



Full wwPDB EM Validation Report ⓘ

Feb 12, 2024 – 04:42 AM EST

PDB ID : 3H3W
EMDB ID : EMD-1048
Title : Fitting of the gp6 crystal structure into 3D cryo-EM reconstruction of bacteriophage T4 dome-shaped baseplate
Authors : Aksyuk, A.A.; Leiman, P.G.; Shneider, M.M.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2009-04-17
Resolution : 12.00 Å (reported)
Based on initial model : 3H2T

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

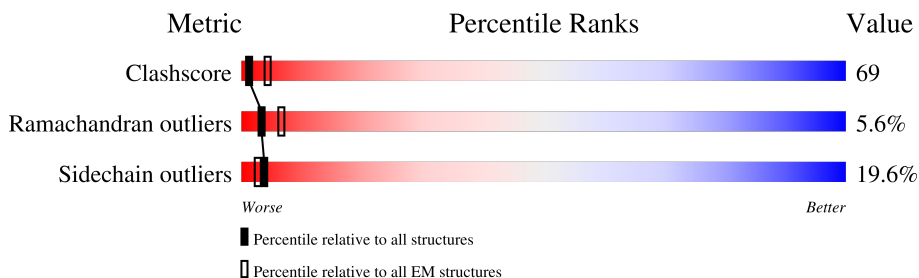
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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.



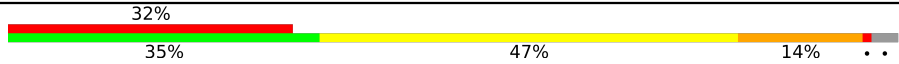

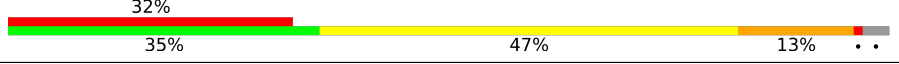
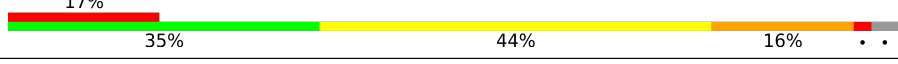
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------|
| 1 | A | 335 | 32% 36% 46% 14% .. |
| 1 | B | 335 | 18% 35% 44% 17% .. |
| 1 | C | 335 | 17% 36% 46% 14% .. |
| 1 | D | 335 | 31% 34% 44% 17% .. |
| 1 | E | 335 | 32% 35% 47% 14% .. |
| 1 | F | 335 | 17% 34% 44% 16% .. |
| 1 | G | 335 | 32% 35% 47% 14% .. |
| 1 | H | 335 | 18% 35% 44% 16% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | I | 335 |  |
| 1 | J | 335 |  |
| 1 | K | 335 |  |
| 1 | L | 335 |  |

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 31380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Baseplate structural protein Gp6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | B | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |
| 1 | C | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | D | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |
| 1 | E | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | F | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |
| 1 | G | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | H | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |
| 1 | I | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | J | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |
| 1 | K | 326 | 2622 | 1667 | 424 | 528 | 3 | 0 | 0 |
| 1 | L | 324 | 2608 | 1658 | 422 | 525 | 3 | 0 | 0 |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 661 | LEU | - | expression tag | UNP P19060 |
| A | 662 | GLU | - | expression tag | UNP P19060 |
| A | 663 | HIS | - | expression tag | UNP P19060 |
| A | 664 | HIS | - | expression tag | UNP P19060 |
| A | 665 | HIS | - | expression tag | UNP P19060 |
| A | 666 | HIS | - | expression tag | UNP P19060 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 667 | HIS | - | expression tag | UNP P19060 |
| A | 668 | HIS | - | expression tag | UNP P19060 |
| B | 661 | LEU | - | expression tag | UNP P19060 |
| B | 662 | GLU | - | expression tag | UNP P19060 |
| B | 663 | HIS | - | expression tag | UNP P19060 |
| B | 664 | HIS | - | expression tag | UNP P19060 |
| B | 665 | HIS | - | expression tag | UNP P19060 |
| B | 666 | HIS | - | expression tag | UNP P19060 |
| B | 667 | HIS | - | expression tag | UNP P19060 |
| B | 668 | HIS | - | expression tag | UNP P19060 |
| C | 661 | LEU | - | expression tag | UNP P19060 |
| C | 662 | GLU | - | expression tag | UNP P19060 |
| C | 663 | HIS | - | expression tag | UNP P19060 |
| C | 664 | HIS | - | expression tag | UNP P19060 |
| C | 665 | HIS | - | expression tag | UNP P19060 |
| C | 666 | HIS | - | expression tag | UNP P19060 |
| C | 667 | HIS | - | expression tag | UNP P19060 |
| C | 668 | HIS | - | expression tag | UNP P19060 |
| D | 661 | LEU | - | expression tag | UNP P19060 |
| D | 662 | GLU | - | expression tag | UNP P19060 |
| D | 663 | HIS | - | expression tag | UNP P19060 |
| D | 664 | HIS | - | expression tag | UNP P19060 |
| D | 665 | HIS | - | expression tag | UNP P19060 |
| D | 666 | HIS | - | expression tag | UNP P19060 |
| D | 667 | HIS | - | expression tag | UNP P19060 |
| D | 668 | HIS | - | expression tag | UNP P19060 |
| E | 661 | LEU | - | expression tag | UNP P19060 |
| E | 662 | GLU | - | expression tag | UNP P19060 |
| E | 663 | HIS | - | expression tag | UNP P19060 |
| E | 664 | HIS | - | expression tag | UNP P19060 |
| E | 665 | HIS | - | expression tag | UNP P19060 |
| E | 666 | HIS | - | expression tag | UNP P19060 |
| E | 667 | HIS | - | expression tag | UNP P19060 |
| E | 668 | HIS | - | expression tag | UNP P19060 |
| F | 661 | LEU | - | expression tag | UNP P19060 |
| F | 662 | GLU | - | expression tag | UNP P19060 |
| F | 663 | HIS | - | expression tag | UNP P19060 |
| F | 664 | HIS | - | expression tag | UNP P19060 |
| F | 665 | HIS | - | expression tag | UNP P19060 |
| F | 666 | HIS | - | expression tag | UNP P19060 |
| F | 667 | HIS | - | expression tag | UNP P19060 |
| F | 668 | HIS | - | expression tag | UNP P19060 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 661 | LEU | - | expression tag | UNP P19060 |
| G | 662 | GLU | - | expression tag | UNP P19060 |
| G | 663 | HIS | - | expression tag | UNP P19060 |
| G | 664 | HIS | - | expression tag | UNP P19060 |
| G | 665 | HIS | - | expression tag | UNP P19060 |
| G | 666 | HIS | - | expression tag | UNP P19060 |
| G | 667 | HIS | - | expression tag | UNP P19060 |
| G | 668 | HIS | - | expression tag | UNP P19060 |
| H | 661 | LEU | - | expression tag | UNP P19060 |
| H | 662 | GLU | - | expression tag | UNP P19060 |
| H | 663 | HIS | - | expression tag | UNP P19060 |
| H | 664 | HIS | - | expression tag | UNP P19060 |
| H | 665 | HIS | - | expression tag | UNP P19060 |
| H | 666 | HIS | - | expression tag | UNP P19060 |
| H | 667 | HIS | - | expression tag | UNP P19060 |
| H | 668 | HIS | - | expression tag | UNP P19060 |
| I | 661 | LEU | - | expression tag | UNP P19060 |
| I | 662 | GLU | - | expression tag | UNP P19060 |
| I | 663 | HIS | - | expression tag | UNP P19060 |
| I | 664 | HIS | - | expression tag | UNP P19060 |
| I | 665 | HIS | - | expression tag | UNP P19060 |
| I | 666 | HIS | - | expression tag | UNP P19060 |
| I | 667 | HIS | - | expression tag | UNP P19060 |
| I | 668 | HIS | - | expression tag | UNP P19060 |
| J | 661 | LEU | - | expression tag | UNP P19060 |
| J | 662 | GLU | - | expression tag | UNP P19060 |
| J | 663 | HIS | - | expression tag | UNP P19060 |
| J | 664 | HIS | - | expression tag | UNP P19060 |
| J | 665 | HIS | - | expression tag | UNP P19060 |
| J | 666 | HIS | - | expression tag | UNP P19060 |
| J | 667 | HIS | - | expression tag | UNP P19060 |
| J | 668 | HIS | - | expression tag | UNP P19060 |
| K | 661 | LEU | - | expression tag | UNP P19060 |
| K | 662 | GLU | - | expression tag | UNP P19060 |
| K | 663 | HIS | - | expression tag | UNP P19060 |
| K | 664 | HIS | - | expression tag | UNP P19060 |
| K | 665 | HIS | - | expression tag | UNP P19060 |
| K | 666 | HIS | - | expression tag | UNP P19060 |
| K | 667 | HIS | - | expression tag | UNP P19060 |
| K | 668 | HIS | - | expression tag | UNP P19060 |
| L | 661 | LEU | - | expression tag | UNP P19060 |
| L | 662 | GLU | - | expression tag | UNP P19060 |

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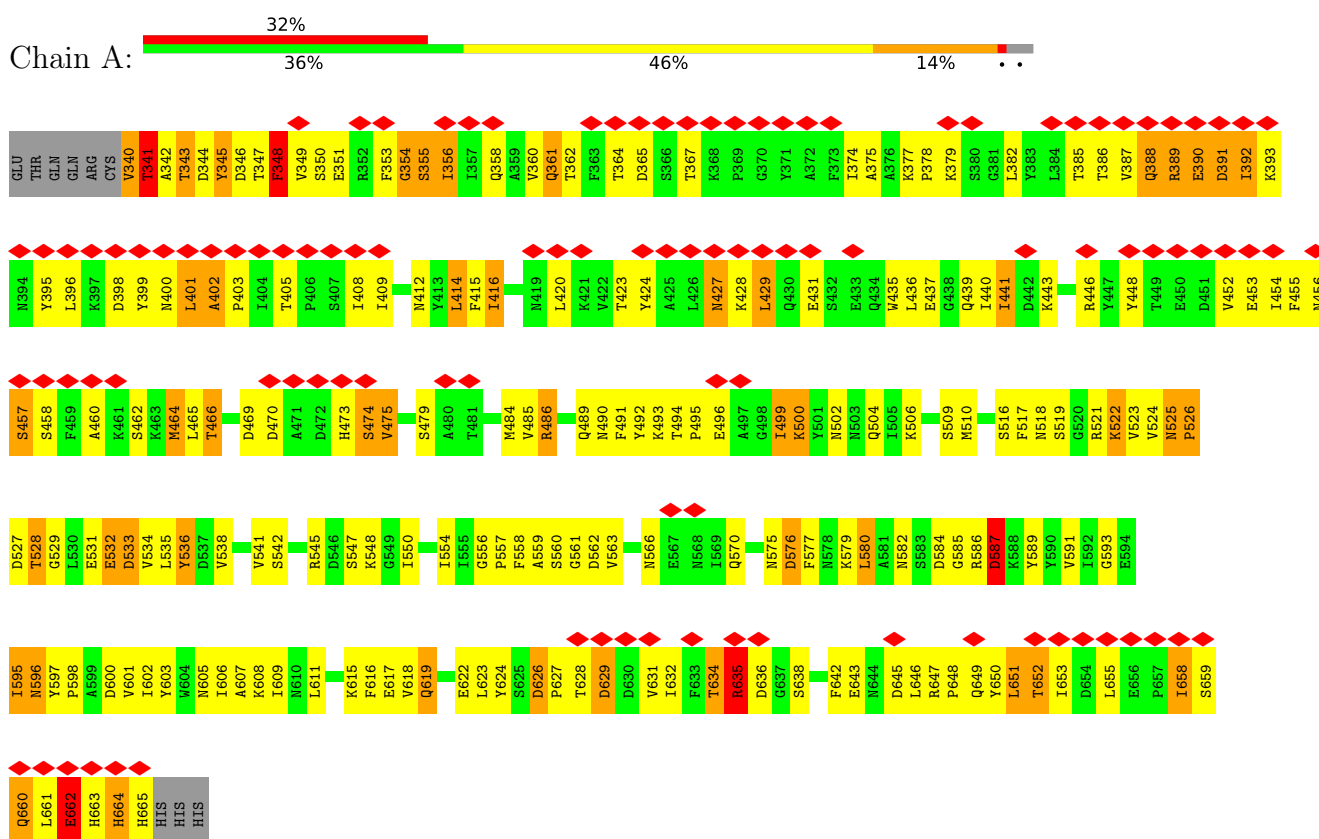
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| L | 663 | HIS | - | expression tag | UNP P19060 |
| L | 664 | HIS | - | expression tag | UNP P19060 |
| L | 665 | HIS | - | expression tag | UNP P19060 |
| L | 666 | HIS | - | expression tag | UNP P19060 |
| L | 667 | HIS | - | expression tag | UNP P19060 |
| L | 668 | HIS | - | expression tag | UNP P19060 |

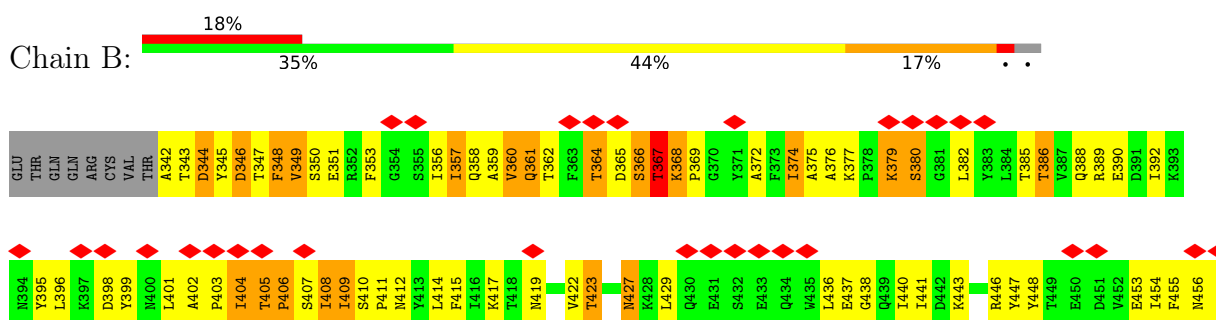
3 Residue-property plots [i](#)

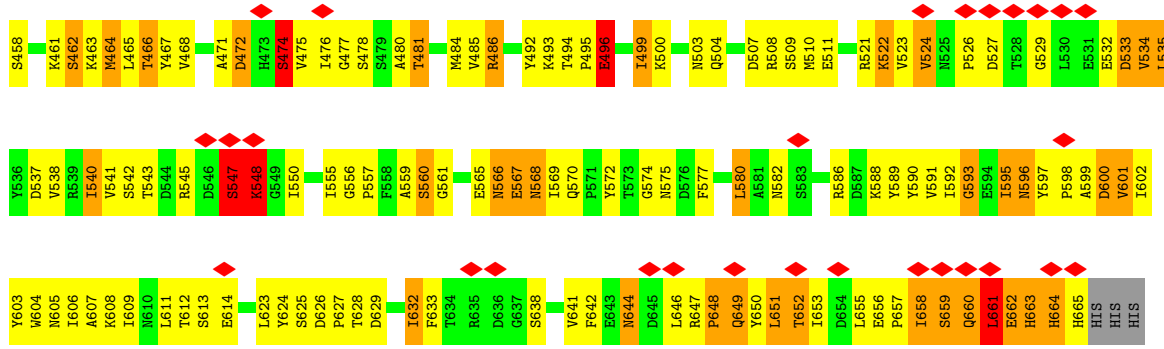
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Baseplate structural protein Gp6

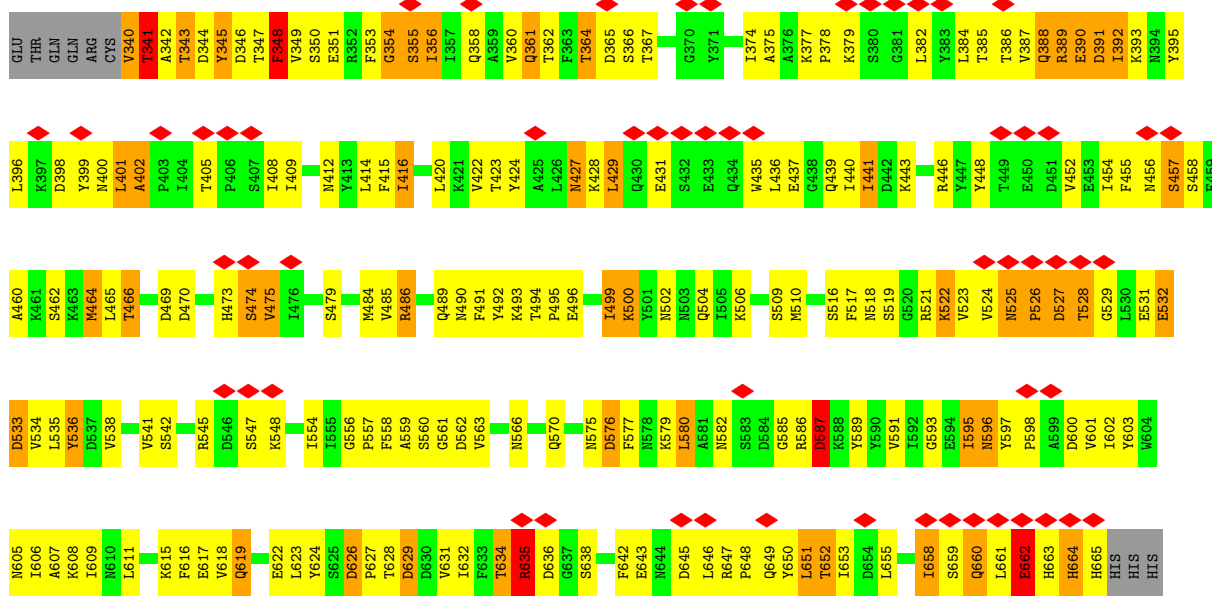


- Molecule 1: Baseplate structural protein Gp6

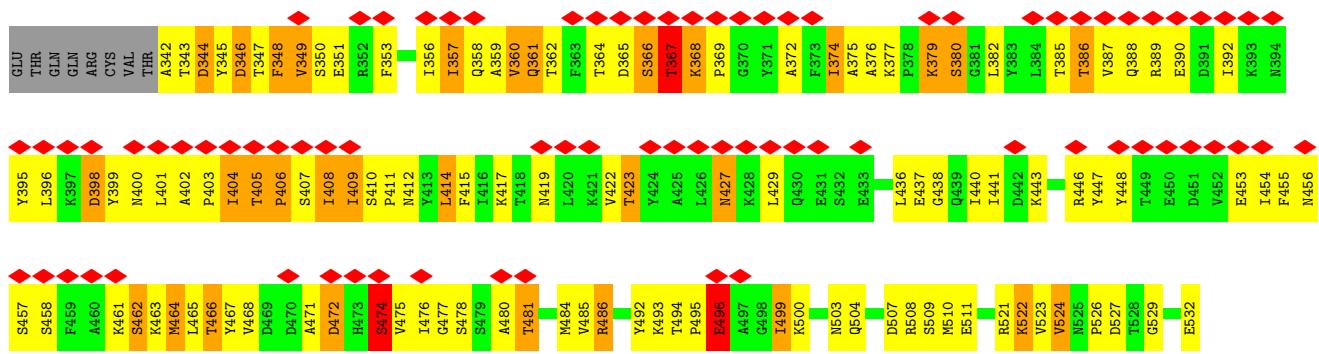


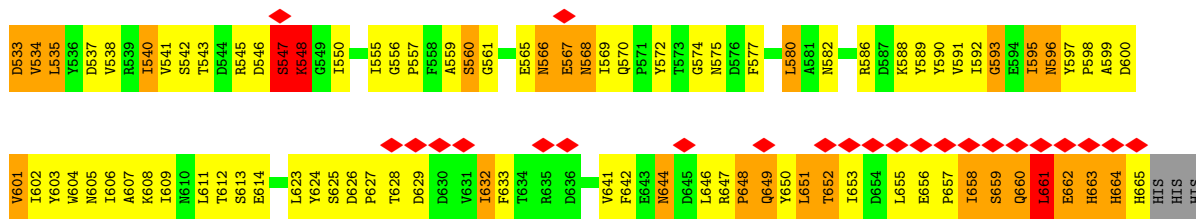


• Molecule 1: Baseplate structural protein Gp6

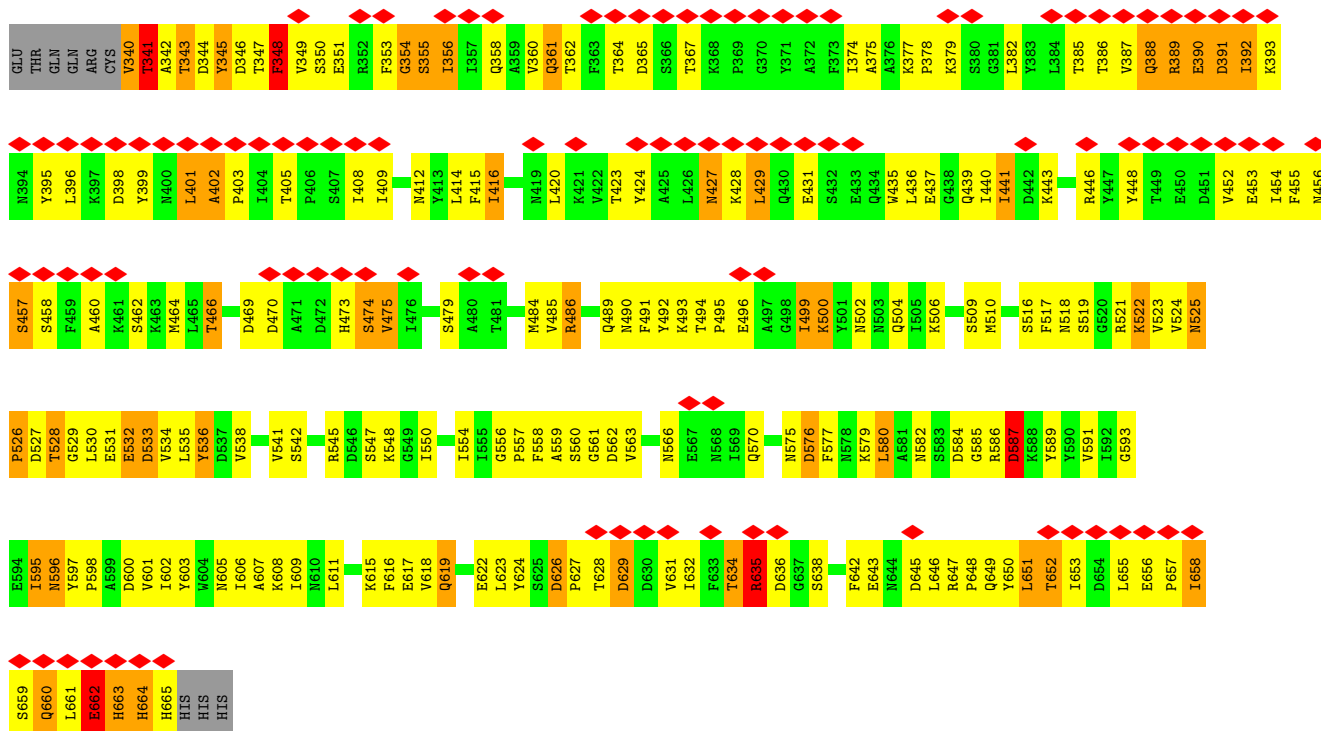


• Molecule 1: Baseplate structural protein Gp6

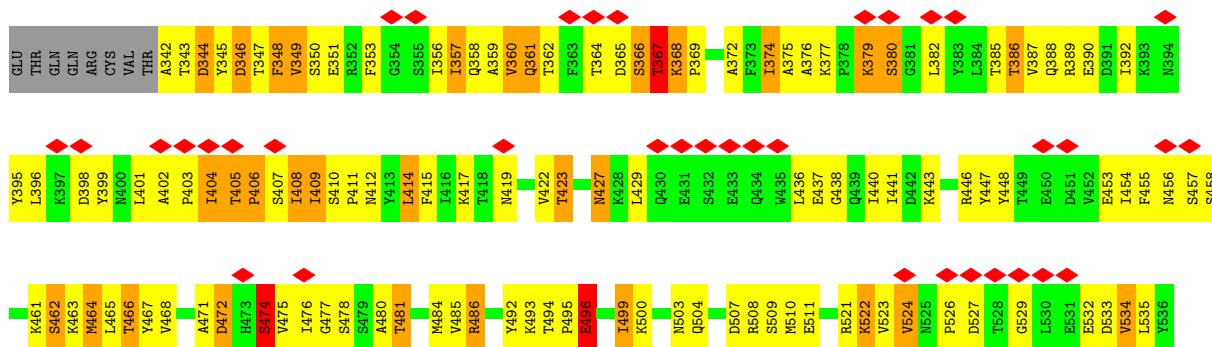


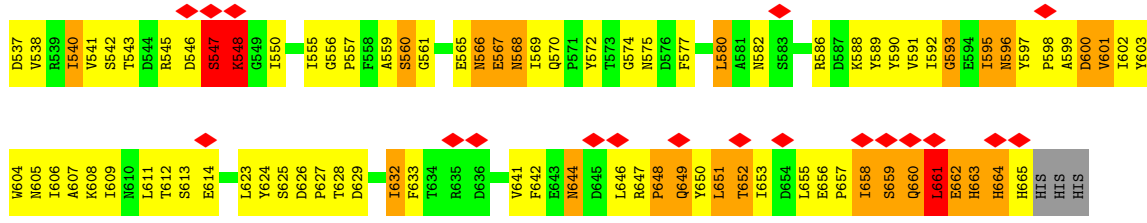


• Molecule 1: Baseplate structural protein Gp6

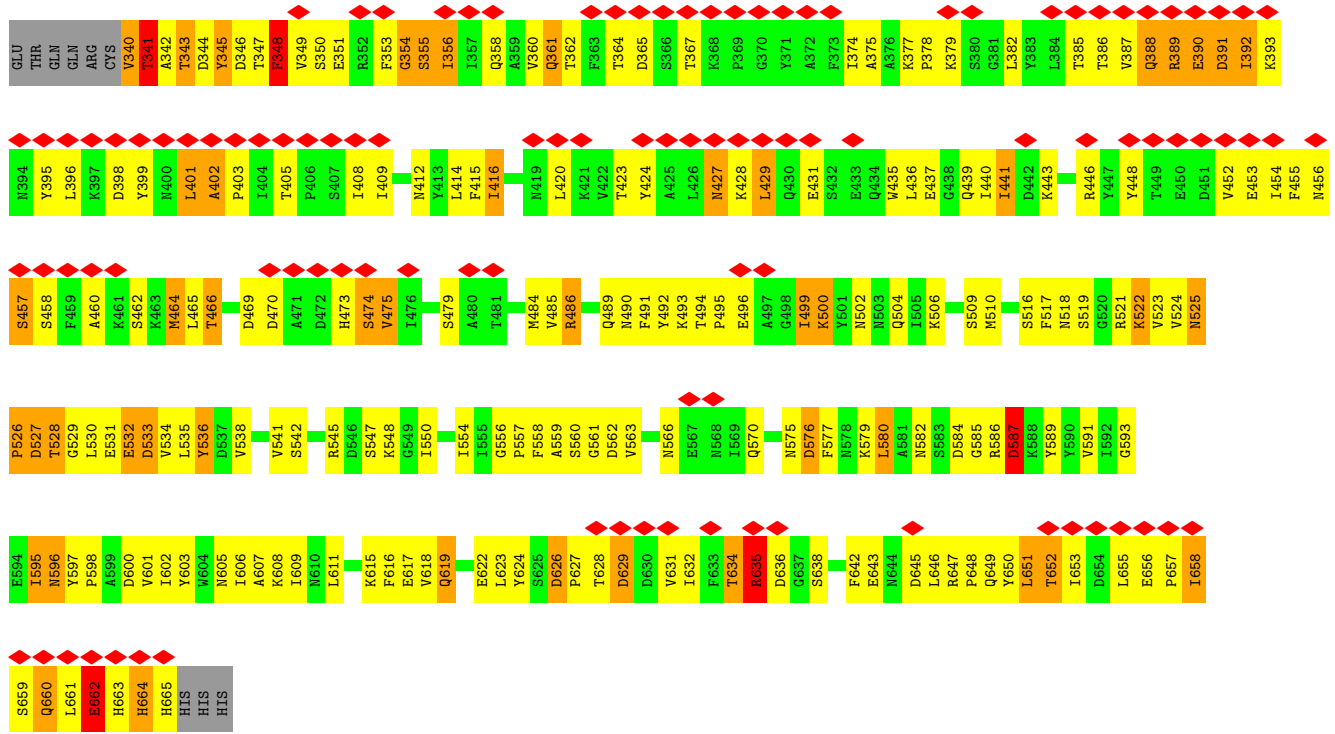


• Molecule 1: Baseplate structural protein Gp6

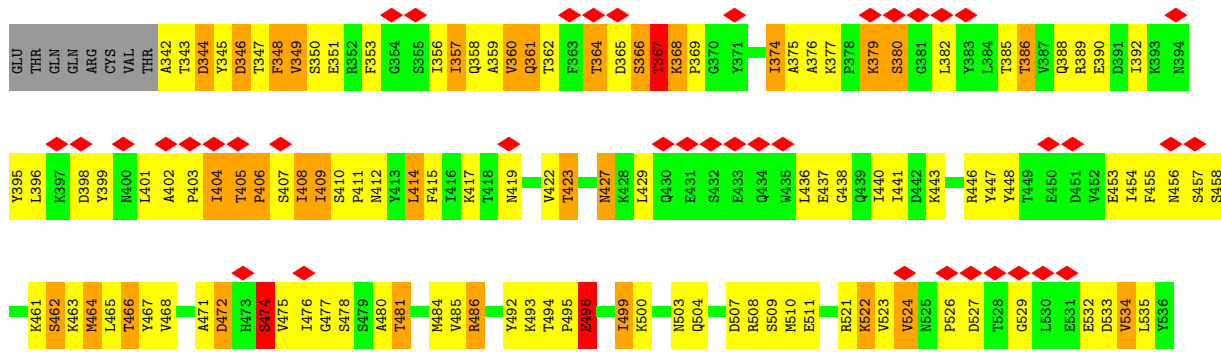


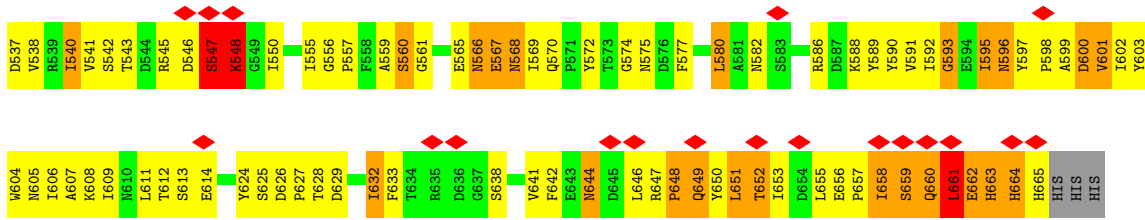


• Molecule 1: Baseplate structural protein Gp6

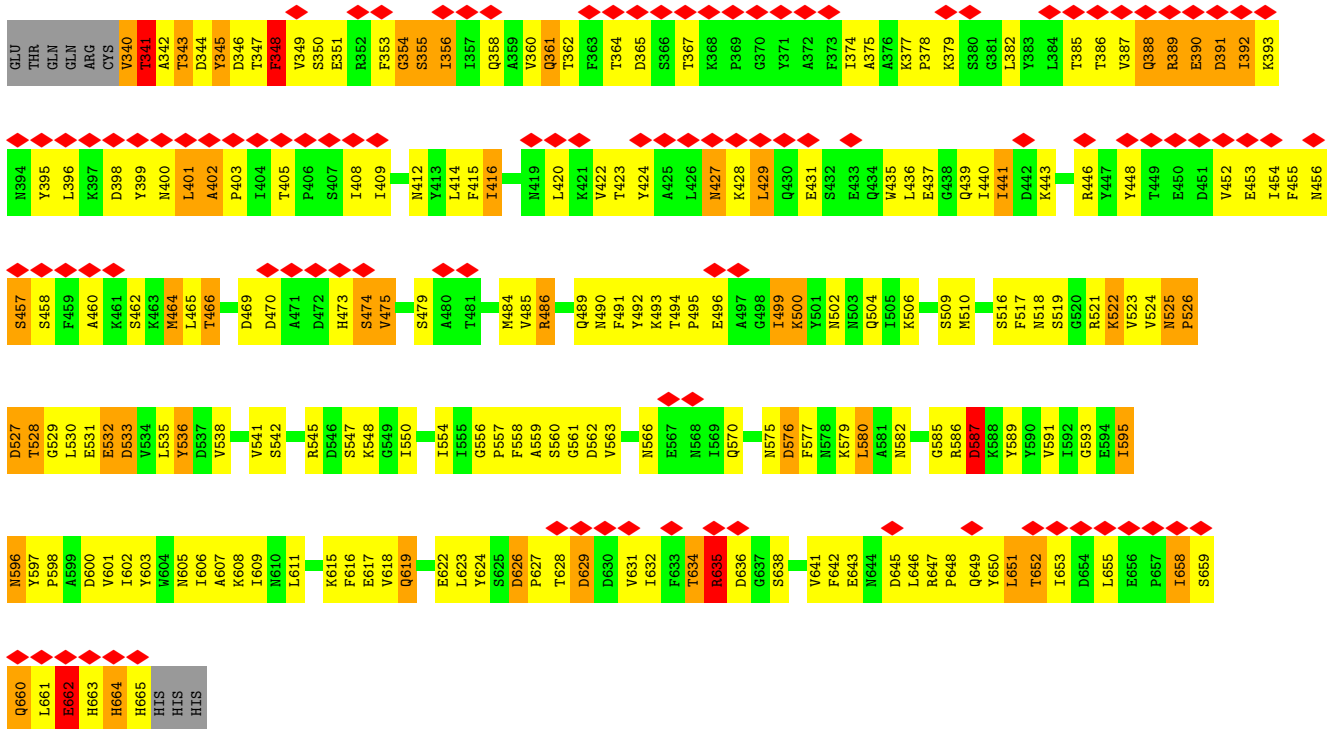


• Molecule 1: Baseplate structural protein Gp6

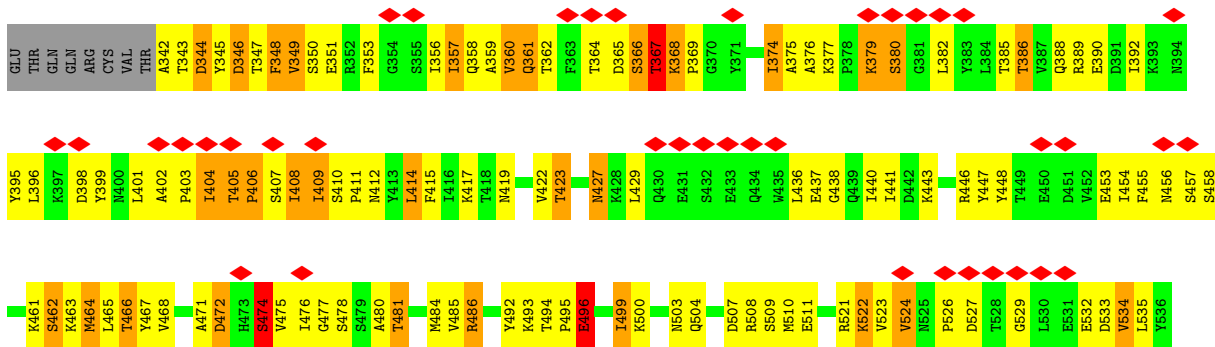


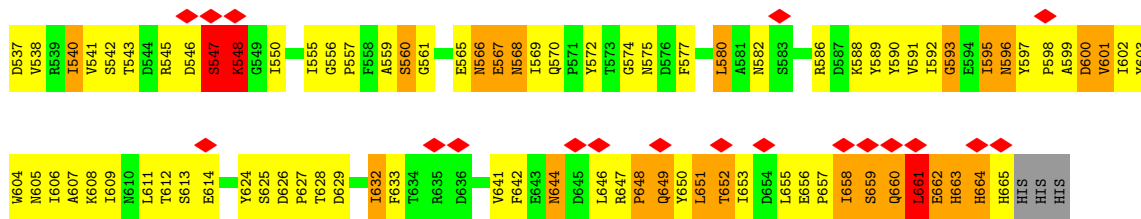


• Molecule 1: Baseplate structural protein Gp6

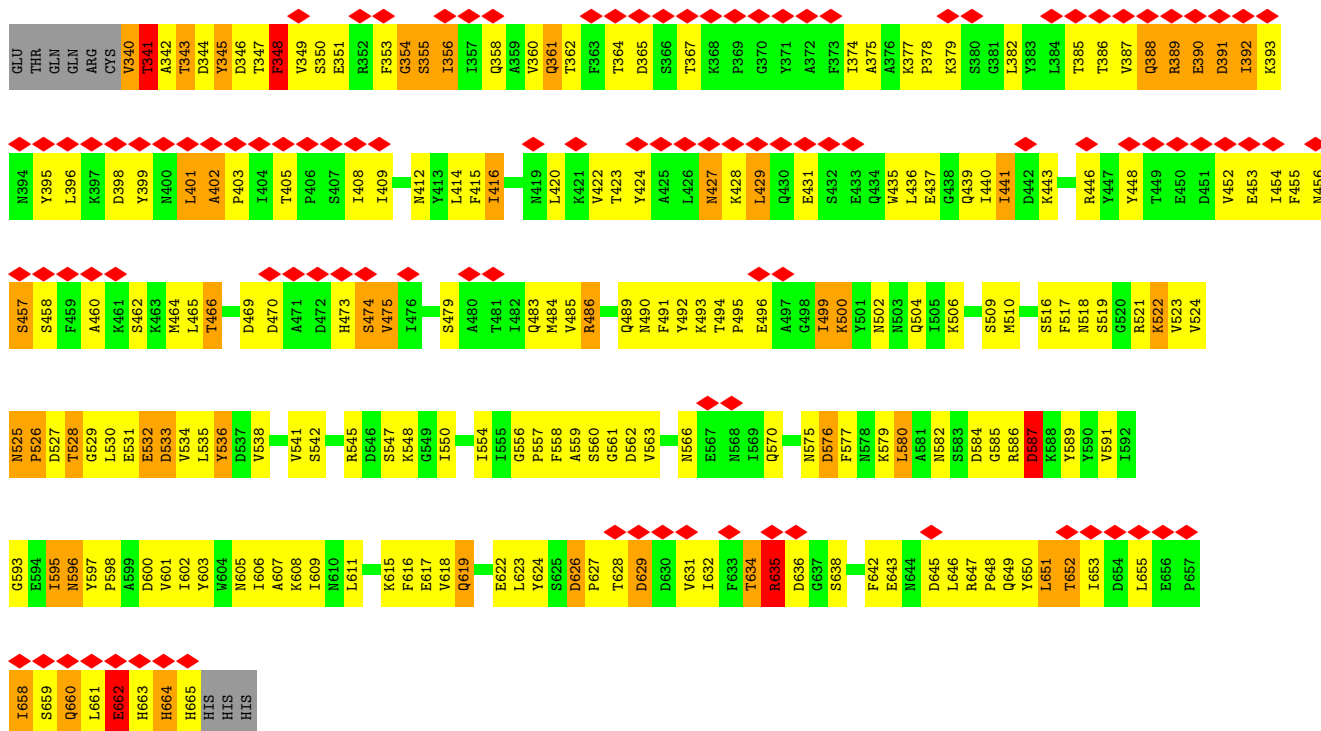


• Molecule 1: Baseplate structural protein Gp6

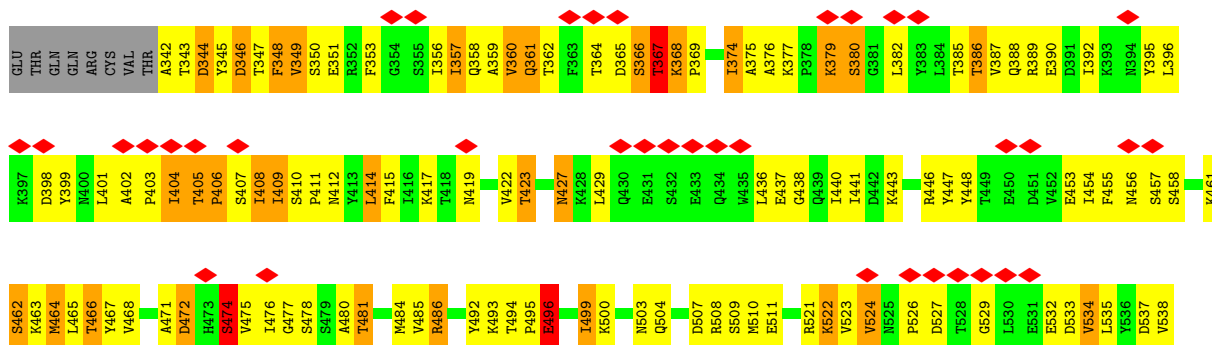


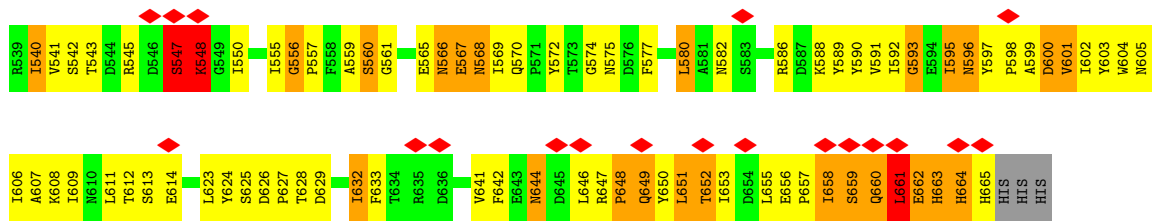


• Molecule 1: Baseplate structural protein Gp6



• Molecule 1: Baseplate structural protein Gp6





4 Experimental information

| Property | Value | Source |
|--------------------------------------|------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C6 | Depositor |
| Number of particles used | 945 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | Not provided | |
| Microscope | FEI/PHILIPS CM300FEG/T | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 47000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum map value | 10.345 | Depositor |
| Minimum map value | -7.648 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 1.45 | Depositor |
| Map size (\AA) | 583.8291, 583.8291, 583.8291 | wwPDB |
| Map dimensions | 196, 196, 196 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 2.97872, 2.97872, 2.97872 | Depositor |

5 Model quality i

5.1 Standard geometry i

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 | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | B | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| 1 | C | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | D | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| 1 | E | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | F | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| 1 | G | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | H | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| 1 | I | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | J | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| 1 | K | 0.50 | 0/2677 | 0.80 | 7/3637 (0.2%) |
| 1 | L | 0.51 | 0/2663 | 0.96 | 11/3617 (0.3%) |
| All | All | 0.51 | 0/32040 | 0.88 | 108/43524 (0.2%) |

There are no bond length outliers.

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | J | 405 | THR | C-N-CD | -29.01 | 56.77 | 120.60 |
| 1 | H | 405 | THR | C-N-CD | -29.01 | 56.77 | 120.60 |
| 1 | D | 405 | THR | C-N-CD | -29.01 | 56.78 | 120.60 |
| 1 | F | 405 | THR | C-N-CD | -29.00 | 56.79 | 120.60 |
| 1 | L | 405 | THR | C-N-CD | -29.00 | 56.80 | 120.60 |
| 1 | B | 405 | THR | C-N-CD | -29.00 | 56.81 | 120.60 |
| 1 | B | 474 | SER | N-CA-CB | -10.98 | 94.03 | 110.50 |
| 1 | L | 474 | SER | N-CA-CB | -10.98 | 94.03 | 110.50 |
| 1 | D | 474 | SER | N-CA-CB | -10.97 | 94.04 | 110.50 |
| 1 | F | 474 | SER | N-CA-CB | -10.97 | 94.05 | 110.50 |
| 1 | H | 474 | SER | N-CA-CB | -10.96 | 94.06 | 110.50 |
| 1 | J | 474 | SER | N-CA-CB | -10.96 | 94.07 | 110.50 |
| 1 | G | 646 | LEU | N-CA-CB | -10.48 | 89.45 | 110.40 |
| 1 | A | 646 | LEU | N-CA-CB | -10.47 | 89.47 | 110.40 |
| 1 | E | 646 | LEU | N-CA-CB | -10.46 | 89.48 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | I | 646 | LEU | N-CA-CB | -10.45 | 89.50 | 110.40 |
| 1 | K | 646 | LEU | N-CA-CB | -10.45 | 89.51 | 110.40 |
| 1 | C | 646 | LEU | N-CA-CB | -10.44 | 89.53 | 110.40 |
| 1 | B | 548 | LYS | N-CA-C | 9.97 | 137.91 | 111.00 |
| 1 | D | 548 | LYS | N-CA-C | 9.96 | 137.88 | 111.00 |
| 1 | L | 548 | LYS | N-CA-C | 9.95 | 137.85 | 111.00 |
| 1 | F | 548 | LYS | N-CA-C | 9.94 | 137.84 | 111.00 |
| 1 | H | 548 | LYS | N-CA-C | 9.94 | 137.83 | 111.00 |
| 1 | J | 548 | LYS | N-CA-C | 9.94 | 137.83 | 111.00 |
| 1 | J | 534 | VAL | N-CA-CB | -9.74 | 90.06 | 111.50 |
| 1 | H | 534 | VAL | N-CA-CB | -9.73 | 90.10 | 111.50 |
| 1 | D | 534 | VAL | N-CA-CB | -9.72 | 90.11 | 111.50 |
| 1 | L | 534 | VAL | N-CA-CB | -9.72 | 90.11 | 111.50 |
| 1 | F | 534 | VAL | N-CA-CB | -9.72 | 90.12 | 111.50 |
| 1 | B | 534 | VAL | N-CA-CB | -9.71 | 90.13 | 111.50 |
| 1 | A | 457 | SER | N-CA-CB | 9.62 | 124.93 | 110.50 |
| 1 | I | 457 | SER | N-CA-CB | 9.62 | 124.93 | 110.50 |
| 1 | E | 457 | SER | N-CA-CB | 9.60 | 124.90 | 110.50 |
| 1 | C | 457 | SER | N-CA-CB | 9.60 | 124.89 | 110.50 |
| 1 | G | 457 | SER | N-CA-CB | 9.59 | 124.88 | 110.50 |
| 1 | K | 457 | SER | N-CA-CB | 9.59 | 124.88 | 110.50 |
| 1 | I | 456 | ASN | CB-CA-C | -8.73 | 92.94 | 110.40 |
| 1 | E | 456 | ASN | CB-CA-C | -8.73 | 92.95 | 110.40 |
| 1 | K | 456 | ASN | CB-CA-C | -8.73 | 92.95 | 110.40 |
| 1 | C | 456 | ASN | CB-CA-C | -8.72 | 92.96 | 110.40 |
| 1 | A | 456 | ASN | CB-CA-C | -8.72 | 92.97 | 110.40 |
| 1 | G | 456 | ASN | CB-CA-C | -8.71 | 92.97 | 110.40 |
| 1 | B | 472 | ASP | CB-CA-C | 8.47 | 127.34 | 110.40 |
| 1 | J | 472 | ASP | CB-CA-C | 8.46 | 127.31 | 110.40 |
| 1 | H | 472 | ASP | CB-CA-C | 8.45 | 127.30 | 110.40 |
| 1 | L | 472 | ASP | CB-CA-C | 8.45 | 127.30 | 110.40 |
| 1 | F | 472 | ASP | CB-CA-C | 8.45 | 127.29 | 110.40 |
| 1 | D | 472 | ASP | CB-CA-C | 8.44 | 127.29 | 110.40 |
| 1 | H | 398 | ASP | CB-CA-C | 7.99 | 126.38 | 110.40 |
| 1 | F | 398 | ASP | CB-CA-C | 7.99 | 126.37 | 110.40 |
| 1 | L | 398 | ASP | CB-CA-C | 7.99 | 126.37 | 110.40 |
| 1 | B | 398 | ASP | CB-CA-C | 7.97 | 126.34 | 110.40 |
| 1 | D | 398 | ASP | CB-CA-C | 7.97 | 126.34 | 110.40 |
| 1 | J | 398 | ASP | CB-CA-C | 7.96 | 126.32 | 110.40 |
| 1 | G | 645 | ASP | CB-CA-C | 7.88 | 126.17 | 110.40 |
| 1 | A | 645 | ASP | CB-CA-C | 7.88 | 126.16 | 110.40 |
| 1 | E | 645 | ASP | CB-CA-C | 7.86 | 126.13 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | I | 645 | ASP | CB-CA-C | 7.86 | 126.12 | 110.40 |
| 1 | K | 645 | ASP | CB-CA-C | 7.85 | 126.10 | 110.40 |
| 1 | C | 645 | ASP | CB-CA-C | 7.84 | 126.09 | 110.40 |
| 1 | C | 527 | ASP | C-N-CA | -6.15 | 106.33 | 121.70 |
| 1 | I | 527 | ASP | C-N-CA | -6.15 | 106.33 | 121.70 |
| 1 | K | 527 | ASP | C-N-CA | -6.14 | 106.35 | 121.70 |
| 1 | A | 527 | ASP | C-N-CA | -6.13 | 106.36 | 121.70 |
| 1 | G | 527 | ASP | C-N-CA | -6.13 | 106.38 | 121.70 |
| 1 | E | 457 | SER | N-CA-C | -6.11 | 94.49 | 111.00 |
| 1 | E | 527 | ASP | C-N-CA | -6.11 | 106.42 | 121.70 |
| 1 | G | 457 | SER | N-CA-C | -6.10 | 94.54 | 111.00 |
| 1 | C | 457 | SER | N-CA-C | -6.09 | 94.54 | 111.00 |
| 1 | K | 457 | SER | N-CA-C | -6.09 | 94.55 | 111.00 |
| 1 | A | 457 | SER | N-CA-C | -6.09 | 94.56 | 111.00 |
| 1 | D | 644 | ASN | CB-CA-C | -6.08 | 98.23 | 110.40 |
| 1 | I | 457 | SER | N-CA-C | -6.08 | 94.57 | 111.00 |
| 1 | J | 644 | ASN | CB-CA-C | -6.08 | 98.24 | 110.40 |
| 1 | F | 644 | ASN | CB-CA-C | -6.08 | 98.24 | 110.40 |
| 1 | L | 644 | ASN | CB-CA-C | -6.08 | 98.24 | 110.40 |
| 1 | B | 644 | ASN | CB-CA-C | -6.08 | 98.25 | 110.40 |
| 1 | H | 644 | ASN | CB-CA-C | -6.07 | 98.26 | 110.40 |
| 1 | J | 547 | SER | N-CA-C | -6.02 | 94.74 | 111.00 |
| 1 | L | 547 | SER | N-CA-C | -6.01 | 94.78 | 111.00 |
| 1 | D | 547 | SER | N-CA-C | -6.00 | 94.79 | 111.00 |
| 1 | F | 547 | SER | N-CA-C | -6.00 | 94.79 | 111.00 |
| 1 | H | 547 | SER | N-CA-C | -6.00 | 94.80 | 111.00 |
| 1 | B | 547 | SER | N-CA-C | -6.00 | 94.80 | 111.00 |
| 1 | C | 525 | ASN | C-N-CD | -5.91 | 107.60 | 120.60 |
| 1 | A | 525 | ASN | C-N-CD | -5.90 | 107.61 | 120.60 |
| 1 | G | 525 | ASN | C-N-CD | -5.88 | 107.66 | 120.60 |
| 1 | I | 525 | ASN | C-N-CD | -5.88 | 107.66 | 120.60 |
| 1 | E | 525 | ASN | C-N-CD | -5.88 | 107.67 | 120.60 |
| 1 | K | 525 | ASN | C-N-CD | -5.88 | 107.67 | 120.60 |
| 1 | F | 533 | ASP | N-CA-C | -5.78 | 95.39 | 111.00 |
| 1 | D | 533 | ASP | N-CA-C | -5.78 | 95.39 | 111.00 |
| 1 | B | 533 | ASP | N-CA-C | -5.76 | 95.43 | 111.00 |
| 1 | J | 533 | ASP | N-CA-C | -5.76 | 95.44 | 111.00 |
| 1 | L | 533 | ASP | N-CA-C | -5.76 | 95.44 | 111.00 |
| 1 | H | 533 | ASP | N-CA-C | -5.76 | 95.45 | 111.00 |
| 1 | L | 533 | ASP | CB-CA-C | -5.66 | 99.09 | 110.40 |
| 1 | J | 533 | ASP | CB-CA-C | -5.63 | 99.13 | 110.40 |
| 1 | H | 533 | ASP | CB-CA-C | -5.63 | 99.14 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | F | 533 | ASP | CB-CA-C | -5.63 | 99.14 | 110.40 |
| 1 | B | 533 | ASP | CB-CA-C | -5.62 | 99.15 | 110.40 |
| 1 | D | 533 | ASP | CB-CA-C | -5.62 | 99.16 | 110.40 |
| 1 | F | 367 | THR | CB-CA-C | -5.36 | 97.13 | 111.60 |
| 1 | B | 367 | THR | CB-CA-C | -5.36 | 97.13 | 111.60 |
| 1 | D | 367 | THR | CB-CA-C | -5.36 | 97.14 | 111.60 |
| 1 | J | 367 | THR | CB-CA-C | -5.35 | 97.14 | 111.60 |
| 1 | H | 367 | THR | CB-CA-C | -5.35 | 97.15 | 111.60 |
| 1 | L | 367 | THR | CB-CA-C | -5.35 | 97.15 | 111.60 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2622 | 0 | 2545 | 394 | 0 |
| 1 | B | 2608 | 0 | 2530 | 369 | 0 |
| 1 | C | 2622 | 0 | 2545 | 396 | 0 |
| 1 | D | 2608 | 0 | 2530 | 375 | 0 |
| 1 | E | 2622 | 0 | 2543 | 440 | 0 |
| 1 | F | 2608 | 0 | 2530 | 338 | 0 |
| 1 | G | 2622 | 0 | 2543 | 376 | 0 |
| 1 | H | 2608 | 0 | 2530 | 367 | 0 |
| 1 | I | 2622 | 0 | 2544 | 376 | 0 |
| 1 | J | 2608 | 0 | 2530 | 334 | 0 |
| 1 | K | 2622 | 0 | 2543 | 414 | 0 |
| 1 | L | 2608 | 0 | 2530 | 339 | 0 |
| All | All | 31380 | 0 | 30443 | 4266 | 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 69.

