 1:B:6:VAL:HG21 | 1.89 | 0.54 |
| 1:A:197:ARG:HD2 | 1:A:277:LYS:O | 2.06 | 0.54 |
| 1:E:99:ILE:HD13 | 1:E:509:ALA:HA | 1.87 | 0.54 |
| 1:H:62:LEU:HD13 | 1:H:67:LYS:HB3 | 1.88 | 0.54 |
| 1:H:69:ILE:HD11 | 1:H:523:THR:HG22 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:293:ALA:O | 1:H:297:GLY:N | 2.27 | 0.54 |
| 2:U:65:VAL:HG22 | 2:U:93:ASP:OD1 | 2.07 | 0.54 |
| 1:M:135:SER:HB2 | 1:M:498:THR:HG21 | 1.87 | 0.54 |
| 1:M:222:LEU:CD2 | 1:M:250:ILE:HB | 2.38 | 0.54 |
| 1:L:385:THR:HG21 | 1:K:506:LEU:HD21 | 1.89 | 0.54 |
| 1:J:293:ALA:O | 1:J:297:GLY:N | 2.29 | 0.54 |
| 1:I:224:GLU:O | 1:I:252:GLU:HB2 | 2.08 | 0.54 |
| 1:I:292:MET:O | 1:I:296:THR:HG22 | 2.08 | 0.54 |
| 1:A:413:VAL:HB | 1:A:498:THR:HG22 | 1.89 | 0.54 |
| 1:E:62:LEU:HD13 | 1:E:67:LYS:HB3 | 1.89 | 0.54 |
| 1:H:292:MET:O | 1:H:296:THR:HG22 | 2.08 | 0.54 |
| 2:Y:3:GLY:HA3 | 2:Y:51:SER:HA | 1.90 | 0.54 |
| 2:R:65:VAL:HG22 | 2:R:93:ASP:OD1 | 2.08 | 0.54 |
| 2:S:31:ILE:HD12 | 1:E:237:LEU:HB3 | 1.89 | 0.54 |
| 1:L:62:LEU:HD13 | 1:L:67:LYS:HB3 | 1.90 | 0.54 |
| 1:J:220:VAL:HG22 | 1:J:248:VAL:CG2 | 2.37 | 0.54 |
| 1:B:260:SER:HA | 1:B:263:VAL:HG22 | 1.90 | 0.54 |
| 1:G:224:GLU:OE1 | 1:G:303:GLU:HA | 2.07 | 0.54 |
| 1:F:22:LEU:HD11 | 1:E:6:VAL:HG21 | 1.89 | 0.54 |
| 1:E:124:VAL:HG21 | 1:E:509:ALA:CB | 2.36 | 0.54 |
| 2:2:15:ARG:NH2 | 2:1:97:LEU:HA | 2.22 | 0.54 |
| 1:N:220:VAL:HG22 | 1:N:248:VAL:CG2 | 2.37 | 0.54 |
| 1:N:512:ALA:O | 1:N:516:THR:HG23 | 2.07 | 0.54 |
| 1:M:73:LEU:HD12 | 1:M:515:LEU:HD13 | 1.90 | 0.54 |
| 1:L:224:GLU:O | 1:L:252:GLU:HB2 | 2.07 | 0.54 |
| 1:J:224:GLU:O | 1:J:252:GLU:HB2 | 2.07 | 0.54 |
| 1:D:224:GLU:OE1 | 1:D:303:GLU:HA | 2.08 | 0.54 |
| 1:D:512:ALA:O | 1:D:516:THR:HG23 | 2.07 | 0.54 |
| 1:B:69:ILE:HD11 | 1:B:523:THR:HG22 | 1.90 | 0.54 |
| 1:A:231:GLN:O | 1:A:234:VAL:HG12 | 2.08 | 0.54 |
| 1:F:13:ARG:HD3 | 1:F:104:PHE:HD1 | 1.73 | 0.54 |
| 1:H:219:TYR:CE2 | 1:H:245:LYS:HD2 | 2.43 | 0.54 |
| 2:Z:32:MET:CE | 1:L:268:LYS:HE3 | 2.37 | 0.54 |
| 2:U:8:LYS:O | 2:T:100:TYR:HA | 2.08 | 0.54 |
| 1:I:89:THR:O | 1:I:93:THR:HG23 | 2.07 | 0.54 |
| 1:D:231:GLN:O | 1:D:234:VAL:HG12 | 2.08 | 0.54 |
| 1:G:89:THR:O | 1:G:93:THR:HG23 | 2.08 | 0.54 |
| 1:F:292:MET:O | 1:F:296:THR:HG22 | 2.08 | 0.54 |
| 1:F:512:ALA:O | 1:F:516:THR:HG23 | 2.08 | 0.54 |
| 1:E:420:LEU:HD11 | 1:E:501:VAL:HG13 | 1.90 | 0.54 |
| 1:M:224:GLU:O | 1:M:252:GLU:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:183:LEU:CD1 | 1:L:385:THR:HG22 | 2.38 | 0.54 |
| 1:K:135:SER:HB2 | 1:K:498:THR:HG21 | 1.88 | 0.54 |
| 1:K:292:MET:O | 1:K:296:THR:HG22 | 2.08 | 0.54 |
| 1:J:393:LYS:O | 1:J:397:VAL:HG23 | 2.08 | 0.54 |
| 1:I:77:VAL:HG22 | 1:I:511:VAL:HB | 1.90 | 0.54 |
| 1:F:220:VAL:HG22 | 1:F:248:VAL:CG2 | 2.38 | 0.54 |
| 1:H:393:LYS:O | 1:H:397:VAL:HG23 | 2.08 | 0.54 |
| 1:L:393:LYS:O | 1:L:397:VAL:HG23 | 2.08 | 0.54 |
| 1:K:228:SER:HA | 1:K:255:ASP:HB2 | 1.90 | 0.54 |
| 1:K:456:ALA:HB3 | 1:K:463:GLY:HA2 | 1.89 | 0.54 |
| 1:J:207:THR:HG23 | 1:J:209:LYS:N | 2.20 | 0.54 |
| 1:D:99:ILE:HD13 | 1:D:509:ALA:HA | 1.89 | 0.54 |
| 1:C:13:ARG:NH2 | 1:C:519:GLU:OE1 | 2.39 | 0.54 |
| 1:A:224:GLU:OE1 | 1:A:303:GLU:HA | 2.08 | 0.54 |
| 1:F:260:SER:HA | 1:F:263:VAL:HG22 | 1.90 | 0.54 |
| 2:R:81:VAL:HG12 | 2:Q:72:LEU:HD21 | 1.89 | 0.53 |
| 1:J:177:VAL:HG11 | 1:J:398:THR:CG2 | 2.39 | 0.53 |
| 1:I:393:LYS:O | 1:I:397:VAL:HG23 | 2.08 | 0.53 |
| 1:A:177:VAL:HG11 | 1:A:398:THR:HG22 | 1.89 | 0.53 |
| 1:E:177:VAL:HG11 | 1:E:398:THR:HG22 | 1.90 | 0.53 |
| 2:Z:46:VAL:HG13 | 2:Z:67:VAL:HA | 1.90 | 0.53 |
| 1:N:89:THR:O | 1:N:93:THR:HG23 | 2.08 | 0.53 |
| 1:M:220:VAL:HG22 | 1:M:248:VAL:CG2 | 2.38 | 0.53 |
| 1:K:224:GLU:O | 1:K:252:GLU:HB2 | 2.08 | 0.53 |
| 1:I:228:SER:HA | 1:I:255:ASP:HB2 | 1.88 | 0.53 |
| 1:D:260:SER:HA | 1:D:263:VAL:HG22 | 1.90 | 0.53 |
| 1:E:219:TYR:CE2 | 1:E:245:LYS:HD2 | 2.44 | 0.53 |
| 1:E:224:GLU:OE1 | 1:E:303:GLU:HA | 2.08 | 0.53 |
| 1:E:393:LYS:O | 1:E:397:VAL:HG23 | 2.08 | 0.53 |
| 2:V:65:VAL:HG22 | 2:V:93:ASP:OD1 | 2.08 | 0.53 |
| 2:2:81:VAL:HG12 | 2:1:72:LEU:HD21 | 1.89 | 0.53 |
| 2:U:13:PHE:CD1 | 2:U:54:LYS:HB2 | 2.44 | 0.53 |
| 1:J:89:THR:O | 1:J:93:THR:HG23 | 2.08 | 0.53 |
| 1:J:203:TYR:HB3 | 1:J:267:LEU:HD11 | 1.91 | 0.53 |
| 1:D:420:LEU:HD11 | 1:D:501:VAL:HG13 | 1.90 | 0.53 |
| 1:B:292:MET:O | 1:B:296:THR:HG22 | 2.09 | 0.53 |
| 1:G:177:VAL:HG11 | 1:G:398:THR:CG2 | 2.38 | 0.53 |
| 1:F:219:TYR:CE2 | 1:F:245:LYS:HD2 | 2.43 | 0.53 |
| 1:E:13:ARG:HD3 | 1:E:104:PHE:HD1 | 1.73 | 0.53 |
| 2:Q:52:GLY:HA3 | 2:Q:60:ILE:HD12 | 1.91 | 0.53 |
| 2:T:65:VAL:HG22 | 2:T:93:ASP:OD1 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:383:GLY:O | 1:N:390:VAL:HG22 | 2.07 | 0.53 |
| 1:J:260:SER:HA | 1:J:263:VAL:HG22 | 1.90 | 0.53 |
| 1:I:512:ALA:O | 1:I:516:THR:HG23 | 2.08 | 0.53 |
| 1:D:124:VAL:HG21 | 1:D:509:ALA:CB | 2.38 | 0.53 |
| 1:C:224:GLU:OE1 | 1:C:303:GLU:HA | 2.08 | 0.53 |
| 1:F:193:MET:HE1 | 1:F:292:MET:HA | 1.90 | 0.53 |
| 2:Z:3:GLY:HA3 | 2:Z:51:SER:HA | 1.91 | 0.53 |
| 1:N:124:VAL:HG21 | 1:N:509:ALA:CB | 2.39 | 0.53 |
| 1:J:206:ASN:HB3 | 1:J:266:ARG:HH21 | 1.74 | 0.53 |
| 1:I:220:VAL:HG22 | 1:I:248:VAL:CG2 | 2.38 | 0.53 |
| 1:C:393:LYS:O | 1:C:397:VAL:HG23 | 2.09 | 0.53 |
| 1:B:220:VAL:HG22 | 1:B:248:VAL:CG2 | 2.38 | 0.53 |
| 1:A:13:ARG:HD3 | 1:A:104:PHE:HD1 | 1.72 | 0.53 |
| 1:F:224:GLU:O | 1:F:252:GLU:HB2 | 2.08 | 0.53 |
| 1:E:233:ILE:HG13 | 1:E:237:LEU:HD13 | 1.90 | 0.53 |
| 2:1:27:THR:HG22 | 2:1:31:ILE:H | 1.73 | 0.53 |
| 2:X:32:MET:HE3 | 1:J:268:LYS:HE3 | 1.90 | 0.53 |
| 2:Q:81:VAL:HG12 | 2:P:72:LEU:HD21 | 1.89 | 0.53 |
| 2:U:5:ALA:HB2 | 2:U:10:LEU:HD13 | 1.90 | 0.53 |
| 1:N:350:ILE:O | 1:N:366:LEU:HD11 | 2.08 | 0.53 |
| 1:K:183:LEU:CD1 | 1:K:385:THR:HG22 | 2.39 | 0.53 |
| 1:K:219:TYR:CE2 | 1:K:245:LYS:HD2 | 2.44 | 0.53 |
| 1:K:220:VAL:HG22 | 1:K:248:VAL:CG2 | 2.38 | 0.53 |
| 1:G:31:MET:SD | 1:G:454:THR:OG1 | 2.62 | 0.53 |
| 1:G:237:LEU:HD21 | 1:G:262:LEU:CD2 | 2.39 | 0.53 |
| 1:F:393:LYS:O | 1:F:397:VAL:HG23 | 2.09 | 0.53 |
| 1:E:195:PHE:CZ | 1:E:331:ALA:HB3 | 2.44 | 0.53 |
| 1:E:220:VAL:HG22 | 1:E:248:VAL:CG2 | 2.39 | 0.53 |
| 1:E:230:ILE:HA | 1:E:233:ILE:HG22 | 1.89 | 0.53 |
| 1:E:410:GLU:HG2 | 1:E:498:THR:OG1 | 2.08 | 0.53 |
| 2:U:80:LYS:HG3 | 2:U:89:PHE:HE1 | 1.74 | 0.53 |
| 1:M:228:SER:HA | 1:M:255:ASP:HB2 | 1.91 | 0.53 |
| 1:L:207:THR:HG23 | 1:L:209:LYS:N | 2.19 | 0.53 |
| 1:K:13:ARG:HD3 | 1:K:104:PHE:HD1 | 1.74 | 0.53 |
| 1:D:219:TYR:CE2 | 1:D:245:LYS:HD2 | 2.44 | 0.53 |
| 1:C:292:MET:O | 1:C:296:THR:HG22 | 2.09 | 0.53 |
| 1:B:177:VAL:HG11 | 1:B:398:THR:HG22 | 1.90 | 0.53 |
| 1:B:219:TYR:CE2 | 1:B:245:LYS:HD2 | 2.43 | 0.53 |
| 1:G:292:MET:O | 1:G:296:THR:HG22 | 2.08 | 0.53 |
| 1:G:301:PHE:CZ | 1:G:313:VAL:HG12 | 2.44 | 0.53 |
| 1:G:393:LYS:O | 1:G:397:VAL:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:224:GLU:O | 1:E:252:GLU:HB2 | 2.08 | 0.53 |
| 1:E:497:PRO:HB2 | 1:E:500:VAL:HG12 | 1.90 | 0.53 |
| 1:N:177:VAL:HG11 | 1:N:398:THR:CG2 | 2.39 | 0.53 |
| 1:N:219:TYR:CE2 | 1:N:245:LYS:HD2 | 2.43 | 0.53 |
| 1:M:22:LEU:HD11 | 1:L:6:VAL:HG21 | 1.90 | 0.53 |
| 1:M:31:MET:SD | 1:M:454:THR:OG1 | 2.61 | 0.53 |
| 1:G:322:GLY:N | 1:G:335:LYS:O | 2.32 | 0.53 |
| 1:H:148:ALA:HB2 | 1:H:404:THR:HG21 | 1.91 | 0.53 |
| 2:O:26:VAL:HG12 | 2:O:32:MET:HG3 | 1.90 | 0.53 |
| 2:T:80:LYS:HG3 | 2:T:89:PHE:HE1 | 1.74 | 0.53 |
| 1:L:220:VAL:HG22 | 1:L:248:VAL:CG2 | 2.39 | 0.53 |
| 1:L:512:ALA:O | 1:L:516:THR:HG23 | 2.09 | 0.53 |
| 1:J:469:LYS:HG2 | 1:J:486:PHE:HE2 | 1.74 | 0.53 |
| 1:I:383:GLY:O | 1:I:390:VAL:HG22 | 2.08 | 0.53 |
| 1:B:385:THR:HG21 | 1:A:506:LEU:HD21 | 1.90 | 0.53 |
| 1:F:188:GLU:OE1 | 1:F:381:LYS:NZ | 2.41 | 0.53 |
| 1:F:197:ARG:H | 1:F:330:ASP:HA | 1.74 | 0.53 |
| 1:E:148:ALA:HB2 | 1:E:404:THR:HG21 | 1.90 | 0.53 |
| 2:V:52:GLY:HA3 | 2:V:60:ILE:HD12 | 1.91 | 0.53 |
| 2:Z:31:ILE:HD12 | 1:L:237:LEU:HB3 | 1.90 | 0.53 |
| 2:W:31:ILE:HD12 | 1:I:237:LEU:HB3 | 1.90 | 0.53 |
| 1:N:69:ILE:HD11 | 1:N:523:THR:HG22 | 1.90 | 0.53 |
| 1:L:228:SER:HA | 1:L:255:ASP:HB2 | 1.91 | 0.53 |
| 1:L:489:MET:O | 1:L:493:GLY:N | 2.32 | 0.53 |
| 1:I:135:SER:CB | 1:I:498:THR:HG21 | 2.38 | 0.53 |
| 1:B:469:LYS:HG2 | 1:B:486:PHE:HE2 | 1.74 | 0.53 |
| 1:F:248:VAL:HG11 | 1:F:324:VAL:HG11 | 1.91 | 0.53 |
| 1:E:260:SER:HA | 1:E:263:VAL:HG22 | 1.91 | 0.53 |
| 1:E:291:ASP:OD1 | 1:E:346:ARG:NE | 2.38 | 0.53 |
| 1:H:420:LEU:HD11 | 1:H:501:VAL:HG13 | 1.90 | 0.52 |
| 2:X:33:LEU:HG | 1:J:230:ILE:HD11 | 1.91 | 0.52 |
| 2:Q:16:VAL:HG13 | 2:Q:46:VAL:HG23 | 1.91 | 0.52 |
| 1:N:237:LEU:HD21 | 1:N:262:LEU:CD2 | 2.39 | 0.52 |
| 1:M:512:ALA:O | 1:M:516:THR:HG23 | 2.10 | 0.52 |
| 1:J:292:MET:O | 1:J:296:THR:HG22 | 2.09 | 0.52 |
| 1:D:177:VAL:HG11 | 1:D:398:THR:CG2 | 2.39 | 0.52 |
| 1:D:373:LEU:O | 1:D:373:LEU:HD23 | 2.09 | 0.52 |
| 1:C:177:VAL:HG11 | 1:C:398:THR:HG22 | 1.90 | 0.52 |
| 1:B:283:ASP:HA | 1:B:286:LYS:HD3 | 1.91 | 0.52 |
| 1:B:456:ALA:HB3 | 1:B:463:GLY:HA2 | 1.90 | 0.52 |
| 1:A:13:ARG:NH2 | 1:A:519:GLU:OE1 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:THR:O | 1:A:93:THR:HG23 | 2.09 | 0.52 |
| 1:G:183:LEU:CD1 | 1:G:385:THR:HG22 | 2.39 | 0.52 |
| 1:G:228:SER:HA | 1:G:255:ASP:HB2 | 1.91 | 0.52 |
| 1:H:52:ASP:OD2 | 5:H:702:HOH:O | 2.19 | 0.52 |
| 1:L:177:VAL:HG11 | 1:L:398:THR:HG22 | 1.92 | 0.52 |
| 1:J:228:SER:HA | 1:J:255:ASP:HB2 | 1.90 | 0.52 |
| 1:B:278:ALA:HB3 | 1:B:285:ARG:NE | 2.24 | 0.52 |
| 1:G:169:VAL:HG21 | 1:G:378:ALA:HB2 | 1.90 | 0.52 |
| 1:G:219:TYR:CE2 | 1:G:245:LYS:HD2 | 2.44 | 0.52 |
| 1:F:525:ILE:HG23 | 1:F:527:LYS:CG | 2.37 | 0.52 |
| 1:E:228:SER:HA | 1:E:255:ASP:HB2 | 1.91 | 0.52 |
| 1:H:410:GLU:HG2 | 1:H:498:THR:OG1 | 2.10 | 0.52 |
| 2:V:73:LEU:HD22 | 2:V:91:PHE:CE2 | 2.45 | 0.52 |
| 2:Q:80:LYS:HG3 | 2:Q:89:PHE:HE1 | 1.74 | 0.52 |
| 2:O:13:PHE:CD1 | 2:O:54:LYS:HB2 | 2.43 | 0.52 |
| 1:N:280:GLY:O | 1:N:285:ARG:HB3 | 2.10 | 0.52 |
| 1:N:489:MET:O | 1:N:493:GLY:N | 2.36 | 0.52 |
| 1:L:264:LEU:CG | 1:L:268:LYS:HE2 | 2.39 | 0.52 |
| 1:J:219:TYR:CE2 | 1:J:245:LYS:HD2 | 2.44 | 0.52 |
| 1:C:69:ILE:HD11 | 1:C:523:THR:HG22 | 1.91 | 0.52 |
| 1:C:194:LYS:HD2 | 1:C:332:MET:HE2 | 1.91 | 0.52 |
| 1:C:220:VAL:HG22 | 1:C:248:VAL:CG2 | 2.39 | 0.52 |
| 1:B:393:LYS:O | 1:B:397:VAL:HG23 | 2.08 | 0.52 |
| 1:F:77:VAL:HG22 | 1:F:511:VAL:HB | 1.92 | 0.52 |
| 1:F:301:PHE:CD1 | 1:F:308:LEU:HB3 | 2.45 | 0.52 |
| 1:E:194:LYS:HD2 | 1:E:332:MET:HE2 | 1.89 | 0.52 |
| 2:V:81:VAL:HG12 | 2:2:72:LEU:HD21 | 1.92 | 0.52 |
| 2:Z:80:LYS:HG3 | 2:Z:89:PHE:HE1 | 1.75 | 0.52 |
| 2:T:56:LYS:HE3 | 2:T:61:GLN:OE1 | 2.10 | 0.52 |
| 1:M:393:LYS:O | 1:M:397:VAL:HG23 | 2.09 | 0.52 |
| 1:J:233:ILE:HG13 | 1:J:237:LEU:CD1 | 2.39 | 0.52 |
| 1:D:427:LEU:HA | 1:D:430:LEU:HD23 | 1.92 | 0.52 |
| 1:B:188:GLU:OE1 | 1:B:381:LYS:NZ | 2.40 | 0.52 |
| 1:B:251:ALA:O | 1:B:277:LYS:HA | 2.10 | 0.52 |
| 1:F:301:PHE:CZ | 1:F:313:VAL:HG12 | 2.44 | 0.52 |
| 1:E:183:LEU:CD1 | 1:E:385:THR:HG22 | 2.40 | 0.52 |
| 2:1:34:PRO:CD | 1:M:261:THR:HG22 | 2.38 | 0.52 |
| 2:X:65:VAL:HG22 | 2:X:93:ASP:OD1 | 2.10 | 0.52 |
| 2:U:73:LEU:HD22 | 2:U:91:PHE:CE2 | 2.45 | 0.52 |
| 1:M:260:SER:HA | 1:M:263:VAL:HG22 | 1.92 | 0.52 |
| 1:I:177:VAL:HG11 | 1:I:398:THR:CG2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:13:ARG:HD3 | 1:B:104:PHE:HD1 | 1.74 | 0.52 |
| 1:A:135:SER:HB2 | 1:A:498:THR:HG21 | 1.91 | 0.52 |
| 1:F:65:LYS:O | 1:F:69:ILE:HG13 | 2.10 | 0.52 |
| 1:E:264:LEU:CD1 | 1:E:268:LYS:HE2 | 2.40 | 0.52 |
| 2:R:80:LYS:HG3 | 2:R:89:PHE:HE1 | 1.74 | 0.52 |
| 1:N:427:LEU:HA | 1:N:430:LEU:HD23 | 1.92 | 0.52 |
| 1:L:195:PHE:CZ | 1:L:331:ALA:HB3 | 2.45 | 0.52 |
| 1:L:469:LYS:HG2 | 1:L:486:PHE:HE2 | 1.74 | 0.52 |
| 1:I:219:TYR:CE2 | 1:I:245:LYS:HD2 | 2.44 | 0.52 |
| 1:D:77:VAL:HG22 | 1:D:511:VAL:HB | 1.91 | 0.52 |
| 1:D:224:GLU:O | 1:D:252:GLU:HB2 | 2.10 | 0.52 |
| 1:C:199:TYR:HD1 | 1:C:326:VAL:HG12 | 1.74 | 0.52 |
| 1:C:228:SER:HA | 1:C:255:ASP:HB2 | 1.90 | 0.52 |
| 1:B:224:GLU:O | 1:B:252:GLU:HB2 | 2.10 | 0.52 |
| 1:B:489:MET:O | 1:B:493:GLY:N | 2.35 | 0.52 |
| 1:F:177:VAL:HG11 | 1:F:398:THR:CG2 | 2.39 | 0.52 |
| 1:H:237:LEU:HD21 | 1:H:262:LEU:CD2 | 2.37 | 0.52 |
| 2:Z:73:LEU:HD22 | 2:Z:91:PHE:CE2 | 2.44 | 0.52 |
| 2:S:73:LEU:HD22 | 2:S:91:PHE:CE2 | 2.45 | 0.52 |
| 1:M:177:VAL:HG11 | 1:M:398:THR:HG22 | 1.92 | 0.52 |
| 1:M:399:ASP:OD1 | 5:M:702:HOH:O | 2.18 | 0.52 |
| 1:K:127:VAL:HG23 | 1:K:423:CYS:CB | 2.39 | 0.52 |
| 1:B:512:ALA:O | 1:B:516:THR:HG23 | 2.09 | 0.52 |
| 1:A:264:LEU:HG | 1:A:268:LYS:CE | 2.33 | 0.52 |
| 2:Y:32:MET:HE3 | 1:K:268:LYS:HE3 | 1.91 | 0.52 |
| 1:M:237:LEU:HD21 | 1:M:262:LEU:CD2 | 2.40 | 0.52 |
| 1:I:237:LEU:HD21 | 1:I:262:LEU:CD2 | 2.39 | 0.52 |
| 1:C:73:LEU:HD12 | 1:C:515:LEU:HD13 | 1.90 | 0.52 |
| 1:C:206:ASN:HB3 | 1:C:266:ARG:HH21 | 1.75 | 0.52 |
| 1:A:220:VAL:HG22 | 1:A:248:VAL:CG2 | 2.39 | 0.52 |
| 1:A:228:SER:HA | 1:A:255:ASP:HB2 | 1.90 | 0.52 |
| 1:A:512:ALA:O | 1:A:516:THR:HG23 | 2.10 | 0.52 |
| 1:E:234:VAL:O | 1:E:238:GLU:HG3 | 2.10 | 0.52 |
| 1:E:292:MET:O | 1:E:296:THR:HG22 | 2.10 | 0.52 |
| 1:E:512:ALA:O | 1:E:516:THR:HG23 | 2.09 | 0.52 |
| 1:H:99:ILE:HD13 | 1:H:509:ALA:HA | 1.91 | 0.52 |
| 2:2:80:LYS:HG3 | 2:2:89:PHE:HE1 | 1.75 | 0.52 |
| 1:L:219:TYR:CE2 | 1:L:245:LYS:HD2 | 2.44 | 0.52 |
| 1:L:292:MET:O | 1:L:296:THR:HG22 | 2.10 | 0.52 |
| 1:D:264:LEU:CD1 | 1:D:268:LYS:HE2 | 2.40 | 0.52 |
| 1:B:291:ASP:OD1 | 1:B:346:ARG:NE | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:219:TYR:CE2 | 1:A:245:LYS:HD2 | 2.44 | 0.52 |
| 1:E:199:TYR:HD1 | 1:E:326:VAL:HG12 | 1.73 | 0.52 |
| 2:X:73:LEU:HD22 | 2:X:91:PHE:CE2 | 2.45 | 0.52 |
| 2:R:3:GLY:HA3 | 2:R:51:SER:HA | 1.91 | 0.52 |
| 2:P:32:MET:CE | 1:B:268:LYS:HE3 | 2.39 | 0.52 |
| 2:O:80:LYS:HG3 | 2:O:89:PHE:HE1 | 1.75 | 0.52 |
| 1:N:373:LEU:O | 1:N:373:LEU:HD23 | 2.10 | 0.52 |
| 1:N:420:LEU:HD11 | 1:N:501:VAL:HG13 | 1.90 | 0.52 |
| 1:M:3:ALA:CB | 1:M:525:ILE:HD12 | 2.40 | 0.52 |
| 1:L:73:LEU:HD12 | 1:L:515:LEU:HD13 | 1.92 | 0.52 |
| 1:K:89:THR:O | 1:K:93:THR:HG23 | 2.10 | 0.52 |
| 1:I:69:ILE:HD11 | 1:I:523:THR:HG22 | 1.92 | 0.52 |
| 1:C:188:GLU:OE1 | 1:C:381:LYS:NZ | 2.41 | 0.52 |
| 1:B:310:LEU:O | 1:B:313:VAL:HG13 | 2.10 | 0.52 |
| 1:G:169:VAL:HG12 | 1:G:173:GLY:HA3 | 1.91 | 0.52 |
| 1:G:512:ALA:O | 1:G:516:THR:HG23 | 2.10 | 0.52 |
| 1:F:183:LEU:CD1 | 1:F:385:THR:HG22 | 2.40 | 0.52 |
| 1:H:220:VAL:HG22 | 1:H:248:VAL:CG2 | 2.39 | 0.51 |
| 2:2:73:LEU:HD22 | 2:2:91:PHE:CE2 | 2.45 | 0.51 |
| 2:R:73:LEU:HD22 | 2:R:91:PHE:CE2 | 2.45 | 0.51 |
| 1:L:413:VAL:HB | 1:L:498:THR:HG22 | 1.91 | 0.51 |
| 1:J:13:ARG:HD3 | 1:J:104:PHE:HD1 | 1.75 | 0.51 |
| 1:J:222:LEU:CD2 | 1:J:250:ILE:HB | 2.39 | 0.51 |
| 1:J:512:ALA:O | 1:J:516:THR:HG23 | 2.09 | 0.51 |
| 1:I:166:MET:HG3 | 1:I:171:ARG:HA | 1.92 | 0.51 |
| 1:D:222:LEU:CD2 | 1:D:250:ILE:HB | 2.39 | 0.51 |
| 1:H:469:LYS:HG2 | 1:H:486:PHE:HE2 | 1.76 | 0.51 |
| 1:H:497:PRO:HD2 | 1:H:500:VAL:HG11 | 1.93 | 0.51 |
| 1:H:512:ALA:O | 1:H:516:THR:HG23 | 2.10 | 0.51 |
| 2:2:27:THR:HG22 | 2:2:31:ILE:H | 1.75 | 0.51 |
| 2:Y:15:ARG:HH22 | 2:X:97:LEU:HA | 1.74 | 0.51 |
| 2:S:65:VAL:HG22 | 2:S:93:ASP:OD1 | 2.10 | 0.51 |
| 1:N:234:VAL:O | 1:N:238:GLU:HG3 | 2.11 | 0.51 |
| 1:M:89:THR:O | 1:M:93:THR:HG23 | 2.10 | 0.51 |
| 1:L:22:LEU:HD11 | 1:K:6:VAL:HG21 | 1.92 | 0.51 |
| 1:I:239:ILE:CD1 | 1:I:313:VAL:HG23 | 2.40 | 0.51 |
| 1:I:350:ILE:O | 1:I:366:LEU:HD11 | 2.10 | 0.51 |
| 1:G:13:ARG:HD3 | 1:G:104:PHE:HD1 | 1.75 | 0.51 |
| 1:G:194:LYS:HD2 | 1:G:332:MET:HE3 | 1.92 | 0.51 |
| 1:F:199:TYR:HD1 | 1:F:326:VAL:HG12 | 1.74 | 0.51 |
| 2:2:3:GLY:HA3 | 2:2:51:SER:HA | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:81:VAL:HG12 | 2:X:72:LEU:HD21 | 1.92 | 0.51 |
| 2:W:80:LYS:HG3 | 2:W:89:PHE:HE1 | 1.74 | 0.51 |
| 1:N:135:SER:CB | 1:N:498:THR:HG21 | 2.40 | 0.51 |
| 1:K:193:MET:HE1 | 1:K:292:MET:HA | 1.91 | 0.51 |
| 1:I:13:ARG:HD3 | 1:I:104:PHE:HD1 | 1.75 | 0.51 |
| 1:I:450:ILE:O | 1:I:454:THR:HG23 | 2.11 | 0.51 |
| 1:D:47:PRO:HG3 | 1:C:69:ILE:HG23 | 1.92 | 0.51 |
| 1:D:410:GLU:HG2 | 1:D:498:THR:OG1 | 2.11 | 0.51 |
| 1:C:89:THR:O | 1:C:93:THR:HG23 | 2.10 | 0.51 |
| 1:B:183:LEU:CD1 | 1:B:385:THR:HG22 | 2.41 | 0.51 |
| 1:B:206:ASN:HB3 | 1:B:266:ARG:NH2 | 2.26 | 0.51 |
| 1:B:237:LEU:HD21 | 1:B:262:LEU:CD2 | 2.37 | 0.51 |
| 1:B:373:LEU:HD23 | 1:B:373:LEU:O | 2.11 | 0.51 |
| 1:F:62:LEU:HD13 | 1:F:67:LYS:HB3 | 1.92 | 0.51 |
| 1:F:450:ILE:O | 1:F:454:THR:HG23 | 2.10 | 0.51 |
| 1:H:22:LEU:HD11 | 1:N:6:VAL:HG21 | 1.91 | 0.51 |
| 2:W:73:LEU:HD22 | 2:W:91:PHE:CE2 | 2.46 | 0.51 |
| 2:Q:33:LEU:HG | 1:C:230:ILE:HD11 | 1.91 | 0.51 |
| 2:Q:73:LEU:HD22 | 2:Q:91:PHE:CE2 | 2.45 | 0.51 |
| 2:P:81:VAL:HG12 | 2:O:72:LEU:HD21 | 1.93 | 0.51 |
| 1:M:62:LEU:HD13 | 1:M:67:LYS:HB3 | 1.92 | 0.51 |
| 1:M:421:LEU:CD2 | 1:M:467:VAL:HG13 | 2.38 | 0.51 |
| 1:L:280:GLY:C | 1:L:285:ARG:HB3 | 2.31 | 0.51 |
| 1:K:13:ARG:NH2 | 1:K:519:GLU:OE1 | 2.42 | 0.51 |
| 1:J:280:GLY:O | 1:J:285:ARG:NE | 2.44 | 0.51 |
| 1:J:420:LEU:HD11 | 1:J:501:VAL:HG13 | 1.91 | 0.51 |
| 1:I:420:LEU:HD11 | 1:I:501:VAL:HG13 | 1.92 | 0.51 |
| 1:D:135:SER:CB | 1:D:498:THR:HG21 | 2.41 | 0.51 |
| 1:F:116:ILE:O | 1:F:120:VAL:HG23 | 2.11 | 0.51 |
| 1:F:234:VAL:O | 1:F:238:GLU:HG3 | 2.10 | 0.51 |
| 1:F:422:ARG:NH1 | 1:F:474:SER:O | 2.43 | 0.51 |
| 1:E:52:ASP:OD2 | 5:E:702:HOH:O | 2.18 | 0.51 |
| 1:E:264:LEU:O | 1:E:268:LYS:HG2 | 2.10 | 0.51 |
| 1:H:239:ILE:CD1 | 1:H:313:VAL:HG23 | 2.40 | 0.51 |
| 1:M:292:MET:O | 1:M:296:THR:HG22 | 2.11 | 0.51 |
| 1:L:525:ILE:HG23 | 1:L:527:LYS:CG | 2.39 | 0.51 |
| 1:K:135:SER:CB | 1:K:498:THR:HG21 | 2.41 | 0.51 |
| 1:D:188:GLU:HB3 | 1:D:379:VAL:HG22 | 1.92 | 0.51 |
| 1:C:183:LEU:CD1 | 1:C:385:THR:HG22 | 2.41 | 0.51 |
| 1:C:410:GLU:HG2 | 1:C:498:THR:OG1 | 2.10 | 0.51 |
| 1:E:135:SER:CB | 1:E:498:THR:HG21 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:1:80:LYS:HG3 | 2:1:89:PHE:HE1 | 1.75 | 0.51 |
| 2:Q:13:PHE:CD1 | 2:Q:54:LYS:HB2 | 2.45 | 0.51 |
| 1:K:71:ALA:O | 1:K:75:GLN:HG3 | 2.11 | 0.51 |
| 1:J:230:ILE:HG13 | 1:J:261:THR:HG21 | 1.93 | 0.51 |
| 1:C:281:PHE:N | 1:C:285:ARG:HG3 | 2.25 | 0.51 |
| 1:C:293:ALA:O | 1:C:297:GLY:N | 2.30 | 0.51 |
| 1:A:420:LEU:HD11 | 1:A:501:VAL:HG13 | 1.91 | 0.51 |
| 1:A:525:ILE:HG23 | 1:A:527:LYS:CG | 2.38 | 0.51 |
| 1:G:52:ASP:OD2 | 5:G:702:HOH:O | 2.18 | 0.51 |
| 1:E:239:ILE:CD1 | 1:E:313:VAL:HG23 | 2.40 | 0.51 |
| 2:P:73:LEU:HD22 | 2:P:91:PHE:CE2 | 2.45 | 0.51 |
| 2:T:73:LEU:HD22 | 2:T:91:PHE:CE2 | 2.46 | 0.51 |
| 1:N:77:VAL:HG22 | 1:N:511:VAL:HB | 1.93 | 0.51 |
| 1:N:169:VAL:HG21 | 1:N:378:ALA:HB2 | 1.93 | 0.51 |
| 1:N:188:GLU:OE1 | 1:N:381:LYS:NZ | 2.39 | 0.51 |
| 1:N:280:GLY:O | 1:N:285:ARG:NE | 2.44 | 0.51 |
| 1:L:206:ASN:HB3 | 1:L:266:ARG:NH2 | 2.26 | 0.51 |
| 1:K:469:LYS:HG2 | 1:K:486:PHE:HE2 | 1.76 | 0.51 |
| 1:J:3:ALA:CB | 1:J:525:ILE:HD12 | 2.40 | 0.51 |
| 1:B:296:THR:OG1 | 1:B:320:LYS:O | 2.27 | 0.51 |
| 1:B:420:LEU:HD11 | 1:B:501:VAL:HG13 | 1.92 | 0.51 |
| 1:A:69:ILE:HD11 | 1:A:523:THR:HG22 | 1.93 | 0.51 |
| 1:A:310:LEU:O | 1:A:313:VAL:HG13 | 2.10 | 0.51 |
| 1:G:233:ILE:HG13 | 1:G:237:LEU:CD1 | 2.40 | 0.51 |
| 1:F:228:SER:HA | 1:F:255:ASP:HB2 | 1.92 | 0.51 |
| 1:H:195:PHE:CZ | 1:H:331:ALA:HB3 | 2.45 | 0.51 |
| 2:1:73:LEU:HD22 | 2:1:91:PHE:CE2 | 2.46 | 0.51 |
| 2:R:72:LEU:HD21 | 2:S:81:VAL:HG12 | 1.92 | 0.51 |
| 1:N:3:ALA:CB | 1:N:525:ILE:HD12 | 2.41 | 0.51 |
| 1:M:195:PHE:CZ | 1:M:331:ALA:HB3 | 2.45 | 0.51 |
| 1:K:3:ALA:CB | 1:K:525:ILE:HD12 | 2.40 | 0.51 |
| 1:K:116:ILE:O | 1:K:120:VAL:HG23 | 2.11 | 0.51 |
| 1:K:206:ASN:HB3 | 1:K:266:ARG:NH2 | 2.26 | 0.51 |
| 1:K:206:ASN:HB3 | 1:K:266:ARG:HH21 | 1.76 | 0.51 |
| 1:D:292:MET:O | 1:D:296:THR:HG22 | 2.10 | 0.51 |
| 1:D:393:LYS:O | 1:D:397:VAL:HG23 | 2.11 | 0.51 |
| 1:D:469:LYS:HG2 | 1:D:486:PHE:HE2 | 1.75 | 0.51 |
| 1:F:73:LEU:HD12 | 1:F:515:LEU:HD13 | 1.93 | 0.51 |
| 1:H:310:LEU:O | 1:H:313:VAL:HG13 | 2.11 | 0.51 |
| 2:Q:65:VAL:HG22 | 2:Q:93:ASP:OD1 | 2.11 | 0.51 |
| 2:P:13:PHE:CD1 | 2:P:54:LYS:HB2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:73:LEU:HD22 | 2:O:91:PHE:CE2 | 2.46 | 0.51 |
| 2:T:81:VAL:HG12 | 2:S:72:LEU:HD21 | 1.92 | 0.51 |
| 1:N:195:PHE:CZ | 1:N:331:ALA:HB3 | 2.45 | 0.51 |
| 1:N:393:LYS:O | 1:N:397:VAL:HG23 | 2.11 | 0.51 |
| 1:M:177:VAL:HG11 | 1:M:398:THR:CG2 | 2.41 | 0.51 |
| 1:L:383:GLY:O | 1:L:390:VAL:HG22 | 2.11 | 0.51 |
| 1:I:410:GLU:HG2 | 1:I:498:THR:OG1 | 2.11 | 0.51 |
| 1:D:310:LEU:O | 1:D:313:VAL:HG13 | 2.11 | 0.51 |
| 1:C:512:ALA:O | 1:C:516:THR:HG23 | 2.09 | 0.51 |
| 1:B:177:VAL:HG11 | 1:B:398:THR:CG2 | 2.40 | 0.51 |
| 1:B:264:LEU:CG | 1:B:268:LYS:HE2 | 2.40 | 0.51 |
| 1:A:22:LEU:HD11 | 1:G:6:VAL:HG21 | 1.92 | 0.51 |
| 1:A:239:ILE:CD1 | 1:A:313:VAL:HG23 | 2.41 | 0.51 |
| 1:E:310:LEU:O | 1:E:313:VAL:HG13 | 2.11 | 0.51 |
| 2:V:26:VAL:HG12 | 2:V:32:MET:CG | 2.41 | 0.51 |
| 1:N:194:LYS:HD2 | 1:N:332:MET:HE2 | 1.92 | 0.51 |
| 1:L:219:TYR:O | 1:L:248:VAL:HG22 | 2.11 | 0.51 |
| 1:K:310:LEU:O | 1:K:313:VAL:HG13 | 2.11 | 0.51 |
| 1:D:31:MET:SD | 1:D:454:THR:OG1 | 2.65 | 0.51 |
| 1:D:195:PHE:CZ | 1:D:331:ALA:HB3 | 2.46 | 0.51 |
| 1:A:410:GLU:HG2 | 1:A:498:THR:OG1 | 2.11 | 0.51 |
| 1:G:224:GLU:OE2 | 1:G:286:LYS:HE3 | 2.11 | 0.51 |
| 1:E:225:LYS:HA | 1:E:252:GLU:OE1 | 2.11 | 0.51 |
| 2:T:27:THR:HG22 | 2:T:31:ILE:H | 1.76 | 0.50 |
| 2:S:80:LYS:HG3 | 2:S:89:PHE:HE1 | 1.76 | 0.50 |
| 1:M:250:ILE:HG12 | 1:M:276:VAL:CG2 | 2.41 | 0.50 |
| 1:L:420:LEU:HD11 | 1:L:501:VAL:HG13 | 1.91 | 0.50 |
| 1:I:3:ALA:CB | 1:I:525:ILE:HD12 | 2.41 | 0.50 |
| 1:D:489:MET:O | 1:D:493:GLY:N | 2.36 | 0.50 |
| 1:A:393:LYS:O | 1:A:397:VAL:HG23 | 2.12 | 0.50 |
| 1:A:427:LEU:HA | 1:A:430:LEU:HD23 | 1.93 | 0.50 |
| 1:G:420:LEU:HD11 | 1:G:501:VAL:HG13 | 1.92 | 0.50 |
| 1:F:206:ASN:HB3 | 1:F:266:ARG:HH21 | 1.76 | 0.50 |
| 1:F:231:GLN:O | 1:F:234:VAL:HG12 | 2.12 | 0.50 |
| 2:V:26:VAL:HA | 2:V:32:MET:HA | 1.93 | 0.50 |
| 2:X:80:LYS:HG3 | 2:X:89:PHE:HE1 | 1.76 | 0.50 |
| 2:R:32:MET:CE | 1:D:268:LYS:HE3 | 2.41 | 0.50 |
| 2:P:80:LYS:HG3 | 2:P:89:PHE:HE1 | 1.75 | 0.50 |
| 1:N:250:ILE:HG12 | 1:N:276:VAL:CG2 | 2.42 | 0.50 |
| 1:N:310:LEU:O | 1:N:313:VAL:HG13 | 2.11 | 0.50 |
| 1:M:183:LEU:CD1 | 1:M:385:THR:HG22 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:280:GLY:C | 1:M:285:ARG:HB3 | 2.31 | 0.50 |
| 1:M:410:GLU:HG2 | 1:M:498:THR:OG1 | 2.11 | 0.50 |
| 1:L:264:LEU:HD11 | 1:L:268:LYS:HE2 | 1.93 | 0.50 |
| 1:I:24:ALA:CB | 1:I:97:ARG:HD3 | 2.40 | 0.50 |
| 1:I:62:LEU:HD13 | 1:I:67:LYS:HB3 | 1.91 | 0.50 |
| 1:I:195:PHE:CZ | 1:I:331:ALA:HB3 | 2.46 | 0.50 |
| 1:I:206:ASN:HB3 | 1:I:266:ARG:NH2 | 2.27 | 0.50 |
| 1:I:222:LEU:CD2 | 1:I:250:ILE:HB | 2.39 | 0.50 |
| 1:D:6:VAL:HG21 | 1:E:22:LEU:HD11 | 1.93 | 0.50 |
| 1:C:296:THR:OG1 | 1:C:320:LYS:O | 2.26 | 0.50 |
| 1:B:73:LEU:HD12 | 1:B:515:LEU:HD13 | 1.92 | 0.50 |
| 1:B:234:VAL:O | 1:B:238:GLU:HG3 | 2.10 | 0.50 |
| 1:A:127:VAL:HG23 | 1:A:423:CYS:CB | 2.40 | 0.50 |
| 1:G:301:PHE:CD1 | 1:G:308:LEU:HB3 | 2.47 | 0.50 |
| 1:F:264:LEU:CG | 1:F:268:LYS:HE2 | 2.40 | 0.50 |
| 1:F:469:LYS:HG2 | 1:F:486:PHE:HE2 | 1.76 | 0.50 |
| 1:K:195:PHE:CZ | 1:K:331:ALA:HB3 | 2.46 | 0.50 |
| 1:G:62:LEU:CD1 | 1:G:67:LYS:HB3 | 2.41 | 0.50 |
| 1:G:193:MET:HE1 | 1:G:292:MET:HA | 1.93 | 0.50 |
| 1:H:123:ALA:HB3 | 1:H:444:ILE:HG13 | 1.94 | 0.50 |
| 2:Y:73:LEU:HD22 | 2:Y:91:PHE:CE2 | 2.46 | 0.50 |
| 2:Y:80:LYS:HG3 | 2:Y:89:PHE:HE1 | 1.75 | 0.50 |
| 2:X:81:VAL:HG12 | 2:W:72:LEU:HD21 | 1.94 | 0.50 |
| 2:R:8:LYS:HA | 2:Q:101:VAL:O | 2.12 | 0.50 |
| 2:Q:31:ILE:HD12 | 1:C:237:LEU:HB3 | 1.92 | 0.50 |
| 2:S:5:ALA:HB2 | 2:S:10:LEU:HD13 | 1.94 | 0.50 |
| 1:M:239:ILE:CD1 | 1:M:313:VAL:HG23 | 2.41 | 0.50 |
| 1:L:310:LEU:O | 1:L:313:VAL:HG13 | 2.11 | 0.50 |
| 1:L:382:VAL:HG23 | 1:L:390:VAL:HG13 | 1.93 | 0.50 |
| 1:F:232:SER:HB2 | 1:F:310:LEU:HD12 | 1.93 | 0.50 |
| 1:H:373:LEU:HD23 | 1:H:373:LEU:O | 2.12 | 0.50 |
| 1:H:421:LEU:CD2 | 1:H:467:VAL:HG13 | 2.37 | 0.50 |
| 1:N:47:PRO:HG3 | 1:M:69:ILE:HG23 | 1.93 | 0.50 |
| 1:N:292:MET:O | 1:N:296:THR:HG22 | 2.11 | 0.50 |
| 1:N:469:LYS:HG2 | 1:N:486:PHE:HE2 | 1.77 | 0.50 |
| 1:M:194:LYS:HD2 | 1:M:332:MET:HE2 | 1.92 | 0.50 |
| 1:M:310:LEU:O | 1:M:313:VAL:HG13 | 2.11 | 0.50 |
| 1:I:73:LEU:HD12 | 1:I:515:LEU:HD13 | 1.92 | 0.50 |
| 1:D:251:ALA:O | 1:D:277:LYS:HA | 2.11 | 0.50 |
| 1:C:62:LEU:HD13 | 1:C:67:LYS:HB3 | 1.93 | 0.50 |
| 1:C:177:VAL:HG11 | 1:C:398:THR:CG2 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:239:ILE:CD1 | 1:C:313:VAL:HG23 | 2.41 | 0.50 |
| 1:C:310:LEU:O | 1:C:313:VAL:HG13 | 2.11 | 0.50 |
| 1:B:228:SER:HA | 1:B:255:ASP:HB2 | 1.91 | 0.50 |
| 1:G:230:ILE:HG13 | 1:G:261:THR:HG21 | 1.94 | 0.50 |
| 1:G:400:ALA:O | 1:G:404:THR:HG23 | 2.12 | 0.50 |
| 1:E:77:VAL:HG22 | 1:E:511:VAL:HB | 1.94 | 0.50 |
| 1:E:373:LEU:HD23 | 1:E:373:LEU:O | 2.11 | 0.50 |
| 1:E:402:ASN:OD1 | 1:E:405:ARG:NH2 | 2.42 | 0.50 |
| 1:H:193:MET:HE1 | 1:H:292:MET:HA | 1.92 | 0.50 |
| 2:V:3:GLY:HA3 | 2:V:51:SER:HA | 1.94 | 0.50 |
| 1:N:228:SER:HA | 1:N:255:ASP:HB2 | 1.92 | 0.50 |
| 1:N:410:GLU:HG2 | 1:N:498:THR:OG1 | 2.11 | 0.50 |
| 1:M:497:PRO:HB2 | 1:M:500:VAL:HG12 | 1.93 | 0.50 |
| 1:L:206:ASN:HB3 | 1:L:266:ARG:HH21 | 1.77 | 0.50 |
| 1:L:239:ILE:CD1 | 1:L:313:VAL:HG23 | 2.42 | 0.50 |
| 1:K:73:LEU:HD12 | 1:K:515:LEU:HD13 | 1.94 | 0.50 |
| 1:J:310:LEU:O | 1:J:313:VAL:HG13 | 2.12 | 0.50 |
| 1:I:206:ASN:HB3 | 1:I:266:ARG:HH21 | 1.77 | 0.50 |
| 1:B:124:VAL:HG21 | 1:B:509:ALA:CB | 2.42 | 0.50 |
| 1:B:264:LEU:HD11 | 1:B:268:LYS:HE2 | 1.93 | 0.50 |
| 1:B:350:ILE:O | 1:B:366:LEU:HD11 | 2.12 | 0.50 |
| 1:E:525:ILE:HG23 | 1:E:527:LYS:CG | 2.40 | 0.50 |
| 1:H:177:VAL:HG11 | 1:H:398:THR:CG2 | 2.41 | 0.50 |
| 2:O:8:LYS:O | 2:U:100:TYR:HA | 2.12 | 0.50 |
| 2:U:44:ALA:HB2 | 2:U:73:LEU:HD11 | 1.94 | 0.50 |
| 1:N:222:LEU:CD2 | 1:N:250:ILE:HB | 2.41 | 0.50 |
| 1:L:169:VAL:HG21 | 1:L:378:ALA:HB2 | 1.93 | 0.50 |
| 1:L:177:VAL:HG11 | 1:L:398:THR:CG2 | 2.41 | 0.50 |
| 1:K:22:LEU:HD11 | 1:J:6:VAL:HG21 | 1.93 | 0.50 |
| 1:K:32:GLY:N | 3:K:601:ADP:O2A | 2.41 | 0.50 |
| 1:K:420:LEU:HD11 | 1:K:501:VAL:HG13 | 1.92 | 0.50 |
| 1:K:512:ALA:O | 1:K:516:THR:HG23 | 2.10 | 0.50 |
| 1:J:252:GLU:HG3 | 1:J:285:ARG:NH1 | 2.27 | 0.50 |
| 1:C:222:LEU:CD2 | 1:C:250:ILE:HB | 2.40 | 0.50 |
| 1:F:120:VAL:O | 1:F:124:VAL:HG23 | 2.12 | 0.50 |
| 1:F:157:GLU:O | 1:F:161:ILE:HG12 | 2.11 | 0.50 |
| 1:E:197:ARG:H | 1:E:330:ASP:HA | 1.76 | 0.50 |
| 1:H:135:SER:CB | 1:H:498:THR:HG21 | 2.42 | 0.50 |
| 1:H:228:SER:HA | 1:H:255:ASP:HB2 | 1.92 | 0.50 |
| 2:2:33:LEU:HG | 1:N:230:ILE:HD11 | 1.94 | 0.50 |
| 2:Y:31:ILE:HD12 | 1:K:237:LEU:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:78:GLY:HA3 | 2:O:91:PHE:CE1 | 2.47 | 0.50 |
| 2:U:20:ARG:HB3 | 2:U:41:VAL:CG1 | 2.41 | 0.50 |
| 1:M:219:TYR:O | 1:M:248:VAL:HG22 | 2.12 | 0.50 |
| 1:K:239:ILE:CD1 | 1:K:313:VAL:HG23 | 2.41 | 0.50 |
| 1:K:393:LYS:O | 1:K:397:VAL:HG23 | 2.11 | 0.50 |
| 1:I:31:MET:SD | 1:I:454:THR:OG1 | 2.65 | 0.50 |
| 1:C:291:ASP:OD1 | 1:C:346:ARG:NE | 2.40 | 0.50 |
| 1:A:73:LEU:HD12 | 1:A:515:LEU:HD13 | 1.93 | 0.50 |
| 1:A:116:ILE:O | 1:A:120:VAL:HG23 | 2.11 | 0.50 |
| 1:A:195:PHE:CZ | 1:A:331:ALA:HB3 | 2.46 | 0.50 |
| 1:G:224:GLU:O | 1:G:252:GLU:HB2 | 2.12 | 0.50 |
| 1:G:227:ILE:HG21 | 1:G:233:ILE:HD13 | 1.94 | 0.50 |
| 1:G:310:LEU:O | 1:G:313:VAL:HG13 | 2.12 | 0.50 |
| 1:G:413:VAL:HB | 1:G:498:THR:HG22 | 1.93 | 0.50 |
| 1:F:166:MET:HG3 | 1:F:171:ARG:HA | 1.94 | 0.50 |
| 2:V:100:TYR:HA | 2:W:8:LYS:O | 2.12 | 0.50 |
| 2:2:8:LYS:HG2 | 2:1:102:ASP:CB | 2.42 | 0.50 |
| 2:S:13:PHE:CD1 | 2:S:54:LYS:HB2 | 2.46 | 0.50 |
| 2:S:44:ALA:HB2 | 2:S:73:LEU:HD11 | 1.94 | 0.50 |
| 1:L:227:ILE:HG21 | 1:L:233:ILE:HD13 | 1.94 | 0.50 |
| 1:K:410:GLU:HG2 | 1:K:498:THR:OG1 | 2.11 | 0.50 |
| 1:I:166:MET:CG | 1:I:171:ARG:HA | 2.42 | 0.50 |
| 1:D:195:PHE:CG | 1:D:279:PRO:HG3 | 2.47 | 0.50 |
| 1:C:206:ASN:HB3 | 1:C:266:ARG:NH2 | 2.27 | 0.50 |
| 1:B:206:ASN:HB3 | 1:B:266:ARG:HH21 | 1.77 | 0.50 |
| 1:B:239:ILE:CD1 | 1:B:313:VAL:HG23 | 2.42 | 0.50 |
| 1:A:169:VAL:HG21 | 1:A:378:ALA:HB2 | 1.93 | 0.50 |
| 1:F:264:LEU:HD11 | 1:F:268:LYS:HE2 | 1.94 | 0.50 |
| 1:F:410:GLU:HG2 | 1:F:498:THR:OG1 | 2.11 | 0.50 |
| 2:V:27:THR:HG22 | 2:V:31:ILE:H | 1.77 | 0.49 |
| 2:1:3:GLY:HA3 | 2:1:51:SER:HA | 1.94 | 0.49 |
| 2:1:44:ALA:HB2 | 2:1:73:LEU:HD11 | 1.94 | 0.49 |
| 2:O:32:MET:HG2 | 1:A:268:LYS:NZ | 2.26 | 0.49 |
| 1:N:239:ILE:CD1 | 1:N:313:VAL:HG23 | 2.42 | 0.49 |
| 1:M:469:LYS:HG2 | 1:M:486:PHE:HE2 | 1.77 | 0.49 |
| 1:L:410:GLU:HG2 | 1:L:498:THR:OG1 | 2.12 | 0.49 |
| 1:K:230:ILE:HG13 | 1:K:261:THR:HG21 | 1.94 | 0.49 |
| 1:K:248:VAL:HG11 | 1:K:324:VAL:HG11 | 1.94 | 0.49 |
| 1:K:251:ALA:O | 1:K:277:LYS:HA | 2.11 | 0.49 |
| 1:I:116:ILE:O | 1:I:120:VAL:HG23 | 2.12 | 0.49 |
| 1:I:157:GLU:O | 1:I:161:ILE:HG12 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:188:GLU:OE1 | 1:D:381:LYS:NZ | 2.41 | 0.49 |
| 1:B:77:VAL:HG22 | 1:B:511:VAL:HB | 1.93 | 0.49 |
| 1:A:255:ASP:OD1 | 1:A:256:GLY:N | 2.45 | 0.49 |
| 1:G:195:PHE:CZ | 1:G:331:ALA:HB3 | 2.47 | 0.49 |
| 1:H:400:ALA:O | 1:H:404:THR:HG23 | 2.12 | 0.49 |
| 2:Q:27:THR:HG22 | 2:Q:31:ILE:H | 1.76 | 0.49 |
| 1:N:224:GLU:O | 1:N:252:GLU:HB2 | 2.12 | 0.49 |
| 1:N:251:ALA:O | 1:N:277:LYS:HA | 2.13 | 0.49 |
| 1:M:47:PRO:HG3 | 1:L:69:ILE:HG23 | 1.94 | 0.49 |
| 1:K:280:GLY:O | 1:K:285:ARG:NE | 2.27 | 0.49 |
| 1:J:138:VAL:HA | 1:J:143:GLU:OE1 | 2.12 | 0.49 |
| 1:D:264:LEU:O | 1:D:268:LYS:HG2 | 2.11 | 0.49 |
| 1:G:116:ILE:O | 1:G:120:VAL:HG23 | 2.12 | 0.49 |
| 1:E:206:ASN:HB3 | 1:E:266:ARG:HH21 | 1.77 | 0.49 |
| 1:E:348:GLN:OE1 | 1:E:351:ILE:HD11 | 2.11 | 0.49 |
| 1:H:136:LYS:HE3 | 1:H:412:ILE:HD11 | 1.92 | 0.49 |
| 1:H:251:ALA:O | 1:H:277:LYS:HA | 2.13 | 0.49 |
| 1:H:303:GLU:HB3 | 1:H:306:LEU:HB3 | 1.95 | 0.49 |
| 2:1:31:ILE:HD12 | 1:M:237:LEU:HB3 | 1.94 | 0.49 |
| 1:N:219:TYR:O | 1:N:248:VAL:HG22 | 2.12 | 0.49 |
| 1:M:135:SER:CB | 1:M:498:THR:HG21 | 2.42 | 0.49 |
| 1:K:194:LYS:HD2 | 1:K:332:MET:HE2 | 1.93 | 0.49 |
| 1:K:350:ILE:O | 1:K:366:LEU:HD11 | 2.12 | 0.49 |
| 1:D:497:PRO:HB2 | 1:D:500:VAL:HG12 | 1.93 | 0.49 |
| 1:B:282:GLY:O | 1:B:285:ARG:HB3 | 2.13 | 0.49 |
| 1:B:525:ILE:HG23 | 1:B:527:LYS:CG | 2.40 | 0.49 |
| 1:A:237:LEU:HD21 | 1:A:262:LEU:CD2 | 2.42 | 0.49 |
| 1:A:469:LYS:HG2 | 1:A:486:PHE:HE2 | 1.76 | 0.49 |
| 1:G:373:LEU:O | 1:G:373:LEU:HD23 | 2.13 | 0.49 |
| 1:F:31:MET:HE1 | 1:F:94:VAL:HG21 | 1.94 | 0.49 |
| 2:V:102:ASP:CB | 2:W:8:LYS:HG2 | 2.42 | 0.49 |
| 1:L:255:ASP:OD1 | 1:L:256:GLY:N | 2.45 | 0.49 |
| 1:L:400:ALA:O | 1:L:404:THR:HG23 | 2.12 | 0.49 |
| 1:J:77:VAL:HG22 | 1:J:511:VAL:HB | 1.94 | 0.49 |
| 1:J:264:LEU:HG | 1:J:268:LYS:HE2 | 1.93 | 0.49 |
| 1:J:410:GLU:HG2 | 1:J:498:THR:OG1 | 2.11 | 0.49 |
| 1:I:14:ALA:O | 1:I:18:GLN:HG3 | 2.12 | 0.49 |
| 1:I:234:VAL:O | 1:I:238:GLU:HG3 | 2.13 | 0.49 |
| 1:C:332:MET:HG2 | 1:C:334:LEU:HD12 | 1.94 | 0.49 |
| 1:F:225:LYS:HA | 1:F:252:GLU:OE1 | 2.12 | 0.49 |
| 1:H:77:VAL:HG22 | 1:H:511:VAL:HB | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:65:VAL:HG22 | 2:2:93:ASP:OD1 | 2.12 | 0.49 |
| 2:W:5:ALA:HB2 | 2:W:10:LEU:HD13 | 1.95 | 0.49 |
| 1:M:394:LYS:O | 1:M:398:THR:HG23 | 2.13 | 0.49 |
| 1:L:230:ILE:HG13 | 1:L:261:THR:HG21 | 1.95 | 0.49 |
| 1:L:237:LEU:HD21 | 1:L:262:LEU:CD2 | 2.40 | 0.49 |
| 1:L:450:ILE:O | 1:L:454:THR:HG23 | 2.13 | 0.49 |
| 1:I:278:ALA:CB | 1:I:289:LEU:HD11 | 2.38 | 0.49 |
| 1:D:350:ILE:HG23 | 1:D:366:LEU:HD22 | 1.95 | 0.49 |
| 1:C:135:SER:CB | 1:C:498:THR:HG21 | 2.42 | 0.49 |
| 1:A:206:ASN:HB3 | 1:A:266:ARG:NH2 | 2.27 | 0.49 |
| 1:G:255:ASP:OD1 | 1:G:256:GLY:N | 2.46 | 0.49 |
| 1:E:13:ARG:NH2 | 1:E:519:GLU:OE1 | 2.40 | 0.49 |
| 1:H:13:ARG:HD3 | 1:H:104:PHE:HD1 | 1.77 | 0.49 |
| 1:H:65:LYS:O | 1:H:69:ILE:HG13 | 2.12 | 0.49 |
| 1:H:222:LEU:CD2 | 1:H:250:ILE:HB | 2.41 | 0.49 |
| 1:H:224:GLU:O | 1:H:252:GLU:HB2 | 2.13 | 0.49 |
| 2:X:27:THR:HG22 | 2:X:31:ILE:H | 1.78 | 0.49 |
| 2:X:90:LEU:CD2 | 2:W:97:LEU:HD12 | 2.34 | 0.49 |
| 2:W:78:GLY:HA3 | 2:W:91:PHE:CE1 | 2.47 | 0.49 |
| 2:O:5:ALA:HB2 | 2:O:10:LEU:HD13 | 1.94 | 0.49 |
| 1:N:350:ILE:HG23 | 1:N:366:LEU:HD22 | 1.94 | 0.49 |
| 1:J:116:ILE:O | 1:J:120:VAL:HG23 | 2.12 | 0.49 |
| 1:J:127:VAL:HG23 | 1:J:423:CYS:CB | 2.41 | 0.49 |
| 1:J:219:TYR:O | 1:J:248:VAL:HG22 | 2.13 | 0.49 |
| 1:C:224:GLU:O | 1:C:252:GLU:HB2 | 2.13 | 0.49 |
| 1:C:348:GLN:OE1 | 1:C:351:ILE:HD11 | 2.13 | 0.49 |
| 1:C:469:LYS:HG2 | 1:C:486:PHE:HE2 | 1.77 | 0.49 |
| 1:B:219:TYR:O | 1:B:248:VAL:HG22 | 2.13 | 0.49 |
| 1:G:24:ALA:CB | 1:G:97:ARG:HD3 | 2.39 | 0.49 |
| 1:G:469:LYS:HG2 | 1:G:486:PHE:HE2 | 1.77 | 0.49 |
| 1:F:346:ARG:O | 1:F:350:ILE:HD12 | 2.11 | 0.49 |
| 2:V:80:LYS:HG3 | 2:V:89:PHE:HE1 | 1.76 | 0.49 |
| 2:Y:27:THR:HG22 | 2:Y:31:ILE:H | 1.78 | 0.49 |
| 2:R:8:LYS:HG2 | 2:Q:102:ASP:CB | 2.42 | 0.49 |
| 2:Q:20:ARG:HB3 | 2:Q:41:VAL:CG1 | 2.43 | 0.49 |
| 1:N:62:LEU:CD1 | 1:N:67:LYS:HB3 | 2.43 | 0.49 |
| 1:N:176:THR:HG22 | 1:N:379:VAL:HG12 | 1.94 | 0.49 |
| 1:N:497:PRO:HB2 | 1:N:500:VAL:HG12 | 1.95 | 0.49 |
| 1:L:32:GLY:N | 3:L:601:ADP:O2A | 2.44 | 0.49 |
| 1:L:127:VAL:HG23 | 1:L:423:CYS:CB | 2.42 | 0.49 |
| 1:C:188:GLU:HB3 | 1:C:379:VAL:HG22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:234:VAL:O | 1:C:238:GLU:HG3 | 2.12 | 0.49 |
| 1:B:99:ILE:HD13 | 1:B:509:ALA:HA | 1.93 | 0.49 |
| 1:B:231:GLN:O | 1:B:234:VAL:HG12 | 2.13 | 0.49 |
| 1:B:255:ASP:OD1 | 1:B:256:GLY:N | 2.46 | 0.49 |
| 1:A:234:VAL:O | 1:A:238:GLU:HG3 | 2.13 | 0.49 |
| 1:A:350:ILE:O | 1:A:366:LEU:HD11 | 2.12 | 0.49 |
| 1:F:140:THR:HG22 | 1:F:143:GLU:HG3 | 1.95 | 0.49 |
| 1:E:65:LYS:O | 1:E:69:ILE:HG13 | 2.13 | 0.49 |
| 1:E:206:ASN:HB3 | 1:E:266:ARG:NH2 | 2.27 | 0.49 |
| 2:S:27:THR:HG22 | 2:S:31:ILE:H | 1.77 | 0.49 |
| 1:M:14:ALA:O | 1:M:18:GLN:HG3 | 2.12 | 0.49 |
| 1:M:54:VAL:O | 1:M:58:LYS:N | 2.22 | 0.49 |
| 1:M:348:GLN:OE1 | 1:M:351:ILE:HD11 | 2.13 | 0.49 |
| 1:L:52:ASP:OD2 | 5:L:702:HOH:O | 2.20 | 0.49 |
| 1:L:124:VAL:HG21 | 1:L:509:ALA:CB | 2.43 | 0.49 |
| 1:L:203:TYR:HB3 | 1:L:267:LEU:HD11 | 1.93 | 0.49 |
| 1:K:394:LYS:O | 1:K:398:THR:HG23 | 2.13 | 0.49 |
| 1:J:24:ALA:CB | 1:J:97:ARG:HD3 | 2.40 | 0.49 |
| 1:D:194:LYS:HD2 | 1:D:332:MET:HE3 | 1.95 | 0.49 |
| 1:C:394:LYS:O | 1:C:398:THR:HG23 | 2.12 | 0.49 |
| 1:A:71:ALA:O | 1:A:75:GLN:HG3 | 2.12 | 0.49 |
| 1:A:157:GLU:O | 1:A:161:ILE:HG12 | 2.12 | 0.49 |
| 1:A:206:ASN:HB3 | 1:A:266:ARG:HH21 | 1.78 | 0.49 |
| 1:A:224:GLU:O | 1:A:252:GLU:HB2 | 2.12 | 0.49 |
| 1:F:135:SER:CB | 1:F:498:THR:HG21 | 2.43 | 0.49 |
| 1:F:400:ALA:O | 1:F:404:THR:HG23 | 2.13 | 0.49 |
| 1:H:230:ILE:HG13 | 1:H:261:THR:HG21 | 1.94 | 0.49 |
| 1:H:347:ILE:O | 1:H:351:ILE:HG23 | 2.13 | 0.49 |
| 2:1:13:PHE:CD1 | 2:1:54:LYS:HB2 | 2.48 | 0.49 |
| 2:O:81:VAL:HG12 | 2:U:72:LEU:HD21 | 1.95 | 0.49 |
| 2:U:34:PRO:CD | 1:G:261:THR:HG22 | 2.42 | 0.49 |
| 2:T:32:MET:CE | 1:F:268:LYS:HE3 | 2.41 | 0.49 |
| 1:N:348:GLN:OE1 | 1:N:351:ILE:HD11 | 2.13 | 0.49 |
| 1:K:131:LEU:HD23 | 1:K:134:GLN:HE21 | 1.77 | 0.49 |
| 1:J:195:PHE:CZ | 1:J:331:ALA:HB3 | 2.48 | 0.49 |
| 1:D:206:ASN:HB3 | 1:D:266:ARG:NH2 | 2.28 | 0.49 |
| 1:D:284:ASN:ND2 | 1:D:365:LYS:HE2 | 2.27 | 0.49 |
| 1:B:194:LYS:HD2 | 1:B:332:MET:HE2 | 1.95 | 0.49 |
| 1:A:135:SER:CB | 1:A:498:THR:HG21 | 2.43 | 0.49 |
| 1:A:285:ARG:HB3 | 1:A:289:LEU:HD13 | 1.94 | 0.49 |
| 1:G:157:GLU:O | 1:G:161:ILE:HG12 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:234:VAL:O | 1:H:238:GLU:HG3 | 2.13 | 0.49 |
| 2:1:56:LYS:HE3 | 2:1:61:GLN:OE1 | 2.13 | 0.49 |
| 2:S:20:ARG:HB3 | 2:S:41:VAL:CG1 | 2.43 | 0.49 |
| 1:M:324:VAL:HG22 | 1:M:333:LEU:CD2 | 2.43 | 0.49 |
| 1:M:450:ILE:O | 1:M:454:THR:HG23 | 2.12 | 0.49 |
| 1:J:20:VAL:HG13 | 1:J:74:VAL:HG21 | 1.95 | 0.49 |
| 1:I:233:ILE:HG13 | 1:I:237:LEU:CD1 | 2.41 | 0.49 |
| 1:I:251:ALA:O | 1:I:277:LYS:HA | 2.13 | 0.49 |
| 1:I:310:LEU:O | 1:I:313:VAL:HG13 | 2.12 | 0.49 |
| 1:D:234:VAL:O | 1:D:238:GLU:HG3 | 2.12 | 0.49 |
| 1:D:394:LYS:O | 1:D:398:THR:HG23 | 2.13 | 0.49 |
| 1:C:230:ILE:HG13 | 1:C:261:THR:HG21 | 1.95 | 0.49 |
| 1:G:234:VAL:O | 1:G:238:GLU:HG3 | 2.13 | 0.49 |
| 1:E:177:VAL:HG11 | 1:E:398:THR:CG2 | 2.42 | 0.49 |
| 1:H:124:VAL:HG21 | 1:H:509:ALA:CB | 2.43 | 0.48 |
| 1:H:138:VAL:CG1 | 1:H:408:VAL:HA | 2.43 | 0.48 |
| 1:H:177:VAL:HG11 | 1:H:398:THR:HG22 | 1.94 | 0.48 |
| 2:2:8:LYS:HA | 2:1:101:VAL:O | 2.13 | 0.48 |
| 2:1:65:VAL:HG22 | 2:1:93:ASP:OD1 | 2.13 | 0.48 |
| 2:R:101:VAL:O | 2:S:8:LYS:HA | 2.13 | 0.48 |
| 2:Q:56:LYS:HE3 | 2:Q:61:GLN:OE1 | 2.13 | 0.48 |
| 1:K:124:VAL:HG21 | 1:K:509:ALA:CB | 2.43 | 0.48 |
| 1:J:234:VAL:O | 1:J:238:GLU:HG3 | 2.13 | 0.48 |
| 1:I:346:ARG:O | 1:I:350:ILE:HD12 | 2.13 | 0.48 |
| 1:I:469:LYS:HG2 | 1:I:486:PHE:HE2 | 1.78 | 0.48 |
| 1:C:193:MET:HE1 | 1:C:292:MET:HA | 1.94 | 0.48 |
| 1:B:278:ALA:CB | 1:B:289:LEU:HD11 | 2.37 | 0.48 |
| 1:A:131:LEU:HD23 | 1:A:134:GLN:HE21 | 1.78 | 0.48 |
| 1:G:77:VAL:HG22 | 1:G:511:VAL:HB | 1.95 | 0.48 |
| 1:G:206:ASN:HB3 | 1:G:266:ARG:NH2 | 2.28 | 0.48 |
| 1:G:250:ILE:HD13 | 1:G:292:MET:HE1 | 1.95 | 0.48 |
| 1:F:140:THR:CG2 | 1:F:143:GLU:HG3 | 2.43 | 0.48 |
| 1:F:373:LEU:O | 1:F:373:LEU:HD23 | 2.13 | 0.48 |
| 1:M:188:GLU:OE1 | 1:M:381:LYS:NZ | 2.41 | 0.48 |
| 1:M:234:VAL:O | 1:M:238:GLU:HG3 | 2.12 | 0.48 |
| 1:K:233:ILE:HG13 | 1:K:237:LEU:CD1 | 2.42 | 0.48 |
| 1:J:251:ALA:O | 1:J:277:LYS:HA | 2.13 | 0.48 |
| 1:J:413:VAL:HB | 1:J:498:THR:HG22 | 1.93 | 0.48 |
| 1:I:230:ILE:HG13 | 1:I:261:THR:HG21 | 1.94 | 0.48 |
| 1:B:127:VAL:HG23 | 1:B:423:CYS:CB | 2.42 | 0.48 |
| 1:B:410:GLU:HG2 | 1:B:498:THR:OG1 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:410:GLU:HG2 | 1:G:498:THR:OG1 | 2.13 | 0.48 |
| 1:G:427:LEU:HA | 1:G:430:LEU:HD23 | 1.95 | 0.48 |
| 1:E:138:VAL:CG1 | 1:E:408:VAL:HA | 2.43 | 0.48 |
| 1:E:350:ILE:HG23 | 1:E:366:LEU:HD22 | 1.95 | 0.48 |
| 1:E:400:ALA:O | 1:E:404:THR:HG23 | 2.13 | 0.48 |
| 1:H:140:THR:HG23 | 1:H:143:GLU:H | 1.79 | 0.48 |
| 1:H:237:LEU:HB3 | 2:V:31:ILE:HD12 | 1.94 | 0.48 |
| 1:H:278:ALA:HB3 | 1:H:285:ARG:NH1 | 2.28 | 0.48 |
| 2:Z:27:THR:HG22 | 2:Z:31:ILE:H | 1.78 | 0.48 |
| 1:N:399:ASP:OD1 | 5:N:702:HOH:O | 2.19 | 0.48 |
| 1:M:255:ASP:OD1 | 1:M:256:GLY:N | 2.46 | 0.48 |
| 1:K:166:MET:HG3 | 1:K:171:ARG:HA | 1.96 | 0.48 |
| 1:K:291:ASP:OD1 | 1:K:346:ARG:NE | 2.40 | 0.48 |
| 1:I:71:ALA:O | 1:I:75:GLN:HG3 | 2.13 | 0.48 |
| 1:I:120:VAL:O | 1:I:124:VAL:HG23 | 2.13 | 0.48 |
| 1:C:255:ASP:OD1 | 1:C:256:GLY:N | 2.46 | 0.48 |
| 1:C:450:ILE:O | 1:C:454:THR:HG23 | 2.14 | 0.48 |
| 1:F:235:PRO:HG3 | 1:F:311:GLU:HA | 1.95 | 0.48 |
| 1:E:219:TYR:O | 1:E:248:VAL:HG22 | 2.14 | 0.48 |
| 1:E:469:LYS:HG2 | 1:E:486:PHE:HE2 | 1.77 | 0.48 |
| 2:W:27:THR:HG22 | 2:W:31:ILE:H | 1.78 | 0.48 |
| 2:T:78:GLY:HA3 | 2:T:91:PHE:CE1 | 2.48 | 0.48 |
| 1:N:324:VAL:HG22 | 1:N:333:LEU:CD2 | 2.43 | 0.48 |
| 1:N:394:LYS:O | 1:N:398:THR:HG23 | 2.13 | 0.48 |
| 1:M:206:ASN:HB3 | 1:M:266:ARG:NH2 | 2.28 | 0.48 |
| 1:L:99:ILE:HD13 | 1:L:509:ALA:HA | 1.94 | 0.48 |
| 1:L:234:VAL:O | 1:L:238:GLU:HG3 | 2.13 | 0.48 |
| 1:K:120:VAL:O | 1:K:124:VAL:HG23 | 2.14 | 0.48 |
| 1:J:52:ASP:OD2 | 5:J:702:HOH:O | 2.20 | 0.48 |
| 1:J:206:ASN:HB3 | 1:J:266:ARG:NH2 | 2.28 | 0.48 |
| 1:C:14:ALA:O | 1:C:18:GLN:HG3 | 2.12 | 0.48 |
| 1:B:348:GLN:OE1 | 1:B:351:ILE:HD11 | 2.13 | 0.48 |
| 1:A:348:GLN:OE1 | 1:A:351:ILE:HD11 | 2.13 | 0.48 |
| 1:G:188:GLU:HB3 | 1:G:379:VAL:HG22 | 1.94 | 0.48 |
| 1:G:206:ASN:HB3 | 1:G:266:ARG:HH21 | 1.79 | 0.48 |
| 1:E:120:VAL:O | 1:E:124:VAL:HG23 | 2.14 | 0.48 |
| 1:E:350:ILE:O | 1:E:366:LEU:HD11 | 2.14 | 0.48 |
| 1:H:271:LEU:HG | 1:H:273:VAL:HG13 | 1.95 | 0.48 |
| 2:V:16:VAL:O | 2:V:90:LEU:HD12 | 2.13 | 0.48 |
| 2:V:44:ALA:HB2 | 2:V:73:LEU:HD11 | 1.96 | 0.48 |
| 2:Y:34:PRO:HD2 | 1:K:230:ILE:HD12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:65:VAL:HG22 | 2:P:93:ASP:OD1 | 2.14 | 0.48 |
| 2:S:32:MET:CE | 1:E:268:LYS:HE3 | 2.43 | 0.48 |
| 1:N:183:LEU:CD1 | 1:N:385:THR:HG22 | 2.43 | 0.48 |
| 1:L:373:LEU:O | 1:L:373:LEU:HD23 | 2.13 | 0.48 |
| 1:K:237:LEU:HD21 | 1:K:262:LEU:CD2 | 2.43 | 0.48 |
| 1:I:248:VAL:HG11 | 1:I:324:VAL:HG11 | 1.96 | 0.48 |
| 1:D:169:VAL:HG21 | 1:D:378:ALA:HB2 | 1.94 | 0.48 |
| 1:C:421:LEU:CD2 | 1:C:467:VAL:HG13 | 2.39 | 0.48 |
| 1:B:188:GLU:HB3 | 1:B:379:VAL:HG22 | 1.94 | 0.48 |
| 1:G:22:LEU:HD11 | 1:F:6:VAL:CG2 | 2.42 | 0.48 |
| 1:F:14:ALA:O | 1:F:18:GLN:HG3 | 2.13 | 0.48 |
| 1:F:206:ASN:HB3 | 1:F:266:ARG:NH2 | 2.28 | 0.48 |
| 1:H:199:TYR:HD1 | 1:H:326:VAL:HG12 | 1.79 | 0.48 |
| 1:H:228:SER:HA | 1:H:255:ASP:HB3 | 1.95 | 0.48 |
| 1:H:322:GLY:N | 1:H:335:LYS:O | 2.35 | 0.48 |
| 2:V:90:LEU:CD2 | 2:2:97:LEU:HD12 | 2.36 | 0.48 |
| 2:X:44:ALA:HB2 | 2:X:73:LEU:HD11 | 1.95 | 0.48 |
| 2:W:13:PHE:CD1 | 2:W:54:LYS:HB3 | 2.48 | 0.48 |
| 1:L:77:VAL:HG22 | 1:L:511:VAL:HB | 1.94 | 0.48 |
| 1:K:24:ALA:CB | 1:K:97:ARG:HD3 | 2.41 | 0.48 |
| 1:K:157:GLU:O | 1:K:161:ILE:HG12 | 2.13 | 0.48 |
| 1:K:348:GLN:OE1 | 1:K:351:ILE:HD11 | 2.14 | 0.48 |
| 1:J:87:ASP:O | 1:J:500:VAL:HG23 | 2.13 | 0.48 |
| 1:J:324:VAL:HG22 | 1:J:333:LEU:CD2 | 2.44 | 0.48 |
| 1:I:373:LEU:O | 1:I:373:LEU:HD23 | 2.13 | 0.48 |
| 1:D:62:LEU:CD1 | 1:D:67:LYS:HB3 | 2.43 | 0.48 |
| 1:D:280:GLY:CA | 1:D:285:ARG:HB3 | 2.43 | 0.48 |
| 1:D:291:ASP:OD1 | 1:D:346:ARG:NE | 2.38 | 0.48 |
| 1:C:124:VAL:HG21 | 1:C:509:ALA:CB | 2.43 | 0.48 |
| 1:B:203:TYR:HB3 | 1:B:267:LEU:HD11 | 1.96 | 0.48 |
| 1:A:394:LYS:O | 1:A:398:THR:HG23 | 2.14 | 0.48 |
| 1:G:166:MET:CG | 1:G:171:ARG:HA | 2.43 | 0.48 |
| 1:E:250:ILE:HG12 | 1:E:276:VAL:CG2 | 2.44 | 0.48 |
| 1:H:233:ILE:HG13 | 1:H:237:LEU:CD1 | 2.42 | 0.48 |
| 1:H:301:PHE:CZ | 1:H:313:VAL:HG12 | 2.49 | 0.48 |
| 1:H:506:LEU:HD21 | 1:I:385:THR:HG21 | 1.95 | 0.48 |
| 2:O:26:VAL:HA | 2:O:32:MET:HA | 1.95 | 0.48 |
| 2:U:8:LYS:HG2 | 2:T:102:ASP:CB | 2.39 | 0.48 |
| 2:U:44:ALA:CB | 2:U:73:LEU:HD11 | 2.44 | 0.48 |
| 1:L:13:ARG:NH2 | 1:L:519:GLU:OE1 | 2.45 | 0.48 |
| 1:L:348:GLN:OE1 | 1:L:351:ILE:HD11 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:371:ALA:HB1 | 1:L:376:GLY:O | 2.13 | 0.48 |
| 1:J:347:ILE:O | 1:J:351:ILE:HG23 | 2.13 | 0.48 |
| 1:J:386:SER:O | 1:J:390:VAL:HG23 | 2.12 | 0.48 |
| 1:I:65:LYS:O | 1:I:69:ILE:HG13 | 2.14 | 0.48 |
| 1:I:400:ALA:O | 1:I:404:THR:HG23 | 2.13 | 0.48 |
| 1:D:120:VAL:HG13 | 1:D:444:ILE:CD1 | 2.40 | 0.48 |
| 1:D:230:ILE:HG13 | 1:D:261:THR:HG21 | 1.96 | 0.48 |
| 1:B:24:ALA:CB | 1:B:97:ARG:HD3 | 2.41 | 0.48 |
| 1:A:233:ILE:HG13 | 1:A:237:LEU:CD1 | 2.43 | 0.48 |
| 1:G:47:PRO:HG3 | 1:F:69:ILE:HG23 | 1.95 | 0.48 |
| 1:G:120:VAL:O | 1:G:124:VAL:HG23 | 2.14 | 0.48 |
| 1:G:421:LEU:CD2 | 1:G:467:VAL:HG13 | 2.41 | 0.48 |
| 1:F:207:THR:OG1 | 1:F:209:LYS:HB3 | 2.13 | 0.48 |
| 1:F:347:ILE:O | 1:F:351:ILE:HG23 | 2.13 | 0.48 |
| 1:E:87:ASP:O | 1:E:500:VAL:HG23 | 2.14 | 0.48 |
| 1:H:219:TYR:O | 1:H:248:VAL:HG22 | 2.13 | 0.48 |
| 2:W:44:ALA:HB2 | 2:W:73:LEU:HD11 | 1.96 | 0.48 |
| 2:R:27:THR:HG22 | 2:R:31:ILE:H | 1.78 | 0.48 |
| 1:N:224:GLU:OE1 | 1:N:303:GLU:HA | 2.14 | 0.48 |
| 1:M:124:VAL:HG21 | 1:M:509:ALA:CB | 2.44 | 0.48 |
| 1:M:371:ALA:HB1 | 1:M:376:GLY:O | 2.14 | 0.48 |
| 1:M:373:LEU:HD23 | 1:M:373:LEU:O | 2.14 | 0.48 |
| 1:M:456:ALA:CB | 1:M:463:GLY:HA2 | 2.42 | 0.48 |
| 1:K:39:ILE:HG12 | 1:K:49:VAL:HG22 | 1.95 | 0.48 |
| 1:K:234:VAL:O | 1:K:238:GLU:HG3 | 2.13 | 0.48 |
| 1:K:278:ALA:HB3 | 1:K:285:ARG:NH1 | 2.29 | 0.48 |
| 1:K:373:LEU:HD23 | 1:K:373:LEU:O | 2.14 | 0.48 |
| 1:J:157:GLU:O | 1:J:161:ILE:HG12 | 2.13 | 0.48 |
| 1:I:394:LYS:O | 1:I:398:THR:HG23 | 2.14 | 0.48 |
| 1:D:227:ILE:HG21 | 1:D:233:ILE:HD13 | 1.96 | 0.48 |
| 1:G:251:ALA:O | 1:G:277:LYS:HA | 2.14 | 0.48 |
| 1:H:116:ILE:O | 1:H:120:VAL:HG23 | 2.13 | 0.48 |
| 1:H:157:GLU:O | 1:H:161:ILE:HG12 | 2.14 | 0.48 |
| 2:V:78:GLY:HA3 | 2:V:91:PHE:CE1 | 2.49 | 0.48 |
| 2:Y:34:PRO:CD | 1:K:261:THR:HG22 | 2.41 | 0.48 |
| 2:X:15:ARG:NH2 | 2:W:97:LEU:HA | 2.29 | 0.48 |
| 2:X:34:PRO:HD2 | 1:J:230:ILE:HD12 | 1.96 | 0.48 |
| 2:S:78:GLY:HA3 | 2:S:91:PHE:CE1 | 2.49 | 0.48 |
| 1:N:52:ASP:OD2 | 5:N:702:HOH:O | 2.20 | 0.48 |
| 1:N:450:ILE:O | 1:N:454:THR:HG23 | 2.14 | 0.48 |
| 1:M:350:ILE:HG23 | 1:M:366:LEU:HD21 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:251:ALA:O | 1:L:277:LYS:HA | 2.14 | 0.48 |
| 1:D:166:MET:HG3 | 1:D:171:ARG:HA | 1.96 | 0.48 |
| 1:C:237:LEU:HD21 | 1:C:262:LEU:CD2 | 2.43 | 0.48 |
| 1:C:347:ILE:O | 1:C:351:ILE:HG23 | 2.13 | 0.48 |
| 1:B:71:ALA:O | 1:B:75:GLN:HG3 | 2.14 | 0.48 |
| 1:B:450:ILE:O | 1:B:454:THR:HG23 | 2.14 | 0.48 |
| 1:A:124:VAL:HG21 | 1:A:509:ALA:CB | 2.44 | 0.48 |
| 1:F:140:THR:HG23 | 1:F:143:GLU:H | 1.78 | 0.48 |
| 1:H:138:VAL:HA | 1:H:143:GLU:OE1 | 2.13 | 0.48 |
| 2:1:20:ARG:HB3 | 2:1:41:VAL:CG1 | 2.44 | 0.48 |
| 2:X:34:PRO:CD | 1:J:261:THR:HG22 | 2.44 | 0.48 |
| 2:Q:44:ALA:HB2 | 2:Q:73:LEU:HD11 | 1.96 | 0.48 |
| 2:U:34:PRO:HD2 | 1:G:230:ILE:HD12 | 1.94 | 0.48 |
| 1:N:127:VAL:HG23 | 1:N:423:CYS:CB | 2.44 | 0.48 |
| 1:N:402:ASN:OD1 | 1:N:405:ARG:NH2 | 2.43 | 0.48 |
| 1:L:71:ALA:O | 1:L:75:GLN:HG3 | 2.14 | 0.48 |
| 1:L:350:ILE:HG23 | 1:L:366:LEU:HD21 | 1.95 | 0.48 |
| 1:D:65:LYS:O | 1:D:69:ILE:HG13 | 2.14 | 0.48 |
| 1:G:324:VAL:HG22 | 1:G:333:LEU:CD2 | 2.44 | 0.48 |
| 1:G:394:LYS:O | 1:G:398:THR:HG23 | 2.14 | 0.48 |
| 1:F:123:ALA:HB3 | 1:F:444:ILE:HG13 | 1.96 | 0.48 |
| 1:E:366:LEU:HD13 | 1:E:370:LEU:CD1 | 2.44 | 0.48 |
| 1:H:348:GLN:OE1 | 1:H:351:ILE:HD11 | 2.14 | 0.47 |
| 1:H:350:ILE:HG23 | 1:H:366:LEU:HD21 | 1.96 | 0.47 |
| 2:2:52:GLY:HA3 | 2:2:60:ILE:HD12 | 1.96 | 0.47 |
| 2:R:53:SER:HB3 | 2:R:61:GLN:HB3 | 1.96 | 0.47 |
| 1:N:166:MET:HG3 | 1:N:171:ARG:HA | 1.95 | 0.47 |
| 1:N:188:GLU:HB3 | 1:N:379:VAL:HG22 | 1.95 | 0.47 |
| 1:M:188:GLU:HB3 | 1:M:379:VAL:HG22 | 1.94 | 0.47 |
| 1:J:280:GLY:O | 1:J:285:ARG:HB3 | 2.13 | 0.47 |
| 1:A:68:ASN:O | 1:A:72:LYS:HG2 | 2.14 | 0.47 |
| 1:A:87:ASP:O | 1:A:500:VAL:HG23 | 2.14 | 0.47 |
| 1:A:148:ALA:HB2 | 1:A:404:THR:CG2 | 2.43 | 0.47 |
| 1:G:350:ILE:HG23 | 1:G:366:LEU:HD21 | 1.96 | 0.47 |
| 1:G:371:ALA:HB1 | 1:G:376:GLY:O | 2.14 | 0.47 |
| 1:H:291:ASP:OD1 | 1:H:346:ARG:NE | 2.42 | 0.47 |
| 2:S:44:ALA:CB | 2:S:73:LEU:HD11 | 2.45 | 0.47 |
| 1:N:157:GLU:O | 1:N:161:ILE:HG12 | 2.14 | 0.47 |
| 1:M:169:VAL:HG21 | 1:M:378:ALA:HB2 | 1.95 | 0.47 |
| 1:M:230:ILE:HG13 | 1:M:261:THR:HG21 | 1.96 | 0.47 |
| 1:M:233:ILE:HG13 | 1:M:237:LEU:CD1 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:194:LYS:HD2 | 1:J:332:MET:HE3 | 1.96 | 0.47 |
| 1:J:239:ILE:CD1 | 1:J:313:VAL:HG23 | 2.43 | 0.47 |
| 1:J:394:LYS:O | 1:J:398:THR:HG23 | 2.14 | 0.47 |
| 1:D:120:VAL:O | 1:D:124:VAL:HG23 | 2.14 | 0.47 |
| 1:C:340:LYS:HA | 1:C:343:ILE:CG1 | 2.38 | 0.47 |
| 1:B:394:LYS:O | 1:B:398:THR:HG23 | 2.15 | 0.47 |
| 1:B:400:ALA:O | 1:B:404:THR:HG23 | 2.14 | 0.47 |
| 1:G:71:ALA:O | 1:G:75:GLN:HG3 | 2.14 | 0.47 |
| 1:G:127:VAL:HG11 | 1:G:505:LEU:HD21 | 1.95 | 0.47 |
| 1:G:525:ILE:HG23 | 1:G:526:PRO:HD2 | 1.96 | 0.47 |
| 1:F:24:ALA:CB | 1:F:97:ARG:HD3 | 2.41 | 0.47 |
| 1:F:62:LEU:CD1 | 1:F:67:LYS:HB3 | 2.44 | 0.47 |
| 1:F:310:LEU:O | 1:F:313:VAL:HG13 | 2.14 | 0.47 |
| 1:E:73:LEU:HD13 | 1:E:515:LEU:HD13 | 1.95 | 0.47 |
| 1:H:120:VAL:O | 1:H:124:VAL:HG23 | 2.14 | 0.47 |
| 2:1:31:ILE:HD11 | 1:M:237:LEU:HD22 | 1.95 | 0.47 |
| 2:O:44:ALA:HB2 | 2:O:73:LEU:HD11 | 1.96 | 0.47 |
| 2:U:16:VAL:CG1 | 2:U:46:VAL:HG23 | 2.45 | 0.47 |
| 1:N:233:ILE:HG13 | 1:N:237:LEU:HD13 | 1.95 | 0.47 |
| 1:N:347:ILE:O | 1:N:351:ILE:HG23 | 2.14 | 0.47 |
| 1:L:31:MET:SD | 1:L:454:THR:OG1 | 2.65 | 0.47 |
| 1:L:322:GLY:N | 1:L:335:LYS:O | 2.32 | 0.47 |
| 1:K:148:ALA:HB2 | 1:K:404:THR:CG2 | 2.43 | 0.47 |
| 1:J:400:ALA:O | 1:J:404:THR:HG23 | 2.14 | 0.47 |
| 1:I:348:GLN:OE1 | 1:I:351:ILE:HD11 | 2.14 | 0.47 |
| 1:C:456:ALA:CB | 1:C:463:GLY:HA2 | 2.44 | 0.47 |
| 1:B:366:LEU:HD13 | 1:B:370:LEU:CD1 | 2.45 | 0.47 |
| 1:G:68:ASN:O | 1:G:72:LYS:HG2 | 2.14 | 0.47 |
| 1:F:394:LYS:O | 1:F:398:THR:HG23 | 2.13 | 0.47 |
| 1:E:347:ILE:O | 1:E:351:ILE:HG23 | 2.13 | 0.47 |
| 2:Y:56:LYS:HE3 | 2:Y:61:GLN:OE1 | 2.14 | 0.47 |
| 2:X:8:LYS:O | 2:W:100:TYR:HA | 2.14 | 0.47 |
| 2:Q:5:ALA:HB2 | 2:Q:10:LEU:HD13 | 1.97 | 0.47 |
| 1:M:248:VAL:HG11 | 1:M:324:VAL:HG11 | 1.97 | 0.47 |
| 1:K:250:ILE:HG12 | 1:K:276:VAL:CG2 | 2.45 | 0.47 |
| 1:J:348:GLN:OE1 | 1:J:351:ILE:HD11 | 2.13 | 0.47 |
| 1:I:203:TYR:HB3 | 1:I:267:LEU:HD11 | 1.96 | 0.47 |
| 1:I:324:VAL:HG22 | 1:I:333:LEU:CD2 | 2.45 | 0.47 |
| 1:C:373:LEU:HD23 | 1:C:373:LEU:O | 2.14 | 0.47 |
| 1:B:157:GLU:O | 1:B:161:ILE:HG12 | 2.14 | 0.47 |
| 1:B:350:ILE:HG23 | 1:B:366:LEU:HD22 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:385:THR:CG2 | 1:A:506:LEU:HD21 | 2.43 | 0.47 |
| 1:A:292:MET:O | 1:A:296:THR:HG22 | 2.14 | 0.47 |
| 1:F:348:GLN:OE1 | 1:F:351:ILE:HD11 | 2.13 | 0.47 |
| 1:E:124:VAL:HG21 | 1:E:509:ALA:HB1 | 1.96 | 0.47 |
| 1:E:340:LYS:CA | 1:E:343:ILE:HG12 | 2.38 | 0.47 |
| 1:H:279:PRO:HB2 | 1:H:288:GLN:OE1 | 2.15 | 0.47 |
| 2:2:20:ARG:HB3 | 2:2:41:VAL:CG1 | 2.44 | 0.47 |
| 2:X:63:VAL:HG13 | 2:X:93:ASP:OD1 | 2.15 | 0.47 |
| 2:P:78:GLY:HA3 | 2:P:91:PHE:CE1 | 2.50 | 0.47 |
| 1:M:166:MET:HG3 | 1:M:171:ARG:HA | 1.97 | 0.47 |
| 1:M:280:GLY:CA | 1:M:285:ARG:HB3 | 2.44 | 0.47 |
| 1:L:13:ARG:HD3 | 1:L:104:PHE:HD1 | 1.78 | 0.47 |
| 1:J:124:VAL:HG21 | 1:J:509:ALA:CB | 2.44 | 0.47 |
| 1:I:301:PHE:CZ | 1:I:313:VAL:HG12 | 2.49 | 0.47 |
| 1:D:348:GLN:OE1 | 1:D:351:ILE:HD11 | 2.13 | 0.47 |
| 1:C:264:LEU:HD11 | 1:C:268:LYS:HE2 | 1.94 | 0.47 |
| 1:A:32:GLY:N | 3:A:601:ADP:O1A | 2.43 | 0.47 |
| 1:A:291:ASP:OD1 | 1:A:346:ARG:NE | 2.40 | 0.47 |
| 1:G:131:LEU:HD23 | 1:G:134:GLN:HE21 | 1.80 | 0.47 |
| 1:G:386:SER:O | 1:G:390:VAL:HG23 | 2.14 | 0.47 |
| 1:G:422:ARG:NH1 | 1:G:474:SER:O | 2.47 | 0.47 |
| 1:F:166:MET:CG | 1:F:171:ARG:HA | 2.44 | 0.47 |
| 1:H:346:ARG:O | 1:H:350:ILE:HD12 | 2.15 | 0.47 |
| 2:V:44:ALA:CB | 2:V:73:LEU:HD11 | 2.44 | 0.47 |
| 2:O:31:ILE:HD12 | 1:A:237:LEU:HB3 | 1.95 | 0.47 |
| 2:T:13:PHE:HA | 2:T:52:GLY:O | 2.14 | 0.47 |
| 1:N:120:VAL:O | 1:N:124:VAL:HG23 | 2.14 | 0.47 |
| 1:N:199:TYR:CE2 | 1:N:202:PRO:HA | 2.50 | 0.47 |
| 1:M:251:ALA:O | 1:M:277:LYS:HA | 2.14 | 0.47 |
| 1:L:65:LYS:O | 1:L:69:ILE:HG13 | 2.15 | 0.47 |
| 1:J:303:GLU:HB3 | 1:J:306:LEU:HB3 | 1.97 | 0.47 |
| 1:J:489:MET:O | 1:J:493:GLY:N | 2.35 | 0.47 |
| 1:D:237:LEU:HD21 | 1:D:262:LEU:CD2 | 2.43 | 0.47 |
| 1:D:450:ILE:O | 1:D:454:THR:HG23 | 2.15 | 0.47 |
| 1:B:99:ILE:CD1 | 1:B:509:ALA:HA | 2.44 | 0.47 |
| 1:B:176:THR:HG22 | 1:B:379:VAL:HG12 | 1.96 | 0.47 |
| 1:A:227:ILE:HG21 | 1:A:233:ILE:HD13 | 1.97 | 0.47 |
| 1:A:373:LEU:O | 1:A:373:LEU:HD23 | 2.14 | 0.47 |
| 1:G:14:ALA:O | 1:G:18:GLN:HG3 | 2.15 | 0.47 |
| 1:F:127:VAL:HG23 | 1:F:423:CYS:HB3 | 1.97 | 0.47 |
| 1:E:161:ILE:CG2 | 1:E:380:LEU:HD22 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:207:THR:OG1 | 1:E:209:LYS:HB3 | 2.15 | 0.47 |
| 1:E:340:LYS:HA | 1:E:343:ILE:CG1 | 2.38 | 0.47 |
| 1:H:31:MET:SD | 1:H:454:THR:OG1 | 2.66 | 0.47 |
| 1:H:140:THR:CG2 | 1:H:143:GLU:HG3 | 2.45 | 0.47 |
| 1:H:140:THR:HG22 | 1:H:143:GLU:HG3 | 1.97 | 0.47 |
| 1:H:255:ASP:OD1 | 1:H:256:GLY:N | 2.45 | 0.47 |
| 1:H:394:LYS:O | 1:H:398:THR:HG23 | 2.14 | 0.47 |
| 2:X:78:GLY:HA3 | 2:X:91:PHE:CE1 | 2.50 | 0.47 |
| 2:P:34:PRO:CD | 1:B:261:THR:HG22 | 2.45 | 0.47 |
| 2:O:8:LYS:HA | 2:U:101:VAL:O | 2.15 | 0.47 |
| 2:U:31:ILE:HD12 | 1:G:237:LEU:CB | 2.45 | 0.47 |
| 1:N:324:VAL:HG22 | 1:N:333:LEU:HD23 | 1.96 | 0.47 |
| 1:M:69:ILE:HD11 | 1:M:523:THR:HG22 | 1.95 | 0.47 |
| 1:M:195:PHE:CG | 1:M:279:PRO:HG3 | 2.49 | 0.47 |
| 1:M:347:ILE:O | 1:M:351:ILE:HG23 | 2.14 | 0.47 |
| 1:M:497:PRO:HD2 | 1:M:500:VAL:HG11 | 1.96 | 0.47 |
| 1:L:24:ALA:CB | 1:L:97:ARG:HD3 | 2.41 | 0.47 |
| 1:K:138:VAL:HA | 1:K:143:GLU:OE1 | 2.15 | 0.47 |
| 1:J:62:LEU:CD1 | 1:J:67:LYS:HB3 | 2.43 | 0.47 |
| 1:J:193:MET:HE1 | 1:J:292:MET:HA | 1.96 | 0.47 |
| 1:J:278:ALA:HB1 | 1:J:289:LEU:HD11 | 1.95 | 0.47 |
| 1:J:373:LEU:O | 1:J:373:LEU:HD23 | 2.14 | 0.47 |
| 1:J:402:ASN:OD1 | 1:J:405:ARG:NH2 | 2.44 | 0.47 |
| 1:I:347:ILE:O | 1:I:351:ILE:HG23 | 2.15 | 0.47 |
| 1:D:124:VAL:HA | 1:D:127:VAL:HG12 | 1.97 | 0.47 |
| 1:D:157:GLU:O | 1:D:161:ILE:HG12 | 2.14 | 0.47 |
| 1:D:239:ILE:CD1 | 1:D:313:VAL:HG23 | 2.44 | 0.47 |
| 1:D:347:ILE:O | 1:D:351:ILE:HG23 | 2.14 | 0.47 |
| 1:C:203:TYR:HB3 | 1:C:267:LEU:HD11 | 1.97 | 0.47 |
| 1:C:233:ILE:HG13 | 1:C:237:LEU:CD1 | 2.44 | 0.47 |
| 1:B:62:LEU:CD1 | 1:B:67:LYS:HB3 | 2.44 | 0.47 |
| 1:B:347:ILE:O | 1:B:351:ILE:HG23 | 2.15 | 0.47 |
| 1:A:77:VAL:HG22 | 1:A:511:VAL:HB | 1.96 | 0.47 |
| 1:A:120:VAL:O | 1:A:124:VAL:HG23 | 2.14 | 0.47 |
| 1:A:223:SER:HB3 | 1:A:251:ALA:HB2 | 1.97 | 0.47 |
| 1:A:228:SER:HA | 1:A:255:ASP:HB3 | 1.96 | 0.47 |
| 1:G:73:LEU:HD12 | 1:G:515:LEU:HD13 | 1.96 | 0.47 |
| 1:G:138:VAL:HA | 1:G:143:GLU:OE1 | 2.14 | 0.47 |
| 1:G:239:ILE:CD1 | 1:G:313:VAL:HG23 | 2.44 | 0.47 |
| 1:G:332:MET:HG2 | 1:G:334:LEU:CD1 | 2.45 | 0.47 |
| 1:G:450:ILE:O | 1:G:454:THR:HG23 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:32:GLY:N | 3:E:601:ADP:O1A | 2.45 | 0.47 |
| 1:E:124:VAL:HA | 1:E:127:VAL:HG12 | 1.97 | 0.47 |
| 1:E:127:VAL:HG23 | 1:E:423:CYS:CB | 2.44 | 0.47 |
| 1:E:169:VAL:HG21 | 1:E:378:ALA:HB2 | 1.97 | 0.47 |
| 1:E:219:TYR:CE2 | 1:E:245:LYS:HB2 | 2.50 | 0.47 |
| 1:E:257:GLU:O | 1:E:261:THR:HG23 | 2.15 | 0.47 |
| 1:E:367:ASN:HA | 1:E:370:LEU:HD13 | 1.95 | 0.47 |
| 2:X:20:ARG:HB3 | 2:X:41:VAL:CG1 | 2.45 | 0.47 |
| 2:Q:13:PHE:HZ | 2:P:64:SER:HG | 1.62 | 0.47 |
| 2:U:27:THR:HG22 | 2:U:31:ILE:H | 1.80 | 0.47 |
| 2:U:78:GLY:HA3 | 2:U:91:PHE:CE1 | 2.49 | 0.47 |
| 2:T:5:ALA:HB2 | 2:T:10:LEU:HD13 | 1.97 | 0.47 |
| 2:T:44:ALA:HB2 | 2:T:73:LEU:HD11 | 1.97 | 0.47 |
| 1:N:127:VAL:HG11 | 1:N:505:LEU:HD21 | 1.97 | 0.47 |
| 1:N:138:VAL:HA | 1:N:143:GLU:OE1 | 2.15 | 0.47 |
| 1:N:413:VAL:HB | 1:N:498:THR:HG22 | 1.96 | 0.47 |
| 1:J:14:ALA:O | 1:J:18:GLN:HG3 | 2.14 | 0.47 |
| 1:J:71:ALA:O | 1:J:75:GLN:HG3 | 2.15 | 0.47 |
| 1:D:138:VAL:HA | 1:D:143:GLU:OE1 | 2.15 | 0.47 |
| 1:C:497:PRO:HB2 | 1:C:500:VAL:HG12 | 1.96 | 0.47 |
| 1:B:350:ILE:HG23 | 1:B:366:LEU:HD21 | 1.97 | 0.47 |
| 1:B:367:ASN:HA | 1:B:370:LEU:HD13 | 1.97 | 0.47 |
| 1:A:47:PRO:HG3 | 1:G:69:ILE:HG23 | 1.95 | 0.47 |
| 1:A:161:ILE:CG2 | 1:A:380:LEU:HD22 | 2.45 | 0.47 |
| 1:A:400:ALA:O | 1:A:404:THR:HG23 | 2.15 | 0.47 |
| 1:G:166:MET:HG3 | 1:G:171:ARG:HA | 1.97 | 0.47 |
| 1:G:347:ILE:O | 1:G:351:ILE:HG23 | 2.14 | 0.47 |
| 1:H:332:MET:HG2 | 1:H:334:LEU:CD1 | 2.45 | 0.47 |
| 1:H:340:LYS:HA | 1:H:343:ILE:CG1 | 2.38 | 0.47 |
| 2:Y:31:ILE:HD11 | 1:K:237:LEU:HD22 | 1.97 | 0.47 |
| 2:Y:78:GLY:HA3 | 2:Y:91:PHE:CE1 | 2.50 | 0.47 |
| 2:R:20:ARG:HB3 | 2:R:41:VAL:CG1 | 2.44 | 0.47 |
| 2:U:31:ILE:HG12 | 2:U:32:MET:H | 1.80 | 0.47 |
| 1:L:62:LEU:CD1 | 1:L:67:LYS:HB3 | 2.44 | 0.47 |
| 1:K:203:TYR:HB3 | 1:K:267:LEU:HD11 | 1.96 | 0.47 |
| 1:K:332:MET:HG2 | 1:K:334:LEU:CD1 | 2.45 | 0.47 |
| 1:K:386:SER:O | 1:K:390:VAL:HG23 | 2.15 | 0.47 |
| 1:J:120:VAL:O | 1:J:124:VAL:HG23 | 2.15 | 0.47 |
| 1:J:382:VAL:HG23 | 1:J:390:VAL:HG13 | 1.97 | 0.47 |
| 1:I:291:ASP:OD1 | 1:I:346:ARG:NE | 2.43 | 0.47 |
| 1:I:332:MET:HG2 | 1:I:334:LEU:HD12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:206:ASN:HB3 | 1:D:266:ARG:HH21 | 1.80 | 0.47 |
| 1:C:138:VAL:HA | 1:C:143:GLU:OE1 | 2.14 | 0.47 |
| 1:C:195:PHE:CD2 | 1:C:197:ARG:HB3 | 2.50 | 0.47 |
| 1:C:219:TYR:O | 1:C:248:VAL:HG22 | 2.14 | 0.47 |
| 1:C:404:THR:O | 1:C:408:VAL:HG13 | 2.15 | 0.47 |
| 1:A:248:VAL:HG11 | 1:A:324:VAL:HG11 | 1.95 | 0.47 |
| 1:A:332:MET:HG2 | 1:A:334:LEU:CD1 | 2.45 | 0.47 |
| 1:A:347:ILE:O | 1:A:351:ILE:HG23 | 2.15 | 0.47 |
| 1:G:197:ARG:NE | 1:G:278:ALA:O | 2.47 | 0.47 |
| 1:G:225:LYS:HA | 1:G:252:GLU:OE1 | 2.15 | 0.47 |
| 1:G:250:ILE:HG12 | 1:G:276:VAL:CG2 | 2.45 | 0.47 |
| 1:F:219:TYR:O | 1:F:248:VAL:HG22 | 2.15 | 0.47 |
| 1:F:264:LEU:O | 1:F:268:LYS:HG2 | 2.15 | 0.47 |
| 1:E:332:MET:HG2 | 1:E:334:LEU:CD1 | 2.45 | 0.47 |
| 1:E:394:LYS:O | 1:E:398:THR:HG23 | 2.14 | 0.47 |
| 1:E:421:LEU:CD2 | 1:E:467:VAL:HG13 | 2.42 | 0.47 |
| 2:Z:8:LYS:HA | 2:Y:101:VAL:O | 2.15 | 0.47 |
| 2:Z:56:LYS:HE3 | 2:Z:61:GLN:OE1 | 2.15 | 0.47 |
| 1:N:22:LEU:HD11 | 1:M:6:VAL:HG21 | 1.96 | 0.47 |
| 1:N:206:ASN:HB3 | 1:N:266:ARG:NH2 | 2.30 | 0.47 |
| 1:M:138:VAL:HA | 1:M:143:GLU:OE1 | 2.14 | 0.47 |
| 1:M:404:THR:O | 1:M:408:VAL:HG13 | 2.14 | 0.47 |
| 1:K:68:ASN:O | 1:K:72:LYS:HG2 | 2.15 | 0.47 |
| 1:K:87:ASP:O | 1:K:500:VAL:HG23 | 2.14 | 0.47 |
| 1:K:332:MET:HG2 | 1:K:334:LEU:HD12 | 1.97 | 0.47 |
| 1:J:166:MET:HG3 | 1:J:171:ARG:HA | 1.97 | 0.47 |
| 1:C:402:ASN:OD1 | 1:C:405:ARG:NH2 | 2.45 | 0.47 |
| 1:B:42:GLN:HG2 | 1:B:47:PRO:HA | 1.97 | 0.47 |
| 1:A:199:TYR:HD1 | 1:A:326:VAL:HG12 | 1.80 | 0.47 |
| 1:A:210:GLY:HA2 | 1:G:356:VAL:HG21 | 1.97 | 0.47 |
| 1:F:161:ILE:HG22 | 1:F:380:LEU:HD22 | 1.97 | 0.47 |
| 1:F:350:ILE:O | 1:F:366:LEU:HD11 | 2.14 | 0.47 |
| 1:E:157:GLU:O | 1:E:161:ILE:HG12 | 2.14 | 0.47 |
| 2:2:32:MET:SD | 1:N:268:LYS:HD3 | 2.55 | 0.46 |
| 2:R:78:GLY:HA3 | 2:R:91:PHE:CE1 | 2.51 | 0.46 |
| 1:L:127:VAL:HG11 | 1:L:505:LEU:HD21 | 1.97 | 0.46 |
| 1:L:195:PHE:CG | 1:L:279:PRO:HG3 | 2.51 | 0.46 |
| 1:K:427:LEU:HA | 1:K:430:LEU:HD23 | 1.97 | 0.46 |
| 1:J:332:MET:HG2 | 1:J:334:LEU:HD12 | 1.97 | 0.46 |
| 1:I:371:ALA:HB1 | 1:I:376:GLY:O | 2.16 | 0.46 |
| 1:D:183:LEU:CD1 | 1:D:385:THR:HG22 | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:399:ASP:OD1 | 5:D:702:HOH:O | 2.19 | 0.46 |
| 1:C:371:ALA:HB1 | 1:C:376:GLY:O | 2.15 | 0.46 |
| 1:C:497:PRO:HD2 | 1:C:500:VAL:HG11 | 1.97 | 0.46 |
| 1:A:39:ILE:HG12 | 1:A:49:VAL:HG22 | 1.97 | 0.46 |
| 1:A:350:ILE:HG23 | 1:A:366:LEU:HD22 | 1.97 | 0.46 |
| 1:G:127:VAL:HG23 | 1:G:423:CYS:CB | 2.46 | 0.46 |
| 1:G:248:VAL:HG11 | 1:G:324:VAL:HG11 | 1.97 | 0.46 |
| 1:G:350:ILE:HG22 | 1:G:370:LEU:HD11 | 1.97 | 0.46 |
| 1:E:166:MET:HG3 | 1:E:171:ARG:HA | 1.97 | 0.46 |
| 1:E:450:ILE:O | 1:E:454:THR:HG23 | 2.15 | 0.46 |
| 1:H:450:ILE:O | 1:H:454:THR:HG23 | 2.16 | 0.46 |
| 2:1:15:ARG:HH22 | 2:Z:97:LEU:HA | 1.80 | 0.46 |
| 2:O:34:PRO:CD | 1:A:261:THR:HG22 | 2.45 | 0.46 |
| 1:N:3:ALA:HB3 | 1:N:525:ILE:HD12 | 1.96 | 0.46 |
| 1:N:366:LEU:HD13 | 1:N:370:LEU:CD1 | 2.45 | 0.46 |
| 1:N:400:ALA:O | 1:N:404:THR:HG23 | 2.16 | 0.46 |
| 1:M:127:VAL:HG23 | 1:M:423:CYS:CB | 2.46 | 0.46 |
| 1:M:157:GLU:O | 1:M:161:ILE:HG12 | 2.15 | 0.46 |
| 1:L:394:LYS:O | 1:L:398:THR:HG23 | 2.14 | 0.46 |
| 1:K:120:VAL:HG13 | 1:K:444:ILE:CD1 | 2.41 | 0.46 |
| 1:K:255:ASP:OD1 | 1:K:256:GLY:N | 2.45 | 0.46 |
| 1:K:347:ILE:O | 1:K:351:ILE:HG23 | 2.15 | 0.46 |
| 1:K:497:PRO:HB2 | 1:K:500:VAL:HG12 | 1.96 | 0.46 |
| 1:J:228:SER:HA | 1:J:255:ASP:HB3 | 1.97 | 0.46 |
| 1:J:264:LEU:CG | 1:J:268:LYS:HE2 | 2.44 | 0.46 |
| 1:J:346:ARG:O | 1:J:350:ILE:HD12 | 2.15 | 0.46 |
| 1:D:332:MET:HG2 | 1:D:334:LEU:HD12 | 1.97 | 0.46 |
| 1:B:14:ALA:O | 1:B:18:GLN:HG3 | 2.15 | 0.46 |
| 1:G:136:LYS:HE3 | 1:G:412:ILE:HD11 | 1.96 | 0.46 |
| 1:G:188:GLU:OE1 | 1:G:381:LYS:NZ | 2.46 | 0.46 |
| 1:G:207:THR:OG1 | 1:G:209:LYS:HB3 | 2.16 | 0.46 |
| 1:G:444:ILE:O | 1:G:448:LEU:HG | 2.15 | 0.46 |
| 1:F:138:VAL:HA | 1:F:143:GLU:OE1 | 2.15 | 0.46 |
| 1:F:413:VAL:HB | 1:F:498:THR:HG22 | 1.98 | 0.46 |
| 1:E:138:VAL:HA | 1:E:143:GLU:OE1 | 2.15 | 0.46 |
| 1:E:231:GLN:O | 1:E:234:VAL:HG12 | 2.16 | 0.46 |
| 1:H:139:THR:O | 1:H:171:ARG:NH2 | 2.33 | 0.46 |
| 1:H:194:LYS:HD2 | 1:H:332:MET:HE3 | 1.97 | 0.46 |
| 2:V:56:LYS:HE3 | 2:V:61:GLN:OE1 | 2.15 | 0.46 |
| 2:1:31:ILE:HD12 | 1:M:237:LEU:CB | 2.46 | 0.46 |
| 2:1:34:PRO:HD2 | 1:M:230:ILE:HD12 | 1.95 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Z:18:VAL:HG12 | 2:Z:46:VAL:CA | 2.37 | 0.46 |
| 1:N:73:LEU:HD12 | 1:N:515:LEU:HD13 | 1.96 | 0.46 |
| 1:N:255:ASP:OD1 | 1:N:256:GLY:N | 2.47 | 0.46 |
| 1:M:71:ALA:O | 1:M:75:GLN:HG3 | 2.16 | 0.46 |
| 1:M:207:THR:OG1 | 1:M:209:LYS:HB3 | 2.15 | 0.46 |
| 1:K:14:ALA:O | 1:K:18:GLN:HG3 | 2.14 | 0.46 |
| 1:D:87:ASP:O | 1:D:500:VAL:HG23 | 2.14 | 0.46 |
| 1:D:127:VAL:HG23 | 1:D:423:CYS:CB | 2.45 | 0.46 |
| 1:C:166:MET:HG3 | 1:C:171:ARG:HA | 1.97 | 0.46 |
| 1:A:230:ILE:HG13 | 1:A:261:THR:HG21 | 1.97 | 0.46 |
| 1:A:346:ARG:O | 1:A:350:ILE:HD12 | 2.15 | 0.46 |
| 1:A:497:PRO:HD2 | 1:A:500:VAL:HG11 | 1.98 | 0.46 |
| 1:G:187:LEU:HD13 | 1:G:380:LEU:CD2 | 2.46 | 0.46 |
| 1:F:219:TYR:HB3 | 1:F:318:LEU:HD23 | 1.98 | 0.46 |
| 1:F:402:ASN:OD1 | 1:F:405:ARG:NH2 | 2.46 | 0.46 |
| 1:E:54:VAL:O | 1:E:58:LYS:N | 2.23 | 0.46 |
| 1:E:116:ILE:O | 1:E:120:VAL:HG23 | 2.16 | 0.46 |
| 1:E:176:THR:HG22 | 1:E:379:VAL:HG12 | 1.96 | 0.46 |
| 1:H:166:MET:HG3 | 1:H:171:ARG:HA | 1.96 | 0.46 |
| 1:H:248:VAL:HG11 | 1:H:324:VAL:HG11 | 1.97 | 0.46 |
| 2:1:27:THR:CG2 | 2:1:31:ILE:H | 2.28 | 0.46 |
| 2:W:44:ALA:CB | 2:W:73:LEU:HD11 | 2.46 | 0.46 |
| 2:T:3:GLY:CA | 2:T:51:SER:HA | 2.44 | 0.46 |
| 2:T:20:ARG:HB3 | 2:T:41:VAL:CG1 | 2.46 | 0.46 |
| 2:S:9:PHE:CD2 | 2:S:17:LEU:HD22 | 2.51 | 0.46 |
| 2:S:33:LEU:HG | 1:E:230:ILE:HD11 | 1.97 | 0.46 |
| 1:N:207:THR:OG1 | 1:N:209:LYS:HB3 | 2.16 | 0.46 |
| 1:N:367:ASN:HA | 1:N:370:LEU:HD13 | 1.97 | 0.46 |
| 1:M:296:THR:OG1 | 1:M:320:LYS:O | 2.32 | 0.46 |
| 1:L:99:ILE:CD1 | 1:L:509:ALA:HA | 2.44 | 0.46 |
| 1:L:385:THR:CG2 | 1:K:506:LEU:HD21 | 2.45 | 0.46 |
| 1:K:127:VAL:HG11 | 1:K:505:LEU:HD21 | 1.98 | 0.46 |
| 1:J:117:ARG:NH1 | 1:J:514:LEU:HB2 | 2.31 | 0.46 |
| 1:J:255:ASP:OD1 | 1:J:256:GLY:N | 2.46 | 0.46 |
| 1:D:73:LEU:HD12 | 1:D:515:LEU:HD13 | 1.96 | 0.46 |
| 1:D:255:ASP:OD1 | 1:D:256:GLY:N | 2.47 | 0.46 |
| 1:C:195:PHE:CZ | 1:C:331:ALA:HB3 | 2.50 | 0.46 |
| 1:E:114:VAL:HG12 | 1:E:118:ARG:NH1 | 2.31 | 0.46 |
| 1:H:332:MET:HG2 | 1:H:334:LEU:HD12 | 1.96 | 0.46 |
| 2:V:10:LEU:HD12 | 2:V:11:PRO:HD2 | 1.98 | 0.46 |
| 2:1:78:GLY:HA3 | 2:1:91:PHE:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:44:ALA:CB | 2:T:73:LEU:HD11 | 2.45 | 0.46 |
| 1:L:280:GLY:CA | 1:L:285:ARG:HB3 | 2.45 | 0.46 |
| 1:L:293:ALA:O | 1:L:297:GLY:N | 2.33 | 0.46 |
| 1:L:347:ILE:O | 1:L:351:ILE:HG23 | 2.15 | 0.46 |
| 1:L:366:LEU:HD13 | 1:L:370:LEU:CD1 | 2.46 | 0.46 |
| 1:C:157:GLU:O | 1:C:161:ILE:HG12 | 2.15 | 0.46 |
| 1:G:346:ARG:O | 1:G:350:ILE:HD12 | 2.14 | 0.46 |
| 1:H:73:LEU:HD13 | 1:H:515:LEU:HD13 | 1.97 | 0.46 |
| 1:H:207:THR:OG1 | 1:H:209:LYS:HB3 | 2.16 | 0.46 |
| 1:H:366:LEU:HD13 | 1:H:370:LEU:CD1 | 2.46 | 0.46 |
| 2:V:8:LYS:HA | 2:2:101:VAL:O | 2.15 | 0.46 |
| 2:V:72:LEU:HD21 | 2:W:81:VAL:HG12 | 1.97 | 0.46 |
| 2:Z:15:ARG:HG2 | 2:Z:90:LEU:HD21 | 1.97 | 0.46 |
| 2:R:31:ILE:HG21 | 1:D:234:VAL:HG23 | 1.98 | 0.46 |
| 2:P:90:LEU:CD2 | 2:O:97:LEU:HD12 | 2.34 | 0.46 |
| 1:N:248:VAL:HG11 | 1:N:324:VAL:HG11 | 1.97 | 0.46 |
| 1:L:350:ILE:O | 1:L:366:LEU:HD11 | 2.15 | 0.46 |
| 1:K:166:MET:CG | 1:K:171:ARG:HA | 2.46 | 0.46 |
| 1:J:68:ASN:O | 1:J:72:LYS:HG2 | 2.16 | 0.46 |
| 1:D:346:ARG:O | 1:D:350:ILE:HD12 | 2.16 | 0.46 |
| 1:D:350:ILE:HG22 | 1:D:370:LEU:HD11 | 1.98 | 0.46 |
| 1:D:386:SER:O | 1:D:390:VAL:HG23 | 2.16 | 0.46 |
| 1:C:71:ALA:O | 1:C:75:GLN:HG3 | 2.16 | 0.46 |
| 1:A:497:PRO:HB2 | 1:A:500:VAL:HG12 | 1.97 | 0.46 |
| 1:F:138:VAL:CG1 | 1:F:408:VAL:HA | 2.46 | 0.46 |
| 1:F:199:TYR:CE2 | 1:F:202:PRO:HA | 2.51 | 0.46 |
| 1:E:255:ASP:OD1 | 1:E:256:GLY:N | 2.46 | 0.46 |
| 1:H:362:GLU:O | 1:H:366:LEU:HB2 | 2.15 | 0.46 |
| 1:H:427:LEU:HA | 1:H:430:LEU:HD23 | 1.98 | 0.46 |
| 2:X:10:LEU:HD12 | 2:X:11:PRO:HD2 | 1.98 | 0.46 |
| 2:Q:44:ALA:CB | 2:Q:73:LEU:HD11 | 2.46 | 0.46 |
| 2:P:16:VAL:C | 2:P:90:LEU:HD12 | 2.36 | 0.46 |
| 2:P:27:THR:HG22 | 2:P:31:ILE:H | 1.80 | 0.46 |
| 2:P:44:ALA:CB | 2:P:73:LEU:HD11 | 2.46 | 0.46 |
| 1:M:291:ASP:OD1 | 1:M:346:ARG:NE | 2.41 | 0.46 |
| 1:K:77:VAL:HG22 | 1:K:511:VAL:HB | 1.96 | 0.46 |
| 1:K:324:VAL:HG22 | 1:K:333:LEU:CD2 | 2.46 | 0.46 |
| 1:K:346:ARG:O | 1:K:350:ILE:HD12 | 2.15 | 0.46 |
| 1:I:194:LYS:HD2 | 1:I:332:MET:HE2 | 1.98 | 0.46 |
| 1:D:219:TYR:O | 1:D:248:VAL:HG22 | 2.16 | 0.46 |
| 1:C:47:PRO:HG3 | 1:B:69:ILE:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:169:VAL:HG21 | 1:C:378:ALA:HB2 | 1.97 | 0.46 |
| 1:C:207:THR:OG1 | 1:C:209:LYS:HB3 | 2.16 | 0.46 |
| 1:C:251:ALA:O | 1:C:277:LYS:HA | 2.15 | 0.46 |
| 1:B:257:GLU:O | 1:B:261:THR:HG23 | 2.15 | 0.46 |
| 1:A:24:ALA:CB | 1:A:97:ARG:HD3 | 2.41 | 0.46 |
| 1:G:280:GLY:O | 1:G:285:ARG:HD3 | 2.16 | 0.46 |
| 1:G:366:LEU:HD13 | 1:G:370:LEU:CD1 | 2.46 | 0.46 |
| 1:F:71:ALA:O | 1:F:75:GLN:HG3 | 2.16 | 0.46 |
| 1:E:251:ALA:O | 1:E:277:LYS:HA | 2.15 | 0.46 |
| 1:E:324:VAL:HG22 | 1:E:333:LEU:HD23 | 1.97 | 0.46 |
| 1:E:346:ARG:O | 1:E:350:ILE:HD12 | 2.15 | 0.46 |
| 1:H:14:ALA:O | 1:H:18:GLN:HG3 | 2.16 | 0.46 |
| 1:H:62:LEU:CD1 | 1:H:67:LYS:HB3 | 2.46 | 0.46 |
| 1:H:127:VAL:HG11 | 1:H:505:LEU:HD21 | 1.97 | 0.46 |
| 2:2:78:GLY:HA3 | 2:2:91:PHE:CE1 | 2.51 | 0.46 |
| 2:1:5:ALA:HB2 | 2:1:10:LEU:HD13 | 1.98 | 0.46 |
| 2:X:44:ALA:CB | 2:X:73:LEU:HD11 | 2.46 | 0.46 |
| 2:O:44:ALA:CB | 2:O:73:LEU:HD11 | 2.45 | 0.46 |
| 1:N:87:ASP:O | 1:N:500:VAL:HG23 | 2.16 | 0.46 |
| 1:N:231:GLN:O | 1:N:234:VAL:HG12 | 2.16 | 0.46 |
| 1:N:285:ARG:HG3 | 1:N:286:LYS:HD2 | 1.97 | 0.46 |
| 1:M:340:LYS:HA | 1:M:343:ILE:CG1 | 2.38 | 0.46 |
| 1:L:157:GLU:O | 1:L:161:ILE:HG12 | 2.15 | 0.46 |
| 1:K:124:VAL:HA | 1:K:127:VAL:HG12 | 1.98 | 0.46 |
| 1:J:207:THR:HG21 | 1:J:212:LYS:H | 1.81 | 0.46 |
| 1:J:227:ILE:HG21 | 1:J:233:ILE:HD13 | 1.98 | 0.46 |
| 1:I:255:ASP:OD1 | 1:I:256:GLY:N | 2.46 | 0.46 |
| 1:B:124:VAL:HA | 1:B:127:VAL:HG12 | 1.98 | 0.46 |
| 1:B:280:GLY:C | 1:B:285:ARG:HB2 | 2.35 | 0.46 |
| 1:G:219:TYR:CE2 | 1:G:245:LYS:HB2 | 2.51 | 0.46 |
| 1:G:348:GLN:OE1 | 1:G:351:ILE:HD11 | 2.15 | 0.46 |
| 1:F:332:MET:HG2 | 1:F:334:LEU:HD12 | 1.96 | 0.46 |
| 1:E:140:THR:HG23 | 1:E:143:GLU:H | 1.81 | 0.46 |
| 1:E:222:LEU:CD2 | 1:E:250:ILE:HB | 2.43 | 0.46 |
| 1:H:131:LEU:HD23 | 1:H:134:GLN:HE21 | 1.81 | 0.46 |
| 2:W:56:LYS:HE3 | 2:W:61:GLN:OE1 | 2.15 | 0.46 |
| 2:Q:27:THR:CG2 | 2:Q:31:ILE:H | 2.29 | 0.46 |
| 1:N:117:ARG:NH1 | 1:N:514:LEU:HB2 | 2.30 | 0.46 |
| 1:N:195:PHE:CG | 1:N:279:PRO:HG3 | 2.51 | 0.46 |
| 1:M:87:ASP:O | 1:M:500:VAL:HG23 | 2.16 | 0.46 |
| 1:L:194:LYS:HD2 | 1:L:332:MET:HE3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:332:MET:HG2 | 1:L:334:LEU:CD1 | 2.46 | 0.46 |
| 1:J:250:ILE:HG12 | 1:J:276:VAL:CG2 | 2.46 | 0.46 |
| 1:J:350:ILE:HG23 | 1:J:366:LEU:HD21 | 1.96 | 0.46 |
| 1:J:399:ASP:OD1 | 5:J:702:HOH:O | 2.18 | 0.46 |
| 1:I:127:VAL:HG23 | 1:I:423:CYS:CB | 2.46 | 0.46 |
| 1:I:350:ILE:HG23 | 1:I:366:LEU:HD21 | 1.98 | 0.46 |
| 1:D:24:ALA:CB | 1:D:97:ARG:HD3 | 2.43 | 0.46 |
| 1:D:400:ALA:O | 1:D:404:THR:HG23 | 2.15 | 0.46 |
| 1:D:413:VAL:HB | 1:D:498:THR:HG22 | 1.97 | 0.46 |
| 1:C:350:ILE:HG23 | 1:C:366:LEU:HD21 | 1.97 | 0.46 |
| 1:C:350:ILE:O | 1:C:366:LEU:HD11 | 2.16 | 0.46 |
| 1:B:197:ARG:N | 1:B:330:ASP:HA | 2.31 | 0.46 |
| 1:A:14:ALA:O | 1:A:18:GLN:HG3 | 2.16 | 0.46 |
| 1:A:138:VAL:CG1 | 1:A:408:VAL:HA | 2.46 | 0.46 |
| 1:G:114:VAL:HG12 | 1:G:118:ARG:NH1 | 2.31 | 0.46 |
| 1:F:340:LYS:HA | 1:F:343:ILE:CG1 | 2.38 | 0.46 |
| 1:H:199:TYR:CE2 | 1:H:202:PRO:HA | 2.51 | 0.46 |
| 1:H:456:ALA:CB | 1:H:463:GLY:HA2 | 2.46 | 0.46 |
| 1:H:462:GLU:O | 1:H:466:ILE:HG12 | 2.16 | 0.46 |
| 2:1:44:ALA:CB | 2:1:73:LEU:HD11 | 2.46 | 0.46 |
| 2:W:63:VAL:HG13 | 2:W:93:ASP:OD1 | 2.16 | 0.46 |
| 2:W:65:VAL:HG22 | 2:W:93:ASP:OD1 | 2.16 | 0.46 |
| 2:Q:78:GLY:HA3 | 2:Q:91:PHE:CE1 | 2.50 | 0.46 |
| 1:M:120:VAL:O | 1:M:124:VAL:HG23 | 2.16 | 0.46 |
| 1:L:161:ILE:CG2 | 1:L:380:LEU:HD22 | 2.46 | 0.46 |
| 1:J:73:LEU:HD13 | 1:J:515:LEU:HD13 | 1.98 | 0.46 |
| 1:J:219:TYR:CE2 | 1:J:245:LYS:HB2 | 2.51 | 0.46 |
| 1:J:350:ILE:O | 1:J:366:LEU:HD11 | 2.16 | 0.46 |
| 1:I:23:LEU:HD22 | 1:I:74:VAL:CG1 | 2.46 | 0.46 |
| 1:I:350:ILE:HG23 | 1:I:366:LEU:HD22 | 1.98 | 0.46 |
| 1:D:127:VAL:HG11 | 1:D:505:LEU:HD21 | 1.98 | 0.46 |
| 1:D:136:LYS:NZ | 1:D:490:VAL:HG11 | 2.30 | 0.46 |
| 1:D:207:THR:OG1 | 1:D:209:LYS:HB3 | 2.16 | 0.46 |
| 1:C:87:ASP:O | 1:C:500:VAL:HG23 | 2.16 | 0.46 |
| 1:A:62:LEU:CD1 | 1:A:67:LYS:HB3 | 2.46 | 0.46 |
| 1:A:324:VAL:HG22 | 1:A:333:LEU:CD2 | 2.46 | 0.46 |
| 1:G:61:ASP:HB2 | 1:F:2:SER:O | 2.16 | 0.46 |
| 1:G:117:ARG:NH1 | 1:G:514:LEU:HB2 | 2.30 | 0.46 |
| 1:G:250:ILE:HD13 | 1:G:292:MET:CE | 2.46 | 0.46 |
| 1:G:362:GLU:O | 1:G:366:LEU:HB2 | 2.15 | 0.46 |
| 1:F:239:ILE:CD1 | 1:F:313:VAL:HG23 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:293:ALA:O | 1:F:297:GLY:N | 2.32 | 0.46 |
| 1:F:324:VAL:HG22 | 1:F:333:LEU:CD2 | 2.46 | 0.46 |
| 1:E:332:MET:HG2 | 1:E:334:LEU:HD12 | 1.98 | 0.46 |
| 1:H:24:ALA:CB | 1:H:97:ARG:HD3 | 2.42 | 0.45 |
| 2:2:34:PRO:HD3 | 1:N:261:THR:HG22 | 1.98 | 0.45 |
| 2:1:8:LYS:HG2 | 2:Z:102:ASP:HB3 | 1.98 | 0.45 |
| 2:Z:63:VAL:HG13 | 2:Z:93:ASP:OD1 | 2.16 | 0.45 |
| 2:X:31:ILE:HG12 | 2:X:32:MET:H | 1.81 | 0.45 |
| 2:Q:8:LYS:HA | 2:P:101:VAL:O | 2.16 | 0.45 |
| 1:N:68:ASN:O | 1:N:72:LYS:HG2 | 2.17 | 0.45 |
| 1:N:136:LYS:NZ | 1:N:490:VAL:HG11 | 2.31 | 0.45 |
| 1:N:386:SER:O | 1:N:390:VAL:HG23 | 2.16 | 0.45 |
| 1:M:427:LEU:HA | 1:M:430:LEU:HD23 | 1.99 | 0.45 |
| 1:J:136:LYS:NZ | 1:J:490:VAL:HG11 | 2.31 | 0.45 |
| 1:J:283:ASP:HA | 1:J:286:LYS:HD3 | 1.98 | 0.45 |
| 1:I:68:ASN:O | 1:I:72:LYS:HG2 | 2.16 | 0.45 |
| 1:I:332:MET:HG2 | 1:I:334:LEU:CD1 | 2.46 | 0.45 |
| 1:I:499:LYS:O | 1:I:503:THR:HG23 | 2.16 | 0.45 |
| 1:D:52:ASP:OD2 | 5:D:702:HOH:O | 2.21 | 0.45 |
| 1:D:117:ARG:NH1 | 1:D:514:LEU:HB2 | 2.30 | 0.45 |
| 1:C:3:ALA:O | 1:C:525:ILE:HG22 | 2.16 | 0.45 |
| 1:C:264:LEU:O | 1:C:268:LYS:HG2 | 2.16 | 0.45 |
| 1:B:138:VAL:HA | 1:B:143:GLU:OE1 | 2.16 | 0.45 |
| 1:A:138:VAL:HA | 1:A:143:GLU:OE1 | 2.15 | 0.45 |
