



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 13, 2017 – 12:06 PM EST

PDB ID : 5KEP
EMDB ID: : EMDB-6620
Title : High resolution cryo-EM maps of Human Papillomavirus 16 reveal L2 location and heparin-induced conformational changes
Authors : Guan, J.; Bywaters, S.M.; Brendle, S.A.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Christensen, N.D.; Hafenstein, S.
Deposited on : 2016-06-10
Resolution : 4.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

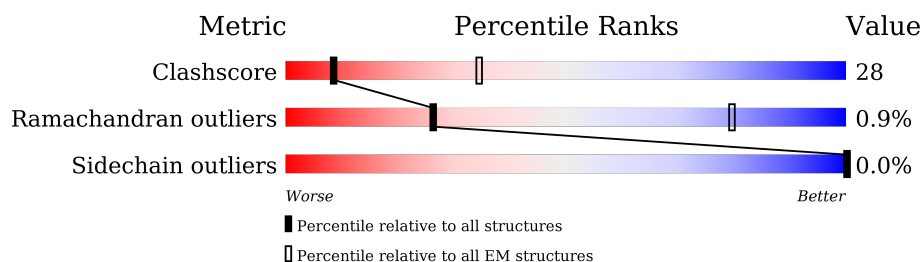
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 483 | |
| 1 | B | 483 | |
| 1 | C | 483 | |
| 1 | D | 483 | |
| 1 | E | 483 | |
| 1 | F | 483 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22267 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.

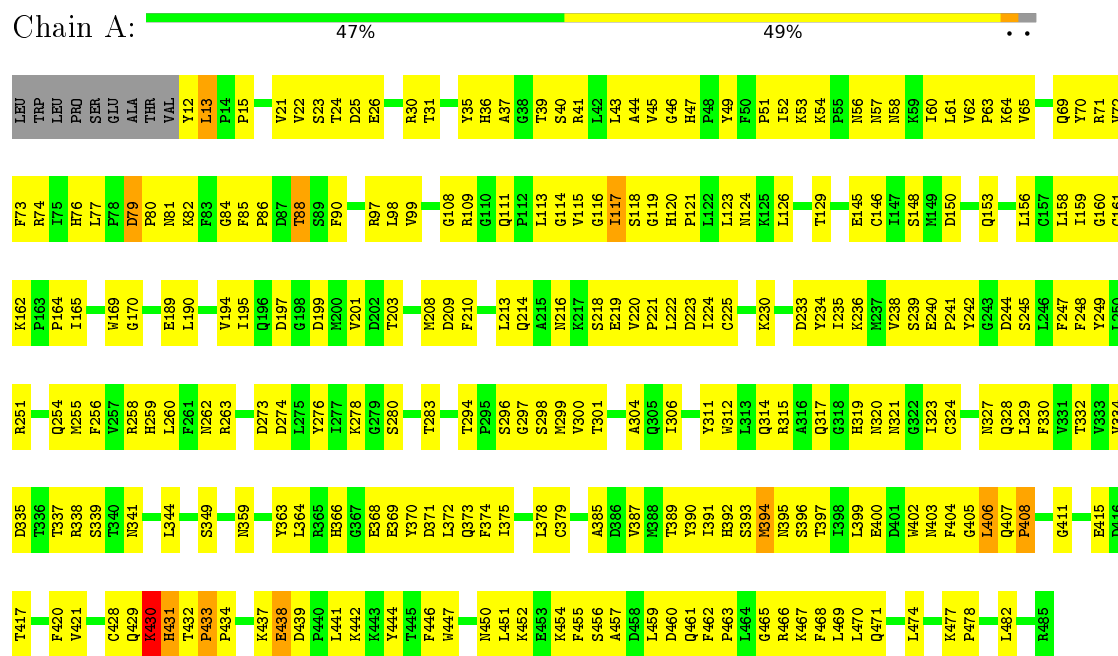
- Molecule 1 is a protein called Major capsid protein L1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 474 | Total | C | N | O | S | 0 | 0 |
| | | | 3725 | 2380 | 627 | 697 | 21 | | |
| 1 | B | 463 | Total | C | N | O | S | 0 | 0 |
| | | | 3638 | 2321 | 612 | 684 | 21 | | |
| 1 | C | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3705 | 2368 | 621 | 695 | 21 | | |
| 1 | D | 471 | Total | C | N | O | S | 0 | 0 |
| | | | 3700 | 2365 | 620 | 694 | 21 | | |
| 1 | E | 482 | Total | C | N | O | S | 0 | 0 |
| | | | 3785 | 2422 | 633 | 709 | 21 | | |
| 1 | F | 473 | Total | C | N | O | S | 0 | 0 |
| | | | 3714 | 2373 | 622 | 698 | 21 | | |

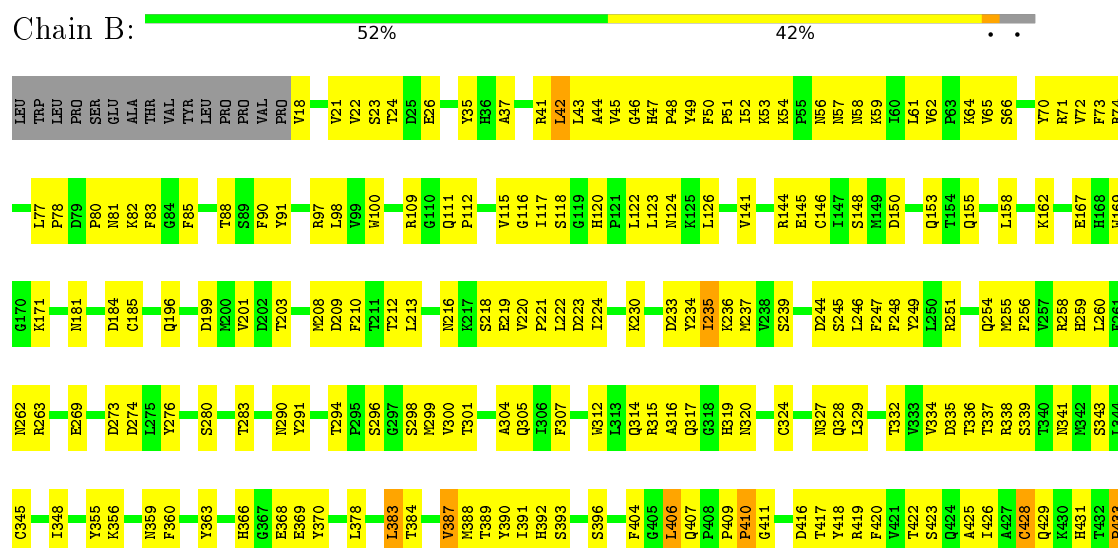
3 Residue-property plots

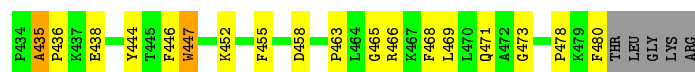
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: Major capsid protein L1