All (4266) 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:B:366:SER:CB | 1:K:403:PRO:HB3 | 1.21 | 1.65 |
| 1:A:664:HIS:NE2 | 1:K:348:PHE:CZ | 1.70 | 1.60 |
| 1:I:400:ASN:ND2 | 1:K:664:HIS:CE1 | 1.69 | 1.58 |
| 1:B:364:THR:CG2 | 1:K:401:LEU:CD1 | 1.79 | 1.58 |
| 1:E:348:PHE:CZ | 1:G:664:HIS:NE2 | 1.68 | 1.57 |
| 1:E:401:LEU:CD1 | 1:H:364:THR:CG2 | 1.78 | 1.56 |
| 1:E:403:PRO:HB3 | 1:H:366:SER:CB | 1.18 | 1.54 |
| 1:E:348:PHE:HZ | 1:G:664:HIS:CD2 | 1.24 | 1.53 |
| 1:E:401:LEU:CD1 | 1:H:364:THR:HG21 | 1.34 | 1.53 |
| 1:A:664:HIS:CD2 | 1:K:348:PHE:HZ | 1.28 | 1.51 |
| 1:B:364:THR:HG21 | 1:K:401:LEU:CD1 | 1.34 | 1.51 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:CD2 | 1.65 | 1.49 |
| 1:E:403:PRO:CB | 1:H:366:SER:HB3 | 1.42 | 1.49 |
| 1:B:366:SER:HB3 | 1:K:403:PRO:CB | 1.45 | 1.47 |
| 1:E:403:PRO:CA | 1:H:366:SER:HB3 | 1.46 | 1.44 |
| 1:D:400:ASN:ND2 | 1:E:662:GLU:HG2 | 1.32 | 1.44 |
| 1:A:403:PRO:CG | 1:C:366:SER:HB2 | 1.45 | 1.42 |
| 1:B:366:SER:HB3 | 1:K:403:PRO:CA | 1.48 | 1.42 |
| 1:E:348:PHE:HZ | 1:G:664:HIS:NE2 | 1.02 | 1.41 |
| 1:D:400:ASN:HD22 | 1:E:662:GLU:CG | 1.33 | 1.39 |
| 1:E:403:PRO:HB3 | 1:H:366:SER:CA | 1.50 | 1.39 |
| 1:I:400:ASN:HD21 | 1:K:664:HIS:CD2 | 1.40 | 1.39 |
| 1:I:400:ASN:ND2 | 1:K:664:HIS:ND1 | 1.62 | 1.39 |
| 1:A:661:LEU:HD13 | 1:A:662:GLU:N | 1.06 | 1.38 |
| 1:B:366:SER:CB | 1:K:403:PRO:CB | 1.99 | 1.38 |
| 1:K:661:LEU:HD13 | 1:K:662:GLU:N | 1.06 | 1.38 |
| 1:B:366:SER:CA | 1:K:403:PRO:HB3 | 1.52 | 1.38 |
| 1:C:661:LEU:HD13 | 1:C:662:GLU:N | 1.06 | 1.38 |
| 1:E:403:PRO:CB | 1:H:366:SER:CB | 1.97 | 1.36 |
| 1:I:400:ASN:ND2 | 1:K:664:HIS:CG | 1.92 | 1.36 |
| 1:I:661:LEU:HD13 | 1:I:662:GLU:N | 1.06 | 1.35 |
| 1:G:661:LEU:HD13 | 1:G:662:GLU:N | 1.06 | 1.34 |
| 1:D:661:LEU:C | 1:D:661:LEU:HD13 | 1.48 | 1.33 |
| 1:E:661:LEU:HD13 | 1:E:662:GLU:N | 1.06 | 1.33 |
| 1:A:664:HIS:NE2 | 1:K:348:PHE:HZ | 1.02 | 1.32 |
| 1:A:559:ALA:C | 1:A:561:GLY:HA3 | 1.49 | 1.32 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:CG | 1.82 | 1.32 |
| 1:F:661:LEU:HD13 | 1:F:661:LEU:C | 1.48 | 1.32 |
| 1:C:559:ALA:C | 1:C:561:GLY:HA3 | 1.49 | 1.31 |
| 1:G:559:ALA:C | 1:G:561:GLY:HA3 | 1.49 | 1.30 |
| 1:H:661:LEU:HD13 | 1:H:661:LEU:C | 1.48 | 1.30 |
| 1:E:559:ALA:C | 1:E:561:GLY:HA3 | 1.49 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:525:ASN:CB | 1:I:526:PRO:HD2 | 1.59 | 1.30 |
| 1:I:559:ALA:C | 1:I:561:GLY:HA3 | 1.49 | 1.29 |
| 1:K:559:ALA:C | 1:K:561:GLY:HA3 | 1.49 | 1.29 |
| 1:G:525:ASN:CB | 1:G:526:PRO:HD2 | 1.59 | 1.29 |
| 1:E:385:THR:OG1 | 1:E:387:VAL:HG23 | 1.33 | 1.28 |
| 1:A:525:ASN:CB | 1:A:526:PRO:HD2 | 1.58 | 1.26 |
| 1:A:401:LEU:CD1 | 1:C:364:THR:HG23 | 1.64 | 1.26 |
| 1:F:408:ILE:C | 1:F:408:ILE:HD12 | 1.56 | 1.26 |
| 1:D:408:ILE:C | 1:D:408:ILE:HD12 | 1.56 | 1.25 |
| 1:D:646:LEU:HD23 | 1:D:646:LEU:O | 1.36 | 1.25 |
| 1:C:385:THR:OG1 | 1:C:387:VAL:HG23 | 1.33 | 1.25 |
| 1:K:401:LEU:C | 1:K:401:LEU:HD23 | 1.55 | 1.25 |
| 1:E:401:LEU:HD23 | 1:E:401:LEU:C | 1.55 | 1.25 |
| 1:D:400:ASN:ND2 | 1:E:662:GLU:CG | 1.91 | 1.24 |
| 1:E:525:ASN:CB | 1:E:526:PRO:HD2 | 1.59 | 1.24 |
| 1:L:661:LEU:C | 1:L:661:LEU:HD13 | 1.48 | 1.24 |
| 1:G:385:THR:OG1 | 1:G:387:VAL:HG23 | 1.33 | 1.24 |
| 1:G:401:LEU:HD23 | 1:G:401:LEU:C | 1.55 | 1.24 |
| 1:J:408:ILE:C | 1:J:408:ILE:HD12 | 1.56 | 1.24 |
| 1:A:401:LEU:HD23 | 1:A:401:LEU:C | 1.55 | 1.23 |
| 1:B:661:LEU:C | 1:B:661:LEU:HD13 | 1.48 | 1.23 |
| 1:H:408:ILE:C | 1:H:408:ILE:HD12 | 1.56 | 1.23 |
| 1:G:559:ALA:O | 1:G:561:GLY:HA3 | 1.40 | 1.23 |
| 1:J:646:LEU:O | 1:J:646:LEU:HD23 | 1.36 | 1.23 |
| 1:A:385:THR:OG1 | 1:A:387:VAL:HG23 | 1.33 | 1.22 |
| 1:L:408:ILE:C | 1:L:408:ILE:HD12 | 1.56 | 1.22 |
| 1:E:559:ALA:O | 1:E:561:GLY:HA3 | 1.40 | 1.22 |
| 1:F:646:LEU:HD23 | 1:F:646:LEU:O | 1.36 | 1.22 |
| 1:I:559:ALA:O | 1:I:561:GLY:HA3 | 1.39 | 1.22 |
| 1:L:661:LEU:O | 1:L:663:HIS:N | 1.72 | 1.22 |
| 1:B:646:LEU:O | 1:B:646:LEU:HD23 | 1.36 | 1.22 |
| 1:G:401:LEU:HD23 | 1:G:402:ALA:N | 1.54 | 1.22 |
| 1:L:409:ILE:C | 1:L:409:ILE:HD12 | 1.59 | 1.22 |
| 1:C:401:LEU:HD23 | 1:C:402:ALA:N | 1.54 | 1.22 |
| 1:K:629:ASP:HA | 1:L:664:HIS:CE1 | 1.75 | 1.22 |
| 1:A:401:LEU:HD23 | 1:A:402:ALA:N | 1.54 | 1.22 |
| 1:I:629:ASP:HA | 1:J:664:HIS:CE1 | 1.75 | 1.22 |
| 1:C:629:ASP:HA | 1:D:664:HIS:CE1 | 1.75 | 1.21 |
| 1:I:401:LEU:HD23 | 1:I:401:LEU:C | 1.55 | 1.21 |
| 1:K:525:ASN:CB | 1:K:526:PRO:HD2 | 1.59 | 1.21 |
| 1:A:661:LEU:HD13 | 1:A:661:LEU:C | 1.58 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:409:ILE:HD12 | 1:H:409:ILE:C | 1.59 | 1.21 |
| 1:A:629:ASP:HA | 1:B:664:HIS:CE1 | 1.75 | 1.21 |
| 1:J:661:LEU:O | 1:J:663:HIS:N | 1.72 | 1.21 |
| 1:K:385:THR:OG1 | 1:K:387:VAL:HG23 | 1.33 | 1.21 |
| 1:B:408:ILE:C | 1:B:408:ILE:HD12 | 1.56 | 1.21 |
| 1:B:661:LEU:O | 1:B:663:HIS:N | 1.72 | 1.21 |
| 1:D:661:LEU:O | 1:D:663:HIS:N | 1.72 | 1.21 |
| 1:E:348:PHE:CZ | 1:G:664:HIS:CD2 | 2.16 | 1.21 |
| 1:E:401:LEU:HD23 | 1:E:402:ALA:N | 1.54 | 1.21 |
| 1:H:646:LEU:O | 1:H:646:LEU:HD23 | 1.36 | 1.21 |
| 1:I:385:THR:OG1 | 1:I:387:VAL:HG23 | 1.33 | 1.21 |
| 1:J:661:LEU:C | 1:J:661:LEU:HD13 | 1.48 | 1.21 |
| 1:I:401:LEU:HD23 | 1:I:402:ALA:N | 1.54 | 1.20 |
| 1:E:629:ASP:HA | 1:F:664:HIS:CE1 | 1.75 | 1.20 |
| 1:L:646:LEU:HD23 | 1:L:646:LEU:O | 1.36 | 1.20 |
| 1:A:664:HIS:CD2 | 1:K:348:PHE:CZ | 2.19 | 1.20 |
| 1:E:661:LEU:CD1 | 1:E:662:GLU:N | 2.03 | 1.20 |
| 1:F:661:LEU:O | 1:F:663:HIS:N | 1.72 | 1.20 |
| 1:J:367:THR:O | 1:J:369:PRO:HD3 | 1.42 | 1.20 |
| 1:B:367:THR:O | 1:B:369:PRO:HD3 | 1.42 | 1.20 |
| 1:G:661:LEU:CD1 | 1:G:662:GLU:N | 2.03 | 1.20 |
| 1:J:409:ILE:C | 1:J:409:ILE:HD12 | 1.59 | 1.20 |
| 1:A:661:LEU:CD1 | 1:A:662:GLU:N | 2.03 | 1.20 |
| 1:C:661:LEU:CD1 | 1:C:662:GLU:N | 2.03 | 1.20 |
| 1:D:367:THR:O | 1:D:369:PRO:HD3 | 1.42 | 1.20 |
| 1:A:340:VAL:HA | 1:A:345:TYR:OH | 1.43 | 1.19 |
| 1:C:502:ASN:HD22 | 1:C:635:ARG:HB3 | 1.08 | 1.19 |
| 1:C:525:ASN:CB | 1:C:526:PRO:HD2 | 1.59 | 1.19 |
| 1:K:401:LEU:HD23 | 1:K:402:ALA:N | 1.54 | 1.19 |
| 1:G:629:ASP:HA | 1:H:664:HIS:CE1 | 1.75 | 1.19 |
| 1:G:525:ASN:O | 1:G:528:THR:HG23 | 1.43 | 1.19 |
| 1:I:661:LEU:CD1 | 1:I:662:GLU:N | 2.03 | 1.19 |
| 1:A:403:PRO:HG3 | 1:C:366:SER:HB2 | 1.24 | 1.19 |
| 1:H:661:LEU:O | 1:H:663:HIS:N | 1.72 | 1.19 |
| 1:K:661:LEU:CD1 | 1:K:662:GLU:N | 2.03 | 1.19 |
| 1:K:559:ALA:O | 1:K:561:GLY:HA3 | 1.39 | 1.19 |
| 1:K:340:VAL:HA | 1:K:345:TYR:OH | 1.43 | 1.18 |
| 1:L:367:THR:O | 1:L:369:PRO:HD3 | 1.42 | 1.18 |
| 1:D:409:ILE:C | 1:D:409:ILE:HD12 | 1.59 | 1.18 |
| 1:H:367:THR:O | 1:H:369:PRO:HD3 | 1.42 | 1.18 |
| 1:C:525:ASN:O | 1:C:528:THR:HG23 | 1.43 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:401:LEU:HD23 | 1:C:401:LEU:C | 1.55 | 1.18 |
| 1:D:409:ILE:HD12 | 1:D:409:ILE:O | 1.44 | 1.18 |
| 1:L:409:ILE:HD12 | 1:L:409:ILE:O | 1.44 | 1.18 |
| 1:C:559:ALA:O | 1:C:561:GLY:HA3 | 1.39 | 1.17 |
| 1:E:340:VAL:HA | 1:E:345:TYR:OH | 1.43 | 1.17 |
| 1:E:525:ASN:O | 1:E:528:THR:HG23 | 1.43 | 1.17 |
| 1:B:409:ILE:HD12 | 1:B:409:ILE:O | 1.44 | 1.17 |
| 1:I:340:VAL:HA | 1:I:345:TYR:OH | 1.43 | 1.17 |
| 1:J:409:ILE:HD12 | 1:J:409:ILE:O | 1.44 | 1.17 |
| 1:K:635:ARG:HG2 | 1:K:636:ASP:H | 1.09 | 1.17 |
| 1:A:525:ASN:O | 1:A:528:THR:HG23 | 1.43 | 1.16 |
| 1:G:340:VAL:HA | 1:G:345:TYR:OH | 1.43 | 1.16 |
| 1:K:525:ASN:O | 1:K:528:THR:HG23 | 1.43 | 1.16 |
| 1:A:403:PRO:CB | 1:C:366:SER:HB2 | 1.76 | 1.16 |
| 1:A:635:ARG:HG2 | 1:A:636:ASP:H | 1.09 | 1.16 |
| 1:E:401:LEU:HD11 | 1:H:364:THR:CG2 | 1.55 | 1.16 |
| 1:C:661:LEU:HD13 | 1:C:661:LEU:C | 1.58 | 1.16 |
| 1:D:647:ARG:NH1 | 1:D:649:GLN:OE1 | 1.78 | 1.16 |
| 1:F:647:ARG:NH1 | 1:F:649:GLN:OE1 | 1.78 | 1.16 |
| 1:I:525:ASN:O | 1:I:528:THR:HG23 | 1.43 | 1.16 |
| 1:A:403:PRO:CD | 1:C:366:SER:HB3 | 1.76 | 1.16 |
| 1:A:559:ALA:O | 1:A:561:GLY:HA3 | 1.40 | 1.16 |
| 1:B:409:ILE:HD12 | 1:B:409:ILE:C | 1.59 | 1.16 |
| 1:E:525:ASN:HB3 | 1:E:526:PRO:HD2 | 1.25 | 1.16 |
| 1:F:409:ILE:C | 1:F:409:ILE:HD12 | 1.59 | 1.16 |
| 1:A:403:PRO:HD3 | 1:C:366:SER:CB | 1.74 | 1.15 |
| 1:A:502:ASN:HD22 | 1:A:635:ARG:HB3 | 1.08 | 1.15 |
| 1:C:340:VAL:C | 1:C:345:TYR:HE1 | 1.49 | 1.15 |
| 1:G:525:ASN:HB3 | 1:G:526:PRO:HD2 | 1.25 | 1.15 |
| 1:E:661:LEU:HD13 | 1:E:661:LEU:C | 1.58 | 1.15 |
| 1:A:403:PRO:CD | 1:C:366:SER:CB | 2.23 | 1.15 |
| 1:F:367:THR:O | 1:F:369:PRO:HD3 | 1.42 | 1.15 |
| 1:A:353:PHE:O | 1:A:355:SER:N | 1.80 | 1.15 |
| 1:E:353:PHE:O | 1:E:355:SER:N | 1.80 | 1.15 |
| 1:G:340:VAL:C | 1:G:345:TYR:HE1 | 1.49 | 1.15 |
| 1:H:409:ILE:HD12 | 1:H:409:ILE:O | 1.44 | 1.15 |
| 1:I:353:PHE:O | 1:I:355:SER:N | 1.80 | 1.15 |
| 1:J:647:ARG:NH1 | 1:J:649:GLN:OE1 | 1.78 | 1.15 |
| 1:E:340:VAL:C | 1:E:345:TYR:HE1 | 1.49 | 1.15 |
| 1:I:502:ASN:HD22 | 1:I:635:ARG:HB3 | 1.08 | 1.15 |
| 1:C:340:VAL:HA | 1:C:345:TYR:OH | 1.43 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:VAL:C | 1:A:345:TYR:HE1 | 1.49 | 1.14 |
| 1:A:525:ASN:HB3 | 1:A:526:PRO:HD2 | 1.25 | 1.14 |
| 1:E:385:THR:HG21 | 1:E:389:ARG:CA | 1.78 | 1.14 |
| 1:J:366:SER:C | 1:J:367:THR:HG22 | 1.68 | 1.14 |
| 1:K:661:LEU:HD13 | 1:K:661:LEU:C | 1.58 | 1.14 |
| 1:K:340:VAL:C | 1:K:345:TYR:HE1 | 1.49 | 1.14 |
| 1:L:647:ARG:NH1 | 1:L:649:GLN:OE1 | 1.78 | 1.14 |
| 1:C:385:THR:HG21 | 1:C:389:ARG:CA | 1.78 | 1.14 |
| 1:I:340:VAL:C | 1:I:345:TYR:HE1 | 1.49 | 1.14 |
| 1:I:385:THR:HG21 | 1:I:389:ARG:CA | 1.78 | 1.14 |
| 1:F:409:ILE:HD12 | 1:F:409:ILE:O | 1.44 | 1.14 |
| 1:G:502:ASN:HD22 | 1:G:635:ARG:HB3 | 1.08 | 1.14 |
| 1:K:353:PHE:O | 1:K:355:SER:N | 1.80 | 1.14 |
| 1:K:385:THR:HG21 | 1:K:389:ARG:CA | 1.78 | 1.14 |
| 1:B:364:THR:CG2 | 1:K:401:LEU:HD11 | 1.58 | 1.13 |
| 1:I:635:ARG:HG2 | 1:I:636:ASP:H | 1.09 | 1.13 |
| 1:C:353:PHE:O | 1:C:355:SER:N | 1.80 | 1.13 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:CB | 1.97 | 1.13 |
| 1:G:385:THR:HG21 | 1:G:389:ARG:CA | 1.78 | 1.13 |
| 1:G:661:LEU:HD13 | 1:G:661:LEU:C | 1.58 | 1.13 |
| 1:B:647:ARG:NH1 | 1:B:649:GLN:OE1 | 1.78 | 1.13 |
| 1:G:353:PHE:O | 1:G:355:SER:N | 1.80 | 1.12 |
| 1:H:647:ARG:NH1 | 1:H:649:GLN:OE1 | 1.78 | 1.12 |
| 1:J:353:PHE:HZ | 1:J:395:TYR:CE2 | 1.67 | 1.12 |
| 1:E:401:LEU:HD12 | 1:H:364:THR:CG2 | 1.63 | 1.12 |
| 1:I:631:VAL:HG21 | 1:J:476:ILE:CG2 | 1.80 | 1.12 |
| 1:G:631:VAL:HG21 | 1:H:476:ILE:CG2 | 1.80 | 1.12 |
| 1:J:367:THR:HG23 | 1:J:368:LYS:H | 1.00 | 1.12 |
| 1:C:631:VAL:HG21 | 1:D:476:ILE:CG2 | 1.80 | 1.11 |
| 1:G:502:ASN:ND2 | 1:G:635:ARG:HB3 | 1.66 | 1.11 |
| 1:H:353:PHE:HZ | 1:H:395:TYR:CE2 | 1.67 | 1.11 |
| 1:A:385:THR:HG21 | 1:A:389:ARG:CA | 1.78 | 1.11 |
| 1:B:353:PHE:HZ | 1:B:395:TYR:CE2 | 1.67 | 1.11 |
| 1:D:353:PHE:HZ | 1:D:395:TYR:CE2 | 1.67 | 1.11 |
| 1:G:385:THR:CG2 | 1:G:389:ARG:H | 1.63 | 1.11 |
| 1:I:661:LEU:HD13 | 1:I:661:LEU:C | 1.58 | 1.11 |
| 1:K:631:VAL:HG21 | 1:L:476:ILE:CG2 | 1.80 | 1.11 |
| 1:L:366:SER:C | 1:L:367:THR:HG22 | 1.68 | 1.11 |
| 1:D:565:GLU:HB3 | 1:D:570:GLN:HE21 | 0.95 | 1.11 |
| 1:E:401:LEU:CG | 1:H:364:THR:CG2 | 2.29 | 1.11 |
| 1:E:502:ASN:ND2 | 1:E:635:ARG:HB3 | 1.66 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:385:THR:CG2 | 1:C:389:ARG:H | 1.63 | 1.11 |
| 1:C:525:ASN:HB3 | 1:C:526:PRO:HD2 | 1.25 | 1.11 |
| 1:E:385:THR:CG2 | 1:E:389:ARG:H | 1.63 | 1.11 |
| 1:E:631:VAL:HG21 | 1:F:476:ILE:CG2 | 1.80 | 1.11 |
| 1:E:635:ARG:HG2 | 1:E:636:ASP:H | 1.09 | 1.11 |
| 1:F:353:PHE:HZ | 1:F:395:TYR:CE2 | 1.67 | 1.11 |
| 1:I:502:ASN:ND2 | 1:I:635:ARG:HB3 | 1.66 | 1.11 |
| 1:A:631:VAL:HG21 | 1:B:476:ILE:CG2 | 1.80 | 1.10 |
| 1:E:502:ASN:HD22 | 1:E:635:ARG:HB3 | 1.08 | 1.10 |
| 1:G:635:ARG:HG2 | 1:G:636:ASP:H | 1.09 | 1.10 |
| 1:K:525:ASN:HB3 | 1:K:526:PRO:HD2 | 1.25 | 1.10 |
| 1:I:385:THR:CG2 | 1:I:389:ARG:H | 1.63 | 1.10 |
| 1:L:353:PHE:HZ | 1:L:395:TYR:CE2 | 1.67 | 1.10 |
| 1:I:400:ASN:ND2 | 1:K:664:HIS:NE2 | 1.98 | 1.10 |
| 1:D:408:ILE:HD12 | 1:D:408:ILE:O | 1.52 | 1.10 |
| 1:K:502:ASN:HD22 | 1:K:635:ARG:HB3 | 1.08 | 1.10 |
| 1:B:364:THR:HG21 | 1:K:401:LEU:CG | 1.82 | 1.09 |
| 1:K:502:ASN:ND2 | 1:K:635:ARG:HB3 | 1.66 | 1.09 |
| 1:A:385:THR:CG2 | 1:A:389:ARG:H | 1.63 | 1.09 |
| 1:K:385:THR:CG2 | 1:K:389:ARG:H | 1.63 | 1.09 |
| 1:A:502:ASN:ND2 | 1:A:635:ARG:HB3 | 1.65 | 1.09 |
| 1:B:366:SER:C | 1:B:367:THR:HG22 | 1.68 | 1.09 |
| 1:B:367:THR:HG23 | 1:B:368:LYS:H | 1.00 | 1.09 |
| 1:B:364:THR:CG2 | 1:K:401:LEU:CG | 2.30 | 1.09 |
| 1:F:565:GLU:HB3 | 1:F:570:GLN:HE21 | 0.95 | 1.08 |
| 1:H:366:SER:C | 1:H:367:THR:HG22 | 1.68 | 1.08 |
| 1:C:502:ASN:ND2 | 1:C:635:ARG:HB3 | 1.66 | 1.08 |
| 1:J:565:GLU:HB3 | 1:J:570:GLN:HE21 | 0.95 | 1.08 |
| 1:E:401:LEU:CG | 1:H:364:THR:HG21 | 1.82 | 1.08 |
| 1:D:399:TYR:HA | 1:E:664:HIS:HB2 | 1.36 | 1.07 |
| 1:A:403:PRO:HD3 | 1:C:366:SER:HB3 | 1.08 | 1.07 |
| 1:L:408:ILE:HD12 | 1:L:408:ILE:O | 1.52 | 1.07 |
| 1:C:635:ARG:HG2 | 1:C:636:ASP:H | 1.09 | 1.07 |
| 1:D:366:SER:C | 1:D:367:THR:HG22 | 1.68 | 1.07 |
| 1:D:367:THR:HG23 | 1:D:368:LYS:H | 1.00 | 1.07 |
| 1:F:366:SER:C | 1:F:367:THR:HG22 | 1.68 | 1.07 |
| 1:F:408:ILE:HD12 | 1:F:408:ILE:O | 1.52 | 1.07 |
| 1:G:525:ASN:CG | 1:G:526:PRO:HD2 | 1.74 | 1.07 |
| 1:J:408:ILE:HD12 | 1:J:408:ILE:O | 1.52 | 1.07 |
| 1:C:385:THR:OG1 | 1:C:387:VAL:CG2 | 2.03 | 1.07 |
| 1:C:525:ASN:CG | 1:C:526:PRO:HD2 | 1.74 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:367:THR:HG23 | 1:F:368:LYS:H | 1.00 | 1.07 |
| 1:H:408:ILE:HD12 | 1:H:408:ILE:O | 1.52 | 1.07 |
| 1:A:385:THR:OG1 | 1:A:387:VAL:CG2 | 2.03 | 1.07 |
| 1:B:565:GLU:HB3 | 1:B:570:GLN:HE21 | 0.94 | 1.07 |
| 1:E:348:PHE:CE2 | 1:G:664:HIS:NE2 | 2.23 | 1.07 |
| 1:B:408:ILE:HD12 | 1:B:408:ILE:O | 1.52 | 1.06 |
| 1:I:525:ASN:HB3 | 1:I:526:PRO:HD2 | 1.25 | 1.06 |
| 1:K:385:THR:OG1 | 1:K:387:VAL:CG2 | 2.03 | 1.06 |
| 1:A:401:LEU:HD12 | 1:C:364:THR:HG23 | 1.32 | 1.06 |
| 1:F:569:ILE:O | 1:F:569:ILE:HG22 | 1.55 | 1.06 |
| 1:A:403:PRO:CG | 1:C:366:SER:CB | 2.32 | 1.06 |
| 1:D:398:ASP:CG | 1:E:663:HIS:CD2 | 2.29 | 1.06 |
| 1:D:398:ASP:HA | 1:E:663:HIS:HB3 | 1.32 | 1.06 |
| 1:H:367:THR:HG23 | 1:H:368:LYS:H | 1.00 | 1.06 |
| 1:E:385:THR:OG1 | 1:E:387:VAL:CG2 | 2.03 | 1.06 |
| 1:I:385:THR:OG1 | 1:I:387:VAL:CG2 | 2.03 | 1.06 |
| 1:A:525:ASN:CG | 1:A:526:PRO:HD2 | 1.74 | 1.06 |
| 1:B:364:THR:CG2 | 1:K:401:LEU:HD12 | 1.63 | 1.06 |
| 1:E:661:LEU:O | 1:E:662:GLU:O | 1.74 | 1.06 |
| 1:G:385:THR:OG1 | 1:G:387:VAL:CG2 | 2.03 | 1.06 |
| 1:K:340:VAL:C | 1:K:345:TYR:CE1 | 2.30 | 1.06 |
| 1:A:401:LEU:HD11 | 1:C:364:THR:HG23 | 1.35 | 1.05 |
| 1:C:661:LEU:O | 1:C:662:GLU:O | 1.74 | 1.05 |
| 1:L:367:THR:HG23 | 1:L:368:LYS:H | 1.00 | 1.05 |
| 1:A:340:VAL:C | 1:A:345:TYR:CE1 | 2.30 | 1.05 |
| 1:E:525:ASN:CG | 1:E:526:PRO:HD2 | 1.74 | 1.05 |
| 1:H:569:ILE:O | 1:H:569:ILE:HG22 | 1.55 | 1.05 |
| 1:K:525:ASN:CG | 1:K:526:PRO:HD2 | 1.74 | 1.05 |
| 1:I:340:VAL:C | 1:I:345:TYR:CE1 | 2.30 | 1.05 |
| 1:C:340:VAL:C | 1:C:345:TYR:CE1 | 2.30 | 1.05 |
| 1:H:565:GLU:HB3 | 1:H:570:GLN:HE21 | 0.95 | 1.05 |
| 1:I:525:ASN:CG | 1:I:526:PRO:HD2 | 1.74 | 1.05 |
| 1:L:565:GLU:HB3 | 1:L:570:GLN:HE21 | 0.95 | 1.05 |
| 1:G:661:LEU:O | 1:G:662:GLU:O | 1.74 | 1.05 |
| 1:E:403:PRO:HA | 1:H:366:SER:HB3 | 1.39 | 1.04 |
| 1:A:661:LEU:O | 1:A:662:GLU:O | 1.74 | 1.04 |
| 1:D:399:TYR:HA | 1:E:664:HIS:CB | 1.88 | 1.04 |
| 1:G:353:PHE:CD1 | 1:G:395:TYR:CE2 | 2.46 | 1.04 |
| 1:D:569:ILE:HG22 | 1:D:569:ILE:O | 1.55 | 1.04 |
| 1:E:353:PHE:CD1 | 1:E:395:TYR:CE2 | 2.46 | 1.04 |
| 1:G:340:VAL:C | 1:G:345:TYR:CE1 | 2.30 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:353:PHE:CD1 | 1:I:395:TYR:CE2 | 2.46 | 1.04 |
| 1:E:340:VAL:C | 1:E:345:TYR:CE1 | 2.30 | 1.03 |
| 1:F:367:THR:HG23 | 1:F:368:LYS:N | 1.70 | 1.03 |
| 1:C:353:PHE:CD1 | 1:C:395:TYR:CE2 | 2.46 | 1.03 |
| 1:F:660:GLN:HA | 1:F:661:LEU:HB2 | 1.41 | 1.03 |
| 1:B:364:THR:HG22 | 1:K:401:LEU:CD1 | 1.87 | 1.03 |
| 1:I:661:LEU:O | 1:I:662:GLU:O | 1.74 | 1.03 |
| 1:K:661:LEU:O | 1:K:662:GLU:O | 1.74 | 1.03 |
| 1:A:353:PHE:CD1 | 1:A:395:TYR:CE2 | 2.46 | 1.03 |
| 1:E:635:ARG:CG | 1:E:636:ASP:H | 1.70 | 1.03 |
| 1:J:569:ILE:HG22 | 1:J:569:ILE:O | 1.55 | 1.03 |
| 1:A:635:ARG:CG | 1:A:636:ASP:H | 1.70 | 1.02 |
| 1:A:664:HIS:NE2 | 1:K:348:PHE:CE2 | 2.27 | 1.02 |
| 1:B:364:THR:HG22 | 1:K:401:LEU:HD12 | 1.38 | 1.02 |
| 1:E:401:LEU:HD12 | 1:H:364:THR:HG22 | 1.38 | 1.02 |
| 1:K:353:PHE:CD1 | 1:K:395:TYR:CE2 | 2.46 | 1.02 |
| 1:F:565:GLU:CB | 1:F:570:GLN:HE21 | 1.73 | 1.02 |
| 1:L:660:GLN:HA | 1:L:661:LEU:HB2 | 1.41 | 1.02 |
| 1:B:565:GLU:CB | 1:B:570:GLN:HE21 | 1.73 | 1.02 |
| 1:A:401:LEU:CD1 | 1:C:364:THR:CG2 | 2.37 | 1.02 |
| 1:E:661:LEU:CD1 | 1:E:662:GLU:HB2 | 1.89 | 1.02 |
| 1:G:661:LEU:CD1 | 1:G:662:GLU:HB2 | 1.89 | 1.02 |
| 1:H:565:GLU:CB | 1:H:570:GLN:HE21 | 1.73 | 1.02 |
| 1:I:661:LEU:CD1 | 1:I:662:GLU:HB2 | 1.89 | 1.02 |
| 1:H:660:GLN:HA | 1:H:661:LEU:HB2 | 1.41 | 1.02 |
| 1:J:565:GLU:CB | 1:J:570:GLN:HE21 | 1.73 | 1.02 |
| 1:J:367:THR:HG23 | 1:J:368:LYS:N | 1.70 | 1.01 |
| 1:K:661:LEU:CD1 | 1:K:662:GLU:HB2 | 1.89 | 1.01 |
| 1:J:661:LEU:O | 1:J:661:LEU:HD22 | 1.60 | 1.01 |
| 1:C:661:LEU:CD1 | 1:C:662:GLU:HB2 | 1.89 | 1.01 |
| 1:F:661:LEU:HD13 | 1:F:661:LEU:O | 1.60 | 1.01 |
| 1:H:661:LEU:HD13 | 1:H:661:LEU:O | 1.60 | 1.01 |
| 1:H:661:LEU:O | 1:H:661:LEU:HD22 | 1.60 | 1.01 |
| 1:L:565:GLU:CB | 1:L:570:GLN:HE21 | 1.73 | 1.01 |
| 1:B:569:ILE:HG22 | 1:B:569:ILE:O | 1.55 | 1.01 |
| 1:F:403:PRO:O | 1:F:405:THR:CG2 | 2.09 | 1.01 |
| 1:F:661:LEU:O | 1:F:661:LEU:HD22 | 1.60 | 1.01 |
| 1:H:403:PRO:O | 1:H:405:THR:CG2 | 2.09 | 1.01 |
| 1:L:569:ILE:HG22 | 1:L:569:ILE:O | 1.55 | 1.01 |
| 1:D:403:PRO:O | 1:D:405:THR:CG2 | 2.09 | 1.01 |
| 1:D:661:LEU:O | 1:D:661:LEU:HD22 | 1.60 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:662:GLU:O | 1:D:663:HIS:HB2 | 1.60 | 1.01 |
| 1:I:400:ASN:ND2 | 1:K:664:HIS:CD2 | 2.11 | 1.01 |
| 1:J:403:PRO:O | 1:J:405:THR:CG2 | 2.09 | 1.01 |
| 1:K:635:ARG:CG | 1:K:636:ASP:H | 1.70 | 1.01 |
| 1:L:661:LEU:O | 1:L:661:LEU:HD22 | 1.60 | 1.01 |
| 1:D:565:GLU:CB | 1:D:570:GLN:HE21 | 1.73 | 1.00 |
| 1:H:662:GLU:O | 1:H:663:HIS:HB2 | 1.60 | 1.00 |
| 1:L:367:THR:HG23 | 1:L:368:LYS:N | 1.70 | 1.00 |
| 1:A:661:LEU:CD1 | 1:A:662:GLU:HB2 | 1.89 | 1.00 |
| 1:E:559:ALA:C | 1:E:561:GLY:CA | 2.30 | 1.00 |
| 1:F:662:GLU:O | 1:F:663:HIS:HB2 | 1.60 | 1.00 |
| 1:E:401:LEU:CD1 | 1:H:364:THR:HG22 | 1.85 | 1.00 |
| 1:G:525:ASN:CG | 1:G:526:PRO:CD | 2.30 | 1.00 |
| 1:K:559:ALA:C | 1:K:561:GLY:CA | 2.30 | 1.00 |
| 1:L:403:PRO:O | 1:L:405:THR:CG2 | 2.09 | 1.00 |
| 1:A:403:PRO:CD | 1:C:366:SER:HB2 | 1.90 | 1.00 |
| 1:B:366:SER:HB3 | 1:K:403:PRO:HA | 1.39 | 1.00 |
| 1:E:525:ASN:CG | 1:E:526:PRO:CD | 2.30 | 1.00 |
| 1:C:525:ASN:CG | 1:C:526:PRO:CD | 2.30 | 1.00 |
| 1:J:661:LEU:O | 1:J:661:LEU:HD13 | 1.60 | 1.00 |
| 1:C:559:ALA:C | 1:C:561:GLY:CA | 2.30 | 1.00 |
| 1:A:525:ASN:CG | 1:A:526:PRO:CD | 2.30 | 0.99 |
| 1:G:665:HIS:CE1 | 1:H:342:ALA:HB3 | 1.97 | 0.99 |
| 1:D:399:TYR:HA | 1:E:664:HIS:CG | 1.88 | 0.99 |
| 1:D:660:GLN:HA | 1:D:661:LEU:HB2 | 1.41 | 0.99 |
| 1:H:367:THR:HG23 | 1:H:368:LYS:N | 1.70 | 0.99 |
| 1:J:660:GLN:HA | 1:J:661:LEU:HB2 | 1.41 | 0.99 |
| 1:A:559:ALA:C | 1:A:561:GLY:CA | 2.30 | 0.99 |
| 1:B:660:GLN:HA | 1:B:661:LEU:HB2 | 1.41 | 0.99 |
| 1:C:635:ARG:CG | 1:C:636:ASP:H | 1.70 | 0.99 |
| 1:G:559:ALA:C | 1:G:561:GLY:CA | 2.30 | 0.99 |
| 1:E:665:HIS:CE1 | 1:F:342:ALA:HB3 | 1.98 | 0.99 |
| 1:G:385:THR:HG23 | 1:G:389:ARG:H | 1.27 | 0.99 |
| 1:B:403:PRO:O | 1:B:405:THR:CG2 | 2.09 | 0.99 |
| 1:B:662:GLU:O | 1:B:663:HIS:HB2 | 1.60 | 0.99 |
| 1:A:665:HIS:CE1 | 1:B:342:ALA:HB3 | 1.97 | 0.99 |
| 1:K:385:THR:HG23 | 1:K:389:ARG:H | 1.27 | 0.99 |
| 1:D:409:ILE:C | 1:D:409:ILE:CD1 | 2.29 | 0.99 |
| 1:H:661:LEU:C | 1:H:661:LEU:CD1 | 2.30 | 0.99 |
| 1:B:661:LEU:HD13 | 1:B:661:LEU:O | 1.60 | 0.99 |
| 1:B:661:LEU:O | 1:B:661:LEU:HD22 | 1.60 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:559:ALA:C | 1:I:561:GLY:CA | 2.30 | 0.99 |
| 1:K:665:HIS:CE1 | 1:L:342:ALA:HB3 | 1.98 | 0.99 |
| 1:D:661:LEU:HD13 | 1:D:661:LEU:O | 1.60 | 0.99 |
| 1:F:661:LEU:C | 1:F:661:LEU:CD1 | 2.30 | 0.99 |
| 1:I:385:THR:HG23 | 1:I:389:ARG:H | 1.27 | 0.99 |
| 1:I:525:ASN:CG | 1:I:526:PRO:CD | 2.30 | 0.98 |
| 1:D:367:THR:HG23 | 1:D:368:LYS:N | 1.70 | 0.98 |
| 1:D:398:ASP:HA | 1:E:663:HIS:CB | 1.92 | 0.98 |
| 1:L:353:PHE:CZ | 1:L:395:TYR:CE2 | 2.51 | 0.98 |
| 1:F:353:PHE:CZ | 1:F:395:TYR:CE2 | 2.51 | 0.98 |
| 1:G:635:ARG:CG | 1:G:636:ASP:H | 1.70 | 0.98 |
| 1:K:401:LEU:C | 1:K:401:LEU:CD2 | 2.30 | 0.98 |
| 1:L:662:GLU:O | 1:L:663:HIS:HB2 | 1.60 | 0.98 |
| 1:I:635:ARG:CG | 1:I:636:ASP:H | 1.70 | 0.98 |
| 1:I:665:HIS:CE1 | 1:J:342:ALA:HB3 | 1.98 | 0.98 |
| 1:K:525:ASN:CG | 1:K:526:PRO:CD | 2.30 | 0.98 |
| 1:L:661:LEU:HD13 | 1:L:661:LEU:O | 1.60 | 0.98 |
| 1:B:353:PHE:CZ | 1:B:395:TYR:CE2 | 2.51 | 0.98 |
| 1:G:661:LEU:CD1 | 1:G:661:LEU:C | 2.29 | 0.98 |
| 1:C:665:HIS:CE1 | 1:D:342:ALA:HB3 | 1.97 | 0.98 |
| 1:B:403:PRO:O | 1:B:405:THR:HG23 | 1.64 | 0.98 |
| 1:L:565:GLU:HB3 | 1:L:570:GLN:NE2 | 1.79 | 0.97 |
| 1:C:389:ARG:HA | 1:C:392:ILE:HG12 | 1.46 | 0.97 |
| 1:I:661:LEU:CD1 | 1:I:661:LEU:C | 2.29 | 0.97 |
| 1:J:353:PHE:CZ | 1:J:395:TYR:CE2 | 2.51 | 0.97 |
| 1:D:353:PHE:CZ | 1:D:395:TYR:CE2 | 2.51 | 0.97 |
| 1:J:565:GLU:HB3 | 1:J:570:GLN:NE2 | 1.79 | 0.97 |
| 1:D:403:PRO:O | 1:D:405:THR:HG23 | 1.64 | 0.97 |
| 1:F:403:PRO:O | 1:F:405:THR:HG23 | 1.64 | 0.97 |
| 1:A:385:THR:HG23 | 1:A:389:ARG:H | 1.27 | 0.97 |
| 1:B:565:GLU:HB3 | 1:B:570:GLN:NE2 | 1.79 | 0.97 |
| 1:A:389:ARG:HA | 1:A:392:ILE:HG12 | 1.46 | 0.97 |
| 1:E:403:PRO:HB3 | 1:H:366:SER:HB2 | 1.43 | 0.97 |
| 1:B:409:ILE:C | 1:B:409:ILE:CD1 | 2.29 | 0.97 |
| 1:H:353:PHE:CZ | 1:H:395:TYR:CE2 | 2.51 | 0.97 |
| 1:D:398:ASP:CA | 1:E:663:HIS:HB3 | 1.94 | 0.97 |
| 1:D:660:GLN:HA | 1:D:661:LEU:CB | 1.95 | 0.97 |
| 1:H:403:PRO:O | 1:H:405:THR:HG23 | 1.64 | 0.97 |
| 1:D:661:LEU:C | 1:D:661:LEU:CD1 | 2.30 | 0.96 |
| 1:J:662:GLU:O | 1:J:663:HIS:HB2 | 1.60 | 0.96 |
| 1:I:389:ARG:HA | 1:I:392:ILE:HG12 | 1.46 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:660:GLN:HA | 1:L:661:LEU:CB | 1.95 | 0.96 |
| 1:B:660:GLN:HA | 1:B:661:LEU:CB | 1.95 | 0.96 |
| 1:D:343:THR:O | 1:D:347:THR:HG23 | 1.65 | 0.96 |
| 1:E:385:THR:HG23 | 1:E:389:ARG:H | 1.27 | 0.96 |
| 1:H:660:GLN:HA | 1:H:661:LEU:CB | 1.95 | 0.96 |
| 1:L:403:PRO:O | 1:L:405:THR:HG23 | 1.64 | 0.96 |
| 1:B:367:THR:HG23 | 1:B:368:LYS:N | 1.70 | 0.96 |
| 1:J:660:GLN:HA | 1:J:661:LEU:CB | 1.95 | 0.96 |
| 1:L:343:THR:O | 1:L:347:THR:HG23 | 1.65 | 0.96 |
| 1:C:340:VAL:HA | 1:C:345:TYR:CZ | 2.01 | 0.96 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:HD2 | 1.32 | 0.96 |
| 1:I:353:PHE:CD1 | 1:I:395:TYR:HE2 | 1.84 | 0.96 |
| 1:J:661:LEU:C | 1:J:661:LEU:CD1 | 2.30 | 0.96 |
| 1:H:565:GLU:HB3 | 1:H:570:GLN:NE2 | 1.79 | 0.96 |
| 1:J:403:PRO:O | 1:J:405:THR:HG23 | 1.64 | 0.96 |
| 1:C:661:LEU:HD13 | 1:C:662:GLU:H | 1.26 | 0.96 |
| 1:D:565:GLU:HB3 | 1:D:570:GLN:NE2 | 1.79 | 0.96 |
| 1:F:503:ASN:HD21 | 1:F:633:PHE:H | 0.96 | 0.96 |
| 1:F:565:GLU:HB3 | 1:F:570:GLN:NE2 | 1.79 | 0.96 |
| 1:I:401:LEU:HD23 | 1:I:402:ALA:CB | 1.96 | 0.96 |
| 1:I:401:LEU:C | 1:I:401:LEU:CD2 | 2.30 | 0.96 |
| 1:K:525:ASN:CB | 1:K:526:PRO:CD | 2.44 | 0.96 |
| 1:E:661:LEU:HD13 | 1:E:662:GLU:H | 1.26 | 0.95 |
| 1:F:660:GLN:HA | 1:F:661:LEU:CB | 1.95 | 0.95 |
| 1:C:401:LEU:HD23 | 1:C:402:ALA:CB | 1.96 | 0.95 |
| 1:B:503:ASN:HD21 | 1:B:633:PHE:H | 0.96 | 0.95 |
| 1:C:401:LEU:CD2 | 1:C:402:ALA:N | 2.29 | 0.95 |
| 1:F:343:THR:O | 1:F:347:THR:HG23 | 1.65 | 0.95 |
| 1:C:661:LEU:CD1 | 1:C:661:LEU:C | 2.29 | 0.95 |
| 1:I:525:ASN:CB | 1:I:526:PRO:CD | 2.44 | 0.95 |
| 1:A:525:ASN:CB | 1:A:526:PRO:CD | 2.44 | 0.95 |
| 1:B:343:THR:O | 1:B:347:THR:HG23 | 1.65 | 0.95 |
| 1:G:389:ARG:HA | 1:G:392:ILE:HG12 | 1.46 | 0.95 |
| 1:H:343:THR:O | 1:H:347:THR:HG23 | 1.65 | 0.95 |
| 1:K:401:LEU:HD23 | 1:K:402:ALA:CB | 1.96 | 0.95 |
| 1:C:385:THR:HG23 | 1:C:389:ARG:H | 1.27 | 0.95 |
| 1:G:401:LEU:CD2 | 1:G:402:ALA:N | 2.30 | 0.95 |
| 1:I:401:LEU:CD2 | 1:I:402:ALA:N | 2.30 | 0.95 |
| 1:L:503:ASN:HD21 | 1:L:633:PHE:H | 0.96 | 0.95 |
| 1:C:353:PHE:CD1 | 1:C:395:TYR:HE2 | 1.83 | 0.95 |
| 1:D:400:ASN:HD22 | 1:E:662:GLU:HG3 | 1.28 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:343:THR:O | 1:J:347:THR:HG23 | 1.65 | 0.95 |
| 1:A:340:VAL:HA | 1:A:345:TYR:CZ | 2.01 | 0.94 |
| 1:A:401:LEU:C | 1:A:401:LEU:CD2 | 2.30 | 0.94 |
| 1:E:340:VAL:HA | 1:E:345:TYR:CZ | 2.01 | 0.94 |
| 1:E:401:LEU:CD2 | 1:E:402:ALA:N | 2.30 | 0.94 |
| 1:J:408:ILE:C | 1:J:408:ILE:CD1 | 2.30 | 0.94 |
| 1:J:409:ILE:C | 1:J:409:ILE:CD1 | 2.29 | 0.94 |
| 1:G:401:LEU:HD23 | 1:G:402:ALA:CB | 1.96 | 0.94 |
| 1:K:340:VAL:HA | 1:K:345:TYR:CZ | 2.01 | 0.94 |
| 1:E:401:LEU:HD23 | 1:E:402:ALA:CB | 1.96 | 0.94 |
| 1:J:503:ASN:HD21 | 1:J:633:PHE:H | 0.96 | 0.94 |
| 1:E:401:LEU:HD23 | 1:E:402:ALA:CA | 1.97 | 0.94 |
| 1:G:525:ASN:CB | 1:G:526:PRO:CD | 2.44 | 0.94 |
| 1:K:389:ARG:HA | 1:K:392:ILE:HG12 | 1.46 | 0.94 |
| 1:C:525:ASN:CB | 1:C:526:PRO:CD | 2.44 | 0.94 |
| 1:I:340:VAL:HA | 1:I:345:TYR:CZ | 2.01 | 0.94 |
| 1:I:385:THR:HG1 | 1:I:387:VAL:HG23 | 1.32 | 0.94 |
| 1:A:401:LEU:CD2 | 1:A:402:ALA:N | 2.30 | 0.94 |
| 1:D:503:ASN:HD21 | 1:D:633:PHE:H | 0.96 | 0.94 |
| 1:E:525:ASN:CB | 1:E:526:PRO:CD | 2.45 | 0.94 |
| 1:A:385:THR:CG2 | 1:A:389:ARG:N | 2.31 | 0.94 |
| 1:A:401:LEU:HD23 | 1:A:402:ALA:CB | 1.96 | 0.94 |
| 1:B:366:SER:HB2 | 1:K:403:PRO:HB3 | 1.45 | 0.94 |
| 1:E:401:LEU:C | 1:E:401:LEU:CD2 | 2.30 | 0.94 |
| 1:G:340:VAL:HA | 1:G:345:TYR:CZ | 2.01 | 0.94 |
| 1:G:353:PHE:CD1 | 1:G:395:TYR:HE2 | 1.84 | 0.94 |
| 1:G:401:LEU:C | 1:G:401:LEU:CD2 | 2.30 | 0.94 |
| 1:H:408:ILE:C | 1:H:408:ILE:CD1 | 2.30 | 0.94 |
| 1:H:503:ASN:HD21 | 1:H:633:PHE:H | 0.96 | 0.94 |
| 1:I:401:LEU:HD23 | 1:I:402:ALA:CA | 1.97 | 0.94 |
| 1:K:401:LEU:HD23 | 1:K:402:ALA:CA | 1.97 | 0.94 |
| 1:L:409:ILE:C | 1:L:409:ILE:CD1 | 2.29 | 0.94 |
| 1:C:401:LEU:C | 1:C:401:LEU:CD2 | 2.30 | 0.94 |
| 1:D:398:ASP:CG | 1:E:663:HIS:HD2 | 1.64 | 0.94 |
| 1:K:353:PHE:CD1 | 1:K:395:TYR:HE2 | 1.84 | 0.94 |
| 1:C:401:LEU:HD23 | 1:C:402:ALA:CA | 1.97 | 0.93 |
| 1:E:389:ARG:HA | 1:E:392:ILE:HG12 | 1.46 | 0.93 |
| 1:E:385:THR:CG2 | 1:E:389:ARG:N | 2.31 | 0.93 |
| 1:B:364:THR:HG23 | 1:K:401:LEU:HG | 1.50 | 0.93 |
| 1:B:661:LEU:C | 1:B:661:LEU:CD1 | 2.30 | 0.93 |
| 1:H:566:ASN:N | 1:H:570:GLN:HE22 | 1.66 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:661:LEU:C | 1:A:661:LEU:CD1 | 2.29 | 0.93 |
| 1:G:401:LEU:HD23 | 1:G:402:ALA:CA | 1.97 | 0.93 |
| 1:K:385:THR:CG2 | 1:K:389:ARG:N | 2.31 | 0.93 |
| 1:E:401:LEU:HG | 1:H:364:THR:HG23 | 1.49 | 0.93 |
| 1:F:408:ILE:C | 1:F:408:ILE:CD1 | 2.30 | 0.93 |
| 1:K:401:LEU:CD2 | 1:K:402:ALA:N | 2.30 | 0.93 |
| 1:A:401:LEU:HD23 | 1:A:402:ALA:CA | 1.97 | 0.93 |
| 1:C:385:THR:HG21 | 1:C:389:ARG:C | 1.89 | 0.93 |
| 1:E:385:THR:HG21 | 1:E:389:ARG:C | 1.89 | 0.93 |
| 1:G:385:THR:HG21 | 1:G:389:ARG:C | 1.89 | 0.93 |
| 1:F:409:ILE:C | 1:F:409:ILE:CD1 | 2.29 | 0.93 |
| 1:F:557:PRO:HG2 | 1:F:580:LEU:HD11 | 1.51 | 0.93 |
| 1:B:557:PRO:HG2 | 1:B:580:LEU:HD11 | 1.51 | 0.93 |
| 1:J:566:ASN:N | 1:J:570:GLN:HE22 | 1.66 | 0.93 |
| 1:E:401:LEU:CD1 | 1:H:364:THR:HG23 | 1.98 | 0.92 |
| 1:E:340:VAL:C | 1:E:341:THR:HG23 | 1.89 | 0.92 |
| 1:G:661:LEU:HD13 | 1:G:662:GLU:H | 1.26 | 0.92 |
| 1:I:340:VAL:C | 1:I:341:THR:HG23 | 1.89 | 0.92 |
| 1:I:385:THR:HG21 | 1:I:389:ARG:C | 1.89 | 0.92 |
| 1:L:408:ILE:C | 1:L:408:ILE:CD1 | 2.30 | 0.92 |
| 1:L:566:ASN:N | 1:L:570:GLN:HE22 | 1.66 | 0.92 |
| 1:A:387:VAL:HG21 | 1:A:390:GLU:OE1 | 1.70 | 0.92 |
| 1:G:385:THR:CG2 | 1:G:389:ARG:N | 2.31 | 0.92 |
| 1:K:340:VAL:C | 1:K:341:THR:HG23 | 1.89 | 0.92 |
| 1:A:353:PHE:CD1 | 1:A:395:TYR:HE2 | 1.84 | 0.92 |
| 1:C:387:VAL:HG21 | 1:C:390:GLU:OE1 | 1.69 | 0.92 |
| 1:K:387:VAL:HG21 | 1:K:390:GLU:OE1 | 1.70 | 0.92 |
| 1:C:385:THR:CG2 | 1:C:389:ARG:N | 2.31 | 0.92 |
| 1:L:647:ARG:CG | 1:L:650:TYR:CD1 | 2.53 | 0.92 |
| 1:B:647:ARG:CG | 1:B:650:TYR:CD1 | 2.53 | 0.92 |
| 1:A:403:PRO:CB | 1:C:366:SER:CB | 2.48 | 0.92 |
| 1:A:661:LEU:HD13 | 1:A:662:GLU:H | 1.26 | 0.92 |
| 1:E:403:PRO:HB3 | 1:H:366:SER:HA | 1.52 | 0.92 |
| 1:F:647:ARG:CG | 1:F:650:TYR:CD1 | 2.53 | 0.92 |
| 1:G:340:VAL:C | 1:G:341:THR:HG23 | 1.89 | 0.92 |
| 1:H:647:ARG:CG | 1:H:650:TYR:CD1 | 2.53 | 0.92 |
| 1:I:385:THR:CG2 | 1:I:389:ARG:N | 2.31 | 0.92 |
| 1:K:401:LEU:CD2 | 1:K:402:ALA:HB2 | 2.00 | 0.92 |
| 1:A:401:LEU:CD2 | 1:A:402:ALA:HB2 | 2.00 | 0.91 |
| 1:B:566:ASN:N | 1:B:570:GLN:HE22 | 1.66 | 0.91 |
| 1:D:647:ARG:CG | 1:D:650:TYR:CD1 | 2.53 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:557:PRO:HG2 | 1:H:580:LEU:HD11 | 1.51 | 0.91 |
| 1:L:557:PRO:HG2 | 1:L:580:LEU:HD11 | 1.51 | 0.91 |
| 1:A:403:PRO:HB3 | 1:C:366:SER:CB | 2.00 | 0.91 |
| 1:C:436:LEU:HD22 | 1:C:655:LEU:HD21 | 1.53 | 0.91 |
| 1:I:401:LEU:CD2 | 1:I:402:ALA:HB2 | 2.00 | 0.91 |
| 1:A:403:PRO:HB3 | 1:C:366:SER:HB2 | 1.52 | 0.91 |
| 1:C:401:LEU:CD2 | 1:C:402:ALA:HB2 | 2.00 | 0.91 |
| 1:H:409:ILE:C | 1:H:409:ILE:CD1 | 2.29 | 0.91 |
| 1:J:557:PRO:HG2 | 1:J:580:LEU:HD11 | 1.52 | 0.91 |
| 1:E:519:SER:HB2 | 1:E:562:ASP:OD1 | 1.71 | 0.91 |
| 1:C:519:SER:HB2 | 1:C:562:ASP:OD1 | 1.71 | 0.91 |
| 1:K:436:LEU:HD22 | 1:K:655:LEU:HD21 | 1.52 | 0.91 |
| 1:I:387:VAL:HG21 | 1:I:390:GLU:OE1 | 1.70 | 0.91 |
| 1:A:385:THR:HG1 | 1:A:387:VAL:HG23 | 1.31 | 0.91 |
| 1:A:635:ARG:CG | 1:A:636:ASP:N | 2.30 | 0.91 |
| 1:B:364:THR:HG23 | 1:K:401:LEU:CD1 | 2.01 | 0.91 |
| 1:G:387:VAL:HG21 | 1:G:390:GLU:OE1 | 1.70 | 0.91 |
| 1:K:661:LEU:CD1 | 1:K:661:LEU:C | 2.29 | 0.91 |
| 1:A:385:THR:HG21 | 1:A:389:ARG:C | 1.89 | 0.91 |
| 1:F:566:ASN:N | 1:F:570:GLN:HE22 | 1.66 | 0.91 |
| 1:G:401:LEU:CD2 | 1:G:402:ALA:HB2 | 2.00 | 0.91 |
| 1:G:519:SER:HB2 | 1:G:562:ASP:OD1 | 1.71 | 0.91 |
| 1:K:635:ARG:CG | 1:K:636:ASP:N | 2.30 | 0.91 |
| 1:C:517:PHE:HD2 | 1:C:536:TYR:HE2 | 1.18 | 0.91 |
| 1:E:401:LEU:CD2 | 1:E:402:ALA:HB2 | 2.00 | 0.91 |
| 1:G:517:PHE:HD2 | 1:G:536:TYR:HE2 | 1.18 | 0.91 |
| 1:K:385:THR:HG21 | 1:K:389:ARG:C | 1.89 | 0.91 |
| 1:D:566:ASN:N | 1:D:570:GLN:HE22 | 1.66 | 0.91 |
| 1:J:647:ARG:CG | 1:J:650:TYR:CD1 | 2.53 | 0.91 |
| 1:I:436:LEU:HD22 | 1:I:655:LEU:HD21 | 1.53 | 0.90 |
| 1:E:387:VAL:HG21 | 1:E:390:GLU:OE1 | 1.70 | 0.90 |
| 1:I:519:SER:HB2 | 1:I:562:ASP:OD1 | 1.71 | 0.90 |
| 1:B:364:THR:CG2 | 1:K:401:LEU:HG | 1.97 | 0.90 |
| 1:D:557:PRO:HG2 | 1:D:580:LEU:HD11 | 1.51 | 0.90 |
| 1:I:635:ARG:HH22 | 1:J:661:LEU:HD12 | 1.36 | 0.90 |
| 1:K:661:LEU:HD13 | 1:K:662:GLU:H | 1.26 | 0.90 |
| 1:A:340:VAL:C | 1:A:341:THR:HG23 | 1.89 | 0.90 |
| 1:B:409:ILE:HD13 | 1:B:410:SER:O | 1.72 | 0.90 |
| 1:D:409:ILE:HD13 | 1:D:410:SER:O | 1.72 | 0.90 |
| 1:E:353:PHE:CD1 | 1:E:395:TYR:HE2 | 1.84 | 0.90 |
| 1:C:635:ARG:HH22 | 1:D:661:LEU:HD12 | 1.36 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:517:PHE:HD2 | 1:E:536:TYR:HE2 | 1.18 | 0.90 |
| 1:E:635:ARG:HH22 | 1:F:661:LEU:HD12 | 1.36 | 0.90 |
| 1:J:409:ILE:HD13 | 1:J:410:SER:O | 1.72 | 0.90 |
| 1:K:385:THR:HG1 | 1:K:387:VAL:HG23 | 1.37 | 0.90 |
| 1:L:409:ILE:HD13 | 1:L:410:SER:O | 1.72 | 0.90 |
| 1:A:436:LEU:HD22 | 1:A:655:LEU:HD21 | 1.53 | 0.90 |
| 1:C:629:ASP:HA | 1:D:664:HIS:NE2 | 1.87 | 0.90 |
| 1:E:631:VAL:HG21 | 1:F:476:ILE:HG21 | 1.53 | 0.90 |
| 1:E:664:HIS:O | 1:E:665:HIS:CG | 2.25 | 0.90 |
| 1:I:635:ARG:CG | 1:I:636:ASP:N | 2.30 | 0.90 |
| 1:I:664:HIS:O | 1:I:665:HIS:CG | 2.25 | 0.90 |
| 1:B:364:THR:HG23 | 1:K:401:LEU:CG | 2.02 | 0.90 |
| 1:C:340:VAL:C | 1:C:341:THR:HG23 | 1.89 | 0.90 |
| 1:G:664:HIS:O | 1:G:665:HIS:CG | 2.25 | 0.90 |
| 1:H:409:ILE:HD13 | 1:H:410:SER:O | 1.72 | 0.90 |
| 1:I:517:PHE:HD2 | 1:I:536:TYR:HE2 | 1.18 | 0.90 |
| 1:I:629:ASP:HA | 1:J:664:HIS:NE2 | 1.87 | 0.90 |
| 1:I:661:LEU:HD13 | 1:I:662:GLU:H | 1.26 | 0.90 |
| 1:B:366:SER:CA | 1:K:403:PRO:CB | 2.41 | 0.90 |
| 1:C:353:PHE:CZ | 1:C:395:TYR:CD2 | 2.60 | 0.90 |
| 1:K:629:ASP:HA | 1:L:664:HIS:NE2 | 1.87 | 0.90 |
| 1:K:631:VAL:HG21 | 1:L:476:ILE:HG21 | 1.53 | 0.90 |
| 1:E:401:LEU:HG | 1:H:364:THR:CG2 | 1.97 | 0.89 |
| 1:F:409:ILE:HD13 | 1:F:410:SER:O | 1.72 | 0.89 |
| 1:K:664:HIS:O | 1:K:665:HIS:CG | 2.25 | 0.89 |
| 1:B:366:SER:HA | 1:K:403:PRO:HB3 | 1.52 | 0.89 |
| 1:G:353:PHE:CZ | 1:G:395:TYR:CD2 | 2.61 | 0.89 |
| 1:I:353:PHE:CZ | 1:I:395:TYR:CD2 | 2.61 | 0.89 |
| 1:B:647:ARG:HG2 | 1:B:650:TYR:CD1 | 2.08 | 0.89 |
| 1:C:631:VAL:HG21 | 1:D:476:ILE:HG21 | 1.53 | 0.89 |
| 1:A:519:SER:HB2 | 1:A:562:ASP:OD1 | 1.71 | 0.89 |
| 1:D:408:ILE:C | 1:D:408:ILE:CD1 | 2.30 | 0.89 |
| 1:J:366:SER:O | 1:J:367:THR:HG22 | 1.73 | 0.89 |
| 1:K:661:LEU:O | 1:K:662:GLU:C | 2.08 | 0.89 |
| 1:F:366:SER:O | 1:F:367:THR:HG22 | 1.73 | 0.89 |
| 1:G:436:LEU:HD22 | 1:G:655:LEU:HD21 | 1.52 | 0.89 |
| 1:K:517:PHE:HD2 | 1:K:536:TYR:HE2 | 1.18 | 0.89 |
| 1:E:353:PHE:CZ | 1:E:395:TYR:CD2 | 2.61 | 0.89 |
| 1:G:635:ARG:CG | 1:G:636:ASP:N | 2.30 | 0.89 |
| 1:H:366:SER:O | 1:H:367:THR:HG22 | 1.73 | 0.89 |
| 1:E:401:LEU:CG | 1:H:364:THR:HG23 | 2.00 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:661:LEU:HG | 1:F:456:ASN:HB3 | 1.55 | 0.89 |
| 1:A:664:HIS:O | 1:A:665:HIS:CG | 2.25 | 0.89 |
| 1:D:366:SER:O | 1:D:367:THR:HG22 | 1.73 | 0.89 |
| 1:H:662:GLU:O | 1:H:663:HIS:CB | 2.20 | 0.89 |
| 1:K:353:PHE:CZ | 1:K:395:TYR:CD2 | 2.60 | 0.89 |
| 1:K:519:SER:HB2 | 1:K:562:ASP:OD1 | 1.71 | 0.89 |
| 1:L:366:SER:O | 1:L:367:THR:HG22 | 1.73 | 0.89 |
| 1:A:353:PHE:CZ | 1:A:395:TYR:CD2 | 2.61 | 0.88 |
| 1:A:517:PHE:HD2 | 1:A:536:TYR:HE2 | 1.18 | 0.88 |
| 1:C:635:ARG:CG | 1:C:636:ASP:N | 2.30 | 0.88 |
| 1:C:664:HIS:O | 1:C:665:HIS:CG | 2.25 | 0.88 |
| 1:G:635:ARG:HH22 | 1:H:661:LEU:HD12 | 1.36 | 0.88 |
| 1:K:340:VAL:O | 1:K:345:TYR:HE1 | 1.55 | 0.88 |
| 1:E:340:VAL:O | 1:E:345:TYR:HE1 | 1.55 | 0.88 |
| 1:G:661:LEU:HG | 1:H:456:ASN:HB3 | 1.55 | 0.88 |
| 1:A:347:THR:OG1 | 1:A:348:PHE:N | 2.05 | 0.88 |
| 1:B:408:ILE:C | 1:B:408:ILE:CD1 | 2.30 | 0.88 |
| 1:G:340:VAL:O | 1:G:345:TYR:HE1 | 1.55 | 0.88 |
| 1:L:647:ARG:HG2 | 1:L:650:TYR:CD1 | 2.08 | 0.88 |
| 1:A:629:ASP:HA | 1:B:664:HIS:NE2 | 1.87 | 0.88 |
| 1:A:635:ARG:HH22 | 1:B:661:LEU:HD12 | 1.36 | 0.88 |
| 1:C:340:VAL:O | 1:C:345:TYR:HE1 | 1.55 | 0.88 |
| 1:E:436:LEU:HD22 | 1:E:655:LEU:HD21 | 1.53 | 0.88 |
| 1:E:401:LEU:HD23 | 1:E:402:ALA:HB2 | 1.55 | 0.88 |
| 1:G:661:LEU:O | 1:G:662:GLU:C | 2.08 | 0.88 |
| 1:I:401:LEU:HD23 | 1:I:402:ALA:HB2 | 1.55 | 0.88 |
| 1:I:661:LEU:HG | 1:J:456:ASN:HB3 | 1.55 | 0.88 |
| 1:C:401:LEU:HD23 | 1:C:402:ALA:HB2 | 1.56 | 0.88 |
| 1:G:631:VAL:HG21 | 1:H:476:ILE:HG21 | 1.53 | 0.88 |
| 1:A:340:VAL:O | 1:A:345:TYR:HE1 | 1.55 | 0.87 |
| 1:C:661:LEU:O | 1:C:662:GLU:C | 2.08 | 0.87 |
| 1:A:661:LEU:O | 1:A:662:GLU:C | 2.08 | 0.87 |
| 1:G:401:LEU:HD23 | 1:G:402:ALA:HB2 | 1.56 | 0.87 |
| 1:E:629:ASP:HA | 1:F:664:HIS:NE2 | 1.87 | 0.87 |
| 1:I:631:VAL:HG21 | 1:J:476:ILE:HG21 | 1.53 | 0.87 |
| 1:I:661:LEU:O | 1:I:662:GLU:C | 2.08 | 0.87 |
| 1:L:661:LEU:C | 1:L:661:LEU:CD1 | 2.30 | 0.87 |
| 1:C:631:VAL:HG21 | 1:D:476:ILE:HG22 | 1.57 | 0.87 |
| 1:D:647:ARG:HG2 | 1:D:650:TYR:CD1 | 2.08 | 0.87 |
| 1:E:635:ARG:CG | 1:E:636:ASP:N | 2.30 | 0.87 |
| 1:G:629:ASP:HA | 1:H:664:HIS:NE2 | 1.87 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:340:VAL:CA | 1:I:345:TYR:CE1 | 2.58 | 0.87 |
| 1:I:347:THR:OG1 | 1:I:348:PHE:N | 2.05 | 0.87 |
| 1:A:631:VAL:HG21 | 1:B:476:ILE:HG21 | 1.53 | 0.87 |
| 1:A:635:ARG:HG2 | 1:A:636:ASP:N | 1.90 | 0.87 |
| 1:G:660:GLN:HG3 | 1:G:661:LEU:N | 1.90 | 0.87 |
| 1:J:647:ARG:HG2 | 1:J:650:TYR:CD1 | 2.08 | 0.87 |
| 1:K:340:VAL:CA | 1:K:345:TYR:CE1 | 2.58 | 0.87 |
| 1:C:385:THR:HG1 | 1:C:387:VAL:HG23 | 1.36 | 0.87 |
| 1:I:340:VAL:O | 1:I:345:TYR:HE1 | 1.55 | 0.87 |
| 1:A:340:VAL:CA | 1:A:345:TYR:CE1 | 2.58 | 0.87 |
| 1:D:367:THR:CG2 | 1:D:368:LYS:H | 1.87 | 0.87 |
| 1:C:340:VAL:CA | 1:C:345:TYR:CE1 | 2.58 | 0.87 |
| 1:B:366:SER:O | 1:B:367:THR:HG22 | 1.73 | 0.86 |
| 1:F:647:ARG:HG2 | 1:F:650:TYR:CD1 | 2.08 | 0.86 |
| 1:C:660:GLN:HG3 | 1:C:661:LEU:N | 1.90 | 0.86 |
| 1:H:647:ARG:HG2 | 1:H:650:TYR:CD1 | 2.08 | 0.86 |
| 1:C:347:THR:OG1 | 1:C:348:PHE:N | 2.05 | 0.86 |
| 1:G:340:VAL:CA | 1:G:345:TYR:CE1 | 2.58 | 0.86 |
| 1:A:661:LEU:HG | 1:B:456:ASN:HB3 | 1.55 | 0.86 |
| 1:I:631:VAL:HG21 | 1:J:476:ILE:HG22 | 1.57 | 0.86 |
| 1:K:661:LEU:HG | 1:L:456:ASN:HB3 | 1.55 | 0.86 |
| 1:E:661:LEU:O | 1:E:662:GLU:C | 2.08 | 0.86 |
| 1:B:364:THR:HG21 | 1:K:401:LEU:HD11 | 0.87 | 0.86 |
| 1:K:635:ARG:HH22 | 1:L:661:LEU:HD12 | 1.37 | 0.86 |
| 1:A:560:SER:N | 1:A:561:GLY:CA | 2.39 | 0.86 |
| 1:K:347:THR:OG1 | 1:K:348:PHE:N | 2.05 | 0.86 |
| 1:A:660:GLN:HG3 | 1:A:661:LEU:N | 1.90 | 0.86 |
| 1:I:341:THR:HG1 | 1:I:344:ASP:HB2 | 1.41 | 0.86 |
| 1:K:341:THR:HG1 | 1:K:344:ASP:HB2 | 1.41 | 0.86 |
| 1:K:560:SER:N | 1:K:561:GLY:CA | 2.39 | 0.86 |
| 1:K:631:VAL:HG21 | 1:L:476:ILE:HG22 | 1.57 | 0.86 |
| 1:L:664:HIS:CG | 1:L:664:HIS:O | 2.29 | 0.86 |
| 1:A:401:LEU:HD12 | 1:C:364:THR:CG2 | 2.05 | 0.85 |
| 1:I:353:PHE:CE1 | 1:I:395:TYR:CE2 | 2.65 | 0.85 |
| 1:C:661:LEU:HG | 1:D:456:ASN:HB3 | 1.55 | 0.85 |
| 1:D:400:ASN:CG | 1:E:662:GLU:HG2 | 1.97 | 0.85 |
| 1:E:340:VAL:CA | 1:E:345:TYR:CE1 | 2.58 | 0.85 |
| 1:K:401:LEU:HD23 | 1:K:402:ALA:HB2 | 1.55 | 0.85 |
| 1:L:353:PHE:HZ | 1:L:395:TYR:HE2 | 1.21 | 0.85 |
| 1:E:560:SER:N | 1:E:561:GLY:CA | 2.39 | 0.85 |
| 1:E:401:LEU:HD11 | 1:H:364:THR:HG21 | 0.86 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:341:THR:O | 1:A:345:TYR:CD1 | 2.30 | 0.85 |
| 1:J:662:GLU:O | 1:J:663:HIS:CB | 2.20 | 0.85 |
| 1:B:353:PHE:HZ | 1:B:395:TYR:HE2 | 1.21 | 0.85 |
| 1:C:341:THR:O | 1:C:345:TYR:CD1 | 2.30 | 0.85 |
| 1:E:341:THR:HG1 | 1:E:344:ASP:HB2 | 1.40 | 0.85 |
| 1:B:664:HIS:CG | 1:B:664:HIS:O | 2.29 | 0.85 |
| 1:E:353:PHE:CE1 | 1:E:395:TYR:CE2 | 2.65 | 0.85 |
| 1:E:660:GLN:HG3 | 1:E:661:LEU:N | 1.90 | 0.85 |
| 1:J:345:TYR:O | 1:J:345:TYR:CD1 | 2.30 | 0.85 |
| 1:L:345:TYR:O | 1:L:345:TYR:CD1 | 2.30 | 0.85 |
| 1:B:662:GLU:O | 1:B:663:HIS:CB | 2.20 | 0.85 |
| 1:G:385:THR:HA | 1:G:387:VAL:HG22 | 1.59 | 0.85 |
| 1:I:660:GLN:HG3 | 1:I:661:LEU:N | 1.90 | 0.85 |
| 1:J:353:PHE:HZ | 1:J:395:TYR:HE2 | 1.21 | 0.85 |
| 1:D:345:TYR:O | 1:D:345:TYR:CD1 | 2.30 | 0.85 |
| 1:H:345:TYR:CD1 | 1:H:345:TYR:O | 2.30 | 0.85 |
| 1:I:635:ARG:HG2 | 1:I:636:ASP:N | 1.90 | 0.85 |
| 1:D:662:GLU:O | 1:D:663:HIS:CB | 2.20 | 0.84 |
| 1:G:631:VAL:HG21 | 1:H:476:ILE:HG22 | 1.57 | 0.84 |
| 1:D:496:GLU:H | 1:D:496:GLU:CD | 1.80 | 0.84 |
| 1:E:341:THR:O | 1:E:345:TYR:CD1 | 2.30 | 0.84 |
| 1:E:347:THR:OG1 | 1:E:348:PHE:N | 2.05 | 0.84 |
| 1:E:385:THR:HA | 1:E:387:VAL:HG22 | 1.59 | 0.84 |
| 1:F:345:TYR:CD1 | 1:F:345:TYR:O | 2.30 | 0.84 |
| 1:I:341:THR:O | 1:I:345:TYR:CD1 | 2.30 | 0.84 |
| 1:I:385:THR:HA | 1:I:387:VAL:HG22 | 1.59 | 0.84 |
| 1:C:353:PHE:CE1 | 1:C:395:TYR:CE2 | 2.65 | 0.84 |
| 1:C:560:SER:N | 1:C:561:GLY:CA | 2.39 | 0.84 |
| 1:G:353:PHE:CE1 | 1:G:395:TYR:CE2 | 2.65 | 0.84 |
| 1:K:341:THR:O | 1:K:345:TYR:CD1 | 2.30 | 0.84 |
| 1:L:367:THR:CG2 | 1:L:368:LYS:H | 1.87 | 0.84 |
| 1:L:496:GLU:H | 1:L:496:GLU:CD | 1.80 | 0.84 |
| 1:B:345:TYR:O | 1:B:345:TYR:CD1 | 2.30 | 0.84 |
| 1:B:496:GLU:CD | 1:B:496:GLU:H | 1.80 | 0.84 |
| 1:F:664:HIS:O | 1:F:664:HIS:CG | 2.29 | 0.84 |
| 1:E:385:THR:HG1 | 1:E:387:VAL:HG23 | 1.37 | 0.84 |
| 1:E:403:PRO:CB | 1:H:366:SER:CA | 2.39 | 0.84 |
| 1:H:664:HIS:CG | 1:H:664:HIS:O | 2.29 | 0.84 |
| 1:K:660:GLN:HG3 | 1:K:661:LEU:N | 1.90 | 0.84 |
| 1:B:567:GLU:HA | 1:B:570:GLN:OE1 | 1.78 | 0.84 |
| 1:D:664:HIS:CG | 1:D:664:HIS:O | 2.29 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:560:SER:N | 1:G:561:GLY:CA | 2.39 | 0.84 |
| 1:I:340:VAL:CA | 1:I:345:TYR:HE1 | 1.90 | 0.84 |
| 1:C:635:ARG:HG2 | 1:C:636:ASP:N | 1.90 | 0.84 |
| 1:A:631:VAL:HG21 | 1:B:476:ILE:HG22 | 1.57 | 0.84 |
| 1:F:567:GLU:HA | 1:F:570:GLN:OE1 | 1.78 | 0.84 |
| 1:F:662:GLU:O | 1:F:663:HIS:CB | 2.20 | 0.84 |
| 1:K:353:PHE:CE1 | 1:K:395:TYR:CE2 | 2.65 | 0.84 |
| 1:A:353:PHE:CE1 | 1:A:395:TYR:CE2 | 2.65 | 0.84 |
| 1:A:401:LEU:HD11 | 1:C:364:THR:CG2 | 2.01 | 0.84 |
| 1:B:543:THR:HG22 | 1:B:577:PHE:HB3 | 1.60 | 0.84 |
| 1:H:353:PHE:HZ | 1:H:395:TYR:HE2 | 1.21 | 0.84 |
| 1:H:543:THR:HG22 | 1:H:577:PHE:HB3 | 1.60 | 0.84 |
| 1:D:353:PHE:HZ | 1:D:395:TYR:HE2 | 1.21 | 0.83 |
| 1:H:366:SER:C | 1:H:367:THR:CG2 | 2.42 | 0.83 |
| 1:I:557:PRO:HB3 | 1:I:587:ASP:HA | 1.60 | 0.83 |
| 1:K:340:VAL:CA | 1:K:345:TYR:HE1 | 1.90 | 0.83 |
| 1:E:661:LEU:CD1 | 1:E:661:LEU:C | 2.29 | 0.83 |
| 1:G:341:THR:O | 1:G:345:TYR:CD1 | 2.30 | 0.83 |
| 1:L:662:GLU:O | 1:L:663:HIS:CB | 2.20 | 0.83 |
| 1:F:582:ASN:HD21 | 1:F:586:ARG:HB2 | 1.44 | 0.83 |
| 1:G:347:THR:OG1 | 1:G:348:PHE:N | 2.05 | 0.83 |
| 1:H:567:GLU:HA | 1:H:570:GLN:OE1 | 1.78 | 0.83 |
| 1:H:657:PRO:C | 1:H:658:ILE:HD13 | 1.99 | 0.83 |
| 1:J:496:GLU:CD | 1:J:496:GLU:H | 1.80 | 0.83 |
| 1:B:582:ASN:HD21 | 1:B:586:ARG:HB2 | 1.43 | 0.83 |
| 1:C:340:VAL:CA | 1:C:345:TYR:HE1 | 1.90 | 0.83 |
| 1:D:582:ASN:HD21 | 1:D:586:ARG:HB2 | 1.44 | 0.83 |
| 1:E:557:PRO:HB3 | 1:E:587:ASP:HA | 1.60 | 0.83 |
| 1:J:664:HIS:CG | 1:J:664:HIS:O | 2.29 | 0.83 |
| 1:F:353:PHE:HZ | 1:F:395:TYR:HE2 | 1.21 | 0.83 |
| 1:F:543:THR:HG22 | 1:F:577:PHE:HB3 | 1.60 | 0.83 |
| 1:L:657:PRO:C | 1:L:658:ILE:HD13 | 1.99 | 0.83 |
| 1:E:345:TYR:N | 1:E:345:TYR:HD1 | 1.77 | 0.83 |
| 1:K:635:ARG:HG2 | 1:K:636:ASP:N | 1.90 | 0.83 |
| 1:L:543:THR:HG22 | 1:L:577:PHE:HB3 | 1.60 | 0.83 |
| 1:E:340:VAL:CA | 1:E:345:TYR:HE1 | 1.90 | 0.83 |
| 1:E:631:VAL:HG21 | 1:F:476:ILE:HG22 | 1.57 | 0.83 |
| 1:F:657:PRO:C | 1:F:658:ILE:HD13 | 1.99 | 0.83 |
| 1:G:345:TYR:N | 1:G:345:TYR:HD1 | 1.77 | 0.83 |
| 1:L:567:GLU:HA | 1:L:570:GLN:OE1 | 1.78 | 0.83 |
| 1:H:367:THR:CG2 | 1:H:368:LYS:H | 1.87 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:345:TYR:CE1 | 1:J:349:VAL:HG23 | 2.14 | 0.83 |
| 1:J:657:PRO:C | 1:J:658:ILE:HD13 | 1.99 | 0.83 |
| 1:D:657:PRO:C | 1:D:658:ILE:HD13 | 1.99 | 0.82 |
| 1:J:567:GLU:HA | 1:J:570:GLN:OE1 | 1.78 | 0.82 |
| 1:A:345:TYR:N | 1:A:345:TYR:HD1 | 1.77 | 0.82 |
| 1:B:379:LYS:HG3 | 1:B:380:SER:N | 1.94 | 0.82 |
| 1:D:345:TYR:CE1 | 1:D:349:VAL:HG23 | 2.14 | 0.82 |
| 1:G:340:VAL:CA | 1:G:345:TYR:HE1 | 1.90 | 0.82 |
| 1:G:557:PRO:HB3 | 1:G:587:ASP:HA | 1.60 | 0.82 |
| 1:H:503:ASN:ND2 | 1:H:633:PHE:H | 1.77 | 0.82 |
| 1:I:560:SER:N | 1:I:561:GLY:CA | 2.39 | 0.82 |
| 1:K:385:THR:HA | 1:K:387:VAL:HG22 | 1.59 | 0.82 |
| 1:D:379:LYS:HG3 | 1:D:380:SER:N | 1.94 | 0.82 |
| 1:H:496:GLU:H | 1:H:496:GLU:CD | 1.80 | 0.82 |
| 1:H:582:ASN:HD21 | 1:H:586:ARG:HB2 | 1.44 | 0.82 |
| 1:J:582:ASN:HD21 | 1:J:586:ARG:HB2 | 1.43 | 0.82 |
| 1:J:659:SER:O | 1:J:660:GLN:HG3 | 1.80 | 0.82 |
| 1:K:661:LEU:HD13 | 1:K:662:GLU:CA | 2.10 | 0.82 |
| 1:A:519:SER:HB2 | 1:A:562:ASP:CG | 2.00 | 0.82 |
| 1:B:345:TYR:CE1 | 1:B:349:VAL:HG23 | 2.14 | 0.82 |
| 1:L:582:ASN:HD21 | 1:L:586:ARG:HB2 | 1.43 | 0.82 |
| 1:C:519:SER:HB2 | 1:C:562:ASP:CG | 2.00 | 0.82 |
| 1:G:519:SER:HB2 | 1:G:562:ASP:CG | 2.00 | 0.82 |
| 1:I:661:LEU:HD13 | 1:I:662:GLU:CA | 2.10 | 0.82 |
| 1:A:385:THR:HA | 1:A:387:VAL:HG22 | 1.59 | 0.82 |
| 1:B:657:PRO:C | 1:B:658:ILE:HD13 | 1.99 | 0.82 |
| 1:F:659:SER:O | 1:F:660:GLN:HG3 | 1.80 | 0.82 |
| 1:G:385:THR:HG1 | 1:G:387:VAL:HG23 | 1.40 | 0.82 |
| 1:A:340:VAL:CA | 1:A:345:TYR:HE1 | 1.90 | 0.82 |
| 1:A:401:LEU:HD23 | 1:A:402:ALA:HB2 | 1.55 | 0.82 |
| 1:D:567:GLU:HA | 1:D:570:GLN:OE1 | 1.78 | 0.82 |
| 1:F:345:TYR:CE1 | 1:F:349:VAL:HG23 | 2.14 | 0.82 |
| 1:F:496:GLU:H | 1:F:496:GLU:CD | 1.80 | 0.82 |
| 1:I:396:LEU:HD22 | 1:I:408:ILE:HD13 | 1.62 | 0.82 |
| 1:C:557:PRO:HB3 | 1:C:587:ASP:HA | 1.60 | 0.82 |
| 1:D:543:THR:HG22 | 1:D:577:PHE:HB3 | 1.60 | 0.82 |
| 1:G:396:LEU:HD22 | 1:G:408:ILE:HD13 | 1.62 | 0.82 |
| 1:L:345:TYR:CE1 | 1:L:349:VAL:HG23 | 2.14 | 0.82 |
| 1:A:661:LEU:HD13 | 1:A:662:GLU:CA | 2.10 | 0.81 |
| 1:J:503:ASN:ND2 | 1:J:633:PHE:H | 1.77 | 0.81 |
| 1:K:519:SER:HB2 | 1:K:562:ASP:CG | 2.00 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:635:ARG:NH2 | 1:D:661:LEU:HD12 | 1.95 | 0.81 |
| 1:D:503:ASN:ND2 | 1:D:633:PHE:H | 1.77 | 0.81 |
| 1:F:379:LYS:HG3 | 1:F:380:SER:N | 1.94 | 0.81 |
| 1:G:661:LEU:HD13 | 1:G:662:GLU:CA | 2.10 | 0.81 |
| 1:J:543:THR:HG22 | 1:J:577:PHE:HB3 | 1.60 | 0.81 |
| 1:C:340:VAL:HA | 1:C:345:TYR:CE1 | 2.15 | 0.81 |
| 1:C:385:THR:HA | 1:C:387:VAL:HG22 | 1.59 | 0.81 |
| 1:D:399:TYR:CA | 1:E:664:HIS:CG | 2.61 | 0.81 |
| 1:D:659:SER:O | 1:D:660:GLN:HG3 | 1.80 | 0.81 |
| 1:G:340:VAL:HA | 1:G:345:TYR:CE1 | 2.15 | 0.81 |
| 1:H:659:SER:O | 1:H:660:GLN:HG3 | 1.80 | 0.81 |
| 1:I:519:SER:HB2 | 1:I:562:ASP:CG | 2.00 | 0.81 |
| 1:L:595:ILE:H | 1:L:595:ILE:HD12 | 1.45 | 0.81 |
| 1:E:519:SER:HB2 | 1:E:562:ASP:CG | 2.00 | 0.81 |
| 1:H:345:TYR:CE1 | 1:H:349:VAL:HG23 | 2.14 | 0.81 |
| 1:I:340:VAL:HA | 1:I:345:TYR:CE1 | 2.15 | 0.81 |
| 1:A:635:ARG:NH2 | 1:B:661:LEU:HD12 | 1.95 | 0.81 |
| 1:E:403:PRO:CA | 1:H:366:SER:CB | 2.42 | 0.81 |
| 1:A:557:PRO:HB3 | 1:A:587:ASP:HA | 1.60 | 0.81 |
| 1:C:345:TYR:N | 1:C:345:TYR:HD1 | 1.77 | 0.81 |
| 1:K:396:LEU:HD22 | 1:K:408:ILE:HD13 | 1.62 | 0.81 |
| 1:I:345:TYR:N | 1:I:345:TYR:HD1 | 1.77 | 0.81 |
| 1:L:379:LYS:HG3 | 1:L:380:SER:N | 1.94 | 0.81 |
| 1:E:396:LEU:HD22 | 1:E:408:ILE:HD13 | 1.62 | 0.81 |
| 1:F:595:ILE:HD12 | 1:F:595:ILE:H | 1.45 | 0.81 |
| 1:K:557:PRO:HB3 | 1:K:587:ASP:HA | 1.60 | 0.81 |
| 1:L:659:SER:O | 1:L:660:GLN:CG | 2.29 | 0.81 |
| 1:A:340:VAL:HA | 1:A:345:TYR:CE1 | 2.15 | 0.80 |
| 1:F:659:SER:O | 1:F:660:GLN:CG | 2.29 | 0.80 |
| 1:G:525:ASN:OD1 | 1:G:526:PRO:CD | 2.30 | 0.80 |
| 1:B:366:SER:O | 1:B:367:THR:CG2 | 2.29 | 0.80 |
| 1:B:595:ILE:H | 1:B:595:ILE:HD12 | 1.45 | 0.80 |
| 1:B:659:SER:O | 1:B:660:GLN:HG3 | 1.80 | 0.80 |
| 1:C:661:LEU:HD13 | 1:C:662:GLU:CA | 2.10 | 0.80 |
| 1:D:661:LEU:O | 1:D:661:LEU:CD1 | 2.29 | 0.80 |
| 1:E:403:PRO:CB | 1:H:366:SER:HA | 2.10 | 0.80 |
| 1:E:635:ARG:NH2 | 1:F:661:LEU:HD12 | 1.95 | 0.80 |
| 1:J:661:LEU:O | 1:J:661:LEU:CD1 | 2.29 | 0.80 |
| 1:D:659:SER:O | 1:D:660:GLN:CG | 2.29 | 0.80 |
| 1:G:388:GLN:O | 1:G:389:ARG:CG | 2.30 | 0.80 |
| 1:J:595:ILE:H | 1:J:595:ILE:HD12 | 1.45 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:525:ASN:OD1 | 1:A:526:PRO:CD | 2.30 | 0.80 |
| 1:E:661:LEU:HD13 | 1:E:662:GLU:CA | 2.10 | 0.80 |
| 1:K:525:ASN:OD1 | 1:K:526:PRO:CD | 2.30 | 0.80 |
| 1:J:659:SER:O | 1:J:660:GLN:CG | 2.29 | 0.80 |
| 1:L:366:SER:O | 1:L:367:THR:CG2 | 2.29 | 0.80 |
| 1:D:400:ASN:ND2 | 1:E:662:GLU:CD | 2.34 | 0.80 |
| 1:H:408:ILE:O | 1:H:408:ILE:CD1 | 2.30 | 0.80 |
| 1:H:659:SER:O | 1:H:660:GLN:CG | 2.29 | 0.80 |
| 1:J:567:GLU:O | 1:J:568:ASN:CB | 2.30 | 0.80 |
| 1:J:661:LEU:O | 1:J:661:LEU:CD2 | 2.29 | 0.80 |
| 1:K:340:VAL:HA | 1:K:345:TYR:CE1 | 2.15 | 0.80 |
| 1:K:388:GLN:O | 1:K:389:ARG:CG | 2.30 | 0.80 |
| 1:L:659:SER:O | 1:L:660:GLN:HG3 | 1.80 | 0.80 |
| 1:A:341:THR:HG1 | 1:A:344:ASP:HB2 | 1.45 | 0.80 |
| 1:B:366:SER:O | 1:B:367:THR:CB | 2.30 | 0.80 |
| 1:B:408:ILE:O | 1:B:408:ILE:CD1 | 2.30 | 0.80 |
| 1:C:385:THR:CG2 | 1:C:389:ARG:CA | 2.60 | 0.80 |
| 1:E:353:PHE:CE1 | 1:E:395:TYR:CD2 | 2.70 | 0.80 |
| 1:I:525:ASN:OD1 | 1:I:526:PRO:CD | 2.30 | 0.80 |
| 1:L:661:LEU:O | 1:L:661:LEU:CD2 | 2.29 | 0.80 |
| 1:A:629:ASP:HA | 1:B:664:HIS:HE1 | 1.47 | 0.80 |
| 1:B:367:THR:CG2 | 1:B:368:LYS:H | 1.87 | 0.80 |
| 1:C:525:ASN:OD1 | 1:C:526:PRO:CD | 2.30 | 0.80 |
| 1:D:366:SER:O | 1:D:367:THR:CB | 2.30 | 0.80 |
| 1:D:567:GLU:O | 1:D:568:ASN:CB | 2.30 | 0.80 |
| 1:E:385:THR:CG2 | 1:E:389:ARG:CA | 2.60 | 0.80 |
| 1:G:635:ARG:NH2 | 1:H:661:LEU:HD12 | 1.95 | 0.80 |
| 1:H:379:LYS:HG3 | 1:H:380:SER:N | 1.94 | 0.80 |
| 1:I:353:PHE:CE1 | 1:I:395:TYR:CD2 | 2.70 | 0.80 |
| 1:I:635:ARG:NH2 | 1:J:661:LEU:HD12 | 1.95 | 0.80 |
| 1:J:366:SER:C | 1:J:367:THR:CG2 | 2.42 | 0.80 |
| 1:J:379:LYS:HG3 | 1:J:380:SER:N | 1.94 | 0.80 |
| 1:K:353:PHE:CE1 | 1:K:395:TYR:CD2 | 2.70 | 0.80 |
| 1:L:503:ASN:HD21 | 1:L:633:PHE:N | 1.79 | 0.80 |
| 1:A:385:THR:CG2 | 1:A:389:ARG:CA | 2.60 | 0.80 |
| 1:A:396:LEU:HD22 | 1:A:408:ILE:HD13 | 1.62 | 0.80 |
| 1:B:659:SER:O | 1:B:660:GLN:CG | 2.29 | 0.80 |
| 1:D:595:ILE:H | 1:D:595:ILE:HD12 | 1.45 | 0.80 |
| 1:K:635:ARG:NH2 | 1:L:661:LEU:HD12 | 1.96 | 0.80 |
| 1:C:396:LEU:HD22 | 1:C:408:ILE:HD13 | 1.62 | 0.80 |
| 1:G:353:PHE:CE1 | 1:G:395:TYR:CD2 | 2.70 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:661:LEU:O | 1:H:661:LEU:CD2 | 2.29 | 0.80 |
| 1:E:340:VAL:HA | 1:E:345:TYR:CE1 | 2.15 | 0.79 |
| 1:F:567:GLU:O | 1:F:568:ASN:CB | 2.30 | 0.79 |
| 1:E:388:GLN:O | 1:E:389:ARG:CB | 2.30 | 0.79 |
| 1:E:388:GLN:O | 1:E:389:ARG:CG | 2.30 | 0.79 |
| 1:H:595:ILE:H | 1:H:595:ILE:HD12 | 1.46 | 0.79 |
| 1:L:503:ASN:ND2 | 1:L:633:PHE:H | 1.77 | 0.79 |
| 1:F:661:LEU:O | 1:F:661:LEU:CD1 | 2.29 | 0.79 |
| 1:I:440:ILE:HD11 | 1:I:653:ILE:HD13 | 1.64 | 0.79 |
| 1:A:353:PHE:CE1 | 1:A:395:TYR:CD2 | 2.70 | 0.79 |
| 1:B:661:LEU:O | 1:B:661:LEU:CD2 | 2.29 | 0.79 |
| 1:I:388:GLN:O | 1:I:389:ARG:CG | 2.30 | 0.79 |
| 1:A:388:GLN:O | 1:A:389:ARG:CG | 2.30 | 0.79 |
| 1:D:661:LEU:O | 1:D:661:LEU:CD2 | 2.29 | 0.79 |
| 1:F:366:SER:O | 1:F:367:THR:CG2 | 2.29 | 0.79 |
| 1:F:503:ASN:HD21 | 1:F:633:PHE:N | 1.79 | 0.79 |
| 1:J:366:SER:O | 1:J:367:THR:CG2 | 2.29 | 0.79 |
| 1:L:567:GLU:O | 1:L:568:ASN:CB | 2.30 | 0.79 |
| 1:C:353:PHE:CE1 | 1:C:395:TYR:CD2 | 2.70 | 0.79 |
| 1:D:366:SER:O | 1:D:367:THR:CG2 | 2.29 | 0.79 |
| 1:D:503:ASN:HD21 | 1:D:633:PHE:N | 1.79 | 0.79 |
| 1:C:385:THR:HG21 | 1:C:389:ARG:HA | 1.64 | 0.79 |
| 1:C:388:GLN:O | 1:C:389:ARG:CG | 2.30 | 0.79 |
| 1:F:661:LEU:O | 1:F:661:LEU:CD2 | 2.30 | 0.79 |
| 1:K:345:TYR:N | 1:K:345:TYR:HD1 | 1.77 | 0.79 |
| 1:K:388:GLN:O | 1:K:389:ARG:CB | 2.30 | 0.79 |
| 1:E:440:ILE:HD11 | 1:E:653:ILE:HD13 | 1.64 | 0.79 |
| 1:G:361:GLN:HG2 | 1:G:455:PHE:CG | 2.18 | 0.79 |
| 1:G:385:THR:HG21 | 1:G:389:ARG:HA | 1.64 | 0.79 |
| 1:H:366:SER:O | 1:H:367:THR:CB | 2.30 | 0.79 |
| 1:I:388:GLN:O | 1:I:389:ARG:CB | 2.30 | 0.79 |
| 1:I:532:GLU:N | 1:I:532:GLU:CD | 2.36 | 0.79 |
| 1:L:408:ILE:O | 1:L:408:ILE:CD1 | 2.30 | 0.79 |
| 1:A:385:THR:CA | 1:A:387:VAL:HG22 | 2.13 | 0.79 |
| 1:B:567:GLU:O | 1:B:568:ASN:CB | 2.30 | 0.79 |
| 1:B:647:ARG:HD2 | 1:B:650:TYR:CE1 | 2.19 | 0.79 |
| 1:K:385:THR:CA | 1:K:387:VAL:HG22 | 2.13 | 0.79 |
| 1:D:374:ILE:HG12 | 1:D:408:ILE:HA | 1.65 | 0.78 |
| 1:E:403:PRO:CG | 1:H:366:SER:HA | 2.13 | 0.78 |
| 1:I:385:THR:CA | 1:I:387:VAL:HG22 | 2.13 | 0.78 |
| 1:J:503:ASN:HD21 | 1:J:633:PHE:N | 1.79 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:385:THR:HG21 | 1:A:389:ARG:HA | 1.64 | 0.78 |
| 1:A:532:GLU:N | 1:A:532:GLU:CD | 2.37 | 0.78 |
| 1:C:388:GLN:O | 1:C:389:ARG:CB | 2.30 | 0.78 |
| 1:G:388:GLN:O | 1:G:389:ARG:CB | 2.30 | 0.78 |
| 1:G:532:GLU:CD | 1:G:532:GLU:N | 2.36 | 0.78 |
| 1:A:457:SER:H | 1:A:634:THR:CG2 | 1.97 | 0.78 |
| 1:G:440:ILE:HD11 | 1:G:653:ILE:HD13 | 1.64 | 0.78 |
| 1:H:503:ASN:HD21 | 1:H:633:PHE:N | 1.79 | 0.78 |
| 1:L:661:LEU:O | 1:L:661:LEU:CD1 | 2.29 | 0.78 |
| 1:B:374:ILE:HG12 | 1:B:408:ILE:HA | 1.65 | 0.78 |
| 1:C:361:GLN:HG2 | 1:C:455:PHE:CG | 2.19 | 0.78 |
| 1:C:457:SER:H | 1:C:634:THR:CG2 | 1.97 | 0.78 |
| 1:I:361:GLN:HG2 | 1:I:455:PHE:CG | 2.19 | 0.78 |
| 1:J:647:ARG:HD2 | 1:J:650:TYR:CE1 | 2.19 | 0.78 |
| 1:B:503:ASN:ND2 | 1:B:633:PHE:H | 1.77 | 0.78 |
| 1:E:361:GLN:HG2 | 1:E:455:PHE:CG | 2.19 | 0.78 |
| 1:F:503:ASN:ND2 | 1:F:633:PHE:H | 1.77 | 0.78 |
| 1:H:374:ILE:HG12 | 1:H:408:ILE:HA | 1.65 | 0.78 |
| 1:I:385:THR:HG21 | 1:I:389:ARG:HA | 1.64 | 0.78 |
| 1:D:408:ILE:O | 1:D:408:ILE:CD1 | 2.30 | 0.78 |
| 1:E:525:ASN:OD1 | 1:E:526:PRO:CD | 2.30 | 0.78 |
| 1:E:629:ASP:HA | 1:F:664:HIS:HE1 | 1.47 | 0.78 |
| 1:J:569:ILE:O | 1:J:569:ILE:CG2 | 2.30 | 0.78 |
| 1:K:532:GLU:CD | 1:K:532:GLU:N | 2.36 | 0.78 |
| 1:C:532:GLU:CD | 1:C:532:GLU:N | 2.37 | 0.78 |
| 1:A:388:GLN:O | 1:A:389:ARG:CB | 2.30 | 0.78 |
| 1:D:366:SER:C | 1:D:367:THR:CG2 | 2.42 | 0.78 |
| 1:F:374:ILE:HG12 | 1:F:408:ILE:HA | 1.65 | 0.78 |
| 1:G:341:THR:HG1 | 1:G:344:ASP:HB2 | 1.48 | 0.78 |
| 1:G:524:VAL:HG22 | 1:G:529:GLY:O | 1.84 | 0.78 |
| 1:H:567:GLU:O | 1:H:568:ASN:CB | 2.30 | 0.78 |
| 1:I:353:PHE:CE2 | 1:I:395:TYR:HD2 | 2.02 | 0.78 |
| 1:K:361:GLN:HG2 | 1:K:455:PHE:CG | 2.18 | 0.78 |
| 1:C:440:ILE:HD11 | 1:C:653:ILE:HD13 | 1.64 | 0.78 |
| 1:H:647:ARG:HD2 | 1:H:650:TYR:CE1 | 2.19 | 0.78 |
| 1:J:374:ILE:HG12 | 1:J:408:ILE:HA | 1.65 | 0.78 |
| 1:K:353:PHE:CE2 | 1:K:395:TYR:HD2 | 2.02 | 0.78 |
| 1:C:385:THR:CA | 1:C:387:VAL:HG22 | 2.14 | 0.78 |
| 1:E:345:TYR:CD1 | 1:E:345:TYR:N | 2.51 | 0.78 |
| 1:J:367:THR:CG2 | 1:J:368:LYS:H | 1.88 | 0.78 |
| 1:L:374:ILE:HG12 | 1:L:408:ILE:HA | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:647:ARG:HD2 | 1:D:650:TYR:CE1 | 2.19 | 0.77 |
| 1:L:647:ARG:HD2 | 1:L:650:TYR:CE1 | 2.19 | 0.77 |
| 1:D:646:LEU:HD23 | 1:D:646:LEU:C | 2.05 | 0.77 |
| 1:G:385:THR:CA | 1:G:387:VAL:HG22 | 2.13 | 0.77 |
| 1:J:366:SER:O | 1:J:367:THR:CB | 2.30 | 0.77 |
| 1:K:440:ILE:HD11 | 1:K:653:ILE:HD13 | 1.64 | 0.77 |
| 1:E:385:THR:HG21 | 1:E:389:ARG:HA | 1.64 | 0.77 |
| 1:H:366:SER:O | 1:H:367:THR:CG2 | 2.29 | 0.77 |
| 1:A:361:GLN:HG2 | 1:A:455:PHE:CG | 2.19 | 0.77 |
| 1:A:403:PRO:HB3 | 1:C:366:SER:OG | 1.85 | 0.77 |
| 1:A:440:ILE:HD11 | 1:A:653:ILE:HD13 | 1.64 | 0.77 |
| 1:E:385:THR:CA | 1:E:387:VAL:HG22 | 2.14 | 0.77 |
| 1:F:646:LEU:HD23 | 1:F:646:LEU:C | 2.05 | 0.77 |
| 1:E:353:PHE:CE2 | 1:E:395:TYR:HD2 | 2.02 | 0.77 |
| 1:F:647:ARG:HD2 | 1:F:650:TYR:CE1 | 2.18 | 0.77 |
| 1:H:403:PRO:O | 1:H:405:THR:HG22 | 1.85 | 0.77 |
| 1:I:524:VAL:HG22 | 1:I:529:GLY:O | 1.84 | 0.77 |
| 1:A:340:VAL:CA | 1:A:345:TYR:OH | 2.30 | 0.77 |
| 1:B:661:LEU:O | 1:B:661:LEU:CD1 | 2.29 | 0.77 |
| 1:A:353:PHE:CE2 | 1:A:395:TYR:HD2 | 2.02 | 0.77 |
| 1:A:524:VAL:HG22 | 1:A:529:GLY:O | 1.84 | 0.77 |
| 1:C:355:SER:OG | 1:C:356:ILE:HG23 | 1.85 | 0.77 |
| 1:D:367:THR:O | 1:D:369:PRO:CD | 2.30 | 0.77 |
| 1:H:646:LEU:HD23 | 1:H:646:LEU:C | 2.05 | 0.77 |
| 1:H:661:LEU:O | 1:H:661:LEU:CD1 | 2.29 | 0.77 |
| 1:L:569:ILE:O | 1:L:569:ILE:CG2 | 2.30 | 0.77 |
| 1:E:355:SER:OG | 1:E:356:ILE:HG23 | 1.85 | 0.77 |
| 1:E:524:VAL:HG22 | 1:E:529:GLY:O | 1.84 | 0.77 |
| 1:K:524:VAL:HG22 | 1:K:529:GLY:O | 1.84 | 0.77 |
| 1:G:353:PHE:CE2 | 1:G:395:TYR:HD2 | 2.02 | 0.77 |
| 1:L:403:PRO:O | 1:L:405:THR:HG22 | 1.85 | 0.77 |
| 1:A:345:TYR:CD1 | 1:A:345:TYR:N | 2.51 | 0.76 |
| 1:C:353:PHE:CE2 | 1:C:395:TYR:HD2 | 2.02 | 0.76 |
| 1:F:367:THR:CG2 | 1:F:368:LYS:H | 1.88 | 0.76 |
| 1:E:532:GLU:CD | 1:E:532:GLU:N | 2.37 | 0.76 |
| 1:G:355:SER:OG | 1:G:356:ILE:HG23 | 1.85 | 0.76 |
| 1:K:457:SER:H | 1:K:634:THR:CG2 | 1.97 | 0.76 |
| 1:B:366:SER:CB | 1:K:403:PRO:CA | 2.44 | 0.76 |
| 1:B:367:THR:O | 1:B:369:PRO:CD | 2.30 | 0.76 |
| 1:D:408:ILE:O | 1:D:409:ILE:CG2 | 2.34 | 0.76 |
| 1:J:403:PRO:O | 1:J:405:THR:HG22 | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:VAL:O | 1:A:345:TYR:CE1 | 2.37 | 0.76 |
| 1:B:366:SER:HA | 1:K:403:PRO:CG | 2.15 | 0.76 |
| 1:J:646:LEU:HD23 | 1:J:646:LEU:C | 2.05 | 0.76 |
| 1:C:629:ASP:HA | 1:D:664:HIS:HE1 | 1.47 | 0.76 |
| 1:J:367:THR:O | 1:J:369:PRO:CD | 2.30 | 0.76 |
| 1:L:408:ILE:O | 1:L:409:ILE:CG2 | 2.34 | 0.76 |
| 1:L:646:LEU:HD23 | 1:L:646:LEU:C | 2.05 | 0.76 |
| 1:B:408:ILE:O | 1:B:409:ILE:CG2 | 2.34 | 0.76 |
| 1:C:524:VAL:HG22 | 1:C:529:GLY:O | 1.84 | 0.76 |
| 1:D:408:ILE:HD12 | 1:D:409:ILE:N | 2.01 | 0.76 |
| 1:D:661:LEU:HD13 | 1:D:662:GLU:N | 2.01 | 0.76 |
| 1:E:457:SER:H | 1:E:634:THR:CG2 | 1.97 | 0.76 |
| 1:B:646:LEU:HD23 | 1:B:646:LEU:C | 2.05 | 0.76 |
| 1:F:661:LEU:HD13 | 1:F:662:GLU:N | 2.01 | 0.76 |
| 1:L:345:TYR:HE1 | 1:L:349:VAL:CG2 | 1.99 | 0.76 |
| 1:L:366:SER:O | 1:L:367:THR:CB | 2.30 | 0.76 |
| 1:A:355:SER:OG | 1:A:356:ILE:HG23 | 1.85 | 0.76 |
| 1:B:408:ILE:HD12 | 1:B:409:ILE:N | 2.01 | 0.76 |
| 1:F:408:ILE:O | 1:F:409:ILE:CG2 | 2.34 | 0.76 |
| 1:G:345:TYR:CD1 | 1:G:345:TYR:N | 2.51 | 0.76 |
| 1:G:401:LEU:O | 1:G:402:ALA:HB3 | 1.84 | 0.76 |
| 1:A:401:LEU:O | 1:A:402:ALA:HB3 | 1.84 | 0.76 |
| 1:B:345:TYR:HE1 | 1:B:349:VAL:CG2 | 1.99 | 0.76 |
| 1:B:427:ASN:ND2 | 1:B:427:ASN:H | 1.84 | 0.76 |
| 1:C:416:ILE:HG13 | 1:C:448:TYR:OH | 1.86 | 0.76 |
| 1:F:403:PRO:O | 1:F:405:THR:HG22 | 1.85 | 0.76 |
| 1:A:560:SER:N | 1:A:561:GLY:HA3 | 2.01 | 0.76 |
| 1:C:340:VAL:CA | 1:C:345:TYR:OH | 2.30 | 0.76 |
| 1:J:408:ILE:O | 1:J:408:ILE:CD1 | 2.30 | 0.76 |
| 1:K:385:THR:HG21 | 1:K:389:ARG:HA | 1.64 | 0.76 |
| 1:J:408:ILE:HD12 | 1:J:409:ILE:N | 2.01 | 0.75 |
| 1:K:401:LEU:O | 1:K:402:ALA:HB3 | 1.84 | 0.75 |
| 1:B:366:SER:HA | 1:K:403:PRO:CB | 2.11 | 0.75 |
| 1:H:408:ILE:O | 1:H:409:ILE:CG2 | 2.34 | 0.75 |
| 1:K:416:ILE:HG13 | 1:K:448:TYR:OH | 1.86 | 0.75 |
| 1:A:416:ILE:HG13 | 1:A:448:TYR:OH | 1.86 | 0.75 |
| 1:B:403:PRO:O | 1:B:405:THR:HG22 | 1.85 | 0.75 |
| 1:B:644:ASN:O | 1:B:644:ASN:ND2 | 2.20 | 0.75 |
| 1:F:366:SER:O | 1:F:367:THR:CB | 2.30 | 0.75 |
| 1:I:355:SER:OG | 1:I:356:ILE:HG23 | 1.85 | 0.75 |
| 1:J:408:ILE:O | 1:J:409:ILE:CG2 | 2.34 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:355:SER:OG | 1:K:356:ILE:HG23 | 1.85 | 0.75 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:HB3 | 1.86 | 0.75 |
| 1:E:340:VAL:CA | 1:E:345:TYR:OH | 2.30 | 0.75 |
| 1:C:401:LEU:O | 1:C:402:ALA:HB3 | 1.85 | 0.75 |
| 1:D:400:ASN:HB3 | 1:E:662:GLU:HA | 1.66 | 0.75 |
| 1:H:345:TYR:HE1 | 1:H:349:VAL:CG2 | 1.99 | 0.75 |
| 1:I:526:PRO:O | 1:I:528:THR:HG22 | 1.87 | 0.75 |
| 1:K:340:VAL:CA | 1:K:345:TYR:OH | 2.30 | 0.75 |
| 1:L:367:THR:O | 1:L:369:PRO:CD | 2.30 | 0.75 |
| 1:C:526:PRO:O | 1:C:528:THR:HG22 | 1.87 | 0.75 |
| 1:D:427:ASN:ND2 | 1:D:427:ASN:H | 1.84 | 0.75 |
| 1:E:416:ILE:HG13 | 1:E:448:TYR:OH | 1.86 | 0.75 |
| 1:G:416:ILE:HG13 | 1:G:448:TYR:OH | 1.86 | 0.75 |
| 1:H:367:THR:O | 1:H:369:PRO:CD | 2.30 | 0.75 |
| 1:H:661:LEU:HD13 | 1:H:662:GLU:N | 2.01 | 0.75 |
| 1:J:345:TYR:HE1 | 1:J:349:VAL:CG2 | 1.99 | 0.75 |
| 1:K:340:VAL:O | 1:K:345:TYR:CE1 | 2.37 | 0.75 |
| 1:K:526:PRO:O | 1:K:528:THR:HG22 | 1.87 | 0.75 |
| 1:L:661:LEU:HD13 | 1:L:662:GLU:N | 2.01 | 0.75 |
| 1:D:345:TYR:HE1 | 1:D:349:VAL:CG2 | 1.99 | 0.75 |
| 1:F:427:ASN:ND2 | 1:F:427:ASN:H | 1.84 | 0.75 |
| 1:F:644:ASN:ND2 | 1:F:644:ASN:O | 2.20 | 0.75 |
| 1:G:526:PRO:O | 1:G:528:THR:HG22 | 1.87 | 0.75 |
| 1:I:401:LEU:O | 1:I:402:ALA:HB3 | 1.84 | 0.75 |
| 1:K:345:TYR:CD1 | 1:K:345:TYR:N | 2.52 | 0.75 |
| 1:L:366:SER:C | 1:L:367:THR:CG2 | 2.42 | 0.75 |
| 1:C:341:THR:HG1 | 1:C:344:ASP:HB2 | 1.48 | 0.75 |
| 1:E:347:THR:O | 1:E:349:VAL:N | 2.20 | 0.75 |
| 1:E:401:LEU:O | 1:E:402:ALA:HB3 | 1.85 | 0.75 |
| 1:H:408:ILE:HD12 | 1:H:409:ILE:N | 2.01 | 0.75 |
| 1:L:408:ILE:HD12 | 1:L:409:ILE:N | 2.01 | 0.75 |
| 1:D:403:PRO:O | 1:D:405:THR:HG22 | 1.85 | 0.75 |
| 1:F:345:TYR:HE1 | 1:F:349:VAL:CG2 | 1.99 | 0.75 |
| 1:B:569:ILE:O | 1:B:569:ILE:CG2 | 2.30 | 0.74 |
| 1:B:661:LEU:HD13 | 1:B:662:GLU:N | 2.01 | 0.74 |
| 1:I:340:VAL:O | 1:I:345:TYR:CE1 | 2.37 | 0.74 |
| 1:L:427:ASN:ND2 | 1:L:427:ASN:H | 1.84 | 0.74 |
| 1:L:644:ASN:O | 1:L:644:ASN:ND2 | 2.20 | 0.74 |
| 1:A:526:PRO:O | 1:A:528:THR:HG22 | 1.87 | 0.74 |
| 1:G:347:THR:O | 1:G:349:VAL:N | 2.20 | 0.74 |
| 1:E:526:PRO:O | 1:E:528:THR:HG22 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:408:ILE:HD12 | 1:F:409:ILE:N | 2.01 | 0.74 |
| 1:G:385:THR:HG21 | 1:G:389:ARG:N | 2.01 | 0.74 |
| 1:G:457:SER:H | 1:G:634:THR:CG2 | 1.97 | 0.74 |
| 1:G:629:ASP:HA | 1:H:664:HIS:HE1 | 1.47 | 0.74 |
| 1:D:644:ASN:O | 1:D:644:ASN:ND2 | 2.20 | 0.74 |
| 1:H:496:GLU:CD | 1:H:496:GLU:N | 2.41 | 0.74 |
| 1:I:416:ILE:HG13 | 1:I:448:TYR:OH | 1.86 | 0.74 |
| 1:J:496:GLU:CD | 1:J:496:GLU:N | 2.41 | 0.74 |
| 1:A:347:THR:O | 1:A:349:VAL:N | 2.20 | 0.74 |
| 1:C:347:THR:O | 1:C:349:VAL:N | 2.20 | 0.74 |
| 1:D:437:GLU:O | 1:D:441:ILE:HG22 | 1.88 | 0.74 |
| 1:I:457:SER:H | 1:I:634:THR:CG2 | 1.97 | 0.74 |
| 1:L:496:GLU:CD | 1:L:496:GLU:N | 2.41 | 0.74 |
| 1:F:437:GLU:O | 1:F:441:ILE:HG22 | 1.88 | 0.74 |
| 1:I:345:TYR:CD1 | 1:I:345:TYR:N | 2.51 | 0.74 |
| 1:B:503:ASN:HD21 | 1:B:633:PHE:N | 1.79 | 0.73 |
| 1:H:437:GLU:O | 1:H:441:ILE:HG22 | 1.88 | 0.73 |
| 1:J:661:LEU:HD13 | 1:J:662:GLU:N | 2.01 | 0.73 |
| 1:L:437:GLU:O | 1:L:441:ILE:HG22 | 1.88 | 0.73 |
| 1:I:347:THR:O | 1:I:349:VAL:N | 2.20 | 0.73 |
| 1:K:347:THR:O | 1:K:349:VAL:N | 2.20 | 0.73 |
| 1:J:437:GLU:O | 1:J:441:ILE:HG22 | 1.88 | 0.73 |
| 1:B:496:GLU:CD | 1:B:496:GLU:N | 2.41 | 0.73 |
| 1:E:635:ARG:HG2 | 1:E:636:ASP:N | 1.90 | 0.73 |
| 1:G:665:HIS:CE1 | 1:H:342:ALA:CB | 2.71 | 0.73 |
| 1:I:665:HIS:CE1 | 1:J:342:ALA:CB | 2.71 | 0.73 |
| 1:K:629:ASP:HB3 | 1:K:631:VAL:O | 1.89 | 0.73 |
| 1:E:665:HIS:CE1 | 1:F:342:ALA:CB | 2.71 | 0.73 |
| 1:H:644:ASN:O | 1:H:644:ASN:ND2 | 2.20 | 0.73 |
| 1:I:340:VAL:CA | 1:I:345:TYR:OH | 2.30 | 0.73 |
| 1:J:644:ASN:O | 1:J:644:ASN:ND2 | 2.20 | 0.73 |
| 1:A:518:ASN:OD1 | 1:A:533:ASP:HB2 | 1.88 | 0.73 |
| 1:B:408:ILE:O | 1:B:409:ILE:HG22 | 1.89 | 0.73 |
| 1:C:665:HIS:CE1 | 1:D:342:ALA:CB | 2.71 | 0.73 |
| 1:G:340:VAL:CA | 1:G:345:TYR:OH | 2.30 | 0.73 |
| 1:I:385:THR:HG21 | 1:I:389:ARG:N | 2.01 | 0.73 |
| 1:I:629:ASP:HB3 | 1:I:631:VAL:O | 1.89 | 0.73 |
| 1:A:629:ASP:HB3 | 1:A:631:VAL:O | 1.89 | 0.73 |
| 1:G:340:VAL:O | 1:G:345:TYR:CE1 | 2.37 | 0.73 |
| 1:E:629:ASP:HB3 | 1:E:631:VAL:O | 1.88 | 0.73 |
| 1:F:408:ILE:O | 1:F:409:ILE:HG22 | 1.89 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:427:ASN:H | 1:H:427:ASN:ND2 | 1.84 | 0.73 |
| 1:L:408:ILE:O | 1:L:409:ILE:HG22 | 1.89 | 0.73 |
| 1:A:665:HIS:CE1 | 1:B:342:ALA:CB | 2.71 | 0.73 |
| 1:C:518:ASN:OD1 | 1:C:533:ASP:HB2 | 1.89 | 0.73 |
| 1:D:496:GLU:CD | 1:D:496:GLU:N | 2.41 | 0.73 |
| 1:G:635:ARG:HG2 | 1:G:636:ASP:N | 1.90 | 0.73 |
| 1:B:437:GLU:O | 1:B:441:ILE:HG22 | 1.88 | 0.72 |
| 1:D:398:ASP:OD1 | 1:E:663:HIS:HD2 | 1.71 | 0.72 |
| 1:K:665:HIS:CE1 | 1:L:342:ALA:CB | 2.71 | 0.72 |
| 1:E:340:VAL:O | 1:E:345:TYR:CE1 | 2.37 | 0.72 |
| 1:C:345:TYR:HD1 | 1:C:345:TYR:H | 1.36 | 0.72 |
| 1:F:367:THR:O | 1:F:369:PRO:CD | 2.30 | 0.72 |
| 1:F:408:ILE:O | 1:F:408:ILE:CD1 | 2.30 | 0.72 |
| 1:H:408:ILE:O | 1:H:409:ILE:HG22 | 1.89 | 0.72 |
| 1:J:427:ASN:ND2 | 1:J:427:ASN:H | 1.84 | 0.72 |
| 1:G:629:ASP:HB3 | 1:G:631:VAL:O | 1.89 | 0.72 |
| 1:I:345:TYR:HD1 | 1:I:345:TYR:H | 1.36 | 0.72 |
| 1:K:518:ASN:OD1 | 1:K:533:ASP:HB2 | 1.88 | 0.72 |
| 1:E:518:ASN:OD1 | 1:E:533:ASP:HB2 | 1.89 | 0.72 |
| 1:E:664:HIS:O | 1:E:665:HIS:ND1 | 2.23 | 0.72 |
| 1:A:385:THR:HG21 | 1:A:389:ARG:N | 2.01 | 0.72 |
| 1:C:340:VAL:O | 1:C:345:TYR:CE1 | 2.37 | 0.72 |
| 1:C:385:THR:HG21 | 1:C:389:ARG:N | 2.01 | 0.72 |
| 1:E:385:THR:HG23 | 1:E:389:ARG:N | 2.02 | 0.72 |
| 1:G:518:ASN:OD1 | 1:G:533:ASP:HB2 | 1.89 | 0.72 |
| 1:I:664:HIS:O | 1:I:665:HIS:ND1 | 2.23 | 0.72 |
| 1:J:408:ILE:O | 1:J:409:ILE:HG22 | 1.89 | 0.72 |
| 1:C:664:HIS:O | 1:C:665:HIS:ND1 | 2.23 | 0.72 |
| 1:A:517:PHE:CD2 | 1:A:536:TYR:HE2 | 2.07 | 0.72 |
| 1:I:518:ASN:OD1 | 1:I:533:ASP:HB2 | 1.89 | 0.72 |
| 1:B:366:SER:C | 1:B:367:THR:CG2 | 2.42 | 0.72 |
| 1:K:385:THR:HG23 | 1:K:389:ARG:N | 2.02 | 0.72 |
| 1:I:385:THR:HG23 | 1:I:389:ARG:N | 2.02 | 0.71 |
| 1:A:664:HIS:O | 1:A:665:HIS:ND1 | 2.23 | 0.71 |
| 1:C:345:TYR:CD1 | 1:C:345:TYR:N | 2.51 | 0.71 |
| 1:C:629:ASP:HB3 | 1:C:631:VAL:O | 1.89 | 0.71 |
| 1:K:664:HIS:O | 1:K:665:HIS:ND1 | 2.23 | 0.71 |
| 1:A:340:VAL:O | 1:A:344:ASP:HB2 | 1.91 | 0.71 |
| 1:E:340:VAL:O | 1:E:344:ASP:HB2 | 1.91 | 0.71 |
| 1:K:345:TYR:HD1 | 1:K:345:TYR:H | 1.36 | 0.71 |
| 1:D:398:ASP:OD1 | 1:E:663:HIS:CD2 | 2.43 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:345:TYR:HD1 | 1:G:345:TYR:H | 1.36 | 0.71 |
| 1:D:408:ILE:O | 1:D:409:ILE:HG22 | 1.89 | 0.71 |
| 1:F:496:GLU:CD | 1:F:496:GLU:N | 2.41 | 0.71 |
| 1:G:664:HIS:O | 1:G:665:HIS:ND1 | 2.23 | 0.71 |
| 1:K:353:PHE:CZ | 1:K:395:TYR:HD2 | 2.09 | 0.71 |
| 1:C:340:VAL:O | 1:C:344:ASP:HB2 | 1.91 | 0.71 |
| 1:D:398:ASP:O | 1:E:663:HIS:N | 2.20 | 0.71 |
| 1:E:358:GLN:HB2 | 1:E:379:LYS:HA | 1.73 | 0.71 |
| 1:H:342:ALA:C | 1:H:346:ASP:OD2 | 2.29 | 0.71 |
| 1:B:342:ALA:O | 1:B:346:ASP:CG | 2.29 | 0.71 |
| 1:I:340:VAL:O | 1:I:344:ASP:HB2 | 1.91 | 0.71 |
| 1:K:340:VAL:O | 1:K:344:ASP:HB2 | 1.91 | 0.71 |
| 1:D:568:ASN:CG | 1:D:569:ILE:H | 1.94 | 0.71 |
| 1:G:661:LEU:CD1 | 1:G:662:GLU:CB | 2.68 | 0.71 |
| 1:K:353:PHE:CG | 1:K:395:TYR:HE2 | 2.09 | 0.71 |
| 1:L:342:ALA:C | 1:L:346:ASP:OD2 | 2.29 | 0.71 |
| 1:A:587:ASP:OD2 | 1:A:587:ASP:C | 2.30 | 0.71 |
| 1:E:517:PHE:CD2 | 1:E:536:TYR:HE2 | 2.07 | 0.71 |
| 1:F:344:ASP:C | 1:F:344:ASP:OD1 | 2.29 | 0.71 |
| 1:F:385:THR:HG23 | 1:F:388:GLN:H | 1.56 | 0.71 |
| 1:I:629:ASP:HA | 1:J:664:HIS:HE1 | 1.47 | 0.71 |
| 1:B:385:THR:HG23 | 1:B:388:GLN:H | 1.56 | 0.70 |
| 1:C:661:LEU:HD12 | 1:C:662:GLU:HB2 | 1.73 | 0.70 |
| 1:H:342:ALA:O | 1:H:346:ASP:CG | 2.30 | 0.70 |
| 1:I:353:PHE:CG | 1:I:395:TYR:HE2 | 2.09 | 0.70 |
| 1:L:344:ASP:C | 1:L:344:ASP:OD1 | 2.29 | 0.70 |
| 1:A:353:PHE:CG | 1:A:395:TYR:HE2 | 2.09 | 0.70 |
| 1:B:342:ALA:C | 1:B:346:ASP:OD2 | 2.29 | 0.70 |
| 1:B:344:ASP:C | 1:B:344:ASP:OD1 | 2.29 | 0.70 |
| 1:G:340:VAL:O | 1:G:344:ASP:HB2 | 1.91 | 0.70 |
| 1:K:385:THR:HG21 | 1:K:389:ARG:N | 2.01 | 0.70 |
| 1:K:587:ASP:C | 1:K:587:ASP:OD2 | 2.30 | 0.70 |
| 1:L:385:THR:HG23 | 1:L:388:GLN:H | 1.56 | 0.70 |
| 1:A:358:GLN:HB2 | 1:A:379:LYS:HA | 1.73 | 0.70 |
| 1:E:522:LYS:N | 1:E:522:LYS:HD3 | 2.07 | 0.70 |
| 1:H:344:ASP:C | 1:H:344:ASP:OD1 | 2.29 | 0.70 |
| 1:I:358:GLN:HB2 | 1:I:379:LYS:HA | 1.73 | 0.70 |
| 1:A:522:LYS:HD3 | 1:A:522:LYS:N | 2.07 | 0.70 |
| 1:A:587:ASP:CG | 1:A:587:ASP:O | 2.30 | 0.70 |
| 1:F:342:ALA:C | 1:F:346:ASP:OD2 | 2.29 | 0.70 |
| 1:G:353:PHE:CG | 1:G:395:TYR:HE2 | 2.09 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:401:LEU:O | 1:G:402:ALA:CB | 2.40 | 0.70 |
| 1:H:385:THR:HG23 | 1:H:388:GLN:H | 1.56 | 0.70 |
| 1:J:385:THR:HG23 | 1:J:388:GLN:H | 1.56 | 0.70 |
| 1:L:342:ALA:O | 1:L:346:ASP:CG | 2.29 | 0.70 |
| 1:L:568:ASN:CG | 1:L:569:ILE:H | 1.94 | 0.70 |
| 1:B:345:TYR:CE1 | 1:B:349:VAL:CG2 | 2.74 | 0.70 |
| 1:E:401:LEU:O | 1:E:402:ALA:CB | 2.40 | 0.70 |
| 1:I:388:GLN:O | 1:I:389:ARG:HB2 | 1.91 | 0.70 |
| 1:J:342:ALA:C | 1:J:346:ASP:OD2 | 2.29 | 0.70 |
| 1:J:342:ALA:O | 1:J:346:ASP:CG | 2.29 | 0.70 |
| 1:J:659:SER:O | 1:J:660:GLN:CD | 2.30 | 0.70 |
| 1:K:522:LYS:HD3 | 1:K:522:LYS:N | 2.07 | 0.70 |
| 1:A:661:LEU:HD12 | 1:A:662:GLU:HB2 | 1.73 | 0.70 |
| 1:B:568:ASN:CG | 1:B:569:ILE:H | 1.94 | 0.70 |
| 1:D:342:ALA:C | 1:D:346:ASP:OD2 | 2.29 | 0.70 |
| 1:D:567:GLU:O | 1:D:568:ASN:CG | 2.30 | 0.70 |
| 1:E:353:PHE:CG | 1:E:395:TYR:HE2 | 2.09 | 0.70 |
| 1:K:661:LEU:CD1 | 1:K:662:GLU:CB | 2.68 | 0.70 |
| 1:A:385:THR:HG23 | 1:A:389:ARG:N | 2.02 | 0.70 |
| 1:B:364:THR:HG23 | 1:K:401:LEU:HD12 | 1.68 | 0.70 |
| 1:D:344:ASP:OD1 | 1:D:344:ASP:C | 2.29 | 0.70 |
| 1:E:388:GLN:O | 1:E:389:ARG:HG3 | 1.92 | 0.70 |
| 1:I:401:LEU:O | 1:I:402:ALA:CB | 2.40 | 0.70 |
| 1:I:440:ILE:HD11 | 1:I:653:ILE:CD1 | 2.21 | 0.70 |
| 1:J:568:ASN:CG | 1:J:569:ILE:H | 1.94 | 0.70 |
| 1:K:385:THR:CG2 | 1:K:389:ARG:CA | 2.60 | 0.70 |
| 1:L:659:SER:O | 1:L:660:GLN:CD | 2.30 | 0.70 |
| 1:A:506:LYS:O | 1:A:509:SER:HB3 | 1.92 | 0.70 |
| 1:C:353:PHE:CZ | 1:C:395:TYR:HD2 | 2.09 | 0.70 |
| 1:C:353:PHE:CG | 1:C:395:TYR:HE2 | 2.09 | 0.70 |
| 1:C:388:GLN:O | 1:C:389:ARG:HG3 | 1.92 | 0.70 |
| 1:D:345:TYR:CE1 | 1:D:349:VAL:CG2 | 2.74 | 0.70 |
| 1:D:567:GLU:O | 1:D:568:ASN:HB3 | 1.92 | 0.70 |
| 1:E:401:LEU:HD23 | 1:E:401:LEU:O | 1.92 | 0.70 |
| 1:E:440:ILE:HD11 | 1:E:653:ILE:CD1 | 2.21 | 0.70 |
| 1:E:587:ASP:CG | 1:E:587:ASP:O | 2.30 | 0.70 |
| 1:G:388:GLN:O | 1:G:389:ARG:HB2 | 1.91 | 0.70 |
| 1:G:440:ILE:HD11 | 1:G:653:ILE:CD1 | 2.21 | 0.70 |
| 1:G:517:PHE:CD2 | 1:G:536:TYR:HE2 | 2.07 | 0.70 |
| 1:J:344:ASP:C | 1:J:344:ASP:OD1 | 2.29 | 0.70 |
| 1:K:358:GLN:HB2 | 1:K:379:LYS:HA | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:567:GLU:O | 1:B:568:ASN:HB3 | 1.92 | 0.70 |
| 1:D:385:THR:HG23 | 1:D:388:GLN:H | 1.56 | 0.70 |
| 1:E:587:ASP:C | 1:E:587:ASP:OD2 | 2.30 | 0.70 |
| 1:F:342:ALA:O | 1:F:346:ASP:CG | 2.29 | 0.70 |
| 1:G:401:LEU:HD23 | 1:G:401:LEU:O | 1.92 | 0.70 |
| 1:G:522:LYS:HD3 | 1:G:522:LYS:N | 2.07 | 0.70 |
| 1:H:567:GLU:O | 1:H:568:ASN:CG | 2.30 | 0.70 |
| 1:H:659:SER:O | 1:H:660:GLN:CD | 2.30 | 0.70 |
| 1:K:440:ILE:HD11 | 1:K:653:ILE:CD1 | 2.21 | 0.70 |
| 1:C:388:GLN:O | 1:C:389:ARG:HB2 | 1.91 | 0.70 |
| 1:E:342:ALA:HB1 | 1:E:362:THR:HB | 1.74 | 0.70 |
| 1:I:506:LYS:O | 1:I:509:SER:HB3 | 1.92 | 0.70 |
| 1:K:457:SER:H | 1:K:634:THR:HG23 | 1.56 | 0.70 |
| 1:L:567:GLU:O | 1:L:568:ASN:CG | 2.30 | 0.70 |
| 1:C:358:GLN:HB2 | 1:C:379:LYS:HA | 1.73 | 0.69 |
| 1:C:587:ASP:C | 1:C:587:ASP:OD2 | 2.30 | 0.69 |
| 1:H:345:TYR:CE1 | 1:H:349:VAL:CG2 | 2.74 | 0.69 |
| 1:K:388:GLN:O | 1:K:389:ARG:HB2 | 1.91 | 0.69 |
| 1:K:506:LYS:O | 1:K:509:SER:HB3 | 1.92 | 0.69 |
| 1:B:567:GLU:O | 1:B:568:ASN:CG | 2.30 | 0.69 |
| 1:D:342:ALA:O | 1:D:346:ASP:CG | 2.29 | 0.69 |
| 1:F:567:GLU:O | 1:F:568:ASN:CG | 2.30 | 0.69 |
| 1:G:358:GLN:HB2 | 1:G:379:LYS:HA | 1.73 | 0.69 |
| 1:I:661:LEU:CD1 | 1:I:662:GLU:CB | 2.68 | 0.69 |
| 1:A:661:LEU:CD1 | 1:A:662:GLU:CB | 2.68 | 0.69 |
| 1:C:342:ALA:HB1 | 1:C:362:THR:HB | 1.74 | 0.69 |
| 1:G:353:PHE:CZ | 1:G:395:TYR:HD2 | 2.09 | 0.69 |
| 1:J:345:TYR:CD1 | 1:J:345:TYR:C | 2.65 | 0.69 |
| 1:J:345:TYR:CE1 | 1:J:349:VAL:CG2 | 2.74 | 0.69 |
| 1:L:345:TYR:CE1 | 1:L:349:VAL:CG2 | 2.74 | 0.69 |
| 1:A:388:GLN:O | 1:A:389:ARG:HB2 | 1.91 | 0.69 |
| 1:B:345:TYR:CD1 | 1:B:345:TYR:C | 2.65 | 0.69 |
| 1:C:440:ILE:HD11 | 1:C:653:ILE:CD1 | 2.21 | 0.69 |
| 1:D:398:ASP:C | 1:E:663:HIS:HB3 | 2.13 | 0.69 |
| 1:E:403:PRO:CB | 1:H:366:SER:HB2 | 2.09 | 0.69 |
| 1:F:659:SER:O | 1:F:660:GLN:CD | 2.30 | 0.69 |
| 1:G:385:THR:HG23 | 1:G:389:ARG:N | 2.02 | 0.69 |
| 1:G:661:LEU:HD12 | 1:G:662:GLU:HB2 | 1.73 | 0.69 |
| 1:H:345:TYR:CD1 | 1:H:345:TYR:C | 2.65 | 0.69 |
| 1:I:522:LYS:HD3 | 1:I:522:LYS:N | 2.07 | 0.69 |
| 1:J:401:LEU:HG | 1:J:403:PRO:HD2 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:345:TYR:HD1 | 1:A:345:TYR:H | 1.36 | 0.69 |
| 1:D:659:SER:O | 1:D:660:GLN:CD | 2.30 | 0.69 |
| 1:E:661:LEU:HD12 | 1:E:662:GLU:HB2 | 1.73 | 0.69 |
| 1:G:342:ALA:HB1 | 1:G:362:THR:HB | 1.74 | 0.69 |
| 1:G:347:THR:O | 1:G:350:SER:N | 2.26 | 0.69 |
| 1:I:347:THR:O | 1:I:350:SER:N | 2.26 | 0.69 |
| 1:J:567:GLU:O | 1:J:568:ASN:CG | 2.30 | 0.69 |
| 1:K:587:ASP:O | 1:K:587:ASP:CG | 2.30 | 0.69 |
| 1:A:440:ILE:HD11 | 1:A:653:ILE:CD1 | 2.21 | 0.69 |
| 1:B:659:SER:O | 1:B:660:GLN:CD | 2.30 | 0.69 |
| 1:C:506:LYS:O | 1:C:509:SER:HB3 | 1.92 | 0.69 |
| 1:D:345:TYR:CD1 | 1:D:345:TYR:C | 2.65 | 0.69 |
| 1:D:566:ASN:N | 1:D:570:GLN:NE2 | 2.41 | 0.69 |
| 1:F:345:TYR:CE1 | 1:F:349:VAL:CG2 | 2.74 | 0.69 |
| 1:F:568:ASN:CG | 1:F:569:ILE:H | 1.94 | 0.69 |
| 1:G:457:SER:H | 1:G:634:THR:HG23 | 1.56 | 0.69 |
| 1:I:342:ALA:HB1 | 1:I:362:THR:HB | 1.74 | 0.69 |
| 1:A:347:THR:O | 1:A:350:SER:N | 2.26 | 0.69 |
| 1:A:401:LEU:HD23 | 1:A:401:LEU:O | 1.92 | 0.69 |
| 1:B:523:VAL:HG12 | 1:B:532:GLU:H | 1.58 | 0.69 |
| 1:C:347:THR:O | 1:C:350:SER:N | 2.26 | 0.69 |
| 1:C:661:LEU:CD1 | 1:C:662:GLU:CB | 2.68 | 0.69 |
| 1:E:388:GLN:O | 1:E:389:ARG:HB2 | 1.91 | 0.69 |
| 1:E:506:LYS:O | 1:E:509:SER:HB3 | 1.92 | 0.69 |
| 1:F:345:TYR:CD1 | 1:F:345:TYR:C | 2.65 | 0.69 |
| 1:H:568:ASN:CG | 1:H:569:ILE:H | 1.94 | 0.69 |
| 1:I:457:SER:H | 1:I:634:THR:HG23 | 1.56 | 0.69 |
| 1:I:587:ASP:CG | 1:I:587:ASP:O | 2.30 | 0.69 |
| 1:K:401:LEU:O | 1:K:402:ALA:CB | 2.40 | 0.69 |
| 1:L:401:LEU:HG | 1:L:403:PRO:HD2 | 1.75 | 0.69 |
| 1:L:567:GLU:O | 1:L:568:ASN:HB3 | 1.92 | 0.69 |
| 1:C:401:LEU:O | 1:C:402:ALA:CB | 2.40 | 0.69 |
| 1:E:345:TYR:HD1 | 1:E:345:TYR:H | 1.36 | 0.69 |
| 1:I:517:PHE:CD2 | 1:I:536:TYR:HE2 | 2.07 | 0.69 |
| 1:K:347:THR:O | 1:K:350:SER:N | 2.26 | 0.69 |
| 1:C:457:SER:H | 1:C:634:THR:HG23 | 1.56 | 0.69 |
| 1:C:522:LYS:HD3 | 1:C:522:LYS:N | 2.07 | 0.69 |
| 1:F:660:GLN:CA | 1:F:661:LEU:CB | 2.71 | 0.69 |
| 1:G:587:ASP:OD2 | 1:G:587:ASP:C | 2.30 | 0.69 |
| 1:H:401:LEU:HG | 1:H:403:PRO:HD2 | 1.75 | 0.69 |
| 1:J:567:GLU:O | 1:J:568:ASN:HB3 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:401:LEU:HD23 | 1:K:401:LEU:O | 1.92 | 0.69 |
| 1:L:345:TYR:CD1 | 1:L:345:TYR:C | 2.65 | 0.69 |
| 1:G:506:LYS:O | 1:G:509:SER:HB3 | 1.92 | 0.68 |
| 1:I:563:VAL:HG22 | 1:I:611:LEU:HD21 | 1.75 | 0.68 |
| 1:K:629:ASP:HA | 1:L:664:HIS:HE1 | 1.47 | 0.68 |
| 1:C:587:ASP:O | 1:C:587:ASP:CG | 2.30 | 0.68 |
| 1:E:563:VAL:HG22 | 1:E:611:LEU:HD21 | 1.75 | 0.68 |
| 1:G:587:ASP:CG | 1:G:587:ASP:O | 2.30 | 0.68 |
| 1:I:388:GLN:O | 1:I:389:ARG:HG3 | 1.92 | 0.68 |
| 1:I:661:LEU:HD12 | 1:I:662:GLU:HB2 | 1.73 | 0.68 |
| 1:D:523:VAL:HG12 | 1:D:532:GLU:H | 1.58 | 0.68 |
| 1:E:347:THR:O | 1:E:350:SER:N | 2.26 | 0.68 |
| 1:G:388:GLN:O | 1:G:389:ARG:HG3 | 1.92 | 0.68 |
| 1:H:523:VAL:HG12 | 1:H:532:GLU:H | 1.58 | 0.68 |
| 1:K:563:VAL:HG22 | 1:K:611:LEU:HD21 | 1.75 | 0.68 |
| 1:A:401:LEU:O | 1:A:402:ALA:CB | 2.40 | 0.68 |
| 1:C:401:LEU:HD23 | 1:C:401:LEU:O | 1.92 | 0.68 |
| 1:A:563:VAL:HG22 | 1:A:611:LEU:HD21 | 1.75 | 0.68 |
| 1:C:563:VAL:HG22 | 1:C:611:LEU:HD21 | 1.75 | 0.68 |
| 1:E:385:THR:HG21 | 1:E:389:ARG:N | 2.01 | 0.68 |
| 1:F:521:ARG:HH22 | 1:F:559:ALA:HB3 | 1.59 | 0.68 |
| 1:G:563:VAL:HG22 | 1:G:611:LEU:HD21 | 1.75 | 0.68 |
| 1:I:587:ASP:OD2 | 1:I:587:ASP:C | 2.30 | 0.68 |
| 1:K:385:THR:HG22 | 1:K:392:ILE:HG23 | 1.76 | 0.68 |
| 1:K:388:GLN:O | 1:K:389:ARG:HG3 | 1.92 | 0.68 |
| 1:D:521:ARG:HH22 | 1:D:559:ALA:HB3 | 1.59 | 0.68 |
| 1:F:401:LEU:HG | 1:F:403:PRO:HD2 | 1.75 | 0.68 |
| 1:I:385:THR:HG22 | 1:I:392:ILE:HG23 | 1.76 | 0.68 |
| 1:K:342:ALA:HB1 | 1:K:362:THR:HB | 1.74 | 0.68 |
| 1:K:395:TYR:HB2 | 1:K:408:ILE:HG12 | 1.76 | 0.68 |
| 1:A:388:GLN:O | 1:A:389:ARG:HG3 | 1.92 | 0.68 |
| 1:B:521:ARG:HH22 | 1:B:559:ALA:HB3 | 1.59 | 0.68 |
| 1:J:647:ARG:HG3 | 1:J:650:TYR:CD1 | 2.29 | 0.68 |
| 1:K:661:LEU:HD12 | 1:K:662:GLU:HB2 | 1.73 | 0.68 |
| 1:I:395:TYR:HB2 | 1:I:408:ILE:HG12 | 1.76 | 0.68 |
| 1:I:401:LEU:HD23 | 1:I:401:LEU:O | 1.92 | 0.68 |
| 1:I:401:LEU:CG | 1:I:402:ALA:N | 2.57 | 0.68 |
| 1:J:523:VAL:HG12 | 1:J:532:GLU:H | 1.58 | 0.68 |
| 1:A:342:ALA:HB1 | 1:A:362:THR:HB | 1.74 | 0.68 |
| 1:A:385:THR:HG22 | 1:A:392:ILE:HG23 | 1.76 | 0.68 |
| 1:D:647:ARG:HG3 | 1:D:650:TYR:CD1 | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:395:TYR:HB2 | 1:E:408:ILE:HG12 | 1.76 | 0.68 |
| 1:H:521:ARG:HH22 | 1:H:559:ALA:HB3 | 1.59 | 0.68 |
| 1:F:523:VAL:HG12 | 1:F:532:GLU:H | 1.58 | 0.67 |
| 1:K:401:LEU:CG | 1:K:402:ALA:N | 2.57 | 0.67 |
| 1:B:401:LEU:HG | 1:B:403:PRO:HD2 | 1.75 | 0.67 |
| 1:D:401:LEU:HG | 1:D:403:PRO:HD2 | 1.75 | 0.67 |
| 1:E:629:ASP:CA | 1:F:664:HIS:NE2 | 2.57 | 0.67 |
| 1:G:440:ILE:HG13 | 1:G:441:ILE:N | 2.09 | 0.67 |
| 1:I:440:ILE:HG13 | 1:I:441:ILE:N | 2.09 | 0.67 |
| 1:F:366:SER:C | 1:F:367:THR:CG2 | 2.42 | 0.67 |
| 1:F:567:GLU:O | 1:F:568:ASN:HB3 | 1.92 | 0.67 |
| 1:L:408:ILE:C | 1:L:409:ILE:HG23 | 2.15 | 0.67 |
| 1:L:566:ASN:N | 1:L:570:GLN:NE2 | 2.41 | 0.67 |
| 1:C:395:TYR:HB2 | 1:C:408:ILE:HG12 | 1.76 | 0.67 |
| 1:G:401:LEU:CG | 1:G:402:ALA:N | 2.57 | 0.67 |
| 1:H:647:ARG:HG3 | 1:H:650:TYR:CD1 | 2.29 | 0.67 |
| 1:I:353:PHE:CZ | 1:I:395:TYR:HD2 | 2.09 | 0.67 |
| 1:L:521:ARG:HH22 | 1:L:559:ALA:HB3 | 1.59 | 0.67 |
| 1:A:340:VAL:O | 1:A:341:THR:HG23 | 1.95 | 0.67 |
| 1:C:440:ILE:HG13 | 1:C:441:ILE:N | 2.09 | 0.67 |
| 1:G:385:THR:CG2 | 1:G:389:ARG:CA | 2.60 | 0.67 |
| 1:H:567:GLU:O | 1:H:568:ASN:HB3 | 1.92 | 0.67 |
| 1:J:521:ARG:HH22 | 1:J:559:ALA:HB3 | 1.59 | 0.67 |
| 1:L:647:ARG:HG3 | 1:L:650:TYR:CD1 | 2.29 | 0.67 |
| 1:F:647:ARG:HG3 | 1:F:650:TYR:CD1 | 2.29 | 0.67 |
| 1:G:340:VAL:O | 1:G:341:THR:HG23 | 1.95 | 0.67 |
| 1:K:340:VAL:O | 1:K:341:THR:HG23 | 1.95 | 0.67 |
| 1:K:517:PHE:CD2 | 1:K:536:TYR:HE2 | 2.07 | 0.67 |
| 1:A:395:TYR:HB2 | 1:A:408:ILE:HG12 | 1.76 | 0.67 |
