



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 12:00 pm GMT

PDB ID : 3S1A
Title : Crystal structure of the phosphorylation-site double mutant S431E/T432E of the KaiC circadian clock protein
Authors : Pattanayek, R.; Williams, D.W.; Rossi, G.; Weigand, S.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.
Deposited on : 2011-05-14
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

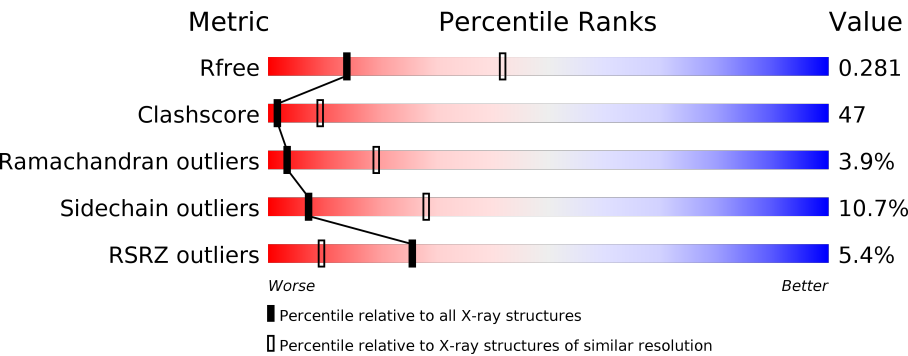
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 111664 | 1851 (3.00-3.00) |
| Clashscore | 122126 | 2167 (3.00-3.00) |
| Ramachandran outliers | 120053 | 2101 (3.00-3.00) |
| Sidechain outliers | 120020 | 2104 (3.00-3.00) |
| RSRZ outliers | 108989 | 1751 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 525 | <div><div>9%</div><div><div></div><div>37%</div><div>50%</div><div>9%</div><div></div></div><div></div></div> |
| 1 | F | 525 | <div><div>6%</div><div><div></div><div>39%</div><div>48%</div><div>9%</div><div></div></div><div></div></div> |
| 2 | B | 525 | <div><div>6%</div><div><div></div><div>31%</div><div>53%</div><div>9%</div><div>6%</div></div><div></div></div> |
| 2 | C | 525 | <div><div>4%</div><div><div></div><div>35%</div><div>49%</div><div>9%</div><div>7%</div></div><div></div></div> |
| 2 | D | 525 | <div><div>2%</div><div><div></div><div>39%</div><div>46%</div><div>6%</div><div>8%</div></div><div></div></div> |
| 2 | E | 525 | <div><div>3%</div><div><div></div><div>39%</div><div>46%</div><div>9%</div><div>6%</div></div><div></div></div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | SEP | A | 320 | - | - | X | X |
| 1 | SEP | F | 320 | - | - | X | - |
| 4 | MG | A | 526 | - | - | - | X |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1 | A | 506 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 3994 | 2512 | 701 | 765 | 1 | 15 | | | |
| 1 | F | 506 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 3994 | 2512 | 701 | 765 | 1 | 15 | | | |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| A | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| A | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| A | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| A | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| A | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| A | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| A | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| F | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| F | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| F | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |

- Molecule 2 is a protein called Circadian clock protein kinase kaiC.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|--|---------|---------|-------|
| 2 | B | 491 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 3875 | 2442 | 678 | 740 | 15 | | | | |
| 2 | C | 488 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 3851 | 2428 | 674 | 734 | 15 | | | | |

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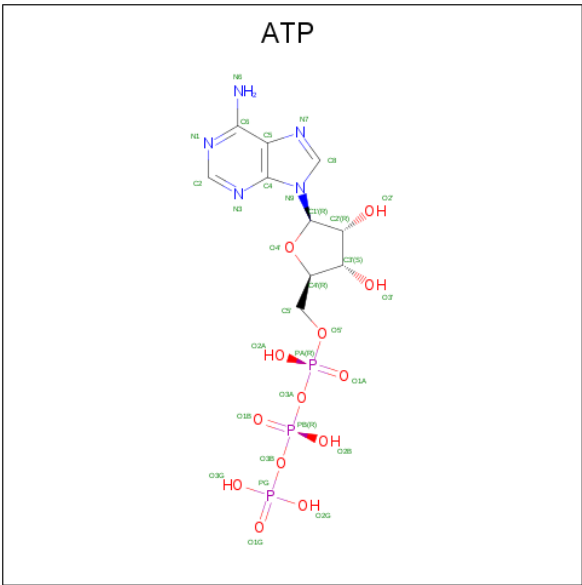
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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | D | 485 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3827 | 2414 | 671 | 727 | 15 | | | |
| 2 | E | 492 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3883 | 2448 | 679 | 741 | 15 | | | |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| B | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| B | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| B | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| B | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| B | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| B | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| B | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| C | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| C | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| C | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| D | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| D | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| D | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 431 | GLU | SER | ENGINEERED MUTATION | UNP Q79PF4 |
| E | 432 | GLU | THR | ENGINEERED MUTATION | UNP Q79PF4 |
| E | 520 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 521 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 522 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 523 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 524 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |
| E | 525 | HIS | - | EXPRESSION TAG | UNP Q79PF4 |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 3 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | D | 4 | Total Mg 4 4 | 0 | 0 |
| 4 | E | 2 | Total Mg 2 2 | 0 | 0 |
| 4 | B | 4 | Total Mg 4 4 | 0 | 0 |
| 4 | C | 4 | Total Mg 4 4 | 0 | 0 |
| 4 | A | 4 | Total Mg 4 4 | 0 | 0 |
| 4 | F | 3 | Total Mg 3 3 | 0 | 0 |

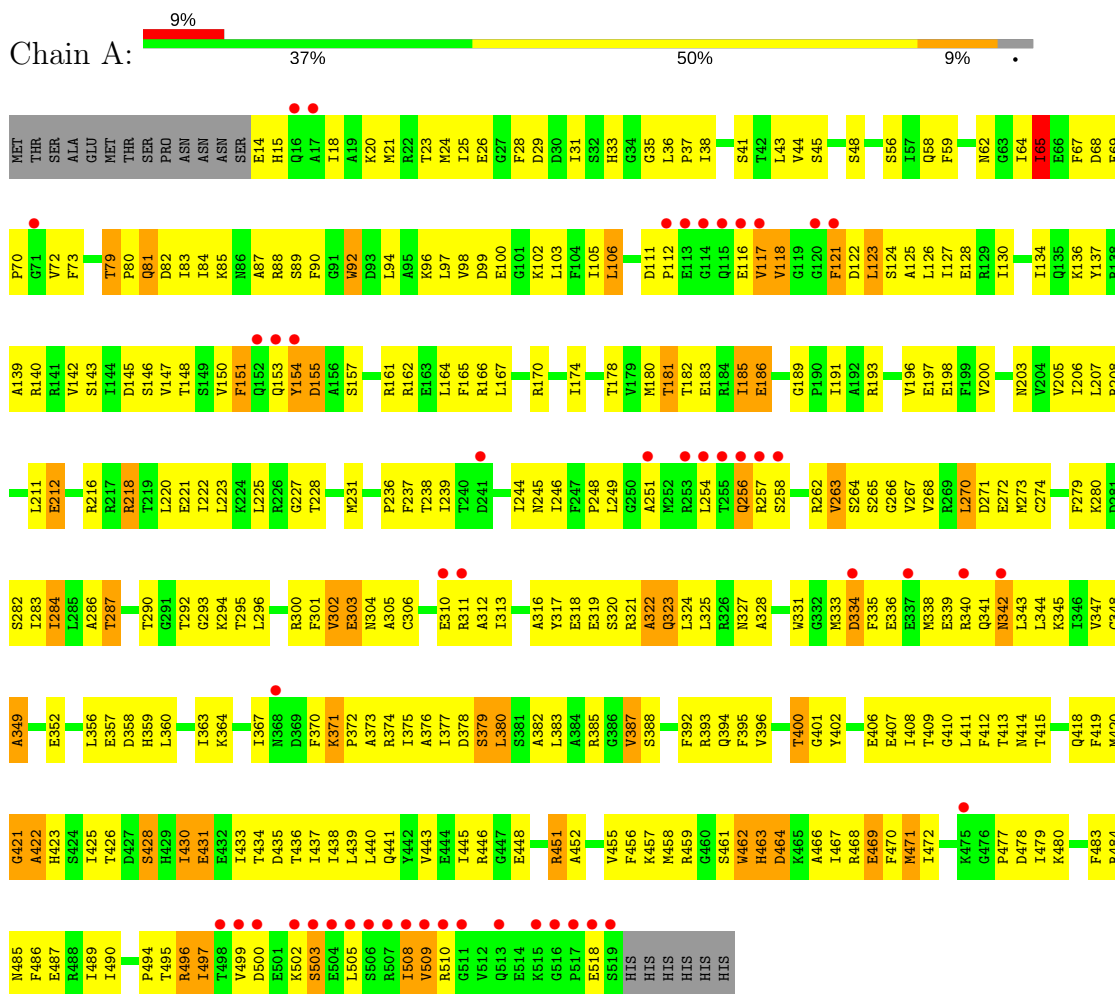
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5 | A | 5 | Total O 5 5 | 0 | 0 |
| 5 | B | 6 | Total O 6 6 | 0 | 0 |
| 5 | C | 10 | Total O 10 10 | 0 | 0 |
| 5 | D | 32 | Total O 32 32 | 0 | 0 |
| 5 | E | 16 | Total O 16 16 | 0 | 0 |
| 5 | F | 12 | Total O 12 12 | 0 | 0 |

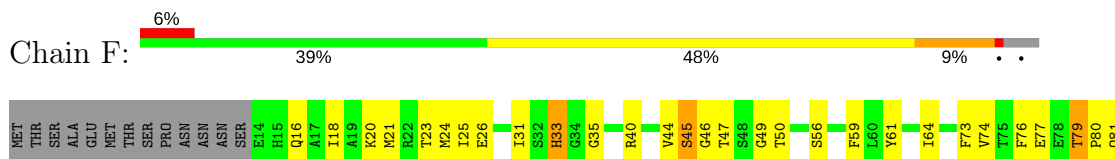
3 Residue-property plots

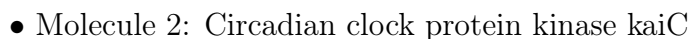
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

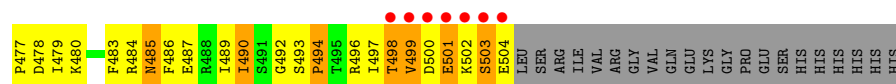
• Molecule 1: Circadian clock protein kinase kaiC



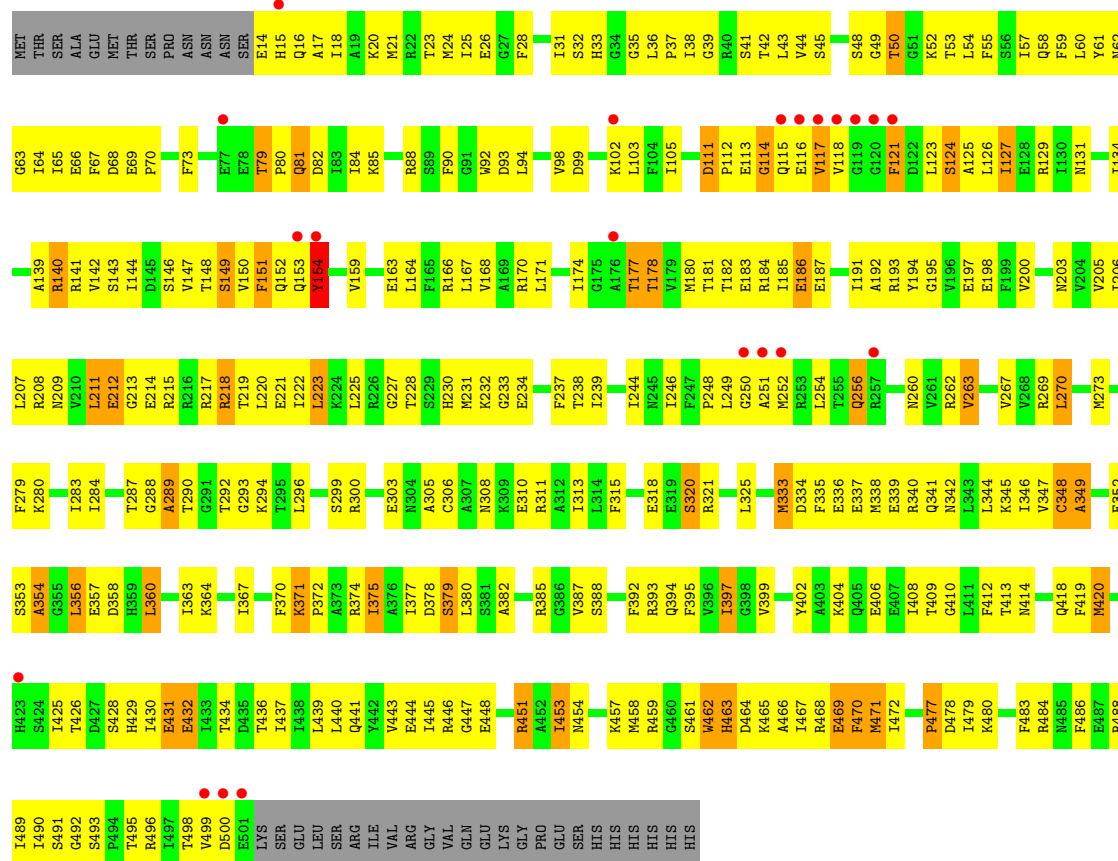
• Molecule 1: Circadian clock protein kinase kaiC



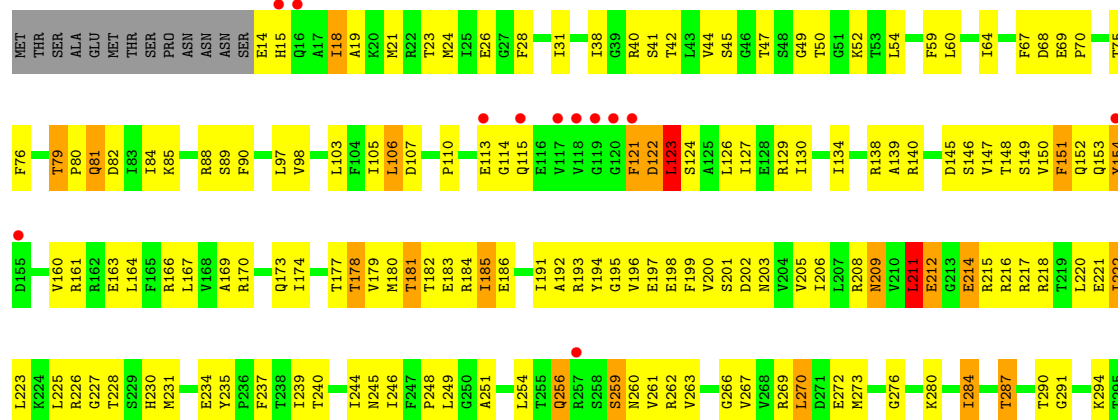




• Molecule 2: Circadian clock protein kinase kaiC



• Molecule 2: Circadian clock protein kinase kaiC



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 132.67Å 135.49Å 204.60Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 17.00 – 3.00 16.96 – 2.89 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (17.00-3.00) 92.3 (16.96-2.89) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.75 (at 2.87Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.242 , 0.288 0.239 , 0.281 | Depositor DCC |
| R_{free} test set | 6459 reflections (7.95%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 65.1 | Xtriage |
| Anisotropy | 0.584 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 60.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.016 for k,h,-l | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 23898 | wwPDB-VP |
| Average B, all atoms (Å ²) | 71.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.43 | 0/4049 | 0.72 | 1/5453 (0.0%) |
| 1 | F | 0.46 | 0/4049 | 0.73 | 0/5453 |
| 2 | B | 0.40 | 0/3940 | 0.67 | 0/5309 |
| 2 | C | 0.41 | 0/3916 | 0.69 | 1/5278 (0.0%) |
| 2 | D | 0.50 | 0/3892 | 0.73 | 0/5245 |
| 2 | E | 0.49 | 0/3948 | 0.75 | 2/5320 (0.0%) |
| All | All | 0.45 | 0/23794 | 0.72 | 4/32058 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | E | 213 | GLY | N-CA-C | -5.96 | 98.21 | 113.10 |
| 2 | E | 106 | LEU | CA-CB-CG | 5.81 | 128.67 | 115.30 |
| 2 | C | 213 | GLY | N-CA-C | -5.28 | 99.90 | 113.10 |
| 1 | A | 380 | LEU | N-CA-C | -5.23 | 96.88 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3994 | 0 | 3985 | 444 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | F | 3994 | 0 | 3983 | 405 | 0 |
| 2 | B | 3875 | 0 | 3863 | 437 | 0 |
| 2 | C | 3851 | 0 | 3839 | 382 | 0 |
| 2 | D | 3827 | 0 | 3819 | 358 | 0 |
| 2 | E | 3883 | 0 | 3875 | 351 | 0 |
| 3 | A | 62 | 0 | 24 | 7 | 0 |
| 3 | B | 62 | 0 | 24 | 8 | 0 |
| 3 | C | 62 | 0 | 24 | 5 | 0 |
| 3 | D | 62 | 0 | 24 | 6 | 0 |
| 3 | E | 62 | 0 | 24 | 11 | 0 |
| 3 | F | 62 | 0 | 24 | 6 | 0 |
| 4 | A | 4 | 0 | 0 | 0 | 0 |
| 4 | B | 4 | 0 | 0 | 0 | 0 |
| 4 | C | 4 | 0 | 0 | 0 | 0 |
| 4 | D | 4 | 0 | 0 | 0 | 0 |
| 4 | E | 2 | 0 | 0 | 0 | 0 |
| 4 | F | 3 | 0 | 0 | 0 | 0 |
| 5 | A | 5 | 0 | 0 | 0 | 0 |
| 5 | B | 6 | 0 | 0 | 1 | 0 |
| 5 | C | 10 | 0 | 0 | 2 | 0 |
| 5 | D | 32 | 0 | 0 | 13 | 0 |
| 5 | E | 16 | 0 | 0 | 0 | 0 |
| 5 | F | 12 | 0 | 0 | 1 | 0 |
| All | All | 23898 | 0 | 23508 | 2227 | 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 47.