| 1:A:161:ILE:HG22 | 1:A:380:LEU:HD22 | 1.99 | 0.45 |
| 1:A:366:LEU:HD13 | 1:A:370:LEU:CD1 | 2.47 | 0.45 |
| 1:E:199:TYR:CE2 | 1:E:202:PRO:HA | 2.51 | 0.45 |
| 1:H:324:VAL:HG22 | 1:H:333:LEU:CD2 | 2.46 | 0.45 |
| 2:Y:31:ILE:HG12 | 2:Y:32:MET:H | 1.82 | 0.45 |
| 2:O:73:LEU:HD13 | 2:O:91:PHE:CE2 | 2.52 | 0.45 |
| 1:N:14:ALA:O | 1:N:18:GLN:HG3 | 2.16 | 0.45 |
| 1:N:161:ILE:CG2 | 1:N:380:LEU:HD22 | 2.45 | 0.45 |
| 1:M:498:THR:O | 1:M:502:ARG:HG2 | 2.17 | 0.45 |
| 1:L:499:LYS:O | 1:L:503:THR:HG23 | 2.16 | 0.45 |
| 1:K:62:LEU:CD1 | 1:K:67:LYS:HB3 | 2.45 | 0.45 |
| 1:K:99:ILE:HD13 | 1:K:509:ALA:HA | 1.99 | 0.45 |
| 1:J:332:MET:HG2 | 1:J:334:LEU:CD1 | 2.46 | 0.45 |
| 1:C:138:VAL:HG21 | 1:C:144:ILE:HD13 | 1.99 | 0.45 |
| 1:C:301:PHE:CZ | 1:C:313:VAL:HG12 | 2.50 | 0.45 |
| 1:B:194:LYS:HD2 | 1:B:332:MET:HE3 | 1.98 | 0.45 |
| 1:B:195:PHE:CZ | 1:B:331:ALA:HB3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:219:TYR:HB3 | 1:B:318:LEU:HD23 | 1.98 | 0.45 |
| 1:A:259:LEU:O | 1:A:263:VAL:HG22 | 2.17 | 0.45 |
| 1:A:386:SER:O | 1:A:390:VAL:HG23 | 2.16 | 0.45 |
| 1:G:23:LEU:HD13 | 1:G:71:ALA:HA | 1.97 | 0.45 |
| 1:G:87:ASP:O | 1:G:500:VAL:HG23 | 2.16 | 0.45 |
| 1:G:332:MET:HG2 | 1:G:334:LEU:HD12 | 1.97 | 0.45 |
| 1:F:161:ILE:CG2 | 1:F:380:LEU:HD22 | 2.46 | 0.45 |
| 1:F:194:LYS:HD2 | 1:F:332:MET:HE2 | 1.97 | 0.45 |
| 1:F:203:TYR:HB3 | 1:F:267:LEU:HD11 | 1.96 | 0.45 |
| 1:F:251:ALA:O | 1:F:277:LYS:HA | 2.16 | 0.45 |
| 1:F:366:LEU:HD13 | 1:F:370:LEU:CD1 | 2.47 | 0.45 |
| 1:E:43:SER:HG | 1:E:44:TRP:HE3 | 1.64 | 0.45 |
| 2:P:56:LYS:HE3 | 2:P:61:GLN:OE1 | 2.16 | 0.45 |
| 2:O:16:VAL:C | 2:O:90:LEU:HD12 | 2.37 | 0.45 |
| 1:M:138:VAL:HG21 | 1:M:144:ILE:HD13 | 1.98 | 0.45 |
| 1:M:228:SER:HA | 1:M:255:ASP:HB3 | 1.98 | 0.45 |
| 1:L:207:THR:OG1 | 1:L:209:LYS:HB3 | 2.16 | 0.45 |
| 1:J:120:VAL:HG13 | 1:J:444:ILE:CD1 | 2.42 | 0.45 |
| 1:D:332:MET:HG2 | 1:D:334:LEU:CD1 | 2.46 | 0.45 |
| 1:C:250:ILE:HG12 | 1:C:276:VAL:CG2 | 2.47 | 0.45 |
| 1:C:253:ASP:OD1 | 1:C:254:VAL:N | 2.49 | 0.45 |
| 1:G:39:ILE:HG12 | 1:G:49:VAL:HG22 | 1.98 | 0.45 |
| 1:G:163:SER:O | 1:G:167:LYS:HG3 | 2.16 | 0.45 |
| 1:H:54:VAL:O | 1:H:58:LYS:N | 2.25 | 0.45 |
| 2:Z:78:GLY:HA3 | 2:Z:91:PHE:CE1 | 2.52 | 0.45 |
| 2:T:16:VAL:CG1 | 2:T:46:VAL:HG23 | 2.47 | 0.45 |
| 1:N:346:ARG:O | 1:N:350:ILE:HD12 | 2.16 | 0.45 |
| 1:L:114:VAL:HG12 | 1:L:118:ARG:NH1 | 2.32 | 0.45 |
| 1:L:117:ARG:NH1 | 1:L:514:LEU:HB2 | 2.31 | 0.45 |
| 1:L:138:VAL:HA | 1:L:143:GLU:OE1 | 2.16 | 0.45 |
| 1:L:324:VAL:HG22 | 1:L:333:LEU:CD2 | 2.47 | 0.45 |
| 1:J:366:LEU:HD13 | 1:J:370:LEU:CD1 | 2.46 | 0.45 |
| 1:I:99:ILE:CD1 | 1:I:509:ALA:HA | 2.46 | 0.45 |
| 1:I:322:GLY:N | 1:I:335:LYS:O | 2.40 | 0.45 |
| 1:D:199:TYR:CE2 | 1:D:202:PRO:HA | 2.51 | 0.45 |
| 1:D:296:THR:OG1 | 1:D:320:LYS:O | 2.31 | 0.45 |
| 1:C:427:LEU:HA | 1:C:430:LEU:HD23 | 1.99 | 0.45 |
| 1:B:207:THR:OG1 | 1:B:209:LYS:HB3 | 2.17 | 0.45 |
| 1:A:166:MET:HG3 | 1:A:171:ARG:HA | 1.98 | 0.45 |
| 1:G:140:THR:CG2 | 1:G:143:GLU:HG3 | 2.47 | 0.45 |
| 1:F:194:LYS:HD2 | 1:F:332:MET:HE3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:350:ILE:O | 1:H:366:LEU:HD11 | 2.17 | 0.45 |
| 1:H:371:ALA:HB1 | 1:H:376:GLY:O | 2.17 | 0.45 |
| 2:Y:8:LYS:HA | 2:X:101:VAL:O | 2.16 | 0.45 |
| 2:X:14:ASP:HB3 | 2:X:92:ARG:NH2 | 2.32 | 0.45 |
| 2:R:97:LEU:HA | 2:S:15:ARG:HH22 | 1.81 | 0.45 |
| 2:S:16:VAL:CG1 | 2:S:46:VAL:HG23 | 2.46 | 0.45 |
| 1:N:65:LYS:O | 1:N:69:ILE:HG13 | 2.16 | 0.45 |
| 1:N:124:VAL:HG21 | 1:N:509:ALA:HB1 | 1.99 | 0.45 |
| 1:M:332:MET:HG2 | 1:M:334:LEU:HD12 | 1.98 | 0.45 |
| 1:I:3:ALA:HB3 | 1:I:525:ILE:HD12 | 1.98 | 0.45 |
| 1:I:123:ALA:HB3 | 1:I:444:ILE:HG13 | 1.99 | 0.45 |
| 1:I:219:TYR:HB3 | 1:I:318:LEU:HD23 | 1.98 | 0.45 |
| 1:I:258:ALA:O | 1:I:262:LEU:HG | 2.17 | 0.45 |
| 1:D:161:ILE:CG2 | 1:D:380:LEU:HD22 | 2.46 | 0.45 |
| 1:C:120:VAL:O | 1:C:124:VAL:HG23 | 2.17 | 0.45 |
| 1:C:161:ILE:CG2 | 1:C:380:LEU:HD22 | 2.47 | 0.45 |
| 1:C:176:THR:HG22 | 1:C:379:VAL:HG12 | 1.98 | 0.45 |
| 1:C:350:ILE:HG23 | 1:C:366:LEU:HD22 | 1.99 | 0.45 |
| 1:A:332:MET:HG2 | 1:A:334:LEU:HD12 | 1.97 | 0.45 |
| 1:A:350:ILE:HG23 | 1:A:366:LEU:HD21 | 1.99 | 0.45 |
| 1:G:199:TYR:CE2 | 1:G:202:PRO:HA | 2.52 | 0.45 |
| 1:F:99:ILE:HD13 | 1:F:509:ALA:HA | 1.98 | 0.45 |
| 1:F:362:GLU:O | 1:F:366:LEU:HB2 | 2.15 | 0.45 |
| 1:H:498:THR:O | 1:H:502:ARG:HG2 | 2.17 | 0.45 |
| 2:2:31:ILE:HG12 | 2:2:32:MET:H | 1.80 | 0.45 |
| 2:W:16:VAL:C | 2:W:90:LEU:HD12 | 2.37 | 0.45 |
| 1:N:527:LYS:O | 1:N:528:GLU:HB2 | 2.16 | 0.45 |
| 1:M:265:ASN:O | 1:M:269:VAL:HG12 | 2.16 | 0.45 |
| 1:M:301:PHE:CZ | 1:M:313:VAL:HG12 | 2.51 | 0.45 |
| 1:L:14:ALA:O | 1:L:18:GLN:HG3 | 2.16 | 0.45 |
| 1:L:332:MET:HG2 | 1:L:334:LEU:HD12 | 1.98 | 0.45 |
| 1:K:47:PRO:HG3 | 1:J:69:ILE:HG23 | 1.98 | 0.45 |
| 1:K:199:TYR:CE2 | 1:K:202:PRO:HA | 2.52 | 0.45 |
| 1:J:187:LEU:HD13 | 1:J:380:LEU:CD2 | 2.46 | 0.45 |
| 1:J:199:TYR:HD1 | 1:J:326:VAL:HG12 | 1.82 | 0.45 |
| 1:I:199:TYR:CE2 | 1:I:202:PRO:HA | 2.52 | 0.45 |
| 1:I:227:ILE:HG21 | 1:I:233:ILE:HD13 | 1.99 | 0.45 |
| 1:D:22:LEU:HD11 | 1:C:6:VAL:HG21 | 1.98 | 0.45 |
| 1:D:114:VAL:HG12 | 1:D:118:ARG:NH1 | 2.32 | 0.45 |
| 1:D:366:LEU:HD13 | 1:D:370:LEU:CD1 | 2.46 | 0.45 |
| 1:B:13:ARG:NH2 | 1:B:519:GLU:OE1 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:371:ALA:HB1 | 1:B:376:GLY:O | 2.17 | 0.45 |
| 1:A:127:VAL:HG11 | 1:A:505:LEU:HD21 | 1.99 | 0.45 |
| 1:A:138:VAL:HG21 | 1:A:144:ILE:HD13 | 1.98 | 0.45 |
| 1:A:207:THR:OG1 | 1:A:209:LYS:HB3 | 2.16 | 0.45 |
| 1:A:293:ALA:O | 1:A:297:GLY:N | 2.29 | 0.45 |
| 1:F:176:THR:O | 1:F:379:VAL:HA | 2.17 | 0.45 |
| 1:F:195:PHE:CG | 1:F:279:PRO:HG3 | 2.52 | 0.45 |
| 1:F:499:LYS:O | 1:F:503:THR:HG23 | 2.16 | 0.45 |
| 1:E:324:VAL:HG22 | 1:E:333:LEU:CD2 | 2.47 | 0.45 |
| 1:H:161:ILE:CG2 | 1:H:380:LEU:HD22 | 2.47 | 0.45 |
| 2:1:16:VAL:CG1 | 2:1:46:VAL:HG23 | 2.47 | 0.45 |
| 2:Y:44:ALA:CB | 2:Y:73:LEU:HD11 | 2.47 | 0.45 |
| 2:Y:44:ALA:HB2 | 2:Y:73:LEU:HD11 | 1.99 | 0.45 |
| 2:Y:63:VAL:HG13 | 2:Y:93:ASP:OD1 | 2.16 | 0.45 |
| 2:X:34:PRO:HD2 | 1:J:230:ILE:CD1 | 2.47 | 0.45 |
| 2:P:8:LYS:O | 2:O:100:TYR:HA | 2.17 | 0.45 |
| 2:P:20:ARG:HB3 | 2:P:41:VAL:CG1 | 2.47 | 0.45 |
| 1:N:23:LEU:HD23 | 1:N:23:LEU:O | 2.16 | 0.45 |
| 1:M:176:THR:O | 1:M:379:VAL:HA | 2.17 | 0.45 |
| 1:M:366:LEU:HD13 | 1:M:370:LEU:CD1 | 2.47 | 0.45 |
| 1:L:42:GLN:HG2 | 1:L:47:PRO:HA | 1.98 | 0.45 |
| 1:L:233:ILE:HG13 | 1:L:237:LEU:CD1 | 2.45 | 0.45 |
| 1:L:340:LYS:HA | 1:L:343:ILE:CG1 | 2.39 | 0.45 |
| 1:L:386:SER:O | 1:L:390:VAL:HG23 | 2.17 | 0.45 |
| 1:K:366:LEU:HD13 | 1:K:370:LEU:CD1 | 2.46 | 0.45 |
| 1:J:39:ILE:HG12 | 1:J:49:VAL:HG22 | 1.98 | 0.45 |
| 1:I:197:ARG:HD2 | 1:I:277:LYS:O | 2.16 | 0.45 |
| 1:I:366:LEU:HD13 | 1:I:370:LEU:CD1 | 2.47 | 0.45 |
| 1:I:386:SER:O | 1:I:390:VAL:HG23 | 2.16 | 0.45 |
| 1:C:8:PHE:CD1 | 1:C:520:VAL:HG22 | 2.51 | 0.45 |
| 1:C:176:THR:O | 1:C:379:VAL:HA | 2.17 | 0.45 |
| 1:C:346:ARG:O | 1:C:350:ILE:HD12 | 2.17 | 0.45 |
| 1:B:120:VAL:HG13 | 1:B:444:ILE:CD1 | 2.38 | 0.45 |
| 1:B:499:LYS:O | 1:B:503:THR:HG23 | 2.16 | 0.45 |
| 1:A:23:LEU:HD22 | 1:A:74:VAL:CG1 | 2.47 | 0.45 |
| 1:A:193:MET:HE2 | 1:A:292:MET:HG2 | 1.99 | 0.45 |
| 1:E:71:ALA:O | 1:E:75:GLN:HG3 | 2.17 | 0.45 |
| 1:E:99:ILE:CD1 | 1:E:509:ALA:HA | 2.47 | 0.45 |
| 1:E:161:ILE:HG22 | 1:E:380:LEU:HD22 | 1.99 | 0.45 |
| 2:P:44:ALA:HB2 | 2:P:73:LEU:HD11 | 1.99 | 0.45 |
| 2:O:4:GLN:OE1 | 2:O:67:VAL:HG11 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:27:THR:HG22 | 2:O:31:ILE:H | 1.81 | 0.45 |
| 1:M:68:ASN:O | 1:M:72:LYS:HG2 | 2.17 | 0.45 |
| 1:M:138:VAL:CG1 | 1:M:408:VAL:HA | 2.47 | 0.45 |
| 1:M:199:TYR:CE2 | 1:M:202:PRO:HA | 2.52 | 0.45 |
| 1:L:285:ARG:HG3 | 1:L:286:LYS:HD2 | 1.98 | 0.45 |
| 1:K:23:LEU:HD22 | 1:K:74:VAL:CG1 | 2.46 | 0.45 |
| 1:J:166:MET:CG | 1:J:171:ARG:HA | 2.47 | 0.45 |
| 1:D:24:ALA:HA | 1:D:27:VAL:HG12 | 1.99 | 0.45 |
| 1:G:350:ILE:O | 1:G:366:LEU:HD11 | 2.16 | 0.45 |
| 1:F:68:ASN:O | 1:F:72:LYS:HG2 | 2.17 | 0.45 |
| 1:F:114:VAL:HG12 | 1:F:118:ARG:NH1 | 2.32 | 0.45 |
| 1:F:332:MET:HG2 | 1:F:334:LEU:CD1 | 2.47 | 0.45 |
| 1:H:71:ALA:O | 1:H:75:GLN:HG3 | 2.16 | 0.45 |
| 2:V:97:LEU:HA | 2:W:15:ARG:HH22 | 1.81 | 0.45 |
| 2:2:56:LYS:HE3 | 2:2:61:GLN:OE1 | 2.17 | 0.45 |
| 2:1:31:ILE:HG12 | 2:1:32:MET:H | 1.82 | 0.45 |
| 2:Z:27:THR:CG2 | 2:Z:31:ILE:H | 2.30 | 0.45 |
| 2:Y:31:ILE:HD12 | 1:K:237:LEU:CB | 2.47 | 0.45 |
| 2:R:25:THR:O | 2:R:33:LEU:HB2 | 2.17 | 0.45 |
| 2:O:56:LYS:HE3 | 2:O:61:GLN:OE1 | 2.17 | 0.45 |
| 2:S:56:LYS:HE3 | 2:S:61:GLN:OE1 | 2.16 | 0.45 |
| 1:M:131:LEU:HD23 | 1:M:134:GLN:HE21 | 1.82 | 0.45 |
| 1:L:228:SER:HA | 1:L:255:ASP:HB3 | 1.98 | 0.45 |
| 1:K:161:ILE:CG2 | 1:K:380:LEU:HD22 | 2.47 | 0.45 |
| 1:K:188:GLU:HB3 | 1:K:379:VAL:HG22 | 1.98 | 0.45 |
| 1:K:301:PHE:CZ | 1:K:313:VAL:HG12 | 2.51 | 0.45 |
| 1:K:350:ILE:HG23 | 1:K:366:LEU:HD21 | 1.97 | 0.45 |
| 1:D:71:ALA:O | 1:D:75:GLN:HG3 | 2.17 | 0.45 |
| 1:D:124:VAL:HG21 | 1:D:509:ALA:HB1 | 1.99 | 0.45 |
| 1:C:77:VAL:HG22 | 1:C:511:VAL:HB | 1.98 | 0.45 |
| 1:C:140:THR:CG2 | 1:C:143:GLU:HG3 | 2.47 | 0.45 |
| 1:C:366:LEU:HD13 | 1:C:370:LEU:CD1 | 2.47 | 0.45 |
| 1:B:68:ASN:O | 1:B:72:LYS:HG2 | 2.17 | 0.45 |
| 1:B:161:ILE:CG2 | 1:B:380:LEU:HD22 | 2.46 | 0.45 |
| 1:G:98:SER:CB | 1:G:450:ILE:HG13 | 2.47 | 0.45 |
| 1:G:456:ALA:CB | 1:G:463:GLY:HA2 | 2.46 | 0.45 |
| 1:F:350:ILE:HG23 | 1:F:366:LEU:HD21 | 1.97 | 0.45 |
| 1:E:24:ALA:CB | 1:E:97:ARG:HD3 | 2.43 | 0.45 |
| 2:W:13:PHE:HA | 2:W:52:GLY:O | 2.17 | 0.45 |
| 2:W:27:THR:CG2 | 2:W:31:ILE:H | 2.30 | 0.45 |
| 2:R:44:ALA:CB | 2:R:73:LEU:HD11 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:13:PHE:HA | 2:O:52:GLY:O | 2.17 | 0.45 |
| 1:N:24:ALA:CB | 1:N:97:ARG:HD3 | 2.43 | 0.45 |
| 1:L:68:ASN:O | 1:L:72:LYS:HG2 | 2.17 | 0.45 |
| 1:L:185:ASP:OD1 | 1:L:382:VAL:HA | 2.17 | 0.45 |
| 1:L:199:TYR:CE2 | 1:L:202:PRO:HA | 2.51 | 0.45 |
| 1:K:497:PRO:HD2 | 1:K:500:VAL:HG11 | 1.98 | 0.45 |
| 1:K:499:LYS:O | 1:K:503:THR:HG23 | 2.17 | 0.45 |
| 1:I:99:ILE:HD13 | 1:I:509:ALA:HA | 1.99 | 0.45 |
| 1:I:138:VAL:HA | 1:I:143:GLU:OE1 | 2.17 | 0.45 |
| 1:D:233:ILE:HG13 | 1:D:237:LEU:CD1 | 2.46 | 0.45 |
| 1:C:27:VAL:O | 1:C:30:THR:OG1 | 2.31 | 0.45 |
| 1:C:127:VAL:HG23 | 1:C:423:CYS:CB | 2.46 | 0.45 |
| 1:C:136:LYS:NZ | 1:C:490:VAL:HG11 | 2.32 | 0.45 |
| 1:B:136:LYS:NZ | 1:B:490:VAL:HG11 | 2.31 | 0.45 |
| 1:A:140:THR:CG2 | 1:A:143:GLU:HG3 | 2.47 | 0.45 |
| 1:F:291:ASP:OD1 | 1:F:346:ARG:NE | 2.43 | 0.45 |
| 1:H:87:ASP:O | 1:H:500:VAL:HG23 | 2.17 | 0.44 |
| 1:H:250:ILE:HG12 | 1:H:276:VAL:CG2 | 2.47 | 0.44 |
| 2:V:15:ARG:NH2 | 2:2:97:LEU:HA | 2.32 | 0.44 |
| 2:1:17:LEU:CB | 2:1:48:ALA:HB3 | 2.34 | 0.44 |
| 2:Z:34:PRO:CD | 1:L:261:THR:HG22 | 2.46 | 0.44 |
| 2:Y:16:VAL:CG1 | 2:Y:46:VAL:HG23 | 2.47 | 0.44 |
| 2:R:56:LYS:HE3 | 2:R:61:GLN:OE1 | 2.17 | 0.44 |
| 2:P:8:LYS:HA | 2:O:101:VAL:O | 2.17 | 0.44 |
| 2:P:16:VAL:CG1 | 2:P:46:VAL:HG23 | 2.47 | 0.44 |
| 2:P:31:ILE:HG12 | 2:P:32:MET:H | 1.82 | 0.44 |
| 2:O:16:VAL:CG1 | 2:O:46:VAL:HG23 | 2.46 | 0.44 |
| 1:K:400:ALA:O | 1:K:404:THR:HG23 | 2.17 | 0.44 |
| 1:J:114:VAL:HG12 | 1:J:118:ARG:NH1 | 2.32 | 0.44 |
| 1:D:68:ASN:O | 1:D:72:LYS:HG2 | 2.16 | 0.44 |
| 1:D:116:ILE:O | 1:D:120:VAL:HG23 | 2.18 | 0.44 |
| 1:D:280:GLY:C | 1:D:285:ARG:HB3 | 2.36 | 0.44 |
| 1:C:99:ILE:HD13 | 1:C:509:ALA:HA | 1.99 | 0.44 |
| 1:B:60:ILE:O | 1:B:75:GLN:NE2 | 2.50 | 0.44 |
| 1:A:199:TYR:CE2 | 1:A:202:PRO:HA | 2.52 | 0.44 |
| 1:A:322:GLY:N | 1:A:335:LYS:O | 2.39 | 0.44 |
| 1:F:127:VAL:HG11 | 1:F:505:LEU:HD21 | 1.98 | 0.44 |
| 1:F:222:LEU:CD2 | 1:F:250:ILE:HB | 2.42 | 0.44 |
| 1:E:14:ALA:O | 1:E:18:GLN:HG3 | 2.16 | 0.44 |
| 1:E:219:TYR:HB3 | 1:E:318:LEU:HD23 | 1.99 | 0.44 |
| 1:H:114:VAL:HG12 | 1:H:118:ARG:NH1 | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:82:VAL:C | 2:2:83:LEU:HD12 | 2.38 | 0.44 |
| 2:R:31:ILE:HG12 | 2:R:32:MET:H | 1.83 | 0.44 |
| 2:O:65:VAL:HG22 | 2:O:93:ASP:OD1 | 2.16 | 0.44 |
| 2:T:8:LYS:HA | 2:S:101:VAL:O | 2.17 | 0.44 |
| 2:T:16:VAL:C | 2:T:90:LEU:HD12 | 2.37 | 0.44 |
| 1:M:123:ALA:HB3 | 1:M:444:ILE:HG13 | 1.99 | 0.44 |
| 1:L:136:LYS:NZ | 1:L:490:VAL:HG11 | 2.32 | 0.44 |
| 1:K:135:SER:OG | 1:K:498:THR:HG21 | 2.17 | 0.44 |
| 1:I:161:ILE:CG2 | 1:I:380:LEU:HD22 | 2.48 | 0.44 |
| 1:I:219:TYR:O | 1:I:248:VAL:HG22 | 2.17 | 0.44 |
| 1:D:176:THR:HG22 | 1:D:379:VAL:HG12 | 1.98 | 0.44 |
| 1:B:23:LEU:O | 1:B:23:LEU:HD23 | 2.17 | 0.44 |
| 1:B:114:VAL:HG12 | 1:B:118:ARG:NH1 | 2.32 | 0.44 |
| 1:A:340:LYS:HA | 1:A:343:ILE:CG1 | 2.39 | 0.44 |
| 1:A:340:LYS:CA | 1:A:343:ILE:HG12 | 2.39 | 0.44 |
| 1:G:187:LEU:HD13 | 1:G:380:LEU:HD21 | 1.99 | 0.44 |
| 1:F:233:ILE:O | 1:F:237:LEU:HD13 | 2.18 | 0.44 |
| 1:E:301:PHE:CZ | 1:E:313:VAL:HG12 | 2.52 | 0.44 |
| 1:H:6:VAL:CG2 | 1:I:22:LEU:HD11 | 2.46 | 0.44 |
| 1:H:22:LEU:HD11 | 1:N:6:VAL:CG2 | 2.48 | 0.44 |
| 2:Z:65:VAL:HG22 | 2:Z:93:ASP:OD1 | 2.17 | 0.44 |
| 2:Y:16:VAL:C | 2:Y:90:LEU:HD12 | 2.38 | 0.44 |
| 2:Q:21:SER:OG | 2:Q:41:VAL:HG21 | 2.17 | 0.44 |
| 2:Q:25:THR:O | 2:Q:33:LEU:HB2 | 2.18 | 0.44 |
| 2:S:13:PHE:HA | 2:S:52:GLY:O | 2.17 | 0.44 |
| 1:N:71:ALA:O | 1:N:75:GLN:HG3 | 2.17 | 0.44 |
| 1:N:124:VAL:HA | 1:N:127:VAL:HG12 | 1.99 | 0.44 |
| 1:N:206:ASN:HB3 | 1:N:266:ARG:HH21 | 1.83 | 0.44 |
| 1:M:114:VAL:HG12 | 1:M:118:ARG:NH1 | 2.32 | 0.44 |
| 1:M:166:MET:CG | 1:M:171:ARG:HA | 2.47 | 0.44 |
| 1:M:386:SER:O | 1:M:390:VAL:HG23 | 2.17 | 0.44 |
| 1:K:69:ILE:HD11 | 1:K:523:THR:HG22 | 1.99 | 0.44 |
| 1:K:176:THR:HG22 | 1:K:379:VAL:HG12 | 1.98 | 0.44 |
| 1:K:199:TYR:HD1 | 1:K:326:VAL:HG12 | 1.82 | 0.44 |
| 1:J:199:TYR:CE2 | 1:J:202:PRO:HA | 2.53 | 0.44 |
| 1:J:499:LYS:O | 1:J:503:THR:HG23 | 2.18 | 0.44 |
| 1:C:197:ARG:N | 1:C:330:ASP:HA | 2.30 | 0.44 |
| 1:B:228:SER:HA | 1:B:255:ASP:HB3 | 1.98 | 0.44 |
| 1:A:499:LYS:O | 1:A:503:THR:HG23 | 2.17 | 0.44 |
| 1:G:12:ALA:HB1 | 1:G:521:VAL:CG2 | 2.47 | 0.44 |
| 1:F:255:ASP:OD1 | 1:F:256:GLY:N | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:343:ILE:O | 1:F:347:ILE:HG13 | 2.18 | 0.44 |
| 1:E:188:GLU:HB3 | 1:E:379:VAL:HG22 | 1.98 | 0.44 |
| 1:H:117:ARG:NH1 | 1:H:514:LEU:HB2 | 2.32 | 0.44 |
| 1:H:343:ILE:O | 1:H:347:ILE:HG13 | 2.17 | 0.44 |
| 1:H:350:ILE:HG22 | 1:H:370:LEU:HD11 | 1.99 | 0.44 |
| 2:X:27:THR:CG2 | 2:X:31:ILE:H | 2.31 | 0.44 |
| 1:N:114:VAL:HG12 | 1:N:118:ARG:NH1 | 2.32 | 0.44 |
| 1:K:228:SER:HA | 1:K:255:ASP:HB3 | 1.98 | 0.44 |
| 1:J:127:VAL:HG11 | 1:J:505:LEU:HD21 | 2.00 | 0.44 |
| 1:I:62:LEU:CD1 | 1:I:67:LYS:HB3 | 2.48 | 0.44 |
| 1:I:176:THR:O | 1:I:379:VAL:HA | 2.17 | 0.44 |
| 1:D:14:ALA:O | 1:D:18:GLN:HG3 | 2.17 | 0.44 |
| 1:D:402:ASN:OD1 | 1:D:405:ARG:NH2 | 2.46 | 0.44 |
| 1:C:68:ASN:O | 1:C:72:LYS:HG2 | 2.17 | 0.44 |
| 1:C:386:SER:O | 1:C:390:VAL:HG23 | 2.17 | 0.44 |
| 1:B:117:ARG:NH1 | 1:B:514:LEU:HB2 | 2.32 | 0.44 |
| 1:F:99:ILE:CD1 | 1:F:509:ALA:HA | 2.46 | 0.44 |
| 1:F:350:ILE:HG22 | 1:F:370:LEU:HD11 | 1.99 | 0.44 |
| 1:E:136:LYS:NZ | 1:E:490:VAL:HG11 | 2.33 | 0.44 |
| 1:E:462:GLU:O | 1:E:466:ILE:HG12 | 2.17 | 0.44 |
| 2:1:52:GLY:HA3 | 2:1:60:ILE:HD12 | 1.99 | 0.44 |
| 2:1:82:VAL:C | 2:1:83:LEU:HD12 | 2.38 | 0.44 |
| 2:O:82:VAL:C | 2:O:83:LEU:HD12 | 2.38 | 0.44 |
| 2:S:4:GLN:OE1 | 2:S:67:VAL:HG11 | 2.18 | 0.44 |
| 1:M:176:THR:HG22 | 1:M:379:VAL:HG12 | 1.98 | 0.44 |
| 1:L:23:LEU:O | 1:L:23:LEU:HD23 | 2.18 | 0.44 |
| 1:L:301:PHE:CZ | 1:L:313:VAL:HG12 | 2.52 | 0.44 |
| 1:L:346:ARG:O | 1:L:350:ILE:HD12 | 2.16 | 0.44 |
| 1:I:250:ILE:HG12 | 1:I:276:VAL:CG2 | 2.48 | 0.44 |
| 1:D:20:VAL:HG13 | 1:D:74:VAL:HG21 | 2.00 | 0.44 |
| 1:C:24:ALA:HA | 1:C:27:VAL:HG12 | 2.00 | 0.44 |
| 1:C:332:MET:HG2 | 1:C:334:LEU:CD1 | 2.47 | 0.44 |
| 1:B:32:GLY:N | 3:B:601:ADP:O1A | 2.44 | 0.44 |
| 1:B:346:ARG:O | 1:B:350:ILE:HD12 | 2.18 | 0.44 |
| 1:B:386:SER:O | 1:B:390:VAL:HG23 | 2.18 | 0.44 |
| 1:F:218:ALA:HB2 | 1:F:246:PRO:HG2 | 2.00 | 0.44 |
| 1:E:140:THR:CG2 | 1:E:143:GLU:HG3 | 2.47 | 0.44 |
| 1:E:203:TYR:HB3 | 1:E:267:LEU:HD11 | 1.98 | 0.44 |
| 1:E:350:ILE:HG22 | 1:E:370:LEU:HD11 | 1.98 | 0.44 |
| 1:E:497:PRO:HD2 | 1:E:500:VAL:HG11 | 1.98 | 0.44 |
| 1:E:499:LYS:O | 1:E:503:THR:HG23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:23:LEU:HD23 | 1:H:23:LEU:O | 2.18 | 0.44 |
| 1:H:207:THR:HG21 | 1:H:212:LYS:H | 1.82 | 0.44 |
| 1:H:250:ILE:HD13 | 1:H:292:MET:CE | 2.48 | 0.44 |
| 1:H:340:LYS:CA | 1:H:343:ILE:HG12 | 2.39 | 0.44 |
| 2:Y:13:PHE:O | 2:Y:53:SER:HA | 2.17 | 0.44 |
| 2:R:27:THR:CG2 | 2:R:31:ILE:H | 2.31 | 0.44 |
| 2:Q:11:PRO:HB2 | 2:Q:15:ARG:HB2 | 2.00 | 0.44 |
| 2:T:4:GLN:OE1 | 2:T:67:VAL:HG11 | 2.17 | 0.44 |
| 2:T:34:PRO:HD3 | 1:F:261:THR:HG22 | 1.99 | 0.44 |
| 1:M:24:ALA:HA | 1:M:27:VAL:HG12 | 2.00 | 0.44 |
| 1:M:161:ILE:CG2 | 1:M:380:LEU:HD22 | 2.47 | 0.44 |
| 1:M:350:ILE:O | 1:M:366:LEU:HD11 | 2.17 | 0.44 |
| 1:M:362:GLU:O | 1:M:366:LEU:HB2 | 2.18 | 0.44 |
| 1:L:138:VAL:CG1 | 1:L:408:VAL:HA | 2.47 | 0.44 |
| 1:L:165:ALA:HB2 | 1:L:187:LEU:CD1 | 2.48 | 0.44 |
| 1:K:219:TYR:O | 1:K:248:VAL:HG22 | 2.18 | 0.44 |
| 1:J:161:ILE:CG2 | 1:J:380:LEU:HD22 | 2.48 | 0.44 |
| 1:C:65:LYS:O | 1:C:69:ILE:HG13 | 2.17 | 0.44 |
| 1:C:120:VAL:HG13 | 1:C:444:ILE:CD1 | 2.38 | 0.44 |
| 1:C:166:MET:CG | 1:C:171:ARG:HA | 2.48 | 0.44 |
| 1:B:64:ASP:OD1 | 1:B:65:LYS:N | 2.51 | 0.44 |
| 1:B:127:VAL:HG11 | 1:B:505:LEU:HD21 | 1.98 | 0.44 |
| 1:B:293:ALA:O | 1:B:297:GLY:N | 2.33 | 0.44 |
| 1:G:69:ILE:HD11 | 1:G:523:THR:HG22 | 1.99 | 0.44 |
| 1:G:73:LEU:HD13 | 1:G:515:LEU:HD13 | 2.00 | 0.44 |
| 1:G:176:THR:HG22 | 1:G:379:VAL:HG12 | 1.98 | 0.44 |
| 2:2:44:ALA:CB | 2:2:73:LEU:HD11 | 2.47 | 0.44 |
| 2:Z:82:VAL:C | 2:Z:83:LEU:HD12 | 2.38 | 0.44 |
| 2:Y:82:VAL:C | 2:Y:83:LEU:HD12 | 2.38 | 0.44 |
| 2:P:82:VAL:C | 2:P:83:LEU:HD12 | 2.38 | 0.44 |
| 2:O:63:VAL:HG13 | 2:O:93:ASP:OD1 | 2.17 | 0.44 |
| 2:U:3:GLY:CA | 2:U:51:SER:HA | 2.45 | 0.44 |
| 1:N:228:SER:HA | 1:N:255:ASP:HB3 | 1.99 | 0.44 |
| 1:M:65:LYS:O | 1:M:69:ILE:HG13 | 2.18 | 0.44 |
| 1:M:120:VAL:HG13 | 1:M:444:ILE:CD1 | 2.37 | 0.44 |
| 1:L:207:THR:HG21 | 1:L:212:LYS:H | 1.82 | 0.44 |
| 1:K:187:LEU:HD13 | 1:K:380:LEU:CD2 | 2.47 | 0.44 |
| 1:K:340:LYS:HA | 1:K:343:ILE:CG1 | 2.38 | 0.44 |
| 1:K:385:THR:HG21 | 1:J:506:LEU:HD21 | 2.00 | 0.44 |
| 1:D:23:LEU:O | 1:D:23:LEU:HD23 | 2.17 | 0.44 |
| 1:C:114:VAL:HG12 | 1:C:118:ARG:NH1 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:138:VAL:CG1 | 1:C:408:VAL:HA | 2.48 | 0.44 |
| 1:A:99:ILE:HD13 | 1:A:509:ALA:HA | 1.99 | 0.44 |
| 1:A:124:VAL:HA | 1:A:127:VAL:HG12 | 1.99 | 0.44 |
| 1:G:175:ILE:CG2 | 1:G:401:LEU:HD11 | 2.48 | 0.44 |
| 1:G:340:LYS:HA | 1:G:343:ILE:CG1 | 2.38 | 0.44 |
| 1:F:253:ASP:OD1 | 1:F:254:VAL:N | 2.51 | 0.44 |
| 1:F:309:ASN:HB2 | 1:F:312:ASP:OD1 | 2.16 | 0.44 |
| 2:Z:31:ILE:HG12 | 2:Z:32:MET:H | 1.82 | 0.44 |
| 2:R:34:PRO:HD3 | 1:D:261:THR:HG22 | 1.98 | 0.44 |
| 2:P:4:GLN:OE1 | 2:P:67:VAL:HG11 | 2.18 | 0.44 |
| 2:S:73:LEU:HB3 | 2:S:91:PHE:CE2 | 2.48 | 0.44 |
| 1:M:77:VAL:HG22 | 1:M:511:VAL:HB | 1.99 | 0.44 |
| 1:L:124:VAL:HA | 1:L:127:VAL:HG12 | 1.99 | 0.44 |
| 1:K:350:ILE:HG23 | 1:K:366:LEU:HD22 | 1.99 | 0.44 |
| 1:K:385:THR:CG2 | 1:J:506:LEU:HD21 | 2.48 | 0.44 |
| 1:J:8:PHE:CD1 | 1:J:520:VAL:HG22 | 2.53 | 0.44 |
| 1:J:343:ILE:O | 1:J:347:ILE:HG13 | 2.17 | 0.44 |
| 1:J:385:THR:CG2 | 1:I:506:LEU:HD21 | 2.48 | 0.44 |
| 1:D:166:MET:CG | 1:D:171:ARG:HA | 2.48 | 0.44 |
| 1:C:140:THR:HG22 | 1:C:143:GLU:HG3 | 2.00 | 0.44 |
| 1:C:280:GLY:CA | 1:C:285:ARG:HG3 | 2.48 | 0.44 |
| 1:C:498:THR:O | 1:C:502:ARG:HG2 | 2.18 | 0.44 |
| 1:B:20:VAL:HG13 | 1:B:74:VAL:HG21 | 2.00 | 0.44 |
| 1:B:148:ALA:HB2 | 1:B:404:THR:CG2 | 2.48 | 0.44 |
| 1:B:253:ASP:OD1 | 1:B:254:VAL:N | 2.51 | 0.44 |
| 1:A:187:LEU:HD13 | 1:A:380:LEU:CD2 | 2.48 | 0.44 |
| 1:G:124:VAL:HG21 | 1:G:509:ALA:CB | 2.48 | 0.44 |
| 1:G:222:LEU:CD2 | 1:G:250:ILE:HB | 2.41 | 0.44 |
| 1:G:499:LYS:O | 1:G:503:THR:HG23 | 2.17 | 0.44 |
| 1:F:227:ILE:HG21 | 1:F:233:ILE:HD13 | 2.00 | 0.44 |
| 1:F:250:ILE:HD13 | 1:F:292:MET:CE | 2.48 | 0.44 |
| 1:H:99:ILE:CD1 | 1:H:509:ALA:HA | 2.47 | 0.44 |
| 2:V:20:ARG:HB3 | 2:V:41:VAL:CG1 | 2.48 | 0.44 |
| 2:W:82:VAL:C | 2:W:83:LEU:HD12 | 2.38 | 0.44 |
| 2:R:14:ASP:HB3 | 2:R:92:ARG:HH21 | 1.83 | 0.44 |
| 2:T:15:ARG:HH22 | 2:S:97:LEU:HA | 1.80 | 0.44 |
| 2:S:27:THR:CG2 | 2:S:31:ILE:H | 2.31 | 0.44 |
| 1:N:138:VAL:CG1 | 1:N:408:VAL:HA | 2.48 | 0.44 |
| 1:M:23:LEU:O | 1:M:23:LEU:HD23 | 2.18 | 0.44 |
| 1:K:23:LEU:HD23 | 1:K:23:LEU:O | 2.18 | 0.44 |
| 1:J:31:MET:SD | 1:J:454:THR:OG1 | 2.68 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:207:THR:OG1 | 1:J:209:LYS:HB3 | 2.17 | 0.44 |
| 1:J:227:ILE:HG12 | 1:J:310:LEU:HD11 | 2.00 | 0.44 |
| 1:J:250:ILE:HD13 | 1:J:292:MET:CE | 2.48 | 0.44 |
| 1:J:362:GLU:O | 1:J:366:LEU:HB2 | 2.18 | 0.44 |
| 1:I:114:VAL:HG12 | 1:I:118:ARG:NH1 | 2.32 | 0.44 |
| 1:I:124:VAL:HG21 | 1:I:509:ALA:CB | 2.48 | 0.44 |
| 1:I:163:SER:O | 1:I:167:LYS:HG3 | 2.18 | 0.44 |
| 1:I:248:VAL:HG12 | 1:I:274:VAL:CG1 | 2.47 | 0.44 |
| 1:D:499:LYS:O | 1:D:503:THR:HG23 | 2.18 | 0.44 |
| 1:C:23:LEU:HD23 | 1:C:23:LEU:O | 2.18 | 0.44 |
| 1:C:257:GLU:O | 1:C:261:THR:HG23 | 2.18 | 0.44 |
| 1:A:248:VAL:HG12 | 1:A:274:VAL:CG1 | 2.47 | 0.44 |
| 1:F:22:LEU:HD11 | 1:E:6:VAL:CG2 | 2.47 | 0.44 |
| 1:F:350:ILE:HG23 | 1:F:366:LEU:HD22 | 1.99 | 0.44 |
| 2:Y:27:THR:CG2 | 2:Y:31:ILE:H | 2.31 | 0.43 |
| 2:X:82:VAL:C | 2:X:83:LEU:HD12 | 2.38 | 0.43 |
| 2:Q:31:ILE:HD12 | 1:C:237:LEU:CB | 2.48 | 0.43 |
| 2:P:13:PHE:HA | 2:P:52:GLY:O | 2.18 | 0.43 |
| 2:P:26:VAL:HA | 2:P:32:MET:HA | 1.99 | 0.43 |
| 2:T:27:THR:CG2 | 2:T:31:ILE:H | 2.30 | 0.43 |
| 1:N:230:ILE:HD12 | 1:N:261:THR:HG21 | 2.00 | 0.43 |
| 1:N:462:GLU:O | 1:N:466:ILE:HG12 | 2.17 | 0.43 |
| 1:K:114:VAL:HG12 | 1:K:118:ARG:NH1 | 2.33 | 0.43 |
| 1:K:371:ALA:HB1 | 1:K:376:GLY:O | 2.17 | 0.43 |
| 1:I:140:THR:CG2 | 1:I:143:GLU:HG3 | 2.48 | 0.43 |
| 1:I:165:ALA:HB2 | 1:I:187:LEU:CD1 | 2.47 | 0.43 |
| 1:C:24:ALA:CB | 1:C:97:ARG:HD3 | 2.45 | 0.43 |
| 1:B:23:LEU:HD22 | 1:B:74:VAL:CG1 | 2.48 | 0.43 |
| 1:B:264:LEU:O | 1:B:268:LYS:HG2 | 2.18 | 0.43 |
| 1:B:332:MET:HG2 | 1:B:334:LEU:HD12 | 2.00 | 0.43 |
| 1:G:219:TYR:O | 1:G:248:VAL:HG22 | 2.18 | 0.43 |
| 1:E:253:ASP:OD1 | 1:E:254:VAL:N | 2.51 | 0.43 |
| 1:H:260:SER:HA | 1:H:263:VAL:HG22 | 1.99 | 0.43 |
| 1:H:506:LEU:HD21 | 1:I:385:THR:CG2 | 2.48 | 0.43 |
| 2:Z:44:ALA:CB | 2:Z:73:LEU:HD11 | 2.48 | 0.43 |
| 2:Y:25:THR:O | 2:Y:33:LEU:HB2 | 2.17 | 0.43 |
| 2:Q:31:ILE:HD11 | 1:C:237:LEU:HD22 | 2.00 | 0.43 |
| 2:O:27:THR:HG22 | 2:O:31:ILE:O | 2.18 | 0.43 |
| 2:U:82:VAL:C | 2:U:83:LEU:HD12 | 2.38 | 0.43 |
| 1:M:98:SER:CB | 1:M:450:ILE:HG13 | 2.48 | 0.43 |
| 1:M:285:ARG:HG3 | 1:M:286:LYS:HD2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:39:ILE:HG12 | 1:L:49:VAL:HG22 | 1.98 | 0.43 |
| 1:L:60:ILE:O | 1:L:75:GLN:NE2 | 2.51 | 0.43 |
| 1:K:138:VAL:HG21 | 1:K:144:ILE:HD13 | 1.99 | 0.43 |
| 1:K:140:THR:CG2 | 1:K:143:GLU:HG3 | 2.48 | 0.43 |
| 1:J:124:VAL:HA | 1:J:127:VAL:HG12 | 2.01 | 0.43 |
| 1:J:291:ASP:OD1 | 1:J:346:ARG:NE | 2.45 | 0.43 |
| 1:I:120:VAL:HG13 | 1:I:444:ILE:CD1 | 2.39 | 0.43 |
| 1:I:148:ALA:HB2 | 1:I:404:THR:CG2 | 2.48 | 0.43 |
| 1:I:362:GLU:O | 1:I:366:LEU:HB2 | 2.18 | 0.43 |
| 1:D:250:ILE:HG12 | 1:D:276:VAL:CG2 | 2.48 | 0.43 |
| 1:C:367:ASN:HA | 1:C:370:LEU:HD13 | 2.00 | 0.43 |
| 1:B:39:ILE:HG12 | 1:B:49:VAL:HG22 | 2.00 | 0.43 |
| 1:A:135:SER:OG | 1:A:498:THR:HG21 | 2.18 | 0.43 |
| 1:F:24:ALA:HA | 1:F:27:VAL:HG12 | 2.01 | 0.43 |
| 1:F:136:LYS:NZ | 1:F:490:VAL:HG11 | 2.33 | 0.43 |
| 1:F:188:GLU:HB3 | 1:F:379:VAL:HG22 | 1.97 | 0.43 |
| 1:H:413:VAL:HB | 1:H:498:THR:HG22 | 2.00 | 0.43 |
| 2:V:27:THR:CG2 | 2:V:31:ILE:H | 2.30 | 0.43 |
| 2:2:27:THR:CG2 | 2:2:31:ILE:H | 2.30 | 0.43 |
| 2:R:82:VAL:C | 2:R:83:LEU:HD12 | 2.38 | 0.43 |
| 2:O:27:THR:CG2 | 2:O:31:ILE:H | 2.31 | 0.43 |
| 2:T:26:VAL:HA | 2:T:32:MET:HA | 2.00 | 0.43 |
| 1:N:116:ILE:O | 1:N:120:VAL:HG23 | 2.17 | 0.43 |
| 1:M:140:THR:CG2 | 1:M:143:GLU:HG3 | 2.48 | 0.43 |
| 1:M:293:ALA:O | 1:M:297:GLY:N | 2.33 | 0.43 |
| 1:L:120:VAL:O | 1:L:124:VAL:HG23 | 2.18 | 0.43 |
| 1:L:253:ASP:OD1 | 1:L:254:VAL:N | 2.51 | 0.43 |
| 1:J:3:ALA:HB3 | 1:J:525:ILE:HD12 | 2.00 | 0.43 |
| 1:J:280:GLY:CA | 1:J:285:ARG:HB3 | 2.48 | 0.43 |
| 1:D:140:THR:CG2 | 1:D:143:GLU:HG3 | 2.48 | 0.43 |
| 1:D:207:THR:HG21 | 1:D:212:LYS:H | 1.82 | 0.43 |
| 1:D:414:LEU:HD22 | 1:D:489:MET:HB2 | 2.01 | 0.43 |
| 1:C:124:VAL:HA | 1:C:127:VAL:HG12 | 2.01 | 0.43 |
| 1:B:87:ASP:O | 1:B:500:VAL:HG23 | 2.18 | 0.43 |
| 1:B:199:TYR:CE2 | 1:B:202:PRO:HA | 2.53 | 0.43 |
| 1:G:498:THR:O | 1:G:502:ARG:HG2 | 2.19 | 0.43 |
| 1:F:20:VAL:HG13 | 1:F:74:VAL:HG21 | 2.00 | 0.43 |
| 1:F:120:VAL:HG13 | 1:F:444:ILE:CD1 | 2.39 | 0.43 |
| 1:F:322:GLY:N | 1:F:335:LYS:O | 2.39 | 0.43 |
| 1:F:371:ALA:HB1 | 1:F:376:GLY:O | 2.18 | 0.43 |
| 1:E:427:LEU:HA | 1:E:430:LEU:HD23 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:82:VAL:C | 2:V:83:LEU:HD12 | 2.38 | 0.43 |
| 2:Y:4:GLN:OE1 | 2:Y:67:VAL:HG11 | 2.18 | 0.43 |
| 2:X:72:LEU:O | 2:X:97:LEU:HB2 | 2.18 | 0.43 |
| 2:W:31:ILE:HG12 | 2:W:32:MET:H | 1.83 | 0.43 |
| 2:U:4:GLN:OE1 | 2:U:67:VAL:HG11 | 2.18 | 0.43 |
| 2:T:82:VAL:C | 2:T:83:LEU:HD12 | 2.38 | 0.43 |
| 2:S:82:VAL:C | 2:S:83:LEU:HD12 | 2.38 | 0.43 |
| 1:N:340:LYS:CA | 1:N:343:ILE:HG12 | 2.39 | 0.43 |
| 1:L:23:LEU:HD22 | 1:L:74:VAL:CG1 | 2.49 | 0.43 |
| 1:K:279:PRO:HB2 | 1:K:288:GLN:OE1 | 2.18 | 0.43 |
| 1:J:195:PHE:CE2 | 1:J:197:ARG:HB3 | 2.54 | 0.43 |
| 1:J:233:ILE:HD11 | 1:J:249:ILE:HD13 | 1.99 | 0.43 |
| 1:J:444:ILE:O | 1:J:448:LEU:HG | 2.19 | 0.43 |
| 1:I:340:LYS:CA | 1:I:343:ILE:HG12 | 2.40 | 0.43 |
| 1:C:327:THR:OG1 | 1:C:330:ASP:O | 2.36 | 0.43 |
| 1:B:140:THR:OG1 | 1:B:141:PRO:HD2 | 2.18 | 0.43 |
| 1:B:222:LEU:CD2 | 1:B:250:ILE:HB | 2.47 | 0.43 |
| 1:A:219:TYR:O | 1:A:248:VAL:HG22 | 2.17 | 0.43 |
| 1:A:301:PHE:CZ | 1:A:313:VAL:HG12 | 2.52 | 0.43 |
| 1:G:32:GLY:N | 3:G:601:ADP:O1A | 2.45 | 0.43 |
| 1:G:199:TYR:HD1 | 1:G:326:VAL:HG12 | 1.84 | 0.43 |
| 1:G:340:LYS:CA | 1:G:343:ILE:HG12 | 2.40 | 0.43 |
| 1:F:87:ASP:O | 1:F:500:VAL:HG23 | 2.18 | 0.43 |
| 1:H:499:LYS:O | 1:H:503:THR:HG23 | 2.18 | 0.43 |
| 2:2:53:SER:HB3 | 2:2:61:GLN:HB3 | 2.00 | 0.43 |
| 2:1:4:GLN:OE1 | 2:1:67:VAL:HG11 | 2.19 | 0.43 |
| 2:Z:73:LEU:HB3 | 2:Z:91:PHE:CE2 | 2.49 | 0.43 |
| 2:X:14:ASP:HB3 | 2:X:92:ARG:HH21 | 1.82 | 0.43 |
| 2:R:14:ASP:HB3 | 2:R:92:ARG:NH2 | 2.34 | 0.43 |
| 2:R:21:SER:OG | 2:R:41:VAL:HG21 | 2.19 | 0.43 |
| 2:P:21:SER:OG | 2:P:41:VAL:HG21 | 2.18 | 0.43 |
| 2:U:17:LEU:HD11 | 2:U:88:TYR:CB | 2.48 | 0.43 |
| 2:T:17:LEU:CB | 2:T:48:ALA:HB3 | 2.36 | 0.43 |
| 2:T:73:LEU:HD13 | 2:T:91:PHE:CE2 | 2.54 | 0.43 |
| 1:N:107:ILE:HD11 | 1:N:516:THR:O | 2.17 | 0.43 |
| 1:N:253:ASP:OD1 | 1:N:254:VAL:N | 2.51 | 0.43 |
| 1:K:3:ALA:HB3 | 1:K:525:ILE:HD12 | 1.99 | 0.43 |
| 1:K:64:ASP:OD1 | 1:K:65:LYS:N | 2.51 | 0.43 |
| 1:K:222:LEU:CD2 | 1:K:250:ILE:HB | 2.42 | 0.43 |
| 1:J:73:LEU:HD12 | 1:J:515:LEU:HD13 | 1.98 | 0.43 |
| 1:B:47:PRO:HG3 | 1:A:69:ILE:HG23 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:99:ILE:CD1 | 1:G:509:ALA:HA | 2.48 | 0.43 |
| 1:G:404:THR:O | 1:G:408:VAL:HG13 | 2.18 | 0.43 |
| 1:F:124:VAL:HG21 | 1:F:509:ALA:CB | 2.49 | 0.43 |
| 1:E:498:THR:O | 1:E:502:ARG:HG2 | 2.19 | 0.43 |
| 1:H:120:VAL:HG13 | 1:H:444:ILE:CD1 | 2.40 | 0.43 |
| 1:H:206:ASN:HB3 | 1:H:266:ARG:NH2 | 2.33 | 0.43 |
| 2:V:26:VAL:HG12 | 2:V:32:MET:HG3 | 2.00 | 0.43 |
| 2:2:4:GLN:OE1 | 2:2:67:VAL:HG11 | 2.18 | 0.43 |
| 2:Z:74:PRO:HD2 | 2:Z:91:PHE:CE2 | 2.53 | 0.43 |
| 2:T:73:LEU:HB3 | 2:T:91:PHE:CE2 | 2.47 | 0.43 |
| 1:N:99:ILE:CD1 | 1:N:509:ALA:HA | 2.48 | 0.43 |
| 1:N:332:MET:HG2 | 1:N:334:LEU:CD1 | 2.48 | 0.43 |
| 1:M:124:VAL:O | 1:M:128:ILE:HG12 | 2.18 | 0.43 |
| 1:M:207:THR:HG21 | 1:M:212:LYS:H | 1.83 | 0.43 |
| 1:M:413:VAL:HB | 1:M:498:THR:HG22 | 2.00 | 0.43 |
| 1:L:194:LYS:HD2 | 1:L:332:MET:HE2 | 1.99 | 0.43 |
| 1:J:350:ILE:HG23 | 1:J:366:LEU:HD22 | 2.00 | 0.43 |
| 1:J:498:THR:O | 1:J:502:ARG:HG2 | 2.18 | 0.43 |
| 1:D:322:GLY:N | 1:D:335:LYS:O | 2.45 | 0.43 |
| 1:B:166:MET:HG3 | 1:B:171:ARG:HA | 1.99 | 0.43 |
| 1:A:371:ALA:HB1 | 1:A:376:GLY:O | 2.19 | 0.43 |
| 1:G:23:LEU:O | 1:G:23:LEU:HD23 | 2.19 | 0.43 |
| 1:G:207:THR:HG21 | 1:G:212:LYS:H | 1.84 | 0.43 |
| 1:G:497:PRO:HD2 | 1:G:500:VAL:HG11 | 2.01 | 0.43 |
| 1:E:350:ILE:HG23 | 1:E:366:LEU:HD21 | 1.99 | 0.43 |
| 1:E:362:GLU:O | 1:E:366:LEU:HB2 | 2.18 | 0.43 |
| 1:E:386:SER:O | 1:E:390:VAL:HG23 | 2.18 | 0.43 |
| 1:H:138:VAL:HG21 | 1:H:144:ILE:HD13 | 2.01 | 0.43 |
| 1:H:259:LEU:O | 1:H:263:VAL:HG22 | 2.19 | 0.43 |
| 2:W:16:VAL:CG1 | 2:W:46:VAL:HG23 | 2.49 | 0.43 |
| 2:Q:16:VAL:CG1 | 2:Q:46:VAL:HG23 | 2.49 | 0.43 |
| 2:U:73:LEU:HD13 | 2:U:91:PHE:CE2 | 2.54 | 0.43 |
| 1:N:195:PHE:CD2 | 1:N:197:ARG:HB3 | 2.54 | 0.43 |
| 1:M:8:PHE:CD1 | 1:M:520:VAL:HG22 | 2.54 | 0.43 |
| 1:M:107:ILE:HD11 | 1:M:516:THR:O | 2.19 | 0.43 |
| 1:M:324:VAL:HG22 | 1:M:333:LEU:HD23 | 1.99 | 0.43 |
| 1:K:227:ILE:HG21 | 1:K:233:ILE:HD13 | 2.01 | 0.43 |
| 1:K:362:GLU:O | 1:K:366:LEU:HB2 | 2.19 | 0.43 |
| 1:I:140:THR:OG1 | 1:I:141:PRO:HD2 | 2.19 | 0.43 |
| 1:D:107:ILE:HD11 | 1:D:516:THR:O | 2.18 | 0.43 |
| 1:D:195:PHE:CD2 | 1:D:197:ARG:HB3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:203:TYR:HB3 | 1:D:267:LEU:HD11 | 2.00 | 0.43 |
| 1:D:219:TYR:CE2 | 1:D:245:LYS:HB2 | 2.54 | 0.43 |
| 1:C:228:SER:HA | 1:C:255:ASP:HB3 | 2.00 | 0.43 |
| 1:C:422:ARG:NH1 | 1:C:474:SER:O | 2.52 | 0.43 |
| 1:B:138:VAL:CG1 | 1:B:408:VAL:HA | 2.48 | 0.43 |
| 1:G:148:ALA:HB2 | 1:G:404:THR:CG2 | 2.48 | 0.43 |
| 1:H:127:VAL:HG23 | 1:H:423:CYS:CB | 2.47 | 0.43 |
| 2:1:73:LEU:HD13 | 2:1:91:PHE:CE2 | 2.54 | 0.43 |
| 2:Y:73:LEU:HD13 | 2:Y:91:PHE:CE2 | 2.53 | 0.43 |
| 2:W:34:PRO:CD | 1:I:261:THR:HG22 | 2.47 | 0.43 |
| 2:R:44:ALA:HB2 | 2:R:73:LEU:HD11 | 2.01 | 0.43 |
| 2:Q:34:PRO:CD | 1:C:261:THR:HG22 | 2.48 | 0.43 |
| 2:U:27:THR:CG2 | 2:U:31:ILE:H | 2.31 | 0.43 |
| 2:S:16:VAL:C | 2:S:90:LEU:HD12 | 2.39 | 0.43 |
| 1:N:24:ALA:HA | 1:N:27:VAL:HG12 | 2.01 | 0.43 |
| 1:N:140:THR:OG1 | 1:N:141:PRO:HD2 | 2.19 | 0.43 |
| 1:N:175:ILE:CG2 | 1:N:401:LEU:HD11 | 2.48 | 0.43 |
| 1:N:340:LYS:HA | 1:N:343:ILE:CG1 | 2.38 | 0.43 |
| 1:M:140:THR:HG22 | 1:M:143:GLU:HG3 | 2.01 | 0.43 |
| 1:M:346:ARG:O | 1:M:350:ILE:HD12 | 2.17 | 0.43 |
| 1:L:222:LEU:CD2 | 1:L:250:ILE:HB | 2.44 | 0.43 |
| 1:K:138:VAL:HG23 | 1:K:143:GLU:HB2 | 2.00 | 0.43 |
| 1:J:163:SER:O | 1:J:167:LYS:HG3 | 2.18 | 0.43 |
| 1:J:248:VAL:HG11 | 1:J:324:VAL:HG11 | 2.01 | 0.43 |
| 1:I:127:VAL:HG11 | 1:I:505:LEU:HD21 | 1.99 | 0.43 |
| 1:I:194:LYS:HD2 | 1:I:332:MET:HE3 | 1.99 | 0.43 |
| 1:D:250:ILE:HD13 | 1:D:292:MET:CE | 2.49 | 0.43 |
| 1:D:350:ILE:HG23 | 1:D:366:LEU:HD21 | 2.00 | 0.43 |
| 1:C:195:PHE:HB2 | 1:C:279:PRO:HB3 | 2.01 | 0.43 |
| 1:A:65:LYS:O | 1:A:69:ILE:HG13 | 2.19 | 0.43 |
| 1:A:166:MET:CG | 1:A:171:ARG:HA | 2.48 | 0.43 |
| 1:A:278:ALA:HB3 | 1:A:285:ARG:HD2 | 2.00 | 0.43 |
| 1:G:228:SER:HA | 1:G:255:ASP:HB3 | 2.00 | 0.43 |
| 1:G:306:LEU:HG | 1:G:308:LEU:CD2 | 2.49 | 0.43 |
| 1:G:343:ILE:O | 1:G:347:ILE:HG13 | 2.18 | 0.43 |
| 1:F:280:GLY:HA3 | 1:F:285:ARG:HB2 | 2.00 | 0.43 |
| 1:F:386:SER:O | 1:F:390:VAL:HG23 | 2.19 | 0.43 |
| 1:E:195:PHE:CG | 1:E:279:PRO:HG3 | 2.53 | 0.43 |
| 1:H:69:ILE:HG23 | 1:I:47:PRO:HG3 | 2.00 | 0.43 |
| 2:V:4:GLN:OE1 | 2:V:67:VAL:HG11 | 2.18 | 0.43 |
| 2:V:73:LEU:HD13 | 2:V:91:PHE:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:25:THR:O | 2:2:33:LEU:HB2 | 2.19 | 0.43 |
| 2:Z:16:VAL:C | 2:Z:90:LEU:HD12 | 2.40 | 0.43 |
| 2:X:26:VAL:HA | 2:X:32:MET:HA | 2.01 | 0.43 |
| 2:W:20:ARG:HB3 | 2:W:41:VAL:CG1 | 2.48 | 0.43 |
| 2:U:25:THR:O | 2:U:33:LEU:HB2 | 2.19 | 0.43 |
| 1:N:350:ILE:HG22 | 1:N:370:LEU:HD11 | 2.00 | 0.43 |
| 1:M:99:ILE:HD13 | 1:M:509:ALA:HA | 2.00 | 0.43 |
| 1:M:138:VAL:HG23 | 1:M:143:GLU:HB2 | 2.00 | 0.43 |
| 1:L:219:TYR:HB3 | 1:L:318:LEU:HD23 | 2.00 | 0.43 |
| 1:K:124:VAL:HG21 | 1:K:509:ALA:HB1 | 2.01 | 0.43 |
| 1:K:138:VAL:CG1 | 1:K:408:VAL:HA | 2.49 | 0.43 |
| 1:K:187:LEU:HD13 | 1:K:380:LEU:HD21 | 2.01 | 0.43 |
| 1:K:322:GLY:N | 1:K:335:LYS:O | 2.39 | 0.43 |
| 1:J:23:LEU:HD13 | 1:J:71:ALA:HA | 2.00 | 0.43 |
| 1:I:207:THR:HG21 | 1:I:212:LYS:H | 1.83 | 0.43 |
| 1:C:227:ILE:HG21 | 1:C:233:ILE:HD13 | 2.01 | 0.43 |
| 1:B:195:PHE:CD2 | 1:B:197:ARG:HB3 | 2.54 | 0.43 |
| 1:B:497:PRO:HD2 | 1:B:500:VAL:HG11 | 2.00 | 0.43 |
| 1:F:8:PHE:CD1 | 1:F:520:VAL:HG22 | 2.54 | 0.43 |
| 1:F:232:SER:HB2 | 1:F:310:LEU:CD1 | 2.49 | 0.43 |
| 1:E:140:THR:HG22 | 1:E:143:GLU:HG3 | 2.01 | 0.43 |
| 1:H:166:MET:CG | 1:H:171:ARG:HA | 2.48 | 0.43 |
| 1:H:350:ILE:HG23 | 1:H:366:LEU:HD22 | 2.01 | 0.43 |
| 2:1:25:THR:O | 2:1:33:LEU:HB2 | 2.19 | 0.43 |
| 2:W:4:GLN:OE1 | 2:W:67:VAL:HG11 | 2.18 | 0.43 |
| 2:R:4:GLN:OE1 | 2:R:67:VAL:HG11 | 2.19 | 0.43 |
| 2:Q:4:GLN:OE1 | 2:Q:67:VAL:HG11 | 2.19 | 0.43 |
| 2:Q:31:ILE:HG12 | 2:Q:32:MET:H | 1.83 | 0.43 |
| 2:Q:82:VAL:C | 2:Q:83:LEU:HD12 | 2.38 | 0.43 |
| 2:P:27:THR:CG2 | 2:P:31:ILE:H | 2.31 | 0.43 |
| 1:N:140:THR:CG2 | 1:N:143:GLU:HG3 | 2.49 | 0.43 |
| 1:M:3:ALA:HB3 | 1:M:525:ILE:HD12 | 2.01 | 0.43 |
| 1:M:250:ILE:HD13 | 1:M:292:MET:HE2 | 2.00 | 0.43 |
| 1:L:188:GLU:HB3 | 1:L:379:VAL:HG22 | 1.99 | 0.43 |
| 1:K:99:ILE:CD1 | 1:K:509:ALA:HA | 2.49 | 0.43 |
| 1:K:253:ASP:OD1 | 1:K:254:VAL:N | 2.52 | 0.43 |
| 1:J:32:GLY:N | 3:J:601:ADP:O2A | 2.44 | 0.43 |
| 1:J:301:PHE:CZ | 1:J:313:VAL:HG12 | 2.54 | 0.43 |
| 1:I:199:TYR:HE2 | 1:I:202:PRO:HA | 1.84 | 0.43 |
| 1:I:225:LYS:HA | 1:I:252:GLU:OE1 | 2.19 | 0.43 |
| 1:I:233:ILE:O | 1:I:237:LEU:HD13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:340:LYS:HA | 1:I:343:ILE:CG1 | 2.39 | 0.43 |
| 1:B:340:LYS:HA | 1:B:343:ILE:CG1 | 2.38 | 0.43 |
| 1:A:30:THR:HG22 | 1:A:36:ARG:O | 2.19 | 0.43 |
| 1:A:343:ILE:O | 1:A:347:ILE:HG13 | 2.19 | 0.43 |
| 1:G:8:PHE:CD1 | 1:G:520:VAL:HG22 | 2.53 | 0.43 |
| 1:G:385:THR:HG21 | 1:F:506:LEU:HD21 | 2.00 | 0.43 |
| 1:F:187:LEU:HD13 | 1:F:380:LEU:CD2 | 2.48 | 0.43 |
| 1:F:427:LEU:HA | 1:F:430:LEU:HD23 | 2.01 | 0.43 |
| 1:H:47:PRO:HG3 | 1:N:69:ILE:HG23 | 2.01 | 0.42 |
| 1:H:68:ASN:O | 1:H:72:LYS:HG2 | 2.18 | 0.42 |
| 2:2:44:ALA:HB2 | 2:2:73:LEU:HD11 | 2.01 | 0.42 |
| 2:1:21:SER:OG | 2:1:41:VAL:HG21 | 2.19 | 0.42 |
| 2:Z:21:SER:OG | 2:Z:41:VAL:HG21 | 2.19 | 0.42 |
| 2:X:4:GLN:OE1 | 2:X:67:VAL:HG11 | 2.19 | 0.42 |
| 2:W:73:LEU:HD13 | 2:W:91:PHE:CE2 | 2.54 | 0.42 |
| 2:O:18:VAL:HG12 | 2:O:46:VAL:CA | 2.44 | 0.42 |
| 2:T:31:ILE:HG12 | 2:T:32:MET:H | 1.83 | 0.42 |
| 1:N:301:PHE:CE1 | 1:N:313:VAL:HG12 | 2.54 | 0.42 |
| 1:N:499:LYS:O | 1:N:503:THR:HG23 | 2.18 | 0.42 |
| 1:M:165:ALA:HB2 | 1:M:187:LEU:CD1 | 2.49 | 0.42 |
| 1:M:332:MET:HG2 | 1:M:334:LEU:CD1 | 2.49 | 0.42 |
| 1:M:480:ASP:O | 1:M:484:GLY:N | 2.52 | 0.42 |
| 1:L:87:ASP:O | 1:L:500:VAL:HG23 | 2.18 | 0.42 |
| 1:J:24:ALA:HA | 1:J:27:VAL:HG12 | 2.01 | 0.42 |
| 1:J:99:ILE:CD1 | 1:J:509:ALA:HA | 2.49 | 0.42 |
| 1:J:309:ASN:HB3 | 1:J:311:GLU:OE1 | 2.19 | 0.42 |
| 1:D:8:PHE:CD1 | 1:D:520:VAL:HG22 | 2.54 | 0.42 |
| 1:D:99:ILE:CD1 | 1:D:509:ALA:HA | 2.49 | 0.42 |
| 1:D:165:ALA:HB2 | 1:D:187:LEU:CD1 | 2.49 | 0.42 |
| 1:C:165:ALA:HB2 | 1:C:187:LEU:CD1 | 2.48 | 0.42 |
| 1:A:199:TYR:HA | 1:A:276:VAL:HG12 | 2.01 | 0.42 |
| 1:E:23:LEU:O | 1:E:23:LEU:HD23 | 2.19 | 0.42 |
| 1:E:140:THR:OG1 | 1:E:141:PRO:HD2 | 2.19 | 0.42 |
| 1:H:32:GLY:N | 3:H:601:ADP:O2A | 2.47 | 0.42 |
| 1:H:185:ASP:OD1 | 1:H:383:GLY:N | 2.38 | 0.42 |
| 1:H:253:ASP:OD1 | 1:H:254:VAL:N | 2.52 | 0.42 |
| 2:X:21:SER:OG | 2:X:41:VAL:HG21 | 2.19 | 0.42 |
| 2:O:20:ARG:HB3 | 2:O:41:VAL:CG1 | 2.49 | 0.42 |
| 2:U:11:PRO:HB2 | 2:U:15:ARG:HB2 | 2.01 | 0.42 |
| 2:T:25:THR:O | 2:T:33:LEU:HB2 | 2.19 | 0.42 |
| 2:S:16:VAL:HG13 | 2:S:46:VAL:HG23 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:23:LEU:HD22 | 1:N:74:VAL:CG1 | 2.49 | 0.42 |
| 1:N:385:THR:HG21 | 1:M:506:LEU:HD21 | 2.01 | 0.42 |
| 1:L:264:LEU:O | 1:L:268:LYS:HG2 | 2.19 | 0.42 |
| 1:J:175:ILE:CG2 | 1:J:401:LEU:HD11 | 2.49 | 0.42 |
| 1:J:194:LYS:HD2 | 1:J:332:MET:HE2 | 2.00 | 0.42 |
| 1:J:350:ILE:HG22 | 1:J:370:LEU:HD11 | 2.01 | 0.42 |
| 1:J:450:ILE:O | 1:J:454:THR:HG23 | 2.19 | 0.42 |
| 1:I:293:ALA:O | 1:I:297:GLY:N | 2.35 | 0.42 |
| 1:I:306:LEU:CG | 1:I:308:LEU:HD23 | 2.40 | 0.42 |
| 1:D:176:THR:O | 1:D:379:VAL:HA | 2.19 | 0.42 |
| 1:D:340:LYS:HA | 1:D:343:ILE:CG1 | 2.38 | 0.42 |
| 1:D:343:ILE:O | 1:D:347:ILE:HG13 | 2.19 | 0.42 |
| 1:B:124:VAL:HG21 | 1:B:509:ALA:HB1 | 2.01 | 0.42 |
| 1:A:23:LEU:O | 1:A:23:LEU:HD23 | 2.18 | 0.42 |
| 1:F:117:ARG:NH1 | 1:F:514:LEU:HB2 | 2.34 | 0.42 |
| 1:E:195:PHE:CD2 | 1:E:197:ARG:HB3 | 2.54 | 0.42 |
| 2:2:73:LEU:HD13 | 2:2:91:PHE:CE2 | 2.55 | 0.42 |
| 2:X:16:VAL:C | 2:X:90:LEU:HD12 | 2.39 | 0.42 |
| 2:U:81:VAL:HG12 | 2:T:72:LEU:HD21 | 2.01 | 0.42 |
| 1:N:435:GLU:O | 1:N:439:ILE:HG13 | 2.18 | 0.42 |
| 1:M:175:ILE:CG2 | 1:M:401:LEU:HD11 | 2.49 | 0.42 |
| 1:M:193:MET:CE | 1:M:292:MET:HG2 | 2.49 | 0.42 |
| 1:M:253:ASP:OD1 | 1:M:254:VAL:N | 2.51 | 0.42 |
| 1:L:64:ASP:OD1 | 1:L:65:LYS:N | 2.52 | 0.42 |
| 1:L:362:GLU:O | 1:L:366:LEU:HB2 | 2.18 | 0.42 |
| 1:K:199:TYR:HE2 | 1:K:202:PRO:HA | 1.85 | 0.42 |
| 1:J:59:SER:O | 1:I:4:LYS:HD2 | 2.20 | 0.42 |
| 1:I:23:LEU:O | 1:I:23:LEU:HD23 | 2.18 | 0.42 |
| 1:I:187:LEU:HD13 | 1:I:380:LEU:CD2 | 2.50 | 0.42 |
| 1:I:350:ILE:HG22 | 1:I:370:LEU:HD11 | 2.02 | 0.42 |
| 1:I:462:GLU:O | 1:I:466:ILE:HG12 | 2.19 | 0.42 |
| 1:D:140:THR:OG1 | 1:D:141:PRO:HD2 | 2.19 | 0.42 |
| 1:D:422:ARG:NH1 | 1:D:474:SER:O | 2.53 | 0.42 |
| 1:C:124:VAL:O | 1:C:128:ILE:HG12 | 2.19 | 0.42 |
| 1:B:239:ILE:HD12 | 1:B:313:VAL:HG23 | 2.01 | 0.42 |
| 1:A:140:THR:HG22 | 1:A:143:GLU:HG3 | 2.02 | 0.42 |
| 1:A:271:LEU:HG | 1:A:273:VAL:HG13 | 2.01 | 0.42 |
| 1:G:279:PRO:HB2 | 1:G:288:GLN:OE1 | 2.19 | 0.42 |
| 1:F:165:ALA:HB2 | 1:F:187:LEU:CD1 | 2.49 | 0.42 |
| 1:F:207:THR:HG21 | 1:F:212:LYS:H | 1.83 | 0.42 |
| 1:E:62:LEU:CD1 | 1:E:67:LYS:HB3 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:290:LYS:O | 1:H:294:ILE:HG12 | 2.19 | 0.42 |
| 2:U:32:MET:SD | 1:G:268:LYS:HE3 | 2.60 | 0.42 |
| 2:S:26:VAL:HA | 2:S:32:MET:HA | 2.00 | 0.42 |
| 2:S:31:ILE:HG12 | 2:S:32:MET:H | 1.84 | 0.42 |
| 1:N:73:LEU:HD13 | 1:N:515:LEU:HD13 | 2.01 | 0.42 |
| 1:N:165:ALA:HB2 | 1:N:187:LEU:CD1 | 2.49 | 0.42 |
| 1:N:166:MET:CG | 1:N:171:ARG:HA | 2.49 | 0.42 |
| 1:N:230:ILE:HD12 | 1:N:261:THR:CG2 | 2.50 | 0.42 |
| 1:N:257:GLU:O | 1:N:261:THR:HG23 | 2.20 | 0.42 |
| 1:M:136:LYS:NZ | 1:M:490:VAL:HG11 | 2.34 | 0.42 |
| 1:M:499:LYS:O | 1:M:503:THR:HG23 | 2.19 | 0.42 |
| 1:L:497:PRO:HD2 | 1:L:500:VAL:HG11 | 2.01 | 0.42 |
| 1:K:197:ARG:NE | 1:K:278:ALA:O | 2.51 | 0.42 |
| 1:J:233:ILE:O | 1:J:237:LEU:HD13 | 2.19 | 0.42 |
| 1:J:439:ILE:O | 1:J:443:ILE:HG13 | 2.18 | 0.42 |
| 1:I:23:LEU:HD13 | 1:I:71:ALA:HA | 2.00 | 0.42 |
| 1:I:188:GLU:HB3 | 1:I:379:VAL:HG23 | 1.98 | 0.42 |
| 1:D:138:VAL:CG1 | 1:D:408:VAL:HA | 2.48 | 0.42 |
| 1:D:324:VAL:HG22 | 1:D:333:LEU:HD23 | 2.01 | 0.42 |
| 1:D:462:GLU:O | 1:D:466:ILE:HG12 | 2.19 | 0.42 |
| 1:C:54:VAL:O | 1:C:58:LYS:N | 2.21 | 0.42 |
| 1:C:127:VAL:HG11 | 1:C:505:LEU:HD21 | 2.02 | 0.42 |
| 1:C:499:LYS:O | 1:C:503:THR:HG23 | 2.19 | 0.42 |
| 1:B:462:GLU:O | 1:B:466:ILE:HG12 | 2.20 | 0.42 |
| 1:A:114:VAL:HG12 | 1:A:118:ARG:NH1 | 2.33 | 0.42 |
| 1:A:136:LYS:NZ | 1:A:490:VAL:HG11 | 2.34 | 0.42 |
| 1:G:138:VAL:HG23 | 1:G:143:GLU:HB2 | 2.01 | 0.42 |
| 1:E:24:ALA:HA | 1:E:27:VAL:HG12 | 2.01 | 0.42 |
| 2:V:9:PHE:CD2 | 2:V:17:LEU:HD22 | 2.54 | 0.42 |
| 2:Q:26:VAL:HA | 2:Q:32:MET:HA | 2.02 | 0.42 |
| 2:O:15:ARG:HH22 | 2:U:97:LEU:HA | 1.84 | 0.42 |
| 2:U:73:LEU:HB3 | 2:U:91:PHE:CE2 | 2.52 | 0.42 |
| 1:N:8:PHE:CD1 | 1:N:520:VAL:HG22 | 2.53 | 0.42 |
| 1:N:207:THR:HG21 | 1:N:212:LYS:H | 1.85 | 0.42 |
| 1:M:23:LEU:HD22 | 1:M:74:VAL:CG1 | 2.49 | 0.42 |
| 1:M:62:LEU:CD1 | 1:M:67:LYS:HB3 | 2.49 | 0.42 |
| 1:M:140:THR:OG1 | 1:M:141:PRO:HD2 | 2.19 | 0.42 |
| 1:M:250:ILE:HD13 | 1:M:292:MET:CE | 2.49 | 0.42 |
| 1:L:497:PRO:HB2 | 1:L:500:VAL:HG12 | 2.01 | 0.42 |
| 1:J:138:VAL:CG1 | 1:J:408:VAL:HA | 2.49 | 0.42 |
| 1:D:73:LEU:HD13 | 1:D:515:LEU:HD13 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:175:ILE:CG2 | 1:D:401:LEU:HD11 | 2.50 | 0.42 |
| 1:B:64:ASP:O | 1:B:68:ASN:HB2 | 2.19 | 0.42 |
| 1:G:350:ILE:HG22 | 1:G:370:LEU:CD1 | 2.50 | 0.42 |
| 1:F:31:MET:SD | 1:F:454:THR:OG1 | 2.69 | 0.42 |
| 1:F:163:SER:O | 1:F:167:LYS:HG3 | 2.19 | 0.42 |
| 1:F:228:SER:HA | 1:F:255:ASP:HB3 | 2.00 | 0.42 |
| 1:E:127:VAL:HG11 | 1:E:505:LEU:HD21 | 2.00 | 0.42 |
| 1:E:343:ILE:O | 1:E:347:ILE:HG13 | 2.18 | 0.42 |
| 1:E:435:GLU:O | 1:E:439:ILE:HG13 | 2.20 | 0.42 |
| 1:H:135:SER:OG | 1:H:498:THR:HG21 | 2.20 | 0.42 |
| 1:H:237:LEU:HD23 | 1:H:271:LEU:HD23 | 2.00 | 0.42 |
| 2:Z:25:THR:O | 2:Z:33:LEU:HB2 | 2.20 | 0.42 |
| 2:Y:34:PRO:HD2 | 1:K:230:ILE:CD1 | 2.49 | 0.42 |
| 2:T:8:LYS:O | 2:S:100:TYR:HA | 2.20 | 0.42 |
| 1:N:147:VAL:HG22 | 1:N:495:ILE:HG13 | 2.01 | 0.42 |
| 1:N:332:MET:HG2 | 1:N:334:LEU:HD12 | 2.01 | 0.42 |
| 1:M:77:VAL:CG2 | 1:M:511:VAL:HB | 2.50 | 0.42 |
| 1:M:478:GLY:O | 1:M:486:PHE:HA | 2.19 | 0.42 |
| 1:K:140:THR:OG1 | 1:K:141:PRO:HD2 | 2.19 | 0.42 |
| 1:I:32:GLY:N | 3:I:601:ADP:O2A | 2.45 | 0.42 |
| 1:I:117:ARG:NH1 | 1:I:514:LEU:HB2 | 2.34 | 0.42 |
| 1:D:135:SER:OG | 1:D:498:THR:HG21 | 2.19 | 0.42 |
| 1:C:62:LEU:CD1 | 1:C:67:LYS:HB3 | 2.49 | 0.42 |
| 1:C:77:VAL:CG2 | 1:C:511:VAL:HB | 2.49 | 0.42 |
| 1:C:98:SER:CB | 1:C:450:ILE:HG13 | 2.49 | 0.42 |
| 1:C:175:ILE:CG2 | 1:C:401:LEU:HD11 | 2.49 | 0.42 |
| 1:B:165:ALA:HB2 | 1:B:187:LEU:CD1 | 2.49 | 0.42 |
| 1:B:233:ILE:O | 1:B:237:LEU:HD13 | 2.20 | 0.42 |
| 1:B:287:ASN:HB3 | 1:B:369:ARG:NH1 | 2.34 | 0.42 |
| 1:A:140:THR:OG1 | 1:A:141:PRO:HD2 | 2.20 | 0.42 |
| 1:F:169:VAL:HG21 | 1:F:378:ALA:HB2 | 2.01 | 0.42 |
| 1:H:237:LEU:HD22 | 2:V:31:ILE:HD11 | 2.02 | 0.42 |
| 1:H:303:GLU:OE1 | 1:H:306:LEU:HD22 | 2.20 | 0.42 |
| 2:2:16:VAL:C | 2:2:90:LEU:HD12 | 2.40 | 0.42 |
| 1:N:120:VAL:HG13 | 1:N:444:ILE:CD1 | 2.40 | 0.42 |
| 1:N:148:ALA:HB2 | 1:N:404:THR:CG2 | 2.49 | 0.42 |
| 1:N:227:ILE:HG21 | 1:N:233:ILE:HD13 | 2.02 | 0.42 |
| 1:N:250:ILE:HD13 | 1:N:292:MET:CE | 2.49 | 0.42 |
| 1:M:462:GLU:O | 1:M:466:ILE:HG12 | 2.20 | 0.42 |
| 1:K:188:GLU:OE1 | 1:K:381:LYS:NZ | 2.46 | 0.42 |
| 1:K:239:ILE:HD11 | 1:K:313:VAL:HG23 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:350:ILE:HG22 | 1:K:370:LEU:HD11 | 2.02 | 0.42 |
| 1:I:39:ILE:HG12 | 1:I:49:VAL:HG22 | 2.02 | 0.42 |
| 1:I:117:ARG:O | 1:I:121:MET:HG2 | 2.20 | 0.42 |
| 1:C:23:LEU:HD22 | 1:C:74:VAL:CG1 | 2.50 | 0.42 |
| 1:C:99:ILE:CD1 | 1:C:509:ALA:HA | 2.50 | 0.42 |
| 1:C:413:VAL:HB | 1:C:498:THR:HG22 | 2.02 | 0.42 |
| 1:A:449:LYS:HE3 | 1:A:471:MET:HE1 | 2.02 | 0.42 |
| 1:F:98:SER:CB | 1:F:450:ILE:HG13 | 2.50 | 0.42 |
| 1:F:117:ARG:O | 1:F:121:MET:HG2 | 2.19 | 0.42 |
| 1:E:54:VAL:HG12 | 1:E:78:ALA:HB1 | 2.02 | 0.42 |
| 1:E:227:ILE:HG21 | 1:E:233:ILE:HD13 | 2.02 | 0.42 |
| 1:H:34:LYS:HD2 | 1:H:459:ALA:HA | 2.02 | 0.42 |
| 2:1:16:VAL:C | 2:1:90:LEU:HD12 | 2.39 | 0.42 |
| 2:U:21:SER:OG | 2:U:41:VAL:HG21 | 2.19 | 0.42 |
| 1:N:456:ALA:CB | 1:N:463:GLY:HA2 | 2.50 | 0.42 |
| 1:M:257:GLU:O | 1:M:261:THR:HG23 | 2.20 | 0.42 |
| 1:L:350:ILE:HG22 | 1:L:370:LEU:HD11 | 2.01 | 0.42 |
| 1:K:250:ILE:HD13 | 1:K:292:MET:CE | 2.50 | 0.42 |
| 1:K:466:ILE:O | 1:K:470:ILE:HG13 | 2.20 | 0.42 |
| 1:J:23:LEU:O | 1:J:23:LEU:HD23 | 2.20 | 0.42 |
| 1:J:98:SER:CB | 1:J:450:ILE:HG13 | 2.50 | 0.42 |
| 1:I:8:PHE:CD1 | 1:I:520:VAL:HG22 | 2.55 | 0.42 |
| 1:I:64:ASP:OD1 | 1:I:65:LYS:N | 2.53 | 0.42 |
| 1:I:161:ILE:HG22 | 1:I:380:LEU:HD22 | 2.02 | 0.42 |
| 1:I:207:THR:OG1 | 1:I:209:LYS:HB3 | 2.19 | 0.42 |
| 1:I:219:TYR:CE2 | 1:I:245:LYS:HB2 | 2.54 | 0.42 |
| 1:D:257:GLU:O | 1:D:261:THR:HG23 | 2.19 | 0.42 |
| 1:C:218:ALA:HB2 | 1:C:246:PRO:HG2 | 2.02 | 0.42 |
| 1:B:350:ILE:HG22 | 1:B:370:LEU:HD11 | 2.01 | 0.42 |
| 1:G:23:LEU:HD22 | 1:G:74:VAL:CG1 | 2.50 | 0.42 |
| 1:G:239:ILE:HD11 | 1:G:313:VAL:HG23 | 2.01 | 0.42 |
| 1:H:73:LEU:HD12 | 1:H:515:LEU:HD13 | 2.01 | 0.42 |
| 1:H:124:VAL:HA | 1:H:127:VAL:HG12 | 2.01 | 0.42 |
| 1:H:239:ILE:HD12 | 1:H:313:VAL:HG23 | 2.02 | 0.42 |
| 2:1:73:LEU:HB3 | 2:1:91:PHE:CE2 | 2.47 | 0.42 |
| 2:P:63:VAL:HG13 | 2:P:93:ASP:OD1 | 2.20 | 0.42 |
| 2:P:73:LEU:HD13 | 2:P:91:PHE:CE2 | 2.55 | 0.42 |
| 2:O:11:PRO:HB2 | 2:O:15:ARG:HB2 | 2.01 | 0.42 |
| 1:N:20:VAL:HG13 | 1:N:74:VAL:HG21 | 2.01 | 0.42 |
| 1:N:350:ILE:HG23 | 1:N:366:LEU:HD21 | 2.00 | 0.42 |
| 1:N:414:LEU:HD22 | 1:N:489:MET:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:498:THR:O | 1:N:502:ARG:HG2 | 2.20 | 0.42 |
| 1:M:127:VAL:HG11 | 1:M:505:LEU:HD21 | 2.02 | 0.42 |
| 1:M:218:ALA:HB2 | 1:M:246:PRO:HG2 | 2.02 | 0.42 |
| 1:M:350:ILE:HG22 | 1:M:370:LEU:HD11 | 2.01 | 0.42 |
| 1:M:422:ARG:NH1 | 1:M:474:SER:O | 2.52 | 0.42 |
| 1:L:346:ARG:NE | 1:L:350:ILE:HD11 | 2.35 | 0.42 |
| 1:K:136:LYS:NZ | 1:K:490:VAL:HG11 | 2.35 | 0.42 |
| 1:K:219:TYR:CE2 | 1:K:245:LYS:HB2 | 2.55 | 0.42 |
| 1:K:224:GLU:OE2 | 1:K:286:LYS:HE3 | 2.19 | 0.42 |
| 1:J:64:ASP:O | 1:J:68:ASN:HB2 | 2.20 | 0.42 |
| 1:J:69:ILE:HD11 | 1:J:523:THR:HG22 | 2.01 | 0.42 |
| 1:J:371:ALA:HB1 | 1:J:376:GLY:O | 2.20 | 0.42 |
| 1:I:239:ILE:HD11 | 1:I:313:VAL:HG23 | 2.01 | 0.42 |
| 1:I:404:THR:O | 1:I:408:VAL:HG13 | 2.20 | 0.42 |
| 1:D:6:VAL:CG2 | 1:E:22:LEU:HD11 | 2.49 | 0.42 |
| 1:D:283:ASP:HA | 1:D:286:LYS:HD3 | 2.02 | 0.42 |
| 1:D:301:PHE:CZ | 1:D:313:VAL:HG12 | 2.54 | 0.42 |
| 1:C:340:LYS:CA | 1:C:343:ILE:HG12 | 2.38 | 0.42 |
| 1:B:4:LYS:HD3 | 1:B:522:VAL:CG1 | 2.50 | 0.42 |
| 1:B:217:ASP:HA | 1:B:321:VAL:O | 2.20 | 0.42 |
| 1:A:188:GLU:O | 1:A:379:VAL:HG22 | 2.19 | 0.42 |
| 1:G:462:GLU:O | 1:G:466:ILE:HG12 | 2.19 | 0.42 |
| 2:Z:4:GLN:OE1 | 2:Z:67:VAL:HG11 | 2.19 | 0.42 |
| 2:X:73:LEU:HD13 | 2:X:91:PHE:CE2 | 2.55 | 0.42 |
| 1:N:135:SER:OG | 1:N:498:THR:HG21 | 2.19 | 0.42 |
| 1:M:52:ASP:OD2 | 5:M:702:HOH:O | 2.22 | 0.42 |
| 1:M:402:ASN:OD1 | 1:M:405:ARG:NH2 | 2.46 | 0.42 |
| 1:L:20:VAL:HG13 | 1:L:74:VAL:HG21 | 2.02 | 0.42 |
| 1:L:476:GLU:OE1 | 1:L:476:GLU:N | 2.52 | 0.42 |
| 1:J:138:VAL:HG23 | 1:J:143:GLU:HB2 | 2.00 | 0.42 |
| 1:J:140:THR:OG1 | 1:J:141:PRO:HD2 | 2.20 | 0.42 |
| 1:J:148:ALA:HB2 | 1:J:404:THR:CG2 | 2.50 | 0.42 |
| 1:I:228:SER:HA | 1:I:255:ASP:HB3 | 2.01 | 0.42 |
| 1:I:253:ASP:OD1 | 1:I:254:VAL:N | 2.52 | 0.42 |
| 1:I:350:ILE:HG22 | 1:I:370:LEU:CD1 | 2.50 | 0.42 |
| 1:D:225:LYS:HA | 1:D:252:GLU:OE1 | 2.20 | 0.42 |
| 1:C:138:VAL:HG23 | 1:C:143:GLU:HB2 | 2.01 | 0.42 |
| 1:C:140:THR:OG1 | 1:C:141:PRO:HD2 | 2.19 | 0.42 |
| 1:C:343:ILE:O | 1:C:347:ILE:HG13 | 2.20 | 0.42 |
| 1:B:120:VAL:O | 1:B:124:VAL:HG23 | 2.19 | 0.42 |
| 1:B:322:GLY:N | 1:B:335:LYS:O | 2.43 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:327:THR:OG1 | 1:B:330:ASP:O | 2.38 | 0.42 |
| 1:B:332:MET:HG2 | 1:B:334:LEU:CD1 | 2.49 | 0.42 |
| 1:B:525:ILE:CG1 | 1:B:526:PRO:HD2 | 2.47 | 0.42 |
| 1:A:8:PHE:CD1 | 1:A:520:VAL:HG22 | 2.54 | 0.42 |
| 1:A:64:ASP:OD1 | 1:A:65:LYS:N | 2.53 | 0.42 |
| 1:A:207:THR:HG21 | 1:A:212:LYS:H | 1.84 | 0.42 |
| 1:A:350:ILE:HG22 | 1:A:370:LEU:HD11 | 2.01 | 0.42 |
| 1:G:199:TYR:HE2 | 1:G:202:PRO:HA | 1.84 | 0.42 |
| 1:F:131:LEU:HD23 | 1:F:134:GLN:HE21 | 1.85 | 0.42 |
| 2:2:10:LEU:HD12 | 2:2:11:PRO:HD2 | 2.02 | 0.41 |
| 2:Q:13:PHE:HA | 2:Q:52:GLY:O | 2.20 | 0.41 |
| 2:O:17:LEU:HD11 | 2:O:88:TYR:CB | 2.49 | 0.41 |
| 2:S:63:VAL:HG13 | 2:S:93:ASP:OD1 | 2.19 | 0.41 |
| 1:N:54:VAL:HG12 | 1:N:78:ALA:HB1 | 2.02 | 0.41 |
| 1:N:233:ILE:O | 1:N:237:LEU:HD13 | 2.20 | 0.41 |
| 1:M:32:GLY:N | 3:M:601:ADP:O2A | 2.47 | 0.41 |
| 1:L:140:THR:OG1 | 1:L:141:PRO:HD2 | 2.19 | 0.41 |
| 1:L:350:ILE:HG23 | 1:L:366:LEU:HD22 | 2.00 | 0.41 |
| 1:K:65:LYS:O | 1:K:69:ILE:HG13 | 2.20 | 0.41 |
| 1:K:225:LYS:HA | 1:K:252:GLU:OE1 | 2.20 | 0.41 |
| 1:J:259:LEU:O | 1:J:263:VAL:HG22 | 2.19 | 0.41 |
| 1:C:258:ALA:O | 1:C:262:LEU:HG | 2.20 | 0.41 |
| 1:A:52:ASP:OD2 | 5:A:702:HOH:O | 2.21 | 0.41 |
| 1:A:140:THR:HG23 | 1:A:143:GLU:H | 1.85 | 0.41 |
| 1:A:176:THR:HG22 | 1:A:379:VAL:HG12 | 2.02 | 0.41 |
| 1:F:195:PHE:CD2 | 1:F:197:ARG:HB3 | 2.54 | 0.41 |
| 1:F:199:TYR:HE2 | 1:F:202:PRO:HA | 1.85 | 0.41 |
| 1:E:68:ASN:O | 1:E:72:LYS:HG2 | 2.20 | 0.41 |
| 1:E:165:ALA:HB2 | 1:E:187:LEU:CD1 | 2.49 | 0.41 |
| 1:H:23:LEU:HD22 | 1:H:74:VAL:CG1 | 2.51 | 0.41 |
| 1:H:98:SER:CB | 1:H:450:ILE:HG13 | 2.49 | 0.41 |
| 1:H:350:ILE:HG22 | 1:H:370:LEU:CD1 | 2.51 | 0.41 |
| 2:1:32:MET:SD | 1:M:268:LYS:HD3 | 2.60 | 0.41 |
| 2:1:34:PRO:HD2 | 1:M:230:ILE:CD1 | 2.50 | 0.41 |
| 2:R:100:TYR:HA | 2:S:8:LYS:O | 2.20 | 0.41 |
| 2:Q:41:VAL:HG22 | 2:Q:43:GLN:H | 1.85 | 0.41 |
| 2:P:17:LEU:HD11 | 2:P:88:TYR:CB | 2.50 | 0.41 |
| 1:N:225:LYS:HA | 1:N:252:GLU:OE1 | 2.19 | 0.41 |
| 1:M:343:ILE:O | 1:M:347:ILE:HG13 | 2.20 | 0.41 |
| 1:J:253:ASP:OD1 | 1:J:254:VAL:N | 2.53 | 0.41 |
| 1:D:147:VAL:HG22 | 1:D:495:ILE:HG13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:324:VAL:HG22 | 1:D:333:LEU:CD2 | 2.50 | 0.41 |
| 1:D:350:ILE:HG22 | 1:D:370:LEU:CD1 | 2.50 | 0.41 |
| 1:C:131:LEU:HD23 | 1:C:134:GLN:HE21 | 1.85 | 0.41 |
| 1:C:207:THR:HG21 | 1:C:212:LYS:H | 1.84 | 0.41 |
| 1:C:362:GLU:O | 1:C:366:LEU:HB2 | 2.19 | 0.41 |
| 1:C:462:GLU:O | 1:C:466:ILE:HG12 | 2.21 | 0.41 |
| 1:B:175:ILE:HG22 | 1:B:401:LEU:HD11 | 2.02 | 0.41 |
| 1:A:24:ALA:HA | 1:A:27:VAL:HG12 | 2.03 | 0.41 |
| 1:A:194:LYS:HD2 | 1:A:332:MET:HE2 | 2.01 | 0.41 |
| 1:G:140:THR:HG22 | 1:G:143:GLU:HG3 | 2.02 | 0.41 |
| 1:H:197:ARG:NE | 1:H:278:ALA:O | 2.53 | 0.41 |
| 1:H:280:GLY:O | 1:H:285:ARG:HB3 | 2.20 | 0.41 |
| 2:Z:26:VAL:HA | 2:Z:32:MET:HA | 2.01 | 0.41 |
| 2:S:53:SER:HB3 | 2:S:61:GLN:HB3 | 2.02 | 0.41 |
| 2:S:73:LEU:HD13 | 2:S:91:PHE:CE2 | 2.55 | 0.41 |
| 1:N:59:SER:O | 1:M:4:LYS:HD2 | 2.20 | 0.41 |
| 1:M:225:LYS:HA | 1:M:252:GLU:OE1 | 2.21 | 0.41 |
| 1:L:124:VAL:HG21 | 1:L:509:ALA:HB1 | 2.03 | 0.41 |
| 1:L:148:ALA:HB2 | 1:L:404:THR:CG2 | 2.49 | 0.41 |
| 1:L:250:ILE:HD13 | 1:L:292:MET:CE | 2.50 | 0.41 |
| 1:L:257:GLU:O | 1:L:261:THR:HG23 | 2.20 | 0.41 |
| 1:L:291:ASP:OD1 | 1:L:346:ARG:NE | 2.44 | 0.41 |
| 1:K:258:ALA:O | 1:K:262:LEU:HG | 2.20 | 0.41 |
| 1:J:385:THR:HG21 | 1:I:506:LEU:HD21 | 2.02 | 0.41 |
| 1:D:148:ALA:HB2 | 1:D:404:THR:CG2 | 2.49 | 0.41 |
| 1:D:253:ASP:OD1 | 1:D:254:VAL:N | 2.52 | 0.41 |
| 1:D:497:PRO:HD2 | 1:D:500:VAL:HG11 | 2.01 | 0.41 |
| 1:D:498:THR:O | 1:D:502:ARG:HG2 | 2.21 | 0.41 |
| 1:B:207:THR:HG21 | 1:B:212:LYS:H | 1.85 | 0.41 |
| 1:A:54:VAL:HG12 | 1:A:78:ALA:HB1 | 2.01 | 0.41 |
| 1:A:124:VAL:HG21 | 1:A:509:ALA:HB1 | 2.03 | 0.41 |
| 1:A:138:VAL:HG23 | 1:A:143:GLU:HB2 | 2.02 | 0.41 |
| 1:A:219:TYR:CE2 | 1:A:245:LYS:HB2 | 2.54 | 0.41 |
| 1:A:384:GLY:N | 1:A:390:VAL:HG22 | 2.34 | 0.41 |
| 1:F:250:ILE:HG12 | 1:F:276:VAL:CG2 | 2.50 | 0.41 |
| 1:E:23:LEU:HD22 | 1:E:74:VAL:CG1 | 2.51 | 0.41 |
| 1:H:138:VAL:HG23 | 1:H:143:GLU:HB2 | 2.03 | 0.41 |
| 2:Z:44:ALA:HB2 | 2:Z:73:LEU:HD11 | 2.03 | 0.41 |
| 2:U:72:LEU:O | 2:U:97:LEU:HB2 | 2.20 | 0.41 |
| 1:N:497:PRO:HD2 | 1:N:500:VAL:HG11 | 2.03 | 0.41 |
| 1:M:197:ARG:HD3 | 1:M:277:LYS:CB | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:64:ASP:O | 1:L:68:ASN:HB2 | 2.21 | 0.41 |
| 1:L:498:THR:O | 1:L:502:ARG:HG2 | 2.21 | 0.41 |
| 1:L:527:LYS:O | 1:L:528:GLU:HB3 | 2.20 | 0.41 |
| 1:K:23:LEU:HD13 | 1:K:71:ALA:HA | 2.01 | 0.41 |
| 1:K:31:MET:SD | 1:K:454:THR:OG1 | 2.68 | 0.41 |
| 1:K:138:VAL:HG23 | 1:K:143:GLU:CB | 2.50 | 0.41 |
| 1:J:188:GLU:HB3 | 1:J:379:VAL:HG22 | 2.02 | 0.41 |
| 1:D:187:LEU:HD13 | 1:D:380:LEU:CD2 | 2.50 | 0.41 |
| 1:D:218:ALA:HB2 | 1:D:246:PRO:HG2 | 2.02 | 0.41 |
| 1:C:107:ILE:HD11 | 1:C:516:THR:O | 2.20 | 0.41 |
| 1:C:350:ILE:HG22 | 1:C:370:LEU:HD11 | 2.01 | 0.41 |
| 1:C:480:ASP:O | 1:C:484:GLY:N | 2.54 | 0.41 |
| 1:G:64:ASP:OD1 | 1:G:65:LYS:N | 2.53 | 0.41 |
| 1:G:253:ASP:OD1 | 1:G:254:VAL:N | 2.54 | 0.41 |
| 1:G:346:ARG:NE | 1:G:350:ILE:HD11 | 2.35 | 0.41 |
| 1:F:281:PHE:N | 1:F:285:ARG:HD3 | 2.18 | 0.41 |
| 1:F:350:ILE:HG22 | 1:F:370:LEU:CD1 | 2.50 | 0.41 |
| 1:E:234:VAL:HG13 | 1:E:235:PRO:HD3 | 2.02 | 0.41 |
| 1:H:4:LYS:HD2 | 1:I:59:SER:O | 2.21 | 0.41 |
| 1:H:140:THR:OG1 | 1:H:141:PRO:HD2 | 2.20 | 0.41 |
| 2:2:14:ASP:HB3 | 2:2:92:ARG:HH21 | 1.86 | 0.41 |
| 2:2:21:SER:OG | 2:2:41:VAL:HG21 | 2.20 | 0.41 |
| 2:1:13:PHE:HA | 2:1:52:GLY:O | 2.21 | 0.41 |
| 2:O:13:PHE:O | 2:O:53:SER:HA | 2.20 | 0.41 |
| 2:U:13:PHE:HA | 2:U:52:GLY:O | 2.21 | 0.41 |
| 1:N:187:LEU:HD13 | 1:N:380:LEU:CD2 | 2.51 | 0.41 |
| 1:M:20:VAL:HG13 | 1:M:74:VAL:HG21 | 2.03 | 0.41 |
| 1:M:239:ILE:HD11 | 1:M:313:VAL:HG23 | 2.02 | 0.41 |
| 1:M:258:ALA:O | 1:M:262:LEU:HG | 2.20 | 0.41 |
| 1:L:175:ILE:HG22 | 1:L:401:LEU:HD11 | 2.01 | 0.41 |
| 1:J:131:LEU:HD23 | 1:J:134:GLN:HE21 | 1.85 | 0.41 |
| 1:J:324:VAL:HG22 | 1:J:333:LEU:HD23 | 2.02 | 0.41 |
| 1:I:31:MET:HE1 | 1:I:94:VAL:HG21 | 2.02 | 0.41 |
| 1:B:497:PRO:HB2 | 1:B:500:VAL:HG12 | 2.01 | 0.41 |
| 1:A:223:SER:HB3 | 1:A:251:ALA:CB | 2.51 | 0.41 |
| 1:A:239:ILE:HD12 | 1:A:313:VAL:HG23 | 2.02 | 0.41 |
| 1:A:466:ILE:O | 1:A:470:ILE:HG13 | 2.20 | 0.41 |
| 1:A:527:LYS:O | 1:A:528:GLU:HB3 | 2.21 | 0.41 |
| 1:G:257:GLU:O | 1:G:261:THR:HG23 | 2.20 | 0.41 |
| 1:F:476:GLU:OE1 | 1:F:476:GLU:N | 2.53 | 0.41 |
| 1:E:195:PHE:HB2 | 1:E:279:PRO:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:227:ILE:HG21 | 1:H:233:ILE:HD13 | 2.03 | 0.41 |
| 1:H:257:GLU:O | 1:H:261:THR:HG23 | 2.21 | 0.41 |
| 2:1:53:SER:HB3 | 2:1:61:GLN:HB3 | 2.03 | 0.41 |
| 2:R:16:VAL:C | 2:R:90:LEU:HD12 | 2.40 | 0.41 |
| 2:R:64:SER:HG | 2:S:13:PHE:HZ | 1.69 | 0.41 |
| 2:R:73:LEU:HD13 | 2:R:91:PHE:CE2 | 2.55 | 0.41 |
| 2:Q:73:LEU:HD13 | 2:Q:91:PHE:CE2 | 2.56 | 0.41 |
| 2:O:26:VAL:HG12 | 2:O:32:MET:SD | 2.60 | 0.41 |
| 2:U:31:ILE:HD12 | 1:G:237:LEU:HB3 | 2.01 | 0.41 |
| 2:S:21:SER:OG | 2:S:41:VAL:HG21 | 2.20 | 0.41 |
| 1:M:124:VAL:HA | 1:M:127:VAL:HG12 | 2.01 | 0.41 |
| 1:L:427:LEU:HA | 1:L:430:LEU:HD23 | 2.03 | 0.41 |
| 1:K:54:VAL:HG12 | 1:K:78:ALA:HB1 | 2.03 | 0.41 |
| 1:K:140:THR:HG22 | 1:K:143:GLU:HG3 | 2.03 | 0.41 |
| 1:J:195:PHE:CD2 | 1:J:197:ARG:HB3 | 2.55 | 0.41 |
| 1:I:444:ILE:O | 1:I:448:LEU:HG | 2.21 | 0.41 |
| 1:I:469:LYS:CG | 1:I:486:PHE:HE2 | 2.34 | 0.41 |
| 1:D:23:LEU:HD22 | 1:D:74:VAL:CG1 | 2.51 | 0.41 |
| 1:C:123:ALA:HB3 | 1:C:444:ILE:HG13 | 2.03 | 0.41 |
| 1:C:250:ILE:HD13 | 1:C:292:MET:CE | 2.51 | 0.41 |
| 1:C:478:GLY:O | 1:C:486:PHE:HA | 2.20 | 0.41 |
| 1:A:120:VAL:HG13 | 1:A:444:ILE:CD1 | 2.41 | 0.41 |
| 1:A:193:MET:CE | 1:A:292:MET:HG2 | 2.50 | 0.41 |
| 1:F:257:GLU:O | 1:F:261:THR:HG23 | 2.20 | 0.41 |
| 1:F:306:LEU:HG | 1:F:308:LEU:CD2 | 2.49 | 0.41 |
| 1:E:103:GLY:HA3 | 1:E:516:THR:HG21 | 2.01 | 0.41 |
| 1:E:239:ILE:HD11 | 1:E:313:VAL:HG23 | 2.02 | 0.41 |
| 1:E:248:VAL:HG11 | 1:E:324:VAL:HG11 | 2.03 | 0.41 |
| 1:E:527:LYS:O | 1:E:528:GLU:HB3 | 2.20 | 0.41 |
| 1:H:24:ALA:HA | 1:H:27:VAL:HG12 | 2.03 | 0.41 |
| 1:H:136:LYS:NZ | 1:H:490:VAL:HG11 | 2.35 | 0.41 |
| 1:H:199:TYR:HE2 | 1:H:202:PRO:HA | 1.85 | 0.41 |
| 1:H:239:ILE:HD11 | 1:H:313:VAL:HG23 | 2.02 | 0.41 |
| 2:W:34:PRO:HD2 | 1:I:230:ILE:HD12 | 2.02 | 0.41 |
| 2:S:16:VAL:HG12 | 2:S:18:VAL:HG13 | 2.02 | 0.41 |
| 1:K:233:ILE:HD11 | 1:K:249:ILE:HD13 | 2.02 | 0.41 |
| 1:K:343:ILE:O | 1:K:347:ILE:HG13 | 2.20 | 0.41 |
| 1:I:136:LYS:NZ | 1:I:490:VAL:HG11 | 2.35 | 0.41 |
| 1:D:54:VAL:HG12 | 1:D:78:ALA:HB1 | 2.03 | 0.41 |
| 1:D:367:ASN:HA | 1:D:370:LEU:HD13 | 2.02 | 0.41 |
| 1:D:435:GLU:O | 1:D:439:ILE:HG13 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:52:ASP:OD1 | 1:B:53:GLY:N | 2.53 | 0.41 |
| 1:B:427:LEU:HA | 1:B:430:LEU:HD23 | 2.03 | 0.41 |
| 1:A:165:ALA:HB2 | 1:A:187:LEU:CD1 | 2.50 | 0.41 |
| 1:A:185:ASP:OD1 | 1:A:382:VAL:HA | 2.21 | 0.41 |
| 1:G:161:ILE:CG2 | 1:G:380:LEU:HD22 | 2.50 | 0.41 |
| 1:F:219:TYR:CE2 | 1:F:245:LYS:HB2 | 2.55 | 0.41 |
| 1:F:382:VAL:HG23 | 1:F:390:VAL:HG13 | 2.02 | 0.41 |
| 1:F:527:LYS:O | 1:F:528:GLU:HB3 | 2.20 | 0.41 |
| 1:H:165:ALA:HB2 | 1:H:187:LEU:CD1 | 2.51 | 0.41 |
| 1:H:169:VAL:HG21 | 1:H:378:ALA:HB2 | 2.03 | 0.41 |
| 1:H:469:LYS:CG | 1:H:486:PHE:HE2 | 2.34 | 0.41 |
| 2:1:13:PHE:HZ | 2:Z:64:SER:HG | 1.68 | 0.41 |
| 2:X:8:LYS:HA | 2:W:101:VAL:O | 2.20 | 0.41 |
| 2:W:73:LEU:HB3 | 2:W:91:PHE:CE2 | 2.47 | 0.41 |
| 1:N:161:ILE:HG22 | 1:N:380:LEU:HD22 | 2.03 | 0.41 |
| 1:N:218:ALA:HA | 1:N:246:PRO:HG2 | 2.03 | 0.41 |
| 1:M:99:ILE:CD1 | 1:M:509:ALA:HA | 2.50 | 0.41 |
| 1:M:367:ASN:HA | 1:M:370:LEU:HD13 | 2.02 | 0.41 |
| 1:L:163:SER:O | 1:L:167:LYS:HG3 | 2.20 | 0.41 |
| 1:L:176:THR:O | 1:L:379:VAL:HA | 2.21 | 0.41 |
| 1:L:513:SER:O | 1:L:517:THR:HG23 | 2.21 | 0.41 |
| 1:J:469:LYS:CG | 1:J:486:PHE:HE2 | 2.33 | 0.41 |
| 1:I:218:ALA:HA | 1:I:246:PRO:HG2 | 2.02 | 0.41 |
| 1:I:250:ILE:HD13 | 1:I:292:MET:CE | 2.51 | 0.41 |
| 1:A:31:MET:HE1 | 1:A:94:VAL:HG21 | 2.03 | 0.41 |
| 1:A:99:ILE:CD1 | 1:A:509:ALA:HA | 2.50 | 0.41 |
| 1:A:212:LYS:HG2 | 1:A:327:THR:CG2 | 2.37 | 0.41 |
| 1:G:64:ASP:O | 1:G:68:ASN:HB2 | 2.21 | 0.41 |
| 1:G:140:THR:OG1 | 1:G:141:PRO:HD2 | 2.20 | 0.41 |
| 1:G:385:THR:CG2 | 1:F:506:LEU:HD21 | 2.51 | 0.41 |
| 1:F:23:LEU:HD23 | 1:F:23:LEU:O | 2.20 | 0.41 |
| 1:F:127:VAL:HG23 | 1:F:423:CYS:CB | 2.51 | 0.41 |
| 1:E:98:SER:HB3 | 1:E:447:THR:HG23 | 2.01 | 0.41 |
| 1:E:207:THR:HG21 | 1:E:212:LYS:H | 1.85 | 0.41 |
| 1:E:228:SER:HA | 1:E:255:ASP:HB3 | 2.01 | 0.41 |
| 1:E:239:ILE:HD12 | 1:E:313:VAL:HG23 | 2.02 | 0.41 |
| 2:Z:20:ARG:HB3 | 2:Z:41:VAL:CG1 | 2.51 | 0.41 |
| 2:W:32:MET:HE3 | 1:I:268:LYS:HE3 | 2.02 | 0.41 |
| 2:P:16:VAL:HG13 | 2:P:46:VAL:HG23 | 2.03 | 0.41 |
| 2:P:31:ILE:HG21 | 1:B:234:VAL:HG23 | 2.03 | 0.41 |
| 1:N:210:GLY:HA2 | 1:M:356:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:219:TYR:CE2 | 1:N:245:LYS:HB2 | 2.55 | 0.41 |
| 1:N:350:ILE:HG22 | 1:N:370:LEU:CD1 | 2.51 | 0.41 |
| 1:M:98:SER:HB2 | 1:M:450:ILE:HG13 | 2.03 | 0.41 |
| 1:M:135:SER:OG | 1:M:498:THR:HG21 | 2.21 | 0.41 |
| 1:M:138:VAL:HG23 | 1:M:143:GLU:CB | 2.50 | 0.41 |
| 1:M:187:LEU:HD13 | 1:M:380:LEU:CD2 | 2.51 | 0.41 |
| 1:M:350:ILE:HG23 | 1:M:366:LEU:HD22 | 2.01 | 0.41 |
| 1:L:175:ILE:CG2 | 1:L:401:LEU:HD11 | 2.51 | 0.41 |
| 1:L:343:ILE:O | 1:L:347:ILE:HG13 | 2.21 | 0.41 |
| 1:J:22:LEU:HD11 | 1:I:6:VAL:CG2 | 2.50 | 0.41 |
| 1:I:87:ASP:O | 1:I:500:VAL:HG23 | 2.21 | 0.41 |
| 1:I:343:ILE:O | 1:I:347:ILE:HG13 | 2.21 | 0.41 |
| 1:D:59:SER:O | 1:C:4:LYS:HD2 | 2.20 | 0.41 |
| 1:D:69:ILE:HG23 | 1:E:47:PRO:HG3 | 2.02 | 0.41 |
| 1:D:469:LYS:CG | 1:D:486:PHE:HE2 | 2.33 | 0.41 |
| 1:D:513:SER:O | 1:D:517:THR:HG23 | 2.21 | 0.41 |
| 1:B:163:SER:O | 1:B:167:LYS:HG3 | 2.21 | 0.41 |
| 1:A:199:TYR:HE2 | 1:A:202:PRO:HA | 1.86 | 0.41 |
| 1:A:253:ASP:OD1 | 1:A:254:VAL:N | 2.52 | 0.41 |
| 1:G:20:VAL:HG13 | 1:G:74:VAL:HG21 | 2.03 | 0.41 |
| 1:G:232:SER:HB2 | 1:G:310:LEU:HD12 | 2.02 | 0.41 |
| 1:G:324:VAL:HG22 | 1:G:333:LEU:HD23 | 2.01 | 0.41 |
| 1:F:54:VAL:HG12 | 1:F:78:ALA:HB1 | 2.03 | 0.41 |
| 1:F:525:ILE:CG1 | 1:F:526:PRO:HD2 | 2.48 | 0.41 |
| 1:E:8:PHE:CD1 | 1:E:520:VAL:HG22 | 2.56 | 0.41 |
| 1:E:20:VAL:HG13 | 1:E:74:VAL:HG21 | 2.02 | 0.41 |
| 1:E:52:ASP:OD1 | 1:E:53:GLY:N | 2.52 | 0.41 |
| 1:E:166:MET:CG | 1:E:171:ARG:HA | 2.51 | 0.41 |
| 1:E:476:GLU:OE1 | 1:E:476:GLU:N | 2.51 | 0.41 |
| 1:H:252:GLU:HG3 | 1:H:285:ARG:NH1 | 2.35 | 0.41 |
| 1:H:346:ARG:NE | 1:H:350:ILE:HD11 | 2.36 | 0.41 |
| 2:V:16:VAL:C | 2:V:90:LEU:HD12 | 2.41 | 0.41 |
| 2:X:31:ILE:HD12 | 1:J:237:LEU:CB | 2.51 | 0.41 |
| 2:Q:10:LEU:HD12 | 2:Q:11:PRO:HD2 | 2.03 | 0.41 |
| 2:P:11:PRO:HB2 | 2:P:15:ARG:HB2 | 2.02 | 0.41 |
| 2:T:63:VAL:HG13 | 2:T:93:ASP:OD1 | 2.21 | 0.41 |
| 1:M:64:ASP:OD1 | 1:M:65:LYS:N | 2.54 | 0.41 |
| 1:L:120:VAL:HG13 | 1:L:444:ILE:CD1 | 2.38 | 0.41 |
| 1:L:176:THR:HG22 | 1:L:379:VAL:HG12 | 2.01 | 0.41 |
| 1:L:340:LYS:CA | 1:L:343:ILE:HG12 | 2.40 | 0.41 |
| 1:K:219:TYR:HB3 | 1:K:318:LEU:HD23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:340:LYS:CA | 1:K:343:ILE:HG12 | 2.39 | 0.41 |
| 1:I:165:ALA:HB2 | 1:I:187:LEU:HD13 | 2.03 | 0.41 |
| 1:C:525:ILE:CG1 | 1:C:526:PRO:HD2 | 2.50 | 0.41 |
| 1:B:175:ILE:CG2 | 1:B:401:LEU:HD11 | 2.51 | 0.41 |
| 1:A:525:ILE:CG1 | 1:A:526:PRO:HD2 | 2.49 | 0.41 |
| 1:G:412:ILE:HG21 | 1:G:495:ILE:HD12 | 2.03 | 0.41 |
| 1:G:466:ILE:O | 1:G:470:ILE:HG13 | 2.21 | 0.41 |
| 1:F:23:LEU:HD22 | 1:F:74:VAL:CG1 | 2.51 | 0.41 |
| 1:E:413:VAL:HB | 1:E:498:THR:HG22 | 2.02 | 0.41 |
| 2:1:41:VAL:HG22 | 2:1:43:GLN:H | 1.86 | 0.40 |
| 2:X:25:THR:O | 2:X:33:LEU:HB2 | 2.21 | 0.40 |
| 2:Q:53:SER:HB3 | 2:Q:61:GLN:HB3 | 2.02 | 0.40 |
| 2:P:25:THR:O | 2:P:33:LEU:HB2 | 2.20 | 0.40 |
| 1:N:469:LYS:CG | 1:N:486:PHE:HE2 | 2.33 | 0.40 |
| 1:L:4:LYS:HD3 | 1:L:522:VAL:CG1 | 2.51 | 0.40 |
| 1:L:52:ASP:OD1 | 1:L:53:GLY:N | 2.53 | 0.40 |
| 1:L:239:ILE:HD11 | 1:L:313:VAL:HG23 | 2.02 | 0.40 |
| 1:L:248:VAL:HG11 | 1:L:324:VAL:HG11 | 2.02 | 0.40 |
| 1:L:525:ILE:CG1 | 1:L:526:PRO:HD2 | 2.48 | 0.40 |
| 1:K:165:ALA:HB2 | 1:K:187:LEU:CD1 | 2.51 | 0.40 |
| 1:K:282:GLY:O | 1:K:286:LYS:HD3 | 2.21 | 0.40 |
| 1:K:303:GLU:HB3 | 1:K:306:LEU:HB3 | 2.02 | 0.40 |
| 1:J:138:VAL:HG23 | 1:J:143:GLU:CB | 2.51 | 0.40 |
| 1:J:462:GLU:O | 1:J:466:ILE:HG12 | 2.21 | 0.40 |
| 1:J:527:LYS:O | 1:J:528:GLU:HB3 | 2.21 | 0.40 |
| 1:D:404:THR:O | 1:D:408:VAL:HG13 | 2.21 | 0.40 |
| 1:C:98:SER:HB2 | 1:C:450:ILE:HG13 | 2.04 | 0.40 |
| 1:C:219:TYR:CE2 | 1:C:245:LYS:HB2 | 2.56 | 0.40 |
| 1:B:165:ALA:HB2 | 1:B:187:LEU:HD13 | 2.03 | 0.40 |
| 1:B:362:GLU:O | 1:B:366:LEU:HB2 | 2.22 | 0.40 |
| 1:A:194:LYS:HD2 | 1:A:332:MET:HE3 | 2.02 | 0.40 |
| 1:G:138:VAL:HG23 | 1:G:143:GLU:CB | 2.51 | 0.40 |
| 1:F:444:ILE:O | 1:F:448:LEU:HG | 2.21 | 0.40 |
| 1:E:185:ASP:OD1 | 1:E:382:VAL:HA | 2.21 | 0.40 |
| 1:E:218:ALA:HB2 | 1:E:246:PRO:HG2 | 2.03 | 0.40 |
| 1:E:230:ILE:HD12 | 1:E:261:THR:CG2 | 2.51 | 0.40 |
| 1:H:163:SER:O | 1:H:167:LYS:HG3 | 2.21 | 0.40 |
| 2:T:31:ILE:HG21 | 1:F:234:VAL:HG23 | 2.03 | 0.40 |
| 1:N:34:LYS:HD2 | 1:N:459:ALA:HA | 2.03 | 0.40 |
| 1:N:64:ASP:OD1 | 1:N:65:LYS:N | 2.54 | 0.40 |
| 1:L:140:THR:CG2 | 1:L:143:GLU:HG3 | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:187:LEU:HD13 | 1:L:380:LEU:CD2 | 2.52 | 0.40 |
| 1:L:324:VAL:HG22 | 1:L:333:LEU:HD23 | 2.02 | 0.40 |
| 1:K:8:PHE:CD1 | 1:K:520:VAL:HG22 | 2.56 | 0.40 |
| 1:K:73:LEU:HD13 | 1:K:515:LEU:HD13 | 2.02 | 0.40 |
| 1:J:199:TYR:HE2 | 1:J:202:PRO:HA | 1.86 | 0.40 |
| 1:I:324:VAL:HG22 | 1:I:333:LEU:HD23 | 2.02 | 0.40 |
| 1:B:59:SER:O | 1:A:4:LYS:HD2 | 2.21 | 0.40 |
| 1:B:107:ILE:HD11 | 1:B:516:THR:O | 2.21 | 0.40 |
| 1:B:324:VAL:HG22 | 1:B:333:LEU:HD23 | 2.03 | 0.40 |
| 1:A:20:VAL:HG13 | 1:A:74:VAL:HG21 | 2.03 | 0.40 |
| 1:A:176:THR:O | 1:A:379:VAL:HA | 2.21 | 0.40 |
| 1:G:98:SER:HB2 | 1:G:450:ILE:HG13 | 2.03 | 0.40 |
| 1:F:422:ARG:HE | 1:F:475:SER:HA | 1.85 | 0.40 |
| 1:E:280:GLY:HA3 | 1:E:285:ARG:N | 2.36 | 0.40 |
| 1:H:280:GLY:H | 1:H:285:ARG:HB3 | 1.86 | 0.40 |
| 1:H:476:GLU:OE1 | 1:H:476:GLU:N | 2.52 | 0.40 |
| 2:2:16:VAL:O | 2:2:90:LEU:HD12 | 2.20 | 0.40 |
| 2:Z:41:VAL:HG22 | 2:Z:43:GLN:H | 1.86 | 0.40 |
| 2:R:63:VAL:HG13 | 2:R:93:ASP:OD1 | 2.21 | 0.40 |
| 2:Q:17:LEU:HD11 | 2:Q:88:TYR:CB | 2.51 | 0.40 |
| 2:P:74:PRO:HD2 | 2:P:91:PHE:CE2 | 2.56 | 0.40 |
| 2:O:3:GLY:CA | 2:O:51:SER:HA | 2.49 | 0.40 |
| 2:U:32:MET:HE1 | 1:G:268:LYS:HG3 | 2.04 | 0.40 |
| 2:T:16:VAL:HG13 | 2:T:46:VAL:HG23 | 2.04 | 0.40 |
| 2:S:25:THR:O | 2:S:33:LEU:HB2 | 2.21 | 0.40 |
| 1:N:32:GLY:N | 3:N:601:ADP:O2A | 2.48 | 0.40 |
| 1:N:476:GLU:OE1 | 1:N:476:GLU:N | 2.53 | 0.40 |
| 1:M:117:ARG:O | 1:M:121:MET:HG2 | 2.21 | 0.40 |
| 1:M:220:VAL:HG22 | 1:M:248:VAL:HG21 | 2.04 | 0.40 |
| 1:M:233:ILE:O | 1:M:237:LEU:HD13 | 2.21 | 0.40 |
| 1:M:321:VAL:HA | 1:M:335:LYS:O | 2.21 | 0.40 |
| 1:L:199:TYR:HE2 | 1:L:202:PRO:HA | 1.86 | 0.40 |
| 1:J:350:ILE:HG22 | 1:J:370:LEU:CD1 | 2.51 | 0.40 |
| 1:I:427:LEU:HA | 1:I:430:LEU:HD23 | 2.04 | 0.40 |
| 1:D:3:ALA:O | 1:D:525:ILE:HG22 | 2.20 | 0.40 |
| 1:C:140:THR:HG23 | 1:C:143:GLU:H | 1.87 | 0.40 |
| 1:C:290:LYS:O | 1:C:294:ILE:HG12 | 2.21 | 0.40 |
| 1:B:36:ARG:NH2 | 1:A:111:ALA:O | 2.54 | 0.40 |
| 1:B:199:TYR:HD1 | 1:B:326:VAL:HG12 | 1.86 | 0.40 |
| 1:B:227:ILE:HG21 | 1:B:233:ILE:HD13 | 2.04 | 0.40 |
| 1:A:73:LEU:HD13 | 1:A:515:LEU:HD13 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:439:ILE:O | 1:G:443:ILE:HG13 | 2.20 | 0.40 |
| 1:F:12:ALA:HB1 | 1:F:521:VAL:CG2 | 2.51 | 0.40 |
| 1:F:59:SER:O | 1:E:4:LYS:HD2 | 2.21 | 0.40 |
| 1:E:230:ILE:HD12 | 1:E:261:THR:HG21 | 2.03 | 0.40 |
| 1:H:52:ASP:OD1 | 1:H:53:GLY:N | 2.53 | 0.40 |
| 1:H:124:VAL:HG21 | 1:H:509:ALA:HB1 | 2.03 | 0.40 |
| 1:H:187:LEU:HD13 | 1:H:380:LEU:CD2 | 2.52 | 0.40 |
| 2:O:9:PHE:CD2 | 2:O:17:LEU:HD22 | 2.57 | 0.40 |
| 2:O:41:VAL:HG22 | 2:O:43:GLN:H | 1.87 | 0.40 |
| 1:M:200:ILE:HD12 | 1:M:275:ALA:O | 2.21 | 0.40 |
| 1:K:161:ILE:HG22 | 1:K:380:LEU:HD22 | 2.04 | 0.40 |
| 1:J:165:ALA:HB2 | 1:J:187:LEU:CD1 | 2.50 | 0.40 |
| 1:J:466:ILE:O | 1:J:470:ILE:HG13 | 2.22 | 0.40 |
| 1:I:98:SER:HB2 | 1:I:450:ILE:HG13 | 2.04 | 0.40 |
| 1:D:52:ASP:OD1 | 1:D:53:GLY:N | 2.52 | 0.40 |
| 1:C:187:LEU:HD13 | 1:C:380:LEU:CD2 | 2.52 | 0.40 |
| 1:C:199:TYR:HB3 | 1:C:326:VAL:HG11 | 2.03 | 0.40 |
| 1:C:239:ILE:HD11 | 1:C:313:VAL:HG23 | 2.03 | 0.40 |
| 1:C:281:PHE:H | 1:C:285:ARG:HG3 | 1.87 | 0.40 |
| 1:C:322:GLY:N | 1:C:335:LYS:O | 2.45 | 0.40 |
| 1:B:176:THR:O | 1:B:379:VAL:HA | 2.21 | 0.40 |
| 1:B:498:THR:O | 1:B:502:ARG:HG2 | 2.21 | 0.40 |
| 1:A:210:GLY:HA2 | 1:G:356:VAL:CG2 | 2.52 | 0.40 |
| 1:A:469:LYS:CG | 1:A:486:PHE:HE2 | 2.34 | 0.40 |
| 1:G:59:SER:O | 1:F:4:LYS:HD2 | 2.22 | 0.40 |
| 1:F:140:THR:OG1 | 1:F:141:PRO:HD2 | 2.21 | 0.40 |
| 1:F:165:ALA:HB2 | 1:F:187:LEU:HD13 | 2.04 | 0.40 |
| 2:Y:10:LEU:HD12 | 2:Y:11:PRO:HD2 | 2.03 | 0.40 |
| 2:R:26:VAL:HA | 2:R:32:MET:HA | 2.03 | 0.40 |
| 2:P:31:ILE:HD12 | 1:B:237:LEU:CB | 2.50 | 0.40 |
| 2:P:41:VAL:HG22 | 2:P:43:GLN:H | 1.87 | 0.40 |
| 2:O:17:LEU:O | 2:O:47:VAL:HG22 | 2.21 | 0.40 |
| 2:U:17:LEU:O | 2:U:47:VAL:HG22 | 2.21 | 0.40 |
| 1:N:371:ALA:HB1 | 1:N:377:VAL:HG12 | 2.02 | 0.40 |
| 1:L:12:ALA:HB1 | 1:L:521:VAL:CG2 | 2.52 | 0.40 |
| 1:L:165:ALA:HB2 | 1:L:187:LEU:HD13 | 2.04 | 0.40 |
| 1:K:350:ILE:HG22 | 1:K:370:LEU:CD1 | 2.52 | 0.40 |
| 1:K:450:ILE:O | 1:K:454:THR:HG23 | 2.22 | 0.40 |
| 1:J:476:GLU:OE1 | 1:J:476:GLU:N | 2.54 | 0.40 |
| 1:I:140:THR:HG22 | 1:I:143:GLU:HG3 | 2.04 | 0.40 |
| 1:I:169:VAL:HG21 | 1:I:378:ALA:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:112:ASN:HB3 | 1:D:436:ASP:OD2 | 2.22 | 0.40 |
| 1:D:161:ILE:HG22 | 1:D:380:LEU:HD22 | 2.03 | 0.40 |
| 1:C:324:VAL:HG22 | 1:C:333:LEU:CD2 | 2.51 | 0.40 |
| 1:B:230:ILE:HD12 | 1:B:261:THR:CG2 | 2.51 | 0.40 |
| 1:G:309:ASN:HB2 | 1:G:312:ASP:OD1 | 2.21 | 0.40 |
| 1:F:176:THR:HG22 | 1:F:379:VAL:HG12 | 2.04 | 0.40 |
| 1:F:230:ILE:HD12 | 1:F:261:THR:CG2 | 2.52 | 0.40 |
| 1:E:98:SER:CB | 1:E:450:ILE:HG13 | 2.51 | 0.40 |
| 1:E:176:THR:O | 1:E:379:VAL:HA | 2.22 | 0.40 |
| 1:E:469:LYS:CG | 1:E:486:PHE:HE2 | 2.34 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 1 | A | 526/528 (100%) | 495 (94%) | 29 (6%) | 2 (0%) | 34 | 66 |
| 1 | B | 526/528 (100%) | 497 (94%) | 28 (5%) | 1 (0%) | 47 | 77 |
| 1 | C | 526/528 (100%) | 492 (94%) | 33 (6%) | 1 (0%) | 47 | 77 |
| 1 | D | 526/528 (100%) | 499 (95%) | 26 (5%) | 1 (0%) | 47 | 77 |
| 1 | E | 526/528 (100%) | 495 (94%) | 30 (6%) | 1 (0%) | 47 | 77 |
| 1 | F | 526/528 (100%) | 493 (94%) | 32 (6%) | 1 (0%) | 47 | 77 |
| 1 | G | 526/528 (100%) | 494 (94%) | 30 (6%) | 2 (0%) | 34 | 66 |
| 1 | H | 526/528 (100%) | 498 (95%) | 26 (5%) | 2 (0%) | 34 | 66 |
| 1 | I | 526/528 (100%) | 496 (94%) | 29 (6%) | 1 (0%) | 47 | 77 |
| 1 | J | 526/528 (100%) | 494 (94%) | 31 (6%) | 1 (0%) | 47 | 77 |
| 1 | K | 526/528 (100%) | 492 (94%) | 32 (6%) | 2 (0%) | 34 | 66 |
| 1 | L | 526/528 (100%) | 493 (94%) | 32 (6%) | 1 (0%) | 47 | 77 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | M | 526/528 (100%) | 494 (94%) | 32 (6%) | 0 | 100 | 100 |
| 1 | N | 526/528 (100%) | 499 (95%) | 27 (5%) | 0 | 100 | 100 |
| 2 | 1 | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | 2 | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | O | 98/100 (98%) | 81 (83%) | 17 (17%) | 0 | 100 | 100 |
| 2 | P | 98/100 (98%) | 79 (81%) | 19 (19%) | 0 | 100 | 100 |
| 2 | Q | 98/100 (98%) | 82 (84%) | 15 (15%) | 1 (1%) | 15 | 47 |
| 2 | R | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | S | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | T | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | U | 98/100 (98%) | 80 (82%) | 18 (18%) | 0 | 100 | 100 |
| 2 | V | 98/100 (98%) | 82 (84%) | 16 (16%) | 0 | 100 | 100 |
| 2 | W | 98/100 (98%) | 82 (84%) | 15 (15%) | 1 (1%) | 15 | 47 |
| 2 | X | 98/100 (98%) | 83 (85%) | 15 (15%) | 0 | 100 | 100 |
| 2 | Y | 98/100 (98%) | 80 (82%) | 17 (17%) | 1 (1%) | 15 | 47 |
| 2 | Z | 98/100 (98%) | 81 (83%) | 17 (17%) | 0 | 100 | 100 |
| All | All | 8736/8792 (99%) | 8061 (92%) | 656 (8%) | 19 (0%) | 50 | 77 |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 269 | VAL |
| 1 | J | 269 | VAL |
| 1 | I | 269 | VAL |
| 1 | A | 269 | VAL |
| 1 | G | 269 | VAL |
| 1 | L | 269 | VAL |
| 1 | K | 269 | VAL |
| 1 | D | 269 | VAL |
| 1 | C | 269 | VAL |
| 1 | B | 269 | VAL |
| 1 | F | 269 | VAL |
| 1 | E | 269 | VAL |
| 1 | H | 281 | PHE |
| 1 | K | 281 | PHE |
| 1 | G | 281 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 279 | PRO |
| 2 | W | 14 | ASP |
| 2 | Y | 14 | ASP |
| 2 | Q | 14 | ASP |

