



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 02:12 PM EDT

PDB ID : 6C3P
EMDB ID : EMD-7339
Title : Cryo-EM structure of human KATP bound to ATP and ADP in propeller form
Authors : Lee, K.P.K.; Chen, J.; MacKinnon, R.
Deposited on : 2018-01-10
Resolution : 5.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

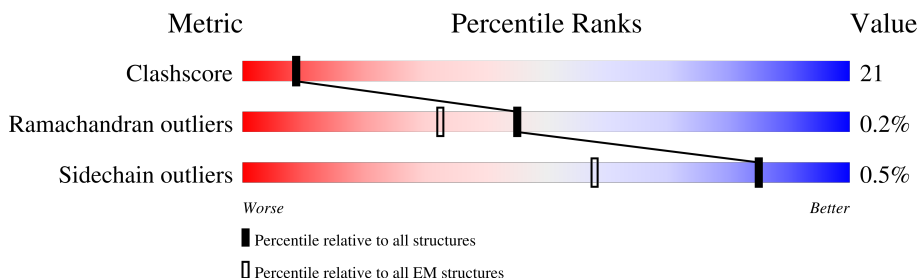
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 406 | |
| 1 | B | 406 | |
| 1 | C | 406 | |
| 1 | D | 406 | |
| 2 | E | 1581 | |
| 2 | F | 1581 | |
| 2 | G | 1581 | |
| 2 | H | 1581 | |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50696 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 ATP-sensitive inward rectifier potassium channel 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2506 | 1619 | 428 | 442 | 17 | | |
| 1 | D | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2506 | 1619 | 428 | 442 | 17 | | |
| 1 | B | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2506 | 1619 | 428 | 442 | 17 | | |
| 1 | C | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2506 | 1619 | 428 | 442 | 17 | | |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -5 | SER | - | expression tag | UNP Q14654 |
| A | -4 | ALA | - | expression tag | UNP Q14654 |
| A | -3 | SER | - | expression tag | UNP Q14654 |
| A | -2 | ALA | - | expression tag | UNP Q14654 |
| A | -1 | SER | - | expression tag | UNP Q14654 |
| A | 0 | ALA | - | expression tag | UNP Q14654 |
| A | 391 | SER | - | expression tag | UNP Q14654 |
| A | 392 | ASN | - | expression tag | UNP Q14654 |
| A | 393 | SER | - | expression tag | UNP Q14654 |
| A | 394 | LEU | - | expression tag | UNP Q14654 |
| A | 395 | GLU | - | expression tag | UNP Q14654 |
| A | 396 | VAL | - | expression tag | UNP Q14654 |
| A | 397 | LEU | - | expression tag | UNP Q14654 |
| A | 398 | PHE | - | expression tag | UNP Q14654 |
| A | 399 | GLN | - | expression tag | UNP Q14654 |
| A | 400 | GLY | - | expression tag | UNP Q14654 |
| D | -5 | SER | - | expression tag | UNP Q14654 |
| D | -4 | ALA | - | expression tag | UNP Q14654 |
| D | -3 | SER | - | expression tag | UNP Q14654 |
| D | -2 | ALA | - | expression tag | UNP Q14654 |
| D | -1 | SER | - | expression tag | UNP Q14654 |
| D | 0 | ALA | - | expression tag | UNP Q14654 |

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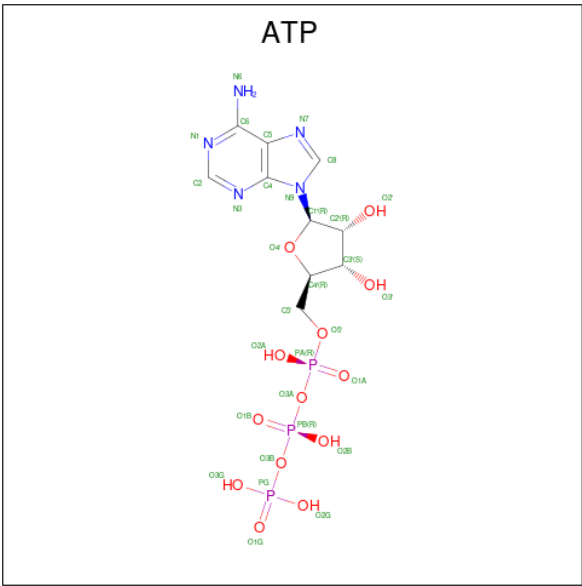
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 391 | SER | - | expression tag | UNP Q14654 |
| D | 392 | ASN | - | expression tag | UNP Q14654 |
| D | 393 | SER | - | expression tag | UNP Q14654 |
| D | 394 | LEU | - | expression tag | UNP Q14654 |
| D | 395 | GLU | - | expression tag | UNP Q14654 |
| D | 396 | VAL | - | expression tag | UNP Q14654 |
| D | 397 | LEU | - | expression tag | UNP Q14654 |
| D | 398 | PHE | - | expression tag | UNP Q14654 |
| D | 399 | GLN | - | expression tag | UNP Q14654 |
| D | 400 | GLY | - | expression tag | UNP Q14654 |
| B | -5 | SER | - | expression tag | UNP Q14654 |
| B | -4 | ALA | - | expression tag | UNP Q14654 |
| B | -3 | SER | - | expression tag | UNP Q14654 |
| B | -2 | ALA | - | expression tag | UNP Q14654 |
| B | -1 | SER | - | expression tag | UNP Q14654 |
| B | 0 | ALA | - | expression tag | UNP Q14654 |
| B | 391 | SER | - | expression tag | UNP Q14654 |
| B | 392 | ASN | - | expression tag | UNP Q14654 |
| B | 393 | SER | - | expression tag | UNP Q14654 |
| B | 394 | LEU | - | expression tag | UNP Q14654 |
| B | 395 | GLU | - | expression tag | UNP Q14654 |
| B | 396 | VAL | - | expression tag | UNP Q14654 |
| B | 397 | LEU | - | expression tag | UNP Q14654 |
| B | 398 | PHE | - | expression tag | UNP Q14654 |
| B | 399 | GLN | - | expression tag | UNP Q14654 |
| B | 400 | GLY | - | expression tag | UNP Q14654 |
| C | -5 | SER | - | expression tag | UNP Q14654 |
| C | -4 | ALA | - | expression tag | UNP Q14654 |
| C | -3 | SER | - | expression tag | UNP Q14654 |
| C | -2 | ALA | - | expression tag | UNP Q14654 |
| C | -1 | SER | - | expression tag | UNP Q14654 |
| C | 0 | ALA | - | expression tag | UNP Q14654 |
| C | 391 | SER | - | expression tag | UNP Q14654 |
| C | 392 | ASN | - | expression tag | UNP Q14654 |
| C | 393 | SER | - | expression tag | UNP Q14654 |
| C | 394 | LEU | - | expression tag | UNP Q14654 |
| C | 395 | GLU | - | expression tag | UNP Q14654 |
| C | 396 | VAL | - | expression tag | UNP Q14654 |
| C | 397 | LEU | - | expression tag | UNP Q14654 |
| C | 398 | PHE | - | expression tag | UNP Q14654 |
| C | 399 | GLN | - | expression tag | UNP Q14654 |
| C | 400 | GLY | - | expression tag | UNP Q14654 |

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2 | E | 1359 | Total | C | N | O | S | 0 | 0 |
| | | | 10077 | 6567 | 1699 | 1760 | 51 | | |
| 2 | H | 1359 | Total | C | N | O | S | 0 | 0 |
| | | | 10077 | 6567 | 1699 | 1760 | 51 | | |
| 2 | G | 1359 | Total | C | N | O | S | 0 | 0 |
| | | | 10077 | 6567 | 1699 | 1760 | 51 | | |
| 2 | F | 1359 | Total | C | N | O | S | 0 | 0 |
| | | | 10077 | 6567 | 1699 | 1760 | 51 | | |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



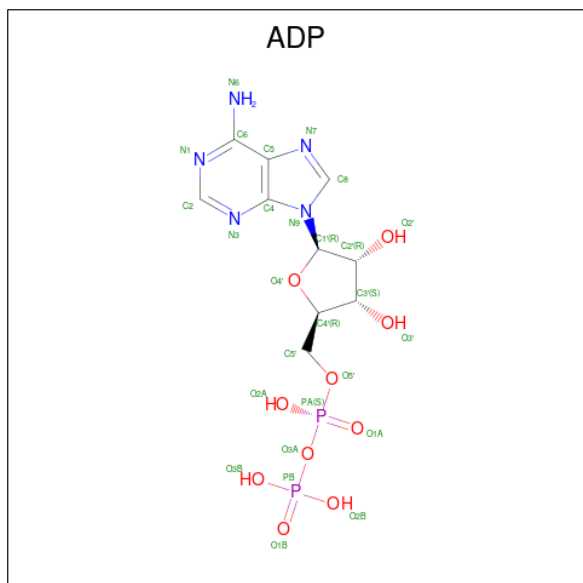
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | A | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | D | 1 | Total | C | N | O | P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

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3 | G | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | F | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 4 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 4 | H | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 4 | G | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 4 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 5 | E | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 5 | H | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 5 | G | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |

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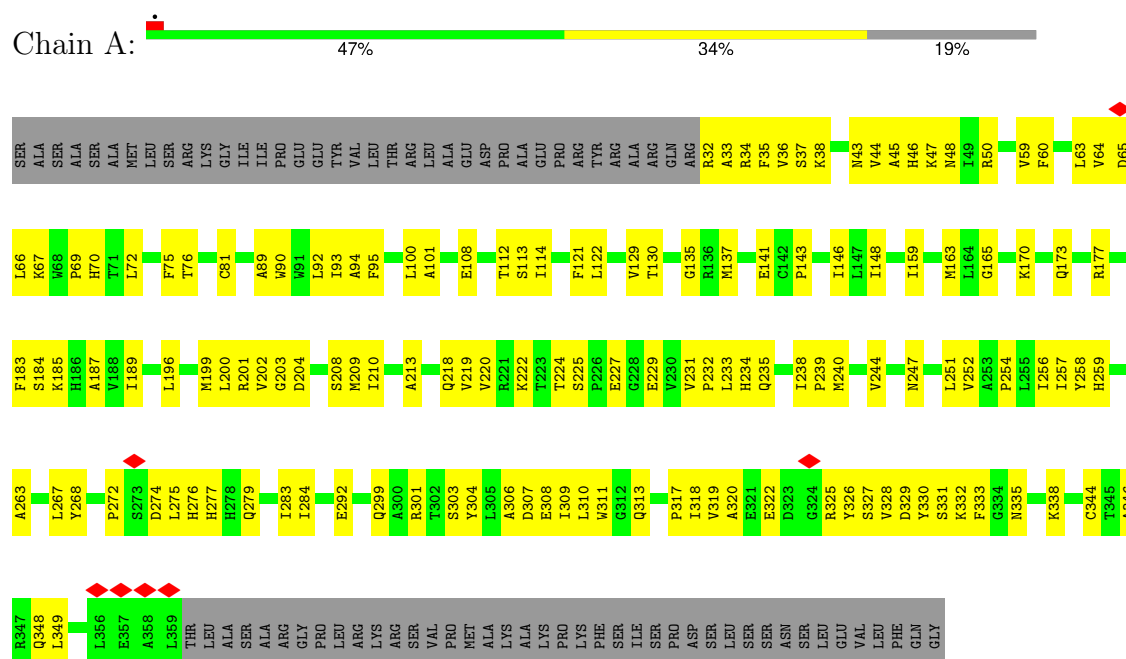
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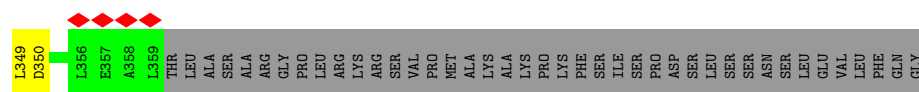
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 5 | F | 2 | 2 | 2 | 0 |

3 Residue-property plots

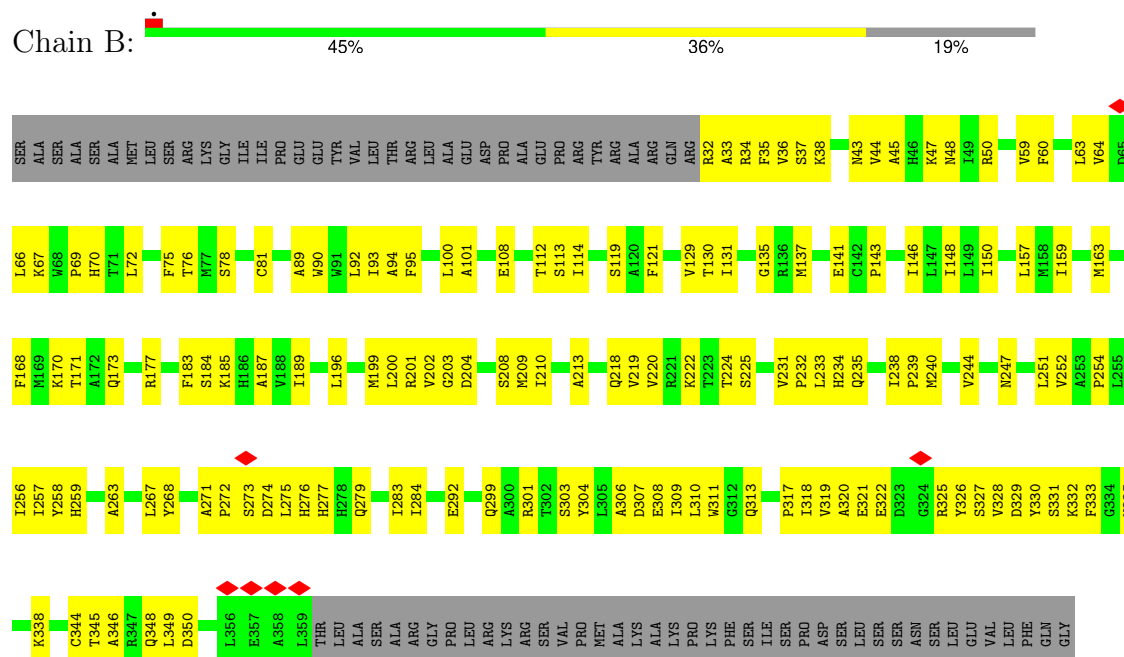
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

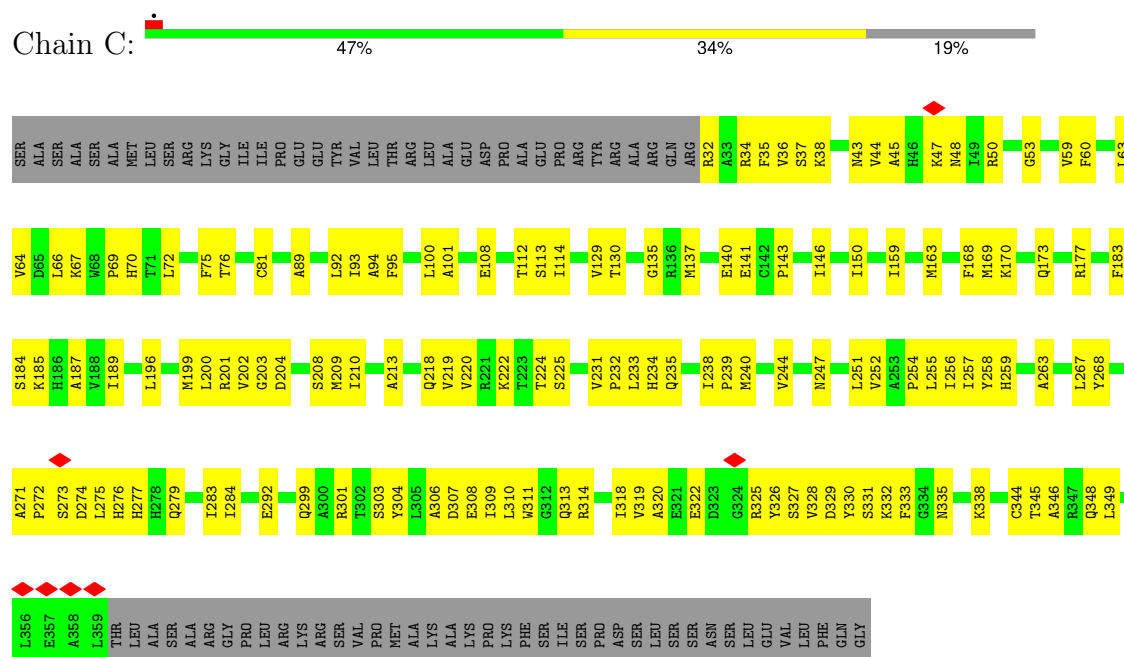




- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



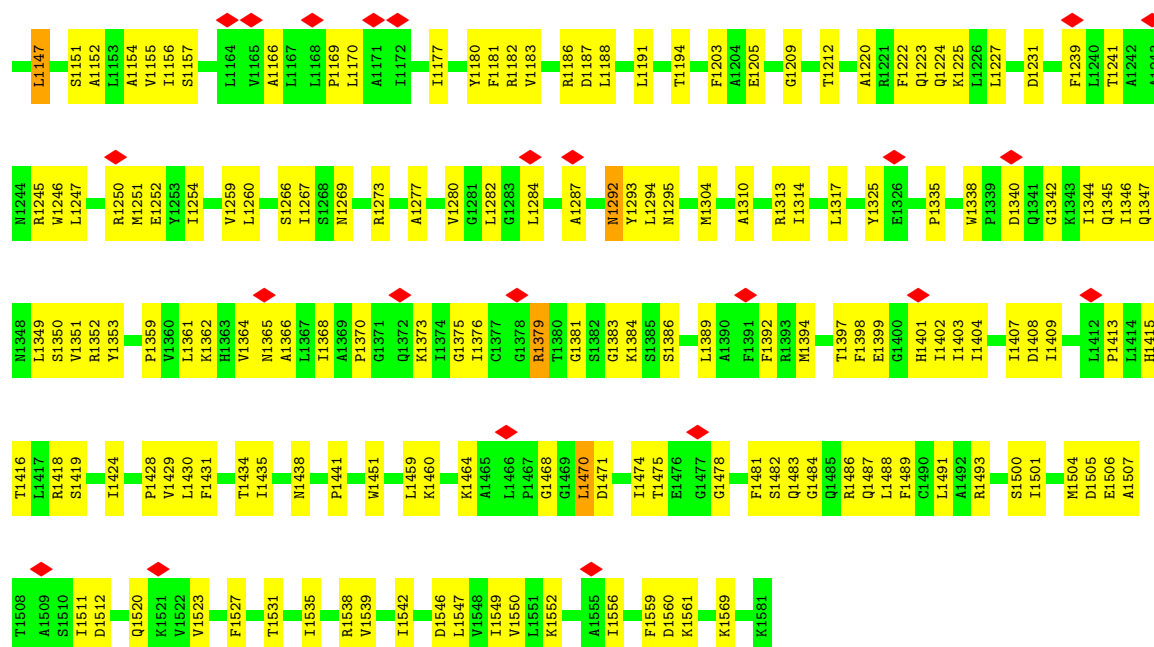
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



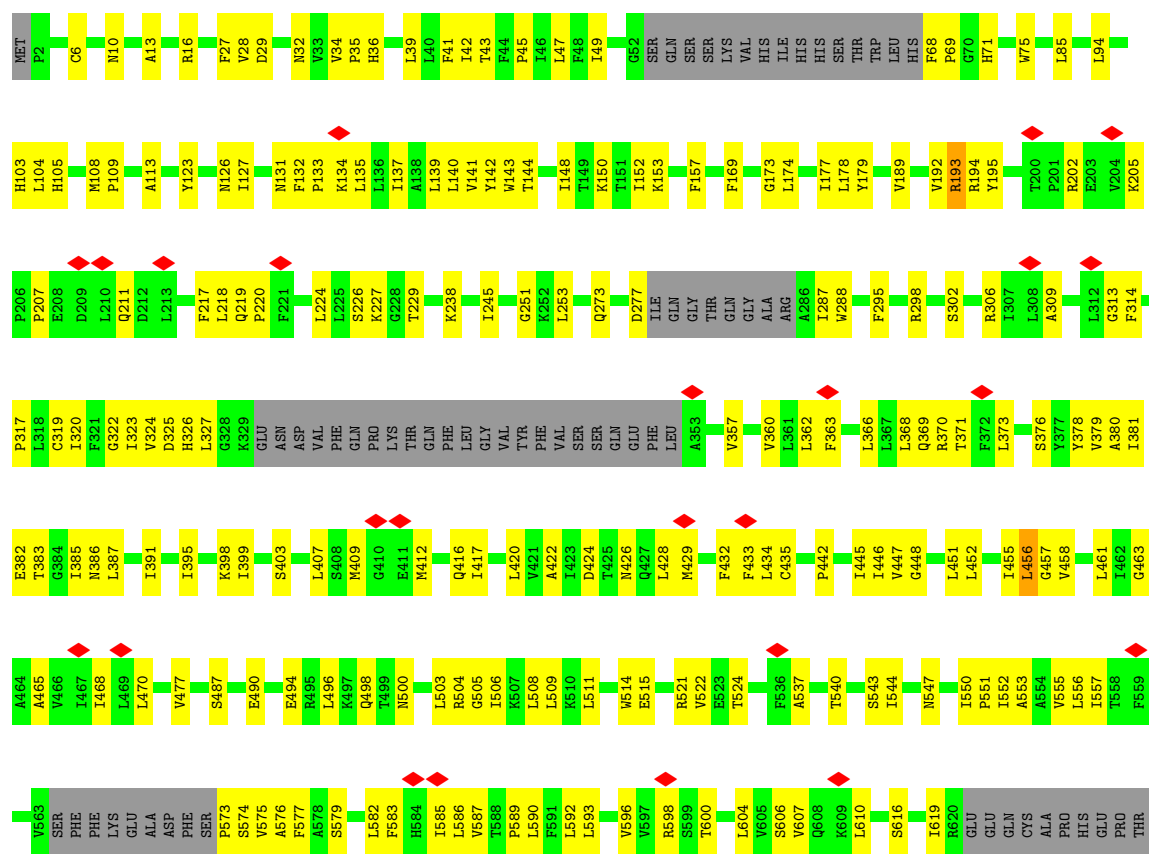
- Molecule 2: ATP-binding cassette sub-family C member 8

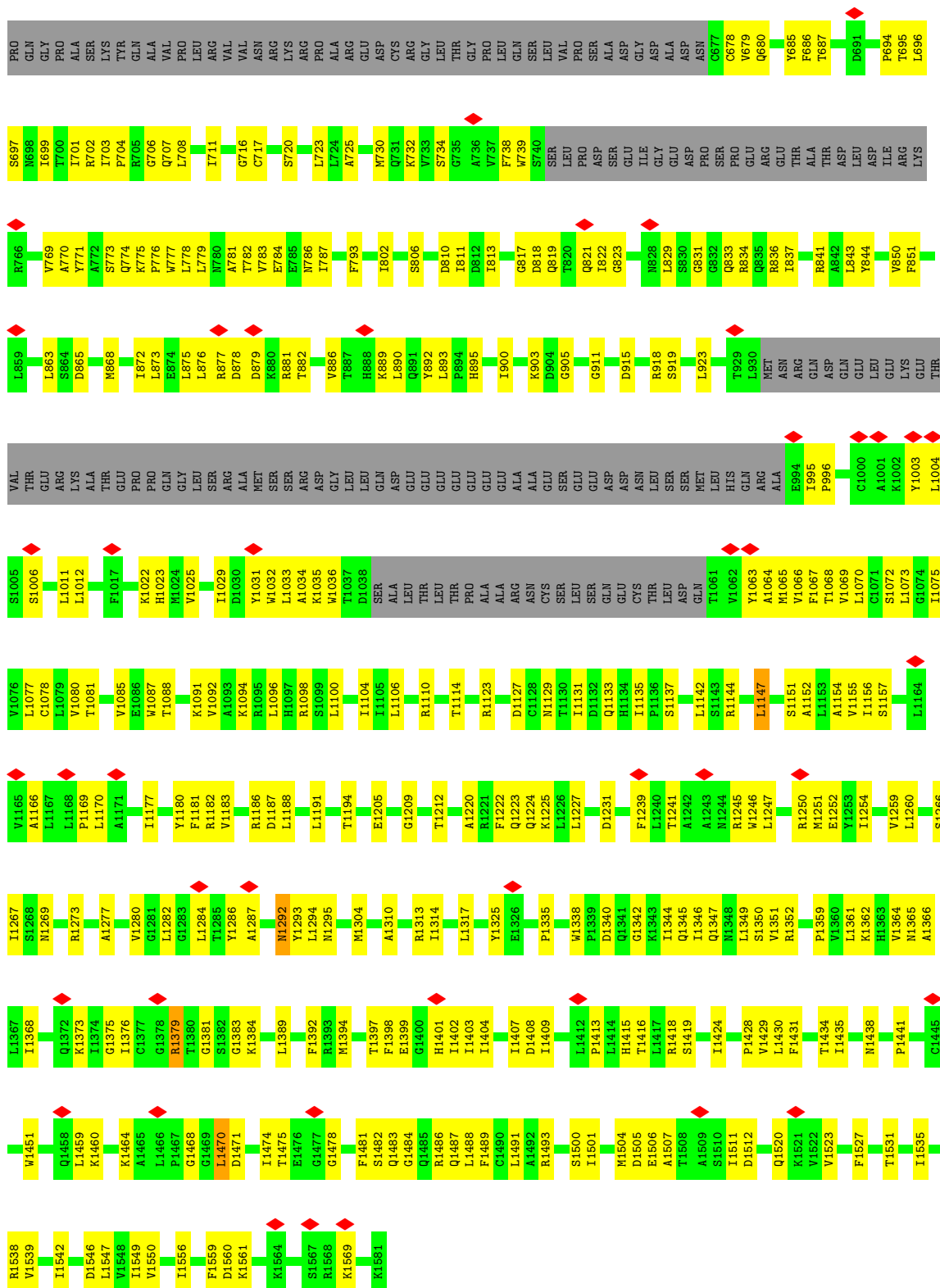




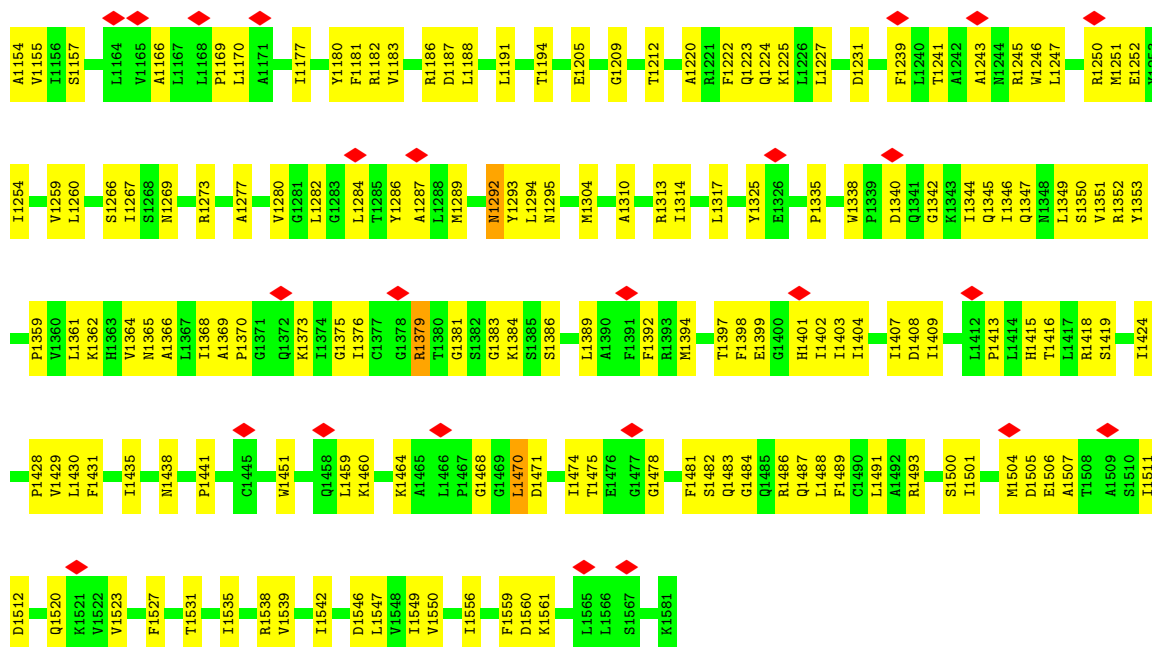


• Molecule 2: ATP-binding cassette sub-family C member 8



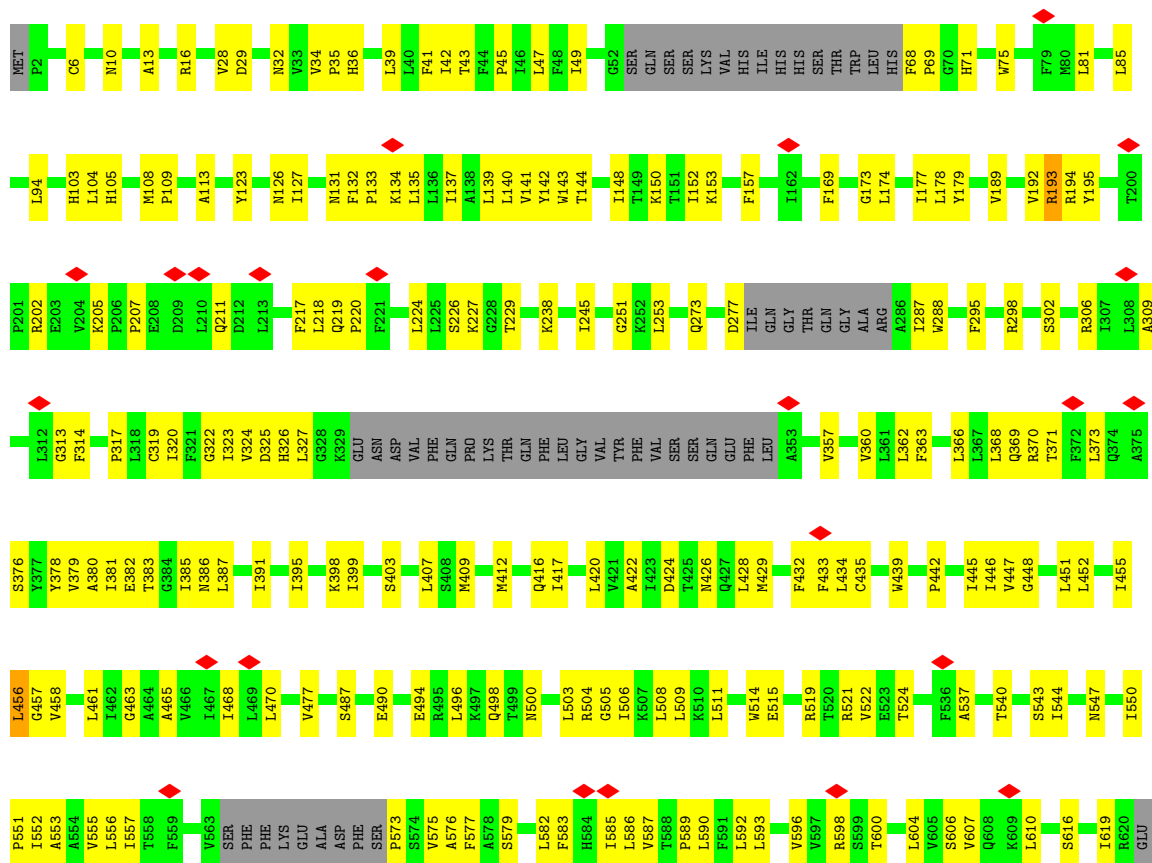






• Molecule 2: ATP-binding cassette sub-family C member 8

Chain F: 53% 32% 14%





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 47282 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.18 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.014 | Depositor |
| Minimum map value | -0.760 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.011 | Depositor |
| Recommended contour level | 0.0343 | Depositor |
| Map size (Å) | 390.0, 390.0, 390.0 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3, 1.3, 1.3 | Depositor |

5 Model quality

5.1 Standard geometry

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

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 | 0.36 | 0/2563 | 0.51 | 0/3490 |
| 1 | B | 0.36 | 0/2563 | 0.51 | 0/3490 |
| 1 | C | 0.36 | 0/2563 | 0.51 | 0/3490 |
| 1 | D | 0.36 | 0/2563 | 0.51 | 0/3490 |
| 2 | E | 0.32 | 0/10282 | 0.50 | 2/14031 (0.0%) |
| 2 | F | 0.32 | 0/10282 | 0.50 | 2/14031 (0.0%) |
| 2 | G | 0.32 | 0/10282 | 0.50 | 2/14031 (0.0%) |
| 2 | H | 0.32 | 0/10282 | 0.50 | 2/14031 (0.0%) |
| All | All | 0.33 | 0/51380 | 0.50 | 8/70084 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | E | 0 | 2 |
| 2 | F | 0 | 2 |
| 2 | G | 0 | 2 |
| 2 | H | 0 | 2 |
| All | All | 0 | 8 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2 | H | 1294 | LEU | CA-CB-CG | 5.39 | 127.69 | 115.30 |
| 2 | G | 1294 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 2 | F | 1294 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 2 | E | 1294 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2 | G | 1470 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |
| 2 | E | 1470 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |
| 2 | F | 1470 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 2 | H | 1470 | LEU | CA-CB-CG | 5.14 | 127.12 | 115.30 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | E | 193 | ARG | Peptide |
| 2 | E | 202 | ARG | Peptide |
| 2 | F | 193 | ARG | Peptide |
| 2 | F | 202 | ARG | Peptide |
| 2 | G | 193 | ARG | Peptide |
| 2 | G | 202 | ARG | Peptide |
| 2 | H | 193 | ARG | Peptide |
| 2 | H | 202 | ARG | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2506 | 0 | 2494 | 129 | 0 |
| 1 | B | 2506 | 0 | 2494 | 130 | 0 |
| 1 | C | 2506 | 0 | 2494 | 120 | 0 |
| 1 | D | 2506 | 0 | 2494 | 122 | 0 |
| 2 | E | 10077 | 0 | 9922 | 408 | 0 |
| 2 | F | 10077 | 0 | 9922 | 407 | 0 |
| 2 | G | 10077 | 0 | 9922 | 406 | 0 |
| 2 | H | 10077 | 0 | 9922 | 404 | 0 |
| 3 | A | 62 | 0 | 24 | 8 | 0 |
| 3 | C | 31 | 0 | 12 | 3 | 0 |
| 3 | D | 31 | 0 | 12 | 4 | 0 |
| 3 | E | 31 | 0 | 12 | 5 | 0 |
| 3 | F | 31 | 0 | 12 | 2 | 0 |
| 3 | G | 31 | 0 | 12 | 4 | 0 |
| 3 | H | 31 | 0 | 12 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | E | 27 | 0 | 12 | 2 | 0 |
| 4 | F | 27 | 0 | 12 | 2 | 0 |
| 4 | G | 27 | 0 | 12 | 2 | 0 |
| 4 | H | 27 | 0 | 12 | 2 | 0 |
| 5 | E | 2 | 0 | 0 | 0 | 0 |
| 5 | F | 2 | 0 | 0 | 0 | 0 |
| 5 | G | 2 | 0 | 0 | 0 | 0 |
| 5 | H | 2 | 0 | 0 | 0 | 0 |
| All | All | 50696 | 0 | 49808 | 2070 | 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 21.