| 1:C:401:LEU:CG | 1:C:402:ALA:N | 2.57 | 0.67 |
| 1:D:540:ILE:HG22 | 1:D:555:ILE:HG13 | 1.77 | 0.67 |
| 1:D:660:GLN:CA | 1:D:661:LEU:CB | 2.71 | 0.67 |
| 1:E:661:LEU:CD1 | 1:E:662:GLU:CB | 2.68 | 0.67 |
| 1:G:385:THR:HG22 | 1:G:392:ILE:HG23 | 1.76 | 0.67 |
| 1:J:408:ILE:C | 1:J:409:ILE:HG23 | 2.15 | 0.67 |
| 1:L:523:VAL:HG12 | 1:L:532:GLU:H | 1.58 | 0.67 |
| 1:A:401:LEU:CG | 1:A:402:ALA:N | 2.57 | 0.67 |
| 1:K:440:ILE:HG13 | 1:K:441:ILE:N | 2.09 | 0.67 |
| 1:A:556:GLY:HA3 | 1:A:589:TYR:CD1 | 2.30 | 0.67 |
| 1:B:566:ASN:N | 1:B:570:GLN:NE2 | 2.41 | 0.67 |
| 1:C:424:TYR:CE2 | 1:C:429:LEU:HD12 | 2.30 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:440:ILE:HG13 | 1:E:441:ILE:N | 2.09 | 0.67 |
| 1:I:424:TYR:CE2 | 1:I:429:LEU:HD12 | 2.30 | 0.67 |
| 1:L:647:ARG:HD2 | 1:L:650:TYR:CZ | 2.30 | 0.67 |
| 1:C:556:GLY:HA3 | 1:C:589:TYR:CD1 | 2.30 | 0.67 |
| 1:D:396:LEU:CD2 | 1:D:406:PRO:HG2 | 2.25 | 0.67 |
| 1:E:340:VAL:O | 1:E:341:THR:HG23 | 1.95 | 0.67 |
| 1:E:385:THR:HG22 | 1:E:392:ILE:HG23 | 1.76 | 0.67 |
| 1:E:556:GLY:HA3 | 1:E:589:TYR:CD1 | 2.30 | 0.67 |
| 1:F:540:ILE:HG22 | 1:F:555:ILE:HG13 | 1.77 | 0.67 |
| 1:J:647:ARG:HD2 | 1:J:650:TYR:CZ | 2.30 | 0.67 |
| 1:D:647:ARG:HD2 | 1:D:650:TYR:CZ | 2.30 | 0.66 |
| 1:E:424:TYR:CE2 | 1:E:429:LEU:HD12 | 2.30 | 0.66 |
| 1:G:629:ASP:CA | 1:H:664:HIS:NE2 | 2.57 | 0.66 |
| 1:H:540:ILE:HG22 | 1:H:555:ILE:HG13 | 1.77 | 0.66 |
| 1:J:540:ILE:HG22 | 1:J:555:ILE:HG13 | 1.77 | 0.66 |
| 1:K:424:TYR:CE2 | 1:K:429:LEU:HD12 | 2.30 | 0.66 |
| 1:K:556:GLY:HA3 | 1:K:589:TYR:CD1 | 2.30 | 0.66 |
| 1:E:401:LEU:CG | 1:E:402:ALA:N | 2.57 | 0.66 |
| 1:F:566:ASN:N | 1:F:570:GLN:NE2 | 2.41 | 0.66 |
| 1:H:647:ARG:HD2 | 1:H:650:TYR:CZ | 2.30 | 0.66 |
| 1:A:424:TYR:CE2 | 1:A:429:LEU:HD12 | 2.30 | 0.66 |
| 1:B:408:ILE:C | 1:B:409:ILE:HG23 | 2.15 | 0.66 |
| 1:D:408:ILE:C | 1:D:409:ILE:HG23 | 2.15 | 0.66 |
| 1:F:365:ASP:OD1 | 1:F:367:THR:HG21 | 1.95 | 0.66 |
| 1:G:424:TYR:CE2 | 1:G:429:LEU:HD12 | 2.30 | 0.66 |
| 1:G:454:ILE:CG2 | 1:G:455:PHE:N | 2.58 | 0.66 |
| 1:I:340:VAL:O | 1:I:341:THR:HG23 | 1.95 | 0.66 |
| 1:A:661:LEU:HD11 | 1:A:662:GLU:HB2 | 1.78 | 0.66 |
| 1:B:396:LEU:CD2 | 1:B:406:PRO:HG2 | 2.25 | 0.66 |
| 1:C:385:THR:HG22 | 1:C:392:ILE:HG23 | 1.76 | 0.66 |
| 1:C:629:ASP:CA | 1:D:664:HIS:NE2 | 2.57 | 0.66 |
| 1:D:365:ASP:OD1 | 1:D:367:THR:HG21 | 1.95 | 0.66 |
| 1:G:395:TYR:HB2 | 1:G:408:ILE:HG12 | 1.76 | 0.66 |
| 1:B:647:ARG:HD2 | 1:B:650:TYR:CZ | 2.30 | 0.66 |
| 1:C:342:ALA:CB | 1:C:362:THR:HG22 | 2.26 | 0.66 |
| 1:F:396:LEU:CD2 | 1:F:406:PRO:HG2 | 2.25 | 0.66 |
| 1:K:661:LEU:HD11 | 1:K:662:GLU:HB2 | 1.78 | 0.66 |
| 1:A:342:ALA:CB | 1:A:362:THR:HG22 | 2.26 | 0.66 |
| 1:B:365:ASP:OD1 | 1:B:367:THR:HG21 | 1.96 | 0.66 |
| 1:B:366:SER:O | 1:B:367:THR:HB | 1.96 | 0.66 |
| 1:C:454:ILE:CG2 | 1:C:455:PHE:N | 2.58 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:454:ILE:CG2 | 1:E:455:PHE:N | 2.59 | 0.66 |
| 1:I:595:ILE:HD13 | 1:I:597:TYR:CE2 | 2.31 | 0.66 |
| 1:I:661:LEU:HD11 | 1:I:662:GLU:HB2 | 1.78 | 0.66 |
| 1:K:595:ILE:HD13 | 1:K:597:TYR:CE2 | 2.31 | 0.66 |
| 1:B:540:ILE:HG22 | 1:B:555:ILE:HG13 | 1.77 | 0.66 |
| 1:C:661:LEU:HD11 | 1:C:662:GLU:HB2 | 1.78 | 0.66 |
| 1:E:353:PHE:CZ | 1:E:395:TYR:HD2 | 2.09 | 0.66 |
| 1:F:366:SER:O | 1:F:367:THR:HB | 1.96 | 0.66 |
| 1:F:408:ILE:C | 1:F:409:ILE:HG23 | 2.15 | 0.66 |
| 1:G:401:LEU:CD2 | 1:G:402:ALA:CA | 2.74 | 0.66 |
| 1:H:348:PHE:O | 1:H:351:GLU:N | 2.21 | 0.66 |
| 1:I:454:ILE:CG2 | 1:I:455:PHE:N | 2.58 | 0.66 |
| 1:I:629:ASP:CA | 1:J:664:HIS:NE2 | 2.57 | 0.66 |
| 1:L:540:ILE:HG22 | 1:L:555:ILE:HG13 | 1.77 | 0.66 |
| 1:B:647:ARG:HG3 | 1:B:650:TYR:CD1 | 2.29 | 0.66 |
| 1:C:595:ILE:HD13 | 1:C:597:TYR:CE2 | 2.31 | 0.66 |
| 1:E:341:THR:OG1 | 1:E:344:ASP:HB2 | 1.96 | 0.66 |
| 1:G:556:GLY:HA3 | 1:G:589:TYR:CD1 | 2.30 | 0.66 |
| 1:H:408:ILE:C | 1:H:409:ILE:HG23 | 2.15 | 0.66 |
| 1:H:569:ILE:O | 1:H:569:ILE:CG2 | 2.30 | 0.66 |
| 1:I:342:ALA:CB | 1:I:362:THR:HG22 | 2.26 | 0.66 |
| 1:J:566:ASN:N | 1:J:570:GLN:NE2 | 2.41 | 0.66 |
| 1:A:629:ASP:CA | 1:B:664:HIS:NE2 | 2.57 | 0.65 |
| 1:E:457:SER:H | 1:E:634:THR:HG23 | 1.56 | 0.65 |
| 1:H:557:PRO:HG2 | 1:H:580:LEU:CD1 | 2.26 | 0.65 |
| 1:I:556:GLY:HA3 | 1:I:589:TYR:CD1 | 2.30 | 0.65 |
| 1:A:387:VAL:HG21 | 1:A:390:GLU:CD | 2.17 | 0.65 |
| 1:A:403:PRO:HG3 | 1:C:366:SER:CB | 2.13 | 0.65 |
| 1:F:647:ARG:HD2 | 1:F:650:TYR:CZ | 2.30 | 0.65 |
| 1:K:387:VAL:HG21 | 1:K:390:GLU:CD | 2.17 | 0.65 |
| 1:C:392:ILE:O | 1:C:396:LEU:HD23 | 1.97 | 0.65 |
| 1:E:548:LYS:O | 1:E:548:LYS:HG2 | 1.96 | 0.65 |
| 1:G:516:SER:HB2 | 1:G:617:GLU:CD | 2.17 | 0.65 |
| 1:G:595:ILE:HD13 | 1:G:597:TYR:CE2 | 2.31 | 0.65 |
| 1:J:557:PRO:HG2 | 1:J:580:LEU:CD1 | 2.26 | 0.65 |
| 1:K:454:ILE:CG2 | 1:K:455:PHE:N | 2.58 | 0.65 |
| 1:L:365:ASP:OD1 | 1:L:367:THR:HG21 | 1.96 | 0.65 |
| 1:L:396:LEU:CD2 | 1:L:406:PRO:HG2 | 2.25 | 0.65 |
| 1:A:385:THR:HG1 | 1:A:387:VAL:CG2 | 1.97 | 0.65 |
| 1:A:440:ILE:HG13 | 1:A:441:ILE:N | 2.09 | 0.65 |
| 1:A:595:ILE:HD13 | 1:A:597:TYR:CE2 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:340:VAL:O | 1:C:341:THR:HG23 | 1.95 | 0.65 |
| 1:K:342:ALA:CB | 1:K:362:THR:HG22 | 2.26 | 0.65 |
| 1:E:392:ILE:O | 1:E:396:LEU:HD23 | 1.97 | 0.65 |
| 1:E:634:THR:OG1 | 1:E:635:ARG:N | 2.30 | 0.65 |
| 1:H:365:ASP:OD1 | 1:H:367:THR:HG21 | 1.96 | 0.65 |
| 1:H:366:SER:O | 1:H:367:THR:HB | 1.96 | 0.65 |
| 1:J:348:PHE:O | 1:J:351:GLU:N | 2.21 | 0.65 |
| 1:J:396:LEU:CD2 | 1:J:406:PRO:HG2 | 2.25 | 0.65 |
| 1:K:516:SER:HB2 | 1:K:617:GLU:CD | 2.17 | 0.65 |
| 1:K:629:ASP:CA | 1:L:664:HIS:NE2 | 2.57 | 0.65 |
| 1:C:341:THR:OG1 | 1:C:344:ASP:HB2 | 1.96 | 0.65 |
| 1:E:595:ILE:HD13 | 1:E:597:TYR:CE2 | 2.31 | 0.65 |
| 1:F:348:PHE:O | 1:F:351:GLU:N | 2.21 | 0.65 |
| 1:H:343:THR:O | 1:H:347:THR:CG2 | 2.44 | 0.65 |
| 1:H:396:LEU:CD2 | 1:H:406:PRO:HG2 | 2.25 | 0.65 |
| 1:L:365:ASP:C | 1:L:367:THR:HG22 | 2.17 | 0.65 |
| 1:A:454:ILE:CG2 | 1:A:455:PHE:N | 2.58 | 0.65 |
| 1:F:557:PRO:HG2 | 1:F:580:LEU:CD1 | 2.26 | 0.65 |
| 1:G:341:THR:OG1 | 1:G:344:ASP:HB2 | 1.96 | 0.65 |
| 1:G:519:SER:CB | 1:G:562:ASP:OD1 | 2.44 | 0.65 |
| 1:I:343:THR:CG2 | 1:I:344:ASP:N | 2.60 | 0.65 |
| 1:I:516:SER:HB2 | 1:I:617:GLU:CD | 2.17 | 0.65 |
| 1:J:646:LEU:O | 1:J:646:LEU:CD2 | 2.30 | 0.65 |
| 1:K:343:THR:CG2 | 1:K:344:ASP:N | 2.60 | 0.65 |
| 1:L:659:SER:O | 1:L:660:GLN:NE2 | 2.30 | 0.65 |
| 1:A:341:THR:OG1 | 1:A:344:ASP:HB2 | 1.96 | 0.65 |
| 1:D:398:ASP:O | 1:E:663:HIS:CB | 2.41 | 0.65 |
| 1:E:516:SER:HB2 | 1:E:617:GLU:CD | 2.17 | 0.65 |
| 1:G:392:ILE:O | 1:G:396:LEU:HD23 | 1.97 | 0.65 |
| 1:I:341:THR:OG1 | 1:I:344:ASP:HB2 | 1.96 | 0.65 |
| 1:J:365:ASP:C | 1:J:367:THR:HG22 | 2.17 | 0.65 |
| 1:J:440:ILE:HG22 | 1:J:471:ALA:HB3 | 1.79 | 0.65 |
| 1:L:366:SER:O | 1:L:367:THR:HB | 1.96 | 0.65 |
| 1:B:659:SER:O | 1:B:660:GLN:NE2 | 2.30 | 0.65 |
| 1:C:385:THR:HG23 | 1:C:389:ARG:N | 2.02 | 0.65 |
| 1:D:366:SER:O | 1:D:367:THR:HB | 1.96 | 0.65 |
| 1:H:566:ASN:O | 1:H:570:GLN:NE2 | 2.30 | 0.65 |
| 1:J:366:SER:O | 1:J:367:THR:HB | 1.96 | 0.65 |
| 1:K:548:LYS:HG2 | 1:K:548:LYS:O | 1.96 | 0.65 |
| 1:L:440:ILE:HG22 | 1:L:471:ALA:HB3 | 1.79 | 0.65 |
| 1:B:440:ILE:HG22 | 1:B:471:ALA:HB3 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:548:LYS:HG2 | 1:C:548:LYS:O | 1.96 | 0.65 |
| 1:C:634:THR:OG1 | 1:C:635:ARG:N | 2.30 | 0.65 |
| 1:D:398:ASP:HA | 1:E:663:HIS:HB2 | 1.79 | 0.65 |
| 1:D:659:SER:O | 1:D:660:GLN:NE2 | 2.30 | 0.65 |
| 1:F:566:ASN:O | 1:F:570:GLN:NE2 | 2.30 | 0.65 |
| 1:J:659:SER:O | 1:J:660:GLN:NE2 | 2.30 | 0.65 |
| 1:A:343:THR:CG2 | 1:A:344:ASP:N | 2.60 | 0.64 |
| 1:D:365:ASP:C | 1:D:367:THR:HG22 | 2.17 | 0.64 |
| 1:E:545:ARG:HB3 | 1:E:597:TYR:CD2 | 2.32 | 0.64 |
| 1:J:365:ASP:OD1 | 1:J:367:THR:HG21 | 1.96 | 0.64 |
| 1:K:519:SER:CB | 1:K:562:ASP:OD1 | 2.44 | 0.64 |
| 1:L:557:PRO:HG2 | 1:L:580:LEU:CD1 | 2.26 | 0.64 |
| 1:A:516:SER:HB2 | 1:A:617:GLU:CD | 2.17 | 0.64 |
| 1:D:566:ASN:O | 1:D:570:GLN:NE2 | 2.30 | 0.64 |
| 1:E:342:ALA:CB | 1:E:362:THR:HG22 | 2.26 | 0.64 |
| 1:G:545:ARG:HB3 | 1:G:597:TYR:CD2 | 2.32 | 0.64 |
| 1:I:548:LYS:HG2 | 1:I:548:LYS:O | 1.96 | 0.64 |
| 1:A:392:ILE:O | 1:A:396:LEU:HD23 | 1.97 | 0.64 |
| 1:F:647:ARG:HH11 | 1:F:649:GLN:CD | 1.99 | 0.64 |
| 1:G:342:ALA:CB | 1:G:362:THR:HG22 | 2.26 | 0.64 |
| 1:H:422:VAL:CG1 | 1:H:475:VAL:HG13 | 2.27 | 0.64 |
| 1:J:347:THR:OG1 | 1:J:348:PHE:N | 2.30 | 0.64 |
| 1:J:566:ASN:O | 1:J:570:GLN:NE2 | 2.30 | 0.64 |
| 1:J:660:GLN:CA | 1:J:661:LEU:CB | 2.71 | 0.64 |
| 1:K:341:THR:OG1 | 1:K:344:ASP:HB2 | 1.96 | 0.64 |
| 1:A:519:SER:CB | 1:A:562:ASP:OD1 | 2.44 | 0.64 |
| 1:C:343:THR:CG2 | 1:C:344:ASP:N | 2.60 | 0.64 |
| 1:C:387:VAL:HG21 | 1:C:390:GLU:CD | 2.16 | 0.64 |
| 1:C:516:SER:HB2 | 1:C:617:GLU:CD | 2.17 | 0.64 |
| 1:F:659:SER:O | 1:F:660:GLN:NE2 | 2.30 | 0.64 |
| 1:G:343:THR:CG2 | 1:G:344:ASP:N | 2.60 | 0.64 |
| 1:B:347:THR:OG1 | 1:B:348:PHE:N | 2.30 | 0.64 |
| 1:B:365:ASP:C | 1:B:367:THR:HG22 | 2.17 | 0.64 |
| 1:C:517:PHE:CD2 | 1:C:536:TYR:HE2 | 2.07 | 0.64 |
| 1:E:343:THR:HG22 | 1:E:344:ASP:N | 2.13 | 0.64 |
| 1:F:422:VAL:CG1 | 1:F:475:VAL:HG13 | 2.27 | 0.64 |
| 1:H:365:ASP:C | 1:H:367:THR:HG22 | 2.17 | 0.64 |
| 1:H:440:ILE:HG22 | 1:H:471:ALA:HB3 | 1.79 | 0.64 |
| 1:H:566:ASN:N | 1:H:570:GLN:NE2 | 2.41 | 0.64 |
| 1:A:597:TYR:HB2 | 1:A:598:PRO:HD3 | 1.80 | 0.64 |
| 1:F:440:ILE:HG22 | 1:F:471:ALA:HB3 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:392:ILE:O | 1:I:396:LEU:HD23 | 1.97 | 0.64 |
| 1:I:545:ARG:HB3 | 1:I:597:TYR:CD2 | 2.32 | 0.64 |
| 1:L:345:TYR:HE1 | 1:L:349:VAL:HG21 | 1.62 | 0.64 |
| 1:C:518:ASN:HA | 1:C:535:LEU:HD22 | 1.80 | 0.64 |
| 1:D:557:PRO:HG2 | 1:D:580:LEU:CD1 | 2.26 | 0.64 |
| 1:G:387:VAL:HG21 | 1:G:390:GLU:CD | 2.17 | 0.64 |
| 1:G:597:TYR:HB2 | 1:G:598:PRO:HD3 | 1.80 | 0.64 |
| 1:H:344:ASP:OD1 | 1:H:345:TYR:N | 2.31 | 0.64 |
| 1:K:634:THR:OG1 | 1:K:635:ARG:N | 2.30 | 0.64 |
| 1:L:422:VAL:CG1 | 1:L:475:VAL:HG13 | 2.27 | 0.64 |
| 1:L:566:ASN:O | 1:L:570:GLN:NE2 | 2.30 | 0.64 |
| 1:B:345:TYR:HE1 | 1:B:349:VAL:HG21 | 1.62 | 0.64 |
| 1:B:557:PRO:HG2 | 1:B:580:LEU:CD1 | 2.26 | 0.64 |
| 1:D:347:THR:OG1 | 1:D:348:PHE:N | 2.30 | 0.64 |
| 1:E:518:ASN:HA | 1:E:535:LEU:HD22 | 1.80 | 0.64 |
| 1:G:661:LEU:HD11 | 1:G:662:GLU:HB2 | 1.78 | 0.64 |
| 1:H:659:SER:O | 1:H:660:GLN:NE2 | 2.30 | 0.64 |
| 1:I:387:VAL:HG21 | 1:I:390:GLU:CD | 2.17 | 0.64 |
| 1:J:422:VAL:CG1 | 1:J:475:VAL:HG13 | 2.27 | 0.64 |
| 1:K:392:ILE:O | 1:K:396:LEU:HD23 | 1.97 | 0.64 |
| 1:B:422:VAL:CG1 | 1:B:475:VAL:HG13 | 2.27 | 0.64 |
| 1:D:343:THR:O | 1:D:347:THR:CG2 | 2.44 | 0.64 |
| 1:G:401:LEU:CD2 | 1:G:402:ALA:CB | 2.69 | 0.64 |
| 1:L:646:LEU:O | 1:L:646:LEU:CD2 | 2.30 | 0.64 |
| 1:A:343:THR:HG22 | 1:A:344:ASP:N | 2.13 | 0.64 |
| 1:A:548:LYS:HG2 | 1:A:548:LYS:O | 1.96 | 0.64 |
| 1:B:566:ASN:O | 1:B:570:GLN:NE2 | 2.30 | 0.64 |
| 1:C:401:LEU:CD2 | 1:C:402:ALA:CA | 2.74 | 0.64 |
| 1:G:343:THR:HG22 | 1:G:344:ASP:N | 2.13 | 0.64 |
| 1:G:385:THR:HG21 | 1:G:392:ILE:H | 1.63 | 0.64 |
| 1:J:404:ILE:HD13 | 1:J:404:ILE:H | 1.63 | 0.64 |
| 1:L:343:THR:O | 1:L:347:THR:CG2 | 2.44 | 0.64 |
| 1:D:465:LEU:HD21 | 1:D:480:ALA:HB2 | 1.81 | 0.63 |
| 1:I:385:THR:HG21 | 1:I:392:ILE:H | 1.63 | 0.63 |
| 1:I:519:SER:CB | 1:I:562:ASP:OD1 | 2.44 | 0.63 |
| 1:I:634:THR:OG1 | 1:I:635:ARG:N | 2.30 | 0.63 |
| 1:K:545:ARG:HB3 | 1:K:597:TYR:CD2 | 2.32 | 0.63 |
| 1:L:465:LEU:HD21 | 1:L:480:ALA:HB2 | 1.81 | 0.63 |
| 1:A:545:ARG:HB3 | 1:A:597:TYR:CD2 | 2.32 | 0.63 |
| 1:C:385:THR:HG21 | 1:C:392:ILE:H | 1.63 | 0.63 |
| 1:D:440:ILE:HG22 | 1:D:471:ALA:HB3 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:340:VAL:C | 1:G:341:THR:CG2 | 2.62 | 0.63 |
| 1:G:518:ASN:HA | 1:G:535:LEU:HD22 | 1.80 | 0.63 |
| 1:J:344:ASP:OD1 | 1:J:345:TYR:N | 2.31 | 0.63 |
| 1:J:345:TYR:HE1 | 1:J:349:VAL:HG21 | 1.62 | 0.63 |
| 1:J:647:ARG:CD | 1:J:650:TYR:CE1 | 2.81 | 0.63 |
| 1:K:597:TYR:HB2 | 1:K:598:PRO:HD3 | 1.80 | 0.63 |
| 1:L:344:ASP:OD1 | 1:L:345:TYR:N | 2.31 | 0.63 |
| 1:C:545:ARG:HB3 | 1:C:597:TYR:CD2 | 2.32 | 0.63 |
| 1:D:404:ILE:HD13 | 1:D:404:ILE:H | 1.63 | 0.63 |
| 1:D:422:VAL:CG1 | 1:D:475:VAL:HG13 | 2.27 | 0.63 |
| 1:E:403:PRO:HA | 1:H:366:SER:CB | 2.22 | 0.63 |
| 1:F:344:ASP:OD1 | 1:F:345:TYR:N | 2.31 | 0.63 |
| 1:H:499:ILE:HD12 | 1:H:500:LYS:N | 2.14 | 0.63 |
| 1:B:366:SER:HB2 | 1:K:403:PRO:CB | 2.12 | 0.63 |
| 1:B:396:LEU:O | 1:B:399:TYR:O | 2.17 | 0.63 |
| 1:B:465:LEU:HD21 | 1:B:480:ALA:HB2 | 1.81 | 0.63 |
| 1:B:657:PRO:C | 1:B:658:ILE:CD1 | 2.67 | 0.63 |
| 1:D:344:ASP:OD1 | 1:D:345:TYR:N | 2.31 | 0.63 |
| 1:E:385:THR:HG21 | 1:E:392:ILE:H | 1.63 | 0.63 |
| 1:F:365:ASP:C | 1:F:367:THR:HG22 | 2.17 | 0.63 |
| 1:H:647:ARG:CD | 1:H:650:TYR:CE1 | 2.81 | 0.63 |
| 1:I:343:THR:HG22 | 1:I:344:ASP:N | 2.13 | 0.63 |
| 1:I:385:THR:CG2 | 1:I:389:ARG:CA | 2.60 | 0.63 |
| 1:A:385:THR:CG2 | 1:A:392:ILE:H | 2.12 | 0.63 |
| 1:C:517:PHE:HD2 | 1:C:536:TYR:CE2 | 2.09 | 0.63 |
| 1:C:597:TYR:HB2 | 1:C:598:PRO:HD3 | 1.80 | 0.63 |
| 1:E:340:VAL:HG12 | 1:E:345:TYR:OH | 1.99 | 0.63 |
| 1:E:387:VAL:HG21 | 1:E:390:GLU:CD | 2.17 | 0.63 |
| 1:J:499:ILE:HD12 | 1:J:500:LYS:N | 2.14 | 0.63 |
| 1:A:524:VAL:HG13 | 1:A:529:GLY:O | 1.99 | 0.63 |
| 1:C:519:SER:CB | 1:C:562:ASP:OD1 | 2.44 | 0.63 |
| 1:E:436:LEU:HD23 | 1:E:436:LEU:C | 2.19 | 0.63 |
| 1:E:597:TYR:HB2 | 1:E:598:PRO:HD3 | 1.80 | 0.63 |
| 1:G:340:VAL:HG12 | 1:G:345:TYR:OH | 1.99 | 0.63 |
| 1:I:385:THR:CG2 | 1:I:392:ILE:H | 2.12 | 0.63 |
| 1:E:385:THR:CG2 | 1:E:392:ILE:H | 2.12 | 0.63 |
| 1:G:548:LYS:O | 1:G:548:LYS:HG2 | 1.96 | 0.63 |
| 1:I:378:PRO:O | 1:I:379:LYS:HB3 | 1.99 | 0.63 |
| 1:I:597:TYR:HB2 | 1:I:598:PRO:HD3 | 1.80 | 0.63 |
| 1:L:396:LEU:O | 1:L:399:TYR:O | 2.17 | 0.63 |
| 1:L:404:ILE:HD13 | 1:L:404:ILE:H | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:345:TYR:HE1 | 1:D:349:VAL:HG21 | 1.62 | 0.63 |
| 1:E:343:THR:CG2 | 1:E:344:ASP:N | 2.60 | 0.63 |
| 1:E:519:SER:CB | 1:E:562:ASP:OD1 | 2.44 | 0.63 |
| 1:G:378:PRO:O | 1:G:379:LYS:HB3 | 1.99 | 0.63 |
| 1:I:525:ASN:OD1 | 1:I:526:PRO:HD3 | 1.99 | 0.63 |
| 1:J:396:LEU:O | 1:J:399:TYR:O | 2.17 | 0.63 |
| 1:L:499:ILE:HD12 | 1:L:500:LYS:N | 2.14 | 0.63 |
| 1:E:661:LEU:HD11 | 1:E:662:GLU:HB2 | 1.78 | 0.63 |
| 1:F:465:LEU:HD21 | 1:F:480:ALA:HB2 | 1.81 | 0.63 |
| 1:F:647:ARG:CD | 1:F:650:TYR:CE1 | 2.81 | 0.63 |
| 1:I:436:LEU:HD23 | 1:I:436:LEU:C | 2.19 | 0.63 |
| 1:L:647:ARG:CD | 1:L:650:TYR:CE1 | 2.81 | 0.63 |
| 1:A:340:VAL:HG12 | 1:A:345:TYR:OH | 1.99 | 0.62 |
| 1:B:344:ASP:OD1 | 1:B:345:TYR:N | 2.31 | 0.62 |
| 1:C:340:VAL:HG12 | 1:C:345:TYR:OH | 1.99 | 0.62 |
| 1:C:378:PRO:O | 1:C:379:LYS:HB3 | 1.99 | 0.62 |
| 1:C:524:VAL:HG13 | 1:C:529:GLY:O | 1.99 | 0.62 |
| 1:D:647:ARG:HH11 | 1:D:649:GLN:CD | 2.00 | 0.62 |
| 1:B:499:ILE:HD12 | 1:B:500:LYS:N | 2.14 | 0.62 |
| 1:C:385:THR:CG2 | 1:C:392:ILE:H | 2.12 | 0.62 |
| 1:H:404:ILE:H | 1:H:404:ILE:HD13 | 1.63 | 0.62 |
| 1:H:465:LEU:HD21 | 1:H:480:ALA:HB2 | 1.81 | 0.62 |
| 1:I:533:ASP:OD2 | 1:I:533:ASP:N | 2.32 | 0.62 |
| 1:K:340:VAL:HG12 | 1:K:345:TYR:OH | 1.99 | 0.62 |
| 1:K:385:THR:HG21 | 1:K:392:ILE:H | 1.63 | 0.62 |
| 1:A:634:THR:OG1 | 1:A:635:ARG:N | 2.30 | 0.62 |
| 1:D:499:ILE:HD12 | 1:D:500:LYS:N | 2.14 | 0.62 |
| 1:E:408:ILE:H | 1:E:408:ILE:HD12 | 1.64 | 0.62 |
| 1:F:499:ILE:HD12 | 1:F:500:LYS:N | 2.14 | 0.62 |
| 1:G:385:THR:CG2 | 1:G:392:ILE:H | 2.12 | 0.62 |
| 1:H:660:GLN:CA | 1:H:661:LEU:CB | 2.71 | 0.62 |
| 1:K:517:PHE:HD2 | 1:K:536:TYR:CE2 | 2.09 | 0.62 |
| 1:K:525:ASN:OD1 | 1:K:526:PRO:HD3 | 1.98 | 0.62 |
| 1:A:517:PHE:HD2 | 1:A:536:TYR:CE2 | 2.09 | 0.62 |
| 1:A:518:ASN:HA | 1:A:535:LEU:HD22 | 1.80 | 0.62 |
| 1:A:533:ASP:OD2 | 1:A:533:ASP:N | 2.32 | 0.62 |
| 1:C:343:THR:HG22 | 1:C:344:ASP:N | 2.13 | 0.62 |
| 1:C:415:PHE:HB2 | 1:C:485:VAL:HB | 1.81 | 0.62 |
| 1:D:376:ALA:O | 1:D:411:PRO:HD3 | 2.00 | 0.62 |
| 1:E:358:GLN:HB2 | 1:E:379:LYS:CA | 2.30 | 0.62 |
| 1:G:356:ILE:O | 1:G:356:ILE:HG12 | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:408:ILE:HD12 | 1:G:408:ILE:H | 1.64 | 0.62 |
| 1:G:533:ASP:OD2 | 1:G:533:ASP:N | 2.32 | 0.62 |
| 1:J:465:LEU:HD21 | 1:J:480:ALA:HB2 | 1.81 | 0.62 |
| 1:A:378:PRO:O | 1:A:379:LYS:HB3 | 1.99 | 0.62 |
| 1:B:376:ALA:O | 1:B:411:PRO:HD3 | 1.99 | 0.62 |
| 1:D:647:ARG:CD | 1:D:650:TYR:CE1 | 2.81 | 0.62 |
| 1:E:389:ARG:O | 1:E:392:ILE:N | 2.31 | 0.62 |
| 1:G:436:LEU:HD23 | 1:G:436:LEU:C | 2.19 | 0.62 |
| 1:I:340:VAL:CG1 | 1:I:345:TYR:OH | 2.48 | 0.62 |
| 1:J:647:ARG:HH11 | 1:J:649:GLN:CD | 1.99 | 0.62 |
| 1:J:657:PRO:C | 1:J:658:ILE:CD1 | 2.67 | 0.62 |
| 1:K:436:LEU:C | 1:K:436:LEU:HD23 | 2.19 | 0.62 |
| 1:L:657:PRO:C | 1:L:658:ILE:CD1 | 2.67 | 0.62 |
| 1:A:385:THR:HG21 | 1:A:392:ILE:H | 1.63 | 0.62 |
| 1:A:408:ILE:H | 1:A:408:ILE:HD12 | 1.64 | 0.62 |
| 1:C:340:VAL:CG1 | 1:C:345:TYR:OH | 2.48 | 0.62 |
| 1:E:533:ASP:OD2 | 1:E:533:ASP:N | 2.32 | 0.62 |
| 1:F:404:ILE:HD13 | 1:F:404:ILE:H | 1.63 | 0.62 |
| 1:F:566:ASN:C | 1:F:570:GLN:HE22 | 2.03 | 0.62 |
| 1:F:657:PRO:C | 1:F:658:ILE:CD1 | 2.67 | 0.62 |
| 1:G:415:PHE:HB2 | 1:G:485:VAL:HB | 1.81 | 0.62 |
| 1:H:660:GLN:CA | 1:H:661:LEU:HB2 | 2.26 | 0.62 |
| 1:I:340:VAL:HG12 | 1:I:345:TYR:OH | 1.99 | 0.62 |
| 1:I:518:ASN:HA | 1:I:535:LEU:HD22 | 1.80 | 0.62 |
| 1:D:415:PHE:HB2 | 1:D:485:VAL:HB | 1.82 | 0.62 |
| 1:G:341:THR:O | 1:G:345:TYR:CE1 | 2.53 | 0.62 |
| 1:G:389:ARG:O | 1:G:392:ILE:N | 2.31 | 0.62 |
| 1:H:647:ARG:HG2 | 1:H:650:TYR:CE1 | 2.35 | 0.62 |
| 1:J:660:GLN:CA | 1:J:661:LEU:HB2 | 2.26 | 0.62 |
| 1:K:340:VAL:CG1 | 1:K:345:TYR:OH | 2.48 | 0.62 |
| 1:K:353:PHE:CG | 1:K:395:TYR:CE2 | 2.87 | 0.62 |
| 1:K:524:VAL:HG13 | 1:K:529:GLY:O | 1.99 | 0.62 |
| 1:B:647:ARG:CD | 1:B:650:TYR:CE1 | 2.81 | 0.62 |
| 1:D:396:LEU:O | 1:D:399:TYR:O | 2.17 | 0.62 |
| 1:G:525:ASN:OD1 | 1:G:526:PRO:HD3 | 1.98 | 0.62 |
| 1:H:657:PRO:C | 1:H:658:ILE:CD1 | 2.67 | 0.62 |
| 1:L:647:ARG:HG2 | 1:L:650:TYR:CE1 | 2.35 | 0.62 |
| 1:B:647:ARG:HH11 | 1:B:649:GLN:CD | 1.99 | 0.62 |
| 1:E:401:LEU:CD2 | 1:E:402:ALA:CA | 2.74 | 0.62 |
| 1:E:525:ASN:OD1 | 1:E:526:PRO:HD3 | 1.99 | 0.62 |
| 1:I:408:ILE:H | 1:I:408:ILE:HD12 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:647:ARG:HG2 | 1:J:650:TYR:CE1 | 2.35 | 0.62 |
| 1:K:356:ILE:O | 1:K:356:ILE:HG12 | 1.98 | 0.62 |
| 1:L:647:ARG:HH11 | 1:L:649:GLN:CD | 2.00 | 0.62 |
| 1:A:340:VAL:CG1 | 1:A:345:TYR:OH | 2.48 | 0.62 |
| 1:B:404:ILE:HD13 | 1:B:404:ILE:H | 1.63 | 0.62 |
| 1:B:647:ARG:HG2 | 1:B:650:TYR:CE1 | 2.35 | 0.62 |
| 1:B:660:GLN:CA | 1:B:661:LEU:CB | 2.71 | 0.62 |
| 1:C:408:ILE:H | 1:C:408:ILE:HD12 | 1.64 | 0.62 |
| 1:F:646:LEU:O | 1:F:646:LEU:CD2 | 2.30 | 0.62 |
| 1:F:647:ARG:HG2 | 1:F:650:TYR:CE1 | 2.35 | 0.62 |
| 1:G:358:GLN:HB2 | 1:G:379:LYS:CA | 2.30 | 0.62 |
| 1:G:524:VAL:HG13 | 1:G:529:GLY:O | 1.99 | 0.62 |
| 1:H:376:ALA:O | 1:H:411:PRO:HD3 | 2.00 | 0.62 |
| 1:H:396:LEU:O | 1:H:399:TYR:O | 2.17 | 0.62 |
| 1:I:356:ILE:O | 1:I:356:ILE:HG12 | 1.99 | 0.62 |
| 1:J:376:ALA:O | 1:J:411:PRO:HD3 | 2.00 | 0.62 |
| 1:K:343:THR:HG22 | 1:K:344:ASP:N | 2.13 | 0.62 |
| 1:K:378:PRO:O | 1:K:379:LYS:HB3 | 1.99 | 0.62 |
| 1:K:385:THR:CG2 | 1:K:392:ILE:H | 2.12 | 0.62 |
| 1:A:341:THR:O | 1:A:345:TYR:CE1 | 2.53 | 0.61 |
| 1:C:341:THR:O | 1:C:345:TYR:CE1 | 2.53 | 0.61 |
| 1:C:353:PHE:CG | 1:C:395:TYR:CE2 | 2.87 | 0.61 |
| 1:C:436:LEU:C | 1:C:436:LEU:HD23 | 2.19 | 0.61 |
| 1:C:525:ASN:OD1 | 1:C:526:PRO:HD3 | 1.98 | 0.61 |
| 1:E:415:PHE:HB2 | 1:E:485:VAL:HB | 1.81 | 0.61 |
| 1:E:427:ASN:ND2 | 1:E:660:GLN:HB2 | 2.15 | 0.61 |
| 1:E:521:ARG:O | 1:E:533:ASP:HA | 2.00 | 0.61 |
| 1:G:521:ARG:O | 1:G:533:ASP:HA | 2.00 | 0.61 |
| 1:J:566:ASN:C | 1:J:570:GLN:HE22 | 2.03 | 0.61 |
| 1:L:408:ILE:C | 1:L:409:ILE:CG2 | 2.68 | 0.61 |
| 1:L:566:ASN:C | 1:L:570:GLN:HE22 | 2.03 | 0.61 |
| 1:L:660:GLN:CA | 1:L:661:LEU:HB2 | 2.25 | 0.61 |
| 1:A:415:PHE:HB2 | 1:A:485:VAL:HB | 1.81 | 0.61 |
| 1:A:427:ASN:ND2 | 1:A:660:GLN:HB2 | 2.15 | 0.61 |
| 1:A:521:ARG:O | 1:A:533:ASP:HA | 2.00 | 0.61 |
| 1:B:408:ILE:C | 1:B:409:ILE:CG2 | 2.68 | 0.61 |
| 1:C:401:LEU:CD2 | 1:C:402:ALA:CB | 2.69 | 0.61 |
| 1:C:427:ASN:ND2 | 1:C:660:GLN:HB2 | 2.15 | 0.61 |
| 1:E:340:VAL:CG1 | 1:E:345:TYR:OH | 2.48 | 0.61 |
| 1:F:345:TYR:HE1 | 1:F:349:VAL:HG21 | 1.62 | 0.61 |
| 1:F:396:LEU:O | 1:F:399:TYR:O | 2.17 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:537:ASP:O | 1:F:538:VAL:HG23 | 2.00 | 0.61 |
| 1:H:408:ILE:C | 1:H:409:ILE:CG2 | 2.68 | 0.61 |
| 1:I:341:THR:O | 1:I:345:TYR:CE1 | 2.53 | 0.61 |
| 1:L:347:THR:OG1 | 1:L:348:PHE:N | 2.30 | 0.61 |
| 1:B:646:LEU:O | 1:B:646:LEU:CD2 | 2.30 | 0.61 |
| 1:C:389:ARG:CA | 1:C:392:ILE:HG12 | 2.28 | 0.61 |
| 1:E:341:THR:O | 1:E:345:TYR:CE1 | 2.53 | 0.61 |
| 1:E:524:VAL:HG13 | 1:E:529:GLY:O | 1.99 | 0.61 |
| 1:F:343:THR:O | 1:F:347:THR:CG2 | 2.44 | 0.61 |
| 1:G:427:ASN:ND2 | 1:G:660:GLN:HB2 | 2.15 | 0.61 |
| 1:H:345:TYR:HE1 | 1:H:349:VAL:HG21 | 1.62 | 0.61 |
| 1:H:347:THR:OG1 | 1:H:348:PHE:N | 2.30 | 0.61 |
| 1:I:385:THR:HG1 | 1:I:387:VAL:CG2 | 1.98 | 0.61 |
| 1:I:500:LYS:HB3 | 1:I:600:ASP:O | 2.00 | 0.61 |
| 1:K:521:ARG:O | 1:K:533:ASP:HA | 2.00 | 0.61 |
| 1:L:660:GLN:CA | 1:L:661:LEU:CB | 2.71 | 0.61 |
| 1:C:533:ASP:OD2 | 1:C:533:ASP:N | 2.32 | 0.61 |
| 1:D:408:ILE:C | 1:D:409:ILE:CG2 | 2.68 | 0.61 |
| 1:D:647:ARG:HG2 | 1:D:650:TYR:CE1 | 2.35 | 0.61 |
| 1:F:568:ASN:OD1 | 1:F:569:ILE:N | 2.30 | 0.61 |
| 1:G:525:ASN:CG | 1:G:526:PRO:HD3 | 2.20 | 0.61 |
| 1:I:342:ALA:HB1 | 1:I:362:THR:CB | 2.30 | 0.61 |
| 1:I:517:PHE:HD2 | 1:I:536:TYR:CE2 | 2.09 | 0.61 |
| 1:K:408:ILE:H | 1:K:408:ILE:HD12 | 1.64 | 0.61 |
| 1:K:415:PHE:HB2 | 1:K:485:VAL:HB | 1.81 | 0.61 |
| 1:K:500:LYS:HB3 | 1:K:600:ASP:O | 2.00 | 0.61 |
| 1:K:518:ASN:HA | 1:K:535:LEU:HD22 | 1.80 | 0.61 |
| 1:L:415:PHE:HB2 | 1:L:485:VAL:HB | 1.82 | 0.61 |
| 1:A:342:ALA:HB1 | 1:A:362:THR:CB | 2.30 | 0.61 |
| 1:A:436:LEU:HD23 | 1:A:436:LEU:C | 2.19 | 0.61 |
| 1:E:356:ILE:HG12 | 1:E:356:ILE:O | 1.98 | 0.61 |
| 1:E:378:PRO:O | 1:E:379:LYS:HB3 | 1.99 | 0.61 |
| 1:G:634:THR:OG1 | 1:G:635:ARG:N | 2.30 | 0.61 |
| 1:I:415:PHE:HB2 | 1:I:485:VAL:HB | 1.81 | 0.61 |
| 1:I:436:LEU:HD22 | 1:I:655:LEU:CD2 | 2.29 | 0.61 |
| 1:I:524:VAL:HG13 | 1:I:529:GLY:O | 1.99 | 0.61 |
| 1:K:358:GLN:HB2 | 1:K:379:LYS:CA | 2.30 | 0.61 |
| 1:K:533:ASP:OD2 | 1:K:533:ASP:N | 2.32 | 0.61 |
| 1:A:353:PHE:CG | 1:A:395:TYR:CE2 | 2.87 | 0.61 |
| 1:B:348:PHE:O | 1:B:351:GLU:N | 2.21 | 0.61 |
| 1:D:657:PRO:C | 1:D:658:ILE:CD1 | 2.67 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:340:VAL:CG1 | 1:G:345:TYR:OH | 2.48 | 0.61 |
| 1:J:348:PHE:O | 1:J:349:VAL:C | 2.39 | 0.61 |
| 1:J:537:ASP:O | 1:J:538:VAL:HG23 | 2.00 | 0.61 |
| 1:K:342:ALA:HB1 | 1:K:362:THR:CB | 2.30 | 0.61 |
| 1:A:401:LEU:CD2 | 1:A:402:ALA:CA | 2.74 | 0.61 |
| 1:C:521:ARG:O | 1:C:533:ASP:HA | 2.00 | 0.61 |
| 1:D:348:PHE:O | 1:D:351:GLU:N | 2.21 | 0.61 |
| 1:E:500:LYS:HB3 | 1:E:600:ASP:O | 2.00 | 0.61 |
| 1:G:342:ALA:HB1 | 1:G:362:THR:CB | 2.30 | 0.61 |
| 1:G:517:PHE:HD2 | 1:G:536:TYR:CE2 | 2.09 | 0.61 |
| 1:K:401:LEU:CD2 | 1:K:402:ALA:CA | 2.74 | 0.61 |
| 1:K:427:ASN:ND2 | 1:K:660:GLN:HB2 | 2.15 | 0.61 |
| 1:L:376:ALA:O | 1:L:411:PRO:HD3 | 2.00 | 0.61 |
| 1:A:647:ARG:HG3 | 1:A:650:TYR:CD1 | 2.36 | 0.61 |
| 1:B:566:ASN:C | 1:B:570:GLN:HE22 | 2.03 | 0.61 |
| 1:C:358:GLN:HB2 | 1:C:379:LYS:CA | 2.30 | 0.61 |
| 1:C:525:ASN:CG | 1:C:526:PRO:HD3 | 2.20 | 0.61 |
| 1:D:566:ASN:C | 1:D:570:GLN:HE22 | 2.03 | 0.61 |
| 1:G:436:LEU:HD22 | 1:G:655:LEU:CD2 | 2.29 | 0.61 |
| 1:G:500:LYS:HB3 | 1:G:600:ASP:O | 2.00 | 0.61 |
| 1:H:647:ARG:HH11 | 1:H:649:GLN:CD | 2.00 | 0.61 |
| 1:A:389:ARG:CA | 1:A:392:ILE:HG12 | 2.28 | 0.61 |
| 1:A:457:SER:H | 1:A:634:THR:HG23 | 1.56 | 0.61 |
| 1:A:500:LYS:HB3 | 1:A:600:ASP:O | 2.00 | 0.61 |
| 1:B:415:PHE:HB2 | 1:B:485:VAL:HB | 1.82 | 0.61 |
| 1:E:517:PHE:HD2 | 1:E:536:TYR:CE2 | 2.09 | 0.61 |
| 1:G:504:GLN:HE22 | 1:G:598:PRO:HA | 1.66 | 0.61 |
| 1:I:353:PHE:CG | 1:I:395:TYR:CE2 | 2.87 | 0.61 |
| 1:I:504:GLN:HE22 | 1:I:598:PRO:HA | 1.66 | 0.61 |
| 1:I:521:ARG:O | 1:I:533:ASP:HA | 2.00 | 0.61 |
| 1:L:537:ASP:O | 1:L:538:VAL:HG23 | 2.00 | 0.61 |
| 1:A:525:ASN:CG | 1:A:526:PRO:HD3 | 2.20 | 0.61 |
| 1:A:525:ASN:OD1 | 1:A:526:PRO:HD3 | 1.98 | 0.61 |
| 1:C:385:THR:HG1 | 1:C:387:VAL:CG2 | 2.04 | 0.61 |
| 1:H:566:ASN:C | 1:H:570:GLN:HE22 | 2.03 | 0.61 |
| 1:I:427:ASN:ND2 | 1:I:660:GLN:HB2 | 2.15 | 0.61 |
| 1:J:415:PHE:HB2 | 1:J:485:VAL:HB | 1.81 | 0.61 |
| 1:K:389:ARG:CA | 1:K:392:ILE:HG12 | 2.28 | 0.61 |
| 1:K:647:ARG:HG3 | 1:K:650:TYR:CD1 | 2.36 | 0.61 |
| 1:A:358:GLN:HB2 | 1:A:379:LYS:CA | 2.30 | 0.60 |
| 1:C:443:LYS:HE3 | 1:C:470:ASP:O | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:647:ARG:HG3 | 1:C:650:TYR:CD1 | 2.36 | 0.60 |
| 1:F:376:ALA:O | 1:F:411:PRO:HD3 | 2.00 | 0.60 |
| 1:E:443:LYS:HE3 | 1:E:470:ASP:O | 2.01 | 0.60 |
| 1:H:348:PHE:O | 1:H:349:VAL:C | 2.39 | 0.60 |
| 1:J:408:ILE:C | 1:J:409:ILE:CG2 | 2.68 | 0.60 |
| 1:K:443:LYS:HE3 | 1:K:470:ASP:O | 2.01 | 0.60 |
| 1:A:353:PHE:CZ | 1:A:395:TYR:HD2 | 2.09 | 0.60 |
| 1:C:342:ALA:HB1 | 1:C:362:THR:CB | 2.30 | 0.60 |
| 1:E:429:LEU:HD22 | 1:E:431:GLU:O | 2.01 | 0.60 |
| 1:E:457:SER:H | 1:E:634:THR:HG21 | 1.66 | 0.60 |
| 1:H:415:PHE:HB2 | 1:H:485:VAL:HB | 1.81 | 0.60 |
| 1:I:358:GLN:HB2 | 1:I:379:LYS:CA | 2.30 | 0.60 |
| 1:K:341:THR:O | 1:K:345:TYR:CE1 | 2.53 | 0.60 |
| 1:K:429:LEU:HD22 | 1:K:431:GLU:O | 2.01 | 0.60 |
| 1:A:504:GLN:HE22 | 1:A:598:PRO:HA | 1.66 | 0.60 |
| 1:E:342:ALA:HB1 | 1:E:362:THR:CB | 2.30 | 0.60 |
| 1:E:504:GLN:HE22 | 1:E:598:PRO:HA | 1.66 | 0.60 |
| 1:H:537:ASP:O | 1:H:538:VAL:HG23 | 2.01 | 0.60 |
| 1:I:525:ASN:CG | 1:I:526:PRO:HD3 | 2.20 | 0.60 |
| 1:I:647:ARG:HG3 | 1:I:650:TYR:CD1 | 2.36 | 0.60 |
| 1:J:593:GLY:HA3 | 1:J:603:TYR:O | 2.02 | 0.60 |
| 1:B:348:PHE:O | 1:B:349:VAL:C | 2.39 | 0.60 |
| 1:D:398:ASP:CG | 1:E:663:HIS:HB3 | 2.22 | 0.60 |
| 1:D:537:ASP:O | 1:D:538:VAL:HG23 | 2.00 | 0.60 |
| 1:F:347:THR:OG1 | 1:F:348:PHE:N | 2.30 | 0.60 |
| 1:I:443:LYS:HE3 | 1:I:470:ASP:O | 2.01 | 0.60 |
| 1:E:647:ARG:HG3 | 1:E:650:TYR:CD1 | 2.36 | 0.60 |
| 1:G:647:ARG:HG3 | 1:G:650:TYR:CD1 | 2.36 | 0.60 |
| 1:J:664:HIS:O | 1:J:664:HIS:CD2 | 2.54 | 0.60 |
| 1:L:656:GLU:OE1 | 1:L:664:HIS:O | 2.20 | 0.60 |
| 1:B:664:HIS:O | 1:B:664:HIS:CD2 | 2.54 | 0.60 |
| 1:C:500:LYS:HB3 | 1:C:600:ASP:O | 2.00 | 0.60 |
| 1:C:504:GLN:HE22 | 1:C:598:PRO:HA | 1.66 | 0.60 |
| 1:G:429:LEU:HD22 | 1:G:431:GLU:O | 2.02 | 0.60 |
| 1:A:429:LEU:HD22 | 1:A:431:GLU:O | 2.02 | 0.60 |
| 1:A:443:LYS:HE3 | 1:A:470:ASP:O | 2.02 | 0.60 |
| 1:C:342:ALA:HB1 | 1:C:362:THR:O | 2.02 | 0.60 |
| 1:J:343:THR:O | 1:J:347:THR:CG2 | 2.44 | 0.60 |
| 1:B:656:GLU:OE1 | 1:B:664:HIS:O | 2.20 | 0.60 |
| 1:C:356:ILE:O | 1:C:356:ILE:HG12 | 1.98 | 0.60 |
| 1:F:593:GLY:HA3 | 1:F:603:TYR:O | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:647:ARG:CG | 1:F:650:TYR:CE1 | 2.85 | 0.60 |
| 1:G:443:LYS:HE3 | 1:G:470:ASP:O | 2.01 | 0.60 |
| 1:G:457:SER:H | 1:G:634:THR:HG21 | 1.66 | 0.60 |
| 1:K:342:ALA:HB1 | 1:K:362:THR:O | 2.02 | 0.60 |
| 1:C:566:ASN:O | 1:C:570:GLN:NE2 | 2.35 | 0.60 |
| 1:D:350:SER:HA | 1:D:357:ILE:HD11 | 1.84 | 0.60 |
| 1:D:409:ILE:HD12 | 1:D:410:SER:N | 2.17 | 0.60 |
| 1:E:342:ALA:HB1 | 1:E:362:THR:O | 2.02 | 0.60 |
| 1:E:525:ASN:CG | 1:E:526:PRO:HD3 | 2.20 | 0.60 |
| 1:F:415:PHE:HB2 | 1:F:485:VAL:HB | 1.81 | 0.60 |
| 1:J:409:ILE:HD12 | 1:J:410:SER:N | 2.16 | 0.60 |
| 1:J:464:MET:HG3 | 1:J:465:LEU:N | 2.17 | 0.60 |
| 1:K:436:LEU:HD22 | 1:K:655:LEU:CD2 | 2.29 | 0.60 |
| 1:L:348:PHE:O | 1:L:349:VAL:C | 2.39 | 0.60 |
| 1:L:593:GLY:HA3 | 1:L:603:TYR:O | 2.02 | 0.60 |
| 1:L:664:HIS:O | 1:L:664:HIS:CD2 | 2.55 | 0.60 |
| 1:B:343:THR:O | 1:B:347:THR:CG2 | 2.44 | 0.59 |
| 1:B:359:ALA:HB1 | 1:B:455:PHE:CE2 | 2.37 | 0.59 |
| 1:D:647:ARG:CG | 1:D:650:TYR:CE1 | 2.85 | 0.59 |
| 1:D:656:GLU:OE1 | 1:D:664:HIS:O | 2.20 | 0.59 |
| 1:L:359:ALA:HB1 | 1:L:455:PHE:CE2 | 2.37 | 0.59 |
| 1:L:464:MET:HG3 | 1:L:465:LEU:N | 2.17 | 0.59 |
| 1:D:359:ALA:HB1 | 1:D:455:PHE:CE2 | 2.37 | 0.59 |
| 1:F:409:ILE:HD12 | 1:F:410:SER:N | 2.17 | 0.59 |
| 1:H:359:ALA:HB1 | 1:H:455:PHE:CE2 | 2.37 | 0.59 |
| 1:H:409:ILE:HD12 | 1:H:410:SER:N | 2.17 | 0.59 |
| 1:H:568:ASN:OD1 | 1:H:569:ILE:N | 2.30 | 0.59 |
| 1:J:550:ILE:HD13 | 1:J:596:ASN:HA | 1.84 | 0.59 |
| 1:B:537:ASP:O | 1:B:538:VAL:HG23 | 2.00 | 0.59 |
| 1:B:593:GLY:HA3 | 1:B:603:TYR:O | 2.02 | 0.59 |
| 1:B:660:GLN:CA | 1:B:661:LEU:HB2 | 2.26 | 0.59 |
| 1:C:429:LEU:HD22 | 1:C:431:GLU:O | 2.02 | 0.59 |
| 1:D:664:HIS:O | 1:D:664:HIS:CD2 | 2.55 | 0.59 |
| 1:E:385:THR:O | 1:E:388:GLN:N | 2.35 | 0.59 |
| 1:F:359:ALA:HB1 | 1:F:455:PHE:CE2 | 2.37 | 0.59 |
| 1:G:509:SER:OG | 1:G:626:ASP:N | 2.34 | 0.59 |
| 1:H:646:LEU:O | 1:H:646:LEU:CD2 | 2.30 | 0.59 |
| 1:I:385:THR:O | 1:I:388:GLN:N | 2.35 | 0.59 |
| 1:K:531:GLU:C | 1:K:532:GLU:CD | 2.61 | 0.59 |
| 1:A:342:ALA:HB1 | 1:A:362:THR:O | 2.02 | 0.59 |
| 1:A:356:ILE:O | 1:A:356:ILE:HG12 | 1.98 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:557:PRO:HG3 | 1:B:589:TYR:CZ | 2.38 | 0.59 |
| 1:D:398:ASP:O | 1:E:663:HIS:HB3 | 2.02 | 0.59 |
| 1:G:385:THR:O | 1:G:388:GLN:N | 2.35 | 0.59 |
| 1:H:464:MET:HG3 | 1:H:465:LEU:N | 2.17 | 0.59 |
| 1:H:593:GLY:HA3 | 1:H:603:TYR:O | 2.02 | 0.59 |
| 1:A:457:SER:H | 1:A:634:THR:HG21 | 1.66 | 0.59 |
| 1:A:531:GLU:C | 1:A:532:GLU:CD | 2.61 | 0.59 |
| 1:B:440:ILE:HG22 | 1:B:471:ALA:CB | 2.33 | 0.59 |
| 1:E:436:LEU:HD22 | 1:E:655:LEU:CD2 | 2.29 | 0.59 |
| 1:F:408:ILE:C | 1:F:409:ILE:CG2 | 2.68 | 0.59 |
| 1:F:464:MET:HG3 | 1:F:465:LEU:N | 2.17 | 0.59 |
| 1:F:557:PRO:HG3 | 1:F:589:TYR:CZ | 2.38 | 0.59 |
| 1:F:664:HIS:O | 1:F:664:HIS:CD2 | 2.54 | 0.59 |
| 1:H:647:ARG:CG | 1:H:650:TYR:CE1 | 2.85 | 0.59 |
| 1:I:389:ARG:O | 1:I:392:ILE:N | 2.31 | 0.59 |
| 1:L:647:ARG:CG | 1:L:650:TYR:CE1 | 2.85 | 0.59 |
| 1:D:453:GLU:CD | 1:D:641:VAL:HG23 | 2.23 | 0.59 |
| 1:E:340:VAL:C | 1:E:341:THR:CG2 | 2.62 | 0.59 |
| 1:F:656:GLU:OE1 | 1:F:664:HIS:O | 2.20 | 0.59 |
| 1:I:342:ALA:HB1 | 1:I:362:THR:O | 2.02 | 0.59 |
| 1:I:429:LEU:HD22 | 1:I:431:GLU:O | 2.01 | 0.59 |
| 1:J:656:GLU:OE1 | 1:J:664:HIS:O | 2.20 | 0.59 |
| 1:L:550:ILE:HD13 | 1:L:596:ASN:HA | 1.84 | 0.59 |
| 1:L:557:PRO:HG3 | 1:L:589:TYR:CZ | 2.38 | 0.59 |
| 1:B:568:ASN:OD1 | 1:B:569:ILE:N | 2.30 | 0.59 |
| 1:D:402:ALA:N | 1:D:403:PRO:CD | 2.66 | 0.59 |
| 1:D:440:ILE:HG22 | 1:D:471:ALA:CB | 2.33 | 0.59 |
| 1:D:646:LEU:O | 1:D:646:LEU:CD2 | 2.30 | 0.59 |
| 1:F:350:SER:HA | 1:F:357:ILE:HD11 | 1.84 | 0.59 |
| 1:F:440:ILE:HG22 | 1:F:471:ALA:CB | 2.33 | 0.59 |
| 1:F:509:SER:OG | 1:F:626:ASP:N | 2.32 | 0.59 |
| 1:G:353:PHE:CG | 1:G:395:TYR:CE2 | 2.87 | 0.59 |
| 1:G:566:ASN:O | 1:G:570:GLN:NE2 | 2.35 | 0.59 |
| 1:I:531:GLU:C | 1:I:532:GLU:CD | 2.61 | 0.59 |
| 1:L:440:ILE:HG22 | 1:L:471:ALA:CB | 2.33 | 0.59 |
| 1:C:509:SER:OG | 1:C:626:ASP:N | 2.34 | 0.59 |
| 1:D:348:PHE:O | 1:D:349:VAL:C | 2.39 | 0.59 |
| 1:E:531:GLU:C | 1:E:532:GLU:CD | 2.61 | 0.59 |
| 1:H:664:HIS:O | 1:H:664:HIS:CD2 | 2.54 | 0.59 |
| 1:K:504:GLN:HE22 | 1:K:598:PRO:HA | 1.66 | 0.59 |
| 1:L:350:SER:HA | 1:L:357:ILE:HD11 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:350:SER:HA | 1:B:357:ILE:HD11 | 1.84 | 0.59 |
| 1:B:367:THR:CG2 | 1:B:368:LYS:N | 2.44 | 0.59 |
| 1:D:593:GLY:HA3 | 1:D:603:TYR:O | 2.02 | 0.59 |
| 1:G:531:GLU:C | 1:G:532:GLU:CD | 2.61 | 0.59 |
| 1:H:557:PRO:HG3 | 1:H:589:TYR:CZ | 2.38 | 0.59 |
| 1:J:359:ALA:HB1 | 1:J:455:PHE:CE2 | 2.37 | 0.59 |
| 1:J:453:GLU:CD | 1:J:641:VAL:HG23 | 2.23 | 0.59 |
| 1:L:346:ASP:OD2 | 1:L:361:GLN:HA | 2.03 | 0.59 |
| 1:B:550:ILE:HD13 | 1:B:596:ASN:HA | 1.84 | 0.59 |
| 1:B:464:MET:HG3 | 1:B:465:LEU:N | 2.17 | 0.58 |
| 1:F:453:GLU:CD | 1:F:641:VAL:HG23 | 2.23 | 0.58 |
| 1:G:342:ALA:HB1 | 1:G:362:THR:O | 2.02 | 0.58 |
| 1:J:647:ARG:CG | 1:J:650:TYR:CE1 | 2.85 | 0.58 |
| 1:A:385:THR:O | 1:A:388:GLN:N | 2.35 | 0.58 |
| 1:C:385:THR:O | 1:C:388:GLN:N | 2.35 | 0.58 |
| 1:C:389:ARG:O | 1:C:392:ILE:N | 2.31 | 0.58 |
| 1:C:617:GLU:HG3 | 1:C:618:VAL:HG13 | 1.85 | 0.58 |
| 1:D:464:MET:HG3 | 1:D:465:LEU:N | 2.17 | 0.58 |
| 1:F:346:ASP:OD2 | 1:F:361:GLN:HA | 2.03 | 0.58 |
| 1:F:550:ILE:HD13 | 1:F:596:ASN:HA | 1.84 | 0.58 |
| 1:H:402:ALA:N | 1:H:403:PRO:CD | 2.66 | 0.58 |
| 1:H:440:ILE:HG22 | 1:H:471:ALA:CB | 2.33 | 0.58 |
| 1:H:550:ILE:HD13 | 1:H:596:ASN:HA | 1.84 | 0.58 |
| 1:L:409:ILE:HD12 | 1:L:410:SER:N | 2.17 | 0.58 |
| 1:A:385:THR:OG1 | 1:A:389:ARG:N | 2.37 | 0.58 |
| 1:A:436:LEU:HD22 | 1:A:655:LEU:CD2 | 2.29 | 0.58 |
| 1:D:396:LEU:HD21 | 1:D:406:PRO:HG2 | 1.85 | 0.58 |
| 1:H:509:SER:OG | 1:H:626:ASP:N | 2.32 | 0.58 |
| 1:I:524:VAL:HG13 | 1:I:529:GLY:H | 1.69 | 0.58 |
| 1:J:346:ASP:OD2 | 1:J:361:GLN:HA | 2.03 | 0.58 |
| 1:J:557:PRO:HG3 | 1:J:589:TYR:CZ | 2.38 | 0.58 |
| 1:K:385:THR:O | 1:K:388:GLN:N | 2.35 | 0.58 |
| 1:L:453:GLU:CD | 1:L:641:VAL:HG23 | 2.23 | 0.58 |
| 1:A:524:VAL:HG13 | 1:A:529:GLY:H | 1.69 | 0.58 |
| 1:B:647:ARG:CG | 1:B:650:TYR:CE1 | 2.85 | 0.58 |
| 1:C:531:GLU:C | 1:C:532:GLU:CD | 2.61 | 0.58 |
| 1:C:664:HIS:O | 1:C:665:HIS:CB | 2.51 | 0.58 |
| 1:D:346:ASP:OD2 | 1:D:361:GLN:HA | 2.03 | 0.58 |
| 1:E:524:VAL:HG13 | 1:E:529:GLY:H | 1.68 | 0.58 |
| 1:G:385:THR:OG1 | 1:G:389:ARG:N | 2.37 | 0.58 |
| 1:G:524:VAL:HG13 | 1:G:529:GLY:H | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:440:ILE:HG22 | 1:J:471:ALA:CB | 2.33 | 0.58 |
| 1:K:524:VAL:HG13 | 1:K:529:GLY:H | 1.69 | 0.58 |
| 1:K:664:HIS:O | 1:K:665:HIS:CB | 2.51 | 0.58 |
| 1:L:402:ALA:N | 1:L:403:PRO:CD | 2.66 | 0.58 |
| 1:A:664:HIS:O | 1:A:665:HIS:CB | 2.51 | 0.58 |
| 1:C:385:THR:OG1 | 1:C:389:ARG:N | 2.37 | 0.58 |
| 1:D:557:PRO:HG3 | 1:D:589:TYR:CZ | 2.38 | 0.58 |
| 1:I:457:SER:H | 1:I:634:THR:HG21 | 1.66 | 0.58 |
| 1:K:389:ARG:O | 1:K:392:ILE:N | 2.31 | 0.58 |
| 1:K:499:ILE:HD11 | 1:K:623:LEU:HD23 | 1.86 | 0.58 |
| 1:L:504:GLN:NE2 | 1:L:597:TYR:O | 2.37 | 0.58 |
| 1:A:408:ILE:HD12 | 1:A:408:ILE:N | 2.19 | 0.58 |
| 1:B:346:ASP:OD2 | 1:B:361:GLN:HA | 2.03 | 0.58 |
| 1:B:402:ALA:N | 1:B:403:PRO:CD | 2.66 | 0.58 |
| 1:E:389:ARG:CA | 1:E:392:ILE:HG12 | 2.28 | 0.58 |
| 1:H:453:GLU:CD | 1:H:641:VAL:HG23 | 2.23 | 0.58 |
| 1:I:385:THR:OG1 | 1:I:389:ARG:N | 2.37 | 0.58 |
| 1:I:386:THR:C | 1:I:388:GLN:H | 2.07 | 0.58 |
| 1:I:499:ILE:HD11 | 1:I:623:LEU:HD23 | 1.86 | 0.58 |
| 1:K:408:ILE:HD12 | 1:K:408:ILE:N | 2.19 | 0.58 |
| 1:C:385:THR:CB | 1:C:389:ARG:H | 2.17 | 0.58 |
| 1:D:476:ILE:HG22 | 1:D:477:GLY:N | 2.18 | 0.58 |
| 1:E:353:PHE:CG | 1:E:395:TYR:CE2 | 2.87 | 0.58 |
| 1:G:486:ARG:NH1 | 1:G:500:LYS:O | 2.36 | 0.58 |
| 1:H:656:GLU:OE1 | 1:H:664:HIS:O | 2.20 | 0.58 |
| 1:I:401:LEU:CD2 | 1:I:402:ALA:CA | 2.74 | 0.58 |
| 1:K:617:GLU:HG3 | 1:K:618:VAL:HG13 | 1.85 | 0.58 |
| 1:B:453:GLU:CD | 1:B:641:VAL:HG23 | 2.23 | 0.58 |
| 1:D:504:GLN:NE2 | 1:D:597:TYR:O | 2.37 | 0.58 |
| 1:F:389:ARG:NH2 | 1:F:410:SER:OG | 2.37 | 0.58 |
| 1:G:408:ILE:HD12 | 1:G:408:ILE:N | 2.19 | 0.58 |
| 1:G:499:ILE:HD11 | 1:G:623:LEU:HD23 | 1.86 | 0.58 |
| 1:J:350:SER:HA | 1:J:357:ILE:HD11 | 1.84 | 0.58 |
| 1:J:396:LEU:HD21 | 1:J:406:PRO:HG2 | 1.85 | 0.58 |
| 1:K:525:ASN:CG | 1:K:526:PRO:HD3 | 2.20 | 0.58 |
| 1:K:635:ARG:HG3 | 1:K:636:ASP:N | 2.19 | 0.58 |
| 1:L:409:ILE:CD1 | 1:L:410:SER:O | 2.50 | 0.58 |
| 1:L:593:GLY:HA3 | 1:L:604:TRP:HA | 1.86 | 0.58 |
| 1:A:566:ASN:O | 1:A:570:GLN:NE2 | 2.35 | 0.58 |
| 1:A:635:ARG:HG3 | 1:A:636:ASP:N | 2.19 | 0.58 |
| 1:C:424:TYR:CB | 1:C:475:VAL:H | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:389:ARG:NH2 | 1:D:410:SER:OG | 2.37 | 0.58 |
| 1:D:593:GLY:HA3 | 1:D:604:TRP:HA | 1.86 | 0.58 |
| 1:F:348:PHE:O | 1:F:349:VAL:C | 2.39 | 0.58 |
| 1:G:525:ASN:HB3 | 1:G:526:PRO:CD | 2.17 | 0.58 |
| 1:H:346:ASP:OD2 | 1:H:361:GLN:HA | 2.03 | 0.58 |
| 1:C:408:ILE:HD12 | 1:C:408:ILE:N | 2.19 | 0.58 |
| 1:C:524:VAL:HG13 | 1:C:529:GLY:H | 1.69 | 0.58 |
| 1:E:349:VAL:C | 1:E:351:GLU:H | 2.08 | 0.58 |
| 1:E:566:ASN:O | 1:E:570:GLN:NE2 | 2.35 | 0.58 |
| 1:H:350:SER:HA | 1:H:357:ILE:HD11 | 1.84 | 0.58 |
| 1:K:385:THR:OG1 | 1:K:389:ARG:N | 2.37 | 0.58 |
| 1:A:499:ILE:HD11 | 1:A:623:LEU:HD23 | 1.86 | 0.57 |
| 1:A:536:TYR:CD1 | 1:A:586:ARG:HD3 | 2.39 | 0.57 |
| 1:B:565:GLU:C | 1:B:570:GLN:NE2 | 2.58 | 0.57 |
| 1:C:536:TYR:CD1 | 1:C:586:ARG:HD3 | 2.39 | 0.57 |
| 1:E:493:LYS:HE2 | 1:E:494:THR:O | 2.04 | 0.57 |
| 1:F:402:ALA:N | 1:F:403:PRO:CD | 2.66 | 0.57 |
| 1:F:504:GLN:NE2 | 1:F:597:TYR:O | 2.37 | 0.57 |
| 1:L:389:ARG:NH2 | 1:L:410:SER:OG | 2.37 | 0.57 |
| 1:L:396:LEU:HD13 | 1:L:406:PRO:HD2 | 1.86 | 0.57 |
| 1:A:386:THR:C | 1:A:388:GLN:H | 2.07 | 0.57 |
| 1:A:389:ARG:O | 1:A:392:ILE:N | 2.31 | 0.57 |
| 1:C:486:ARG:NH1 | 1:C:500:LYS:O | 2.36 | 0.57 |
| 1:E:385:THR:OG1 | 1:E:389:ARG:N | 2.37 | 0.57 |
| 1:E:408:ILE:HD12 | 1:E:408:ILE:N | 2.19 | 0.57 |
| 1:F:396:LEU:HD21 | 1:F:406:PRO:HG2 | 1.85 | 0.57 |
| 1:F:593:GLY:HA3 | 1:F:604:TRP:HA | 1.86 | 0.57 |
| 1:G:424:TYR:CB | 1:G:475:VAL:H | 2.17 | 0.57 |
| 1:H:389:ARG:NH2 | 1:H:410:SER:OG | 2.37 | 0.57 |
| 1:H:656:GLU:OE1 | 1:H:664:HIS:HB2 | 2.04 | 0.57 |
| 1:I:617:GLU:HG3 | 1:I:618:VAL:HG13 | 1.86 | 0.57 |
| 1:L:565:GLU:C | 1:L:570:GLN:NE2 | 2.58 | 0.57 |
| 1:A:424:TYR:CB | 1:A:475:VAL:H | 2.17 | 0.57 |
| 1:B:396:LEU:HD21 | 1:B:406:PRO:HG2 | 1.85 | 0.57 |
| 1:C:499:ILE:HD11 | 1:C:623:LEU:HD23 | 1.86 | 0.57 |
| 1:D:396:LEU:HD13 | 1:D:406:PRO:HD2 | 1.87 | 0.57 |
| 1:E:385:THR:CG2 | 1:E:392:ILE:HG23 | 2.35 | 0.57 |
| 1:F:657:PRO:O | 1:F:658:ILE:CD1 | 2.53 | 0.57 |
| 1:H:504:GLN:NE2 | 1:H:597:TYR:O | 2.37 | 0.57 |
| 1:I:424:TYR:CB | 1:I:475:VAL:H | 2.17 | 0.57 |
| 1:J:389:ARG:NH2 | 1:J:410:SER:OG | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:593:GLY:HA3 | 1:J:604:TRP:HA | 1.86 | 0.57 |
| 1:K:457:SER:H | 1:K:634:THR:HG21 | 1.66 | 0.57 |
| 1:K:509:SER:OG | 1:K:626:ASP:N | 2.34 | 0.57 |
| 1:K:536:TYR:CD1 | 1:K:586:ARG:HD3 | 2.39 | 0.57 |
| 1:L:656:GLU:OE1 | 1:L:664:HIS:HB2 | 2.04 | 0.57 |
| 1:B:389:ARG:NH2 | 1:B:410:SER:OG | 2.37 | 0.57 |
| 1:B:657:PRO:O | 1:B:658:ILE:CD1 | 2.53 | 0.57 |
| 1:E:424:TYR:CB | 1:E:475:VAL:H | 2.17 | 0.57 |
| 1:F:409:ILE:CD1 | 1:F:410:SER:N | 2.67 | 0.57 |
| 1:F:656:GLU:OE1 | 1:F:664:HIS:HB2 | 2.04 | 0.57 |
| 1:H:565:GLU:C | 1:H:570:GLN:NE2 | 2.58 | 0.57 |
| 1:J:656:GLU:OE1 | 1:J:664:HIS:HB2 | 2.04 | 0.57 |
| 1:K:424:TYR:CB | 1:K:475:VAL:H | 2.17 | 0.57 |
| 1:A:509:SER:OG | 1:A:626:ASP:N | 2.34 | 0.57 |
| 1:A:617:GLU:HG3 | 1:A:618:VAL:HG13 | 1.86 | 0.57 |
| 1:B:409:ILE:HD12 | 1:B:410:SER:N | 2.16 | 0.57 |
| 1:C:386:THR:C | 1:C:388:GLN:H | 2.07 | 0.57 |
| 1:C:436:LEU:HD22 | 1:C:655:LEU:CD2 | 2.29 | 0.57 |
| 1:D:656:GLU:OE1 | 1:D:664:HIS:HB2 | 2.04 | 0.57 |
| 1:G:349:VAL:C | 1:G:351:GLU:H | 2.08 | 0.57 |
| 1:H:646:LEU:C | 1:H:646:LEU:CD2 | 2.72 | 0.57 |
| 1:I:385:THR:HG21 | 1:I:389:ARG:O | 2.04 | 0.57 |
| 1:I:664:HIS:O | 1:I:665:HIS:CB | 2.51 | 0.57 |
| 1:K:385:THR:HG21 | 1:K:389:ARG:O | 2.04 | 0.57 |
| 1:K:566:ASN:O | 1:K:570:GLN:NE2 | 2.35 | 0.57 |
| 1:C:349:VAL:C | 1:C:351:GLU:H | 2.08 | 0.57 |
| 1:C:493:LYS:HE2 | 1:C:494:THR:O | 2.04 | 0.57 |
| 1:D:550:ILE:HD13 | 1:D:596:ASN:HA | 1.84 | 0.57 |
| 1:D:657:PRO:O | 1:D:658:ILE:CD1 | 2.53 | 0.57 |
| 1:E:499:ILE:HD11 | 1:E:623:LEU:HD23 | 1.86 | 0.57 |
| 1:F:656:GLU:OE1 | 1:F:664:HIS:CB | 2.53 | 0.57 |
| 1:G:493:LYS:HE2 | 1:G:494:THR:O | 2.04 | 0.57 |
| 1:H:657:PRO:O | 1:H:658:ILE:CD1 | 2.53 | 0.57 |
| 1:I:566:ASN:O | 1:I:570:GLN:NE2 | 2.35 | 0.57 |
| 1:K:387:VAL:C | 1:K:388:GLN:CG | 2.73 | 0.57 |
| 1:L:656:GLU:OE1 | 1:L:664:HIS:CB | 2.53 | 0.57 |
| 1:B:504:GLN:NE2 | 1:B:597:TYR:O | 2.37 | 0.57 |
| 1:B:656:GLU:OE1 | 1:B:664:HIS:HB2 | 2.04 | 0.57 |
| 1:D:565:GLU:C | 1:D:570:GLN:NE2 | 2.58 | 0.57 |
| 1:E:486:ARG:NH1 | 1:E:500:LYS:O | 2.36 | 0.57 |
| 1:F:346:ASP:OD1 | 1:F:362:THR:OG1 | 2.23 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:385:THR:HG21 | 1:G:389:ARG:O | 2.04 | 0.57 |
| 1:I:408:ILE:HD12 | 1:I:408:ILE:N | 2.19 | 0.57 |
| 1:I:493:LYS:HE2 | 1:I:494:THR:O | 2.04 | 0.57 |
| 1:J:565:GLU:C | 1:J:570:GLN:NE2 | 2.58 | 0.57 |
| 1:J:656:GLU:OE1 | 1:J:664:HIS:CB | 2.53 | 0.57 |
| 1:K:493:LYS:HE2 | 1:K:494:THR:O | 2.04 | 0.57 |
| 1:L:409:ILE:CD1 | 1:L:410:SER:N | 2.67 | 0.57 |
| 1:L:646:LEU:C | 1:L:646:LEU:CD2 | 2.72 | 0.57 |
| 1:C:635:ARG:HH22 | 1:D:661:LEU:CD1 | 2.14 | 0.57 |
| 1:G:379:LYS:O | 1:G:379:LYS:HG2 | 2.05 | 0.57 |
| 1:I:536:TYR:CD1 | 1:I:586:ARG:HD3 | 2.39 | 0.57 |
| 1:B:509:SER:OG | 1:B:626:ASP:N | 2.32 | 0.57 |
| 1:D:409:ILE:CD1 | 1:D:410:SER:N | 2.67 | 0.57 |
| 1:D:656:GLU:OE1 | 1:D:664:HIS:CB | 2.53 | 0.57 |
| 1:E:536:TYR:CD1 | 1:E:586:ARG:HD3 | 2.39 | 0.57 |
| 1:F:565:GLU:C | 1:F:570:GLN:NE2 | 2.58 | 0.57 |
| 1:G:386:THR:C | 1:G:388:GLN:H | 2.07 | 0.57 |
| 1:G:536:TYR:CD1 | 1:G:586:ARG:HD3 | 2.39 | 0.57 |
| 1:I:385:THR:CG2 | 1:I:392:ILE:HG23 | 2.35 | 0.57 |
| 1:J:657:PRO:O | 1:J:658:ILE:CD1 | 2.53 | 0.57 |
| 1:A:385:THR:CB | 1:A:389:ARG:H | 2.17 | 0.57 |
| 1:C:385:THR:CG2 | 1:C:392:ILE:HG23 | 2.35 | 0.57 |
| 1:C:387:VAL:C | 1:C:388:GLN:CG | 2.73 | 0.57 |
| 1:E:382:LEU:HD21 | 1:E:643:GLU:HG3 | 1.87 | 0.57 |
| 1:F:405:THR:O | 1:F:406:PRO:O | 2.23 | 0.57 |
| 1:G:385:THR:CG2 | 1:G:392:ILE:HG23 | 2.35 | 0.57 |
| 1:H:656:GLU:OE1 | 1:H:664:HIS:CB | 2.53 | 0.57 |
| 1:I:349:VAL:C | 1:I:351:GLU:H | 2.08 | 0.57 |
| 1:I:387:VAL:C | 1:I:388:GLN:CG | 2.73 | 0.57 |
| 1:J:504:GLN:NE2 | 1:J:597:TYR:O | 2.37 | 0.57 |
| 1:K:385:THR:CG2 | 1:K:392:ILE:HG23 | 2.35 | 0.57 |
| 1:L:396:LEU:HD21 | 1:L:406:PRO:HG2 | 1.85 | 0.57 |
| 1:A:493:LYS:HE2 | 1:A:494:THR:O | 2.04 | 0.56 |
| 1:B:346:ASP:OD1 | 1:B:362:THR:OG1 | 2.23 | 0.56 |
| 1:G:617:GLU:HG3 | 1:G:618:VAL:HG13 | 1.85 | 0.56 |
| 1:H:396:LEU:HD21 | 1:H:406:PRO:HG2 | 1.85 | 0.56 |
| 1:I:387:VAL:O | 1:I:388:GLN:CD | 2.44 | 0.56 |
| 1:K:379:LYS:HG2 | 1:K:379:LYS:O | 2.05 | 0.56 |
| 1:K:454:ILE:HG22 | 1:K:455:PHE:N | 2.20 | 0.56 |
| 1:A:385:THR:HG21 | 1:A:389:ARG:O | 2.05 | 0.56 |
| 1:A:387:VAL:O | 1:A:388:GLN:CD | 2.44 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:405:THR:O | 1:B:406:PRO:O | 2.23 | 0.56 |
| 1:D:568:ASN:OD1 | 1:D:569:ILE:N | 2.30 | 0.56 |
| 1:G:388:GLN:O | 1:G:389:ARG:NE | 2.39 | 0.56 |
| 1:G:389:ARG:CA | 1:G:392:ILE:HG12 | 2.28 | 0.56 |
| 1:G:664:HIS:O | 1:G:665:HIS:CB | 2.51 | 0.56 |
| 1:H:409:ILE:CD1 | 1:H:410:SER:N | 2.67 | 0.56 |
| 1:H:593:GLY:HA3 | 1:H:604:TRP:HA | 1.86 | 0.56 |
| 1:J:402:ALA:N | 1:J:403:PRO:CD | 2.66 | 0.56 |
| 1:L:568:ASN:OD1 | 1:L:569:ILE:N | 2.30 | 0.56 |
| 1:A:349:VAL:C | 1:A:351:GLU:H | 2.08 | 0.56 |
| 1:A:385:THR:CG2 | 1:A:392:ILE:HG23 | 2.35 | 0.56 |
| 1:A:387:VAL:C | 1:A:388:GLN:CG | 2.73 | 0.56 |
| 1:A:525:ASN:HB3 | 1:A:526:PRO:CD | 2.17 | 0.56 |
| 1:B:499:ILE:HG23 | 1:B:602:ILE:HB | 1.87 | 0.56 |
| 1:C:427:ASN:ND2 | 1:C:427:ASN:H | 2.03 | 0.56 |
| 1:D:409:ILE:CD1 | 1:D:410:SER:O | 2.50 | 0.56 |
| 1:E:386:THR:C | 1:E:388:GLN:H | 2.07 | 0.56 |
| 1:E:635:ARG:HH22 | 1:F:661:LEU:CD1 | 2.14 | 0.56 |
| 1:G:387:VAL:O | 1:G:388:GLN:CD | 2.44 | 0.56 |
| 1:H:405:THR:O | 1:H:406:PRO:O | 2.23 | 0.56 |
| 1:I:427:ASN:ND2 | 1:I:427:ASN:H | 2.03 | 0.56 |
| 1:K:349:VAL:C | 1:K:351:GLU:H | 2.08 | 0.56 |
| 1:K:387:VAL:O | 1:K:388:GLN:CD | 2.44 | 0.56 |
| 1:K:388:GLN:O | 1:K:389:ARG:NE | 2.39 | 0.56 |
| 1:L:476:ILE:HG22 | 1:L:477:GLY:N | 2.18 | 0.56 |
| 1:B:656:GLU:OE1 | 1:B:664:HIS:CB | 2.53 | 0.56 |
| 1:C:385:THR:HG21 | 1:C:389:ARG:O | 2.04 | 0.56 |
| 1:C:457:SER:H | 1:C:634:THR:HG21 | 1.66 | 0.56 |
| 1:D:346:ASP:OD1 | 1:D:362:THR:OG1 | 2.23 | 0.56 |
| 1:E:385:THR:HG21 | 1:E:389:ARG:O | 2.04 | 0.56 |
| 1:G:403:PRO:CD | 1:J:366:SER:HA | 2.24 | 0.56 |
| 1:H:596:ASN:HD22 | 1:H:599:ALA:H | 1.54 | 0.56 |
| 1:J:396:LEU:HD13 | 1:J:406:PRO:HD2 | 1.86 | 0.56 |
| 1:J:509:SER:OG | 1:J:626:ASP:N | 2.32 | 0.56 |
| 1:K:382:LEU:HD21 | 1:K:643:GLU:HG3 | 1.87 | 0.56 |
| 1:K:387:VAL:HG21 | 1:K:390:GLU:HB2 | 1.88 | 0.56 |
| 1:K:486:ARG:NH1 | 1:K:500:LYS:O | 2.36 | 0.56 |
| 1:A:486:ARG:NH1 | 1:A:500:LYS:O | 2.36 | 0.56 |
| 1:C:387:VAL:O | 1:C:388:GLN:CD | 2.44 | 0.56 |
| 1:D:499:ILE:HG23 | 1:D:602:ILE:HB | 1.87 | 0.56 |
| 1:G:387:VAL:C | 1:G:388:GLN:CG | 2.73 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:427:ASN:ND2 | 1:G:427:ASN:H | 2.03 | 0.56 |
| 1:I:385:THR:CB | 1:I:389:ARG:H | 2.17 | 0.56 |
| 1:K:385:THR:CB | 1:K:389:ARG:H | 2.17 | 0.56 |
| 1:K:525:ASN:HB3 | 1:K:526:PRO:CD | 2.17 | 0.56 |
| 1:L:657:PRO:O | 1:L:658:ILE:CD1 | 2.53 | 0.56 |
| 1:A:342:ALA:CB | 1:A:362:THR:CG2 | 2.84 | 0.56 |
| 1:A:388:GLN:O | 1:A:389:ARG:NE | 2.38 | 0.56 |
| 1:B:409:ILE:CD1 | 1:B:410:SER:N | 2.67 | 0.56 |
| 1:B:409:ILE:CD1 | 1:B:410:SER:O | 2.50 | 0.56 |
| 1:B:593:GLY:HA3 | 1:B:604:TRP:HA | 1.86 | 0.56 |
| 1:B:644:ASN:ND2 | 1:B:644:ASN:C | 2.59 | 0.56 |
| 1:D:568:ASN:CG | 1:D:569:ILE:N | 2.59 | 0.56 |
| 1:E:389:ARG:HA | 1:E:392:ILE:CG1 | 2.29 | 0.56 |
| 1:F:396:LEU:HD13 | 1:F:406:PRO:HD2 | 1.86 | 0.56 |
| 1:I:387:VAL:HG21 | 1:I:390:GLU:HB2 | 1.88 | 0.56 |
| 1:I:509:SER:OG | 1:I:626:ASP:N | 2.34 | 0.56 |
| 1:J:646:LEU:C | 1:J:646:LEU:CD2 | 2.72 | 0.56 |
| 1:L:346:ASP:OD1 | 1:L:362:THR:OG1 | 2.23 | 0.56 |
| 1:A:387:VAL:HG21 | 1:A:390:GLU:HB2 | 1.88 | 0.56 |
| 1:B:396:LEU:HD13 | 1:B:406:PRO:HD2 | 1.86 | 0.56 |
| 1:E:664:HIS:O | 1:E:665:HIS:CB | 2.51 | 0.56 |
| 1:G:560:SER:N | 1:G:561:GLY:HA2 | 2.20 | 0.56 |
| 1:H:568:ASN:CG | 1:H:569:ILE:N | 2.59 | 0.56 |
| 1:L:405:THR:O | 1:L:406:PRO:O | 2.23 | 0.56 |
| 1:L:568:ASN:CG | 1:L:569:ILE:N | 2.59 | 0.56 |
| 1:E:379:LYS:HG2 | 1:E:379:LYS:O | 2.05 | 0.56 |
| 1:E:387:VAL:O | 1:E:388:GLN:CD | 2.44 | 0.56 |
| 1:E:509:SER:OG | 1:E:626:ASP:N | 2.34 | 0.56 |
| 1:F:596:ASN:HD22 | 1:F:599:ALA:H | 1.54 | 0.56 |
| 1:F:644:ASN:ND2 | 1:F:644:ASN:C | 2.59 | 0.56 |
| 1:G:387:VAL:HG21 | 1:G:390:GLU:HB2 | 1.88 | 0.56 |
| 1:I:379:LYS:O | 1:I:379:LYS:HG2 | 2.05 | 0.56 |
| 1:I:389:ARG:HA | 1:I:392:ILE:CG1 | 2.29 | 0.56 |
| 1:J:405:THR:O | 1:J:406:PRO:O | 2.23 | 0.56 |
| 1:K:347:THR:O | 1:K:348:PHE:C | 2.44 | 0.56 |
| 1:K:386:THR:C | 1:K:388:GLN:H | 2.07 | 0.56 |
| 1:A:379:LYS:O | 1:A:379:LYS:HG2 | 2.05 | 0.56 |
| 1:E:387:VAL:HG21 | 1:E:390:GLU:HB2 | 1.88 | 0.56 |
| 1:E:617:GLU:HG3 | 1:E:618:VAL:HG13 | 1.85 | 0.56 |
| 1:K:448:TYR:CD1 | 1:K:642:PHE:HB2 | 2.41 | 0.56 |
| 1:L:596:ASN:HD22 | 1:L:599:ALA:H | 1.54 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:427:ASN:ND2 | 1:A:427:ASN:H | 2.03 | 0.56 |
| 1:B:366:SER:CB | 1:K:403:PRO:HA | 2.22 | 0.56 |
| 1:B:658:ILE:HD13 | 1:B:658:ILE:N | 2.21 | 0.56 |
| 1:C:388:GLN:O | 1:C:389:ARG:NE | 2.39 | 0.56 |
| 1:D:359:ALA:O | 1:D:376:ALA:HA | 2.06 | 0.56 |
| 1:D:647:ARG:HD3 | 1:D:649:GLN:HG3 | 1.88 | 0.56 |
| 1:E:401:LEU:HD12 | 1:H:364:THR:HG23 | 1.67 | 0.56 |
| 1:E:448:TYR:CD1 | 1:E:642:PHE:HB2 | 2.41 | 0.56 |
| 1:E:454:ILE:HG22 | 1:E:455:PHE:N | 2.20 | 0.56 |
| 1:H:396:LEU:HD13 | 1:H:406:PRO:HD2 | 1.87 | 0.56 |
| 1:I:342:ALA:CB | 1:I:362:THR:CG2 | 2.84 | 0.56 |
| 1:A:454:ILE:HG22 | 1:A:455:PHE:N | 2.20 | 0.55 |
| 1:B:596:ASN:HD22 | 1:B:599:ALA:H | 1.54 | 0.55 |
| 1:D:644:ASN:ND2 | 1:D:644:ASN:C | 2.59 | 0.55 |
| 1:E:385:THR:HG1 | 1:E:387:VAL:CG2 | 2.05 | 0.55 |
| 1:E:427:ASN:ND2 | 1:E:427:ASN:H | 2.03 | 0.55 |
| 1:I:388:GLN:O | 1:I:389:ARG:NE | 2.39 | 0.55 |
| 1:J:596:ASN:HD22 | 1:J:599:ALA:H | 1.54 | 0.55 |
| 1:K:385:THR:HG1 | 1:K:387:VAL:CG2 | 2.05 | 0.55 |
| 1:L:359:ALA:O | 1:L:376:ALA:HA | 2.06 | 0.55 |
| 1:A:382:LEU:HD21 | 1:A:643:GLU:HG3 | 1.87 | 0.55 |
| 1:B:359:ALA:O | 1:B:376:ALA:HA | 2.06 | 0.55 |
| 1:D:405:THR:O | 1:D:406:PRO:O | 2.23 | 0.55 |
| 1:G:342:ALA:CB | 1:G:362:THR:CG2 | 2.84 | 0.55 |
| 1:I:342:ALA:HB1 | 1:I:362:THR:CG2 | 2.37 | 0.55 |
| 1:I:358:GLN:OE1 | 1:I:377:LYS:HE3 | 2.07 | 0.55 |
| 1:I:448:TYR:CD1 | 1:I:642:PHE:HB2 | 2.41 | 0.55 |
| 1:J:346:ASP:OD1 | 1:J:362:THR:OG1 | 2.23 | 0.55 |
| 1:J:568:ASN:CG | 1:J:569:ILE:N | 2.59 | 0.55 |
| 1:K:358:GLN:OE1 | 1:K:377:LYS:HE3 | 2.07 | 0.55 |
| 1:A:560:SER:N | 1:A:561:GLY:HA2 | 2.20 | 0.55 |
| 1:C:382:LEU:HD21 | 1:C:643:GLU:HG3 | 1.87 | 0.55 |
| 1:C:385:THR:HB | 1:C:391:ASP:CG | 2.27 | 0.55 |
| 1:D:356:ILE:O | 1:D:379:LYS:HB3 | 2.06 | 0.55 |
| 1:D:509:SER:OG | 1:D:626:ASP:N | 2.32 | 0.55 |
| 1:D:658:ILE:HD13 | 1:D:658:ILE:N | 2.21 | 0.55 |
| 1:G:382:LEU:HD21 | 1:G:643:GLU:HG3 | 1.87 | 0.55 |
| 1:G:454:ILE:HG22 | 1:G:455:PHE:N | 2.20 | 0.55 |
| 1:J:409:ILE:CD1 | 1:J:410:SER:N | 2.67 | 0.55 |
| 1:K:342:ALA:CB | 1:K:362:THR:CG2 | 2.84 | 0.55 |
| 1:L:644:ASN:ND2 | 1:L:644:ASN:C | 2.59 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:347:THR:O | 1:A:348:PHE:C | 2.44 | 0.55 |
| 1:A:448:TYR:CD1 | 1:A:642:PHE:HB2 | 2.41 | 0.55 |
| 1:D:398:ASP:OD2 | 1:E:663:HIS:HB2 | 2.00 | 0.55 |
| 1:D:398:ASP:CG | 1:E:663:HIS:CG | 2.71 | 0.55 |
| 1:E:388:GLN:O | 1:E:389:ARG:NE | 2.39 | 0.55 |
| 1:E:526:PRO:O | 1:E:528:THR:CG2 | 2.55 | 0.55 |
| 1:I:560:SER:N | 1:I:561:GLY:HA2 | 2.20 | 0.55 |
| 1:J:356:ILE:O | 1:J:379:LYS:HB3 | 2.06 | 0.55 |
| 1:A:358:GLN:OE1 | 1:A:377:LYS:HE3 | 2.07 | 0.55 |
| 1:C:342:ALA:CB | 1:C:362:THR:CG2 | 2.84 | 0.55 |
| 1:C:448:TYR:CD1 | 1:C:642:PHE:HB2 | 2.41 | 0.55 |
| 1:C:454:ILE:HG22 | 1:C:455:PHE:N | 2.20 | 0.55 |
| 1:H:499:ILE:HG23 | 1:H:602:ILE:HB | 1.87 | 0.55 |
| 1:I:347:THR:O | 1:I:348:PHE:C | 2.44 | 0.55 |
| 1:I:382:LEU:HD21 | 1:I:643:GLU:HG3 | 1.87 | 0.55 |
| 1:I:486:ARG:NH1 | 1:I:500:LYS:O | 2.36 | 0.55 |
| 1:I:532:GLU:N | 1:I:532:GLU:OE2 | 2.39 | 0.55 |
| 1:K:427:ASN:ND2 | 1:K:427:ASN:H | 2.03 | 0.55 |
| 1:E:342:ALA:CB | 1:E:362:THR:CG2 | 2.84 | 0.55 |
| 1:E:403:PRO:HG3 | 1:H:366:SER:HA | 1.87 | 0.55 |
| 1:H:644:ASN:ND2 | 1:H:644:ASN:C | 2.59 | 0.55 |
| 1:K:389:ARG:HA | 1:K:392:ILE:CG1 | 2.29 | 0.55 |
| 1:C:379:LYS:HG2 | 1:C:379:LYS:O | 2.05 | 0.55 |
| 1:C:387:VAL:HG21 | 1:C:390:GLU:HB2 | 1.88 | 0.55 |
| 1:E:348:PHE:CZ | 1:G:664:HIS:HD2 | 2.13 | 0.55 |
| 1:F:499:ILE:HG23 | 1:F:602:ILE:HB | 1.87 | 0.55 |
| 1:F:647:ARG:HD3 | 1:F:649:GLN:HG3 | 1.88 | 0.55 |
| 1:H:346:ASP:OD1 | 1:H:362:THR:OG1 | 2.23 | 0.55 |
| 1:K:385:THR:HB | 1:K:391:ASP:CG | 2.27 | 0.55 |
| 1:K:532:GLU:N | 1:K:532:GLU:OE2 | 2.39 | 0.55 |
| 1:K:560:SER:N | 1:K:561:GLY:HA2 | 2.20 | 0.55 |
| 1:C:342:ALA:HB1 | 1:C:362:THR:CG2 | 2.37 | 0.55 |
| 1:E:525:ASN:HB3 | 1:E:526:PRO:CD | 2.17 | 0.55 |
| 1:G:342:ALA:HB1 | 1:G:362:THR:CG2 | 2.37 | 0.55 |
| 1:G:385:THR:CB | 1:G:389:ARG:H | 2.17 | 0.55 |
| 1:G:448:TYR:CD1 | 1:G:642:PHE:HB2 | 2.41 | 0.55 |
| 1:G:526:PRO:O | 1:G:528:THR:CG2 | 2.55 | 0.55 |
| 1:J:499:ILE:HG23 | 1:J:602:ILE:HB | 1.87 | 0.55 |
| 1:J:647:ARG:HD3 | 1:J:649:GLN:HG3 | 1.88 | 0.55 |
| 1:B:365:ASP:O | 1:B:367:THR:N | 2.40 | 0.55 |
| 1:D:400:ASN:HD21 | 1:E:662:GLU:CD | 2.10 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:648:PRO:HD2 | 1:D:649:GLN:HG2 | 1.89 | 0.55 |
| 1:E:387:VAL:C | 1:E:388:GLN:CG | 2.73 | 0.55 |
| 1:F:534:VAL:O | 1:F:534:VAL:HG12 | 2.07 | 0.55 |
| 1:G:358:GLN:OE1 | 1:G:377:LYS:HE3 | 2.07 | 0.55 |
| 1:I:454:ILE:HG22 | 1:I:455:PHE:N | 2.20 | 0.55 |
| 1:K:631:VAL:CG2 | 1:L:476:ILE:CG2 | 2.72 | 0.55 |
| 1:L:648:PRO:HD2 | 1:L:649:GLN:HG2 | 1.89 | 0.55 |
| 1:B:568:ASN:CG | 1:B:569:ILE:N | 2.59 | 0.55 |
| 1:B:648:PRO:HD2 | 1:B:649:GLN:HG2 | 1.89 | 0.55 |
| 1:G:347:THR:O | 1:G:348:PHE:C | 2.44 | 0.55 |
| 1:G:532:GLU:N | 1:G:532:GLU:OE2 | 2.39 | 0.55 |
| 1:H:365:ASP:OD1 | 1:H:367:THR:CG2 | 2.55 | 0.55 |
| 1:L:658:ILE:HD13 | 1:L:658:ILE:N | 2.21 | 0.55 |
| 1:A:403:PRO:N | 1:C:366:SER:HB3 | 2.21 | 0.54 |
| 1:B:347:THR:O | 1:B:348:PHE:C | 2.45 | 0.54 |
| 1:B:647:ARG:HD3 | 1:B:649:GLN:HG3 | 1.88 | 0.54 |
| 1:C:532:GLU:N | 1:C:532:GLU:OE2 | 2.40 | 0.54 |
| 1:C:560:SER:N | 1:C:561:GLY:HA2 | 2.20 | 0.54 |
| 1:D:596:ASN:HD22 | 1:D:599:ALA:H | 1.54 | 0.54 |
| 1:F:646:LEU:C | 1:F:646:LEU:CD2 | 2.72 | 0.54 |
| 1:G:631:VAL:CG2 | 1:H:476:ILE:HG22 | 2.34 | 0.54 |
| 1:H:356:ILE:O | 1:H:379:LYS:HB3 | 2.07 | 0.54 |
| 1:I:385:THR:HB | 1:I:391:ASP:CG | 2.27 | 0.54 |
| 1:K:342:ALA:HB1 | 1:K:362:THR:CG2 | 2.37 | 0.54 |
| 1:L:365:ASP:OD1 | 1:L:367:THR:CG2 | 2.55 | 0.54 |
| 1:L:365:ASP:O | 1:L:367:THR:N | 2.40 | 0.54 |
| 1:L:499:ILE:HG23 | 1:L:602:ILE:HB | 1.88 | 0.54 |
| 1:A:532:GLU:N | 1:A:532:GLU:OE2 | 2.39 | 0.54 |
| 1:A:605:ASN:HB3 | 1:A:608:LYS:HG3 | 1.89 | 0.54 |
| 1:C:526:PRO:O | 1:C:528:THR:CG2 | 2.55 | 0.54 |
| 1:F:568:ASN:CG | 1:F:569:ILE:N | 2.59 | 0.54 |
| 1:G:385:THR:HB | 1:G:391:ASP:CG | 2.27 | 0.54 |
| 1:G:389:ARG:HA | 1:G:392:ILE:CG1 | 2.29 | 0.54 |
| 1:J:359:ALA:O | 1:J:376:ALA:HA | 2.06 | 0.54 |
| 1:J:644:ASN:ND2 | 1:J:644:ASN:C | 2.59 | 0.54 |
| 1:L:509:SER:OG | 1:L:626:ASP:N | 2.32 | 0.54 |
| 1:A:342:ALA:HB1 | 1:A:362:THR:CG2 | 2.37 | 0.54 |
| 1:A:385:THR:HB | 1:A:391:ASP:CG | 2.27 | 0.54 |
| 1:C:605:ASN:HB3 | 1:C:608:LYS:HG3 | 1.89 | 0.54 |
| 1:E:342:ALA:HB1 | 1:E:362:THR:CG2 | 2.37 | 0.54 |
| 1:E:532:GLU:N | 1:E:532:GLU:OE2 | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:658:ILE:HD13 | 1:F:658:ILE:N | 2.21 | 0.54 |
| 1:H:658:ILE:HD13 | 1:H:658:ILE:N | 2.21 | 0.54 |
| 1:L:356:ILE:O | 1:L:379:LYS:HB3 | 2.06 | 0.54 |
| 1:A:389:ARG:HA | 1:A:392:ILE:CG1 | 2.29 | 0.54 |
| 1:D:657:PRO:O | 1:D:658:ILE:HD12 | 2.08 | 0.54 |
| 1:E:385:THR:HB | 1:E:391:ASP:CG | 2.27 | 0.54 |
| 1:F:359:ALA:O | 1:F:376:ALA:HA | 2.06 | 0.54 |
| 1:H:365:ASP:O | 1:H:367:THR:N | 2.40 | 0.54 |
| 1:J:534:VAL:O | 1:J:534:VAL:HG12 | 2.07 | 0.54 |
| 1:K:631:VAL:CG2 | 1:L:476:ILE:HG22 | 2.34 | 0.54 |
| 1:L:534:VAL:O | 1:L:534:VAL:HG12 | 2.07 | 0.54 |
| 1:B:427:ASN:ND2 | 1:B:427:ASN:N | 2.54 | 0.54 |
| 1:E:358:GLN:OE1 | 1:E:377:LYS:HE3 | 2.07 | 0.54 |
| 1:E:385:THR:CB | 1:E:389:ARG:H | 2.17 | 0.54 |
| 1:G:635:ARG:HH22 | 1:H:661:LEU:CD1 | 2.15 | 0.54 |
| 1:I:631:VAL:CG2 | 1:J:476:ILE:HG22 | 2.34 | 0.54 |
| 1:J:657:PRO:O | 1:J:658:ILE:HD12 | 2.08 | 0.54 |
| 1:B:356:ILE:O | 1:B:379:LYS:HB3 | 2.07 | 0.54 |
| 1:D:365:ASP:O | 1:D:367:THR:N | 2.40 | 0.54 |
| 1:E:347:THR:O | 1:E:348:PHE:C | 2.44 | 0.54 |
| 1:E:560:SER:N | 1:E:561:GLY:HA2 | 2.20 | 0.54 |
| 1:H:647:ARG:HD3 | 1:H:649:GLN:HG3 | 1.88 | 0.54 |
| 1:I:353:PHE:CE2 | 1:I:395:TYR:CD2 | 2.86 | 0.54 |
| 1:K:526:PRO:O | 1:K:528:THR:CG2 | 2.55 | 0.54 |
| 1:K:605:ASN:HB3 | 1:K:608:LYS:HG3 | 1.89 | 0.54 |
| 1:C:347:THR:O | 1:C:348:PHE:C | 2.44 | 0.54 |
| 1:C:358:GLN:OE1 | 1:C:377:LYS:HE3 | 2.07 | 0.54 |
| 1:F:365:ASP:O | 1:F:367:THR:N | 2.40 | 0.54 |
| 1:H:359:ALA:O | 1:H:376:ALA:HA | 2.07 | 0.54 |
| 1:I:526:PRO:O | 1:I:528:THR:CG2 | 2.55 | 0.54 |
| 1:L:647:ARG:HD3 | 1:L:649:GLN:HG3 | 1.88 | 0.54 |
| 1:B:534:VAL:O | 1:B:534:VAL:HG12 | 2.07 | 0.54 |
| 1:H:347:THR:O | 1:H:348:PHE:C | 2.46 | 0.54 |
| 1:H:657:PRO:O | 1:H:658:ILE:HD12 | 2.08 | 0.54 |
| 1:J:648:PRO:HD2 | 1:J:649:GLN:HG2 | 1.89 | 0.54 |
| 1:L:657:PRO:O | 1:L:658:ILE:HD12 | 2.08 | 0.54 |
| 1:A:536:TYR:HB2 | 1:A:586:ARG:NH1 | 2.23 | 0.54 |
| 1:B:365:ASP:OD1 | 1:B:367:THR:CG2 | 2.55 | 0.54 |
| 1:B:646:LEU:C | 1:B:646:LEU:CD2 | 2.72 | 0.54 |
| 1:D:595:ILE:HD12 | 1:D:595:ILE:N | 2.21 | 0.54 |
| 1:I:389:ARG:CA | 1:I:392:ILE:HG12 | 2.28 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:359:ALA:HB1 | 1:B:455:PHE:HE2 | 1.73 | 0.54 |
| 1:E:635:ARG:HG3 | 1:E:636:ASP:N | 2.19 | 0.54 |
| 1:F:356:ILE:O | 1:F:379:LYS:HB3 | 2.06 | 0.54 |
| 1:F:409:ILE:CD1 | 1:F:410:SER:O | 2.50 | 0.54 |
| 1:G:605:ASN:HB3 | 1:G:608:LYS:HG3 | 1.89 | 0.54 |
| 1:G:635:ARG:HG3 | 1:G:636:ASP:N | 2.19 | 0.54 |
| 1:H:596:ASN:ND2 | 1:H:599:ALA:H | 2.06 | 0.54 |
| 1:A:526:PRO:O | 1:A:528:THR:CG2 | 2.55 | 0.53 |
| 1:C:389:ARG:HA | 1:C:392:ILE:CG1 | 2.29 | 0.53 |
| 1:D:365:ASP:OD1 | 1:D:367:THR:CG2 | 2.55 | 0.53 |
| 1:D:396:LEU:HD22 | 1:D:406:PRO:HG2 | 1.90 | 0.53 |
| 1:D:534:VAL:O | 1:D:534:VAL:HG12 | 2.07 | 0.53 |
| 1:D:646:LEU:C | 1:D:646:LEU:CD2 | 2.72 | 0.53 |
| 1:I:631:VAL:CG2 | 1:J:476:ILE:CG2 | 2.72 | 0.53 |
| 1:J:365:ASP:OD1 | 1:J:367:THR:CG2 | 2.55 | 0.53 |
| 1:J:658:ILE:HD13 | 1:J:658:ILE:N | 2.21 | 0.53 |
| 1:K:412:ASN:O | 1:K:638:SER:HA | 2.08 | 0.53 |
| 1:B:526:PRO:HA | 1:B:529:GLY:O | 2.09 | 0.53 |
| 1:B:657:PRO:O | 1:B:658:ILE:HD12 | 2.08 | 0.53 |
| 1:D:359:ALA:HB1 | 1:D:455:PHE:HE2 | 1.73 | 0.53 |
| 1:D:526:PRO:HA | 1:D:529:GLY:O | 2.09 | 0.53 |
| 1:D:596:ASN:HB3 | 1:D:601:VAL:HG23 | 1.90 | 0.53 |
| 1:F:359:ALA:HB1 | 1:F:455:PHE:HE2 | 1.73 | 0.53 |
| 1:F:526:PRO:HA | 1:F:529:GLY:O | 2.08 | 0.53 |
| 1:J:365:ASP:O | 1:J:367:THR:N | 2.40 | 0.53 |
| 1:F:559:ALA:O | 1:F:561:GLY:N | 2.42 | 0.53 |
| 1:H:559:ALA:O | 1:H:561:GLY:N | 2.41 | 0.53 |
| 1:I:605:ASN:HB3 | 1:I:608:LYS:HG3 | 1.89 | 0.53 |
| 1:I:635:ARG:HH22 | 1:J:661:LEU:CD1 | 2.14 | 0.53 |
| 1:K:382:LEU:HD12 | 1:K:647:ARG:HH21 | 1.74 | 0.53 |
| 1:K:536:TYR:HB2 | 1:K:586:ARG:NH1 | 2.23 | 0.53 |
| 1:L:526:PRO:HA | 1:L:529:GLY:O | 2.08 | 0.53 |
| 1:L:559:ALA:O | 1:L:561:GLY:N | 2.42 | 0.53 |
| 1:A:631:VAL:CG2 | 1:B:476:ILE:CG2 | 2.72 | 0.53 |
| 1:B:542:SER:HB2 | 1:B:595:ILE:HG12 | 1.91 | 0.53 |
| 1:E:412:ASN:O | 1:E:638:SER:HA | 2.09 | 0.53 |
| 1:E:536:TYR:HB2 | 1:E:586:ARG:NH1 | 2.23 | 0.53 |
| 1:F:365:ASP:OD1 | 1:F:367:THR:CG2 | 2.55 | 0.53 |
| 1:H:526:PRO:HA | 1:H:529:GLY:O | 2.09 | 0.53 |
| 1:H:534:VAL:HG12 | 1:H:534:VAL:O | 2.07 | 0.53 |
| 1:H:596:ASN:HB3 | 1:H:601:VAL:HG23 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:412:ASN:O | 1:I:638:SER:HA | 2.08 | 0.53 |
| 1:K:635:ARG:HH22 | 1:L:661:LEU:CD1 | 2.15 | 0.53 |
| 1:L:542:SER:HB2 | 1:L:595:ILE:HG12 | 1.91 | 0.53 |
| 1:A:382:LEU:HD12 | 1:A:647:ARG:HH21 | 1.74 | 0.53 |
| 1:B:476:ILE:HG22 | 1:B:477:GLY:N | 2.18 | 0.53 |
| 1:E:605:ASN:HB3 | 1:E:608:LYS:HG3 | 1.89 | 0.53 |
| 1:G:428:LYS:HD2 | 1:G:473:HIS:HD2 | 1.74 | 0.53 |
| 1:H:648:PRO:HD2 | 1:H:649:GLN:HG2 | 1.89 | 0.53 |
| 1:J:542:SER:HB2 | 1:J:595:ILE:HG12 | 1.91 | 0.53 |
| 1:J:596:ASN:ND2 | 1:J:599:ALA:H | 2.06 | 0.53 |
| 1:C:382:LEU:HD12 | 1:C:647:ARG:HH21 | 1.74 | 0.53 |
| 1:D:400:ASN:H | 1:E:664:HIS:HB2 | 1.74 | 0.53 |
| 1:F:657:PRO:O | 1:F:658:ILE:HD12 | 2.08 | 0.53 |
| 1:G:412:ASN:O | 1:G:638:SER:HA | 2.08 | 0.53 |
| 1:A:428:LYS:HD2 | 1:A:473:HIS:HD2 | 1.74 | 0.53 |
| 1:A:619:GLN:HA | 1:A:619:GLN:HE21 | 1.74 | 0.53 |
| 1:B:565:GLU:C | 1:B:570:GLN:HE22 | 2.12 | 0.53 |
| 1:C:619:GLN:HA | 1:C:619:GLN:HE21 | 1.74 | 0.53 |
| 1:D:559:ALA:O | 1:D:561:GLY:N | 2.41 | 0.53 |
| 1:E:385:THR:CG2 | 1:E:389:ARG:C | 2.73 | 0.53 |
| 1:F:453:GLU:O | 1:F:454:ILE:HG13 | 2.09 | 0.53 |
| 1:G:343:THR:O | 1:G:347:THR:HG23 | 2.09 | 0.53 |
| 1:G:536:TYR:HB2 | 1:G:586:ARG:NH1 | 2.23 | 0.53 |
| 1:H:409:ILE:CD1 | 1:H:410:SER:O | 2.50 | 0.53 |
| 1:I:635:ARG:HG3 | 1:I:636:ASP:N | 2.19 | 0.53 |
| 1:L:348:PHE:O | 1:L:351:GLU:N | 2.21 | 0.53 |
| 1:L:565:GLU:C | 1:L:570:GLN:HE22 | 2.12 | 0.53 |
| 1:A:387:VAL:C | 1:A:388:GLN:CD | 2.68 | 0.53 |
| 1:A:631:VAL:CG2 | 1:B:476:ILE:HG22 | 2.34 | 0.53 |
| 1:B:596:ASN:ND2 | 1:B:599:ALA:H | 2.06 | 0.53 |
| 1:B:596:ASN:HB3 | 1:B:601:VAL:HG23 | 1.90 | 0.53 |
| 1:C:387:VAL:C | 1:C:388:GLN:CD | 2.68 | 0.53 |
| 1:C:536:TYR:HB2 | 1:C:586:ARG:NH1 | 2.23 | 0.53 |
| 1:D:343:THR:HB | 1:D:347:THR:CG2 | 2.39 | 0.53 |
| 1:D:542:SER:HB2 | 1:D:595:ILE:HG12 | 1.91 | 0.53 |
| 1:D:596:ASN:ND2 | 1:D:599:ALA:H | 2.06 | 0.53 |
| 1:F:648:PRO:HD2 | 1:F:649:GLN:HG2 | 1.89 | 0.53 |
| 1:I:343:THR:O | 1:I:347:THR:HG23 | 2.09 | 0.53 |
| 1:J:559:ALA:O | 1:J:561:GLY:N | 2.41 | 0.53 |
| 1:J:565:GLU:C | 1:J:570:GLN:HE22 | 2.12 | 0.53 |
| 1:K:387:VAL:C | 1:K:388:GLN:CD | 2.68 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:428:LYS:HD2 | 1:K:473:HIS:HD2 | 1.74 | 0.53 |
| 1:C:412:ASN:O | 1:C:638:SER:HA | 2.08 | 0.53 |
| 1:D:347:THR:O | 1:D:348:PHE:C | 2.45 | 0.53 |
| 1:H:453:GLU:O | 1:H:454:ILE:HG13 | 2.09 | 0.53 |
| 1:I:382:LEU:HD12 | 1:I:647:ARG:HH21 | 1.74 | 0.53 |
| 1:I:536:TYR:HB2 | 1:I:586:ARG:NH1 | 2.23 | 0.53 |
| 1:K:385:THR:CG2 | 1:K:389:ARG:C | 2.73 | 0.53 |
| 1:B:396:LEU:HD22 | 1:B:406:PRO:HG2 | 1.90 | 0.53 |
| 1:D:547:SER:O | 1:D:548:LYS:HG2 | 2.09 | 0.53 |
| 1:E:651:LEU:CD2 | 1:E:653:ILE:HG13 | 2.39 | 0.53 |
| 1:F:565:GLU:C | 1:F:570:GLN:HE22 | 2.12 | 0.53 |
| 1:F:596:ASN:HB3 | 1:F:601:VAL:HG23 | 1.90 | 0.53 |
| 1:H:343:THR:HB | 1:H:347:THR:CG2 | 2.39 | 0.53 |
| 1:J:343:THR:HB | 1:J:347:THR:CG2 | 2.39 | 0.53 |
| 1:J:568:ASN:OD1 | 1:J:569:ILE:N | 2.30 | 0.53 |
| 1:A:343:THR:O | 1:A:347:THR:HG23 | 2.09 | 0.52 |
| 1:B:440:ILE:HD11 | 1:B:653:ILE:HD13 | 1.91 | 0.52 |
| 1:B:547:SER:O | 1:B:548:LYS:HG2 | 2.09 | 0.52 |
| 1:B:559:ALA:O | 1:B:561:GLY:N | 2.41 | 0.52 |
| 1:E:631:VAL:CG2 | 1:F:476:ILE:HG22 | 2.34 | 0.52 |
| 1:F:343:THR:HB | 1:F:347:THR:CG2 | 2.39 | 0.52 |
| 1:G:382:LEU:HD12 | 1:G:647:ARG:HH21 | 1.74 | 0.52 |
| 1:G:385:THR:CB | 1:G:387:VAL:CG2 | 2.88 | 0.52 |
| 1:G:619:GLN:HE21 | 1:G:619:GLN:HA | 1.74 | 0.52 |
| 1:H:565:GLU:C | 1:H:570:GLN:HE22 | 2.12 | 0.52 |
| 1:I:385:THR:CB | 1:I:387:VAL:CG2 | 2.88 | 0.52 |
| 1:I:525:ASN:HB3 | 1:I:526:PRO:CD | 2.17 | 0.52 |
| 1:J:408:ILE:O | 1:J:409:ILE:HG23 | 2.09 | 0.52 |
| 1:L:343:THR:HB | 1:L:347:THR:CG2 | 2.39 | 0.52 |
| 1:L:408:ILE:HD12 | 1:L:409:ILE:CA | 2.40 | 0.52 |
| 1:C:452:VAL:HG22 | 1:C:458:SER:O | 2.10 | 0.52 |
| 1:D:565:GLU:C | 1:D:570:GLN:HE22 | 2.12 | 0.52 |
| 1:E:556:GLY:HA3 | 1:E:589:TYR:HD1 | 1.74 | 0.52 |
| 1:G:353:PHE:CE2 | 1:G:395:TYR:CD2 | 2.86 | 0.52 |
| 1:H:542:SER:HB2 | 1:H:595:ILE:HG12 | 1.91 | 0.52 |
| 1:I:491:PHE:CZ | 1:I:616:PHE:HB2 | 2.45 | 0.52 |
| 1:K:343:THR:O | 1:K:347:THR:HG23 | 2.09 | 0.52 |
| 1:L:547:SER:O | 1:L:548:LYS:HG2 | 2.09 | 0.52 |
| 1:C:631:VAL:CG2 | 1:D:476:ILE:HG22 | 2.34 | 0.52 |
| 1:D:400:ASN:CB | 1:E:662:GLU:HG2 | 2.39 | 0.52 |
| 1:D:453:GLU:O | 1:D:454:ILE:HG13 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:408:ILE:O | 1:F:409:ILE:HG23 | 2.09 | 0.52 |
| 1:H:408:ILE:O | 1:H:409:ILE:HG23 | 2.09 | 0.52 |
| 1:H:565:GLU:CB | 1:H:570:GLN:NE2 | 2.55 | 0.52 |
| 1:I:619:GLN:HA | 1:I:619:GLN:HE21 | 1.74 | 0.52 |
| 1:I:651:LEU:CD2 | 1:I:653:ILE:HG13 | 2.39 | 0.52 |
| 1:J:347:THR:O | 1:J:348:PHE:C | 2.46 | 0.52 |
| 1:J:453:GLU:O | 1:J:454:ILE:HG13 | 2.09 | 0.52 |
| 1:K:556:GLY:HA3 | 1:K:589:TYR:HD1 | 1.74 | 0.52 |
| 1:K:619:GLN:HA | 1:K:619:GLN:HE21 | 1.74 | 0.52 |
| 1:D:440:ILE:HD11 | 1:D:653:ILE:HD13 | 1.91 | 0.52 |
| 1:E:382:LEU:HD12 | 1:E:647:ARG:HH21 | 1.74 | 0.52 |
| 1:F:408:ILE:HD12 | 1:F:409:ILE:CA | 2.40 | 0.52 |
| 1:F:476:ILE:HG22 | 1:F:477:GLY:N | 2.18 | 0.52 |
| 1:F:547:SER:O | 1:F:548:LYS:HG2 | 2.09 | 0.52 |
| 1:I:428:LYS:HD2 | 1:I:473:HIS:HD2 | 1.74 | 0.52 |
| 1:J:359:ALA:HB1 | 1:J:455:PHE:HE2 | 1.73 | 0.52 |
| 1:L:440:ILE:HD11 | 1:L:653:ILE:HD13 | 1.91 | 0.52 |
| 1:L:596:ASN:ND2 | 1:L:599:ALA:H | 2.07 | 0.52 |
| 1:A:635:ARG:HH22 | 1:B:661:LEU:CD1 | 2.14 | 0.52 |
| 1:C:651:LEU:CD2 | 1:C:653:ILE:HG13 | 2.39 | 0.52 |
| 1:E:343:THR:O | 1:E:347:THR:HG23 | 2.09 | 0.52 |
| 1:E:619:GLN:HA | 1:E:619:GLN:HE21 | 1.74 | 0.52 |
| 1:F:472:ASP:OD2 | 1:F:474:SER:HB3 | 2.10 | 0.52 |
| 1:F:542:SER:HB2 | 1:F:595:ILE:HG12 | 1.91 | 0.52 |
| 1:G:452:VAL:HG22 | 1:G:458:SER:O | 2.10 | 0.52 |
| 1:G:651:LEU:CD2 | 1:G:653:ILE:HG13 | 2.39 | 0.52 |
| 1:I:387:VAL:C | 1:I:388:GLN:CD | 2.68 | 0.52 |
| 1:J:472:ASP:OD2 | 1:J:474:SER:HB3 | 2.10 | 0.52 |
| 1:J:596:ASN:HB3 | 1:J:601:VAL:HG23 | 1.90 | 0.52 |
| 1:L:359:ALA:HB1 | 1:L:455:PHE:HE2 | 1.73 | 0.52 |
| 1:L:453:GLU:O | 1:L:454:ILE:HG13 | 2.09 | 0.52 |
| 1:L:486:ARG:HG2 | 1:L:499:ILE:CD1 | 2.40 | 0.52 |
| 1:A:385:THR:CB | 1:A:387:VAL:CG2 | 2.88 | 0.52 |
| 1:A:412:ASN:O | 1:A:638:SER:HA | 2.08 | 0.52 |
| 1:C:343:THR:O | 1:C:347:THR:HG23 | 2.09 | 0.52 |
| 1:D:660:GLN:CA | 1:D:661:LEU:HB2 | 2.26 | 0.52 |
| 1:F:486:ARG:HG2 | 1:F:499:ILE:CD1 | 2.40 | 0.52 |
| 1:H:396:LEU:HD22 | 1:H:406:PRO:HG2 | 1.90 | 0.52 |
| 1:K:385:THR:CB | 1:K:387:VAL:CG2 | 2.88 | 0.52 |
| 1:A:491:PHE:CZ | 1:A:616:PHE:HB2 | 2.45 | 0.52 |
| 1:D:486:ARG:HG2 | 1:D:499:ILE:CD1 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:387:VAL:C | 1:E:388:GLN:CD | 2.68 | 0.52 |
| 1:F:596:ASN:ND2 | 1:F:599:ALA:H | 2.06 | 0.52 |
| 1:L:595:ILE:HD12 | 1:L:595:ILE:N | 2.21 | 0.52 |
| 1:B:408:ILE:HD12 | 1:B:409:ILE:CA | 2.40 | 0.52 |
| 1:C:533:ASP:O | 1:C:535:LEU:HD23 | 2.10 | 0.52 |
| 1:C:556:GLY:HA3 | 1:C:589:TYR:HD1 | 1.74 | 0.52 |
| 1:E:342:ALA:CB | 1:E:362:THR:O | 2.58 | 0.52 |
| 1:F:348:PHE:O | 1:F:350:SER:N | 2.43 | 0.52 |
| 1:F:382:LEU:HD12 | 1:F:646:LEU:HD13 | 1.92 | 0.52 |
| 1:F:440:ILE:HD11 | 1:F:653:ILE:HD13 | 1.91 | 0.52 |
| 1:F:660:GLN:CA | 1:F:661:LEU:HB2 | 2.26 | 0.52 |
| 1:G:387:VAL:C | 1:G:388:GLN:CD | 2.68 | 0.52 |
| 1:G:448:TYR:CE1 | 1:G:642:PHE:HB2 | 2.45 | 0.52 |
| 1:G:491:PHE:CZ | 1:G:616:PHE:HB2 | 2.45 | 0.52 |
| 1:J:526:PRO:HA | 1:J:529:GLY:O | 2.09 | 0.52 |
| 1:L:596:ASN:HB3 | 1:L:601:VAL:HG23 | 1.90 | 0.52 |
| 1:A:388:GLN:C | 1:A:389:ARG:HG3 | 2.30 | 0.52 |
| 1:A:651:LEU:CD2 | 1:A:653:ILE:HG13 | 2.39 | 0.52 |
| 1:B:343:THR:HB | 1:B:347:THR:CG2 | 2.39 | 0.52 |
| 1:B:453:GLU:O | 1:B:454:ILE:HG13 | 2.09 | 0.52 |
| 1:J:348:PHE:O | 1:J:350:SER:N | 2.43 | 0.52 |
| 1:J:486:ARG:HG2 | 1:J:499:ILE:CD1 | 2.40 | 0.52 |
| 1:K:554:ILE:HG22 | 1:K:591:VAL:HA | 1.92 | 0.52 |
| 1:A:342:ALA:CB | 1:A:362:THR:O | 2.58 | 0.52 |
| 1:B:472:ASP:OD2 | 1:B:474:SER:HB3 | 2.10 | 0.52 |
| 1:B:628:THR:HG22 | 1:B:629:ASP:OD1 | 2.10 | 0.52 |
| 1:E:388:GLN:C | 1:E:389:ARG:HG3 | 2.30 | 0.52 |
| 1:E:428:LYS:HD2 | 1:E:473:HIS:HD2 | 1.74 | 0.52 |
| 1:E:448:TYR:CE1 | 1:E:642:PHE:HB2 | 2.45 | 0.52 |
| 1:F:661:LEU:O | 1:F:661:LEU:CG | 2.58 | 0.52 |
| 1:H:359:ALA:HB1 | 1:H:455:PHE:HE2 | 1.73 | 0.52 |
| 1:J:396:LEU:HD22 | 1:J:406:PRO:HG2 | 1.90 | 0.52 |
| 1:J:409:ILE:CD1 | 1:J:410:SER:O | 2.50 | 0.52 |
| 1:A:342:ALA:HA | 1:A:362:THR:HG21 | 1.93 | 0.51 |
| 1:B:348:PHE:O | 1:B:350:SER:N | 2.43 | 0.51 |
| 1:B:523:VAL:HG11 | 1:B:532:GLU:HB2 | 1.92 | 0.51 |
| 1:C:342:ALA:CB | 1:C:362:THR:O | 2.58 | 0.51 |
| 1:C:448:TYR:CE1 | 1:C:642:PHE:HB2 | 2.45 | 0.51 |
| 1:C:491:PHE:CZ | 1:C:616:PHE:HB2 | 2.45 | 0.51 |
| 1:D:427:ASN:ND2 | 1:D:427:ASN:N | 2.54 | 0.51 |
| 1:D:523:VAL:HG11 | 1:D:532:GLU:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:491:PHE:CZ | 1:E:616:PHE:HB2 | 2.45 | 0.51 |
| 1:G:556:GLY:HA3 | 1:G:589:TYR:HD1 | 1.74 | 0.51 |
| 1:H:382:LEU:HD12 | 1:H:646:LEU:HD13 | 1.92 | 0.51 |
| 1:H:486:ARG:HG2 | 1:H:499:ILE:CD1 | 2.40 | 0.51 |
| 1:I:448:TYR:CE1 | 1:I:642:PHE:HB2 | 2.45 | 0.51 |
| 1:K:491:PHE:CZ | 1:K:616:PHE:HB2 | 2.45 | 0.51 |
| 1:L:348:PHE:O | 1:L:350:SER:N | 2.43 | 0.51 |
| 1:B:365:ASP:HB3 | 1:B:368:LYS:HB2 | 1.92 | 0.51 |
| 1:C:635:ARG:HG3 | 1:C:636:ASP:N | 2.19 | 0.51 |
| 1:E:452:VAL:HG22 | 1:E:458:SER:O | 2.10 | 0.51 |
| 1:E:554:ILE:HG22 | 1:E:591:VAL:HA | 1.92 | 0.51 |
| 1:I:533:ASP:O | 1:I:535:LEU:HD23 | 2.10 | 0.51 |
| 1:J:408:ILE:HD12 | 1:J:409:ILE:CA | 2.40 | 0.51 |
| 1:K:462:SER:HB3 | 1:L:478:SER:O | 2.11 | 0.51 |
| 1:B:409:ILE:HD13 | 1:B:410:SER:C | 2.31 | 0.51 |
| 1:B:486:ARG:HG2 | 1:B:499:ILE:CD1 | 2.40 | 0.51 |
| 1:E:462:SER:HB3 | 1:F:478:SER:O | 2.11 | 0.51 |
| 1:E:533:ASP:O | 1:E:535:LEU:HD23 | 2.10 | 0.51 |
| 1:G:388:GLN:C | 1:G:389:ARG:HG3 | 2.30 | 0.51 |
| 1:H:661:LEU:O | 1:H:661:LEU:CG | 2.58 | 0.51 |
| 1:I:342:ALA:HA | 1:I:362:THR:HG21 | 1.93 | 0.51 |
| 1:I:554:ILE:HG22 | 1:I:591:VAL:HA | 1.92 | 0.51 |
| 1:J:409:ILE:CD1 | 1:J:410:SER:C | 2.79 | 0.51 |
| 1:J:547:SER:O | 1:J:548:LYS:HG2 | 2.10 | 0.51 |
| 1:J:567:GLU:CA | 1:J:570:GLN:OE1 | 2.56 | 0.51 |
| 1:J:595:ILE:HD12 | 1:J:595:ILE:N | 2.21 | 0.51 |
| 1:K:533:ASP:O | 1:K:535:LEU:HD23 | 2.10 | 0.51 |
| 1:C:387:VAL:CG2 | 1:C:390:GLU:CD | 2.79 | 0.51 |
| 1:C:522:LYS:N | 1:C:522:LYS:CD | 2.72 | 0.51 |
| 1:F:365:ASP:CG | 1:F:367:THR:HG21 | 2.31 | 0.51 |
| 1:F:628:THR:HG22 | 1:F:629:ASP:OD1 | 2.10 | 0.51 |
| 1:H:348:PHE:O | 1:H:350:SER:N | 2.43 | 0.51 |
| 1:H:440:ILE:HD11 | 1:H:653:ILE:HD13 | 1.91 | 0.51 |
| 1:H:547:SER:O | 1:H:548:LYS:HG2 | 2.09 | 0.51 |
| 1:I:342:ALA:CB | 1:I:362:THR:O | 2.58 | 0.51 |
| 1:J:440:ILE:HD11 | 1:J:653:ILE:HD13 | 1.91 | 0.51 |
| 1:K:388:GLN:C | 1:K:389:ARG:HG3 | 2.30 | 0.51 |
| 1:L:472:ASP:OD2 | 1:L:474:SER:HB3 | 2.10 | 0.51 |
| 1:B:658:ILE:CD1 | 1:B:658:ILE:N | 2.73 | 0.51 |
| 1:C:428:LYS:HD2 | 1:C:473:HIS:HD2 | 1.74 | 0.51 |
| 1:E:353:PHE:CE2 | 1:E:395:TYR:CD2 | 2.86 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:385:THR:CG2 | 1:G:389:ARG:C | 2.73 | 0.51 |
| 1:G:462:SER:HB3 | 1:H:478:SER:O | 2.11 | 0.51 |
| 1:G:492:TYR:O | 1:G:606:ILE:HG13 | 2.11 | 0.51 |
| 1:G:533:ASP:O | 1:G:535:LEU:HD23 | 2.10 | 0.51 |
| 1:H:443:LYS:HG3 | 1:H:471:ALA:HB2 | 1.93 | 0.51 |
| 1:H:476:ILE:HG22 | 1:H:477:GLY:N | 2.18 | 0.51 |
| 1:K:342:ALA:HA | 1:K:362:THR:HG21 | 1.93 | 0.51 |
| 1:A:448:TYR:CE1 | 1:A:642:PHE:HB2 | 2.45 | 0.51 |
| 1:A:457:SER:N | 1:A:634:THR:HG23 | 2.26 | 0.51 |
| 1:A:462:SER:HB3 | 1:B:478:SER:O | 2.11 | 0.51 |
| 1:C:492:TYR:O | 1:C:606:ILE:HG13 | 2.11 | 0.51 |
| 1:C:554:ILE:HG22 | 1:C:591:VAL:HA | 1.92 | 0.51 |
| 1:F:443:LYS:HG3 | 1:F:471:ALA:HB2 | 1.93 | 0.51 |
| 1:F:565:GLU:CB | 1:F:570:GLN:NE2 | 2.55 | 0.51 |
| 1:H:409:ILE:HD13 | 1:H:410:SER:C | 2.31 | 0.51 |
| 1:I:452:VAL:HG22 | 1:I:458:SER:O | 2.10 | 0.51 |
| 1:I:462:SER:HB3 | 1:J:478:SER:O | 2.11 | 0.51 |
| 1:L:365:ASP:HB3 | 1:L:368:LYS:HB2 | 1.92 | 0.51 |
| 1:A:387:VAL:CG2 | 1:A:390:GLU:CD | 2.79 | 0.51 |
| 1:A:403:PRO:N | 1:C:366:SER:CB | 2.73 | 0.51 |
| 1:B:365:ASP:CG | 1:B:367:THR:HG21 | 2.31 | 0.51 |
| 1:B:595:ILE:HD12 | 1:B:595:ILE:N | 2.21 | 0.51 |
| 1:C:385:THR:CB | 1:C:387:VAL:CG2 | 2.88 | 0.51 |
| 1:D:348:PHE:O | 1:D:350:SER:N | 2.43 | 0.51 |
| 1:D:408:ILE:HD12 | 1:D:409:ILE:CA | 2.40 | 0.51 |
| 1:D:660:GLN:HA | 1:D:661:LEU:HB3 | 1.90 | 0.51 |
| 1:I:388:GLN:C | 1:I:389:ARG:HG3 | 2.30 | 0.51 |
| 1:J:628:THR:HG22 | 1:J:629:ASP:OD1 | 2.10 | 0.51 |
| 1:K:387:VAL:CG2 | 1:K:390:GLU:CD | 2.79 | 0.51 |
| 1:K:452:VAL:HG22 | 1:K:458:SER:O | 2.10 | 0.51 |
| 1:A:340:VAL:O | 1:A:341:THR:O | 2.29 | 0.51 |
| 1:A:492:TYR:O | 1:A:606:ILE:HG13 | 2.11 | 0.51 |
| 1:A:533:ASP:O | 1:A:535:LEU:HD23 | 2.10 | 0.51 |
| 1:A:554:ILE:HG22 | 1:A:591:VAL:HA | 1.92 | 0.51 |
| 1:A:651:LEU:HD23 | 1:A:652:THR:N | 2.26 | 0.51 |
| 1:C:353:PHE:O | 1:C:354:GLY:C | 2.48 | 0.51 |
| 1:C:388:GLN:C | 1:C:389:ARG:HG3 | 2.30 | 0.51 |
| 1:D:472:ASP:OD2 | 1:D:474:SER:HB3 | 2.10 | 0.51 |
| 1:D:492:TYR:CE1 | 1:D:606:ILE:HB | 2.46 | 0.51 |
| 1:E:340:VAL:O | 1:E:341:THR:O | 2.29 | 0.51 |
| 1:F:396:LEU:HD22 | 1:F:406:PRO:HG2 | 1.90 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:402:ALA:H | 1:H:403:PRO:CD | 2.24 | 0.51 |
| 1:J:661:LEU:O | 1:J:661:LEU:CG | 2.58 | 0.51 |
| 1:K:448:TYR:CE1 | 1:K:642:PHE:HB2 | 2.45 | 0.51 |
| 1:K:492:TYR:O | 1:K:606:ILE:HG13 | 2.11 | 0.51 |
| 1:K:651:LEU:HD23 | 1:K:652:THR:N | 2.26 | 0.51 |
| 1:L:402:ALA:H | 1:L:403:PRO:CD | 2.24 | 0.51 |
| 1:L:409:ILE:CD1 | 1:L:410:SER:C | 2.79 | 0.51 |
| 1:L:523:VAL:HG11 | 1:L:532:GLU:HB2 | 1.92 | 0.51 |
| 1:B:366:SER:HA | 1:K:403:PRO:HG3 | 1.89 | 0.51 |
| 1:B:409:ILE:CD1 | 1:B:410:SER:C | 2.79 | 0.51 |
| 1:C:340:VAL:O | 1:C:341:THR:O | 2.29 | 0.51 |
| 1:C:651:LEU:HD23 | 1:C:652:THR:N | 2.26 | 0.51 |
| 1:F:365:ASP:HB3 | 1:F:368:LYS:HB2 | 1.93 | 0.51 |
| 1:H:365:ASP:CG | 1:H:367:THR:HG21 | 2.31 | 0.51 |
| 1:H:408:ILE:HD12 | 1:H:409:ILE:CA | 2.40 | 0.51 |
| 1:H:409:ILE:CD1 | 1:H:410:SER:C | 2.79 | 0.51 |
| 1:H:628:THR:HG22 | 1:H:629:ASP:OD1 | 2.10 | 0.51 |
| 1:J:361:GLN:HE22 | 1:J:456:ASN:HD21 | 1.57 | 0.51 |
| 1:J:409:ILE:HD13 | 1:J:410:SER:C | 2.31 | 0.51 |
| 1:K:353:PHE:CE2 | 1:K:395:TYR:CD2 | 2.86 | 0.51 |
| 1:K:651:LEU:CD2 | 1:K:653:ILE:HG13 | 2.39 | 0.51 |
| 1:A:452:VAL:HG22 | 1:A:458:SER:O | 2.10 | 0.51 |
| 1:D:402:ALA:H | 1:D:403:PRO:CD | 2.24 | 0.51 |
| 1:F:396:LEU:HD13 | 1:F:405:THR:O | 2.11 | 0.51 |
| 1:F:567:GLU:O | 1:F:568:ASN:OD1 | 2.29 | 0.51 |
| 1:G:342:ALA:CB | 1:G:362:THR:O | 2.58 | 0.51 |
| 1:G:554:ILE:HG22 | 1:G:591:VAL:HA | 1.92 | 0.51 |
| 1:G:559:ALA:O | 1:G:561:GLY:CA | 2.34 | 0.51 |
| 1:H:361:GLN:HE22 | 1:H:456:ASN:HD21 | 1.57 | 0.51 |
| 1:H:595:ILE:HD12 | 1:H:595:ILE:N | 2.21 | 0.51 |
| 1:I:387:VAL:CG2 | 1:I:390:GLU:CD | 2.79 | 0.51 |
| 1:J:342:ALA:O | 1:J:346:ASP:OD2 | 2.29 | 0.51 |
| 1:K:340:VAL:O | 1:K:341:THR:O | 2.29 | 0.51 |
| 1:L:396:LEU:HD22 | 1:L:406:PRO:HG2 | 1.90 | 0.51 |
| 1:L:628:THR:HG22 | 1:L:629:ASP:OD1 | 2.10 | 0.51 |
| 1:B:382:LEU:HD12 | 1:B:646:LEU:HD13 | 1.92 | 0.50 |
| 1:B:443:LYS:HG3 | 1:B:471:ALA:HB2 | 1.93 | 0.50 |
| 1:B:661:LEU:O | 1:B:661:LEU:CG | 2.58 | 0.50 |
| 1:D:342:ALA:O | 1:D:346:ASP:OD2 | 2.29 | 0.50 |
| 1:D:361:GLN:HE22 | 1:D:456:ASN:HD21 | 1.57 | 0.50 |
| 1:D:409:ILE:HD13 | 1:D:410:SER:C | 2.31 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:628:THR:HG22 | 1:D:629:ASP:OD1 | 2.10 | 0.50 |
| 1:F:402:ALA:H | 1:F:403:PRO:CD | 2.24 | 0.50 |
| 1:H:492:TYR:CE1 | 1:H:606:ILE:HB | 2.46 | 0.50 |
| 1:H:523:VAL:HG11 | 1:H:532:GLU:HB2 | 1.92 | 0.50 |
| 1:J:382:LEU:HD12 | 1:J:646:LEU:HD13 | 1.92 | 0.50 |
| 1:K:342:ALA:CB | 1:K:362:THR:O | 2.58 | 0.50 |
| 1:L:382:LEU:HD12 | 1:L:646:LEU:HD13 | 1.92 | 0.50 |
| 1:L:408:ILE:O | 1:L:409:ILE:HG23 | 2.09 | 0.50 |
| 1:A:556:GLY:HA3 | 1:A:589:TYR:HD1 | 1.74 | 0.50 |
| 1:B:402:ALA:H | 1:B:403:PRO:CD | 2.24 | 0.50 |
| 1:D:510:MET:HB3 | 1:D:542:SER:HB3 | 1.94 | 0.50 |
| 1:E:387:VAL:CG2 | 1:E:390:GLU:CD | 2.79 | 0.50 |
| 1:E:492:TYR:O | 1:E:606:ILE:HG13 | 2.11 | 0.50 |
| 1:F:409:ILE:CD1 | 1:F:410:SER:C | 2.79 | 0.50 |
| 1:F:565:GLU:OE2 | 1:F:590:TYR:OH | 2.28 | 0.50 |
| 1:G:340:VAL:O | 1:G:341:THR:O | 2.29 | 0.50 |
| 1:H:472:ASP:OD2 | 1:H:474:SER:HB3 | 2.10 | 0.50 |
| 1:H:567:GLU:O | 1:H:568:ASN:OD1 | 2.29 | 0.50 |
| 1:I:466:THR:HB | 1:J:466:THR:HB | 1.94 | 0.50 |
| 1:I:651:LEU:HD23 | 1:I:652:THR:N | 2.26 | 0.50 |
| 1:J:492:TYR:CE1 | 1:J:606:ILE:HB | 2.46 | 0.50 |
| 1:J:565:GLU:OE2 | 1:J:590:TYR:OH | 2.28 | 0.50 |
| 1:K:457:SER:N | 1:K:634:THR:HG23 | 2.26 | 0.50 |
| 1:L:342:ALA:O | 1:L:346:ASP:OD2 | 2.29 | 0.50 |
| 1:L:443:LYS:HG3 | 1:L:471:ALA:HB2 | 1.93 | 0.50 |
| 1:L:660:GLN:HA | 1:L:661:LEU:HB3 | 1.90 | 0.50 |
| 1:A:342:ALA:HB1 | 1:A:362:THR:HG22 | 1.94 | 0.50 |
| 1:A:495:PRO:HD2 | 1:A:499:ILE:HG22 | 1.93 | 0.50 |
| 1:D:365:ASP:CG | 1:D:367:THR:HG21 | 2.31 | 0.50 |
| 1:D:365:ASP:HB3 | 1:D:368:LYS:HB2 | 1.93 | 0.50 |
| 1:D:396:LEU:HD13 | 1:D:405:THR:O | 2.11 | 0.50 |
| 1:D:409:ILE:CD1 | 1:D:410:SER:C | 2.79 | 0.50 |
| 1:D:423:THR:HB | 1:D:656:GLU:HB3 | 1.94 | 0.50 |
| 1:D:661:LEU:O | 1:D:661:LEU:CG | 2.58 | 0.50 |
| 1:F:361:GLN:HE22 | 1:F:456:ASN:HD21 | 1.57 | 0.50 |
| 1:F:409:ILE:HD13 | 1:F:410:SER:C | 2.31 | 0.50 |
| 1:G:342:ALA:HA | 1:G:362:THR:HG21 | 1.93 | 0.50 |
| 1:H:342:ALA:O | 1:H:346:ASP:OD2 | 2.29 | 0.50 |
| 1:H:396:LEU:HD13 | 1:H:405:THR:O | 2.11 | 0.50 |
| 1:H:565:GLU:OE2 | 1:H:590:TYR:OH | 2.28 | 0.50 |
| 1:I:403:PRO:CD | 1:L:366:SER:HA | 2.28 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:423:THR:HB | 1:L:656:GLU:HB3 | 1.94 | 0.50 |
| 1:L:510:MET:HB3 | 1:L:542:SER:HB3 | 1.93 | 0.50 |
| 1:A:348:PHE:HZ | 1:A:400:ASN:HD21 | 1.58 | 0.50 |
| 1:B:492:TYR:CE1 | 1:B:606:ILE:HB | 2.46 | 0.50 |
| 1:B:567:GLU:O | 1:B:568:ASN:OD1 | 2.29 | 0.50 |
| 1:C:340:VAL:O | 1:C:341:THR:OG1 | 2.30 | 0.50 |
| 1:D:342:ALA:O | 1:D:346:ASP:OD1 | 2.30 | 0.50 |
| 1:D:382:LEU:HD12 | 1:D:646:LEU:HD13 | 1.92 | 0.50 |
| 1:D:566:ASN:O | 1:D:570:GLN:OE1 | 2.30 | 0.50 |
| 1:E:495:PRO:HD2 | 1:E:499:ILE:HG22 | 1.93 | 0.50 |
| 1:I:340:VAL:O | 1:I:341:THR:O | 2.29 | 0.50 |
| 1:J:566:ASN:O | 1:J:568:ASN:OD1 | 2.30 | 0.50 |
| 1:K:466:THR:HB | 1:L:466:THR:HB | 1.94 | 0.50 |
| 1:L:347:THR:O | 1:L:348:PHE:C | 2.46 | 0.50 |
| 1:L:661:LEU:O | 1:L:661:LEU:CG | 2.58 | 0.50 |
| 1:A:517:PHE:HE1 | 1:A:615:LYS:HD2 | 1.77 | 0.50 |
| 1:C:342:ALA:HA | 1:C:362:THR:HG21 | 1.93 | 0.50 |
| 1:C:385:THR:CG2 | 1:C:389:ARG:C | 2.73 | 0.50 |
| 1:C:631:VAL:CG2 | 1:D:476:ILE:CG2 | 2.72 | 0.50 |
| 1:D:567:GLU:O | 1:D:568:ASN:OD1 | 2.29 | 0.50 |
| 1:E:466:THR:HB | 1:F:466:THR:HB | 1.94 | 0.50 |
| 1:E:510:MET:HB3 | 1:E:542:SER:OG | 2.12 | 0.50 |