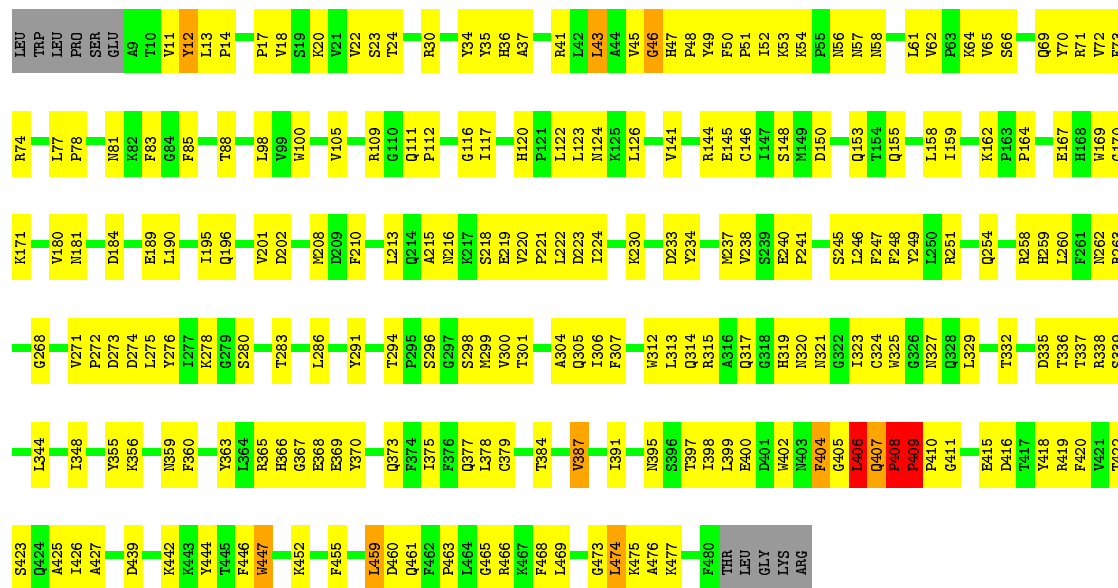
• Molecule 1: Major capsid protein L1





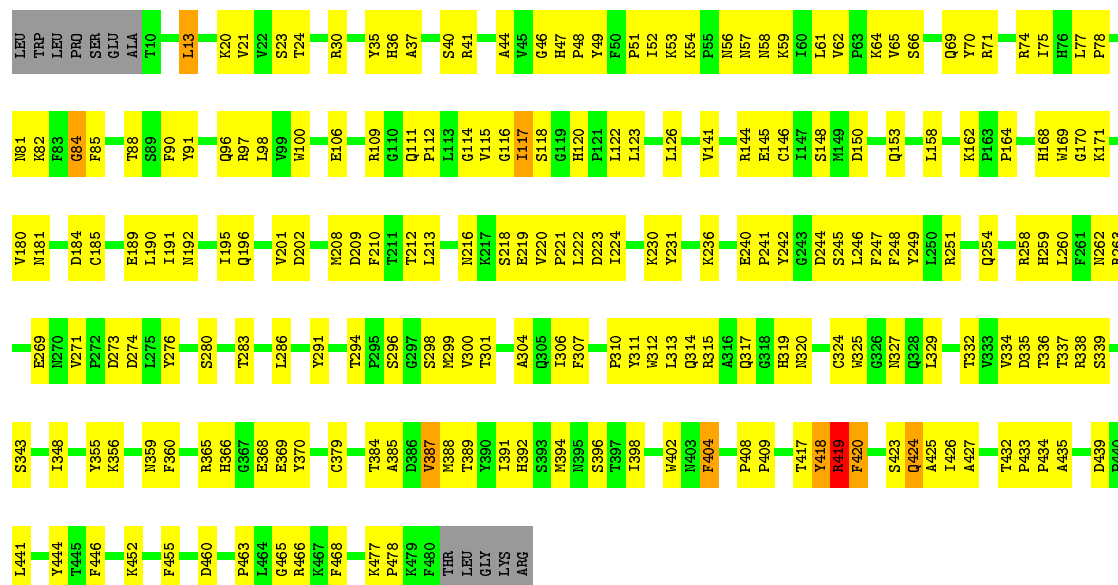
• Molecule 1: Major capsid protein L1

Chain C: 52% 43%



• Molecule 1: Major capsid protein L1

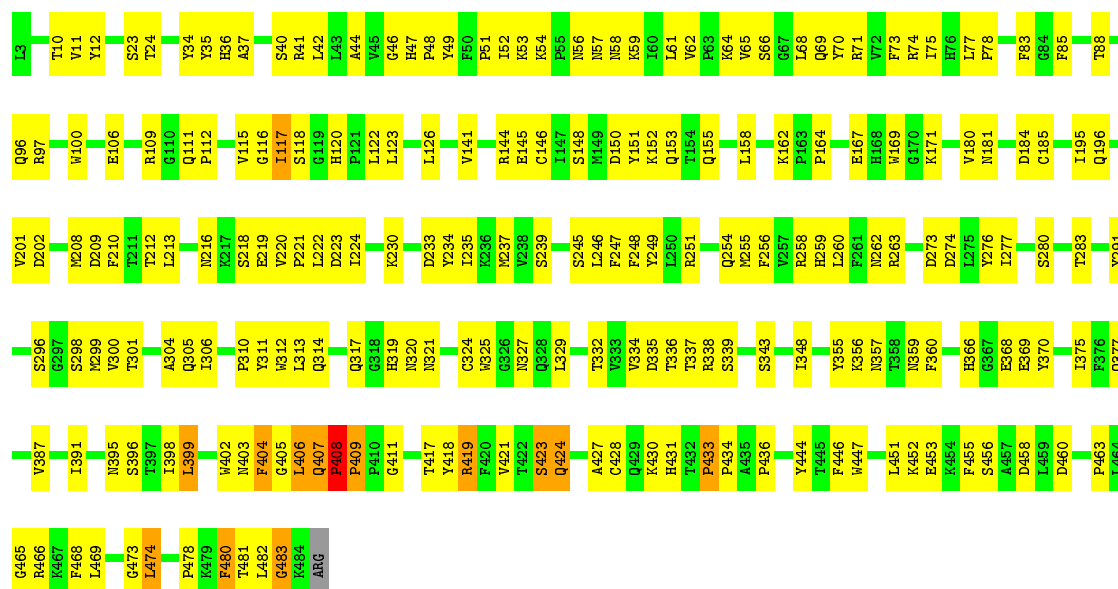
Chain D: 54% 41%



• Molecule 1: Major capsid protein L1

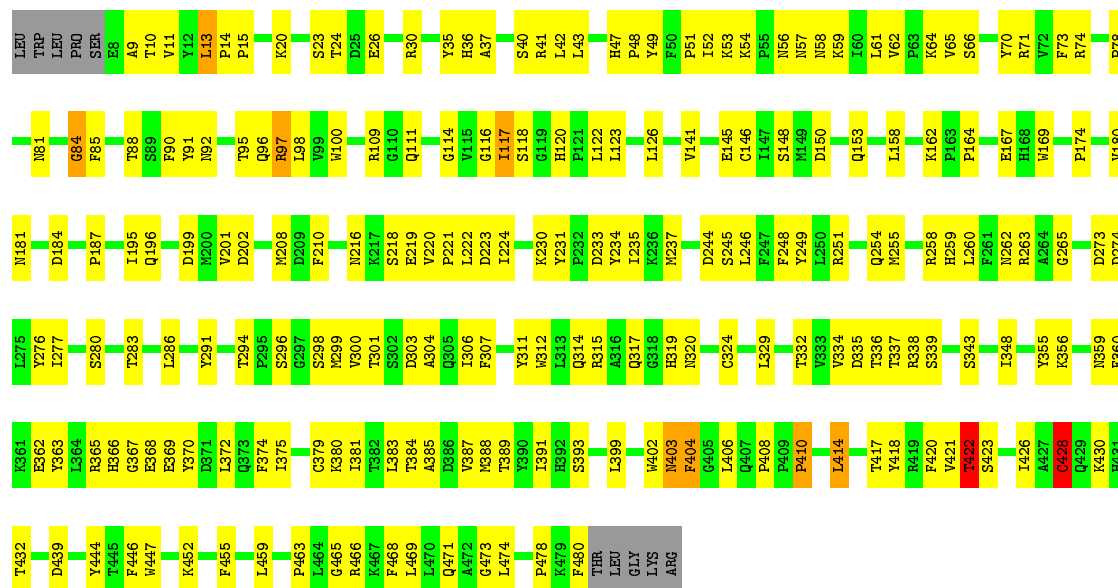
Chain E: 56% 41%





• Molecule 1: Major capsid protein L1

Chain F: 55% 41%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 57556 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.50 | 0/3827 | 0.66 | 4/5209 (0.1%) |
| 1 | B | 0.62 | 4/3736 (0.1%) | 0.69 | 5/5083 (0.1%) |
| 1 | C | 0.66 | 4/3807 (0.1%) | 0.70 | 5/5185 (0.1%) |
| 1 | D | 0.65 | 3/3802 (0.1%) | 0.73 | 6/5178 (0.1%) |
| 1 | E | 0.63 | 1/3890 (0.0%) | 0.65 | 5/5299 (0.1%) |
| 1 | F | 0.60 | 2/3816 (0.1%) | 0.68 | 6/5197 (0.1%) |
| All | All | 0.61 | 14/22878 (0.1%) | 0.69 | 31/31151 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 11 |
| 1 | B | 0 | 6 |
| 1 | C | 0 | 4 |
| 1 | D | 0 | 7 |
| 1 | E | 0 | 11 |
| 1 | F | 0 | 3 |
| All | All | 0 | 42 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | D | 435 | ALA | C-N | -10.16 | 1.15 | 1.34 |
| 1 | F | 404 | PHE | CE1-CZ | -9.70 | 1.19 | 1.37 |
| 1 | C | 46 | GLY | C-N | -8.66 | 1.14 | 1.34 |
| 1 | B | 447 | TRP | CB-CG | -8.18 | 1.35 | 1.50 |
| 1 | E | 407 | GLN | C-O | 7.07 | 1.36 | 1.23 |
| 1 | F | 404 | PHE | CG-CD1 | -7.02 | 1.28 | 1.38 |
| 1 | B | 447 | TRP | CE2-CZ2 | -6.89 | 1.28 | 1.39 |
| 1 | C | 404 | PHE | CB-CG | -6.85 | 1.39 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 408 | PRO | CB-CG | -6.57 | 1.17 | 1.50 |
| 1 | D | 84 | GLY | C-N | -5.88 | 1.20 | 1.34 |
| 1 | D | 420 | PHE | CB-CG | -5.82 | 1.41 | 1.51 |
| 1 | B | 428 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 1 | C | 447 | TRP | CB-CG | -5.32 | 1.40 | 1.50 |
| 1 | B | 447 | TRP | CE3-CZ3 | -5.21 | 1.29 | 1.38 |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | D | 419 | ARG | NE-CZ-NH2 | 17.08 | 128.84 | 120.30 |
| 1 | B | 42 | LEU | CA-CB-CG | 15.47 | 150.89 | 115.30 |
| 1 | B | 383 | LEU | CB-CG-CD1 | -10.49 | 93.16 | 111.00 |
| 1 | E | 405 | GLY | N-CA-C | -9.03 | 90.52 | 113.10 |
| 1 | F | 428 | CYS | CA-CB-SG | -8.46 | 98.76 | 114.00 |
| 1 | D | 13 | LEU | CA-CB-CG | -8.46 | 95.84 | 115.30 |
| 1 | C | 43 | LEU | CA-CB-CG | 7.85 | 133.36 | 115.30 |
| 1 | F | 13 | LEU | CB-CG-CD1 | -7.83 | 97.68 | 111.00 |
| 1 | C | 406 | LEU | CA-CB-CG | 7.76 | 133.16 | 115.30 |
| 1 | B | 383 | LEU | CA-CB-CG | 7.72 | 133.05 | 115.30 |
| 1 | C | 476 | ALA | N-CA-C | -7.53 | 90.68 | 111.00 |
| 1 | E | 474 | LEU | CA-CB-CG | 7.12 | 131.68 | 115.30 |
| 1 | D | 419 | ARG | NH1-CZ-NH2 | -6.90 | 111.81 | 119.40 |
| 1 | E | 408 | PRO | N-CA-C | 6.82 | 129.84 | 112.10 |
| 1 | A | 79 | ASP | CB-CG-OD1 | 6.52 | 124.17 | 118.30 |
| 1 | D | 420 | PHE | CB-CA-C | -6.28 | 97.84 | 110.40 |
| 1 | C | 474 | LEU | CA-CB-CG | 5.87 | 128.79 | 115.30 |
| 1 | F | 13 | LEU | CA-CB-CG | 5.81 | 128.66 | 115.30 |
| 1 | F | 414 | LEU | CA-CB-CG | -5.71 | 102.17 | 115.30 |
| 1 | F | 97 | ARG | CG-CD-NE | 5.67 | 123.72 | 111.80 |
| 1 | B | 428 | CYS | CA-CB-SG | 5.61 | 124.11 | 114.00 |
| 1 | A | 430 | LYS | N-CA-C | -5.39 | 96.45 | 111.00 |
| 1 | C | 459 | LEU | CA-CB-CG | -5.37 | 102.94 | 115.30 |
| 1 | E | 483 | GLY | N-CA-C | -5.33 | 99.78 | 113.10 |
| 1 | A | 482 | LEU | C-N-CA | -5.33 | 111.11 | 122.30 |
| 1 | B | 411 | GLY | N-CA-C | 5.20 | 126.09 | 113.10 |
| 1 | D | 419 | ARG | CG-CD-NE | 5.18 | 122.68 | 111.80 |
| 1 | E | 399 | LEU | CB-CG-CD1 | -5.10 | 102.33 | 111.00 |
| 1 | D | 84 | GLY | C-N-CA | 5.09 | 134.43 | 121.70 |
| 1 | F | 84 | GLY | C-N-CA | 5.06 | 134.35 | 121.70 |
| 1 | A | 378 | LEU | CB-CG-CD1 | -5.04 | 102.43 | 111.00 |

There are no chirality outliers.

All (42) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 13 | LEU | Peptide |
| 1 | A | 15 | PRO | Peptide |
| 1 | A | 408 | PRO | Peptide |
| 1 | A | 415 | GLU | Peptide |
| 1 | A | 417 | THR | Peptide |
| 1 | A | 429 | GLN | Peptide |
| 1 | A | 430 | LYS | Peptide |
| 1 | A | 431 | HIS | Peptide |
| 1 | A | 433 | PRO | Peptide |
| 1 | A | 438 | GLU | Peptide |
| 1 | A | 88 | THR | Peptide |
| 1 | B | 406 | LEU | Peptide |
| 1 | B | 423 | SER | Peptide |
| 1 | B | 425 | ALA | Peptide |
| 1 | B | 428 | CYS | Peptide |
| 1 | B | 433 | PRO | Peptide |
| 1 | B | 435 | ALA | Peptide |
| 1 | C | 12 | TYR | Peptide |
| 1 | C | 17 | PRO | Peptide |
| 1 | C | 409 | PRO | Peptide |
| 1 | C | 475 | LYS | Peptide |
| 1 | D | 404 | PHE | Peptide |
| 1 | D | 418 | TYR | Peptide |
| 1 | D | 419 | ARG | Peptide |
| 1 | D | 420 | PHE | Peptide |
| 1 | D | 424 | GLN | Peptide |
| 1 | D | 425 | ALA | Peptide |
| 1 | D | 477 | LYS | Peptide |
| 1 | E | 10 | THR | Peptide |
| 1 | E | 403 | ASN | Peptide |
| 1 | E | 404 | PHE | Peptide |
| 1 | E | 406 | LEU | Peptide |
| 1 | E | 408 | PRO | Peptide |
| 1 | E | 418 | TYR | Peptide |
| 1 | E | 419 | ARG | Peptide |
| 1 | E | 423 | SER | Peptide |
| 1 | E | 433 | PRO | Peptide |
| 1 | E | 434 | PRO | Peptide |
| 1 | E | 480 | PHE | Peptide |
| 1 | F | 406 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | F | 422 | THR | Peptide |
| 1 | F | 428 | CYS | 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 | 3725 | 0 | 3648 | 231 | 0 |
| 1 | B | 3638 | 0 | 3551 | 221 | 0 |
| 1 | C | 3705 | 0 | 3621 | 251 | 0 |
| 1 | D | 3700 | 0 | 3616 | 201 | 0 |
| 1 | E | 3785 | 0 | 3706 | 211 | 0 |
| 1 | F | 3714 | 0 | 3628 | 215 | 0 |
| All | All | 22267 | 0 | 21770 | 1225 | 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 28.