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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | B | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | C | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | D | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | E | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | F | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | G | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | H | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | I | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | J | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | K | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | L | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | M | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 1 | N | 427/427 (100%) | 427 (100%) | 0 | 100 | 100 |
| 2 | 1 | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | 2 | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | O | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | P | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | Q | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | R | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 2 | S | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | T | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | U | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | V | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | W | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | X | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | Y | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 2 | Z | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| All | All | 7112/7112 (100%) | 7112 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 367 | ASN |
| 1 | N | 367 | ASN |
| 1 | M | 284 | ASN |
| 1 | M | 367 | ASN |
| 1 | L | 284 | ASN |
| 1 | L | 367 | ASN |
| 1 | K | 134 | GLN |
| 1 | K | 367 | ASN |
| 1 | J | 284 | ASN |
| 1 | I | 367 | ASN |
| 1 | D | 284 | ASN |
| 1 | D | 367 | ASN |
| 1 | C | 367 | ASN |
| 1 | B | 284 | ASN |
| 1 | B | 367 | ASN |
| 1 | A | 134 | GLN |
| 1 | A | 265 | ASN |
| 1 | A | 367 | ASN |
| 1 | G | 134 | GLN |
| 1 | G | 367 | ASN |
| 1 | F | 367 | ASN |
| 1 | E | 367 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 3 | ADP | B | 601 | 4 | 24,29,29 | 4.72 | 9 (37%) | 29,45,45 | 2.48 | 4 (13%) |
| 3 | ADP | C | 601 | 4 | 24,29,29 | 4.73 | 8 (33%) | 29,45,45 | 2.49 | 4 (13%) |
| 3 | ADP | I | 601 | 4 | 24,29,29 | 4.71 | 8 (33%) | 29,45,45 | 2.49 | 4 (13%) |
| 3 | ADP | F | 601 | 4 | 24,29,29 | 4.73 | 9 (37%) | 29,45,45 | 2.46 | 4 (13%) |
| 3 | ADP | N | 601 | 4 | 24,29,29 | 4.71 | 9 (37%) | 29,45,45 | 2.48 | 4 (13%) |
| 3 | ADP | M | 601 | 4 | 24,29,29 | 4.71 | 8 (33%) | 29,45,45 | 2.50 | 4 (13%) |
| 3 | ADP | L | 601 | 4 | 24,29,29 | 4.70 | 8 (33%) | 29,45,45 | 2.48 | 4 (13%) |
| 3 | ADP | H | 601 | 4 | 24,29,29 | 4.72 | 8 (33%) | 29,45,45 | 2.50 | 4 (13%) |
| 3 | ADP | D | 601 | 4 | 24,29,29 | 4.71 | 9 (37%) | 29,45,45 | 2.47 | 4 (13%) |
| 3 | ADP | E | 601 | 4 | 24,29,29 | 4.73 | 8 (33%) | 29,45,45 | 2.48 | 4 (13%) |
| 3 | ADP | A | 601 | 4 | 24,29,29 | 4.71 | 8 (33%) | 29,45,45 | 2.47 | 4 (13%) |
| 3 | ADP | G | 601 | 4 | 24,29,29 | 4.72 | 8 (33%) | 29,45,45 | 2.47 | 4 (13%) |
| 3 | ADP | K | 601 | 4 | 24,29,29 | 4.71 | 8 (33%) | 29,45,45 | 2.49 | 4 (13%) |
| 3 | ADP | J | 601 | 4 | 24,29,29 | 4.71 | 9 (37%) | 29,45,45 | 2.49 | 4 (13%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | ADP | B | 601 | 4 | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ADP | C | 601 | 4 | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ADP | I | 601 | 4 | - | 3/12/32/32 | 0/3/3/3 |
| 3 | ADP | F | 601 | 4 | - | 6/12/32/32 | 0/3/3/3 |
| 3 | ADP | N | 601 | 4 | - | 3/12/32/32 | 0/3/3/3 |
| 3 | ADP | M | 601 | 4 | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ADP | L | 601 | 4 | - | 2/12/32/32 | 0/3/3/3 |
| 3 | ADP | H | 601 | 4 | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ADP | D | 601 | 4 | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ADP | E | 601 | 4 | - | 6/12/32/32 | 0/3/3/3 |
| 3 | ADP | A | 601 | 4 | - | 4/12/32/32 | 0/3/3/3 |
| 3 | ADP | G | 601 | 4 | - | 4/12/32/32 | 0/3/3/3 |
| 3 | ADP | K | 601 | 4 | - | 2/12/32/32 | 0/3/3/3 |
| 3 | ADP | J | 601 | 4 | - | 4/12/32/32 | 0/3/3/3 |