All (2227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:455:VAL:HG12 | 1:A:463:HIS:CD2 | 1.63 | 1.30 |
| 1:A:320:SEP:HB2 | 2:B:254:LEU:O | 1.42 | 1.17 |
| 1:A:254:LEU:CD2 | 1:F:320:SEP:HA | 1.74 | 1.16 |
| 1:A:321:ARG:O | 1:A:324:LEU:HB2 | 1.45 | 1.14 |
| 1:F:263:VAL:HG12 | 1:F:374:ARG:HH21 | 1.10 | 1.14 |
| 1:A:455:VAL:CG1 | 1:A:463:HIS:HD2 | 1.61 | 1.13 |
| 1:A:254:LEU:HD21 | 1:F:320:SEP:HA | 1.15 | 1.13 |
| 2:D:123:LEU:HG | 2:D:163:GLU:OE2 | 1.49 | 1.13 |
| 1:F:305:ALA:HB2 | 1:F:374:ARG:HD2 | 1.21 | 1.13 |
| 1:F:509:VAL:HG12 | 1:F:510:ARG:H | 1.07 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:305:ALA:HB2 | 2:B:374:ARG:HD2 | 1.33 | 1.11 |
| 2:E:305:ALA:HB2 | 2:E:374:ARG:HD2 | 1.26 | 1.11 |
| 1:A:320:SEP:CA | 2:B:254:LEU:HG | 1.83 | 1.08 |
| 2:E:263:VAL:HG12 | 2:E:374:ARG:HH21 | 1.12 | 1.07 |
| 1:A:14:GLU:HG3 | 1:A:15:HIS:H | 1.19 | 1.07 |
| 2:B:269:ARG:HB3 | 2:B:479:ILE:HD13 | 1.37 | 1.06 |
| 1:A:320:SEP:HA | 2:B:254:LEU:HG | 1.30 | 1.06 |
| 2:D:123:LEU:O | 2:D:127:ILE:HD13 | 1.54 | 1.05 |
| 2:B:263:VAL:HG12 | 2:B:374:ARG:HH21 | 1.20 | 1.05 |
| 1:A:455:VAL:HG12 | 1:A:463:HIS:HD2 | 0.88 | 1.04 |
| 2:C:205:VAL:HG22 | 2:C:222:ILE:HD13 | 1.38 | 1.04 |
| 2:B:497:ILE:HD12 | 2:B:499:VAL:H | 1.22 | 1.03 |
| 1:A:455:VAL:CG1 | 1:A:463:HIS:CD2 | 2.39 | 1.02 |
| 2:D:445:ILE:HD13 | 2:D:450:SER:OG | 1.58 | 1.02 |
| 2:D:123:LEU:HD12 | 2:D:166:ARG:HD2 | 1.41 | 1.02 |
| 1:A:305:ALA:HB2 | 1:A:374:ARG:HD2 | 1.39 | 1.02 |
| 2:D:371:LYS:HD2 | 2:D:371:LYS:O | 1.60 | 1.02 |
| 1:F:18:ILE:HD12 | 1:F:227:GLY:HA3 | 1.44 | 0.99 |
| 2:D:311:ARG:HD2 | 2:D:371:LYS:HE3 | 1.42 | 0.99 |
| 2:E:313:ILE:HD12 | 2:E:367:ILE:HD13 | 1.45 | 0.98 |
| 1:A:41:SER:HB3 | 1:A:178:THR:HB | 1.46 | 0.97 |
| 1:F:263:VAL:CG1 | 1:F:374:ARG:HH21 | 1.76 | 0.97 |
| 2:D:335:PHE:HA | 2:D:338:MET:HG3 | 1.45 | 0.96 |
| 1:F:79:THR:HG22 | 1:F:82:ASP:H | 1.30 | 0.96 |
| 2:B:325:LEU:HD23 | 2:B:335:PHE:CB | 1.94 | 0.96 |
| 2:B:147:VAL:HG11 | 2:B:180:MET:HE3 | 1.47 | 0.96 |
| 2:B:434:THR:HG21 | 2:B:437:ILE:HD11 | 1.48 | 0.95 |
| 1:A:31:ILE:HD11 | 1:A:246:ILE:HG21 | 1.45 | 0.95 |
| 2:B:385:ARG:HG2 | 2:C:393:ARG:NH1 | 1.80 | 0.95 |
| 2:C:305:ALA:HB2 | 2:C:374:ARG:HD2 | 1.48 | 0.95 |
| 2:E:356:LEU:HD22 | 2:E:387:VAL:HG11 | 1.48 | 0.94 |
| 2:C:371:LYS:HD2 | 2:C:371:LYS:O | 1.67 | 0.94 |
| 2:E:311:ARG:HD2 | 2:E:371:LYS:HE3 | 1.50 | 0.94 |
| 1:F:509:VAL:HG12 | 1:F:510:ARG:N | 1.83 | 0.93 |
| 2:C:434:THR:HG23 | 2:C:437:ILE:HD11 | 1.47 | 0.93 |
| 2:B:285:LEU:HD23 | 2:B:437:ILE:HD12 | 1.51 | 0.93 |
| 2:D:146:SER:H | 2:D:181:THR:HG22 | 1.34 | 0.93 |
| 2:B:73:PHE:HB3 | 2:B:105:ILE:HD13 | 1.50 | 0.93 |
| 2:C:367:ILE:HG12 | 2:C:375:ILE:HD11 | 1.51 | 0.93 |
| 2:B:170:ARG:O | 2:B:174:ILE:HG12 | 1.69 | 0.92 |
| 2:B:325:LEU:HD23 | 2:B:335:PHE:HB2 | 1.47 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:21:MET:HE3 | 2:C:141:ARG:NE | 1.84 | 0.92 |
| 2:B:54:LEU:HD23 | 2:B:244:ILE:HD11 | 1.51 | 0.92 |
| 1:F:263:VAL:HG12 | 1:F:374:ARG:NH2 | 1.85 | 0.92 |
| 1:F:508:ILE:O | 1:F:509:VAL:HG23 | 1.69 | 0.91 |
| 2:D:333:MET:HA | 5:D:913:HOH:O | 1.70 | 0.91 |
| 2:C:437:ILE:CD1 | 2:C:457:LYS:HE2 | 2.01 | 0.91 |
| 2:E:79:THR:HG23 | 2:E:81:GLN:HG2 | 1.52 | 0.91 |
| 1:F:18:ILE:CD1 | 1:F:227:GLY:HA3 | 2.01 | 0.90 |
| 1:A:25:ILE:HD12 | 1:A:58:GLN:HG2 | 1.51 | 0.90 |
| 2:B:483:PHE:HB3 | 2:B:486:PHE:HD1 | 1.36 | 0.90 |
| 2:C:123:LEU:HD23 | 2:C:127:ILE:HD11 | 1.54 | 0.89 |
| 2:C:287:THR:HG23 | 2:C:414:ASN:HD22 | 1.36 | 0.89 |
| 2:E:313:ILE:HB | 2:E:375:ILE:HD11 | 1.54 | 0.89 |
| 1:A:462:TRP:O | 1:A:463:HIS:HB3 | 1.73 | 0.89 |
| 2:B:45:SER:HB3 | 2:B:182:THR:HB | 1.54 | 0.89 |
| 1:A:79:THR:CG2 | 1:A:81:GLN:HG2 | 2.02 | 0.89 |
| 2:C:344:LEU:HD22 | 2:C:345:LYS:H | 1.37 | 0.89 |
| 1:A:79:THR:HG23 | 1:A:81:GLN:HE21 | 1.36 | 0.88 |
| 2:D:79:THR:HG22 | 2:D:82:ASP:H | 1.36 | 0.88 |
| 1:A:203:ASN:HB3 | 1:A:225:LEU:HD23 | 1.55 | 0.88 |
| 2:D:60:LEU:O | 2:D:64:ILE:HD13 | 1.74 | 0.88 |
| 2:C:206:ILE:HD11 | 2:C:223:LEU:HB2 | 1.54 | 0.88 |
| 2:B:147:VAL:HG11 | 2:B:180:MET:CE | 2.05 | 0.87 |
| 2:E:287:THR:HG23 | 2:E:414:ASN:HD22 | 1.36 | 0.87 |
| 2:B:148:THR:HG21 | 2:B:193:ARG:HD2 | 1.57 | 0.87 |
| 1:F:509:VAL:CG1 | 1:F:510:ARG:H | 1.86 | 0.87 |
| 1:A:396:VAL:HG11 | 1:A:430:ILE:HG21 | 1.56 | 0.87 |
| 2:E:79:THR:CG2 | 2:E:81:GLN:HG2 | 2.05 | 0.87 |
| 2:C:182:THR:HG21 | 2:C:192:ALA:HB1 | 1.56 | 0.86 |
| 2:E:303:GLU:OE2 | 2:E:333:MET:HB3 | 1.76 | 0.86 |
| 2:C:493:SER:HB3 | 2:D:488:ARG:HG2 | 1.56 | 0.86 |
| 1:F:299:SER:C | 1:F:333:MET:HE1 | 1.95 | 0.86 |
| 2:C:45:SER:HB3 | 2:C:182:THR:HB | 1.56 | 0.85 |
| 2:C:287:THR:HG21 | 2:C:425:ILE:O | 1.76 | 0.85 |
| 2:E:269:ARG:HG2 | 2:E:479:ILE:HB | 1.55 | 0.85 |
| 2:C:437:ILE:HD13 | 2:C:457:LYS:HE2 | 1.58 | 0.85 |
| 1:A:318:GLU:OE1 | 2:B:432:GLU:HG2 | 1.76 | 0.85 |
| 1:F:18:ILE:HD13 | 1:F:40:ARG:NH1 | 1.91 | 0.85 |
| 1:A:14:GLU:CG | 1:A:15:HIS:H | 1.88 | 0.85 |
| 1:A:451:ARG:HH11 | 1:A:451:ARG:HG2 | 1.41 | 0.85 |
| 2:E:293:GLY:HA2 | 3:E:901:ATP:O1A | 1.77 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:363:ILE:O | 1:F:367:ILE:HG12 | 1.76 | 0.85 |
| 1:F:287:THR:HG23 | 1:F:414:ASN:HD22 | 1.39 | 0.85 |
| 1:F:123:LEU:O | 1:F:127:ILE:HD13 | 1.76 | 0.85 |
| 2:B:426:THR:HB | 2:B:431:GLU:OE2 | 1.77 | 0.84 |
| 2:B:140:ARG:NH1 | 2:B:140:ARG:HB3 | 1.91 | 0.84 |
| 2:C:25:ILE:HG23 | 2:C:58:GLN:NE2 | 1.90 | 0.84 |
| 2:C:140:ARG:HB3 | 2:C:140:ARG:NH1 | 1.93 | 0.84 |
| 2:C:269:ARG:HB3 | 2:C:479:ILE:HD12 | 1.59 | 0.84 |
| 2:B:503:SER:O | 2:B:504:GLU:HB2 | 1.74 | 0.84 |
| 2:E:435:ASP:HA | 2:E:459:ARG:HD2 | 1.58 | 0.84 |
| 1:F:293:GLY:HA2 | 3:F:901:ATP:O1A | 1.78 | 0.84 |
| 1:A:257:ARG:NH2 | 1:A:407:GLU:HG2 | 1.93 | 0.84 |
| 2:B:263:VAL:HG12 | 2:B:374:ARG:NH2 | 1.93 | 0.84 |
| 2:B:263:VAL:CG1 | 2:B:374:ARG:HH21 | 1.90 | 0.84 |
| 2:B:300:ARG:HA | 2:B:333:MET:CE | 2.07 | 0.83 |
| 1:F:191:ILE:HB | 1:F:198:GLU:CG | 2.08 | 0.83 |
| 2:B:116:GLU:HG2 | 2:B:117:VAL:H | 1.44 | 0.83 |
| 2:C:147:VAL:O | 2:C:150:VAL:HG12 | 1.78 | 0.83 |
| 1:F:313:ILE:HB | 1:F:375:ILE:HD11 | 1.61 | 0.83 |
| 2:C:25:ILE:HG12 | 2:C:58:GLN:HE21 | 1.43 | 0.83 |
| 2:D:287:THR:HG23 | 2:D:414:ASN:HD22 | 1.41 | 0.83 |
| 1:A:396:VAL:HG11 | 1:A:430:ILE:CG2 | 2.08 | 0.82 |
| 1:F:269:ARG:HG2 | 1:F:479:ILE:HB | 1.60 | 0.82 |
| 2:D:248:PRO:HB2 | 2:D:251:ALA:HB3 | 1.61 | 0.82 |
| 2:E:125:ALA:O | 2:E:129:ARG:HG3 | 1.79 | 0.82 |
| 1:A:320:SEP:C | 1:A:348:CYS:SG | 2.68 | 0.82 |
| 2:B:451:ARG:HH11 | 2:B:451:ARG:HG2 | 1.43 | 0.82 |
| 1:A:21:MET:HB2 | 1:A:38:ILE:HD11 | 1.62 | 0.82 |
| 2:B:300:ARG:HA | 2:B:333:MET:HE3 | 1.59 | 0.82 |
| 2:C:31:ILE:HD11 | 2:C:246:ILE:HG21 | 1.62 | 0.82 |
| 2:B:300:ARG:N | 2:B:333:MET:HE1 | 1.95 | 0.81 |
| 2:E:313:ILE:HB | 2:E:375:ILE:CD1 | 2.10 | 0.81 |
| 1:F:283:ILE:HG23 | 1:F:412:PHE:CE1 | 2.15 | 0.81 |
| 2:B:285:LEU:HB3 | 2:B:437:ILE:HD13 | 1.62 | 0.81 |
| 2:B:296:LEU:HD21 | 2:B:477:PRO:HD3 | 1.62 | 0.81 |
| 1:F:455:VAL:HG11 | 1:F:463:HIS:HB2 | 1.62 | 0.81 |
| 1:A:254:LEU:HD22 | 1:F:348:CYS:HB3 | 1.62 | 0.81 |
| 2:C:140:ARG:HB3 | 2:C:140:ARG:HH11 | 1.45 | 0.81 |
| 1:A:254:LEU:HD21 | 1:F:320:SEP:CA | 2.04 | 0.81 |
| 2:D:147:VAL:HG11 | 2:D:180:MET:HE3 | 1.62 | 0.81 |
| 2:E:263:VAL:HG12 | 2:E:374:ARG:NH2 | 1.95 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:169:ALA:O | 2:B:173:GLN:HG3 | 1.81 | 0.81 |
| 2:B:334:ASP:OD1 | 2:B:336:GLU:HB2 | 1.80 | 0.81 |
| 1:A:462:TRP:O | 1:A:463:HIS:CB | 2.30 | 0.80 |
| 2:B:46:GLY:HA3 | 2:B:50:THR:HG21 | 1.64 | 0.80 |
| 2:E:263:VAL:CG1 | 2:E:374:ARG:HH21 | 1.94 | 0.80 |
| 2:E:446:ARG:NH2 | 2:E:496:ARG:NH2 | 2.29 | 0.80 |
| 2:B:311:ARG:HD2 | 2:B:371:LYS:HE3 | 1.63 | 0.80 |
| 1:A:462:TRP:CE3 | 1:A:463:HIS:N | 2.49 | 0.80 |
| 2:B:479:ILE:HD12 | 2:B:479:ILE:H | 1.44 | 0.80 |
| 1:A:273:MET:O | 1:A:274:CYS:HB2 | 1.79 | 0.80 |
| 2:C:28:PHE:CE1 | 2:C:222:ILE:HD11 | 2.17 | 0.79 |
| 2:D:315:PHE:HB2 | 2:D:377:ILE:HD13 | 1.64 | 0.79 |
| 1:F:313:ILE:O | 1:F:375:ILE:HD13 | 1.82 | 0.79 |
| 2:B:299:SER:C | 2:B:333:MET:HE1 | 2.02 | 0.79 |
| 2:E:426:THR:HG21 | 2:E:430:ILE:HG12 | 1.65 | 0.79 |
| 1:A:318:GLU:CD | 2:B:432:GLU:HG2 | 2.02 | 0.79 |
| 2:B:379:SER:HA | 2:B:413:THR:HG22 | 1.65 | 0.79 |
| 1:F:471:MET:HG3 | 1:F:478:ASP:HB3 | 1.61 | 0.79 |
| 1:A:320:SEP:HA | 2:B:254:LEU:CG | 2.12 | 0.79 |
| 2:C:123:LEU:HD13 | 2:C:166:ARG:HD2 | 1.65 | 0.79 |
| 2:D:44:VAL:HG22 | 2:D:205:VAL:HB | 1.64 | 0.79 |
| 2:E:379:SER:H | 2:E:413:THR:HB | 1.47 | 0.79 |
| 2:D:140:ARG:NH1 | 2:D:140:ARG:HB3 | 1.98 | 0.78 |
| 1:F:453:ILE:HG21 | 1:F:479:ILE:HD12 | 1.64 | 0.78 |
| 2:D:445:ILE:HD13 | 2:D:450:SER:HG | 1.48 | 0.78 |
| 1:A:164:LEU:HD11 | 1:A:197:GLU:HG3 | 1.63 | 0.78 |
| 2:E:371:LYS:HD2 | 2:E:371:LYS:O | 1.83 | 0.78 |
| 2:E:18:ILE:HD11 | 2:E:228:THR:OG1 | 1.83 | 0.78 |
| 2:E:382:ALA:O | 2:E:385:ARG:HG3 | 1.83 | 0.78 |
| 1:F:508:ILE:C | 1:F:509:VAL:HG23 | 2.00 | 0.78 |
| 1:A:205:VAL:HG22 | 1:A:222:ILE:HD13 | 1.63 | 0.78 |
| 2:B:191:ILE:HB | 2:B:198:GLU:CG | 2.14 | 0.78 |
| 2:D:267:VAL:HG23 | 2:D:300:ARG:HG2 | 1.65 | 0.78 |
| 2:E:38:ILE:HA | 2:E:177:THR:HG23 | 1.66 | 0.78 |
| 1:A:147:VAL:O | 1:A:150:VAL:HG12 | 1.83 | 0.77 |
| 1:A:471:MET:SD | 1:A:478:ASP:HB3 | 2.24 | 0.77 |
| 1:F:122:ASP:HA | 1:F:125:ALA:HB3 | 1.66 | 0.77 |
| 1:A:227:GLY:O | 1:F:89:SER:HB2 | 1.84 | 0.77 |
| 2:B:182:THR:HG21 | 2:B:192:ALA:HB1 | 1.66 | 0.77 |
| 2:C:262:ARG:HH22 | 2:C:461:SER:HB2 | 1.49 | 0.77 |
| 2:D:70:PRO:HB2 | 2:D:139:ALA:HA | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:313:ILE:HB | 2:D:375:ILE:CD1 | 2.14 | 0.77 |
| 2:D:496:ARG:HG2 | 2:E:487:GLU:OE1 | 1.85 | 0.77 |
| 1:F:203:ASN:HB3 | 1:F:225:LEU:HD23 | 1.66 | 0.77 |
| 2:B:140:ARG:HH11 | 2:B:140:ARG:HB3 | 1.49 | 0.77 |
| 1:A:256:GLN:HG3 | 1:F:320:SEP:O1P | 1.85 | 0.77 |
| 1:A:370:PHE:HD2 | 1:A:372:PRO:HG3 | 1.49 | 0.76 |
| 2:E:14:GLU:HG3 | 2:E:16:GLN:H | 1.49 | 0.76 |
| 2:D:451:ARG:HH11 | 2:D:451:ARG:HG2 | 1.50 | 0.76 |
| 1:F:287:THR:CG2 | 1:F:414:ASN:HD22 | 1.98 | 0.76 |
| 1:F:486:PHE:CE2 | 1:F:496:ARG:HD2 | 2.19 | 0.76 |
| 1:A:263:VAL:HG12 | 1:A:374:ARG:HH21 | 1.49 | 0.76 |
| 2:E:356:LEU:CD2 | 2:E:387:VAL:HG11 | 2.16 | 0.76 |
| 1:A:375:ILE:HD13 | 1:A:408:ILE:HG21 | 1.68 | 0.76 |
| 1:A:140:ARG:HB3 | 1:A:140:ARG:NH1 | 2.00 | 0.76 |
| 2:C:170:ARG:O | 2:C:174:ILE:HG12 | 1.86 | 0.76 |
| 1:F:508:ILE:O | 1:F:509:VAL:CG2 | 2.33 | 0.76 |
| 2:C:205:VAL:CG2 | 2:C:222:ILE:HD13 | 2.16 | 0.75 |
| 2:D:182:THR:HG22 | 2:D:183:GLU:N | 2.01 | 0.75 |
| 2:D:18:ILE:CD1 | 2:D:227:GLY:HA3 | 2.16 | 0.75 |
| 1:A:14:GLU:HG3 | 1:A:15:HIS:N | 1.99 | 0.75 |
| 2:B:492:GLY:O | 2:B:494:PRO:HD3 | 1.86 | 0.75 |
| 2:D:444:GLU:OE2 | 2:E:489:ILE:HD13 | 1.87 | 0.75 |
| 1:A:318:GLU:OE2 | 2:B:432:GLU:HG2 | 1.86 | 0.75 |
| 2:D:311:ARG:HD2 | 2:D:371:LYS:CE | 2.17 | 0.75 |
| 1:A:325:LEU:HD23 | 1:A:335:PHE:HB2 | 1.69 | 0.75 |
| 2:C:299:SER:C | 2:C:333:MET:HE1 | 2.06 | 0.75 |
| 2:D:148:THR:OG1 | 2:D:182:THR:HG23 | 1.86 | 0.75 |
| 2:E:79:THR:HG22 | 2:E:82:ASP:H | 1.51 | 0.75 |
| 2:B:325:LEU:HD23 | 2:B:335:PHE:HB3 | 1.68 | 0.75 |
| 2:B:25:ILE:HG12 | 2:B:58:GLN:HE21 | 1.50 | 0.75 |
| 2:D:212:GLU:O | 2:D:212:GLU:HG2 | 1.86 | 0.75 |
| 2:E:453:ILE:HG21 | 2:E:479:ILE:HD12 | 1.68 | 0.75 |
| 2:B:356:LEU:HD13 | 2:B:387:VAL:HG21 | 1.69 | 0.74 |
| 3:B:901:ATP:H3' | 2:C:458:MET:O | 1.87 | 0.74 |
| 2:E:273:MET:O | 2:E:463:HIS:HA | 1.87 | 0.74 |
| 2:D:18:ILE:HD12 | 2:D:227:GLY:HA3 | 1.68 | 0.74 |
| 1:A:25:ILE:CD1 | 1:A:58:GLN:HG2 | 2.17 | 0.74 |
| 2:D:443:VAL:O | 2:D:445:ILE:HD12 | 1.88 | 0.74 |
| 2:E:148:THR:OG1 | 2:E:182:THR:HG23 | 1.86 | 0.74 |
| 2:E:93:ASP:OD2 | 2:E:96:LYS:HB2 | 1.87 | 0.74 |
| 2:E:123:LEU:HD23 | 2:E:127:ILE:HD11 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:MET:HB2 | 1:A:38:ILE:CD1 | 2.17 | 0.74 |
| 1:F:500:ASP:O | 1:F:501:GLU:HB3 | 1.87 | 0.74 |
| 1:A:321:ARG:O | 1:A:324:LEU:CB | 2.32 | 0.74 |
| 2:C:335:PHE:HA | 2:C:338:MET:HG3 | 1.68 | 0.74 |
| 1:A:254:LEU:HD21 | 1:F:319:GLU:O | 1.87 | 0.74 |
| 1:A:508:ILE:H | 1:A:508:ILE:HD13 | 1.51 | 0.74 |
| 1:F:170:ARG:O | 1:F:174:ILE:HG12 | 1.88 | 0.74 |
| 2:B:148:THR:CG2 | 2:B:193:ARG:HD2 | 2.18 | 0.73 |
| 1:A:96:LYS:O | 1:A:100:GLU:HG3 | 1.88 | 0.73 |
| 2:C:344:LEU:HD22 | 2:C:345:LYS:N | 2.03 | 0.73 |
| 2:C:495:THR:HA | 2:D:487:GLU:OE2 | 1.88 | 0.73 |
| 2:E:377:ILE:HD11 | 2:E:399:VAL:HG11 | 1.69 | 0.73 |
| 2:B:295:THR:HG21 | 2:B:319:GLU:OE2 | 1.87 | 0.73 |
| 2:B:21:MET:HB2 | 2:B:38:ILE:HG12 | 1.70 | 0.73 |
| 1:A:290:THR:HG21 | 2:B:425:ILE:HD12 | 1.69 | 0.73 |
| 2:B:61:TYR:CE1 | 2:B:92:TRP:HB2 | 2.24 | 0.73 |
| 2:D:431:GLU:O | 2:D:434:THR:HG22 | 1.87 | 0.73 |
| 1:A:254:LEU:O | 1:A:254:LEU:HD23 | 1.89 | 0.73 |
| 2:D:344:LEU:HD22 | 2:D:345:LYS:H | 1.53 | 0.73 |
| 2:B:127:ILE:HG21 | 2:B:170:ARG:HG3 | 1.69 | 0.73 |
| 2:E:304:ASN:HB3 | 2:E:374:ARG:HH12 | 1.53 | 0.73 |
| 1:A:371:LYS:O | 1:A:371:LYS:HD2 | 1.87 | 0.73 |
| 1:A:266:GLY:HA3 | 1:A:300:ARG:O | 1.88 | 0.73 |
| 2:C:262:ARG:NH2 | 2:C:461:SER:HB2 | 2.04 | 0.73 |
| 2:C:36:LEU:HD12 | 2:C:59:PHE:CE1 | 2.23 | 0.73 |
| 2:E:319:GLU:O | 1:F:254:LEU:HD21 | 1.89 | 0.73 |
| 1:F:283:ILE:HG23 | 1:F:412:PHE:HE1 | 1.53 | 0.73 |
| 2:B:25:ILE:HG12 | 2:B:58:GLN:NE2 | 2.04 | 0.73 |
| 2:D:478:ASP:HB2 | 5:D:555:HOH:O | 1.89 | 0.73 |
| 1:F:489:ILE:HA | 1:F:494:PRO:HG3 | 1.70 | 0.73 |
| 1:A:89:SER:HB2 | 2:B:227:GLY:O | 1.89 | 0.73 |
| 1:A:320:SEP:O | 1:A:348:CYS:SG | 2.47 | 0.72 |
| 2:C:28:PHE:CZ | 2:C:222:ILE:HD11 | 2.24 | 0.72 |
| 2:C:182:THR:HG22 | 2:C:183:GLU:N | 2.04 | 0.72 |
| 2:B:493:SER:HB3 | 2:C:488:ARG:HG2 | 1.71 | 0.72 |
| 1:F:347:VAL:O | 1:F:348:CYS:HB2 | 1.88 | 0.72 |
| 2:E:191:ILE:HD12 | 2:E:206:ILE:CD1 | 2.19 | 0.72 |
| 1:F:514:GLU:O | 1:F:515:LYS:HB3 | 1.89 | 0.72 |
| 1:A:147:VAL:HG11 | 1:A:180:MET:HE3 | 1.71 | 0.72 |
| 1:F:305:ALA:CB | 1:F:374:ARG:HD2 | 2.11 | 0.72 |
| 1:A:462:TRP:CD2 | 1:A:463:HIS:N | 2.52 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:140:ARG:HH11 | 2:D:140:ARG:HB3 | 1.55 | 0.72 |
| 2:E:191:ILE:HB | 2:E:198:GLU:CG | 2.20 | 0.72 |
| 2:B:285:LEU:HB3 | 2:B:437:ILE:CD1 | 2.18 | 0.72 |
| 2:B:287:THR:HG23 | 2:B:414:ASN:HD22 | 1.55 | 0.72 |
| 2:E:159:VAL:O | 2:E:163:GLU:HG2 | 1.90 | 0.72 |
| 2:D:332:GLY:C | 2:D:333:MET:HG2 | 2.09 | 0.72 |
| 1:F:379:SER:H | 1:F:413:THR:HB | 1.55 | 0.72 |
| 1:A:248:PRO:HB2 | 1:A:251:ALA:HB3 | 1.72 | 0.71 |
| 2:D:446:ARG:N | 2:D:496:ARG:HH12 | 1.87 | 0.71 |
| 1:F:111:ASP:OD1 | 1:F:112:PRO:HD2 | 1.90 | 0.71 |
| 2:C:269:ARG:HG2 | 2:C:479:ILE:HB | 1.72 | 0.71 |
| 1:F:31:ILE:HG21 | 1:F:222:ILE:HD13 | 1.73 | 0.71 |
| 1:F:248:PRO:HB2 | 1:F:251:ALA:HB3 | 1.71 | 0.71 |
| 2:B:191:ILE:HB | 2:B:198:GLU:HG3 | 1.71 | 0.71 |
| 2:B:54:LEU:HD23 | 2:B:244:ILE:CD1 | 2.20 | 0.71 |
| 2:E:248:PRO:HB2 | 2:E:251:ALA:HB3 | 1.70 | 0.71 |
| 2:C:123:LEU:HD21 | 2:C:167:LEU:HB2 | 1.73 | 0.71 |
| 2:D:191:ILE:HB | 2:D:198:GLU:CG | 2.20 | 0.71 |
| 2:B:178:THR:HG22 | 2:B:179:VAL:H | 1.55 | 0.71 |
| 2:C:191:ILE:HB | 2:C:198:GLU:CG | 2.21 | 0.71 |
| 2:E:436:THR:HG23 | 2:E:458:MET:HG2 | 1.73 | 0.71 |
| 2:B:284:ILE:HG23 | 2:B:436:THR:HB | 1.71 | 0.71 |
| 2:C:50:THR:HG21 | 2:C:207:LEU:O | 1.91 | 0.71 |
| 2:E:313:ILE:HG13 | 2:E:372:PRO:CG | 2.20 | 0.71 |
| 2:E:426:THR:HG22 | 2:E:428:SER:H | 1.55 | 0.71 |
| 1:A:116:GLU:C | 1:A:117:VAL:HG23 | 2.09 | 0.71 |
| 2:B:453:ILE:HD13 | 2:B:454:ASN:N | 2.06 | 0.71 |
| 2:D:344:LEU:HD22 | 2:D:345:LYS:N | 2.06 | 0.71 |
| 2:D:439:LEU:HD12 | 2:D:440:LEU:N | 2.06 | 0.71 |
| 2:D:446:ARG:H | 2:D:496:ARG:HH12 | 1.39 | 0.71 |
| 2:E:462:TRP:CE2 | 2:E:463:HIS:O | 2.44 | 0.71 |
| 1:F:379:SER:OG | 1:F:382:ALA:HB2 | 1.91 | 0.71 |
| 1:A:263:VAL:CG1 | 1:A:374:ARG:HH21 | 2.03 | 0.71 |
| 2:C:140:ARG:HH11 | 2:C:140:ARG:CB | 2.04 | 0.70 |
| 2:C:377:ILE:HD12 | 2:C:412:PHE:CE2 | 2.26 | 0.70 |
| 1:F:96:LYS:O | 1:F:100:GLU:HG3 | 1.91 | 0.70 |
| 2:B:425:ILE:HD11 | 2:B:456:PHE:CE2 | 2.26 | 0.70 |
| 1:F:515:LYS:HG3 | 1:F:516:GLY:H | 1.56 | 0.70 |
| 2:C:393:ARG:O | 2:C:397:ILE:HD13 | 1.90 | 0.70 |
| 2:C:25:ILE:HG23 | 2:C:58:GLN:HE22 | 1.54 | 0.70 |
| 1:F:31:ILE:CG2 | 1:F:222:ILE:HD13 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:359:HIS:O | 2:D:363:ILE:HG12 | 1.91 | 0.70 |
| 2:E:446:ARG:NH2 | 2:E:496:ARG:HH22 | 1.88 | 0.70 |
| 2:E:317:TYR:OH | 2:E:363:ILE:HD11 | 1.90 | 0.70 |
| 1:A:318:GLU:OE1 | 2:B:432:GLU:HB3 | 1.91 | 0.70 |
| 2:E:453:ILE:HB | 2:E:470:PHE:CD2 | 2.27 | 0.70 |
| 1:A:321:ARG:HA | 1:A:324:LEU:HD12 | 1.71 | 0.70 |
| 2:E:266:GLY:HA2 | 2:E:304:ASN:HD22 | 1.55 | 0.70 |
| 1:A:458:MET:O | 3:F:901:ATP:H3' | 1.91 | 0.70 |
| 1:F:147:VAL:O | 1:F:150:VAL:HG12 | 1.92 | 0.70 |
| 2:C:283:ILE:HD11 | 2:C:404:LYS:HG3 | 1.74 | 0.70 |
| 2:C:379:SER:H | 2:C:413:THR:HB | 1.56 | 0.70 |
| 2:E:418:GLN:HB2 | 1:F:423:HIS:O | 1.91 | 0.70 |
| 2:B:434:THR:CG2 | 2:B:437:ILE:HD11 | 2.21 | 0.69 |
| 1:F:18:ILE:HD13 | 1:F:40:ARG:HH12 | 1.53 | 0.69 |
| 2:D:478:ASP:CB | 5:D:555:HOH:O | 2.40 | 0.69 |
| 2:E:300:ARG:HA | 2:E:333:MET:HE1 | 1.72 | 0.69 |
| 1:A:154:TYR:O | 1:A:155:ASP:CG | 2.30 | 0.69 |
| 2:E:43:LEU:HD11 | 2:E:182:THR:OG1 | 1.92 | 0.69 |
| 1:F:208:ARG:NH2 | 1:F:221:GLU:OE2 | 2.24 | 0.69 |
| 1:F:338:MET:HB3 | 1:F:344:LEU:HB3 | 1.74 | 0.69 |
| 1:F:317:TYR:OH | 1:F:363:ILE:HD11 | 1.92 | 0.69 |
| 2:C:221:GLU:HG3 | 2:C:233:GLY:O | 1.92 | 0.69 |
| 2:D:147:VAL:O | 2:D:150:VAL:HG12 | 1.92 | 0.69 |
| 2:D:161:ARG:HB2 | 2:D:196:VAL:HG11 | 1.74 | 0.69 |
| 2:D:284:ILE:HD12 | 2:D:410:GLY:O | 1.92 | 0.69 |
| 1:F:515:LYS:HG3 | 1:F:516:GLY:N | 2.08 | 0.69 |
| 2:B:218:ARG:CZ | 2:B:239:ILE:HD12 | 2.22 | 0.69 |
| 2:D:387:VAL:HG12 | 2:D:388:SER:N | 2.08 | 0.69 |
| 2:D:269:ARG:HG2 | 2:D:479:ILE:HB | 1.74 | 0.69 |
| 1:F:462:TRP:O | 1:F:463:HIS:CD2 | 2.46 | 0.69 |
| 1:A:484:ARG:NH1 | 1:A:484:ARG:HB3 | 2.07 | 0.69 |
| 2:B:84:ILE:HD12 | 2:B:94:LEU:HB2 | 1.74 | 0.69 |
| 2:E:126:LEU:O | 2:E:130:ILE:HG12 | 1.92 | 0.69 |
| 2:E:294:LYS:HG2 | 2:E:413:THR:HG23 | 1.75 | 0.69 |
| 1:A:451:ARG:HD2 | 1:A:451:ARG:N | 2.08 | 0.69 |
| 1:A:425:ILE:HD12 | 1:F:290:THR:HG21 | 1.73 | 0.69 |
| 2:C:94:LEU:O | 2:C:98:VAL:HG23 | 1.92 | 0.69 |
| 2:D:147:VAL:HG11 | 2:D:180:MET:CE | 2.23 | 0.69 |
| 2:D:220:LEU:HD13 | 2:D:246:ILE:HD11 | 1.73 | 0.69 |
| 1:F:264:SER:O | 1:F:374:ARG:NH2 | 2.25 | 0.69 |
| 1:A:287:THR:HG23 | 1:A:414:ASN:HD22 | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:320:SEP:HB2 | 2:B:254:LEU:C | 2.13 | 0.69 |
| 2:C:218:ARG:CZ | 2:C:239:ILE:HD12 | 2.23 | 0.69 |
| 2:C:287:THR:HG23 | 2:C:414:ASN:ND2 | 2.07 | 0.69 |
| 2:C:419:PHE:O | 2:C:420:MET:HB2 | 1.92 | 0.69 |
| 2:C:393:ARG:HH21 | 2:C:429:HIS:HB2 | 1.58 | 0.69 |
| 1:A:320:SEP:O1P | 2:B:256:GLN:HG3 | 1.92 | 0.68 |
| 1:A:396:VAL:O | 1:A:400:THR:HB | 1.94 | 0.68 |
| 2:B:51:GLY:O | 2:B:54:LEU:N | 2.26 | 0.68 |
| 1:A:254:LEU:HD23 | 1:F:320:SEP:HA | 1.74 | 0.68 |
| 1:A:318:GLU:OE1 | 2:B:432:GLU:CG | 2.42 | 0.68 |
| 2:B:225:LEU:HD12 | 2:B:230:HIS:HB3 | 1.74 | 0.68 |
| 2:C:159:VAL:O | 2:C:163:GLU:HG2 | 1.93 | 0.68 |
| 2:C:453:ILE:HD13 | 2:C:454:ASN:N | 2.07 | 0.68 |
| 2:E:320:SER:HA | 1:F:254:LEU:HG | 1.75 | 0.68 |
| 1:A:264:SER:HA | 1:A:271:ASP:OD1 | 1.94 | 0.68 |
| 2:B:315:PHE:CE2 | 2:B:347:VAL:HG21 | 2.29 | 0.68 |
| 2:E:74:VAL:HG21 | 2:E:130:ILE:HD12 | 1.76 | 0.68 |
| 2:B:325:LEU:CD2 | 2:B:335:PHE:HB3 | 2.23 | 0.68 |
| 2:C:45:SER:CB | 2:C:182:THR:HB | 2.23 | 0.68 |
| 2:E:377:ILE:HD12 | 2:E:412:PHE:CE2 | 2.28 | 0.68 |
| 1:A:191:ILE:HB | 1:A:198:GLU:CG | 2.24 | 0.68 |
| 1:A:372:PRO:O | 1:A:408:ILE:HD12 | 1.94 | 0.68 |
| 1:A:88:ARG:HH11 | 1:A:88:ARG:HG2 | 1.58 | 0.68 |
| 2:C:111:ASP:OD1 | 2:C:113:GLU:HG2 | 1.92 | 0.68 |
| 2:D:122:ASP:O | 2:D:123:LEU:HB2 | 1.92 | 0.68 |
| 2:D:301:PHE:CZ | 2:D:374:ARG:HD3 | 2.28 | 0.68 |
| 1:F:508:ILE:O | 1:F:509:VAL:CB | 2.42 | 0.68 |
| 2:C:447:GLY:HA2 | 2:D:489:ILE:HD12 | 1.76 | 0.68 |
| 2:E:287:THR:HG23 | 2:E:414:ASN:ND2 | 2.08 | 0.68 |
| 2:D:347:VAL:O | 2:D:348:CYS:HB2 | 1.94 | 0.68 |
| 2:E:123:LEU:O | 2:E:127:ILE:HG12 | 1.93 | 0.68 |
| 1:A:84:ILE:HG23 | 1:A:94:LEU:HB2 | 1.76 | 0.68 |
| 2:B:502:LYS:HG3 | 2:B:504:GLU:O | 1.94 | 0.68 |
| 1:A:266:GLY:HA3 | 1:A:300:ARG:HG3 | 1.74 | 0.68 |
| 2:D:478:ASP:CA | 5:D:555:HOH:O | 2.41 | 0.68 |
| 2:B:140:ARG:CB | 2:B:140:ARG:HH11 | 2.07 | 0.67 |
| 2:C:470:PHE:HB2 | 2:C:478:ASP:O | 1.94 | 0.67 |
| 2:D:475:LYS:HA | 5:D:553:HOH:O | 1.93 | 0.67 |
| 2:E:140:ARG:NH1 | 2:E:140:ARG:HB3 | 2.09 | 0.67 |
| 2:E:344:LEU:HD11 | 2:E:346:ILE:HG13 | 1.76 | 0.67 |
| 1:F:471:MET:CG | 1:F:478:ASP:HB3 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:486:PHE:CB | 1:F:489:ILE:HD11 | 2.24 | 0.67 |
| 2:C:431:GLU:HG2 | 2:C:431:GLU:O | 1.94 | 0.67 |
| 2:E:363:ILE:O | 2:E:367:ILE:HG12 | 1.93 | 0.67 |
| 1:A:211:LEU:HB2 | 1:A:216:ARG:NE | 2.09 | 0.67 |
| 2:E:171:LEU:HA | 2:E:174:ILE:HD12 | 1.76 | 0.67 |
| 1:A:208:ARG:NH2 | 1:A:221:GLU:OE2 | 2.28 | 0.67 |
| 1:A:79:THR:HG21 | 1:A:81:GLN:HG2 | 1.74 | 0.67 |
| 2:B:56:SER:O | 2:B:59:PHE:HB3 | 1.94 | 0.67 |
| 2:C:451:ARG:HH11 | 2:C:451:ARG:HG2 | 1.59 | 0.67 |
| 2:D:222:ILE:HD12 | 2:D:222:ILE:N | 2.09 | 0.67 |
| 2:E:377:ILE:HD12 | 2:E:412:PHE:HE2 | 1.57 | 0.67 |
| 2:E:445:ILE:O | 2:E:446:ARG:HB2 | 1.93 | 0.67 |
| 1:A:311:ARG:HA | 1:A:343:LEU:O | 1.95 | 0.67 |
| 1:A:323:GLN:HG3 | 1:A:324:LEU:N | 2.10 | 0.67 |
| 2:D:400:THR:HG22 | 2:D:401:GLY:N | 2.08 | 0.67 |
| 2:D:287:THR:CG2 | 2:D:414:ASN:HD22 | 2.06 | 0.67 |
| 2:D:81:GLN:NE2 | 2:D:81:GLN:H | 1.93 | 0.67 |
| 1:F:191:ILE:HB | 1:F:198:GLU:CD | 2.14 | 0.67 |
| 1:A:484:ARG:HB3 | 1:A:484:ARG:HH11 | 1.58 | 0.66 |
| 2:B:497:ILE:HD12 | 2:B:499:VAL:N | 2.03 | 0.66 |
| 2:C:54:LEU:HD23 | 2:C:244:ILE:HG12 | 1.77 | 0.66 |
| 2:C:151:PHE:C | 2:C:153:GLN:H | 1.95 | 0.66 |
| 2:E:496:ARG:O | 2:E:497:ILE:HD13 | 1.95 | 0.66 |
| 1:F:426:THR:HG22 | 1:F:428:SER:H | 1.61 | 0.66 |
| 2:B:79:THR:CG2 | 2:B:81:GLN:HG2 | 2.25 | 0.66 |
| 2:B:287:THR:HG21 | 2:B:425:ILE:O | 1.95 | 0.66 |
| 2:D:313:ILE:HB | 2:D:375:ILE:HD13 | 1.76 | 0.66 |
| 2:E:289:ALA:HB2 | 2:E:419:PHE:HA | 1.77 | 0.66 |
| 2:B:325:LEU:CD2 | 2:B:335:PHE:CB | 2.72 | 0.66 |
| 2:B:52:LYS:N | 3:B:903:ATP:O1B | 2.28 | 0.66 |
| 2:C:436:THR:C | 2:C:437:ILE:HD12 | 2.16 | 0.66 |
| 1:A:73:PHE:HB3 | 1:A:105:ILE:HD13 | 1.77 | 0.66 |
| 1:A:359:HIS:O | 1:A:363:ILE:HG12 | 1.95 | 0.66 |
| 1:A:421:GLY:O | 1:A:422:ALA:C | 2.34 | 0.66 |
| 1:A:487:GLU:HG3 | 1:A:497:ILE:HD11 | 1.77 | 0.66 |
| 2:B:246:ILE:O | 2:B:248:PRO:HD3 | 1.95 | 0.66 |
| 2:B:425:ILE:HD11 | 2:B:456:PHE:CD2 | 2.31 | 0.66 |
| 2:C:28:PHE:HA | 2:C:246:ILE:HD12 | 1.78 | 0.66 |
| 2:C:31:ILE:CD1 | 2:C:246:ILE:HG21 | 2.24 | 0.66 |
| 2:E:487:GLU:O | 2:E:488:ARG:HB2 | 1.96 | 0.66 |
| 1:F:18:ILE:CD1 | 1:F:40:ARG:HH12 | 2.08 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:345:LYS:HE2 | 1:F:366:GLU:OE1 | 1.95 | 0.66 |
| 1:F:46:GLY:HA2 | 1:F:184:ARG:HD2 | 1.76 | 0.66 |
| 2:D:31:ILE:HG21 | 2:D:222:ILE:CD1 | 2.25 | 0.66 |
| 2:B:44:VAL:HG22 | 2:B:205:VAL:CG1 | 2.26 | 0.66 |
| 2:E:170:ARG:O | 2:E:174:ILE:HG13 | 1.94 | 0.66 |
| 1:F:49:GLY:HA2 | 3:F:903:ATP:O2B | 1.96 | 0.66 |
| 2:C:79:THR:CG2 | 2:C:82:ASP:H | 2.08 | 0.66 |
| 1:A:406:GLU:HB3 | 1:A:408:ILE:HG12 | 1.78 | 0.65 |
| 2:B:462:TRP:O | 2:B:463:HIS:CG | 2.49 | 0.65 |
| 2:C:439:LEU:HD12 | 2:C:440:LEU:N | 2.10 | 0.65 |
| 2:D:21:MET:HE1 | 2:D:177:THR:HB | 1.78 | 0.65 |
| 2:D:379:SER:H | 2:D:413:THR:HB | 1.61 | 0.65 |
| 2:E:121:PHE:CD1 | 2:E:121:PHE:N | 2.63 | 0.65 |
| 2:B:145:ASP:OD2 | 2:B:181:THR:HG21 | 1.96 | 0.65 |
| 2:C:121:PHE:H | 2:C:121:PHE:HD1 | 1.44 | 0.65 |
| 2:C:25:ILE:HG12 | 2:C:58:GLN:NE2 | 2.12 | 0.65 |
| 2:C:437:ILE:HD13 | 2:C:457:LYS:HG2 | 1.79 | 0.65 |
| 2:E:451:ARG:HD2 | 2:E:451:ARG:H | 1.62 | 0.65 |
| 2:B:43:LEU:HD11 | 2:B:182:THR:OG1 | 1.97 | 0.65 |
| 2:B:79:THR:HG23 | 2:B:81:GLN:HG2 | 1.78 | 0.65 |
| 1:F:505:LEU:O | 1:F:506:SER:HB3 | 1.96 | 0.65 |
| 2:B:20:LYS:HE3 | 2:B:228:THR:HG21 | 1.78 | 0.65 |
| 2:B:311:ARG:HD2 | 2:B:371:LYS:CE | 2.26 | 0.65 |
| 2:B:65:ILE:HG22 | 2:B:65:ILE:O | 1.94 | 0.65 |
| 2:C:182:THR:HG22 | 2:C:183:GLU:H | 1.59 | 0.65 |
| 2:D:18:ILE:HD13 | 2:D:40:ARG:NH1 | 2.12 | 0.65 |
| 2:E:147:VAL:O | 2:E:150:VAL:HG12 | 1.97 | 0.65 |
| 2:D:194:TYR:O | 2:D:196:VAL:HG23 | 1.97 | 0.65 |
| 2:E:191:ILE:HB | 2:E:198:GLU:HG2 | 1.78 | 0.65 |
| 1:F:151:PHE:C | 1:F:153:GLN:H | 2.00 | 0.65 |
| 2:C:335:PHE:O | 2:C:339:GLU:HG3 | 1.96 | 0.65 |
| 2:D:49:GLY:O | 2:D:218:ARG:NH2 | 2.30 | 0.65 |
| 2:E:334:ASP:OD1 | 2:E:336:GLU:HB2 | 1.97 | 0.65 |
| 1:F:378:ASP:OD1 | 1:F:413:THR:HG21 | 1.97 | 0.65 |
| 2:D:170:ARG:O | 2:D:174:ILE:HG13 | 1.97 | 0.65 |
| 1:F:20:LYS:HD3 | 1:F:35:GLY:O | 1.96 | 0.65 |
| 2:C:367:ILE:HG12 | 2:C:375:ILE:CD1 | 2.26 | 0.64 |
| 2:E:106:LEU:HD21 | 2:E:130:ILE:HD13 | 1.79 | 0.64 |
| 2:E:359:HIS:HA | 2:E:362:ILE:HD12 | 1.78 | 0.64 |
| 1:A:338:MET:HB3 | 1:A:344:LEU:HB3 | 1.79 | 0.64 |
| 1:A:436:THR:CG2 | 1:A:458:MET:HG2 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:41:SER:CB | 2:D:178:THR:HB | 2.26 | 0.64 |
| 2:E:449:MET:HE3 | 1:F:490:ILE:HD11 | 1.78 | 0.64 |
| 2:D:81:GLN:H | 2:D:81:GLN:CD | 1.98 | 0.64 |
| 2:E:311:ARG:HD2 | 2:E:371:LYS:CE | 2.26 | 0.64 |
| 3:E:901:ATP:H3' | 1:F:458:MET:O | 1.96 | 0.64 |
| 1:F:504:GLU:HA | 1:F:507:ARG:NE | 2.13 | 0.64 |
| 1:F:79:THR:HG23 | 1:F:81:GLN:H | 1.61 | 0.64 |
| 1:A:320:SEP:N | 2:B:254:LEU:HG | 2.12 | 0.64 |
| 2:C:284:ILE:HD12 | 2:C:410:GLY:O | 1.98 | 0.64 |
| 2:D:383:LEU:HD13 | 2:D:395:PHE:CE2 | 2.31 | 0.64 |
| 2:C:448:GLU:HG2 | 2:D:466:ALA:HA | 1.79 | 0.64 |
| 1:A:321:ARG:O | 1:A:324:LEU:N | 2.30 | 0.64 |
| 2:C:123:LEU:CD2 | 2:C:127:ILE:HD11 | 2.27 | 0.64 |
| 2:C:61:TYR:CE1 | 2:C:92:TRP:HB2 | 2.32 | 0.64 |
| 2:D:146:SER:N | 2:D:181:THR:HG22 | 2.11 | 0.64 |
| 1:A:379:SER:H | 1:A:413:THR:HB | 1.62 | 0.64 |
| 2:B:497:ILE:CD1 | 2:B:499:VAL:H | 2.06 | 0.64 |
| 2:D:383:LEU:HD13 | 2:D:395:PHE:HE2 | 1.63 | 0.64 |
| 2:E:23:THR:O | 2:E:24:MET:HB2 | 1.98 | 0.64 |
| 2:D:197:GLU:CD | 2:D:197:GLU:H | 1.99 | 0.64 |
| 2:B:283:ILE:CD1 | 2:B:404:LYS:HG3 | 2.28 | 0.64 |
| 2:C:123:LEU:HD11 | 2:C:163:GLU:O | 1.98 | 0.64 |
| 1:A:328:ALA:O | 1:A:333:MET:CG | 2.46 | 0.63 |
| 2:B:294:LYS:HB3 | 2:B:413:THR:OG1 | 1.98 | 0.63 |
| 2:B:62:ASN:O | 2:B:66:GLU:HB2 | 1.98 | 0.63 |
| 2:E:455:VAL:HG11 | 2:E:463:HIS:HB2 | 1.80 | 0.63 |
| 2:E:94:LEU:O | 2:E:98:VAL:HG23 | 1.98 | 0.63 |
| 1:F:104:PHE:CE2 | 1:F:106:LEU:HB2 | 2.33 | 0.63 |
| 1:F:140:ARG:HB3 | 1:F:140:ARG:HH11 | 1.61 | 0.63 |
| 2:C:344:LEU:HD11 | 2:C:346:ILE:HG13 | 1.79 | 0.63 |
| 2:D:328:ALA:HB2 | 5:D:552:HOH:O | 1.97 | 0.63 |
| 2:E:344:LEU:HD22 | 2:E:345:LYS:H | 1.63 | 0.63 |
| 2:D:208:ARG:NH2 | 2:D:221:GLU:OE2 | 2.31 | 0.63 |
| 2:D:446:ARG:H | 2:D:496:ARG:NH1 | 1.97 | 0.63 |
| 1:F:382:ALA:O | 1:F:385:ARG:HG3 | 1.97 | 0.63 |
| 1:A:147:VAL:HG11 | 1:A:180:MET:CE | 2.27 | 0.63 |
| 1:A:25:ILE:HD12 | 1:A:58:GLN:CG | 2.28 | 0.63 |
| 2:C:293:GLY:HA2 | 3:C:901:ATP:O1A | 1.98 | 0.63 |
| 2:E:38:ILE:HA | 2:E:177:THR:CG2 | 2.28 | 0.63 |
| 1:F:356:LEU:HD13 | 1:F:387:VAL:HG21 | 1.79 | 0.63 |
| 1:A:218:ARG:CZ | 1:A:239:ILE:HD12 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:447:GLY:HA2 | 2:D:489:ILE:CD1 | 2.29 | 0.63 |
| 1:F:372:PRO:O | 1:F:408:ILE:HD12 | 1.99 | 0.63 |
| 2:B:147:VAL:O | 2:B:150:VAL:HG12 | 1.98 | 0.63 |
| 2:B:239:ILE:HG12 | 2:B:244:ILE:HD13 | 1.81 | 0.63 |
| 2:B:273:MET:O | 2:B:463:HIS:HA | 1.98 | 0.63 |
| 2:D:353:SER:O | 2:D:354:ALA:HB2 | 1.98 | 0.63 |
| 2:E:202:ASP:HA | 2:E:226:ARG:HD2 | 1.80 | 0.63 |
| 2:E:84:ILE:HG21 | 2:E:95:ALA:HB2 | 1.81 | 0.63 |
| 1:F:182:THR:HG21 | 1:F:192:ALA:HB1 | 1.80 | 0.63 |
| 2:B:387:VAL:HG12 | 2:B:388:SER:N | 2.13 | 0.63 |
| 2:B:80:PRO:O | 2:B:84:ILE:HG12 | 1.99 | 0.63 |
| 2:B:360:LEU:HD22 | 2:B:360:LEU:O | 1.97 | 0.63 |
| 2:C:146:SER:H | 2:C:181:THR:HB | 1.64 | 0.63 |
| 2:C:313:ILE:HG12 | 2:C:345:LYS:HB3 | 1.81 | 0.63 |
| 2:D:123:LEU:CD1 | 2:D:166:ARG:HD2 | 2.24 | 0.63 |
| 1:F:311:ARG:HD2 | 1:F:371:LYS:CE | 2.29 | 0.63 |
| 1:A:45:SER:HB3 | 1:A:182:THR:HB | 1.80 | 0.62 |
| 2:B:203:ASN:HB3 | 2:B:225:LEU:HD23 | 1.81 | 0.62 |
| 2:C:43:LEU:HD11 | 2:C:182:THR:OG1 | 1.98 | 0.62 |
| 2:D:114:GLY:O | 2:D:115:GLN:HG3 | 1.98 | 0.62 |
| 1:F:191:ILE:HB | 1:F:198:GLU:HG3 | 1.80 | 0.62 |
| 1:A:254:LEU:HD22 | 1:F:348:CYS:CB | 2.29 | 0.62 |
| 2:C:81:GLN:NE2 | 2:C:81:GLN:H | 1.96 | 0.62 |
| 2:D:393:ARG:O | 2:D:397:ILE:HG13 | 1.99 | 0.62 |
| 2:E:313:ILE:HG13 | 2:E:372:PRO:HG3 | 1.81 | 0.62 |
| 1:A:24:MET:HB2 | 1:A:62:ASN:HD22 | 1.63 | 0.62 |
| 2:B:45:SER:CB | 2:B:182:THR:HB | 2.29 | 0.62 |
| 2:C:80:PRO:O | 2:C:84:ILE:HG12 | 1.99 | 0.62 |
| 2:E:461:SER:OG | 2:E:462:TRP:N | 2.32 | 0.62 |
| 1:A:433:ILE:HG22 | 1:A:433:ILE:O | 1.99 | 0.62 |
| 2:C:206:ILE:CD1 | 2:C:223:LEU:HB2 | 2.27 | 0.62 |
| 2:E:150:VAL:HG13 | 2:E:151:PHE:N | 2.13 | 0.62 |
| 2:E:431:GLU:O | 2:E:434:THR:HG22 | 2.00 | 0.62 |
| 1:F:486:PHE:HB3 | 1:F:489:ILE:HD11 | 1.79 | 0.62 |
| 1:A:335:PHE:O | 1:A:338:MET:N | 2.32 | 0.62 |
| 1:A:451:ARG:NH1 | 1:A:451:ARG:HG2 | 2.13 | 0.62 |
| 1:A:273:MET:HG2 | 1:A:464:ASP:OD2 | 1.99 | 0.62 |
| 2:C:441:GLN:HE22 | 2:C:490:ILE:HD13 | 1.64 | 0.62 |
| 2:D:231:MET:CE | 2:D:251:ALA:HB2 | 2.30 | 0.62 |
| 2:D:453:ILE:HG21 | 2:D:479:ILE:HD12 | 1.79 | 0.62 |
| 1:F:287:THR:HG21 | 1:F:425:ILE:O | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:MET:CB | 2:B:62:ASN:HD22 | 2.12 | 0.62 |
| 2:B:305:ALA:CB | 2:B:374:ARG:HD2 | 2.21 | 0.62 |
| 2:D:356:LEU:HD22 | 2:D:387:VAL:HG11 | 1.80 | 0.62 |
| 1:F:320:SEP:N | 1:F:320:SEP:O2P | 2.33 | 0.62 |
| 1:F:186:GLU:OE2 | 1:F:187:GLU:N | 2.32 | 0.62 |
| 1:A:379:SER:OG | 1:A:382:ALA:CB | 2.48 | 0.62 |
| 2:B:356:LEU:HD22 | 2:B:387:VAL:HG11 | 1.81 | 0.62 |
| 2:B:471:MET:HE2 | 2:B:478:ASP:HB3 | 1.81 | 0.62 |
| 2:D:148:THR:CG2 | 2:D:193:ARG:HD2 | 2.29 | 0.62 |
| 2:D:18:ILE:HD13 | 2:D:40:ARG:HH12 | 1.64 | 0.62 |
| 2:E:437:ILE:CD1 | 2:E:457:LYS:HE2 | 2.29 | 0.62 |
| 1:A:499:VAL:O | 1:A:499:VAL:HG12 | 1.99 | 0.62 |
| 2:E:287:THR:HG22 | 2:E:288:GLY:H | 1.63 | 0.62 |
| 1:A:258:SER:OG | 1:F:326:ARG:HD3 | 1.99 | 0.62 |
| 2:C:148:THR:CG2 | 2:C:193:ARG:HD2 | 2.29 | 0.62 |
| 2:D:344:LEU:HD13 | 2:D:344:LEU:C | 2.20 | 0.62 |
| 2:E:182:THR:HG21 | 2:E:192:ALA:HB1 | 1.82 | 0.62 |
| 2:E:439:LEU:HD12 | 2:E:440:LEU:N | 2.14 | 0.62 |
| 1:A:256:GLN:HG3 | 1:F:320:SEP:P | 2.40 | 0.62 |
| 2:C:232:LYS:N | 2:C:232:LYS:HD2 | 2.14 | 0.61 |
| 1:F:134:ILE:HD11 | 1:F:142:VAL:CG2 | 2.29 | 0.61 |
| 1:F:315:PHE:CE1 | 1:F:375:ILE:HD11 | 2.35 | 0.61 |
| 1:F:298:VAL:HG22 | 1:F:411:LEU:HD23 | 1.80 | 0.61 |
| 2:B:300:ARG:CA | 2:B:333:MET:HE1 | 2.30 | 0.61 |
| 2:C:371:LYS:CD | 2:C:371:LYS:O | 2.47 | 0.61 |
| 2:E:444:GLU:OE1 | 1:F:490:ILE:HG12 | 1.99 | 0.61 |
| 2:E:296:LEU:HD13 | 2:E:331:TRP:CD2 | 2.36 | 0.61 |
| 2:E:304:ASN:HB3 | 2:E:374:ARG:NH1 | 2.14 | 0.61 |
| 1:A:356:LEU:HD13 | 1:A:387:VAL:HG21 | 1.81 | 0.61 |
| 1:A:274:CYS:N | 1:A:463:HIS:O | 2.31 | 0.61 |
| 2:B:31:ILE:HA | 2:B:231:MET:SD | 2.41 | 0.61 |
| 2:E:485:ASN:ND2 | 2:E:496:ARG:HH11 | 1.99 | 0.61 |
| 1:F:344:LEU:HD22 | 1:F:345:LYS:N | 2.15 | 0.61 |
| 1:A:89:SER:CB | 2:B:227:GLY:O | 2.48 | 0.61 |
| 2:D:41:SER:HB3 | 2:D:178:THR:HB | 1.83 | 0.61 |
| 2:D:222:ILE:N | 2:D:222:ILE:CD1 | 2.63 | 0.61 |
| 2:D:445:ILE:HA | 2:D:496:ARG:HH12 | 1.65 | 0.61 |
| 2:E:356:LEU:HD13 | 2:E:387:VAL:HG21 | 1.81 | 0.61 |
| 2:E:451:ARG:HD2 | 2:E:451:ARG:N | 2.16 | 0.61 |
| 1:A:148:THR:HG21 | 1:A:183:GLU:HG3 | 1.81 | 0.61 |
| 1:A:327:ASN:ND2 | 1:A:331:TRP:CH2 | 2.69 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:LYS:HG2 | 1:A:402:TYR:CE2 | 2.35 | 0.61 |
| 2:D:426:THR:HG21 | 2:D:430:ILE:HG12 | 1.82 | 0.61 |
| 1:A:183:GLU:HB2 | 2:B:199:PHE:CE1 | 2.35 | 0.61 |
| 1:A:377:ILE:HD13 | 1:A:412:PHE:CE2 | 2.36 | 0.61 |
| 2:B:117:VAL:O | 2:B:117:VAL:HG12 | 2.01 | 0.61 |
| 2:C:20:LYS:HE3 | 2:C:228:THR:HG21 | 1.82 | 0.61 |
| 1:F:311:ARG:HD2 | 1:F:371:LYS:HE3 | 1.83 | 0.61 |
| 2:B:379:SER:CA | 2:B:413:THR:HG22 | 2.31 | 0.61 |
| 2:D:79:THR:CG2 | 2:D:82:ASP:H | 2.12 | 0.61 |
| 1:F:106:LEU:C | 1:F:106:LEU:HD12 | 2.21 | 0.61 |
| 1:F:200:VAL:O | 1:F:200:VAL:HG12 | 2.00 | 0.61 |
| 1:F:296:LEU:HD13 | 1:F:331:TRP:CD2 | 2.35 | 0.61 |
| 1:F:499:VAL:HG13 | 1:F:500:ASP:OD1 | 2.01 | 0.61 |
| 1:A:441:GLN:HE22 | 1:A:490:ILE:HD13 | 1.65 | 0.61 |
| 2:C:28:PHE:CA | 2:C:246:ILE:HD12 | 2.31 | 0.61 |
| 2:C:469:GLU:HG3 | 2:C:480:LYS:HE3 | 1.81 | 0.61 |
| 2:E:496:ARG:HG3 | 2:E:497:ILE:N | 2.14 | 0.61 |
| 2:B:335:PHE:O | 2:B:339:GLU:HG3 | 2.01 | 0.60 |
| 2:B:221:GLU:HG3 | 2:B:233:GLY:O | 2.01 | 0.60 |
| 2:B:284:ILE:HD12 | 2:B:410:GLY:O | 2.01 | 0.60 |
| 2:C:269:ARG:O | 2:C:273:MET:HG3 | 2.01 | 0.60 |
| 1:F:170:ARG:HB3 | 1:F:170:ARG:NH1 | 2.16 | 0.60 |
| 1:F:300:ARG:N | 1:F:333:MET:HE1 | 2.17 | 0.60 |
| 1:A:140:ARG:HH11 | 1:A:140:ARG:HB3 | 1.64 | 0.60 |
| 1:A:316:ALA:O | 1:A:348:CYS:HA | 2.01 | 0.60 |
| 2:B:80:PRO:HB3 | 2:B:105:ILE:HG21 | 1.82 | 0.60 |
| 2:D:433:ILE:HG22 | 2:D:433:ILE:O | 2.00 | 0.60 |
| 2:E:287:THR:CG2 | 2:E:414:ASN:HD22 | 2.10 | 0.60 |
| 1:F:451:ARG:HH11 | 1:F:451:ARG:HG2 | 1.66 | 0.60 |
| 1:A:462:TRP:O | 1:A:463:HIS:ND1 | 2.34 | 0.60 |
| 2:C:418:GLN:HB2 | 2:D:423:HIS:O | 2.01 | 0.60 |
| 1:A:161:ARG:NH2 | 1:F:149:SER:HB3 | 2.17 | 0.60 |
| 2:C:164:LEU:HB3 | 2:C:200:VAL:HG11 | 1.83 | 0.60 |
| 2:B:195:GLY:HA2 | 2:B:198:GLU:OE1 | 2.00 | 0.60 |
| 2:C:24:MET:HB2 | 2:C:62:ASN:HD22 | 1.66 | 0.60 |
| 2:E:344:LEU:C | 2:E:344:LEU:HD13 | 2.22 | 0.60 |
| 2:D:151:PHE:C | 2:D:153:GLN:H | 2.05 | 0.60 |
| 2:E:441:GLN:HE22 | 2:E:490:ILE:HD13 | 1.66 | 0.60 |
| 2:B:344:LEU:HD11 | 2:B:346:ILE:HD11 | 1.83 | 0.60 |
| 2:B:283:ILE:HD11 | 2:B:404:LYS:HG3 | 1.84 | 0.60 |
| 2:C:24:MET:HB2 | 2:C:62:ASN:ND2 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:88:ARG:HD3 | 2:D:15:HIS:O | 2.01 | 0.60 |
| 1:A:471:MET:HB3 | 1:A:480:LYS:NZ | 2.15 | 0.60 |
| 2:B:237:PHE:CB | 2:B:246:ILE:HG12 | 2.32 | 0.60 |
| 1:A:31:ILE:CD1 | 1:A:246:ILE:HG21 | 2.26 | 0.59 |
| 2:C:287:THR:CG2 | 2:C:414:ASN:HD22 | 2.12 | 0.59 |
| 2:E:164:LEU:HB3 | 2:E:200:VAL:HG11 | 1.84 | 0.59 |
| 2:E:284:ILE:HD12 | 2:E:284:ILE:N | 2.17 | 0.59 |
| 2:E:499:VAL:HG12 | 2:E:499:VAL:O | 2.02 | 0.59 |
| 2:B:219:THR:HB | 2:B:234:GLU:HB3 | 1.84 | 0.59 |
| 2:B:382:ALA:O | 2:B:385:ARG:HB2 | 2.02 | 0.59 |
| 2:C:239:ILE:HG12 | 2:C:244:ILE:HD13 | 1.84 | 0.59 |
| 2:D:169:ALA:O | 2:D:173:GLN:HG3 | 2.02 | 0.59 |
| 2:D:267:VAL:CG2 | 2:D:300:ARG:HG2 | 2.30 | 0.59 |
| 2:D:47:THR:O | 2:D:50:THR:HG23 | 2.02 | 0.59 |
| 2:E:426:THR:HG22 | 2:E:428:SER:N | 2.17 | 0.59 |
| 1:A:98:VAL:HA | 1:A:103:LEU:O | 2.01 | 0.59 |
| 2:B:448:GLU:HG2 | 2:C:466:ALA:HA | 1.84 | 0.59 |
| 2:C:182:THR:HG21 | 2:C:192:ALA:CB | 2.31 | 0.59 |
| 2:D:130:ILE:O | 2:D:134:ILE:HG12 | 2.02 | 0.59 |
| 2:D:356:LEU:CD2 | 2:D:387:VAL:HG11 | 2.33 | 0.59 |
| 1:A:164:LEU:CD1 | 1:A:197:GLU:HG3 | 2.32 | 0.59 |
| 1:A:495:THR:HG22 | 1:A:497:ILE:HG23 | 1.84 | 0.59 |
| 2:C:454:ASN:HB2 | 2:C:467:ILE:HD13 | 1.84 | 0.59 |
| 1:A:392:PHE:HE2 | 1:A:430:ILE:HD11 | 1.67 | 0.59 |
| 2:B:377:ILE:HD13 | 2:B:412:PHE:CE2 | 2.37 | 0.59 |
| 2:C:395:PHE:O | 2:C:399:VAL:HG23 | 2.02 | 0.59 |
| 2:D:122:ASP:O | 2:D:123:LEU:CB | 2.51 | 0.59 |
| 2:E:294:LYS:HB2 | 3:E:901:ATP:O1B | 2.02 | 0.59 |
| 1:A:370:PHE:CD2 | 1:A:372:PRO:HG3 | 2.34 | 0.59 |
| 2:C:437:ILE:HD11 | 2:C:457:LYS:HE2 | 1.84 | 0.59 |
| 2:C:471:MET:HG3 | 2:C:478:ASP:HB3 | 1.85 | 0.59 |
| 1:F:461:SER:OG | 1:F:462:TRP:N | 2.34 | 0.59 |
| 1:A:161:ARG:HB2 | 1:A:196:VAL:HG11 | 1.83 | 0.59 |
| 2:D:317:TYR:OH | 2:D:363:ILE:HD11 | 2.02 | 0.59 |
| 1:A:203:ASN:HB3 | 1:A:225:LEU:CD2 | 2.28 | 0.59 |
| 1:A:318:GLU:OE1 | 2:B:432:GLU:CB | 2.50 | 0.59 |
| 2:D:220:LEU:HD13 | 2:D:246:ILE:CD1 | 2.32 | 0.59 |
| 2:D:287:THR:HG21 | 2:D:425:ILE:O | 2.03 | 0.59 |
| 2:D:478:ASP:HA | 5:D:555:HOH:O | 2.01 | 0.59 |
| 2:E:269:ARG:O | 2:E:273:MET:HG3 | 2.03 | 0.59 |
| 2:C:387:VAL:HG12 | 2:C:388:SER:N | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:417:ASP:HB3 | 2:C:429:HIS:CE1 | 2.38 | 0.58 |
| 2:C:262:ARG:HH22 | 2:C:461:SER:CB | 2.15 | 0.58 |
| 2:C:340:ARG:O | 2:C:342:ASN:N | 2.36 | 0.58 |
| 2:D:182:THR:HG21 | 2:D:192:ALA:HB1 | 1.84 | 0.58 |
| 1:A:325:LEU:HD23 | 1:A:335:PHE:CB | 2.32 | 0.58 |
| 1:A:311:ARG:HB3 | 1:A:370:PHE:CE2 | 2.39 | 0.58 |
| 2:C:21:MET:HE3 | 2:C:141:ARG:CZ | 2.31 | 0.58 |
| 1:F:313:ILE:HD12 | 1:F:367:ILE:HD13 | 1.85 | 0.58 |
| 1:A:257:ARG:HH22 | 1:A:407:GLU:HG2 | 1.66 | 0.58 |
| 1:A:402:TYR:O | 1:A:406:GLU:HB2 | 2.03 | 0.58 |
| 1:A:287:THR:CG2 | 1:A:414:ASN:HD22 | 2.16 | 0.58 |
| 2:D:161:ARG:HD2 | 2:D:196:VAL:HG13 | 1.85 | 0.58 |
| 2:D:31:ILE:HG21 | 2:D:222:ILE:HD13 | 1.86 | 0.58 |
| 2:D:363:ILE:O | 2:D:367:ILE:HG12 | 2.03 | 0.58 |
| 1:F:31:ILE:CD1 | 1:F:246:ILE:HG21 | 2.33 | 0.58 |
| 1:A:371:LYS:N | 1:A:372:PRO:HD3 | 2.17 | 0.58 |
| 2:C:70:PRO:HD2 | 2:C:140:ARG:HG2 | 1.85 | 0.58 |
| 2:C:79:THR:HG22 | 2:C:82:ASP:HB2 | 1.86 | 0.58 |
| 2:E:184:ARG:C | 2:E:185:ILE:HD13 | 2.24 | 0.58 |
| 1:A:265:SER:O | 1:A:301:PHE:HA | 2.04 | 0.58 |
| 1:A:284:ILE:HD12 | 1:A:284:ILE:H | 1.67 | 0.58 |
| 2:B:300:ARG:HA | 2:B:333:MET:HE1 | 1.84 | 0.58 |
| 2:B:451:ARG:NH1 | 2:B:451:ARG:HG2 | 2.12 | 0.58 |
| 2:C:311:ARG:HD2 | 2:C:371:LYS:HE3 | 1.86 | 0.58 |
| 2:C:313:ILE:HD11 | 2:C:370:PHE:HB3 | 1.84 | 0.58 |
| 2:D:79:THR:CG2 | 2:D:81:GLN:HG2 | 2.33 | 0.58 |
| 2:E:344:LEU:HD22 | 2:E:345:LYS:N | 2.18 | 0.58 |
| 1:F:375:ILE:O | 1:F:410:GLY:HA2 | 2.04 | 0.58 |
| 1:F:484:ARG:HH11 | 1:F:484:ARG:HB3 | 1.68 | 0.58 |
| 2:D:396:VAL:O | 2:D:400:THR:HB | 2.04 | 0.58 |
| 1:F:148:THR:HG21 | 1:F:193:ARG:HD2 | 1.84 | 0.58 |
| 2:C:451:ARG:NH1 | 2:C:451:ARG:HG2 | 2.18 | 0.58 |
| 2:D:182:THR:HG22 | 2:D:183:GLU:H | 1.67 | 0.58 |
| 1:A:127:ILE:HD11 | 1:A:167:LEU:CD1 | 2.33 | 0.58 |
| 1:A:305:ALA:CB | 1:A:374:ARG:HD2 | 2.25 | 0.58 |
| 2:B:151:PHE:C | 2:B:153:GLN:H | 2.07 | 0.58 |
| 2:D:418:GLN:HB2 | 2:E:423:HIS:O | 2.04 | 0.58 |
| 2:E:140:ARG:HB3 | 2:E:140:ARG:HH11 | 1.68 | 0.58 |
| 1:F:426:THR:HB | 1:F:431:GLU:OE2 | 2.03 | 0.58 |
| 2:B:51:GLY:N | 3:B:903:ATP:O1B | 2.36 | 0.58 |
| 2:E:377:ILE:CD1 | 2:E:399:VAL:HG11 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:280:LYS:NZ | 1:F:407:GLU:HB3 | 2.19 | 0.58 |
| 1:F:352:GLU:CD | 1:F:352:GLU:H | 2.07 | 0.58 |
| 1:F:357:GLU:HG3 | 1:F:358:ASP:N | 2.18 | 0.58 |
| 1:A:64:ILE:HG22 | 1:A:65:ILE:HD13 | 1.86 | 0.58 |
| 2:B:496:ARG:HG2 | 2:B:498:THR:HG23 | 1.86 | 0.58 |
| 2:D:192:ALA:HB3 | 2:D:197:GLU:OE2 | 2.04 | 0.58 |
| 2:D:266:GLY:O | 2:D:300:ARG:HG3 | 2.04 | 0.58 |
| 1:F:287:THR:HG23 | 1:F:414:ASN:ND2 | 2.14 | 0.58 |
| 1:A:272:GLU:C | 1:A:273:MET:O | 2.36 | 0.57 |
| 2:B:305:ALA:HB2 | 2:B:374:ARG:CD | 2.21 | 0.57 |
| 2:E:123:LEU:CD2 | 2:E:127:ILE:HD11 | 2.33 | 0.57 |
| 2:E:50:THR:HG22 | 2:E:209:ASN:HB2 | 1.86 | 0.57 |
| 1:A:371:LYS:O | 1:A:371:LYS:CD | 2.52 | 0.57 |
| 1:A:379:SER:OG | 1:A:382:ALA:HB2 | 2.04 | 0.57 |
| 2:B:285:LEU:HD23 | 2:B:437:ILE:CD1 | 2.31 | 0.57 |
| 2:C:147:VAL:HG11 | 2:C:180:MET:HE3 | 1.85 | 0.57 |
| 2:D:218:ARG:CZ | 2:D:239:ILE:HD12 | 2.34 | 0.57 |
| 1:F:306:CYS:SG | 1:F:344:LEU:HB2 | 2.44 | 0.57 |
| 2:B:194:TYR:O | 2:B:196:VAL:HG23 | 2.05 | 0.57 |
| 2:C:353:SER:O | 2:C:354:ALA:HB2 | 2.04 | 0.57 |
| 2:C:79:THR:HG23 | 2:C:82:ASP:H | 1.69 | 0.57 |
| 2:D:191:ILE:HB | 2:D:198:GLU:HG3 | 1.85 | 0.57 |
| 2:E:140:ARG:HH11 | 2:E:140:ARG:CB | 2.17 | 0.57 |
| 2:E:283:ILE:HG23 | 2:E:412:PHE:CE1 | 2.39 | 0.57 |
| 1:A:150:VAL:HG13 | 1:A:151:PHE:N | 2.18 | 0.57 |
| 1:A:483:PHE:HB3 | 1:A:486:PHE:CD1 | 2.40 | 0.57 |
| 2:B:191:ILE:HB | 2:B:198:GLU:CD | 2.25 | 0.57 |
| 2:C:486:PHE:CB | 2:C:489:ILE:HD11 | 2.34 | 0.57 |
| 2:D:47:THR:HG22 | 2:D:184:ARG:O | 2.03 | 0.57 |
| 1:F:118:VAL:O | 1:F:118:VAL:HG13 | 2.03 | 0.57 |
| 1:A:254:LEU:HD22 | 1:F:348:CYS:SG | 2.45 | 0.57 |
| 1:A:363:ILE:O | 1:A:367:ILE:HG12 | 2.05 | 0.57 |
| 2:C:14:GLU:HG3 | 2:C:16:GLN:H | 1.69 | 0.57 |
| 2:C:334:ASP:OD1 | 2:C:336:GLU:HB2 | 2.05 | 0.57 |