All (2070) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:1501:ILE:HG22 | 2:H:1531:THR:HB | 1.55 | 0.88 |
| 2:G:1501:ILE:HG22 | 2:G:1531:THR:HB | 1.55 | 0.88 |
| 2:F:1501:ILE:HG22 | 2:F:1531:THR:HB | 1.55 | 0.87 |
| 2:H:1459:LEU:HD21 | 2:H:1488:LEU:HB3 | 1.58 | 0.86 |
| 2:E:1501:ILE:HG22 | 2:E:1531:THR:HB | 1.55 | 0.85 |
| 2:E:1459:LEU:HD21 | 2:E:1488:LEU:HB3 | 1.58 | 0.85 |
| 2:F:1459:LEU:HD21 | 2:F:1488:LEU:HB3 | 1.58 | 0.85 |
| 2:H:1350:SER:HB2 | 2:H:1399:GLU:HB2 | 1.58 | 0.84 |
| 2:H:193:ARG:O | 2:H:195:TYR:N | 2.11 | 0.84 |
| 2:E:193:ARG:O | 2:E:195:TYR:N | 2.10 | 0.84 |
| 2:F:1350:SER:HB2 | 2:F:1399:GLU:HB2 | 1.58 | 0.84 |
| 2:E:1350:SER:HB2 | 2:E:1399:GLU:HB2 | 1.58 | 0.83 |
| 2:G:1459:LEU:HD21 | 2:G:1488:LEU:HB3 | 1.58 | 0.83 |
| 2:G:1350:SER:HB2 | 2:G:1399:GLU:HB2 | 1.58 | 0.83 |
| 1:A:67:LYS:HG2 | 1:A:69:PRO:HD2 | 1.61 | 0.83 |
| 1:D:67:LYS:HG2 | 1:D:69:PRO:HD2 | 1.61 | 0.82 |
| 2:F:193:ARG:O | 2:F:195:TYR:N | 2.10 | 0.82 |
| 2:G:193:ARG:O | 2:G:195:TYR:N | 2.11 | 0.82 |
| 1:B:67:LYS:HG2 | 1:B:69:PRO:HD2 | 1.61 | 0.82 |
| 1:C:81:CYS:HB2 | 2:G:41:PHE:HB3 | 1.60 | 0.82 |
| 1:A:101:ALA:HB2 | 2:E:16:ARG:HB2 | 1.60 | 0.82 |
| 1:C:67:LYS:HG2 | 1:C:69:PRO:HD2 | 1.61 | 0.81 |
| 2:H:424:ASP:OD1 | 2:H:606:SER:OG | 2.00 | 0.79 |
| 2:E:424:ASP:OD1 | 2:E:606:SER:OG | 2.00 | 0.79 |
| 2:G:424:ASP:OD1 | 2:G:606:SER:OG | 2.00 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:810:ASP:OD2 | 2:G:836:ARG:NH2 | 2.16 | 0.79 |
| 2:E:810:ASP:OD2 | 2:E:836:ARG:NH2 | 2.16 | 0.78 |
| 2:F:424:ASP:OD1 | 2:F:606:SER:OG | 2.00 | 0.78 |
| 1:A:81:CYS:HB2 | 2:E:41:PHE:HB3 | 1.65 | 0.78 |
| 2:E:309:ALA:O | 2:E:369:GLN:NE2 | 2.17 | 0.78 |
| 2:E:218:LEU:HD23 | 2:E:219:GLN:H | 1.48 | 0.77 |
| 2:H:810:ASP:OD2 | 2:H:836:ARG:NH2 | 2.16 | 0.77 |
| 2:E:412:MET:HA | 2:E:416:GLN:HE21 | 1.49 | 0.77 |
| 2:G:412:MET:HA | 2:G:416:GLN:HE21 | 1.49 | 0.77 |
| 2:F:810:ASP:OD2 | 2:F:836:ARG:NH2 | 2.16 | 0.77 |
| 2:G:218:LEU:HD23 | 2:G:219:GLN:H | 1.48 | 0.77 |
| 2:G:309:ALA:O | 2:G:369:GLN:NE2 | 2.18 | 0.77 |
| 2:F:865:ASP:OD1 | 2:F:892:TYR:OH | 2.03 | 0.77 |
| 2:H:412:MET:HA | 2:H:416:GLN:HE21 | 1.50 | 0.77 |
| 2:F:218:LEU:HD23 | 2:F:219:GLN:H | 1.48 | 0.76 |
| 2:H:218:LEU:HD23 | 2:H:219:GLN:H | 1.48 | 0.76 |
| 2:G:380:ALA:O | 2:G:383:THR:OG1 | 2.03 | 0.76 |
| 2:F:380:ALA:O | 2:F:383:THR:OG1 | 2.03 | 0.76 |
| 2:H:380:ALA:O | 2:H:383:THR:OG1 | 2.03 | 0.76 |
| 2:F:309:ALA:O | 2:F:369:GLN:NE2 | 2.18 | 0.76 |
| 2:H:865:ASP:OD1 | 2:H:892:TYR:OH | 2.03 | 0.76 |
| 2:E:380:ALA:O | 2:E:383:THR:OG1 | 2.03 | 0.75 |
| 2:H:309:ALA:O | 2:H:369:GLN:NE2 | 2.18 | 0.75 |
| 1:A:44:VAL:HG22 | 1:D:326:TYR:HB2 | 1.67 | 0.75 |
| 2:H:432:PHE:HA | 2:H:435:CYS:HB2 | 1.69 | 0.75 |
| 2:F:412:MET:HA | 2:F:416:GLN:HE21 | 1.49 | 0.75 |
| 2:G:432:PHE:HA | 2:G:435:CYS:HB2 | 1.69 | 0.75 |
| 2:E:711:ILE:HB | 2:E:886:VAL:HG12 | 1.69 | 0.75 |
| 2:E:865:ASP:OD1 | 2:E:892:TYR:OH | 2.03 | 0.74 |
| 1:D:44:VAL:HG22 | 1:C:326:TYR:HB2 | 1.68 | 0.74 |
| 2:F:711:ILE:HB | 2:F:886:VAL:HG12 | 1.69 | 0.74 |
| 2:E:773:SER:OG | 2:E:775:LYS:O | 2.06 | 0.74 |
| 2:G:456:LEU:HD11 | 2:G:579:SER:HB2 | 1.70 | 0.74 |
| 2:G:773:SER:OG | 2:G:775:LYS:O | 2.06 | 0.74 |
| 2:G:865:ASP:OD1 | 2:G:892:TYR:OH | 2.03 | 0.74 |
| 1:C:218:GLN:HE21 | 1:C:235:GLN:HB3 | 1.54 | 0.73 |
| 2:E:432:PHE:HA | 2:E:435:CYS:HB2 | 1.69 | 0.73 |
| 2:F:432:PHE:HA | 2:F:435:CYS:HB2 | 1.69 | 0.73 |
| 1:D:218:GLN:HE21 | 1:D:235:GLN:HB3 | 1.54 | 0.73 |
| 2:G:711:ILE:HB | 2:G:886:VAL:HG12 | 1.69 | 0.73 |
| 2:H:711:ILE:HB | 2:H:886:VAL:HG12 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:218:GLN:HE21 | 1:B:235:GLN:HB3 | 1.54 | 0.72 |
| 3:A:502:ATP:N6 | 1:D:330:TYR:O | 2.23 | 0.72 |
| 1:D:81:CYS:HB2 | 2:H:41:PHE:HB3 | 1.69 | 0.72 |
| 2:F:456:LEU:HD11 | 2:F:579:SER:HB2 | 1.70 | 0.72 |
| 2:H:456:LEU:HD11 | 2:H:579:SER:HB2 | 1.70 | 0.72 |
| 1:D:101:ALA:HB2 | 2:H:16:ARG:HB2 | 1.71 | 0.72 |
| 2:G:1031:TYR:HA | 2:G:1282:LEU:HD11 | 1.71 | 0.71 |
| 2:G:1259:VAL:HA | 2:G:1287:ALA:HB1 | 1.72 | 0.71 |
| 2:H:1031:TYR:HA | 2:H:1282:LEU:HD11 | 1.71 | 0.71 |
| 2:F:773:SER:OG | 2:F:775:LYS:O | 2.06 | 0.71 |
| 2:F:1259:VAL:HA | 2:F:1287:ALA:HB1 | 1.72 | 0.71 |
| 2:H:773:SER:OG | 2:H:775:LYS:O | 2.06 | 0.71 |
| 1:A:218:GLN:HE21 | 1:A:235:GLN:HB3 | 1.54 | 0.71 |
| 2:E:1031:TYR:HA | 2:E:1282:LEU:HD11 | 1.71 | 0.71 |
| 2:E:456:LEU:HD11 | 2:E:579:SER:HB2 | 1.70 | 0.71 |
| 2:E:1259:VAL:HA | 2:E:1287:ALA:HB1 | 1.72 | 0.70 |
| 2:E:420:LEU:O | 2:E:424:ASP:HB3 | 1.92 | 0.70 |
| 2:F:1031:TYR:HA | 2:F:1282:LEU:HD11 | 1.71 | 0.70 |
| 2:E:370:ARG:HG3 | 2:E:373:LEU:HD12 | 1.73 | 0.70 |
| 2:H:219:GLN:HB3 | 2:H:227:LYS:HG2 | 1.73 | 0.70 |
| 2:H:1259:VAL:HA | 2:H:1287:ALA:HB1 | 1.72 | 0.70 |
| 2:F:370:ARG:HG3 | 2:F:373:LEU:HD12 | 1.74 | 0.70 |
| 2:H:370:ARG:HG3 | 2:H:373:LEU:HD12 | 1.73 | 0.70 |
| 2:G:420:LEU:O | 2:G:424:ASP:HB3 | 1.92 | 0.70 |
| 2:H:420:LEU:O | 2:H:424:ASP:HB3 | 1.92 | 0.70 |
| 2:G:452:LEU:HB3 | 2:G:461:LEU:HD22 | 1.75 | 0.69 |
| 2:E:132:PHE:O | 2:E:135:LEU:N | 2.23 | 0.69 |
| 2:H:29:ASP:OD2 | 2:H:105:HIS:ND1 | 2.20 | 0.69 |
| 2:E:193:ARG:O | 2:E:195:TYR:HD1 | 1.75 | 0.69 |
| 2:F:420:LEU:O | 2:F:424:ASP:HB3 | 1.92 | 0.69 |
| 2:G:1491:LEU:HD11 | 2:G:1507:ALA:HB1 | 1.74 | 0.69 |
| 2:F:193:ARG:O | 2:F:195:TYR:HD1 | 1.75 | 0.69 |
| 2:F:219:GLN:HB3 | 2:F:227:LYS:HG2 | 1.73 | 0.69 |
| 2:F:1481:PHE:O | 2:F:1486:ARG:NH2 | 2.26 | 0.69 |
| 2:E:29:ASP:OD2 | 2:E:105:HIS:ND1 | 2.21 | 0.69 |
| 2:H:10:ASN:HA | 2:H:13:ALA:HB3 | 1.74 | 0.69 |
| 1:B:32:ARG:NE | 1:B:277:HIS:O | 2.26 | 0.69 |
| 2:E:1491:LEU:HD11 | 2:E:1507:ALA:HB1 | 1.74 | 0.69 |
| 2:H:193:ARG:O | 2:H:195:TYR:HD1 | 1.75 | 0.69 |
| 2:G:193:ARG:O | 2:G:195:TYR:HD1 | 1.75 | 0.69 |
| 2:H:1491:LEU:HD11 | 2:H:1507:ALA:HB1 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:370:ARG:HG3 | 2:G:373:LEU:HD12 | 1.74 | 0.69 |
| 2:E:1389:LEU:HB3 | 2:E:1394:MET:HB2 | 1.74 | 0.69 |
| 1:D:276:HIS:CE1 | 1:D:279:GLN:HB2 | 2.28 | 0.68 |
| 2:E:1481:PHE:O | 2:E:1486:ARG:NH2 | 2.26 | 0.68 |
| 2:G:1389:LEU:HB3 | 2:G:1394:MET:HB2 | 1.74 | 0.68 |
| 1:A:32:ARG:NE | 1:A:277:HIS:O | 2.26 | 0.68 |
| 1:B:313:GLN:HG2 | 1:B:338:LYS:HA | 1.75 | 0.68 |
| 1:C:32:ARG:NE | 1:C:277:HIS:O | 2.26 | 0.68 |
| 1:C:276:HIS:CE1 | 1:C:279:GLN:HB2 | 2.29 | 0.68 |
| 2:G:1353:TYR:HH | 2:G:1386:SER:HG | 1.41 | 0.68 |
| 1:A:313:GLN:HG2 | 1:A:338:LYS:HA | 1.75 | 0.68 |
| 1:B:326:TYR:HB2 | 1:C:44:VAL:HG22 | 1.75 | 0.68 |
| 1:C:313:GLN:HG2 | 1:C:338:LYS:HA | 1.75 | 0.68 |
| 2:F:10:ASN:HA | 2:F:13:ALA:HB3 | 1.75 | 0.68 |
| 2:H:1481:PHE:O | 2:H:1486:ARG:NH2 | 2.26 | 0.68 |
| 2:G:1481:PHE:O | 2:G:1486:ARG:NH2 | 2.26 | 0.68 |
| 2:H:456:LEU:HD22 | 2:H:575:VAL:HA | 1.76 | 0.68 |
| 2:G:219:GLN:HB3 | 2:G:227:LYS:HG2 | 1.74 | 0.68 |
| 2:F:1389:LEU:HB3 | 2:F:1394:MET:HB2 | 1.74 | 0.68 |
| 1:D:32:ARG:NE | 1:D:277:HIS:O | 2.26 | 0.68 |
| 1:B:276:HIS:CE1 | 1:B:279:GLN:HB2 | 2.28 | 0.68 |
| 2:E:10:ASN:HA | 2:E:13:ALA:HB3 | 1.75 | 0.68 |
| 2:E:219:GLN:HB3 | 2:E:227:LYS:HG2 | 1.74 | 0.68 |
| 2:G:456:LEU:HD22 | 2:G:575:VAL:HA | 1.76 | 0.68 |
| 2:F:1491:LEU:HD11 | 2:F:1507:ALA:HB1 | 1.74 | 0.68 |
| 1:A:276:HIS:CE1 | 1:A:279:GLN:HB2 | 2.28 | 0.68 |
| 2:G:29:ASP:OD2 | 2:G:105:HIS:ND1 | 2.21 | 0.68 |
| 1:C:201:ARG:HA | 1:C:256:ILE:HA | 1.76 | 0.68 |
| 2:H:132:PHE:O | 2:H:135:LEU:N | 2.23 | 0.68 |
| 2:H:1376:ILE:HG12 | 2:H:1549:ILE:HB | 1.76 | 0.68 |
| 2:G:1376:ILE:HG12 | 2:G:1549:ILE:HB | 1.76 | 0.68 |
| 2:F:452:LEU:HB3 | 2:F:461:LEU:HD22 | 1.75 | 0.68 |
| 2:E:498:GLN:HB3 | 2:E:522:VAL:HG22 | 1.76 | 0.67 |
| 2:G:498:GLN:HB3 | 2:G:522:VAL:HG22 | 1.76 | 0.67 |
| 2:E:452:LEU:HB3 | 2:E:461:LEU:HD22 | 1.75 | 0.67 |
| 2:G:302:SER:OG | 2:G:376:SER:O | 2.12 | 0.67 |
| 2:F:498:GLN:HB3 | 2:F:522:VAL:HG22 | 1.76 | 0.67 |
| 1:B:201:ARG:HA | 1:B:256:ILE:HA | 1.77 | 0.67 |
| 2:H:452:LEU:HB3 | 2:H:461:LEU:HD22 | 1.75 | 0.67 |
| 2:G:10:ASN:HA | 2:G:13:ALA:HB3 | 1.74 | 0.67 |
| 2:E:434:LEU:HD13 | 2:E:596:VAL:HA | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:829:LEU:HD13 | 2:E:833:GLN:HB2 | 1.77 | 0.67 |
| 2:H:1389:LEU:HB3 | 2:H:1394:MET:HB2 | 1.74 | 0.67 |
| 2:E:456:LEU:HD22 | 2:E:575:VAL:HA | 1.76 | 0.67 |
| 2:G:132:PHE:O | 2:G:135:LEU:N | 2.23 | 0.67 |
| 2:G:320:ILE:HG23 | 2:G:1284:LEU:HD11 | 1.77 | 0.67 |
| 2:F:434:LEU:HD13 | 2:F:596:VAL:HA | 1.77 | 0.67 |
| 2:F:1004:LEU:HB2 | 2:F:1012:LEU:HD21 | 1.77 | 0.67 |
| 1:D:313:GLN:HG2 | 1:D:338:LYS:HA | 1.74 | 0.67 |
| 3:D:501:ATP:N6 | 1:C:330:TYR:O | 2.27 | 0.67 |
| 2:H:829:LEU:HD13 | 2:H:833:GLN:HB2 | 1.77 | 0.67 |
| 2:G:1004:LEU:HB2 | 2:G:1012:LEU:HD21 | 1.77 | 0.67 |
| 2:F:132:PHE:O | 2:F:135:LEU:N | 2.23 | 0.67 |
| 2:G:455:ILE:HG13 | 2:G:456:LEU:H | 1.60 | 0.66 |
| 2:E:1004:LEU:HB2 | 2:E:1012:LEU:HD21 | 1.77 | 0.66 |
| 2:E:1376:ILE:HG12 | 2:E:1549:ILE:HB | 1.76 | 0.66 |
| 2:E:1353:TYR:HH | 2:E:1386:SER:HG | 1.42 | 0.66 |
| 2:H:704:PRO:HB2 | 2:H:707:GLN:HG3 | 1.78 | 0.66 |
| 2:H:1011:LEU:HD11 | 2:H:1091:LYS:HD3 | 1.78 | 0.66 |
| 1:D:184:SER:O | 1:D:304:TYR:OH | 2.09 | 0.66 |
| 2:H:498:GLN:HB3 | 2:H:522:VAL:HG22 | 1.77 | 0.66 |
| 2:F:302:SER:OG | 2:F:376:SER:O | 2.12 | 0.66 |
| 2:F:456:LEU:HD22 | 2:F:575:VAL:HA | 1.76 | 0.66 |
| 2:E:1131:ILE:HA | 2:E:1135:ILE:HG12 | 1.77 | 0.66 |
| 2:F:29:ASP:OD2 | 2:F:105:HIS:ND1 | 2.20 | 0.66 |
| 2:H:434:LEU:HD13 | 2:H:596:VAL:HA | 1.77 | 0.66 |
| 2:G:1131:ILE:HA | 2:G:1135:ILE:HG12 | 1.77 | 0.66 |
| 1:A:201:ARG:HA | 1:A:256:ILE:HA | 1.76 | 0.66 |
| 1:D:201:ARG:HA | 1:D:256:ILE:HA | 1.76 | 0.66 |
| 2:H:320:ILE:HG23 | 2:H:1284:LEU:HD11 | 1.77 | 0.66 |
| 1:D:50:ARG:HB2 | 3:D:501:ATP:C6 | 2.30 | 0.66 |
| 2:E:302:SER:OG | 2:E:376:SER:O | 2.12 | 0.66 |
| 2:G:704:PRO:HB2 | 2:G:707:GLN:HG3 | 1.78 | 0.66 |
| 2:F:1011:LEU:HD11 | 2:F:1091:LYS:HD3 | 1.78 | 0.66 |
| 2:H:302:SER:OG | 2:H:376:SER:O | 2.12 | 0.66 |
| 2:H:717:CYS:O | 2:H:905:GLY:N | 2.28 | 0.66 |
| 2:F:829:LEU:HD13 | 2:F:833:GLN:HB2 | 1.77 | 0.66 |
| 1:B:274:ASP:OD1 | 1:B:279:GLN:NE2 | 2.29 | 0.65 |
| 1:C:274:ASP:OD1 | 1:C:279:GLN:NE2 | 2.29 | 0.65 |
| 2:H:1004:LEU:HB2 | 2:H:1012:LEU:HD21 | 1.77 | 0.65 |
| 2:G:717:CYS:O | 2:G:905:GLY:N | 2.28 | 0.65 |
| 2:F:320:ILE:HG23 | 2:F:1284:LEU:HD11 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1376:ILE:HG12 | 2:F:1549:ILE:HB | 1.76 | 0.65 |
| 1:A:274:ASP:OD1 | 1:A:279:GLN:NE2 | 2.29 | 0.65 |
| 1:D:274:ASP:OD1 | 1:D:279:GLN:NE2 | 2.29 | 0.65 |
| 2:G:829:LEU:HD13 | 2:G:833:GLN:HB2 | 1.77 | 0.65 |
| 2:G:1011:LEU:HD11 | 2:G:1091:LYS:HD3 | 1.78 | 0.65 |
| 2:F:1131:ILE:HA | 2:F:1135:ILE:HG12 | 1.77 | 0.65 |
| 2:H:1131:ILE:HA | 2:H:1135:ILE:HG12 | 1.77 | 0.65 |
| 2:G:434:LEU:HD13 | 2:G:596:VAL:HA | 1.77 | 0.65 |
| 2:F:455:ILE:HG13 | 2:F:456:LEU:H | 1.60 | 0.65 |
| 1:C:184:SER:O | 1:C:304:TYR:OH | 2.09 | 0.65 |
| 2:E:309:ALA:C | 2:E:369:GLN:HE22 | 2.00 | 0.65 |
| 3:A:501:ATP:C6 | 1:B:50:ARG:HB2 | 2.32 | 0.65 |
| 2:E:1011:LEU:HD11 | 2:E:1091:LYS:HD3 | 1.78 | 0.65 |
| 2:F:309:ALA:C | 2:F:369:GLN:HE22 | 2.00 | 0.65 |
| 2:E:320:ILE:HG23 | 2:E:1284:LEU:HD11 | 1.77 | 0.65 |
| 2:E:455:ILE:HG13 | 2:E:456:LEU:H | 1.61 | 0.65 |
| 2:E:577:PHE:CZ | 2:E:1282:LEU:HA | 2.32 | 0.65 |
| 2:H:1389:LEU:HD22 | 2:H:1394:MET:HG3 | 1.79 | 0.65 |
| 2:G:1389:LEU:HD22 | 2:G:1394:MET:HG3 | 1.79 | 0.65 |
| 2:H:455:ILE:HG13 | 2:H:456:LEU:H | 1.61 | 0.64 |
| 2:H:577:PHE:CZ | 2:H:1282:LEU:HA | 2.32 | 0.64 |
| 2:F:577:PHE:CZ | 2:F:1282:LEU:HA | 2.32 | 0.64 |
| 2:G:226:SER:HA | 2:G:229:THR:HG22 | 1.79 | 0.64 |
| 2:E:704:PRO:HB2 | 2:E:707:GLN:HG3 | 1.78 | 0.64 |
| 2:E:1389:LEU:HD22 | 2:E:1394:MET:HG3 | 1.79 | 0.64 |
| 2:F:226:SER:HA | 2:F:229:THR:HG22 | 1.79 | 0.64 |
| 1:A:184:SER:O | 1:A:304:TYR:OH | 2.09 | 0.64 |
| 1:B:177:ARG:NH2 | 1:B:208:SER:O | 2.31 | 0.64 |
| 1:B:244:VAL:HG22 | 1:C:239:PRO:HB3 | 1.79 | 0.64 |
| 2:G:577:PHE:CZ | 2:G:1282:LEU:HA | 2.32 | 0.64 |
| 2:F:717:CYS:O | 2:F:905:GLY:N | 2.28 | 0.64 |
| 2:F:1389:LEU:HD22 | 2:F:1394:MET:HG3 | 1.79 | 0.64 |
| 2:F:704:PRO:HB2 | 2:F:707:GLN:HG3 | 1.78 | 0.64 |
| 1:A:177:ARG:NH2 | 1:A:208:SER:O | 2.31 | 0.63 |
| 1:D:177:ARG:NH2 | 1:D:208:SER:O | 2.31 | 0.63 |
| 1:D:218:GLN:O | 1:D:284:ILE:N | 2.24 | 0.63 |
| 2:H:309:ALA:C | 2:H:369:GLN:HE22 | 2.00 | 0.63 |
| 2:F:94:LEU:HD11 | 2:F:357:VAL:HG21 | 1.80 | 0.63 |
| 1:D:38:LYS:HZ3 | 1:D:185:LYS:HG3 | 1.62 | 0.63 |
| 1:B:200:LEU:O | 1:B:257:ILE:N | 2.31 | 0.63 |
| 1:A:50:ARG:HB2 | 3:A:502:ATP:C6 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:38:LYS:HZ3 | 1:C:185:LYS:HG3 | 1.62 | 0.63 |
| 2:E:226:SER:HA | 2:E:229:THR:HG22 | 1.79 | 0.63 |
| 2:F:686:PHE:HB2 | 2:F:696:LEU:HB2 | 1.81 | 0.63 |
| 2:H:452:LEU:HA | 2:H:455:ILE:HG22 | 1.81 | 0.63 |
| 2:G:1424:ILE:HD12 | 2:G:1504:MET:HG2 | 1.81 | 0.63 |
| 2:F:452:LEU:HA | 2:F:455:ILE:HG22 | 1.81 | 0.63 |
| 2:E:94:LEU:HD11 | 2:E:357:VAL:HG21 | 1.80 | 0.63 |
| 2:H:850:VAL:HG21 | 2:H:881:ARG:HE | 1.64 | 0.63 |
| 2:G:309:ALA:C | 2:G:369:GLN:HE22 | 2.00 | 0.63 |
| 2:E:686:PHE:HB2 | 2:E:696:LEU:HB2 | 1.81 | 0.63 |
| 2:H:226:SER:HA | 2:H:229:THR:HG22 | 1.79 | 0.63 |
| 2:H:1342:GLY:HA3 | 2:H:1501:ILE:HG21 | 1.81 | 0.63 |
| 1:A:33:ALA:O | 1:D:326:TYR:OH | 2.06 | 0.62 |
| 2:G:94:LEU:HD11 | 2:G:357:VAL:HG21 | 1.80 | 0.62 |
| 1:A:227:GLU:OE2 | 1:D:194:GLY:N | 2.31 | 0.62 |
| 1:B:81:CYS:HB2 | 2:F:41:PHE:HB3 | 1.80 | 0.62 |
| 1:C:200:LEU:O | 1:C:257:ILE:N | 2.31 | 0.62 |
| 2:H:1424:ILE:HD12 | 2:H:1504:MET:HG2 | 1.81 | 0.62 |
| 2:G:1023:HIS:HB2 | 2:G:1147:LEU:HD12 | 1.81 | 0.62 |
| 2:G:1342:GLY:HA3 | 2:G:1501:ILE:HG21 | 1.81 | 0.62 |
| 2:G:1379:ARG:O | 2:G:1384:LYS:NZ | 2.32 | 0.62 |
| 2:E:850:VAL:HG21 | 2:E:881:ARG:HE | 1.64 | 0.62 |
| 2:E:1342:GLY:HA3 | 2:E:1501:ILE:HG21 | 1.81 | 0.62 |
| 2:F:295:PHE:CZ | 2:F:383:THR:HB | 2.35 | 0.62 |
| 1:A:34:ARG:NH2 | 1:A:303:SER:OG | 2.32 | 0.62 |
| 2:E:717:CYS:O | 2:E:905:GLY:N | 2.28 | 0.62 |
| 2:H:1379:ARG:O | 2:H:1384:LYS:NZ | 2.32 | 0.62 |
| 2:G:850:VAL:HG21 | 2:G:881:ARG:HE | 1.64 | 0.62 |
| 2:F:1023:HIS:HB2 | 2:F:1147:LEU:HD12 | 1.81 | 0.62 |
| 2:E:295:PHE:CZ | 2:E:383:THR:HB | 2.34 | 0.62 |
| 2:E:452:LEU:HA | 2:E:455:ILE:HG22 | 1.81 | 0.62 |
| 2:E:1023:HIS:HB2 | 2:E:1147:LEU:HD12 | 1.81 | 0.62 |
| 2:G:295:PHE:CZ | 2:G:383:THR:HB | 2.35 | 0.62 |
| 2:F:295:PHE:HZ | 2:F:383:THR:HB | 1.65 | 0.62 |
| 2:F:1379:ARG:O | 2:F:1384:LYS:NZ | 2.32 | 0.62 |
| 1:A:94:ALA:HB2 | 1:A:114:ILE:HD11 | 1.82 | 0.62 |
| 2:H:295:PHE:CZ | 2:H:383:THR:HB | 2.35 | 0.62 |
| 2:G:573:PRO:HG2 | 2:G:575:VAL:HG22 | 1.82 | 0.62 |
| 1:B:94:ALA:HB2 | 1:B:114:ILE:HD11 | 1.82 | 0.62 |
| 2:F:379:VAL:O | 2:F:383:THR:HG23 | 1.99 | 0.62 |
| 1:C:201:ARG:NH1 | 1:C:333:PHE:O | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:295:PHE:HZ | 2:E:383:THR:HB | 1.65 | 0.62 |
| 2:H:379:VAL:O | 2:H:383:THR:HG23 | 1.99 | 0.62 |
| 2:H:573:PRO:HG2 | 2:H:575:VAL:HG22 | 1.82 | 0.62 |
| 2:H:686:PHE:HB2 | 2:H:696:LEU:HB2 | 1.81 | 0.62 |
| 2:G:686:PHE:HB2 | 2:G:696:LEU:HB2 | 1.81 | 0.62 |
| 1:A:251:LEU:HD11 | 1:A:254:PRO:HA | 1.82 | 0.61 |
| 1:C:251:LEU:HD11 | 1:C:254:PRO:HA | 1.82 | 0.61 |
| 2:E:573:PRO:HG2 | 2:E:575:VAL:HG22 | 1.82 | 0.61 |
| 2:G:379:VAL:O | 2:G:383:THR:HG23 | 1.99 | 0.61 |
| 2:G:600:THR:O | 2:G:604:LEU:HG | 2.00 | 0.61 |
| 1:B:251:LEU:HD11 | 1:B:254:PRO:HA | 1.82 | 0.61 |
| 2:E:379:VAL:O | 2:E:383:THR:HG23 | 1.99 | 0.61 |
| 2:E:1424:ILE:HD12 | 2:E:1504:MET:HG2 | 1.81 | 0.61 |
| 2:F:1342:GLY:HA3 | 2:F:1501:ILE:HG21 | 1.81 | 0.61 |
| 2:F:1424:ILE:HD12 | 2:F:1504:MET:HG2 | 1.81 | 0.61 |
| 1:B:201:ARG:NH1 | 1:B:333:PHE:O | 2.33 | 0.61 |
| 1:C:50:ARG:HB2 | 3:C:501:ATP:C6 | 2.34 | 0.61 |
| 2:H:600:THR:O | 2:H:604:LEU:HG | 2.00 | 0.61 |
| 2:H:1023:HIS:HB2 | 2:H:1147:LEU:HD12 | 1.81 | 0.61 |
| 1:A:329:ASP:OD1 | 1:A:331:SER:OG | 2.14 | 0.61 |
| 2:E:403:SER:HA | 2:E:619:ILE:HG12 | 1.83 | 0.61 |
| 2:E:774:GLN:HG2 | 2:E:1483:GLN:HG3 | 1.83 | 0.61 |
| 2:E:1379:ARG:O | 2:E:1384:LYS:NZ | 2.32 | 0.61 |
| 2:H:94:LEU:HD11 | 2:H:357:VAL:HG21 | 1.80 | 0.61 |
| 2:H:723:LEU:HB3 | 2:H:851:PHE:CZ | 2.36 | 0.61 |
| 1:A:200:LEU:O | 1:A:257:ILE:N | 2.31 | 0.61 |
| 1:D:177:ARG:NH1 | 1:D:208:SER:OG | 2.34 | 0.61 |
| 2:F:403:SER:HA | 2:F:619:ILE:HG12 | 1.83 | 0.61 |
| 1:A:219:VAL:HA | 1:A:283:ILE:HA | 1.83 | 0.61 |
| 2:H:403:SER:HA | 2:H:619:ILE:HG12 | 1.83 | 0.61 |
| 2:H:774:GLN:HG2 | 2:H:1483:GLN:HG3 | 1.83 | 0.61 |
| 2:G:403:SER:HA | 2:G:619:ILE:HG12 | 1.83 | 0.61 |
| 2:G:1430:LEU:HD23 | 2:G:1474:ILE:HD13 | 1.83 | 0.61 |
| 2:F:723:LEU:HB3 | 2:F:851:PHE:CZ | 2.36 | 0.61 |
| 2:F:1403:ILE:HD13 | 2:F:1408:ASP:HA | 1.82 | 0.61 |
| 1:D:201:ARG:NH1 | 1:D:333:PHE:O | 2.33 | 0.61 |
| 1:B:177:ARG:NH1 | 1:B:208:SER:OG | 2.34 | 0.61 |
| 1:D:200:LEU:O | 1:D:257:ILE:N | 2.31 | 0.61 |
| 2:G:774:GLN:HG2 | 2:G:1483:GLN:HG3 | 1.83 | 0.61 |
| 2:F:850:VAL:HG21 | 2:F:881:ARG:HE | 1.64 | 0.61 |
| 1:C:177:ARG:NH2 | 1:C:208:SER:O | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:600:THR:O | 2:E:604:LEU:HG | 2.00 | 0.60 |
| 1:A:330:TYR:O | 3:A:501:ATP:N6 | 2.34 | 0.60 |
| 2:E:723:LEU:HB3 | 2:E:851:PHE:CZ | 2.36 | 0.60 |
| 2:F:1110:ARG:HE | 2:F:1114:THR:HG1 | 1.47 | 0.60 |
| 1:A:229:GLU:HB3 | 1:D:314:ARG:HH11 | 1.67 | 0.60 |
| 2:F:573:PRO:HG2 | 2:F:575:VAL:HG22 | 1.82 | 0.60 |
| 2:F:600:THR:O | 2:F:604:LEU:HG | 2.00 | 0.60 |
| 2:F:1430:LEU:HD23 | 2:F:1474:ILE:HD13 | 1.83 | 0.60 |
| 1:D:251:LEU:HD11 | 1:D:254:PRO:HA | 1.82 | 0.60 |
| 2:H:295:PHE:HZ | 2:H:383:THR:HB | 1.65 | 0.60 |
| 1:A:177:ARG:NH1 | 1:A:208:SER:OG | 2.34 | 0.60 |
| 1:A:326:TYR:HB2 | 1:B:44:VAL:HG22 | 1.81 | 0.60 |
| 1:B:34:ARG:NH2 | 1:B:303:SER:OG | 2.32 | 0.60 |
| 1:B:101:ALA:HB2 | 2:F:16:ARG:HB2 | 1.83 | 0.60 |
| 1:B:219:VAL:HA | 1:B:283:ILE:HA | 1.83 | 0.60 |
| 1:C:34:ARG:NH2 | 1:C:303:SER:OG | 2.32 | 0.60 |
| 1:C:94:ALA:HB2 | 1:C:114:ILE:HD11 | 1.82 | 0.60 |
| 1:C:177:ARG:NH1 | 1:C:208:SER:OG | 2.34 | 0.60 |
| 2:G:452:LEU:HA | 2:G:455:ILE:HG22 | 1.81 | 0.60 |
| 2:G:521:ARG:O | 2:G:524:THR:OG1 | 2.17 | 0.60 |
| 2:F:322:GLY:O | 2:F:326:HIS:ND1 | 2.30 | 0.60 |
| 1:A:203:GLY:HA2 | 1:A:254:PRO:HB3 | 1.84 | 0.60 |
| 1:D:94:ALA:HB2 | 1:D:114:ILE:HD11 | 1.82 | 0.60 |
| 1:B:38:LYS:HZ3 | 1:B:185:LYS:HG3 | 1.65 | 0.60 |
| 2:E:1110:ARG:HE | 2:E:1114:THR:HG1 | 1.47 | 0.60 |
| 1:B:203:GLY:HA2 | 1:B:254:PRO:HB3 | 1.84 | 0.60 |
| 1:C:101:ALA:HB2 | 2:G:16:ARG:HB2 | 1.83 | 0.60 |
| 2:E:314:PHE:CZ | 2:E:448:GLY:HA2 | 2.37 | 0.60 |
| 2:E:1403:ILE:HD13 | 2:E:1408:ASP:HA | 1.83 | 0.60 |
| 2:H:314:PHE:CZ | 2:H:448:GLY:HA2 | 2.37 | 0.60 |
| 2:G:295:PHE:HZ | 2:G:383:THR:HB | 1.65 | 0.60 |
| 2:G:1110:ARG:HE | 2:G:1114:THR:HG1 | 1.48 | 0.60 |
| 2:F:774:GLN:HG2 | 2:F:1483:GLN:HG3 | 1.83 | 0.60 |
| 2:H:133:PRO:HB2 | 2:H:195:TYR:CZ | 2.36 | 0.60 |
| 2:H:1403:ILE:HD13 | 2:H:1408:ASP:HA | 1.82 | 0.60 |
| 2:H:1430:LEU:HD23 | 2:H:1474:ILE:HD13 | 1.83 | 0.60 |
| 2:F:133:PRO:HB2 | 2:F:195:TYR:CZ | 2.36 | 0.60 |
| 1:C:219:VAL:HA | 1:C:283:ILE:HA | 1.83 | 0.60 |
| 2:E:133:PRO:HB2 | 2:E:195:TYR:CZ | 2.36 | 0.60 |
| 2:G:314:PHE:CZ | 2:G:448:GLY:HA2 | 2.37 | 0.60 |
| 2:F:1424:ILE:HD13 | 2:F:1491:LEU:HG | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:521:ARG:O | 2:F:524:THR:OG1 | 2.17 | 0.60 |
| 2:H:508:LEU:HD22 | 2:H:1431:PHE:HZ | 1.67 | 0.59 |
| 2:F:1154:ALA:O | 2:F:1157:SER:OG | 2.19 | 0.59 |
| 1:A:38:LYS:HZ3 | 1:A:185:LYS:HG3 | 1.66 | 0.59 |
| 2:E:1424:ILE:HD13 | 2:E:1491:LEU:HG | 1.84 | 0.59 |
| 2:F:1500:SER:O | 2:F:1531:THR:N | 2.28 | 0.59 |
| 1:D:203:GLY:HA2 | 1:D:254:PRO:HB3 | 1.84 | 0.59 |
| 1:C:203:GLY:HA2 | 1:C:254:PRO:HB3 | 1.84 | 0.59 |
| 2:H:494:GLU:O | 2:H:498:GLN:HG2 | 2.02 | 0.59 |
| 2:G:133:PRO:HB2 | 2:G:195:TYR:CZ | 2.36 | 0.59 |
| 2:G:723:LEU:HB3 | 2:G:851:PHE:CZ | 2.36 | 0.59 |
| 1:C:231:VAL:HG23 | 1:C:234:HIS:HB2 | 1.84 | 0.59 |
| 2:H:422:ALA:O | 2:H:426:ASN:ND2 | 2.36 | 0.59 |
| 2:G:508:LEU:HD22 | 2:G:1431:PHE:HZ | 1.67 | 0.59 |
| 2:F:314:PHE:CZ | 2:F:448:GLY:HA2 | 2.37 | 0.59 |
| 2:F:422:ALA:O | 2:F:426:ASN:ND2 | 2.36 | 0.59 |
| 1:B:59:VAL:O | 1:B:63:LEU:HB2 | 2.02 | 0.59 |
| 2:E:521:ARG:O | 2:E:524:THR:OG1 | 2.17 | 0.59 |
| 2:H:1154:ALA:O | 2:H:1157:SER:OG | 2.19 | 0.59 |
| 2:G:1269:ASN:O | 2:G:1273:ARG:N | 2.28 | 0.59 |
| 2:G:1403:ILE:HD13 | 2:G:1408:ASP:HA | 1.82 | 0.59 |
| 2:F:442:PRO:HA | 2:F:445:ILE:HG22 | 1.84 | 0.59 |
| 2:F:494:GLU:O | 2:F:498:GLN:HG2 | 2.02 | 0.59 |
| 1:B:231:VAL:HG23 | 1:B:234:HIS:HB2 | 1.84 | 0.59 |
| 2:E:1430:LEU:HD23 | 2:E:1474:ILE:HD13 | 1.83 | 0.59 |
| 1:C:238:ILE:HD11 | 1:C:259:HIS:CD2 | 2.38 | 0.59 |
| 1:A:59:VAL:O | 1:A:63:LEU:HB2 | 2.02 | 0.59 |
| 1:A:201:ARG:NH1 | 1:A:333:PHE:O | 2.33 | 0.59 |
| 1:D:219:VAL:HA | 1:D:283:ILE:HA | 1.83 | 0.59 |
| 1:D:231:VAL:HG23 | 1:D:234:HIS:HB2 | 1.84 | 0.59 |
| 2:E:322:GLY:O | 2:E:326:HIS:ND1 | 2.30 | 0.59 |
| 2:E:494:GLU:O | 2:E:498:GLN:HG2 | 2.02 | 0.59 |
| 2:G:422:ALA:O | 2:G:426:ASN:ND2 | 2.35 | 0.59 |
| 1:B:307:ASP:OD1 | 1:B:308:GLU:N | 2.36 | 0.59 |
| 2:H:1375:GLY:N | 2:H:1547:LEU:O | 2.32 | 0.59 |
| 2:G:1424:ILE:HD13 | 2:G:1491:LEU:HG | 1.84 | 0.59 |
| 1:C:59:VAL:O | 1:C:63:LEU:HB2 | 2.02 | 0.59 |
| 2:E:323:ILE:HG23 | 2:E:1267:ILE:HD11 | 1.85 | 0.59 |
| 2:F:508:LEU:HD22 | 2:F:1431:PHE:HZ | 1.67 | 0.59 |
| 1:A:66:LEU:O | 1:A:170:LYS:NZ | 2.32 | 0.58 |
| 1:D:59:VAL:O | 1:D:63:LEU:HB2 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:307:ASP:OD1 | 1:D:308:GLU:N | 2.36 | 0.58 |
| 1:C:307:ASP:OD1 | 1:C:308:GLU:N | 2.36 | 0.58 |
| 2:E:442:PRO:HA | 2:E:445:ILE:HG22 | 1.84 | 0.58 |
| 2:H:1424:ILE:HD13 | 2:H:1491:LEU:HG | 1.84 | 0.58 |
| 2:H:1500:SER:O | 2:H:1531:THR:N | 2.28 | 0.58 |
| 2:G:494:GLU:O | 2:G:498:GLN:HG2 | 2.02 | 0.58 |
| 2:E:422:ALA:O | 2:E:426:ASN:ND2 | 2.36 | 0.58 |
| 2:H:1501:ILE:HA | 2:H:1531:THR:O | 2.03 | 0.58 |
| 1:B:32:ARG:NH2 | 1:B:279:GLN:O | 2.30 | 0.58 |
| 2:H:878:ASP:OD1 | 2:H:879:ASP:N | 2.36 | 0.58 |
| 2:F:555:VAL:HG12 | 2:F:583:PHE:HD2 | 1.69 | 0.58 |
| 2:E:890:LEU:HA | 2:E:893:LEU:HD23 | 1.84 | 0.58 |
| 2:E:1501:ILE:HA | 2:E:1531:THR:O | 2.04 | 0.58 |
| 2:H:711:ILE:HG13 | 2:H:900:ILE:HB | 1.86 | 0.58 |
| 2:G:442:PRO:HA | 2:G:445:ILE:HG22 | 1.84 | 0.58 |
| 2:F:878:ASP:OD1 | 2:F:879:ASP:N | 2.36 | 0.58 |
| 1:D:329:ASP:OD1 | 1:D:331:SER:OG | 2.14 | 0.58 |
| 2:H:322:GLY:O | 2:H:326:HIS:ND1 | 2.30 | 0.58 |
| 2:G:890:LEU:HA | 2:G:893:LEU:HD23 | 1.85 | 0.58 |
| 2:F:711:ILE:HG13 | 2:F:900:ILE:HB | 1.86 | 0.58 |
| 2:F:786:ASN:ND2 | 2:F:822:ILE:HD11 | 2.19 | 0.58 |
| 2:F:1501:ILE:HA | 2:F:1531:THR:O | 2.04 | 0.58 |
| 1:A:218:GLN:O | 1:A:284:ILE:N | 2.24 | 0.58 |
| 1:A:231:VAL:HG23 | 1:A:234:HIS:HB2 | 1.84 | 0.58 |
| 1:D:34:ARG:NH2 | 1:D:303:SER:OG | 2.32 | 0.58 |
| 1:D:238:ILE:HD11 | 1:D:259:HIS:CD2 | 2.38 | 0.58 |
| 2:E:508:LEU:HD22 | 2:E:1431:PHE:HZ | 1.67 | 0.58 |
| 2:E:598:ARG:NH1 | 2:E:1137:SER:OG | 2.37 | 0.58 |
| 2:H:1110:ARG:HE | 2:H:1114:THR:HG1 | 1.49 | 0.58 |
| 2:F:1032:TRP:CH2 | 2:F:1066:VAL:HG13 | 2.39 | 0.58 |
| 2:H:442:PRO:HA | 2:H:445:ILE:HG22 | 1.84 | 0.58 |
| 2:H:1032:TRP:CH2 | 2:H:1066:VAL:HG13 | 2.39 | 0.58 |
| 1:A:346:ALA:HA | 1:A:349:LEU:HB2 | 1.86 | 0.58 |
| 1:B:238:ILE:HD11 | 1:B:259:HIS:CD2 | 2.38 | 0.58 |
| 2:E:555:VAL:HG12 | 2:E:583:PHE:HD2 | 1.69 | 0.58 |
| 2:G:323:ILE:HG23 | 2:G:1267:ILE:HD11 | 1.85 | 0.58 |
| 2:G:555:VAL:HG12 | 2:G:583:PHE:HD2 | 1.69 | 0.58 |
| 2:G:711:ILE:HG13 | 2:G:900:ILE:HB | 1.86 | 0.58 |
| 2:F:323:ILE:HG23 | 2:F:1267:ILE:HD11 | 1.85 | 0.58 |
| 2:F:1353:TYR:HH | 2:F:1386:SER:HG | 1.48 | 0.58 |
| 1:D:66:LEU:O | 1:D:170:LYS:NZ | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:346:ALA:HA | 1:C:349:LEU:HB2 | 1.86 | 0.58 |
| 2:G:598:ARG:NH1 | 2:G:1137:SER:OG | 2.37 | 0.58 |
| 2:F:509:LEU:HB3 | 2:F:515:GLU:HG2 | 1.86 | 0.58 |
| 2:F:890:LEU:HA | 2:F:893:LEU:HD23 | 1.84 | 0.58 |
| 1:A:238:ILE:HD11 | 1:A:259:HIS:CD2 | 2.38 | 0.57 |
| 1:B:184:SER:O | 1:B:304:TYR:OH | 2.09 | 0.57 |
| 2:E:786:ASN:ND2 | 2:E:822:ILE:HD11 | 2.19 | 0.57 |
| 2:H:786:ASN:ND2 | 2:H:822:ILE:HD11 | 2.19 | 0.57 |
| 2:G:1032:TRP:CH2 | 2:G:1066:VAL:HG13 | 2.39 | 0.57 |
| 1:A:307:ASP:OD1 | 1:A:308:GLU:N | 2.36 | 0.57 |
| 2:E:1032:TRP:CH2 | 2:E:1066:VAL:HG13 | 2.39 | 0.57 |
| 2:H:890:LEU:HA | 2:H:893:LEU:HD23 | 1.84 | 0.57 |
| 2:G:878:ASP:OD1 | 2:G:879:ASP:N | 2.36 | 0.57 |
| 2:G:1154:ALA:O | 2:G:1157:SER:OG | 2.19 | 0.57 |
| 1:A:229:GLU:HB3 | 1:D:314:ARG:NH1 | 2.18 | 0.57 |
| 1:B:346:ALA:HA | 1:B:349:LEU:HB2 | 1.86 | 0.57 |
| 2:H:521:ARG:O | 2:H:524:THR:OG1 | 2.17 | 0.57 |
| 2:G:412:MET:HA | 2:G:416:GLN:NE2 | 2.19 | 0.57 |
| 2:F:836:ARG:HD3 | 2:F:863:LEU:HD23 | 1.87 | 0.57 |
| 1:B:218:GLN:O | 1:B:284:ILE:N | 2.24 | 0.57 |
| 1:A:189:ILE:HD11 | 1:A:309:ILE:HG22 | 1.87 | 0.57 |
| 2:G:1500:SER:O | 2:G:1531:THR:N | 2.28 | 0.57 |
| 2:G:1501:ILE:HA | 2:G:1531:THR:O | 2.04 | 0.57 |
| 2:G:381:ILE:HG13 | 2:G:433:PHE:CE1 | 2.40 | 0.57 |
| 2:F:378:TYR:HA | 2:F:381:ILE:HG22 | 1.87 | 0.57 |
| 1:A:121:PHE:HE2 | 1:B:150:ILE:HD11 | 1.70 | 0.57 |
| 1:D:346:ALA:HA | 1:D:349:LEU:HB2 | 1.86 | 0.57 |
| 1:B:330:TYR:O | 3:C:501:ATP:N6 | 2.38 | 0.57 |
| 2:E:711:ILE:HG13 | 2:E:900:ILE:HB | 1.86 | 0.57 |
| 2:H:1269:ASN:O | 2:H:1273:ARG:N | 2.28 | 0.57 |
| 1:B:329:ASP:OD1 | 1:B:331:SER:OG | 2.14 | 0.57 |
| 2:E:836:ARG:HD3 | 2:E:863:LEU:HD23 | 1.87 | 0.57 |
| 2:E:878:ASP:OD1 | 2:E:879:ASP:N | 2.36 | 0.57 |
| 2:E:1065:MET:O | 2:E:1068:THR:OG1 | 2.20 | 0.57 |
| 2:G:786:ASN:ND2 | 2:G:822:ILE:HD11 | 2.19 | 0.57 |
| 1:D:189:ILE:HD11 | 1:D:309:ILE:HG22 | 1.87 | 0.57 |
| 2:H:323:ILE:HG23 | 2:H:1267:ILE:HD11 | 1.85 | 0.57 |
| 2:H:555:VAL:HG12 | 2:H:583:PHE:HD2 | 1.69 | 0.57 |
| 2:G:378:TYR:HA | 2:G:381:ILE:HG22 | 1.87 | 0.57 |
| 2:G:679:VAL:HG22 | 2:G:739:TRP:CD1 | 2.40 | 0.57 |
| 1:A:218:GLN:NE2 | 1:A:235:GLN:HB3 | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:159:ILE:O | 1:B:163:MET:HG2 | 2.05 | 0.57 |
| 1:C:329:ASP:OD1 | 1:C:331:SER:OG | 2.14 | 0.57 |
| 2:E:412:MET:HA | 2:E:416:GLN:NE2 | 2.19 | 0.57 |
| 2:E:509:LEU:HB3 | 2:E:515:GLU:HG2 | 1.86 | 0.57 |
| 2:E:1123:ARG:HA | 2:E:1127:ASP:HB2 | 1.87 | 0.57 |
| 2:H:412:MET:HA | 2:H:416:GLN:NE2 | 2.19 | 0.57 |
| 2:G:509:LEU:HB3 | 2:G:515:GLU:HG2 | 1.86 | 0.57 |
| 2:F:381:ILE:HG13 | 2:F:433:PHE:CE1 | 2.40 | 0.57 |
| 1:A:92:LEU:HD22 | 2:E:34:VAL:HG21 | 1.87 | 0.56 |
| 2:H:381:ILE:HG13 | 2:H:433:PHE:CE1 | 2.40 | 0.56 |
| 2:F:775:LYS:HB3 | 2:F:1483:GLN:HE22 | 1.70 | 0.56 |
| 1:D:159:ILE:O | 1:D:163:MET:HG2 | 2.05 | 0.56 |
| 2:H:378:TYR:HA | 2:H:381:ILE:HG22 | 1.87 | 0.56 |
| 2:G:1182:ARG:HH22 | 2:G:1186:ARG:HH21 | 1.53 | 0.56 |
| 2:F:598:ARG:NH1 | 2:F:1137:SER:OG | 2.37 | 0.56 |
| 1:A:95:PHE:HE2 | 2:E:27:PHE:HA | 1.70 | 0.56 |
| 1:B:189:ILE:HD11 | 1:B:309:ILE:HG22 | 1.87 | 0.56 |
| 2:H:679:VAL:HG22 | 2:H:739:TRP:CD1 | 2.40 | 0.56 |
| 2:H:775:LYS:HB3 | 2:H:1483:GLN:HE22 | 1.71 | 0.56 |
| 2:H:1415:HIS:O | 2:H:1419:SER:OG | 2.18 | 0.56 |
| 2:G:1431:PHE:HB2 | 2:G:1438:ASN:HD22 | 1.70 | 0.56 |
| 2:F:1065:MET:O | 2:F:1068:THR:OG1 | 2.20 | 0.56 |
| 2:F:1123:ARG:HA | 2:F:1127:ASP:HB2 | 1.87 | 0.56 |
| 2:F:1338:TRP:O | 2:F:1340:ASP:N | 2.39 | 0.56 |
| 2:F:1431:PHE:HB2 | 2:F:1438:ASN:HD22 | 1.70 | 0.56 |
| 2:E:378:TYR:HA | 2:E:381:ILE:HG22 | 1.87 | 0.56 |
| 2:H:509:LEU:HB3 | 2:H:515:GLU:HG2 | 1.86 | 0.56 |
| 2:G:322:GLY:O | 2:G:326:HIS:ND1 | 2.30 | 0.56 |
| 1:C:177:ARG:NH2 | 1:C:204:ASP:OD2 | 2.38 | 0.56 |
| 2:H:598:ARG:NH1 | 2:H:1137:SER:OG | 2.37 | 0.56 |
| 2:H:1431:PHE:HB2 | 2:H:1438:ASN:HD22 | 1.70 | 0.56 |
| 2:F:1182:ARG:HH22 | 2:F:1186:ARG:HH21 | 1.53 | 0.56 |
| 1:B:218:GLN:NE2 | 1:B:235:GLN:HB3 | 2.20 | 0.56 |
| 1:C:218:GLN:O | 1:C:284:ILE:N | 2.24 | 0.56 |
| 2:E:775:LYS:HB3 | 2:E:1483:GLN:HE22 | 1.70 | 0.56 |
| 1:B:171:THR:HG23 | 1:C:169:MET:HE1 | 1.88 | 0.56 |
| 2:E:217:PHE:HB2 | 2:E:251:GLY:HA3 | 1.88 | 0.56 |
| 2:E:319:CYS:SG | 2:E:362:LEU:HB2 | 2.46 | 0.56 |
| 2:E:381:ILE:HG13 | 2:E:433:PHE:CE1 | 2.40 | 0.56 |
| 2:G:1506:GLU:H | 2:G:1535:ILE:HB | 1.71 | 0.56 |
| 1:B:177:ARG:NH2 | 1:B:204:ASP:OD2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:209:MET:HE1 | 1:B:252:VAL:HG22 | 1.88 | 0.56 |
| 2:E:679:VAL:HG22 | 2:E:739:TRP:CD1 | 2.40 | 0.56 |
| 2:E:1338:TRP:O | 2:E:1340:ASP:N | 2.39 | 0.56 |
| 2:H:1506:GLU:H | 2:H:1535:ILE:HB | 1.71 | 0.56 |
| 2:G:775:LYS:HB3 | 2:G:1483:GLN:HE22 | 1.71 | 0.56 |