All (117) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | C | 601 | ADP | C2'-C1' | -15.47 | 1.30 | 1.53 |
| 3 | H | 601 | ADP | C2'-C1' | -15.47 | 1.30 | 1.53 |
| 3 | F | 601 | ADP | C2'-C1' | -15.47 | 1.30 | 1.53 |
| 3 | G | 601 | ADP | C2'-C1' | -15.46 | 1.30 | 1.53 |
| 3 | I | 601 | ADP | C2'-C1' | -15.46 | 1.30 | 1.53 |
| 3 | B | 601 | ADP | C2'-C1' | -15.46 | 1.30 | 1.53 |
| 3 | J | 601 | ADP | C2'-C1' | -15.45 | 1.30 | 1.53 |
| 3 | D | 601 | ADP | C2'-C1' | -15.44 | 1.30 | 1.53 |
| 3 | E | 601 | ADP | C2'-C1' | -15.43 | 1.30 | 1.53 |
| 3 | N | 601 | ADP | C2'-C1' | -15.41 | 1.30 | 1.53 |
| 3 | M | 601 | ADP | C2'-C1' | -15.40 | 1.30 | 1.53 |
| 3 | A | 601 | ADP | C2'-C1' | -15.39 | 1.30 | 1.53 |
| 3 | K | 601 | ADP | C2'-C1' | -15.36 | 1.30 | 1.53 |
| 3 | L | 601 | ADP | C2'-C1' | -15.34 | 1.30 | 1.53 |
| 3 | C | 601 | ADP | O4'-C1' | 14.19 | 1.60 | 1.41 |
| 3 | H | 601 | ADP | O4'-C1' | 14.18 | 1.60 | 1.41 |
| 3 | E | 601 | ADP | O4'-C1' | 14.18 | 1.60 | 1.41 |
| 3 | M | 601 | ADP | O4'-C1' | 14.14 | 1.60 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | B | 601 | ADP | O4'-C1' | 14.13 | 1.60 | 1.41 |
| 3 | F | 601 | ADP | O4'-C1' | 14.13 | 1.60 | 1.41 |
| 3 | L | 601 | ADP | O4'-C1' | 14.12 | 1.60 | 1.41 |
| 3 | A | 601 | ADP | O4'-C1' | 14.12 | 1.60 | 1.41 |
| 3 | N | 601 | ADP | O4'-C1' | 14.12 | 1.60 | 1.41 |
| 3 | K | 601 | ADP | O4'-C1' | 14.11 | 1.60 | 1.41 |
| 3 | G | 601 | ADP | O4'-C1' | 14.09 | 1.60 | 1.41 |
| 3 | I | 601 | ADP | O4'-C1' | 14.07 | 1.60 | 1.41 |
| 3 | J | 601 | ADP | O4'-C1' | 14.03 | 1.60 | 1.41 |
| 3 | D | 601 | ADP | O4'-C1' | 13.99 | 1.60 | 1.41 |
| 3 | B | 601 | ADP | O4'-C4' | -6.38 | 1.30 | 1.45 |
| 3 | A | 601 | ADP | O4'-C4' | -6.37 | 1.30 | 1.45 |
| 3 | K | 601 | ADP | O4'-C4' | -6.37 | 1.30 | 1.45 |
| 3 | J | 601 | ADP | O4'-C4' | -6.36 | 1.30 | 1.45 |
| 3 | F | 601 | ADP | O4'-C4' | -6.36 | 1.30 | 1.45 |
| 3 | N | 601 | ADP | O4'-C4' | -6.36 | 1.30 | 1.45 |
| 3 | L | 601 | ADP | O4'-C4' | -6.35 | 1.30 | 1.45 |
| 3 | D | 601 | ADP | O4'-C4' | -6.34 | 1.30 | 1.45 |
| 3 | G | 601 | ADP | O4'-C4' | -6.33 | 1.30 | 1.45 |
| 3 | I | 601 | ADP | O4'-C4' | -6.33 | 1.30 | 1.45 |
| 3 | E | 601 | ADP | O4'-C4' | -6.32 | 1.30 | 1.45 |
| 3 | C | 601 | ADP | O4'-C4' | -6.29 | 1.30 | 1.45 |
| 3 | M | 601 | ADP | O4'-C4' | -6.28 | 1.31 | 1.45 |
| 3 | H | 601 | ADP | O4'-C4' | -6.27 | 1.31 | 1.45 |
| 3 | F | 601 | ADP | O2'-C2' | 3.71 | 1.51 | 1.43 |
| 3 | K | 601 | ADP | O2'-C2' | 3.71 | 1.51 | 1.43 |
| 3 | A | 601 | ADP | O2'-C2' | 3.70 | 1.51 | 1.43 |
| 3 | I | 601 | ADP | O2'-C2' | 3.69 | 1.51 | 1.43 |
| 3 | E | 601 | ADP | O2'-C2' | 3.68 | 1.51 | 1.43 |
| 3 | H | 601 | ADP | O2'-C2' | 3.68 | 1.51 | 1.43 |
| 3 | G | 601 | ADP | O2'-C2' | 3.68 | 1.51 | 1.43 |
| 3 | M | 601 | ADP | O2'-C2' | 3.67 | 1.51 | 1.43 |
| 3 | N | 601 | ADP | O2'-C2' | 3.67 | 1.51 | 1.43 |
| 3 | C | 601 | ADP | O2'-C2' | 3.66 | 1.51 | 1.43 |
| 3 | B | 601 | ADP | O2'-C2' | 3.66 | 1.51 | 1.43 |
| 3 | D | 601 | ADP | O2'-C2' | 3.66 | 1.51 | 1.43 |
| 3 | J | 601 | ADP | O2'-C2' | 3.66 | 1.51 | 1.43 |
| 3 | L | 601 | ADP | O2'-C2' | 3.65 | 1.51 | 1.43 |
| 3 | D | 601 | ADP | C4-N3 | -2.64 | 1.32 | 1.35 |
| 3 | B | 601 | ADP | C4-N3 | -2.63 | 1.32 | 1.35 |
| 3 | K | 601 | ADP | O3'-C3' | -2.62 | 1.36 | 1.43 |
| 3 | N | 601 | ADP | C4-N3 | -2.62 | 1.32 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | D | 601 | ADP | O3'-C3' | -2.61 | 1.36 | 1.43 |
| 3 | E | 601 | ADP | C4-N3 | -2.60 | 1.32 | 1.35 |
| 3 | C | 601 | ADP | O3'-C3' | -2.60 | 1.36 | 1.43 |
| 3 | H | 601 | ADP | C4-N3 | -2.60 | 1.32 | 1.35 |
| 3 | M | 601 | ADP | C4-N3 | -2.59 | 1.32 | 1.35 |
| 3 | A | 601 | ADP | O3'-C3' | -2.59 | 1.36 | 1.43 |
| 3 | F | 601 | ADP | C4-N3 | -2.58 | 1.32 | 1.35 |
| 3 | J | 601 | ADP | O3'-C3' | -2.58 | 1.36 | 1.43 |
| 3 | I | 601 | ADP | C4-N3 | -2.57 | 1.32 | 1.35 |
| 3 | N | 601 | ADP | O3'-C3' | -2.57 | 1.36 | 1.43 |
| 3 | E | 601 | ADP | O3'-C3' | -2.56 | 1.36 | 1.43 |
| 3 | H | 601 | ADP | O3'-C3' | -2.56 | 1.36 | 1.43 |
| 3 | G | 601 | ADP | C2-N3 | 2.56 | 1.36 | 1.32 |
| 3 | F | 601 | ADP | C2-N3 | 2.56 | 1.36 | 1.32 |
| 3 | K | 601 | ADP | C4-N3 | -2.55 | 1.32 | 1.35 |
| 3 | L | 601 | ADP | O3'-C3' | -2.55 | 1.37 | 1.43 |
| 3 | F | 601 | ADP | O3'-C3' | -2.55 | 1.37 | 1.43 |
| 3 | M | 601 | ADP | C2-N3 | 2.55 | 1.36 | 1.32 |
| 3 | G | 601 | ADP | O3'-C3' | -2.54 | 1.37 | 1.43 |
| 3 | I | 601 | ADP | O3'-C3' | -2.54 | 1.37 | 1.43 |
| 3 | B | 601 | ADP | O3'-C3' | -2.54 | 1.37 | 1.43 |
| 3 | E | 601 | ADP | C2-N3 | 2.54 | 1.36 | 1.32 |
| 3 | J | 601 | ADP | C4-N3 | -2.54 | 1.32 | 1.35 |
| 3 | J | 601 | ADP | C2-N3 | 2.53 | 1.36 | 1.32 |
| 3 | C | 601 | ADP | C4-N3 | -2.53 | 1.32 | 1.35 |
| 3 | L | 601 | ADP | C4-N3 | -2.53 | 1.32 | 1.35 |
| 3 | M | 601 | ADP | O3'-C3' | -2.53 | 1.37 | 1.43 |
| 3 | C | 601 | ADP | C2-N3 | 2.53 | 1.36 | 1.32 |
| 3 | H | 601 | ADP | C2-N3 | 2.52 | 1.36 | 1.32 |
| 3 | A | 601 | ADP | C2-N3 | 2.52 | 1.36 | 1.32 |
| 3 | G | 601 | ADP | C4-N3 | -2.52 | 1.32 | 1.35 |
| 3 | I | 601 | ADP | C2-N3 | 2.52 | 1.36 | 1.32 |
| 3 | D | 601 | ADP | C2-N3 | 2.50 | 1.36 | 1.32 |
| 3 | A | 601 | ADP | C4-N3 | -2.50 | 1.32 | 1.35 |
| 3 | L | 601 | ADP | C2-N3 | 2.47 | 1.36 | 1.32 |
| 3 | B | 601 | ADP | C2-N3 | 2.47 | 1.36 | 1.32 |
| 3 | K | 601 | ADP | C2-N3 | 2.47 | 1.36 | 1.32 |
| 3 | N | 601 | ADP | C2-N3 | 2.45 | 1.36 | 1.32 |
| 3 | L | 601 | ADP | C6-N6 | 2.34 | 1.42 | 1.34 |
| 3 | H | 601 | ADP | C6-N6 | 2.34 | 1.42 | 1.34 |
| 3 | A | 601 | ADP | C6-N6 | 2.34 | 1.42 | 1.34 |
| 3 | J | 601 | ADP | C6-N6 | 2.34 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | C | 601 | ADP | C6-N6 | 2.34 | 1.42 | 1.34 |
| 3 | B | 601 | ADP | C6-N6 | 2.33 | 1.42 | 1.34 |
| 3 | I | 601 | ADP | C6-N6 | 2.33 | 1.42 | 1.34 |
| 3 | E | 601 | ADP | C6-N6 | 2.33 | 1.42 | 1.34 |
| 3 | N | 601 | ADP | C6-N6 | 2.32 | 1.42 | 1.34 |
| 3 | G | 601 | ADP | C6-N6 | 2.32 | 1.42 | 1.34 |
| 3 | K | 601 | ADP | C6-N6 | 2.32 | 1.42 | 1.34 |
| 3 | F | 601 | ADP | C6-N6 | 2.31 | 1.42 | 1.34 |
| 3 | M | 601 | ADP | C6-N6 | 2.31 | 1.42 | 1.34 |
| 3 | D | 601 | ADP | C6-N6 | 2.30 | 1.42 | 1.34 |
| 3 | D | 601 | ADP | C5-C4 | -2.06 | 1.35 | 1.40 |
| 3 | N | 601 | ADP | C5-C4 | -2.01 | 1.35 | 1.40 |
| 3 | B | 601 | ADP | C5-C4 | -2.01 | 1.35 | 1.40 |
| 3 | J | 601 | ADP | C5-C4 | -2.01 | 1.35 | 1.40 |
| 3 | F | 601 | ADP | C5-C4 | -2.00 | 1.35 | 1.40 |