| 2:D:31:ILE:HD11 | 2:D:246:ILE:HG21 | 1.85 | 0.57 |
| 2:D:79:THR:HG22 | 2:D:82:ASP:N | 2.15 | 0.57 |
| 2:D:183:GLU:HB2 | 2:E:199:PHE:CE1 | 2.39 | 0.57 |
| 1:F:74:VAL:HB | 1:F:144:ILE:HD13 | 1.86 | 0.57 |
| 2:D:296:LEU:HD12 | 2:D:296:LEU:O | 2.05 | 0.57 |
| 2:D:79:THR:HG23 | 2:D:81:GLN:HG2 | 1.86 | 0.57 |
| 1:F:76:PHE:O | 1:F:109:SER:HA | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:148:THR:OG1 | 1:F:182:THR:HG23 | 2.04 | 0.57 |
| 1:F:321:ARG:O | 1:F:325:LEU:HD12 | 2.05 | 0.57 |
| 1:A:311:ARG:HD2 | 1:A:371:LYS:CE | 2.35 | 0.57 |
| 1:A:469:GLU:HB2 | 1:A:483:PHE:CZ | 2.39 | 0.57 |
| 2:D:182:THR:CG2 | 2:D:183:GLU:N | 2.67 | 0.57 |
| 1:A:266:GLY:CA | 1:A:300:ARG:HG3 | 2.35 | 0.57 |
| 1:A:302:VAL:HG12 | 1:A:303:GLU:N | 2.20 | 0.57 |
| 1:A:311:ARG:HD2 | 1:A:371:LYS:HE3 | 1.86 | 0.57 |
| 2:B:81:GLN:CD | 2:B:81:GLN:H | 2.08 | 0.57 |
| 2:C:353:SER:O | 2:C:354:ALA:CB | 2.53 | 0.57 |
| 2:C:377:ILE:HD12 | 2:C:412:PHE:HE2 | 1.68 | 0.57 |
| 1:A:313:ILE:CD1 | 1:A:372:PRO:HG2 | 2.34 | 0.57 |
| 2:B:334:ASP:O | 2:B:338:MET:HG2 | 2.04 | 0.57 |
| 2:B:294:LYS:N | 3:B:901:ATP:O1B | 2.37 | 0.57 |
| 2:E:441:GLN:NE2 | 2:E:490:ILE:HD13 | 2.20 | 0.57 |
| 2:E:214:GLU:HB3 | 1:F:234:GLU:HB2 | 1.86 | 0.57 |
| 2:B:264:SER:HA | 2:B:271:ASP:OD1 | 2.05 | 0.57 |
| 2:C:397:ILE:H | 2:C:397:ILE:HD13 | 1.69 | 0.57 |
| 2:D:296:LEU:HA | 2:D:331:TRP:CZ3 | 2.40 | 0.57 |
| 2:E:379:SER:N | 2:E:413:THR:HB | 2.17 | 0.57 |
| 1:A:439:LEU:HD12 | 1:A:440:LEU:N | 2.20 | 0.56 |
| 2:B:150:VAL:O | 2:B:153:GLN:HG3 | 2.05 | 0.56 |
| 1:F:16:GLN:HE22 | 1:F:33:HIS:HB3 | 1.70 | 0.56 |
| 1:A:263:VAL:HG12 | 1:A:374:ARG:NH2 | 2.18 | 0.56 |
| 1:A:479:ILE:H | 1:A:479:ILE:HD12 | 1.69 | 0.56 |
| 2:E:287:THR:HG21 | 2:E:425:ILE:O | 2.06 | 0.56 |
| 1:A:487:GLU:HG3 | 1:A:497:ILE:CD1 | 2.34 | 0.56 |
| 2:C:33:HIS:CD2 | 2:C:230:HIS:HA | 2.41 | 0.56 |
| 2:C:325:LEU:HD23 | 2:C:335:PHE:HB2 | 1.87 | 0.56 |
| 2:D:31:ILE:CG2 | 2:D:222:ILE:CD1 | 2.84 | 0.56 |
| 2:E:163:GLU:HA | 2:E:163:GLU:OE2 | 2.05 | 0.56 |
| 2:E:302:VAL:CG1 | 2:E:344:LEU:HD23 | 2.35 | 0.56 |
| 2:E:441:GLN:HE22 | 2:E:490:ILE:HA | 1.70 | 0.56 |
| 1:F:371:LYS:CD | 1:F:371:LYS:O | 2.54 | 0.56 |
| 2:B:264:SER:HB3 | 2:B:304:ASN:HD21 | 1.70 | 0.56 |
| 2:C:431:GLU:HA | 2:C:434:THR:HG22 | 1.87 | 0.56 |
| 2:D:487:GLU:OE1 | 2:D:497:ILE:HD13 | 2.05 | 0.56 |
| 2:E:23:THR:OG1 | 2:E:29:ASP:OD1 | 2.24 | 0.56 |
| 1:F:273:MET:O | 1:F:463:HIS:HA | 2.05 | 0.56 |
| 1:A:271:ASP:C | 1:A:273:MET:O | 2.44 | 0.56 |
| 1:A:328:ALA:O | 1:A:333:MET:HG2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:SER:HA | 1:A:178:THR:O | 2.06 | 0.56 |
| 2:B:248:PRO:HB2 | 2:B:251:ALA:HB3 | 1.87 | 0.56 |
| 2:B:88:ARG:HG2 | 2:B:88:ARG:HH11 | 1.70 | 0.56 |
| 2:E:148:THR:CG2 | 2:E:193:ARG:HD2 | 2.35 | 0.56 |
| 1:F:352:GLU:N | 1:F:352:GLU:CD | 2.59 | 0.56 |
| 1:F:484:ARG:CB | 1:F:484:ARG:NH1 | 2.68 | 0.56 |
| 1:F:504:GLU:O | 1:F:505:LEU:HB2 | 2.03 | 0.56 |
| 1:A:463:HIS:O | 1:A:464:ASP:HB3 | 2.06 | 0.56 |
| 2:B:205:VAL:CG2 | 2:B:222:ILE:HD13 | 2.35 | 0.56 |
| 2:B:41:SER:OG | 2:B:168:VAL:HG13 | 2.05 | 0.56 |
| 2:B:444:GLU:OE2 | 2:C:489:ILE:HG12 | 2.05 | 0.56 |
| 2:C:444:GLU:OE2 | 2:D:489:ILE:HG13 | 2.06 | 0.56 |
| 1:A:14:GLU:CG | 1:A:15:HIS:N | 2.60 | 0.56 |
| 1:A:153:GLN:O | 1:A:154:TYR:HD2 | 1.87 | 0.56 |
| 2:B:418:GLN:HG3 | 2:B:418:GLN:O | 2.06 | 0.56 |
| 2:C:18:ILE:HB | 2:C:228:THR:HG23 | 1.88 | 0.56 |
| 2:E:497:ILE:HG22 | 2:E:498:THR:H | 1.70 | 0.56 |
| 2:B:185:ILE:H | 2:B:185:ILE:HD12 | 1.71 | 0.56 |
| 2:C:283:ILE:HD13 | 2:C:404:LYS:HE3 | 1.87 | 0.56 |
| 2:E:70:PRO:HB2 | 2:E:139:ALA:HA | 1.88 | 0.56 |
| 2:E:356:LEU:CD1 | 2:E:387:VAL:HG21 | 2.36 | 0.56 |
| 1:F:134:ILE:HD13 | 1:F:139:ALA:HB3 | 1.88 | 0.56 |
| 1:A:88:ARG:NH1 | 1:A:88:ARG:HG2 | 2.20 | 0.56 |
| 2:C:393:ARG:NH2 | 2:C:429:HIS:HB2 | 2.21 | 0.56 |
| 2:D:347:VAL:HG12 | 2:D:348:CYS:N | 2.20 | 0.56 |
| 2:E:462:TRP:CD2 | 2:E:463:HIS:O | 2.59 | 0.56 |
| 1:F:144:ILE:CG2 | 1:F:147:VAL:HG12 | 2.36 | 0.56 |
| 2:B:196:VAL:O | 2:B:200:VAL:HG23 | 2.06 | 0.55 |
| 2:C:54:LEU:CD2 | 2:C:244:ILE:HG12 | 2.36 | 0.55 |
| 2:D:76:PHE:CZ | 2:D:126:LEU:HD21 | 2.41 | 0.55 |
| 1:A:347:VAL:O | 1:A:348:CYS:HB2 | 2.06 | 0.55 |
| 2:B:462:TRP:O | 2:B:463:HIS:CD2 | 2.60 | 0.55 |
| 2:B:64:ILE:HG21 | 2:B:97:LEU:HD13 | 1.88 | 0.55 |
| 2:C:238:THR:HG22 | 2:C:239:ILE:N | 2.21 | 0.55 |
| 1:F:344:LEU:HD13 | 1:F:344:LEU:C | 2.27 | 0.55 |
| 1:A:121:PHE:O | 1:A:125:ALA:HB2 | 2.05 | 0.55 |
| 1:A:333:MET:O | 1:A:334:ASP:HB2 | 2.06 | 0.55 |
| 1:A:471:MET:CE | 1:A:478:ASP:HB3 | 2.36 | 0.55 |
| 2:C:21:MET:O | 2:C:35:GLY:HA3 | 2.07 | 0.55 |
| 2:D:340:ARG:O | 2:D:342:ASN:N | 2.38 | 0.55 |
| 2:E:191:ILE:HD12 | 2:E:206:ILE:HD11 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:291:GLY:HA3 | 1:F:442:TYR:OH | 2.07 | 0.55 |
| 1:A:323:GLN:CB | 2:B:258:SER:OG | 2.54 | 0.55 |
| 2:B:90:PHE:HB2 | 2:B:92:TRP:CE2 | 2.41 | 0.55 |
| 2:C:238:THR:HG22 | 2:C:239:ILE:H | 1.70 | 0.55 |
| 2:D:191:ILE:CD1 | 2:D:198:GLU:HG2 | 2.36 | 0.55 |
| 2:D:76:PHE:HZ | 2:D:126:LEU:HD21 | 1.70 | 0.55 |
| 2:D:89:SER:HB2 | 2:E:227:GLY:O | 2.07 | 0.55 |
| 2:E:396:VAL:HG11 | 2:E:430:ILE:HG21 | 1.89 | 0.55 |
| 1:F:191:ILE:CB | 1:F:198:GLU:CG | 2.84 | 0.55 |
| 2:B:150:VAL:HG13 | 2:B:151:PHE:N | 2.22 | 0.55 |
| 2:C:144:ILE:CG2 | 2:C:147:VAL:HG12 | 2.36 | 0.55 |
| 2:C:471:MET:CG | 2:C:478:ASP:HB3 | 2.37 | 0.55 |
| 2:C:67:PHE:HB2 | 2:C:69:GLU:HG3 | 1.88 | 0.55 |
| 2:E:150:VAL:CG1 | 2:E:151:PHE:N | 2.69 | 0.55 |
| 2:E:193:ARG:NH2 | 1:F:195:GLY:O | 2.32 | 0.55 |
| 1:A:18:ILE:CD1 | 1:F:85:LYS:HG3 | 2.36 | 0.55 |
| 1:A:317:TYR:OH | 1:A:363:ILE:HD11 | 2.07 | 0.55 |
| 2:C:225:LEU:HD12 | 2:C:230:HIS:HB3 | 1.89 | 0.55 |
| 2:E:348:CYS:HB3 | 1:F:254:LEU:HD23 | 1.89 | 0.55 |
| 1:F:443:VAL:CG1 | 1:F:445:ILE:HD11 | 2.37 | 0.55 |
| 2:C:336:GLU:OE1 | 2:C:336:GLU:HA | 2.07 | 0.55 |
| 1:F:316:ALA:O | 1:F:348:CYS:HA | 2.06 | 0.55 |
| 1:F:486:PHE:HE2 | 1:F:496:ARG:HD2 | 1.68 | 0.55 |
| 1:F:508:ILE:O | 1:F:509:VAL:HB | 2.06 | 0.55 |
| 1:A:505:LEU:O | 1:A:508:ILE:HD11 | 2.06 | 0.55 |
| 2:B:313:ILE:HG13 | 2:B:372:PRO:CG | 2.37 | 0.55 |
| 2:C:340:ARG:C | 2:C:342:ASN:H | 2.09 | 0.55 |
| 2:E:20:LYS:HE3 | 2:E:228:THR:HG21 | 1.88 | 0.55 |
| 2:E:313:ILE:HG13 | 2:E:372:PRO:HG2 | 1.89 | 0.55 |
| 1:F:371:LYS:HD2 | 1:F:371:LYS:O | 2.07 | 0.55 |
| 1:A:287:THR:HG23 | 1:A:414:ASN:HB3 | 1.89 | 0.55 |
| 1:A:400:THR:HG22 | 1:A:401:GLY:N | 2.22 | 0.55 |
| 2:E:294:LYS:N | 3:E:901:ATP:O1B | 2.39 | 0.55 |
| 1:F:336:GLU:HB3 | 1:F:340:ARG:NH2 | 2.21 | 0.55 |
| 1:F:501:GLU:HG3 | 1:F:502:LYS:N | 2.22 | 0.55 |
| 1:A:448:GLU:HG2 | 2:B:466:ALA:HB2 | 1.89 | 0.55 |
| 2:C:397:ILE:N | 2:C:397:ILE:CD1 | 2.69 | 0.55 |
| 2:E:145:ASP:OD2 | 2:E:181:THR:HG21 | 2.06 | 0.55 |
| 2:E:336:GLU:HA | 2:E:336:GLU:OE1 | 2.05 | 0.55 |
| 2:E:451:ARG:HH11 | 2:E:451:ARG:HG2 | 1.72 | 0.55 |
| 1:A:200:VAL:HG12 | 1:A:200:VAL:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:296:LEU:HD22 | 1:A:472:ILE:HD12 | 1.87 | 0.54 |
| 2:B:205:VAL:HG23 | 2:B:222:ILE:HD13 | 1.89 | 0.54 |
| 1:A:322:ALA:HB3 | 2:B:256:GLN:O | 2.06 | 0.54 |
| 2:B:265:SER:HB2 | 2:B:270:LEU:HD13 | 1.90 | 0.54 |
| 2:B:81:GLN:H | 2:B:81:GLN:NE2 | 2.04 | 0.54 |
| 2:D:215:ARG:HA | 2:D:215:ARG:NE | 2.22 | 0.54 |
| 2:D:387:VAL:CG1 | 2:D:388:SER:N | 2.70 | 0.54 |
| 2:D:443:VAL:HG12 | 2:D:445:ILE:HD11 | 1.89 | 0.54 |
| 2:E:86:ASN:OD1 | 1:F:18:ILE:HD11 | 2.06 | 0.54 |
| 1:F:280:LYS:HZ3 | 1:F:407:GLU:HB3 | 1.73 | 0.54 |
| 1:F:486:PHE:HB2 | 1:F:489:ILE:HD11 | 1.89 | 0.54 |
| 1:A:43:LEU:HD11 | 1:A:182:THR:OG1 | 2.07 | 0.54 |
| 2:B:129:ARG:O | 2:B:132:TYR:HB3 | 2.07 | 0.54 |
| 2:B:202:ASP:HA | 2:B:226:ARG:HD2 | 1.89 | 0.54 |
| 2:B:93:ASP:OD1 | 2:B:95:ALA:HB3 | 2.07 | 0.54 |
| 2:C:206:ILE:N | 2:C:206:ILE:HD12 | 2.22 | 0.54 |
| 2:D:484:ARG:HH11 | 2:D:484:ARG:HB3 | 1.72 | 0.54 |
| 2:E:347:VAL:HG12 | 2:E:348:CYS:N | 2.21 | 0.54 |
| 2:E:79:THR:HG21 | 2:E:81:GLN:HG2 | 1.88 | 0.54 |
| 1:F:169:ALA:O | 1:F:173:GLN:HG3 | 2.07 | 0.54 |
| 1:F:23:THR:HB | 1:F:25:ILE:HG12 | 1.88 | 0.54 |
| 2:B:479:ILE:N | 2:B:479:ILE:HD12 | 2.20 | 0.54 |
| 2:E:169:ALA:O | 2:E:173:GLN:HG3 | 2.07 | 0.54 |
| 2:B:286:ALA:HA | 2:B:438:ILE:O | 2.08 | 0.54 |
| 2:C:464:ASP:OD1 | 2:C:465:LYS:N | 2.40 | 0.54 |
| 2:D:323:GLN:NE2 | 2:E:459:ARG:HD3 | 2.22 | 0.54 |
| 2:D:426:THR:HG22 | 2:D:428:SER:H | 1.72 | 0.54 |
| 1:A:56:SER:HB2 | 1:A:143:SER:HB3 | 1.89 | 0.54 |
| 2:B:178:THR:HG22 | 2:B:179:VAL:N | 2.22 | 0.54 |
| 2:C:111:ASP:O | 2:C:113:GLU:N | 2.34 | 0.54 |
| 2:C:127:ILE:CD1 | 2:C:167:LEU:HD13 | 2.37 | 0.54 |
| 2:C:426:THR:HG22 | 2:C:428:SER:H | 1.72 | 0.54 |
| 2:C:437:ILE:HD12 | 2:C:437:ILE:N | 2.22 | 0.54 |
| 2:C:461:SER:OG | 2:C:462:TRP:N | 2.39 | 0.54 |
| 2:D:443:VAL:CG1 | 2:D:445:ILE:HD11 | 2.38 | 0.54 |
| 1:F:117:VAL:O | 1:F:118:VAL:HB | 2.07 | 0.54 |
| 2:B:273:MET:O | 2:B:464:ASP:N | 2.36 | 0.54 |
| 2:C:127:ILE:HD13 | 2:C:127:ILE:N | 2.23 | 0.54 |
| 2:D:195:GLY:HA2 | 2:D:198:GLU:OE1 | 2.08 | 0.54 |
| 2:D:263:VAL:HG12 | 2:D:374:ARG:NH2 | 2.22 | 0.54 |
| 2:E:54:LEU:HD23 | 2:E:244:ILE:HD11 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:508:ILE:HD13 | 1:A:508:ILE:N | 2.19 | 0.54 |
| 2:B:24:MET:HB2 | 2:B:62:ASN:HD22 | 1.72 | 0.54 |
| 2:B:256:GLN:HE21 | 2:B:404:LYS:HB3 | 1.72 | 0.54 |
| 1:F:126:LEU:O | 1:F:130:ILE:HG12 | 2.06 | 0.54 |
| 1:F:45:SER:HB2 | 1:F:182:THR:HB | 1.89 | 0.54 |
| 1:A:455:VAL:HG11 | 1:A:463:HIS:CD2 | 2.40 | 0.54 |
| 1:A:502:LYS:O | 1:A:503:SER:HB3 | 2.08 | 0.54 |
| 2:B:38:ILE:HA | 2:B:177:THR:CG2 | 2.38 | 0.54 |
| 2:B:21:MET:CB | 2:B:38:ILE:HG12 | 2.37 | 0.54 |
| 2:B:46:GLY:CA | 2:B:50:THR:HG21 | 2.35 | 0.54 |
| 2:D:31:ILE:CG2 | 2:D:222:ILE:HD13 | 2.38 | 0.54 |
| 2:D:394:GLN:HA | 2:D:397:ILE:HD12 | 1.88 | 0.54 |
| 1:F:469:GLU:HG3 | 1:F:470:PHE:N | 2.23 | 0.54 |
| 2:B:31:ILE:HD13 | 2:B:231:MET:SD | 2.47 | 0.54 |
| 2:B:372:PRO:O | 2:B:408:ILE:HD12 | 2.08 | 0.54 |
| 1:F:197:GLU:H | 1:F:197:GLU:CD | 2.11 | 0.54 |
| 1:F:313:ILE:HB | 1:F:375:ILE:CD1 | 2.35 | 0.54 |
| 1:A:296:LEU:HD13 | 1:A:331:TRP:CE2 | 2.42 | 0.54 |
| 1:A:470:PHE:HE1 | 1:A:472:ILE:HD11 | 1.73 | 0.54 |
| 2:B:264:SER:HB3 | 2:B:304:ASN:ND2 | 2.22 | 0.54 |
| 2:B:67:PHE:HB2 | 2:B:69:GLU:HG3 | 1.89 | 0.54 |
| 2:D:443:VAL:O | 2:D:445:ILE:CD1 | 2.54 | 0.54 |
| 1:A:20:LYS:HD3 | 1:A:35:GLY:O | 2.07 | 0.53 |
| 2:D:225:LEU:HD12 | 2:D:230:HIS:HB3 | 1.90 | 0.53 |
| 2:E:127:ILE:CD1 | 2:E:167:LEU:HD13 | 2.38 | 0.53 |
| 2:E:325:LEU:CD2 | 2:E:335:PHE:HB2 | 2.38 | 0.53 |
| 1:F:294:LYS:N | 3:F:901:ATP:O1B | 2.41 | 0.53 |
| 1:A:378:ASP:O | 1:A:379:SER:CB | 2.57 | 0.53 |
| 2:C:31:ILE:HA | 2:C:231:MET:SD | 2.48 | 0.53 |
| 2:D:317:TYR:CE2 | 2:D:383:LEU:HD21 | 2.43 | 0.53 |
| 2:E:152:GLN:HG3 | 1:F:161:ARG:HH11 | 1.73 | 0.53 |
| 1:A:123:LEU:O | 1:A:127:ILE:HG12 | 2.09 | 0.53 |
| 1:A:372:PRO:HB2 | 1:A:375:ILE:CD1 | 2.38 | 0.53 |
| 2:C:283:ILE:CD1 | 2:C:404:LYS:HG3 | 2.37 | 0.53 |
| 2:D:106:LEU:CD1 | 2:D:129:ARG:NH2 | 2.72 | 0.53 |
| 2:D:256:GLN:HG3 | 2:D:404:LYS:HD3 | 1.90 | 0.53 |
| 2:D:419:PHE:O | 2:D:420:MET:HB2 | 2.08 | 0.53 |
| 2:E:347:VAL:O | 2:E:348:CYS:HB2 | 2.08 | 0.53 |
| 1:A:41:SER:CB | 1:A:178:THR:HB | 2.29 | 0.53 |
| 1:A:336:GLU:O | 1:A:339:GLU:HB2 | 2.08 | 0.53 |
| 1:A:462:TRP:O | 1:A:463:HIS:CG | 2.61 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:206:ILE:N | 2:B:206:ILE:HD12 | 2.24 | 0.53 |
| 2:D:151:PHE:O | 2:D:153:GLN:N | 2.38 | 0.53 |
| 2:D:80:PRO:O | 2:D:84:ILE:HG12 | 2.08 | 0.53 |
| 2:E:79:THR:CG2 | 2:E:82:ASP:H | 2.21 | 0.53 |
| 1:F:178:THR:HG22 | 1:F:179:VAL:N | 2.23 | 0.53 |
| 1:F:414:ASN:ND2 | 1:F:426:THR:HG23 | 2.23 | 0.53 |
| 2:E:449:MET:HE3 | 1:F:467:ILE:HD11 | 1.90 | 0.53 |
| 1:A:183:GLU:CB | 2:B:199:PHE:CE1 | 2.91 | 0.53 |
| 2:B:469:GLU:HG3 | 2:B:470:PHE:N | 2.23 | 0.53 |
| 2:B:483:PHE:HB3 | 2:B:486:PHE:CD1 | 2.29 | 0.53 |
| 2:B:84:ILE:HA | 2:B:94:LEU:HD12 | 1.89 | 0.53 |
| 2:C:248:PRO:HB2 | 2:C:251:ALA:HB3 | 1.90 | 0.53 |
| 1:A:374:ARG:O | 1:A:375:ILE:HD12 | 2.08 | 0.53 |
| 2:B:191:ILE:CB | 2:B:198:GLU:HG3 | 2.39 | 0.53 |
| 2:C:356:LEU:HD22 | 2:C:387:VAL:HG11 | 1.91 | 0.53 |
| 2:D:178:THR:HG22 | 2:D:179:VAL:N | 2.23 | 0.53 |
| 2:D:468:ARG:HH11 | 2:D:468:ARG:HG2 | 1.74 | 0.53 |
| 2:E:287:THR:HG22 | 2:E:288:GLY:N | 2.23 | 0.53 |
| 1:F:125:ALA:O | 1:F:129:ARG:HG3 | 2.07 | 0.53 |
| 1:F:443:VAL:O | 1:F:445:ILE:HD12 | 2.07 | 0.53 |
| 1:F:56:SER:HB2 | 1:F:143:SER:HB3 | 1.90 | 0.53 |
| 1:A:170:ARG:O | 1:A:174:ILE:HG12 | 2.09 | 0.53 |
| 1:A:327:ASN:OD1 | 2:B:459:ARG:O | 2.27 | 0.53 |
| 1:A:376:ALA:HA | 1:A:411:LEU:O | 2.09 | 0.53 |
| 2:B:18:ILE:HB | 2:B:228:THR:CG2 | 2.38 | 0.53 |
| 2:C:308:ASN:O | 2:C:310:GLU:HG3 | 2.08 | 0.53 |
| 2:D:446:ARG:H | 2:D:496:ARG:HH22 | 1.57 | 0.53 |
| 2:C:123:LEU:HA | 2:C:127:ILE:CD1 | 2.39 | 0.53 |
| 2:D:150:VAL:O | 2:D:153:GLN:HG3 | 2.09 | 0.53 |
| 2:D:21:MET:HE3 | 2:D:59:PHE:CZ | 2.44 | 0.53 |
| 2:B:123:LEU:O | 2:B:123:LEU:HD13 | 2.09 | 0.53 |
| 2:C:347:VAL:O | 2:C:348:CYS:HB2 | 2.08 | 0.53 |
| 2:D:31:ILE:HG21 | 2:D:222:ILE:HD11 | 1.90 | 0.53 |
| 1:A:280:LYS:O | 1:A:409:THR:OG1 | 2.23 | 0.53 |
| 1:A:31:ILE:HD11 | 1:A:246:ILE:CG2 | 2.30 | 0.53 |
| 1:A:296:LEU:CD2 | 1:A:472:ILE:HD12 | 2.39 | 0.53 |
| 2:C:378:ASP:O | 2:C:379:SER:HB3 | 2.09 | 0.53 |
| 2:D:140:ARG:HH11 | 2:D:140:ARG:CB | 2.20 | 0.53 |
| 2:D:150:VAL:HG13 | 2:D:151:PHE:N | 2.23 | 0.53 |
| 2:D:315:PHE:HE1 | 2:D:375:ILE:HD12 | 1.73 | 0.53 |
| 2:E:259:SER:N | 2:E:281:ASP:OD2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:344:LEU:HD11 | 1:F:346:ILE:HG13 | 1.89 | 0.53 |
| 1:F:504:GLU:HA | 1:F:507:ARG:HG3 | 1.90 | 0.53 |
| 2:B:220:LEU:HD13 | 2:B:246:ILE:HD13 | 1.91 | 0.52 |
| 2:B:64:ILE:HG22 | 2:B:65:ILE:HD13 | 1.90 | 0.52 |
| 2:C:123:LEU:HD12 | 2:C:163:GLU:OE2 | 2.09 | 0.52 |
| 2:C:126:LEU:O | 2:C:129:ARG:HB2 | 2.10 | 0.52 |
| 2:C:182:THR:CG2 | 2:C:183:GLU:N | 2.72 | 0.52 |
| 2:C:42:THR:HA | 2:C:203:ASN:HB2 | 1.91 | 0.52 |
| 1:A:320:SEP:O1P | 2:B:256:GLN:CG | 2.57 | 0.52 |
| 2:B:318:GLU:OE2 | 2:C:432:GLU:HG2 | 2.10 | 0.52 |
| 2:C:146:SER:HA | 2:C:181:THR:O | 2.08 | 0.52 |
| 2:C:18:ILE:HD12 | 2:C:18:ILE:N | 2.24 | 0.52 |
| 2:C:486:PHE:CE2 | 2:C:496:ARG:HG2 | 2.44 | 0.52 |
| 1:F:115:GLN:HG3 | 1:F:116:GLU:N | 2.23 | 0.52 |
| 1:F:338:MET:HB3 | 1:F:344:LEU:CB | 2.37 | 0.52 |
| 1:F:467:ILE:HG22 | 1:F:467:ILE:O | 2.09 | 0.52 |
| 1:A:306:CYS:SG | 1:A:338:MET:SD | 3.08 | 0.52 |
| 2:B:298:VAL:HG11 | 2:B:314:LEU:HD11 | 1.89 | 0.52 |
| 2:B:320:SER:HA | 2:C:254:LEU:HG | 1.91 | 0.52 |
| 2:C:267:VAL:HB | 2:C:270:LEU:HB2 | 1.92 | 0.52 |
| 2:D:266:GLY:HA3 | 2:D:300:ARG:O | 2.08 | 0.52 |
| 2:D:451:ARG:HH11 | 2:D:451:ARG:CG | 2.19 | 0.52 |
| 2:D:468:ARG:NH1 | 2:D:468:ARG:HG2 | 2.25 | 0.52 |
| 2:E:72:VAL:HG21 | 2:E:134:ILE:HD13 | 1.91 | 0.52 |
| 1:A:153:GLN:O | 1:A:154:TYR:HB3 | 2.10 | 0.52 |
| 2:B:379:SER:N | 2:B:413:THR:HG22 | 2.24 | 0.52 |
| 2:B:89:SER:HB2 | 2:C:227:GLY:O | 2.09 | 0.52 |
| 2:C:73:PHE:HD1 | 2:C:143:SER:HB2 | 1.74 | 0.52 |
| 2:C:262:ARG:NE | 2:C:279:PHE:CE2 | 2.77 | 0.52 |
| 2:D:470:PHE:CE1 | 2:D:472:ILE:HD11 | 2.44 | 0.52 |
| 3:D:903:ATP:O3' | 2:E:224:LYS:HB2 | 2.09 | 0.52 |
| 1:F:170:ARG:HD2 | 1:F:173:GLN:OE1 | 2.10 | 0.52 |
| 1:F:291:GLY:HA3 | 1:F:442:TYR:HH | 1.75 | 0.52 |
| 1:F:303:GLU:OE2 | 1:F:333:MET:HB3 | 2.10 | 0.52 |
| 1:F:468:ARG:NH1 | 1:F:468:ARG:HG2 | 2.25 | 0.52 |
| 1:A:379:SER:OG | 1:A:382:ALA:N | 2.43 | 0.52 |
| 1:A:510:ARG:HA | 1:A:510:ARG:NE | 2.25 | 0.52 |
| 2:C:356:LEU:CD2 | 2:C:387:VAL:HG11 | 2.39 | 0.52 |
| 2:B:38:ILE:HA | 2:B:177:THR:HG23 | 1.92 | 0.52 |
| 2:B:220:LEU:HD13 | 2:B:246:ILE:CD1 | 2.40 | 0.52 |
| 2:C:111:ASP:CG | 2:C:113:GLU:HG2 | 2.30 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:142:VAL:O | 2:C:178:THR:HA | 2.09 | 0.52 |
| 2:C:144:ILE:HG21 | 2:C:147:VAL:HG12 | 1.92 | 0.52 |
| 2:C:348:CYS:HB3 | 2:D:254:LEU:HB3 | 1.89 | 0.52 |
| 2:C:79:THR:HG22 | 2:C:82:ASP:CB | 2.39 | 0.52 |
| 2:E:439:LEU:HD12 | 2:E:440:LEU:H | 1.74 | 0.52 |
| 2:E:437:ILE:HD11 | 2:E:457:LYS:HE2 | 1.92 | 0.52 |
| 1:F:161:ARG:HB2 | 1:F:196:VAL:HG11 | 1.92 | 0.52 |
| 1:F:445:ILE:HD13 | 1:F:450:SER:OG | 2.08 | 0.52 |
| 1:A:45:SER:CB | 1:A:182:THR:HB | 2.40 | 0.52 |
| 1:A:479:ILE:HD12 | 1:A:479:ILE:N | 2.25 | 0.52 |
| 1:A:82:ASP:O | 1:A:85:LYS:HB3 | 2.10 | 0.52 |
| 2:B:471:MET:HB3 | 2:B:480:LYS:HZ1 | 1.75 | 0.52 |
| 2:D:301:PHE:CE1 | 2:D:374:ARG:HD3 | 2.44 | 0.52 |
| 2:E:203:ASN:HB3 | 2:E:225:LEU:HD23 | 1.91 | 0.52 |
| 1:F:23:THR:CB | 1:F:25:ILE:HG12 | 2.39 | 0.52 |
| 1:A:206:ILE:N | 1:A:206:ILE:HD12 | 2.24 | 0.52 |
| 1:A:320:SEP:O | 1:A:324:LEU:HD12 | 2.10 | 0.52 |
| 1:A:456:PHE:HE2 | 1:F:290:THR:HG23 | 1.73 | 0.52 |
| 1:A:471:MET:HB3 | 1:A:480:LYS:HZ1 | 1.73 | 0.52 |
| 2:B:209:ASN:HD21 | 2:B:216:ARG:HB3 | 1.74 | 0.52 |
| 2:B:289:ALA:HB2 | 2:B:419:PHE:HA | 1.92 | 0.52 |
| 2:B:51:GLY:O | 2:B:52:LYS:C | 2.47 | 0.52 |
| 2:E:184:ARG:HD2 | 2:E:191:ILE:O | 2.10 | 0.52 |
| 2:E:469:GLU:HB3 | 2:E:483:PHE:CZ | 2.44 | 0.52 |
| 1:F:500:ASP:O | 1:F:501:GLU:CB | 2.57 | 0.52 |
| 2:B:145:ASP:HA | 2:B:181:THR:HB | 1.92 | 0.52 |
| 2:B:232:LYS:N | 2:B:232:LYS:HD2 | 2.24 | 0.52 |
| 2:C:148:THR:HG21 | 2:C:193:ARG:HD2 | 1.92 | 0.52 |
| 2:E:160:VAL:HG21 | 2:E:194:TYR:CD2 | 2.44 | 0.52 |
| 2:E:299:SER:O | 2:E:333:MET:HE2 | 2.09 | 0.52 |
| 1:A:151:PHE:C | 1:A:153:GLN:H | 2.14 | 0.52 |
| 1:A:218:ARG:NH1 | 1:A:239:ILE:HD12 | 2.25 | 0.52 |
| 2:C:150:VAL:HG13 | 2:C:151:PHE:N | 2.24 | 0.52 |
| 2:C:65:ILE:N | 2:C:65:ILE:HD12 | 2.25 | 0.52 |
| 2:E:313:ILE:HG22 | 2:E:314:LEU:N | 2.25 | 0.52 |
| 1:F:74:VAL:HG21 | 1:F:130:ILE:HD12 | 1.91 | 0.52 |
| 1:F:191:ILE:CB | 1:F:198:GLU:HG3 | 2.39 | 0.52 |
| 1:A:284:ILE:HB | 1:A:411:LEU:HD12 | 1.91 | 0.51 |
| 1:A:455:VAL:HG11 | 1:A:463:HIS:HB2 | 1.91 | 0.51 |
| 2:C:182:THR:CG2 | 2:C:183:GLU:H | 2.23 | 0.51 |
| 2:C:61:TYR:CD2 | 2:C:65:ILE:HD13 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:153:GLN:C | 1:F:158:SER:HB2 | 2.30 | 0.51 |
| 1:F:516:GLY:N | 1:F:517:PRO:HD2 | 2.24 | 0.51 |
| 1:A:254:LEU:O | 1:A:254:LEU:CD2 | 2.57 | 0.51 |
| 1:A:377:ILE:N | 1:A:377:ILE:HD12 | 2.25 | 0.51 |
| 2:B:316:ALA:O | 2:B:348:CYS:HA | 2.11 | 0.51 |
| 1:A:415:THR:HB | 2:B:432:GLU:OE1 | 2.11 | 0.51 |
| 2:C:495:THR:HG22 | 2:D:487:GLU:OE2 | 2.10 | 0.51 |
| 2:C:48:SER:HB2 | 2:D:199:PHE:CE1 | 2.46 | 0.51 |
| 2:E:98:VAL:HA | 2:E:103:LEU:O | 2.10 | 0.51 |
| 2:E:413:THR:HG22 | 2:E:414:ASN:N | 2.25 | 0.51 |
| 2:E:454:ASN:HD21 | 2:E:456:PHE:HA | 1.75 | 0.51 |
| 1:F:220:LEU:C | 1:F:220:LEU:HD23 | 2.30 | 0.51 |
| 1:F:462:TRP:CE3 | 1:F:463:HIS:N | 2.73 | 0.51 |
| 1:A:446:ARG:HA | 1:A:496:ARG:NH2 | 2.25 | 0.51 |
| 1:F:360:LEU:O | 1:F:360:LEU:HD22 | 2.10 | 0.51 |
| 1:A:161:ARG:CB | 1:A:196:VAL:HG11 | 2.40 | 0.51 |
| 1:A:425:ILE:HD13 | 1:A:437:ILE:HD13 | 1.92 | 0.51 |
| 1:A:467:ILE:N | 1:A:467:ILE:HD12 | 2.25 | 0.51 |
| 1:A:87:ALA:O | 1:A:92:TRP:CD1 | 2.62 | 0.51 |
| 2:B:315:PHE:CD2 | 2:B:347:VAL:HG21 | 2.46 | 0.51 |
| 2:C:123:LEU:CD2 | 2:C:167:LEU:HB2 | 2.38 | 0.51 |
| 2:D:203:ASN:HB3 | 2:D:225:LEU:HD23 | 1.92 | 0.51 |
| 2:E:496:ARG:C | 2:E:497:ILE:HD13 | 2.31 | 0.51 |
| 1:F:104:PHE:HE2 | 1:F:106:LEU:HB2 | 1.76 | 0.51 |
| 1:A:296:LEU:HD13 | 1:A:331:TRP:CD2 | 2.46 | 0.51 |
| 2:B:371:LYS:N | 2:B:372:PRO:HD3 | 2.25 | 0.51 |
| 2:D:145:ASP:OD2 | 2:D:181:THR:HG21 | 2.11 | 0.51 |
| 2:E:151:PHE:C | 2:E:153:GLN:H | 2.14 | 0.51 |
| 1:F:270:LEU:O | 1:F:273:MET:HB2 | 2.10 | 0.51 |
| 1:F:315:PHE:HE1 | 1:F:375:ILE:HD11 | 1.74 | 0.51 |
| 1:A:279:PHE:HB2 | 1:A:282:SER:HB3 | 1.93 | 0.51 |
| 2:B:240:THR:HG21 | 2:B:361:GLN:HE22 | 1.76 | 0.51 |
| 2:C:206:ILE:H | 2:C:206:ILE:HD12 | 1.76 | 0.51 |
| 2:C:21:MET:HB2 | 2:C:38:ILE:HG12 | 1.93 | 0.51 |
| 2:C:220:LEU:C | 2:C:220:LEU:HD23 | 2.31 | 0.51 |
| 2:C:54:LEU:O | 2:C:57:ILE:N | 2.44 | 0.51 |
| 2:D:185:ILE:HD12 | 2:D:185:ILE:H | 1.76 | 0.51 |
| 2:D:461:SER:OG | 2:D:462:TRP:N | 2.43 | 0.51 |
| 2:E:127:ILE:HD12 | 2:E:167:LEU:CD1 | 2.41 | 0.51 |
| 1:F:73:PHE:HB3 | 1:F:105:ILE:HD13 | 1.91 | 0.51 |
| 1:F:380:LEU:O | 1:F:382:ALA:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:ILE:HB | 2:B:228:THR:HG23 | 1.93 | 0.51 |
| 2:B:80:PRO:CB | 2:B:105:ILE:HG21 | 2.41 | 0.51 |
| 2:C:121:PHE:N | 2:C:121:PHE:CD1 | 2.79 | 0.51 |
| 2:D:31:ILE:HA | 2:D:231:MET:SD | 2.51 | 0.51 |
| 2:D:445:ILE:HD12 | 2:D:445:ILE:N | 2.26 | 0.51 |
| 1:F:468:ARG:HH11 | 1:F:468:ARG:HG2 | 1.75 | 0.51 |
| 2:B:187:GLU:O | 2:B:208:ARG:HD3 | 2.11 | 0.51 |
| 2:B:161:ARG:NH2 | 2:B:199:PHE:HB2 | 2.26 | 0.51 |
| 2:B:469:GLU:HB2 | 2:B:483:PHE:CZ | 2.46 | 0.51 |
| 2:C:85:LYS:NZ | 2:D:14:GLU:HB3 | 2.25 | 0.51 |
| 2:E:52:LYS:HD3 | 2:E:182:THR:O | 2.10 | 0.51 |
| 1:F:451:ARG:HB3 | 1:F:470:PHE:CE2 | 2.46 | 0.51 |
| 1:A:433:ILE:CG2 | 1:A:433:ILE:O | 2.59 | 0.51 |
| 1:A:463:HIS:O | 1:A:464:ASP:CB | 2.59 | 0.51 |
| 1:A:470:PHE:CE1 | 1:A:472:ILE:HD11 | 2.45 | 0.51 |
| 2:B:381:SER:HB3 | 2:B:414:ASN:OD1 | 2.10 | 0.51 |
| 2:C:151:PHE:C | 2:C:153:GLN:N | 2.63 | 0.51 |
| 2:C:184:ARG:HG2 | 2:C:191:ILE:O | 2.11 | 0.51 |
| 2:C:431:GLU:O | 2:C:432:GLU:HB2 | 2.09 | 0.51 |
| 2:E:359:HIS:O | 2:E:363:ILE:HG12 | 2.10 | 0.51 |
| 1:A:254:LEU:HD11 | 1:F:319:GLU:O | 2.11 | 0.51 |
| 1:A:70:PRO:HB2 | 1:A:139:ALA:HA | 1.93 | 0.51 |
| 2:B:451:ARG:CG | 2:B:451:ARG:NH1 | 2.74 | 0.51 |
| 2:C:214:GLU:OE2 | 2:D:217:ARG:NH1 | 2.44 | 0.51 |
| 2:C:252:MET:HE3 | 2:C:397:ILE:HG22 | 1.92 | 0.51 |
| 2:D:437:ILE:CD1 | 2:D:457:LYS:HE2 | 2.41 | 0.51 |
| 1:F:320:SEP:O | 1:F:324:LEU:HB2 | 2.10 | 0.51 |
| 1:F:284:ILE:HD12 | 1:F:410:GLY:O | 2.11 | 0.51 |
| 1:A:140:ARG:HH11 | 1:A:140:ARG:CB | 2.23 | 0.50 |
| 2:E:123:LEU:HD23 | 2:E:127:ILE:CD1 | 2.37 | 0.50 |
| 2:E:28:PHE:N | 2:E:246:ILE:HD12 | 2.26 | 0.50 |
| 1:F:148:THR:HG21 | 1:F:183:GLU:HG3 | 1.93 | 0.50 |
| 1:A:67:PHE:HB2 | 1:A:69:GLU:HG3 | 1.93 | 0.50 |
| 2:D:214:GLU:HA | 2:E:234:GLU:OE1 | 2.12 | 0.50 |
| 1:F:312:ALA:HA | 1:F:374:ARG:O | 2.12 | 0.50 |
| 2:B:147:VAL:HG11 | 2:B:180:MET:HE2 | 1.90 | 0.50 |
| 1:A:320:SEP:CB | 2:B:254:LEU:O | 2.36 | 0.50 |
| 2:B:280:LYS:NZ | 2:B:407:GLU:HB3 | 2.26 | 0.50 |
| 2:B:440:LEU:CD2 | 2:B:453:ILE:HG12 | 2.40 | 0.50 |
| 2:C:38:ILE:HA | 2:C:177:THR:HG23 | 1.94 | 0.50 |
| 2:C:28:PHE:HE1 | 2:C:222:ILE:HD11 | 1.71 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:150:VAL:CG1 | 2:D:151:PHE:N | 2.75 | 0.50 |
| 2:D:446:ARG:HB3 | 2:E:484:ARG:HG3 | 1.93 | 0.50 |
| 2:D:451:ARG:HB3 | 2:D:470:PHE:CE2 | 2.45 | 0.50 |
| 2:D:385:ARG:HG2 | 2:E:393:ARG:NH1 | 2.26 | 0.50 |
| 1:F:203:ASN:HB3 | 1:F:225:LEU:CD2 | 2.40 | 0.50 |
| 1:F:79:THR:HG23 | 1:F:81:GLN:HG2 | 1.92 | 0.50 |
| 1:A:116:GLU:O | 1:A:117:VAL:HG23 | 2.10 | 0.50 |
| 1:A:79:THR:HG22 | 1:A:82:ASP:H | 1.76 | 0.50 |
| 2:C:360:LEU:HA | 2:C:363:ILE:HD12 | 1.93 | 0.50 |
| 2:D:211:LEU:HA | 2:D:216:ARG:HD3 | 1.93 | 0.50 |
| 2:D:323:GLN:HE22 | 2:E:459:ARG:HD3 | 1.75 | 0.50 |
| 2:D:371:LYS:CD | 2:D:371:LYS:O | 2.48 | 0.50 |
| 2:E:191:ILE:HD12 | 2:E:206:ILE:HG13 | 1.93 | 0.50 |
| 1:A:118:VAL:HG23 | 1:A:153:GLN:OE1 | 2.11 | 0.50 |
| 1:A:148:THR:HG21 | 1:A:183:GLU:CG | 2.41 | 0.50 |
| 2:B:485:ASN:N | 2:B:485:ASN:OD1 | 2.44 | 0.50 |
| 2:D:161:ARG:HB2 | 2:D:196:VAL:CG1 | 2.41 | 0.50 |
| 2:D:402:TYR:O | 2:D:405:GLN:HG2 | 2.12 | 0.50 |
| 1:F:140:ARG:CB | 1:F:140:ARG:HH11 | 2.24 | 0.50 |
| 1:A:271:ASP:O | 1:A:273:MET:O | 2.30 | 0.50 |
| 1:A:335:PHE:O | 1:A:336:GLU:C | 2.48 | 0.50 |
| 2:B:249:LEU:CD1 | 2:B:394:GLN:HG2 | 2.42 | 0.50 |
| 2:E:118:VAL:O | 2:E:118:VAL:HG12 | 2.12 | 0.50 |
| 2:E:255:THR:O | 2:E:255:THR:HG22 | 2.11 | 0.50 |
| 1:F:123:LEU:O | 1:F:123:LEU:HD13 | 2.10 | 0.50 |
| 1:F:151:PHE:O | 1:F:153:GLN:N | 2.42 | 0.50 |
| 1:A:456:PHE:CE2 | 1:F:290:THR:HG23 | 2.46 | 0.50 |
| 1:F:313:ILE:HG13 | 1:F:372:PRO:CG | 2.41 | 0.50 |
| 1:A:435:ASP:HA | 1:A:459:ARG:HD2 | 1.93 | 0.50 |
| 2:D:446:ARG:H | 2:D:496:ARG:NH2 | 2.10 | 0.50 |
| 2:E:148:THR:HG21 | 2:E:183:GLU:CG | 2.42 | 0.50 |
| 1:F:18:ILE:HD11 | 1:F:227:GLY:HA3 | 1.87 | 0.50 |
| 1:F:462:TRP:CD2 | 1:F:463:HIS:N | 2.80 | 0.50 |
| 1:A:64:ILE:HD12 | 1:A:102:LYS:HB3 | 1.94 | 0.50 |
| 1:A:267:VAL:HB | 1:A:270:LEU:HB2 | 1.94 | 0.50 |
| 2:B:68:ASP:OD1 | 2:B:102:LYS:NZ | 2.44 | 0.50 |
| 2:B:106:LEU:HD12 | 2:B:106:LEU:C | 2.32 | 0.50 |
| 2:B:237:PHE:HB2 | 2:B:246:ILE:HG12 | 1.93 | 0.50 |
| 2:B:248:PRO:O | 2:B:251:ALA:N | 2.45 | 0.50 |
| 2:B:433:ILE:O | 2:B:433:ILE:HG22 | 2.12 | 0.50 |
| 2:C:393:ARG:HH21 | 2:C:429:HIS:CB | 2.22 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:334:ASP:OD1 | 2:D:336:GLU:HB2 | 2.11 | 0.50 |
| 2:E:440:LEU:CD2 | 2:E:453:ILE:HG12 | 2.41 | 0.50 |
| 2:E:54:LEU:HD23 | 2:E:244:ILE:CD1 | 2.42 | 0.50 |
| 1:F:425:ILE:HD11 | 1:F:456:PHE:CD2 | 2.46 | 0.50 |
| 1:F:79:THR:CG2 | 1:F:81:GLN:HG2 | 2.42 | 0.50 |
| 1:A:153:GLN:O | 1:A:154:TYR:CD2 | 2.64 | 0.50 |
| 2:B:358:ASP:O | 2:B:362:ILE:HG12 | 2.11 | 0.50 |
| 2:C:127:ILE:HD13 | 2:C:127:ILE:H | 1.77 | 0.50 |
| 2:C:41:SER:OG | 2:C:168:VAL:HG13 | 2.11 | 0.50 |
| 2:C:54:LEU:HD13 | 2:C:90:PHE:CZ | 2.47 | 0.50 |
| 1:F:151:PHE:C | 1:F:153:GLN:N | 2.65 | 0.50 |
| 1:F:353:SER:O | 1:F:354:ALA:HB2 | 2.11 | 0.50 |
| 1:F:317:TYR:CD2 | 1:F:383:LEU:HD21 | 2.47 | 0.50 |
| 1:A:136:LYS:HD3 | 1:A:137:TYR:CE1 | 2.47 | 0.49 |
| 1:A:45:SER:HA | 1:A:182:THR:O | 2.12 | 0.49 |
| 1:A:467:ILE:HD13 | 1:F:447:GLY:C | 2.32 | 0.49 |
| 2:C:116:GLU:O | 2:C:117:VAL:HB | 2.11 | 0.49 |
| 2:C:214:GLU:C | 2:C:215:ARG:HE | 2.15 | 0.49 |
| 2:D:127:ILE:HD11 | 2:D:167:LEU:HD13 | 1.94 | 0.49 |
| 2:D:81:GLN:N | 2:D:81:GLN:CD | 2.66 | 0.49 |
| 2:E:385:ARG:HA | 1:F:393:ARG:NH1 | 2.27 | 0.49 |
| 1:F:504:GLU:HA | 1:F:507:ARG:CG | 2.41 | 0.49 |
| 1:A:419:PHE:O | 1:A:420:MET:HB2 | 2.12 | 0.49 |
| 1:A:484:ARG:NH1 | 1:A:484:ARG:CB | 2.74 | 0.49 |
| 2:C:117:VAL:HG12 | 2:C:117:VAL:O | 2.11 | 0.49 |
| 2:C:313:ILE:HD12 | 2:C:372:PRO:HG2 | 1.93 | 0.49 |
| 2:C:52:LYS:HD2 | 2:C:182:THR:O | 2.12 | 0.49 |
| 2:E:396:VAL:HG11 | 2:E:430:ILE:CG2 | 2.42 | 0.49 |
| 1:F:49:GLY:CA | 3:F:903:ATP:O2B | 2.59 | 0.49 |
| 1:A:377:ILE:HG22 | 1:A:379:SER:O | 2.13 | 0.49 |
| 1:A:426:THR:HG22 | 1:A:428:SER:H | 1.77 | 0.49 |
| 1:A:436:THR:HG23 | 1:A:457:LYS:O | 2.12 | 0.49 |
| 2:C:289:ALA:HB2 | 2:C:419:PHE:HA | 1.93 | 0.49 |
| 2:C:18:ILE:HG21 | 2:C:37:PRO:HB3 | 1.95 | 0.49 |
| 2:C:252:MET:CE | 2:C:397:ILE:HG22 | 2.42 | 0.49 |
| 2:C:52:LYS:N | 3:C:903:ATP:O1B | 2.45 | 0.49 |
| 2:D:121:PHE:O | 2:D:124:SER:OG | 2.26 | 0.49 |
| 2:E:309:LYS:HA | 2:E:343:LEU:HD13 | 1.94 | 0.49 |
| 1:F:33:HIS:CD2 | 1:F:229:SER:OG | 2.65 | 0.49 |
| 1:F:287:THR:HG23 | 1:F:414:ASN:HB3 | 1.93 | 0.49 |
| 1:F:514:GLU:HG2 | 1:F:519:SER:HB3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:ARG:O | 1:A:236:PRO:HA | 2.12 | 0.49 |
| 1:A:448:GLU:HG2 | 2:B:466:ALA:CB | 2.43 | 0.49 |
| 2:B:126:LEU:HD12 | 2:B:129:ARG:HD3 | 1.95 | 0.49 |
| 2:B:162:ARG:HB2 | 2:B:162:ARG:NH1 | 2.27 | 0.49 |
| 2:B:340:ARG:C | 2:B:342:ASN:H | 2.15 | 0.49 |
| 2:C:191:ILE:HB | 2:C:198:GLU:HG3 | 1.91 | 0.49 |
| 2:C:486:PHE:HB2 | 2:C:489:ILE:HD11 | 1.94 | 0.49 |
| 2:D:333:MET:CG | 5:D:910:HOH:O | 2.60 | 0.49 |
| 2:E:140:ARG:HH11 | 2:E:140:ARG:CA | 2.25 | 0.49 |
| 1:F:144:ILE:HG22 | 1:F:147:VAL:HG12 | 1.94 | 0.49 |
| 1:F:148:THR:CG2 | 1:F:193:ARG:HD2 | 2.43 | 0.49 |
| 1:A:284:ILE:N | 1:A:284:ILE:HD12 | 2.26 | 0.49 |
| 1:A:344:LEU:HD13 | 1:A:344:LEU:C | 2.33 | 0.49 |
| 1:A:436:THR:HG23 | 1:A:458:MET:HG2 | 1.93 | 0.49 |
| 2:B:318:GLU:HG3 | 5:B:528:HOH:O | 2.13 | 0.49 |
| 2:B:376:ALA:HA | 2:B:411:LEU:O | 2.13 | 0.49 |
| 2:C:225:LEU:HB2 | 2:C:230:HIS:HD2 | 1.77 | 0.49 |
| 2:C:149:SER:HB3 | 2:D:161:ARG:NH2 | 2.26 | 0.49 |
| 2:D:179:VAL:HG12 | 2:D:179:VAL:O | 2.12 | 0.49 |
| 2:D:191:ILE:HG12 | 2:D:206:ILE:HD11 | 1.95 | 0.49 |
| 2:D:273:MET:CE | 2:D:468:ARG:HD2 | 2.41 | 0.49 |
| 1:A:441:GLN:NE2 | 1:A:490:ILE:HD13 | 2.27 | 0.49 |
| 2:B:23:THR:O | 2:B:24:MET:HB2 | 2.12 | 0.49 |
| 2:B:273:MET:CE | 2:B:468:ARG:HD2 | 2.42 | 0.49 |
| 2:B:344:LEU:HD11 | 2:B:346:ILE:CD1 | 2.42 | 0.49 |
| 2:B:377:ILE:N | 2:B:377:ILE:HD12 | 2.28 | 0.49 |
| 2:C:147:VAL:HG11 | 2:C:180:MET:CE | 2.41 | 0.49 |
| 2:C:163:GLU:HA | 2:C:163:GLU:OE2 | 2.13 | 0.49 |
| 2:C:397:ILE:H | 2:C:397:ILE:CD1 | 2.25 | 0.49 |
| 2:D:446:ARG:N | 2:D:496:ARG:NH1 | 2.57 | 0.49 |
| 2:D:67:PHE:HB2 | 2:D:69:GLU:HG3 | 1.93 | 0.49 |
| 2:E:262:ARG:NH2 | 2:E:461:SER:HB2 | 2.28 | 0.49 |
| 2:E:79:THR:HG23 | 2:E:81:GLN:H | 1.77 | 0.49 |
| 2:B:486:PHE:CE2 | 2:B:496:ARG:HB2 | 2.48 | 0.49 |
| 2:C:121:PHE:HB3 | 2:C:125:ALA:HB3 | 1.94 | 0.49 |
| 2:C:334:ASP:O | 2:C:338:MET:HG2 | 2.13 | 0.49 |
| 2:C:340:ARG:C | 2:C:342:ASN:N | 2.65 | 0.49 |
| 2:D:60:LEU:O | 2:D:64:ILE:CD1 | 2.55 | 0.49 |
| 2:E:315:PHE:CE2 | 2:E:363:ILE:HD13 | 2.48 | 0.49 |
| 1:A:284:ILE:HD12 | 1:A:410:GLY:O | 2.13 | 0.49 |
| 2:B:194:TYR:O | 2:B:196:VAL:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:209:ASN:ND2 | 2:B:216:ARG:HD2 | 2.28 | 0.49 |
| 2:C:98:VAL:HA | 2:C:103:LEU:O | 2.12 | 0.49 |
| 2:C:211:LEU:HD12 | 2:C:215:ARG:O | 2.13 | 0.49 |
| 2:C:218:ARG:NH1 | 2:C:239:ILE:HD12 | 2.27 | 0.49 |
| 2:D:335:PHE:HA | 2:D:338:MET:CG | 2.30 | 0.49 |
| 2:D:412:PHE:N | 2:D:412:PHE:CD1 | 2.80 | 0.49 |
| 1:F:289:ALA:HB2 | 1:F:419:PHE:HA | 1.95 | 0.49 |
| 1:A:244:ILE:HG22 | 1:A:246:ILE:CD1 | 2.43 | 0.49 |
| 1:A:82:ASP:O | 1:A:83:ILE:C | 2.51 | 0.49 |
| 2:D:79:THR:HG22 | 2:D:82:ASP:HB2 | 1.94 | 0.49 |
| 2:E:273:MET:O | 2:E:463:HIS:CA | 2.60 | 0.49 |
| 1:F:218:ARG:CZ | 1:F:239:ILE:HD12 | 2.43 | 0.49 |
| 2:E:123:LEU:HD23 | 2:E:127:ILE:CG1 | 2.43 | 0.49 |
| 1:F:21:MET:HE3 | 1:F:141:ARG:CZ | 2.43 | 0.49 |
| 1:F:245:ASN:HD22 | 1:F:361:GLN:HE21 | 1.60 | 0.49 |
| 1:F:507:ARG:CD | 1:F:507:ARG:O | 2.61 | 0.49 |
| 1:A:205:VAL:HG22 | 1:A:222:ILE:CD1 | 2.37 | 0.48 |
| 2:B:436:THR:HG23 | 2:B:458:MET:HG3 | 1.95 | 0.48 |
| 2:C:93:ASP:OD1 | 2:C:93:ASP:C | 2.50 | 0.48 |
| 2:D:237:PHE:HB3 | 2:D:246:ILE:HG12 | 1.95 | 0.48 |
| 2:D:85:LYS:NZ | 2:E:14:GLU:HB3 | 2.27 | 0.48 |
| 2:E:302:VAL:HG13 | 2:E:344:LEU:HD23 | 1.94 | 0.48 |
| 2:E:387:VAL:HG12 | 2:E:388:SER:N | 2.28 | 0.48 |
| 1:F:393:ARG:O | 1:F:397:ILE:HG13 | 2.12 | 0.48 |
| 1:A:237:PHE:HB3 | 1:A:246:ILE:HG13 | 1.95 | 0.48 |
| 1:A:338:MET:HB3 | 1:A:344:LEU:CB | 2.42 | 0.48 |
| 2:D:21:MET:CE | 2:D:177:THR:HB | 2.42 | 0.48 |
| 2:D:231:MET:HB3 | 2:D:235:TYR:OH | 2.13 | 0.48 |
| 2:D:385:ARG:NH2 | 2:E:433:ILE:HD11 | 2.27 | 0.48 |
| 2:E:96:LYS:O | 2:E:100:GLU:HG3 | 2.12 | 0.48 |
| 2:E:271:ASP:OD1 | 2:E:277:GLY:HA2 | 2.13 | 0.48 |
| 2:E:486:PHE:HA | 2:E:495:THR:O | 2.13 | 0.48 |
| 2:E:93:ASP:OD2 | 2:E:96:LYS:CB | 2.59 | 0.48 |
| 2:C:239:ILE:CG1 | 2:C:244:ILE:HD13 | 2.44 | 0.48 |
| 2:D:121:PHE:N | 2:D:121:PHE:CD1 | 2.81 | 0.48 |
| 2:D:336:GLU:OE1 | 2:D:336:GLU:HA | 2.13 | 0.48 |
| 2:D:445:ILE:CA | 2:D:496:ARG:HH12 | 2.27 | 0.48 |
| 2:E:299:SER:C | 2:E:333:MET:HE2 | 2.33 | 0.48 |
| 2:E:53:THR:OG1 | 3:E:903:ATP:O2G | 2.31 | 0.48 |
| 1:F:115:GLN:CG | 1:F:116:GLU:N | 2.74 | 0.48 |
| 1:F:182:THR:HG22 | 1:F:183:GLU:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:197:GLU:N | 1:F:197:GLU:OE2 | 2.41 | 0.48 |
| 1:F:284:ILE:N | 1:F:284:ILE:HD12 | 2.28 | 0.48 |
| 1:F:325:LEU:HD23 | 1:F:335:PHE:HB2 | 1.96 | 0.48 |
| 1:A:186:GLU:HB3 | 1:A:189:GLY:HA3 | 1.94 | 0.48 |
| 2:C:123:LEU:O | 2:C:124:SER:C | 2.51 | 0.48 |
| 2:C:214:GLU:HB3 | 2:D:234:GLU:HB2 | 1.95 | 0.48 |
| 2:D:433:ILE:CG2 | 2:D:433:ILE:O | 2.60 | 0.48 |
| 2:D:486:PHE:CE2 | 2:D:496:ARG:HB3 | 2.49 | 0.48 |
| 1:F:220:LEU:HD21 | 1:F:222:ILE:CD1 | 2.43 | 0.48 |
| 1:A:106:LEU:HD12 | 1:A:106:LEU:C | 2.34 | 0.48 |
| 2:C:123:LEU:O | 2:C:126:LEU:N | 2.46 | 0.48 |
| 2:C:364:LYS:HE2 | 2:C:402:TYR:CD1 | 2.49 | 0.48 |
| 2:C:454:ASN:CB | 2:C:467:ILE:HD13 | 2.43 | 0.48 |
| 2:C:54:LEU:O | 2:C:55:PHE:C | 2.52 | 0.48 |
| 2:D:149:SER:HA | 2:D:152:GLN:HB2 | 1.95 | 0.48 |
| 2:E:49:GLY:O | 2:E:218:ARG:NH2 | 2.47 | 0.48 |
| 2:E:303:GLU:HB2 | 2:E:333:MET:CE | 2.43 | 0.48 |
| 2:E:316:ALA:O | 2:E:348:CYS:HA | 2.14 | 0.48 |
| 2:E:81:GLN:NE2 | 2:E:81:GLN:H | 2.10 | 0.48 |
| 1:F:305:ALA:O | 1:F:310:GLU:HB2 | 2.13 | 0.48 |
| 1:F:484:ARG:NH1 | 1:F:484:ARG:HB3 | 2.27 | 0.48 |
| 2:B:56:SER:HB2 | 2:B:143:SER:HB3 | 1.96 | 0.48 |
| 2:B:222:ILE:HG22 | 2:B:230:HIS:CE1 | 2.49 | 0.48 |
| 2:D:451:ARG:N | 2:D:451:ARG:HD2 | 2.28 | 0.48 |
| 2:E:148:THR:HG21 | 2:E:193:ARG:HD2 | 1.94 | 0.48 |
| 1:F:182:THR:CG2 | 1:F:192:ALA:HB1 | 2.44 | 0.48 |
| 1:F:23:THR:O | 1:F:24:MET:HB2 | 2.14 | 0.48 |
| 1:F:380:LEU:C | 1:F:382:ALA:H | 2.16 | 0.48 |
| 2:B:237:PHE:HB3 | 2:B:246:ILE:HG12 | 1.94 | 0.48 |
| 2:B:438:ILE:HG23 | 2:B:453:ILE:HD11 | 1.94 | 0.48 |
| 2:C:218:ARG:HB3 | 5:C:528:HOH:O | 2.13 | 0.48 |
| 2:D:262:ARG:HD2 | 2:D:276:GLY:O | 2.14 | 0.48 |
| 1:A:256:GLN:CG | 1:F:320:SEP:P | 3.01 | 0.48 |
| 1:F:431:GLU:O | 1:F:434:THR:HG22 | 2.13 | 0.48 |
| 1:A:313:ILE:HD12 | 1:A:367:ILE:HD13 | 1.94 | 0.48 |
| 2:B:503:SER:O | 2:B:504:GLU:CB | 2.55 | 0.48 |
| 2:D:197:GLU:OE2 | 2:D:197:GLU:N | 2.35 | 0.48 |
| 2:D:270:LEU:O | 2:D:270:LEU:HD23 | 2.13 | 0.48 |
| 2:D:443:VAL:C | 2:D:445:ILE:HD12 | 2.34 | 0.48 |
| 2:E:148:THR:HG21 | 2:E:183:GLU:HG3 | 1.96 | 0.48 |
| 1:F:446:ARG:H | 1:F:496:ARG:NH2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:509:VAL:CG1 | 1:F:510:ARG:N | 2.54 | 0.48 |
| 2:B:215:ARG:NH2 | 2:C:234:GLU:O | 2.47 | 0.48 |
| 2:C:284:ILE:H | 2:C:284:ILE:HD12 | 1.79 | 0.48 |
| 2:C:371:LYS:N | 2:C:372:PRO:HD3 | 2.28 | 0.48 |
| 2:C:431:GLU:CG | 2:C:431:GLU:O | 2.61 | 0.48 |
| 2:D:212:GLU:CG | 2:D:212:GLU:O | 2.60 | 0.48 |
| 2:E:273:MET:CE | 2:E:468:ARG:HD2 | 2.44 | 0.48 |
| 1:A:317:TYR:CD2 | 1:A:383:LEU:HD21 | 2.49 | 0.48 |
| 2:B:72:VAL:HG23 | 2:B:139:ALA:CB | 2.44 | 0.48 |
| 2:C:434:THR:CG2 | 2:C:437:ILE:HD11 | 2.31 | 0.48 |
| 2:C:464:ASP:OD1 | 2:C:464:ASP:C | 2.52 | 0.48 |
| 2:D:182:THR:CG2 | 2:D:183:GLU:H | 2.24 | 0.48 |
| 2:D:352:GLU:C | 2:D:354:ALA:H | 2.18 | 0.48 |
| 3:E:901:ATP:O3' | 1:F:457:LYS:HB2 | 2.14 | 0.48 |
| 1:A:150:VAL:CG1 | 1:A:151:PHE:N | 2.76 | 0.47 |
| 1:A:344:LEU:HD13 | 1:A:345:LYS:N | 2.29 | 0.47 |
| 2:B:184:ARG:NH2 | 2:B:186:GLU:O | 2.47 | 0.47 |
| 2:B:296:LEU:HD21 | 2:B:477:PRO:CD | 2.38 | 0.47 |
| 2:C:249:LEU:HD13 | 2:C:394:GLN:O | 2.14 | 0.47 |
| 2:D:151:PHE:C | 2:D:153:GLN:N | 2.67 | 0.47 |
| 2:D:68:ASP:O | 2:D:68:ASP:OD1 | 2.31 | 0.47 |
| 2:E:203:ASN:ND2 | 2:E:203:ASN:N | 2.61 | 0.47 |
| 2:E:336:GLU:O | 2:E:339:GLU:HB2 | 2.14 | 0.47 |
| 2:E:485:ASN:OD1 | 2:E:485:ASN:N | 2.47 | 0.47 |
| 1:F:20:LYS:HB3 | 1:F:35:GLY:O | 2.13 | 0.47 |
| 1:F:302:VAL:HG12 | 1:F:303:GLU:N | 2.28 | 0.47 |
| 1:F:283:ILE:HD11 | 1:F:404:LYS:HG3 | 1.96 | 0.47 |
| 1:F:452:ALA:HA | 1:F:469:GLU:HA | 1.96 | 0.47 |
| 1:A:162:ARG:NH1 | 1:F:116:GLU:HG2 | 2.29 | 0.47 |
| 1:A:320:SEP:O | 1:A:324:LEU:CD1 | 2.63 | 0.47 |
| 1:A:294:LYS:N | 3:A:901:ATP:O1B | 2.47 | 0.47 |
| 2:B:125:ALA:O | 2:B:129:ARG:HG3 | 2.13 | 0.47 |
| 1:A:425:ILE:CD1 | 1:F:290:THR:HG21 | 2.42 | 0.47 |
| 1:A:118:VAL:HG12 | 1:A:122:ASP:HB3 | 1.95 | 0.47 |
| 1:A:249:LEU:HD12 | 1:A:394:GLN:OE1 | 2.15 | 0.47 |
| 2:B:284:ILE:N | 2:B:284:ILE:HD12 | 2.29 | 0.47 |
| 2:C:197:GLU:CD | 2:C:197:GLU:H | 2.14 | 0.47 |
| 2:C:462:TRP:CE2 | 2:C:463:HIS:O | 2.68 | 0.47 |
| 2:D:266:GLY:O | 2:D:300:ARG:CG | 2.62 | 0.47 |
| 2:D:315:PHE:CE1 | 2:D:375:ILE:HD12 | 2.50 | 0.47 |
| 2:D:334:ASP:O | 2:D:338:MET:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:451:ARG:HG2 | 2:D:451:ARG:NH1 | 2.23 | 0.47 |
| 2:D:471:MET:HG3 | 2:D:478:ASP:HB3 | 1.96 | 0.47 |
| 2:E:167:LEU:HG | 2:E:171:LEU:HD12 | 1.96 | 0.47 |
| 2:E:344:LEU:HD11 | 2:E:346:ILE:CG1 | 2.42 | 0.47 |
| 2:E:49:GLY:N | 3:E:903:ATP:O2B | 2.48 | 0.47 |
| 1:F:338:MET:CB | 1:F:344:LEU:HB3 | 2.43 | 0.47 |
| 1:A:111:ASP:CG | 1:A:112:PRO:HD2 | 2.34 | 0.47 |
| 1:A:451:ARG:CG | 1:A:451:ARG:NH1 | 2.76 | 0.47 |
| 1:A:90:PHE:HB2 | 1:A:92:TRP:CE2 | 2.49 | 0.47 |
| 2:B:104:PHE:HD2 | 2:B:133:ALA:HB1 | 1.79 | 0.47 |
| 2:B:419:PHE:O | 2:B:420:MET:HB2 | 2.14 | 0.47 |
| 2:D:304:ASN:OD1 | 2:D:374:ARG:NH2 | 2.47 | 0.47 |
| 2:D:332:GLY:O | 2:D:333:MET:O | 2.31 | 0.47 |
| 2:D:370:PHE:O | 2:D:371:LYS:HG3 | 2.13 | 0.47 |
| 2:D:64:ILE:HD12 | 2:D:64:ILE:N | 2.29 | 0.47 |
| 2:D:385:ARG:HH22 | 2:E:433:ILE:CD1 | 2.28 | 0.47 |
| 1:F:106:LEU:HD13 | 1:F:129:ARG:CZ | 2.44 | 0.47 |
| 1:F:336:GLU:OE1 | 1:F:336:GLU:HA | 2.14 | 0.47 |
| 1:F:370:PHE:C | 1:F:372:PRO:HD3 | 2.34 | 0.47 |
| 1:A:457:LYS:HB2 | 3:F:901:ATP:O3' | 2.14 | 0.47 |
| 2:B:371:LYS:O | 2:B:371:LYS:HD2 | 2.14 | 0.47 |
| 2:C:191:ILE:HB | 2:C:198:GLU:HG2 | 1.96 | 0.47 |
| 2:D:425:ILE:CD1 | 2:D:439:LEU:HD22 | 2.45 | 0.47 |
| 2:E:142:VAL:HB | 2:E:178:THR:HG23 | 1.96 | 0.47 |
| 2:D:110:PRO:HD2 | 2:E:165:PHE:CE2 | 2.49 | 0.47 |
| 2:E:52:LYS:HE3 | 3:E:903:ATP:O1B | 2.14 | 0.47 |
| 1:A:467:ILE:HD11 | 1:F:449:MET:HG2 | 1.95 | 0.47 |
| 1:A:154:TYR:O | 1:A:155:ASP:CB | 2.62 | 0.47 |
| 1:A:421:GLY:O | 1:A:422:ALA:O | 2.32 | 0.47 |
| 1:A:462:TRP:CG | 1:A:463:HIS:N | 2.76 | 0.47 |
| 2:B:22:ARG:NH2 | 2:B:24:MET:SD | 2.87 | 0.47 |
| 2:B:25:ILE:HG23 | 2:B:58:GLN:NE2 | 2.29 | 0.47 |
| 3:A:901:ATP:O3' | 2:B:457:LYS:HB2 | 2.14 | 0.47 |
| 2:B:73:PHE:HD2 | 2:B:105:ILE:HD12 | 1.80 | 0.47 |
| 2:C:334:ASP:OD1 | 2:C:336:GLU:N | 2.48 | 0.47 |
| 2:C:419:PHE:O | 2:C:420:MET:CB | 2.61 | 0.47 |
| 2:D:42:THR:HA | 2:D:203:ASN:HB2 | 1.97 | 0.47 |
| 2:D:225:LEU:HB2 | 2:D:230:HIS:HD2 | 1.79 | 0.47 |
| 2:D:231:MET:HE1 | 2:D:251:ALA:HB2 | 1.96 | 0.47 |
| 2:D:98:VAL:HA | 2:D:103:LEU:O | 2.15 | 0.47 |
| 2:E:123:LEU:HD13 | 2:E:166:ARG:HD2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:147:VAL:HG23 | 2:E:148:THR:N | 2.30 | 0.47 |
| 2:E:127:ILE:HD12 | 2:E:167:LEU:HD13 | 1.96 | 0.47 |
| 1:F:31:ILE:HD11 | 1:F:246:ILE:HG21 | 1.95 | 0.47 |
| 1:A:370:PHE:C | 1:A:372:PRO:HD3 | 2.35 | 0.47 |
| 2:B:150:VAL:CG1 | 2:B:151:PHE:N | 2.77 | 0.47 |
| 2:C:419:PHE:CG | 2:C:419:PHE:O | 2.67 | 0.47 |
| 2:C:437:ILE:HD13 | 2:C:457:LYS:CE | 2.38 | 0.47 |
| 2:D:328:ALA:CA | 5:D:552:HOH:O | 2.62 | 0.47 |
| 2:E:417:ASP:O | 1:F:424:SER:HB3 | 2.15 | 0.47 |
| 1:F:430:ILE:O | 1:F:432:GLU:N | 2.47 | 0.47 |
| 1:A:262:ARG:O | 1:A:263:VAL:HG22 | 2.15 | 0.47 |
| 2:B:118:VAL:HG12 | 2:B:121:PHE:HB2 | 1.96 | 0.47 |
| 2:B:184:ARG:HG2 | 2:B:191:ILE:O | 2.14 | 0.47 |
| 2:B:313:ILE:CD1 | 2:B:372:PRO:HG2 | 2.45 | 0.47 |
| 2:C:263:VAL:HG21 | 2:C:280:LYS:HA | 1.96 | 0.47 |
| 2:C:294:LYS:HB2 | 3:C:901:ATP:O1B | 2.15 | 0.47 |
| 2:E:371:LYS:N | 2:E:372:PRO:HD3 | 2.29 | 0.47 |
| 1:A:256:GLN:CG | 1:F:320:SEP:O1P | 2.60 | 0.47 |
| 1:A:244:ILE:HG22 | 1:A:246:ILE:HD11 | 1.96 | 0.47 |
| 2:B:269:ARG:O | 2:B:273:MET:HG3 | 2.15 | 0.47 |
| 2:B:350:TYR:HE1 | 2:C:252:MET:HG2 | 1.80 | 0.47 |
| 2:B:80:PRO:HG3 | 2:B:105:ILE:CG2 | 2.44 | 0.47 |
| 2:C:294:LYS:N | 3:C:901:ATP:O1B | 2.46 | 0.47 |
| 2:D:18:ILE:CD1 | 2:D:40:ARG:HH12 | 2.27 | 0.47 |
| 2:D:451:ARG:NH1 | 2:D:451:ARG:CG | 2.75 | 0.47 |
| 2:E:150:VAL:CG1 | 2:E:151:PHE:H | 2.28 | 0.47 |
| 1:F:380:LEU:C | 1:F:382:ALA:N | 2.68 | 0.47 |
| 1:F:269:ARG:CG | 1:F:479:ILE:HB | 2.40 | 0.47 |
| 1:F:61:TYR:O | 1:F:64:ILE:N | 2.48 | 0.47 |
| 1:A:452:ALA:HA | 1:A:468:ARG:O | 2.15 | 0.47 |
| 2:B:217:ARG:HG3 | 2:B:357:GLU:OE2 | 2.15 | 0.47 |
| 2:E:344:LEU:HD13 | 2:E:345:LYS:N | 2.29 | 0.47 |
| 1:F:98:VAL:HA | 1:F:103:LEU:O | 2.15 | 0.47 |
| 1:F:115:GLN:CG | 1:F:116:GLU:H | 2.27 | 0.47 |
| 1:F:504:GLU:OE2 | 1:F:505:LEU:HD13 | 2.15 | 0.47 |
| 1:F:507:ARG:O | 1:F:507:ARG:HD3 | 2.15 | 0.47 |
| 1:A:134:ILE:HA | 1:A:139:ALA:HB3 | 1.97 | 0.47 |
| 1:A:270:LEU:O | 1:A:273:MET:O | 2.33 | 0.47 |
| 2:B:74:VAL:HG13 | 2:B:106:LEU:HG | 1.97 | 0.47 |
| 2:B:501:GLU:HB2 | 2:B:502:LYS:H | 1.36 | 0.47 |
| 2:C:313:ILE:HD11 | 2:C:370:PHE:CB | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:164:LEU:HD11 | 1:F:197:GLU:HG3 | 1.96 | 0.47 |
| 1:F:287:THR:CG2 | 1:F:414:ASN:ND2 | 2.74 | 0.47 |