All (1225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:404:PHE:HB2 | 1:C:405:GLY:HA2 | 1.34 | 1.08 |
| 1:C:400:GLU:HA | 1:C:404:PHE:CZ | 1.97 | 1.00 |
| 1:D:97:ARG:HH22 | 1:D:404:PHE:HB2 | 1.26 | 0.98 |
| 1:A:46:GLY:HA3 | 1:A:65:VAL:HB | 1.47 | 0.95 |
| 1:B:44:ALA:HB3 | 1:B:368:GLU:HB2 | 1.46 | 0.95 |
| 1:E:399:LEU:HB3 | 1:E:404:PHE:CZ | 2.01 | 0.94 |
| 1:C:406:LEU:C | 1:C:408:PRO:HA | 1.87 | 0.93 |
| 1:A:407:GLN:HB2 | 1:A:411:GLY:HA2 | 1.49 | 0.93 |
| 1:E:424:GLN:NE2 | 1:E:428:CYS:O | 2.01 | 0.93 |
| 1:F:11:VAL:HG11 | 1:F:14:PRO:HD2 | 1.50 | 0.92 |
| 1:F:97:ARG:HH21 | 1:F:403:ASN:HB2 | 1.37 | 0.90 |
| 1:E:97:ARG:NH2 | 1:E:404:PHE:O | 2.04 | 0.90 |
| 1:E:417:THR:HB | 1:E:419:ARG:HE | 1.37 | 0.88 |
| 1:E:399:LEU:HB3 | 1:E:404:PHE:CE1 | 2.09 | 0.88 |
| 1:C:219:GLU:OE1 | 1:C:263:ARG:NH1 | 2.07 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:460:ASP:O | 1:A:466:ARG:NH2 | 2.07 | 0.87 |
| 1:B:219:GLU:OE1 | 1:B:263:ARG:NH1 | 2.07 | 0.87 |
| 1:F:422:THR:OG1 | 1:F:430:LYS:NZ | 2.08 | 0.86 |
| 1:F:219:GLU:OE1 | 1:F:263:ARG:NH1 | 2.08 | 0.86 |
| 1:E:109:ARG:NH1 | 1:E:369:GLU:O | 2.08 | 0.85 |
| 1:C:43:LEU:HA | 1:C:368:GLU:O | 1.76 | 0.85 |
| 1:A:259:HIS:H | 1:A:294:THR:HB | 1.41 | 0.85 |
| 1:E:219:GLU:OE1 | 1:E:263:ARG:NH1 | 2.08 | 0.85 |
| 1:E:37:ALA:HB2 | 1:E:455:PHE:HA | 1.57 | 0.85 |
| 1:B:406:LEU:HA | 1:B:407:GLN:HB2 | 1.56 | 0.84 |
| 1:F:109:ARG:NH1 | 1:F:369:GLU:O | 2.09 | 0.84 |
| 1:D:219:GLU:OE1 | 1:D:263:ARG:NH1 | 2.11 | 0.84 |
| 1:E:74:ARG:HB2 | 1:E:446:PHE:HE1 | 1.43 | 0.83 |
| 1:F:97:ARG:NH2 | 1:F:403:ASN:HB2 | 1.93 | 0.83 |
| 1:A:80:PRO:HB2 | 1:A:98:LEU:HB2 | 1.58 | 0.83 |
| 1:A:306:ILE:O | 1:A:311:TYR:OH | 1.95 | 0.83 |
| 1:B:419:ARG:O | 1:B:422:THR:OG1 | 1.96 | 0.82 |
| 1:F:74:ARG:HB2 | 1:F:446:PHE:HE1 | 1.44 | 0.82 |
| 1:E:421:VAL:HB | 1:E:430:LYS:HZ1 | 1.45 | 0.82 |
| 1:F:74:ARG:NH1 | 1:F:439:ASP:OD2 | 2.12 | 0.82 |
| 1:D:258:ARG:NH2 | 1:D:296:SER:OG | 2.14 | 0.81 |
| 1:B:83:PHE:HE1 | 1:C:13:LEU:HD22 | 1.45 | 0.81 |
| 1:E:258:ARG:NH2 | 1:E:296:SER:OG | 2.14 | 0.80 |
| 1:F:51:PRO:HD3 | 1:F:64:LYS:HD2 | 1.62 | 0.80 |
| 1:D:460:ASP:OD1 | 1:E:319:HIS:NE2 | 2.14 | 0.80 |
| 1:F:158:LEU:HB2 | 1:F:332:THR:HB | 1.63 | 0.80 |
| 1:B:383:LEU:HD11 | 1:B:404:PHE:CE1 | 2.17 | 0.80 |
| 1:B:258:ARG:NH2 | 1:B:296:SER:OG | 2.16 | 0.79 |
| 1:E:51:PRO:HD3 | 1:E:64:LYS:HD2 | 1.64 | 0.79 |
| 1:E:126:LEU:HB3 | 1:E:262:ASN:HB2 | 1.64 | 0.79 |
| 1:A:52:ILE:HB | 1:A:62:VAL:HB | 1.63 | 0.78 |
| 1:D:74:ARG:HB2 | 1:D:446:PHE:HE1 | 1.48 | 0.78 |
| 1:C:53:LYS:HA | 1:C:61:LEU:H | 1.48 | 0.78 |
| 1:E:53:LYS:HA | 1:E:61:LEU:H | 1.48 | 0.78 |
| 1:D:111:GLN:HB2 | 1:D:338:ARG:HD3 | 1.65 | 0.78 |
| 1:E:404:PHE:HE2 | 1:E:409:PRO:HG3 | 1.49 | 0.78 |
| 1:A:37:ALA:HB2 | 1:A:455:PHE:HA | 1.65 | 0.78 |
| 1:D:109:ARG:NH1 | 1:D:369:GLU:O | 2.17 | 0.78 |
| 1:A:117:ILE:HG12 | 1:A:118:SER:H | 1.49 | 0.77 |
| 1:A:241:PRO:O | 1:A:319:HIS:ND1 | 2.15 | 0.77 |
| 1:B:74:ARG:HB2 | 1:B:446:PHE:HE1 | 1.47 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:47:HIS:HE1 | 1:F:49:TYR:HB2 | 1.48 | 0.77 |
| 1:C:74:ARG:HB2 | 1:C:446:PHE:HE1 | 1.49 | 0.77 |
| 1:D:418:TYR:HB3 | 1:D:419:ARG:HA | 1.67 | 0.77 |
| 1:F:258:ARG:NH2 | 1:F:296:SER:OG | 2.17 | 0.77 |
| 1:C:109:ARG:NH1 | 1:C:369:GLU:O | 2.19 | 0.76 |
| 1:B:82:LYS:HB3 | 1:C:12:TYR:CE1 | 2.20 | 0.76 |
| 1:C:52:ILE:HB | 1:C:62:VAL:HB | 1.68 | 0.76 |
| 1:E:404:PHE:CE2 | 1:E:409:PRO:HG3 | 2.21 | 0.76 |
| 1:C:111:GLN:HB2 | 1:C:338:ARG:HD3 | 1.68 | 0.76 |
| 1:B:120:HIS:HB2 | 1:B:221:PRO:HA | 1.67 | 0.76 |
| 1:B:244:ASP:OD1 | 1:B:320:ASN:ND2 | 2.19 | 0.75 |
| 1:F:116:GLY:N | 1:F:339:SER:OG | 2.20 | 0.75 |
| 1:B:126:LEU:HB3 | 1:B:262:ASN:HB2 | 1.67 | 0.75 |
| 1:B:109:ARG:NH1 | 1:B:369:GLU:O | 2.20 | 0.75 |
| 1:F:478:PRO:HG2 | 1:F:480:PHE:HE2 | 1.52 | 0.74 |
| 1:A:97:ARG:HG3 | 1:A:404:PHE:HB3 | 1.70 | 0.74 |
| 1:B:312:TRP:CH2 | 1:B:468:PHE:HD1 | 2.05 | 0.74 |
| 1:D:385:ALA:HA | 1:D:388:MET:HB2 | 1.68 | 0.74 |
| 1:F:126:LEU:HB3 | 1:F:262:ASN:HB2 | 1.70 | 0.73 |
| 1:A:235:ILE:O | 1:A:239:SER:OG | 2.05 | 0.73 |
| 1:B:158:LEU:HB2 | 1:B:332:THR:HB | 1.68 | 0.73 |
| 1:E:463:PRO:HA | 1:E:466:ARG:HH12 | 1.52 | 0.73 |
| 1:E:111:GLN:HB2 | 1:E:338:ARG:HD3 | 1.68 | 0.73 |
| 1:E:57:ASN:OD1 | 1:E:58:ASN:N | 2.22 | 0.73 |
| 1:B:51:PRO:HD3 | 1:B:64:LYS:HD2 | 1.70 | 0.73 |
| 1:D:70:TYR:OH | 1:D:230:LYS:O | 2.06 | 0.73 |
| 1:B:53:LYS:HA | 1:B:61:LEU:H | 1.53 | 0.72 |
| 1:D:57:ASN:OD1 | 1:D:58:ASN:N | 2.23 | 0.72 |
| 1:C:11:VAL:HG13 | 1:C:13:LEU:HD11 | 1.70 | 0.72 |
| 1:A:120:HIS:HB2 | 1:A:221:PRO:HA | 1.70 | 0.72 |
| 1:C:57:ASN:OD1 | 1:C:58:ASN:N | 2.23 | 0.72 |
| 1:E:52:ILE:HB | 1:E:62:VAL:HB | 1.70 | 0.72 |
| 1:F:57:ASN:OD1 | 1:F:58:ASN:N | 2.22 | 0.72 |
| 1:B:384:THR:H | 1:B:387:VAL:HB | 1.55 | 0.71 |
| 1:E:74:ARG:HB2 | 1:E:446:PHE:CE1 | 2.25 | 0.71 |
| 1:F:95:THR:O | 1:F:383:LEU:HD12 | 1.90 | 0.71 |
| 1:A:392:HIS:HB2 | 1:A:399:LEU:HD12 | 1.72 | 0.71 |
| 1:D:126:LEU:HB3 | 1:D:262:ASN:HB2 | 1.73 | 0.71 |
| 1:E:162:LYS:HB2 | 1:E:245:SER:HA | 1.71 | 0.71 |
| 1:F:463:PRO:HA | 1:F:466:ARG:HH12 | 1.54 | 0.71 |
| 1:A:407:GLN:HB3 | 1:A:408:PRO:HD2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:VAL:HG13 | 1:F:426:ILE:HD11 | 1.73 | 0.71 |
| 1:D:47:HIS:HE1 | 1:D:49:TYR:HB2 | 1.54 | 0.71 |
| 1:B:46:GLY:HA3 | 1:B:65:VAL:HB | 1.71 | 0.70 |
| 1:E:120:HIS:HB2 | 1:E:221:PRO:HA | 1.73 | 0.70 |
| 1:F:70:TYR:OH | 1:F:230:LYS:O | 2.09 | 0.70 |
| 1:A:244:ASP:HA | 1:A:320:ASN:HD22 | 1.56 | 0.70 |
| 1:A:450:ASN:OD1 | 1:A:452:LYS:N | 2.22 | 0.70 |
| 1:F:312:TRP:CH2 | 1:F:468:PHE:HD1 | 2.09 | 0.70 |
| 1:D:51:PRO:HD3 | 1:D:64:LYS:HD2 | 1.73 | 0.70 |
| 1:F:53:LYS:HA | 1:F:61:LEU:H | 1.56 | 0.70 |
| 1:A:240:GLU:OE1 | 1:A:245:SER:N | 2.16 | 0.70 |
| 1:C:126:LEU:HB3 | 1:C:262:ASN:HB2 | 1.73 | 0.70 |
| 1:F:408:PRO:O | 1:F:410:PRO:HD2 | 1.91 | 0.70 |
| 1:B:54:LYS:HB3 | 1:B:57:ASN:HB3 | 1.72 | 0.69 |
| 1:E:463:PRO:HA | 1:E:466:ARG:NH1 | 2.07 | 0.69 |
| 1:D:324:CYS:SG | 1:D:329:LEU:HD12 | 2.31 | 0.69 |
| 1:C:407:GLN:N | 1:C:408:PRO:HA | 2.06 | 0.69 |
| 1:E:196:GLN:HE21 | 1:E:444:TYR:HD1 | 1.39 | 0.69 |
| 1:C:65:VAL:HG13 | 1:C:71:ARG:HH22 | 1.58 | 0.69 |
| 1:F:324:CYS:SG | 1:F:329:LEU:HD12 | 2.32 | 0.69 |
| 1:B:57:ASN:OD1 | 1:B:58:ASN:N | 2.26 | 0.69 |
| 1:C:408:PRO:HB2 | 1:C:409:PRO:CD | 2.22 | 0.69 |
| 1:D:116:GLY:N | 1:D:339:SER:OG | 2.20 | 0.69 |
| 1:E:474:LEU:HD13 | 1:E:478:PRO:HD3 | 1.75 | 0.69 |
| 1:A:437:LYS:O | 1:A:438:GLU:HG3 | 1.92 | 0.69 |
| 1:C:158:LEU:HB2 | 1:C:332:THR:HB | 1.73 | 0.69 |
| 1:A:62:VAL:HG22 | 1:F:426:ILE:HG12 | 1.74 | 0.69 |
| 1:A:162:LYS:HB2 | 1:A:245:SER:HA | 1.72 | 0.69 |
| 1:B:70:TYR:OH | 1:B:230:LYS:O | 2.10 | 0.69 |
| 1:A:39:THR:HG23 | 1:A:451:LEU:HD21 | 1.75 | 0.69 |
| 1:B:111:GLN:HB2 | 1:B:338:ARG:HD3 | 1.74 | 0.69 |
| 1:E:70:TYR:OH | 1:E:230:LYS:O | 2.10 | 0.69 |
| 1:C:324:CYS:SG | 1:C:329:LEU:HD12 | 2.34 | 0.68 |
| 1:F:210:PHE:HE2 | 1:F:224:ILE:HD12 | 1.59 | 0.68 |
| 1:D:210:PHE:HE2 | 1:D:224:ILE:HD12 | 1.58 | 0.68 |
| 1:C:18:VAL:HG12 | 1:C:20:LYS:H | 1.58 | 0.68 |
| 1:C:455:PHE:HB2 | 1:D:13:LEU:HD11 | 1.75 | 0.68 |
| 1:D:463:PRO:HA | 1:D:466:ARG:HH12 | 1.56 | 0.68 |
| 1:C:210:PHE:HE2 | 1:C:224:ILE:HD12 | 1.59 | 0.68 |
| 1:C:258:ARG:NH2 | 1:C:296:SER:OG | 2.24 | 0.68 |
| 1:C:81:ASN:HD21 | 1:C:98:LEU:H | 1.39 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:41:ARG:HH21 | 1:C:369:GLU:HG3 | 1.59 | 0.68 |
| 1:F:162:LYS:HB2 | 1:F:245:SER:HA | 1.76 | 0.68 |