All (56) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3 | C | 601 | ADP | C5-C6-N6 | 9.16 | 134.28 | 120.35 |
| 3 | M | 601 | ADP | C5-C6-N6 | 9.11 | 134.20 | 120.35 |
| 3 | K | 601 | ADP | C5-C6-N6 | 9.07 | 134.14 | 120.35 |
| 3 | I | 601 | ADP | C5-C6-N6 | 9.06 | 134.12 | 120.35 |
| 3 | H | 601 | ADP | C5-C6-N6 | 9.05 | 134.10 | 120.35 |
| 3 | E | 601 | ADP | C5-C6-N6 | 9.04 | 134.09 | 120.35 |
| 3 | G | 601 | ADP | C5-C6-N6 | 9.03 | 134.08 | 120.35 |
| 3 | J | 601 | ADP | C5-C6-N6 | 9.03 | 134.08 | 120.35 |
| 3 | N | 601 | ADP | C5-C6-N6 | 9.02 | 134.07 | 120.35 |
| 3 | F | 601 | ADP | C5-C6-N6 | 9.02 | 134.06 | 120.35 |
| 3 | L | 601 | ADP | C5-C6-N6 | 9.01 | 134.04 | 120.35 |
| 3 | D | 601 | ADP | C5-C6-N6 | 9.00 | 134.03 | 120.35 |
| 3 | A | 601 | ADP | C5-C6-N6 | 9.00 | 134.03 | 120.35 |
| 3 | B | 601 | ADP | C5-C6-N6 | 9.00 | 134.02 | 120.35 |
| 3 | C | 601 | ADP | N6-C6-N1 | -6.38 | 105.33 | 118.57 |
| 3 | M | 601 | ADP | N6-C6-N1 | -6.34 | 105.41 | 118.57 |
| 3 | K | 601 | ADP | N6-C6-N1 | -6.27 | 105.56 | 118.57 |
| 3 | I | 601 | ADP | N6-C6-N1 | -6.26 | 105.58 | 118.57 |
| 3 | N | 601 | ADP | N6-C6-N1 | -6.25 | 105.60 | 118.57 |
| 3 | E | 601 | ADP | N6-C6-N1 | -6.25 | 105.60 | 118.57 |
| 3 | A | 601 | ADP | N6-C6-N1 | -6.25 | 105.61 | 118.57 |
| 3 | F | 601 | ADP | N6-C6-N1 | -6.24 | 105.62 | 118.57 |
| 3 | L | 601 | ADP | N6-C6-N1 | -6.24 | 105.63 | 118.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | D | 601 | ADP | N6-C6-N1 | -6.23 | 105.64 | 118.57 |
| 3 | B | 601 | ADP | N6-C6-N1 | -6.23 | 105.65 | 118.57 |
| 3 | H | 601 | ADP | N6-C6-N1 | -6.23 | 105.65 | 118.57 |
| 3 | G | 601 | ADP | N6-C6-N1 | -6.22 | 105.66 | 118.57 |
| 3 | J | 601 | ADP | N6-C6-N1 | -6.22 | 105.67 | 118.57 |
| 3 | B | 601 | ADP | N3-C2-N1 | -5.77 | 119.65 | 128.68 |
| 3 | E | 601 | ADP | N3-C2-N1 | -5.77 | 119.66 | 128.68 |
| 3 | A | 601 | ADP | N3-C2-N1 | -5.74 | 119.71 | 128.68 |
| 3 | K | 601 | ADP | N3-C2-N1 | -5.73 | 119.72 | 128.68 |
| 3 | H | 601 | ADP | N3-C2-N1 | -5.72 | 119.73 | 128.68 |
| 3 | M | 601 | ADP | N3-C2-N1 | -5.72 | 119.74 | 128.68 |
| 3 | J | 601 | ADP | N3-C2-N1 | -5.70 | 119.76 | 128.68 |
| 3 | C | 601 | ADP | N3-C2-N1 | -5.70 | 119.78 | 128.68 |
| 3 | L | 601 | ADP | N3-C2-N1 | -5.69 | 119.78 | 128.68 |
| 3 | D | 601 | ADP | N3-C2-N1 | -5.69 | 119.78 | 128.68 |
| 3 | G | 601 | ADP | N3-C2-N1 | -5.65 | 119.85 | 128.68 |
| 3 | F | 601 | ADP | N3-C2-N1 | -5.61 | 119.91 | 128.68 |
| 3 | N | 601 | ADP | N3-C2-N1 | -5.61 | 119.91 | 128.68 |
| 3 | I | 601 | ADP | N3-C2-N1 | -5.55 | 120.01 | 128.68 |
| 3 | B | 601 | ADP | PA-O3A-PB | -3.73 | 120.03 | 132.83 |
| 3 | G | 601 | ADP | PA-O3A-PB | -3.66 | 120.25 | 132.83 |
| 3 | I | 601 | ADP | PA-O3A-PB | -3.66 | 120.27 | 132.83 |
| 3 | D | 601 | ADP | PA-O3A-PB | -3.62 | 120.40 | 132.83 |
| 3 | J | 601 | ADP | PA-O3A-PB | -3.59 | 120.49 | 132.83 |
| 3 | H | 601 | ADP | PA-O3A-PB | -3.58 | 120.54 | 132.83 |
| 3 | N | 601 | ADP | PA-O3A-PB | -3.56 | 120.62 | 132.83 |
| 3 | F | 601 | ADP | PA-O3A-PB | -3.55 | 120.64 | 132.83 |
| 3 | E | 601 | ADP | PA-O3A-PB | -3.49 | 120.85 | 132.83 |
| 3 | L | 601 | ADP | PA-O3A-PB | -3.48 | 120.90 | 132.83 |
| 3 | M | 601 | ADP | PA-O3A-PB | -3.40 | 121.15 | 132.83 |
| 3 | A | 601 | ADP | PA-O3A-PB | -3.39 | 121.21 | 132.83 |
| 3 | K | 601 | ADP | PA-O3A-PB | -3.34 | 121.37 | 132.83 |
| 3 | C | 601 | ADP | PA-O3A-PB | -3.32 | 121.44 | 132.83 |