| 2:G:1065:MET:O | 2:G:1068:THR:OG1 | 2.20 | 0.56 |
| 2:F:319:CYS:SG | 2:F:362:LEU:HB2 | 2.46 | 0.56 |
| 1:A:159:ILE:O | 1:A:163:MET:HG2 | 2.05 | 0.56 |
| 1:D:218:GLN:NE2 | 1:D:235:GLN:HB3 | 2.20 | 0.56 |
| 2:H:319:CYS:SG | 2:H:362:LEU:HB2 | 2.46 | 0.56 |
| 2:G:1123:ARG:HA | 2:G:1127:ASP:HB2 | 1.87 | 0.56 |
| 2:F:217:PHE:HB2 | 2:F:251:GLY:HA3 | 1.88 | 0.56 |
| 1:A:244:VAL:HG22 | 1:B:239:PRO:HB3 | 1.88 | 0.56 |
| 1:C:159:ILE:O | 1:C:163:MET:HG2 | 2.05 | 0.56 |
| 2:G:706:GLY:N | 2:G:882:THR:OG1 | 2.38 | 0.56 |
| 1:D:92:LEU:HD22 | 2:H:34:VAL:HG21 | 1.88 | 0.55 |
| 2:H:429:MET:HG2 | 2:H:433:PHE:CZ | 2.42 | 0.55 |
| 2:H:836:ARG:HD3 | 2:H:863:LEU:HD23 | 1.87 | 0.55 |
| 2:F:429:MET:HG2 | 2:F:433:PHE:CZ | 2.41 | 0.55 |
| 2:E:1032:TRP:HH2 | 2:E:1066:VAL:HG13 | 1.72 | 0.55 |
| 2:H:831:GLY:HA2 | 2:H:834:ARG:HD3 | 1.89 | 0.55 |
| 2:F:679:VAL:HG22 | 2:F:739:TRP:CD1 | 2.40 | 0.55 |
| 1:C:189:ILE:HD11 | 1:C:309:ILE:HG22 | 1.87 | 0.55 |
| 1:D:32:ARG:NH2 | 1:D:279:GLN:O | 2.30 | 0.55 |
| 1:D:177:ARG:NH2 | 1:D:204:ASP:OD2 | 2.38 | 0.55 |
| 2:H:1246:TRP:HE1 | 2:H:1250:ARG:NH2 | 2.04 | 0.55 |
| 2:G:429:MET:HG2 | 2:G:433:PHE:CZ | 2.41 | 0.55 |
| 2:F:775:LYS:HB3 | 2:F:1483:GLN:NE2 | 2.21 | 0.55 |
| 2:E:412:MET:HB2 | 2:E:417:ILE:HD11 | 1.89 | 0.55 |
| 2:H:217:PHE:HB2 | 2:H:251:GLY:HA3 | 1.88 | 0.55 |
| 2:H:1123:ARG:HA | 2:H:1127:ASP:HB2 | 1.87 | 0.55 |
| 2:G:686:PHE:HB3 | 2:G:730:MET:SD | 2.47 | 0.55 |
| 2:G:1351:VAL:HA | 2:G:1397:THR:HA | 1.89 | 0.55 |
| 2:F:412:MET:HB2 | 2:F:417:ILE:HD11 | 1.89 | 0.55 |
| 1:A:32:ARG:NH2 | 1:A:279:GLN:O | 2.30 | 0.55 |
| 1:A:35:PHE:CD2 | 1:A:36:VAL:HG23 | 2.42 | 0.55 |
| 1:A:177:ARG:NH2 | 1:A:204:ASP:OD2 | 2.38 | 0.55 |
| 1:C:218:GLN:NE2 | 1:C:235:GLN:HB3 | 2.20 | 0.55 |
| 2:E:775:LYS:HB3 | 2:E:1483:GLN:NE2 | 2.21 | 0.55 |
| 2:E:1431:PHE:HB2 | 2:E:1438:ASN:HD22 | 1.70 | 0.55 |
| 2:G:141:VAL:O | 2:G:144:THR:OG1 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:319:CYS:SG | 2:G:362:LEU:HB2 | 2.46 | 0.55 |
| 2:F:1351:VAL:HA | 2:F:1397:THR:HA | 1.89 | 0.55 |
| 2:H:686:PHE:HB3 | 2:H:730:MET:SD | 2.47 | 0.55 |
| 2:H:1182:ARG:HH22 | 2:H:1186:ARG:HH21 | 1.53 | 0.55 |
| 2:H:1338:TRP:O | 2:H:1340:ASP:N | 2.38 | 0.55 |
| 2:G:1246:TRP:HE1 | 2:G:1250:ARG:NH2 | 2.04 | 0.55 |
| 2:G:1338:TRP:O | 2:G:1340:ASP:N | 2.39 | 0.55 |
| 2:E:313:GLY:H | 2:E:369:GLN:NE2 | 2.05 | 0.55 |
| 2:E:1154:ALA:O | 2:E:1157:SER:OG | 2.19 | 0.55 |
| 2:E:1246:TRP:HE1 | 2:E:1250:ARG:NH2 | 2.04 | 0.55 |
| 2:H:1032:TRP:HH2 | 2:H:1066:VAL:HG13 | 1.72 | 0.55 |
| 2:F:686:PHE:HB3 | 2:F:730:MET:SD | 2.47 | 0.55 |
| 2:E:429:MET:HG2 | 2:E:433:PHE:CZ | 2.41 | 0.55 |
| 2:H:133:PRO:HB2 | 2:H:195:TYR:CE1 | 2.42 | 0.55 |
| 2:H:412:MET:HB2 | 2:H:417:ILE:HD11 | 1.89 | 0.55 |
| 2:H:775:LYS:HB3 | 2:H:1483:GLN:NE2 | 2.21 | 0.55 |
| 2:F:313:GLY:H | 2:F:369:GLN:NE2 | 2.05 | 0.55 |
| 2:E:141:VAL:O | 2:E:144:THR:OG1 | 2.21 | 0.55 |
| 2:E:686:PHE:HB3 | 2:E:730:MET:SD | 2.47 | 0.55 |
| 2:E:1182:ARG:HH22 | 2:E:1186:ARG:HH21 | 1.53 | 0.55 |
| 2:E:1560:ASP:OD1 | 2:E:1561:LYS:N | 2.39 | 0.55 |
| 2:G:836:ARG:HD3 | 2:G:863:LEU:HD23 | 1.87 | 0.55 |
| 2:G:1560:ASP:OD1 | 2:G:1561:LYS:N | 2.39 | 0.55 |
| 2:F:1269:ASN:O | 2:F:1273:ARG:N | 2.28 | 0.55 |
| 1:D:129:VAL:O | 1:D:130:THR:OG1 | 2.23 | 0.54 |
| 1:B:35:PHE:CD2 | 1:B:36:VAL:HG23 | 2.42 | 0.54 |
| 2:G:217:PHE:HB2 | 2:G:251:GLY:HA3 | 1.88 | 0.54 |
| 2:G:775:LYS:HB3 | 2:G:1483:GLN:NE2 | 2.21 | 0.54 |
| 2:F:509:LEU:HB3 | 2:F:515:GLU:CG | 2.38 | 0.54 |
| 2:G:1180:TYR:O | 2:G:1183:VAL:HG12 | 2.08 | 0.54 |
| 2:F:1032:TRP:HH2 | 2:F:1066:VAL:HG13 | 1.72 | 0.54 |
| 1:C:35:PHE:CD2 | 1:C:36:VAL:HG23 | 2.42 | 0.54 |
| 2:H:313:GLY:H | 2:H:369:GLN:NE2 | 2.05 | 0.54 |
| 2:H:782:THR:HG23 | 2:H:819:GLN:HA | 1.89 | 0.54 |
| 2:G:137:ILE:HG23 | 2:G:195:TYR:OH | 2.08 | 0.54 |
| 2:G:509:LEU:HB3 | 2:G:515:GLU:CG | 2.38 | 0.54 |
| 2:G:723:LEU:HB3 | 2:G:851:PHE:HZ | 1.73 | 0.54 |
| 2:F:782:THR:HG22 | 2:F:784:GLU:H | 1.73 | 0.54 |
| 2:E:716:GLY:N | 3:E:2004:ATP:O3G | 2.34 | 0.54 |
| 2:H:723:LEU:HB3 | 2:H:851:PHE:HZ | 1.72 | 0.54 |
| 2:H:1180:TYR:O | 2:H:1183:VAL:HG12 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1351:VAL:HA | 2:H:1397:THR:HA | 1.89 | 0.54 |
| 2:G:831:GLY:HA2 | 2:G:834:ARG:HD3 | 1.89 | 0.54 |
| 2:E:133:PRO:HB2 | 2:E:195:TYR:CE1 | 2.42 | 0.54 |
| 2:E:1351:VAL:HA | 2:E:1397:THR:HA | 1.89 | 0.54 |
| 2:G:514:TRP:CD2 | 2:G:1441:PRO:HG2 | 2.42 | 0.54 |
| 2:F:141:VAL:O | 2:F:144:THR:OG1 | 2.21 | 0.54 |
| 2:E:370:ARG:HG2 | 2:E:1252:GLU:CD | 2.28 | 0.54 |
| 2:E:514:TRP:CD2 | 2:E:1441:PRO:HG2 | 2.42 | 0.54 |
| 2:G:782:THR:HG23 | 2:G:819:GLN:HA | 1.89 | 0.54 |
| 2:F:412:MET:HA | 2:F:416:GLN:NE2 | 2.19 | 0.54 |
| 2:H:514:TRP:CD2 | 2:H:1441:PRO:HG2 | 2.42 | 0.54 |
| 2:G:47:LEU:HD21 | 2:G:126:ASN:HD22 | 1.73 | 0.54 |
| 2:G:1032:TRP:HH2 | 2:G:1066:VAL:HG13 | 1.72 | 0.54 |
| 2:F:1180:TYR:O | 2:F:1183:VAL:HG12 | 2.08 | 0.54 |
| 1:A:46:HIS:O | 1:D:330:TYR:HD2 | 1.91 | 0.54 |
| 1:D:35:PHE:CD2 | 1:D:36:VAL:HG23 | 2.42 | 0.54 |
| 1:C:129:VAL:O | 1:C:130:THR:OG1 | 2.23 | 0.54 |
| 2:E:47:LEU:HD21 | 2:E:126:ASN:HD22 | 1.73 | 0.54 |
| 2:H:137:ILE:HG23 | 2:H:195:TYR:OH | 2.08 | 0.54 |
| 2:H:782:THR:HG22 | 2:H:784:GLU:H | 1.73 | 0.54 |
| 2:H:1129:ASN:OD1 | 2:H:1133:GLN:NE2 | 2.41 | 0.54 |
| 2:G:412:MET:HB2 | 2:G:417:ILE:HD11 | 1.89 | 0.54 |
| 2:F:514:TRP:CD2 | 2:F:1441:PRO:HG2 | 2.42 | 0.54 |
| 2:F:1506:GLU:H | 2:F:1535:ILE:HB | 1.71 | 0.54 |
| 2:E:509:LEU:HB3 | 2:E:515:GLU:CG | 2.38 | 0.54 |
| 2:E:1011:LEU:HD22 | 2:E:1088:THR:HB | 1.90 | 0.54 |
| 2:G:1431:PHE:O | 2:G:1438:ASN:ND2 | 2.34 | 0.54 |
| 2:F:1246:TRP:HE1 | 2:F:1250:ARG:NH2 | 2.04 | 0.54 |
| 2:H:47:LEU:HD21 | 2:H:126:ASN:HD22 | 1.73 | 0.54 |
| 2:H:509:LEU:HB3 | 2:H:515:GLU:CG | 2.38 | 0.54 |
| 2:H:1011:LEU:HD22 | 2:H:1088:THR:HB | 1.90 | 0.54 |
| 2:G:586:LEU:O | 2:G:589:PRO:HD2 | 2.08 | 0.54 |
| 2:G:1129:ASN:OD1 | 2:G:1133:GLN:NE2 | 2.41 | 0.54 |
| 1:B:317:PRO:HB3 | 1:C:232:PRO:HD3 | 1.89 | 0.53 |
| 1:C:32:ARG:NH2 | 1:C:279:GLN:O | 2.30 | 0.53 |
| 2:E:706:GLY:N | 2:E:882:THR:OG1 | 2.38 | 0.53 |
| 2:H:1431:PHE:O | 2:H:1438:ASN:ND2 | 2.35 | 0.53 |
| 2:F:137:ILE:HG23 | 2:F:195:TYR:OH | 2.08 | 0.53 |
| 2:F:370:ARG:HG2 | 2:F:1252:GLU:CD | 2.29 | 0.53 |
| 2:F:586:LEU:O | 2:F:589:PRO:HD2 | 2.08 | 0.53 |
| 2:F:1129:ASN:OD1 | 2:F:1133:GLN:NE2 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1180:TYR:O | 2:E:1183:VAL:HG12 | 2.08 | 0.53 |
| 2:E:1500:SER:O | 2:E:1531:THR:N | 2.28 | 0.53 |
| 2:G:133:PRO:HB2 | 2:G:195:TYR:CE1 | 2.42 | 0.53 |
| 2:G:313:GLY:H | 2:G:369:GLN:NE2 | 2.05 | 0.53 |
| 2:F:47:LEU:HD21 | 2:F:126:ASN:HD22 | 1.73 | 0.53 |
| 2:F:831:GLY:HA2 | 2:F:834:ARG:HD3 | 1.89 | 0.53 |
| 1:A:112:THR:OG1 | 1:A:137:MET:N | 2.42 | 0.53 |
| 2:E:782:THR:HG23 | 2:E:819:GLN:HA | 1.89 | 0.53 |
| 2:E:1269:ASN:O | 2:E:1273:ARG:N | 2.28 | 0.53 |
| 2:H:451:LEU:O | 2:H:455:ILE:N | 2.42 | 0.53 |
| 2:H:1344:ILE:O | 2:H:1368:ILE:N | 2.29 | 0.53 |
| 2:G:1398:PHE:CD2 | 2:G:1399:GLU:HG2 | 2.44 | 0.53 |
| 2:F:133:PRO:HB2 | 2:F:195:TYR:CE1 | 2.42 | 0.53 |
| 2:F:782:THR:HG23 | 2:F:819:GLN:HA | 1.89 | 0.53 |
| 2:H:586:LEU:O | 2:H:589:PRO:HD2 | 2.08 | 0.53 |
| 1:B:275:LEU:HD21 | 1:B:311:TRP:HB2 | 1.91 | 0.53 |
| 2:E:137:ILE:HG23 | 2:E:195:TYR:OH | 2.08 | 0.53 |
| 2:E:1460:LYS:HG2 | 2:E:1464:LYS:HZ2 | 1.74 | 0.53 |
| 2:E:1506:GLU:H | 2:E:1535:ILE:HB | 1.71 | 0.53 |
| 2:H:370:ARG:HG2 | 2:H:1252:GLU:CD | 2.29 | 0.53 |
| 1:A:275:LEU:HD21 | 1:A:311:TRP:HB2 | 1.91 | 0.53 |
| 2:E:451:LEU:O | 2:E:455:ILE:N | 2.41 | 0.53 |
| 2:E:831:GLY:HA2 | 2:E:834:ARG:HD3 | 1.89 | 0.53 |
| 2:E:1129:ASN:OD1 | 2:E:1133:GLN:NE2 | 2.41 | 0.53 |
| 2:E:1383:GLY:HA2 | 4:E:2001:ADP:H5'1 | 1.91 | 0.53 |
| 2:H:1398:PHE:CD2 | 2:H:1399:GLU:HG2 | 2.44 | 0.53 |
| 2:G:1011:LEU:HD22 | 2:G:1088:THR:HB | 1.90 | 0.53 |
| 2:F:723:LEU:HB3 | 2:F:851:PHE:HZ | 1.72 | 0.53 |
| 2:E:1398:PHE:CD2 | 2:E:1399:GLU:HG2 | 2.44 | 0.53 |
| 2:H:71:HIS:O | 2:H:75:TRP:HD1 | 1.92 | 0.53 |
| 2:G:193:ARG:O | 2:G:195:TYR:CD1 | 2.59 | 0.53 |
| 2:F:1011:LEU:HD22 | 2:F:1088:THR:HB | 1.91 | 0.53 |
| 2:E:586:LEU:O | 2:E:589:PRO:HD2 | 2.08 | 0.53 |
| 2:E:779:LEU:HA | 2:E:1205:GLU:OE1 | 2.09 | 0.53 |
| 2:H:500:ASN:O | 2:H:504:ARG:HG2 | 2.09 | 0.53 |
| 2:G:782:THR:HG22 | 2:G:784:GLU:H | 1.73 | 0.53 |
| 2:G:1383:GLY:HA2 | 4:G:2001:ADP:H5'1 | 1.91 | 0.53 |
| 2:F:71:HIS:O | 2:F:75:TRP:HD1 | 1.92 | 0.53 |
| 1:D:199:MET:HG2 | 1:D:258:TYR:CB | 2.39 | 0.53 |
| 1:B:199:MET:HG2 | 1:B:258:TYR:CB | 2.39 | 0.53 |
| 2:E:500:ASN:O | 2:E:504:ARG:HG2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1375:GLY:N | 2:G:1547:LEU:O | 2.32 | 0.53 |
| 2:F:193:ARG:O | 2:F:195:TYR:CD1 | 2.59 | 0.53 |
| 2:E:782:THR:HG22 | 2:E:784:GLU:H | 1.73 | 0.53 |
| 2:H:706:GLY:N | 2:H:882:THR:OG1 | 2.38 | 0.53 |
| 2:H:1383:GLY:HA2 | 4:H:2001:ADP:H5'1 | 1.91 | 0.53 |
| 2:G:500:ASN:O | 2:G:504:ARG:HG2 | 2.09 | 0.53 |
| 2:F:1383:GLY:HA2 | 4:F:2001:ADP:H5'1 | 1.91 | 0.53 |
| 2:H:686:PHE:HA | 2:H:732:LYS:HA | 1.91 | 0.52 |
| 1:A:199:MET:HG2 | 1:A:258:TYR:CB | 2.39 | 0.52 |
| 2:E:71:HIS:O | 2:E:75:TRP:HD1 | 1.92 | 0.52 |
| 2:E:1344:ILE:O | 2:E:1368:ILE:N | 2.29 | 0.52 |
| 2:H:317:PRO:HA | 2:H:320:ILE:HD12 | 1.92 | 0.52 |
| 2:G:71:HIS:O | 2:G:75:TRP:HD1 | 1.92 | 0.52 |
| 2:G:317:PRO:HA | 2:G:320:ILE:HD12 | 1.92 | 0.52 |
| 2:G:451:LEU:O | 2:G:455:ILE:N | 2.41 | 0.52 |
| 2:F:369:GLN:HG3 | 2:F:370:ARG:HD2 | 1.92 | 0.52 |
| 2:F:451:LEU:O | 2:F:455:ILE:N | 2.42 | 0.52 |
| 2:F:500:ASN:O | 2:F:504:ARG:HG2 | 2.09 | 0.52 |
| 2:F:1398:PHE:CD2 | 2:F:1399:GLU:HG2 | 2.44 | 0.52 |
| 1:C:199:MET:HG2 | 1:C:258:TYR:CB | 2.39 | 0.52 |
| 2:E:723:LEU:HB3 | 2:E:851:PHE:HZ | 1.73 | 0.52 |
| 2:G:868:MET:O | 2:G:872:ILE:HB | 2.10 | 0.52 |
| 2:F:395:ILE:O | 2:F:399:ILE:HG12 | 2.09 | 0.52 |
| 2:F:779:LEU:HA | 2:F:1205:GLU:OE1 | 2.09 | 0.52 |
| 1:B:199:MET:HG2 | 1:B:258:TYR:HB2 | 1.92 | 0.52 |
| 2:E:1370:PRO:O | 2:E:1531:THR:OG1 | 2.16 | 0.52 |
| 2:G:1351:VAL:HG22 | 2:G:1361:LEU:HB3 | 1.91 | 0.52 |
| 2:F:139:LEU:HD12 | 2:F:143:TRP:HE1 | 1.74 | 0.52 |
| 2:E:193:ARG:O | 2:E:195:TYR:CD1 | 2.60 | 0.52 |
| 2:H:369:GLN:HG3 | 2:H:370:ARG:HD2 | 1.92 | 0.52 |
| 2:H:779:LEU:HA | 2:H:1205:GLU:OE1 | 2.09 | 0.52 |
| 1:A:199:MET:HG2 | 1:A:258:TYR:HB2 | 1.92 | 0.52 |
| 1:D:275:LEU:HD21 | 1:D:311:TRP:HB2 | 1.91 | 0.52 |
| 2:E:139:LEU:HD12 | 2:E:143:TRP:HE1 | 1.74 | 0.52 |
| 2:E:369:GLN:HG3 | 2:E:370:ARG:HD2 | 1.92 | 0.52 |
| 2:G:369:GLN:HG3 | 2:G:370:ARG:HD2 | 1.92 | 0.52 |
| 2:G:370:ARG:HG2 | 2:G:1252:GLU:CD | 2.29 | 0.52 |
| 2:G:779:LEU:HA | 2:G:1205:GLU:OE1 | 2.09 | 0.52 |
| 2:G:1556:ILE:HG21 | 2:G:1559:PHE:HB3 | 1.91 | 0.52 |
| 2:F:686:PHE:HA | 2:F:732:LYS:HA | 1.91 | 0.52 |
| 2:E:686:PHE:HA | 2:E:732:LYS:HA | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1556:ILE:HG21 | 2:E:1559:PHE:HB3 | 1.92 | 0.52 |
| 2:H:395:ILE:O | 2:H:399:ILE:HG12 | 2.09 | 0.52 |
| 2:G:1408:ASP:OD1 | 2:G:1409:ILE:N | 2.40 | 0.52 |
| 2:G:395:ILE:O | 2:G:399:ILE:HG12 | 2.09 | 0.52 |
| 2:F:771:TYR:HD2 | 2:F:1212:THR:HG22 | 1.75 | 0.52 |
| 1:C:275:LEU:HD21 | 1:C:311:TRP:HB2 | 1.91 | 0.52 |
| 2:E:317:PRO:HA | 2:E:320:ILE:HD12 | 1.92 | 0.52 |
| 2:E:1351:VAL:HG22 | 2:E:1361:LEU:HB3 | 1.91 | 0.52 |
| 2:E:1431:PHE:O | 2:E:1438:ASN:ND2 | 2.35 | 0.52 |
| 2:H:868:MET:O | 2:H:872:ILE:HB | 2.10 | 0.52 |
| 2:H:1310:ALA:HA | 2:H:1313:ARG:NH2 | 2.25 | 0.52 |
| 2:F:587:VAL:HA | 2:F:590:LEU:HD12 | 1.92 | 0.52 |
| 2:F:1310:ALA:HA | 2:F:1313:ARG:NH2 | 2.25 | 0.52 |
| 2:F:1375:GLY:O | 2:F:1549:ILE:N | 2.43 | 0.52 |
| 1:B:121:PHE:HE2 | 1:C:150:ILE:HD11 | 1.75 | 0.52 |
| 1:C:199:MET:HG2 | 1:C:258:TYR:HB2 | 1.92 | 0.52 |
| 2:E:587:VAL:HA | 2:E:590:LEU:HD12 | 1.92 | 0.52 |
| 2:G:1004:LEU:HD22 | 2:G:1012:LEU:HD11 | 1.92 | 0.52 |
| 1:D:112:THR:OG1 | 1:D:137:MET:N | 2.41 | 0.51 |
| 2:E:1375:GLY:N | 2:E:1547:LEU:O | 2.32 | 0.51 |
| 2:G:1310:ALA:HA | 2:G:1313:ARG:NH2 | 2.25 | 0.51 |
| 2:H:139:LEU:HD12 | 2:H:143:TRP:HE1 | 1.74 | 0.51 |
| 2:H:382:GLU:OE2 | 2:H:386:ASN:ND2 | 2.37 | 0.51 |
| 2:F:1351:VAL:HG22 | 2:F:1361:LEU:HB3 | 1.91 | 0.51 |
| 2:F:1375:GLY:N | 2:F:1547:LEU:O | 2.32 | 0.51 |
| 2:E:42:ILE:HG23 | 2:E:43:THR:HG23 | 1.92 | 0.51 |
| 2:E:395:ILE:O | 2:E:399:ILE:HG12 | 2.09 | 0.51 |
| 2:E:868:MET:O | 2:E:872:ILE:HB | 2.10 | 0.51 |
| 2:H:42:ILE:HG23 | 2:H:43:THR:HG23 | 1.92 | 0.51 |
| 2:H:587:VAL:HA | 2:H:590:LEU:HD12 | 1.92 | 0.51 |
| 2:G:139:LEU:HD12 | 2:G:143:TRP:HE1 | 1.74 | 0.51 |
| 2:F:317:PRO:HA | 2:F:320:ILE:HD12 | 1.92 | 0.51 |
| 2:F:706:GLY:N | 2:F:882:THR:OG1 | 2.38 | 0.51 |
| 2:F:1004:LEU:HD22 | 2:F:1012:LEU:HD11 | 1.92 | 0.51 |
| 1:A:95:PHE:HD1 | 1:A:100:LEU:HD12 | 1.75 | 0.51 |
| 1:A:272:PRO:HD3 | 1:A:311:TRP:CZ2 | 2.46 | 0.51 |
| 2:E:1310:ALA:HA | 2:E:1313:ARG:NH2 | 2.25 | 0.51 |
| 2:H:1375:GLY:O | 2:H:1549:ILE:N | 2.43 | 0.51 |
| 2:H:1560:ASP:OD1 | 2:H:1561:LYS:N | 2.39 | 0.51 |
| 1:D:272:PRO:HD3 | 1:D:311:TRP:CZ2 | 2.46 | 0.51 |
| 2:E:771:TYR:HD2 | 2:E:1212:THR:HG22 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1004:LEU:HD22 | 2:E:1012:LEU:HD11 | 1.92 | 0.51 |
| 2:E:1375:GLY:O | 2:E:1549:ILE:N | 2.43 | 0.51 |
| 2:H:1004:LEU:HD22 | 2:H:1012:LEU:HD11 | 1.93 | 0.51 |
| 2:H:1065:MET:O | 2:H:1068:THR:OG1 | 2.20 | 0.51 |
| 2:G:686:PHE:HA | 2:G:732:LYS:HA | 1.91 | 0.51 |
| 1:B:272:PRO:HD3 | 1:B:311:TRP:CZ2 | 2.46 | 0.51 |
| 1:C:112:THR:OG1 | 1:C:137:MET:N | 2.42 | 0.51 |
| 2:H:253:LEU:HD11 | 2:H:1231:ASP:HB3 | 1.93 | 0.51 |
| 2:H:1408:ASP:OD1 | 2:H:1409:ILE:N | 2.40 | 0.51 |
| 2:F:868:MET:O | 2:F:872:ILE:HB | 2.10 | 0.51 |
| 1:A:47:LYS:HE3 | 1:D:327:SER:HB2 | 1.93 | 0.51 |
| 1:D:199:MET:HG2 | 1:D:258:TYR:HB2 | 1.92 | 0.51 |
| 1:B:275:LEU:HA | 1:B:306:ALA:HB1 | 1.93 | 0.51 |
| 2:H:193:ARG:O | 2:H:195:TYR:CD1 | 2.59 | 0.51 |
| 2:H:777:TRP:CZ3 | 2:H:1209:GLY:HA3 | 2.46 | 0.51 |
| 2:G:273:GLN:O | 2:G:277:ASP:N | 2.39 | 0.51 |
| 2:G:587:VAL:HA | 2:G:590:LEU:HD12 | 1.92 | 0.51 |
| 2:G:771:TYR:HD2 | 2:G:1212:THR:HG22 | 1.75 | 0.51 |
| 2:F:218:LEU:HD23 | 2:F:219:GLN:N | 2.23 | 0.51 |
| 2:F:598:ARG:HH12 | 2:F:1137:SER:HG | 1.56 | 0.51 |
| 2:F:1560:ASP:OD1 | 2:F:1561:LYS:N | 2.39 | 0.51 |
| 1:A:46:HIS:HD2 | 1:D:330:TYR:CZ | 2.29 | 0.51 |
| 2:H:716:GLY:N | 3:H:2004:ATP:O3G | 2.34 | 0.51 |
| 2:G:39:LEU:HD22 | 2:G:142:TYR:CE2 | 2.46 | 0.51 |
| 2:G:1375:GLY:O | 2:G:1549:ILE:N | 2.43 | 0.51 |
| 1:A:209:MET:HE1 | 1:A:252:VAL:HG22 | 1.92 | 0.51 |
| 1:D:344:CYS:SG | 1:D:349:LEU:HD22 | 2.51 | 0.51 |
| 1:B:108:GLU:HB2 | 1:B:141:GLU:HG3 | 1.93 | 0.51 |
| 1:C:108:GLU:HB2 | 1:C:141:GLU:HG3 | 1.93 | 0.51 |
| 2:E:253:LEU:HD11 | 2:E:1231:ASP:HB3 | 1.93 | 0.51 |
| 2:E:1451:TRP:CE3 | 2:E:1460:LYS:HG3 | 2.46 | 0.51 |
| 2:H:704:PRO:HB2 | 2:H:707:GLN:CG | 2.41 | 0.51 |
| 2:H:771:TYR:HD2 | 2:H:1212:THR:HG22 | 1.75 | 0.51 |
| 2:G:777:TRP:CZ3 | 2:G:1209:GLY:HA3 | 2.46 | 0.51 |
| 1:B:95:PHE:HD1 | 1:B:100:LEU:HD12 | 1.75 | 0.50 |
| 1:C:272:PRO:HD3 | 1:C:311:TRP:CZ2 | 2.46 | 0.50 |
| 2:E:1482:SER:OG | 3:E:2004:ATP:O3A | 2.26 | 0.50 |
| 2:H:1351:VAL:HG22 | 2:H:1361:LEU:HB3 | 1.91 | 0.50 |
| 2:H:1478:GLY:HA3 | 2:H:1486:ARG:HD3 | 1.94 | 0.50 |
| 2:G:104:LEU:HD23 | 2:G:104:LEU:H | 1.76 | 0.50 |
| 2:F:42:ILE:HG23 | 2:F:43:THR:HG23 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1451:TRP:CE3 | 2:F:1460:LYS:HG3 | 2.46 | 0.50 |
| 2:F:1556:ILE:HG21 | 2:F:1559:PHE:HB3 | 1.91 | 0.50 |
| 1:C:66:LEU:O | 1:C:170:LYS:NZ | 2.32 | 0.50 |
| 2:H:511:LEU:HD22 | 2:H:1392:PHE:HD2 | 1.76 | 0.50 |
| 2:H:1556:ILE:HG21 | 2:H:1559:PHE:HB3 | 1.91 | 0.50 |
| 2:G:777:TRP:CH2 | 2:G:1209:GLY:HA3 | 2.46 | 0.50 |
| 1:A:344:CYS:SG | 1:A:349:LEU:HD22 | 2.51 | 0.50 |
| 1:C:95:PHE:HD1 | 1:C:100:LEU:HD12 | 1.75 | 0.50 |
| 2:E:1064:ALA:O | 2:E:1068:THR:HG23 | 2.12 | 0.50 |
| 2:H:1460:LYS:HG2 | 2:H:1464:LYS:HZ2 | 1.76 | 0.50 |
| 2:G:452:LEU:HD21 | 2:G:582:LEU:HD22 | 1.93 | 0.50 |
| 2:G:1478:GLY:HA3 | 2:G:1486:ARG:HD3 | 1.94 | 0.50 |
| 2:F:357:VAL:HA | 2:F:360:VAL:HG12 | 1.94 | 0.50 |
| 1:D:238:ILE:HD12 | 1:D:267:LEU:HD13 | 1.93 | 0.50 |
| 2:E:39:LEU:HD22 | 2:E:142:TYR:CE2 | 2.46 | 0.50 |
| 2:E:777:TRP:CZ3 | 2:E:1209:GLY:HA3 | 2.46 | 0.50 |
| 2:G:704:PRO:HB2 | 2:G:707:GLN:CG | 2.41 | 0.50 |
| 2:F:253:LEU:HD11 | 2:F:1231:ASP:HB3 | 1.93 | 0.50 |
| 2:F:1344:ILE:O | 2:F:1368:ILE:N | 2.29 | 0.50 |
| 1:B:344:CYS:SG | 1:B:349:LEU:HD22 | 2.51 | 0.50 |
| 1:C:275:LEU:HA | 1:C:306:ALA:HB1 | 1.94 | 0.50 |
| 2:E:777:TRP:CH2 | 2:E:1209:GLY:HA3 | 2.47 | 0.50 |
| 2:H:452:LEU:HD21 | 2:H:582:LEU:HD22 | 1.93 | 0.50 |
| 2:H:1451:TRP:CE3 | 2:H:1460:LYS:HG3 | 2.47 | 0.50 |
| 2:G:511:LEU:HD22 | 2:G:1392:PHE:HD2 | 1.76 | 0.50 |
| 2:F:1353:TYR:OH | 2:F:1386:SER:OG | 2.23 | 0.50 |
| 2:E:287:ILE:HD11 | 2:E:607:VAL:HG13 | 1.94 | 0.50 |
| 2:E:452:LEU:HD21 | 2:E:582:LEU:HD22 | 1.92 | 0.50 |
| 2:E:1408:ASP:OD1 | 2:E:1409:ILE:N | 2.40 | 0.50 |
| 2:H:287:ILE:HD11 | 2:H:607:VAL:HG13 | 1.94 | 0.50 |
| 2:F:39:LEU:HD22 | 2:F:142:TYR:CE2 | 2.46 | 0.50 |
| 2:F:1408:ASP:OD1 | 2:F:1409:ILE:N | 2.40 | 0.50 |
| 1:A:108:GLU:HB2 | 1:A:141:GLU:HG3 | 1.93 | 0.50 |
| 1:A:275:LEU:HA | 1:A:306:ALA:HB1 | 1.94 | 0.50 |
| 1:D:108:GLU:HB2 | 1:D:141:GLU:HG3 | 1.93 | 0.50 |
| 1:C:209:MET:O | 1:C:292:GLU:HB2 | 2.12 | 0.50 |
| 2:E:39:LEU:HA | 2:E:42:ILE:HG22 | 1.94 | 0.50 |
| 2:E:357:VAL:HA | 2:E:360:VAL:HG12 | 1.94 | 0.50 |
| 2:E:1478:GLY:HA3 | 2:E:1486:ARG:HD3 | 1.94 | 0.50 |
| 2:H:363:PHE:CD1 | 2:H:1260:LEU:HB2 | 2.47 | 0.50 |
| 2:H:777:TRP:CH2 | 2:H:1209:GLY:HA3 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:253:LEU:HD11 | 2:G:1231:ASP:HB3 | 1.93 | 0.50 |
| 2:G:1100:LEU:HD22 | 2:G:1314:ILE:HG23 | 1.94 | 0.50 |
| 2:F:777:TRP:CZ3 | 2:F:1209:GLY:HA3 | 2.46 | 0.50 |
| 1:A:238:ILE:HD12 | 1:A:267:LEU:HD13 | 1.93 | 0.50 |
| 1:D:95:PHE:HD1 | 1:D:100:LEU:HD12 | 1.76 | 0.50 |
| 1:B:66:LEU:O | 1:B:170:LYS:NZ | 2.32 | 0.50 |
| 2:E:382:GLU:OE2 | 2:E:386:ASN:ND2 | 2.37 | 0.50 |
| 2:E:704:PRO:HB2 | 2:E:707:GLN:CG | 2.41 | 0.50 |
| 2:G:357:VAL:HA | 2:G:360:VAL:HG12 | 1.93 | 0.50 |
| 2:F:39:LEU:HA | 2:F:42:ILE:HG22 | 1.94 | 0.50 |
| 2:F:1064:ALA:O | 2:F:1068:THR:HG23 | 2.12 | 0.50 |
| 1:A:187:ALA:O | 1:A:310:LEU:N | 2.45 | 0.50 |
| 2:H:141:VAL:O | 2:H:144:THR:OG1 | 2.21 | 0.50 |
| 2:H:686:PHE:HE2 | 2:H:699:ILE:HD11 | 1.77 | 0.50 |
| 2:H:1346:ILE:HD11 | 2:H:1364:VAL:HG22 | 1.94 | 0.50 |
| 2:G:42:ILE:HG23 | 2:G:43:THR:HG23 | 1.92 | 0.50 |
| 2:G:317:PRO:HG3 | 2:G:585:ILE:HD12 | 1.94 | 0.50 |
| 2:G:552:ILE:HA | 2:G:555:VAL:HG22 | 1.94 | 0.50 |
| 2:F:687:THR:HB | 2:F:694:PRO:HA | 1.94 | 0.50 |
| 2:F:1478:GLY:HA3 | 2:F:1486:ARG:HD3 | 1.94 | 0.50 |
| 1:D:60:PHE:O | 1:D:64:VAL:HG23 | 2.12 | 0.49 |
| 1:C:344:CYS:SG | 1:C:349:LEU:HD22 | 2.51 | 0.49 |
| 2:E:1346:ILE:HD11 | 2:E:1364:VAL:HG22 | 1.93 | 0.49 |
| 2:G:1064:ALA:O | 2:G:1068:THR:HG23 | 2.12 | 0.49 |
| 2:F:287:ILE:HD11 | 2:F:607:VAL:HG13 | 1.94 | 0.49 |
| 2:F:452:LEU:HD21 | 2:F:582:LEU:HD22 | 1.93 | 0.49 |
| 2:F:704:PRO:HB2 | 2:F:707:GLN:CG | 2.41 | 0.49 |
| 2:F:716:GLY:N | 3:F:2004:ATP:O3G | 2.33 | 0.49 |
| 1:D:220:VAL:HG12 | 1:D:235:GLN:HG2 | 1.94 | 0.49 |
| 1:D:275:LEU:HA | 1:D:306:ALA:HB1 | 1.93 | 0.49 |
| 1:B:72:LEU:O | 1:B:76:THR:HG23 | 2.13 | 0.49 |
| 1:C:60:PHE:O | 1:C:64:VAL:HG23 | 2.12 | 0.49 |
| 1:C:220:VAL:HG12 | 1:C:235:GLN:HG2 | 1.94 | 0.49 |
| 1:C:239:PRO:O | 1:C:259:HIS:ND1 | 2.34 | 0.49 |
| 2:H:39:LEU:HA | 2:H:42:ILE:HG22 | 1.94 | 0.49 |
| 2:H:39:LEU:HD22 | 2:H:142:TYR:CE2 | 2.46 | 0.49 |
| 2:H:1100:LEU:HD22 | 2:H:1314:ILE:HG23 | 1.94 | 0.49 |
| 2:G:686:PHE:HE2 | 2:G:699:ILE:HD11 | 1.77 | 0.49 |
| 2:G:687:THR:HB | 2:G:694:PRO:HA | 1.95 | 0.49 |
| 2:G:1451:TRP:CE3 | 2:G:1460:LYS:HG3 | 2.46 | 0.49 |
| 2:F:104:LEU:HD23 | 2:F:104:LEU:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:45:ALA:HB3 | 1:A:47:LYS:HZ2 | 1.76 | 0.49 |
| 1:C:238:ILE:HD12 | 1:C:267:LEU:HD13 | 1.93 | 0.49 |
| 2:E:686:PHE:HE2 | 2:E:699:ILE:HD11 | 1.77 | 0.49 |
| 2:E:1539:VAL:O | 2:E:1542:ILE:HG22 | 2.13 | 0.49 |
| 2:H:317:PRO:HG3 | 2:H:585:ILE:HD12 | 1.94 | 0.49 |
| 2:H:1064:ALA:O | 2:H:1068:THR:HG23 | 2.12 | 0.49 |
| 1:D:187:ALA:O | 1:D:310:LEU:N | 2.45 | 0.49 |
| 2:E:363:PHE:CD1 | 2:E:1260:LEU:HB2 | 2.47 | 0.49 |
| 2:H:104:LEU:HD23 | 2:H:104:LEU:H | 1.77 | 0.49 |
| 2:G:1415:HIS:O | 2:G:1419:SER:OG | 2.18 | 0.49 |
| 2:F:317:PRO:HG3 | 2:F:585:ILE:HD12 | 1.94 | 0.49 |
| 2:F:777:TRP:CH2 | 2:F:1209:GLY:HA3 | 2.47 | 0.49 |
| 1:A:60:PHE:O | 1:A:64:VAL:HG23 | 2.12 | 0.49 |
| 1:C:322:GLU:N | 1:C:325:ARG:O | 2.46 | 0.49 |
| 2:H:1151:SER:O | 2:H:1155:VAL:HG23 | 2.13 | 0.49 |
| 2:F:511:LEU:HD22 | 2:F:1392:PHE:HD2 | 1.76 | 0.49 |
| 2:F:1100:LEU:HD22 | 2:F:1314:ILE:HG23 | 1.94 | 0.49 |
| 2:F:1539:VAL:O | 2:F:1542:ILE:HG22 | 2.13 | 0.49 |
| 1:A:220:VAL:HG12 | 1:A:235:GLN:HG2 | 1.94 | 0.49 |
| 1:A:319:VAL:HB | 1:B:232:PRO:HG2 | 1.95 | 0.49 |
| 1:A:322:GLU:N | 1:A:325:ARG:O | 2.46 | 0.49 |
| 1:B:209:MET:O | 1:B:292:GLU:HB2 | 2.12 | 0.49 |
| 1:C:72:LEU:O | 1:C:76:THR:HG23 | 2.13 | 0.49 |
| 2:E:317:PRO:HG3 | 2:E:585:ILE:HD12 | 1.94 | 0.49 |
| 2:E:511:LEU:HD22 | 2:E:1392:PHE:HD2 | 1.76 | 0.49 |
| 2:E:778:LEU:HA | 2:E:841:ARG:NH1 | 2.28 | 0.49 |
| 2:H:381:ILE:HG21 | 2:H:1241:THR:HG21 | 1.95 | 0.49 |
| 1:D:322:GLU:N | 1:D:325:ARG:O | 2.46 | 0.49 |
| 1:B:187:ALA:O | 1:B:310:LEU:N | 2.45 | 0.49 |
| 1:B:238:ILE:HD12 | 1:B:267:LEU:HD13 | 1.93 | 0.49 |
| 1:C:272:PRO:O | 1:C:273:SER:OG | 2.27 | 0.49 |
| 2:E:1003:TYR:CE1 | 2:E:1092:VAL:HG11 | 2.48 | 0.49 |
| 2:E:1100:LEU:HD22 | 2:E:1314:ILE:HG23 | 1.94 | 0.49 |
| 2:E:1373:LYS:O | 2:E:1546:ASP:N | 2.31 | 0.49 |
| 2:G:363:PHE:CD1 | 2:G:1260:LEU:HB2 | 2.47 | 0.49 |
| 2:G:686:PHE:O | 2:G:695:THR:N | 2.46 | 0.49 |
| 2:F:363:PHE:CD1 | 2:F:1260:LEU:HB2 | 2.47 | 0.49 |
| 2:F:461:LEU:O | 2:F:463:GLY:N | 2.46 | 0.49 |
| 2:F:1066:VAL:O | 2:F:1069:VAL:HG12 | 2.13 | 0.49 |
| 1:C:113:SER:OG | 1:C:135:GLY:O | 2.29 | 0.49 |
| 1:C:209:MET:HE1 | 1:C:252:VAL:HG22 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:771:TYR:CD2 | 2:E:1212:THR:HG22 | 2.48 | 0.49 |
| 2:E:1151:SER:O | 2:E:1155:VAL:HG23 | 2.13 | 0.49 |
| 2:E:1392:PHE:HB3 | 2:E:1418:ARG:NE | 2.28 | 0.49 |
| 2:H:1381:GLY:HA2 | 4:H:2001:ADP:H5'2 | 1.94 | 0.49 |
| 2:G:381:ILE:HG21 | 2:G:1241:THR:HG21 | 1.95 | 0.49 |
| 2:G:1151:SER:O | 2:G:1155:VAL:HG23 | 2.13 | 0.49 |
| 2:G:1381:GLY:HA2 | 4:G:2001:ADP:H5'2 | 1.94 | 0.49 |
| 2:G:1460:LYS:HG2 | 2:G:1464:LYS:NZ | 2.28 | 0.49 |
| 2:F:552:ILE:HA | 2:F:555:VAL:HG22 | 1.94 | 0.49 |
| 1:A:72:LEU:O | 1:A:76:THR:HG23 | 2.13 | 0.49 |
| 1:B:112:THR:OG1 | 1:B:137:MET:N | 2.42 | 0.49 |
| 1:C:318:ILE:O | 1:C:329:ASP:N | 2.45 | 0.49 |
| 1:C:320:ALA:O | 1:C:327:SER:OG | 2.31 | 0.49 |
| 2:E:552:ILE:HA | 2:E:555:VAL:HG22 | 1.94 | 0.49 |
| 2:E:1478:GLY:O | 2:E:1486:ARG:NH2 | 2.46 | 0.49 |
| 2:H:1550:VAL:O | 2:H:1556:ILE:HA | 2.13 | 0.49 |
| 2:G:461:LEU:O | 2:G:463:GLY:N | 2.46 | 0.49 |
| 2:G:778:LEU:HD13 | 2:G:823:GLY:HA2 | 1.95 | 0.49 |
| 2:G:1460:LYS:HG2 | 2:G:1464:LYS:HZ2 | 1.77 | 0.49 |
| 2:F:382:GLU:OE2 | 2:F:386:ASN:ND2 | 2.37 | 0.49 |
| 2:F:1003:TYR:CE1 | 2:F:1092:VAL:HG11 | 2.48 | 0.49 |
| 2:F:1550:VAL:O | 2:F:1556:ILE:HA | 2.13 | 0.49 |
| 1:A:209:MET:O | 1:A:292:GLU:HB2 | 2.12 | 0.49 |
| 1:D:209:MET:O | 1:D:292:GLU:HB2 | 2.12 | 0.49 |
| 1:B:60:PHE:O | 1:B:64:VAL:HG23 | 2.12 | 0.49 |
| 2:E:686:PHE:O | 2:E:695:THR:N | 2.46 | 0.49 |
| 2:E:778:LEU:HD13 | 2:E:823:GLY:HA2 | 1.95 | 0.49 |
| 2:E:1381:GLY:HA2 | 4:E:2001:ADP:H5'2 | 1.94 | 0.49 |
| 2:H:1003:TYR:CE1 | 2:H:1092:VAL:HG11 | 2.48 | 0.49 |
| 2:G:778:LEU:HA | 2:G:841:ARG:NH1 | 2.28 | 0.49 |
| 2:G:1066:VAL:O | 2:G:1069:VAL:HG12 | 2.13 | 0.49 |
| 2:F:381:ILE:HG21 | 2:F:1241:THR:HG21 | 1.95 | 0.49 |
| 2:F:1451:TRP:HE3 | 2:F:1460:LYS:HG3 | 1.78 | 0.49 |
| 2:E:381:ILE:HG21 | 2:E:1241:THR:HG21 | 1.95 | 0.48 |
| 2:H:357:VAL:HA | 2:H:360:VAL:HG12 | 1.94 | 0.48 |
| 2:H:461:LEU:O | 2:H:463:GLY:N | 2.46 | 0.48 |
| 2:H:679:VAL:HG13 | 2:H:739:TRP:CD1 | 2.48 | 0.48 |
| 2:H:1392:PHE:HB3 | 2:H:1418:ARG:NE | 2.28 | 0.48 |
| 2:G:287:ILE:HD11 | 2:G:607:VAL:HG13 | 1.94 | 0.48 |
| 2:G:1266:SER:HB3 | 2:G:1280:VAL:HG13 | 1.95 | 0.48 |
| 2:G:1484:GLY:O | 2:G:1488:LEU:HD23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:320:ILE:O | 2:F:324:VAL:HG23 | 2.13 | 0.48 |
| 2:F:417:ILE:O | 2:F:420:LEU:HG | 2.13 | 0.48 |
| 1:A:129:VAL:O | 1:A:130:THR:OG1 | 2.23 | 0.48 |
| 1:B:220:VAL:HG12 | 1:B:235:GLN:HG2 | 1.94 | 0.48 |
| 1:B:322:GLU:N | 1:B:325:ARG:O | 2.46 | 0.48 |
| 1:C:187:ALA:O | 1:C:310:LEU:N | 2.45 | 0.48 |
| 2:H:774:GLN:NE2 | 3:H:2004:ATP:O2G | 2.47 | 0.48 |
| 2:H:1003:TYR:CZ | 2:H:1135:ILE:HG21 | 2.48 | 0.48 |
| 2:H:1451:TRP:HE3 | 2:H:1460:LYS:HG3 | 1.78 | 0.48 |
| 2:F:679:VAL:HG13 | 2:F:739:TRP:CD1 | 2.48 | 0.48 |
| 2:F:686:PHE:O | 2:F:695:THR:N | 2.46 | 0.48 |
| 2:F:1003:TYR:CZ | 2:F:1135:ILE:HG21 | 2.49 | 0.48 |
| 2:F:1151:SER:O | 2:F:1155:VAL:HG23 | 2.13 | 0.48 |
| 2:F:1346:ILE:HD11 | 2:F:1364:VAL:HG22 | 1.93 | 0.48 |
| 2:E:774:GLN:NE2 | 3:E:2004:ATP:O2G | 2.47 | 0.48 |
| 2:E:1451:TRP:HE3 | 2:E:1460:LYS:HG3 | 1.78 | 0.48 |
| 2:E:1460:LYS:HG2 | 2:E:1464:LYS:NZ | 2.28 | 0.48 |
| 2:G:39:LEU:HA | 2:G:42:ILE:HG22 | 1.94 | 0.48 |
| 2:G:774:GLN:NE2 | 3:G:2004:ATP:O2G | 2.46 | 0.48 |
| 2:G:1003:TYR:CE1 | 2:G:1092:VAL:HG11 | 2.48 | 0.48 |
| 2:G:1550:VAL:O | 2:G:1556:ILE:HA | 2.13 | 0.48 |
| 2:F:1029:ILE:HD12 | 2:F:1070:LEU:HB3 | 1.95 | 0.48 |
| 2:E:104:LEU:HD23 | 2:E:104:LEU:H | 1.77 | 0.48 |
| 2:E:461:LEU:O | 2:E:463:GLY:N | 2.46 | 0.48 |
| 2:E:679:VAL:HG13 | 2:E:739:TRP:CD1 | 2.48 | 0.48 |
| 2:E:687:THR:HB | 2:E:694:PRO:HA | 1.95 | 0.48 |
| 2:E:1029:ILE:HD12 | 2:E:1070:LEU:HB3 | 1.95 | 0.48 |
| 2:H:1094:LYS:HE2 | 2:H:1098:ARG:HH22 | 1.79 | 0.48 |
| 2:G:771:TYR:CD2 | 2:G:1212:THR:HG22 | 2.48 | 0.48 |
| 2:G:1451:TRP:HE3 | 2:G:1460:LYS:HG3 | 1.78 | 0.48 |
| 2:F:778:LEU:HA | 2:F:841:ARG:NH1 | 2.28 | 0.48 |
| 1:A:326:TYR:OH | 1:B:33:ALA:O | 2.22 | 0.48 |
| 1:D:72:LEU:O | 1:D:76:THR:HG23 | 2.13 | 0.48 |
| 2:H:314:PHE:CE2 | 2:H:447:VAL:HG12 | 2.49 | 0.48 |
| 2:H:687:THR:HB | 2:H:694:PRO:HA | 1.95 | 0.48 |
| 2:H:771:TYR:CD2 | 2:H:1212:THR:HG22 | 2.48 | 0.48 |
| 2:H:1373:LYS:O | 2:H:1546:ASP:N | 2.31 | 0.48 |
| 2:H:1478:GLY:O | 2:H:1486:ARG:NH2 | 2.46 | 0.48 |
| 2:G:1346:ILE:HD11 | 2:G:1364:VAL:HG22 | 1.93 | 0.48 |
| 2:F:686:PHE:HE2 | 2:F:699:ILE:HD11 | 1.77 | 0.48 |
| 2:F:1392:PHE:HB3 | 2:F:1418:ARG:NE | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:239:PRO:O | 1:B:259:HIS:ND1 | 2.34 | 0.48 |
| 2:E:218:LEU:HD23 | 2:E:219:GLN:N | 2.23 | 0.48 |
| 2:E:417:ILE:O | 2:E:420:LEU:HG | 2.13 | 0.48 |
| 2:E:1066:VAL:O | 2:E:1069:VAL:HG12 | 2.13 | 0.48 |
| 2:E:1468:GLY:O | 2:E:1471:ASP:HB2 | 2.14 | 0.48 |
| 2:H:782:THR:OG1 | 2:H:821:GLN:OE1 | 2.16 | 0.48 |
| 2:H:889:LYS:HB3 | 2:H:1538:ARG:HH12 | 1.78 | 0.48 |
| 2:H:1468:GLY:O | 2:H:1471:ASP:HB2 | 2.14 | 0.48 |
| 2:G:314:PHE:CE2 | 2:G:447:VAL:HG12 | 2.49 | 0.48 |
| 2:G:716:GLY:N | 3:G:2004:ATP:O3G | 2.33 | 0.48 |
| 2:G:1392:PHE:HB3 | 2:G:1418:ARG:NE | 2.28 | 0.48 |
| 2:F:771:TYR:CD2 | 2:F:1212:THR:HG22 | 2.48 | 0.48 |
| 2:F:1460:LYS:HG2 | 2:F:1464:LYS:NZ | 2.28 | 0.48 |
| 1:D:318:ILE:O | 1:D:329:ASP:N | 2.45 | 0.48 |
| 2:E:1292:ASN:HB3 | 2:E:1293:TYR:CD2 | 2.49 | 0.48 |
| 2:H:1222:PHE:HD1 | 2:H:1225:LYS:HD3 | 1.79 | 0.48 |
| 2:H:1266:SER:HB3 | 2:H:1280:VAL:HG13 | 1.95 | 0.48 |
| 2:H:1539:VAL:O | 2:H:1542:ILE:HG22 | 2.13 | 0.48 |
| 1:A:46:HIS:O | 1:D:328:VAL:O | 2.32 | 0.48 |
| 2:E:320:ILE:O | 2:E:324:VAL:HG23 | 2.13 | 0.48 |
| 2:E:1003:TYR:CZ | 2:E:1135:ILE:HG21 | 2.49 | 0.48 |
| 2:E:1415:HIS:O | 2:E:1419:SER:OG | 2.18 | 0.48 |
| 2:E:1550:VAL:O | 2:E:1556:ILE:HA | 2.13 | 0.48 |
| 2:H:598:ARG:HH12 | 2:H:1137:SER:HG | 1.61 | 0.48 |
| 2:H:686:PHE:O | 2:H:695:THR:N | 2.46 | 0.48 |
| 2:G:1003:TYR:CZ | 2:G:1135:ILE:HG21 | 2.48 | 0.48 |
| 2:G:1182:ARG:NH2 | 2:G:1186:ARG:HH21 | 2.12 | 0.48 |
| 2:G:1468:GLY:O | 2:G:1471:ASP:HB2 | 2.14 | 0.48 |
| 2:F:1381:GLY:HA2 | 4:F:2001:ADP:H5'2 | 1.94 | 0.48 |
| 2:E:680:GLN:HB2 | 2:E:701:ILE:O | 2.14 | 0.48 |
| 2:E:1484:GLY:O | 2:E:1488:LEU:HD23 | 2.14 | 0.48 |
| 2:H:552:ILE:HA | 2:H:555:VAL:HG22 | 1.94 | 0.48 |
| 2:G:417:ILE:O | 2:G:420:LEU:HG | 2.13 | 0.48 |
| 2:G:505:GLY:HA3 | 2:G:1429:VAL:HG11 | 1.96 | 0.48 |
| 2:G:1344:ILE:O | 2:G:1368:ILE:N | 2.29 | 0.48 |