| 1:C:124:ASN:HA | 1:C:144:ARG:HG2 | 1.76 | 0.68 |
| 1:A:117:ILE:HG13 | 1:A:150:ASP:HA | 1.76 | 0.68 |
| 1:D:312:TRP:CH2 | 1:D:468:PHE:HD1 | 2.12 | 0.68 |
| 1:E:150:ASP:OD1 | 1:E:296:SER:HA | 1.94 | 0.68 |
| 1:C:162:LYS:HB2 | 1:C:245:SER:HA | 1.76 | 0.68 |
| 1:C:460:ASP:OD1 | 1:D:319:HIS:NE2 | 2.21 | 0.68 |
| 1:F:463:PRO:HA | 1:F:466:ARG:NH1 | 2.08 | 0.68 |
| 1:B:150:ASP:OD1 | 1:B:296:SER:HA | 1.93 | 0.67 |
| 1:E:399:LEU:HB3 | 1:E:404:PHE:HZ | 1.57 | 0.67 |
| 1:A:385:ALA:O | 1:A:389:THR:N | 2.21 | 0.67 |
| 1:A:81:ASN:HD21 | 1:A:97:ARG:HD2 | 1.58 | 0.67 |
| 1:D:162:LYS:HB2 | 1:D:245:SER:HA | 1.76 | 0.67 |
| 1:A:439:ASP:HB3 | 1:A:442:LYS:HB2 | 1.76 | 0.67 |
| 1:A:69:GLN:OE1 | 1:A:71:ARG:NH2 | 2.27 | 0.67 |
| 1:B:37:ALA:HB2 | 1:B:455:PHE:HA | 1.76 | 0.67 |
| 1:C:399:LEU:HB3 | 1:C:404:PHE:HE1 | 1.59 | 0.67 |
| 1:C:312:TRP:CH2 | 1:C:468:PHE:HD1 | 2.13 | 0.67 |
| 1:D:301:THR:HG23 | 1:D:304:ALA:H | 1.60 | 0.67 |
| 1:E:324:CYS:SG | 1:E:329:LEU:HD12 | 2.35 | 0.67 |
| 1:E:355:TYR:HE1 | 1:E:360:PHE:CE2 | 2.13 | 0.67 |
| 1:F:111:GLN:HB2 | 1:F:338:ARG:HD3 | 1.77 | 0.67 |
| 1:D:47:HIS:CE1 | 1:D:49:TYR:HB2 | 2.30 | 0.66 |
| 1:B:429:GLN:O | 1:B:431:HIS:ND1 | 2.25 | 0.66 |
| 1:B:42:LEU:HG | 1:B:370:TYR:HB2 | 1.77 | 0.66 |
| 1:D:54:LYS:HB3 | 1:D:57:ASN:HB3 | 1.77 | 0.66 |
| 1:B:210:PHE:HE2 | 1:B:224:ILE:HD12 | 1.59 | 0.66 |
| 1:C:54:LYS:HB3 | 1:C:57:ASN:HB3 | 1.77 | 0.66 |
| 1:E:37:ALA:HB2 | 1:E:455:PHE:HD1 | 1.60 | 0.66 |
| 1:E:46:GLY:HA3 | 1:E:65:VAL:HB | 1.78 | 0.66 |
| 1:B:324:CYS:SG | 1:B:329:LEU:HD12 | 2.35 | 0.66 |
| 1:C:150:ASP:OD1 | 1:C:296:SER:HA | 1.95 | 0.65 |
| 1:D:74:ARG:HB2 | 1:D:446:PHE:CE1 | 2.30 | 0.65 |
| 1:F:71:ARG:HG3 | 1:F:370:TYR:OH | 1.96 | 0.65 |
| 1:F:74:ARG:HB2 | 1:F:446:PHE:CE1 | 2.29 | 0.65 |
| 1:E:455:PHE:O | 1:F:13:LEU:HD21 | 1.97 | 0.65 |
| 1:F:150:ASP:OD1 | 1:F:296:SER:HA | 1.96 | 0.65 |
| 1:A:421:VAL:HG22 | 1:A:430:LYS:HB3 | 1.78 | 0.65 |
| 1:C:116:GLY:N | 1:C:339:SER:OG | 2.21 | 0.65 |
| 1:B:83:PHE:HD2 | 1:B:85:PHE:HE1 | 1.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:466:ARG:HH21 | 1:E:319:HIS:CE1 | 2.14 | 0.65 |
| 1:E:234:TYR:HA | 1:E:237:MET:HE3 | 1.79 | 0.65 |
| 1:C:120:HIS:HB2 | 1:C:221:PRO:HA | 1.79 | 0.65 |
| 1:D:97:ARG:NH2 | 1:D:404:PHE:HB2 | 2.05 | 0.65 |
| 1:B:109:ARG:HD3 | 1:B:370:TYR:HD1 | 1.62 | 0.65 |
| 1:A:158:LEU:HB2 | 1:A:332:THR:HB | 1.77 | 0.65 |
| 1:A:169:TRP:HB2 | 1:A:208:MET:HB3 | 1.79 | 0.64 |
| 1:B:223:ASP:OD1 | 1:B:224:ILE:N | 2.30 | 0.64 |
| 1:C:463:PRO:HA | 1:C:466:ARG:NH1 | 2.11 | 0.64 |
| 1:D:169:TRP:HB2 | 1:D:208:MET:HB3 | 1.79 | 0.64 |
| 1:D:223:ASP:OD1 | 1:D:224:ILE:N | 2.30 | 0.64 |
| 1:F:54:LYS:HB3 | 1:F:57:ASN:HB3 | 1.80 | 0.64 |
| 1:A:156:LEU:HG | 1:A:334:VAL:HB | 1.78 | 0.64 |
| 1:C:408:PRO:HB2 | 1:C:409:PRO:HD2 | 1.79 | 0.64 |
| 1:B:109:ARG:NH2 | 1:B:338:ARG:HD2 | 2.13 | 0.64 |
| 1:D:85:PHE:HB2 | 1:D:88:THR:HG22 | 1.79 | 0.64 |
| 1:A:153:GLN:OE1 | 1:A:254:GLN:NE2 | 2.30 | 0.64 |
| 1:A:402:TRP:HE3 | 1:A:404:PHE:CE1 | 2.16 | 0.64 |
| 1:C:399:LEU:HB3 | 1:C:404:PHE:CE1 | 2.32 | 0.64 |
| 1:E:71:ARG:HG3 | 1:E:370:TYR:OH | 1.98 | 0.64 |
| 1:C:465:GLY:O | 1:C:468:PHE:N | 2.30 | 0.64 |
| 1:D:52:ILE:HB | 1:D:62:VAL:HB | 1.80 | 0.64 |
| 1:B:234:TYR:HA | 1:B:237:MET:HE3 | 1.78 | 0.63 |
| 1:B:355:TYR:HE1 | 1:B:360:PHE:CE2 | 2.16 | 0.63 |
| 1:D:463:PRO:HA | 1:D:466:ARG:NH1 | 2.11 | 0.63 |
| 1:B:162:LYS:HB2 | 1:B:245:SER:HA | 1.80 | 0.63 |
| 1:F:96:GLN:HA | 1:F:383:LEU:HD12 | 1.81 | 0.63 |
| 1:A:53:LYS:HA | 1:A:61:LEU:H | 1.64 | 0.63 |
| 1:B:85:PHE:H | 1:B:88:THR:HG22 | 1.63 | 0.63 |
| 1:C:223:ASP:OD1 | 1:C:224:ILE:N | 2.32 | 0.63 |
| 1:A:52:ILE:O | 1:A:62:VAL:N | 2.25 | 0.63 |
| 1:C:397:THR:HA | 1:C:400:GLU:CD | 2.19 | 0.63 |
| 1:D:158:LEU:HB2 | 1:D:332:THR:HB | 1.79 | 0.63 |
| 1:D:65:VAL:HG13 | 1:D:71:ARG:HH22 | 1.63 | 0.63 |
| 1:F:301:THR:HG23 | 1:F:304:ALA:H | 1.64 | 0.63 |
| 1:C:51:PRO:HD3 | 1:C:64:LYS:HD2 | 1.81 | 0.63 |
| 1:D:71:ARG:HG3 | 1:D:370:TYR:OH | 1.98 | 0.63 |
| 1:F:52:ILE:HB | 1:F:62:VAL:HB | 1.81 | 0.63 |
| 1:F:96:GLN:O | 1:F:97:ARG:NH1 | 2.28 | 0.63 |
| 1:A:40:SER:OG | 1:A:41:ARG:N | 2.31 | 0.63 |
| 1:B:65:VAL:HG13 | 1:B:71:ARG:HH22 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:37:ALA:HB2 | 1:C:455:PHE:HD1 | 1.63 | 0.63 |
| 1:E:169:TRP:HB2 | 1:E:208:MET:HB3 | 1.80 | 0.63 |
| 1:E:335:ASP:OD1 | 1:E:336:THR:N | 2.32 | 0.63 |
| 1:B:466:ARG:HH21 | 1:C:319:HIS:CE1 | 2.17 | 0.63 |
| 1:D:385:ALA:O | 1:D:389:THR:N | 2.28 | 0.63 |
| 1:E:406:LEU:HA | 1:E:408:PRO:HD2 | 1.81 | 0.63 |
| 1:A:428:CYS:HB3 | 1:A:432:THR:HG23 | 1.79 | 0.62 |
| 1:E:223:ASP:OD1 | 1:E:224:ILE:N | 2.32 | 0.62 |
| 1:F:37:ALA:HB2 | 1:F:455:PHE:HA | 1.82 | 0.62 |
| 1:A:161:CYS:SG | 1:A:244:ASP:HB3 | 2.39 | 0.62 |
| 1:B:301:THR:HG23 | 1:B:304:ALA:H | 1.64 | 0.62 |
| 1:E:404:PHE:CD2 | 1:E:406:LEU:HD12 | 2.34 | 0.62 |
| 1:E:301:THR:HG23 | 1:E:304:ALA:H | 1.63 | 0.62 |
| 1:C:70:TYR:OH | 1:C:230:LYS:O | 2.16 | 0.62 |
| 1:D:196:GLN:HE21 | 1:D:444:TYR:HD1 | 1.48 | 0.62 |
| 1:F:387:VAL:O | 1:F:391:ILE:HD12 | 2.00 | 0.62 |
| 1:A:197:ASP:HB2 | 1:A:446:PHE:HA | 1.82 | 0.62 |
| 1:C:301:THR:HG23 | 1:C:304:ALA:H | 1.64 | 0.62 |
| 1:E:65:VAL:HG13 | 1:E:71:ARG:HH22 | 1.65 | 0.62 |
| 1:A:164:PRO:HB2 | 1:A:195:ILE:HD12 | 1.82 | 0.62 |
| 1:D:81:ASN:HD21 | 1:D:97:ARG:HB3 | 1.64 | 0.62 |
| 1:F:372:LEU:HD22 | 1:F:374:PHE:CZ | 2.35 | 0.62 |
| 1:F:234:TYR:HA | 1:F:237:MET:HE3 | 1.80 | 0.61 |
| 1:B:18:VAL:HG11 | 1:F:480:PHE:HE1 | 1.64 | 0.61 |
| 1:A:242:TYR:CE1 | 1:A:394:MET:HG3 | 2.35 | 0.61 |
| 1:B:72:VAL:O | 1:B:447:TRP:HB3 | 2.01 | 0.61 |
| 1:B:263:ARG:NH2 | 1:F:343:SER:OG | 2.32 | 0.61 |
| 1:E:56:ASN:OD1 | 1:E:57:ASN:N | 2.34 | 0.61 |
| 1:A:258:ARG:NH2 | 1:A:296:SER:OG | 2.34 | 0.61 |
| 1:B:169:TRP:HB2 | 1:B:208:MET:HB3 | 1.81 | 0.61 |
| 1:C:404:PHE:HB3 | 1:C:407:GLN:HA | 1.83 | 0.61 |
| 1:B:22:VAL:HG11 | 1:F:480:PHE:CD2 | 2.35 | 0.61 |
| 1:C:47:HIS:HE1 | 1:C:49:TYR:HB2 | 1.64 | 0.61 |
| 1:E:65:VAL:HG13 | 1:E:71:ARG:NH2 | 2.15 | 0.61 |
| 1:F:78:PRO:HD3 | 1:F:452:LYS:HG2 | 1.82 | 0.61 |
| 1:F:47:HIS:CE1 | 1:F:49:TYR:HB2 | 2.31 | 0.61 |
| 1:A:301:THR:HG23 | 1:A:304:ALA:H | 1.65 | 0.60 |
| 1:C:469:LEU:O | 1:C:473:GLY:N | 2.32 | 0.60 |
| 1:E:54:LYS:HB3 | 1:E:57:ASN:HB3 | 1.82 | 0.60 |
| 1:C:169:TRP:HB2 | 1:C:208:MET:HB3 | 1.83 | 0.60 |
| 1:D:120:HIS:ND1 | 1:D:122:LEU:O | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:240:GLU:OE1 | 1:D:245:SER:N | 2.33 | 0.60 |
| 1:D:53:LYS:HA | 1:D:61:LEU:H | 1.66 | 0.60 |
| 1:F:420:PHE:HB3 | 1:F:430:LYS:CE | 2.31 | 0.60 |
| 1:B:41:ARG:HG2 | 1:B:42:LEU:N | 2.16 | 0.60 |
| 1:E:78:PRO:HD3 | 1:E:452:LYS:HA | 1.82 | 0.60 |
| 1:F:120:HIS:ND1 | 1:F:122:LEU:O | 2.34 | 0.60 |
| 1:F:312:TRP:CZ3 | 1:F:468:PHE:HD1 | 2.20 | 0.60 |
| 1:A:56:ASN:OD1 | 1:A:57:ASN:N | 2.34 | 0.60 |
| 1:C:356:LYS:HA | 1:D:141:VAL:HG13 | 1.83 | 0.60 |
| 1:D:37:ALA:HB2 | 1:D:455:PHE:HA | 1.81 | 0.60 |
| 1:C:37:ALA:HB2 | 1:C:455:PHE:HA | 1.83 | 0.60 |
| 1:F:223:ASP:OD1 | 1:F:224:ILE:N | 2.34 | 0.60 |
| 1:A:390:TYR:O | 1:A:394:MET:N | 2.21 | 0.60 |
| 1:B:416:ASP:HB3 | 1:B:418:TYR:CE2 | 2.36 | 0.60 |
| 1:C:117:ILE:HD11 | 1:D:260:LEU:HG | 1.84 | 0.60 |
| 1:F:420:PHE:HB3 | 1:F:430:LYS:HE2 | 1.84 | 0.60 |
| 1:B:47:HIS:HE1 | 1:B:49:TYR:HB2 | 1.66 | 0.59 |
| 1:C:463:PRO:HA | 1:C:466:ARG:HH12 | 1.67 | 0.59 |
| 1:E:120:HIS:ND1 | 1:E:122:LEU:O | 2.35 | 0.59 |
| 1:E:70:TYR:HD1 | 1:E:334:VAL:HG21 | 1.67 | 0.59 |
| 1:E:421:VAL:HB | 1:E:430:LYS:NZ | 2.15 | 0.59 |