| 1:F:347:THR:O | 1:F:348:PHE:O | 2.30 | 0.50 |
| 1:H:342:ALA:O | 1:H:346:ASP:OD1 | 2.30 | 0.50 |
| 1:I:437:GLU:C | 1:I:439:GLN:H | 2.15 | 0.50 |
| 1:J:402:ALA:H | 1:J:403:PRO:CD | 2.24 | 0.50 |
| 1:J:523:VAL:HG11 | 1:J:532:GLU:HB2 | 1.92 | 0.50 |
| 1:L:566:ASN:O | 1:L:568:ASN:OD1 | 2.30 | 0.50 |
| 1:A:437:GLU:C | 1:A:439:GLN:H | 2.15 | 0.50 |
| 1:B:342:ALA:O | 1:B:346:ASP:OD2 | 2.29 | 0.50 |
| 1:C:387:VAL:O | 1:C:388:GLN:OE1 | 2.30 | 0.50 |
| 1:E:385:THR:CB | 1:E:387:VAL:CG2 | 2.88 | 0.50 |
| 1:F:523:VAL:HG11 | 1:F:532:GLU:HB2 | 1.92 | 0.50 |
| 1:G:651:LEU:HD23 | 1:G:652:THR:N | 2.26 | 0.50 |
| 1:H:567:GLU:CA | 1:H:570:GLN:OE1 | 2.56 | 0.50 |
| 1:J:347:THR:O | 1:J:348:PHE:O | 2.30 | 0.50 |
| 1:J:443:LYS:HG3 | 1:J:471:ALA:HB2 | 1.93 | 0.50 |
| 1:J:476:ILE:HG22 | 1:J:477:GLY:N | 2.18 | 0.50 |
| 1:J:510:MET:HB3 | 1:J:542:SER:HB3 | 1.94 | 0.50 |
| 1:K:340:VAL:C | 1:K:341:THR:CG2 | 2.62 | 0.50 |
| 1:K:517:PHE:HE1 | 1:K:615:LYS:HD2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:361:GLN:HE22 | 1:B:456:ASN:HD21 | 1.57 | 0.50 |
| 1:B:423:THR:HB | 1:B:656:GLU:HB3 | 1.94 | 0.50 |
| 1:B:448:TYR:O | 1:B:453:GLU:HG3 | 2.12 | 0.50 |
| 1:E:517:PHE:HE1 | 1:E:615:LYS:HD2 | 1.77 | 0.50 |
| 1:F:492:TYR:CE1 | 1:F:606:ILE:HB | 2.46 | 0.50 |
| 1:G:437:GLU:C | 1:G:439:GLN:H | 2.15 | 0.50 |
| 1:G:510:MET:HB3 | 1:G:542:SER:OG | 2.12 | 0.50 |
| 1:I:517:PHE:HE1 | 1:I:615:LYS:HD2 | 1.77 | 0.50 |
| 1:J:567:GLU:O | 1:J:568:ASN:OD1 | 2.29 | 0.50 |
| 1:J:655:LEU:HD12 | 1:J:655:LEU:N | 2.27 | 0.50 |
| 1:K:387:VAL:O | 1:K:388:GLN:OE1 | 2.30 | 0.50 |
| 1:L:448:TYR:O | 1:L:453:GLU:HG3 | 2.12 | 0.50 |
| 1:A:466:THR:HB | 1:B:466:THR:HB | 1.94 | 0.50 |
| 1:B:507:ASP:OD1 | 1:B:545:ARG:HG3 | 2.12 | 0.50 |
| 1:C:462:SER:HB3 | 1:D:478:SER:O | 2.11 | 0.50 |
| 1:C:525:ASN:HB3 | 1:C:526:PRO:CD | 2.17 | 0.50 |
| 1:E:342:ALA:HA | 1:E:362:THR:HG21 | 1.93 | 0.50 |
| 1:G:387:VAL:CG2 | 1:G:390:GLU:CD | 2.79 | 0.50 |
| 1:H:365:ASP:HB3 | 1:H:368:LYS:HB2 | 1.92 | 0.50 |
| 1:I:492:TYR:O | 1:I:606:ILE:HG13 | 2.11 | 0.50 |
| 1:I:510:MET:HB3 | 1:I:542:SER:OG | 2.12 | 0.50 |
| 1:J:396:LEU:HD13 | 1:J:405:THR:O | 2.11 | 0.50 |
| 1:K:495:PRO:HD2 | 1:K:499:ILE:HG22 | 1.93 | 0.50 |
| 1:L:365:ASP:CG | 1:L:367:THR:HG21 | 2.31 | 0.50 |
| 1:L:409:ILE:HD13 | 1:L:410:SER:C | 2.31 | 0.50 |
| 1:B:566:ASN:O | 1:B:570:GLN:OE1 | 2.30 | 0.50 |
| 1:D:655:LEU:HD12 | 1:D:655:LEU:N | 2.27 | 0.50 |
| 1:E:342:ALA:HB2 | 1:E:362:THR:HG22 | 1.94 | 0.50 |
| 1:E:607:ALA:O | 1:E:609:ILE:O | 2.30 | 0.50 |
| 1:G:466:THR:HB | 1:H:466:THR:HB | 1.94 | 0.50 |
| 1:H:347:THR:O | 1:H:348:PHE:O | 2.30 | 0.50 |
| 1:I:587:ASP:O | 1:I:587:ASP:OD2 | 2.30 | 0.50 |
| 1:I:607:ALA:O | 1:I:609:ILE:O | 2.30 | 0.50 |
| 1:J:365:ASP:HB3 | 1:J:368:LYS:HB2 | 1.93 | 0.50 |
| 1:K:401:LEU:HG | 1:K:402:ALA:N | 2.27 | 0.50 |
| 1:K:437:GLU:C | 1:K:439:GLN:H | 2.15 | 0.50 |
| 1:L:347:THR:O | 1:L:348:PHE:O | 2.30 | 0.50 |
| 1:L:492:TYR:CE1 | 1:L:606:ILE:HB | 2.46 | 0.50 |
| 1:L:567:GLU:O | 1:L:568:ASN:OD1 | 2.29 | 0.50 |
| 1:A:361:GLN:NE2 | 1:A:361:GLN:HA | 2.27 | 0.49 |
| 1:C:466:THR:HB | 1:D:466:THR:HB | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:510:MET:HB3 | 1:C:542:SER:OG | 2.12 | 0.49 |
| 1:D:448:TYR:O | 1:D:453:GLU:HG3 | 2.12 | 0.49 |
| 1:D:566:ASN:O | 1:D:568:ASN:OD1 | 2.30 | 0.49 |
| 1:E:651:LEU:HD23 | 1:E:652:THR:N | 2.26 | 0.49 |
| 1:F:347:THR:O | 1:F:348:PHE:C | 2.46 | 0.49 |
| 1:F:567:GLU:CA | 1:F:570:GLN:OE1 | 2.56 | 0.49 |
| 1:G:340:VAL:O | 1:G:341:THR:OG1 | 2.30 | 0.49 |
| 1:J:365:ASP:CG | 1:J:367:THR:HG21 | 2.31 | 0.49 |
| 1:J:566:ASN:O | 1:J:570:GLN:OE1 | 2.30 | 0.49 |
| 1:K:342:ALA:HB1 | 1:K:362:THR:HG22 | 1.94 | 0.49 |
| 1:A:342:ALA:HB2 | 1:A:362:THR:HG22 | 1.93 | 0.49 |
| 1:B:492:TYR:CE1 | 1:B:611:LEU:O | 2.66 | 0.49 |
| 1:B:510:MET:HB3 | 1:B:542:SER:HB3 | 1.94 | 0.49 |
| 1:C:342:ALA:HB2 | 1:C:362:THR:HG22 | 1.93 | 0.49 |
| 1:C:353:PHE:CE2 | 1:C:395:TYR:CD2 | 2.86 | 0.49 |
| 1:D:443:LYS:HG3 | 1:D:471:ALA:HB2 | 1.93 | 0.49 |
| 1:D:567:GLU:C | 1:D:568:ASN:OD1 | 2.51 | 0.49 |
| 1:F:566:ASN:O | 1:F:568:ASN:OD1 | 2.30 | 0.49 |
| 1:G:387:VAL:O | 1:G:388:GLN:OE1 | 2.30 | 0.49 |
| 1:H:655:LEU:HD12 | 1:H:655:LEU:N | 2.27 | 0.49 |
| 1:I:391:ASP:OD1 | 1:I:391:ASP:N | 2.46 | 0.49 |
| 1:I:556:GLY:HA3 | 1:I:589:TYR:HD1 | 1.74 | 0.49 |
| 1:L:361:GLN:HE22 | 1:L:456:ASN:HD21 | 1.57 | 0.49 |
| 1:A:387:VAL:O | 1:A:388:GLN:OE1 | 2.30 | 0.49 |
| 1:A:510:MET:HB3 | 1:A:542:SER:OG | 2.12 | 0.49 |
| 1:B:347:THR:O | 1:B:348:PHE:O | 2.30 | 0.49 |
| 1:B:566:ASN:O | 1:B:568:ASN:OD1 | 2.30 | 0.49 |
| 1:B:566:ASN:CA | 1:B:570:GLN:HE22 | 2.26 | 0.49 |
| 1:B:567:GLU:C | 1:B:568:ASN:OD1 | 2.51 | 0.49 |
| 1:C:348:PHE:HZ | 1:C:400:ASN:HD21 | 1.59 | 0.49 |
| 1:C:517:PHE:HE1 | 1:C:615:LYS:HD2 | 1.77 | 0.49 |
| 1:C:607:ALA:O | 1:C:609:ILE:O | 2.30 | 0.49 |
| 1:D:492:TYR:CE1 | 1:D:611:LEU:O | 2.65 | 0.49 |
| 1:E:361:GLN:HA | 1:E:361:GLN:NE2 | 2.27 | 0.49 |
| 1:E:457:SER:N | 1:E:634:THR:HG23 | 2.26 | 0.49 |
| 1:F:567:GLU:C | 1:F:568:ASN:OD1 | 2.51 | 0.49 |
| 1:G:361:GLN:NE2 | 1:G:361:GLN:HA | 2.27 | 0.49 |
| 1:G:495:PRO:HD2 | 1:G:499:ILE:HG22 | 1.93 | 0.49 |
| 1:J:507:ASP:OD1 | 1:J:545:ARG:HG3 | 2.12 | 0.49 |
| 1:K:607:ALA:O | 1:K:609:ILE:O | 2.30 | 0.49 |
| 1:L:492:TYR:CE1 | 1:L:611:LEU:O | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:507:ASP:OD1 | 1:L:545:ARG:HG3 | 2.12 | 0.49 |
| 1:L:655:LEU:HD12 | 1:L:655:LEU:N | 2.27 | 0.49 |
| 1:B:567:GLU:CA | 1:B:570:GLN:OE1 | 2.56 | 0.49 |
| 1:C:437:GLU:C | 1:C:439:GLN:H | 2.15 | 0.49 |
| 1:E:437:GLU:C | 1:E:439:GLN:H | 2.15 | 0.49 |
| 1:F:507:ASP:OD1 | 1:F:545:ARG:HG3 | 2.12 | 0.49 |
| 1:H:566:ASN:O | 1:H:568:ASN:OD1 | 2.30 | 0.49 |
| 1:H:566:ASN:O | 1:H:570:GLN:OE1 | 2.30 | 0.49 |
| 1:I:457:SER:N | 1:I:634:THR:HG23 | 2.26 | 0.49 |
| 1:J:342:ALA:O | 1:J:346:ASP:OD1 | 2.30 | 0.49 |
| 1:J:565:GLU:CB | 1:J:570:GLN:NE2 | 2.55 | 0.49 |
| 1:K:510:MET:HB3 | 1:K:542:SER:OG | 2.12 | 0.49 |
| 1:A:401:LEU:HG | 1:A:402:ALA:N | 2.28 | 0.49 |
| 1:B:353:PHE:CZ | 1:B:395:TYR:HE2 | 2.11 | 0.49 |
| 1:B:396:LEU:HD13 | 1:B:405:THR:O | 2.11 | 0.49 |
| 1:D:566:ASN:CA | 1:D:570:GLN:HE22 | 2.26 | 0.49 |
| 1:D:567:GLU:CA | 1:D:570:GLN:OE1 | 2.56 | 0.49 |
| 1:E:342:ALA:HB1 | 1:E:362:THR:HG22 | 1.94 | 0.49 |
| 1:F:342:ALA:O | 1:F:346:ASP:OD1 | 2.30 | 0.49 |
| 1:F:566:ASN:O | 1:F:570:GLN:OE1 | 2.30 | 0.49 |
| 1:F:655:LEU:N | 1:F:655:LEU:HD12 | 2.27 | 0.49 |
| 1:G:342:ALA:HB2 | 1:G:362:THR:HG22 | 1.93 | 0.49 |
| 1:K:361:GLN:HA | 1:K:361:GLN:NE2 | 2.27 | 0.49 |
| 1:B:342:ALA:O | 1:B:346:ASP:OD1 | 2.30 | 0.49 |
| 1:B:366:SER:HB3 | 1:K:403:PRO:N | 2.17 | 0.49 |
| 1:B:448:TYR:CD1 | 1:B:642:PHE:HB2 | 2.48 | 0.49 |
| 1:C:495:PRO:HD2 | 1:C:499:ILE:HG22 | 1.93 | 0.49 |
| 1:E:522:LYS:N | 1:E:522:LYS:CD | 2.72 | 0.49 |
| 1:G:607:ALA:O | 1:G:609:ILE:O | 2.30 | 0.49 |
| 1:I:387:VAL:O | 1:I:388:GLN:OE1 | 2.30 | 0.49 |
| 1:I:495:PRO:HD2 | 1:I:499:ILE:HG22 | 1.93 | 0.49 |
| 1:J:427:ASN:ND2 | 1:J:427:ASN:N | 2.54 | 0.49 |
| 1:K:342:ALA:HB2 | 1:K:362:THR:HG22 | 1.94 | 0.49 |
| 1:L:396:LEU:HD13 | 1:L:405:THR:O | 2.11 | 0.49 |
| 1:L:567:GLU:CA | 1:L:570:GLN:OE1 | 2.56 | 0.49 |
| 1:B:447:TYR:HB2 | 1:B:467:TYR:CG | 2.48 | 0.49 |
| 1:C:587:ASP:OD2 | 1:C:587:ASP:O | 2.30 | 0.49 |
| 1:D:408:ILE:HD12 | 1:D:409:ILE:HA | 1.95 | 0.49 |
| 1:D:507:ASP:OD1 | 1:D:545:ARG:HG3 | 2.12 | 0.49 |
| 1:E:587:ASP:O | 1:E:587:ASP:OD2 | 2.30 | 0.49 |
| 1:F:492:TYR:CE1 | 1:F:611:LEU:O | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:401:LEU:HG | 1:G:402:ALA:N | 2.27 | 0.49 |
| 1:G:466:THR:CG2 | 1:H:466:THR:HB | 2.43 | 0.49 |
| 1:H:346:ASP:HB3 | 1:H:360:VAL:HB | 1.95 | 0.49 |
| 1:H:448:TYR:O | 1:H:453:GLU:HG3 | 2.12 | 0.49 |
| 1:H:510:MET:HB3 | 1:H:542:SER:HB3 | 1.94 | 0.49 |
| 1:J:540:ILE:HG22 | 1:J:555:ILE:CG1 | 2.43 | 0.49 |
| 1:L:597:TYR:HB2 | 1:L:598:PRO:HD3 | 1.95 | 0.49 |
| 1:C:385:THR:C | 1:C:387:VAL:N | 2.66 | 0.49 |
| 1:D:347:THR:O | 1:D:348:PHE:O | 2.30 | 0.49 |
| 1:E:387:VAL:O | 1:E:388:GLN:OE1 | 2.30 | 0.49 |
| 1:F:566:ASN:CA | 1:F:570:GLN:HE22 | 2.26 | 0.49 |
| 1:J:448:TYR:CD1 | 1:J:642:PHE:HB2 | 2.48 | 0.49 |
| 1:L:567:GLU:C | 1:L:568:ASN:OD1 | 2.51 | 0.49 |
| 1:A:385:THR:HG23 | 1:A:385:THR:O | 2.12 | 0.49 |
| 1:A:522:LYS:N | 1:A:522:LYS:CD | 2.72 | 0.49 |
| 1:A:607:ALA:O | 1:A:609:ILE:O | 2.30 | 0.49 |
| 1:B:412:ASN:ND2 | 1:B:486:ARG:NH2 | 2.61 | 0.49 |
| 1:C:340:VAL:C | 1:C:341:THR:CG2 | 2.62 | 0.49 |
| 1:C:361:GLN:HA | 1:C:361:GLN:NE2 | 2.27 | 0.49 |
| 1:D:401:LEU:CG | 1:D:403:PRO:HD2 | 2.42 | 0.49 |
| 1:D:448:TYR:CD1 | 1:D:642:PHE:HB2 | 2.48 | 0.49 |
| 1:F:346:ASP:HB3 | 1:F:360:VAL:HB | 1.95 | 0.49 |
| 1:F:423:THR:HB | 1:F:656:GLU:HB3 | 1.94 | 0.49 |
| 1:G:391:ASP:N | 1:G:391:ASP:OD1 | 2.46 | 0.49 |
| 1:G:457:SER:N | 1:G:634:THR:HG23 | 2.26 | 0.49 |
| 1:G:587:ASP:OD2 | 1:G:587:ASP:O | 2.30 | 0.49 |
| 1:G:631:VAL:CG2 | 1:H:476:ILE:CG2 | 2.72 | 0.49 |
| 1:H:507:ASP:OD1 | 1:H:545:ARG:HG3 | 2.12 | 0.49 |
| 1:I:361:GLN:NE2 | 1:I:361:GLN:HA | 2.27 | 0.49 |
| 1:J:412:ASN:ND2 | 1:J:486:ARG:NH2 | 2.61 | 0.49 |
| 1:L:447:TYR:HB2 | 1:L:467:TYR:CG | 2.48 | 0.49 |
| 1:L:448:TYR:CD1 | 1:L:642:PHE:HB2 | 2.48 | 0.49 |
| 1:L:566:ASN:CA | 1:L:570:GLN:HE22 | 2.26 | 0.49 |
| 1:A:391:ASP:OD1 | 1:A:391:ASP:N | 2.46 | 0.49 |
| 1:C:385:THR:HG23 | 1:C:385:THR:O | 2.12 | 0.49 |
| 1:C:401:LEU:HG | 1:C:402:ALA:N | 2.27 | 0.49 |
| 1:D:662:GLU:O | 1:D:662:GLU:HG2 | 2.13 | 0.49 |
| 1:E:340:VAL:HA | 1:E:345:TYR:HH | 1.68 | 0.49 |
| 1:F:540:ILE:HG22 | 1:F:555:ILE:CG1 | 2.43 | 0.49 |
| 1:H:412:ASN:ND2 | 1:H:486:ARG:NH2 | 2.61 | 0.49 |
| 1:H:447:TYR:HB2 | 1:H:467:TYR:CG | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:423:THR:HB | 1:J:656:GLU:HB3 | 1.94 | 0.49 |
| 1:J:447:TYR:HB2 | 1:J:467:TYR:CG | 2.48 | 0.49 |
| 1:J:448:TYR:O | 1:J:453:GLU:HG3 | 2.12 | 0.49 |
| 1:J:662:GLU:O | 1:J:662:GLU:HG2 | 2.13 | 0.49 |
| 1:K:358:GLN:HB2 | 1:K:379:LYS:CB | 2.43 | 0.49 |
| 1:K:385:THR:HG23 | 1:K:385:THR:O | 2.12 | 0.49 |
| 1:K:466:THR:CG2 | 1:L:466:THR:HB | 2.43 | 0.49 |
| 1:L:566:ASN:O | 1:L:570:GLN:OE1 | 2.30 | 0.49 |
| 1:A:531:GLU:C | 1:A:532:GLU:OE1 | 2.52 | 0.48 |
| 1:A:536:TYR:CD1 | 1:A:586:ARG:CD | 2.96 | 0.48 |
| 1:C:391:ASP:OD1 | 1:C:391:ASP:N | 2.46 | 0.48 |
| 1:C:466:THR:CG2 | 1:D:466:THR:HB | 2.43 | 0.48 |
| 1:C:518:ASN:OD1 | 1:C:533:ASP:CB | 2.60 | 0.48 |
| 1:E:403:PRO:N | 1:H:366:SER:HB3 | 2.16 | 0.48 |
| 1:G:385:THR:HG23 | 1:G:385:THR:O | 2.12 | 0.48 |
| 1:G:518:ASN:OD1 | 1:G:533:ASP:CB | 2.60 | 0.48 |
| 1:H:448:TYR:CD1 | 1:H:642:PHE:HB2 | 2.48 | 0.48 |
| 1:H:567:GLU:C | 1:H:568:ASN:OD1 | 2.51 | 0.48 |
| 1:I:353:PHE:O | 1:I:354:GLY:C | 2.48 | 0.48 |
| 1:I:385:THR:HG23 | 1:I:385:THR:O | 2.12 | 0.48 |
| 1:I:466:THR:CG2 | 1:J:466:THR:HB | 2.43 | 0.48 |
| 1:I:558:PHE:O | 1:I:586:ARG:HB3 | 2.13 | 0.48 |
| 1:J:597:TYR:HB2 | 1:J:598:PRO:HD3 | 1.95 | 0.48 |
| 1:K:536:TYR:CD1 | 1:K:586:ARG:CD | 2.96 | 0.48 |
| 1:B:346:ASP:HB3 | 1:B:360:VAL:HB | 1.95 | 0.48 |
| 1:B:401:LEU:CG | 1:B:403:PRO:HD2 | 2.42 | 0.48 |
| 1:D:414:LEU:HD23 | 1:D:414:LEU:HA | 1.70 | 0.48 |
| 1:E:536:TYR:CD1 | 1:E:586:ARG:CD | 2.96 | 0.48 |
| 1:F:510:MET:HB3 | 1:F:542:SER:HB3 | 1.94 | 0.48 |
| 1:F:661:LEU:C | 1:F:663:HIS:N | 2.61 | 0.48 |
| 1:H:492:TYR:CE1 | 1:H:611:LEU:O | 2.66 | 0.48 |
| 1:K:531:GLU:C | 1:K:532:GLU:OE1 | 2.52 | 0.48 |
| 1:A:358:GLN:HB2 | 1:A:379:LYS:CB | 2.43 | 0.48 |
| 1:C:358:GLN:HB2 | 1:C:379:LYS:CB | 2.43 | 0.48 |
| 1:D:508:ARG:HG2 | 1:D:577:PHE:HA | 1.96 | 0.48 |
| 1:E:358:GLN:HB2 | 1:E:379:LYS:CB | 2.43 | 0.48 |
| 1:F:412:ASN:ND2 | 1:F:486:ARG:NH2 | 2.61 | 0.48 |
| 1:F:447:TYR:HB2 | 1:F:467:TYR:CG | 2.48 | 0.48 |
| 1:G:342:ALA:HB1 | 1:G:362:THR:HG22 | 1.94 | 0.48 |
| 1:G:517:PHE:HE1 | 1:G:615:LYS:HD2 | 1.77 | 0.48 |
| 1:H:423:THR:HB | 1:H:656:GLU:HB3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:342:ALA:HB1 | 1:I:362:THR:HG22 | 1.94 | 0.48 |
| 1:I:358:GLN:HB2 | 1:I:379:LYS:CB | 2.43 | 0.48 |
| 1:I:385:THR:C | 1:I:387:VAL:N | 2.66 | 0.48 |
| 1:J:346:ASP:HB3 | 1:J:360:VAL:HB | 1.95 | 0.48 |
| 1:A:385:THR:C | 1:A:387:VAL:N | 2.66 | 0.48 |
| 1:B:597:TYR:HB2 | 1:B:598:PRO:HD3 | 1.95 | 0.48 |
| 1:B:655:LEU:HD12 | 1:B:655:LEU:N | 2.27 | 0.48 |
| 1:C:342:ALA:HB1 | 1:C:362:THR:HG22 | 1.94 | 0.48 |
| 1:C:361:GLN:CG | 1:C:455:PHE:CD1 | 2.97 | 0.48 |
| 1:C:424:TYR:HB3 | 1:C:475:VAL:H | 1.78 | 0.48 |
| 1:D:658:ILE:CD1 | 1:D:658:ILE:N | 2.74 | 0.48 |
| 1:E:385:THR:HG23 | 1:E:385:THR:O | 2.12 | 0.48 |
| 1:E:466:THR:CG2 | 1:F:466:THR:HB | 2.43 | 0.48 |
| 1:F:662:GLU:O | 1:F:662:GLU:HG2 | 2.13 | 0.48 |
| 1:G:353:PHE:O | 1:G:354:GLY:C | 2.48 | 0.48 |
| 1:J:492:TYR:CE1 | 1:J:611:LEU:O | 2.66 | 0.48 |
| 1:J:567:GLU:C | 1:J:568:ASN:OD1 | 2.51 | 0.48 |
| 1:F:448:TYR:O | 1:F:453:GLU:HG3 | 2.12 | 0.48 |
| 1:F:595:ILE:HD12 | 1:F:595:ILE:N | 2.21 | 0.48 |
| 1:G:358:GLN:HB2 | 1:G:379:LYS:CB | 2.43 | 0.48 |
| 1:G:545:ARG:HB3 | 1:G:597:TYR:CE2 | 2.49 | 0.48 |
| 1:I:342:ALA:HB2 | 1:I:362:THR:HG22 | 1.93 | 0.48 |
| 1:I:401:LEU:HG | 1:I:402:ALA:N | 2.27 | 0.48 |
| 1:J:408:ILE:HD12 | 1:J:409:ILE:HA | 1.95 | 0.48 |
| 1:K:558:PHE:O | 1:K:586:ARG:HB3 | 2.13 | 0.48 |
| 1:L:565:GLU:CB | 1:L:570:GLN:NE2 | 2.55 | 0.48 |
| 1:A:545:ARG:HB3 | 1:A:597:TYR:CE2 | 2.48 | 0.48 |
| 1:B:492:TYR:HE1 | 1:B:611:LEU:O | 1.97 | 0.48 |
| 1:B:662:GLU:O | 1:B:662:GLU:HG2 | 2.13 | 0.48 |
| 1:D:412:ASN:ND2 | 1:D:486:ARG:NH2 | 2.61 | 0.48 |
| 1:D:565:GLU:OE2 | 1:D:590:TYR:OH | 2.28 | 0.48 |
| 1:E:361:GLN:CG | 1:E:455:PHE:CD1 | 2.97 | 0.48 |
| 1:E:545:ARG:HB3 | 1:E:597:TYR:CE2 | 2.49 | 0.48 |
| 1:G:558:PHE:O | 1:G:586:ARG:HB3 | 2.13 | 0.48 |
| 1:H:658:ILE:CD1 | 1:H:658:ILE:N | 2.74 | 0.48 |
| 1:I:385:THR:CG2 | 1:I:389:ARG:C | 2.73 | 0.48 |
| 1:A:466:THR:CG2 | 1:B:466:THR:HB | 2.43 | 0.48 |
| 1:A:518:ASN:OD1 | 1:A:533:ASP:CB | 2.60 | 0.48 |
| 1:C:536:TYR:CD1 | 1:C:586:ARG:CD | 2.96 | 0.48 |
| 1:C:545:ARG:HB3 | 1:C:597:TYR:CE2 | 2.48 | 0.48 |
| 1:E:340:VAL:O | 1:E:341:THR:OG1 | 2.30 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:387:VAL:CG2 | 1:E:390:GLU:OE1 | 2.55 | 0.48 |
| 1:G:531:GLU:C | 1:G:532:GLU:OE1 | 2.52 | 0.48 |
| 1:J:401:LEU:CG | 1:J:403:PRO:HD2 | 2.42 | 0.48 |
| 1:L:342:ALA:O | 1:L:346:ASP:OD1 | 2.30 | 0.48 |
| 1:A:575:ASN:O | 1:A:576:ASP:HB2 | 2.13 | 0.48 |
| 1:E:401:LEU:HG | 1:E:402:ALA:N | 2.27 | 0.48 |
| 1:F:408:ILE:HD12 | 1:F:409:ILE:HA | 1.95 | 0.48 |
| 1:F:448:TYR:CD1 | 1:F:642:PHE:HB2 | 2.48 | 0.48 |
| 1:H:540:ILE:HG22 | 1:H:555:ILE:CG1 | 2.43 | 0.48 |
| 1:J:508:ARG:HG2 | 1:J:577:PHE:HA | 1.96 | 0.48 |
| 1:L:414:LEU:HD23 | 1:L:414:LEU:HA | 1.70 | 0.48 |
| 1:L:508:ARG:HG2 | 1:L:577:PHE:HA | 1.96 | 0.48 |
| 1:A:587:ASP:OD2 | 1:A:587:ASP:O | 2.30 | 0.48 |
| 1:F:651:LEU:HD22 | 1:F:652:THR:N | 2.29 | 0.48 |
| 1:H:597:TYR:HB2 | 1:H:598:PRO:HD3 | 1.95 | 0.48 |
| 1:J:486:ARG:HG2 | 1:J:499:ILE:HD11 | 1.96 | 0.48 |
| 1:J:566:ASN:CA | 1:J:570:GLN:HE22 | 2.26 | 0.48 |
| 1:K:522:LYS:N | 1:K:522:LYS:CD | 2.72 | 0.48 |
| 1:K:575:ASN:O | 1:K:576:ASP:HB2 | 2.13 | 0.48 |
| 1:L:492:TYR:O | 1:L:606:ILE:HG12 | 2.14 | 0.48 |
| 1:L:653:ILE:HG22 | 1:L:655:LEU:HD12 | 1.96 | 0.48 |
| 1:L:662:GLU:O | 1:L:662:GLU:HG2 | 2.13 | 0.48 |
| 1:A:361:GLN:CG | 1:A:455:PHE:CD1 | 2.97 | 0.48 |
| 1:B:486:ARG:HG2 | 1:B:499:ILE:HD11 | 1.96 | 0.48 |
| 1:D:447:TYR:HB2 | 1:D:467:TYR:CG | 2.48 | 0.48 |
| 1:D:492:TYR:O | 1:D:606:ILE:HG12 | 2.14 | 0.48 |
| 1:D:653:ILE:HG22 | 1:D:655:LEU:HD12 | 1.96 | 0.48 |
| 1:F:345:TYR:C | 1:F:345:TYR:HD1 | 2.18 | 0.48 |
| 1:F:508:ARG:HG2 | 1:F:577:PHE:HA | 1.96 | 0.48 |
| 1:H:566:ASN:CA | 1:H:570:GLN:HE22 | 2.26 | 0.48 |
| 1:H:651:LEU:HD22 | 1:H:652:THR:N | 2.29 | 0.48 |
| 1:J:651:LEU:HD22 | 1:J:652:THR:N | 2.29 | 0.48 |
| 1:J:653:ILE:HG22 | 1:J:655:LEU:HD12 | 1.96 | 0.48 |
| 1:L:346:ASP:HB3 | 1:L:360:VAL:HB | 1.95 | 0.48 |
| 1:L:408:ILE:HD12 | 1:L:409:ILE:HA | 1.95 | 0.48 |
| 1:L:412:ASN:ND2 | 1:L:486:ARG:NH2 | 2.61 | 0.48 |
| 1:B:463:LYS:O | 1:B:466:THR:HG23 | 2.14 | 0.47 |
| 1:B:540:ILE:HG22 | 1:B:555:ILE:CG1 | 2.43 | 0.47 |
| 1:B:651:LEU:HD22 | 1:B:652:THR:N | 2.29 | 0.47 |
| 1:C:457:SER:N | 1:C:634:THR:HG23 | 2.26 | 0.47 |
| 1:C:575:ASN:O | 1:C:576:ASP:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:651:LEU:HD22 | 1:D:652:THR:N | 2.29 | 0.47 |
| 1:E:391:ASP:N | 1:E:391:ASP:OD1 | 2.46 | 0.47 |
| 1:E:558:PHE:O | 1:E:586:ARG:HB3 | 2.13 | 0.47 |
| 1:F:492:TYR:HE1 | 1:F:611:LEU:O | 1.97 | 0.47 |
| 1:G:424:TYR:HB3 | 1:G:475:VAL:H | 1.79 | 0.47 |
| 1:G:575:ASN:O | 1:G:576:ASP:HB2 | 2.14 | 0.47 |
| 1:K:545:ARG:HB3 | 1:K:597:TYR:CE2 | 2.49 | 0.47 |
| 1:L:492:TYR:HE1 | 1:L:611:LEU:O | 1.97 | 0.47 |
| 1:C:340:VAL:CA | 1:C:345:TYR:CZ | 2.82 | 0.47 |
| 1:C:448:TYR:CG | 1:C:642:PHE:HB2 | 2.50 | 0.47 |
| 1:E:531:GLU:C | 1:E:532:GLU:OE1 | 2.52 | 0.47 |
| 1:G:579:LYS:HB3 | 1:G:589:TYR:OH | 2.15 | 0.47 |
| 1:H:486:ARG:HG2 | 1:H:499:ILE:HD11 | 1.96 | 0.47 |
| 1:A:424:TYR:HB3 | 1:A:475:VAL:H | 1.79 | 0.47 |
| 1:B:408:ILE:HD12 | 1:B:409:ILE:HA | 1.95 | 0.47 |
| 1:C:387:VAL:CG2 | 1:C:390:GLU:OE1 | 2.54 | 0.47 |
| 1:C:531:GLU:C | 1:C:532:GLU:OE1 | 2.52 | 0.47 |
| 1:C:579:LYS:HB3 | 1:C:589:TYR:OH | 2.15 | 0.47 |
| 1:G:385:THR:C | 1:G:387:VAL:H | 2.16 | 0.47 |
| 1:H:492:TYR:O | 1:H:606:ILE:HG12 | 2.14 | 0.47 |
| 1:H:662:GLU:O | 1:H:662:GLU:HG2 | 2.13 | 0.47 |
| 1:I:361:GLN:CG | 1:I:455:PHE:CD1 | 2.97 | 0.47 |
| 1:I:536:TYR:CD1 | 1:I:586:ARG:CD | 2.96 | 0.47 |
| 1:K:448:TYR:CG | 1:K:642:PHE:HB2 | 2.49 | 0.47 |
| 1:K:518:ASN:OD1 | 1:K:533:ASP:CB | 2.60 | 0.47 |
| 1:L:427:ASN:ND2 | 1:L:427:ASN:N | 2.54 | 0.47 |
| 1:C:558:PHE:O | 1:C:586:ARG:HB3 | 2.13 | 0.47 |
| 1:D:353:PHE:CE2 | 1:D:392:ILE:HD13 | 2.50 | 0.47 |
| 1:D:492:TYR:HE1 | 1:D:611:LEU:O | 1.97 | 0.47 |
| 1:E:361:GLN:HG2 | 1:E:455:PHE:CD1 | 2.50 | 0.47 |
| 1:F:597:TYR:HB2 | 1:F:598:PRO:HD3 | 1.95 | 0.47 |
| 1:G:361:GLN:CG | 1:G:455:PHE:CD1 | 2.97 | 0.47 |
| 1:H:408:ILE:HD12 | 1:H:409:ILE:HA | 1.95 | 0.47 |
| 1:H:448:TYR:CE1 | 1:H:642:PHE:HB2 | 2.50 | 0.47 |
| 1:H:653:ILE:HG22 | 1:H:655:LEU:HD12 | 1.96 | 0.47 |
| 1:I:536:TYR:HD1 | 1:I:586:ARG:HD3 | 1.79 | 0.47 |
| 1:K:361:GLN:CG | 1:K:455:PHE:CD1 | 2.97 | 0.47 |
| 1:L:346:ASP:OD1 | 1:L:346:ASP:N | 2.48 | 0.47 |
| 1:L:353:PHE:CE2 | 1:L:392:ILE:HD13 | 2.50 | 0.47 |
| 1:L:651:LEU:HD22 | 1:L:652:THR:N | 2.29 | 0.47 |
| 1:A:340:VAL:O | 1:A:341:THR:OG1 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:353:PHE:CE2 | 1:A:395:TYR:CD2 | 2.86 | 0.47 |
| 1:D:346:ASP:HB3 | 1:D:360:VAL:HB | 1.95 | 0.47 |
| 1:D:385:THR:HG22 | 1:D:388:GLN:OE1 | 2.15 | 0.47 |
| 1:D:448:TYR:CE1 | 1:D:642:PHE:HB2 | 2.50 | 0.47 |
| 1:E:626:ASP:HA | 1:E:627:PRO:HD3 | 1.65 | 0.47 |
| 1:F:342:ALA:O | 1:F:346:ASP:OD2 | 2.29 | 0.47 |
| 1:F:486:ARG:HG2 | 1:F:499:ILE:HD11 | 1.96 | 0.47 |
| 1:G:626:ASP:HA | 1:G:627:PRO:HD3 | 1.65 | 0.47 |
| 1:I:424:TYR:HB3 | 1:I:475:VAL:H | 1.79 | 0.47 |
| 1:I:545:ARG:HB3 | 1:I:597:TYR:CE2 | 2.49 | 0.47 |
| 1:I:596:ASN:HB3 | 1:I:601:VAL:HG22 | 1.97 | 0.47 |
| 1:J:463:LYS:O | 1:J:466:THR:HG23 | 2.14 | 0.47 |
| 1:L:565:GLU:OE2 | 1:L:590:TYR:OH | 2.28 | 0.47 |
| 1:B:408:ILE:O | 1:B:409:ILE:HG23 | 2.09 | 0.47 |
| 1:F:401:LEU:CG | 1:F:403:PRO:HD2 | 2.42 | 0.47 |
| 1:F:448:TYR:CE1 | 1:F:642:PHE:HB2 | 2.50 | 0.47 |
| 1:F:592:ILE:O | 1:F:593:GLY:O | 2.32 | 0.47 |
| 1:F:653:ILE:HG22 | 1:F:655:LEU:HD12 | 1.96 | 0.47 |
| 1:G:596:ASN:HB3 | 1:G:601:VAL:HG22 | 1.97 | 0.47 |
| 1:I:531:GLU:C | 1:I:532:GLU:OE1 | 2.52 | 0.47 |
| 1:J:353:PHE:CE2 | 1:J:392:ILE:HD13 | 2.50 | 0.47 |
| 1:A:340:VAL:C | 1:A:341:THR:CG2 | 2.62 | 0.47 |
| 1:A:361:GLN:HG2 | 1:A:455:PHE:CD1 | 2.50 | 0.47 |
| 1:B:492:TYR:O | 1:B:606:ILE:HG12 | 2.14 | 0.47 |
| 1:B:508:ARG:HG2 | 1:B:577:PHE:HA | 1.96 | 0.47 |
| 1:B:653:ILE:HG22 | 1:B:655:LEU:HD12 | 1.96 | 0.47 |
| 1:D:592:ILE:O | 1:D:593:GLY:O | 2.32 | 0.47 |
| 1:E:424:TYR:HB3 | 1:E:475:VAL:H | 1.78 | 0.47 |
| 1:E:575:ASN:O | 1:E:576:ASP:HB2 | 2.14 | 0.47 |
| 1:G:385:THR:C | 1:G:387:VAL:N | 2.66 | 0.47 |
| 1:G:536:TYR:CD1 | 1:G:586:ARG:CD | 2.96 | 0.47 |
| 1:H:492:TYR:HE1 | 1:H:611:LEU:O | 1.97 | 0.47 |
| 1:H:592:ILE:O | 1:H:593:GLY:O | 2.32 | 0.47 |
| 1:J:346:ASP:OD1 | 1:J:346:ASP:N | 2.47 | 0.47 |
| 1:J:448:TYR:CE1 | 1:J:642:PHE:HB2 | 2.50 | 0.47 |
| 1:J:492:TYR:HE1 | 1:J:611:LEU:O | 1.97 | 0.47 |
| 1:J:660:GLN:HA | 1:J:661:LEU:HB3 | 1.90 | 0.47 |
| 1:K:579:LYS:HB3 | 1:K:589:TYR:OH | 2.15 | 0.47 |
| 1:K:587:ASP:OD2 | 1:K:587:ASP:O | 2.30 | 0.47 |
| 1:L:401:LEU:CG | 1:L:403:PRO:HD2 | 2.42 | 0.47 |
| 1:L:486:ARG:HG2 | 1:L:499:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:558:PHE:O | 1:A:586:ARG:HB3 | 2.13 | 0.47 |
| 1:B:353:PHE:CE2 | 1:B:392:ILE:HD13 | 2.50 | 0.47 |
| 1:B:385:THR:HG22 | 1:B:388:GLN:OE1 | 2.15 | 0.47 |
| 1:D:597:TYR:HB2 | 1:D:598:PRO:HD3 | 1.95 | 0.47 |
| 1:E:385:THR:C | 1:E:387:VAL:H | 2.16 | 0.47 |
| 1:E:386:THR:C | 1:E:388:GLN:N | 2.67 | 0.47 |
| 1:E:579:LYS:HB3 | 1:E:589:TYR:OH | 2.14 | 0.47 |
| 1:E:596:ASN:HB3 | 1:E:601:VAL:HG22 | 1.97 | 0.47 |
| 1:G:403:PRO:HD3 | 1:J:366:SER:HA | 1.96 | 0.47 |
| 1:G:448:TYR:CG | 1:G:642:PHE:HB2 | 2.50 | 0.47 |
| 1:I:356:ILE:O | 1:I:356:ILE:CG1 | 2.63 | 0.47 |
| 1:I:559:ALA:O | 1:I:561:GLY:CA | 2.34 | 0.47 |
| 1:I:579:LYS:HB3 | 1:I:589:TYR:OH | 2.15 | 0.47 |
| 1:J:592:ILE:O | 1:J:593:GLY:O | 2.32 | 0.47 |
| 1:K:431:GLU:HB2 | 1:K:435:TRP:CE3 | 2.50 | 0.47 |
| 1:A:448:TYR:CG | 1:A:642:PHE:HB2 | 2.50 | 0.47 |
| 1:D:664:HIS:O | 1:D:665:HIS:CB | 2.63 | 0.47 |
| 1:J:492:TYR:O | 1:J:606:ILE:HG12 | 2.14 | 0.47 |
| 1:K:420:LEU:HD12 | 1:K:479:SER:O | 2.15 | 0.47 |
| 1:L:463:LYS:O | 1:L:466:THR:HG23 | 2.14 | 0.47 |
| 1:C:596:ASN:HB3 | 1:C:601:VAL:HG22 | 1.97 | 0.47 |
| 1:D:455:PHE:O | 1:D:456:ASN:HB2 | 2.16 | 0.47 |
| 1:F:463:LYS:O | 1:F:466:THR:HG23 | 2.14 | 0.47 |
| 1:F:522:LYS:HG2 | 1:F:524:VAL:HG23 | 1.97 | 0.47 |
| 1:H:353:PHE:CE2 | 1:H:392:ILE:HD13 | 2.50 | 0.47 |
| 1:H:463:LYS:O | 1:H:466:THR:HG23 | 2.14 | 0.47 |
| 1:H:656:GLU:OE1 | 1:H:664:HIS:CG | 2.68 | 0.47 |
| 1:I:431:GLU:HB2 | 1:I:435:TRP:CE3 | 2.50 | 0.47 |
| 1:L:455:PHE:O | 1:L:456:ASN:HB2 | 2.15 | 0.47 |
| 1:A:420:LEU:HD12 | 1:A:479:SER:O | 2.15 | 0.46 |
| 1:C:420:LEU:HD12 | 1:C:479:SER:O | 2.15 | 0.46 |
| 1:D:398:ASP:CB | 1:E:663:HIS:HB3 | 2.44 | 0.46 |
| 1:D:463:LYS:O | 1:D:466:THR:HG23 | 2.14 | 0.46 |
| 1:E:448:TYR:CG | 1:E:642:PHE:HB2 | 2.49 | 0.46 |
| 1:F:492:TYR:O | 1:F:606:ILE:HG12 | 2.14 | 0.46 |
| 1:H:385:THR:HG22 | 1:H:388:GLN:OE1 | 2.15 | 0.46 |
| 1:H:664:HIS:O | 1:H:665:HIS:CB | 2.63 | 0.46 |
| 1:I:448:TYR:CG | 1:I:642:PHE:HB2 | 2.50 | 0.46 |
| 1:L:540:ILE:HG22 | 1:L:555:ILE:CG1 | 2.43 | 0.46 |
| 1:A:431:GLU:HB2 | 1:A:435:TRP:CE3 | 2.50 | 0.46 |
| 1:B:365:ASP:HB3 | 1:B:367:THR:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:656:GLU:OE1 | 1:B:664:HIS:CG | 2.68 | 0.46 |
| 1:D:399:TYR:CA | 1:E:664:HIS:HB2 | 2.24 | 0.46 |
| 1:D:540:ILE:HG22 | 1:D:555:ILE:CG1 | 2.43 | 0.46 |
| 1:E:431:GLU:HB2 | 1:E:435:TRP:CE3 | 2.50 | 0.46 |
| 1:J:522:LYS:HG2 | 1:J:524:VAL:HG23 | 1.97 | 0.46 |
| 1:K:596:ASN:HB3 | 1:K:601:VAL:HG22 | 1.97 | 0.46 |
| 1:L:656:GLU:OE1 | 1:L:664:HIS:CG | 2.68 | 0.46 |
| 1:A:340:VAL:O | 1:A:341:THR:CG2 | 2.64 | 0.46 |
| 1:B:366:SER:N | 1:B:367:THR:HG22 | 2.31 | 0.46 |
| 1:C:536:TYR:HD1 | 1:C:586:ARG:HD3 | 1.79 | 0.46 |
| 1:C:559:ALA:O | 1:C:561:GLY:CA | 2.34 | 0.46 |
| 1:D:365:ASP:HB3 | 1:D:367:THR:HG23 | 1.97 | 0.46 |
| 1:D:486:ARG:HG2 | 1:D:499:ILE:HD11 | 1.96 | 0.46 |
| 1:D:656:GLU:OE1 | 1:D:664:HIS:CG | 2.68 | 0.46 |
| 1:E:536:TYR:HD1 | 1:E:586:ARG:HD3 | 1.79 | 0.46 |
| 1:F:353:PHE:CE2 | 1:F:392:ILE:HD13 | 2.50 | 0.46 |
| 1:G:431:GLU:HB2 | 1:G:435:TRP:CE3 | 2.50 | 0.46 |
| 1:J:656:GLU:OE1 | 1:J:664:HIS:CG | 2.68 | 0.46 |
| 1:J:664:HIS:O | 1:J:665:HIS:CB | 2.63 | 0.46 |
| 1:K:353:PHE:O | 1:K:354:GLY:C | 2.48 | 0.46 |
| 1:K:424:TYR:HB3 | 1:K:475:VAL:H | 1.79 | 0.46 |
| 1:L:366:SER:N | 1:L:367:THR:HG22 | 2.31 | 0.46 |
| 1:L:448:TYR:CE1 | 1:L:642:PHE:HB2 | 2.50 | 0.46 |
| 1:A:401:LEU:CD2 | 1:A:402:ALA:CB | 2.69 | 0.46 |
| 1:B:448:TYR:CE1 | 1:B:642:PHE:HB2 | 2.50 | 0.46 |
| 1:C:340:VAL:O | 1:C:341:THR:CB | 2.63 | 0.46 |
| 1:C:431:GLU:HB2 | 1:C:435:TRP:CE3 | 2.50 | 0.46 |
| 1:D:408:ILE:O | 1:D:409:ILE:HG23 | 2.09 | 0.46 |
| 1:E:519:SER:O | 1:E:533:ASP:HB2 | 2.16 | 0.46 |
| 1:F:401:LEU:HD12 | 1:F:401:LEU:HA | 1.63 | 0.46 |
| 1:G:361:GLN:HG2 | 1:G:455:PHE:CD1 | 2.49 | 0.46 |
| 1:G:519:SER:O | 1:G:533:ASP:HB2 | 2.16 | 0.46 |
| 1:G:536:TYR:HD1 | 1:G:586:ARG:HD3 | 1.79 | 0.46 |
| 1:H:455:PHE:O | 1:H:456:ASN:HB2 | 2.15 | 0.46 |
| 1:J:596:ASN:ND2 | 1:J:598:PRO:HD2 | 2.31 | 0.46 |
| 1:K:361:GLN:HG2 | 1:K:455:PHE:CD1 | 2.49 | 0.46 |
| 1:L:592:ILE:O | 1:L:593:GLY:O | 2.32 | 0.46 |
| 1:A:385:THR:C | 1:A:387:VAL:H | 2.16 | 0.46 |
| 1:A:396:LEU:O | 1:A:399:TYR:CE1 | 2.69 | 0.46 |
| 1:A:579:LYS:HB3 | 1:A:589:TYR:OH | 2.15 | 0.46 |
| 1:B:592:ILE:O | 1:B:593:GLY:O | 2.32 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:596:ASN:ND2 | 1:B:598:PRO:HD2 | 2.31 | 0.46 |
| 1:C:519:SER:O | 1:C:533:ASP:HB2 | 2.16 | 0.46 |
| 1:D:366:SER:N | 1:D:367:THR:HG22 | 2.31 | 0.46 |
| 1:D:401:LEU:HD12 | 1:D:401:LEU:HA | 1.63 | 0.46 |
| 1:D:565:GLU:CB | 1:D:570:GLN:NE2 | 2.55 | 0.46 |
| 1:E:341:THR:O | 1:E:341:THR:OG1 | 2.33 | 0.46 |
| 1:E:385:THR:C | 1:E:387:VAL:N | 2.66 | 0.46 |
| 1:E:386:THR:O | 1:E:388:GLN:HG3 | 2.16 | 0.46 |
| 1:F:455:PHE:O | 1:F:456:ASN:HB2 | 2.16 | 0.46 |
| 1:F:541:VAL:HG12 | 1:F:542:SER:N | 2.31 | 0.46 |
| 1:G:420:LEU:HD12 | 1:G:479:SER:O | 2.15 | 0.46 |
| 1:I:396:LEU:O | 1:I:399:TYR:CE1 | 2.69 | 0.46 |
| 1:I:401:LEU:CD2 | 1:I:402:ALA:CB | 2.69 | 0.46 |
| 1:J:500:LYS:HB3 | 1:J:500:LYS:HE2 | 1.81 | 0.46 |
| 1:A:596:ASN:HB3 | 1:A:601:VAL:HG22 | 1.97 | 0.46 |
| 1:B:405:THR:OG1 | 1:B:406:PRO:HD2 | 2.15 | 0.46 |
| 1:C:386:THR:O | 1:C:388:GLN:HG3 | 2.16 | 0.46 |
| 1:E:353:PHE:O | 1:E:354:GLY:C | 2.48 | 0.46 |
| 1:E:356:ILE:O | 1:E:356:ILE:CG1 | 2.63 | 0.46 |
| 1:F:385:THR:HG22 | 1:F:388:GLN:OE1 | 2.15 | 0.46 |
| 1:F:386:THR:O | 1:F:390:GLU:HG3 | 2.16 | 0.46 |
| 1:F:656:GLU:OE1 | 1:F:664:HIS:CG | 2.68 | 0.46 |
| 1:G:386:THR:O | 1:G:388:GLN:HG3 | 2.16 | 0.46 |
| 1:G:522:LYS:N | 1:G:522:LYS:CD | 2.72 | 0.46 |
| 1:H:508:ARG:HG2 | 1:H:577:PHE:HA | 1.96 | 0.46 |
| 1:I:522:LYS:N | 1:I:522:LYS:CD | 2.72 | 0.46 |
| 1:I:575:ASN:O | 1:I:576:ASP:HB2 | 2.13 | 0.46 |
| 1:K:536:TYR:HD1 | 1:K:586:ARG:HD3 | 1.79 | 0.46 |
| 1:A:386:THR:O | 1:A:388:GLN:HG3 | 2.16 | 0.46 |
| 1:C:485:VAL:HG22 | 1:C:624:TYR:CD2 | 2.51 | 0.46 |
| 1:E:420:LEU:HD12 | 1:E:479:SER:O | 2.15 | 0.46 |
| 1:F:405:THR:OG1 | 1:F:406:PRO:HD2 | 2.15 | 0.46 |
| 1:F:596:ASN:ND2 | 1:F:598:PRO:HD2 | 2.31 | 0.46 |
| 1:L:522:LYS:HG2 | 1:L:524:VAL:HG23 | 1.97 | 0.46 |
| 1:A:485:VAL:HG22 | 1:A:624:TYR:CD2 | 2.51 | 0.46 |
| 1:A:536:TYR:HD1 | 1:A:586:ARG:HD3 | 1.79 | 0.46 |
| 1:A:559:ALA:O | 1:A:561:GLY:CA | 2.34 | 0.46 |
| 1:B:660:GLN:HA | 1:B:661:LEU:HB3 | 1.90 | 0.46 |
| 1:D:596:ASN:ND2 | 1:D:598:PRO:HD2 | 2.31 | 0.46 |
| 1:E:396:LEU:O | 1:E:399:TYR:CE1 | 2.69 | 0.46 |
| 1:F:607:ALA:C | 1:F:609:ILE:H | 2.20 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:522:LYS:HG2 | 1:H:524:VAL:HG23 | 1.97 | 0.46 |
| 1:I:361:GLN:HG2 | 1:I:455:PHE:CD1 | 2.50 | 0.46 |
| 1:I:626:ASP:HA | 1:I:627:PRO:HD3 | 1.65 | 0.46 |
| 1:J:481:THR:O | 1:J:481:THR:HG22 | 2.16 | 0.46 |
| 1:J:541:VAL:HG12 | 1:J:542:SER:N | 2.31 | 0.46 |
| 1:L:541:VAL:HG12 | 1:L:542:SER:N | 2.30 | 0.46 |
| 1:L:596:ASN:ND2 | 1:L:598:PRO:HD2 | 2.31 | 0.46 |
| 1:A:492:TYR:HA | 1:A:606:ILE:HD12 | 1.98 | 0.46 |
| 1:B:455:PHE:O | 1:B:456:ASN:HB2 | 2.15 | 0.46 |
| 1:B:522:LYS:HG2 | 1:B:524:VAL:HG23 | 1.97 | 0.46 |
| 1:B:565:GLU:OE2 | 1:B:590:TYR:OH | 2.28 | 0.46 |
| 1:C:387:VAL:HB | 1:C:390:GLU:CD | 2.36 | 0.46 |
| 1:D:607:ALA:C | 1:D:609:ILE:H | 2.20 | 0.46 |
| 1:E:559:ALA:O | 1:E:561:GLY:CA | 2.34 | 0.46 |
| 1:H:401:LEU:CD1 | 1:H:403:PRO:HD2 | 2.46 | 0.46 |
| 1:H:541:VAL:HG12 | 1:H:542:SER:N | 2.31 | 0.46 |
| 1:J:366:SER:N | 1:J:367:THR:HG22 | 2.31 | 0.46 |
| 1:J:385:THR:HG22 | 1:J:388:GLN:OE1 | 2.15 | 0.46 |
| 1:K:356:ILE:O | 1:K:356:ILE:CG1 | 2.63 | 0.46 |
| 1:L:365:ASP:HB3 | 1:L:367:THR:HG23 | 1.97 | 0.46 |
| 1:A:387:VAL:HB | 1:A:390:GLU:CD | 2.37 | 0.46 |
| 1:B:386:THR:O | 1:B:390:GLU:HG3 | 2.16 | 0.46 |
| 1:B:644:ASN:C | 1:B:644:ASN:HD22 | 2.20 | 0.46 |
| 1:E:403:PRO:CD | 1:H:366:SER:HA | 2.45 | 0.46 |
| 1:I:386:THR:O | 1:I:388:GLN:HG3 | 2.16 | 0.46 |
| 1:K:385:THR:HG1 | 1:K:388:GLN:N | 2.14 | 0.46 |
| 1:K:391:ASP:C | 1:K:393:LYS:H | 2.20 | 0.46 |
| 1:B:565:GLU:CB | 1:B:570:GLN:NE2 | 2.55 | 0.45 |
| 1:C:391:ASP:C | 1:C:393:LYS:H | 2.20 | 0.45 |
| 1:D:481:THR:O | 1:D:481:THR:HG22 | 2.16 | 0.45 |
| 1:D:522:LYS:HG2 | 1:D:524:VAL:HG23 | 1.97 | 0.45 |
| 1:F:401:LEU:CD1 | 1:F:403:PRO:HD2 | 2.46 | 0.45 |
| 1:F:660:GLN:HA | 1:F:661:LEU:HB3 | 1.90 | 0.45 |
| 1:G:391:ASP:C | 1:G:393:LYS:H | 2.20 | 0.45 |
| 1:H:386:THR:O | 1:H:390:GLU:HG3 | 2.16 | 0.45 |
| 1:K:391:ASP:OD1 | 1:K:391:ASP:N | 2.46 | 0.45 |
| 1:B:401:LEU:CD1 | 1:B:403:PRO:HD2 | 2.46 | 0.45 |
| 1:B:545:ARG:NH1 | 1:B:597:TYR:HB3 | 2.32 | 0.45 |
| 1:C:396:LEU:O | 1:C:399:TYR:CE1 | 2.69 | 0.45 |
| 1:D:346:ASP:OD1 | 1:D:346:ASP:N | 2.47 | 0.45 |
| 1:D:408:ILE:O | 1:D:408:ILE:CG1 | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:492:TYR:HA | 1:E:606:ILE:HD12 | 1.98 | 0.45 |
| 1:E:631:VAL:CG2 | 1:F:476:ILE:CG2 | 2.72 | 0.45 |
| 1:F:365:ASP:HB3 | 1:F:367:THR:HG23 | 1.97 | 0.45 |
| 1:F:500:LYS:HB3 | 1:F:500:LYS:HE2 | 1.80 | 0.45 |
| 1:G:629:ASP:HB2 | 1:G:632:ILE:HD13 | 1.98 | 0.45 |
| 1:H:607:ALA:C | 1:H:609:ILE:H | 2.20 | 0.45 |
| 1:H:644:ASN:C | 1:H:644:ASN:HD22 | 2.20 | 0.45 |
| 1:I:518:ASN:OD1 | 1:I:533:ASP:CB | 2.60 | 0.45 |
| 1:J:345:TYR:C | 1:J:345:TYR:HD1 | 2.18 | 0.45 |
| 1:J:545:ARG:NH1 | 1:J:597:TYR:HB3 | 2.32 | 0.45 |
| 1:K:396:LEU:O | 1:K:399:TYR:CE1 | 2.69 | 0.45 |
| 1:K:485:VAL:HG22 | 1:K:624:TYR:CD2 | 2.51 | 0.45 |
| 1:L:481:THR:O | 1:L:481:THR:HG22 | 2.16 | 0.45 |
| 1:A:502:ASN:ND2 | 1:A:635:ARG:CB | 2.59 | 0.45 |
| 1:D:401:LEU:CD1 | 1:D:403:PRO:HD2 | 2.46 | 0.45 |
| 1:D:545:ARG:NH1 | 1:D:597:TYR:HB3 | 2.32 | 0.45 |
| 1:E:629:ASP:HB2 | 1:E:632:ILE:HD13 | 1.99 | 0.45 |
| 1:F:664:HIS:O | 1:F:665:HIS:CB | 2.63 | 0.45 |
| 1:G:358:GLN:HB2 | 1:G:379:LYS:HB2 | 1.99 | 0.45 |
| 1:G:440:ILE:CG1 | 1:G:441:ILE:N | 2.79 | 0.45 |
| 1:H:481:THR:HG22 | 1:H:481:THR:O | 2.16 | 0.45 |
| 1:J:455:PHE:O | 1:J:456:ASN:HB2 | 2.15 | 0.45 |
| 1:J:644:ASN:C | 1:J:644:ASN:HD22 | 2.20 | 0.45 |
| 1:K:387:VAL:HB | 1:K:390:GLU:CD | 2.37 | 0.45 |
| 1:A:629:ASP:HB2 | 1:A:632:ILE:HD13 | 1.99 | 0.45 |
| 1:B:541:VAL:HG12 | 1:B:542:SER:N | 2.30 | 0.45 |
| 1:D:484:MET:O | 1:D:624:TYR:HA | 2.17 | 0.45 |
| 1:D:541:VAL:HG12 | 1:D:542:SER:N | 2.31 | 0.45 |
| 1:F:566:ASN:O | 1:F:570:GLN:CD | 2.55 | 0.45 |
| 1:G:385:THR:HG1 | 1:G:388:GLN:N | 2.14 | 0.45 |
| 1:H:427:ASN:ND2 | 1:H:427:ASN:N | 2.54 | 0.45 |
| 1:J:484:MET:O | 1:J:624:TYR:HA | 2.17 | 0.45 |
| 1:K:340:VAL:O | 1:K:341:THR:OG1 | 2.30 | 0.45 |
| 1:K:385:THR:C | 1:K:387:VAL:N | 2.66 | 0.45 |
| 1:L:385:THR:HG22 | 1:L:388:GLN:OE1 | 2.15 | 0.45 |
| 1:L:664:HIS:O | 1:L:665:HIS:CB | 2.63 | 0.45 |
| 1:B:366:SER:HA | 1:K:403:PRO:CD | 2.47 | 0.45 |
| 1:B:607:ALA:C | 1:B:609:ILE:H | 2.20 | 0.45 |
| 1:C:346:ASP:OD1 | 1:C:362:THR:HB | 2.17 | 0.45 |
| 1:C:356:ILE:O | 1:C:356:ILE:CG1 | 2.63 | 0.45 |
| 1:C:440:ILE:CG1 | 1:C:441:ILE:N | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:629:ASP:HB2 | 1:C:632:ILE:HD13 | 1.99 | 0.45 |
| 1:F:508:ARG:HA | 1:F:542:SER:O | 2.17 | 0.45 |
| 1:G:340:VAL:O | 1:G:341:THR:CB | 2.63 | 0.45 |
| 1:G:396:LEU:O | 1:G:399:TYR:CE1 | 2.69 | 0.45 |
| 1:G:660:GLN:HG3 | 1:G:661:LEU:H | 1.77 | 0.45 |
| 1:I:485:VAL:HG22 | 1:I:624:TYR:CD2 | 2.51 | 0.45 |
| 1:I:629:ASP:HB2 | 1:I:632:ILE:HD13 | 1.99 | 0.45 |
| 1:J:401:LEU:CD1 | 1:J:403:PRO:HD2 | 2.46 | 0.45 |
| 1:J:566:ASN:O | 1:J:570:GLN:CD | 2.55 | 0.45 |
| 1:K:629:ASP:HB2 | 1:K:632:ILE:HD13 | 1.99 | 0.45 |
| 1:A:519:SER:O | 1:A:533:ASP:HB2 | 2.16 | 0.45 |
| 1:B:648:PRO:HD2 | 1:B:649:GLN:H | 1.81 | 0.45 |
| 1:E:460:ALA:HB2 | 1:E:631:VAL:HG22 | 1.99 | 0.45 |
| 1:E:582:ASN:HB2 | 1:E:585:GLY:C | 2.37 | 0.45 |
| 1:F:484:MET:O | 1:F:624:TYR:HA | 2.17 | 0.45 |
| 1:G:460:ALA:HB2 | 1:G:631:VAL:HG22 | 1.99 | 0.45 |
| 1:G:485:VAL:HG22 | 1:G:624:TYR:CD2 | 2.51 | 0.45 |
| 1:H:366:SER:N | 1:H:367:THR:HG22 | 2.31 | 0.45 |
| 1:H:596:ASN:ND2 | 1:H:598:PRO:HD2 | 2.31 | 0.45 |
| 1:I:420:LEU:HD12 | 1:I:479:SER:O | 2.15 | 0.45 |
| 1:I:582:ASN:HB2 | 1:I:585:GLY:C | 2.37 | 0.45 |
| 1:J:605:ASN:OD1 | 1:J:607:ALA:HB3 | 2.17 | 0.45 |
| 1:K:386:THR:O | 1:K:388:GLN:HG3 | 2.16 | 0.45 |
| 1:K:626:ASP:HA | 1:K:627:PRO:HD3 | 1.65 | 0.45 |
| 1:L:405:THR:OG1 | 1:L:406:PRO:HD2 | 2.15 | 0.45 |
| 1:L:484:MET:O | 1:L:624:TYR:HA | 2.17 | 0.45 |
| 1:A:440:ILE:CG1 | 1:A:441:ILE:N | 2.79 | 0.45 |
| 1:B:605:ASN:OD1 | 1:B:607:ALA:HB3 | 2.17 | 0.45 |
| 1:B:623:LEU:HD12 | 1:B:623:LEU:HA | 1.86 | 0.45 |
| 1:B:664:HIS:O | 1:B:665:HIS:CB | 2.63 | 0.45 |
| 1:D:644:ASN:C | 1:D:644:ASN:HD22 | 2.19 | 0.45 |
| 1:D:658:ILE:CG2 | 1:D:659:SER:N | 2.79 | 0.45 |
| 1:E:391:ASP:C | 1:E:393:LYS:H | 2.20 | 0.45 |
| 1:F:353:PHE:CZ | 1:F:395:TYR:HE2 | 2.11 | 0.45 |
| 1:G:387:VAL:HB | 1:G:390:GLU:CD | 2.37 | 0.45 |
| 1:G:582:ASN:HB2 | 1:G:585:GLY:C | 2.37 | 0.45 |
| 1:H:401:LEU:CG | 1:H:403:PRO:HD2 | 2.42 | 0.45 |
| 1:H:605:ASN:OD1 | 1:H:607:ALA:HB3 | 2.17 | 0.45 |
| 1:H:660:GLN:HA | 1:H:661:LEU:HB3 | 1.90 | 0.45 |
| 1:I:358:GLN:HB2 | 1:I:379:LYS:HB2 | 1.99 | 0.45 |
| 1:K:559:ALA:O | 1:K:561:GLY:CA | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:545:ARG:NH1 | 1:L:597:TYR:HB3 | 2.32 | 0.45 |
| 1:L:644:ASN:C | 1:L:644:ASN:HD22 | 2.20 | 0.45 |
| 1:L:648:PRO:HD2 | 1:L:649:GLN:H | 1.82 | 0.45 |
| 1:A:582:ASN:HB2 | 1:A:585:GLY:C | 2.37 | 0.45 |
| 1:B:511:GLU:HG3 | 1:B:511:GLU:O | 2.17 | 0.45 |
| 1:B:572:TYR:HB2 | 1:B:591:VAL:HG23 | 1.99 | 0.45 |
| 1:D:389:ARG:HA | 1:D:392:ILE:HG22 | 1.99 | 0.45 |
| 1:D:508:ARG:HA | 1:D:542:SER:O | 2.17 | 0.45 |
| 1:E:358:GLN:HB2 | 1:E:379:LYS:HB2 | 1.99 | 0.45 |
| 1:E:387:VAL:HB | 1:E:390:GLU:CD | 2.37 | 0.45 |
| 1:E:485:VAL:HG22 | 1:E:624:TYR:CD2 | 2.51 | 0.45 |
| 1:E:518:ASN:OD1 | 1:E:533:ASP:CB | 2.60 | 0.45 |
| 1:F:366:SER:N | 1:F:367:THR:HG22 | 2.31 | 0.45 |
| 1:F:605:ASN:OD1 | 1:F:607:ALA:HB3 | 2.17 | 0.45 |
| 1:F:648:PRO:HD2 | 1:F:649:GLN:H | 1.82 | 0.45 |
| 1:G:346:ASP:OD1 | 1:G:362:THR:HB | 2.17 | 0.45 |
| 1:H:545:ARG:NH1 | 1:H:597:TYR:HB3 | 2.32 | 0.45 |
| 1:H:566:ASN:O | 1:H:570:GLN:CD | 2.55 | 0.45 |
| 1:J:508:ARG:HA | 1:J:542:SER:O | 2.17 | 0.45 |
| 1:J:607:ALA:C | 1:J:609:ILE:H | 2.20 | 0.45 |
| 1:K:492:TYR:HA | 1:K:606:ILE:HD12 | 1.98 | 0.45 |
| 1:L:605:ASN:OD1 | 1:L:607:ALA:HB3 | 2.17 | 0.45 |
| 1:A:554:ILE:HD11 | 1:A:577:PHE:CD2 | 2.52 | 0.45 |
| 1:C:361:GLN:HG2 | 1:C:455:PHE:CD1 | 2.50 | 0.45 |
| 1:D:572:TYR:HB2 | 1:D:591:VAL:HG23 | 1.99 | 0.45 |
| 1:E:340:VAL:O | 1:E:341:THR:CB | 2.63 | 0.45 |
| 1:G:658:ILE:HA | 1:G:658:ILE:HD13 | 1.52 | 0.45 |
| 1:I:595:ILE:HG23 | 1:I:602:ILE:HG12 | 1.99 | 0.45 |
| 1:J:658:ILE:CD1 | 1:J:658:ILE:N | 2.74 | 0.45 |
| 1:L:658:ILE:CD1 | 1:L:658:ILE:N | 2.74 | 0.45 |
| 1:A:385:THR:CG2 | 1:A:389:ARG:C | 2.73 | 0.45 |
| 1:B:438:GLY:HA2 | 1:B:441:ILE:CG2 | 2.47 | 0.45 |
| 1:G:341:THR:O | 1:G:341:THR:OG1 | 2.33 | 0.45 |
| 1:G:387:VAL:CG2 | 1:G:390:GLU:OE1 | 2.55 | 0.45 |
| 1:G:517:PHE:CE1 | 1:G:615:LYS:HB3 | 2.52 | 0.45 |
| 1:H:346:ASP:OD1 | 1:H:346:ASP:N | 2.48 | 0.45 |
| 1:H:365:ASP:HB3 | 1:H:367:THR:HG23 | 1.97 | 0.45 |
| 1:I:530:LEU:HD23 | 1:I:530:LEU:HA | 1.82 | 0.45 |
| 1:J:648:PRO:HD2 | 1:J:649:GLN:H | 1.82 | 0.45 |
| 1:K:341:THR:O | 1:K:341:THR:OG1 | 2.33 | 0.45 |
| 1:L:508:ARG:HA | 1:L:542:SER:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:517:PHE:CE1 | 1:A:615:LYS:HB3 | 2.52 | 0.44 |
| 1:B:524:VAL:O | 1:B:524:VAL:HG12 | 2.17 | 0.44 |
| 1:B:658:ILE:CG2 | 1:B:659:SER:N | 2.79 | 0.44 |
| 1:C:441:ILE:O | 1:C:441:ILE:HG13 | 2.17 | 0.44 |
| 1:C:582:ASN:HB2 | 1:C:585:GLY:C | 2.37 | 0.44 |
| 1:D:462:SER:O | 1:D:466:THR:CG2 | 2.66 | 0.44 |
| 1:E:595:ILE:HG23 | 1:E:602:ILE:HG12 | 1.99 | 0.44 |
| 1:F:438:GLY:HA2 | 1:F:441:ILE:CG2 | 2.48 | 0.44 |
| 1:F:658:ILE:CG2 | 1:F:659:SER:N | 2.79 | 0.44 |
| 1:H:353:PHE:CZ | 1:H:395:TYR:HE2 | 2.11 | 0.44 |
| 1:H:572:TYR:HB2 | 1:H:591:VAL:HG23 | 1.99 | 0.44 |
| 1:I:340:VAL:O | 1:I:341:THR:CB | 2.63 | 0.44 |
| 1:I:346:ASP:OD1 | 1:I:362:THR:HB | 2.17 | 0.44 |
| 1:I:387:VAL:CG2 | 1:I:390:GLU:HB2 | 2.47 | 0.44 |
| 1:I:387:VAL:HB | 1:I:390:GLU:CD | 2.37 | 0.44 |
| 1:I:441:ILE:O | 1:I:441:ILE:HG13 | 2.17 | 0.44 |
| 1:I:492:TYR:HA | 1:I:606:ILE:HD12 | 1.98 | 0.44 |
| 1:J:365:ASP:HB3 | 1:J:367:THR:HG23 | 1.97 | 0.44 |
| 1:J:401:LEU:HD12 | 1:J:401:LEU:HA | 1.63 | 0.44 |
| 1:K:519:SER:O | 1:K:533:ASP:HB2 | 2.16 | 0.44 |
| 1:L:358:GLN:HB3 | 1:L:379:LYS:HA | 1.99 | 0.44 |
| 1:L:386:THR:O | 1:L:390:GLU:HG3 | 2.16 | 0.44 |
| 1:L:607:ALA:C | 1:L:609:ILE:H | 2.20 | 0.44 |
| 1:A:391:ASP:C | 1:A:393:LYS:H | 2.20 | 0.44 |
| 1:B:377:LYS:HB2 | 1:B:411:PRO:HG2 | 1.99 | 0.44 |
| 1:B:484:MET:O | 1:B:624:TYR:HA | 2.17 | 0.44 |
| 1:B:508:ARG:HA | 1:B:542:SER:O | 2.17 | 0.44 |
| 1:C:385:THR:HG1 | 1:C:388:GLN:N | 2.15 | 0.44 |
| 1:C:492:TYR:HA | 1:C:606:ILE:HD12 | 1.98 | 0.44 |
| 1:D:353:PHE:CZ | 1:D:395:TYR:HE2 | 2.11 | 0.44 |
| 1:E:385:THR:HG1 | 1:E:388:GLN:N | 2.14 | 0.44 |
| 1:F:377:LYS:HB2 | 1:F:411:PRO:HG2 | 1.99 | 0.44 |
| 1:G:510:MET:SD | 1:G:602:ILE:HG21 | 2.58 | 0.44 |
| 1:K:340:VAL:O | 1:K:341:THR:CG2 | 2.64 | 0.44 |
| 1:L:389:ARG:HA | 1:L:392:ILE:HG22 | 1.99 | 0.44 |
| 1:L:566:ASN:O | 1:L:570:GLN:CD | 2.55 | 0.44 |
| 1:A:358:GLN:HB2 | 1:A:379:LYS:HB2 | 1.99 | 0.44 |
| 1:A:460:ALA:HB2 | 1:A:631:VAL:HG22 | 1.99 | 0.44 |
| 1:A:556:GLY:CA | 1:A:589:TYR:CD1 | 3.01 | 0.44 |
| 1:D:605:ASN:OD1 | 1:D:607:ALA:HB3 | 2.17 | 0.44 |
| 1:D:648:PRO:HD2 | 1:D:649:GLN:H | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:510:MET:SD | 1:E:602:ILE:HG21 | 2.57 | 0.44 |
| 1:F:389:ARG:HA | 1:F:392:ILE:HG22 | 1.99 | 0.44 |
| 1:F:427:ASN:ND2 | 1:F:427:ASN:N | 2.54 | 0.44 |
| 1:F:572:TYR:HB2 | 1:F:591:VAL:HG23 | 1.99 | 0.44 |
| 1:G:492:TYR:HA | 1:G:606:ILE:HD12 | 1.98 | 0.44 |
| 1:H:664:HIS:CD2 | 1:H:664:HIS:C | 2.89 | 0.44 |
| 1:I:377:LYS:HA | 1:I:378:PRO:HD3 | 1.84 | 0.44 |
| 1:I:510:MET:SD | 1:I:602:ILE:HG21 | 2.57 | 0.44 |
| 1:I:519:SER:O | 1:I:533:ASP:HB2 | 2.16 | 0.44 |
| 1:J:358:GLN:HB3 | 1:J:379:LYS:HA | 1.99 | 0.44 |
| 1:K:346:ASP:OD1 | 1:K:362:THR:HB | 2.17 | 0.44 |
| 1:K:440:ILE:CG1 | 1:K:441:ILE:N | 2.79 | 0.44 |
| 1:K:582:ASN:HB2 | 1:K:585:GLY:C | 2.37 | 0.44 |
| 1:L:438:GLY:HA2 | 1:L:441:ILE:CG2 | 2.47 | 0.44 |
| 1:B:481:THR:O | 1:B:481:THR:HG22 | 2.16 | 0.44 |
| 1:C:460:ALA:HB2 | 1:C:631:VAL:HG22 | 1.99 | 0.44 |
| 1:D:566:ASN:O | 1:D:570:GLN:CD | 2.55 | 0.44 |
| 1:E:387:VAL:CG2 | 1:E:390:GLU:HB2 | 2.48 | 0.44 |
| 1:E:554:ILE:HD11 | 1:E:577:PHE:CD2 | 2.52 | 0.44 |
| 1:F:511:GLU:O | 1:F:511:GLU:HG3 | 2.17 | 0.44 |
| 1:F:644:ASN:C | 1:F:644:ASN:HD22 | 2.20 | 0.44 |
| 1:H:448:TYR:CG | 1:H:642:PHE:HB2 | 2.53 | 0.44 |
| 1:H:458:SER:HB2 | 1:H:632:ILE:O | 2.17 | 0.44 |
| 1:H:462:SER:O | 1:H:466:THR:CG2 | 2.66 | 0.44 |
| 1:I:502:ASN:ND2 | 1:I:635:ARG:CB | 2.59 | 0.44 |
| 1:K:510:MET:SD | 1:K:602:ILE:HG21 | 2.57 | 0.44 |
| 1:L:658:ILE:CG2 | 1:L:659:SER:N | 2.79 | 0.44 |
| 1:A:346:ASP:OD1 | 1:A:362:THR:HB | 2.17 | 0.44 |
| 1:A:353:PHE:O | 1:A:354:GLY:C | 2.48 | 0.44 |
| 1:B:389:ARG:HA | 1:B:392:ILE:HG22 | 1.99 | 0.44 |
| 1:C:510:MET:SD | 1:C:602:ILE:HG21 | 2.58 | 0.44 |
| 1:C:517:PHE:CE1 | 1:C:615:LYS:HB3 | 2.52 | 0.44 |
| 1:D:511:GLU:HG3 | 1:D:511:GLU:O | 2.17 | 0.44 |
| 1:E:401:LEU:HD21 | 1:E:402:ALA:HB2 | 1.96 | 0.44 |
| 1:E:441:ILE:HG13 | 1:E:441:ILE:O | 2.17 | 0.44 |
| 1:F:458:SER:HB2 | 1:F:632:ILE:O | 2.17 | 0.44 |
| 1:F:545:ARG:NH1 | 1:F:597:TYR:HB3 | 2.32 | 0.44 |
| 1:F:664:HIS:CD2 | 1:F:664:HIS:C | 2.89 | 0.44 |
| 1:G:484:MET:HG3 | 1:G:627:PRO:HG3 | 2.00 | 0.44 |
| 1:H:405:THR:OG1 | 1:H:406:PRO:HD2 | 2.16 | 0.44 |
| 1:H:508:ARG:HA | 1:H:542:SER:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:353:PHE:CZ | 1:J:395:TYR:HE2 | 2.11 | 0.44 |
| 1:J:458:SER:HB2 | 1:J:632:ILE:O | 2.17 | 0.44 |
| 1:J:524:VAL:O | 1:J:524:VAL:HG12 | 2.17 | 0.44 |
| 1:L:462:SER:O | 1:L:466:THR:CG2 | 2.66 | 0.44 |
| 1:C:556:GLY:CA | 1:C:589:TYR:CD1 | 3.01 | 0.44 |
| 1:D:377:LYS:HB2 | 1:D:411:PRO:HG2 | 1.99 | 0.44 |
| 1:E:484:MET:HG3 | 1:E:627:PRO:HG3 | 2.00 | 0.44 |
| 1:F:481:THR:HG22 | 1:F:481:THR:O | 2.16 | 0.44 |
| 1:F:560:SER:HB2 | 1:F:588:LYS:NZ | 2.33 | 0.44 |
| 1:I:391:ASP:C | 1:I:393:LYS:H | 2.20 | 0.44 |
| 1:I:484:MET:HG3 | 1:I:627:PRO:HG3 | 2.00 | 0.44 |
| 1:I:517:PHE:CE1 | 1:I:615:LYS:HB3 | 2.53 | 0.44 |
| 1:J:386:THR:O | 1:J:390:GLU:HG3 | 2.16 | 0.44 |
| 1:K:441:ILE:O | 1:K:441:ILE:HG13 | 2.17 | 0.44 |
| 1:K:460:ALA:HB2 | 1:K:631:VAL:HG22 | 1.99 | 0.44 |
| 1:K:554:ILE:HD11 | 1:K:577:PHE:CD2 | 2.52 | 0.44 |
| 1:L:377:LYS:HB2 | 1:L:411:PRO:HG2 | 1.99 | 0.44 |
| 1:L:401:LEU:CD1 | 1:L:403:PRO:HD2 | 2.46 | 0.44 |
| 1:L:484:MET:HG3 | 1:L:627:PRO:HG3 | 2.00 | 0.44 |
| 1:L:511:GLU:O | 1:L:511:GLU:HG3 | 2.17 | 0.44 |
| 1:A:385:THR:HG1 | 1:A:388:GLN:N | 2.16 | 0.44 |
| 1:A:387:VAL:CG2 | 1:A:390:GLU:HB2 | 2.48 | 0.44 |
| 1:A:510:MET:SD | 1:A:602:ILE:HG21 | 2.57 | 0.44 |
| 1:B:461:LYS:O | 1:B:461:LYS:HG2 | 2.18 | 0.44 |
| 1:E:650:TYR:O | 1:E:651:LEU:HB2 | 2.18 | 0.44 |
| 1:E:658:ILE:HA | 1:E:658:ILE:HD13 | 1.52 | 0.44 |
| 1:F:365:ASP:O | 1:F:366:SER:C | 2.54 | 0.44 |
| 1:F:462:SER:O | 1:F:466:THR:CG2 | 2.66 | 0.44 |
| 1:H:377:LYS:HB2 | 1:H:411:PRO:HG2 | 1.99 | 0.44 |
| 1:H:524:VAL:HG12 | 1:H:524:VAL:O | 2.17 | 0.44 |
| 1:H:648:PRO:HD2 | 1:H:649:GLN:H | 1.81 | 0.44 |
| 1:I:554:ILE:HD11 | 1:I:577:PHE:CD2 | 2.52 | 0.44 |
| 1:J:389:ARG:HA | 1:J:392:ILE:HG22 | 1.99 | 0.44 |
| 1:J:438:GLY:HA2 | 1:J:441:ILE:CG2 | 2.47 | 0.44 |
| 1:K:530:LEU:HD23 | 1:K:530:LEU:HA | 1.82 | 0.44 |
| 1:L:500:LYS:HB3 | 1:L:500:LYS:HE2 | 1.80 | 0.44 |
| 1:L:524:VAL:O | 1:L:524:VAL:HG12 | 2.17 | 0.44 |
| 1:B:462:SER:O | 1:B:466:THR:CG2 | 2.66 | 0.44 |
| 1:B:484:MET:HG3 | 1:B:627:PRO:HG3 | 2.00 | 0.44 |
| 1:B:500:LYS:HB3 | 1:B:500:LYS:HE2 | 1.80 | 0.44 |
| 1:B:566:ASN:O | 1:B:570:GLN:CD | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:358:GLN:HB2 | 1:C:379:LYS:HB2 | 1.99 | 0.44 |
| 1:C:660:GLN:HG3 | 1:C:661:LEU:H | 1.77 | 0.44 |
| 1:D:367:THR:CG2 | 1:D:368:LYS:N | 2.45 | 0.44 |
| 1:D:405:THR:OG1 | 1:D:406:PRO:HD2 | 2.15 | 0.44 |
| 1:D:524:VAL:O | 1:D:524:VAL:HG12 | 2.17 | 0.44 |
| 1:D:560:SER:HB2 | 1:D:588:LYS:NZ | 2.33 | 0.44 |
| 1:E:517:PHE:CE1 | 1:E:615:LYS:HB3 | 2.52 | 0.44 |
| 1:F:658:ILE:HD12 | 1:F:658:ILE:HA | 1.67 | 0.44 |
| 1:G:375:ALA:HA | 1:G:409:ILE:HD12 | 2.00 | 0.44 |
| 1:G:441:ILE:HG13 | 1:G:441:ILE:O | 2.17 | 0.44 |
| 1:H:661:LEU:C | 1:H:663:HIS:N | 2.61 | 0.44 |
| 1:I:341:THR:O | 1:I:341:THR:OG1 | 2.33 | 0.44 |
| 1:I:385:THR:HG1 | 1:I:388:GLN:N | 2.15 | 0.44 |
| 1:I:403:PRO:HD3 | 1:L:366:SER:HA | 2.00 | 0.44 |
| 1:K:379:LYS:O | 1:K:379:LYS:CG | 2.66 | 0.44 |
| 1:B:458:SER:HB2 | 1:B:632:ILE:O | 2.17 | 0.44 |
| 1:C:582:ASN:C | 1:C:585:GLY:H | 2.21 | 0.44 |
| 1:C:595:ILE:HG23 | 1:C:602:ILE:HG12 | 1.99 | 0.44 |
| 1:D:358:GLN:HB3 | 1:D:379:LYS:HA | 1.99 | 0.44 |
| 1:E:379:LYS:O | 1:E:379:LYS:CG | 2.66 | 0.44 |
| 1:F:346:ASP:OD1 | 1:F:346:ASP:N | 2.48 | 0.44 |
| 1:G:365:ASP:OD2 | 1:G:367:THR:HB | 2.18 | 0.44 |
| 1:G:607:ALA:C | 1:G:609:ILE:O | 2.57 | 0.44 |
| 1:H:438:GLY:HA2 | 1:H:441:ILE:CG2 | 2.47 | 0.44 |
| 1:I:340:VAL:O | 1:I:341:THR:OG1 | 2.30 | 0.44 |
| 1:I:379:LYS:O | 1:I:379:LYS:CG | 2.66 | 0.44 |
| 1:I:635:ARG:HE | 1:I:635:ARG:HB2 | 1.66 | 0.44 |
| 1:J:405:THR:OG1 | 1:J:406:PRO:HD2 | 2.15 | 0.44 |
| 1:J:658:ILE:CG2 | 1:J:659:SER:N | 2.79 | 0.44 |
| 1:K:517:PHE:CE1 | 1:K:615:LYS:HB3 | 2.52 | 0.44 |
| 1:K:556:GLY:CA | 1:K:589:TYR:CD1 | 3.01 | 0.44 |
| 1:L:458:SER:HB2 | 1:L:632:ILE:O | 2.17 | 0.44 |
| 1:A:516:SER:HB2 | 1:A:617:GLU:OE1 | 2.18 | 0.43 |
| 1:D:386:THR:O | 1:D:390:GLU:HG3 | 2.16 | 0.43 |
| 1:E:530:LEU:HD23 | 1:E:530:LEU:HA | 1.82 | 0.43 |
| 1:E:607:ALA:C | 1:E:609:ILE:O | 2.57 | 0.43 |
| 1:F:464:MET:O | 1:F:468:VAL:HG23 | 2.18 | 0.43 |
| 1:G:650:TYR:O | 1:G:651:LEU:HB2 | 2.18 | 0.43 |
| 1:H:484:MET:O | 1:H:624:TYR:HA | 2.17 | 0.43 |
| 1:H:560:SER:HB2 | 1:H:588:LYS:NZ | 2.33 | 0.43 |
| 1:I:460:ALA:HB2 | 1:I:631:VAL:HG22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:607:ALA:C | 1:I:609:ILE:O | 2.57 | 0.43 |
| 1:K:358:GLN:HB2 | 1:K:379:LYS:HB2 | 1.99 | 0.43 |
| 1:K:484:MET:HG3 | 1:K:627:PRO:HG3 | 2.00 | 0.43 |
| 1:L:461:LYS:O | 1:L:461:LYS:HG2 | 2.18 | 0.43 |
| 1:L:557:PRO:CG | 1:L:580:LEU:HD11 | 2.37 | 0.43 |
| 1:A:650:TYR:O | 1:A:651:LEU:HB2 | 2.18 | 0.43 |
| 1:B:560:SER:HB2 | 1:B:588:LYS:NZ | 2.33 | 0.43 |
| 1:C:650:TYR:O | 1:C:651:LEU:HB2 | 2.18 | 0.43 |
| 1:D:438:GLY:HA2 | 1:D:441:ILE:CG2 | 2.47 | 0.43 |
| 1:E:408:ILE:H | 1:E:408:ILE:CD1 | 2.30 | 0.43 |
| 1:E:635:ARG:HE | 1:E:635:ARG:HB2 | 1.66 | 0.43 |
| 1:F:461:LYS:O | 1:F:461:LYS:HG2 | 2.18 | 0.43 |
| 1:F:484:MET:HG3 | 1:F:627:PRO:HG3 | 2.00 | 0.43 |
| 1:G:541:VAL:CG1 | 1:G:542:SER:N | 2.82 | 0.43 |
| 1:G:554:ILE:HD11 | 1:G:577:PHE:CD2 | 2.52 | 0.43 |
| 1:H:648:PRO:CD | 1:H:649:GLN:H | 2.32 | 0.43 |
| 1:H:658:ILE:CG2 | 1:H:659:SER:N | 2.79 | 0.43 |
| 1:I:340:VAL:O | 1:I:341:THR:CG2 | 2.64 | 0.43 |
| 1:I:375:ALA:HA | 1:I:409:ILE:HD12 | 2.00 | 0.43 |
| 1:J:462:SER:O | 1:J:466:THR:CG2 | 2.66 | 0.43 |
| 1:K:387:VAL:CG2 | 1:K:390:GLU:HB2 | 2.47 | 0.43 |
| 1:K:595:ILE:HG23 | 1:K:602:ILE:HG12 | 1.99 | 0.43 |
| 1:A:356:ILE:O | 1:A:356:ILE:CG1 | 2.63 | 0.43 |
| 1:A:361:GLN:HA | 1:A:361:GLN:HE21 | 1.84 | 0.43 |
| 1:A:379:LYS:O | 1:A:379:LYS:CG | 2.66 | 0.43 |
| 1:A:541:VAL:CG1 | 1:A:542:SER:N | 2.81 | 0.43 |
| 1:A:664:HIS:HD2 | 1:K:348:PHE:CZ | 2.17 | 0.43 |
| 1:B:377:LYS:CE | 1:B:641:VAL:HG21 | 2.48 | 0.43 |
| 1:C:365:ASP:OD2 | 1:C:367:THR:HB | 2.18 | 0.43 |
| 1:C:385:THR:C | 1:C:387:VAL:H | 2.16 | 0.43 |
| 1:C:401:LEU:HD21 | 1:C:402:ALA:HB2 | 1.96 | 0.43 |
| 1:C:541:VAL:CG1 | 1:C:542:SER:N | 2.82 | 0.43 |
| 1:C:635:ARG:HE | 1:C:635:ARG:HB2 | 1.66 | 0.43 |
| 1:D:623:LEU:HD12 | 1:D:623:LEU:HA | 1.86 | 0.43 |
| 1:E:375:ALA:HA | 1:E:409:ILE:HD12 | 2.00 | 0.43 |
| 1:E:656:GLU:HA | 1:E:657:PRO:HD3 | 1.82 | 0.43 |
| 1:H:464:MET:O | 1:H:468:VAL:HG23 | 2.18 | 0.43 |
| 1:H:557:PRO:CG | 1:H:580:LEU:HD11 | 2.37 | 0.43 |
| 1:I:385:THR:OG1 | 1:I:387:VAL:HG22 | 2.11 | 0.43 |
| 1:K:516:SER:HB2 | 1:K:617:GLU:OE1 | 2.18 | 0.43 |
| 1:K:541:VAL:CG1 | 1:K:542:SER:N | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:484:MET:HG3 | 1:C:627:PRO:HG3 | 2.00 | 0.43 |
| 1:D:458:SER:HB2 | 1:D:632:ILE:O | 2.17 | 0.43 |
| 1:E:346:ASP:OD1 | 1:E:362:THR:HB | 2.17 | 0.43 |
| 1:E:365:ASP:OD2 | 1:E:367:THR:HB | 2.18 | 0.43 |
| 1:E:661:LEU:HD13 | 1:E:662:GLU:CB | 2.42 | 0.43 |
| 1:F:524:VAL:O | 1:F:524:VAL:HG12 | 2.17 | 0.43 |
| 1:H:389:ARG:HA | 1:H:392:ILE:HG22 | 1.99 | 0.43 |
| 1:I:541:VAL:CG1 | 1:I:542:SER:N | 2.82 | 0.43 |
| 1:J:377:LYS:CE | 1:J:641:VAL:HG21 | 2.48 | 0.43 |
| 1:J:448:TYR:CG | 1:J:642:PHE:HB2 | 2.53 | 0.43 |
| 1:K:375:ALA:HA | 1:K:409:ILE:HD12 | 2.00 | 0.43 |
| 1:L:353:PHE:CZ | 1:L:395:TYR:CD2 | 3.05 | 0.43 |
| 1:A:365:ASP:OD2 | 1:A:367:THR:HB | 2.18 | 0.43 |
| 1:B:358:GLN:HB3 | 1:B:379:LYS:HA | 1.99 | 0.43 |
| 1:B:366:SER:C | 1:K:403:PRO:HB3 | 2.29 | 0.43 |
| 1:B:664:HIS:CD2 | 1:B:664:HIS:C | 2.90 | 0.43 |
| 1:D:464:MET:O | 1:D:468:VAL:HG23 | 2.18 | 0.43 |
| 1:F:375:ALA:HA | 1:F:409:ILE:O | 2.19 | 0.43 |
| 1:F:448:TYR:C | 1:F:453:GLU:HG3 | 2.39 | 0.43 |
| 1:F:648:PRO:CD | 1:F:649:GLN:H | 2.32 | 0.43 |
| 1:G:516:SER:HB2 | 1:G:617:GLU:OE1 | 2.18 | 0.43 |
| 1:H:375:ALA:HA | 1:H:409:ILE:O | 2.19 | 0.43 |
| 1:H:511:GLU:HG3 | 1:H:511:GLU:O | 2.17 | 0.43 |
| 1:I:658:ILE:HD13 | 1:I:658:ILE:HA | 1.52 | 0.43 |
| 1:J:353:PHE:CZ | 1:J:395:TYR:CD2 | 3.05 | 0.43 |
| 1:J:511:GLU:HG3 | 1:J:511:GLU:O | 2.17 | 0.43 |
| 1:K:385:THR:C | 1:K:387:VAL:H | 2.16 | 0.43 |
| 1:K:650:TYR:O | 1:K:651:LEU:HB2 | 2.18 | 0.43 |
| 1:K:661:LEU:HA | 1:K:661:LEU:HD22 | 1.75 | 0.43 |
| 1:L:560:SER:HB2 | 1:L:588:LYS:NZ | 2.33 | 0.43 |
| 1:A:349:VAL:C | 1:A:351:GLU:N | 2.71 | 0.43 |
| 1:A:484:MET:HG3 | 1:A:627:PRO:HG3 | 2.00 | 0.43 |
| 1:A:582:ASN:C | 1:A:585:GLY:H | 2.21 | 0.43 |
| 1:B:447:TYR:HB2 | 1:B:467:TYR:CD1 | 2.54 | 0.43 |
| 1:C:387:VAL:CG2 | 1:C:390:GLU:HB2 | 2.47 | 0.43 |
| 1:C:607:ALA:C | 1:C:609:ILE:O | 2.57 | 0.43 |
| 1:D:345:TYR:C | 1:D:345:TYR:HD1 | 2.18 | 0.43 |
| 1:D:664:HIS:CD2 | 1:D:664:HIS:C | 2.90 | 0.43 |
| 1:E:349:VAL:C | 1:E:351:GLU:N | 2.71 | 0.43 |
| 1:E:541:VAL:CG1 | 1:E:542:SER:N | 2.82 | 0.43 |
| 1:G:595:ILE:HG23 | 1:G:602:ILE:HG12 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:377:LYS:CE | 1:H:641:VAL:HG21 | 2.48 | 0.43 |
| 1:H:461:LYS:O | 1:H:461:LYS:HG2 | 2.18 | 0.43 |
| 1:I:361:GLN:HA | 1:I:361:GLN:HE21 | 1.84 | 0.43 |
| 1:I:582:ASN:C | 1:I:585:GLY:H | 2.21 | 0.43 |
| 1:I:593:GLY:HA3 | 1:I:603:TYR:O | 2.19 | 0.43 |
| 1:J:572:TYR:HB2 | 1:J:591:VAL:CG2 | 2.49 | 0.43 |
| 1:J:572:TYR:HB2 | 1:J:591:VAL:HG23 | 1.99 | 0.43 |
| 1:K:401:LEU:CD2 | 1:K:402:ALA:CB | 2.68 | 0.43 |
| 1:L:448:TYR:C | 1:L:453:GLU:HG3 | 2.39 | 0.43 |
| 1:L:572:TYR:HB2 | 1:L:591:VAL:CG2 | 2.49 | 0.43 |
| 1:A:375:ALA:HA | 1:A:409:ILE:HD12 | 2.00 | 0.43 |
| 1:A:533:ASP:O | 1:A:535:LEU:CD2 | 2.67 | 0.43 |
| 1:B:448:TYR:CG | 1:B:642:PHE:HB2 | 2.53 | 0.43 |
| 1:B:653:ILE:HG22 | 1:B:655:LEU:CD1 | 2.49 | 0.43 |
| 1:C:375:ALA:HA | 1:C:409:ILE:HD12 | 2.00 | 0.43 |
| 1:C:379:LYS:O | 1:C:379:LYS:CG | 2.66 | 0.43 |
| 1:C:661:LEU:HA | 1:C:661:LEU:HD22 | 1.75 | 0.43 |
| 1:D:448:TYR:C | 1:D:453:GLU:HG3 | 2.39 | 0.43 |
| 1:E:361:GLN:HA | 1:E:361:GLN:HE21 | 1.84 | 0.43 |
| 1:E:469:ASP:HA | 1:E:475:VAL:HG11 | 2.01 | 0.43 |
| 1:F:358:GLN:HB3 | 1:F:379:LYS:HA | 1.99 | 0.43 |
| 1:F:448:TYR:CG | 1:F:642:PHE:HB2 | 2.53 | 0.43 |
| 1:G:593:GLY:HA3 | 1:G:603:TYR:O | 2.19 | 0.43 |
| 1:I:408:ILE:H | 1:I:408:ILE:CD1 | 2.30 | 0.43 |
| 1:J:365:ASP:O | 1:J:366:SER:C | 2.54 | 0.43 |
| 1:J:377:LYS:HB2 | 1:J:411:PRO:HG2 | 1.99 | 0.43 |
| 1:K:469:ASP:HA | 1:K:475:VAL:HG11 | 2.00 | 0.43 |
| 1:K:607:ALA:C | 1:K:609:ILE:O | 2.57 | 0.43 |
| 1:K:623:LEU:HD12 | 1:K:623:LEU:HA | 1.79 | 0.43 |
| 1:L:377:LYS:CE | 1:L:641:VAL:HG21 | 2.48 | 0.43 |
| 1:L:494:THR:HG22 | 1:L:499:ILE:HG22 | 2.01 | 0.43 |
| 1:L:572:TYR:HB2 | 1:L:591:VAL:HG23 | 1.99 | 0.43 |
| 1:L:592:ILE:CD1 | 1:L:606:ILE:HD13 | 2.49 | 0.43 |
| 1:L:653:ILE:HG22 | 1:L:655:LEU:CD1 | 2.49 | 0.43 |
| 1:L:664:HIS:CD2 | 1:L:664:HIS:C | 2.90 | 0.43 |
| 1:A:626:ASP:HA | 1:A:627:PRO:HD3 | 1.65 | 0.43 |
| 1:B:410:SER:HA | 1:B:411:PRO:HD3 | 1.81 | 0.43 |
| 1:B:494:THR:HG22 | 1:B:499:ILE:HG22 | 2.01 | 0.43 |
| 1:C:516:SER:HB2 | 1:C:617:GLU:OE1 | 2.18 | 0.43 |
| 1:C:554:ILE:HD11 | 1:C:577:PHE:CD2 | 2.52 | 0.43 |
| 1:D:377:LYS:CE | 1:D:641:VAL:HG21 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:448:TYR:CG | 1:D:642:PHE:HB2 | 2.53 | 0.43 |
| 1:E:492:TYR:CE1 | 1:E:606:ILE:HB | 2.54 | 0.43 |
| 1:E:533:ASP:O | 1:E:535:LEU:CD2 | 2.67 | 0.43 |
| 1:F:377:LYS:CE | 1:F:641:VAL:HG21 | 2.48 | 0.43 |
| 1:F:592:ILE:CD1 | 1:F:606:ILE:HD13 | 2.49 | 0.43 |
| 1:G:379:LYS:O | 1:G:379:LYS:CG | 2.66 | 0.43 |
| 1:G:387:VAL:CG2 | 1:G:390:GLU:HB2 | 2.48 | 0.43 |
| 1:H:388:GLN:O | 1:H:392:ILE:HG22 | 2.19 | 0.43 |
| 1:H:484:MET:HG3 | 1:H:627:PRO:HG3 | 2.00 | 0.43 |
| 1:K:533:ASP:O | 1:K:535:LEU:CD2 | 2.67 | 0.43 |
| 1:K:593:GLY:HA3 | 1:K:603:TYR:O | 2.19 | 0.43 |
| 1:L:353:PHE:CZ | 1:L:395:TYR:HE2 | 2.11 | 0.43 |
| 1:L:375:ALA:HA | 1:L:409:ILE:O | 2.19 | 0.43 |
| 1:A:441:ILE:O | 1:A:441:ILE:HG13 | 2.17 | 0.43 |
| 1:C:349:VAL:C | 1:C:351:GLU:N | 2.71 | 0.43 |
| 1:C:386:THR:C | 1:C:388:GLN:N | 2.67 | 0.43 |
| 1:C:408:ILE:H | 1:C:408:ILE:CD1 | 2.30 | 0.43 |
| 1:C:593:GLY:HA3 | 1:C:603:TYR:O | 2.19 | 0.43 |
| 1:D:353:PHE:CZ | 1:D:395:TYR:CD2 | 3.05 | 0.43 |
| 1:F:465:LEU:HD21 | 1:F:480:ALA:CB | 2.49 | 0.43 |
| 1:G:530:LEU:HD23 | 1:G:530:LEU:HA | 1.82 | 0.43 |
| 1:H:401:LEU:HD12 | 1:H:401:LEU:HA | 1.62 | 0.43 |
| 1:H:572:TYR:HB2 | 1:H:591:VAL:CG2 | 2.49 | 0.43 |
| 1:H:653:ILE:HG22 | 1:H:655:LEU:CD1 | 2.49 | 0.43 |
| 1:I:492:TYR:CE1 | 1:I:606:ILE:HB | 2.54 | 0.43 |
| 1:I:533:ASP:O | 1:I:535:LEU:CD2 | 2.67 | 0.43 |
| 1:I:557:PRO:HD3 | 1:I:580:LEU:HD11 | 2.01 | 0.43 |
| 1:K:557:PRO:HD3 | 1:K:580:LEU:HD11 | 2.01 | 0.43 |
| 1:A:408:ILE:H | 1:A:408:ILE:CD1 | 2.30 | 0.43 |
| 1:A:607:ALA:C | 1:A:609:ILE:O | 2.57 | 0.43 |
| 1:B:464:MET:O | 1:B:468:VAL:HG23 | 2.19 | 0.43 |
| 1:B:592:ILE:CD1 | 1:B:606:ILE:HD13 | 2.49 | 0.43 |
| 1:D:365:ASP:CG | 1:D:367:THR:CG2 | 2.88 | 0.43 |
| 1:D:422:VAL:HG11 | 1:D:475:VAL:HG13 | 2.01 | 0.43 |
| 1:D:447:TYR:HB2 | 1:D:467:TYR:CD1 | 2.54 | 0.43 |
| 1:D:484:MET:HG3 | 1:D:627:PRO:HG3 | 2.00 | 0.43 |
| 1:D:557:PRO:CG | 1:D:580:LEU:HD11 | 2.37 | 0.43 |
| 1:D:592:ILE:CD1 | 1:D:606:ILE:HD13 | 2.49 | 0.43 |
| 1:E:440:ILE:CG1 | 1:E:441:ILE:N | 2.79 | 0.43 |
| 1:F:388:GLN:O | 1:F:392:ILE:HG22 | 2.19 | 0.43 |
| 1:G:533:ASP:O | 1:G:535:LEU:CD2 | 2.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:386:THR:C | 1:I:388:GLN:N | 2.67 | 0.43 |
| 1:J:388:GLN:O | 1:J:392:ILE:HG22 | 2.19 | 0.43 |
| 1:J:648:PRO:CD | 1:J:649:GLN:H | 2.32 | 0.43 |
| 1:K:340:VAL:O | 1:K:341:THR:CB | 2.63 | 0.43 |
| 1:K:365:ASP:OD2 | 1:K:367:THR:HB | 2.18 | 0.43 |
| 1:K:377:LYS:HA | 1:K:378:PRO:HD3 | 1.84 | 0.43 |
| 1:L:388:GLN:O | 1:L:392:ILE:HG22 | 2.19 | 0.43 |
| 1:B:401:LEU:HA | 1:B:401:LEU:HD12 | 1.62 | 0.42 |
| 1:B:448:TYR:C | 1:B:453:GLU:HG3 | 2.39 | 0.42 |
| 1:B:465:LEU:HD21 | 1:B:480:ALA:CB | 2.49 | 0.42 |
| 1:B:572:TYR:HB2 | 1:B:591:VAL:CG2 | 2.49 | 0.42 |
| 1:C:458:SER:HB2 | 1:C:632:ILE:O | 2.19 | 0.42 |
| 1:D:465:LEU:HD21 | 1:D:480:ALA:CB | 2.49 | 0.42 |
| 1:D:607:ALA:O | 1:D:609:ILE:N | 2.52 | 0.42 |
| 1:E:340:VAL:O | 1:E:341:THR:CG2 | 2.64 | 0.42 |
| 1:E:516:SER:HB2 | 1:E:617:GLU:OE1 | 2.18 | 0.42 |
| 1:F:447:TYR:HB2 | 1:F:467:TYR:CD1 | 2.54 | 0.42 |
| 1:H:358:GLN:HB3 | 1:H:379:LYS:HA | 1.99 | 0.42 |
| 1:H:542:SER:HB2 | 1:H:595:ILE:CD1 | 2.49 | 0.42 |
| 1:H:607:ALA:O | 1:H:609:ILE:N | 2.52 | 0.42 |
| 1:I:650:TYR:O | 1:I:651:LEU:HB2 | 2.18 | 0.42 |
| 1:J:375:ALA:HA | 1:J:409:ILE:O | 2.19 | 0.42 |
| 1:J:414:LEU:HD23 | 1:J:414:LEU:HA | 1.70 | 0.42 |
| 1:J:448:TYR:C | 1:J:453:GLU:HG3 | 2.39 | 0.42 |
| 1:K:582:ASN:C | 1:K:585:GLY:H | 2.21 | 0.42 |
| 1:L:448:TYR:CG | 1:L:642:PHE:HB2 | 2.53 | 0.42 |
| 1:A:464:MET:CG | 1:A:465:LEU:N | 2.82 | 0.42 |
| 1:B:345:TYR:C | 1:B:345:TYR:HD1 | 2.18 | 0.42 |
| 1:C:387:VAL:CB | 1:C:390:GLU:CD | 2.87 | 0.42 |
| 1:C:469:ASP:HA | 1:C:475:VAL:HG11 | 2.00 | 0.42 |
| 1:C:533:ASP:O | 1:C:535:LEU:CD2 | 2.67 | 0.42 |
| 1:C:647:ARG:N | 1:C:648:PRO:HD3 | 2.34 | 0.42 |
| 1:D:375:ALA:HA | 1:D:409:ILE:O | 2.19 | 0.42 |
| 1:F:492:TYR:OH | 1:F:611:LEU:O | 2.34 | 0.42 |
| 1:F:653:ILE:HG22 | 1:F:655:LEU:CD1 | 2.49 | 0.42 |
| 1:G:388:GLN:C | 1:G:389:ARG:CG | 2.88 | 0.42 |
| 1:G:623:LEU:HD12 | 1:G:623:LEU:HA | 1.79 | 0.42 |
| 1:H:345:TYR:C | 1:H:345:TYR:HD1 | 2.18 | 0.42 |
| 1:H:422:VAL:HG11 | 1:H:475:VAL:HG13 | 2.01 | 0.42 |
| 1:I:454:ILE:HG23 | 1:I:455:PHE:N | 2.34 | 0.42 |
| 1:I:660:GLN:HG3 | 1:I:661:LEU:H | 1.77 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:464:MET:O | 1:J:468:VAL:HG23 | 2.18 | 0.42 |
| 1:J:592:ILE:CD1 | 1:J:606:ILE:HD13 | 2.49 | 0.42 |
| 1:L:607:ALA:O | 1:L:609:ILE:N | 2.52 | 0.42 |
| 1:A:469:ASP:HA | 1:A:475:VAL:HG11 | 2.01 | 0.42 |
| 1:A:595:ILE:HG23 | 1:A:602:ILE:HG12 | 1.99 | 0.42 |
| 1:A:661:LEU:CD1 | 1:A:662:GLU:CA | 2.85 | 0.42 |
| 1:D:572:TYR:HB2 | 1:D:591:VAL:CG2 | 2.49 | 0.42 |
| 1:E:458:SER:HB2 | 1:E:632:ILE:O | 2.19 | 0.42 |
| 1:E:661:LEU:HD22 | 1:E:661:LEU:HA | 1.75 | 0.42 |
| 1:G:340:VAL:CA | 1:G:345:TYR:CZ | 2.82 | 0.42 |
| 1:G:454:ILE:HG23 | 1:G:455:PHE:N | 2.34 | 0.42 |
| 1:H:365:ASP:CG | 1:H:367:THR:CG2 | 2.88 | 0.42 |
| 1:I:346:ASP:OD1 | 1:I:362:THR:CB | 2.67 | 0.42 |
| 1:I:365:ASP:OD2 | 1:I:367:THR:HB | 2.18 | 0.42 |
| 1:J:365:ASP:CG | 1:J:367:THR:CG2 | 2.88 | 0.42 |
| 1:J:461:LYS:HG2 | 1:J:461:LYS:O | 2.18 | 0.42 |
| 1:J:484:MET:HG3 | 1:J:627:PRO:HG3 | 1.99 | 0.42 |
| 1:J:560:SER:HB2 | 1:J:588:LYS:NZ | 2.33 | 0.42 |
| 1:K:647:ARG:N | 1:K:648:PRO:HD3 | 2.34 | 0.42 |
| 1:L:365:ASP:CG | 1:L:367:THR:CG2 | 2.88 | 0.42 |
| 1:L:464:MET:O | 1:L:468:VAL:HG23 | 2.18 | 0.42 |
| 1:L:542:SER:HB2 | 1:L:595:ILE:CD1 | 2.50 | 0.42 |
| 1:C:492:TYR:CE1 | 1:C:606:ILE:HB | 2.54 | 0.42 |
| 1:D:658:ILE:HD12 | 1:D:658:ILE:HA | 1.67 | 0.42 |
| 1:E:556:GLY:CA | 1:E:589:TYR:CD1 | 3.01 | 0.42 |
| 1:F:365:ASP:CG | 1:F:367:THR:CG2 | 2.87 | 0.42 |
| 1:F:557:PRO:CG | 1:F:580:LEU:HD11 | 2.37 | 0.42 |
| 1:G:408:ILE:H | 1:G:408:ILE:CD1 | 2.30 | 0.42 |
| 1:G:469:ASP:HA | 1:G:475:VAL:HG11 | 2.00 | 0.42 |
| 1:G:582:ASN:C | 1:G:585:GLY:H | 2.21 | 0.42 |
| 1:G:661:LEU:HD22 | 1:G:661:LEU:HA | 1.75 | 0.42 |
| 1:H:592:ILE:CD1 | 1:H:606:ILE:HD13 | 2.49 | 0.42 |
| 1:I:469:ASP:HA | 1:I:475:VAL:HG11 | 2.01 | 0.42 |
| 1:I:516:SER:HB2 | 1:I:617:GLU:OE1 | 2.18 | 0.42 |
| 1:A:347:THR:C | 1:A:349:VAL:N | 2.73 | 0.42 |
| 1:A:492:TYR:CE1 | 1:A:606:ILE:HB | 2.54 | 0.42 |
| 1:C:454:ILE:HG23 | 1:C:455:PHE:N | 2.34 | 0.42 |
| 1:D:388:GLN:O | 1:D:392:ILE:HG22 | 2.19 | 0.42 |
| 1:D:400:ASN:HD22 | 1:E:662:GLU:HG2 | 1.02 | 0.42 |
| 1:D:495:PRO:O | 1:D:496:GLU:C | 2.57 | 0.42 |
| 1:E:593:GLY:HA3 | 1:E:603:TYR:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:414:LEU:HD23 | 1:F:414:LEU:HA | 1.70 | 0.42 |
| 1:G:492:TYR:CE1 | 1:G:606:ILE:HB | 2.54 | 0.42 |
| 1:H:448:TYR:C | 1:H:453:GLU:HG3 | 2.39 | 0.42 |
| 1:I:448:TYR:CZ | 1:I:642:PHE:HB2 | 2.55 | 0.42 |
| 1:I:521:ARG:HE | 1:I:521:ARG:HB2 | 1.71 | 0.42 |
| 1:J:494:THR:HG22 | 1:J:499:ILE:HG22 | 2.01 | 0.42 |
| 1:J:495:PRO:O | 1:J:496:GLU:C | 2.57 | 0.42 |
| 1:J:607:ALA:O | 1:J:609:ILE:N | 2.52 | 0.42 |
| 1:A:593:GLY:HA3 | 1:A:603:TYR:O | 2.19 | 0.42 |
| 1:D:545:ARG:CZ | 1:D:597:TYR:HB3 | 2.50 | 0.42 |
| 1:F:495:PRO:O | 1:F:496:GLU:C | 2.57 | 0.42 |
| 1:F:607:ALA:O | 1:F:609:ILE:N | 2.52 | 0.42 |
| 1:F:623:LEU:HD12 | 1:F:623:LEU:HA | 1.86 | 0.42 |
| 1:G:448:TYR:CZ | 1:G:642:PHE:HB2 | 2.55 | 0.42 |
| 1:I:387:VAL:CB | 1:I:390:GLU:CD | 2.88 | 0.42 |
| 1:K:349:VAL:C | 1:K:351:GLU:N | 2.71 | 0.42 |
| 1:L:465:LEU:HD21 | 1:L:480:ALA:CB | 2.49 | 0.42 |
| 1:L:545:ARG:CZ | 1:L:597:TYR:HB3 | 2.50 | 0.42 |
| 1:B:365:ASP:CG | 1:B:367:THR:CG2 | 2.88 | 0.42 |
| 1:B:542:SER:HB2 | 1:B:595:ILE:CD1 | 2.49 | 0.42 |
| 1:B:607:ALA:O | 1:B:609:ILE:N | 2.52 | 0.42 |
| 1:D:648:PRO:CD | 1:D:649:GLN:H | 2.32 | 0.42 |
| 1:E:556:GLY:CA | 1:E:589:TYR:HD1 | 2.32 | 0.42 |
| 1:G:346:ASP:OD1 | 1:G:362:THR:CB | 2.67 | 0.42 |
| 1:I:556:GLY:CA | 1:I:589:TYR:CD1 | 3.01 | 0.42 |
| 1:I:661:LEU:HA | 1:I:661:LEU:HD22 | 1.75 | 0.42 |
| 1:J:447:TYR:HB2 | 1:J:467:TYR:CD1 | 2.54 | 0.42 |
| 1:J:542:SER:HB2 | 1:J:595:ILE:CD1 | 2.50 | 0.42 |
| 1:K:361:GLN:HA | 1:K:361:GLN:HE21 | 1.84 | 0.42 |
| 1:K:386:THR:C | 1:K:388:GLN:N | 2.67 | 0.42 |
| 1:C:388:GLN:C | 1:C:389:ARG:CG | 2.88 | 0.42 |
| 1:D:461:LYS:O | 1:D:461:LYS:HG2 | 2.18 | 0.42 |
| 1:E:448:TYR:HA | 1:E:452:VAL:HB | 2.02 | 0.42 |
| 1:E:448:TYR:CZ | 1:E:642:PHE:HB2 | 2.55 | 0.42 |
| 1:F:422:VAL:HG11 | 1:F:475:VAL:HG13 | 2.01 | 0.42 |
| 1:G:386:THR:C | 1:G:388:GLN:N | 2.67 | 0.42 |
| 1:G:387:VAL:CB | 1:G:390:GLU:CD | 2.88 | 0.42 |
| 1:I:647:ARG:N | 1:I:648:PRO:HD3 | 2.34 | 0.42 |
| 1:J:405:THR:HB | 1:J:406:PRO:HD3 | 1.43 | 0.42 |
| 1:K:387:VAL:CB | 1:K:390:GLU:CD | 2.88 | 0.42 |
| 1:A:458:SER:HB2 | 1:A:632:ILE:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:595:ILE:HG23 | 1:A:602:ILE:HG23 | 2.02 | 0.42 |
| 1:B:388:GLN:O | 1:B:392:ILE:HG22 | 2.19 | 0.42 |
| 1:B:648:PRO:CD | 1:B:649:GLN:H | 2.32 | 0.42 |
| 1:C:346:ASP:OD1 | 1:C:362:THR:CB | 2.67 | 0.42 |
| 1:C:502:ASN:ND2 | 1:C:635:ARG:CB | 2.59 | 0.42 |
| 1:E:346:ASP:OD1 | 1:E:362:THR:CB | 2.67 | 0.42 |
| 1:E:647:ARG:N | 1:E:648:PRO:HD3 | 2.34 | 0.42 |
| 1:F:545:ARG:CZ | 1:F:597:TYR:HB3 | 2.50 | 0.42 |
| 1:F:572:TYR:HB2 | 1:F:591:VAL:CG2 | 2.49 | 0.42 |
| 1:G:349:VAL:C | 1:G:351:GLU:N | 2.71 | 0.42 |
| 1:G:377:LYS:HA | 1:G:378:PRO:HD3 | 1.84 | 0.42 |
| 1:H:408:ILE:O | 1:H:408:ILE:CG1 | 2.64 | 0.42 |
| 1:H:545:ARG:CZ | 1:H:597:TYR:HB3 | 2.50 | 0.42 |
| 1:K:346:ASP:OD1 | 1:K:362:THR:CB | 2.67 | 0.42 |
| 1:K:454:ILE:HG23 | 1:K:455:PHE:N | 2.34 | 0.42 |
| 1:K:458:SER:HB2 | 1:K:632:ILE:O | 2.19 | 0.42 |
| 1:K:492:TYR:CE1 | 1:K:606:ILE:HB | 2.54 | 0.42 |
| 1:L:345:TYR:C | 1:L:345:TYR:HD1 | 2.18 | 0.42 |
| 1:L:448:TYR:CZ | 1:L:642:PHE:HB2 | 2.55 | 0.42 |
| 1:A:346:ASP:OD1 | 1:A:362:THR:CB | 2.67 | 0.42 |
| 1:A:651:LEU:HD23 | 1:A:651:LEU:C | 2.40 | 0.42 |
| 1:B:346:ASP:OD1 | 1:B:346:ASP:N | 2.47 | 0.42 |
| 1:B:658:ILE:HD12 | 1:B:658:ILE:HA | 1.67 | 0.42 |
| 1:C:424:TYR:O | 1:C:658:ILE:HB | 2.20 | 0.42 |
| 1:D:358:GLN:HE21 | 1:D:377:LYS:HZ2 | 1.67 | 0.42 |
| 1:E:387:VAL:CB | 1:E:390:GLU:CD | 2.88 | 0.42 |
| 1:E:557:PRO:HD3 | 1:E:580:LEU:HD11 | 2.01 | 0.42 |
| 1:E:660:GLN:HG3 | 1:E:661:LEU:H | 1.77 | 0.42 |
| 1:G:556:GLY:CA | 1:G:589:TYR:HD1 | 2.32 | 0.42 |
| 1:H:495:PRO:O | 1:H:496:GLU:C | 2.57 | 0.42 |
| 1:I:440:ILE:CG1 | 1:I:441:ILE:N | 2.79 | 0.42 |
| 1:J:653:ILE:HG22 | 1:J:655:LEU:CD1 | 2.49 | 0.42 |
| 1:K:465:LEU:HD23 | 1:K:465:LEU:HA | 1.84 | 0.42 |
| 1:L:422:VAL:HG11 | 1:L:475:VAL:HG13 | 2.01 | 0.42 |
| 1:A:340:VAL:O | 1:A:341:THR:CB | 2.63 | 0.41 |
| 1:A:424:TYR:O | 1:A:658:ILE:HB | 2.20 | 0.41 |
| 1:A:557:PRO:HD3 | 1:A:580:LEU:HD11 | 2.01 | 0.41 |
| 1:A:660:GLN:HG3 | 1:A:661:LEU:H | 1.77 | 0.41 |
| 1:B:375:ALA:HA | 1:B:409:ILE:O | 2.19 | 0.41 |
| 1:B:448:TYR:CZ | 1:B:642:PHE:HB2 | 2.55 | 0.41 |
| 1:B:545:ARG:CZ | 1:B:597:TYR:HB3 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:557:PRO:HD3 | 1:C:580:LEU:HD11 | 2.01 | 0.41 |
| 1:D:494:THR:HG22 | 1:D:499:ILE:HG22 | 2.01 | 0.41 |
| 1:F:448:TYR:CZ | 1:F:642:PHE:HB2 | 2.55 | 0.41 |
| 1:I:525:ASN:OD1 | 1:I:526:PRO:N | 2.53 | 0.41 |
| 1:J:545:ARG:CZ | 1:J:597:TYR:HB3 | 2.50 | 0.41 |
| 1:K:408:ILE:H | 1:K:408:ILE:CD1 | 2.30 | 0.41 |
| 1:K:448:TYR:CZ | 1:K:642:PHE:HB2 | 2.55 | 0.41 |
| 1:A:387:VAL:CG2 | 1:A:390:GLU:OE1 | 2.55 | 0.41 |
| 1:A:387:VAL:CB | 1:A:390:GLU:CD | 2.88 | 0.41 |
| 1:C:448:TYR:HA | 1:C:452:VAL:HB | 2.02 | 0.41 |
| 1:C:556:GLY:CA | 1:C:589:TYR:HD1 | 2.32 | 0.41 |
| 1:D:653:ILE:HG22 | 1:D:655:LEU:CD1 | 2.49 | 0.41 |
| 1:F:353:PHE:CZ | 1:F:395:TYR:CD2 | 3.05 | 0.41 |
| 1:F:494:THR:HG22 | 1:F:499:ILE:HG22 | 2.01 | 0.41 |
| 1:F:642:PHE:CZ | 1:F:644:ASN:HB2 | 2.55 | 0.41 |
| 1:G:525:ASN:OD1 | 1:G:526:PRO:N | 2.53 | 0.41 |
| 1:G:651:LEU:HD23 | 1:G:651:LEU:C | 2.40 | 0.41 |
| 1:I:465:LEU:HD23 | 1:I:465:LEU:HA | 1.84 | 0.41 |
| 1:I:493:LYS:HE3 | 1:I:493:LYS:HB2 | 1.91 | 0.41 |
| 1:J:496:GLU:N | 1:J:496:GLU:OE1 | 2.30 | 0.41 |
| 1:L:401:LEU:HD12 | 1:L:401:LEU:HA | 1.63 | 0.41 |
| 1:A:550:ILE:HG12 | 1:A:596:ASN:HA | 2.02 | 0.41 |
| 1:B:495:PRO:O | 1:B:496:GLU:C | 2.57 | 0.41 |
| 1:C:361:GLN:HA | 1:C:361:GLN:HE21 | 1.84 | 0.41 |
| 1:C:595:ILE:HG23 | 1:C:602:ILE:HG23 | 2.02 | 0.41 |
| 1:E:377:LYS:HA | 1:E:378:PRO:HD3 | 1.84 | 0.41 |
| 1:E:525:ASN:OD1 | 1:E:526:PRO:N | 2.53 | 0.41 |
| 1:G:361:GLN:HG2 | 1:G:455:PHE:CB | 2.50 | 0.41 |
| 1:G:502:ASN:ND2 | 1:G:635:ARG:CB | 2.59 | 0.41 |
| 1:G:557:PRO:HD3 | 1:G:580:LEU:HD11 | 2.01 | 0.41 |
| 1:H:494:THR:HG22 | 1:H:499:ILE:HG22 | 2.01 | 0.41 |
| 1:H:642:PHE:CZ | 1:H:644:ASN:HB2 | 2.55 | 0.41 |
| 1:I:401:LEU:HD21 | 1:I:402:ALA:HB2 | 1.96 | 0.41 |
| 1:I:458:SER:HB2 | 1:I:632:ILE:O | 2.19 | 0.41 |
| 1:I:550:ILE:HG12 | 1:I:596:ASN:HA | 2.02 | 0.41 |
| 1:I:556:GLY:CA | 1:I:589:TYR:HD1 | 2.32 | 0.41 |
| 1:K:502:ASN:ND2 | 1:K:635:ARG:CB | 2.59 | 0.41 |
| 1:A:382:LEU:CD1 | 1:A:647:ARG:HH21 | 2.33 | 0.41 |
| 1:C:384:LEU:HD23 | 1:C:384:LEU:HA | 1.85 | 0.41 |
| 1:C:448:TYR:CZ | 1:C:642:PHE:HB2 | 2.55 | 0.41 |
| 1:E:454:ILE:HG23 | 1:E:455:PHE:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:448:TYR:HA | 1:G:452:VAL:HB | 2.02 | 0.41 |
| 1:G:458:SER:HB2 | 1:G:632:ILE:O | 2.19 | 0.41 |
| 1:G:556:GLY:CA | 1:G:589:TYR:CD1 | 3.01 | 0.41 |
| 1:H:365:ASP:O | 1:H:366:SER:C | 2.54 | 0.41 |
| 1:H:447:TYR:HB2 | 1:H:467:TYR:CD1 | 2.54 | 0.41 |
| 1:I:349:VAL:C | 1:I:351:GLU:N | 2.71 | 0.41 |
| 1:I:387:VAL:CG2 | 1:I:390:GLU:OE1 | 2.55 | 0.41 |
| 1:I:651:LEU:HD23 | 1:I:651:LEU:C | 2.40 | 0.41 |
| 1:K:525:ASN:OD1 | 1:K:526:PRO:N | 2.53 | 0.41 |
| 1:A:453:GLU:O | 1:A:454:ILE:HG13 | 2.21 | 0.41 |
| 1:C:382:LEU:CD1 | 1:C:647:ARG:HH21 | 2.33 | 0.41 |
| 1:C:464:MET:CG | 1:C:465:LEU:N | 2.82 | 0.41 |
| 1:D:542:SER:HB2 | 1:D:595:ILE:CD1 | 2.50 | 0.41 |
| 1:E:453:GLU:O | 1:E:454:ILE:HG13 | 2.21 | 0.41 |
| 1:E:651:LEU:HD23 | 1:E:651:LEU:C | 2.40 | 0.41 |
| 1:G:647:ARG:N | 1:G:648:PRO:HD3 | 2.34 | 0.41 |
| 1:G:656:GLU:HA | 1:G:657:PRO:HD3 | 1.82 | 0.41 |
| 1:H:476:ILE:CG2 | 1:H:476:ILE:O | 2.60 | 0.41 |
| 1:J:422:VAL:HG11 | 1:J:475:VAL:HG13 | 2.01 | 0.41 |
| 1:K:550:ILE:HG12 | 1:K:596:ASN:HA | 2.02 | 0.41 |
| 1:K:556:GLY:CA | 1:K:589:TYR:HD1 | 2.32 | 0.41 |
| 1:K:595:ILE:HG23 | 1:K:602:ILE:HG23 | 2.02 | 0.41 |
| 1:L:365:ASP:O | 1:L:366:SER:C | 2.54 | 0.41 |
| 1:L:642:PHE:CZ | 1:L:644:ASN:HB2 | 2.55 | 0.41 |
| 1:A:448:TYR:CZ | 1:A:642:PHE:HB2 | 2.55 | 0.41 |
| 1:B:396:LEU:HD13 | 1:B:405:THR:OG1 | 2.21 | 0.41 |
| 1:B:642:PHE:CZ | 1:B:644:ASN:HB2 | 2.55 | 0.41 |
| 1:C:651:LEU:HD23 | 1:C:651:LEU:C | 2.40 | 0.41 |
| 1:G:526:PRO:O | 1:G:527:ASP:C | 2.59 | 0.41 |
| 1:G:595:ILE:HG23 | 1:G:602:ILE:HG23 | 2.02 | 0.41 |
| 1:H:375:ALA:HA | 1:H:409:ILE:CD1 | 2.51 | 0.41 |
| 1:H:396:LEU:HD13 | 1:H:405:THR:OG1 | 2.21 | 0.41 |
| 1:H:448:TYR:CZ | 1:H:642:PHE:HB2 | 2.55 | 0.41 |
| 1:J:448:TYR:CZ | 1:J:642:PHE:HB2 | 2.55 | 0.41 |
| 1:L:367:THR:CG2 | 1:L:368:LYS:N | 2.44 | 0.41 |
| 1:L:402:ALA:O | 1:L:403:PRO:C | 2.59 | 0.41 |
| 1:L:447:TYR:HB2 | 1:L:467:TYR:CD1 | 2.54 | 0.41 |
| 1:A:361:GLN:HG2 | 1:A:455:PHE:CB | 2.50 | 0.41 |
| 1:A:647:ARG:N | 1:A:648:PRO:HD3 | 2.34 | 0.41 |
| 1:B:408:ILE:O | 1:B:408:ILE:CG1 | 2.64 | 0.41 |
| 1:B:455:PHE:O | 1:B:456:ASN:CB | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:647:ARG:HD3 | 1:B:649:GLN:CG | 2.51 | 0.41 |
| 1:C:377:LYS:HA | 1:C:378:PRO:HD3 | 1.84 | 0.41 |
| 1:C:521:ARG:HE | 1:C:521:ARG:HB2 | 1.71 | 0.41 |
| 1:E:361:GLN:HG2 | 1:E:455:PHE:CB | 2.50 | 0.41 |
| 1:H:358:GLN:HE21 | 1:H:377:LYS:NZ | 2.19 | 0.41 |
| 1:I:424:TYR:O | 1:I:658:ILE:HB | 2.20 | 0.41 |
| 1:I:424:TYR:HB2 | 1:I:475:VAL:H | 1.85 | 0.41 |
| 1:I:595:ILE:HG23 | 1:I:602:ILE:HG23 | 2.02 | 0.41 |
| 1:J:642:PHE:CZ | 1:J:644:ASN:HB2 | 2.55 | 0.41 |
| 1:K:361:GLN:HG2 | 1:K:455:PHE:CB | 2.50 | 0.41 |
| 1:K:382:LEU:CD1 | 1:K:647:ARG:HH21 | 2.33 | 0.41 |
| 1:K:424:TYR:HB2 | 1:K:475:VAL:H | 1.85 | 0.41 |
| 1:K:651:LEU:HD23 | 1:K:651:LEU:C | 2.40 | 0.41 |
| 1:L:375:ALA:HA | 1:L:409:ILE:CD1 | 2.51 | 0.41 |
| 1:L:455:PHE:O | 1:L:456:ASN:CB | 2.69 | 0.41 |
| 1:L:663:HIS:HE1 | 1:L:665:HIS:O | 2.04 | 0.41 |
| 1:B:375:ALA:HA | 1:B:409:ILE:CD1 | 2.51 | 0.41 |
| 1:B:663:HIS:HE1 | 1:B:665:HIS:O | 2.04 | 0.41 |
| 1:C:341:THR:O | 1:C:341:THR:OG1 | 2.33 | 0.41 |
| 1:C:361:GLN:HG2 | 1:C:455:PHE:CB | 2.50 | 0.41 |
| 1:E:523:VAL:HG12 | 1:E:534:VAL:HG22 | 2.03 | 0.41 |
| 1:E:582:ASN:C | 1:E:585:GLY:H | 2.21 | 0.41 |
| 1:F:542:SER:HB2 | 1:F:595:ILE:CD1 | 2.50 | 0.41 |
| 1:G:453:GLU:O | 1:G:454:ILE:HG13 | 2.21 | 0.41 |
| 1:G:595:ILE:CG2 | 1:G:602:ILE:HG12 | 2.51 | 0.41 |
| 1:I:526:PRO:O | 1:I:527:ASP:C | 2.59 | 0.41 |
| 1:K:448:TYR:HA | 1:K:452:VAL:HB | 2.02 | 0.41 |
| 1:A:414:LEU:HD23 | 1:A:414:LEU:HA | 1.91 | 0.41 |
| 1:A:448:TYR:HA | 1:A:452:VAL:HB | 2.02 | 0.41 |
| 1:A:523:VAL:HG22 | 1:A:524:VAL:H | 1.86 | 0.41 |
| 1:B:448:TYR:CD2 | 1:B:642:PHE:HB2 | 2.56 | 0.41 |
| 1:C:420:LEU:HG | 1:C:422:VAL:HG23 | 2.03 | 0.41 |
| 1:C:523:VAL:HG12 | 1:C:534:VAL:HG22 | 2.03 | 0.41 |
| 1:D:396:LEU:HD13 | 1:D:405:THR:OG1 | 2.21 | 0.41 |
| 1:D:448:TYR:CZ | 1:D:642:PHE:HB2 | 2.55 | 0.41 |
| 1:D:455:PHE:O | 1:D:456:ASN:CB | 2.69 | 0.41 |
| 1:D:492:TYR:OH | 1:D:611:LEU:O | 2.34 | 0.41 |
| 1:D:546:ASP:CG | 1:D:547:SER:O | 2.59 | 0.41 |
| 1:D:642:PHE:CZ | 1:D:644:ASN:HB2 | 2.55 | 0.41 |
| 1:E:353:PHE:O | 1:E:355:SER:HB3 | 2.21 | 0.41 |
| 1:E:523:VAL:HG22 | 1:E:524:VAL:H | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:358:GLN:HE21 | 1:F:377:LYS:NZ | 2.19 | 0.41 |
| 1:G:361:GLN:HA | 1:G:361:GLN:HE21 | 1.84 | 0.41 |
| 1:G:382:LEU:CD1 | 1:G:647:ARG:HH21 | 2.33 | 0.41 |
| 1:G:523:VAL:HG12 | 1:G:534:VAL:HG22 | 2.03 | 0.41 |
| 1:H:448:TYR:CD2 | 1:H:642:PHE:HB2 | 2.56 | 0.41 |
| 1:H:546:ASP:CG | 1:H:547:SER:O | 2.59 | 0.41 |
| 1:J:455:PHE:O | 1:J:456:ASN:CB | 2.69 | 0.41 |
| 1:J:546:ASP:CG | 1:J:547:SER:O | 2.59 | 0.41 |
| 1:K:660:GLN:HG3 | 1:K:661:LEU:H | 1.77 | 0.41 |
| 1:L:495:PRO:O | 1:L:496:GLU:C | 2.57 | 0.41 |
| 1:L:651:LEU:HD23 | 1:L:651:LEU:HA | 1.83 | 0.41 |
| 1:A:454:ILE:HG23 | 1:A:455:PHE:N | 2.34 | 0.41 |
| 1:B:353:PHE:CZ | 1:B:395:TYR:CD2 | 3.05 | 0.41 |
| 1:C:353:PHE:O | 1:C:355:SER:HB3 | 2.21 | 0.41 |
| 1:C:647:ARG:CG | 1:C:650:TYR:CD1 | 3.04 | 0.41 |
| 1:D:385:THR:HG23 | 1:D:387:VAL:HG13 | 2.03 | 0.41 |
| 1:E:424:TYR:O | 1:E:658:ILE:HB | 2.20 | 0.41 |
| 1:H:410:SER:HA | 1:H:411:PRO:HD3 | 1.81 | 0.41 |
| 1:H:599:ALA:O | 1:H:600:ASP:C | 2.59 | 0.41 |
| 1:J:541:VAL:HG12 | 1:J:542:SER:H | 1.86 | 0.41 |
| 1:K:523:VAL:HG12 | 1:K:534:VAL:HG22 | 2.03 | 0.41 |
| 1:L:396:LEU:HD13 | 1:L:405:THR:OG1 | 2.21 | 0.41 |
| 1:L:410:SER:HA | 1:L:411:PRO:HD3 | 1.81 | 0.41 |
| 1:A:582:ASN:C | 1:A:584:ASP:N | 2.74 | 0.40 |
| 1:B:365:ASP:O | 1:B:366:SER:C | 2.54 | 0.40 |
| 1:C:525:ASN:OD1 | 1:C:526:PRO:N | 2.53 | 0.40 |
| 1:C:526:PRO:O | 1:C:527:ASP:C | 2.59 | 0.40 |
| 1:D:476:ILE:CG2 | 1:D:476:ILE:O | 2.60 | 0.40 |
| 1:D:663:HIS:HE1 | 1:D:665:HIS:O | 2.04 | 0.40 |
| 1:E:582:ASN:C | 1:E:584:ASP:N | 2.74 | 0.40 |
| 1:F:358:GLN:HE21 | 1:F:377:LYS:HZ2 | 1.69 | 0.40 |
| 1:F:396:LEU:HD13 | 1:F:405:THR:OG1 | 2.21 | 0.40 |
| 1:F:402:ALA:O | 1:F:403:PRO:C | 2.59 | 0.40 |
| 1:H:455:PHE:O | 1:H:456:ASN:CB | 2.69 | 0.40 |
| 1:H:658:ILE:HD12 | 1:H:658:ILE:HA | 1.67 | 0.40 |
| 1:I:347:THR:C | 1:I:349:VAL:N | 2.73 | 0.40 |
| 1:I:420:LEU:HG | 1:I:422:VAL:HG23 | 2.03 | 0.40 |
| 1:J:599:ALA:O | 1:J:600:ASP:C | 2.59 | 0.40 |
| 1:J:664:HIS:CD2 | 1:J:664:HIS:C | 2.90 | 0.40 |
| 1:K:424:TYR:O | 1:K:658:ILE:HB | 2.20 | 0.40 |
| 1:K:523:VAL:HG22 | 1:K:524:VAL:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:556:GLY:HA2 | 1:L:557:PRO:HD3 | 1.90 | 0.40 |
| 1:A:355:SER:OG | 1:A:356:ILE:N | 2.55 | 0.40 |
| 1:A:623:LEU:HD12 | 1:A:623:LEU:HA | 1.79 | 0.40 |
| 1:B:533:ASP:O | 1:B:535:LEU:HG | 2.22 | 0.40 |
| 1:B:557:PRO:CG | 1:B:580:LEU:HD11 | 2.37 | 0.40 |
| 1:C:347:THR:C | 1:C:349:VAL:N | 2.73 | 0.40 |
| 1:D:358:GLN:HE21 | 1:D:377:LYS:NZ | 2.19 | 0.40 |
| 1:D:372:ALA:O | 1:D:406:PRO:HA | 2.21 | 0.40 |
| 1:F:372:ALA:O | 1:F:406:PRO:HA | 2.21 | 0.40 |
| 1:F:546:ASP:CG | 1:F:547:SER:O | 2.59 | 0.40 |
| 1:G:550:ILE:HG12 | 1:G:596:ASN:HA | 2.02 | 0.40 |
| 1:H:647:ARG:HD3 | 1:H:649:GLN:CG | 2.51 | 0.40 |
| 1:I:453:GLU:O | 1:I:454:ILE:HG13 | 2.21 | 0.40 |
| 1:J:375:ALA:HA | 1:J:409:ILE:CD1 | 2.51 | 0.40 |
| 1:J:448:TYR:CD2 | 1:J:642:PHE:HB2 | 2.56 | 0.40 |
| 1:K:353:PHE:O | 1:K:355:SER:HB3 | 2.21 | 0.40 |
| 1:K:420:LEU:HG | 1:K:422:VAL:HG23 | 2.03 | 0.40 |
| 1:K:453:GLU:O | 1:K:454:ILE:HG13 | 2.21 | 0.40 |
| 1:K:483:GLN:HG2 | 1:K:626:ASP:HB3 | 2.04 | 0.40 |
| 1:K:629:ASP:N | 1:K:629:ASP:OD1 | 2.55 | 0.40 |
| 1:L:385:THR:HG23 | 1:L:387:VAL:HG13 | 2.04 | 0.40 |
| 1:L:405:THR:OG1 | 1:L:406:PRO:CD | 2.66 | 0.40 |
| 1:L:599:ALA:O | 1:L:600:ASP:C | 2.59 | 0.40 |
| 1:L:623:LEU:HA | 1:L:623:LEU:HD12 | 1.86 | 0.40 |
| 1:A:424:TYR:HB2 | 1:A:475:VAL:H | 1.85 | 0.40 |
| 1:A:595:ILE:CG2 | 1:A:602:ILE:HG12 | 2.51 | 0.40 |
| 1:B:372:ALA:O | 1:B:406:PRO:HA | 2.21 | 0.40 |
| 1:B:422:VAL:HG11 | 1:B:475:VAL:HG13 | 2.01 | 0.40 |
| 1:C:626:ASP:HA | 1:C:627:PRO:HD3 | 1.65 | 0.40 |
| 1:C:629:ASP:N | 1:C:629:ASP:OD1 | 2.55 | 0.40 |
| 1:D:375:ALA:HA | 1:D:409:ILE:CD1 | 2.51 | 0.40 |
| 1:D:448:TYR:CD2 | 1:D:642:PHE:HB2 | 2.56 | 0.40 |
| 1:D:647:ARG:HD3 | 1:D:649:GLN:CG | 2.51 | 0.40 |
| 1:E:550:ILE:HG12 | 1:E:596:ASN:HA | 2.02 | 0.40 |
| 1:E:647:ARG:CG | 1:E:650:TYR:CD1 | 3.04 | 0.40 |
| 1:F:385:THR:HG23 | 1:F:387:VAL:HG13 | 2.04 | 0.40 |
| 1:F:448:TYR:CD2 | 1:F:642:PHE:HB2 | 2.56 | 0.40 |
| 1:F:663:HIS:HE1 | 1:F:665:HIS:O | 2.04 | 0.40 |
| 1:G:424:TYR:O | 1:G:658:ILE:HB | 2.20 | 0.40 |
| 1:G:465:LEU:HA | 1:G:465:LEU:HD23 | 1.84 | 0.40 |
| 1:G:582:ASN:C | 1:G:584:ASP:N | 2.74 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:629:ASP:OD1 | 1:I:629:ASP:N | 2.55 | 0.40 |
| 1:J:358:GLN:HE21 | 1:J:377:LYS:NZ | 2.19 | 0.40 |
| 1:J:396:LEU:HD13 | 1:J:405:THR:OG1 | 2.21 | 0.40 |
| 1:K:582:ASN:C | 1:K:584:ASP:N | 2.74 | 0.40 |
| 1:L:448:TYR:CD2 | 1:L:642:PHE:HB2 | 2.56 | 0.40 |
| 1:L:648:PRO:CD | 1:L:649:GLN:H | 2.32 | 0.40 |
| 1:L:659:SER:HB3 | 1:L:660:GLN:H | 1.78 | 0.40 |
| 1:A:523:VAL:HG12 | 1:A:534:VAL:HG22 | 2.03 | 0.40 |
| 1:A:525:ASN:OD1 | 1:A:526:PRO:N | 2.53 | 0.40 |
| 1:A:556:GLY:CA | 1:A:589:TYR:HD1 | 2.32 | 0.40 |
| 1:B:486:ARG:HH22 | 1:B:638:SER:HB3 | 1.86 | 0.40 |
| 1:B:599:ALA:O | 1:B:600:ASP:C | 2.59 | 0.40 |
| 1:C:340:VAL:O | 1:C:341:THR:CG2 | 2.64 | 0.40 |
| 1:D:441:ILE:HD11 | 1:D:644:ASN:CG | 2.42 | 0.40 |
| 1:D:533:ASP:O | 1:D:535:LEU:HG | 2.22 | 0.40 |
| 1:F:356:ILE:O | 1:F:379:LYS:N | 2.48 | 0.40 |
| 1:F:441:ILE:HD11 | 1:F:644:ASN:CG | 2.42 | 0.40 |
| 1:G:340:VAL:O | 1:G:341:THR:CG2 | 2.64 | 0.40 |
| 1:H:402:ALA:O | 1:H:403:PRO:C | 2.59 | 0.40 |
| 1:H:414:LEU:HD23 | 1:H:414:LEU:HA | 1.70 | 0.40 |
| 1:H:486:ARG:HH22 | 1:H:638:SER:HB3 | 1.86 | 0.40 |
| 1:H:663:HIS:HE1 | 1:H:665:HIS:O | 2.04 | 0.40 |
| 1:I:453:GLU:HG2 | 1:I:641:VAL:HA | 2.04 | 0.40 |
| 1:I:523:VAL:HG22 | 1:I:524:VAL:H | 1.86 | 0.40 |
| 1:K:347:THR:C | 1:K:349:VAL:N | 2.73 | 0.40 |
| 1:K:387:VAL:CG2 | 1:K:390:GLU:OE1 | 2.55 | 0.40 |
| 1:B:441:ILE:HD11 | 1:B:644:ASN:CG | 2.42 | 0.40 |
| 1:C:424:TYR:HB2 | 1:C:475:VAL:H | 1.85 | 0.40 |
| 1:C:523:VAL:HG22 | 1:C:524:VAL:H | 1.86 | 0.40 |
| 1:C:595:ILE:CG2 | 1:C:602:ILE:HG12 | 2.51 | 0.40 |
| 1:C:658:ILE:HD13 | 1:C:658:ILE:HA | 1.52 | 0.40 |
| 1:E:595:ILE:HG23 | 1:E:602:ILE:HG23 | 2.02 | 0.40 |
| 1:F:375:ALA:HA | 1:F:409:ILE:CD1 | 2.51 | 0.40 |
| 1:F:455:PHE:O | 1:F:456:ASN:CB | 2.69 | 0.40 |
| 1:F:599:ALA:O | 1:F:600:ASP:C | 2.59 | 0.40 |
| 1:G:424:TYR:HB2 | 1:G:475:VAL:H | 1.85 | 0.40 |
| 1:G:464:MET:CG | 1:G:465:LEU:N | 2.82 | 0.40 |
| 1:H:465:LEU:HD21 | 1:H:480:ALA:CB | 2.49 | 0.40 |
| 1:I:464:MET:CG | 1:I:465:LEU:N | 2.82 | 0.40 |
| 1:J:465:LEU:HD21 | 1:J:480:ALA:CB | 2.49 | 0.40 |
| 1:J:658:ILE:HD12 | 1:J:658:ILE:HA | 1.67 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:K:355:SER:OG | 1:K:356:ILE:N | 2.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | B | 322/335 (96%) | 261 (81%) | 42 (13%) | 19 (6%) | 1 | 17 |
| 1 | C | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | D | 322/335 (96%) | 262 (81%) | 41 (13%) | 19 (6%) | 1 | 17 |
| 1 | E | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | F | 322/335 (96%) | 262 (81%) | 41 (13%) | 19 (6%) | 1 | 17 |
| 1 | G | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | H | 322/335 (96%) | 262 (81%) | 41 (13%) | 19 (6%) | 1 | 17 |
| 1 | I | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | J | 322/335 (96%) | 261 (81%) | 42 (13%) | 19 (6%) | 1 | 17 |
| 1 | K | 324/335 (97%) | 260 (80%) | 47 (14%) | 17 (5%) | 2 | 19 |
| 1 | L | 322/335 (96%) | 261 (81%) | 42 (13%) | 19 (6%) | 1 | 17 |
| All | All | 3876/4020 (96%) | 3129 (81%) | 531 (14%) | 216 (6%) | 3 | 19 |