| 1:F:458:MET:SD | 1:F:461:SER:HB3 | 2.55 | 0.47 |
| 1:A:237:PHE:CB | 1:A:246:ILE:HG13 | 2.44 | 0.46 |
| 1:A:28:PHE:CE1 | 1:A:222:ILE:HD11 | 2.50 | 0.46 |
| 1:A:313:ILE:HG13 | 1:A:372:PRO:CG | 2.45 | 0.46 |
| 1:A:65:ILE:HD11 | 1:A:97:LEU:HD21 | 1.97 | 0.46 |
| 1:A:79:THR:HB | 1:A:82:ASP:OD2 | 2.14 | 0.46 |
| 2:B:170:ARG:HH12 | 2:B:174:ILE:HD11 | 1.80 | 0.46 |
| 2:B:222:ILE:O | 2:B:230:HIS:CE1 | 2.69 | 0.46 |
| 2:C:144:ILE:HD11 | 2:C:171:LEU:HD11 | 1.96 | 0.46 |
| 2:C:144:ILE:HD13 | 2:C:167:LEU:HD21 | 1.97 | 0.46 |
| 2:B:193:ARG:NH2 | 2:C:195:GLY:O | 2.42 | 0.46 |
| 2:E:468:ARG:HH11 | 2:E:468:ARG:HG2 | 1.80 | 0.46 |
| 1:F:315:PHE:CE1 | 1:F:375:ILE:CD1 | 2.97 | 0.46 |
| 1:A:153:GLN:O | 1:A:154:TYR:CB | 2.63 | 0.46 |
| 1:A:357:GLU:HG3 | 1:A:358:ASP:N | 2.29 | 0.46 |
| 1:A:356:LEU:CD1 | 1:A:387:VAL:HG21 | 2.45 | 0.46 |
| 2:B:327:ASN:HD21 | 2:C:459:ARG:HB3 | 1.79 | 0.46 |
| 2:B:463:HIS:ND1 | 2:B:463:HIS:C | 2.68 | 0.46 |
| 2:B:52:LYS:HE2 | 3:B:903:ATP:O1B | 2.16 | 0.46 |
| 2:C:315:PHE:CE2 | 2:C:363:ILE:HA | 2.50 | 0.46 |
| 2:C:249:LEU:HD12 | 2:C:394:GLN:OE1 | 2.15 | 0.46 |
| 2:D:147:VAL:CG2 | 2:D:148:THR:N | 2.77 | 0.46 |
| 2:D:211:LEU:HD12 | 2:D:215:ARG:O | 2.15 | 0.46 |
| 2:D:486:PHE:CE2 | 2:D:496:ARG:HD3 | 2.51 | 0.46 |
| 2:E:318:GLU:OE2 | 1:F:432:GLU:HB3 | 2.15 | 0.46 |
| 2:E:453:ILE:HB | 2:E:470:PHE:HD2 | 1.80 | 0.46 |
| 1:A:340:ARG:C | 1:A:342:ASN:H | 2.18 | 0.46 |
| 2:C:215:ARG:NE | 2:C:215:ARG:HA | 2.30 | 0.46 |
| 2:C:49:GLY:O | 2:C:218:ARG:NH2 | 2.48 | 0.46 |
| 2:C:64:ILE:CD1 | 2:C:103:LEU:HB2 | 2.46 | 0.46 |
| 2:D:181:THR:HG22 | 2:D:181:THR:O | 2.14 | 0.46 |
| 2:E:219:THR:HA | 2:E:235:TYR:O | 2.15 | 0.46 |
| 2:D:348:CYS:HB3 | 2:E:254:LEU:HB3 | 1.98 | 0.46 |
| 1:F:255:THR:O | 1:F:255:THR:HG22 | 2.15 | 0.46 |
| 1:F:436:THR:OG1 | 1:F:458:MET:HG2 | 2.15 | 0.46 |
| 1:A:68:ASP:CG | 1:A:102:LYS:HZ2 | 2.18 | 0.46 |
| 2:B:127:ILE:HG22 | 2:B:127:ILE:O | 2.16 | 0.46 |
| 2:B:184:ARG:HH22 | 2:B:187:GLU:C | 2.19 | 0.46 |
| 2:B:208:ARG:O | 2:B:218:ARG:HA | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:269:ARG:HG2 | 2:B:479:ILE:HB | 1.96 | 0.46 |
| 2:B:313:ILE:HG13 | 2:B:372:PRO:HG3 | 1.97 | 0.46 |
| 2:B:454:ASN:HB2 | 2:B:467:ILE:HD13 | 1.96 | 0.46 |
| 2:C:333:MET:H | 2:C:333:MET:HG2 | 1.42 | 0.46 |
| 2:C:49:GLY:CA | 3:C:903:ATP:O2B | 2.63 | 0.46 |
| 2:D:28:PHE:HA | 2:D:31:ILE:HD12 | 1.98 | 0.46 |
| 2:E:191:ILE:HG23 | 2:E:206:ILE:CD1 | 2.45 | 0.46 |
| 2:E:221:GLU:HG3 | 2:E:222:ILE:N | 2.31 | 0.46 |
| 2:E:281:ASP:O | 2:E:282:SER:HB3 | 2.16 | 0.46 |
| 1:F:147:VAL:HG11 | 1:F:180:MET:HE3 | 1.97 | 0.46 |
| 1:F:471:MET:O | 1:F:471:MET:HE2 | 2.16 | 0.46 |
| 1:A:145:ASP:OD2 | 1:A:181:THR:HG21 | 2.15 | 0.46 |
| 1:A:292:THR:HB | 1:A:440:LEU:HB3 | 1.96 | 0.46 |
| 1:A:423:HIS:O | 1:F:418:GLN:HB2 | 2.16 | 0.46 |
| 1:A:440:LEU:HD22 | 1:A:470:PHE:CE2 | 2.51 | 0.46 |
| 2:B:387:VAL:CG1 | 2:B:388:SER:N | 2.78 | 0.46 |
| 2:B:469:GLU:HG2 | 2:B:480:LYS:HB2 | 1.97 | 0.46 |
| 2:C:232:LYS:N | 2:C:232:LYS:CD | 2.79 | 0.46 |
| 2:B:353:SER:HA | 2:C:250:GLY:O | 2.16 | 0.46 |
| 2:C:357:GLU:HG3 | 2:C:358:ASP:N | 2.30 | 0.46 |
| 2:D:185:ILE:N | 2:D:185:ILE:HD12 | 2.31 | 0.46 |
| 2:E:191:ILE:HD12 | 2:E:206:ILE:CG1 | 2.45 | 0.46 |
| 1:F:207:LEU:HD21 | 1:F:220:LEU:HD12 | 1.96 | 0.46 |
| 1:F:414:ASN:HD21 | 1:F:426:THR:HG23 | 1.80 | 0.46 |
| 1:F:455:VAL:HG12 | 1:F:463:HIS:ND1 | 2.31 | 0.46 |
| 1:F:505:LEU:O | 1:F:506:SER:CB | 2.63 | 0.46 |
| 2:B:122:ASP:C | 2:B:124:SER:H | 2.19 | 0.46 |
| 2:B:489:ILE:O | 2:B:492:GLY:N | 2.49 | 0.46 |
| 2:C:31:ILE:HD11 | 2:C:246:ILE:CG2 | 2.41 | 0.46 |
| 2:C:426:THR:HG21 | 2:C:430:ILE:HG12 | 1.97 | 0.46 |
| 2:E:283:ILE:HG13 | 2:E:400:THR:HG23 | 1.98 | 0.46 |
| 2:E:396:VAL:O | 2:E:400:THR:HB | 2.16 | 0.46 |
| 2:E:453:ILE:O | 2:E:453:ILE:HG23 | 2.15 | 0.46 |
| 2:E:454:ASN:ND2 | 2:E:456:PHE:HA | 2.30 | 0.46 |
| 1:F:149:SER:HA | 1:F:152:GLN:HB2 | 1.96 | 0.46 |
| 1:F:319:GLU:HA | 1:F:320:SEP:O2P | 2.16 | 0.46 |
| 1:A:333:MET:O | 1:A:334:ASP:CB | 2.63 | 0.46 |
| 1:A:392:PHE:HE2 | 1:A:430:ILE:CD1 | 2.29 | 0.46 |
| 2:B:213:GLY:O | 2:B:214:GLU:HB2 | 2.16 | 0.46 |
| 2:B:265:SER:CB | 2:B:270:LEU:HD13 | 2.46 | 0.46 |
| 2:B:363:ILE:HG22 | 2:B:367:ILE:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:79:THR:HG23 | 2:B:82:ASP:H | 1.80 | 0.46 |
| 3:B:901:ATP:O3' | 2:C:457:LYS:HB2 | 2.15 | 0.46 |
| 2:C:38:ILE:HG22 | 2:C:39:GLY:N | 2.31 | 0.46 |
| 1:F:315:PHE:CE2 | 1:F:347:VAL:HG21 | 2.50 | 0.46 |
| 1:A:466:ALA:HA | 1:F:448:GLU:HG2 | 1.98 | 0.46 |
| 1:F:514:GLU:CB | 1:F:519:SER:HB3 | 2.46 | 0.46 |
| 2:B:360:LEU:HD23 | 2:B:399:VAL:CG2 | 2.46 | 0.46 |
| 2:B:57:ILE:C | 2:B:59:PHE:N | 2.69 | 0.46 |
| 2:C:283:ILE:N | 2:C:283:ILE:HD12 | 2.31 | 0.46 |
| 2:C:430:ILE:O | 2:C:432:GLU:N | 2.48 | 0.46 |
| 2:D:123:LEU:HA | 2:D:123:LEU:HD22 | 1.83 | 0.46 |
| 2:D:356:LEU:HD13 | 2:D:387:VAL:HG21 | 1.98 | 0.46 |
| 2:D:294:LYS:N | 3:D:901:ATP:O1B | 2.46 | 0.46 |
| 2:E:223:LEU:HD22 | 2:E:223:LEU:O | 2.16 | 0.46 |
| 2:E:269:ARG:NH2 | 2:E:468:ARG:NH2 | 2.64 | 0.46 |
| 1:F:270:LEU:CD2 | 1:F:274:CYS:SG | 3.04 | 0.46 |
| 1:F:484:ARG:CZ | 1:F:484:ARG:HB2 | 2.46 | 0.46 |
| 1:A:191:ILE:CG2 | 1:A:198:GLU:HG3 | 2.46 | 0.46 |
| 1:A:207:LEU:HD22 | 1:A:237:PHE:HE2 | 1.81 | 0.46 |
| 1:A:231:MET:CE | 1:A:251:ALA:HB2 | 2.45 | 0.46 |
| 2:B:20:LYS:HG2 | 2:B:35:GLY:O | 2.16 | 0.46 |
| 2:B:462:TRP:CE3 | 2:B:463:HIS:N | 2.84 | 0.46 |
| 2:C:249:LEU:HD12 | 2:C:394:GLN:HG2 | 1.97 | 0.46 |
| 2:D:211:LEU:O | 2:D:215:ARG:O | 2.34 | 0.46 |
| 2:E:46:GLY:HA2 | 2:E:184:ARG:HD3 | 1.97 | 0.46 |
| 2:E:501:GLU:O | 2:E:502:LYS:HG3 | 2.16 | 0.46 |
| 1:F:122:ASP:O | 1:F:126:LEU:HB2 | 2.16 | 0.46 |
| 1:F:191:ILE:CG2 | 1:F:198:GLU:HG3 | 2.46 | 0.46 |
| 1:A:393:ARG:NH1 | 1:F:385:ARG:HA | 2.31 | 0.46 |
| 1:A:375:ILE:O | 1:A:410:GLY:HA2 | 2.15 | 0.46 |
| 2:C:150:VAL:O | 2:C:153:GLN:HG3 | 2.16 | 0.46 |
| 2:C:197:GLU:N | 2:C:197:GLU:OE2 | 2.39 | 0.46 |
| 2:D:287:THR:HG23 | 2:D:414:ASN:ND2 | 2.22 | 0.46 |
| 2:D:382:ALA:O | 2:D:385:ARG:HG3 | 2.16 | 0.46 |
| 2:E:123:LEU:HD22 | 2:E:166:ARG:HD2 | 1.98 | 0.46 |
| 1:A:116:GLU:O | 1:A:117:VAL:CB | 2.63 | 0.45 |
| 1:A:185:ILE:HD12 | 1:A:185:ILE:N | 2.31 | 0.45 |
| 1:A:364:LYS:HG2 | 1:A:402:TYR:CD2 | 2.50 | 0.45 |
| 2:C:50:THR:HA | 5:C:528:HOH:O | 2.15 | 0.45 |
| 2:C:88:ARG:HD3 | 2:D:15:HIS:C | 2.36 | 0.45 |
| 2:D:191:ILE:HD12 | 2:D:198:GLU:HG2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:262:ARG:HH22 | 2:E:461:SER:HB2 | 1.81 | 0.45 |
| 1:F:387:VAL:CG1 | 1:F:388:SER:N | 2.79 | 0.45 |
| 1:F:420:MET:HE3 | 1:F:492:GLY:HA3 | 1.98 | 0.45 |
| 1:F:292:THR:HB | 1:F:440:LEU:HB3 | 1.98 | 0.45 |
| 2:B:123:LEU:HD12 | 2:B:166:ARG:HD2 | 1.98 | 0.45 |
| 2:B:84:ILE:HG23 | 2:B:94:LEU:HB2 | 1.97 | 0.45 |
| 2:E:385:ARG:HA | 1:F:393:ARG:HH12 | 1.81 | 0.45 |
| 2:E:495:THR:HA | 1:F:487:GLU:OE1 | 2.17 | 0.45 |
| 2:E:504:GLU:HG2 | 2:E:505:LEU:N | 2.30 | 0.45 |
| 1:A:420:MET:O | 1:A:422:ALA:N | 2.41 | 0.45 |
| 2:C:334:ASP:C | 2:C:334:ASP:OD1 | 2.55 | 0.45 |
| 2:C:462:TRP:CD2 | 2:C:463:HIS:O | 2.69 | 0.45 |
| 2:D:313:ILE:HG21 | 2:D:315:PHE:CZ | 2.50 | 0.45 |
| 2:D:305:ALA:HB2 | 2:D:374:ARG:HD2 | 1.98 | 0.45 |
| 2:D:471:MET:HE2 | 2:D:478:ASP:HB2 | 1.98 | 0.45 |
| 1:F:222:ILE:HD12 | 1:F:222:ILE:N | 2.31 | 0.45 |
| 1:F:356:LEU:CD1 | 1:F:387:VAL:HG21 | 2.44 | 0.45 |
| 1:F:284:ILE:HB | 1:F:411:LEU:HD12 | 1.97 | 0.45 |
| 1:A:262:ARG:NH2 | 1:A:461:SER:HB2 | 2.31 | 0.45 |
| 1:A:496:ARG:HG3 | 2:B:487:GLU:OE1 | 2.16 | 0.45 |
| 1:A:295:THR:HB | 3:A:901:ATP:PA | 2.57 | 0.45 |
| 2:B:140:ARG:CB | 2:B:140:ARG:NH1 | 2.69 | 0.45 |
| 2:B:379:SER:H | 2:B:413:THR:HG22 | 1.81 | 0.45 |
| 2:C:150:VAL:CG1 | 2:C:151:PHE:N | 2.80 | 0.45 |
| 2:D:218:ARG:NH1 | 2:D:239:ILE:HD12 | 2.31 | 0.45 |
| 2:D:298:VAL:HG13 | 2:D:376:ALA:HB1 | 1.98 | 0.45 |
| 2:E:74:VAL:CG2 | 2:E:130:ILE:HD12 | 2.46 | 0.45 |
| 2:E:315:PHE:CE2 | 2:E:347:VAL:HG21 | 2.51 | 0.45 |
| 2:E:392:PHE:O | 2:E:395:PHE:N | 2.49 | 0.45 |
| 2:E:56:SER:OG | 2:E:73:PHE:HE1 | 1.99 | 0.45 |
| 1:F:134:ILE:HD11 | 1:F:142:VAL:HG22 | 1.97 | 0.45 |
| 1:A:293:GLY:HA2 | 3:A:901:ATP:O1A | 2.16 | 0.45 |
| 1:A:311:ARG:O | 1:A:373:ALA:N | 2.40 | 0.45 |
| 1:A:387:VAL:HG12 | 1:A:388:SER:N | 2.31 | 0.45 |
| 1:A:380:LEU:N | 1:A:413:THR:O | 2.48 | 0.45 |
| 1:A:286:ALA:HA | 1:A:438:ILE:O | 2.16 | 0.45 |
| 2:B:218:ARG:NH2 | 2:B:239:ILE:HD12 | 2.31 | 0.45 |
| 2:C:73:PHE:HB3 | 2:C:105:ILE:HD13 | 1.97 | 0.45 |
| 2:C:127:ILE:HD12 | 2:C:167:LEU:HD13 | 1.98 | 0.45 |
| 2:C:127:ILE:HG21 | 2:C:170:ARG:HG3 | 1.97 | 0.45 |
| 2:C:60:LEU:O | 2:C:61:TYR:C | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:445:ILE:HA | 2:D:496:ARG:NH1 | 2.32 | 0.45 |
| 2:E:140:ARG:HH11 | 2:E:140:ARG:HA | 1.81 | 0.45 |
| 2:E:145:ASP:O | 2:E:146:SER:OG | 2.32 | 0.45 |
| 1:F:122:ASP:O | 1:F:126:LEU:N | 2.50 | 0.45 |
| 1:F:299:SER:CB | 1:F:333:MET:HE1 | 2.46 | 0.45 |
| 1:F:296:LEU:HD13 | 1:F:331:TRP:CE2 | 2.51 | 0.45 |
| 1:A:164:LEU:HD11 | 1:A:197:GLU:CG | 2.41 | 0.45 |
| 1:A:287:THR:HG21 | 1:A:425:ILE:O | 2.16 | 0.45 |
| 2:C:287:THR:HG22 | 2:C:288:GLY:N | 2.31 | 0.45 |
| 2:C:311:ARG:HD2 | 2:C:371:LYS:CE | 2.46 | 0.45 |
| 2:D:263:VAL:HG21 | 2:D:280:LYS:HA | 1.98 | 0.45 |
| 2:E:14:GLU:HG3 | 2:E:16:GLN:N | 2.26 | 0.45 |
| 2:E:193:ARG:HH11 | 2:E:193:ARG:HG2 | 1.82 | 0.45 |
| 2:E:400:THR:HG22 | 2:E:401:GLY:N | 2.30 | 0.45 |
| 2:E:283:ILE:HG23 | 2:E:412:PHE:HE1 | 1.79 | 0.45 |
| 1:F:31:ILE:HG22 | 1:F:222:ILE:HD13 | 1.97 | 0.45 |
| 1:F:387:VAL:HG12 | 1:F:388:SER:N | 2.32 | 0.45 |
| 1:A:246:ILE:O | 1:A:248:PRO:HD3 | 2.17 | 0.45 |
| 1:A:296:LEU:HA | 1:A:331:TRP:CZ3 | 2.51 | 0.45 |
| 2:B:314:LEU:HB3 | 2:B:346:ILE:HD13 | 1.98 | 0.45 |
| 2:B:356:LEU:HD21 | 2:B:392:PHE:HA | 1.99 | 0.45 |
| 2:C:300:ARG:N | 2:C:333:MET:HE1 | 2.31 | 0.45 |
| 2:D:259:SER:OG | 2:D:261:VAL:HG23 | 2.17 | 0.45 |
| 2:D:316:ALA:O | 2:D:348:CYS:HA | 2.16 | 0.45 |
| 2:E:121:PHE:O | 2:E:122:ASP:C | 2.55 | 0.45 |
| 1:F:497:ILE:HG13 | 1:F:497:ILE:O | 2.14 | 0.45 |
| 1:A:18:ILE:HD11 | 1:F:85:LYS:HG3 | 1.99 | 0.45 |
| 1:A:211:LEU:HB2 | 1:A:216:ARG:CD | 2.46 | 0.45 |
| 2:B:122:ASP:C | 2:B:124:SER:N | 2.70 | 0.45 |
| 2:B:147:VAL:CG2 | 2:B:148:THR:N | 2.79 | 0.45 |
| 2:B:284:ILE:H | 2:B:284:ILE:HD12 | 1.81 | 0.45 |
| 2:B:445:ILE:HD12 | 2:B:486:PHE:CZ | 2.52 | 0.45 |
| 2:C:406:GLU:O | 2:C:408:ILE:HG13 | 2.17 | 0.45 |
| 2:D:325:LEU:HD23 | 2:D:335:PHE:HB2 | 1.98 | 0.45 |
| 1:F:178:THR:CG2 | 1:F:179:VAL:N | 2.79 | 0.45 |
| 1:F:256:GLN:HG2 | 1:F:256:GLN:H | 1.50 | 0.45 |
| 1:A:127:ILE:HD11 | 1:A:167:LEU:HD13 | 1.98 | 0.45 |
| 1:A:268:VAL:O | 1:A:271:ASP:HB2 | 2.17 | 0.45 |
| 1:A:352:GLU:CD | 1:A:352:GLU:N | 2.70 | 0.45 |
| 1:A:489:ILE:HD13 | 1:A:494:PRO:HB3 | 1.99 | 0.45 |
| 2:B:116:GLU:HG2 | 2:B:117:VAL:N | 2.23 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:140:ARG:CA | 2:B:140:ARG:HH11 | 2.30 | 0.45 |
| 2:B:212:GLU:HG2 | 2:B:212:GLU:O | 2.16 | 0.45 |
| 2:B:88:ARG:HG2 | 2:B:88:ARG:NH1 | 2.32 | 0.45 |
| 2:C:79:THR:HG22 | 2:C:82:ASP:H | 1.79 | 0.45 |
| 2:D:202:ASP:HA | 2:D:226:ARG:HD2 | 1.99 | 0.45 |
| 2:D:333:MET:HG2 | 5:D:910:HOH:O | 2.17 | 0.45 |
| 2:D:315:PHE:CD2 | 2:D:347:VAL:HG21 | 2.52 | 0.45 |
| 1:F:129:ARG:O | 1:F:132:TYR:HB3 | 2.17 | 0.45 |
| 1:F:471:MET:SD | 1:F:478:ASP:HB3 | 2.56 | 0.45 |
| 1:A:183:GLU:OE2 | 2:B:161:ARG:NH1 | 2.49 | 0.45 |
| 2:B:298:VAL:HG12 | 2:B:299:SER:N | 2.32 | 0.45 |
| 2:D:23:THR:O | 2:D:24:MET:HB2 | 2.17 | 0.45 |
| 2:E:144:ILE:HD11 | 2:E:171:LEU:HD11 | 1.98 | 0.45 |
| 1:F:131:ASN:OD1 | 1:F:174:ILE:HD12 | 2.16 | 0.45 |
| 1:F:504:GLU:HB2 | 1:F:505:LEU:H | 1.48 | 0.45 |
| 1:A:207:LEU:HD22 | 1:A:237:PHE:CE2 | 2.52 | 0.44 |
| 1:A:428:SER:OG | 1:A:430:ILE:HD11 | 2.17 | 0.44 |
| 2:B:302:VAL:HG13 | 2:B:344:LEU:HD23 | 1.98 | 0.44 |
| 2:B:492:GLY:C | 2:B:494:PRO:HD3 | 2.36 | 0.44 |
| 2:D:67:PHE:CB | 2:D:69:GLU:HG3 | 2.47 | 0.44 |
| 1:F:231:MET:SD | 1:F:251:ALA:HB2 | 2.56 | 0.44 |
| 1:F:379:SER:HA | 1:F:413:THR:HG22 | 1.99 | 0.44 |
| 1:F:514:GLU:O | 1:F:515:LYS:CB | 2.60 | 0.44 |
| 1:A:146:SER:H | 1:A:181:THR:HG22 | 1.81 | 0.44 |
| 1:A:182:THR:HG22 | 1:A:183:GLU:N | 2.32 | 0.44 |
| 1:A:24:MET:N | 1:A:29:ASP:OD2 | 2.44 | 0.44 |
| 1:A:311:ARG:NH1 | 1:A:371:LYS:HE3 | 2.32 | 0.44 |
| 3:A:901:ATP:H3' | 2:B:458:MET:O | 2.17 | 0.44 |
| 2:B:105:ILE:O | 2:B:105:ILE:HG22 | 2.16 | 0.44 |
| 2:B:295:THR:HG23 | 2:B:378:ASP:OD2 | 2.18 | 0.44 |
| 2:B:57:ILE:C | 2:B:59:PHE:H | 2.20 | 0.44 |
| 2:C:337:GLU:OE1 | 2:C:340:ARG:NH1 | 2.50 | 0.44 |
| 2:C:68:ASP:CG | 2:C:102:LYS:HZ1 | 2.20 | 0.44 |
| 2:D:191:ILE:HB | 2:D:198:GLU:HG2 | 1.97 | 0.44 |
| 2:E:161:ARG:CA | 2:E:196:VAL:HG11 | 2.47 | 0.44 |
| 2:E:191:ILE:CB | 2:E:198:GLU:HG2 | 2.46 | 0.44 |
| 2:E:315:PHE:CD2 | 2:E:363:ILE:HD13 | 2.52 | 0.44 |
| 1:F:121:PHE:HD2 | 1:F:121:PHE:HA | 1.69 | 0.44 |
| 1:F:315:PHE:HE1 | 1:F:375:ILE:CD1 | 2.30 | 0.44 |
| 1:F:515:LYS:HG3 | 1:F:517:PRO:HD2 | 1.98 | 0.44 |
| 1:A:44:VAL:HG22 | 1:A:205:VAL:HB | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:ILE:HG13 | 1:A:372:PRO:HG2 | 1.98 | 0.44 |
| 1:A:441:GLN:O | 1:A:441:GLN:HG3 | 2.18 | 0.44 |
| 2:B:44:VAL:HA | 2:B:205:VAL:O | 2.17 | 0.44 |
| 2:B:360:LEU:HD23 | 2:B:399:VAL:HG23 | 1.99 | 0.44 |
| 2:B:371:LYS:O | 2:B:371:LYS:CD | 2.66 | 0.44 |
| 2:D:47:THR:HG22 | 2:D:184:ARG:C | 2.36 | 0.44 |
| 1:F:116:GLU:O | 1:F:117:VAL:HB | 2.16 | 0.44 |
| 1:A:462:TRP:C | 1:A:463:HIS:HD1 | 2.21 | 0.44 |
| 2:B:126:LEU:C | 2:B:128:GLU:H | 2.19 | 0.44 |
| 2:B:79:THR:HG22 | 2:B:82:ASP:OD2 | 2.17 | 0.44 |
| 2:C:263:VAL:CG2 | 2:C:280:LYS:HA | 2.47 | 0.44 |
| 2:C:469:GLU:CG | 2:C:480:LYS:HE3 | 2.47 | 0.44 |
| 2:D:340:ARG:C | 2:D:342:ASN:N | 2.71 | 0.44 |
| 2:D:378:ASP:O | 2:D:379:SER:HB3 | 2.18 | 0.44 |
| 2:D:464:ASP:OD1 | 2:D:465:LYS:N | 2.50 | 0.44 |
| 2:E:130:ILE:O | 2:E:134:ILE:HG12 | 2.17 | 0.44 |
| 2:E:443:VAL:HG12 | 2:E:445:ILE:HG13 | 2.00 | 0.44 |
| 2:E:489:ILE:HD12 | 2:E:489:ILE:N | 2.32 | 0.44 |
| 1:F:123:LEU:HD12 | 1:F:166:ARG:HD2 | 1.99 | 0.44 |
| 1:F:80:PRO:HB2 | 1:F:81:GLN:NE2 | 2.32 | 0.44 |
| 1:A:31:ILE:HD13 | 1:A:220:LEU:HD22 | 1.98 | 0.44 |
| 1:A:320:SEP:C | 1:A:348:CYS:HG | 2.27 | 0.44 |
| 1:A:420:MET:CE | 2:B:490:ILE:HG21 | 2.48 | 0.44 |
| 2:C:126:LEU:O | 2:C:129:ARG:N | 2.50 | 0.44 |
| 2:C:284:ILE:HD11 | 2:C:409:THR:HG22 | 2.00 | 0.44 |
| 2:D:41:SER:HB2 | 2:D:178:THR:HB | 1.98 | 0.44 |
| 2:E:104:PHE:CE2 | 2:E:106:LEU:HB2 | 2.53 | 0.44 |
| 1:F:106:LEU:HD13 | 1:F:129:ARG:NH2 | 2.32 | 0.44 |
| 1:F:504:GLU:HB3 | 1:F:507:ARG:NH2 | 2.32 | 0.44 |
| 1:A:127:ILE:HD11 | 1:A:167:LEU:HD12 | 1.99 | 0.44 |
| 2:B:47:THR:O | 2:B:50:THR:HB | 2.17 | 0.44 |
| 2:B:497:ILE:HD12 | 2:B:498:THR:N | 2.33 | 0.44 |
| 2:C:41:SER:HA | 2:C:178:THR:O | 2.18 | 0.44 |
| 2:D:353:SER:O | 2:D:354:ALA:CB | 2.61 | 0.44 |
| 2:D:311:ARG:CD | 2:D:371:LYS:HE3 | 2.29 | 0.44 |
| 2:D:385:ARG:NH2 | 2:E:433:ILE:CD1 | 2.80 | 0.44 |
| 1:F:191:ILE:HD13 | 1:F:198:GLU:HG2 | 1.99 | 0.44 |
| 1:A:418:GLN:HB2 | 2:B:423:HIS:O | 2.17 | 0.44 |
| 2:B:280:LYS:HZ3 | 2:B:407:GLU:HB3 | 1.83 | 0.44 |
| 2:B:461:SER:OG | 2:B:462:TRP:N | 2.50 | 0.44 |
| 2:D:148:THR:HG21 | 2:D:193:ARG:HD2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:291:GLY:CA | 3:D:901:ATP:O2B | 2.65 | 0.44 |
| 2:D:458:MET:HB2 | 2:D:463:HIS:HD2 | 1.83 | 0.44 |
| 2:E:202:ASP:HB2 | 2:E:203:ASN:ND2 | 2.33 | 0.44 |
| 2:E:212:GLU:HG2 | 2:E:212:GLU:O | 2.17 | 0.44 |
| 2:E:451:ARG:HH11 | 2:E:451:ARG:CG | 2.30 | 0.44 |
| 2:E:469:GLU:CB | 2:E:483:PHE:CZ | 3.01 | 0.44 |
| 1:F:21:MET:HE3 | 1:F:141:ARG:NE | 2.33 | 0.44 |
| 1:F:468:ARG:HD3 | 1:F:479:ILE:HG22 | 1.99 | 0.44 |
| 1:F:504:GLU:HA | 1:F:507:ARG:HE | 1.81 | 0.44 |
| 1:A:79:THR:HG23 | 1:A:81:GLN:HG2 | 1.92 | 0.44 |
| 2:B:194:TYR:C | 2:B:196:VAL:N | 2.67 | 0.44 |
| 2:B:266:GLY:O | 2:B:300:ARG:CG | 2.66 | 0.44 |
| 2:B:327:ASN:ND2 | 2:C:459:ARG:HB3 | 2.33 | 0.44 |
| 2:C:239:ILE:HG12 | 2:C:244:ILE:CD1 | 2.48 | 0.44 |
| 2:C:284:ILE:N | 2:C:284:ILE:HD12 | 2.33 | 0.44 |
| 2:C:325:LEU:CD2 | 2:C:335:PHE:HB2 | 2.47 | 0.44 |
| 2:E:451:ARG:HB3 | 2:E:470:PHE:CE2 | 2.53 | 0.44 |
| 2:D:495:THR:HA | 2:E:487:GLU:OE2 | 2.18 | 0.44 |
| 1:F:462:TRP:O | 1:F:463:HIS:CG | 2.70 | 0.44 |
| 1:A:448:GLU:HG2 | 2:B:466:ALA:HA | 2.00 | 0.44 |
| 2:B:353:SER:O | 2:B:354:ALA:HB2 | 2.17 | 0.44 |
| 2:B:44:VAL:HG22 | 2:B:205:VAL:HG12 | 1.99 | 0.44 |
| 2:B:500:ASP:C | 2:B:501:GLU:HG3 | 2.38 | 0.44 |
| 2:B:84:ILE:HD12 | 2:B:94:LEU:CB | 2.44 | 0.44 |
| 2:C:140:ARG:CA | 2:C:140:ARG:HH11 | 2.31 | 0.44 |
| 2:C:420:MET:HE3 | 2:C:492:GLY:HA3 | 2.00 | 0.44 |
| 2:D:333:MET:CA | 5:D:913:HOH:O | 2.44 | 0.44 |
| 2:D:426:THR:HB | 2:D:431:GLU:OE2 | 2.18 | 0.44 |
| 2:E:192:ALA:HB3 | 2:E:197:GLU:OE2 | 2.18 | 0.44 |
| 2:E:489:ILE:HA | 2:E:494:PRO:HG3 | 1.99 | 0.44 |
| 2:E:504:GLU:CG | 2:E:505:LEU:H | 2.30 | 0.44 |
| 1:F:44:VAL:O | 1:F:181:THR:HA | 2.18 | 0.44 |
| 1:F:313:ILE:HG13 | 1:F:372:PRO:HG2 | 2.00 | 0.44 |
| 1:A:124:SER:O | 1:A:128:GLU:HG3 | 2.18 | 0.43 |
| 2:B:199:PHE:CD2 | 2:B:199:PHE:N | 2.86 | 0.43 |
| 2:B:93:ASP:OD2 | 2:B:96:LYS:HB2 | 2.18 | 0.43 |
| 2:D:19:ALA:HB1 | 2:D:38:ILE:HD12 | 1.99 | 0.43 |
| 2:E:148:THR:HG1 | 2:E:182:THR:HG23 | 1.83 | 0.43 |
| 1:F:231:MET:CE | 1:F:251:ALA:HB2 | 2.48 | 0.43 |
| 1:F:445:ILE:HG22 | 1:F:446:ARG:HD2 | 2.00 | 0.43 |
| 1:F:513:GLN:HA | 1:F:513:GLN:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:486:PHE:CB | 1:A:489:ILE:HD11 | 2.48 | 0.43 |
| 2:B:126:LEU:C | 2:B:128:GLU:N | 2.71 | 0.43 |
| 2:B:283:ILE:HG12 | 2:B:400:THR:HG23 | 2.00 | 0.43 |
| 2:C:134:ILE:HG23 | 2:C:139:ALA:HB3 | 1.99 | 0.43 |
| 2:C:164:LEU:HD11 | 2:C:197:GLU:HG3 | 2.00 | 0.43 |
| 2:D:123:LEU:HD21 | 2:D:163:GLU:HB3 | 2.00 | 0.43 |
| 2:D:273:MET:O | 2:D:463:HIS:HA | 2.17 | 0.43 |
| 2:E:419:PHE:O | 2:E:420:MET:HB2 | 2.18 | 0.43 |
| 1:F:111:ASP:HA | 1:F:112:PRO:HD3 | 1.92 | 0.43 |
| 1:F:127:ILE:CD1 | 1:F:167:LEU:HD13 | 2.48 | 0.43 |
| 1:F:185:ILE:N | 1:F:185:ILE:HD13 | 2.33 | 0.43 |
| 1:A:377:ILE:HD13 | 1:A:412:PHE:CD2 | 2.53 | 0.43 |
| 2:B:146:SER:H | 2:B:181:THR:CG2 | 2.31 | 0.43 |
| 2:B:87:ALA:HB1 | 2:B:92:TRP:CD1 | 2.53 | 0.43 |
| 2:C:292:THR:HB | 2:C:440:LEU:HB3 | 1.99 | 0.43 |
| 2:C:453:ILE:HD13 | 2:C:453:ILE:C | 2.38 | 0.43 |
| 2:C:81:GLN:CD | 2:C:81:GLN:H | 2.20 | 0.43 |
| 2:D:350:TYR:CE1 | 2:E:252:MET:HE2 | 2.53 | 0.43 |
| 2:E:313:ILE:HB | 2:E:375:ILE:HD13 | 1.94 | 0.43 |
| 2:E:438:ILE:N | 2:E:438:ILE:HD12 | 2.33 | 0.43 |
| 1:F:406:GLU:HB3 | 1:F:408:ILE:HG12 | 1.99 | 0.43 |
| 2:B:131:ASN:OD1 | 2:B:174:ILE:HD12 | 2.18 | 0.43 |
| 2:B:377:ILE:HB | 2:B:412:PHE:HD2 | 1.82 | 0.43 |
| 2:B:426:THR:HG22 | 2:B:429:HIS:H | 1.83 | 0.43 |
| 2:C:131:ASN:OD1 | 2:C:174:ILE:HD12 | 2.17 | 0.43 |
| 2:C:387:VAL:CG1 | 2:C:388:SER:N | 2.82 | 0.43 |
| 2:D:350:TYR:O | 2:D:351:PRO:C | 2.56 | 0.43 |
| 2:E:444:GLU:O | 2:E:494:PRO:HD2 | 2.17 | 0.43 |
| 1:F:496:ARG:HD3 | 1:F:496:ARG:N | 2.33 | 0.43 |
| 1:A:136:LYS:HD3 | 1:A:137:TYR:HE1 | 1.83 | 0.43 |
| 1:A:153:GLN:C | 1:A:154:TYR:CD2 | 2.92 | 0.43 |
| 1:A:305:ALA:O | 1:A:310:GLU:HB2 | 2.19 | 0.43 |
| 1:A:312:ALA:HA | 1:A:374:ARG:O | 2.19 | 0.43 |
| 1:A:378:ASP:OD1 | 1:A:413:THR:HG21 | 2.19 | 0.43 |
| 1:A:274:CYS:HA | 1:A:463:HIS:HB2 | 1.99 | 0.43 |
| 1:A:471:MET:HE2 | 1:A:471:MET:O | 2.18 | 0.43 |
| 1:A:72:VAL:HB | 1:A:142:VAL:HG22 | 2.00 | 0.43 |
| 1:A:211:LEU:HD21 | 2:B:188:TYR:HE2 | 1.84 | 0.43 |
| 2:C:121:PHE:O | 2:C:125:ALA:HB3 | 2.18 | 0.43 |
| 2:C:392:PHE:CE2 | 2:C:430:ILE:HD11 | 2.54 | 0.43 |
| 2:C:66:GLU:C | 2:C:67:PHE:CD1 | 2.92 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:79:THR:HG23 | 2:C:81:GLN:HG2 | 2.01 | 0.43 |
| 2:C:318:GLU:OE2 | 2:D:432:GLU:HG2 | 2.19 | 0.43 |
| 2:E:184:ARG:CD | 2:E:191:ILE:O | 2.66 | 0.43 |
| 2:E:22:ARG:HB3 | 2:E:29:ASP:OD2 | 2.19 | 0.43 |
| 1:F:281:ASP:OD1 | 1:F:407:GLU:OE1 | 2.37 | 0.43 |
| 1:F:284:ILE:HD12 | 1:F:284:ILE:H | 1.83 | 0.43 |
| 2:B:123:LEU:O | 2:B:127:ILE:HG13 | 2.19 | 0.43 |
| 2:B:164:LEU:HD11 | 2:B:197:GLU:HG3 | 2.00 | 0.43 |
| 2:B:52:LYS:HD2 | 2:B:182:THR:O | 2.19 | 0.43 |
| 2:C:256:GLN:HG2 | 2:C:256:GLN:H | 1.54 | 0.43 |
| 2:D:203:ASN:HB3 | 2:D:225:LEU:CD2 | 2.48 | 0.43 |
| 2:D:387:VAL:CG1 | 2:D:388:SER:H | 2.32 | 0.43 |
| 2:E:313:ILE:CD1 | 2:E:372:PRO:HG2 | 2.48 | 0.43 |
| 2:B:51:GLY:H | 3:B:903:ATP:PB | 2.42 | 0.43 |
| 2:B:79:THR:HG21 | 2:B:81:GLN:HG2 | 1.99 | 0.43 |
| 2:C:471:MET:HB3 | 2:C:480:LYS:NZ | 2.34 | 0.43 |
| 2:D:148:THR:HG23 | 2:D:193:ARG:HD2 | 1.99 | 0.43 |
| 2:D:203:ASN:CB | 2:D:225:LEU:HD23 | 2.49 | 0.43 |
| 2:D:296:LEU:HD11 | 2:D:477:PRO:HD3 | 2.01 | 0.43 |
| 1:F:464:ASP:OD2 | 1:F:466:ALA:HB3 | 2.19 | 0.43 |
| 1:A:18:ILE:HG21 | 1:A:37:PRO:HB3 | 2.00 | 0.43 |
| 1:A:65:ILE:HG12 | 1:A:65:ILE:H | 1.62 | 0.43 |
| 2:B:136:LYS:HE2 | 2:B:137:TYR:CE1 | 2.54 | 0.43 |
| 2:B:142:VAL:HG23 | 2:B:176:ALA:HB1 | 2.01 | 0.43 |
| 2:B:333:MET:HG2 | 2:B:333:MET:H | 1.34 | 0.43 |
| 2:B:455:VAL:HG11 | 2:B:463:HIS:HB2 | 2.01 | 0.43 |
| 2:B:92:TRP:HD1 | 2:B:92:TRP:O | 2.02 | 0.43 |
| 2:B:89:SER:CB | 2:C:227:GLY:O | 2.67 | 0.43 |
| 2:D:230:HIS:C | 2:D:230:HIS:HD1 | 2.22 | 0.43 |
| 2:D:446:ARG:H | 2:D:496:ARG:CZ | 2.31 | 0.43 |
| 2:E:486:PHE:CB | 2:E:489:ILE:HD11 | 2.49 | 0.43 |
| 1:F:109:SER:HA | 1:F:110:PRO:HD3 | 1.84 | 0.43 |
| 1:F:126:LEU:HD11 | 1:F:130:ILE:HD11 | 2.01 | 0.43 |
| 1:F:455:VAL:HG11 | 1:F:463:HIS:CB | 2.40 | 0.43 |
| 2:B:21:MET:HB2 | 2:B:38:ILE:CG1 | 2.43 | 0.43 |
| 2:C:44:VAL:HA | 2:C:205:VAL:O | 2.18 | 0.43 |
| 2:D:469:GLU:HG3 | 2:D:470:PHE:N | 2.31 | 0.43 |
| 1:F:247:PHE:HB3 | 1:F:249:LEU:HD21 | 2.01 | 0.43 |
| 1:F:248:PRO:HB2 | 1:F:251:ALA:CB | 2.45 | 0.43 |
| 1:F:94:LEU:O | 1:F:97:LEU:N | 2.51 | 0.43 |
| 1:A:126:LEU:HG | 1:A:130:ILE:CD1 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:TYR:N | 1:A:137:TYR:CD1 | 2.86 | 0.43 |
| 1:A:148:THR:CG2 | 1:A:193:ARG:HD2 | 2.49 | 0.43 |
| 1:A:317:TYR:CE2 | 1:A:383:LEU:HD21 | 2.54 | 0.43 |
| 1:A:471:MET:HG3 | 1:A:471:MET:H | 1.67 | 0.43 |
| 2:B:127:ILE:HD13 | 2:B:170:ARG:HG3 | 2.01 | 0.43 |
| 2:C:113:GLU:O | 2:C:114:GLY:C | 2.58 | 0.43 |
| 2:C:127:ILE:N | 2:C:127:ILE:CD1 | 2.82 | 0.43 |
| 2:C:446:ARG:HG2 | 2:C:496:ARG:CZ | 2.49 | 0.43 |
| 2:C:61:TYR:CG | 2:C:65:ILE:HD13 | 2.53 | 0.43 |
| 2:D:209:ASN:HD22 | 2:D:209:ASN:HA | 1.61 | 0.43 |
| 1:F:329:TYR:C | 1:F:331:TRP:N | 2.72 | 0.43 |
| 1:F:515:LYS:CG | 1:F:517:PRO:HD2 | 2.49 | 0.43 |
| 1:F:93:ASP:OD2 | 1:F:96:LYS:HB2 | 2.18 | 0.43 |
| 1:A:267:VAL:CG1 | 1:A:270:LEU:HB2 | 2.48 | 0.42 |
| 1:A:356:LEU:HD23 | 1:A:395:PHE:HB2 | 2.01 | 0.42 |
| 2:B:162:ARG:HH11 | 2:B:162:ARG:CB | 2.31 | 0.42 |
| 2:C:348:CYS:O | 2:C:349:ALA:HB2 | 2.19 | 0.42 |
| 2:C:483:PHE:N | 2:C:483:PHE:CD1 | 2.87 | 0.42 |
| 2:E:147:VAL:CG2 | 2:E:148:THR:N | 2.82 | 0.42 |
| 1:F:380:LEU:O | 1:F:383:LEU:N | 2.50 | 0.42 |
| 1:A:340:ARG:O | 1:A:342:ASN:N | 2.53 | 0.42 |
| 1:A:379:SER:H | 1:A:413:THR:CB | 2.32 | 0.42 |
| 2:C:425:ILE:HD12 | 2:C:425:ILE:H | 1.84 | 0.42 |
| 2:C:44:VAL:HG12 | 2:C:44:VAL:O | 2.19 | 0.42 |
| 2:D:394:GLN:NE2 | 5:D:530:HOH:O | 2.51 | 0.42 |
| 2:D:471:MET:HE2 | 2:D:478:ASP:CB | 2.49 | 0.42 |
| 2:E:296:LEU:HD13 | 2:E:331:TRP:CE3 | 2.54 | 0.42 |
| 2:E:371:LYS:CD | 2:E:371:LYS:O | 2.62 | 0.42 |
| 1:F:134:ILE:CD1 | 1:F:139:ALA:HB3 | 2.50 | 0.42 |
| 1:F:289:ALA:O | 1:F:292:THR:HG23 | 2.18 | 0.42 |
| 1:F:375:ILE:HA | 1:F:375:ILE:HD13 | 1.87 | 0.42 |
| 1:F:387:VAL:CG1 | 1:F:391:ALA:HB3 | 2.49 | 0.42 |
| 1:A:304:ASN:OD1 | 1:A:304:ASN:O | 2.38 | 0.42 |
| 1:A:82:ASP:O | 1:A:85:LYS:N | 2.52 | 0.42 |
| 2:B:451:ARG:HB3 | 2:B:470:PHE:CE2 | 2.54 | 0.42 |
| 2:C:378:ASP:O | 2:C:379:SER:CB | 2.66 | 0.42 |
| 2:C:443:VAL:HG12 | 2:C:445:ILE:HG12 | 2.02 | 0.42 |
| 2:C:472:ILE:HD12 | 2:C:472:ILE:N | 2.34 | 0.42 |
| 2:D:18:ILE:HD12 | 2:D:227:GLY:CA | 2.42 | 0.42 |
| 2:D:385:ARG:HG2 | 2:E:393:ARG:CZ | 2.48 | 0.42 |
| 2:E:69:GLU:HA | 2:E:70:PRO:HD3 | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:164:LEU:O | 1:F:167:LEU:N | 2.52 | 0.42 |
| 1:F:212:GLU:OE2 | 1:F:212:GLU:O | 2.36 | 0.42 |
| 1:A:212:GLU:CG | 1:A:212:GLU:O | 2.68 | 0.42 |
| 1:A:266:GLY:C | 1:A:300:ARG:HG3 | 2.39 | 0.42 |
| 1:A:36:LEU:HA | 1:A:37:PRO:HD3 | 1.87 | 0.42 |
| 1:A:64:ILE:CD1 | 1:A:70:PRO:HA | 2.48 | 0.42 |
| 2:B:98:VAL:HA | 2:B:103:LEU:O | 2.19 | 0.42 |
| 2:B:393:ARG:O | 2:B:397:ILE:HG13 | 2.19 | 0.42 |
| 2:B:451:ARG:HD2 | 2:B:451:ARG:N | 2.34 | 0.42 |
| 2:C:486:PHE:HE2 | 2:C:496:ARG:HG2 | 1.84 | 0.42 |
| 2:D:244:ILE:HG22 | 2:D:245:ASN:N | 2.34 | 0.42 |
| 2:D:64:ILE:HG21 | 2:D:97:LEU:HD13 | 2.00 | 0.42 |
| 2:E:348:CYS:O | 2:E:349:ALA:HB2 | 2.19 | 0.42 |
| 2:E:289:ALA:CB | 2:E:419:PHE:HA | 2.46 | 0.42 |
| 2:E:462:TRP:O | 2:E:463:HIS:CD2 | 2.72 | 0.42 |
| 2:E:331:TRP:NE1 | 3:E:901:ATP:N7 | 2.59 | 0.42 |
| 1:F:18:ILE:HB | 1:F:228:THR:CG2 | 2.48 | 0.42 |
| 1:F:313:ILE:CD1 | 1:F:372:PRO:HG2 | 2.49 | 0.42 |
| 1:A:320:SEP:O2P | 2:B:256:GLN:O | 2.37 | 0.42 |
| 1:A:336:GLU:OE1 | 1:A:336:GLU:HA | 2.19 | 0.42 |
| 2:D:420:MET:HE3 | 2:D:420:MET:HB3 | 1.83 | 0.42 |
| 2:D:52:LYS:N | 3:D:903:ATP:O1B | 2.43 | 0.42 |
| 2:E:223:LEU:HD23 | 2:E:223:LEU:HA | 1.45 | 0.42 |
| 2:E:315:PHE:CD2 | 2:E:347:VAL:HG21 | 2.54 | 0.42 |
| 2:E:445:ILE:HD11 | 2:E:483:PHE:CE2 | 2.54 | 0.42 |
| 1:F:484:ARG:CB | 1:F:484:ARG:HH11 | 2.29 | 0.42 |
| 1:F:47:THR:O | 1:F:50:THR:HG23 | 2.20 | 0.42 |
| 3:A:901:ATP:O2G | 2:B:459:ARG:NH2 | 2.51 | 0.42 |
| 2:B:73:PHE:CD2 | 2:B:105:ILE:HD12 | 2.54 | 0.42 |
| 2:B:204:VAL:HG23 | 2:B:224:LYS:HG2 | 2.00 | 0.42 |
| 2:B:36:LEU:HD12 | 2:B:59:PHE:CE1 | 2.54 | 0.42 |
| 2:B:24:MET:HB3 | 2:B:62:ASN:HD22 | 1.84 | 0.42 |
| 2:C:486:PHE:HB3 | 2:C:489:ILE:HD11 | 2.01 | 0.42 |
| 2:D:160:VAL:O | 2:D:164:LEU:HB2 | 2.19 | 0.42 |
| 2:D:127:ILE:CD1 | 2:D:167:LEU:HD13 | 2.50 | 0.42 |
| 2:D:52:LYS:HB2 | 2:D:52:LYS:HE3 | 1.85 | 0.42 |
| 1:F:191:ILE:HG21 | 1:F:198:GLU:HG3 | 2.02 | 0.42 |
| 1:F:484:ARG:HB2 | 1:F:484:ARG:NH1 | 2.34 | 0.42 |
| 1:A:148:THR:OG1 | 1:A:182:THR:HG23 | 2.20 | 0.42 |
| 1:A:325:LEU:HD22 | 1:A:336:GLU:HG2 | 2.02 | 0.42 |
| 1:A:485:ASN:N | 1:A:485:ASN:OD1 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:164:LEU:HB3 | 2:B:200:VAL:HG11 | 2.02 | 0.42 |
| 2:B:453:ILE:HD13 | 2:B:454:ASN:H | 1.83 | 0.42 |
| 2:C:186:GLU:OE2 | 2:C:187:GLU:N | 2.53 | 0.42 |
| 2:C:208:ARG:NH2 | 2:C:221:GLU:OE2 | 2.52 | 0.42 |
| 2:C:363:ILE:HG22 | 2:C:367:ILE:HD11 | 2.02 | 0.42 |
| 2:D:367:ILE:HG23 | 2:D:372:PRO:HD2 | 2.01 | 0.42 |
| 2:D:384:ALA:HB2 | 2:D:392:PHE:CE1 | 2.54 | 0.42 |
| 2:E:413:THR:CG2 | 2:E:414:ASN:N | 2.83 | 0.42 |
| 1:F:269:ARG:O | 1:F:272:GLU:HB2 | 2.20 | 0.42 |
| 1:F:367:ILE:HD11 | 1:F:375:ILE:HG13 | 2.00 | 0.42 |
| 1:A:393:ARG:HH12 | 1:F:385:ARG:HA | 1.85 | 0.42 |
| 1:A:306:CYS:HB2 | 1:A:338:MET:SD | 2.59 | 0.42 |
| 1:A:311:ARG:CZ | 1:A:371:LYS:HE3 | 2.50 | 0.42 |
| 1:A:382:ALA:O | 1:A:385:ARG:HG3 | 2.20 | 0.42 |
| 1:A:81:GLN:H | 1:A:81:GLN:NE2 | 2.18 | 0.42 |
| 1:A:348:CYS:HB3 | 2:B:254:LEU:HD23 | 2.02 | 0.42 |
| 2:B:445:ILE:HD11 | 2:B:494:PRO:HG2 | 2.01 | 0.42 |
| 2:C:439:LEU:HD12 | 2:C:439:LEU:C | 2.40 | 0.42 |
| 2:E:220:LEU:C | 2:E:220:LEU:HD23 | 2.40 | 0.42 |
| 2:E:225:LEU:HD12 | 2:E:230:HIS:HB3 | 2.00 | 0.42 |
| 2:E:23:THR:O | 2:E:24:MET:CB | 2.68 | 0.42 |
| 1:A:166:ARG:HG3 | 1:F:112:PRO:O | 2.20 | 0.42 |
| 2:B:436:THR:HG23 | 2:B:458:MET:CG | 2.50 | 0.42 |
| 2:C:62:ASN:O | 2:C:66:GLU:N | 2.47 | 0.42 |
| 2:D:332:GLY:O | 2:D:333:MET:HG2 | 2.19 | 0.42 |
| 2:D:325:LEU:CD2 | 2:D:335:PHE:HB2 | 2.50 | 0.42 |
| 2:E:106:LEU:HD13 | 2:E:129:ARG:NH2 | 2.34 | 0.42 |
| 2:E:164:LEU:HD23 | 2:E:164:LEU:HA | 1.81 | 0.42 |
| 2:E:217:ARG:HH21 | 2:E:236:PRO:HB3 | 1.85 | 0.42 |
| 2:E:344:LEU:CD1 | 2:E:346:ILE:HG13 | 2.48 | 0.42 |
| 2:E:360:LEU:HD22 | 2:E:360:LEU:O | 2.20 | 0.42 |
| 2:E:445:ILE:HG22 | 2:E:445:ILE:O | 2.20 | 0.42 |
| 2:E:486:PHE:HB2 | 2:E:489:ILE:HD11 | 2.00 | 0.42 |
| 2:E:326:ARG:HD3 | 1:F:258:SER:OG | 2.20 | 0.42 |
| 1:F:433:ILE:N | 1:F:433:ILE:HD12 | 2.34 | 0.42 |
| 1:A:319:GLU:O | 2:B:254:LEU:HD21 | 2.20 | 0.42 |
| 1:A:348:CYS:O | 1:A:349:ALA:HB2 | 2.20 | 0.42 |
| 1:A:426:THR:HB | 1:A:431:GLU:OE1 | 2.20 | 0.42 |
| 1:A:451:ARG:CD | 1:A:451:ARG:N | 2.81 | 0.42 |
| 2:B:350:TYR:CE1 | 2:C:252:MET:HE2 | 2.55 | 0.42 |
| 2:C:54:LEU:HD23 | 2:C:244:ILE:CG1 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:117:VAL:O | 1:F:118:VAL:CB | 2.67 | 0.42 |
| 1:F:451:ARG:NH1 | 1:F:451:ARG:HG2 | 2.33 | 0.42 |
| 1:A:323:GLN:HA | 2:B:258:SER:OG | 2.19 | 0.41 |
| 1:A:367:ILE:HD12 | 1:A:375:ILE:HD11 | 2.01 | 0.41 |
| 2:B:125:ALA:O | 2:B:128:GLU:HB2 | 2.20 | 0.41 |
| 2:B:282:SER:C | 2:B:283:ILE:HD12 | 2.41 | 0.41 |
| 2:B:471:MET:HB3 | 2:B:480:LYS:NZ | 2.34 | 0.41 |
| 2:B:50:THR:HG22 | 2:B:52:LYS:HE2 | 2.02 | 0.41 |
| 2:B:61:TYR:CZ | 2:B:92:TRP:HB2 | 2.55 | 0.41 |
| 2:C:142:VAL:HG12 | 2:C:178:THR:HG23 | 2.02 | 0.41 |
| 2:D:70:PRO:HG2 | 2:D:138:ARG:O | 2.20 | 0.41 |
| 2:D:19:ALA:CB | 2:D:38:ILE:HD12 | 2.49 | 0.41 |
| 2:D:439:LEU:HD12 | 2:D:439:LEU:C | 2.40 | 0.41 |
| 2:D:54:LEU:HD13 | 2:D:90:PHE:CZ | 2.55 | 0.41 |
| 2:E:489:ILE:H | 2:E:489:ILE:HD12 | 1.85 | 0.41 |
| 1:F:150:VAL:O | 1:F:153:GLN:HG3 | 2.20 | 0.41 |
| 1:F:249:LEU:HD12 | 1:F:394:GLN:CD | 2.39 | 0.41 |
| 1:F:344:LEU:HD13 | 1:F:344:LEU:O | 2.20 | 0.41 |
| 1:F:371:LYS:N | 1:F:372:PRO:HD3 | 2.35 | 0.41 |
| 1:F:438:ILE:O | 1:F:438:ILE:HG22 | 2.19 | 0.41 |
| 1:F:49:GLY:O | 1:F:218:ARG:NH2 | 2.52 | 0.41 |
| 1:A:283:ILE:HD12 | 1:A:412:PHE:CE1 | 2.55 | 0.41 |
| 3:A:903:ATP:O3' | 2:B:224:LYS:HB2 | 2.21 | 0.41 |
| 2:B:73:PHE:HE2 | 2:B:83:ILE:HD13 | 1.85 | 0.41 |
| 2:C:290:THR:HG23 | 2:C:290:THR:O | 2.21 | 0.41 |
| 2:E:180:MET:HB3 | 2:E:180:MET:HE2 | 1.82 | 0.41 |
| 2:E:200:VAL:O | 2:E:200:VAL:CG1 | 2.67 | 0.41 |
| 1:F:161:ARG:HB2 | 1:F:196:VAL:CG1 | 2.49 | 0.41 |
| 1:F:486:PHE:HD2 | 1:F:494:PRO:HB2 | 1.84 | 0.41 |
| 1:A:244:ILE:CG2 | 1:A:246:ILE:HD11 | 2.50 | 0.41 |
| 1:A:79:THR:HG23 | 1:A:81:GLN:NE2 | 2.17 | 0.41 |
| 2:B:336:GLU:OE1 | 2:B:336:GLU:HA | 2.21 | 0.41 |
| 2:B:249:LEU:HD13 | 2:B:394:GLN:HG2 | 2.02 | 0.41 |
| 2:C:42:THR:HG23 | 2:C:203:ASN:HB2 | 2.01 | 0.41 |
| 2:D:106:LEU:HD11 | 2:D:129:ARG:CZ | 2.50 | 0.41 |
| 2:E:443:VAL:HG11 | 2:E:445:ILE:HD11 | 2.02 | 0.41 |
| 1:F:21:MET:HE1 | 1:F:141:ARG:HG2 | 2.02 | 0.41 |
| 1:F:433:ILE:HG22 | 1:F:433:ILE:O | 2.19 | 0.41 |
| 1:A:20:LYS:HE3 | 1:A:228:THR:HG21 | 2.01 | 0.41 |
| 2:B:51:GLY:C | 3:B:903:ATP:O1B | 2.59 | 0.41 |
| 2:C:219:THR:O | 2:C:237:PHE:HE2 | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:32:SER:OG | 2:C:35:GLY:HA2 | 2.20 | 0.41 |
| 2:C:380:LEU:HA | 2:C:380:LEU:HD23 | 1.90 | 0.41 |
| 2:C:25:ILE:CG1 | 2:C:58:GLN:HE21 | 2.24 | 0.41 |
| 2:D:45:SER:HB3 | 2:D:182:THR:HB | 2.02 | 0.41 |
| 2:E:49:GLY:HA2 | 3:E:903:ATP:O2B | 2.21 | 0.41 |
| 1:F:220:LEU:HD21 | 1:F:222:ILE:HD11 | 2.03 | 0.41 |
| 1:A:489:ILE:HD13 | 1:A:494:PRO:CG | 2.50 | 0.41 |
| 2:B:182:THR:HG21 | 2:B:192:ALA:CB | 2.41 | 0.41 |
| 2:B:194:TYR:O | 2:B:195:GLY:C | 2.57 | 0.41 |
| 2:B:452:ALA:O | 2:B:470:PHE:HE2 | 2.03 | 0.41 |
| 2:B:499:VAL:C | 2:B:501:GLU:H | 2.23 | 0.41 |
| 2:C:382:ALA:O | 2:C:385:ARG:HG3 | 2.19 | 0.41 |
| 2:C:70:PRO:HB2 | 2:C:139:ALA:HA | 2.02 | 0.41 |
| 2:D:344:LEU:HD13 | 2:D:345:LYS:N | 2.36 | 0.41 |
| 1:F:396:VAL:O | 1:F:400:THR:HB | 2.19 | 0.41 |
| 1:A:396:VAL:O | 1:A:400:THR:CB | 2.67 | 0.41 |
| 2:B:347:VAL:O | 2:B:348:CYS:HB2 | 2.21 | 0.41 |
| 2:B:36:LEU:HD12 | 2:B:59:PHE:CZ | 2.56 | 0.41 |
| 2:B:471:MET:HG2 | 2:B:480:LYS:HZ3 | 1.84 | 0.41 |
| 2:B:73:PHE:HB3 | 2:B:105:ILE:CD1 | 2.36 | 0.41 |
| 2:B:326:ARG:HG3 | 2:C:260:ASN:ND2 | 2.35 | 0.41 |
| 2:C:63:GLY:CA | 2:C:141:ARG:CZ | 2.98 | 0.41 |
| 2:D:328:ALA:N | 5:D:552:HOH:O | 2.53 | 0.41 |
| 2:D:88:ARG:HD3 | 2:E:15:HIS:O | 2.20 | 0.41 |
| 2:E:18:ILE:HD12 | 2:E:18:ILE:O | 2.21 | 0.41 |
| 2:E:353:SER:O | 2:E:354:ALA:HB2 | 2.20 | 0.41 |
| 2:E:468:ARG:NH1 | 2:E:468:ARG:HG2 | 2.36 | 0.41 |
| 1:F:266:GLY:HA3 | 1:F:300:ARG:HG3 | 2.02 | 0.41 |
| 1:F:312:ALA:HB2 | 1:F:374:ARG:HB2 | 2.01 | 0.41 |
| 1:A:94:LEU:HD22 | 1:A:103:LEU:CD2 | 2.51 | 0.41 |
| 1:A:323:GLN:HA | 2:B:258:SER:CB | 2.51 | 0.41 |
| 1:A:319:GLU:OE1 | 1:A:324:LEU:HD23 | 2.21 | 0.41 |
| 1:A:36:LEU:HD12 | 1:A:59:PHE:CE1 | 2.56 | 0.41 |
| 2:B:151:PHE:C | 2:B:153:GLN:N | 2.74 | 0.41 |
| 2:B:182:THR:HG22 | 2:B:183:GLU:H | 1.86 | 0.41 |
| 2:B:311:ARG:CD | 2:B:371:LYS:HE3 | 2.41 | 0.41 |
| 1:A:448:GLU:HG2 | 2:B:466:ALA:CA | 2.50 | 0.41 |
| 2:B:80:PRO:HA | 2:B:83:ILE:HD12 | 2.03 | 0.41 |
| 2:C:468:ARG:HG2 | 2:C:468:ARG:NH1 | 2.35 | 0.41 |
| 2:C:61:TYR:CZ | 2:C:92:TRP:HB2 | 2.56 | 0.41 |
| 2:D:84:ILE:HD11 | 2:D:105:ILE:CD1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:49:GLY:CA | 3:D:903:ATP:O2B | 2.68 | 0.41 |
| 2:E:152:GLN:HG3 | 1:F:161:ARG:NH1 | 2.34 | 0.41 |
| 2:E:211:LEU:HD12 | 2:E:211:LEU:HA | 1.88 | 0.41 |
| 1:F:299:SER:HB3 | 1:F:333:MET:HE1 | 2.01 | 0.41 |
| 1:A:304:ASN:HB3 | 1:A:374:ARG:HH12 | 1.86 | 0.41 |
| 1:A:461:SER:OG | 1:A:462:TRP:N | 2.54 | 0.41 |
| 1:A:64:ILE:HG21 | 1:A:97:LEU:HD22 | 2.02 | 0.41 |
| 1:A:320:SEP:CB | 2:B:254:LEU:HG | 2.46 | 0.41 |
| 2:B:51:GLY:O | 2:B:54:LEU:HB3 | 2.21 | 0.41 |
| 2:C:127:ILE:HD11 | 2:C:167:LEU:HD13 | 2.02 | 0.41 |
| 2:C:23:THR:O | 2:C:24:MET:HB2 | 2.21 | 0.41 |
| 2:C:306:CYS:SG | 2:C:344:LEU:HB2 | 2.61 | 0.41 |
| 2:D:106:LEU:C | 2:D:106:LEU:HD12 | 2.41 | 0.41 |
| 2:E:269:ARG:HH22 | 2:E:468:ARG:NH2 | 2.18 | 0.41 |
| 2:E:291:GLY:C | 2:E:442:TYR:OH | 2.59 | 0.41 |
| 2:E:325:LEU:HD23 | 2:E:335:PHE:HB2 | 2.03 | 0.41 |
| 1:A:467:ILE:HD13 | 1:F:447:GLY:O | 2.20 | 0.41 |
| 2:B:161:ARG:HB2 | 2:B:196:VAL:HG11 | 2.01 | 0.41 |
| 2:B:479:ILE:CD1 | 2:B:479:ILE:H | 2.21 | 0.41 |
| 2:B:76:PHE:CZ | 2:B:126:LEU:HD21 | 2.56 | 0.41 |
| 2:B:92:TRP:CD1 | 2:B:92:TRP:O | 2.74 | 0.41 |
| 2:C:448:GLU:HG2 | 2:D:466:ALA:CA | 2.48 | 0.41 |
| 2:D:21:MET:CE | 2:D:59:PHE:HZ | 2.33 | 0.41 |
| 2:D:246:ILE:O | 2:D:248:PRO:HD3 | 2.20 | 0.41 |
| 2:D:54:LEU:CD2 | 2:D:239:ILE:HG23 | 2.51 | 0.41 |
| 2:E:419:PHE:O | 2:E:420:MET:O | 2.39 | 0.41 |
| 2:E:445:ILE:O | 2:E:446:ARG:CB | 2.65 | 0.41 |
| 1:F:299:SER:C | 1:F:333:MET:CE | 2.79 | 0.41 |
| 1:A:162:ARG:O | 1:A:165:PHE:HB3 | 2.20 | 0.41 |
| 1:A:284:ILE:HG22 | 1:A:438:ILE:HD13 | 2.03 | 0.41 |
| 2:B:111:ASP:O | 2:B:113:GLU:N | 2.54 | 0.41 |
| 2:B:45:SER:HB3 | 2:B:182:THR:CB | 2.39 | 0.41 |
| 2:B:96:LYS:O | 2:B:100:GLU:HG3 | 2.21 | 0.41 |
| 2:C:118:VAL:O | 2:C:118:VAL:HG12 | 2.21 | 0.41 |
| 2:C:20:LYS:HE2 | 2:C:228:THR:OG1 | 2.21 | 0.41 |
| 2:C:231:MET:CE | 2:C:251:ALA:HB2 | 2.51 | 0.41 |
| 2:D:294:LYS:O | 2:D:298:VAL:HG23 | 2.20 | 0.41 |
| 2:D:387:VAL:HG12 | 2:D:388:SER:H | 1.83 | 0.41 |
| 2:E:264:SER:O | 2:E:374:ARG:NH2 | 2.53 | 0.41 |
| 2:E:265:SER:HB3 | 2:E:278:PHE:CZ | 2.55 | 0.41 |
| 2:E:362:ILE:O | 2:E:365:SER:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:269:ARG:CG | 2:E:479:ILE:HB | 2.40 | 0.41 |
| 2:E:84:ILE:O | 2:E:87:ALA:HB3 | 2.20 | 0.41 |
| 1:A:116:GLU:O | 1:A:117:VAL:HB | 2.21 | 0.41 |
| 1:A:23:THR:OG1 | 1:A:25:ILE:HG12 | 2.21 | 0.41 |
| 2:B:116:GLU:HG2 | 2:B:154:TYR:HE2 | 1.86 | 0.41 |
| 2:B:213:GLY:O | 2:B:214:GLU:CB | 2.68 | 0.41 |
| 2:B:211:LEU:O | 2:B:215:ARG:O | 2.39 | 0.41 |
| 2:B:451:ARG:NH1 | 2:B:472:ILE:HD12 | 2.35 | 0.41 |
| 2:C:53:THR:O | 2:C:57:ILE:HG12 | 2.20 | 0.41 |
| 2:E:443:VAL:CG1 | 2:E:494:PRO:HG2 | 2.50 | 0.41 |
| 1:F:126:LEU:O | 1:F:127:ILE:C | 2.58 | 0.41 |
| 1:F:194:TYR:O | 1:F:195:GLY:C | 2.58 | 0.41 |
| 1:F:443:VAL:HG12 | 1:F:445:ILE:HD11 | 2.03 | 0.41 |
| 1:A:116:GLU:C | 1:A:117:VAL:CG2 | 2.79 | 0.40 |
| 1:A:443:VAL:CG1 | 1:A:445:ILE:HD11 | 2.51 | 0.40 |
| 1:A:296:LEU:HD21 | 1:A:477:PRO:HD3 | 2.03 | 0.40 |
| 1:A:496:ARG:O | 1:A:497:ILE:HG23 | 2.21 | 0.40 |
| 1:A:80:PRO:HD2 | 1:A:81:GLN:NE2 | 2.36 | 0.40 |
| 2:B:429:HIS:HA | 2:B:431:GLU:OE2 | 2.20 | 0.40 |
| 2:B:81:GLN:CD | 2:B:81:GLN:N | 2.73 | 0.40 |
| 2:C:194:TYR:CD1 | 2:C:194:TYR:N | 2.89 | 0.40 |
| 2:C:21:MET:HE3 | 2:C:141:ARG:CD | 2.51 | 0.40 |
| 2:C:352:GLU:N | 2:C:352:GLU:CD | 2.74 | 0.40 |
| 2:C:296:LEU:HD21 | 2:C:477:PRO:HB3 | 2.03 | 0.40 |
| 2:D:443:VAL:HG12 | 2:D:445:ILE:CD1 | 2.51 | 0.40 |
| 2:D:484:ARG:NH1 | 2:D:484:ARG:CB | 2.84 | 0.40 |
| 2:E:148:THR:HG23 | 2:E:193:ARG:HD2 | 2.03 | 0.40 |
| 2:E:306:CYS:SG | 2:E:338:MET:SD | 3.20 | 0.40 |
| 2:E:392:PHE:O | 2:E:395:PHE:HB3 | 2.20 | 0.40 |
| 2:E:451:ARG:CG | 2:E:451:ARG:NH1 | 2.84 | 0.40 |
| 1:F:21:MET:CE | 1:F:59:PHE:CE1 | 3.04 | 0.40 |
| 1:A:112:PRO:O | 2:B:166:ARG:HG3 | 2.21 | 0.40 |
| 1:A:237:PHE:HA | 1:A:245:ASN:O | 2.21 | 0.40 |
| 1:A:24:MET:CB | 1:A:62:ASN:HD22 | 2.31 | 0.40 |
| 2:B:161:ARG:HB2 | 2:B:196:VAL:CG1 | 2.50 | 0.40 |
| 1:A:420:MET:HE1 | 2:B:490:ILE:HG21 | 2.02 | 0.40 |
| 2:B:497:ILE:O | 2:B:498:THR:C | 2.59 | 0.40 |
| 2:C:153:GLN:O | 2:C:154:TYR:CB | 2.69 | 0.40 |
| 2:C:320:SER:HA | 2:D:254:LEU:HG | 2.02 | 0.40 |
| 2:D:200:VAL:O | 2:D:200:VAL:HG12 | 2.20 | 0.40 |
| 2:D:64:ILE:HD12 | 2:D:69:GLU:O | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:49:GLY:HA2 | 3:D:903:ATP:O2B | 2.21 | 0.40 |
| 2:E:143:SER:HA | 2:E:179:VAL:O | 2.20 | 0.40 |
| 1:F:393:ARG:NH2 | 5:F:527:HOH:O | 2.45 | 0.40 |
| 1:A:237:PHE:C | 1:A:237:PHE:CD1 | 2.94 | 0.40 |
| 1:A:340:ARG:C | 1:A:342:ASN:N | 2.75 | 0.40 |
| 1:A:489:ILE:HD13 | 1:A:494:PRO:HG3 | 2.04 | 0.40 |
| 2:B:47:THR:HG23 | 2:B:187:GLU:OE2 | 2.21 | 0.40 |
| 2:B:267:VAL:HB | 2:B:270:LEU:HB2 | 2.04 | 0.40 |
| 2:B:326:ARG:HG3 | 2:C:260:ASN:HD21 | 1.87 | 0.40 |
| 2:B:249:LEU:HD12 | 2:B:394:GLN:HG2 | 2.02 | 0.40 |
| 2:B:25:ILE:HG23 | 2:B:58:GLN:HE22 | 1.86 | 0.40 |
| 2:C:123:LEU:HA | 2:C:127:ILE:HD13 | 2.02 | 0.40 |
| 2:C:28:PHE:N | 2:C:246:ILE:HD12 | 2.36 | 0.40 |
| 2:C:468:ARG:HG2 | 2:C:468:ARG:HH11 | 1.85 | 0.40 |
| 2:C:484:ARG:HB3 | 2:C:484:ARG:NH1 | 2.35 | 0.40 |
| 2:D:396:VAL:HG11 | 2:D:430:ILE:CG2 | 2.51 | 0.40 |
| 2:D:472:ILE:N | 2:D:472:ILE:HD12 | 2.37 | 0.40 |
| 2:D:75:THR:HG22 | 2:D:107:ASP:HA | 2.04 | 0.40 |
| 1:F:18:ILE:HD12 | 1:F:227:GLY:CA | 2.33 | 0.40 |
| 1:F:362:ILE:O | 1:F:365:SER:HB3 | 2.21 | 0.40 |
| 1:A:487:GLU:OE1 | 1:F:496:ARG:HG2 | 2.22 | 0.40 |
| 2:B:134:ILE:HA | 2:B:139:ALA:HB3 | 2.02 | 0.40 |
| 1:A:290:THR:CG2 | 2:B:425:ILE:HD12 | 2.44 | 0.40 |
| 2:C:149:SER:HA | 2:C:152:GLN:HB2 | 2.03 | 0.40 |
| 2:D:315:PHE:HA | 2:D:347:VAL:HB | 2.04 | 0.40 |
| 2:E:186:GLU:OE2 | 2:E:187:GLU:N | 2.54 | 0.40 |
| 2:E:262:ARG:HD2 | 2:E:276:GLY:O | 2.21 | 0.40 |
| 2:E:436:THR:HG23 | 2:E:458:MET:CG | 2.47 | 0.40 |
| 1:F:357:GLU:CG | 1:F:358:ASP:N | 2.84 | 0.40 |
| 1:F:425:ILE:HD13 | 1:F:437:ILE:HG21 | 2.03 | 0.40 |
| 2:B:119:GLY:C | 2:B:121:PHE:N | 2.75 | 0.40 |
| 2:B:363:ILE:O | 2:B:367:ILE:HG13 | 2.21 | 0.40 |
| 2:C:111:ASP:OD2 | 2:C:113:GLU:HG2 | 2.21 | 0.40 |
| 2:C:121:PHE:HB3 | 2:C:125:ALA:CB | 2.51 | 0.40 |
| 2:C:65:ILE:HG22 | 2:C:65:ILE:O | 2.21 | 0.40 |
| 2:D:249:LEU:CD1 | 2:D:394:GLN:HG2 | 2.51 | 0.40 |
| 2:D:269:ARG:O | 2:D:272:GLU:HB2 | 2.20 | 0.40 |
| 2:D:357:GLU:HG3 | 2:D:358:ASP:N | 2.36 | 0.40 |
| 2:D:44:VAL:O | 2:D:44:VAL:HG12 | 2.21 | 0.40 |
| 2:E:333:MET:HB2 | 2:E:333:MET:HE3 | 1.96 | 0.40 |
| 2:E:428:SER:CB | 2:E:430:ILE:HD11 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:E:428:SER:OG | 2:E:430:ILE:HD11 | 2.22 | 0.40 |
| 2:E:49:GLY:CA | 3:E:903:ATP:O2B | 2.70 | 0.40 |
| 1:F:172:LYS:HE3 | 1:F:172:LYS:HB2 | 1.92 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 503/525 (96%) | 406 (81%) | 76 (15%) | 21 (4%) | 3 | 17 |
| 1 | F | 503/525 (96%) | 422 (84%) | 61 (12%) | 20 (4%) | 3 | 18 |
| 2 | B | 489/525 (93%) | 389 (80%) | 82 (17%) | 18 (4%) | 4 | 21 |
| 2 | C | 486/525 (93%) | 419 (86%) | 45 (9%) | 22 (4%) | 3 | 16 |
| 2 | D | 483/525 (92%) | 415 (86%) | 52 (11%) | 16 (3%) | 4 | 23 |
| 2 | E | 490/525 (93%) | 402 (82%) | 69 (14%) | 19 (4%) | 3 | 19 |
| All | All | 2954/3150 (94%) | 2453 (83%) | 385 (13%) | 116 (4%) | 3 | 19 |