| 1:A:324:CYS:SG | 1:A:329:LEU:HD12 | 2.42 | 0.59 |
| 1:A:97:ARG:HG3 | 1:A:404:PHE:CB | 2.31 | 0.59 |
| 1:E:258:ARG:HG2 | 1:E:259:HIS:ND1 | 2.17 | 0.59 |
| 1:A:97:ARG:HH21 | 1:A:405:GLY:HA3 | 1.67 | 0.59 |
| 1:C:144:ARG:NH1 | 1:C:216:ASN:OD1 | 2.36 | 0.59 |
| 1:D:97:ARG:HH22 | 1:D:404:PHE:CB | 2.07 | 0.59 |
| 1:B:109:ARG:HD3 | 1:B:370:TYR:CD1 | 2.38 | 0.59 |
| 1:E:469:LEU:O | 1:E:473:GLY:N | 2.36 | 0.59 |
| 1:B:258:ARG:HG2 | 1:B:259:HIS:ND1 | 2.17 | 0.59 |
| 1:B:82:LYS:HB3 | 1:C:12:TYR:HE1 | 1.68 | 0.59 |
| 1:F:169:TRP:HB2 | 1:F:208:MET:HB3 | 1.84 | 0.59 |
| 1:F:469:LEU:O | 1:F:473:GLY:N | 2.36 | 0.59 |
| 1:B:148:SER:OG | 1:C:260:LEU:HD23 | 2.03 | 0.59 |
| 1:B:56:ASN:OD1 | 1:B:57:ASN:N | 2.36 | 0.59 |
| 1:E:47:HIS:HE1 | 1:E:49:TYR:HB2 | 1.68 | 0.59 |
| 1:F:48:PRO:HA | 1:F:66:SER:HB2 | 1.83 | 0.59 |
| 1:A:402:TRP:N | 1:A:402:TRP:CD1 | 2.70 | 0.58 |
| 1:B:254:GLN:NE2 | 1:B:298:SER:HB3 | 2.17 | 0.58 |
| 1:B:109:ARG:HH21 | 1:B:338:ARG:HD2 | 1.67 | 0.58 |
| 1:D:81:ASN:OD1 | 1:D:98:LEU:N | 2.35 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:335:ASP:OD2 | 1:F:337:THR:OG1 | 2.19 | 0.58 |
| 1:C:418:TYR:HB3 | 1:C:420:PHE:CE2 | 2.38 | 0.58 |
| 1:C:196:GLN:HE21 | 1:C:444:TYR:HD1 | 1.51 | 0.58 |
| 1:D:117:ILE:HG12 | 1:D:118:SER:H | 1.68 | 0.58 |
| 1:F:117:ILE:HG13 | 1:F:118:SER:H | 1.68 | 0.58 |
| 1:B:463:PRO:HA | 1:B:466:ARG:HH12 | 1.68 | 0.58 |
| 1:B:57:ASN:OD1 | 1:B:59:LYS:N | 2.32 | 0.58 |
| 1:D:258:ARG:HG2 | 1:D:259:HIS:ND1 | 2.18 | 0.58 |
| 1:A:115:VAL:HA | 1:A:339:SER:OG | 2.03 | 0.58 |
| 1:E:466:ARG:HH21 | 1:F:319:HIS:CE1 | 2.21 | 0.58 |
| 1:D:65:VAL:HG13 | 1:D:71:ARG:NH2 | 2.17 | 0.58 |
| 1:D:171:LYS:HB2 | 1:D:213:LEU:HD11 | 1.85 | 0.58 |
| 1:A:41:ARG:HA | 1:A:370:TYR:O | 2.02 | 0.58 |
| 1:A:437:LYS:HG2 | 1:A:438:GLU:H | 1.69 | 0.58 |
| 1:B:78:PRO:HD2 | 1:B:455:PHE:CZ | 2.39 | 0.58 |
| 1:D:150:ASP:OD1 | 1:D:296:SER:HA | 2.03 | 0.58 |
| 1:B:120:HIS:CD2 | 1:B:222:LEU:HD12 | 2.38 | 0.58 |
| 1:B:312:TRP:CZ3 | 1:B:468:PHE:HD1 | 2.20 | 0.58 |
| 1:B:83:PHE:CE1 | 1:C:13:LEU:HD22 | 2.33 | 0.58 |
| 1:B:83:PHE:HD2 | 1:B:85:PHE:CE1 | 2.22 | 0.58 |
| 1:E:109:ARG:HH21 | 1:E:338:ARG:HD2 | 1.68 | 0.58 |
| 1:A:85:PHE:CE1 | 1:A:88:THR:HA | 2.39 | 0.58 |
| 1:B:463:PRO:HA | 1:B:466:ARG:NH1 | 2.19 | 0.58 |
| 1:E:417:THR:HB | 1:E:419:ARG:NE | 2.14 | 0.58 |
| 1:D:355:TYR:HE1 | 1:D:360:PHE:CE2 | 2.22 | 0.58 |
| 1:E:158:LEU:HB2 | 1:E:332:THR:HB | 1.86 | 0.58 |
| 1:F:90:PHE:HD1 | 1:F:380:LYS:HZ3 | 1.51 | 0.58 |
| 1:A:123:LEU:N | 1:A:145:GLU:O | 2.36 | 0.57 |
| 1:D:423:SER:OG | 1:D:424:GLN:N | 2.36 | 0.57 |
| 1:E:83:PHE:HA | 1:F:11:VAL:CG2 | 2.34 | 0.57 |
| 1:D:335:ASP:OD1 | 1:D:336:THR:N | 2.37 | 0.57 |
| 1:E:41:ARG:NH2 | 1:E:369:GLU:OE2 | 2.37 | 0.57 |
| 1:C:43:LEU:HD12 | 1:C:368:GLU:C | 2.24 | 0.57 |
| 1:D:120:HIS:HB2 | 1:D:221:PRO:HA | 1.86 | 0.57 |
| 1:C:460:ASP:O | 1:C:466:ARG:NH2 | 2.37 | 0.57 |
| 1:C:74:ARG:HB2 | 1:C:446:PHE:CE1 | 2.37 | 0.57 |
| 1:D:56:ASN:OD1 | 1:D:57:ASN:N | 2.38 | 0.57 |
| 1:E:117:ILE:HG13 | 1:E:118:SER:H | 1.68 | 0.57 |
| 1:E:48:PRO:HA | 1:E:66:SER:HB2 | 1.86 | 0.57 |
| 1:A:45:VAL:HA | 1:A:366:HIS:O | 2.04 | 0.57 |
| 1:B:335:ASP:OD1 | 1:B:336:THR:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:247:PHE:HE1 | 1:C:313:LEU:HD13 | 1.68 | 0.57 |
| 1:C:35:TYR:HD2 | 1:C:100:TRP:HH2 | 1.53 | 0.57 |
| 1:E:148:SER:OG | 1:F:260:LEU:HD23 | 2.04 | 0.57 |
| 1:C:71:ARG:HG3 | 1:C:370:TYR:OH | 2.04 | 0.57 |
| 1:C:41:ARG:NH2 | 1:C:369:GLU:OE2 | 2.36 | 0.57 |
| 1:E:109:ARG:NH2 | 1:E:338:ARG:HD2 | 2.20 | 0.57 |
| 1:A:54:LYS:HD2 | 1:A:57:ASN:HB2 | 1.86 | 0.57 |
| 1:B:260:LEU:HD23 | 1:F:148:SER:OG | 2.05 | 0.57 |
| 1:C:387:VAL:O | 1:C:391:ILE:HD12 | 2.05 | 0.57 |
| 1:D:48:PRO:HA | 1:D:66:SER:HB2 | 1.87 | 0.57 |
| 1:A:116:GLY:HA3 | 1:A:341:ASN:HD22 | 1.69 | 0.57 |
| 1:A:47:HIS:HE2 | 1:A:364:LEU:HD12 | 1.70 | 0.57 |
| 1:E:424:GLN:OE1 | 1:E:427:ALA:HB3 | 2.03 | 0.57 |
| 1:A:70:TYR:N | 1:A:199:ASP:O | 2.32 | 0.57 |
| 1:A:223:ASP:OD1 | 1:A:223:ASP:N | 2.36 | 0.57 |
| 1:A:242:TYR:CZ | 1:A:394:MET:HG3 | 2.40 | 0.57 |
| 1:B:343:SER:OG | 1:C:263:ARG:NH2 | 2.37 | 0.57 |
| 1:C:335:ASP:OD1 | 1:C:336:THR:N | 2.37 | 0.57 |
| 1:C:384:THR:H | 1:C:387:VAL:HB | 1.70 | 0.57 |
| 1:D:37:ALA:HB2 | 1:D:455:PHE:HD1 | 1.69 | 0.57 |
| 1:E:70:TYR:CD1 | 1:E:334:VAL:HG21 | 2.40 | 0.57 |
| 1:C:56:ASN:OD1 | 1:C:57:ASN:N | 2.37 | 0.56 |
| 1:D:78:PRO:HD3 | 1:D:452:LYS:HA | 1.86 | 0.56 |
| 1:B:312:TRP:CE2 | 1:B:471:GLN:NE2 | 2.73 | 0.56 |
| 1:B:74:ARG:HB2 | 1:B:446:PHE:CE1 | 2.36 | 0.56 |
| 1:B:78:PRO:HD3 | 1:B:452:LYS:HA | 1.87 | 0.56 |
| 1:F:109:ARG:NH2 | 1:F:338:ARG:HD2 | 2.20 | 0.56 |
| 1:B:42:LEU:CG | 1:B:370:TYR:HB2 | 2.35 | 0.56 |
| 1:C:404:PHE:HB3 | 1:C:407:GLN:N | 2.20 | 0.56 |
| 1:F:120:HIS:HB2 | 1:F:221:PRO:HA | 1.86 | 0.56 |
| 1:A:194:VAL:O | 1:A:230:LYS:NZ | 2.38 | 0.56 |
| 1:D:96:GLN:O | 1:D:97:ARG:NH1 | 2.34 | 0.56 |
| 1:A:88:THR:O | 1:A:90:PHE:N | 2.39 | 0.56 |
| 1:E:41:ARG:HH21 | 1:E:369:GLU:HG3 | 1.69 | 0.56 |
| 1:A:317:GLN:N | 1:A:317:GLN:OE1 | 2.31 | 0.56 |
| 1:C:259:HIS:H | 1:C:294:THR:HB | 1.69 | 0.56 |
| 1:C:409:PRO:C | 1:C:411:GLY:H | 2.07 | 0.56 |
| 1:D:109:ARG:NH2 | 1:D:338:ARG:HD2 | 2.20 | 0.56 |
| 1:D:84:GLY:HA3 | 1:E:12:TYR:HB3 | 1.87 | 0.56 |
| 1:A:391:ILE:O | 1:A:395:ASN:N | 2.38 | 0.56 |
| 1:D:169:TRP:HA | 1:D:189:GLU:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:109:ARG:HH21 | 1:F:338:ARG:HD2 | 1.71 | 0.56 |
| 1:C:466:ARG:HH21 | 1:D:319:HIS:CE1 | 2.24 | 0.56 |
| 1:D:216:ASN:ND2 | 1:D:219:GLU:OE2 | 2.36 | 0.56 |
| 1:B:216:ASN:ND2 | 1:B:219:GLU:OE2 | 2.36 | 0.56 |
| 1:F:196:GLN:HE21 | 1:F:444:TYR:HD1 | 1.54 | 0.56 |
| 1:C:41:ARG:NH2 | 1:C:369:GLU:HG3 | 2.21 | 0.56 |
| 1:E:460:ASP:OD1 | 1:F:319:HIS:NE2 | 2.30 | 0.56 |
| 1:A:210:PHE:O | 1:A:214:GLN:N | 2.22 | 0.55 |
| 1:A:402:TRP:HE3 | 1:A:404:PHE:HE1 | 1.54 | 0.55 |
| 1:C:366:HIS:CE1 | 1:C:368:GLU:OE2 | 2.58 | 0.55 |
| 1:D:312:TRP:HH2 | 1:D:468:PHE:HD1 | 1.52 | 0.55 |
| 1:E:97:ARG:HG3 | 1:E:402:TRP:CE3 | 2.41 | 0.55 |
| 1:F:335:ASP:OD1 | 1:F:336:THR:N | 2.38 | 0.55 |
| 1:A:119:GLY:HA3 | 1:A:148:SER:HA | 1.88 | 0.55 |
| 1:B:387:VAL:O | 1:B:391:ILE:HD12 | 2.06 | 0.55 |
| 1:B:52:ILE:HB | 1:B:62:VAL:HB | 1.86 | 0.55 |
| 1:B:356:LYS:HA | 1:C:141:VAL:HG13 | 1.88 | 0.55 |
| 1:C:148:SER:OG | 1:D:260:LEU:HD23 | 2.06 | 0.55 |
| 1:D:109:ARG:HH21 | 1:D:338:ARG:HD2 | 1.71 | 0.55 |
| 1:E:144:ARG:HH12 | 1:F:277:ILE:HB | 1.71 | 0.55 |
| 1:F:164:PRO:HB2 | 1:F:195:ILE:HD12 | 1.88 | 0.55 |
| 1:F:167:GLU:CD | 1:F:233:ASP:HB2 | 2.26 | 0.55 |
| 1:D:144:ARG:HH12 | 1:E:277:ILE:HB | 1.72 | 0.55 |
| 1:B:319:HIS:CE1 | 1:F:466:ARG:HH21 | 2.23 | 0.55 |
| 1:B:167:GLU:CD | 1:B:233:ASP:HB2 | 2.25 | 0.55 |
| 1:C:109:ARG:HH21 | 1:C:338:ARG:HD2 | 1.71 | 0.55 |
| 1:A:97:ARG:HG3 | 1:A:404:PHE:CG | 2.42 | 0.55 |
| 1:C:78:PRO:HD3 | 1:C:452:LYS:HA | 1.89 | 0.55 |
| 1:A:31:THR:HG23 | 1:A:379:CYS:HA | 1.89 | 0.55 |
| 1:C:47:HIS:CE1 | 1:C:49:TYR:HB2 | 2.41 | 0.55 |
| 1:D:254:GLN:NE2 | 1:D:298:SER:HB3 | 2.22 | 0.55 |
| 1:E:210:PHE:HE2 | 1:E:224:ILE:HD12 | 1.71 | 0.55 |
| 1:E:78:PRO:HD2 | 1:E:455:PHE:CZ | 2.42 | 0.55 |
| 1:F:13:LEU:HB2 | 1:F:14:PRO:CD | 2.36 | 0.55 |
| 1:C:404:PHE:HB2 | 1:C:405:GLY:CA | 2.20 | 0.55 |
| 1:C:404:PHE:CB | 1:C:406:LEU:C | 2.75 | 0.55 |
| 1:C:81:ASN:ND2 | 1:C:98:LEU:H | 2.04 | 0.55 |
| 1:B:469:LEU:O | 1:B:473:GLY:N | 2.39 | 0.55 |
| 1:A:36:HIS:HB2 | 1:A:375:ILE:HD13 | 1.89 | 0.55 |
| 1:F:306:ILE:O | 1:F:311:TYR:OH | 2.20 | 0.55 |