| 2:G:1539:VAL:O | 2:G:1542:ILE:HG22 | 2.12 | 0.48 |
| 2:F:1478:GLY:O | 2:F:1486:ARG:NH2 | 2.47 | 0.48 |
| 1:A:38:LYS:NZ | 1:A:185:LYS:HG3 | 2.29 | 0.48 |
| 1:B:38:LYS:NZ | 1:B:185:LYS:HG3 | 2.29 | 0.48 |
| 2:H:273:GLN:O | 2:H:277:ASP:N | 2.39 | 0.48 |
| 2:H:320:ILE:O | 2:H:324:VAL:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1292:ASN:HB3 | 2:H:1293:TYR:CD2 | 2.49 | 0.48 |
| 2:H:1460:LYS:HG2 | 2:H:1464:LYS:NZ | 2.28 | 0.48 |
| 2:G:32:ASN:ND2 | 2:G:153:LYS:HD2 | 2.29 | 0.48 |
| 2:G:1222:PHE:HD1 | 2:G:1225:LYS:HD3 | 1.79 | 0.48 |
| 1:D:240:MET:HG2 | 1:D:247:ASN:HD22 | 1.79 | 0.47 |
| 1:B:171:THR:HG23 | 1:C:169:MET:CE | 2.44 | 0.47 |
| 2:G:1006:SER:HB2 | 2:G:1092:VAL:HG13 | 1.96 | 0.47 |
| 2:G:1292:ASN:HB3 | 2:G:1293:TYR:CD2 | 2.49 | 0.47 |
| 2:F:1032:TRP:CZ2 | 2:F:1063:TYR:HD1 | 2.32 | 0.47 |
| 2:F:1346:ILE:HG13 | 2:F:1365:ASN:HA | 1.96 | 0.47 |
| 2:F:1468:GLY:O | 2:F:1471:ASP:HB2 | 2.13 | 0.47 |
| 1:D:272:PRO:HB3 | 1:D:311:TRP:CE2 | 2.49 | 0.47 |
| 1:C:272:PRO:HB3 | 1:C:311:TRP:CE2 | 2.49 | 0.47 |
| 2:E:1094:LYS:HE2 | 2:E:1098:ARG:HH22 | 1.79 | 0.47 |
| 2:E:1266:SER:HB3 | 2:E:1280:VAL:HG13 | 1.95 | 0.47 |
| 2:E:1346:ILE:HG13 | 2:E:1365:ASN:HA | 1.96 | 0.47 |
| 2:H:455:ILE:O | 2:H:457:GLY:N | 2.47 | 0.47 |
| 2:H:680:GLN:HB2 | 2:H:701:ILE:O | 2.14 | 0.47 |
| 2:H:1032:TRP:CZ2 | 2:H:1063:TYR:HD1 | 2.32 | 0.47 |
| 2:G:320:ILE:O | 2:G:324:VAL:HG23 | 2.13 | 0.47 |
| 2:G:1036:TRP:HZ3 | 2:G:1063:TYR:HB2 | 1.80 | 0.47 |
| 2:G:1094:LYS:HE2 | 2:G:1098:ARG:HH22 | 1.79 | 0.47 |
| 2:G:1478:GLY:O | 2:G:1486:ARG:NH2 | 2.46 | 0.47 |
| 2:F:778:LEU:HD13 | 2:F:823:GLY:HA2 | 1.95 | 0.47 |
| 2:F:1036:TRP:CZ3 | 2:F:1063:TYR:HB2 | 2.49 | 0.47 |
| 2:F:1182:ARG:NH2 | 2:F:1186:ARG:HH21 | 2.12 | 0.47 |
| 2:F:1222:PHE:HD1 | 2:F:1225:LYS:HD3 | 1.79 | 0.47 |
| 1:A:122:LEU:HD21 | 1:B:146:ILE:HG12 | 1.97 | 0.47 |
| 1:D:209:MET:HE1 | 1:D:252:VAL:HG22 | 1.96 | 0.47 |
| 1:B:272:PRO:HB3 | 1:B:311:TRP:CE2 | 2.49 | 0.47 |
| 1:C:170:LYS:O | 1:C:173:GLN:HB2 | 2.15 | 0.47 |
| 2:E:455:ILE:O | 2:E:457:GLY:N | 2.48 | 0.47 |
| 2:E:1100:LEU:O | 2:E:1104:ILE:HG12 | 2.15 | 0.47 |
| 2:H:32:ASN:ND2 | 2:H:153:LYS:HD2 | 2.29 | 0.47 |
| 2:H:417:ILE:O | 2:H:420:LEU:HG | 2.13 | 0.47 |
| 2:H:778:LEU:HA | 2:H:841:ARG:NH1 | 2.28 | 0.47 |
| 2:H:1031:TYR:O | 2:H:1034:ALA:HB3 | 2.14 | 0.47 |
| 2:H:1100:LEU:O | 2:H:1104:ILE:HG12 | 2.15 | 0.47 |
| 2:H:1484:GLY:O | 2:H:1488:LEU:HD23 | 2.13 | 0.47 |
| 2:G:455:ILE:O | 2:G:457:GLY:N | 2.48 | 0.47 |
| 2:G:679:VAL:HG13 | 2:G:739:TRP:CD1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1029:ILE:HD12 | 2:G:1070:LEU:HB3 | 1.95 | 0.47 |
| 2:G:1036:TRP:CZ3 | 2:G:1063:TYR:HB2 | 2.49 | 0.47 |
| 2:F:1031:TYR:O | 2:F:1034:ALA:HB3 | 2.14 | 0.47 |
| 2:F:1266:SER:HB3 | 2:F:1280:VAL:HG13 | 1.95 | 0.47 |
| 2:E:314:PHE:CE2 | 2:E:447:VAL:HG12 | 2.49 | 0.47 |
| 2:E:889:LYS:HB3 | 2:E:1538:ARG:HH22 | 1.80 | 0.47 |
| 2:E:1511:ILE:HG22 | 2:E:1512:ASP:O | 2.15 | 0.47 |
| 2:H:505:GLY:HA3 | 2:H:1429:VAL:HG11 | 1.96 | 0.47 |
| 2:F:1292:ASN:HB3 | 2:F:1293:TYR:CD2 | 2.49 | 0.47 |
| 1:C:196:LEU:HD21 | 1:C:311:TRP:CH2 | 2.50 | 0.47 |
| 2:E:1031:TYR:O | 2:E:1034:ALA:HB3 | 2.15 | 0.47 |
| 2:H:1170:LEU:HD12 | 2:H:1254:ILE:HG23 | 1.97 | 0.47 |
| 2:G:889:LYS:HB3 | 2:G:1538:ARG:HH12 | 1.79 | 0.47 |
| 2:G:1170:LEU:HD12 | 2:G:1254:ILE:HG23 | 1.97 | 0.47 |
| 2:G:1482:SER:OG | 3:G:2004:ATP:O3A | 2.26 | 0.47 |
| 2:F:32:ASN:ND2 | 2:F:153:LYS:HD2 | 2.29 | 0.47 |
| 2:F:314:PHE:CE2 | 2:F:447:VAL:HG12 | 2.49 | 0.47 |
| 2:F:1094:LYS:HE2 | 2:F:1098:ARG:HH22 | 1.79 | 0.47 |
| 2:F:1484:GLY:O | 2:F:1488:LEU:HD23 | 2.14 | 0.47 |
| 1:D:38:LYS:NZ | 1:D:185:LYS:HG3 | 2.29 | 0.47 |
| 1:B:196:LEU:HD21 | 1:B:311:TRP:CH2 | 2.50 | 0.47 |
| 2:E:1006:SER:HB2 | 2:E:1092:VAL:HG13 | 1.97 | 0.47 |
| 2:E:1036:TRP:CZ3 | 2:E:1063:TYR:HB2 | 2.49 | 0.47 |
| 2:H:1006:SER:HB2 | 2:H:1092:VAL:HG13 | 1.97 | 0.47 |
| 2:H:1346:ILE:HG22 | 2:H:1402:ILE:HG13 | 1.97 | 0.47 |
| 2:H:1511:ILE:HG22 | 2:H:1512:ASP:O | 2.14 | 0.47 |
| 2:G:850:VAL:CG2 | 2:G:881:ARG:HE | 2.28 | 0.47 |
| 2:F:774:GLN:NE2 | 3:F:2004:ATP:O2G | 2.47 | 0.47 |
| 1:A:50:ARG:NH1 | 3:A:502:ATP:H2' | 2.30 | 0.47 |
| 1:A:121:PHE:CE2 | 1:B:150:ILE:HD11 | 2.48 | 0.47 |
| 1:A:272:PRO:HB3 | 1:A:311:TRP:CE2 | 2.49 | 0.47 |
| 1:D:320:ALA:O | 1:D:327:SER:OG | 2.31 | 0.47 |
| 1:B:170:LYS:O | 1:B:173:GLN:HB2 | 2.15 | 0.47 |
| 1:B:319:VAL:HB | 1:C:232:PRO:HG2 | 1.97 | 0.47 |
| 1:C:38:LYS:NZ | 1:C:185:LYS:HG3 | 2.29 | 0.47 |
| 1:C:53:GLY:C | 2:G:132:PHE:HZ | 2.18 | 0.47 |
| 1:C:240:MET:HG2 | 1:C:247:ASN:HD22 | 1.79 | 0.47 |
| 2:H:455:ILE:O | 2:H:458:VAL:N | 2.48 | 0.47 |
| 2:H:778:LEU:HD13 | 2:H:823:GLY:HA2 | 1.95 | 0.47 |
| 2:H:786:ASN:HB2 | 2:H:841:ARG:HH11 | 1.79 | 0.47 |
| 2:H:1036:TRP:CZ3 | 2:H:1063:TYR:HB2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1066:VAL:O | 2:H:1069:VAL:HG12 | 2.13 | 0.47 |
| 2:H:1182:ARG:NH2 | 2:H:1186:ARG:HH21 | 2.12 | 0.47 |
| 2:G:150:LYS:HG3 | 2:G:179:TYR:HE2 | 1.80 | 0.47 |
| 2:G:218:LEU:HD22 | 2:G:220:PRO:HD3 | 1.97 | 0.47 |
| 2:G:680:GLN:HB2 | 2:G:701:ILE:O | 2.14 | 0.47 |
| 2:G:1031:TYR:O | 2:G:1034:ALA:HB3 | 2.15 | 0.47 |
| 2:G:1032:TRP:CZ2 | 2:G:1063:TYR:HD1 | 2.32 | 0.47 |
| 2:F:273:GLN:O | 2:F:277:ASP:N | 2.39 | 0.47 |
| 2:F:455:ILE:O | 2:F:458:VAL:N | 2.48 | 0.47 |
| 2:F:496:LEU:O | 2:F:500:ASN:ND2 | 2.48 | 0.47 |
| 2:F:850:VAL:CG2 | 2:F:881:ARG:HE | 2.28 | 0.47 |
| 2:F:1511:ILE:HG22 | 2:F:1512:ASP:O | 2.14 | 0.47 |
| 2:E:889:LYS:HB3 | 2:E:1538:ARG:HH12 | 1.79 | 0.47 |
| 2:E:1032:TRP:CZ2 | 2:E:1063:TYR:HD1 | 2.32 | 0.47 |
| 2:E:1188:LEU:HD21 | 2:E:1239:PHE:HB3 | 1.96 | 0.47 |
| 2:H:1029:ILE:HD12 | 2:H:1070:LEU:HB3 | 1.95 | 0.47 |
| 2:F:1036:TRP:HZ3 | 2:F:1063:TYR:HB2 | 1.79 | 0.47 |
| 2:F:1100:LEU:O | 2:F:1104:ILE:HG12 | 2.15 | 0.47 |
| 1:A:165:GLY:HA2 | 1:D:168:PHE:HD1 | 1.79 | 0.47 |
| 1:A:240:MET:HG2 | 1:A:247:ASN:HD22 | 1.79 | 0.47 |
| 2:E:32:ASN:ND2 | 2:E:153:LYS:HD2 | 2.29 | 0.47 |
| 2:E:69:PRO:HG3 | 2:E:192:VAL:HG11 | 1.97 | 0.47 |
| 2:E:786:ASN:HB2 | 2:E:841:ARG:HH11 | 1.79 | 0.47 |
| 2:H:218:LEU:HD22 | 2:H:220:PRO:HD3 | 1.97 | 0.47 |
| 2:H:537:ALA:HA | 2:H:540:THR:HG22 | 1.97 | 0.47 |
| 2:H:1036:TRP:HZ3 | 2:H:1063:TYR:HB2 | 1.80 | 0.47 |
| 2:G:1011:LEU:HD21 | 2:G:1087:TRP:CE3 | 2.50 | 0.47 |
| 1:D:170:LYS:O | 1:D:173:GLN:HB2 | 2.15 | 0.47 |
| 2:H:850:VAL:CG2 | 2:H:881:ARG:HE | 2.28 | 0.47 |
| 2:H:1188:LEU:HD21 | 2:H:1239:PHE:HB3 | 1.96 | 0.47 |
| 2:G:434:LEU:HD22 | 2:G:596:VAL:HG22 | 1.97 | 0.47 |
| 2:G:786:ASN:HB2 | 2:G:841:ARG:HH11 | 1.79 | 0.47 |
| 2:F:218:LEU:HD22 | 2:F:220:PRO:HD3 | 1.97 | 0.47 |
| 1:A:277:HIS:O | 1:A:277:HIS:ND1 | 2.49 | 0.46 |
| 1:A:317:PRO:HB3 | 1:B:232:PRO:HD3 | 1.97 | 0.46 |
| 1:D:196:LEU:HD21 | 1:D:311:TRP:CH2 | 2.49 | 0.46 |
| 1:B:45:ALA:HB3 | 1:B:47:LYS:NZ | 2.31 | 0.46 |
| 2:E:782:THR:HG22 | 2:E:784:GLU:N | 2.30 | 0.46 |
| 2:E:1170:LEU:HD12 | 2:E:1254:ILE:HG23 | 1.97 | 0.46 |
| 2:H:496:LEU:O | 2:H:500:ASN:ND2 | 2.48 | 0.46 |
| 2:G:150:LYS:HG3 | 2:G:179:TYR:CE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1188:LEU:HD21 | 2:G:1239:PHE:HB3 | 1.96 | 0.46 |
| 2:F:69:PRO:HD2 | 2:F:189:VAL:HG23 | 1.98 | 0.46 |
| 2:F:680:GLN:HB2 | 2:F:701:ILE:O | 2.14 | 0.46 |
| 2:F:1006:SER:HB2 | 2:F:1092:VAL:HG13 | 1.97 | 0.46 |
| 2:E:218:LEU:HD22 | 2:E:220:PRO:HD3 | 1.97 | 0.46 |
| 2:E:505:GLY:HA3 | 2:E:1429:VAL:HG11 | 1.96 | 0.46 |
| 2:E:850:VAL:CG2 | 2:E:881:ARG:HE | 2.28 | 0.46 |
| 2:H:288:TRP:NE1 | 2:H:607:VAL:HG11 | 2.31 | 0.46 |
| 2:H:434:LEU:HD22 | 2:H:596:VAL:HG22 | 1.98 | 0.46 |
| 2:G:288:TRP:NE1 | 2:G:607:VAL:HG11 | 2.31 | 0.46 |
| 2:F:69:PRO:HG3 | 2:F:192:VAL:HG11 | 1.97 | 0.46 |
| 2:F:723:LEU:HD22 | 2:F:851:PHE:HE1 | 1.80 | 0.46 |
| 1:A:170:LYS:O | 1:A:173:GLN:HB2 | 2.15 | 0.46 |
| 1:D:45:ALA:HB3 | 1:D:47:LYS:NZ | 2.30 | 0.46 |
| 1:B:240:MET:HG2 | 1:B:247:ASN:HD22 | 1.79 | 0.46 |
| 2:G:782:THR:HG22 | 2:G:784:GLU:N | 2.30 | 0.46 |
| 2:F:434:LEU:HD22 | 2:F:596:VAL:HG22 | 1.98 | 0.46 |
| 2:F:455:ILE:O | 2:F:457:GLY:N | 2.48 | 0.46 |
| 2:F:786:ASN:HB2 | 2:F:841:ARG:HH11 | 1.79 | 0.46 |
| 2:F:1181:PHE:CD2 | 2:F:1247:LEU:HD22 | 2.50 | 0.46 |
| 1:B:37:SER:HB2 | 1:B:43:ASN:HD21 | 1.81 | 0.46 |
| 1:B:277:HIS:O | 1:B:277:HIS:ND1 | 2.49 | 0.46 |
| 1:C:45:ALA:HB3 | 1:C:47:LYS:NZ | 2.30 | 0.46 |
| 2:E:496:LEU:O | 2:E:500:ASN:ND2 | 2.48 | 0.46 |
| 2:E:537:ALA:HA | 2:E:540:THR:HG22 | 1.97 | 0.46 |
| 2:E:723:LEU:HD22 | 2:E:851:PHE:HE1 | 1.81 | 0.46 |
| 2:E:1222:PHE:HD1 | 2:E:1225:LYS:HD3 | 1.79 | 0.46 |
| 2:H:723:LEU:HD22 | 2:H:851:PHE:HE1 | 1.81 | 0.46 |
| 2:H:1338:TRP:HH2 | 2:H:1404:ILE:HB | 1.81 | 0.46 |
| 2:G:45:PRO:O | 2:G:49:ILE:HG23 | 2.16 | 0.46 |
| 2:G:69:PRO:HD2 | 2:G:189:VAL:HG23 | 1.98 | 0.46 |
| 2:G:409:MET:O | 2:G:1475:THR:HG21 | 2.16 | 0.46 |
| 2:G:1100:LEU:O | 2:G:1104:ILE:HG12 | 2.15 | 0.46 |
| 2:G:1346:ILE:HG13 | 2:G:1365:ASN:HA | 1.96 | 0.46 |
| 2:F:150:LYS:HG3 | 2:F:179:TYR:HE2 | 1.80 | 0.46 |
| 1:A:196:LEU:HD21 | 1:A:311:TRP:CH2 | 2.50 | 0.46 |
| 1:D:95:PHE:HE2 | 2:H:27:PHE:HA | 1.80 | 0.46 |
| 2:E:679:VAL:HG22 | 2:E:739:TRP:HD1 | 1.81 | 0.46 |
| 2:E:1072:SER:O | 2:E:1075:ILE:HG22 | 2.16 | 0.46 |
| 2:E:1338:TRP:HH2 | 2:E:1404:ILE:HB | 1.81 | 0.46 |
| 2:E:1346:ILE:HG22 | 2:E:1402:ILE:HG13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:218:LEU:HD23 | 2:H:219:GLN:N | 2.23 | 0.46 |
| 2:H:409:MET:O | 2:H:1475:THR:HG21 | 2.16 | 0.46 |
| 2:H:1066:VAL:HA | 2:H:1069:VAL:HG12 | 1.98 | 0.46 |
| 2:H:1181:PHE:CD2 | 2:H:1247:LEU:HD22 | 2.51 | 0.46 |
| 2:G:833:GLN:HG2 | 2:G:836:ARG:NH2 | 2.31 | 0.46 |
| 2:F:1147:LEU:HD22 | 2:F:1147:LEU:HA | 1.83 | 0.46 |
| 2:F:1188:LEU:HD21 | 2:F:1239:PHE:HB3 | 1.96 | 0.46 |
| 2:E:843:LEU:O | 2:E:881:ARG:NH2 | 2.41 | 0.46 |
| 2:E:1142:LEU:HD13 | 2:E:1304:MET:SD | 2.56 | 0.46 |
| 2:E:1182:ARG:NH2 | 2:E:1186:ARG:HH21 | 2.12 | 0.46 |
| 2:H:150:LYS:HG3 | 2:H:179:TYR:HE2 | 1.80 | 0.46 |
| 2:H:679:VAL:HG22 | 2:H:739:TRP:HD1 | 1.81 | 0.46 |
| 2:H:782:THR:HG22 | 2:H:784:GLU:N | 2.30 | 0.46 |
| 2:H:889:LYS:HB3 | 2:H:1538:ARG:HH22 | 1.80 | 0.46 |
| 2:H:1142:LEU:HD13 | 2:H:1304:MET:SD | 2.56 | 0.46 |
| 2:H:1346:ILE:HG13 | 2:H:1365:ASN:HA | 1.96 | 0.46 |
| 2:H:1403:ILE:HA | 2:H:1407:ILE:O | 2.16 | 0.46 |
| 2:G:889:LYS:HB3 | 2:G:1538:ARG:HH22 | 1.80 | 0.46 |
| 2:G:1403:ILE:HA | 2:G:1407:ILE:O | 2.16 | 0.46 |
| 2:G:1430:LEU:HD23 | 2:G:1474:ILE:HG21 | 1.98 | 0.46 |
| 2:G:1511:ILE:HG22 | 2:G:1512:ASP:O | 2.15 | 0.46 |
| 2:F:889:LYS:HB3 | 2:F:1538:ARG:HH22 | 1.80 | 0.46 |
| 2:F:889:LYS:HB3 | 2:F:1538:ARG:HH12 | 1.78 | 0.46 |
| 2:F:1072:SER:O | 2:F:1075:ILE:HG22 | 2.16 | 0.46 |
| 2:H:45:PRO:O | 2:H:49:ILE:HG23 | 2.16 | 0.46 |
| 2:H:833:GLN:HG2 | 2:H:836:ARG:NH2 | 2.31 | 0.46 |
| 2:G:455:ILE:O | 2:G:458:VAL:N | 2.48 | 0.46 |
| 2:G:678:CYS:HB2 | 2:G:703:ILE:O | 2.16 | 0.46 |
| 2:F:288:TRP:NE1 | 2:F:607:VAL:HG11 | 2.31 | 0.46 |
| 2:F:717:CYS:HB2 | 2:F:903:LYS:HA | 1.98 | 0.46 |
| 2:F:1011:LEU:HD21 | 2:F:1087:TRP:CE3 | 2.50 | 0.46 |
| 2:F:1170:LEU:HD12 | 2:F:1254:ILE:HG23 | 1.97 | 0.46 |
| 1:D:37:SER:HB2 | 1:D:43:ASN:HD21 | 1.81 | 0.46 |
| 2:E:45:PRO:O | 2:E:49:ILE:HG23 | 2.16 | 0.46 |
| 2:E:150:LYS:HG3 | 2:E:179:TYR:HE2 | 1.80 | 0.46 |
| 2:E:455:ILE:O | 2:E:458:VAL:N | 2.48 | 0.46 |
| 2:E:782:THR:OG1 | 2:E:821:GLN:OE1 | 2.16 | 0.46 |
| 2:E:1022:LYS:HE2 | 2:E:1078:CYS:HA | 1.97 | 0.46 |
| 2:H:717:CYS:HB2 | 2:H:903:LYS:HA | 1.98 | 0.46 |
| 2:G:496:LEU:O | 2:G:500:ASN:ND2 | 2.48 | 0.46 |
| 2:G:717:CYS:HB2 | 2:G:903:LYS:HA | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1142:LEU:HD13 | 2:F:1304:MET:SD | 2.56 | 0.46 |
| 1:B:318:ILE:O | 1:B:329:ASP:N | 2.45 | 0.46 |
| 1:C:37:SER:HB2 | 1:C:43:ASN:HD21 | 1.81 | 0.46 |
| 1:C:92:LEU:HD22 | 2:G:34:VAL:HG21 | 1.98 | 0.46 |
| 1:C:277:HIS:O | 1:C:277:HIS:ND1 | 2.49 | 0.46 |
| 2:E:69:PRO:HD2 | 2:E:189:VAL:HG23 | 1.97 | 0.46 |
| 2:E:434:LEU:HD22 | 2:E:596:VAL:HG22 | 1.98 | 0.46 |
| 2:E:833:GLN:HG2 | 2:E:836:ARG:NH2 | 2.31 | 0.46 |
| 2:H:1430:LEU:HD23 | 2:H:1474:ILE:HG21 | 1.98 | 0.46 |
| 2:F:505:GLY:HA3 | 2:F:1429:VAL:HG11 | 1.96 | 0.46 |
| 2:F:843:LEU:O | 2:F:881:ARG:NH2 | 2.41 | 0.46 |
| 2:E:555:VAL:HG12 | 2:E:583:PHE:CD2 | 2.50 | 0.46 |
| 2:E:717:CYS:HB2 | 2:E:903:LYS:HA | 1.98 | 0.46 |
| 2:E:1011:LEU:HD21 | 2:E:1087:TRP:CE3 | 2.50 | 0.46 |
| 2:E:1181:PHE:CD2 | 2:E:1247:LEU:HD22 | 2.51 | 0.46 |
| 2:E:1345:GLN:HA | 2:E:1366:ALA:O | 2.16 | 0.46 |
| 2:E:1349:LEU:HB3 | 2:E:1364:VAL:HG13 | 1.98 | 0.46 |
| 2:H:150:LYS:HG3 | 2:H:179:TYR:CE2 | 2.51 | 0.46 |
| 2:H:1022:LYS:HE2 | 2:H:1078:CYS:HA | 1.97 | 0.46 |
| 2:G:537:ALA:HA | 2:G:540:THR:HG22 | 1.97 | 0.46 |
| 2:G:1072:SER:O | 2:G:1075:ILE:HG22 | 2.16 | 0.46 |
| 2:G:1181:PHE:CD2 | 2:G:1247:LEU:HD22 | 2.50 | 0.46 |
| 2:F:85:LEU:HA | 2:F:85:LEU:HD13 | 1.82 | 0.46 |
| 2:F:150:LYS:HG3 | 2:F:179:TYR:CE2 | 2.51 | 0.46 |
| 2:F:782:THR:HG22 | 2:F:784:GLU:N | 2.30 | 0.46 |
| 2:F:1346:ILE:HG22 | 2:F:1402:ILE:HG13 | 1.97 | 0.46 |
| 1:A:232:PRO:HD3 | 1:D:317:PRO:HB3 | 1.98 | 0.45 |
| 1:D:277:HIS:O | 1:D:277:HIS:ND1 | 2.49 | 0.45 |
| 1:B:119:SER:OG | 1:C:140:GLU:OE2 | 2.27 | 0.45 |
| 1:C:143:PRO:HA | 1:C:146:ILE:HD12 | 1.98 | 0.45 |
| 1:C:263:ALA:HA | 1:C:268:TYR:CG | 2.51 | 0.45 |
| 1:C:272:PRO:HB3 | 1:C:311:TRP:CD1 | 2.52 | 0.45 |
| 2:H:1011:LEU:HD21 | 2:H:1087:TRP:CE3 | 2.50 | 0.45 |
| 2:H:1335:PRO:HD2 | 2:H:1338:TRP:CD1 | 2.52 | 0.45 |
| 2:G:1335:PRO:HD2 | 2:G:1338:TRP:CD1 | 2.52 | 0.45 |
| 2:F:679:VAL:HG22 | 2:F:739:TRP:HD1 | 1.81 | 0.45 |
| 2:F:1338:TRP:HH2 | 2:F:1404:ILE:HB | 1.81 | 0.45 |
| 1:A:89:ALA:O | 1:A:93:ILE:HG12 | 2.17 | 0.45 |
| 1:A:318:ILE:O | 1:A:329:ASP:N | 2.45 | 0.45 |
| 1:A:318:ILE:HA | 1:A:332:LYS:HZ1 | 1.80 | 0.45 |
| 1:D:272:PRO:HB3 | 1:D:311:TRP:CD1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:273:GLN:O | 2:E:277:ASP:N | 2.39 | 0.45 |
| 2:G:69:PRO:HG3 | 2:G:192:VAL:HG11 | 1.97 | 0.45 |
| 2:G:382:GLU:OE2 | 2:G:386:ASN:ND2 | 2.37 | 0.45 |
| 2:G:723:LEU:HD22 | 2:G:851:PHE:HE1 | 1.81 | 0.45 |
| 1:A:45:ALA:HB3 | 1:A:47:LYS:NZ | 2.31 | 0.45 |
| 1:A:332:LYS:HA | 1:A:335:ASN:OD1 | 2.16 | 0.45 |
| 1:D:229:GLU:HB3 | 1:C:314:ARG:NH1 | 2.31 | 0.45 |
| 1:D:263:ALA:HA | 1:D:268:TYR:CG | 2.51 | 0.45 |
| 2:H:1072:SER:O | 2:H:1075:ILE:HG22 | 2.16 | 0.45 |
| 2:H:1345:GLN:HA | 2:H:1366:ALA:O | 2.17 | 0.45 |
| 2:F:45:PRO:O | 2:F:49:ILE:HG23 | 2.16 | 0.45 |
| 2:F:409:MET:O | 2:F:1475:THR:HG21 | 2.16 | 0.45 |
| 2:F:678:CYS:HB2 | 2:F:703:ILE:O | 2.16 | 0.45 |
| 2:F:833:GLN:HG2 | 2:F:836:ARG:NH2 | 2.31 | 0.45 |
| 2:F:1347:GLN:HE21 | 2:F:1401:HIS:CE1 | 2.35 | 0.45 |
| 2:F:1403:ILE:HA | 2:F:1407:ILE:O | 2.16 | 0.45 |
| 1:A:183:PHE:CE1 | 1:A:202:VAL:HG23 | 2.52 | 0.45 |
| 2:E:1430:LEU:HD23 | 2:E:1474:ILE:HG21 | 1.98 | 0.45 |
| 2:E:1435:ILE:HB | 2:E:1470:LEU:HB2 | 1.99 | 0.45 |
| 2:H:1482:SER:OG | 3:H:2004:ATP:O3A | 2.26 | 0.45 |
| 2:G:1066:VAL:HA | 2:G:1069:VAL:HG12 | 1.98 | 0.45 |
| 2:G:1346:ILE:HG22 | 2:G:1402:ILE:HG13 | 1.97 | 0.45 |
| 2:F:28:VAL:O | 2:F:32:ASN:ND2 | 2.50 | 0.45 |
| 2:F:465:ALA:HA | 2:F:468:ILE:HD12 | 1.98 | 0.45 |
| 2:F:1335:PRO:HD2 | 2:F:1338:TRP:CD1 | 2.52 | 0.45 |
| 2:F:1430:LEU:HD23 | 2:F:1474:ILE:HG21 | 1.98 | 0.45 |
| 1:D:200:LEU:N | 1:D:257:ILE:O | 2.47 | 0.45 |
| 1:D:239:PRO:HB3 | 1:C:244:VAL:HG22 | 1.98 | 0.45 |
| 1:B:272:PRO:HB3 | 1:B:311:TRP:CD1 | 2.52 | 0.45 |
| 2:E:150:LYS:HG3 | 2:E:179:TYR:CE2 | 2.51 | 0.45 |
| 2:E:686:PHE:CD1 | 2:E:725:ALA:HB1 | 2.52 | 0.45 |
| 2:E:837:ILE:HG22 | 2:E:841:ARG:NH2 | 2.32 | 0.45 |
| 2:E:1036:TRP:HZ3 | 2:E:1063:TYR:HB2 | 1.80 | 0.45 |
| 2:E:1347:GLN:HE21 | 2:E:1401:HIS:CE1 | 2.35 | 0.45 |
| 2:H:69:PRO:HD2 | 2:H:189:VAL:HG23 | 1.98 | 0.45 |
| 2:G:680:GLN:OE1 | 2:G:702:ARG:NE | 2.50 | 0.45 |
| 2:G:837:ILE:HG22 | 2:G:841:ARG:NH2 | 2.32 | 0.45 |
| 2:G:1022:LYS:HE2 | 2:G:1078:CYS:HA | 1.97 | 0.45 |
| 2:G:1142:LEU:HD13 | 2:G:1304:MET:SD | 2.56 | 0.45 |
| 2:F:1431:PHE:O | 2:F:1438:ASN:ND2 | 2.35 | 0.45 |
| 1:A:263:ALA:HA | 1:A:268:TYR:CG | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:332:LYS:HA | 1:D:335:ASN:OD1 | 2.17 | 0.45 |
| 2:E:678:CYS:HB2 | 2:E:703:ILE:O | 2.16 | 0.45 |
| 2:H:28:VAL:O | 2:H:32:ASN:ND2 | 2.50 | 0.45 |
| 2:H:678:CYS:HB2 | 2:H:703:ILE:O | 2.16 | 0.45 |
| 2:G:555:VAL:HG12 | 2:G:583:PHE:CD2 | 2.50 | 0.45 |
| 2:F:1349:LEU:HB3 | 2:F:1364:VAL:HG13 | 1.98 | 0.45 |
| 1:D:183:PHE:CE1 | 1:D:202:VAL:HG23 | 2.52 | 0.45 |
| 1:B:89:ALA:O | 1:B:93:ILE:HG12 | 2.17 | 0.45 |
| 1:B:263:ALA:HA | 1:B:268:TYR:CG | 2.51 | 0.45 |
| 1:B:332:LYS:HA | 1:B:335:ASN:OD1 | 2.17 | 0.45 |
| 2:E:1359:PRO:HB3 | 2:E:1398:PHE:CZ | 2.52 | 0.45 |
| 2:H:720:SER:N | 3:H:2004:ATP:O2B | 2.35 | 0.45 |
| 2:F:298:ARG:HD2 | 2:F:383:THR:HG22 | 1.99 | 0.45 |
| 2:F:442:PRO:O | 2:F:446:ILE:HG12 | 2.17 | 0.45 |
| 1:A:37:SER:HB2 | 1:A:43:ASN:HD21 | 1.81 | 0.45 |
| 1:A:47:LYS:NZ | 1:D:327:SER:HA | 2.32 | 0.45 |
| 1:A:272:PRO:HB3 | 1:A:311:TRP:CD1 | 2.51 | 0.45 |
| 3:A:501:ATP:H2' | 1:B:50:ARG:NH1 | 2.31 | 0.45 |
| 1:D:89:ALA:O | 1:D:93:ILE:HG12 | 2.17 | 0.45 |
| 1:C:89:ALA:O | 1:C:93:ILE:HG12 | 2.17 | 0.45 |
| 1:C:332:LYS:HA | 1:C:335:ASN:OD1 | 2.17 | 0.45 |
| 2:E:288:TRP:NE1 | 2:E:607:VAL:HG11 | 2.31 | 0.45 |
| 2:E:1335:PRO:HD2 | 2:E:1338:TRP:CD1 | 2.52 | 0.45 |
| 2:H:686:PHE:CD1 | 2:H:725:ALA:HB1 | 2.52 | 0.45 |
| 2:H:1359:PRO:HB3 | 2:H:1398:PHE:CZ | 2.52 | 0.45 |
| 2:F:537:ALA:HA | 2:F:540:THR:HG22 | 1.97 | 0.45 |
| 2:F:686:PHE:CD1 | 2:F:725:ALA:HB1 | 2.52 | 0.45 |
| 1:B:92:LEU:HD22 | 2:F:34:VAL:HG21 | 1.99 | 0.45 |
| 2:E:409:MET:O | 2:E:1475:THR:HG21 | 2.16 | 0.45 |
| 2:E:680:GLN:OE1 | 2:E:702:ARG:NE | 2.50 | 0.45 |
| 2:H:69:PRO:HG3 | 2:H:192:VAL:HG11 | 1.97 | 0.45 |
| 2:H:442:PRO:O | 2:H:446:ILE:HG12 | 2.17 | 0.45 |
| 2:H:1335:PRO:HD2 | 2:H:1338:TRP:HD1 | 1.82 | 0.45 |
| 2:G:28:VAL:O | 2:G:32:ASN:ND2 | 2.50 | 0.45 |
| 2:G:218:LEU:HD23 | 2:G:219:GLN:N | 2.23 | 0.45 |
| 2:G:298:ARG:HD2 | 2:G:383:THR:HG22 | 1.98 | 0.45 |
| 2:G:1335:PRO:HD2 | 2:G:1338:TRP:HD1 | 1.82 | 0.45 |
| 2:G:1338:TRP:HH2 | 2:G:1404:ILE:HB | 1.81 | 0.45 |
| 2:G:1345:GLN:HA | 2:G:1366:ALA:O | 2.16 | 0.45 |
| 2:F:1022:LYS:HE2 | 2:F:1078:CYS:HA | 1.98 | 0.45 |
| 2:F:1066:VAL:HA | 2:F:1069:VAL:HG12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1345:GLN:HA | 2:F:1366:ALA:O | 2.17 | 0.45 |
| 1:B:143:PRO:HA | 1:B:146:ILE:HD12 | 1.98 | 0.45 |
| 1:B:183:PHE:CE1 | 1:B:202:VAL:HG23 | 2.52 | 0.45 |
| 1:B:200:LEU:N | 1:B:257:ILE:O | 2.47 | 0.45 |
| 2:E:28:VAL:O | 2:E:32:ASN:ND2 | 2.50 | 0.45 |
| 2:H:428:LEU:HD11 | 2:H:610:LEU:HD11 | 1.99 | 0.45 |
| 2:H:465:ALA:HA | 2:H:468:ILE:HD12 | 1.99 | 0.45 |
| 2:H:680:GLN:OE1 | 2:H:702:ARG:NE | 2.50 | 0.45 |
| 2:H:1106:LEU:HG | 2:H:1325:TYR:CE2 | 2.52 | 0.45 |
| 2:G:1269:ASN:OD1 | 2:G:1273:ARG:HB3 | 2.17 | 0.45 |
| 2:G:1347:GLN:HE21 | 2:G:1401:HIS:CE1 | 2.35 | 0.45 |
| 1:A:143:PRO:HA | 1:A:146:ILE:HD12 | 1.99 | 0.44 |
| 1:D:67:LYS:HD3 | 1:D:70:HIS:CE1 | 2.52 | 0.44 |
| 2:E:919:SER:O | 2:E:923:LEU:HB2 | 2.18 | 0.44 |
| 2:E:1403:ILE:HA | 2:E:1407:ILE:O | 2.16 | 0.44 |
| 2:E:1486:ARG:HA | 2:E:1489:PHE:HD2 | 1.82 | 0.44 |
| 2:H:457:GLY:O | 2:H:461:LEU:HD23 | 2.17 | 0.44 |
| 2:H:777:TRP:CG | 2:H:778:LEU:N | 2.86 | 0.44 |
| 2:G:131:ASN:O | 2:G:133:PRO:HD3 | 2.17 | 0.44 |
| 2:G:593:LEU:HA | 2:G:596:VAL:HB | 1.99 | 0.44 |
| 2:F:889:LYS:HB3 | 2:F:1538:ARG:NH1 | 2.32 | 0.44 |
| 2:F:1222:PHE:CD1 | 2:F:1225:LYS:HD3 | 2.53 | 0.44 |
| 1:B:67:LYS:HD3 | 1:B:70:HIS:CE1 | 2.52 | 0.44 |
| 1:B:218:GLN:N | 1:B:284:ILE:O | 2.51 | 0.44 |
| 2:E:298:ARG:HD2 | 2:E:383:THR:HG22 | 1.98 | 0.44 |
| 2:E:556:LEU:HD11 | 2:E:1068:THR:HG22 | 1.99 | 0.44 |
| 2:E:592:LEU:O | 2:E:596:VAL:HG23 | 2.18 | 0.44 |
| 2:E:1222:PHE:CD1 | 2:E:1225:LYS:HD3 | 2.52 | 0.44 |
| 2:E:1335:PRO:HD2 | 2:E:1338:TRP:HD1 | 1.83 | 0.44 |
| 2:G:85:LEU:HD13 | 2:G:85:LEU:HA | 1.82 | 0.44 |
| 2:G:442:PRO:O | 2:G:446:ILE:HG12 | 2.17 | 0.44 |
| 2:G:457:GLY:O | 2:G:461:LEU:HD23 | 2.17 | 0.44 |
| 2:G:777:TRP:CG | 2:G:778:LEU:N | 2.85 | 0.44 |
| 2:G:1106:LEU:HG | 2:G:1325:TYR:CE2 | 2.52 | 0.44 |
| 2:F:435:CYS:HG | 2:F:439:TRP:HZ3 | 1.64 | 0.44 |
| 2:F:1486:ARG:HA | 2:F:1489:PHE:HD2 | 1.82 | 0.44 |
| 1:A:67:LYS:HD3 | 1:A:70:HIS:CE1 | 2.52 | 0.44 |
| 1:D:143:PRO:HA | 1:D:146:ILE:HD12 | 1.98 | 0.44 |
| 1:D:319:VAL:HG22 | 1:D:328:VAL:HG22 | 1.99 | 0.44 |
| 2:E:123:TYR:O | 2:E:127:ILE:HG12 | 2.17 | 0.44 |
| 2:H:123:TYR:O | 2:H:127:ILE:HG12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:503:LEU:HD23 | 2:H:506:ILE:HD13 | 1.99 | 0.44 |
| 2:G:428:LEU:HD11 | 2:G:610:LEU:HD11 | 2.00 | 0.44 |
| 2:G:810:ASP:O | 2:G:813:ILE:HG22 | 2.18 | 0.44 |
| 2:G:1359:PRO:HB3 | 2:G:1398:PHE:CZ | 2.52 | 0.44 |
| 2:F:131:ASN:O | 2:F:133:PRO:HD3 | 2.17 | 0.44 |
| 2:F:556:LEU:HD11 | 2:F:1068:THR:HG22 | 1.99 | 0.44 |
| 1:D:276:HIS:O | 1:D:306:ALA:HB3 | 2.18 | 0.44 |
| 1:D:318:ILE:HB | 1:D:329:ASP:O | 2.18 | 0.44 |
| 1:C:45:ALA:HB3 | 1:C:47:LYS:HZ2 | 1.83 | 0.44 |
| 1:C:183:PHE:CE1 | 1:C:202:VAL:HG23 | 2.52 | 0.44 |
| 2:H:306:ARG:HB2 | 2:H:376:SER:OG | 2.18 | 0.44 |
| 2:H:776:PRO:HG2 | 2:H:834:ARG:NH1 | 2.32 | 0.44 |
| 2:H:1222:PHE:CD1 | 2:H:1225:LYS:HD3 | 2.52 | 0.44 |
| 2:G:1349:LEU:HB3 | 2:G:1364:VAL:HG13 | 1.98 | 0.44 |
| 2:F:123:TYR:O | 2:F:127:ILE:HG12 | 2.17 | 0.44 |
| 2:F:593:LEU:HA | 2:F:596:VAL:HB | 1.99 | 0.44 |
| 2:F:777:TRP:CG | 2:F:778:LEU:N | 2.85 | 0.44 |
| 2:F:1269:ASN:OD1 | 2:F:1273:ARG:HB3 | 2.17 | 0.44 |
| 2:F:1373:LYS:O | 2:F:1546:ASP:N | 2.31 | 0.44 |
| 1:C:67:LYS:HD3 | 1:C:70:HIS:CE1 | 2.52 | 0.44 |
| 2:E:131:ASN:O | 2:E:133:PRO:HD3 | 2.17 | 0.44 |
| 2:E:140:LEU:O | 2:E:144:THR:HG23 | 2.18 | 0.44 |
| 2:E:306:ARG:HB2 | 2:E:376:SER:OG | 2.18 | 0.44 |
| 2:E:810:ASP:O | 2:E:813:ILE:HG22 | 2.18 | 0.44 |
| 2:E:889:LYS:HB3 | 2:E:1538:ARG:NH1 | 2.33 | 0.44 |
| 2:E:1087:TRP:CE2 | 2:E:1091:LYS:HD2 | 2.53 | 0.44 |
| 2:E:1106:LEU:HG | 2:E:1325:TYR:CE2 | 2.52 | 0.44 |
| 2:H:810:ASP:O | 2:H:813:ILE:HG22 | 2.18 | 0.44 |
| 2:H:1347:GLN:HE21 | 2:H:1401:HIS:CE1 | 2.35 | 0.44 |
| 2:F:457:GLY:O | 2:F:461:LEU:HD23 | 2.17 | 0.44 |
| 2:F:776:PRO:HG2 | 2:F:834:ARG:NH1 | 2.32 | 0.44 |
| 2:F:837:ILE:HG22 | 2:F:841:ARG:NH2 | 2.32 | 0.44 |
| 2:F:1106:LEU:HG | 2:F:1325:TYR:CE2 | 2.52 | 0.44 |
| 2:G:776:PRO:HG2 | 2:G:834:ARG:NH1 | 2.32 | 0.44 |
| 2:G:782:THR:OG1 | 2:G:821:GLN:OE1 | 2.15 | 0.44 |
| 2:G:889:LYS:HB3 | 2:G:1538:ARG:NH1 | 2.33 | 0.44 |
| 2:G:1087:TRP:CE2 | 2:G:1091:LYS:HD2 | 2.53 | 0.44 |
| 2:F:1335:PRO:HD2 | 2:F:1338:TRP:HD1 | 1.82 | 0.44 |
| 1:A:276:HIS:O | 1:A:306:ALA:HB3 | 2.18 | 0.44 |
| 1:D:272:PRO:O | 1:D:273:SER:OG | 2.27 | 0.44 |
| 1:B:129:VAL:O | 1:B:130:THR:OG1 | 2.23 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:132:PHE:O | 2:E:134:LYS:N | 2.51 | 0.44 |
| 2:E:428:LEU:HD11 | 2:E:610:LEU:HD11 | 1.99 | 0.44 |
| 2:E:777:TRP:CG | 2:E:778:LEU:N | 2.86 | 0.44 |
| 2:H:370:ARG:CB | 2:H:1252:GLU:HG2 | 2.48 | 0.44 |
| 2:H:837:ILE:HG22 | 2:H:841:ARG:NH2 | 2.32 | 0.44 |
| 2:H:1191:LEU:HA | 2:H:1194:THR:HG22 | 2.00 | 0.44 |
| 2:H:1486:ARG:HA | 2:H:1489:PHE:HD2 | 1.82 | 0.44 |
| 2:G:148:ILE:O | 2:G:152:ILE:HG12 | 2.18 | 0.44 |
| 2:G:514:TRP:CZ3 | 2:G:1493:ARG:HD2 | 2.53 | 0.44 |
| 2:G:1123:ARG:HG2 | 2:G:1317:LEU:HD12 | 2.00 | 0.44 |
| 2:F:592:LEU:O | 2:F:596:VAL:HG23 | 2.18 | 0.44 |
| 1:A:113:SER:OG | 1:A:135:GLY:O | 2.30 | 0.44 |
| 2:E:544:ILE:HG23 | 2:E:1144:ARG:HH22 | 1.83 | 0.44 |
| 2:E:573:PRO:HB2 | 2:E:574:SER:H | 1.64 | 0.44 |
| 2:E:1191:LEU:HA | 2:E:1194:THR:HG22 | 2.00 | 0.44 |
| 2:E:1269:ASN:OD1 | 2:E:1273:ARG:HB3 | 2.17 | 0.44 |
| 2:H:132:PHE:O | 2:H:134:LYS:N | 2.51 | 0.44 |
| 2:H:544:ILE:HG23 | 2:H:1144:ARG:HH22 | 1.83 | 0.44 |
| 2:H:1123:ARG:HG2 | 2:H:1317:LEU:HD12 | 2.00 | 0.44 |
| 2:H:1435:ILE:HB | 2:H:1470:LEU:HB2 | 1.99 | 0.44 |
| 2:G:140:LEU:O | 2:G:144:THR:HG23 | 2.18 | 0.44 |
| 2:G:465:ALA:HA | 2:G:468:ILE:HD12 | 1.99 | 0.44 |
| 2:G:556:LEU:HD11 | 2:G:1068:THR:HG22 | 1.99 | 0.44 |
| 2:G:679:VAL:HG22 | 2:G:739:TRP:HD1 | 1.81 | 0.44 |
| 2:G:1222:PHE:CD1 | 2:G:1225:LYS:HD3 | 2.53 | 0.44 |
| 2:F:555:VAL:HG12 | 2:F:583:PHE:CD2 | 2.50 | 0.44 |
| 2:F:1177:ILE:HD11 | 2:F:1251:MET:SD | 2.58 | 0.44 |
| 2:F:1191:LEU:HA | 2:F:1194:THR:HG22 | 2.00 | 0.44 |
| 2:F:1434:THR:O | 2:F:1438:ASN:N | 2.39 | 0.44 |
| 1:D:66:LEU:HD21 | 1:D:70:HIS:HB2 | 2.00 | 0.44 |
| 1:B:113:SER:OG | 1:B:135:GLY:O | 2.30 | 0.44 |
| 1:C:276:HIS:O | 1:C:306:ALA:HB3 | 2.18 | 0.44 |
| 2:E:720:SER:N | 3:E:2004:ATP:O2B | 2.35 | 0.44 |
| 2:E:776:PRO:HG2 | 2:E:834:ARG:NH1 | 2.32 | 0.44 |
| 2:H:148:ILE:O | 2:H:152:ILE:HG12 | 2.18 | 0.44 |
| 2:H:555:VAL:HG12 | 2:H:583:PHE:CD2 | 2.50 | 0.44 |
| 2:G:123:TYR:O | 2:G:127:ILE:HG12 | 2.17 | 0.44 |
| 2:G:370:ARG:CB | 2:G:1252:GLU:HG2 | 2.48 | 0.44 |
| 2:G:783:VAL:HB | 2:G:818:ASP:O | 2.18 | 0.44 |
| 2:G:1191:LEU:HA | 2:G:1194:THR:HG22 | 2.00 | 0.44 |
| 2:G:1435:ILE:HB | 2:G:1470:LEU:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:132:PHE:O | 2:F:134:LYS:N | 2.51 | 0.44 |
| 2:F:306:ARG:HB2 | 2:F:376:SER:OG | 2.18 | 0.44 |
| 2:F:680:GLN:OE1 | 2:F:702:ARG:NE | 2.50 | 0.44 |
| 2:F:1081:THR:O | 2:F:1085:VAL:HG23 | 2.18 | 0.44 |
| 2:F:1123:ARG:HG2 | 2:F:1317:LEU:HD12 | 2.00 | 0.44 |
| 1:B:121:PHE:CE2 | 1:C:150:ILE:HD11 | 2.52 | 0.43 |
| 1:B:222:LYS:HG3 | 1:B:232:PRO:HA | 2.00 | 0.43 |
| 1:C:318:ILE:HB | 1:C:329:ASP:O | 2.18 | 0.43 |
| 2:E:6:CYS:HA | 2:E:103:HIS:HB2 | 2.00 | 0.43 |
| 2:E:370:ARG:CB | 2:E:1252:GLU:HG2 | 2.48 | 0.43 |
| 2:E:465:ALA:HA | 2:E:468:ILE:HD12 | 1.99 | 0.43 |
| 2:E:514:TRP:CZ3 | 2:E:1493:ARG:HD2 | 2.53 | 0.43 |
| 2:E:1066:VAL:HA | 2:E:1069:VAL:HG12 | 1.98 | 0.43 |
| 2:E:1123:ARG:HG2 | 2:E:1317:LEU:HD12 | 2.00 | 0.43 |
| 2:H:550:ILE:N | 2:H:551:PRO:HD2 | 2.33 | 0.43 |
| 2:H:593:LEU:HA | 2:H:596:VAL:HB | 1.99 | 0.43 |
| 2:G:1081:THR:O | 2:G:1085:VAL:HG23 | 2.18 | 0.43 |
| 2:F:140:LEU:O | 2:F:144:THR:HG23 | 2.18 | 0.43 |
| 2:F:148:ILE:O | 2:F:152:ILE:HG12 | 2.18 | 0.43 |
| 2:F:428:LEU:HD11 | 2:F:610:LEU:HD11 | 2.00 | 0.43 |
| 2:F:783:VAL:HB | 2:F:818:ASP:O | 2.18 | 0.43 |
| 2:F:1087:TRP:CE2 | 2:F:1091:LYS:HD2 | 2.53 | 0.43 |
| 2:F:1359:PRO:HB3 | 2:F:1398:PHE:CZ | 2.52 | 0.43 |
| 1:D:218:GLN:N | 1:D:284:ILE:O | 2.50 | 0.43 |
| 1:D:318:ILE:HA | 1:D:332:LYS:HZ1 | 1.83 | 0.43 |
| 1:B:94:ALA:CB | 1:B:114:ILE:HD11 | 2.48 | 0.43 |
| 1:B:319:VAL:HG22 | 1:B:328:VAL:HG22 | 1.99 | 0.43 |
| 1:C:318:ILE:HA | 1:C:332:LYS:HZ2 | 1.84 | 0.43 |
| 2:H:327:LEU:HD22 | 2:H:1277:ALA:HB2 | 2.01 | 0.43 |
| 2:H:556:LEU:HD11 | 2:H:1068:THR:HG22 | 1.99 | 0.43 |
| 2:H:919:SER:O | 2:H:923:LEU:HB2 | 2.18 | 0.43 |
| 2:H:1087:TRP:CE2 | 2:H:1091:LYS:HD2 | 2.53 | 0.43 |
| 2:G:6:CYS:HA | 2:G:103:HIS:HB2 | 2.01 | 0.43 |
| 2:G:306:ARG:HB2 | 2:G:376:SER:OG | 2.18 | 0.43 |
| 2:G:592:LEU:O | 2:G:596:VAL:HG23 | 2.17 | 0.43 |
| 2:G:686:PHE:CD1 | 2:G:725:ALA:HB1 | 2.52 | 0.43 |
| 2:G:1031:TYR:HA | 2:G:1282:LEU:CD1 | 2.45 | 0.43 |
| 2:G:1177:ILE:HD11 | 2:G:1251:MET:SD | 2.58 | 0.43 |
| 1:A:94:ALA:CB | 1:A:114:ILE:HD11 | 2.49 | 0.43 |
| 1:A:177:ARG:HH21 | 1:A:204:ASP:CG | 2.22 | 0.43 |
| 1:A:318:ILE:HB | 1:A:329:ASP:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:131:ILE:HG12 | 1:C:130:THR:HA | 2.01 | 0.43 |
| 2:E:148:ILE:O | 2:E:152:ILE:HG12 | 2.18 | 0.43 |
| 2:E:550:ILE:N | 2:E:551:PRO:HD2 | 2.33 | 0.43 |
| 2:E:593:LEU:HA | 2:E:596:VAL:HB | 1.99 | 0.43 |
| 2:H:131:ASN:O | 2:H:133:PRO:HD3 | 2.17 | 0.43 |
| 2:H:1081:THR:O | 2:H:1085:VAL:HG23 | 2.18 | 0.43 |
| 2:H:1177:ILE:HD11 | 2:H:1251:MET:SD | 2.58 | 0.43 |
| 2:H:1269:ASN:OD1 | 2:H:1273:ARG:HB3 | 2.17 | 0.43 |
| 2:G:132:PHE:O | 2:G:134:LYS:N | 2.51 | 0.43 |
| 2:G:309:ALA:HB1 | 2:G:369:GLN:OE1 | 2.18 | 0.43 |
| 2:G:1413:PRO:HB2 | 2:G:1416:THR:HG23 | 2.01 | 0.43 |
| 2:F:919:SER:O | 2:F:923:LEU:HB2 | 2.18 | 0.43 |
| 1:A:222:LYS:HG3 | 1:A:232:PRO:HA | 2.00 | 0.43 |
| 1:A:319:VAL:HG22 | 1:A:328:VAL:HG22 | 2.00 | 0.43 |
| 1:B:177:ARG:HH21 | 1:B:204:ASP:CG | 2.22 | 0.43 |
| 1:C:66:LEU:HD21 | 1:C:70:HIS:HB2 | 2.00 | 0.43 |
| 2:E:108:MET:N | 2:E:109:PRO:HD2 | 2.33 | 0.43 |
| 2:E:783:VAL:HB | 2:E:818:ASP:O | 2.18 | 0.43 |
| 2:E:1081:THR:O | 2:E:1085:VAL:HG23 | 2.18 | 0.43 |
| 2:E:1177:ILE:HD11 | 2:E:1251:MET:SD | 2.58 | 0.43 |
| 2:E:1350:SER:HA | 2:E:1361:LEU:O | 2.19 | 0.43 |
| 2:H:368:LEU:HA | 2:H:371:THR:HG22 | 2.01 | 0.43 |