All (116) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 154 | TYR |
| 1 | A | 334 | ASP |
| 1 | A | 462 | TRP |
| 1 | A | 463 | HIS |
| 1 | A | 503 | SER |
| 2 | B | 52 | LYS |
| 2 | B | 154 | TYR |
| 2 | B | 211 | LEU |
| 2 | C | 17 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 117 | VAL |
| 2 | C | 154 | TYR |
| 2 | C | 354 | ALA |
| 2 | C | 432 | GLU |
| 2 | C | 463 | HIS |
| 2 | D | 113 | GLU |
| 2 | D | 154 | TYR |
| 2 | D | 211 | LEU |
| 2 | D | 463 | HIS |
| 2 | E | 122 | ASP |
| 2 | E | 154 | TYR |
| 2 | E | 157 | SER |
| 2 | E | 211 | LEU |
| 2 | E | 387 | VAL |
| 1 | F | 118 | VAL |
| 1 | F | 154 | TYR |
| 1 | F | 211 | LEU |
| 1 | F | 431 | GLU |
| 1 | F | 504 | GLU |
| 1 | F | 506 | SER |
| 1 | F | 509 | VAL |
| 1 | A | 117 | VAL |
| 1 | A | 155 | ASP |
| 1 | A | 322 | ALA |
| 1 | A | 422 | ALA |
| 2 | B | 119 | GLY |
| 2 | B | 341 | GLN |
| 2 | B | 484 | ARG |
| 2 | C | 112 | PRO |
| 2 | C | 124 | SER |
| 2 | C | 211 | LEU |
| 2 | C | 341 | GLN |
| 2 | C | 431 | GLU |
| 2 | D | 123 | LEU |
| 2 | D | 333 | MET |
| 2 | D | 341 | GLN |
| 2 | D | 354 | ALA |
| 2 | D | 494 | PRO |
| 2 | E | 420 | MET |
| 2 | E | 463 | HIS |
| 2 | E | 494 | PRO |
| 2 | E | 502 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 117 | VAL |
| 1 | F | 214 | GLU |
| 1 | F | 420 | MET |
| 1 | F | 500 | ASP |
| 1 | F | 501 | GLU |
| 1 | A | 341 | GLN |
| 1 | A | 387 | VAL |
| 1 | A | 464 | ASP |
| 1 | A | 500 | ASP |
| 2 | B | 420 | MET |
| 2 | C | 379 | SER |
| 2 | D | 214 | GLU |
| 2 | E | 304 | ASN |
| 2 | E | 446 | ARG |
| 1 | F | 189 | GLY |
| 1 | F | 379 | SER |
| 1 | F | 381 | SER |
| 1 | A | 157 | SER |
| 1 | A | 379 | SER |
| 2 | B | 149 | SER |
| 2 | B | 348 | CYS |
| 2 | B | 379 | SER |
| 2 | B | 498 | THR |
| 2 | C | 289 | ALA |
| 2 | C | 349 | ALA |
| 2 | D | 353 | SER |
| 2 | D | 387 | VAL |
| 2 | D | 420 | MET |
| 2 | D | 496 | ARG |
| 2 | E | 52 | LYS |
| 2 | E | 189 | GLY |
| 2 | E | 379 | SER |
| 1 | F | 152 | GLN |
| 1 | F | 515 | LYS |
| 2 | B | 17 | ALA |
| 2 | B | 87 | ALA |
| 2 | B | 112 | PRO |
| 2 | B | 167 | LEU |
| 2 | C | 114 | GLY |
| 2 | C | 115 | GLN |
| 2 | C | 149 | SER |
| 2 | C | 348 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 348 | CYS |
| 2 | E | 372 | PRO |
| 2 | E | 480 | LYS |
| 2 | E | 488 | ARG |
| 1 | F | 157 | SER |
| 1 | F | 348 | CYS |
| 1 | F | 517 | PRO |
| 1 | A | 48 | SER |
| 1 | A | 349 | ALA |
| 1 | A | 421 | GLY |
| 1 | A | 509 | VAL |
| 2 | B | 494 | PRO |
| 2 | C | 212 | GLU |
| 2 | C | 420 | MET |
| 2 | E | 113 | GLU |
| 2 | C | 477 | PRO |
| 2 | E | 117 | VAL |
| 2 | B | 117 | VAL |
| 1 | A | 65 | ILE |
| 1 | A | 497 | ILE |
| 2 | B | 195 | GLY |
| 2 | C | 499 | VAL |
| 2 | D | 18 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 431/449 (96%) | 389 (90%) | 42 (10%) | 9 | 33 |
| 1 | F | 431/449 (96%) | 383 (89%) | 48 (11%) | 7 | 27 |
| 2 | B | 419/450 (93%) | 370 (88%) | 49 (12%) | 6 | 24 |
| 2 | C | 416/450 (92%) | 374 (90%) | 42 (10%) | 8 | 31 |
| 2 | D | 413/450 (92%) | 367 (89%) | 46 (11%) | 7 | 27 |
| 2 | E | 420/450 (93%) | 377 (90%) | 43 (10%) | 8 | 30 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-------------|
| All | All | 2530/2698 (94%) | 2260 (89%) | 270 (11%) | 7 28 |