There are no chirality outliers.

All (59) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 3 | H | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | H | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | N | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | N | 601 | ADP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 3 | M | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | M | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | L | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | K | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | J | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | J | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | I | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | I | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | D | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | D | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | C | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | C | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | B | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | B | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | A | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | A | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | G | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | G | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | G | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | F | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | F | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | F | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | E | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | E | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | E | 601 | ADP | C4'-C5'-O5'-PA |
| 3 | C | 601 | ADP | PB-O3A-PA-O1A |
| 3 | A | 601 | ADP | PB-O3A-PA-O1A |
| 3 | L | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | K | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | D | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | C | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | B | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | A | 601 | ADP | C5'-O5'-PA-O3A |
| 3 | D | 601 | ADP | PB-O3A-PA-O1A |
| 3 | B | 601 | ADP | PB-O3A-PA-O1A |
| 3 | H | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | N | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | M | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | J | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | G | 601 | ADP | PB-O3A-PA-O1A |
| 3 | E | 601 | ADP | PB-O3A-PA-O2A |
| 3 | D | 601 | ADP | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 3 | F | 601 | ADP | PB-O3A-PA-O1A |
| 3 | F | 601 | ADP | PB-O3A-PA-O2A |
| 3 | H | 601 | ADP | PB-O3A-PA-O2A |
| 3 | M | 601 | ADP | PB-O3A-PA-O2A |
| 3 | C | 601 | ADP | PB-O3A-PA-O2A |
| 3 | B | 601 | ADP | PB-O3A-PA-O2A |
| 3 | E | 601 | ADP | PB-O3A-PA-O1A |
| 3 | H | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | M | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | J | 601 | ADP | C5'-O5'-PA-O1A |
| 3 | I | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | F | 601 | ADP | C5'-O5'-PA-O2A |
| 3 | E | 601 | ADP | C5'-O5'-PA-O2A |