All (216) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 348 | PHE |
| 1 | A | 354 | GLY |
| 1 | A | 389 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 390 | GLU |
| 1 | A | 526 | PRO |
| 1 | A | 576 | ASP |
| 1 | A | 635 | ARG |
| 1 | A | 662 | GLU |
| 1 | B | 368 | LYS |
| 1 | B | 406 | PRO |
| 1 | B | 556 | GLY |
| 1 | B | 568 | ASN |
| 1 | B | 593 | GLY |
| 1 | B | 660 | GLN |
| 1 | B | 661 | LEU |
| 1 | B | 662 | GLU |
| 1 | C | 348 | PHE |
| 1 | C | 354 | GLY |
| 1 | C | 389 | ARG |
| 1 | C | 390 | GLU |
| 1 | C | 526 | PRO |
| 1 | C | 576 | ASP |
| 1 | C | 635 | ARG |
| 1 | C | 662 | GLU |
| 1 | D | 368 | LYS |
| 1 | D | 406 | PRO |
| 1 | D | 556 | GLY |
| 1 | D | 568 | ASN |
| 1 | D | 593 | GLY |
| 1 | D | 660 | GLN |
| 1 | D | 661 | LEU |
| 1 | D | 662 | GLU |
| 1 | E | 348 | PHE |
| 1 | E | 354 | GLY |
| 1 | E | 389 | ARG |
| 1 | E | 390 | GLU |
| 1 | E | 526 | PRO |
| 1 | E | 576 | ASP |
| 1 | E | 635 | ARG |
| 1 | E | 662 | GLU |
| 1 | F | 368 | LYS |
| 1 | F | 406 | PRO |
| 1 | F | 556 | GLY |
| 1 | F | 568 | ASN |
| 1 | F | 593 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | F | 660 | GLN |
| 1 | F | 661 | LEU |
| 1 | F | 662 | GLU |
| 1 | G | 348 | PHE |
| 1 | G | 354 | GLY |
| 1 | G | 389 | ARG |
| 1 | G | 390 | GLU |
| 1 | G | 526 | PRO |
| 1 | G | 576 | ASP |
| 1 | G | 635 | ARG |
| 1 | G | 662 | GLU |
| 1 | H | 368 | LYS |
| 1 | H | 406 | PRO |
| 1 | H | 556 | GLY |
| 1 | H | 568 | ASN |
| 1 | H | 593 | GLY |
| 1 | H | 660 | GLN |
| 1 | H | 661 | LEU |
| 1 | H | 662 | GLU |
| 1 | I | 348 | PHE |
| 1 | I | 354 | GLY |
| 1 | I | 389 | ARG |
| 1 | I | 390 | GLU |
| 1 | I | 526 | PRO |
| 1 | I | 576 | ASP |
| 1 | I | 635 | ARG |
| 1 | I | 662 | GLU |
| 1 | J | 368 | LYS |
| 1 | J | 406 | PRO |
| 1 | J | 556 | GLY |
| 1 | J | 568 | ASN |
| 1 | J | 593 | GLY |
| 1 | J | 660 | GLN |
| 1 | J | 661 | LEU |
| 1 | J | 662 | GLU |
| 1 | K | 348 | PHE |
| 1 | K | 354 | GLY |
| 1 | K | 389 | ARG |
| 1 | K | 390 | GLU |
| 1 | K | 526 | PRO |
| 1 | K | 576 | ASP |
| 1 | K | 635 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | K | 662 | GLU |
| 1 | L | 368 | LYS |
| 1 | L | 406 | PRO |
| 1 | L | 556 | GLY |
| 1 | L | 568 | ASN |
| 1 | L | 593 | GLY |
| 1 | L | 660 | GLN |
| 1 | L | 661 | LEU |
| 1 | L | 662 | GLU |
| 1 | A | 402 | ALA |
| 1 | A | 474 | SER |
| 1 | A | 490 | ASN |
| 1 | A | 664 | HIS |
| 1 | B | 367 | THR |
| 1 | B | 560 | SER |
| 1 | B | 600 | ASP |
| 1 | C | 402 | ALA |
| 1 | C | 474 | SER |
| 1 | C | 490 | ASN |
| 1 | C | 664 | HIS |
| 1 | D | 367 | THR |
| 1 | D | 560 | SER |
| 1 | D | 600 | ASP |
| 1 | E | 402 | ALA |
| 1 | E | 474 | SER |
| 1 | E | 490 | ASN |
| 1 | E | 664 | HIS |
| 1 | F | 367 | THR |
| 1 | F | 560 | SER |
| 1 | F | 600 | ASP |
| 1 | G | 402 | ALA |
| 1 | G | 474 | SER |
| 1 | G | 490 | ASN |
| 1 | G | 664 | HIS |
| 1 | H | 367 | THR |
| 1 | H | 560 | SER |
| 1 | H | 600 | ASP |
| 1 | I | 402 | ALA |
| 1 | I | 474 | SER |
| 1 | I | 490 | ASN |
| 1 | I | 664 | HIS |
| 1 | J | 367 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | J | 560 | SER |
| 1 | J | 600 | ASP |
| 1 | K | 402 | ALA |
| 1 | K | 474 | SER |
| 1 | K | 490 | ASN |
| 1 | K | 664 | HIS |
| 1 | L | 367 | THR |
| 1 | L | 560 | SER |
| 1 | L | 600 | ASP |
| 1 | A | 341 | THR |
| 1 | A | 587 | ASP |
| 1 | A | 651 | LEU |
| 1 | B | 348 | PHE |
| 1 | B | 574 | GLY |
| 1 | B | 608 | LYS |
| 1 | B | 663 | HIS |
| 1 | C | 341 | THR |
| 1 | C | 587 | ASP |
| 1 | C | 651 | LEU |
| 1 | D | 348 | PHE |
| 1 | D | 574 | GLY |
| 1 | D | 608 | LYS |
| 1 | D | 663 | HIS |
| 1 | E | 341 | THR |
| 1 | E | 587 | ASP |
| 1 | E | 651 | LEU |
| 1 | F | 348 | PHE |
| 1 | F | 574 | GLY |
| 1 | F | 608 | LYS |
| 1 | F | 663 | HIS |
| 1 | G | 341 | THR |
| 1 | G | 587 | ASP |
| 1 | G | 651 | LEU |
| 1 | H | 348 | PHE |
| 1 | H | 574 | GLY |
| 1 | H | 608 | LYS |
| 1 | H | 663 | HIS |
| 1 | I | 341 | THR |
| 1 | I | 587 | ASP |
| 1 | I | 651 | LEU |
| 1 | J | 348 | PHE |
| 1 | J | 574 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | J | 608 | LYS |
| 1 | J | 663 | HIS |
| 1 | K | 341 | THR |
| 1 | K | 587 | ASP |
| 1 | K | 651 | LEU |
| 1 | L | 348 | PHE |
| 1 | L | 574 | GLY |
| 1 | L | 608 | LYS |
| 1 | L | 663 | HIS |
| 1 | B | 349 | VAL |
| 1 | B | 625 | SER |
| 1 | D | 349 | VAL |
| 1 | D | 625 | SER |
| 1 | F | 349 | VAL |
| 1 | F | 625 | SER |
| 1 | H | 349 | VAL |
| 1 | H | 625 | SER |
| 1 | J | 349 | VAL |
| 1 | J | 625 | SER |
| 1 | L | 349 | VAL |
| 1 | L | 625 | SER |
| 1 | B | 496 | GLU |
| 1 | D | 496 | GLU |
| 1 | J | 496 | GLU |
| 1 | L | 496 | GLU |
| 1 | A | 475 | VAL |
| 1 | C | 475 | VAL |
| 1 | E | 475 | VAL |
| 1 | F | 496 | GLU |
| 1 | G | 475 | VAL |
| 1 | H | 496 | GLU |
| 1 | I | 475 | VAL |
| 1 | K | 475 | VAL |
| 1 | B | 524 | VAL |
| 1 | D | 524 | VAL |
| 1 | F | 524 | VAL |
| 1 | H | 524 | VAL |
| 1 | J | 524 | VAL |
| 1 | L | 524 | VAL |
| 1 | A | 392 | ILE |
| 1 | C | 392 | ILE |
| 1 | E | 392 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 392 | ILE |
| 1 | I | 392 | ILE |
| 1 | K | 392 | ILE |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-------------|
| 1 | A | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | B | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| 1 | C | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | D | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| 1 | E | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | F | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| 1 | G | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | H | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| 1 | I | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | J | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| 1 | K | 295/304 (97%) | 239 (81%) | 56 (19%) | 1 8 |
| 1 | L | 293/304 (96%) | 234 (80%) | 59 (20%) | 1 7 |
| All | All | 3528/3648 (97%) | 2838 (80%) | 690 (20%) | 4 8 |