All (270) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 26 | GLU |
| 1 | A | 33 | HIS |
| 1 | A | 65 | ILE |
| 1 | A | 79 | THR |
| 1 | A | 81 | GLN |
| 1 | A | 92 | TRP |
| 1 | A | 99 | ASP |
| 1 | A | 106 | LEU |
| 1 | A | 118 | VAL |
| 1 | A | 121 | PHE |
| 1 | A | 123 | LEU |
| 1 | A | 151 | PHE |
| 1 | A | 181 | THR |
| 1 | A | 185 | ILE |
| 1 | A | 186 | GLU |
| 1 | A | 212 | GLU |
| 1 | A | 218 | ARG |
| 1 | A | 223 | LEU |
| 1 | A | 238 | THR |
| 1 | A | 256 | GLN |
| 1 | A | 263 | VAL |
| 1 | A | 270 | LEU |
| 1 | A | 284 | ILE |
| 1 | A | 287 | THR |
| 1 | A | 302 | VAL |
| 1 | A | 303 | GLU |
| 1 | A | 323 | GLN |
| 1 | A | 342 | ASN |
| 1 | A | 360 | LEU |
| 1 | A | 371 | LYS |
| 1 | A | 400 | THR |
| 1 | A | 428 | SER |
| 1 | A | 430 | ILE |
| 1 | A | 431 | GLU |
| 1 | A | 434 | THR |
| 1 | A | 451 | ARG |
| 1 | A | 469 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 471 | MET |
| 1 | A | 496 | ARG |
| 1 | A | 508 | ILE |
| 1 | A | 509 | VAL |
| 1 | A | 518 | GLU |
| 2 | B | 26 | GLU |
| 2 | B | 52 | LYS |
| 2 | B | 81 | GLN |
| 2 | B | 92 | TRP |
| 2 | B | 99 | ASP |
| 2 | B | 106 | LEU |
| 2 | B | 111 | ASP |
| 2 | B | 112 | PRO |
| 2 | B | 123 | LEU |
| 2 | B | 128 | GLU |
| 2 | B | 140 | ARG |
| 2 | B | 151 | PHE |
| 2 | B | 154 | TYR |
| 2 | B | 178 | THR |
| 2 | B | 181 | THR |
| 2 | B | 183 | GLU |
| 2 | B | 185 | ILE |
| 2 | B | 186 | GLU |
| 2 | B | 198 | GLU |
| 2 | B | 209 | ASN |
| 2 | B | 212 | GLU |
| 2 | B | 223 | LEU |
| 2 | B | 256 | GLN |
| 2 | B | 270 | LEU |
| 2 | B | 284 | ILE |
| 2 | B | 303 | GLU |
| 2 | B | 320 | SER |
| 2 | B | 333 | MET |
| 2 | B | 360 | LEU |
| 2 | B | 366 | GLU |
| 2 | B | 369 | ASP |
| 2 | B | 371 | LYS |
| 2 | B | 375 | ILE |
| 2 | B | 380 | LEU |
| 2 | B | 413 | THR |
| 2 | B | 432 | GLU |
| 2 | B | 450 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 451 | ARG |
| 2 | B | 453 | ILE |
| 2 | B | 462 | TRP |
| 2 | B | 463 | HIS |
| 2 | B | 469 | GLU |
| 2 | B | 471 | MET |
| 2 | B | 474 | ASP |
| 2 | B | 485 | ASN |
| 2 | B | 490 | ILE |
| 2 | B | 499 | VAL |
| 2 | B | 501 | GLU |
| 2 | B | 503 | SER |
| 2 | C | 15 | HIS |
| 2 | C | 26 | GLU |
| 2 | C | 50 | THR |
| 2 | C | 79 | THR |
| 2 | C | 81 | GLN |
| 2 | C | 99 | ASP |
| 2 | C | 111 | ASP |
| 2 | C | 121 | PHE |
| 2 | C | 127 | ILE |
| 2 | C | 140 | ARG |
| 2 | C | 151 | PHE |
| 2 | C | 154 | TYR |
| 2 | C | 177 | THR |
| 2 | C | 178 | THR |
| 2 | C | 185 | ILE |
| 2 | C | 186 | GLU |
| 2 | C | 209 | ASN |
| 2 | C | 212 | GLU |
| 2 | C | 217 | ARG |
| 2 | C | 218 | ARG |
| 2 | C | 223 | LEU |
| 2 | C | 256 | GLN |
| 2 | C | 263 | VAL |
| 2 | C | 270 | LEU |
| 2 | C | 303 | GLU |
| 2 | C | 320 | SER |
| 2 | C | 321 | ARG |
| 2 | C | 333 | MET |
| 2 | C | 356 | LEU |
| 2 | C | 360 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 371 | LYS |
| 2 | C | 375 | ILE |
| 2 | C | 397 | ILE |
| 2 | C | 451 | ARG |
| 2 | C | 453 | ILE |
| 2 | C | 462 | TRP |
| 2 | C | 469 | GLU |
| 2 | C | 470 | PHE |
| 2 | C | 471 | MET |
| 2 | C | 491 | SER |
| 2 | C | 498 | THR |
| 2 | C | 500 | ASP |
| 2 | D | 26 | GLU |
| 2 | D | 79 | THR |
| 2 | D | 81 | GLN |
| 2 | D | 106 | LEU |
| 2 | D | 121 | PHE |
| 2 | D | 122 | ASP |
| 2 | D | 123 | LEU |
| 2 | D | 151 | PHE |
| 2 | D | 154 | TYR |
| 2 | D | 178 | THR |
| 2 | D | 181 | THR |
| 2 | D | 185 | ILE |
| 2 | D | 186 | GLU |
| 2 | D | 201 | SER |
| 2 | D | 209 | ASN |
| 2 | D | 211 | LEU |
| 2 | D | 212 | GLU |
| 2 | D | 222 | ILE |
| 2 | D | 223 | LEU |
| 2 | D | 228 | THR |
| 2 | D | 240 | THR |
| 2 | D | 256 | GLN |
| 2 | D | 259 | SER |
| 2 | D | 260 | ASN |
| 2 | D | 270 | LEU |
| 2 | D | 284 | ILE |
| 2 | D | 287 | THR |
| 2 | D | 290 | THR |
| 2 | D | 321 | ARG |
| 2 | D | 333 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 338 | MET |
| 2 | D | 342 | ASN |
| 2 | D | 360 | LEU |
| 2 | D | 366 | GLU |
| 2 | D | 369 | ASP |
| 2 | D | 371 | LYS |
| 2 | D | 400 | THR |
| 2 | D | 416 | SER |
| 2 | D | 451 | ARG |
| 2 | D | 469 | GLU |
| 2 | D | 471 | MET |
| 2 | D | 474 | ASP |
| 2 | D | 487 | GLU |
| 2 | D | 490 | ILE |
| 2 | D | 496 | ARG |
| 2 | D | 498 | THR |
| 2 | E | 26 | GLU |
| 2 | E | 79 | THR |
| 2 | E | 81 | GLN |
| 2 | E | 99 | ASP |
| 2 | E | 106 | LEU |
| 2 | E | 113 | GLU |
| 2 | E | 121 | PHE |
| 2 | E | 140 | ARG |
| 2 | E | 151 | PHE |
| 2 | E | 154 | TYR |
| 2 | E | 171 | LEU |
| 2 | E | 177 | THR |
| 2 | E | 178 | THR |
| 2 | E | 181 | THR |
| 2 | E | 183 | GLU |
| 2 | E | 185 | ILE |
| 2 | E | 186 | GLU |
| 2 | E | 203 | ASN |
| 2 | E | 209 | ASN |
| 2 | E | 212 | GLU |
| 2 | E | 216 | ARG |
| 2 | E | 223 | LEU |
| 2 | E | 228 | THR |
| 2 | E | 256 | GLN |
| 2 | E | 270 | LEU |
| 2 | E | 300 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 320 | SER |
| 2 | E | 321 | ARG |
| 2 | E | 325 | LEU |
| 2 | E | 333 | MET |
| 2 | E | 342 | ASN |
| 2 | E | 360 | LEU |
| 2 | E | 371 | LYS |
| 2 | E | 375 | ILE |
| 2 | E | 417 | ASP |
| 2 | E | 451 | ARG |
| 2 | E | 453 | ILE |
| 2 | E | 458 | MET |
| 2 | E | 464 | ASP |
| 2 | E | 471 | MET |
| 2 | E | 474 | ASP |
| 2 | E | 501 | GLU |
| 2 | E | 505 | LEU |
| 1 | F | 26 | GLU |
| 1 | F | 33 | HIS |
| 1 | F | 45 | SER |
| 1 | F | 77 | GLU |
| 1 | F | 79 | THR |
| 1 | F | 99 | ASP |
| 1 | F | 106 | LEU |
| 1 | F | 116 | GLU |
| 1 | F | 121 | PHE |
| 1 | F | 123 | LEU |
| 1 | F | 140 | ARG |
| 1 | F | 151 | PHE |
| 1 | F | 154 | TYR |
| 1 | F | 181 | THR |
| 1 | F | 183 | GLU |
| 1 | F | 184 | ARG |
| 1 | F | 185 | ILE |
| 1 | F | 186 | GLU |
| 1 | F | 198 | GLU |
| 1 | F | 203 | ASN |
| 1 | F | 212 | GLU |
| 1 | F | 223 | LEU |
| 1 | F | 256 | GLN |
| 1 | F | 287 | THR |
| 1 | F | 300 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 302 | VAL |
| 1 | F | 314 | LEU |
| 1 | F | 321 | ARG |
| 1 | F | 325 | LEU |
| 1 | F | 333 | MET |
| 1 | F | 342 | ASN |
| 1 | F | 360 | LEU |
| 1 | F | 369 | ASP |
| 1 | F | 371 | LYS |
| 1 | F | 375 | ILE |
| 1 | F | 381 | SER |
| 1 | F | 417 | ASP |
| 1 | F | 451 | ARG |
| 1 | F | 458 | MET |
| 1 | F | 462 | TRP |
| 1 | F | 469 | GLU |
| 1 | F | 471 | MET |
| 1 | F | 496 | ARG |
| 1 | F | 501 | GLU |
| 1 | F | 504 | GLU |
| 1 | F | 507 | ARG |
| 1 | F | 514 | GLU |
| 1 | F | 515 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 15 | HIS |
| 1 | A | 33 | HIS |
| 1 | A | 62 | ASN |
| 1 | A | 81 | GLN |
| 1 | A | 209 | ASN |
| 1 | A | 304 | ASN |
| 1 | A | 368 | ASN |
| 1 | A | 414 | ASN |
| 1 | A | 441 | GLN |
| 1 | A | 463 | HIS |
| 2 | B | 58 | GLN |
| 2 | B | 62 | ASN |
| 2 | B | 81 | GLN |
| 2 | B | 209 | ASN |
| 2 | B | 256 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 260 | ASN |
| 2 | B | 323 | GLN |
| 2 | B | 361 | GLN |
| 2 | B | 368 | ASN |
| 2 | B | 414 | ASN |
| 2 | B | 441 | GLN |
| 2 | B | 454 | ASN |
| 2 | C | 33 | HIS |
| 2 | C | 58 | GLN |
| 2 | C | 81 | GLN |
| 2 | C | 209 | ASN |
| 2 | C | 256 | GLN |
| 2 | C | 260 | ASN |
| 2 | C | 304 | ASN |
| 2 | C | 368 | ASN |
| 2 | C | 389 | ASN |
| 2 | C | 414 | ASN |
| 2 | C | 429 | HIS |
| 2 | C | 441 | GLN |
| 2 | D | 33 | HIS |
| 2 | D | 81 | GLN |
| 2 | D | 209 | ASN |
| 2 | D | 327 | ASN |
| 2 | D | 414 | ASN |
| 2 | E | 81 | GLN |
| 2 | E | 203 | ASN |
| 2 | E | 209 | ASN |
| 2 | E | 256 | GLN |
| 2 | E | 304 | ASN |
| 2 | E | 361 | GLN |
| 2 | E | 368 | ASN |
| 2 | E | 414 | ASN |
| 2 | E | 441 | GLN |
| 2 | E | 454 | ASN |
| 1 | F | 16 | GLN |
| 1 | F | 33 | HIS |
| 1 | F | 81 | GLN |
| 1 | F | 209 | ASN |
| 1 | F | 260 | ASN |
| 1 | F | 323 | GLN |
| 1 | F | 361 | GLN |
| 1 | F | 368 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 414 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | SEP | A | 320 | 1 | 9,9,10 | 2.05 | 2 (22%) | 9,12,14 | 2.81 | 2 (22%) |
| 1 | SEP | F | 320 | 1 | 9,9,10 | 1.93 | 3 (33%) | 9,12,14 | 2.96 | 3 (33%) |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | SEP | A | 320 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | SEP | F | 320 | 1 | - | 0/5/8/10 | 0/0/0/0 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | F | 320 | SEP | P-O2P | 2.51 | 1.65 | 1.54 |
| 1 | F | 320 | SEP | CB-CA | 2.56 | 1.59 | 1.52 |
| 1 | A | 320 | SEP | CA-C | 3.43 | 1.54 | 1.50 |
| 1 | F | 320 | SEP | P-O1P | 4.27 | 1.65 | 1.50 |
| 1 | A | 320 | SEP | P-O1P | 4.61 | 1.66 | 1.50 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | F | 320 | SEP | OG-CB-CA | -5.39 | 102.85 | 108.17 |
| 1 | F | 320 | SEP | P-OG-CB | -5.23 | 103.89 | 118.30 |
| 1 | A | 320 | SEP | P-OG-CB | -4.99 | 104.56 | 118.30 |
| 1 | F | 320 | SEP | O3P-P-OG | 3.99 | 117.36 | 106.73 |
| 1 | A | 320 | SEP | OG-CB-CA | 5.94 | 114.02 | 108.17 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 27 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 320 | SEP | 16 | 0 |
| 1 | F | 320 | SEP | 11 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 21 are monoatomic - leaving 12 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 | ATP | A | 901 | 4 | 27,33,33 | 1.27 | 3 (11%) | 27,52,52 | 2.40 | 5 (18%) |
| 3 | ATP | A | 903 | 4 | 27,33,33 | 1.23 | 3 (11%) | 27,52,52 | 2.38 | 5 (18%) |
| 3 | ATP | B | 901 | 4 | 27,33,33 | 1.30 | 4 (14%) | 27,52,52 | 2.39 | 3 (11%) |
| 3 | ATP | B | 903 | 4 | 27,33,33 | 1.29 | 4 (14%) | 27,52,52 | 2.49 | 6 (22%) |
| 3 | ATP | C | 901 | 4 | 27,33,33 | 1.32 | 3 (11%) | 27,52,52 | 2.43 | 4 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | ATP | C | 903 | 4 | 27,33,33 | 1.19 | 2 (7%) | 27,52,52 | 2.51 | 4 (14%) |
| 3 | ATP | D | 901 | 4 | 27,33,33 | 1.21 | 2 (7%) | 27,52,52 | 2.42 | 3 (11%) |
| 3 | ATP | D | 903 | 4 | 27,33,33 | 1.03 | 1 (3%) | 27,52,52 | 2.45 | 4 (14%) |
| 3 | ATP | E | 901 | 4 | 27,33,33 | 1.29 | 3 (11%) | 27,52,52 | 2.45 | 5 (18%) |
| 3 | ATP | E | 903 | - | 27,33,33 | 1.27 | 2 (7%) | 27,52,52 | 2.30 | 5 (18%) |
| 3 | ATP | F | 901 | 4 | 27,33,33 | 1.29 | 4 (14%) | 27,52,52 | 2.37 | 6 (22%) |
| 3 | ATP | F | 903 | 4 | 27,33,33 | 1.36 | 2 (7%) | 27,52,52 | 2.36 | 3 (11%) |