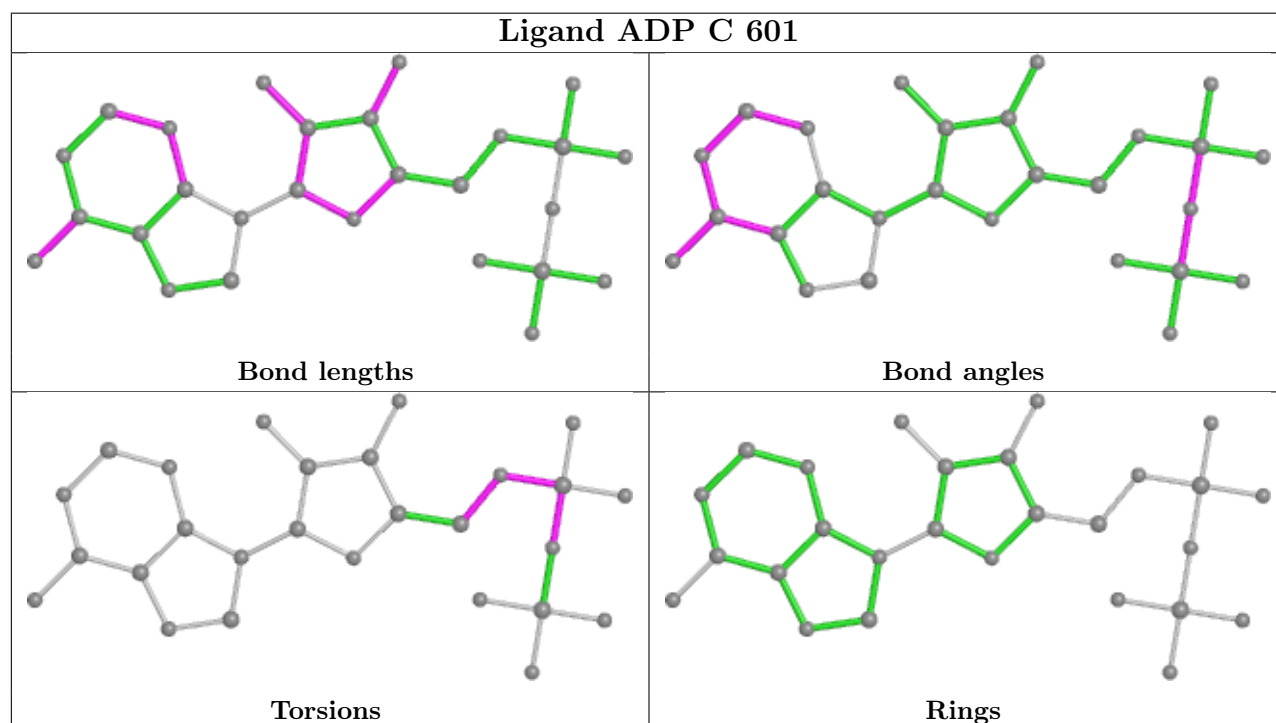
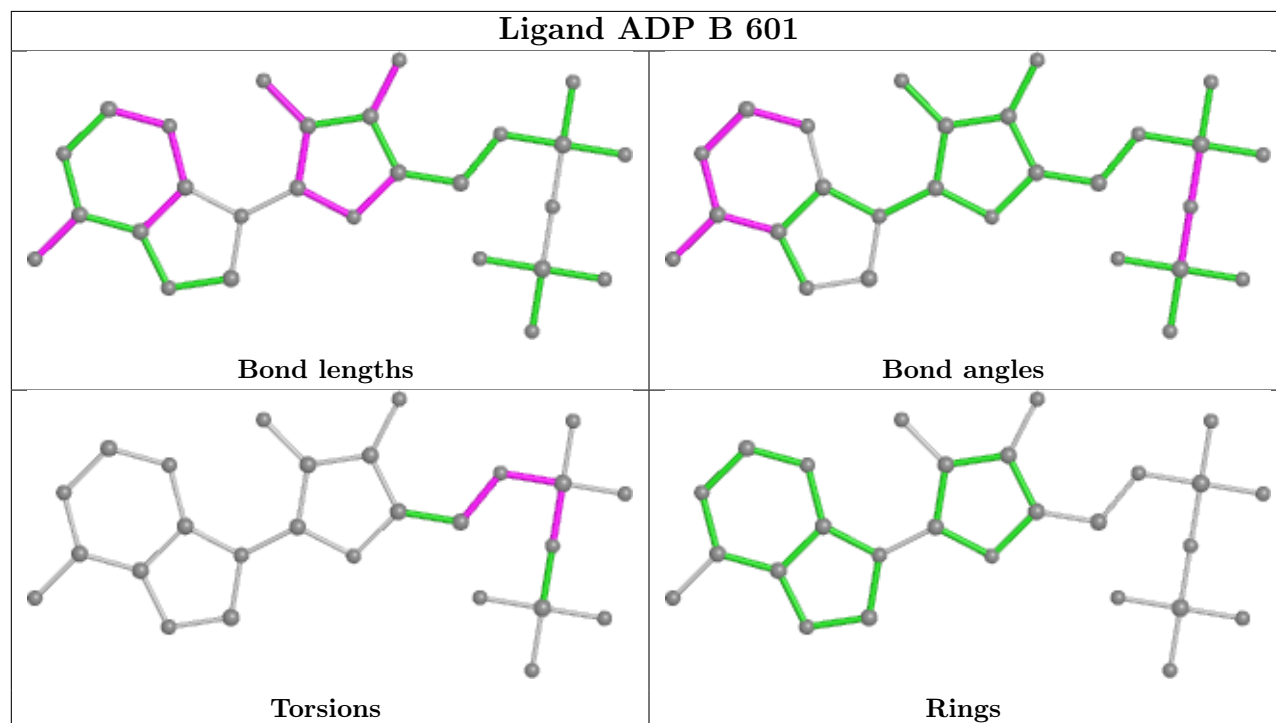
There are no ring outliers.

14 monomers are involved in 26 short contacts:

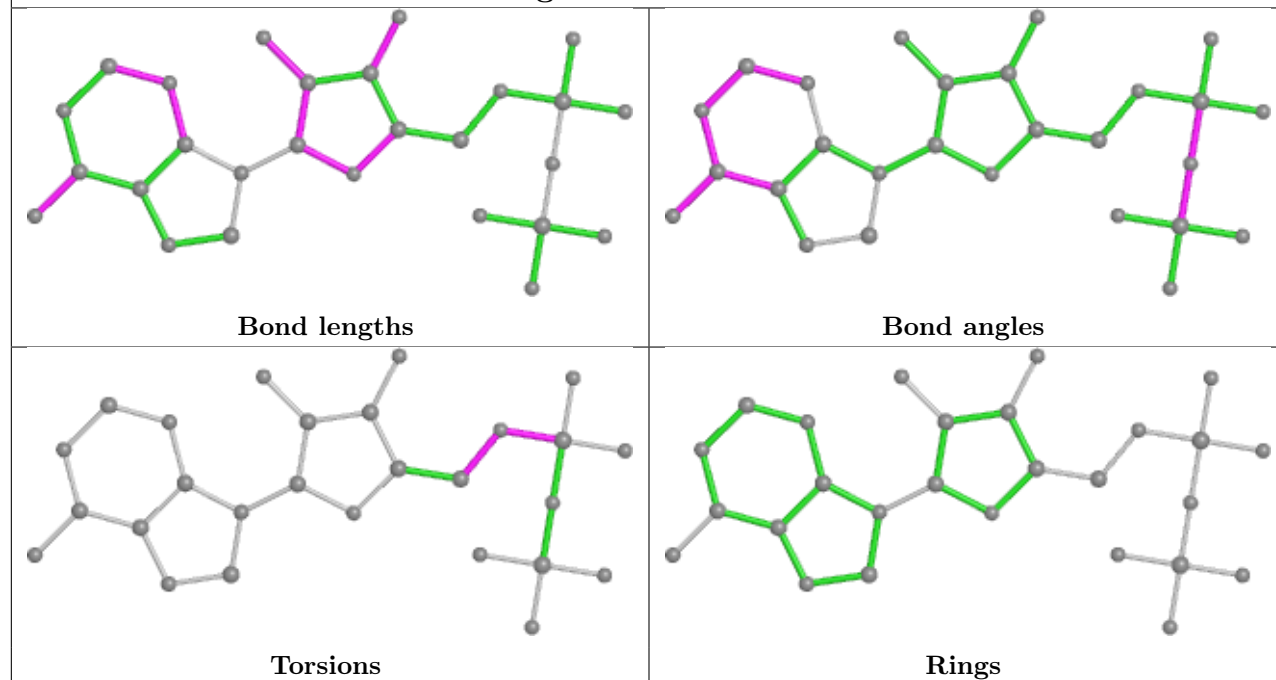
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | B | 601 | ADP | 2 | 0 |
| 3 | C | 601 | ADP | 1 | 0 |
| 3 | I | 601 | ADP | 2 | 0 |
| 3 | F | 601 | ADP | 1 | 0 |
| 3 | N | 601 | ADP | 2 | 0 |
| 3 | M | 601 | ADP | 2 | 0 |
| 3 | L | 601 | ADP | 2 | 0 |
| 3 | H | 601 | ADP | 2 | 0 |
| 3 | D | 601 | ADP | 2 | 0 |
| 3 | E | 601 | ADP | 2 | 0 |
| 3 | A | 601 | ADP | 2 | 0 |
| 3 | G | 601 | ADP | 2 | 0 |
| 3 | K | 601 | ADP | 2 | 0 |
| 3 | J | 601 | ADP | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

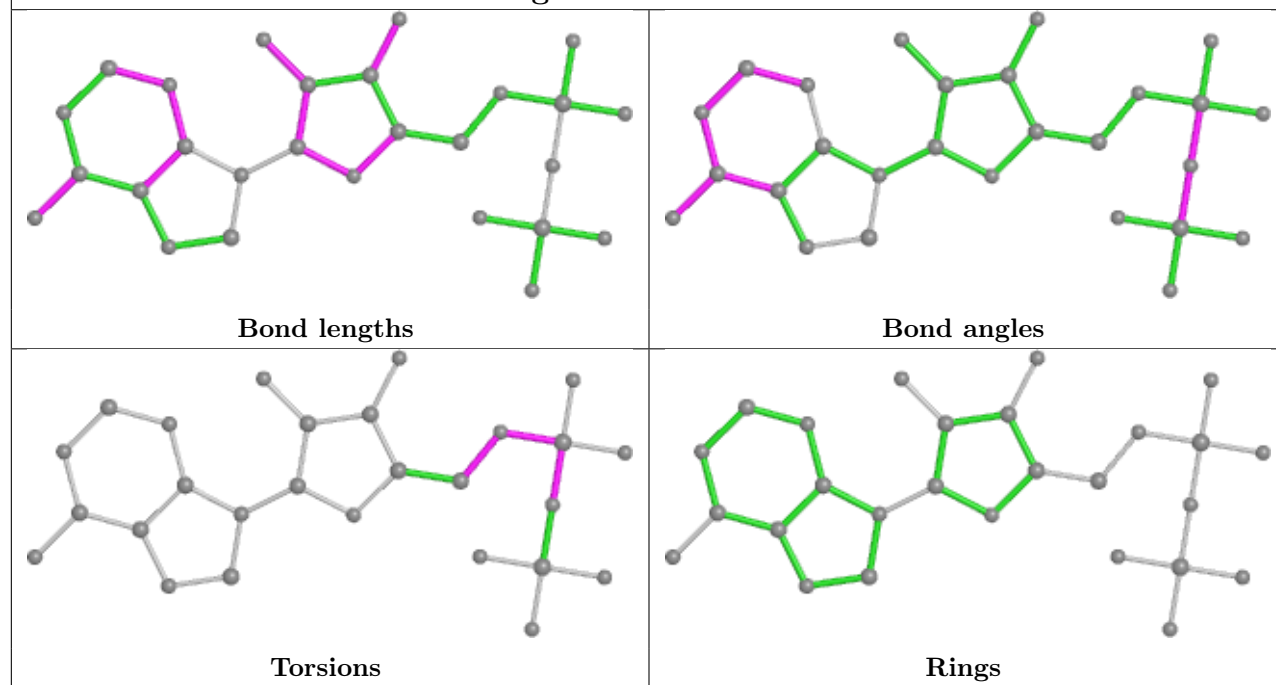
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

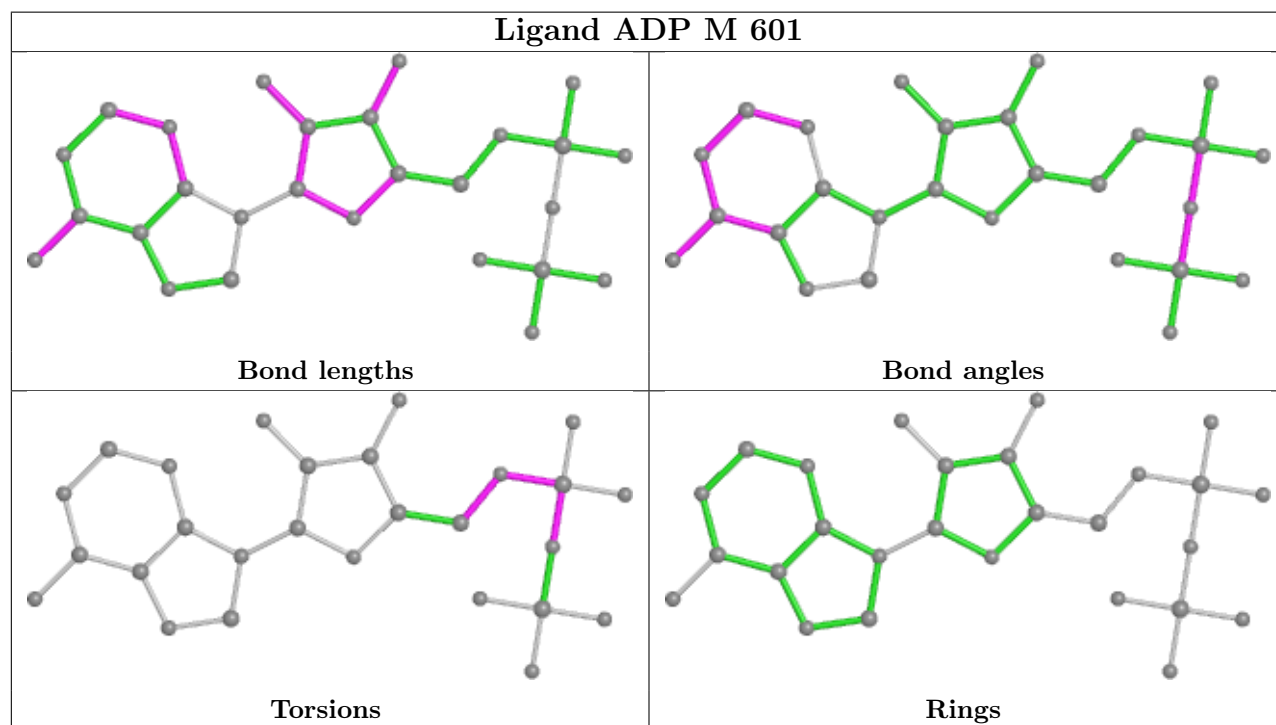
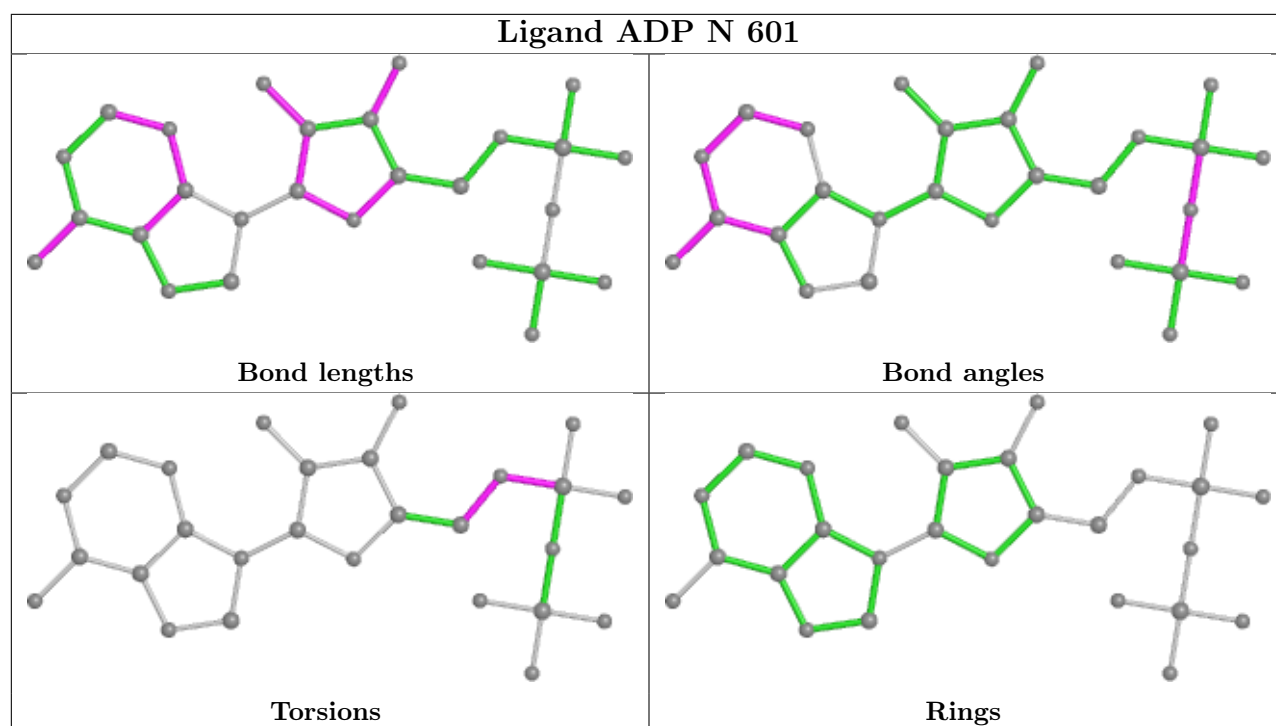


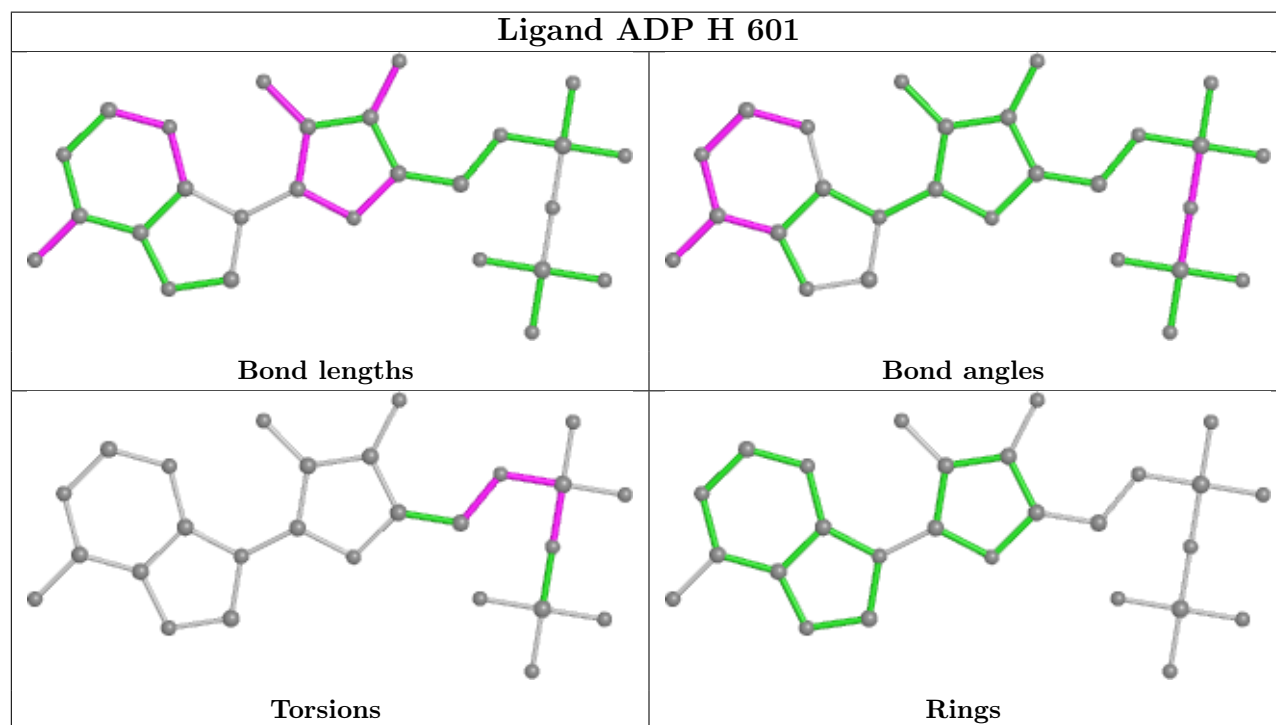
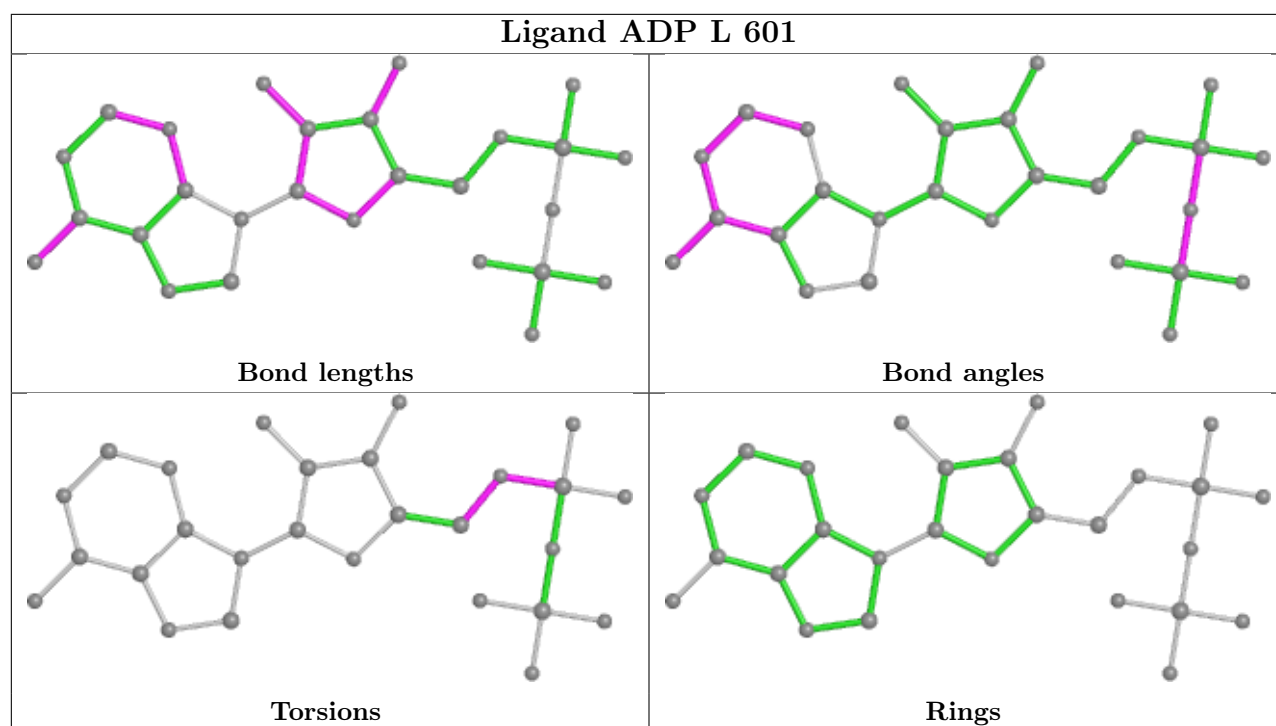
Ligand ADP I 601