| 2:H:508:LEU:HD22 | 2:H:1431:PHE:CZ | 2.51 | 0.43 |
| 2:F:544:ILE:HG23 | 2:F:1144:ARG:HH22 | 1.83 | 0.43 |
| 2:F:873:LEU:O | 2:F:877:ARG:HB2 | 2.18 | 0.43 |
| 1:A:239:PRO:O | 1:A:259:HIS:ND1 | 2.34 | 0.43 |
| 1:A:320:ALA:O | 1:A:327:SER:OG | 2.31 | 0.43 |
| 1:B:272:PRO:O | 1:B:273:SER:OG | 2.27 | 0.43 |
| 1:C:94:ALA:CB | 1:C:114:ILE:HD11 | 2.48 | 0.43 |
| 2:E:309:ALA:HB1 | 2:E:369:GLN:OE1 | 2.19 | 0.43 |
| 2:E:327:LEU:HD23 | 2:E:327:LEU:O | 2.19 | 0.43 |
| 2:E:442:PRO:O | 2:E:446:ILE:HG12 | 2.17 | 0.43 |
| 2:H:140:LEU:O | 2:H:144:THR:HG23 | 2.18 | 0.43 |
| 2:G:708:LEU:HB2 | 2:G:876:LEU:HD21 | 2.01 | 0.43 |
| 2:G:1223:GLN:O | 2:G:1227:LEU:HD13 | 2.19 | 0.43 |
| 2:G:1486:ARG:HA | 2:G:1489:PHE:HD2 | 1.82 | 0.43 |
| 2:F:6:CYS:HA | 2:F:103:HIS:HB2 | 2.01 | 0.43 |
| 2:F:108:MET:N | 2:F:109:PRO:HD2 | 2.33 | 0.43 |
| 2:F:503:LEU:HD23 | 2:F:506:ILE:HD13 | 1.99 | 0.43 |
| 2:F:708:LEU:HB2 | 2:F:876:LEU:HD21 | 2.01 | 0.43 |
| 2:F:802:ILE:O | 2:F:806:SER:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:889:LYS:HB3 | 2:F:1538:ARG:NH2 | 2.34 | 0.43 |
| 2:F:1350:SER:HA | 2:F:1361:LEU:O | 2.19 | 0.43 |
| 1:A:50:ARG:HB2 | 3:A:502:ATP:C5 | 2.53 | 0.43 |
| 1:A:50:ARG:NH1 | 3:A:502:ATP:O2B | 2.48 | 0.43 |
| 1:A:66:LEU:HD21 | 1:A:70:HIS:HB2 | 2.00 | 0.43 |
| 1:C:177:ARG:HH21 | 1:C:204:ASP:CG | 2.22 | 0.43 |
| 2:E:368:LEU:HA | 2:E:371:THR:HG22 | 2.01 | 0.43 |
| 2:E:802:ILE:O | 2:E:806:SER:N | 2.52 | 0.43 |
| 2:E:1223:GLN:O | 2:E:1227:LEU:HD13 | 2.19 | 0.43 |
| 2:H:6:CYS:HA | 2:H:103:HIS:HB2 | 2.00 | 0.43 |
| 2:H:139:LEU:O | 2:H:143:TRP:HD1 | 2.02 | 0.43 |
| 2:H:298:ARG:HD2 | 2:H:383:THR:HG22 | 1.98 | 0.43 |
| 2:H:514:TRP:CZ3 | 2:H:1493:ARG:HD2 | 2.53 | 0.43 |
| 2:H:573:PRO:HB2 | 2:H:574:SER:H | 1.64 | 0.43 |
| 2:H:592:LEU:O | 2:H:596:VAL:HG23 | 2.18 | 0.43 |
| 2:H:783:VAL:HB | 2:H:818:ASP:O | 2.18 | 0.43 |
| 2:H:1223:GLN:O | 2:H:1227:LEU:HD13 | 2.19 | 0.43 |
| 2:H:1349:LEU:HB3 | 2:H:1364:VAL:HG13 | 1.99 | 0.43 |
| 1:A:299:GLN:O | 1:A:301:ARG:NH1 | 2.52 | 0.43 |
| 1:D:224:THR:HG22 | 1:D:225:SER:O | 2.19 | 0.43 |
| 1:B:276:HIS:O | 1:B:306:ALA:HB3 | 2.18 | 0.43 |
| 2:E:327:LEU:HD22 | 2:E:1277:ALA:HB2 | 2.01 | 0.43 |
| 2:E:575:VAL:HG23 | 2:E:576:ALA:N | 2.34 | 0.43 |
| 2:E:868:MET:HG3 | 2:E:872:ILE:HG13 | 2.01 | 0.43 |
| 2:G:553:ALA:O | 2:G:557:ILE:HG12 | 2.19 | 0.43 |
| 2:G:575:VAL:HG23 | 2:G:576:ALA:N | 2.34 | 0.43 |
| 2:G:1064:ALA:O | 2:G:1067:PHE:HB3 | 2.19 | 0.43 |
| 2:F:370:ARG:CB | 2:F:1252:GLU:HG2 | 2.48 | 0.43 |
| 2:F:810:ASP:O | 2:F:813:ILE:HG22 | 2.18 | 0.43 |
| 2:F:1223:GLN:O | 2:F:1227:LEU:HD13 | 2.18 | 0.43 |
| 1:B:168:PHE:CZ | 1:C:168:PHE:CD2 | 3.07 | 0.43 |
| 1:C:35:PHE:CE1 | 1:C:233:LEU:HD13 | 2.54 | 0.43 |
| 1:C:319:VAL:HG22 | 1:C:328:VAL:HG22 | 2.00 | 0.43 |
| 2:E:68:PHE:N | 2:E:69:PRO:CD | 2.82 | 0.43 |
| 2:E:139:LEU:O | 2:E:143:TRP:HD1 | 2.02 | 0.43 |
| 2:E:173:GLY:O | 2:E:177:ILE:HG12 | 2.19 | 0.43 |
| 2:E:457:GLY:O | 2:E:461:LEU:HD23 | 2.18 | 0.43 |
| 2:E:470:LEU:HD13 | 2:E:550:ILE:HG21 | 2.01 | 0.43 |
| 2:E:1166:ALA:O | 2:E:1169:PRO:HD2 | 2.19 | 0.43 |
| 2:H:108:MET:N | 2:H:109:PRO:HD2 | 2.33 | 0.43 |
| 2:H:238:LYS:HA | 2:H:1180:TYR:OH | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:366:LEU:HA | 2:H:369:GLN:HB3 | 2.00 | 0.43 |
| 2:H:553:ALA:O | 2:H:557:ILE:HG12 | 2.19 | 0.43 |
| 2:H:1245:ARG:NE | 2:H:1245:ARG:HA | 2.34 | 0.43 |
| 2:G:108:MET:N | 2:G:109:PRO:HD2 | 2.33 | 0.43 |
| 2:G:327:LEU:HD23 | 2:G:327:LEU:O | 2.19 | 0.43 |
| 2:G:544:ILE:HG23 | 2:G:1144:ARG:HH22 | 1.83 | 0.43 |
| 2:F:309:ALA:HB1 | 2:F:369:GLN:OE1 | 2.18 | 0.43 |
| 2:F:514:TRP:CZ3 | 2:F:1493:ARG:HD2 | 2.53 | 0.43 |
| 2:F:1166:ALA:O | 2:F:1169:PRO:HD2 | 2.19 | 0.43 |
| 1:D:239:PRO:O | 1:D:259:HIS:ND1 | 2.34 | 0.43 |
| 1:B:157:LEU:HA | 1:B:157:LEU:HD23 | 1.85 | 0.43 |
| 1:B:224:THR:HG22 | 1:B:225:SER:O | 2.19 | 0.43 |
| 1:B:318:ILE:HB | 1:B:329:ASP:O | 2.18 | 0.43 |
| 1:C:224:THR:HG22 | 1:C:225:SER:O | 2.19 | 0.43 |
| 2:E:708:LEU:HB2 | 2:E:876:LEU:HD21 | 2.01 | 0.43 |
| 2:H:327:LEU:HD23 | 2:H:327:LEU:O | 2.19 | 0.43 |
| 2:H:889:LYS:HB3 | 2:H:1538:ARG:NH1 | 2.33 | 0.43 |
| 2:G:245:ILE:N | 2:G:1187:ASP:OD2 | 2.52 | 0.43 |
| 2:G:253:LEU:HD21 | 2:G:1231:ASP:CG | 2.39 | 0.43 |
| 2:G:720:SER:N | 3:G:2004:ATP:O2B | 2.35 | 0.43 |
| 2:G:802:ILE:O | 2:G:806:SER:N | 2.52 | 0.43 |
| 2:G:873:LEU:O | 2:G:877:ARG:HB2 | 2.18 | 0.43 |
| 2:G:919:SER:O | 2:G:923:LEU:HB2 | 2.17 | 0.43 |
| 2:G:1092:VAL:O | 2:G:1096:LEU:HG | 2.19 | 0.43 |
| 2:F:253:LEU:HD21 | 2:F:1231:ASP:CG | 2.39 | 0.43 |
| 2:F:550:ILE:N | 2:F:551:PRO:HD2 | 2.33 | 0.43 |
| 2:F:892:TYR:HD1 | 2:F:895:HIS:ND1 | 2.17 | 0.43 |
| 1:D:35:PHE:CE1 | 1:D:233:LEU:HD13 | 2.54 | 0.43 |
| 1:D:299:GLN:O | 1:D:301:ARG:NH1 | 2.52 | 0.43 |
| 2:E:553:ALA:O | 2:E:557:ILE:HG12 | 2.19 | 0.43 |
| 2:E:911:GLY:HA3 | 2:E:915:ASP:OD2 | 2.19 | 0.43 |
| 2:H:174:LEU:HD13 | 2:H:178:LEU:HD13 | 2.01 | 0.43 |
| 2:H:575:VAL:HG23 | 2:H:576:ALA:N | 2.34 | 0.43 |
| 2:H:802:ILE:O | 2:H:806:SER:N | 2.52 | 0.43 |
| 2:H:892:TYR:HD1 | 2:H:895:HIS:ND1 | 2.17 | 0.43 |
| 2:H:1032:TRP:CD1 | 2:H:1035:LYS:HD3 | 2.54 | 0.43 |
| 2:G:327:LEU:HD22 | 2:G:1277:ALA:HB2 | 2.01 | 0.43 |
| 2:G:366:LEU:HA | 2:G:369:GLN:HB3 | 2.01 | 0.43 |
| 2:G:487:SER:HA | 2:G:490:GLU:HG2 | 2.01 | 0.43 |
| 2:G:892:TYR:HD1 | 2:G:895:HIS:ND1 | 2.17 | 0.43 |
| 2:G:1123:ARG:HE | 2:G:1317:LEU:HD11 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:1350:SER:HA | 2:G:1361:LEU:O | 2.19 | 0.43 |
| 2:F:139:LEU:O | 2:F:143:TRP:HD1 | 2.02 | 0.43 |
| 2:F:366:LEU:HA | 2:F:369:GLN:HB3 | 2.00 | 0.43 |
| 2:F:508:LEU:HD22 | 2:F:1431:PHE:CZ | 2.51 | 0.43 |
| 2:F:553:ALA:O | 2:F:557:ILE:HG12 | 2.19 | 0.43 |
| 2:F:1032:TRP:CD1 | 2:F:1035:LYS:HD3 | 2.54 | 0.43 |
| 2:F:1123:ARG:HE | 2:F:1317:LEU:HD11 | 1.84 | 0.43 |
| 1:A:65:ASP:HB2 | 1:D:293:THR:HG22 | 2.00 | 0.42 |
| 1:A:218:GLN:N | 1:A:284:ILE:O | 2.51 | 0.42 |
| 1:D:268:TYR:OH | 1:D:350:ASP:OD2 | 2.22 | 0.42 |
| 1:B:35:PHE:CE1 | 1:B:233:LEU:HD13 | 2.54 | 0.42 |
| 2:E:205:LYS:O | 2:E:207:PRO:HD3 | 2.19 | 0.42 |
| 2:E:1092:VAL:O | 2:E:1096:LEU:HG | 2.19 | 0.42 |
| 2:E:1350:SER:HA | 2:E:1362:LYS:HA | 2.01 | 0.42 |
| 2:H:309:ALA:HB1 | 2:H:369:GLN:OE1 | 2.18 | 0.42 |
| 2:H:1166:ALA:O | 2:H:1169:PRO:HD2 | 2.19 | 0.42 |
| 2:H:1413:PRO:HB2 | 2:H:1416:THR:HG23 | 2.01 | 0.42 |
| 2:G:174:LEU:HD13 | 2:G:178:LEU:HD13 | 2.01 | 0.42 |
| 2:G:868:MET:HG3 | 2:G:872:ILE:HG13 | 2.01 | 0.42 |
| 2:G:1166:ALA:O | 2:G:1169:PRO:HD2 | 2.19 | 0.42 |
| 2:F:470:LEU:HD13 | 2:F:550:ILE:HG21 | 2.01 | 0.42 |
| 2:F:685:TYR:CD1 | 2:F:697:SER:HA | 2.55 | 0.42 |
| 2:F:1245:ARG:NE | 2:F:1245:ARG:HA | 2.34 | 0.42 |
| 2:E:174:LEU:HD13 | 2:E:178:LEU:HD13 | 2.01 | 0.42 |
| 2:E:253:LEU:HD21 | 2:E:1231:ASP:CG | 2.39 | 0.42 |
| 2:E:892:TYR:HD1 | 2:E:895:HIS:ND1 | 2.17 | 0.42 |
| 2:E:1031:TYR:HA | 2:E:1282:LEU:CD1 | 2.45 | 0.42 |
| 2:E:1123:ARG:HE | 2:E:1317:LEU:HD11 | 1.84 | 0.42 |
| 2:H:173:GLY:O | 2:H:177:ILE:HG12 | 2.19 | 0.42 |
| 2:H:889:LYS:HB3 | 2:H:1538:ARG:NH2 | 2.34 | 0.42 |
| 2:H:1092:VAL:O | 2:H:1096:LEU:HG | 2.19 | 0.42 |
| 2:G:173:GLY:O | 2:G:177:ILE:HG12 | 2.19 | 0.42 |
| 2:G:889:LYS:HB3 | 2:G:1538:ARG:NH2 | 2.34 | 0.42 |
| 2:G:1032:TRP:CD1 | 2:G:1035:LYS:HD3 | 2.54 | 0.42 |
| 2:G:1106:LEU:HG | 2:G:1325:TYR:HE2 | 1.85 | 0.42 |
| 2:G:1245:ARG:HA | 2:G:1245:ARG:NE | 2.34 | 0.42 |
| 2:F:205:LYS:O | 2:F:207:PRO:HD3 | 2.19 | 0.42 |
| 2:F:238:LYS:HA | 2:F:1180:TYR:OH | 2.19 | 0.42 |
| 2:F:487:SER:HA | 2:F:490:GLU:HG2 | 2.01 | 0.42 |
| 2:F:1106:LEU:HG | 2:F:1325:TYR:HE2 | 1.85 | 0.42 |
| 1:D:113:SER:OG | 1:D:135:GLY:O | 2.30 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:35:PHE:CD1 | 1:B:233:LEU:HD13 | 2.54 | 0.42 |
| 1:B:66:LEU:HD21 | 1:B:70:HIS:HB2 | 2.00 | 0.42 |
| 1:C:222:LYS:HG3 | 1:C:232:PRO:HA | 2.00 | 0.42 |
| 2:E:685:TYR:CD1 | 2:E:697:SER:HA | 2.55 | 0.42 |
| 2:H:1064:ALA:O | 2:H:1067:PHE:HB3 | 2.19 | 0.42 |
| 2:G:503:LEU:HD23 | 2:G:506:ILE:HD13 | 2.00 | 0.42 |
| 2:F:327:LEU:HD22 | 2:F:1277:ALA:HB2 | 2.01 | 0.42 |
| 2:F:575:VAL:HG23 | 2:F:576:ALA:N | 2.34 | 0.42 |
| 2:F:850:VAL:HG21 | 2:F:881:ARG:NE | 2.32 | 0.42 |
| 2:F:1092:VAL:O | 2:F:1096:LEU:HG | 2.19 | 0.42 |
| 2:F:1435:ILE:HB | 2:F:1470:LEU:HB2 | 1.99 | 0.42 |
| 1:A:63:LEU:HD11 | 1:A:75:PHE:CZ | 2.55 | 0.42 |
| 1:A:267:LEU:HD21 | 1:A:283:ILE:HD11 | 2.01 | 0.42 |
| 1:A:344:CYS:HB2 | 1:A:348:GLN:OE1 | 2.20 | 0.42 |
| 1:C:200:LEU:N | 1:C:257:ILE:O | 2.47 | 0.42 |
| 2:E:889:LYS:HB3 | 2:E:1538:ARG:NH2 | 2.34 | 0.42 |
| 2:E:1064:ALA:O | 2:E:1067:PHE:HB3 | 2.19 | 0.42 |
| 2:H:708:LEU:HB2 | 2:H:876:LEU:HD21 | 2.01 | 0.42 |
| 2:G:238:LYS:HA | 2:G:1180:TYR:OH | 2.19 | 0.42 |
| 2:G:325:ASP:OD1 | 2:G:326:HIS:N | 2.53 | 0.42 |
| 2:G:550:ILE:N | 2:G:551:PRO:HD2 | 2.34 | 0.42 |
| 2:G:911:GLY:HA3 | 2:G:915:ASP:OD2 | 2.20 | 0.42 |
| 2:G:1460:LYS:O | 2:G:1464:LYS:HG3 | 2.20 | 0.42 |
| 2:F:398:LYS:NZ | 2:F:616:SER:HB2 | 2.35 | 0.42 |
| 2:F:868:MET:HG3 | 2:F:872:ILE:HG13 | 2.01 | 0.42 |
| 2:F:1064:ALA:O | 2:F:1067:PHE:HB3 | 2.19 | 0.42 |
| 2:F:1413:PRO:HB2 | 2:F:1416:THR:HG23 | 2.01 | 0.42 |
| 1:A:35:PHE:CE1 | 1:A:233:LEU:HD13 | 2.54 | 0.42 |
| 1:D:177:ARG:HH21 | 1:D:204:ASP:CG | 2.22 | 0.42 |
| 1:D:222:LYS:HG3 | 1:D:232:PRO:HA | 2.00 | 0.42 |
| 1:B:272:PRO:C | 1:B:274:ASP:H | 2.23 | 0.42 |
| 1:C:35:PHE:CD1 | 1:C:233:LEU:HD13 | 2.54 | 0.42 |
| 2:E:207:PRO:HA | 2:E:211:GLN:H | 1.85 | 0.42 |
| 2:E:238:LYS:HA | 2:E:1180:TYR:OH | 2.19 | 0.42 |
| 2:E:366:LEU:HA | 2:E:369:GLN:HB3 | 2.00 | 0.42 |
| 2:E:503:LEU:HD23 | 2:E:506:ILE:HD13 | 2.00 | 0.42 |
| 2:E:873:LEU:O | 2:E:877:ARG:HB2 | 2.18 | 0.42 |
| 2:E:1147:LEU:HD22 | 2:E:1147:LEU:HA | 1.83 | 0.42 |
| 2:H:68:PHE:N | 2:H:69:PRO:CD | 2.82 | 0.42 |
| 2:H:1033:LEU:HD12 | 2:H:1036:TRP:HB3 | 2.02 | 0.42 |
| 2:H:1350:SER:HA | 2:H:1361:LEU:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:68:PHE:N | 2:G:69:PRO:CD | 2.82 | 0.42 |
| 2:F:911:GLY:HA3 | 2:F:915:ASP:OD2 | 2.19 | 0.42 |
| 1:A:35:PHE:CD1 | 1:A:233:LEU:HD13 | 2.54 | 0.42 |
| 1:C:344:CYS:HB2 | 1:C:348:GLN:OE1 | 2.20 | 0.42 |
| 2:E:1352:ARG:HB3 | 2:E:1359:PRO:HA | 2.02 | 0.42 |
| 2:H:36:HIS:CE1 | 2:H:113:ALA:HB2 | 2.55 | 0.42 |
| 2:H:85:LEU:HA | 2:H:85:LEU:HD13 | 1.82 | 0.42 |
| 2:H:253:LEU:HD21 | 2:H:1231:ASP:CG | 2.39 | 0.42 |
| 2:G:1033:LEU:HD12 | 2:G:1036:TRP:HB3 | 2.02 | 0.42 |
| 2:F:68:PHE:N | 2:F:69:PRO:CD | 2.82 | 0.42 |
| 2:F:477:VAL:HG11 | 2:F:543:SER:HB2 | 2.02 | 0.42 |
| 2:F:1466:LEU:HA | 2:F:1467:PRO:HD3 | 1.95 | 0.42 |
| 1:D:63:LEU:HD11 | 1:D:75:PHE:CZ | 2.55 | 0.42 |
| 1:B:299:GLN:O | 1:B:301:ARG:NH1 | 2.52 | 0.42 |
| 1:C:218:GLN:N | 1:C:284:ILE:O | 2.50 | 0.42 |
| 2:E:36:HIS:CE1 | 2:E:113:ALA:HB2 | 2.55 | 0.42 |
| 2:E:477:VAL:HG11 | 2:E:543:SER:HB2 | 2.02 | 0.42 |
| 2:E:508:LEU:HD22 | 2:E:1431:PHE:CZ | 2.51 | 0.42 |
| 2:E:1032:TRP:CD1 | 2:E:1035:LYS:HD3 | 2.54 | 0.42 |
| 2:E:1413:PRO:HB2 | 2:E:1416:THR:HG23 | 2.01 | 0.42 |
| 2:H:205:LYS:O | 2:H:207:PRO:HD3 | 2.19 | 0.42 |
| 2:H:207:PRO:HA | 2:H:211:GLN:H | 1.85 | 0.42 |
| 2:G:36:HIS:CE1 | 2:G:113:ALA:HB2 | 2.55 | 0.42 |
| 2:G:1147:LEU:HD22 | 2:G:1147:LEU:HA | 1.83 | 0.42 |
| 2:G:1347:GLN:HA | 2:G:1365:ASN:HB3 | 2.02 | 0.42 |
| 2:F:245:ILE:N | 2:F:1187:ASP:OD2 | 2.52 | 0.42 |
| 2:F:1352:ARG:HB3 | 2:F:1359:PRO:HA | 2.02 | 0.42 |
| 1:A:224:THR:HG22 | 1:A:225:SER:O | 2.19 | 0.42 |
| 1:A:239:PRO:HB3 | 1:D:244:VAL:HG22 | 2.02 | 0.42 |
| 1:B:268:TYR:OH | 1:B:350:ASP:OD2 | 2.22 | 0.42 |
| 1:B:330:TYR:O | 1:B:333:PHE:HB2 | 2.20 | 0.42 |
| 2:E:325:ASP:OD1 | 2:E:326:HIS:N | 2.53 | 0.42 |
| 2:E:1106:LEU:HG | 2:E:1325:TYR:HE2 | 1.84 | 0.42 |
| 2:E:1220:ALA:O | 2:E:1224:GLN:HG2 | 2.20 | 0.42 |
| 2:H:477:VAL:HG11 | 2:H:543:SER:HB2 | 2.02 | 0.42 |
| 2:H:1077:LEU:HA | 2:H:1080:VAL:HG12 | 2.01 | 0.42 |
| 2:H:1349:LEU:HB3 | 2:H:1364:VAL:CG1 | 2.50 | 0.42 |
| 2:G:205:LYS:O | 2:G:207:PRO:HD3 | 2.19 | 0.42 |
| 2:G:1220:ALA:O | 2:G:1224:GLN:HG2 | 2.20 | 0.42 |
| 2:G:1373:LYS:O | 2:G:1546:ASP:N | 2.31 | 0.42 |
| 2:G:1392:PHE:O | 2:G:1418:ARG:NH1 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:368:LEU:HA | 2:F:371:THR:HG22 | 2.01 | 0.42 |
| 2:F:1031:TYR:HA | 2:F:1282:LEU:CD1 | 2.46 | 0.42 |
| 1:A:95:PHE:CD1 | 1:A:100:LEU:HD12 | 2.54 | 0.42 |
| 1:A:272:PRO:C | 1:A:274:ASP:H | 2.23 | 0.42 |
| 1:D:35:PHE:CD1 | 1:D:233:LEU:HD13 | 2.54 | 0.42 |
| 1:C:330:TYR:O | 1:C:333:PHE:HB2 | 2.20 | 0.42 |
| 2:E:685:TYR:CD2 | 2:E:734:SER:HB3 | 2.55 | 0.42 |
| 2:E:1520:GLN:HA | 2:E:1523:VAL:HG12 | 2.02 | 0.42 |
| 2:H:381:ILE:O | 2:H:385:ILE:HG12 | 2.20 | 0.42 |
| 2:H:1520:GLN:HA | 2:H:1523:VAL:HG12 | 2.02 | 0.42 |
| 2:G:850:VAL:HG21 | 2:G:881:ARG:NE | 2.32 | 0.42 |
| 1:B:63:LEU:HD11 | 1:B:75:PHE:CZ | 2.55 | 0.42 |
| 1:B:183:PHE:O | 3:C:501:ATP:H5'1 | 2.20 | 0.42 |
| 1:B:321:GLU:OE2 | 1:C:32:ARG:N | 2.53 | 0.42 |
| 1:C:299:GLN:O | 1:C:301:ARG:NH1 | 2.52 | 0.42 |
| 2:E:85:LEU:HD13 | 2:E:85:LEU:HA | 1.82 | 0.42 |
| 2:H:1123:ARG:HE | 2:H:1317:LEU:HD11 | 1.84 | 0.42 |
| 2:H:1350:SER:HA | 2:H:1362:LYS:HA | 2.01 | 0.42 |
| 2:H:1523:VAL:O | 2:H:1527:PHE:HB2 | 2.20 | 0.42 |
| 2:G:139:LEU:O | 2:G:143:TRP:HD1 | 2.02 | 0.42 |
| 2:G:1352:ARG:HB3 | 2:G:1359:PRO:HA | 2.02 | 0.42 |
| 2:F:174:LEU:HD13 | 2:F:178:LEU:HD13 | 2.01 | 0.42 |
| 2:F:872:ILE:HD13 | 2:F:875:LEU:HD12 | 2.02 | 0.42 |
| 2:F:1033:LEU:HD12 | 2:F:1036:TRP:HB3 | 2.02 | 0.42 |
| 2:F:1505:ASP:HA | 2:F:1535:ILE:HB | 2.02 | 0.42 |
| 1:D:344:CYS:HB2 | 1:D:348:GLN:OE1 | 2.20 | 0.41 |
| 1:B:344:CYS:HB2 | 1:B:348:GLN:OE1 | 2.20 | 0.41 |
| 2:E:1245:ARG:NE | 2:E:1245:ARG:HA | 2.34 | 0.41 |
| 2:E:1460:LYS:O | 2:E:1464:LYS:HG3 | 2.20 | 0.41 |
| 2:H:245:ILE:N | 2:H:1187:ASP:OD2 | 2.52 | 0.41 |
| 2:H:470:LEU:HD13 | 2:H:550:ILE:HG21 | 2.01 | 0.41 |
| 2:H:685:TYR:CD2 | 2:H:734:SER:HB3 | 2.55 | 0.41 |
| 2:H:911:GLY:HA3 | 2:H:915:ASP:OD2 | 2.19 | 0.41 |
| 2:H:1220:ALA:O | 2:H:1224:GLN:HG2 | 2.20 | 0.41 |
| 2:H:1352:ARG:HB3 | 2:H:1359:PRO:HA | 2.02 | 0.41 |
| 2:G:470:LEU:HD13 | 2:G:550:ILE:HG21 | 2.01 | 0.41 |
| 2:G:685:TYR:CD2 | 2:G:734:SER:HB3 | 2.55 | 0.41 |
| 2:F:173:GLY:O | 2:F:177:ILE:HG12 | 2.19 | 0.41 |
| 2:F:322:GLY:C | 2:F:326:HIS:HD1 | 2.21 | 0.41 |
| 2:F:327:LEU:O | 2:F:327:LEU:HD23 | 2.19 | 0.41 |
| 2:F:1032:TRP:HD1 | 2:F:1035:LYS:HD3 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1350:SER:HA | 2:F:1362:LYS:HA | 2.01 | 0.41 |
| 1:B:95:PHE:CD1 | 1:B:100:LEU:HD12 | 2.54 | 0.41 |
| 2:E:398:LYS:NZ | 2:E:616:SER:HB2 | 2.35 | 0.41 |
| 2:E:1033:LEU:HD12 | 2:E:1036:TRP:HB3 | 2.02 | 0.41 |
| 2:H:325:ASP:OD1 | 2:H:326:HIS:N | 2.53 | 0.41 |
| 2:H:381:ILE:HD13 | 2:H:1241:THR:HG23 | 2.02 | 0.41 |
| 2:H:685:TYR:CD1 | 2:H:697:SER:HA | 2.55 | 0.41 |
| 2:H:873:LEU:O | 2:H:877:ARG:HB2 | 2.19 | 0.41 |
| 2:H:1434:THR:O | 2:H:1438:ASN:N | 2.39 | 0.41 |
| 2:G:685:TYR:CD1 | 2:G:697:SER:HA | 2.55 | 0.41 |
| 2:G:781:ALA:HA | 2:G:821:GLN:HE22 | 1.86 | 0.41 |
| 2:G:1032:TRP:HD1 | 2:G:1035:LYS:HD3 | 1.86 | 0.41 |
| 2:G:1077:LEU:HA | 2:G:1080:VAL:HG12 | 2.02 | 0.41 |
| 2:F:387:LEU:O | 2:F:391:ILE:HG12 | 2.20 | 0.41 |
| 2:F:781:ALA:HA | 2:F:821:GLN:HE22 | 1.85 | 0.41 |
| 2:F:1077:LEU:HA | 2:F:1080:VAL:HG12 | 2.02 | 0.41 |
| 1:A:254:PRO:HD2 | 1:A:328:VAL:HG11 | 2.03 | 0.41 |
| 1:A:299:GLN:NE2 | 1:A:301:ARG:HD2 | 2.36 | 0.41 |
| 1:D:267:LEU:HD21 | 1:D:283:ILE:HD11 | 2.01 | 0.41 |
| 1:B:313:GLN:HE21 | 1:B:338:LYS:HG2 | 1.86 | 0.41 |
| 1:C:63:LEU:HD11 | 1:C:75:PHE:CZ | 2.55 | 0.41 |
| 1:C:202:VAL:N | 1:C:255:LEU:O | 2.40 | 0.41 |
| 2:E:387:LEU:O | 2:E:391:ILE:HG12 | 2.20 | 0.41 |
| 2:E:850:VAL:HG21 | 2:E:881:ARG:NE | 2.32 | 0.41 |
| 2:E:1434:THR:O | 2:E:1438:ASN:N | 2.39 | 0.41 |
| 2:H:1147:LEU:HA | 2:H:1147:LEU:HD22 | 1.83 | 0.41 |
| 2:G:1520:GLN:HA | 2:G:1523:VAL:HG12 | 2.02 | 0.41 |
| 2:G:1523:VAL:O | 2:G:1527:PHE:HB2 | 2.21 | 0.41 |
| 2:F:381:ILE:O | 2:F:385:ILE:HG12 | 2.20 | 0.41 |
| 2:F:451:LEU:HD13 | 2:F:455:ILE:HB | 2.03 | 0.41 |
| 1:D:50:ARG:NH1 | 3:D:501:ATP:H2' | 2.36 | 0.41 |
| 1:D:229:GLU:HB3 | 1:C:314:ARG:HH11 | 1.86 | 0.41 |
| 1:C:299:GLN:NE2 | 1:C:301:ARG:HD2 | 2.36 | 0.41 |
| 2:E:157:PHE:HE2 | 2:E:169:PHE:HB2 | 1.85 | 0.41 |
| 2:E:245:ILE:N | 2:E:1187:ASP:OD2 | 2.52 | 0.41 |
| 2:E:381:ILE:O | 2:E:385:ILE:HG12 | 2.20 | 0.41 |
| 2:E:407:LEU:HD12 | 2:E:412:MET:O | 2.21 | 0.41 |
| 2:E:781:ALA:HA | 2:E:821:GLN:HE22 | 1.86 | 0.41 |
| 2:H:157:PHE:HE2 | 2:H:169:PHE:HB2 | 1.85 | 0.41 |
| 2:H:407:LEU:HD12 | 2:H:412:MET:O | 2.21 | 0.41 |
| 2:G:477:VAL:HG11 | 2:G:543:SER:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:325:ASP:OD1 | 2:F:326:HIS:N | 2.53 | 0.41 |
| 2:F:407:LEU:HD12 | 2:F:412:MET:O | 2.20 | 0.41 |
| 2:F:767:GLY:O | 2:F:769:VAL:N | 2.52 | 0.41 |
| 2:F:1025:VAL:HG21 | 2:F:1073:LEU:HD22 | 2.03 | 0.41 |
| 2:F:1317:LEU:HD23 | 2:F:1317:LEU:HA | 1.85 | 0.41 |
| 1:A:46:HIS:CD2 | 1:D:330:TYR:CE2 | 3.09 | 0.41 |
| 1:D:299:GLN:NE2 | 1:D:301:ARG:HD2 | 2.36 | 0.41 |
| 1:B:299:GLN:NE2 | 1:B:301:ARG:HD2 | 2.36 | 0.41 |
| 1:B:320:ALA:O | 1:B:327:SER:OG | 2.31 | 0.41 |
| 2:E:487:SER:HA | 2:E:490:GLU:HG2 | 2.01 | 0.41 |
| 2:E:1379:ARG:NE | 2:E:1552:LYS:O | 2.47 | 0.41 |
| 2:H:387:LEU:O | 2:H:391:ILE:HG12 | 2.20 | 0.41 |
| 2:H:398:LYS:NZ | 2:H:616:SER:HB2 | 2.35 | 0.41 |
| 2:H:487:SER:HA | 2:H:490:GLU:HG2 | 2.02 | 0.41 |
| 2:H:781:ALA:HA | 2:H:821:GLN:HE22 | 1.86 | 0.41 |
| 2:H:1031:TYR:HA | 2:H:1282:LEU:CD1 | 2.46 | 0.41 |
| 2:G:207:PRO:HA | 2:G:211:GLN:H | 1.85 | 0.41 |
| 2:G:322:GLY:C | 2:G:326:HIS:HD1 | 2.21 | 0.41 |
| 2:G:1088:THR:O | 2:G:1092:VAL:HG23 | 2.20 | 0.41 |
| 2:G:1349:LEU:HB3 | 2:G:1364:VAL:CG1 | 2.50 | 0.41 |
| 2:F:36:HIS:CE1 | 2:F:113:ALA:HB2 | 2.55 | 0.41 |
| 2:F:207:PRO:HA | 2:F:211:GLN:H | 1.85 | 0.41 |
| 2:F:679:VAL:HA | 2:F:738:PHE:O | 2.21 | 0.41 |
| 1:A:313:GLN:HE21 | 1:A:338:LYS:HG2 | 1.86 | 0.41 |
| 1:D:95:PHE:CD1 | 1:D:100:LEU:HD12 | 2.54 | 0.41 |
| 1:D:272:PRO:C | 1:D:274:ASP:H | 2.23 | 0.41 |
| 1:B:267:LEU:HD21 | 1:B:283:ILE:HD11 | 2.01 | 0.41 |
| 1:B:271:ALA:HB2 | 1:B:345:THR:HG22 | 2.02 | 0.41 |
| 2:E:811:ILE:O | 2:E:817:GLY:HA2 | 2.21 | 0.41 |
| 2:H:868:MET:HG3 | 2:H:872:ILE:HG13 | 2.01 | 0.41 |
| 2:H:1025:VAL:HG21 | 2:H:1073:LEU:HD22 | 2.03 | 0.41 |
| 2:G:157:PHE:HE2 | 2:G:169:PHE:HB2 | 1.85 | 0.41 |
| 2:G:381:ILE:O | 2:G:385:ILE:HG12 | 2.20 | 0.41 |
| 2:G:398:LYS:NZ | 2:G:616:SER:HB2 | 2.35 | 0.41 |
| 2:G:1033:LEU:O | 2:G:1036:TRP:HB3 | 2.21 | 0.41 |
| 2:G:1505:ASP:HA | 2:G:1535:ILE:HB | 2.02 | 0.41 |
| 2:F:685:TYR:CD2 | 2:F:734:SER:HB3 | 2.55 | 0.41 |
| 2:F:1088:THR:O | 2:F:1092:VAL:HG23 | 2.20 | 0.41 |
| 2:F:1347:GLN:HA | 2:F:1365:ASN:HB3 | 2.02 | 0.41 |
| 1:A:240:MET:HG2 | 1:A:247:ASN:ND2 | 2.36 | 0.41 |
| 1:A:330:TYR:O | 1:A:333:PHE:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:50:ARG:HB2 | 3:D:501:ATP:C5 | 2.56 | 0.41 |
| 1:B:75:PHE:O | 1:B:78:SER:OG | 2.27 | 0.41 |
| 1:B:254:PRO:HD2 | 1:B:328:VAL:HG11 | 2.03 | 0.41 |
| 1:C:254:PRO:HD2 | 1:C:328:VAL:HG11 | 2.02 | 0.41 |
| 2:E:1349:LEU:HB3 | 2:E:1364:VAL:CG1 | 2.50 | 0.41 |
| 2:E:1402:ILE:HG23 | 2:E:1409:ILE:HB | 2.03 | 0.41 |
| 2:E:1523:VAL:O | 2:E:1527:PHE:HB2 | 2.20 | 0.41 |
| 2:H:575:VAL:HG23 | 2:H:576:ALA:H | 1.86 | 0.41 |
| 2:H:679:VAL:HA | 2:H:738:PHE:O | 2.21 | 0.41 |
| 2:H:811:ILE:O | 2:H:817:GLY:HA2 | 2.21 | 0.41 |
| 2:H:850:VAL:HG21 | 2:H:881:ARG:NE | 2.32 | 0.41 |
| 2:G:368:LEU:HA | 2:G:371:THR:HG22 | 2.01 | 0.41 |
| 2:G:793:PHE:HA | 2:G:844:TYR:OH | 2.21 | 0.41 |
| 2:G:811:ILE:O | 2:G:817:GLY:HA2 | 2.21 | 0.41 |
| 2:F:1392:PHE:O | 2:F:1418:ARG:NH1 | 2.47 | 0.41 |
| 2:F:1460:LYS:O | 2:F:1464:LYS:HG3 | 2.20 | 0.41 |
| 1:D:165:GLY:HA2 | 1:C:168:PHE:HD1 | 1.85 | 0.41 |
| 1:D:254:PRO:HD2 | 1:D:328:VAL:HG11 | 2.02 | 0.41 |
| 1:D:330:TYR:O | 1:D:333:PHE:HB2 | 2.20 | 0.41 |
| 1:B:240:MET:HG2 | 1:B:247:ASN:ND2 | 2.36 | 0.41 |
| 1:C:271:ALA:HB2 | 1:C:345:THR:HG22 | 2.02 | 0.41 |
| 2:E:769:VAL:HG12 | 2:E:770:ALA:O | 2.21 | 0.41 |
| 2:H:137:ILE:O | 2:H:140:LEU:HB3 | 2.21 | 0.41 |
| 2:H:793:PHE:HA | 2:H:844:TYR:OH | 2.21 | 0.41 |
| 2:G:872:ILE:HD13 | 2:G:875:LEU:HD12 | 2.02 | 0.41 |
| 2:G:1350:SER:HA | 2:G:1362:LYS:HA | 2.01 | 0.41 |
| 2:F:224:LEU:HA | 2:F:227:LYS:HB2 | 2.03 | 0.41 |
| 2:F:769:VAL:HG12 | 2:F:770:ALA:O | 2.21 | 0.41 |
| 2:F:811:ILE:O | 2:F:817:GLY:HA2 | 2.21 | 0.41 |
| 1:A:200:LEU:N | 1:A:257:ILE:O | 2.47 | 0.41 |
| 1:D:210:ILE:HG23 | 1:D:213:ALA:HB2 | 2.03 | 0.41 |
| 1:D:240:MET:HG2 | 1:D:247:ASN:ND2 | 2.36 | 0.41 |
| 1:B:45:ALA:HB3 | 1:B:47:LYS:HZ2 | 1.85 | 0.41 |
| 1:C:313:GLN:HE21 | 1:C:338:LYS:HG2 | 1.86 | 0.41 |
| 2:E:381:ILE:HD13 | 2:E:1241:THR:HG23 | 2.02 | 0.41 |
| 2:E:424:ASP:OD2 | 2:E:610:LEU:HD21 | 2.21 | 0.41 |
| 2:E:435:CYS:HG | 2:E:439:TRP:HZ3 | 1.67 | 0.41 |
| 2:E:451:LEU:HD13 | 2:E:455:ILE:HB | 2.03 | 0.41 |
| 2:E:774:GLN:HE22 | 3:E:2004:ATP:PG | 2.44 | 0.41 |
| 2:E:1025:VAL:HG21 | 2:E:1073:LEU:HD22 | 2.03 | 0.41 |
| 2:E:1428:PRO:HB3 | 2:E:1487:GLN:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:1505:ASP:HA | 2:E:1535:ILE:HB | 2.02 | 0.41 |
| 2:E:1569:LYS:HD2 | 2:E:1569:LYS:O | 2.21 | 0.41 |
| 2:H:511:LEU:O | 2:H:1418:ARG:HB3 | 2.21 | 0.41 |
| 2:H:769:VAL:HG12 | 2:H:770:ALA:O | 2.21 | 0.41 |
| 2:H:1033:LEU:O | 2:H:1036:TRP:HB3 | 2.21 | 0.41 |
| 2:H:1106:LEU:HG | 2:H:1325:TYR:HE2 | 1.84 | 0.41 |
| 2:G:137:ILE:O | 2:G:140:LEU:HB3 | 2.21 | 0.41 |
| 2:G:387:LEU:O | 2:G:391:ILE:HG12 | 2.20 | 0.41 |
| 2:G:424:ASP:OD2 | 2:G:610:LEU:HD21 | 2.21 | 0.41 |
| 2:G:709:THR:HG22 | 2:G:884:VAL:HG22 | 2.03 | 0.41 |
| 2:G:780:ASN:ND2 | 2:G:1205:GLU:OE2 | 2.54 | 0.41 |
| 2:F:157:PHE:HE2 | 2:F:169:PHE:HB2 | 1.85 | 0.41 |
| 2:F:381:ILE:HD13 | 2:F:1241:THR:HG23 | 2.02 | 0.41 |
| 2:F:709:THR:HG22 | 2:F:884:VAL:HG22 | 2.03 | 0.41 |
| 2:F:781:ALA:HA | 2:F:821:GLN:NE2 | 2.36 | 0.41 |
| 2:F:782:THR:OG1 | 2:F:821:GLN:OE1 | 2.16 | 0.41 |
| 2:F:1349:LEU:HB3 | 2:F:1364:VAL:CG1 | 2.50 | 0.41 |
| 2:F:1520:GLN:HA | 2:F:1523:VAL:HG12 | 2.02 | 0.41 |
| 1:B:210:ILE:HG23 | 1:B:213:ALA:HB2 | 2.03 | 0.41 |
| 1:C:240:MET:HG2 | 1:C:247:ASN:ND2 | 2.36 | 0.41 |
| 2:E:81:LEU:HD11 | 2:E:179:TYR:HE1 | 1.86 | 0.41 |
| 2:E:137:ILE:O | 2:E:140:LEU:HB3 | 2.21 | 0.41 |
| 2:E:679:VAL:HA | 2:E:738:PHE:O | 2.21 | 0.41 |
| 2:E:1033:LEU:O | 2:E:1036:TRP:HB3 | 2.21 | 0.41 |
| 2:E:1088:THR:O | 2:E:1092:VAL:HG23 | 2.20 | 0.41 |
| 2:E:1317:LEU:HA | 2:E:1317:LEU:HD23 | 1.85 | 0.41 |
| 2:H:224:LEU:HA | 2:H:227:LYS:HB2 | 2.03 | 0.41 |
| 2:H:424:ASP:OD2 | 2:H:610:LEU:HD21 | 2.21 | 0.41 |
| 2:H:1428:PRO:HB3 | 2:H:1487:GLN:HA | 2.03 | 0.41 |
| 2:H:1569:LYS:HD2 | 2:H:1569:LYS:O | 2.21 | 0.41 |
| 2:G:368:LEU:O | 2:G:371:THR:HG22 | 2.21 | 0.41 |
| 2:G:843:LEU:O | 2:G:881:ARG:NH2 | 2.41 | 0.41 |
| 2:F:575:VAL:HG23 | 2:F:576:ALA:H | 1.86 | 0.41 |
| 1:A:95:PHE:CD2 | 2:E:27:PHE:HD1 | 2.39 | 0.40 |
| 1:C:210:ILE:HG23 | 1:C:213:ALA:HB2 | 2.03 | 0.40 |
| 1:C:267:LEU:HD21 | 1:C:283:ILE:HD11 | 2.01 | 0.40 |
| 1:C:272:PRO:C | 1:C:274:ASP:H | 2.23 | 0.40 |
| 2:H:774:GLN:HE22 | 3:H:2004:ATP:PG | 2.44 | 0.40 |
| 2:H:1032:TRP:HD1 | 2:H:1035:LYS:HD3 | 1.86 | 0.40 |
| 2:G:35:PRO:O | 2:G:142:TYR:HE1 | 2.05 | 0.40 |
| 2:G:451:LEU:HD13 | 2:G:455:ILE:HB | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1438:ASN:OD1 | 2:G:1474:ILE:HD12 | 2.22 | 0.40 |
| 2:F:29:ASP:OD1 | 2:F:109:PRO:HG3 | 2.21 | 0.40 |
| 2:F:81:LEU:HD11 | 2:F:179:TYR:HE1 | 1.86 | 0.40 |
| 2:F:424:ASP:OD2 | 2:F:610:LEU:HD21 | 2.21 | 0.40 |
| 2:F:1423:ILE:HG13 | 2:F:1503:ILE:HG23 | 2.03 | 0.40 |
| 2:F:1438:ASN:OD1 | 2:F:1474:ILE:HD12 | 2.21 | 0.40 |
| 1:A:90:TRP:CZ2 | 1:A:148:ILE:HG22 | 2.56 | 0.40 |
| 1:B:90:TRP:CZ2 | 1:B:148:ILE:HG22 | 2.56 | 0.40 |
| 1:B:275:LEU:HB2 | 1:B:306:ALA:O | 2.22 | 0.40 |
| 2:E:515:GLU:O | 2:E:519:ARG:CB | 2.70 | 0.40 |
| 2:E:767:GLY:O | 2:E:769:VAL:N | 2.52 | 0.40 |
| 2:E:872:ILE:HD13 | 2:E:875:LEU:HD12 | 2.02 | 0.40 |
| 2:H:368:LEU:O | 2:H:371:THR:HG22 | 2.21 | 0.40 |
| 2:H:786:ASN:OD1 | 2:H:787:ILE:N | 2.54 | 0.40 |
| 2:H:872:ILE:HD13 | 2:H:875:LEU:HD12 | 2.02 | 0.40 |
| 2:H:1155:VAL:HG11 | 2:H:1286:TYR:CE2 | 2.57 | 0.40 |
| 2:G:381:ILE:HD13 | 2:G:1241:THR:HG23 | 2.03 | 0.40 |
| 2:G:575:VAL:HG23 | 2:G:576:ALA:H | 1.86 | 0.40 |
| 2:G:1181:PHE:HE1 | 2:G:1243:ALA:HB1 | 1.86 | 0.40 |
| 2:G:1369:ALA:HB1 | 2:G:1370:PRO:HD2 | 2.04 | 0.40 |
| 2:G:1402:ILE:HG23 | 2:G:1409:ILE:HB | 2.03 | 0.40 |
| 2:F:368:LEU:O | 2:F:371:THR:HG22 | 2.22 | 0.40 |
| 2:F:793:PHE:HA | 2:F:844:TYR:OH | 2.21 | 0.40 |
| 2:F:861:ILE:H | 2:F:861:ILE:HG13 | 1.72 | 0.40 |
| 2:F:1033:LEU:O | 2:F:1036:TRP:HB3 | 2.21 | 0.40 |
| 2:F:1220:ALA:O | 2:F:1224:GLN:HG2 | 2.20 | 0.40 |
| 2:F:1523:VAL:O | 2:F:1527:PHE:HB2 | 2.20 | 0.40 |
| 1:A:210:ILE:HG23 | 1:A:213:ALA:HB2 | 2.03 | 0.40 |
| 1:B:318:ILE:HA | 1:B:332:LYS:HZ2 | 1.86 | 0.40 |
| 2:E:469:LEU:O | 2:E:472:PRO:HD2 | 2.21 | 0.40 |
| 2:E:575:VAL:HG23 | 2:E:576:ALA:H | 1.86 | 0.40 |
| 2:E:770:ALA:HB3 | 2:E:850:VAL:HA | 2.04 | 0.40 |
| 2:H:35:PRO:O | 2:H:142:TYR:HE1 | 2.05 | 0.40 |
| 2:H:770:ALA:HB3 | 2:H:850:VAL:HA | 2.04 | 0.40 |
| 2:H:781:ALA:HA | 2:H:821:GLN:NE2 | 2.36 | 0.40 |
| 2:H:843:LEU:O | 2:H:881:ARG:NH2 | 2.41 | 0.40 |
| 2:H:995:ILE:N | 2:H:996:PRO:HD2 | 2.36 | 0.40 |
| 2:H:1088:THR:O | 2:H:1092:VAL:HG23 | 2.20 | 0.40 |
| 2:H:1392:PHE:O | 2:H:1418:ARG:NH1 | 2.47 | 0.40 |
| 2:H:1505:ASP:HA | 2:H:1535:ILE:HB | 2.03 | 0.40 |
| 2:G:511:LEU:O | 2:G:1418:ARG:HB3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:573:PRO:HB2 | 2:G:574:SER:H | 1.64 | 0.40 |
| 2:G:769:VAL:HG12 | 2:G:770:ALA:O | 2.21 | 0.40 |
| 2:G:1289:MET:O | 2:G:1293:TYR:HD2 | 2.05 | 0.40 |
| 2:G:1431:PHE:HB2 | 2:G:1438:ASN:ND2 | 2.36 | 0.40 |
| 2:F:515:GLU:O | 2:F:519:ARG:CB | 2.69 | 0.40 |
| 2:F:780:ASN:ND2 | 2:F:1205:GLU:OE2 | 2.54 | 0.40 |
| 2:E:793:PHE:HA | 2:E:844:TYR:OH | 2.21 | 0.40 |
| 2:E:995:ILE:N | 2:E:996:PRO:HD2 | 2.36 | 0.40 |
| 2:E:1032:TRP:HD1 | 2:E:1035:LYS:HD3 | 1.86 | 0.40 |
| 2:E:1077:LEU:HA | 2:E:1080:VAL:HG12 | 2.02 | 0.40 |
| 2:E:1392:PHE:O | 2:E:1418:ARG:NH1 | 2.47 | 0.40 |
| 2:H:1152:ALA:O | 2:H:1156:ILE:HG12 | 2.21 | 0.40 |
| 2:G:81:LEU:HD11 | 2:G:179:TYR:HE1 | 1.86 | 0.40 |
| 2:G:224:LEU:HA | 2:G:227:LYS:HB2 | 2.03 | 0.40 |
| 2:G:685:TYR:HB2 | 2:G:734:SER:N | 2.36 | 0.40 |
| 2:G:1012:LEU:HD13 | 2:G:1012:LEU:HA | 1.95 | 0.40 |
| 2:G:1428:PRO:HB3 | 2:G:1487:GLN:HA | 2.03 | 0.40 |
| 2:F:35:PRO:O | 2:F:142:TYR:HE1 | 2.05 | 0.40 |
| 2:F:137:ILE:O | 2:F:140:LEU:HB3 | 2.21 | 0.40 |
| 1:B:271:ALA:HB2 | 1:B:345:THR:CG2 | 2.52 | 0.40 |
| 2:E:421:VAL:HG11 | 2:E:1203:PHE:CD2 | 2.57 | 0.40 |
| 2:E:781:ALA:HA | 2:E:821:GLN:NE2 | 2.36 | 0.40 |
| 2:E:869:GLN:O | 2:E:873:LEU:HB3 | 2.22 | 0.40 |
| 2:E:1152:ALA:O | 2:E:1156:ILE:HG12 | 2.21 | 0.40 |
| 2:H:1347:GLN:HA | 2:H:1365:ASN:HB3 | 2.02 | 0.40 |
| 2:H:1402:ILE:HG23 | 2:H:1409:ILE:HB | 2.03 | 0.40 |
| 2:H:1438:ASN:OD1 | 2:H:1474:ILE:HD12 | 2.21 | 0.40 |
| 2:H:1460:LYS:O | 2:H:1464:LYS:HG3 | 2.20 | 0.40 |
| 2:G:407:LEU:HD12 | 2:G:412:MET:O | 2.21 | 0.40 |
| 2:G:995:ILE:N | 2:G:996:PRO:HD2 | 2.36 | 0.40 |
| 2:G:1025:VAL:HG21 | 2:G:1073:LEU:HD22 | 2.03 | 0.40 |
| 2:G:1155:VAL:HG11 | 2:G:1286:TYR:CE2 | 2.57 | 0.40 |
| 2:F:370:ARG:HB3 | 2:F:1252:GLU:HG2 | 2.03 | 0.40 |
| 2:F:457:GLY:O | 2:F:461:LEU:HB3 | 2.22 | 0.40 |
| 2:F:709:THR:HA | 2:F:898:TRP:O | 2.22 | 0.40 |
| 2:F:1289:MET:O | 2:F:1293:TYR:HD2 | 2.05 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 326/406 (80%) | 293 (90%) | 32 (10%) | 1 (0%) | 37 | 72 |
| 1 | B | 326/406 (80%) | 293 (90%) | 32 (10%) | 1 (0%) | 37 | 72 |
| 1 | C | 326/406 (80%) | 293 (90%) | 32 (10%) | 1 (0%) | 37 | 72 |
| 1 | D | 326/406 (80%) | 292 (90%) | 33 (10%) | 1 (0%) | 37 | 72 |
| 2 | E | 1341/1581 (85%) | 1242 (93%) | 97 (7%) | 2 (0%) | 48 | 83 |
| 2 | F | 1341/1581 (85%) | 1241 (92%) | 98 (7%) | 2 (0%) | 48 | 83 |
| 2 | G | 1341/1581 (85%) | 1240 (92%) | 99 (7%) | 2 (0%) | 48 | 83 |
| 2 | H | 1341/1581 (85%) | 1241 (92%) | 98 (7%) | 2 (0%) | 48 | 83 |
| All | All | 6668/7948 (84%) | 6135 (92%) | 521 (8%) | 12 (0%) | 45 | 78 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 194 | ARG |
| 2 | H | 194 | ARG |
| 2 | G | 194 | ARG |
| 2 | F | 194 | ARG |
| 1 | A | 48 | ASN |
| 1 | D | 48 | ASN |
| 1 | B | 48 | ASN |
| 1 | C | 48 | ASN |
| 2 | E | 456 | LEU |
| 2 | H | 456 | LEU |
| 2 | G | 456 | LEU |
| 2 | F | 456 | LEU |