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 | ATP | A | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | A | 903 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | B | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | B | 903 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | C | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | C | 903 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | D | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | D | 903 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | E | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | E | 903 | - | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | F | 901 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ATP | F | 903 | 4 | - | 0/18/38/38 | 0/3/3/3 |

All (33) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | E | 903 | ATP | C2'-C3' | -2.27 | 1.47 | 1.53 |
| 3 | C | 903 | ATP | O4'-C4' | -2.15 | 1.40 | 1.45 |
| 3 | C | 901 | ATP | C4-N3 | 2.06 | 1.38 | 1.35 |
| 3 | F | 901 | ATP | C4-N3 | 2.09 | 1.38 | 1.35 |
| 3 | A | 901 | ATP | C2-N1 | 2.11 | 1.37 | 1.33 |
| 3 | C | 901 | ATP | O4'-C1' | 2.12 | 1.44 | 1.41 |
| 3 | B | 901 | ATP | C4-N3 | 2.15 | 1.38 | 1.35 |
| 3 | B | 903 | ATP | C2-N1 | 2.18 | 1.38 | 1.33 |
| 3 | A | 903 | ATP | C2-N1 | 2.20 | 1.38 | 1.33 |
| 3 | E | 901 | ATP | C4-N3 | 2.24 | 1.38 | 1.35 |
| 3 | B | 903 | ATP | C4-N3 | 2.24 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | E | 901 | ATP | C2-N1 | 2.25 | 1.38 | 1.33 |
| 3 | F | 901 | ATP | C2-N1 | 2.34 | 1.38 | 1.33 |
| 3 | D | 901 | ATP | O4'-C1' | 2.36 | 1.44 | 1.41 |
| 3 | A | 903 | ATP | O4'-C1' | 2.40 | 1.44 | 1.41 |
| 3 | B | 901 | ATP | O4'-C1' | 2.45 | 1.44 | 1.41 |
| 3 | B | 901 | ATP | C2-N1 | 2.49 | 1.38 | 1.33 |
| 3 | F | 903 | ATP | C2-N1 | 2.52 | 1.38 | 1.33 |
| 3 | F | 901 | ATP | O4'-C1' | 2.61 | 1.44 | 1.41 |
| 3 | A | 901 | ATP | O4'-C1' | 2.68 | 1.45 | 1.41 |
| 3 | B | 903 | ATP | O4'-C1' | 3.00 | 1.45 | 1.41 |
| 3 | C | 903 | ATP | C2-N3 | 3.31 | 1.37 | 1.32 |
| 3 | D | 903 | ATP | C2-N3 | 3.35 | 1.37 | 1.32 |
| 3 | A | 903 | ATP | C2-N3 | 3.71 | 1.38 | 1.32 |
| 3 | D | 901 | ATP | C2-N3 | 3.72 | 1.38 | 1.32 |
| 3 | B | 901 | ATP | C2-N3 | 3.73 | 1.38 | 1.32 |
| 3 | B | 903 | ATP | C2-N3 | 3.95 | 1.38 | 1.32 |
| 3 | E | 903 | ATP | C2-N3 | 4.04 | 1.38 | 1.32 |
| 3 | F | 901 | ATP | C2-N3 | 4.10 | 1.38 | 1.32 |
| 3 | A | 901 | ATP | C2-N3 | 4.16 | 1.38 | 1.32 |
| 3 | E | 901 | ATP | C2-N3 | 4.21 | 1.39 | 1.32 |
| 3 | C | 901 | ATP | C2-N3 | 4.37 | 1.39 | 1.32 |
| 3 | F | 903 | ATP | C2-N3 | 4.72 | 1.39 | 1.32 |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 3 | D | 901 | ATP | N3-C2-N1 | -10.72 | 119.69 | 128.86 |
| 3 | C | 903 | ATP | N3-C2-N1 | -10.69 | 119.71 | 128.86 |
| 3 | C | 901 | ATP | N3-C2-N1 | -10.39 | 119.97 | 128.86 |
| 3 | B | 903 | ATP | N3-C2-N1 | -10.28 | 120.06 | 128.86 |
| 3 | B | 901 | ATP | N3-C2-N1 | -10.26 | 120.08 | 128.86 |
| 3 | A | 903 | ATP | N3-C2-N1 | -10.13 | 120.19 | 128.86 |
| 3 | D | 903 | ATP | N3-C2-N1 | -10.06 | 120.25 | 128.86 |
| 3 | E | 901 | ATP | N3-C2-N1 | -9.95 | 120.35 | 128.86 |
| 3 | F | 903 | ATP | N3-C2-N1 | -9.93 | 120.37 | 128.86 |
| 3 | F | 901 | ATP | N3-C2-N1 | -9.84 | 120.44 | 128.86 |
| 3 | A | 901 | ATP | N3-C2-N1 | -9.75 | 120.51 | 128.86 |
| 3 | E | 903 | ATP | N3-C2-N1 | -9.67 | 120.59 | 128.86 |
| 3 | D | 903 | ATP | C4-C5-N7 | -5.03 | 104.55 | 109.41 |
| 3 | E | 901 | ATP | C4-C5-N7 | -4.76 | 104.81 | 109.41 |
| 3 | A | 901 | ATP | C4-C5-N7 | -4.60 | 104.97 | 109.41 |
| 3 | E | 903 | ATP | C4-C5-N7 | -4.51 | 105.06 | 109.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | F | 901 | ATP | C4-C5-N7 | -4.47 | 105.09 | 109.41 |
| 3 | B | 903 | ATP | C4-C5-N7 | -4.38 | 105.17 | 109.41 |
| 3 | C | 903 | ATP | C4-C5-N7 | -4.25 | 105.30 | 109.41 |
| 3 | F | 903 | ATP | C4-C5-N7 | -4.24 | 105.31 | 109.41 |
| 3 | C | 901 | ATP | C4-C5-N7 | -4.19 | 105.37 | 109.41 |
| 3 | B | 901 | ATP | C4-C5-N7 | -4.17 | 105.38 | 109.41 |
| 3 | A | 903 | ATP | C4-C5-N7 | -4.12 | 105.43 | 109.41 |
| 3 | D | 901 | ATP | C4-C5-N7 | -3.90 | 105.64 | 109.41 |
| 3 | B | 903 | ATP | PB-O3B-PG | -2.69 | 123.60 | 132.63 |
| 3 | E | 901 | ATP | N6-C6-N1 | -2.33 | 113.74 | 118.57 |
| 3 | D | 903 | ATP | N6-C6-N1 | -2.32 | 113.76 | 118.57 |
| 3 | A | 903 | ATP | PB-O3B-PG | -2.27 | 125.00 | 132.63 |
| 3 | A | 901 | ATP | N6-C6-N1 | -2.25 | 113.89 | 118.57 |
| 3 | B | 903 | ATP | N6-C6-N1 | -2.20 | 114.01 | 118.57 |
| 3 | F | 901 | ATP | PB-O3B-PG | -2.19 | 125.28 | 132.63 |
| 3 | F | 901 | ATP | N6-C6-N1 | -2.17 | 114.06 | 118.57 |
| 3 | C | 903 | ATP | N6-C6-N1 | -2.08 | 114.25 | 118.57 |
| 3 | A | 901 | ATP | PB-O3B-PG | -2.06 | 125.70 | 132.63 |
| 3 | A | 903 | ATP | N6-C6-N1 | -2.05 | 114.31 | 118.57 |
| 3 | E | 903 | ATP | PB-O3B-PG | -2.01 | 125.86 | 132.63 |
| 3 | F | 901 | ATP | O2'-C2'-C3' | 2.10 | 118.55 | 111.83 |
| 3 | E | 903 | ATP | PA-O3A-PB | 2.15 | 139.86 | 132.63 |
| 3 | E | 901 | ATP | O2'-C2'-C3' | 2.23 | 118.96 | 111.83 |
| 3 | B | 903 | ATP | O2'-C2'-C3' | 2.33 | 119.30 | 111.83 |
| 3 | C | 901 | ATP | C5-C6-N6 | 2.44 | 125.44 | 120.47 |
| 3 | D | 901 | ATP | C5-C6-N6 | 2.45 | 125.46 | 120.47 |
| 3 | F | 903 | ATP | C5-C6-N6 | 2.52 | 125.60 | 120.47 |
| 3 | E | 903 | ATP | C5-C6-N6 | 2.54 | 125.65 | 120.47 |
| 3 | C | 901 | ATP | O2'-C2'-C3' | 2.62 | 120.23 | 111.83 |
| 3 | A | 903 | ATP | C5-C6-N6 | 2.78 | 126.14 | 120.47 |
| 3 | B | 901 | ATP | C5-C6-N6 | 2.80 | 126.17 | 120.47 |
| 3 | B | 903 | ATP | C5-C6-N6 | 2.86 | 126.29 | 120.47 |
| 3 | F | 901 | ATP | C5-C6-N6 | 2.91 | 126.39 | 120.47 |
| 3 | C | 903 | ATP | C5-C6-N6 | 2.92 | 126.42 | 120.47 |
| 3 | E | 901 | ATP | C5-C6-N6 | 3.06 | 126.72 | 120.47 |
| 3 | A | 901 | ATP | C5-C6-N6 | 3.07 | 126.73 | 120.47 |
| 3 | D | 903 | ATP | C5-C6-N6 | 3.21 | 127.02 | 120.47 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | A | 901 | ATP | 6 | 0 |
| 3 | A | 903 | ATP | 1 | 0 |
| 3 | B | 901 | ATP | 3 | 0 |
| 3 | B | 903 | ATP | 5 | 0 |
| 3 | C | 901 | ATP | 3 | 0 |
| 3 | C | 903 | ATP | 2 | 0 |
| 3 | D | 901 | ATP | 2 | 0 |
| 3 | D | 903 | ATP | 4 | 0 |
| 3 | E | 901 | ATP | 6 | 0 |
| 3 | E | 903 | ATP | 5 | 0 |
| 3 | F | 901 | ATP | 4 | 0 |
| 3 | F | 903 | ATP | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ > 2 | | OWAB(Å ²) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1 | A | 505/525 (96%) | 0.17 | 49 (9%) | 8 2 | 31, 77, 121, 154 | 0 |
| 1 | F | 505/525 (96%) | -0.10 | 31 (6%) | 21 7 | 18, 66, 113, 145 | 0 |
| 2 | B | 491/525 (93%) | 0.13 | 32 (6%) | 19 6 | 43, 82, 126, 158 | 0 |
| 2 | C | 488/525 (92%) | -0.17 | 21 (4%) | 35 13 | 30, 69, 122, 160 | 0 |
| 2 | D | 485/525 (92%) | -0.37 | 13 (2%) | 54 26 | 20, 53, 106, 152 | 0 |
| 2 | E | 492/525 (93%) | -0.26 | 15 (3%) | 50 22 | 15, 59, 104, 148 | 0 |
| All | All | 2966/3150 (94%) | -0.10 | 161 (5%) | 26 9 | 15, 69, 117, 160 | 0 |