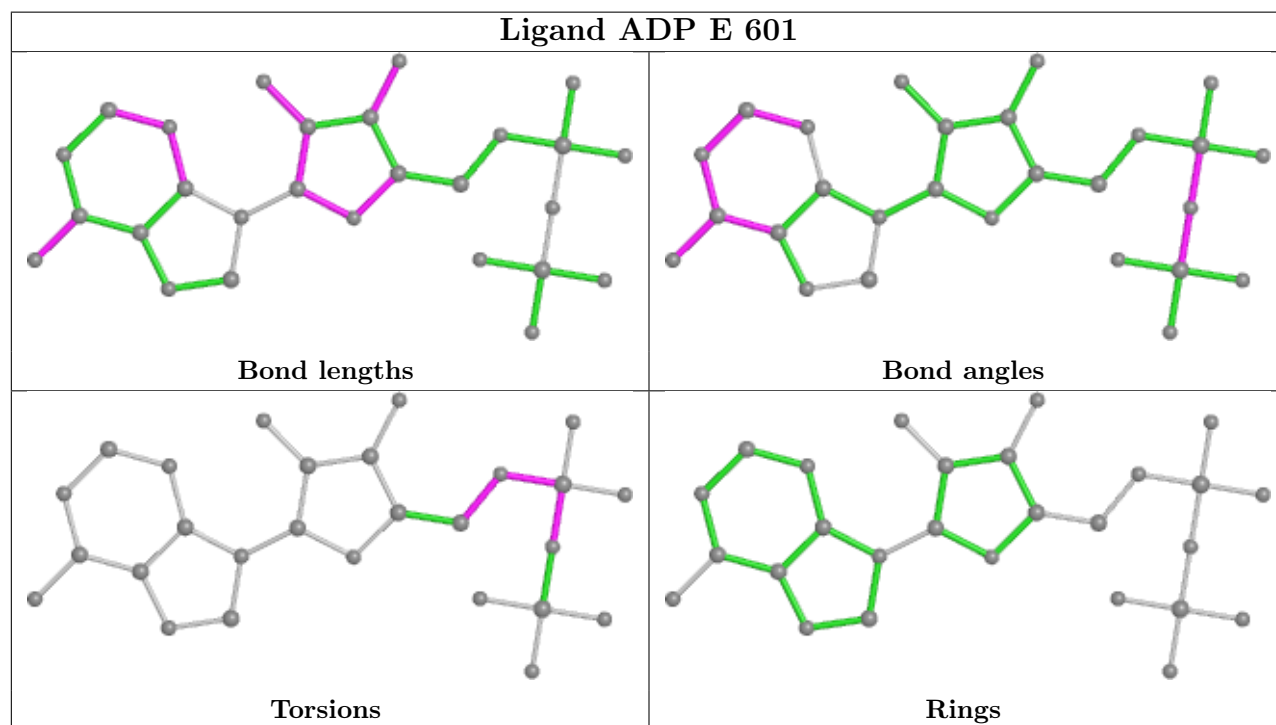
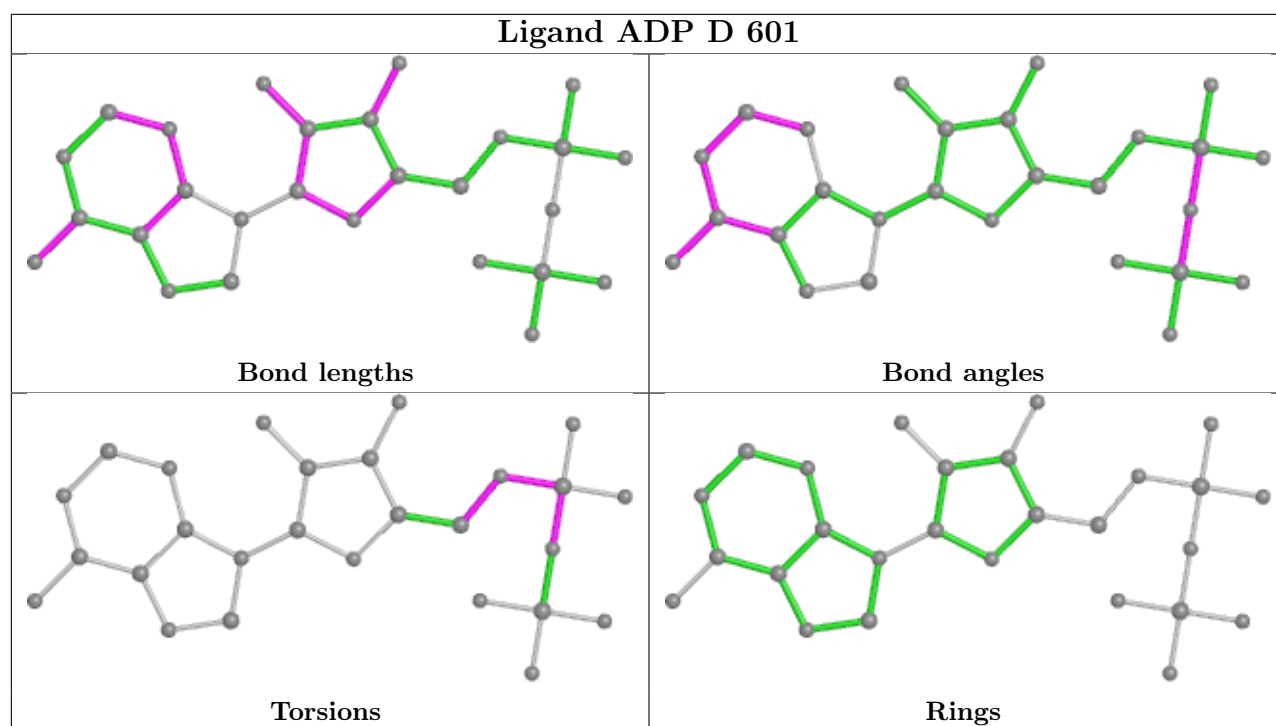


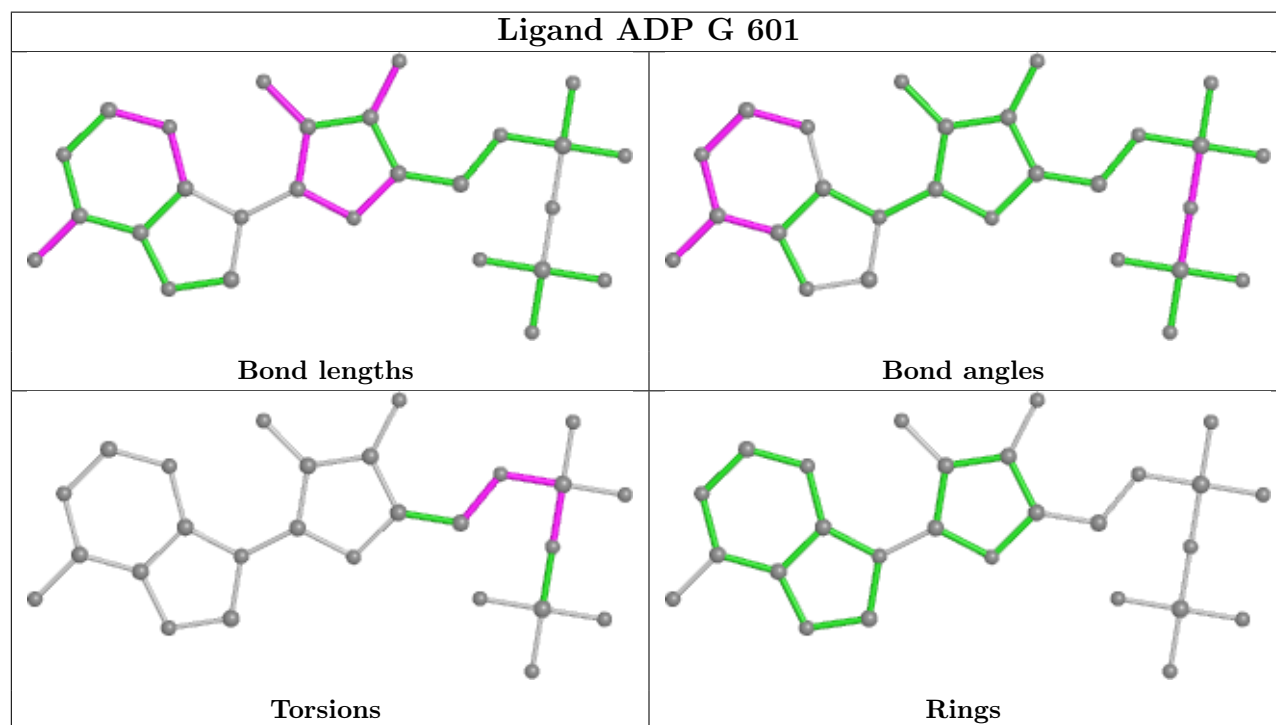
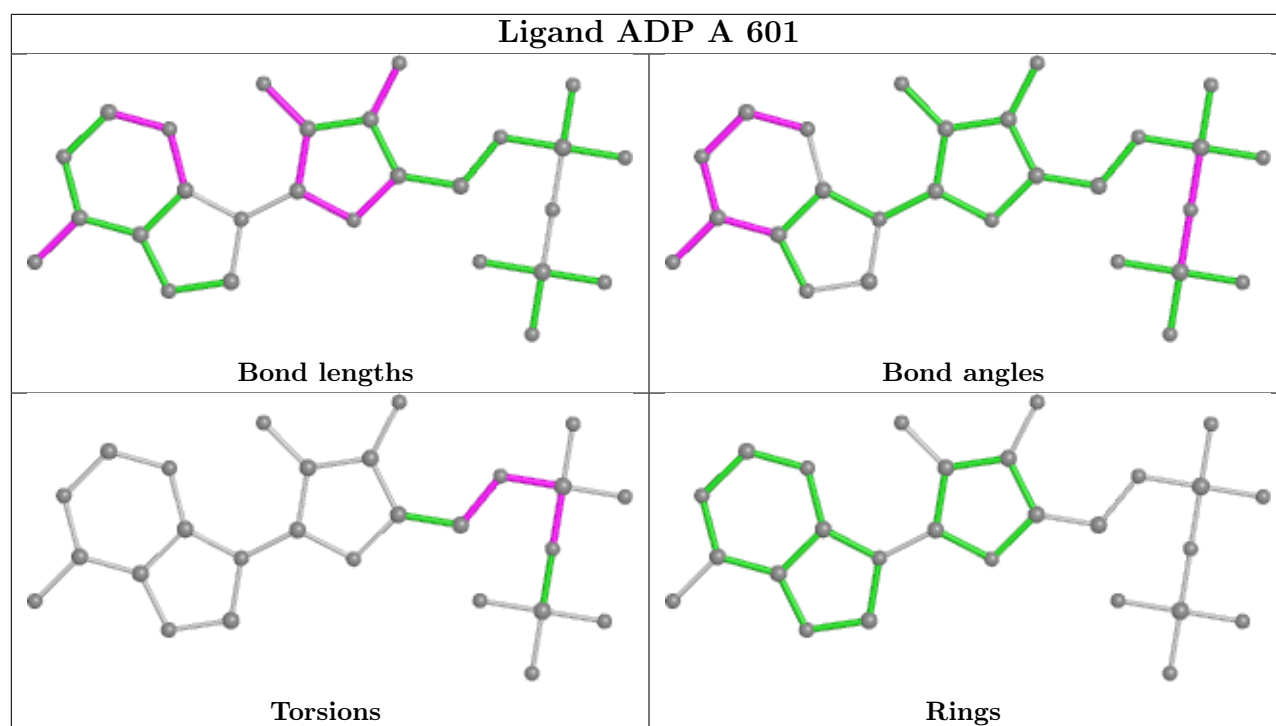
Ligand ADP F 601

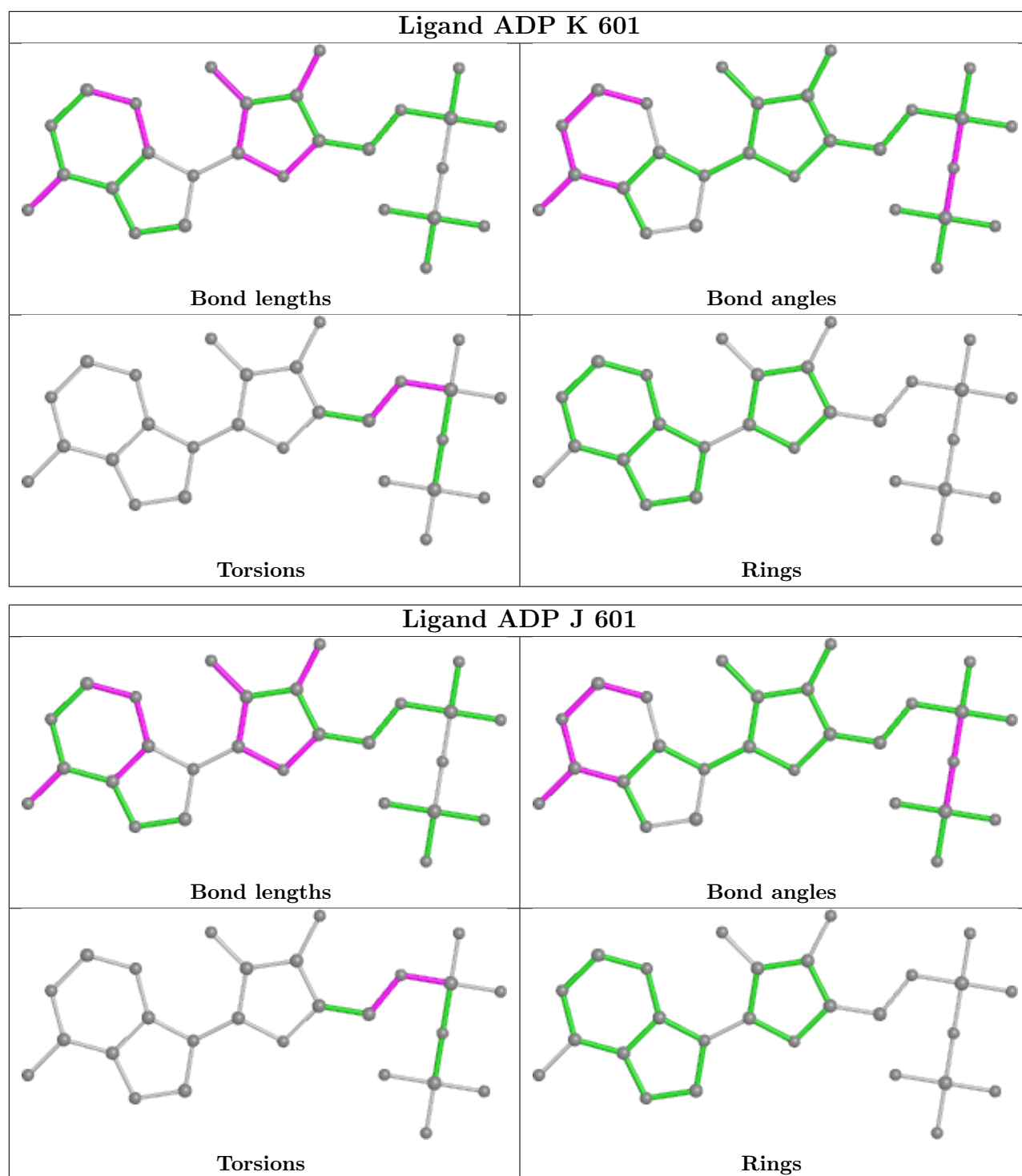












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

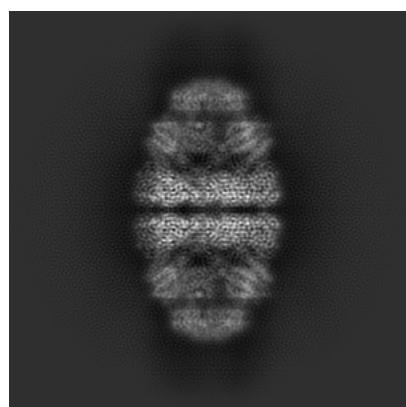
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9195. These allow visual inspection of the internal detail of the map and identification of artifacts.

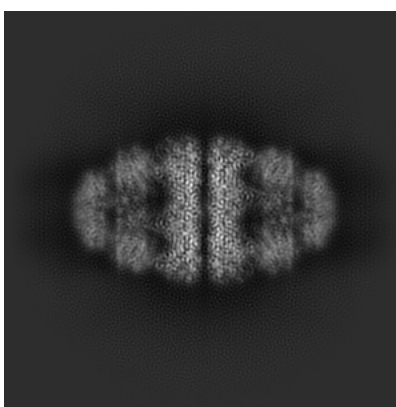
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

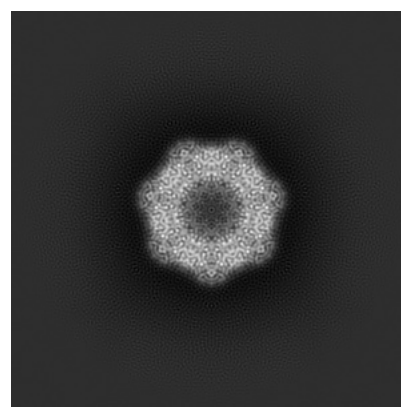
6.1.1 Primary map



X



Y

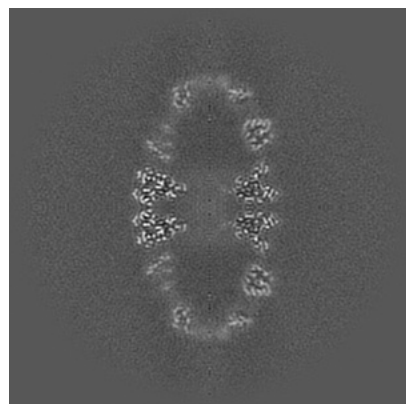


Z

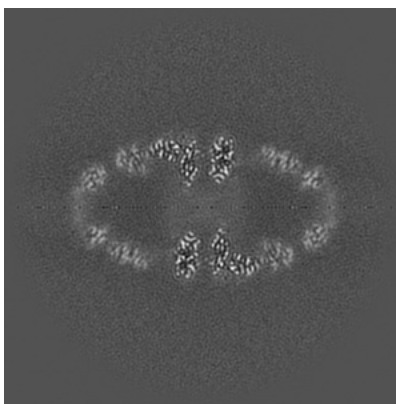
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

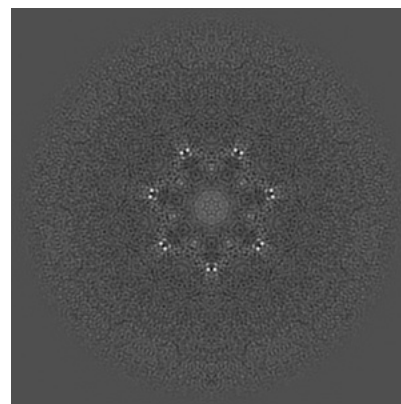
6.2.1 Primary map



X Index: 176



Y Index: 176

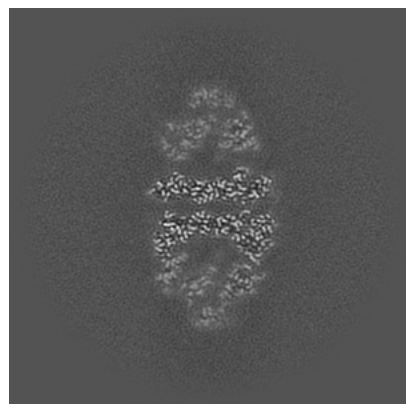


Z Index: 176

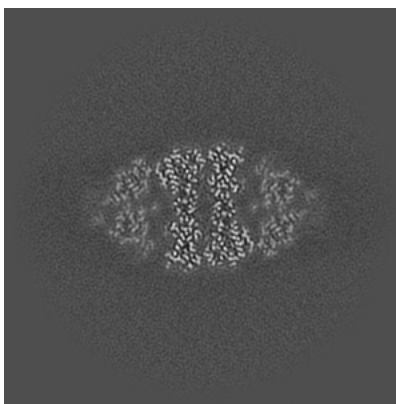
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

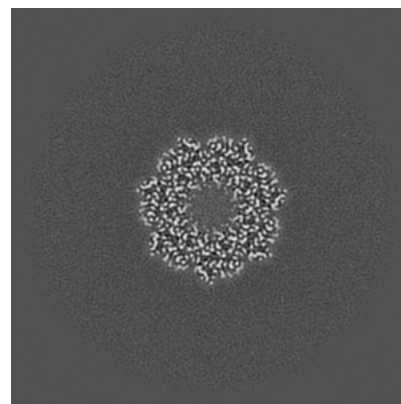
6.3.1 Primary map



X Index: 208



Y Index: 140

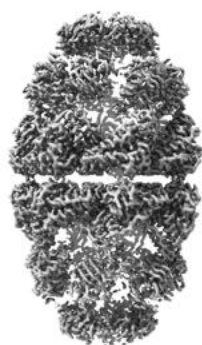


Z Index: 164

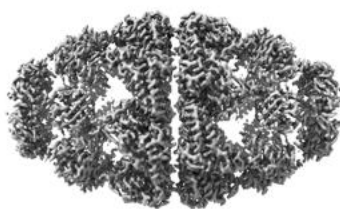
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

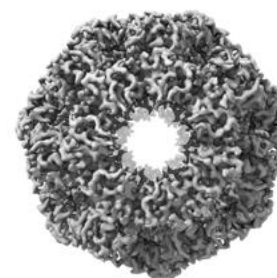
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

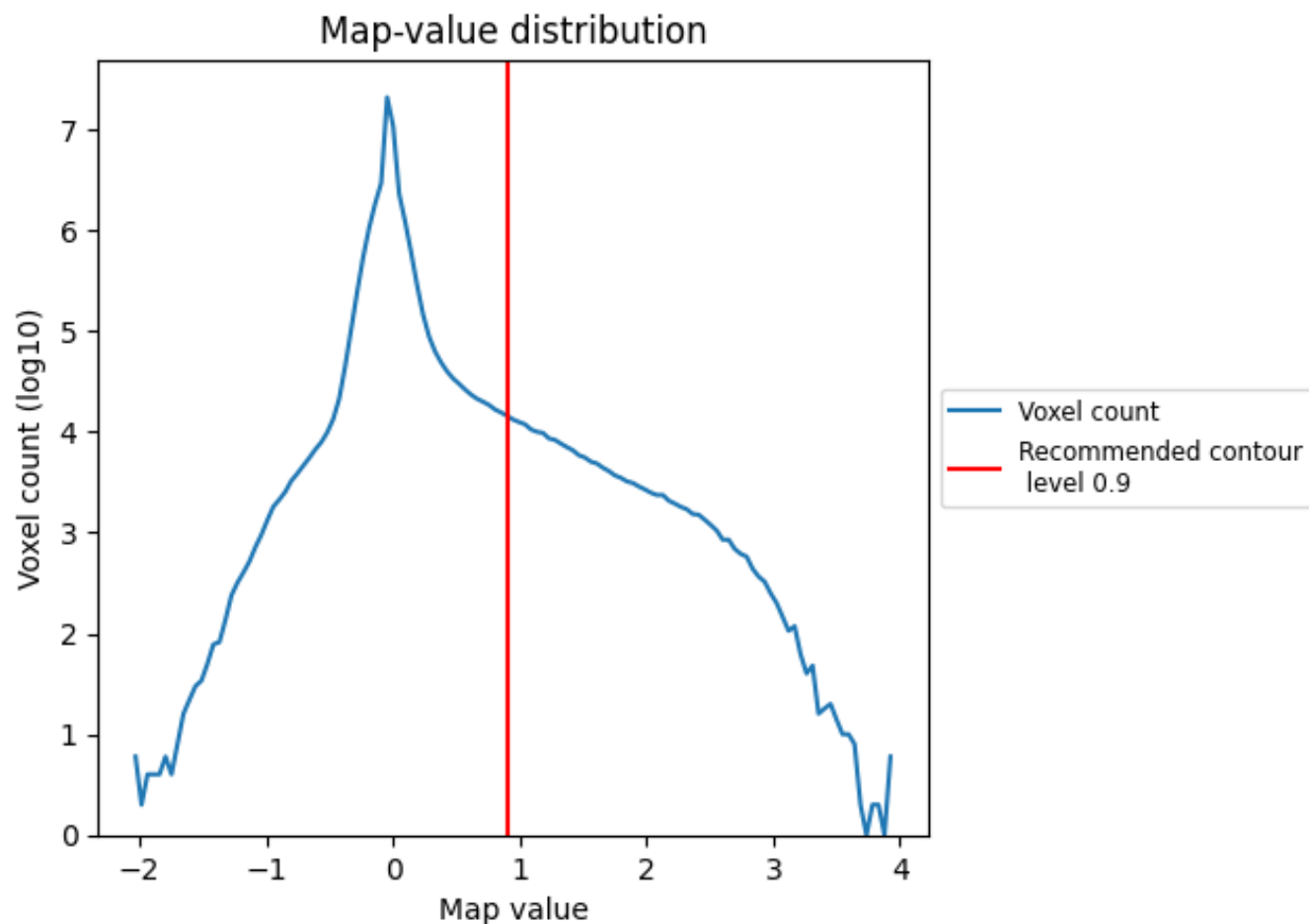
6.5 Mask visualisation

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

7 Map analysis [i](#)

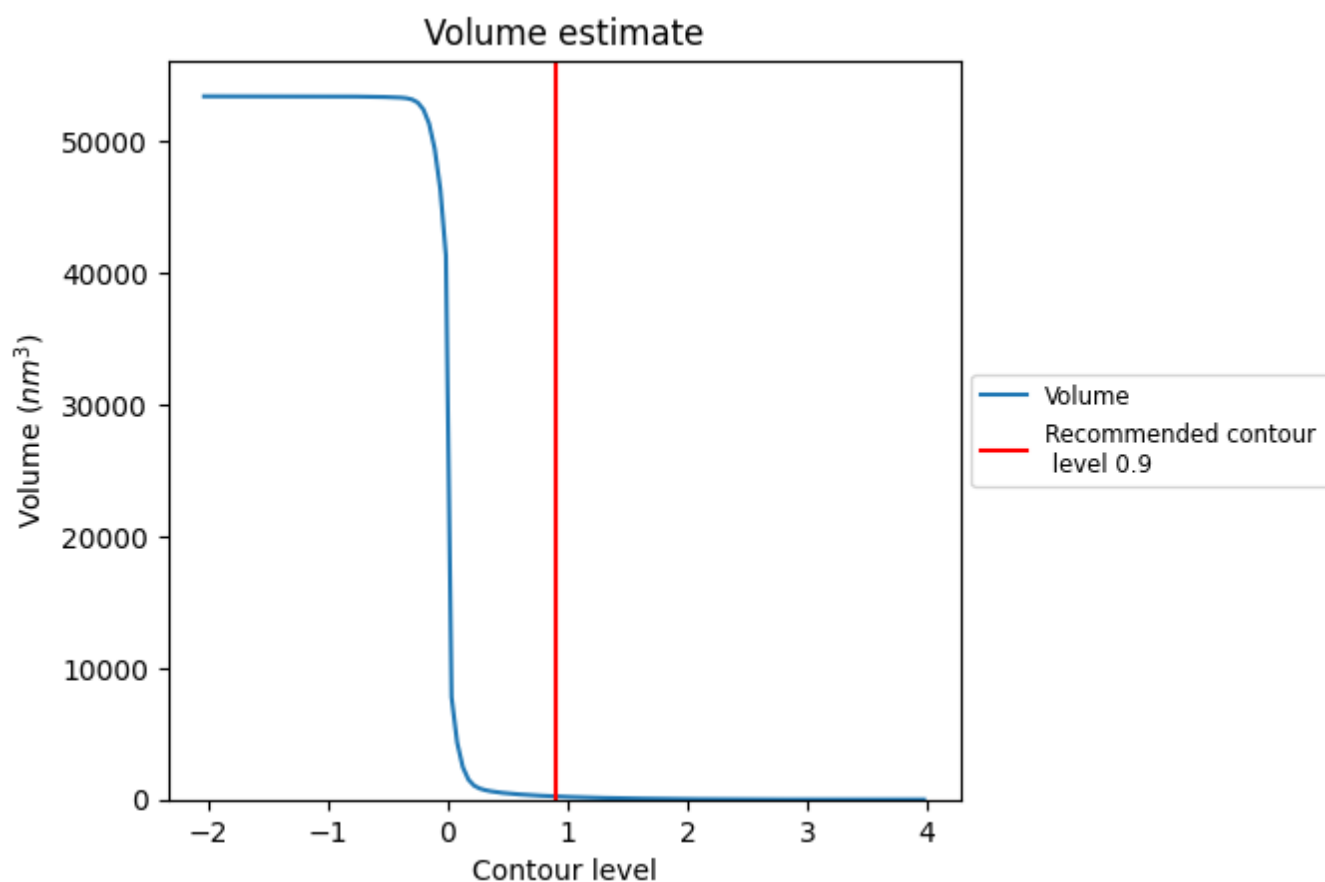
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

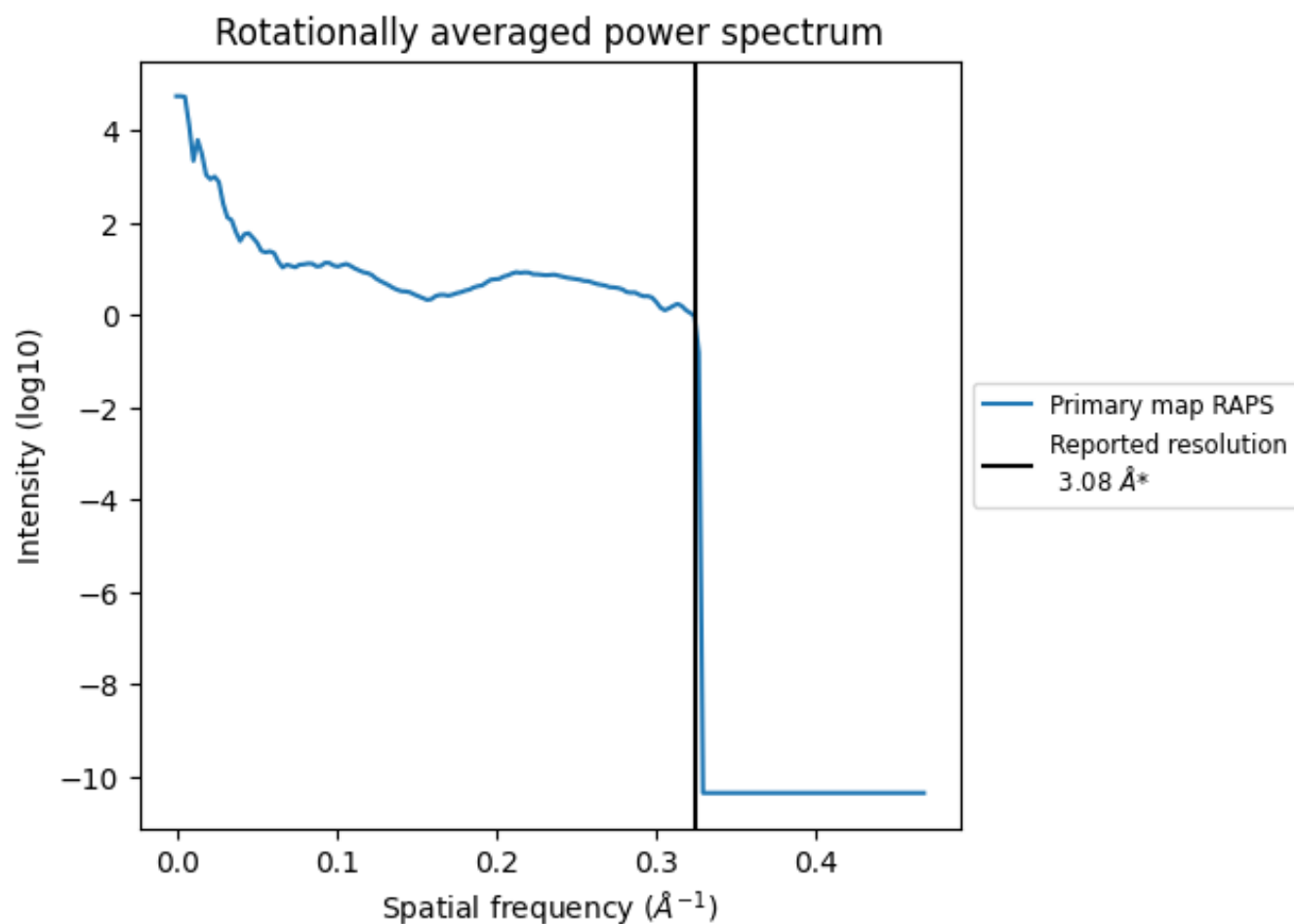
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm³; this corresponds to an approximate mass of 218 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

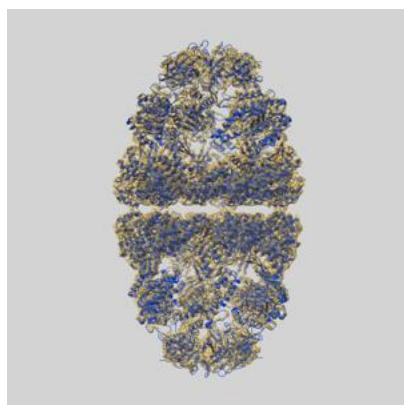
8 Fourier-Shell correlation

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

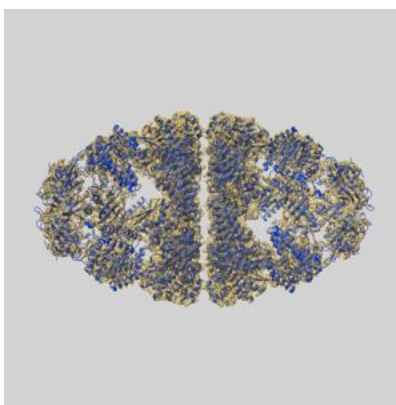
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9195 and PDB model 6MRC. Per-residue inclusion information can be found in section [3](#) on page [10](#).

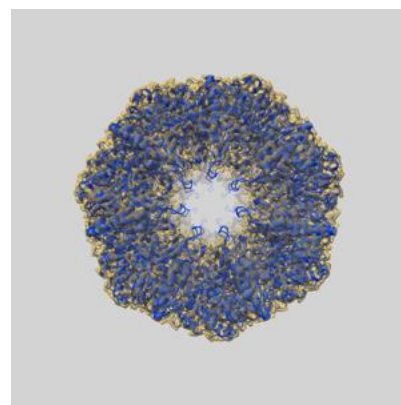
9.1 Map-model overlay [i](#)



X



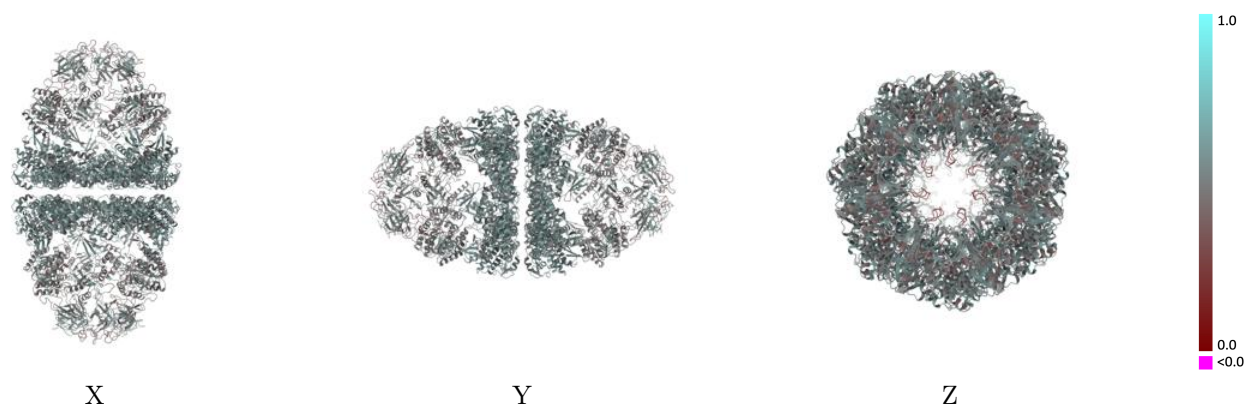
Y



Z

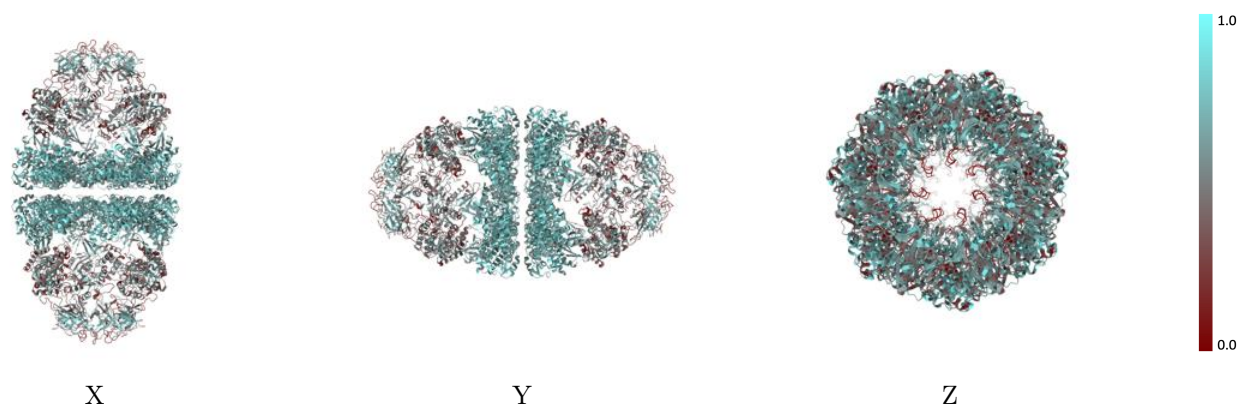
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



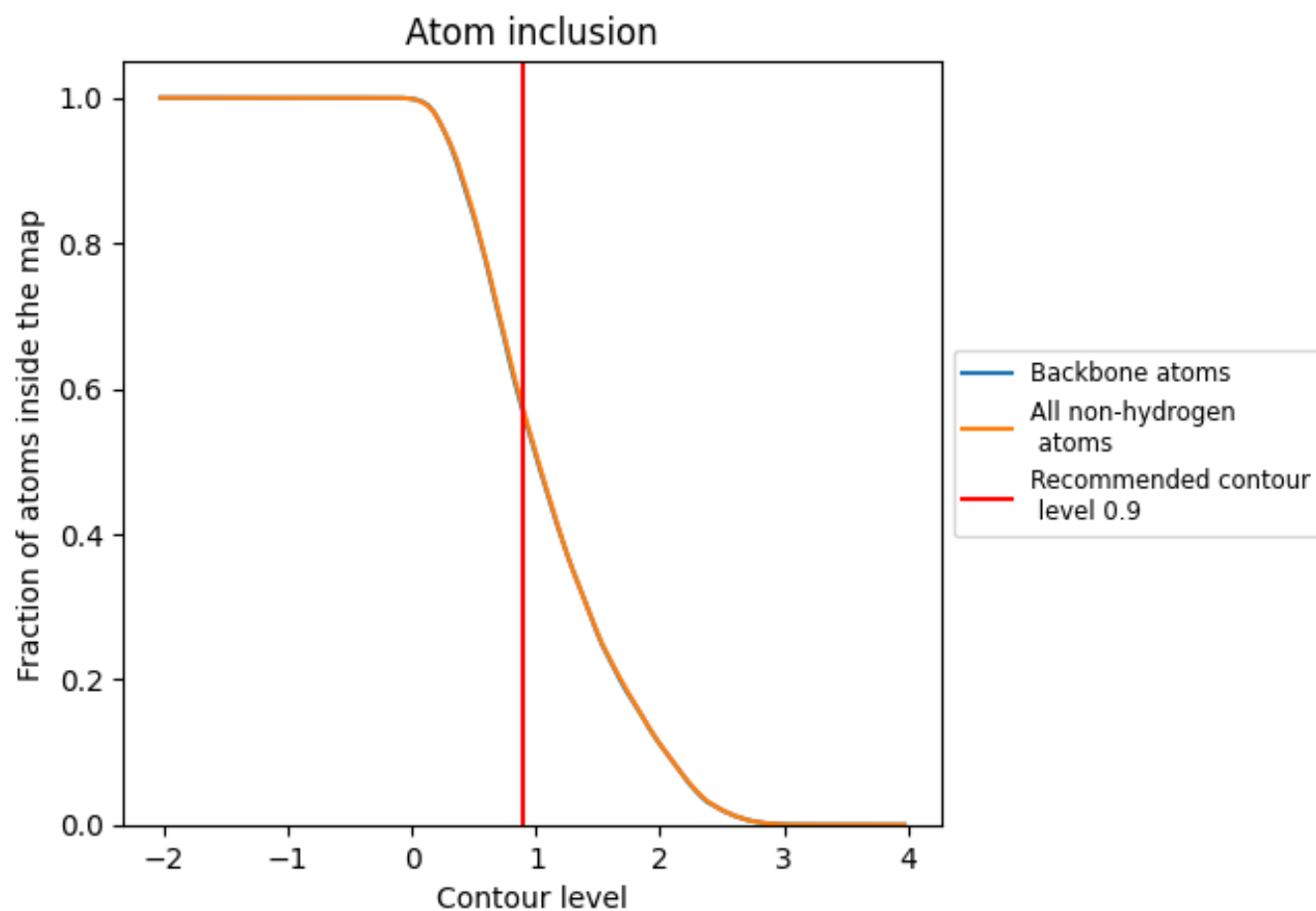
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.5686 |  0.5080 |
| 1 |  0.4376 |  0.4620 |
| 2 |  0.4456 |  0.4660 |
| A |  0.5972 |  0.5180 |
| B |  0.5975 |  0.5150 |
| C |  0.5983 |  0.5170 |
| D |  0.6003 |  0.5190 |
| E |  0.5980 |  0.5170 |
| F |  0.5980 |  0.5170 |
| G |  0.5950 |  0.5160 |
| H |  0.6013 |  0.5180 |
| I |  0.5957 |  0.5140 |
| J |  0.5972 |  0.5160 |
| K |  0.5970 |  0.5180 |
| L |  0.6001 |  0.5180 |
| M |  0.5965 |  0.5190 |
| N |  0.5983 |  0.5160 |
| O |  0.4376 |  0.4570 |
| P |  0.4376 |  0.4590 |
| Q |  0.4349 |  0.4590 |
| R |  0.4362 |  0.4630 |
| S |  0.4376 |  0.4650 |
| T |  0.4349 |  0.4590 |
| U |  0.4322 |  0.4570 |
| V |  0.4403 |  0.4590 |
| W |  0.4443 |  0.4570 |
| X |  0.4389 |  0.4580 |
| Y |  0.4376 |  0.4590 |
| Z |  0.4349 |  0.4600 |