5.3.2 Protein sidechains

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

entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1 | A | 265/348 (76%) | 265 (100%) | 0 | 100 | 100 |
| 1 | B | 265/348 (76%) | 265 (100%) | 0 | 100 | 100 |
| 1 | C | 265/348 (76%) | 265 (100%) | 0 | 100 | 100 |
| 1 | D | 265/348 (76%) | 265 (100%) | 0 | 100 | 100 |
| 2 | E | 1004/1368 (73%) | 998 (99%) | 6 (1%) | 84 | 88 |
| 2 | F | 1004/1368 (73%) | 998 (99%) | 6 (1%) | 84 | 88 |
| 2 | G | 1004/1368 (73%) | 998 (99%) | 6 (1%) | 84 | 88 |
| 2 | H | 1004/1368 (73%) | 998 (99%) | 6 (1%) | 84 | 88 |
| All | All | 5076/6864 (74%) | 5052 (100%) | 24 (0%) | 85 | 89 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | E | 547 | ASN |
| 2 | E | 918 | ARG |
| 2 | E | 1147 | LEU |
| 2 | E | 1292 | ASN |
| 2 | E | 1295 | ASN |
| 2 | E | 1379 | ARG |
| 2 | H | 547 | ASN |
| 2 | H | 918 | ARG |
| 2 | H | 1147 | LEU |
| 2 | H | 1292 | ASN |
| 2 | H | 1295 | ASN |
| 2 | H | 1379 | ARG |
| 2 | G | 547 | ASN |
| 2 | G | 918 | ARG |
| 2 | G | 1147 | LEU |
| 2 | G | 1292 | ASN |
| 2 | G | 1295 | ASN |
| 2 | G | 1379 | ARG |
| 2 | F | 547 | ASN |
| 2 | F | 918 | ARG |
| 2 | F | 1147 | LEU |
| 2 | F | 1292 | ASN |
| 2 | F | 1295 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 1379 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 43 | ASN |
| 1 | A | 46 | HIS |
| 1 | A | 193 | HIS |
| 1 | A | 247 | ASN |
| 1 | A | 276 | HIS |
| 1 | A | 278 | HIS |
| 1 | A | 279 | GLN |
| 1 | D | 43 | ASN |
| 1 | D | 46 | HIS |
| 1 | D | 193 | HIS |
| 1 | D | 247 | ASN |
| 1 | D | 276 | HIS |
| 1 | D | 278 | HIS |
| 1 | D | 279 | GLN |
| 1 | B | 43 | ASN |
| 1 | B | 46 | HIS |
| 1 | B | 247 | ASN |
| 1 | B | 276 | HIS |
| 1 | B | 278 | HIS |
| 1 | B | 279 | GLN |
| 1 | C | 43 | ASN |
| 1 | C | 46 | HIS |
| 1 | C | 247 | ASN |
| 1 | C | 276 | HIS |
| 1 | C | 278 | HIS |
| 1 | C | 279 | GLN |
| 2 | E | 36 | HIS |
| 2 | E | 103 | HIS |
| 2 | E | 126 | ASN |
| 2 | E | 188 | ASN |
| 2 | E | 416 | GLN |
| 2 | E | 426 | ASN |
| 2 | E | 474 | GLN |
| 2 | E | 498 | GLN |
| 2 | E | 926 | HIS |
| 2 | E | 1129 | ASN |
| 2 | E | 1133 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | E | 1272 | HIS |
| 2 | E | 1292 | ASN |
| 2 | E | 1483 | GLN |
| 2 | H | 32 | ASN |
| 2 | H | 36 | HIS |
| 2 | H | 103 | HIS |
| 2 | H | 126 | ASN |
| 2 | H | 188 | ASN |
| 2 | H | 416 | GLN |
| 2 | H | 426 | ASN |
| 2 | H | 474 | GLN |
| 2 | H | 498 | GLN |
| 2 | H | 926 | HIS |
| 2 | H | 1129 | ASN |
| 2 | H | 1133 | GLN |
| 2 | H | 1272 | HIS |
| 2 | H | 1292 | ASN |
| 2 | H | 1483 | GLN |
| 2 | G | 32 | ASN |
| 2 | G | 36 | HIS |
| 2 | G | 103 | HIS |
| 2 | G | 126 | ASN |
| 2 | G | 188 | ASN |
| 2 | G | 416 | GLN |
| 2 | G | 426 | ASN |
| 2 | G | 474 | GLN |
| 2 | G | 498 | GLN |
| 2 | G | 926 | HIS |
| 2 | G | 1102 | ASN |
| 2 | G | 1129 | ASN |
| 2 | G | 1133 | GLN |
| 2 | G | 1272 | HIS |
| 2 | G | 1292 | ASN |
| 2 | G | 1483 | GLN |
| 2 | F | 36 | HIS |
| 2 | F | 103 | HIS |
| 2 | F | 126 | ASN |
| 2 | F | 188 | ASN |
| 2 | F | 416 | GLN |
| 2 | F | 426 | ASN |
| 2 | F | 474 | GLN |
| 2 | F | 498 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 926 | HIS |
| 2 | F | 1102 | ASN |
| 2 | F | 1129 | ASN |
| 2 | F | 1133 | GLN |
| 2 | F | 1272 | HIS |
| 2 | F | 1292 | ASN |
| 2 | F | 1483 | GLN |