All (690) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 340 | VAL |
| 1 | A | 341 | THR |
| 1 | A | 343 | THR |
| 1 | A | 345 | TYR |
| 1 | A | 348 | PHE |
| 1 | A | 355 | SER |
| 1 | A | 356 | ILE |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 360 | VAL |
| 1 | A | 361 | GLN |
| 1 | A | 364 | THR |
| 1 | A | 374 | ILE |
| 1 | A | 388 | GLN |
| 1 | A | 391 | ASP |
| 1 | A | 398 | ASP |
| 1 | A | 401 | LEU |
| 1 | A | 405 | THR |
| 1 | A | 414 | LEU |
| 1 | A | 416 | ILE |
| 1 | A | 423 | THR |
| 1 | A | 427 | ASN |
| 1 | A | 429 | LEU |
| 1 | A | 441 | ILE |
| 1 | A | 446 | ARG |
| 1 | A | 464 | MET |
| 1 | A | 466 | THR |
| 1 | A | 474 | SER |
| 1 | A | 486 | ARG |
| 1 | A | 489 | GLN |
| 1 | A | 496 | GLU |
| 1 | A | 499 | ILE |
| 1 | A | 500 | LYS |
| 1 | A | 522 | LYS |
| 1 | A | 528 | THR |
| 1 | A | 532 | GLU |
| 1 | A | 533 | ASP |
| 1 | A | 536 | TYR |
| 1 | A | 538 | VAL |
| 1 | A | 547 | SER |
| 1 | A | 580 | LEU |
| 1 | A | 587 | ASP |
| 1 | A | 595 | ILE |
| 1 | A | 596 | ASN |
| 1 | A | 619 | GLN |
| 1 | A | 622 | GLU |
| 1 | A | 626 | ASP |
| 1 | A | 628 | THR |
| 1 | A | 629 | ASP |
| 1 | A | 634 | THR |
| 1 | A | 635 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 649 | GLN |
| 1 | A | 652 | THR |
| 1 | A | 658 | ILE |
| 1 | A | 659 | SER |
| 1 | A | 660 | GLN |
| 1 | A | 662 | GLU |
| 1 | A | 663 | HIS |
| 1 | B | 344 | ASP |
| 1 | B | 346 | ASP |
| 1 | B | 357 | ILE |
| 1 | B | 360 | VAL |
| 1 | B | 361 | GLN |
| 1 | B | 364 | THR |
| 1 | B | 366 | SER |
| 1 | B | 367 | THR |
| 1 | B | 374 | ILE |
| 1 | B | 379 | LYS |
| 1 | B | 380 | SER |
| 1 | B | 386 | THR |
| 1 | B | 404 | ILE |
| 1 | B | 407 | SER |
| 1 | B | 408 | ILE |
| 1 | B | 409 | ILE |
| 1 | B | 414 | LEU |
| 1 | B | 417 | LYS |
| 1 | B | 419 | ASN |
| 1 | B | 423 | THR |
| 1 | B | 427 | ASN |
| 1 | B | 429 | LEU |
| 1 | B | 436 | LEU |
| 1 | B | 446 | ARG |
| 1 | B | 457 | SER |
| 1 | B | 462 | SER |
| 1 | B | 464 | MET |
| 1 | B | 466 | THR |
| 1 | B | 474 | SER |
| 1 | B | 481 | THR |
| 1 | B | 486 | ARG |
| 1 | B | 493 | LYS |
| 1 | B | 496 | GLU |
| 1 | B | 499 | ILE |
| 1 | B | 522 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 527 | ASP |
| 1 | B | 535 | LEU |
| 1 | B | 540 | ILE |
| 1 | B | 547 | SER |
| 1 | B | 548 | LYS |
| 1 | B | 566 | ASN |
| 1 | B | 567 | GLU |
| 1 | B | 575 | ASN |
| 1 | B | 580 | LEU |
| 1 | B | 595 | ILE |
| 1 | B | 596 | ASN |
| 1 | B | 601 | VAL |
| 1 | B | 612 | THR |
| 1 | B | 613 | SER |
| 1 | B | 614 | GLU |
| 1 | B | 632 | ILE |
| 1 | B | 648 | PRO |
| 1 | B | 649 | GLN |
| 1 | B | 651 | LEU |
| 1 | B | 652 | THR |
| 1 | B | 658 | ILE |
| 1 | B | 659 | SER |
| 1 | B | 661 | LEU |
| 1 | B | 664 | HIS |
| 1 | C | 340 | VAL |
| 1 | C | 341 | THR |
| 1 | C | 343 | THR |
| 1 | C | 345 | TYR |
| 1 | C | 348 | PHE |
| 1 | C | 355 | SER |
| 1 | C | 356 | ILE |
| 1 | C | 360 | VAL |
| 1 | C | 361 | GLN |
| 1 | C | 364 | THR |
| 1 | C | 374 | ILE |
| 1 | C | 388 | GLN |
| 1 | C | 391 | ASP |
| 1 | C | 398 | ASP |
| 1 | C | 401 | LEU |
| 1 | C | 405 | THR |
| 1 | C | 414 | LEU |
| 1 | C | 416 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 423 | THR |
| 1 | C | 427 | ASN |
| 1 | C | 429 | LEU |
| 1 | C | 441 | ILE |
| 1 | C | 446 | ARG |
| 1 | C | 464 | MET |
| 1 | C | 466 | THR |
| 1 | C | 474 | SER |
| 1 | C | 486 | ARG |
| 1 | C | 489 | GLN |
| 1 | C | 496 | GLU |
| 1 | C | 499 | ILE |
| 1 | C | 500 | LYS |
| 1 | C | 522 | LYS |
| 1 | C | 528 | THR |
| 1 | C | 532 | GLU |
| 1 | C | 533 | ASP |
| 1 | C | 536 | TYR |
| 1 | C | 538 | VAL |
| 1 | C | 547 | SER |
| 1 | C | 580 | LEU |
| 1 | C | 587 | ASP |
| 1 | C | 595 | ILE |
| 1 | C | 596 | ASN |
| 1 | C | 619 | GLN |
| 1 | C | 622 | GLU |
| 1 | C | 626 | ASP |
| 1 | C | 628 | THR |
| 1 | C | 629 | ASP |
| 1 | C | 634 | THR |
| 1 | C | 635 | ARG |
| 1 | C | 649 | GLN |
| 1 | C | 652 | THR |
| 1 | C | 658 | ILE |
| 1 | C | 659 | SER |
| 1 | C | 660 | GLN |
| 1 | C | 662 | GLU |
| 1 | C | 663 | HIS |
| 1 | D | 344 | ASP |
| 1 | D | 346 | ASP |
| 1 | D | 357 | ILE |
| 1 | D | 360 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 361 | GLN |
| 1 | D | 364 | THR |
| 1 | D | 366 | SER |
| 1 | D | 367 | THR |
| 1 | D | 374 | ILE |
| 1 | D | 379 | LYS |
| 1 | D | 380 | SER |
| 1 | D | 386 | THR |
| 1 | D | 404 | ILE |
| 1 | D | 407 | SER |
| 1 | D | 408 | ILE |
| 1 | D | 409 | ILE |
| 1 | D | 414 | LEU |
| 1 | D | 417 | LYS |
| 1 | D | 419 | ASN |
| 1 | D | 423 | THR |
| 1 | D | 427 | ASN |
| 1 | D | 429 | LEU |
| 1 | D | 436 | LEU |
| 1 | D | 446 | ARG |
| 1 | D | 457 | SER |
| 1 | D | 462 | SER |
| 1 | D | 464 | MET |
| 1 | D | 466 | THR |
| 1 | D | 474 | SER |
| 1 | D | 481 | THR |
| 1 | D | 486 | ARG |
| 1 | D | 493 | LYS |
| 1 | D | 496 | GLU |
| 1 | D | 499 | ILE |
| 1 | D | 522 | LYS |
| 1 | D | 527 | ASP |
| 1 | D | 535 | LEU |
| 1 | D | 540 | ILE |
| 1 | D | 547 | SER |
| 1 | D | 548 | LYS |
| 1 | D | 566 | ASN |
| 1 | D | 567 | GLU |
| 1 | D | 575 | ASN |
| 1 | D | 580 | LEU |
| 1 | D | 595 | ILE |
| 1 | D | 596 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 601 | VAL |
| 1 | D | 612 | THR |
| 1 | D | 613 | SER |
| 1 | D | 614 | GLU |
| 1 | D | 632 | ILE |
| 1 | D | 648 | PRO |
| 1 | D | 649 | GLN |
| 1 | D | 651 | LEU |
| 1 | D | 652 | THR |
| 1 | D | 658 | ILE |
| 1 | D | 659 | SER |
| 1 | D | 661 | LEU |
| 1 | D | 664 | HIS |
| 1 | E | 340 | VAL |
| 1 | E | 341 | THR |
| 1 | E | 343 | THR |
| 1 | E | 345 | TYR |
| 1 | E | 348 | PHE |
| 1 | E | 355 | SER |
| 1 | E | 356 | ILE |
| 1 | E | 360 | VAL |
| 1 | E | 361 | GLN |
| 1 | E | 364 | THR |
| 1 | E | 374 | ILE |
| 1 | E | 388 | GLN |
| 1 | E | 391 | ASP |
| 1 | E | 398 | ASP |
| 1 | E | 401 | LEU |
| 1 | E | 405 | THR |
| 1 | E | 414 | LEU |
| 1 | E | 416 | ILE |
| 1 | E | 423 | THR |
| 1 | E | 427 | ASN |
| 1 | E | 429 | LEU |
| 1 | E | 441 | ILE |
| 1 | E | 446 | ARG |
| 1 | E | 464 | MET |
| 1 | E | 466 | THR |
| 1 | E | 474 | SER |
| 1 | E | 486 | ARG |
| 1 | E | 489 | GLN |
| 1 | E | 496 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | E | 499 | ILE |
| 1 | E | 500 | LYS |
| 1 | E | 522 | LYS |
| 1 | E | 528 | THR |
| 1 | E | 532 | GLU |
| 1 | E | 533 | ASP |
| 1 | E | 536 | TYR |
| 1 | E | 538 | VAL |
| 1 | E | 547 | SER |
| 1 | E | 580 | LEU |
| 1 | E | 587 | ASP |
| 1 | E | 595 | ILE |
| 1 | E | 596 | ASN |
| 1 | E | 619 | GLN |
| 1 | E | 622 | GLU |
| 1 | E | 626 | ASP |
| 1 | E | 628 | THR |
| 1 | E | 629 | ASP |
| 1 | E | 634 | THR |
| 1 | E | 635 | ARG |
| 1 | E | 649 | GLN |
| 1 | E | 652 | THR |
| 1 | E | 658 | ILE |
| 1 | E | 659 | SER |
| 1 | E | 660 | GLN |
| 1 | E | 662 | GLU |
| 1 | E | 663 | HIS |
| 1 | F | 344 | ASP |
| 1 | F | 346 | ASP |
| 1 | F | 357 | ILE |
| 1 | F | 360 | VAL |
| 1 | F | 361 | GLN |
| 1 | F | 364 | THR |
| 1 | F | 366 | SER |
| 1 | F | 367 | THR |
| 1 | F | 374 | ILE |
| 1 | F | 379 | LYS |
| 1 | F | 380 | SER |
| 1 | F | 386 | THR |
| 1 | F | 404 | ILE |
| 1 | F | 407 | SER |
| 1 | F | 408 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | F | 409 | ILE |
| 1 | F | 414 | LEU |
| 1 | F | 417 | LYS |
| 1 | F | 419 | ASN |
| 1 | F | 423 | THR |
| 1 | F | 427 | ASN |
| 1 | F | 429 | LEU |
| 1 | F | 436 | LEU |
| 1 | F | 446 | ARG |
| 1 | F | 457 | SER |
| 1 | F | 462 | SER |
| 1 | F | 464 | MET |
| 1 | F | 466 | THR |
| 1 | F | 474 | SER |
| 1 | F | 481 | THR |
| 1 | F | 486 | ARG |
| 1 | F | 493 | LYS |
| 1 | F | 496 | GLU |
| 1 | F | 499 | ILE |
| 1 | F | 522 | LYS |
| 1 | F | 527 | ASP |
| 1 | F | 535 | LEU |
| 1 | F | 540 | ILE |
| 1 | F | 547 | SER |
| 1 | F | 548 | LYS |
| 1 | F | 566 | ASN |
| 1 | F | 567 | GLU |
| 1 | F | 575 | ASN |
| 1 | F | 580 | LEU |
| 1 | F | 595 | ILE |
| 1 | F | 596 | ASN |
| 1 | F | 601 | VAL |
| 1 | F | 612 | THR |
| 1 | F | 613 | SER |
| 1 | F | 614 | GLU |
| 1 | F | 632 | ILE |
| 1 | F | 648 | PRO |
| 1 | F | 649 | GLN |
| 1 | F | 651 | LEU |
| 1 | F | 652 | THR |
| 1 | F | 658 | ILE |
| 1 | F | 659 | SER |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | F | 661 | LEU |
| 1 | F | 664 | HIS |
| 1 | G | 340 | VAL |
| 1 | G | 341 | THR |
| 1 | G | 343 | THR |
| 1 | G | 345 | TYR |
| 1 | G | 348 | PHE |
| 1 | G | 355 | SER |
| 1 | G | 356 | ILE |
| 1 | G | 360 | VAL |
| 1 | G | 361 | GLN |
| 1 | G | 364 | THR |
| 1 | G | 374 | ILE |
| 1 | G | 388 | GLN |
| 1 | G | 391 | ASP |
| 1 | G | 398 | ASP |
| 1 | G | 401 | LEU |
| 1 | G | 405 | THR |
| 1 | G | 414 | LEU |
| 1 | G | 416 | ILE |
| 1 | G | 423 | THR |
| 1 | G | 427 | ASN |
| 1 | G | 429 | LEU |
| 1 | G | 441 | ILE |
| 1 | G | 446 | ARG |
| 1 | G | 464 | MET |
| 1 | G | 466 | THR |
| 1 | G | 474 | SER |
| 1 | G | 486 | ARG |
| 1 | G | 489 | GLN |
| 1 | G | 496 | GLU |
| 1 | G | 499 | ILE |
| 1 | G | 500 | LYS |
| 1 | G | 522 | LYS |
| 1 | G | 528 | THR |
| 1 | G | 532 | GLU |
| 1 | G | 533 | ASP |
| 1 | G | 536 | TYR |
| 1 | G | 538 | VAL |
| 1 | G | 547 | SER |
| 1 | G | 580 | LEU |
| 1 | G | 587 | ASP |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | G | 595 | ILE |
| 1 | G | 596 | ASN |
| 1 | G | 619 | GLN |
| 1 | G | 622 | GLU |
| 1 | G | 626 | ASP |
| 1 | G | 628 | THR |
| 1 | G | 629 | ASP |
| 1 | G | 634 | THR |
| 1 | G | 635 | ARG |
| 1 | G | 649 | GLN |
| 1 | G | 652 | THR |
| 1 | G | 658 | ILE |
| 1 | G | 659 | SER |
| 1 | G | 660 | GLN |
| 1 | G | 662 | GLU |
| 1 | G | 663 | HIS |
| 1 | H | 344 | ASP |
| 1 | H | 346 | ASP |
| 1 | H | 357 | ILE |
| 1 | H | 360 | VAL |
| 1 | H | 361 | GLN |
| 1 | H | 364 | THR |
| 1 | H | 366 | SER |
| 1 | H | 367 | THR |
| 1 | H | 374 | ILE |
| 1 | H | 379 | LYS |
| 1 | H | 380 | SER |
| 1 | H | 386 | THR |
| 1 | H | 404 | ILE |
| 1 | H | 407 | SER |
| 1 | H | 408 | ILE |
| 1 | H | 409 | ILE |
| 1 | H | 414 | LEU |
| 1 | H | 417 | LYS |
| 1 | H | 419 | ASN |
| 1 | H | 423 | THR |
| 1 | H | 427 | ASN |
| 1 | H | 429 | LEU |
| 1 | H | 436 | LEU |
| 1 | H | 446 | ARG |
| 1 | H | 457 | SER |
| 1 | H | 462 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | H | 464 | MET |
| 1 | H | 466 | THR |
| 1 | H | 474 | SER |
| 1 | H | 481 | THR |
| 1 | H | 486 | ARG |
| 1 | H | 493 | LYS |
| 1 | H | 496 | GLU |
| 1 | H | 499 | ILE |
| 1 | H | 522 | LYS |
| 1 | H | 527 | ASP |
| 1 | H | 535 | LEU |
| 1 | H | 540 | ILE |
| 1 | H | 547 | SER |
| 1 | H | 548 | LYS |
| 1 | H | 566 | ASN |
| 1 | H | 567 | GLU |
| 1 | H | 575 | ASN |
| 1 | H | 580 | LEU |
| 1 | H | 595 | ILE |
| 1 | H | 596 | ASN |
| 1 | H | 601 | VAL |
| 1 | H | 612 | THR |
| 1 | H | 613 | SER |
| 1 | H | 614 | GLU |
| 1 | H | 632 | ILE |
| 1 | H | 648 | PRO |
| 1 | H | 649 | GLN |
| 1 | H | 651 | LEU |
| 1 | H | 652 | THR |
| 1 | H | 658 | ILE |
| 1 | H | 659 | SER |
| 1 | H | 661 | LEU |
| 1 | H | 664 | HIS |
| 1 | I | 340 | VAL |
| 1 | I | 341 | THR |
| 1 | I | 343 | THR |
| 1 | I | 345 | TYR |
| 1 | I | 348 | PHE |
| 1 | I | 355 | SER |
| 1 | I | 356 | ILE |
| 1 | I | 360 | VAL |
| 1 | I | 361 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | I | 364 | THR |
| 1 | I | 374 | ILE |
| 1 | I | 388 | GLN |
| 1 | I | 391 | ASP |
| 1 | I | 398 | ASP |
| 1 | I | 401 | LEU |
| 1 | I | 405 | THR |
| 1 | I | 414 | LEU |
| 1 | I | 416 | ILE |
| 1 | I | 423 | THR |
| 1 | I | 427 | ASN |
| 1 | I | 429 | LEU |
| 1 | I | 441 | ILE |
| 1 | I | 446 | ARG |
| 1 | I | 464 | MET |
| 1 | I | 466 | THR |
| 1 | I | 474 | SER |
| 1 | I | 486 | ARG |
| 1 | I | 489 | GLN |
| 1 | I | 496 | GLU |
| 1 | I | 499 | ILE |
| 1 | I | 500 | LYS |
| 1 | I | 522 | LYS |
| 1 | I | 528 | THR |
| 1 | I | 532 | GLU |
| 1 | I | 533 | ASP |
| 1 | I | 536 | TYR |
| 1 | I | 538 | VAL |
| 1 | I | 547 | SER |
| 1 | I | 580 | LEU |
| 1 | I | 587 | ASP |
| 1 | I | 595 | ILE |
| 1 | I | 596 | ASN |
| 1 | I | 619 | GLN |
| 1 | I | 622 | GLU |
| 1 | I | 626 | ASP |
| 1 | I | 628 | THR |
| 1 | I | 629 | ASP |
| 1 | I | 634 | THR |
| 1 | I | 635 | ARG |
| 1 | I | 649 | GLN |
| 1 | I | 652 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | I | 658 | ILE |
| 1 | I | 659 | SER |
| 1 | I | 660 | GLN |
| 1 | I | 662 | GLU |
| 1 | I | 663 | HIS |
| 1 | J | 344 | ASP |
| 1 | J | 346 | ASP |
| 1 | J | 357 | ILE |
| 1 | J | 360 | VAL |
| 1 | J | 361 | GLN |
| 1 | J | 364 | THR |
| 1 | J | 366 | SER |
| 1 | J | 367 | THR |
| 1 | J | 374 | ILE |
| 1 | J | 379 | LYS |
| 1 | J | 380 | SER |
| 1 | J | 386 | THR |
| 1 | J | 404 | ILE |
| 1 | J | 407 | SER |
| 1 | J | 408 | ILE |
| 1 | J | 409 | ILE |
| 1 | J | 414 | LEU |
| 1 | J | 417 | LYS |
| 1 | J | 419 | ASN |
| 1 | J | 423 | THR |
| 1 | J | 427 | ASN |
| 1 | J | 429 | LEU |
| 1 | J | 436 | LEU |
| 1 | J | 446 | ARG |
| 1 | J | 457 | SER |
| 1 | J | 462 | SER |
| 1 | J | 464 | MET |
| 1 | J | 466 | THR |
| 1 | J | 474 | SER |
| 1 | J | 481 | THR |
| 1 | J | 486 | ARG |
| 1 | J | 493 | LYS |
| 1 | J | 496 | GLU |
| 1 | J | 499 | ILE |
| 1 | J | 522 | LYS |
| 1 | J | 527 | ASP |
| 1 | J | 535 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | J | 540 | ILE |
| 1 | J | 547 | SER |
| 1 | J | 548 | LYS |
| 1 | J | 566 | ASN |
| 1 | J | 567 | GLU |
| 1 | J | 575 | ASN |
| 1 | J | 580 | LEU |
| 1 | J | 595 | ILE |
| 1 | J | 596 | ASN |
| 1 | J | 601 | VAL |
| 1 | J | 612 | THR |
| 1 | J | 613 | SER |
| 1 | J | 614 | GLU |
| 1 | J | 632 | ILE |
| 1 | J | 648 | PRO |
| 1 | J | 649 | GLN |
| 1 | J | 651 | LEU |
| 1 | J | 652 | THR |
| 1 | J | 658 | ILE |
| 1 | J | 659 | SER |
| 1 | J | 661 | LEU |
| 1 | J | 664 | HIS |
| 1 | K | 340 | VAL |
| 1 | K | 341 | THR |
| 1 | K | 343 | THR |
| 1 | K | 345 | TYR |
| 1 | K | 348 | PHE |
| 1 | K | 355 | SER |
| 1 | K | 356 | ILE |
| 1 | K | 360 | VAL |
| 1 | K | 361 | GLN |
| 1 | K | 364 | THR |
| 1 | K | 374 | ILE |
| 1 | K | 388 | GLN |
| 1 | K | 391 | ASP |
| 1 | K | 398 | ASP |
| 1 | K | 401 | LEU |
| 1 | K | 405 | THR |
| 1 | K | 414 | LEU |
| 1 | K | 416 | ILE |
| 1 | K | 423 | THR |
| 1 | K | 427 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | K | 429 | LEU |
| 1 | K | 441 | ILE |
| 1 | K | 446 | ARG |
| 1 | K | 464 | MET |
| 1 | K | 466 | THR |
| 1 | K | 474 | SER |
| 1 | K | 486 | ARG |
| 1 | K | 489 | GLN |
| 1 | K | 496 | GLU |
| 1 | K | 499 | ILE |
| 1 | K | 500 | LYS |
| 1 | K | 522 | LYS |
| 1 | K | 528 | THR |
| 1 | K | 532 | GLU |
| 1 | K | 533 | ASP |
| 1 | K | 536 | TYR |
| 1 | K | 538 | VAL |
| 1 | K | 547 | SER |
| 1 | K | 580 | LEU |
| 1 | K | 587 | ASP |
| 1 | K | 595 | ILE |
| 1 | K | 596 | ASN |
| 1 | K | 619 | GLN |
| 1 | K | 622 | GLU |
| 1 | K | 626 | ASP |
| 1 | K | 628 | THR |
| 1 | K | 629 | ASP |
| 1 | K | 634 | THR |
| 1 | K | 635 | ARG |
| 1 | K | 649 | GLN |
| 1 | K | 652 | THR |
| 1 | K | 658 | ILE |
| 1 | K | 659 | SER |
| 1 | K | 660 | GLN |
| 1 | K | 662 | GLU |
| 1 | K | 663 | HIS |
| 1 | L | 344 | ASP |
| 1 | L | 346 | ASP |
| 1 | L | 357 | ILE |
| 1 | L | 360 | VAL |
| 1 | L | 361 | GLN |
| 1 | L | 364 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | L | 366 | SER |
| 1 | L | 367 | THR |
| 1 | L | 374 | ILE |
| 1 | L | 379 | LYS |
| 1 | L | 380 | SER |
| 1 | L | 386 | THR |
| 1 | L | 404 | ILE |
| 1 | L | 407 | SER |
| 1 | L | 408 | ILE |
| 1 | L | 409 | ILE |
| 1 | L | 414 | LEU |
| 1 | L | 417 | LYS |
| 1 | L | 419 | ASN |
| 1 | L | 423 | THR |
| 1 | L | 427 | ASN |
| 1 | L | 429 | LEU |
| 1 | L | 436 | LEU |
| 1 | L | 446 | ARG |
| 1 | L | 457 | SER |
| 1 | L | 462 | SER |
| 1 | L | 464 | MET |
| 1 | L | 466 | THR |
| 1 | L | 474 | SER |
| 1 | L | 481 | THR |
| 1 | L | 486 | ARG |
| 1 | L | 493 | LYS |
| 1 | L | 496 | GLU |
| 1 | L | 499 | ILE |
| 1 | L | 522 | LYS |
| 1 | L | 527 | ASP |
| 1 | L | 535 | LEU |
| 1 | L | 540 | ILE |
| 1 | L | 547 | SER |
| 1 | L | 548 | LYS |
| 1 | L | 566 | ASN |
| 1 | L | 567 | GLU |
| 1 | L | 575 | ASN |
| 1 | L | 580 | LEU |
| 1 | L | 595 | ILE |
| 1 | L | 596 | ASN |
| 1 | L | 601 | VAL |
| 1 | L | 612 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 613 | SER |
| 1 | L | 614 | GLU |
| 1 | L | 632 | ILE |
| 1 | L | 648 | PRO |
| 1 | L | 649 | GLN |
| 1 | L | 651 | LEU |
| 1 | L | 652 | THR |
| 1 | L | 658 | ILE |
| 1 | L | 659 | SER |
| 1 | L | 661 | LEU |
| 1 | L | 664 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 361 | GLN |
| 1 | A | 427 | ASN |
| 1 | A | 473 | HIS |
| 1 | A | 504 | GLN |
| 1 | A | 596 | ASN |
| 1 | A | 610 | ASN |
| 1 | A | 619 | GLN |
| 1 | B | 358 | GLN |
| 1 | B | 394 | ASN |
| 1 | B | 412 | ASN |
| 1 | B | 427 | ASN |
| 1 | B | 456 | ASN |
| 1 | B | 490 | ASN |
| 1 | B | 503 | ASN |
| 1 | B | 504 | GLN |
| 1 | B | 570 | GLN |
| 1 | B | 575 | ASN |
| 1 | B | 578 | ASN |
| 1 | B | 582 | ASN |
| 1 | B | 596 | ASN |
| 1 | B | 644 | ASN |
| 1 | B | 663 | HIS |
| 1 | C | 361 | GLN |
| 1 | C | 427 | ASN |
| 1 | C | 473 | HIS |
| 1 | C | 504 | GLN |
| 1 | C | 596 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 610 | ASN |
| 1 | C | 619 | GLN |
| 1 | D | 358 | GLN |
| 1 | D | 394 | ASN |
| 1 | D | 400 | ASN |
| 1 | D | 412 | ASN |
| 1 | D | 427 | ASN |
| 1 | D | 456 | ASN |
| 1 | D | 490 | ASN |
| 1 | D | 503 | ASN |
| 1 | D | 570 | GLN |
| 1 | D | 575 | ASN |
| 1 | D | 578 | ASN |
| 1 | D | 582 | ASN |
| 1 | D | 596 | ASN |
| 1 | D | 644 | ASN |
| 1 | D | 663 | HIS |
| 1 | E | 361 | GLN |
| 1 | E | 427 | ASN |
| 1 | E | 473 | HIS |
| 1 | E | 504 | GLN |
| 1 | E | 596 | ASN |
| 1 | E | 610 | ASN |
| 1 | E | 619 | GLN |
| 1 | E | 663 | HIS |
| 1 | F | 358 | GLN |
| 1 | F | 394 | ASN |
| 1 | F | 412 | ASN |
| 1 | F | 427 | ASN |
| 1 | F | 456 | ASN |
| 1 | F | 490 | ASN |
| 1 | F | 503 | ASN |
| 1 | F | 504 | GLN |
| 1 | F | 570 | GLN |
| 1 | F | 575 | ASN |
| 1 | F | 578 | ASN |
| 1 | F | 582 | ASN |
| 1 | F | 596 | ASN |
| 1 | F | 644 | ASN |
| 1 | F | 663 | HIS |
| 1 | G | 361 | GLN |
| 1 | G | 427 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | G | 473 | HIS |
| 1 | G | 504 | GLN |
| 1 | G | 596 | ASN |
| 1 | G | 610 | ASN |
| 1 | G | 619 | GLN |
| 1 | H | 358 | GLN |
| 1 | H | 394 | ASN |
| 1 | H | 412 | ASN |
| 1 | H | 427 | ASN |
| 1 | H | 456 | ASN |
| 1 | H | 490 | ASN |
| 1 | H | 503 | ASN |
| 1 | H | 570 | GLN |
| 1 | H | 575 | ASN |
| 1 | H | 578 | ASN |
| 1 | H | 582 | ASN |
| 1 | H | 596 | ASN |
| 1 | H | 644 | ASN |
| 1 | H | 663 | HIS |
| 1 | I | 361 | GLN |
| 1 | I | 427 | ASN |
| 1 | I | 473 | HIS |
| 1 | I | 504 | GLN |
| 1 | I | 596 | ASN |
| 1 | I | 610 | ASN |
| 1 | I | 619 | GLN |
| 1 | J | 358 | GLN |
| 1 | J | 394 | ASN |
| 1 | J | 412 | ASN |
| 1 | J | 427 | ASN |
| 1 | J | 456 | ASN |
| 1 | J | 490 | ASN |
| 1 | J | 503 | ASN |
| 1 | J | 504 | GLN |
| 1 | J | 570 | GLN |
| 1 | J | 575 | ASN |
| 1 | J | 578 | ASN |
| 1 | J | 582 | ASN |
| 1 | J | 596 | ASN |
| 1 | J | 644 | ASN |
| 1 | J | 663 | HIS |
| 1 | K | 361 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 427 | ASN |
| 1 | K | 473 | HIS |
| 1 | K | 502 | ASN |
| 1 | K | 504 | GLN |
| 1 | K | 596 | ASN |
| 1 | K | 610 | ASN |
| 1 | K | 619 | GLN |
| 1 | L | 358 | GLN |
| 1 | L | 394 | ASN |
| 1 | L | 412 | ASN |
| 1 | L | 427 | ASN |
| 1 | L | 456 | ASN |
| 1 | L | 490 | ASN |
| 1 | L | 503 | ASN |
| 1 | L | 504 | GLN |
| 1 | L | 570 | GLN |
| 1 | L | 575 | ASN |
| 1 | L | 578 | ASN |
| 1 | L | 582 | ASN |
| 1 | L | 596 | ASN |
| 1 | L | 644 | ASN |
| 1 | L | 663 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