| 1:C:111:GLN:N | 1:C:369:GLU:OE1 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:312:TRP:CH2 | 1:D:468:PHE:CD1 | 2.95 | 0.54 |
| 1:E:85:PHE:H | 1:E:88:THR:HG22 | 1.71 | 0.54 |
| 1:A:43:LEU:HD12 | 1:A:368:GLU:O | 2.08 | 0.54 |
| 1:C:273:ASP:OD1 | 1:C:274:ASP:N | 2.40 | 0.54 |
| 1:D:387:VAL:O | 1:D:391:ILE:HD12 | 2.08 | 0.54 |
| 1:E:343:SER:OG | 1:F:263:ARG:NH2 | 2.38 | 0.54 |
| 1:A:170:GLY:O | 1:A:189:GLU:N | 2.38 | 0.54 |
| 1:A:238:VAL:HG13 | 1:A:317:GLN:HG3 | 1.89 | 0.54 |
| 1:C:120:HIS:ND1 | 1:C:122:LEU:O | 2.41 | 0.54 |
| 1:C:234:TYR:HA | 1:C:237:MET:HE3 | 1.89 | 0.54 |
| 1:D:181:ASN:N | 1:D:184:ASP:OD2 | 2.38 | 0.54 |
| 1:E:482:LEU:HD13 | 1:F:26:GLU:OE1 | 2.08 | 0.54 |
| 1:F:249:TYR:HE1 | 1:F:251:ARG:NH1 | 2.05 | 0.54 |
| 1:F:280:SER:O | 1:F:283:THR:OG1 | 2.21 | 0.54 |
| 1:B:466:ARG:NH2 | 1:C:319:HIS:CE1 | 2.76 | 0.54 |
| 1:C:404:PHE:HB2 | 1:C:406:LEU:C | 2.27 | 0.54 |
| 1:F:123:LEU:N | 1:F:145:GLU:O | 2.39 | 0.54 |
| 1:A:466:ARG:O | 1:A:470:LEU:N | 2.36 | 0.54 |
| 1:C:85:PHE:H | 1:C:88:THR:HG22 | 1.72 | 0.54 |
| 1:E:273:ASP:OD1 | 1:E:274:ASP:N | 2.40 | 0.54 |
| 1:B:45:VAL:HA | 1:B:366:HIS:O | 2.07 | 0.54 |
| 1:B:383:LEU:HD22 | 1:B:388:MET:HG2 | 1.88 | 0.54 |
| 1:D:417:THR:O | 1:D:418:TYR:CD1 | 2.61 | 0.54 |
| 1:E:36:HIS:O | 1:E:456:SER:N | 2.40 | 0.54 |
| 1:A:57:ASN:OD1 | 1:A:58:ASN:N | 2.41 | 0.54 |
| 1:D:259:HIS:H | 1:D:294:THR:HB | 1.73 | 0.54 |
| 1:A:22:VAL:HB | 1:A:26:GLU:HG3 | 1.87 | 0.54 |
| 1:B:458:ASP:OD2 | 1:C:20:LYS:HE2 | 2.07 | 0.54 |
| 1:E:35:TYR:HD2 | 1:E:100:TRP:CH2 | 2.26 | 0.54 |
| 1:E:421:VAL:O | 1:E:430:LYS:NZ | 2.41 | 0.54 |
| 1:A:169:TRP:CZ3 | 1:A:190:LEU:HB2 | 2.43 | 0.54 |
| 1:A:248:PHE:CG | 1:A:249:TYR:N | 2.75 | 0.54 |
| 1:C:123:LEU:H | 1:C:145:GLU:H | 1.56 | 0.54 |
| 1:D:384:THR:O | 1:D:387:VAL:HB | 2.08 | 0.53 |
| 1:F:37:ALA:HB2 | 1:F:455:PHE:HD1 | 1.73 | 0.53 |
| 1:A:160:GLY:HA2 | 1:A:247:PHE:CE2 | 2.43 | 0.53 |
| 1:C:52:ILE:O | 1:C:61:LEU:N | 2.41 | 0.53 |
| 1:D:273:ASP:OD1 | 1:D:274:ASP:N | 2.40 | 0.53 |
| 1:F:120:HIS:CD2 | 1:F:222:LEU:HD12 | 2.43 | 0.53 |
| 1:A:53:LYS:HA | 1:A:60:ILE:HA | 1.89 | 0.53 |
| 1:F:65:VAL:HG13 | 1:F:71:ARG:NH2 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:159:ILE:HD12 | 1:A:248:PHE:HD2 | 1.73 | 0.53 |
| 1:C:54:LYS:HD2 | 1:C:57:ASN:HB2 | 1.89 | 0.53 |
| 1:D:70:TYR:HD1 | 1:D:334:VAL:HG21 | 1.74 | 0.53 |
| 1:D:78:PRO:HD2 | 1:D:455:PHE:CZ | 2.44 | 0.53 |
| 1:F:244:ASP:OD1 | 1:F:320:ASN:ND2 | 2.33 | 0.53 |
| 1:A:23:SER:HA | 1:A:319:HIS:HB3 | 1.90 | 0.53 |
| 1:A:47:HIS:NE2 | 1:A:364:LEU:HD12 | 2.23 | 0.53 |
| 1:C:312:TRP:HH2 | 1:C:468:PHE:HD1 | 1.53 | 0.53 |
| 1:C:395:ASN:HB3 | 1:C:398:ILE:CD1 | 2.38 | 0.53 |
| 1:A:85:PHE:CE1 | 1:A:88:THR:HG22 | 2.43 | 0.53 |
| 1:C:171:LYS:HB2 | 1:C:213:LEU:HD11 | 1.90 | 0.53 |
| 1:E:52:ILE:HG22 | 1:E:61:LEU:HB3 | 1.90 | 0.53 |
| 1:A:54:LYS:HB3 | 1:A:57:ASN:HB3 | 1.91 | 0.53 |
| 1:B:417:THR:HG21 | 1:B:426:ILE:HG21 | 1.90 | 0.53 |
| 1:C:399:LEU:CB | 1:C:404:PHE:HE1 | 2.22 | 0.53 |
| 1:C:83:PHE:HD2 | 1:C:85:PHE:CE1 | 2.26 | 0.53 |
| 1:E:395:ASN:HB3 | 1:E:398:ILE:HD12 | 1.91 | 0.53 |
| 1:F:11:VAL:HG12 | 1:F:13:LEU:N | 2.24 | 0.53 |
| 1:F:421:VAL:O | 1:F:422:THR:HG23 | 2.08 | 0.53 |
| 1:A:371:ASP:OD1 | 1:A:373:GLN:HG3 | 2.09 | 0.53 |
| 1:B:65:VAL:HG13 | 1:B:71:ARG:NH2 | 2.24 | 0.53 |
| 1:C:312:TRP:CH2 | 1:C:468:PHE:CD1 | 2.96 | 0.53 |
| 1:C:43:LEU:HD13 | 1:C:369:GLU:HB2 | 1.91 | 0.53 |
| 1:E:44:ALA:HB3 | 1:E:368:GLU:HB2 | 1.91 | 0.53 |
| 1:A:24:THR:HG21 | 1:A:320:ASN:HA | 1.90 | 0.53 |
| 1:A:273:ASP:HA | 1:A:276:TYR:CE2 | 2.45 | 0.52 |
| 1:A:85:PHE:CD1 | 1:A:88:THR:HG22 | 2.44 | 0.52 |
| 1:B:123:LEU:N | 1:B:145:GLU:O | 2.42 | 0.52 |
| 1:B:141:VAL:HG13 | 1:F:356:LYS:HA | 1.90 | 0.52 |
| 1:D:97:ARG:HG3 | 1:D:402:TRP:CE3 | 2.43 | 0.52 |
| 1:E:52:ILE:O | 1:E:61:LEU:N | 2.43 | 0.52 |
| 1:A:441:LEU:HG | 1:A:444:TYR:CD2 | 2.43 | 0.52 |
| 1:A:53:LYS:HB3 | 1:A:60:ILE:HG22 | 1.91 | 0.52 |
| 1:B:44:ALA:O | 1:B:368:GLU:N | 2.42 | 0.52 |
| 1:E:96:GLN:O | 1:E:97:ARG:NH1 | 2.40 | 0.52 |
| 1:F:56:ASN:OD1 | 1:F:57:ASN:N | 2.42 | 0.52 |
| 1:A:392:HIS:HA | 1:A:396:SER:HA | 1.91 | 0.52 |
| 1:A:463:PRO:HA | 1:A:466:ARG:NH1 | 2.24 | 0.52 |
| 1:A:84:GLY:HA3 | 1:F:84:GLY:HA3 | 1.92 | 0.52 |
| 1:B:155:GLN:NE2 | 1:B:305:GLN:OE1 | 2.42 | 0.52 |
| 1:D:164:PRO:HB2 | 1:D:195:ILE:HD12 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:35:TYR:HD2 | 1:D:100:TRP:HH2 | 1.55 | 0.52 |
| 1:A:195:ILE:HA | 1:A:230:LYS:NZ | 2.24 | 0.52 |
| 1:B:335:ASP:OD1 | 1:B:337:THR:HG23 | 2.10 | 0.52 |
| 1:C:109:ARG:NH2 | 1:C:338:ARG:HD2 | 2.25 | 0.52 |
| 1:F:258:ARG:HG2 | 1:F:259:HIS:ND1 | 2.24 | 0.52 |
| 1:C:399:LEU:C | 1:C:404:PHE:HE1 | 2.13 | 0.52 |
| 1:D:220:VAL:HB | 1:D:224:ILE:HD11 | 1.91 | 0.52 |
| 1:E:431:HIS:HB3 | 1:E:433:PRO:HD2 | 1.89 | 0.52 |
| 1:E:65:VAL:HA | 1:E:69:GLN:OE1 | 2.10 | 0.52 |
| 1:F:11:VAL:CG1 | 1:F:14:PRO:HD2 | 2.33 | 0.52 |
| 1:F:408:PRO:C | 1:F:410:PRO:HD2 | 2.29 | 0.52 |
| 1:F:78:PRO:HD2 | 1:F:455:PHE:CZ | 2.45 | 0.52 |
| 1:B:348:ILE:HG22 | 1:B:359:ASN:O | 2.09 | 0.52 |
| 1:D:384:THR:O | 1:D:388:MET:HG3 | 2.10 | 0.52 |
| 1:A:51:PRO:HB3 | 1:A:64:LYS:H | 1.74 | 0.52 |
| 1:C:419:ARG:C | 1:C:420:PHE:CD1 | 2.83 | 0.52 |
| 1:A:335:ASP:CG | 1:A:337:THR:HG1 | 2.12 | 0.52 |
| 1:A:408:PRO:O | 1:A:411:GLY:N | 2.43 | 0.52 |
| 1:D:392:HIS:O | 1:D:396:SER:OG | 2.25 | 0.52 |
| 1:D:312:TRP:HH2 | 1:D:468:PHE:CD1 | 2.27 | 0.52 |
| 1:F:335:ASP:OD1 | 1:F:337:THR:HG23 | 2.09 | 0.52 |
| 1:C:312:TRP:HH2 | 1:C:468:PHE:CD1 | 2.28 | 0.52 |
| 1:A:234:TYR:OH | 1:A:251:ARG:HD3 | 2.09 | 0.52 |
| 1:B:120:HIS:ND1 | 1:B:122:LEU:O | 2.41 | 0.52 |
| 1:B:41:ARG:NH2 | 1:C:190:LEU:HD21 | 2.25 | 0.52 |
| 1:B:480:PHE:CE2 | 1:C:22:VAL:HG11 | 2.45 | 0.52 |
| 1:D:335:ASP:OD1 | 1:D:337:THR:HG23 | 2.10 | 0.52 |
| 1:D:148:SER:OG | 1:E:260:LEU:HD23 | 2.09 | 0.52 |
| 1:F:312:TRP:CE2 | 1:F:471:GLN:NE2 | 2.78 | 0.52 |
| 1:F:478:PRO:HG2 | 1:F:480:PHE:CE2 | 2.40 | 0.52 |
| 1:D:343:SER:OG | 1:E:263:ARG:NH2 | 2.43 | 0.51 |
| 1:D:391:ILE:O | 1:D:394:MET:N | 2.43 | 0.51 |
| 1:F:123:LEU:H | 1:F:145:GLU:H | 1.58 | 0.51 |
| 1:F:24:THR:HG21 | 1:F:320:ASN:HA | 1.91 | 0.51 |
| 1:F:52:ILE:O | 1:F:61:LEU:N | 2.43 | 0.51 |
| 1:A:258:ARG:HB2 | 1:A:296:SER:HB2 | 1.93 | 0.51 |
| 1:A:85:PHE:HB2 | 1:A:86:PRO:HD2 | 1.92 | 0.51 |
| 1:D:97:ARG:HG3 | 1:D:402:TRP:CZ3 | 2.45 | 0.51 |
| 1:E:306:ILE:O | 1:E:311:TYR:OH | 2.18 | 0.51 |
| 1:A:387:VAL:O | 1:A:391:ILE:HD12 | 2.10 | 0.51 |
| 1:A:45:VAL:HG12 | 1:A:46:GLY:N | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:466:ARG:HH21 | 1:F:319:HIS:HE1 | 1.58 | 0.51 |
| 1:F:92:ASN:O | 1:F:96:GLN:HB2 | 2.10 | 0.51 |
| 1:A:240:GLU:OE2 | 1:A:242:TYR:HB2 | 2.10 | 0.51 |
| 1:C:238:VAL:HG13 | 1:C:317:GLN:HG3 | 1.91 | 0.51 |
| 1:C:43:LEU:HD12 | 1:C:368:GLU:H | 1.75 | 0.51 |
| 1:D:249:TYR:HE1 | 1:D:251:ARG:NH1 | 2.08 | 0.51 |
| 1:E:407:GLN:N | 1:E:408:PRO:CD | 2.74 | 0.51 |
| 1:A:47:HIS:CD2 | 1:A:364:LEU:HB2 | 2.46 | 0.51 |
| 1:B:35:TYR:HD2 | 1:B:100:TRP:CH2 | 2.29 | 0.51 |
| 1:C:70:TYR:HE1 | 1:C:201:VAL:HG22 | 1.75 | 0.51 |
| 1:D:170:GLY:O | 1:D:189:GLU:N | 2.43 | 0.51 |
| 1:F:42:LEU:HD13 | 1:F:447:TRP:HE1 | 1.76 | 0.51 |
| 1:A:244:ASP:OD1 | 1:A:320:ASN:HB2 | 2.11 | 0.51 |
| 1:C:35:TYR:HD2 | 1:C:100:TRP:CH2 | 2.28 | 0.51 |
| 1:C:43:LEU:HD12 | 1:C:368:GLU:N | 2.25 | 0.51 |
| 1:C:78:PRO:HD2 | 1:C:455:PHE:CZ | 2.46 | 0.51 |
| 1:D:52:ILE:O | 1:D:61:LEU:N | 2.43 | 0.51 |
| 1:E:70:TYR:HE1 | 1:E:201:VAL:HG22 | 1.75 | 0.51 |