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 3 | ATP | H | 2004 | 5 | 28,33,33 | 0.86 | 0 | 34,52,52 | 1.19 | 3 (8%) |
| 4 | ADP | E | 2001 | 5 | 24,29,29 | 0.86 | 0 | 29,45,45 | 1.21 | 2 (6%) |
| 3 | ATP | A | 501 | - | 28,33,33 | 0.78 | 0 | 34,52,52 | 1.23 | 3 (8%) |
| 3 | ATP | E | 2004 | 5 | 28,33,33 | 0.85 | 0 | 34,52,52 | 1.20 | 3 (8%) |
| 4 | ADP | F | 2001 | 5 | 24,29,29 | 0.86 | 0 | 29,45,45 | 1.22 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | ADP | G | 2001 | 5 | 24,29,29 | 0.86 | 0 | 29,45,45 | 1.21 | 2 (6%) |
| 3 | ATP | A | 502 | - | 28,33,33 | 0.78 | 0 | 34,52,52 | 1.24 | 4 (11%) |
| 4 | ADP | H | 2001 | 5 | 24,29,29 | 0.85 | 0 | 29,45,45 | 1.22 | 2 (6%) |
| 3 | ATP | D | 501 | - | 28,33,33 | 0.79 | 0 | 34,52,52 | 1.23 | 3 (8%) |
| 3 | ATP | F | 2004 | 5 | 28,33,33 | 0.86 | 0 | 34,52,52 | 1.20 | 3 (8%) |
| 3 | ATP | C | 501 | - | 28,33,33 | 0.79 | 0 | 34,52,52 | 1.24 | 3 (8%) |
| 3 | ATP | G | 2004 | 5 | 28,33,33 | 0.85 | 0 | 34,52,52 | 1.20 | 3 (8%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 3 | ATP | H | 2004 | 5 | - | 3/18/38/38 | 0/3/3/3 |
| 4 | ADP | E | 2001 | 5 | - | 4/12/32/32 | 0/3/3/3 |
| 3 | ATP | A | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 3 | ATP | E | 2004 | 5 | - | 3/18/38/38 | 0/3/3/3 |
| 4 | ADP | F | 2001 | 5 | - | 4/12/32/32 | 0/3/3/3 |
| 4 | ADP | G | 2001 | 5 | - | 4/12/32/32 | 0/3/3/3 |
| 3 | ATP | A | 502 | - | - | 4/18/38/38 | 0/3/3/3 |
| 4 | ADP | H | 2001 | 5 | - | 4/12/32/32 | 0/3/3/3 |
| 3 | ATP | D | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 3 | ATP | F | 2004 | 5 | - | 3/18/38/38 | 0/3/3/3 |
| 3 | ATP | C | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 3 | ATP | G | 2004 | 5 | - | 3/18/38/38 | 0/3/3/3 |

There are no bond length outliers.

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | H | 2001 | ADP | N3-C2-N1 | -3.82 | 123.49 | 128.67 |
| 4 | E | 2001 | ADP | N3-C2-N1 | -3.80 | 123.51 | 128.67 |
| 4 | F | 2001 | ADP | N3-C2-N1 | -3.79 | 123.53 | 128.67 |
| 4 | G | 2001 | ADP | N3-C2-N1 | -3.77 | 123.56 | 128.67 |
| 3 | C | 501 | ATP | N3-C2-N1 | -3.55 | 123.85 | 128.67 |
| 3 | E | 2004 | ATP | N3-C2-N1 | -3.51 | 123.91 | 128.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3 | A | 502 | ATP | N3-C2-N1 | -3.50 | 123.92 | 128.67 |
| 3 | G | 2004 | ATP | N3-C2-N1 | -3.49 | 123.93 | 128.67 |
| 3 | F | 2004 | ATP | N3-C2-N1 | -3.48 | 123.94 | 128.67 |
| 3 | H | 2004 | ATP | N3-C2-N1 | -3.48 | 123.95 | 128.67 |
| 3 | A | 501 | ATP | N3-C2-N1 | -3.47 | 123.97 | 128.67 |
| 3 | D | 501 | ATP | N3-C2-N1 | -3.43 | 124.02 | 128.67 |
| 3 | C | 501 | ATP | C4-C5-N7 | -2.74 | 106.44 | 109.34 |
| 3 | A | 501 | ATP | C4-C5-N7 | -2.72 | 106.47 | 109.34 |
| 3 | A | 502 | ATP | C4-C5-N7 | -2.66 | 106.53 | 109.34 |
| 3 | D | 501 | ATP | C4-C5-N7 | -2.58 | 106.61 | 109.34 |
| 4 | F | 2001 | ADP | C4-C5-N7 | -2.51 | 106.68 | 109.34 |
| 4 | G | 2001 | ADP | C4-C5-N7 | -2.45 | 106.75 | 109.34 |
| 4 | H | 2001 | ADP | C4-C5-N7 | -2.44 | 106.76 | 109.34 |
| 4 | E | 2001 | ADP | C4-C5-N7 | -2.43 | 106.77 | 109.34 |
| 3 | E | 2004 | ATP | C4-C5-N7 | -2.37 | 106.83 | 109.34 |
| 3 | F | 2004 | ATP | C4-C5-N7 | -2.36 | 106.84 | 109.34 |
| 3 | H | 2004 | ATP | C4-C5-N7 | -2.36 | 106.84 | 109.34 |
| 3 | G | 2004 | ATP | C4-C5-N7 | -2.30 | 106.91 | 109.34 |
| 3 | H | 2004 | ATP | C2'-C3'-C4' | 2.10 | 106.66 | 102.61 |
| 3 | E | 2004 | ATP | C2'-C3'-C4' | 2.09 | 106.66 | 102.61 |
| 3 | F | 2004 | ATP | C2'-C3'-C4' | 2.09 | 106.64 | 102.61 |
| 3 | G | 2004 | ATP | C2'-C3'-C4' | 2.07 | 106.62 | 102.61 |
| 3 | C | 501 | ATP | O2A-PA-O1A | 2.06 | 122.00 | 112.44 |
| 3 | A | 501 | ATP | O2A-PA-O1A | 2.04 | 121.92 | 112.44 |
| 3 | D | 501 | ATP | O2A-PA-O1A | 2.03 | 121.89 | 112.44 |
| 3 | A | 502 | ATP | O2A-PA-O1A | 2.03 | 121.87 | 112.44 |
| 3 | A | 502 | ATP | O3G-PG-O2G | 2.00 | 115.31 | 107.80 |

There are no chirality outliers.

All (45) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 3 | A | 501 | ATP | C5'-O5'-PA-O1A |
| 3 | A | 501 | ATP | C5'-O5'-PA-O3A |
| 3 | A | 502 | ATP | C5'-O5'-PA-O3A |
| 3 | D | 501 | ATP | C5'-O5'-PA-O1A |
| 3 | D | 501 | ATP | C5'-O5'-PA-O3A |
| 3 | C | 501 | ATP | C5'-O5'-PA-O1A |
| 3 | C | 501 | ATP | C5'-O5'-PA-O3A |
| 3 | E | 2004 | ATP | C5'-O5'-PA-O2A |
| 3 | E | 2004 | ATP | C5'-O5'-PA-O3A |
| 3 | H | 2004 | ATP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 3 | H | 2004 | ATP | C5'-O5'-PA-O3A |
| 3 | G | 2004 | ATP | C5'-O5'-PA-O2A |
| 3 | G | 2004 | ATP | C5'-O5'-PA-O3A |
| 3 | F | 2004 | ATP | C5'-O5'-PA-O2A |
| 3 | F | 2004 | ATP | C5'-O5'-PA-O3A |
| 3 | A | 501 | ATP | O4'-C4'-C5'-O5' |
| 3 | A | 502 | ATP | O4'-C4'-C5'-O5' |
| 3 | D | 501 | ATP | O4'-C4'-C5'-O5' |
| 3 | C | 501 | ATP | O4'-C4'-C5'-O5' |
| 4 | E | 2001 | ADP | O4'-C4'-C5'-O5' |
| 4 | H | 2001 | ADP | O4'-C4'-C5'-O5' |
| 4 | G | 2001 | ADP | O4'-C4'-C5'-O5' |
| 4 | F | 2001 | ADP | O4'-C4'-C5'-O5' |
| 3 | A | 501 | ATP | C3'-C4'-C5'-O5' |
| 3 | D | 501 | ATP | C3'-C4'-C5'-O5' |
| 3 | C | 501 | ATP | C3'-C4'-C5'-O5' |
| 4 | E | 2001 | ADP | C3'-C4'-C5'-O5' |
| 4 | H | 2001 | ADP | C3'-C4'-C5'-O5' |
| 4 | G | 2001 | ADP | C3'-C4'-C5'-O5' |
| 4 | F | 2001 | ADP | C3'-C4'-C5'-O5' |
| 3 | A | 502 | ATP | C3'-C4'-C5'-O5' |
| 3 | E | 2004 | ATP | PB-O3A-PA-O1A |
| 3 | H | 2004 | ATP | PB-O3A-PA-O1A |
| 3 | G | 2004 | ATP | PB-O3A-PA-O1A |
| 3 | F | 2004 | ATP | PB-O3A-PA-O1A |
| 4 | E | 2001 | ADP | PB-O3A-PA-O1A |
| 4 | H | 2001 | ADP | PB-O3A-PA-O1A |
| 4 | G | 2001 | ADP | PB-O3A-PA-O1A |
| 4 | F | 2001 | ADP | PB-O3A-PA-O1A |
| 3 | A | 502 | ATP | C5'-O5'-PA-O1A |
| 3 | A | 501 | ATP | PB-O3A-PA-O1A |
| 4 | E | 2001 | ADP | PB-O3A-PA-O2A |
| 4 | H | 2001 | ADP | PB-O3A-PA-O2A |
| 4 | G | 2001 | ADP | PB-O3A-PA-O2A |
| 4 | F | 2001 | ADP | PB-O3A-PA-O2A |

There are no ring outliers.

12 monomers are involved in 39 short contacts:

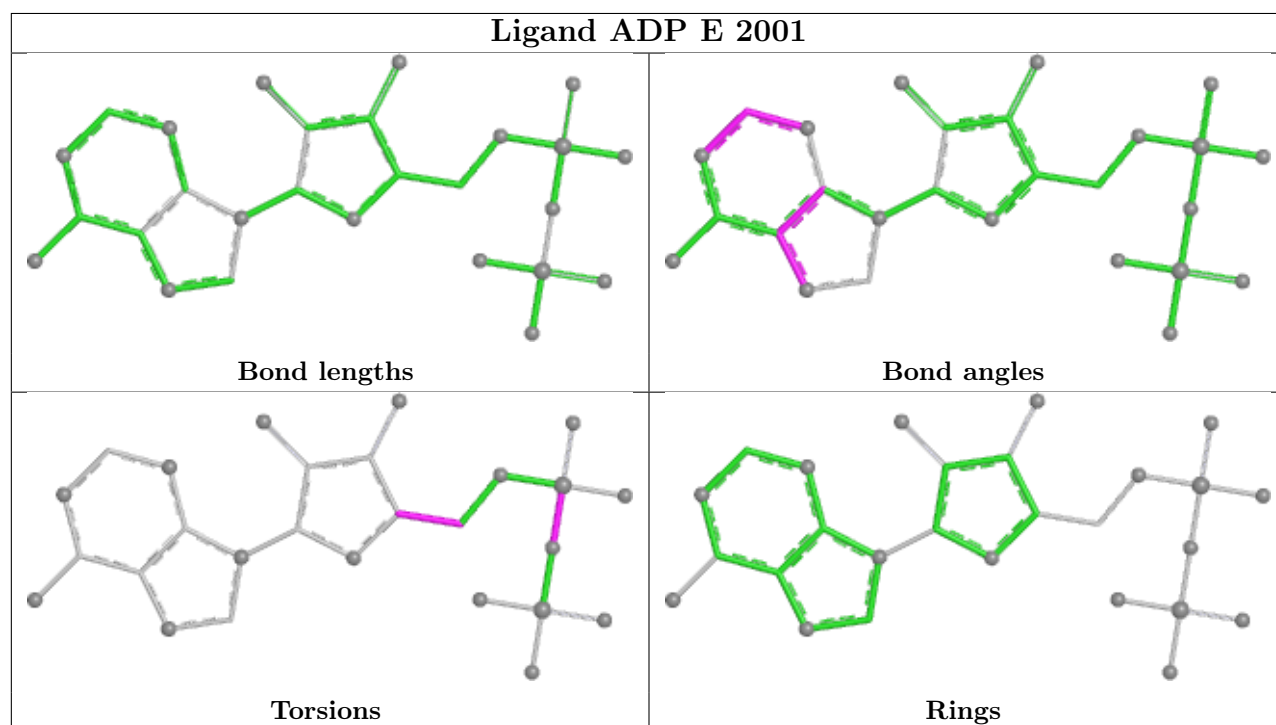
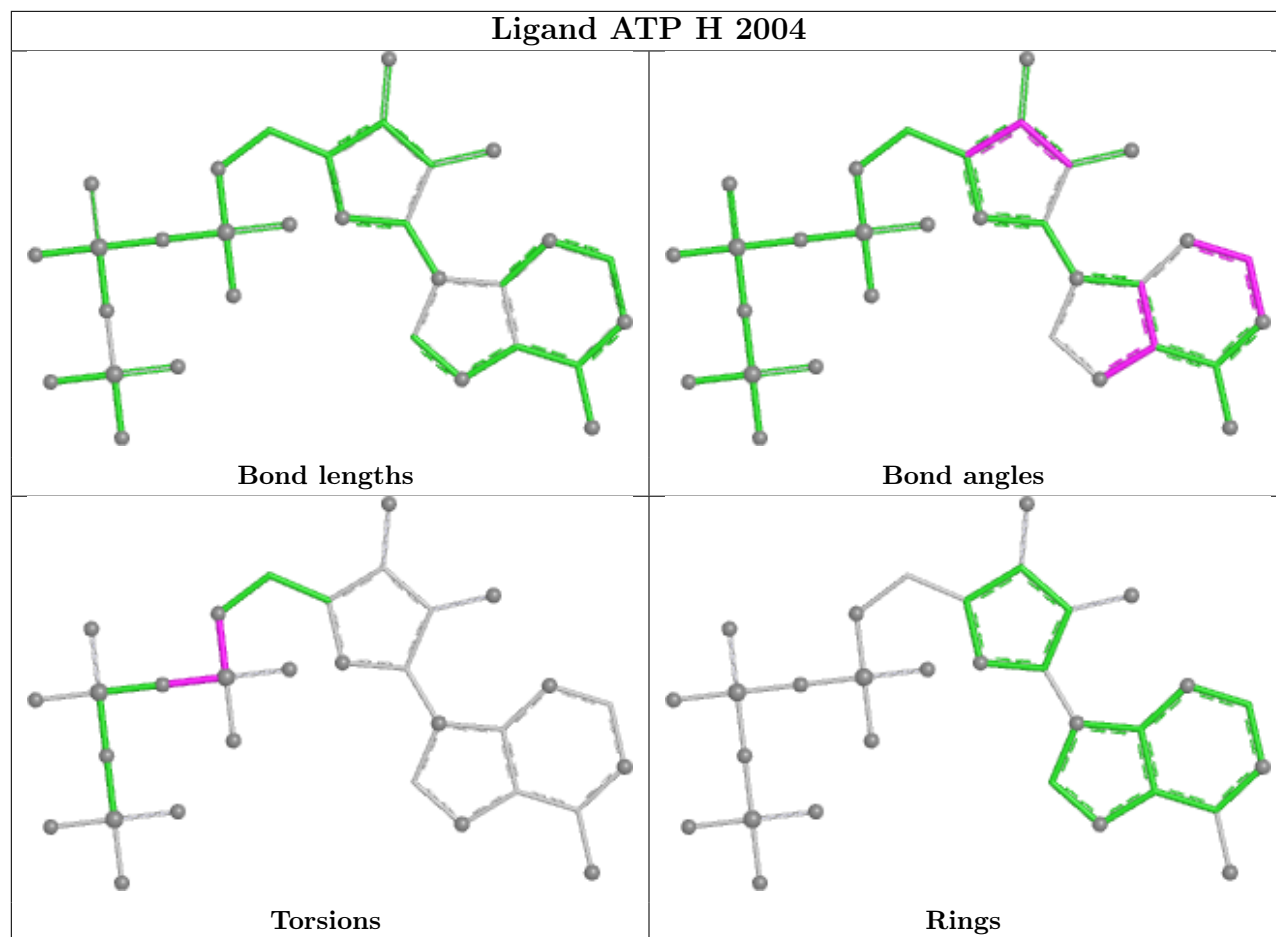
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | H | 2004 | ATP | 5 | 0 |
| 4 | E | 2001 | ADP | 2 | 0 |

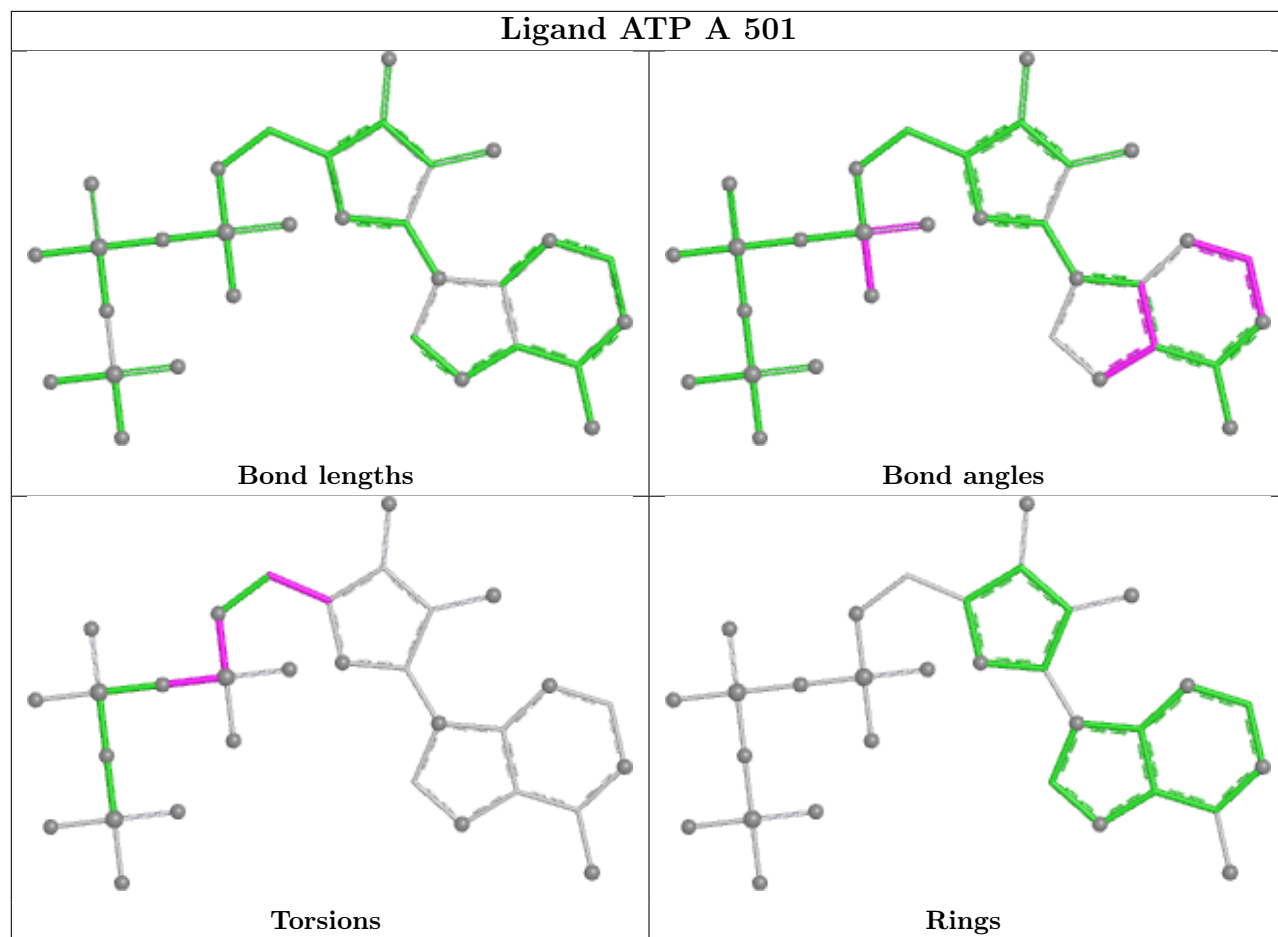
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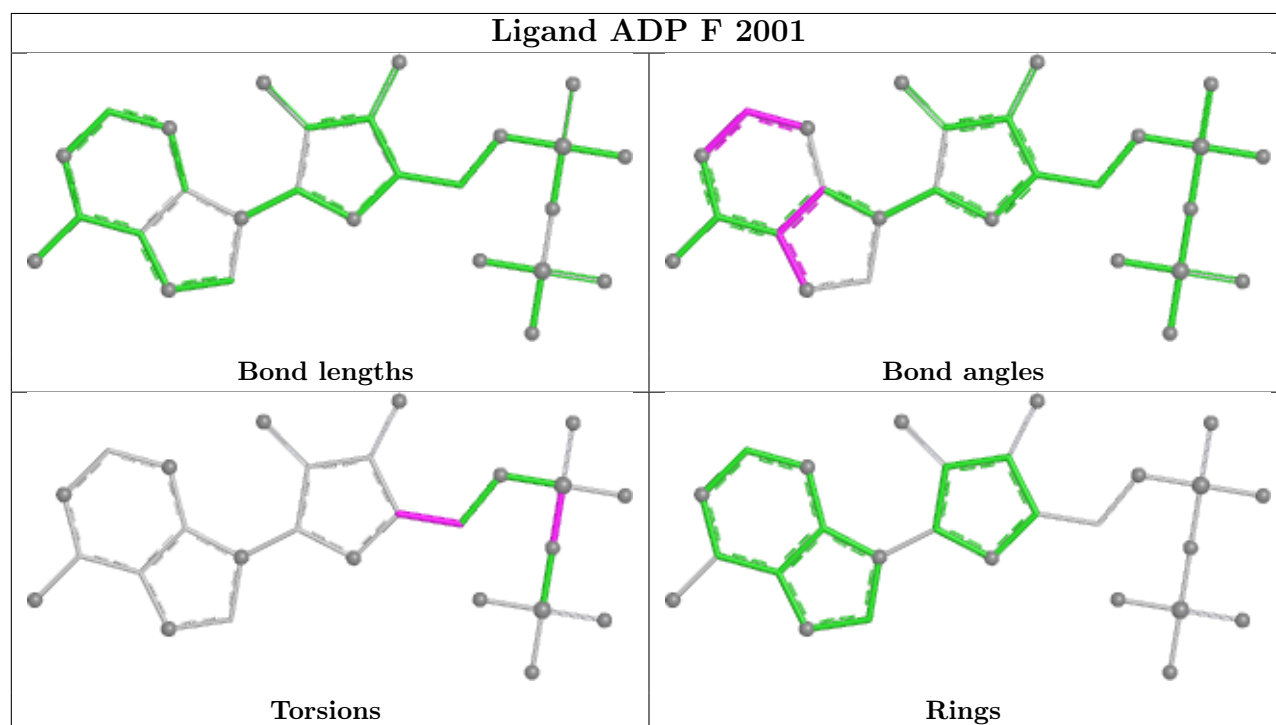
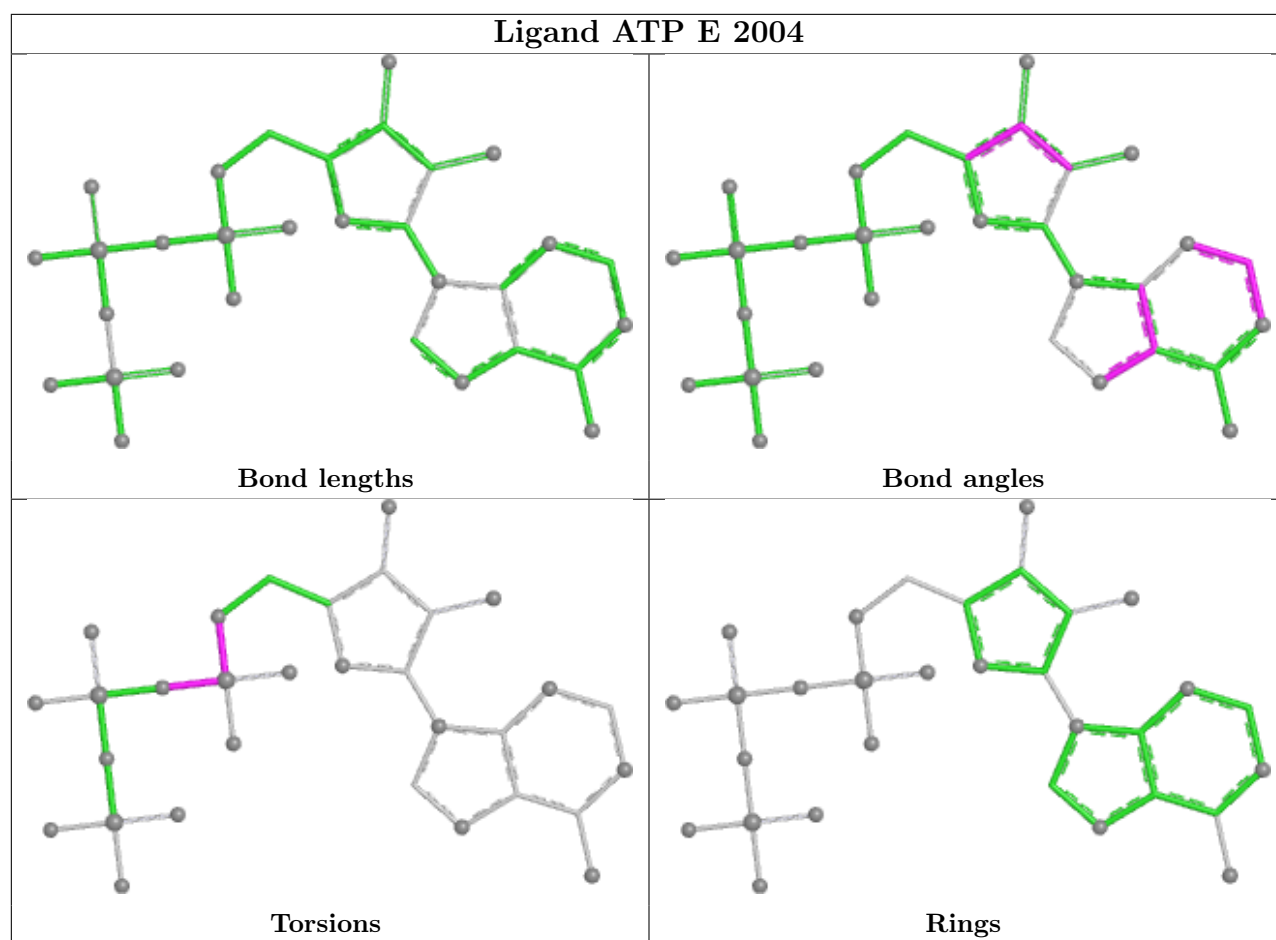
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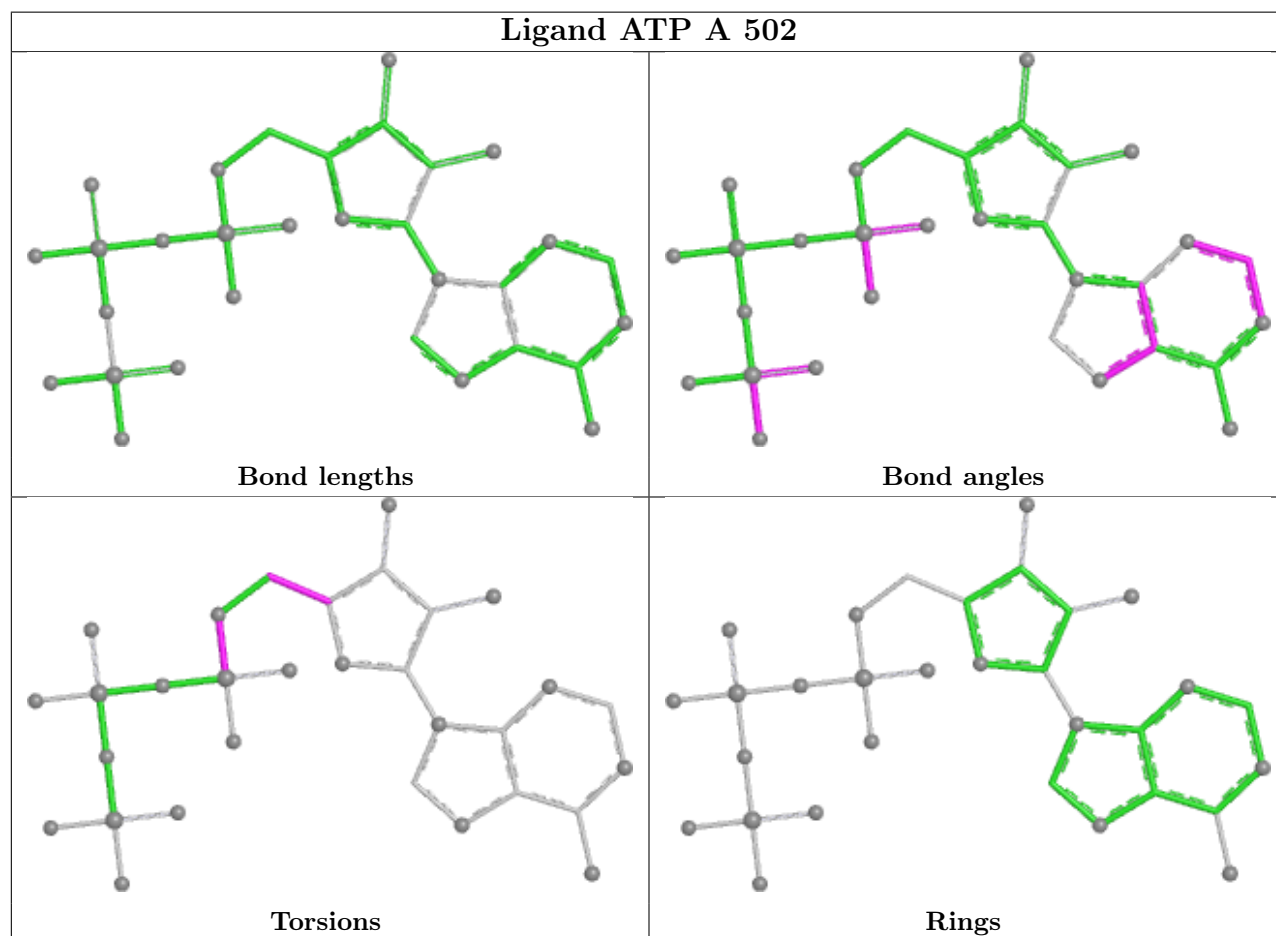
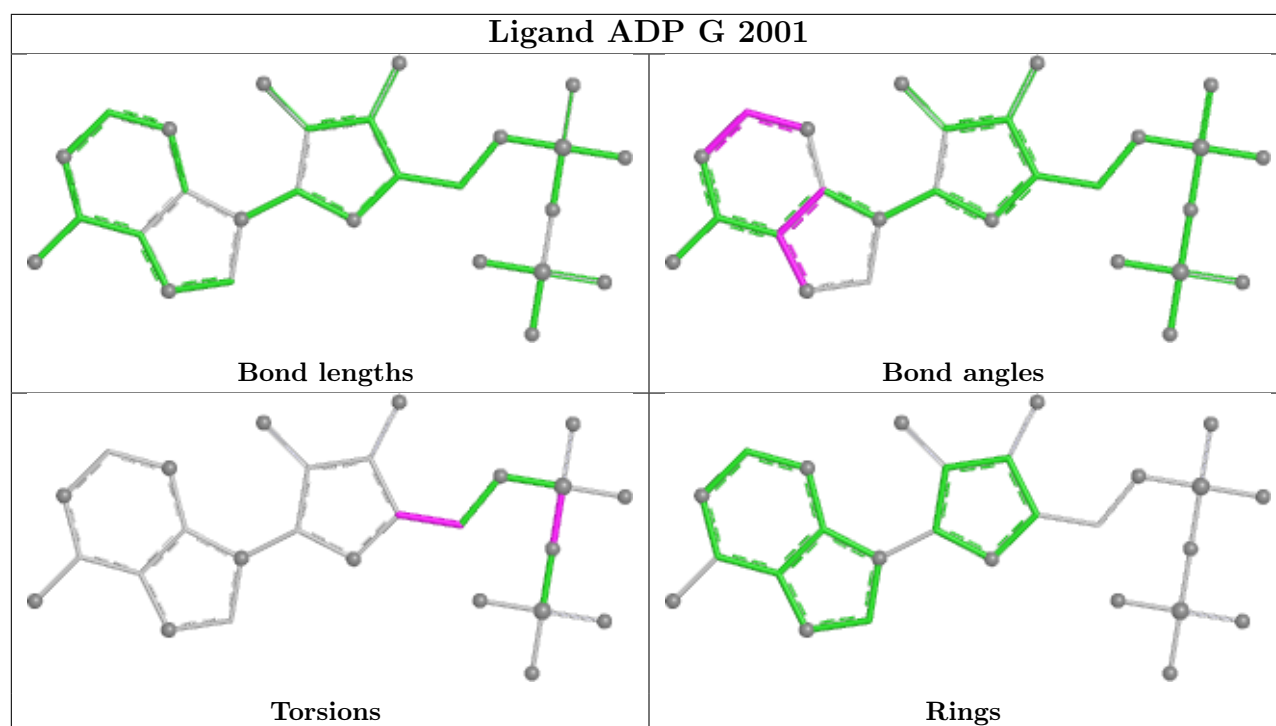
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | A | 501 | ATP | 3 | 0 |
| 3 | E | 2004 | ATP | 5 | 0 |
| 4 | F | 2001 | ADP | 2 | 0 |
| 4 | G | 2001 | ADP | 2 | 0 |
| 3 | A | 502 | ATP | 5 | 0 |
| 4 | H | 2001 | ADP | 2 | 0 |
| 3 | D | 501 | ATP | 4 | 0 |
| 3 | F | 2004 | ATP | 2 | 0 |
| 3 | C | 501 | ATP | 3 | 0 |
| 3 | G | 2004 | ATP | 4 | 0 |

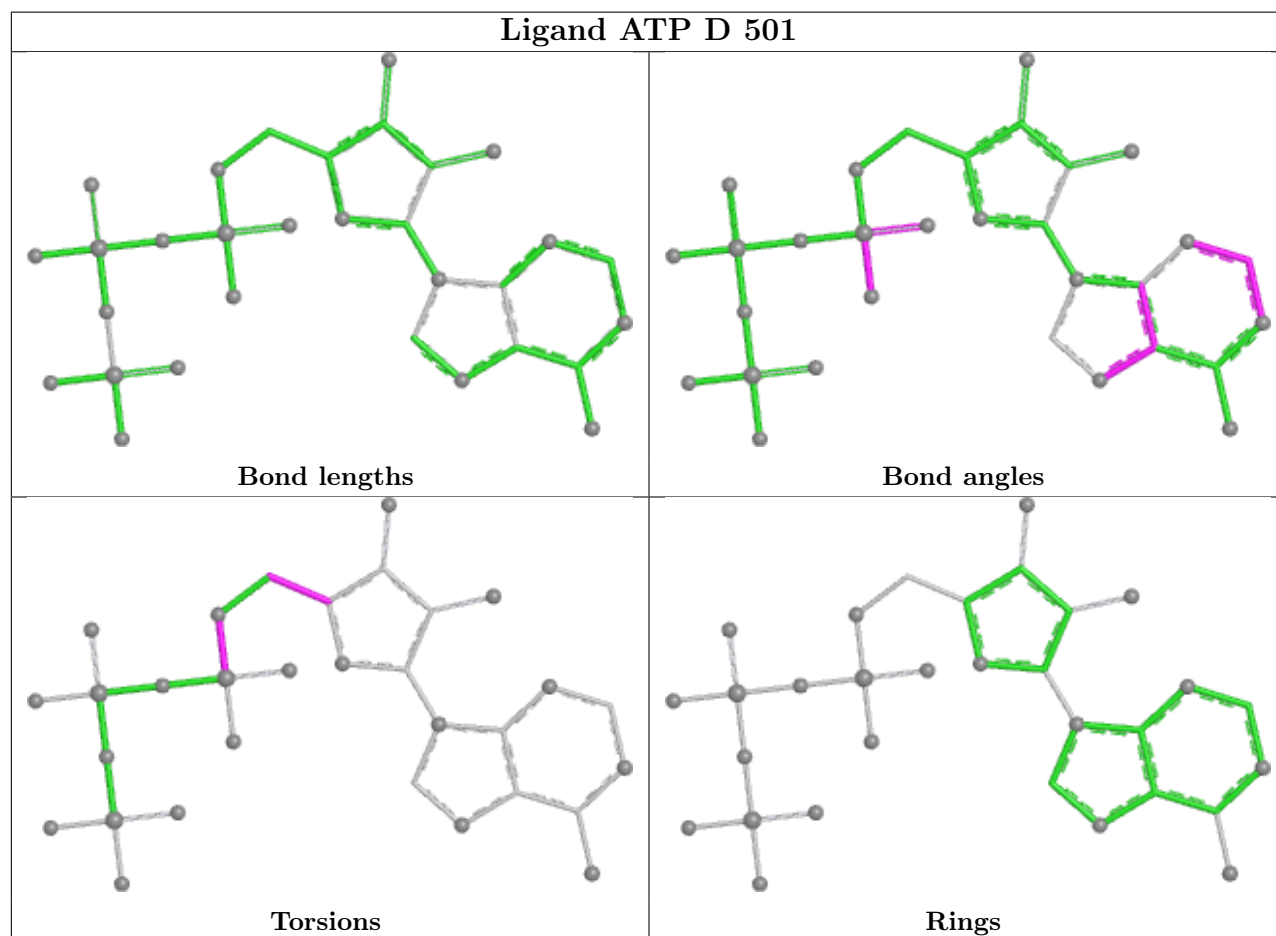
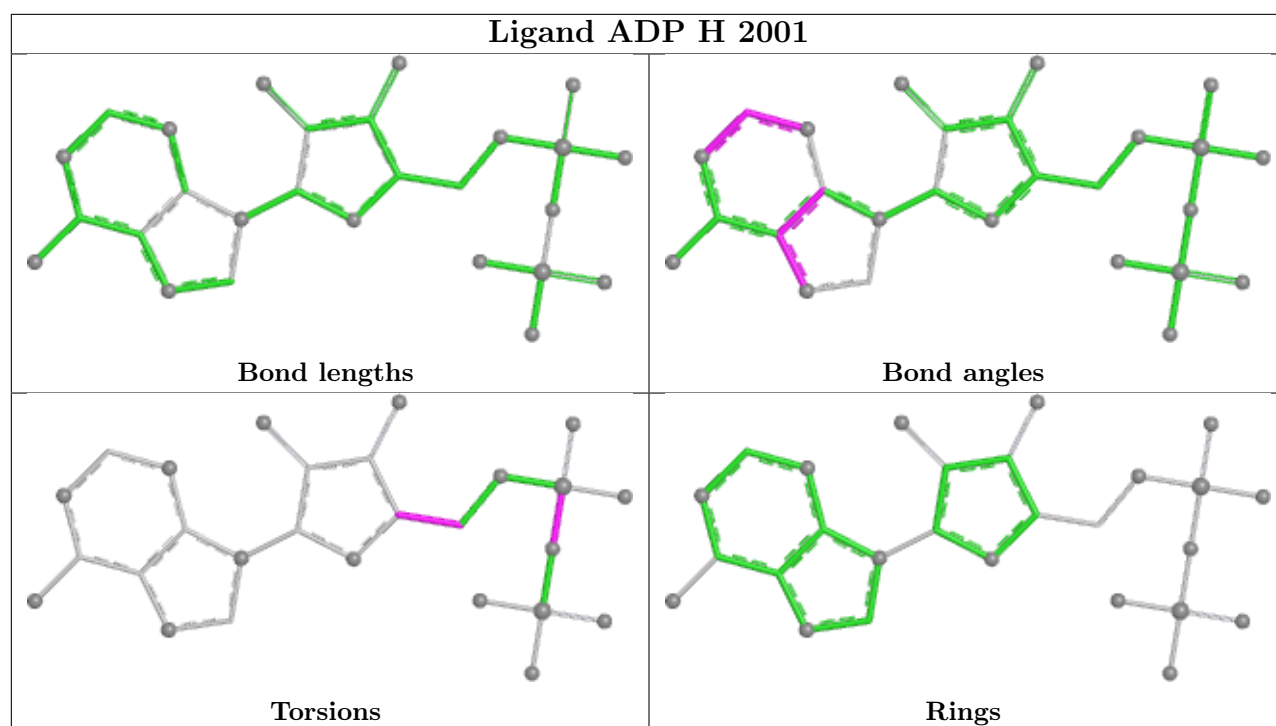
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