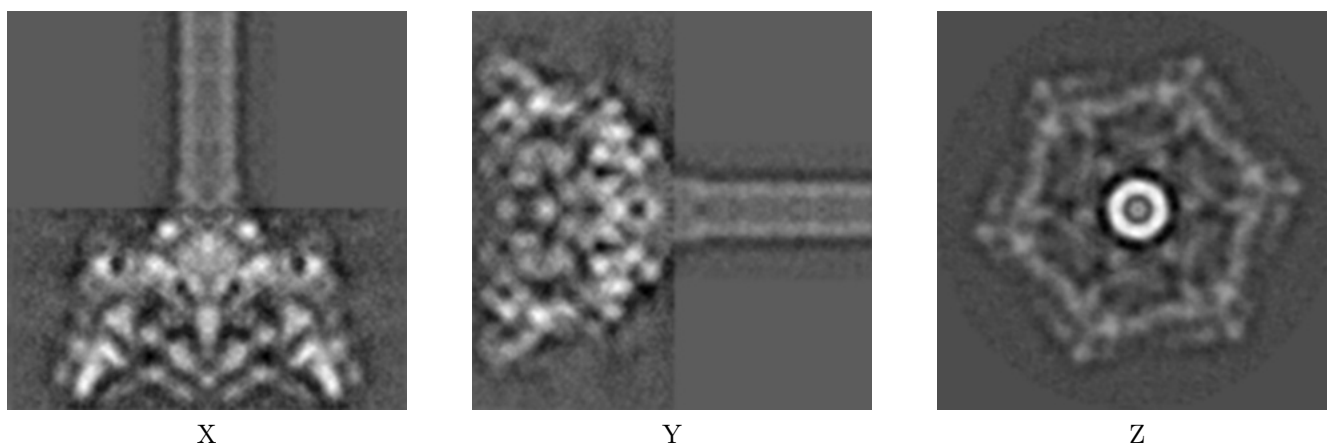
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1048. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