| 1:F:57:ASN:CG | 1:F:59:LYS:H | 2.13 | 0.51 |
| 1:D:24:THR:HG21 | 1:D:320:ASN:HA | 1.92 | 0.51 |
| 1:D:23:SER:HA | 1:D:319:HIS:HB3 | 1.93 | 0.51 |
| 1:E:85:PHE:H | 1:E:88:THR:CG2 | 2.24 | 0.51 |
| 1:E:356:LYS:HA | 1:F:141:VAL:HG13 | 1.93 | 0.51 |
| 1:F:57:ASN:OD1 | 1:F:59:LYS:N | 2.40 | 0.51 |
| 1:D:465:GLY:O | 1:D:468:PHE:N | 2.43 | 0.51 |
| 1:F:41:ARG:HH21 | 1:F:369:GLU:HG3 | 1.76 | 0.51 |
| 1:C:20:LYS:O | 1:C:22:VAL:HG13 | 2.11 | 0.51 |
| 1:E:35:TYR:HD2 | 1:E:100:TRP:HH2 | 1.57 | 0.51 |
| 1:A:99:VAL:N | 1:A:379:CYS:O | 2.39 | 0.51 |
| 1:A:84:GLY:HA3 | 1:F:84:GLY:CA | 2.41 | 0.51 |
| 1:C:220:VAL:HB | 1:C:224:ILE:HD11 | 1.93 | 0.51 |
| 1:C:280:SER:O | 1:C:283:THR:OG1 | 2.24 | 0.51 |
| 1:A:312:TRP:CZ3 | 1:A:468:PHE:HB2 | 2.46 | 0.50 |
| 1:E:120:HIS:CD2 | 1:E:222:LEU:HD12 | 2.46 | 0.50 |
| 1:E:273:ASP:HA | 1:E:276:TYR:CE2 | 2.46 | 0.50 |
| 1:E:335:ASP:OD1 | 1:E:337:THR:HG23 | 2.11 | 0.50 |
| 1:E:83:PHE:CD2 | 1:E:85:PHE:HE1 | 2.29 | 0.50 |
| 1:C:23:SER:HA | 1:C:319:HIS:HB3 | 1.93 | 0.50 |
| 1:D:216:ASN:C | 1:D:218:SER:H | 2.13 | 0.50 |
| 1:E:249:TYR:HE1 | 1:E:251:ARG:NH1 | 2.09 | 0.50 |
| 1:A:37:ALA:HB3 | 1:A:455:PHE:HD1 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:44:ALA:N | 1:B:368:GLU:O | 2.39 | 0.50 |
| 1:B:73:PHE:HZ | 1:B:370:TYR:CD2 | 2.29 | 0.50 |
| 1:F:117:ILE:HG13 | 1:F:118:SER:N | 2.26 | 0.50 |
| 1:A:36:HIS:CG | 1:A:37:ALA:N | 2.79 | 0.50 |
| 1:A:45:VAL:HG12 | 1:A:46:GLY:H | 1.76 | 0.50 |
| 1:D:180:VAL:HG13 | 1:D:184:ASP:HB2 | 1.93 | 0.50 |
| 1:E:180:VAL:HG13 | 1:E:184:ASP:HB2 | 1.93 | 0.50 |
| 1:A:51:PRO:HD3 | 1:A:64:LYS:HB2 | 1.92 | 0.50 |
| 1:C:335:ASP:OD1 | 1:C:337:THR:HG23 | 2.11 | 0.50 |
| 1:C:461:GLN:HE22 | 1:D:21:VAL:HG23 | 1.75 | 0.50 |
| 1:D:335:ASP:OD2 | 1:D:337:THR:OG1 | 2.24 | 0.50 |
| 1:A:220:VAL:HB | 1:A:224:ILE:HD11 | 1.93 | 0.50 |
| 1:A:258:ARG:HG2 | 1:A:259:HIS:ND1 | 2.27 | 0.50 |
| 1:D:97:ARG:NH2 | 1:D:404:PHE:HD2 | 2.10 | 0.50 |
| 1:A:280:SER:N | 1:A:283:THR:OG1 | 2.44 | 0.50 |
| 1:A:247:PHE:HA | 1:A:317:GLN:HE22 | 1.77 | 0.50 |
| 1:A:80:PRO:CB | 1:A:98:LEU:HB2 | 2.38 | 0.50 |
| 1:E:348:ILE:HG22 | 1:E:359:ASN:O | 2.11 | 0.50 |
| 1:C:181:ASN:N | 1:C:184:ASP:OD2 | 2.38 | 0.50 |
| 1:C:24:THR:HG21 | 1:C:320:ASN:HA | 1.94 | 0.50 |
| 1:E:210:PHE:CE2 | 1:E:220:VAL:HG11 | 2.45 | 0.50 |
| 1:E:40:SER:OG | 1:E:41:ARG:N | 2.45 | 0.50 |
| 1:F:90:PHE:CE1 | 1:F:91:TYR:HD2 | 2.29 | 0.50 |
| 1:C:111:GLN:HG2 | 1:C:369:GLU:HB3 | 1.94 | 0.50 |
| 1:D:249:TYR:HE1 | 1:D:251:ARG:HH11 | 1.60 | 0.50 |
| 1:A:403:ASN:HB2 | 1:A:404:PHE:C | 2.32 | 0.49 |
| 1:B:269:GLU:HG3 | 1:F:363:TYR:HE1 | 1.77 | 0.49 |
| 1:B:416:ASP:HB3 | 1:B:418:TYR:CZ | 2.46 | 0.49 |
| 1:B:420:PHE:CE1 | 1:B:429:GLN:NE2 | 2.79 | 0.49 |
| 1:B:57:ASN:CG | 1:B:59:LYS:H | 2.15 | 0.49 |
| 1:C:65:VAL:HG13 | 1:C:71:ARG:NH2 | 2.24 | 0.49 |
| 1:C:77:LEU:O | 1:C:327:ASN:HB3 | 2.12 | 0.49 |
| 1:E:117:ILE:HG13 | 1:E:118:SER:N | 2.27 | 0.49 |
| 1:E:480:PHE:O | 1:E:481:THR:HG23 | 2.12 | 0.49 |
| 1:F:273:ASP:OD1 | 1:F:274:ASP:N | 2.45 | 0.49 |
| 1:B:273:ASP:OD1 | 1:B:274:ASP:N | 2.45 | 0.49 |
| 1:D:120:HIS:CD2 | 1:D:222:LEU:HD12 | 2.47 | 0.49 |
| 1:E:116:GLY:N | 1:E:339:SER:OG | 2.19 | 0.49 |
| 1:F:372:LEU:HD22 | 1:F:374:PHE:HZ | 1.73 | 0.49 |
| 1:F:78:PRO:HD3 | 1:F:452:LYS:HA | 1.94 | 0.49 |
| 1:C:109:ARG:HD2 | 1:C:369:GLU:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:418:TYR:CB | 1:D:419:ARG:HA | 2.40 | 0.49 |
| 1:E:482:LEU:HD12 | 1:E:483:GLY:H | 1.76 | 0.49 |
| 1:F:348:ILE:HG22 | 1:F:359:ASN:O | 2.12 | 0.49 |
| 1:B:23:SER:HA | 1:B:319:HIS:HB3 | 1.95 | 0.49 |
| 1:B:259:HIS:H | 1:B:294:THR:HB | 1.76 | 0.49 |
| 1:D:366:HIS:CE1 | 1:D:368:GLU:OE2 | 2.65 | 0.49 |
| 1:E:71:ARG:HG3 | 1:E:370:TYR:CZ | 2.46 | 0.49 |
| 1:E:117:ILE:HD11 | 1:F:260:LEU:HD21 | 1.93 | 0.49 |
| 1:A:203:THR:HG21 | 1:A:224:ILE:HD13 | 1.94 | 0.49 |
| 1:B:112:PRO:HB2 | 1:C:202:ASP:OD2 | 2.12 | 0.49 |
| 1:B:235:ILE:O | 1:B:239:SER:N | 2.45 | 0.49 |
| 1:B:465:GLY:O | 1:B:468:PHE:N | 2.45 | 0.49 |
| 1:C:216:ASN:C | 1:C:218:SER:H | 2.16 | 0.49 |
| 1:D:70:TYR:CD1 | 1:D:334:VAL:HG21 | 2.47 | 0.49 |
| 1:E:23:SER:HA | 1:E:319:HIS:HB3 | 1.93 | 0.49 |
| 1:A:25:ASP:OD2 | 1:A:321:ASN:ND2 | 2.40 | 0.49 |
| 1:A:344:LEU:O | 1:A:363:TYR:N | 2.43 | 0.49 |
| 1:C:258:ARG:HG2 | 1:C:259:HIS:ND1 | 2.28 | 0.49 |
| 1:A:30:ARG:HD3 | 1:A:379:CYS:SG | 2.53 | 0.49 |
| 1:C:120:HIS:CE1 | 1:C:122:LEU:H | 2.30 | 0.49 |
| 1:C:153:GLN:NE2 | 1:C:300:VAL:HG12 | 2.27 | 0.49 |
| 1:C:249:TYR:HE1 | 1:C:251:ARG:NH1 | 2.10 | 0.49 |
| 1:C:325:TRP:CE3 | 1:C:398:ILE:HG21 | 2.47 | 0.49 |
| 1:C:466:ARG:NH2 | 1:D:319:HIS:CE1 | 2.81 | 0.49 |
| 1:D:35:TYR:HD2 | 1:D:100:TRP:CH2 | 2.31 | 0.49 |
| 1:D:97:ARG:HE | 1:D:402:TRP:HB3 | 1.78 | 0.49 |
| 1:A:129:THR:OG1 | 1:A:260:LEU:HB3 | 2.12 | 0.49 |
| 1:E:153:GLN:NE2 | 1:E:300:VAL:HG12 | 2.28 | 0.49 |
| 1:D:306:ILE:O | 1:D:311:TYR:OH | 2.29 | 0.49 |
| 1:F:428:CYS:HB3 | 1:F:432:THR:HG21 | 1.95 | 0.49 |
| 1:C:112:PRO:HB2 | 1:D:202:ASP:OD2 | 2.13 | 0.49 |
| 1:E:181:ASN:N | 1:E:184:ASP:OD2 | 2.42 | 0.49 |
| 1:F:70:TYR:HE1 | 1:F:201:VAL:HG22 | 1.78 | 0.49 |
| 1:F:366:HIS:CE1 | 1:F:368:GLU:OE2 | 2.66 | 0.49 |
| 1:A:77:LEU:O | 1:A:452:LYS:HE2 | 2.13 | 0.48 |
| 1:C:123:LEU:N | 1:C:145:GLU:O | 2.46 | 0.48 |
| 1:D:120:HIS:CE1 | 1:D:122:LEU:H | 2.31 | 0.48 |
| 1:D:153:GLN:NE2 | 1:D:300:VAL:HG12 | 2.28 | 0.48 |
| 1:D:348:ILE:HG22 | 1:D:359:ASN:O | 2.12 | 0.48 |
| 1:E:47:HIS:CE1 | 1:E:49:TYR:HB2 | 2.48 | 0.48 |
| 1:F:233:ASP:N | 1:F:237:MET:HE2 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:30:ARG:HD3 | 1:F:379:CYS:SG | 2.53 | 0.48 |
| 1:A:120:HIS:CD2 | 1:A:222:LEU:HD12 | 2.48 | 0.48 |
| 1:A:465:GLY:O | 1:A:468:PHE:N | 2.47 | 0.48 |
| 1:B:181:ASN:N | 1:B:184:ASP:OD2 | 2.42 | 0.48 |
| 1:B:233:ASP:N | 1:B:237:MET:HE2 | 2.28 | 0.48 |
| 1:B:478:PRO:HG2 | 1:B:480:PHE:CE2 | 2.48 | 0.48 |
| 1:E:314:GLN:O | 1:E:321:ASN:ND2 | 2.46 | 0.48 |
| 1:E:42:LEU:HD13 | 1:E:447:TRP:HE1 | 1.78 | 0.48 |
| 1:A:372:LEU:HB3 | 1:A:374:PHE:CZ | 2.49 | 0.48 |
| 1:B:291:TYR:OH | 1:F:146:CYS:SG | 2.65 | 0.48 |
| 1:C:422:THR:HG22 | 1:C:426:ILE:HD12 | 1.95 | 0.48 |
| 1:E:396:SER:O | 1:E:399:LEU:HB2 | 2.14 | 0.48 |
| 1:F:153:GLN:NE2 | 1:F:300:VAL:HG12 | 2.28 | 0.48 |
| 1:C:355:TYR:HE1 | 1:C:360:PHE:CE2 | 2.31 | 0.48 |
| 1:E:280:SER:O | 1:E:283:THR:OG1 | 2.21 | 0.48 |
| 1:B:171:LYS:HB2 | 1:B:213:LEU:HD11 | 1.94 | 0.48 |
| 1:B:109:ARG:CZ | 1:B:338:ARG:HD2 | 2.43 | 0.48 |
| 1:B:466:ARG:HH21 | 1:C:319:HIS:HE1 | 1.60 | 0.48 |
| 1:C:120:HIS:CD2 | 1:C:222:LEU:HD12 | 2.49 | 0.48 |
| 1:E:77:LEU:O | 1:E:327:ASN:HB3 | 2.13 | 0.48 |
| 1:F:180:VAL:HG13 | 1:F:184:ASP:HB2 | 1.95 | 0.48 |
| 1:F:216:ASN:C | 1:F:218:SER:H | 2.16 | 0.48 |
| 1:A:114:GLY:N | 1:A:337:THR:O | 2.45 | 0.48 |
| 1:A:372:LEU:HD22 | 1:A:374:PHE:CZ | 2.48 | 0.48 |
| 1:A:441:LEU:HG | 1:A:444:TYR:HD2 | 1.77 | 0.48 |
| 1:B:120:HIS:CE1 | 1:B:122:LEU:H | 2.31 | 0.48 |
| 1:B:43:LEU:HD11 | 1:C:169:TRP:CH2 | 2.49 | 0.48 |
| 1:C:72:VAL:O | 1:C:447:TRP:HB3 | 2.14 | 0.48 |
| 1:C:83:PHE:HE1 | 1:D:13:LEU:HD12 | 1.78 | 0.48 |
| 1:D:189:GLU:HG2 | 1:D:190:LEU:N | 2.28 | 0.48 |
| 1:E:118:SER:O | 1:E:148:SER:HB2 | 2.13 | 0.48 |
| 1:E:254:GLN:NE2 | 1:E:298:SER:HB3 | 2.29 | 0.48 |
| 1:A:35:TYR:HD1 | 1:A:456:SER:O | 1.96 | 0.48 |
| 1:B:124:ASN:HA | 1:B:144:ARG:HG2 | 1.96 | 0.48 |
| 1:C:404:PHE:CB | 1:C:405:GLY:HA2 | 2.22 | 0.48 |
| 1:F:417:THR:HG1 | 1:F:418:TYR:HD2 | 1.62 | 0.48 |