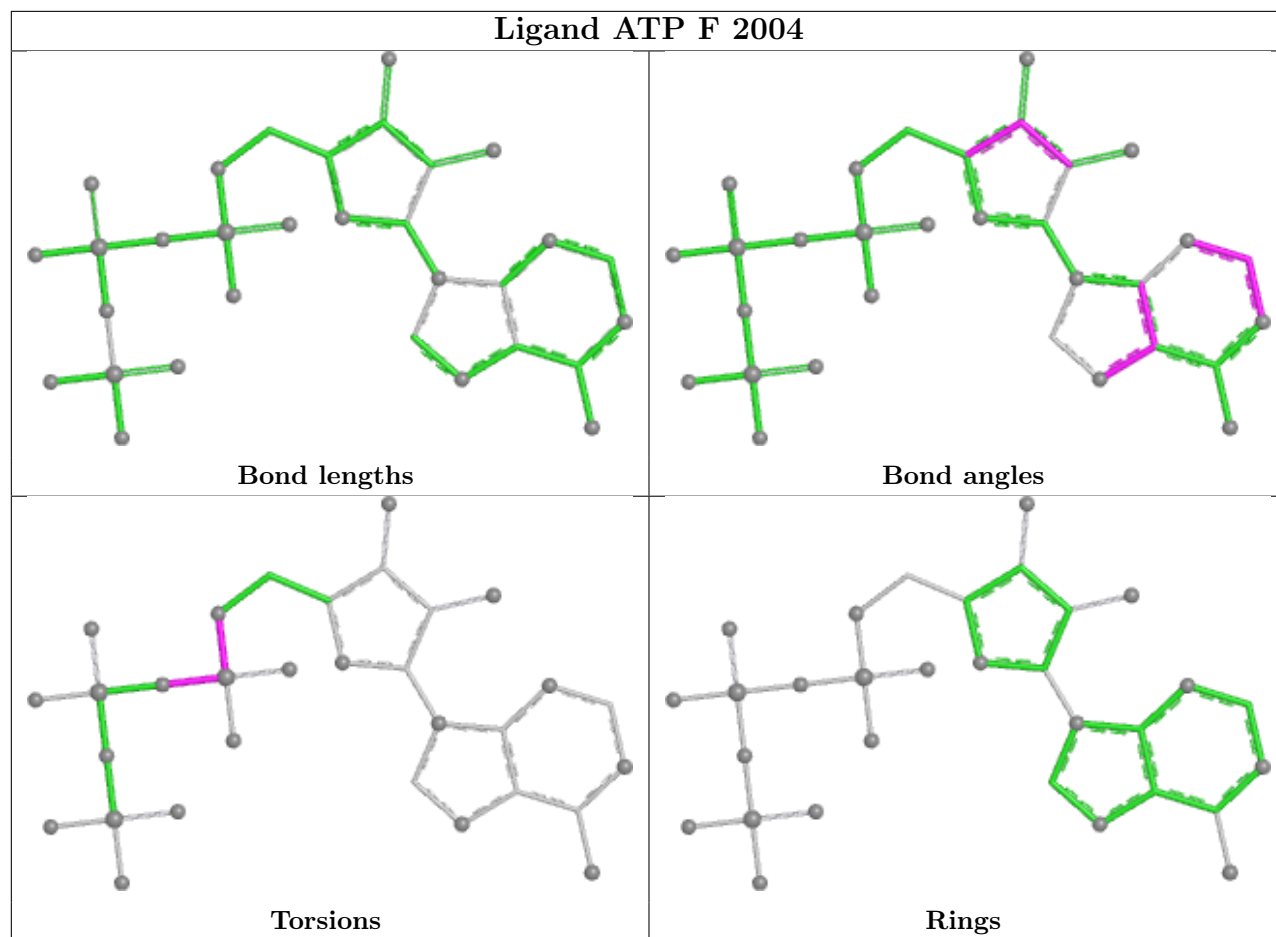


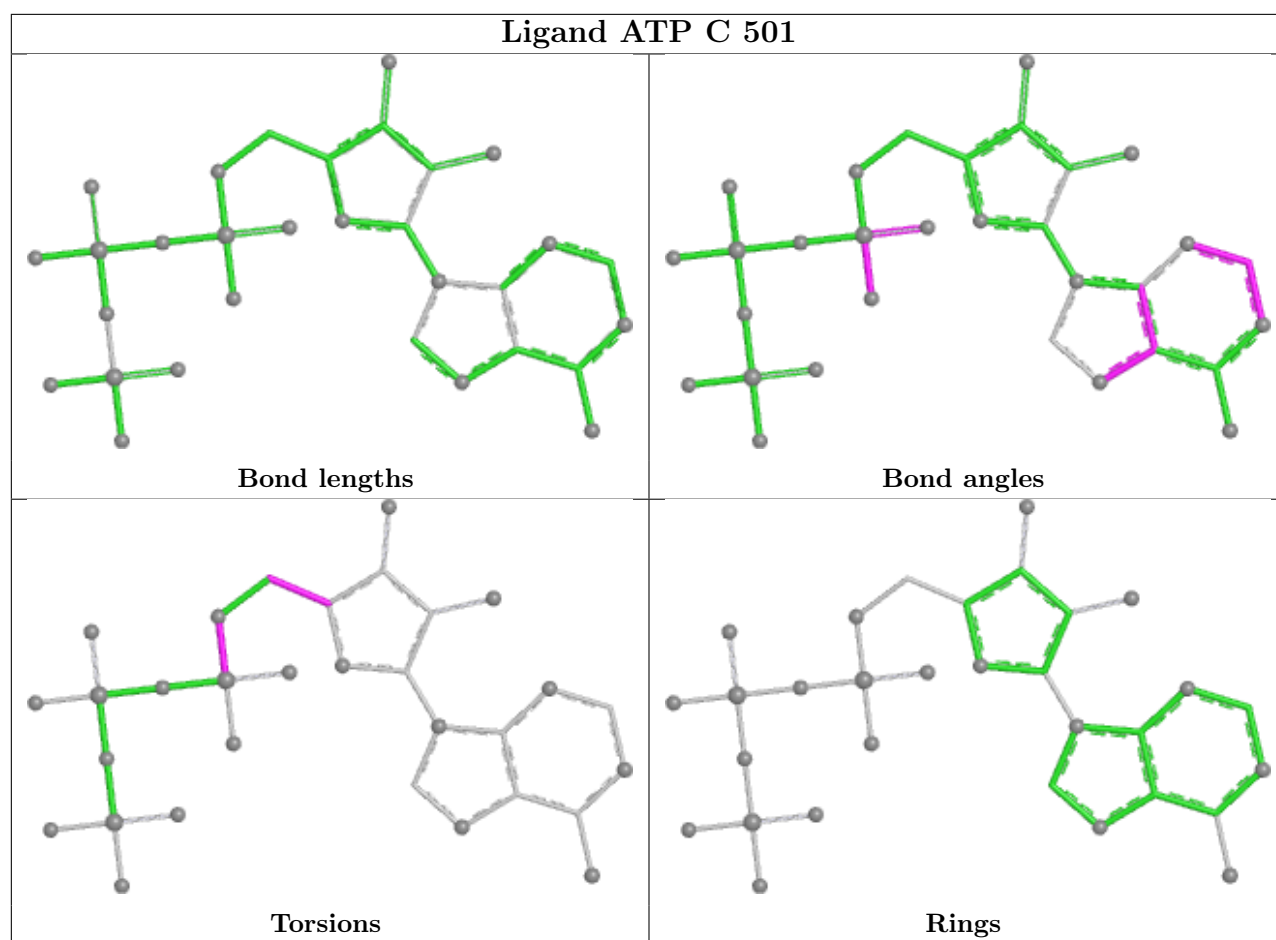


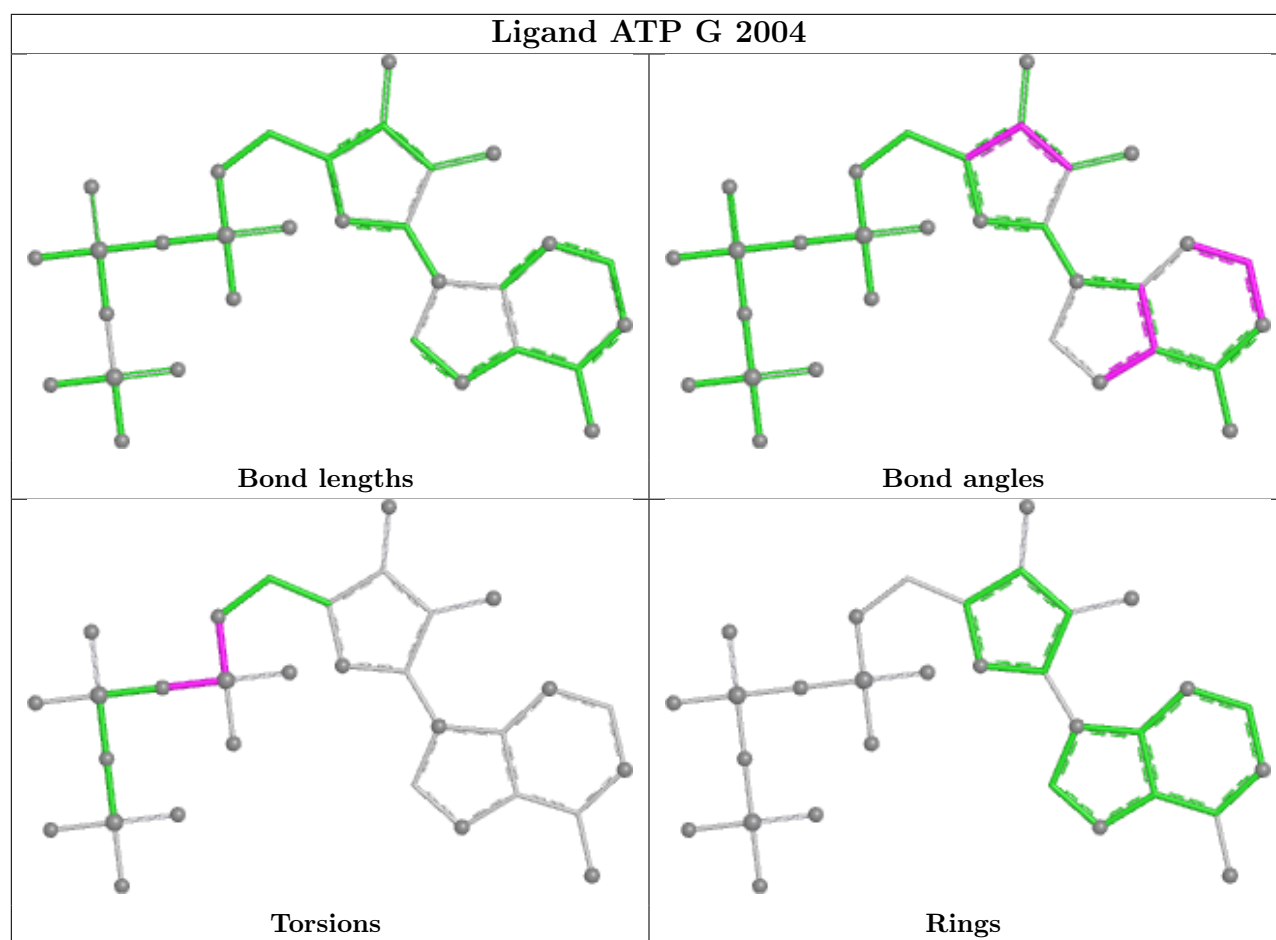












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

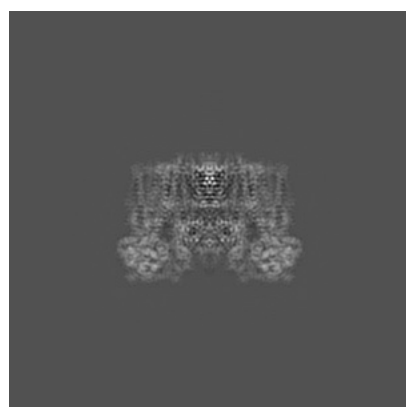
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7339. These allow visual inspection of the internal detail of the map and identification of artifacts.

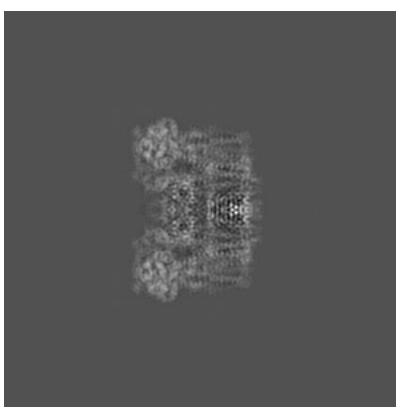
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

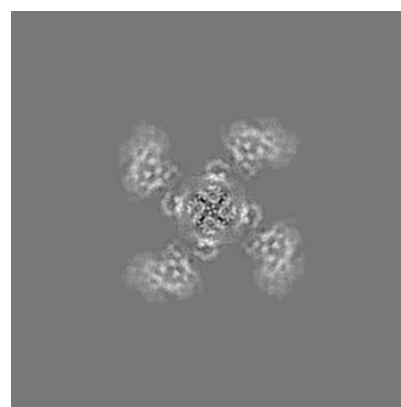
6.1.1 Primary map



X



Y

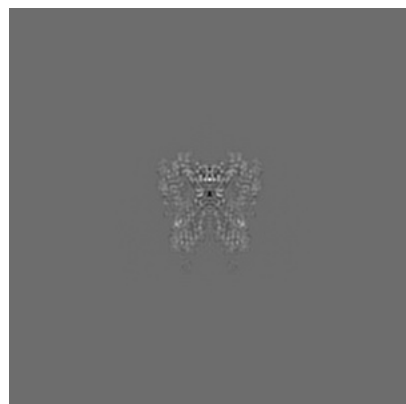


Z

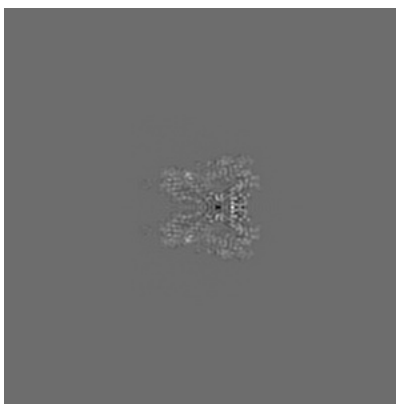
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

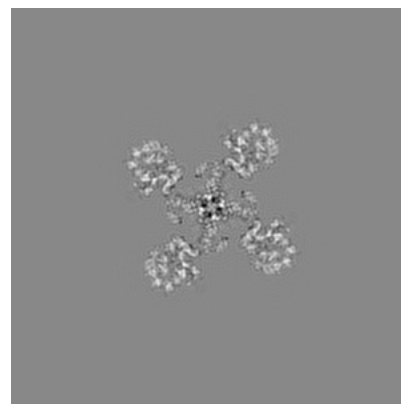
6.2.1 Primary map



X Index: 150



Y Index: 150

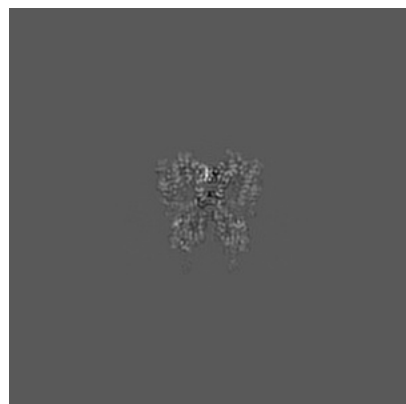


Z Index: 150

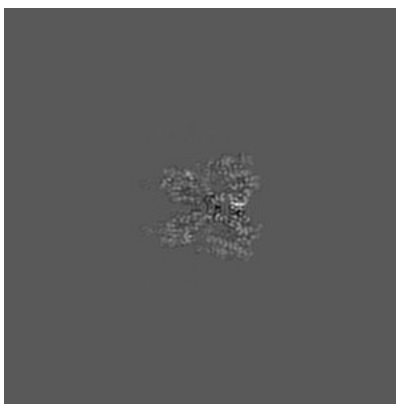
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

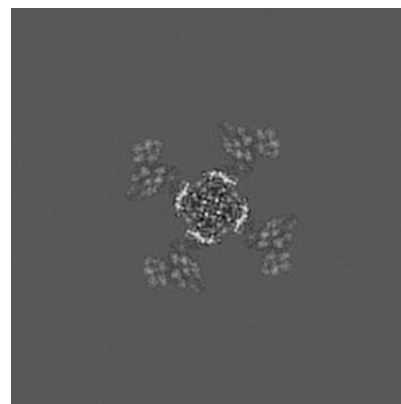
6.3.1 Primary map



X Index: 149



Y Index: 149

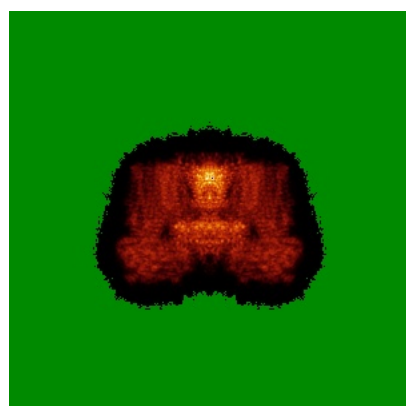


Z Index: 138

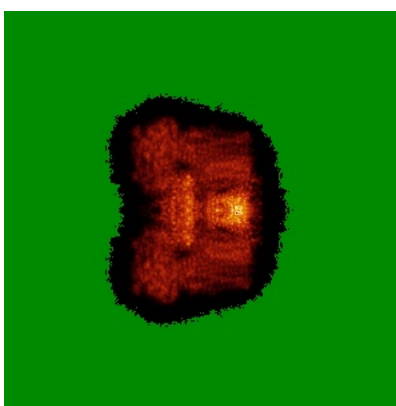
The images above show the largest variance slices of the map in three orthogonal directions.

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

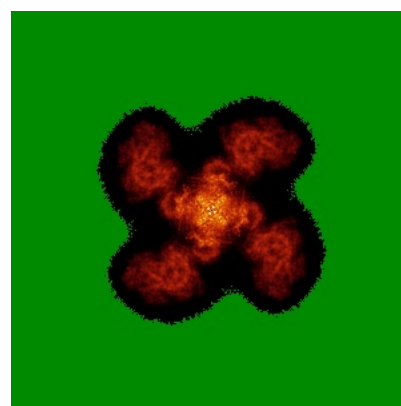
6.4.1 Primary map



X



Y

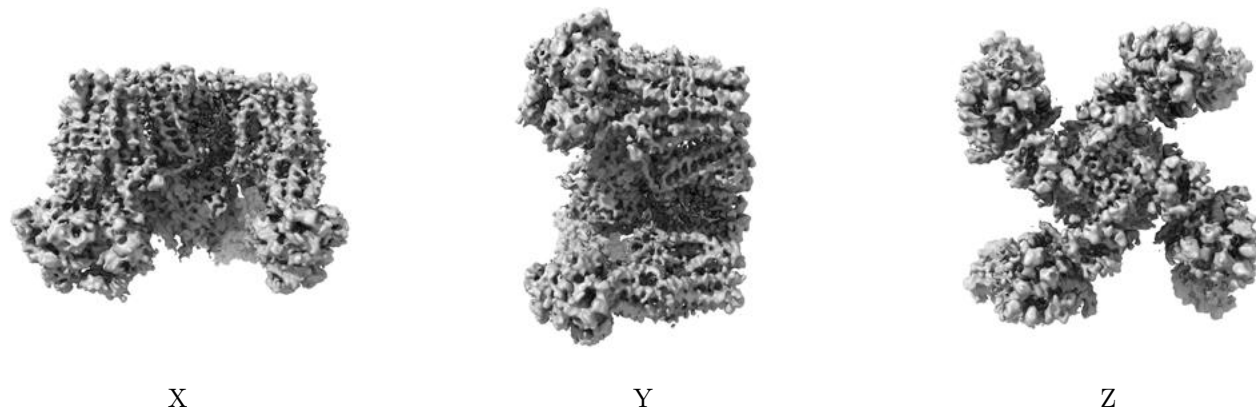


Z

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 0.0343. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

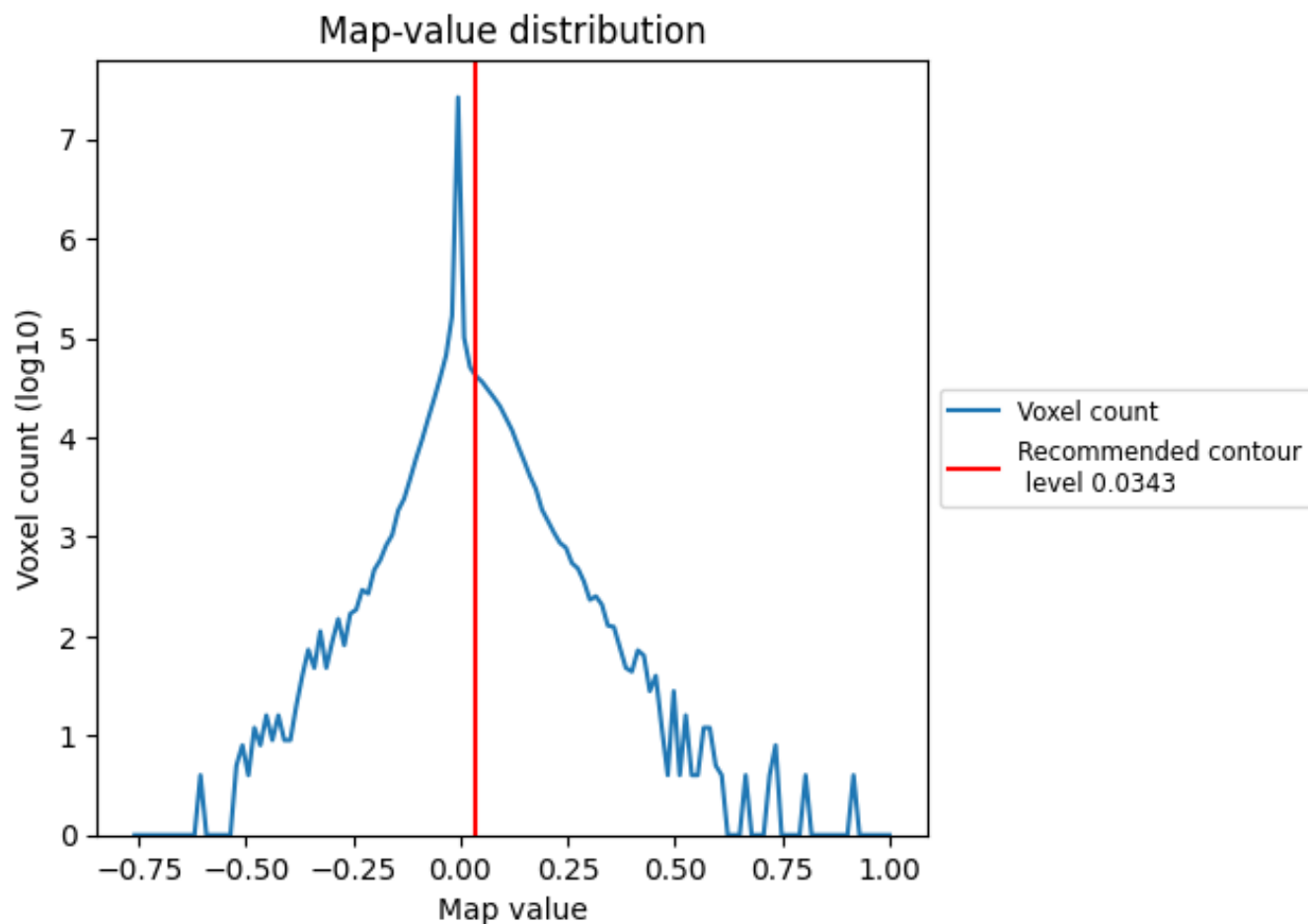
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

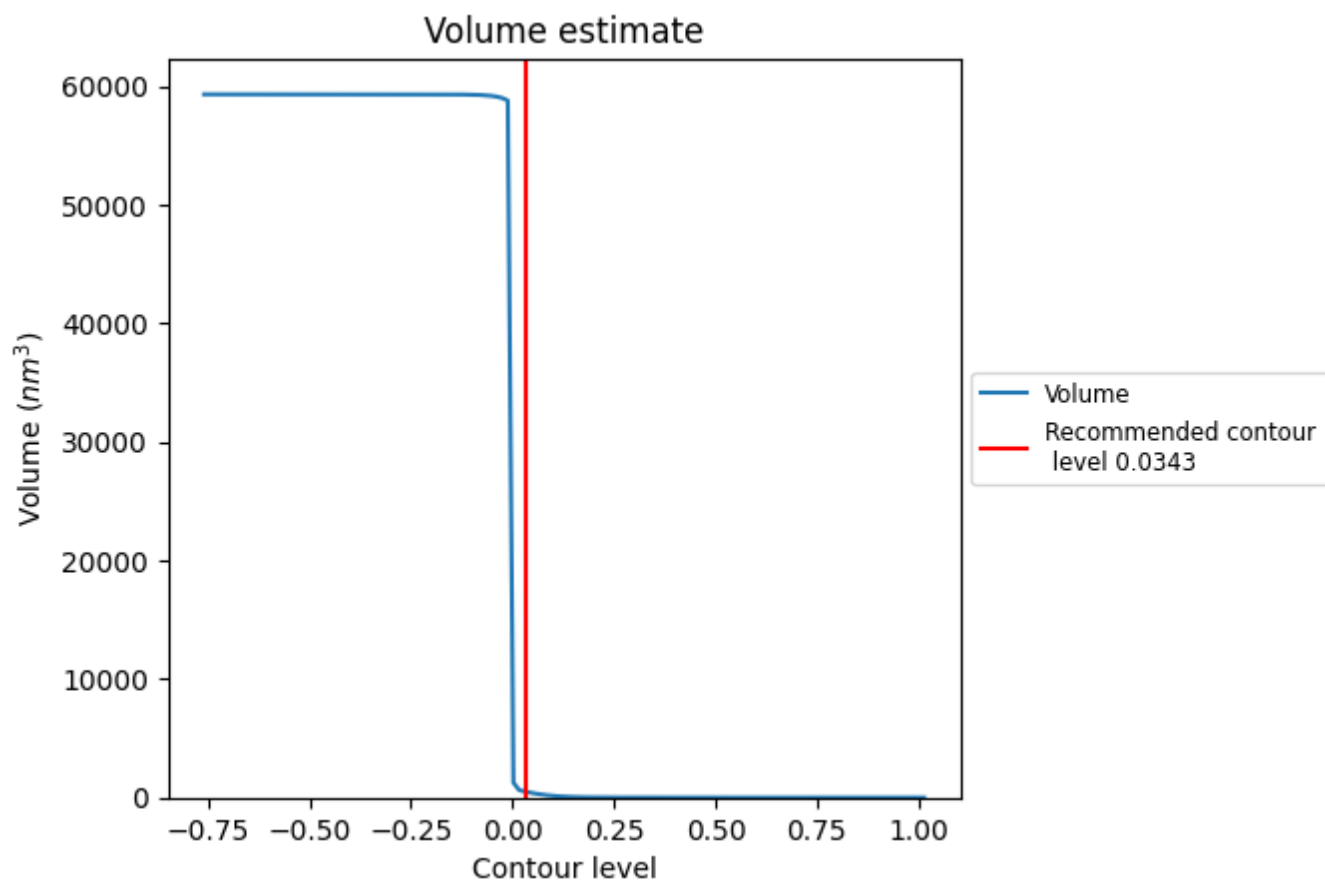
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

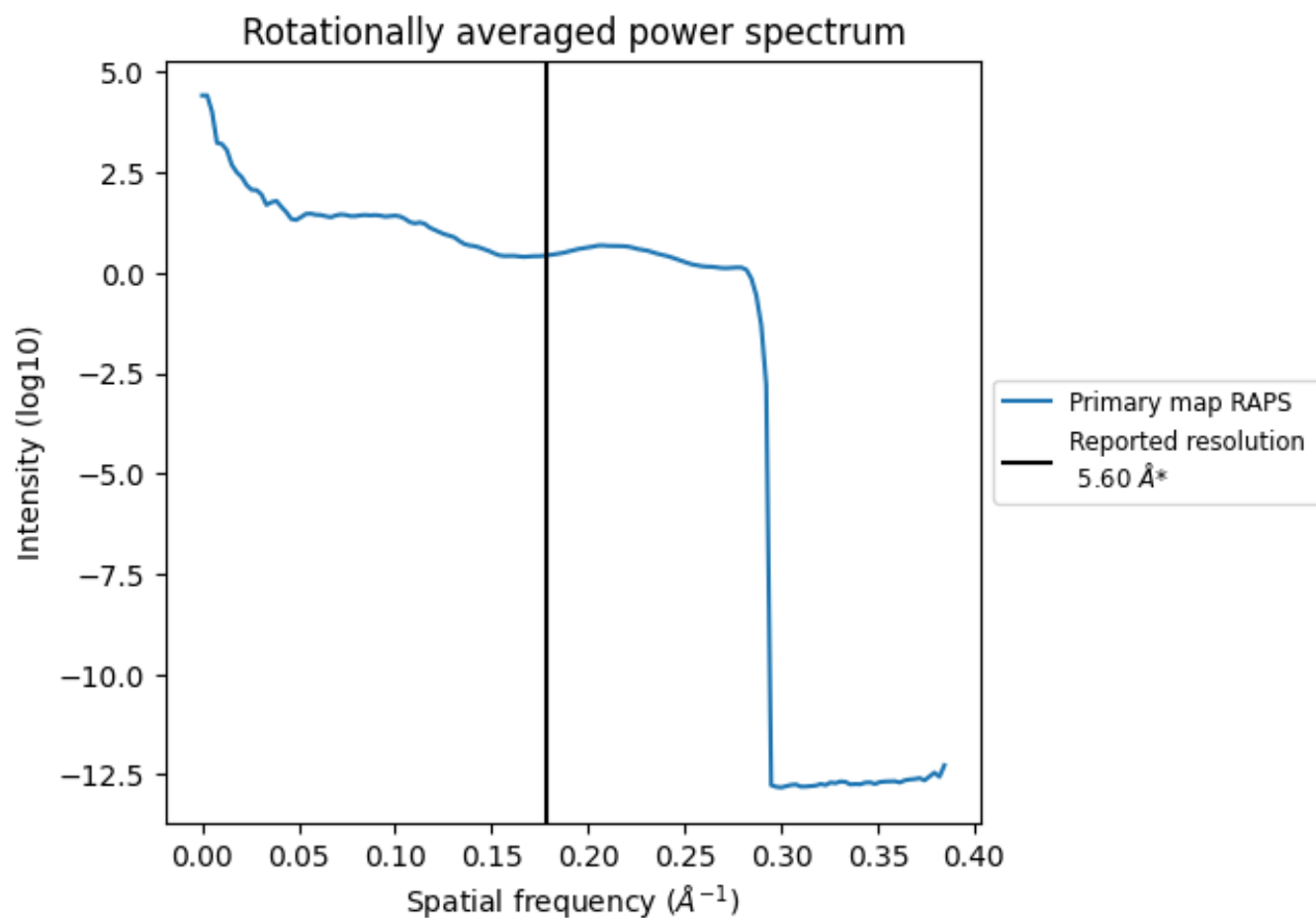
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 479 nm^3 ; this corresponds to an approximate mass of 433 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

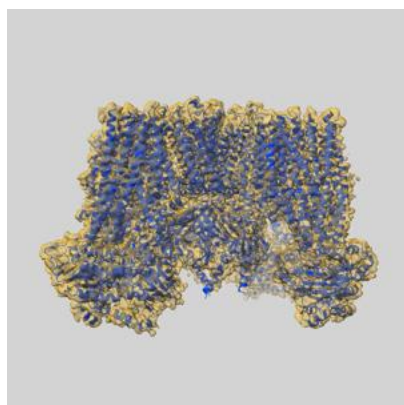
8 Fourier-Shell correlation ⓘ

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

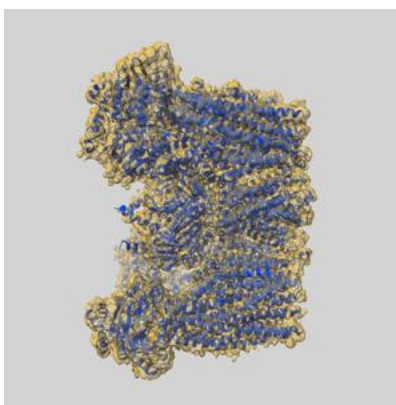
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7339 and PDB model 6C3P. Per-residue inclusion information can be found in section [3](#) on page [8](#).

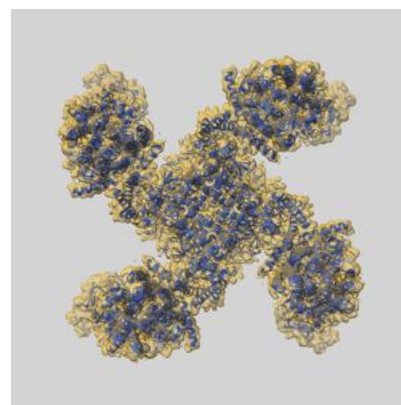
9.1 Map-model overlay [i](#)



X



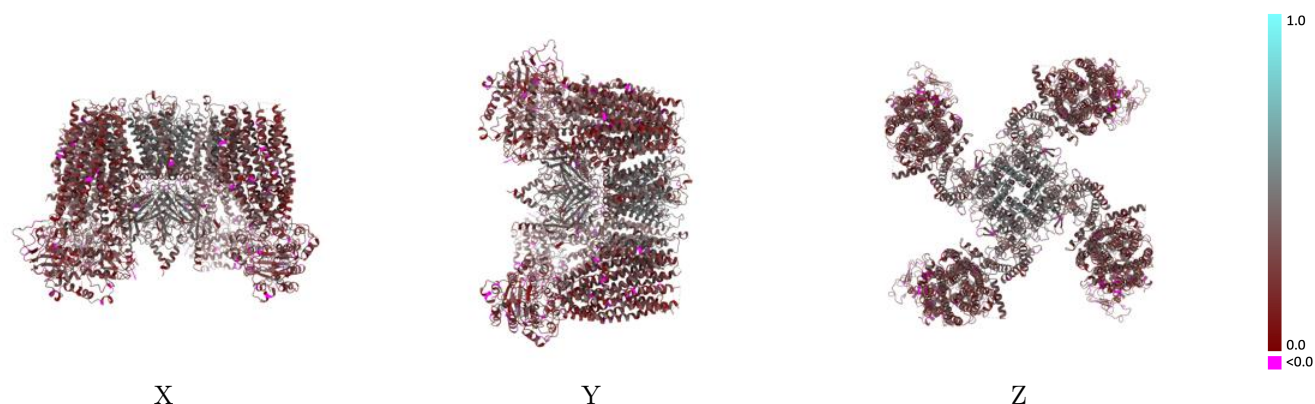
Y



Z

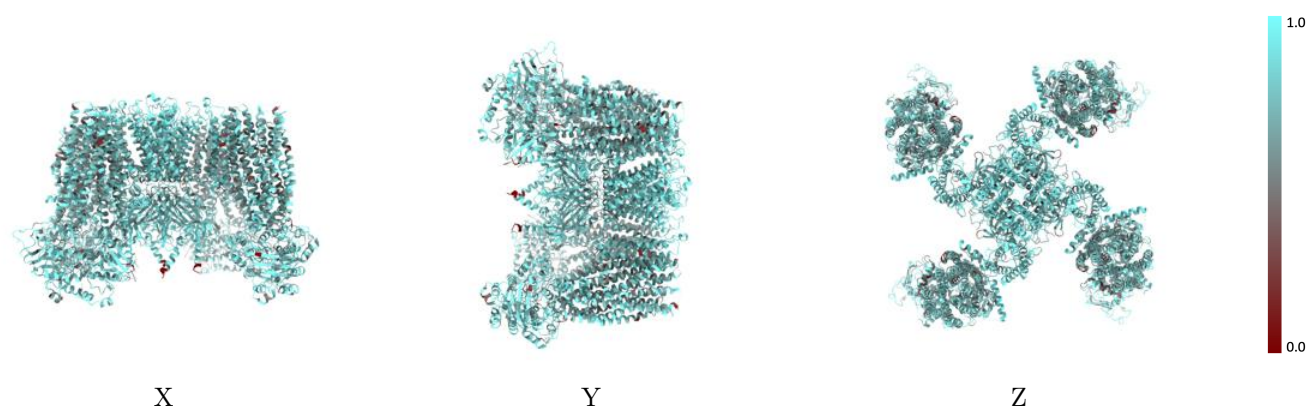
The images above show the 3D surface view of the map at the recommended contour level 0.0343 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



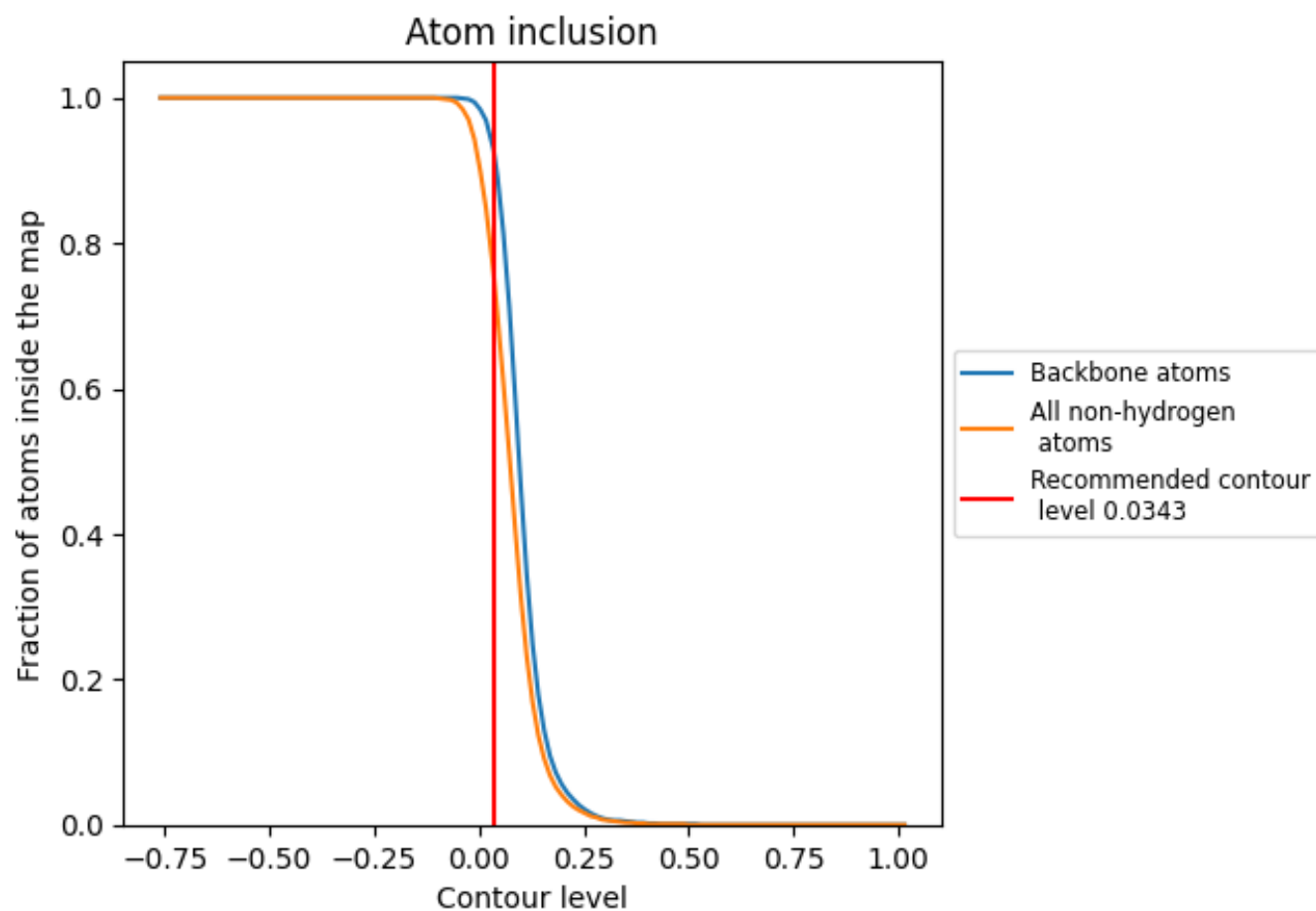
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0343).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0343) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|-------------------------------|-------------------------------|
| All | <div><div></div></div> 0.7590 | <div><div></div></div> 0.2940 |
| A | <div><div></div></div> 0.8320 | <div><div></div></div> 0.3920 |
| B | <div><div></div></div> 0.8270 | <div><div></div></div> 0.3930 |
| C | <div><div></div></div> 0.8310 | <div><div></div></div> 0.3920 |
| D | <div><div></div></div> 0.8350 | <div><div></div></div> 0.3950 |
| E | <div><div></div></div> 0.7420 | <div><div></div></div> 0.2720 |
| F | <div><div></div></div> 0.7420 | <div><div></div></div> 0.2680 |
| G | <div><div></div></div> 0.7420 | <div><div></div></div> 0.2710 |
| H | <div><div></div></div> 0.7400 | <div><div></div></div> 0.2670 |

1.0

0.0

<0.0