All (161) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 118 | VAL | 7.7 |
| 1 | F | 516 | GLY | 6.9 |
| 2 | D | 119 | GLY | 6.4 |
| 1 | A | 509 | VAL | 5.8 |
| 2 | D | 117 | VAL | 5.6 |
| 2 | D | 121 | PHE | 5.4 |
| 1 | F | 517 | PRO | 5.4 |
| 2 | B | 500 | ASP | 5.3 |
| 1 | F | 500 | ASP | 5.1 |
| 2 | C | 117 | VAL | 5.1 |
| 1 | F | 506 | SER | 5.1 |
| 2 | E | 500 | ASP | 5.1 |
| 2 | C | 119 | GLY | 4.9 |
| 1 | A | 519 | SER | 4.9 |
| 1 | A | 513 | GLN | 4.8 |
| 1 | A | 500 | ASP | 4.7 |
| 1 | A | 258 | SER | 4.7 |
| 2 | B | 503 | SER | 4.7 |
| 1 | F | 509 | VAL | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 504 | GLU | 4.7 |
| 1 | F | 515 | LYS | 4.7 |
| 1 | F | 507 | ARG | 4.6 |
| 1 | A | 120 | GLY | 4.6 |
| 2 | B | 255 | THR | 4.5 |
| 1 | A | 16 | GLN | 4.5 |
| 1 | A | 506 | SER | 4.5 |
| 2 | D | 120 | GLY | 4.4 |
| 2 | C | 118 | VAL | 4.4 |
| 2 | B | 501 | GLU | 4.4 |
| 2 | B | 117 | VAL | 4.4 |
| 1 | F | 154 | TYR | 4.3 |
| 1 | A | 503 | SER | 4.2 |
| 1 | A | 257 | ARG | 4.2 |
| 1 | A | 507 | ARG | 4.1 |
| 2 | B | 15 | HIS | 4.1 |
| 1 | F | 508 | ILE | 4.0 |
| 1 | A | 518 | GLU | 4.0 |
| 2 | C | 120 | GLY | 4.0 |
| 1 | A | 508 | ILE | 4.0 |
| 2 | C | 499 | VAL | 3.9 |
| 2 | E | 154 | TYR | 3.9 |
| 2 | E | 504 | GLU | 3.9 |
| 1 | F | 121 | PHE | 3.8 |
| 2 | B | 251 | ALA | 3.8 |
| 1 | F | 519 | SER | 3.8 |
| 1 | A | 511 | GLY | 3.8 |
| 2 | B | 254 | LEU | 3.8 |
| 1 | A | 517 | PRO | 3.7 |
| 2 | E | 121 | PHE | 3.7 |
| 2 | E | 501 | GLU | 3.6 |
| 1 | A | 254 | LEU | 3.6 |
| 1 | A | 117 | VAL | 3.5 |
| 2 | B | 158 | SER | 3.5 |
| 2 | B | 307 | ALA | 3.4 |
| 1 | A | 516 | GLY | 3.4 |
| 1 | F | 511 | GLY | 3.4 |
| 2 | B | 498 | THR | 3.4 |
| 1 | F | 501 | GLU | 3.4 |
| 2 | E | 499 | VAL | 3.3 |
| 2 | C | 154 | TYR | 3.3 |
| 2 | C | 251 | ALA | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | E | 503 | SER | 3.3 |
| 1 | A | 121 | PHE | 3.3 |
| 2 | B | 175 | GLY | 3.3 |
| 1 | A | 115 | GLN | 3.3 |
| 2 | B | 499 | VAL | 3.3 |
| 2 | B | 157 | SER | 3.2 |
| 2 | D | 154 | TYR | 3.2 |
| 1 | F | 518 | GLU | 3.2 |
| 2 | C | 500 | ASP | 3.1 |
| 2 | B | 153 | GLN | 3.1 |
| 1 | F | 512 | VAL | 3.0 |
| 1 | A | 510 | ARG | 3.0 |
| 1 | A | 251 | ALA | 3.0 |
| 1 | F | 498 | THR | 3.0 |
| 1 | A | 498 | THR | 3.0 |
| 1 | F | 257 | ARG | 2.9 |
| 2 | D | 113 | GLU | 2.9 |
| 2 | B | 119 | GLY | 2.9 |
| 2 | E | 505 | LEU | 2.9 |
| 1 | A | 334 | ASP | 2.9 |
| 1 | F | 255 | THR | 2.9 |
| 2 | B | 257 | ARG | 2.9 |
| 2 | B | 407 | GLU | 2.9 |
| 2 | C | 252 | MET | 2.9 |
| 1 | F | 513 | GLN | 2.8 |
| 2 | D | 498 | THR | 2.8 |
| 1 | F | 514 | GLU | 2.8 |
| 2 | B | 116 | GLU | 2.8 |
| 1 | A | 502 | LYS | 2.8 |
| 2 | B | 135 | GLN | 2.8 |
| 1 | A | 241 | ASP | 2.8 |
| 2 | B | 118 | VAL | 2.8 |
| 1 | F | 504 | GLU | 2.8 |
| 2 | E | 113 | GLU | 2.8 |
| 2 | D | 16 | GLN | 2.8 |
| 2 | B | 502 | LYS | 2.8 |
| 2 | E | 116 | GLU | 2.7 |
| 1 | A | 505 | LEU | 2.7 |
| 1 | F | 503 | SER | 2.7 |
| 2 | C | 77 | GLU | 2.7 |
| 2 | C | 257 | ARG | 2.6 |
| 2 | E | 118 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 117 | VAL | 2.6 |
| 2 | C | 116 | GLU | 2.6 |
| 1 | A | 152 | GLN | 2.6 |
| 2 | C | 115 | GLN | 2.6 |
| 1 | A | 253 | ARG | 2.6 |
| 1 | A | 256 | GLN | 2.6 |
| 2 | B | 253 | ARG | 2.6 |
| 2 | B | 16 | GLN | 2.5 |
| 2 | D | 15 | HIS | 2.5 |
| 2 | D | 155 | ASP | 2.5 |
| 2 | C | 15 | HIS | 2.5 |
| 2 | B | 132 | TYR | 2.5 |
| 1 | A | 499 | VAL | 2.5 |
| 2 | B | 154 | TYR | 2.5 |
| 2 | B | 504 | GLU | 2.5 |
| 2 | C | 423 | HIS | 2.5 |
| 1 | F | 510 | ARG | 2.5 |
| 1 | A | 255 | THR | 2.5 |
| 1 | A | 337 | GLU | 2.5 |
| 2 | C | 501 | GLU | 2.5 |
| 1 | A | 116 | GLU | 2.5 |
| 1 | F | 155 | ASP | 2.5 |
| 1 | F | 499 | VAL | 2.4 |
| 1 | A | 17 | ALA | 2.4 |
| 1 | A | 112 | PRO | 2.4 |
| 2 | E | 332 | GLY | 2.4 |
| 1 | A | 153 | GLN | 2.4 |
| 1 | A | 71 | GLY | 2.4 |
| 1 | F | 311 | ARG | 2.4 |
| 2 | B | 121 | PHE | 2.4 |
| 1 | F | 251 | ALA | 2.3 |
| 1 | A | 310 | GLU | 2.3 |
| 1 | A | 311 | ARG | 2.3 |
| 1 | A | 154 | TYR | 2.3 |
| 1 | A | 114 | GLY | 2.3 |
| 2 | E | 310 | GLU | 2.3 |
| 1 | A | 475 | LYS | 2.2 |
| 1 | F | 502 | LYS | 2.2 |
| 2 | B | 14 | GLU | 2.2 |
| 1 | A | 342 | ASN | 2.2 |
| 2 | B | 342 | ASN | 2.2 |
| 2 | B | 250 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 256 | GLN | 2.2 |
| 2 | C | 121 | PHE | 2.2 |
| 2 | C | 153 | GLN | 2.2 |
| 1 | F | 120 | GLY | 2.2 |
| 2 | C | 102 | LYS | 2.1 |
| 2 | D | 257 | ARG | 2.1 |
| 1 | A | 113 | GLU | 2.1 |
| 2 | B | 115 | GLN | 2.1 |
| 2 | C | 176 | ALA | 2.1 |
| 2 | E | 115 | GLN | 2.1 |
| 1 | A | 368 | ASN | 2.1 |
| 1 | A | 515 | LYS | 2.1 |
| 2 | D | 115 | GLN | 2.0 |
| 2 | E | 155 | ASP | 2.0 |
| 2 | C | 250 | GLY | 2.0 |
| 1 | A | 340 | ARG | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1 | SEP | A | 320 | 10/11 | 0.58 | 0.54 | 49,59,66,68 | 0 |
| 1 | SEP | F | 320 | 10/11 | 0.60 | 0.39 | 45,57,63,66 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MG | B | 801 | 1/1 | 0.68 | 0.12 | 45,45,45,45 | 0 |
| 4 | MG | A | 526 | 1/1 | 0.74 | 0.48 | 58,58,58,58 | 0 |
| 4 | MG | C | 701 | 1/1 | 0.82 | 0.26 | 70,70,70,70 | 0 |
| 4 | MG | B | 701 | 1/1 | 0.83 | 0.23 | 58,58,58,58 | 0 |
| 4 | MG | D | 701 | 1/1 | 0.85 | 0.35 | 59,59,59,59 | 0 |
| 4 | MG | C | 702 | 1/1 | 0.85 | 0.49 | 65,65,65,65 | 0 |
| 4 | MG | B | 702 | 1/1 | 0.88 | 0.24 | 79,79,79,79 | 0 |
| 4 | MG | F | 701 | 1/1 | 0.89 | 0.19 | 45,45,45,45 | 0 |
| 3 | ATP | B | 903 | 31/31 | 0.91 | 0.17 | 77,81,94,95 | 0 |
| 3 | ATP | B | 901 | 31/31 | 0.92 | 0.20 | 67,70,85,87 | 0 |
| 3 | ATP | C | 903 | 31/31 | 0.92 | 0.19 | 42,52,85,85 | 0 |
| 3 | ATP | A | 903 | 31/31 | 0.92 | 0.19 | 61,66,76,77 | 0 |
| 3 | ATP | A | 901 | 31/31 | 0.93 | 0.19 | 84,86,89,90 | 0 |
| 4 | MG | F | 802 | 1/1 | 0.93 | 0.26 | 53,53,53,53 | 0 |
| 4 | MG | D | 801 | 1/1 | 0.94 | 0.34 | 44,44,44,44 | 0 |
| 4 | MG | A | 802 | 1/1 | 0.94 | 0.31 | 82,82,82,82 | 0 |
| 3 | ATP | F | 903 | 31/31 | 0.94 | 0.15 | 44,48,62,62 | 0 |
| 3 | ATP | F | 901 | 31/31 | 0.94 | 0.18 | 74,83,88,89 | 0 |
| 4 | MG | D | 702 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 4 | MG | A | 701 | 1/1 | 0.94 | 0.33 | 63,63,63,63 | 0 |
| 4 | MG | A | 801 | 1/1 | 0.94 | 0.14 | 46,46,46,46 | 0 |
| 3 | ATP | E | 901 | 31/31 | 0.95 | 0.16 | 65,72,81,81 | 0 |
| 3 | ATP | D | 901 | 31/31 | 0.95 | 0.17 | 50,54,60,62 | 0 |
| 4 | MG | E | 801 | 1/1 | 0.95 | 0.18 | 38,38,38,38 | 0 |
| 3 | ATP | D | 903 | 31/31 | 0.95 | 0.15 | 26,35,60,62 | 0 |
| 4 | MG | E | 802 | 1/1 | 0.95 | 0.18 | 46,46,46,46 | 0 |
| 3 | ATP | E | 903 | 31/31 | 0.96 | 0.14 | 22,28,60,62 | 0 |
| 4 | MG | D | 802 | 1/1 | 0.96 | 0.12 | 17,17,17,17 | 0 |
| 3 | ATP | C | 901 | 31/31 | 0.96 | 0.17 | 36,47,56,56 | 0 |
| 4 | MG | F | 702 | 1/1 | 0.96 | 0.24 | 68,68,68,68 | 0 |
| 4 | MG | C | 802 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 4 | MG | C | 801 | 1/1 | 0.97 | 0.08 | 25,25,25,25 | 0 |
| 4 | MG | B | 802 | 1/1 | 0.98 | 0.18 | 64,64,64,64 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.