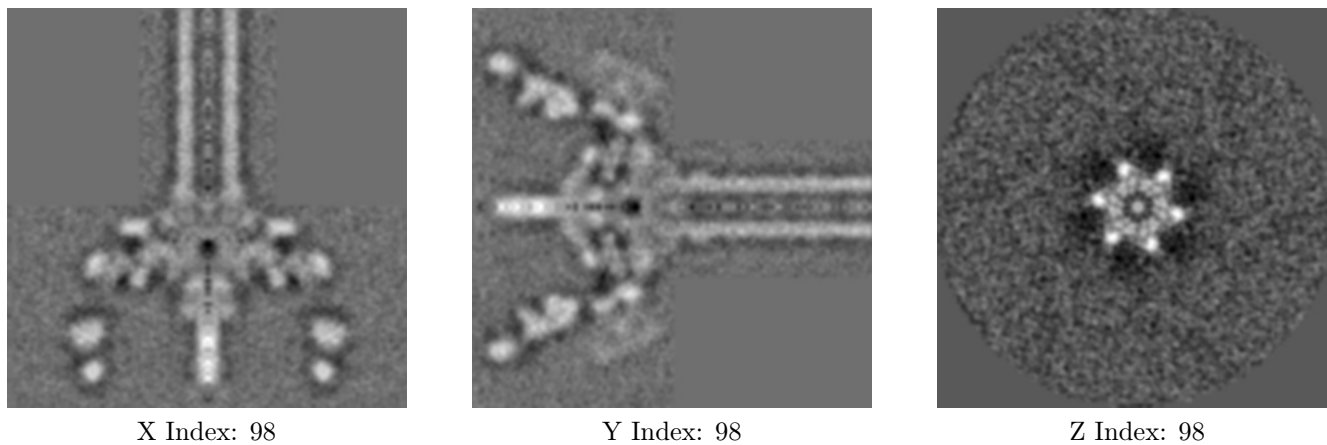
6.1.1 Primary map



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

6.2 Central slices [i](#)

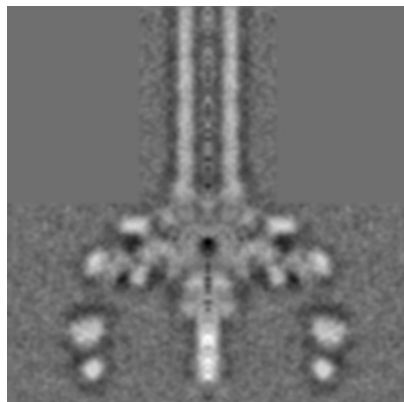
6.2.1 Primary map



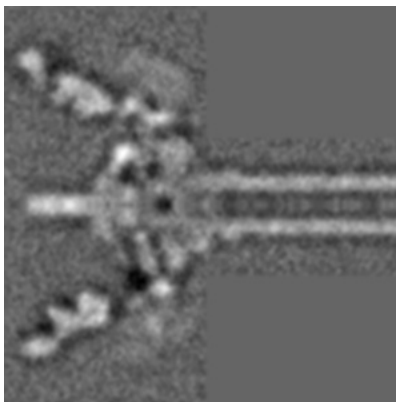
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

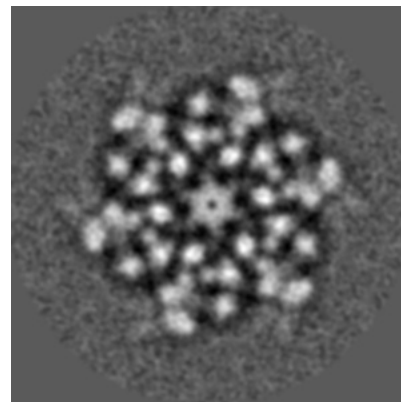
6.3.1 Primary map



X Index: 98



Y Index: 100

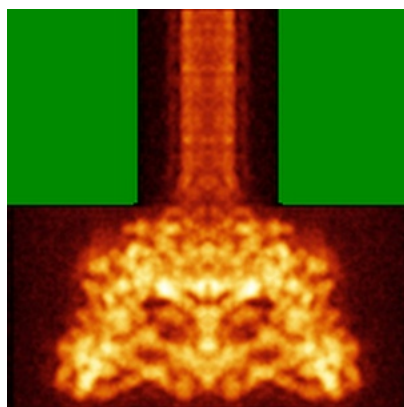


Z Index: 60

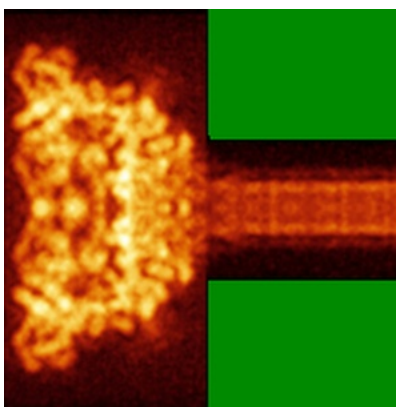
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

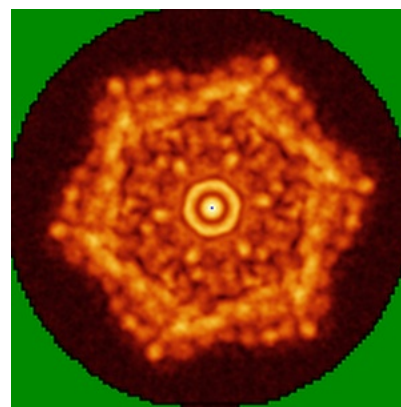
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

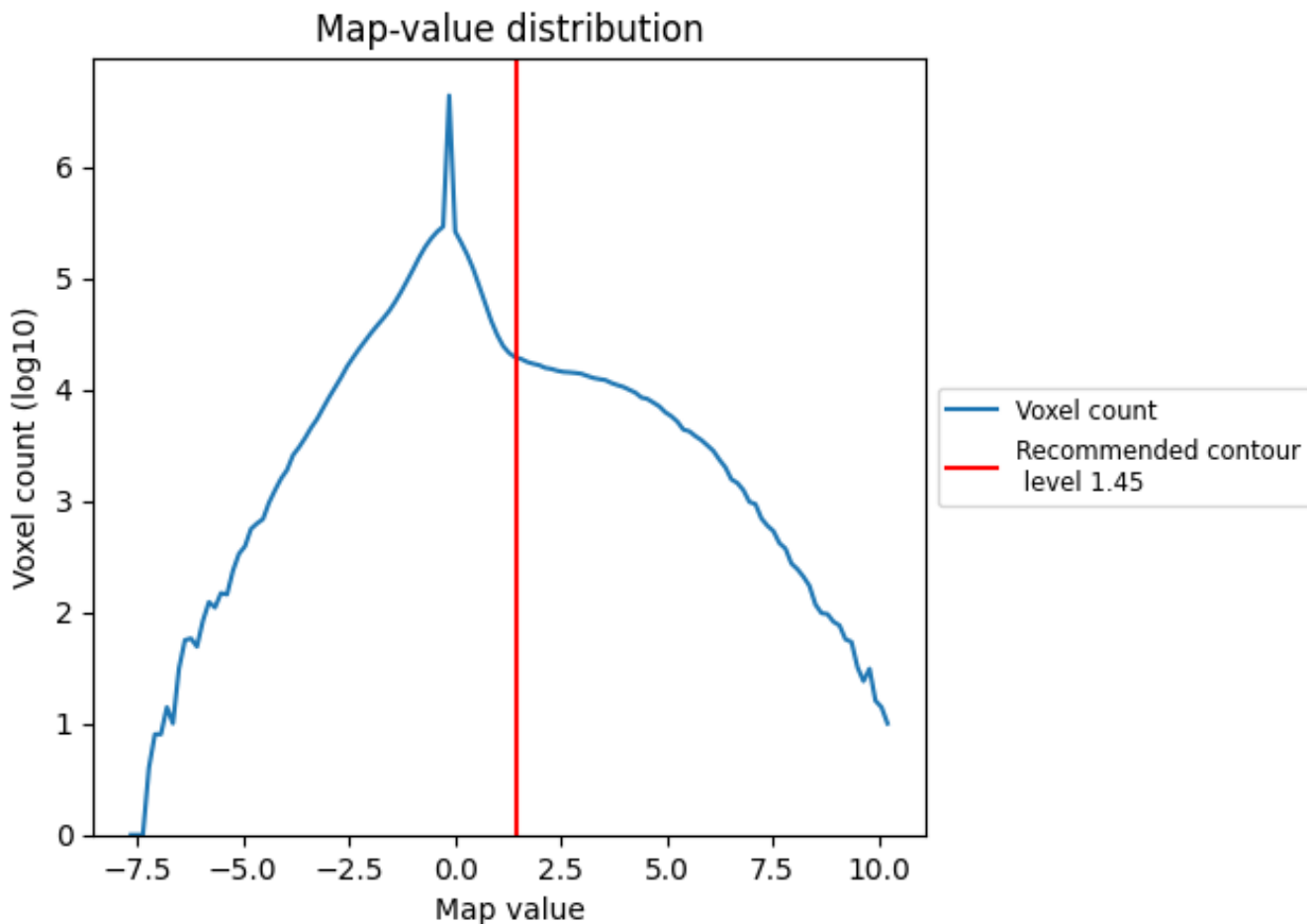
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

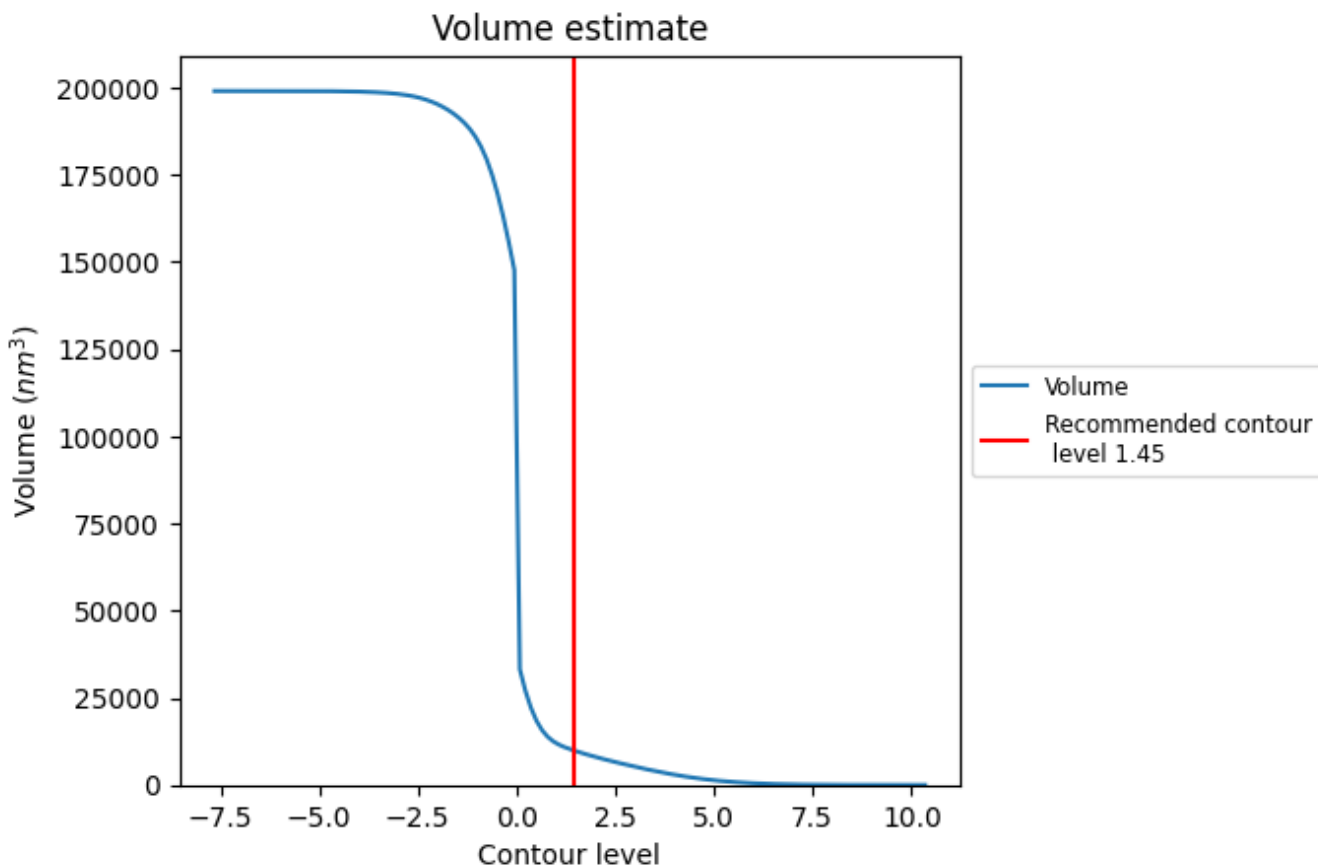
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

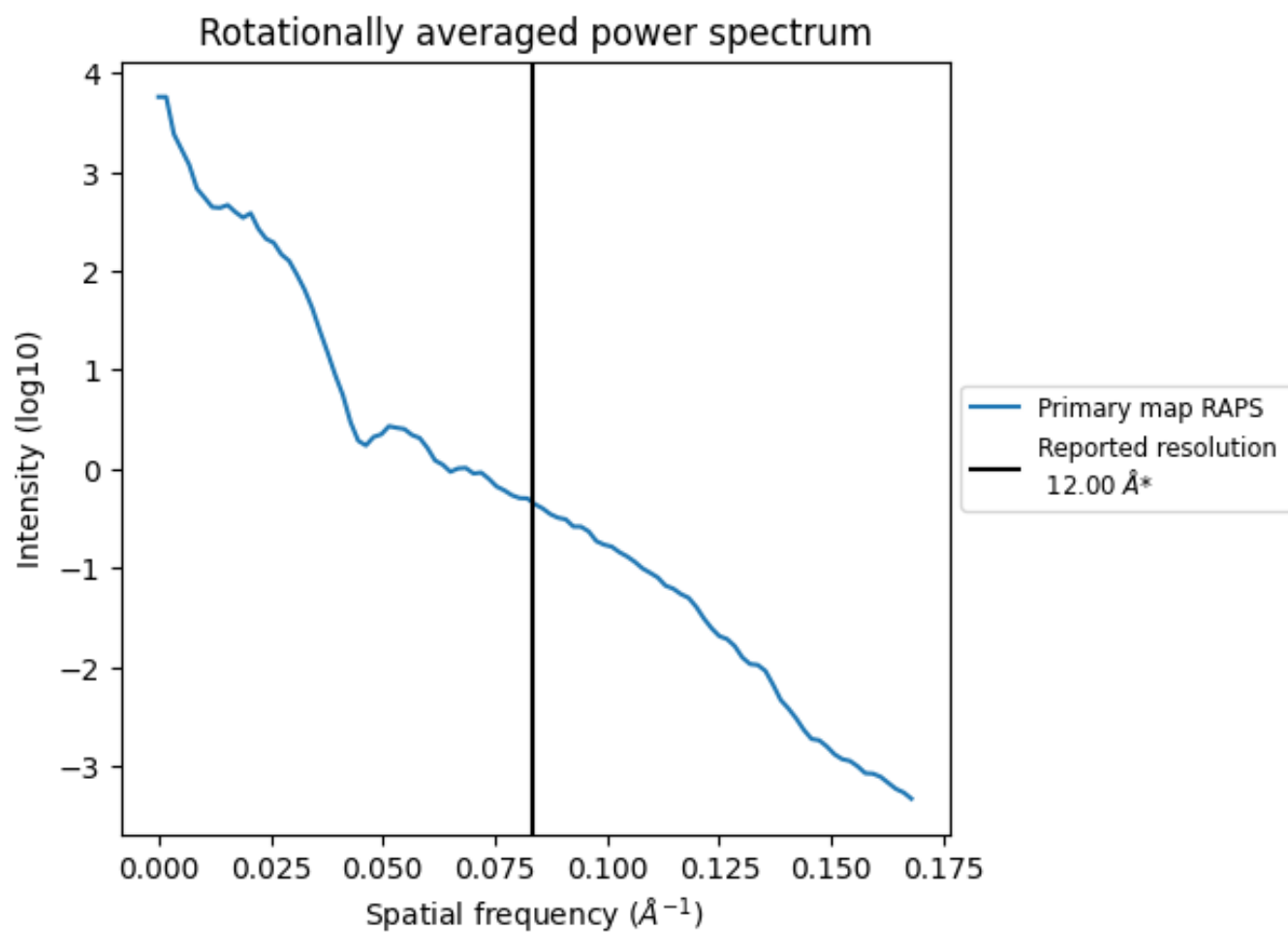
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9896 nm^3 ; this corresponds to an approximate mass of 8939 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.083 Å⁻¹

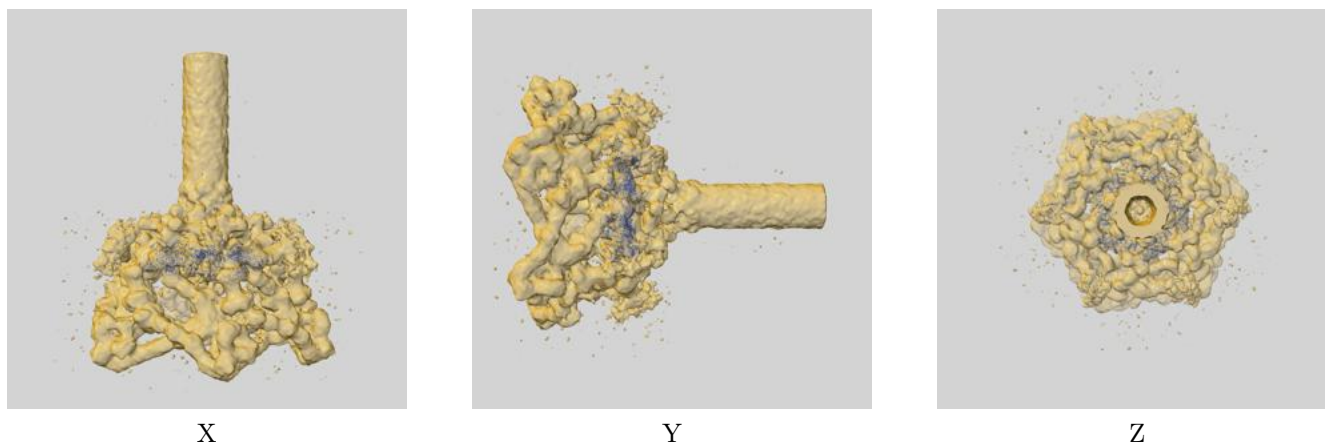
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

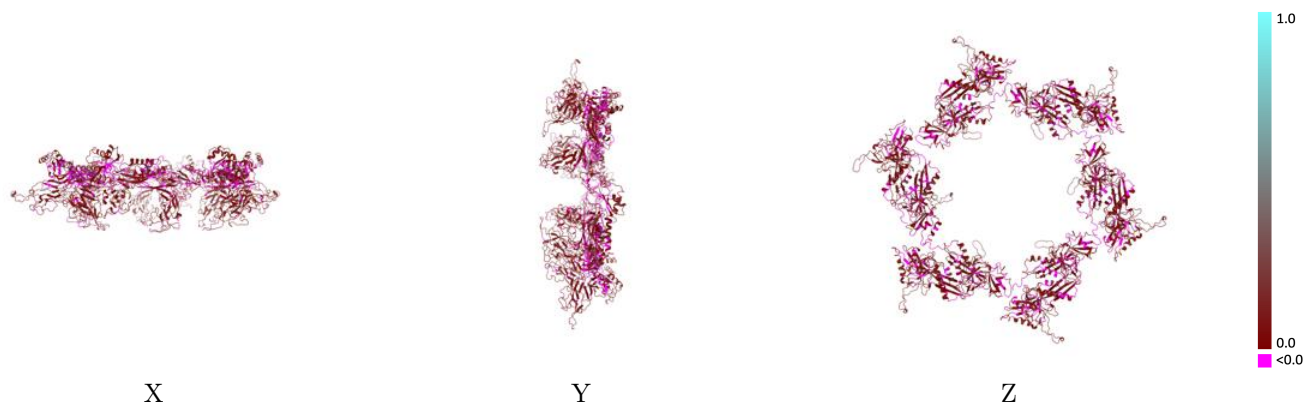
This section contains information regarding the fit between EMDB map EMD-1048 and PDB model 3H3W. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



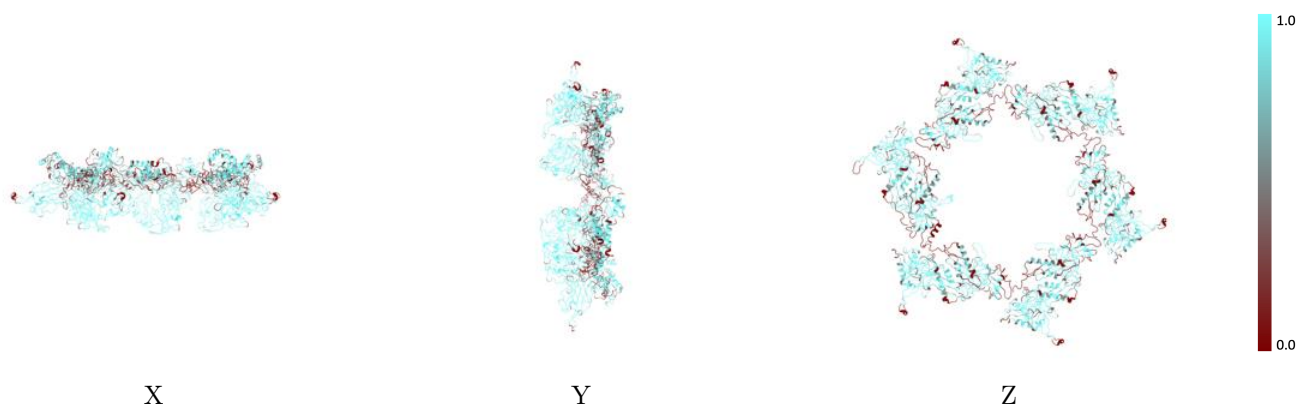
The images above show the 3D surface view of the map at the recommended contour level 1.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



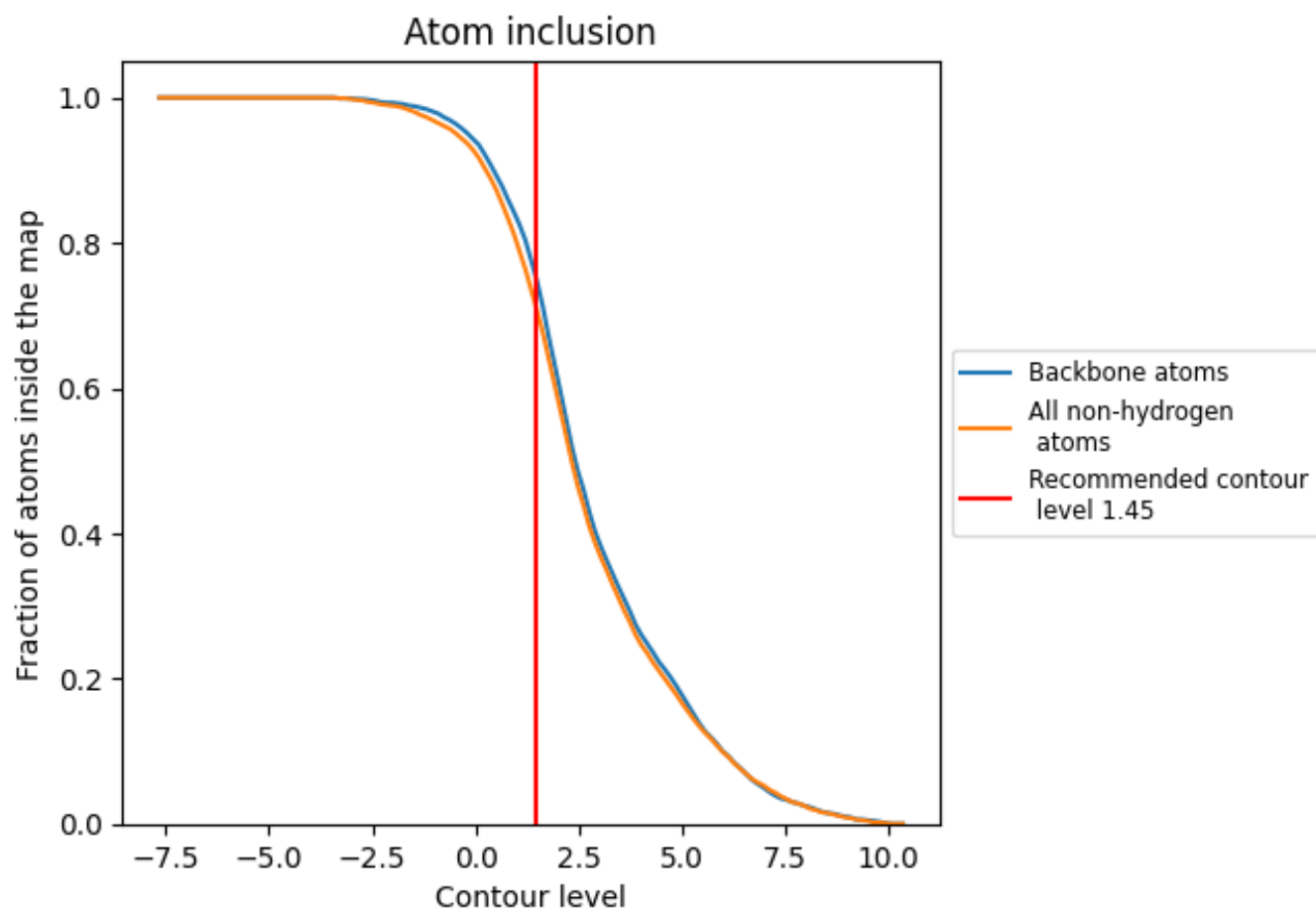
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.45).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.45) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7150 |  0.0680 |
| A |  0.6560 |  0.0630 |
| B |  0.7730 |  0.0750 |
| C |  0.7700 |  0.0760 |
| D |  0.6550 |  0.0630 |
| E |  0.6540 |  0.0630 |
| F |  0.7800 |  0.0730 |
| G |  0.6550 |  0.0600 |
| H |  0.7730 |  0.0740 |
| I |  0.6540 |  0.0630 |
| J |  0.7740 |  0.0720 |
| K |  0.6540 |  0.0640 |
| L |  0.7800 |  0.0750 |