| 1:B:209:ASP:OD2 | 1:B:212:THR:HG23 | 2.14 | 0.48 |
| 1:B:196:GLN:HE21 | 1:B:444:TYR:HD1 | 1.60 | 0.48 |
| 1:B:70:TYR:HE1 | 1:B:201:VAL:HG22 | 1.79 | 0.48 |
| 1:D:242:TYR:CZ | 1:D:394:MET:HG3 | 2.48 | 0.48 |
| 1:D:432:THR:HA | 1:D:434:PRO:HD2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:46:GLY:HA3 | 1:D:65:VAL:HB | 1.95 | 0.48 |
| 1:F:35:TYR:HD2 | 1:F:100:TRP:CH2 | 2.31 | 0.48 |
| 1:F:43:LEU:HD12 | 1:F:368:GLU:O | 2.14 | 0.48 |
| 1:A:349:SER:O | 1:A:359:ASN:ND2 | 2.45 | 0.48 |
| 1:B:85:PHE:H | 1:B:88:THR:CG2 | 2.26 | 0.48 |
| 1:D:123:LEU:N | 1:D:145:GLU:O | 2.47 | 0.48 |
| 1:D:71:ARG:HG3 | 1:D:370:TYR:CZ | 2.49 | 0.48 |
| 1:E:298:SER:OG | 1:E:299:MET:N | 2.46 | 0.48 |
| 1:A:244:ASP:OD1 | 1:A:320:ASN:ND2 | 2.47 | 0.48 |
| 1:B:47:HIS:CE1 | 1:B:49:TYR:HB2 | 2.48 | 0.48 |
| 1:C:77:LEU:HD22 | 1:C:455:PHE:HZ | 1.78 | 0.48 |
| 1:D:40:SER:OG | 1:D:41:ARG:N | 2.47 | 0.48 |
| 1:E:57:ASN:CG | 1:E:59:LYS:H | 2.16 | 0.48 |
| 1:A:402:TRP:CE3 | 1:A:404:PHE:HE1 | 2.32 | 0.47 |
| 1:B:41:ARG:HG2 | 1:B:42:LEU:H | 1.78 | 0.47 |
| 1:B:77:LEU:HD22 | 1:B:455:PHE:CZ | 2.49 | 0.47 |
| 1:D:247:PHE:HE1 | 1:D:313:LEU:HD13 | 1.79 | 0.47 |
| 1:E:115:VAL:H | 1:F:255:MET:HE1 | 1.79 | 0.47 |
| 1:F:312:TRP:HH2 | 1:F:468:PHE:HD1 | 1.59 | 0.47 |
| 1:A:469:LEU:HD22 | 1:A:474:LEU:HD23 | 1.96 | 0.47 |
| 1:A:65:VAL:HG13 | 1:A:71:ARG:HH22 | 1.78 | 0.47 |
| 1:B:109:ARG:NE | 1:B:338:ARG:HD2 | 2.29 | 0.47 |
| 1:C:459:LEU:HB2 | 1:C:477:LYS:NZ | 2.29 | 0.47 |
| 1:D:81:ASN:ND2 | 1:D:97:ARG:HD2 | 2.29 | 0.47 |
| 1:E:57:ASN:OD1 | 1:E:59:LYS:N | 2.43 | 0.47 |
| 1:F:36:HIS:HD2 | 1:F:375:ILE:HD13 | 1.78 | 0.47 |
| 1:B:42:LEU:HD21 | 1:B:370:TYR:HD2 | 1.78 | 0.47 |
| 1:C:109:ARG:HG3 | 1:C:307:PHE:HD2 | 1.79 | 0.47 |
| 1:C:405:GLY:N | 1:C:406:LEU:O | 2.48 | 0.47 |
| 1:F:23:SER:HA | 1:F:319:HIS:HB3 | 1.95 | 0.47 |
| 1:A:150:ASP:OD1 | 1:A:296:SER:HA | 2.14 | 0.47 |
| 1:A:165:ILE:HG21 | 1:A:236:LYS:NZ | 2.29 | 0.47 |
| 1:A:431:HIS:HB3 | 1:A:433:PRO:O | 2.14 | 0.47 |
| 1:A:37:ALA:CB | 1:A:455:PHE:HD1 | 2.27 | 0.47 |
| 1:F:181:ASN:N | 1:F:184:ASP:OD2 | 2.40 | 0.47 |
| 1:F:40:SER:OG | 1:F:41:ARG:N | 2.47 | 0.47 |
| 1:C:249:TYR:HE1 | 1:C:251:ARG:HH11 | 1.62 | 0.47 |
| 1:C:109:ARG:NH1 | 1:C:370:TYR:CE1 | 2.82 | 0.47 |
| 1:B:269:GLU:HG3 | 1:F:363:TYR:CE1 | 2.50 | 0.47 |
| 1:A:158:LEU:HD12 | 1:A:332:THR:HB | 1.97 | 0.47 |
| 1:A:73:PHE:CD1 | 1:A:447:TRP:HD1 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:111:GLN:HG2 | 1:B:369:GLU:HB3 | 1.97 | 0.47 |
| 1:C:46:GLY:HA3 | 1:C:65:VAL:HB | 1.96 | 0.47 |
| 1:C:77:LEU:HD22 | 1:C:455:PHE:CZ | 2.50 | 0.47 |
| 1:E:258:ARG:HG2 | 1:E:259:HIS:CE1 | 2.50 | 0.47 |
| 1:E:51:PRO:HB3 | 1:E:64:LYS:HB2 | 1.97 | 0.47 |
| 1:F:96:GLN:HA | 1:F:383:LEU:CD1 | 2.44 | 0.47 |
| 1:D:426:ILE:HG22 | 1:D:427:ALA:N | 2.30 | 0.47 |
| 1:E:123:LEU:N | 1:E:145:GLU:O | 2.47 | 0.47 |
| 1:F:118:SER:O | 1:F:148:SER:HB2 | 2.15 | 0.47 |
| 1:E:455:PHE:HB2 | 1:F:13:LEU:HD11 | 1.96 | 0.47 |
| 1:F:254:GLN:OE1 | 1:F:298:SER:HB3 | 2.15 | 0.47 |
| 1:B:216:ASN:C | 1:B:218:SER:H | 2.18 | 0.47 |
| 1:F:109:ARG:HG3 | 1:F:307:PHE:HD2 | 1.79 | 0.47 |
| 1:A:349:SER:N | 1:A:359:ASN:OD1 | 2.37 | 0.47 |
| 1:B:109:ARG:HG3 | 1:B:307:PHE:HD2 | 1.80 | 0.47 |
| 1:B:70:TYR:HD1 | 1:B:334:VAL:HG21 | 1.80 | 0.47 |
| 1:D:90:PHE:CE1 | 1:D:91:TYR:HD2 | 2.33 | 0.47 |
| 1:E:70:TYR:CE1 | 1:E:201:VAL:HG22 | 2.49 | 0.47 |
| 1:E:247:PHE:HE1 | 1:E:313:LEU:HD13 | 1.80 | 0.47 |
| 1:A:24:THR:OG1 | 1:A:321:ASN:N | 2.48 | 0.47 |
| 1:C:34:TYR:HE1 | 1:C:377:GLN:HG3 | 1.80 | 0.47 |
| 1:C:50:PHE:CE2 | 1:D:271:VAL:HG22 | 2.50 | 0.47 |
| 1:D:312:TRP:CZ3 | 1:D:468:PHE:HD1 | 2.32 | 0.47 |
| 1:B:21:VAL:HG13 | 1:B:390:TYR:OH | 2.15 | 0.47 |
| 1:C:233:ASP:N | 1:C:237:MET:HE2 | 2.29 | 0.47 |
| 1:D:210:PHE:CE2 | 1:D:220:VAL:HG11 | 2.50 | 0.47 |
| 1:E:395:ASN:HB3 | 1:E:398:ILE:CD1 | 2.45 | 0.47 |
| 1:E:68:LEU:HD11 | 1:E:151:TYR:HD2 | 1.80 | 0.47 |
| 1:A:126:LEU:HB3 | 1:A:262:ASN:HB2 | 1.96 | 0.46 |
| 1:A:35:TYR:CE1 | 1:A:457:ALA:HA | 2.50 | 0.46 |
| 1:B:216:ASN:HA | 1:F:360:PHE:CE2 | 2.50 | 0.46 |
| 1:C:312:TRP:CZ3 | 1:C:468:PHE:HD1 | 2.33 | 0.46 |
| 1:D:77:LEU:O | 1:D:327:ASN:HB3 | 2.14 | 0.46 |
| 1:B:153:GLN:NE2 | 1:B:300:VAL:HG12 | 2.31 | 0.46 |
| 1:B:169:TRP:O | 1:B:208:MET:HA | 2.15 | 0.46 |
| 1:C:180:VAL:HG13 | 1:C:184:ASP:HB2 | 1.96 | 0.46 |
| 1:C:366:HIS:CE1 | 1:C:367:GLY:O | 2.69 | 0.46 |
| 1:C:73:PHE:CD1 | 1:C:447:TRP:CD1 | 3.03 | 0.46 |
| 1:A:312:TRP:CH2 | 1:A:468:PHE:HB2 | 2.50 | 0.46 |
| 1:A:37:ALA:HB3 | 1:A:455:PHE:CD1 | 2.50 | 0.46 |
| 1:B:258:ARG:HG2 | 1:B:259:HIS:CE1 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:339:SER:O | 1:B:366:HIS:NE2 | 2.48 | 0.46 |
| 1:B:392:HIS:O | 1:B:396:SER:OG | 2.26 | 0.46 |
| 1:B:418:TYR:HB3 | 1:B:419:ARG:HG2 | 1.98 | 0.46 |
| 1:C:272:PRO:HD2 | 1:C:275:LEU:HD12 | 1.97 | 0.46 |
| 1:C:81:ASN:OD1 | 1:C:98:LEU:N | 2.48 | 0.46 |
| 1:A:170:GLY:N | 1:A:189:GLU:O | 2.46 | 0.46 |
| 1:A:242:TYR:HE1 | 1:A:390:TYR:HH | 1.64 | 0.46 |
| 1:A:74:ARG:HG3 | 1:A:330:PHE:HE1 | 1.80 | 0.46 |
| 1:A:65:VAL:HG13 | 1:A:71:ARG:NH2 | 2.31 | 0.46 |
| 1:A:73:PHE:CE1 | 1:A:447:TRP:HD1 | 2.34 | 0.46 |
| 1:E:458:ASP:OD2 | 1:F:20:LYS:HE2 | 2.15 | 0.46 |
| 1:F:246:LEU:HD12 | 1:F:246:LEU:O | 2.15 | 0.46 |
| 1:B:383:LEU:HA | 1:B:387:VAL:HG11 | 1.97 | 0.46 |
| 1:C:399:LEU:C | 1:C:404:PHE:CE1 | 2.89 | 0.46 |
| 1:C:48:PRO:HA | 1:C:66:SER:HB2 | 1.98 | 0.46 |
| 1:C:71:ARG:HG3 | 1:C:370:TYR:CZ | 2.50 | 0.46 |
| 1:D:246:LEU:O | 1:D:246:LEU:HD12 | 2.16 | 0.46 |
| 1:E:482:LEU:HG | 1:E:483:GLY:N | 2.31 | 0.46 |
| 1:A:124:ASN:ND2 | 1:A:263:ARG:HD2 | 2.30 | 0.46 |
| 1:B:259:HIS:C | 1:B:260:LEU:HD12 | 2.36 | 0.46 |
| 1:A:254:GLN:NE2 | 1:A:298:SER:HB3 | 2.31 | 0.46 |
| 1:A:298:SER:OG | 1:A:299:MET:N | 2.47 | 0.46 |
| 1:B:298:SER:OG | 1:B:299:MET:N | 2.48 | 0.46 |
| 1:B:70:TYR:CD1 | 1:B:334:VAL:HG21 | 2.51 | 0.46 |
| 1:B:116:GLY:N | 1:B:339:SER:OG | 2.20 | 0.46 |
| 1:B:355:TYR:CG | 1:C:144:ARG:NH2 | 2.83 | 0.46 |
| 1:C:50:PHE:HA | 1:C:64:LYS:HD2 | 1.97 | 0.46 |
| 1:C:85:PHE:H | 1:C:88:THR:CG2 | 2.29 | 0.46 |
| 1:A:240:GLU:OE1 | 1:A:244:ASP:N | 2.49 | 0.46 |
| 1:A:341:ASN:OD1 | 1:A:366:HIS:HB2 | 2.16 | 0.46 |
| 1:B:23:SER:O | 1:B:26:GLU:HG2 | 2.16 | 0.46 |
| 1:B:41:ARG:CG | 1:B:42:LEU:N | 2.79 | 0.46 |
| 1:B:48:PRO:HA | 1:B:66:SER:HB2 | 1.98 | 0.46 |
| 1:D:117:ILE:HG12 | 1:D:118:SER:N | 2.29 | 0.46 |
| 1:E:115:VAL:HG12 | 1:E:116:GLY:O | 2.16 | 0.46 |
| 1:B:42:LEU:CD2 | 1:B:370:TYR:HB2 | 2.46 | 0.46 |
| 1:C:164:PRO:HB2 | 1:C:195:ILE:HD12 | 1.97 | 0.46 |
| 1:D:114:GLY:HA2 | 1:E:255:MET:CE | 2.46 | 0.46 |
| 1:F:109:ARG:HG3 | 1:F:307:PHE:CD2 | 2.51 | 0.46 |
| 1:B:81:ASN:HD21 | 1:B:97:ARG:HB3 | 1.81 | 0.46 |
| 1:C:30:ARG:HD3 | 1:C:379:CYS:SG | 2.56 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:TYR:HE1 | 1:E:377:GLN:HG3 | 1.80 | 0.46 |
| 1:C:45:VAL:HA | 1:C:366:HIS:O | 2.14 | 0.45 |
| 1:C:459:LEU:HB2 | 1:C:477:LYS:HZ3 | 1.81 | 0.45 |
| 1:E:466:ARG:NH2 | 1:F:319:HIS:CE1 | 2.84 | 0.45 |
| 1:A:150:ASP:OD2 | 1:A:297:GLY:N | 2.48 | 0.45 |
| 1:A:329:LEU:HD23 | 1:A:330:PHE:N | 2.31 | 0.45 |
| 1:A:385:ALA:O | 1:A:389:THR:OG1 | 2.33 | 0.45 |
| 1:B:144:ARG:NH1 | 1:B:218:SER:OG | 2.49 | 0.45 |
| 1:C:109:ARG:HE | 1:C:338:ARG:HD2 | 1.80 | 0.45 |
| 1:E:112:PRO:HB2 | 1:F:202:ASP:OD2 | 2.16 | 0.45 |
| 1:E:164:PRO:HB2 | 1:E:195:ILE:HD12 | 1.98 | 0.45 |
| 1:E:83:PHE:HD2 | 1:E:85:PHE:HE1 | 1.64 | 0.45 |
| 1:F:70:TYR:HD1 | 1:F:334:VAL:HG21 | 1.80 | 0.45 |
| 1:C:400:GLU:HA | 1:C:404:PHE:HZ | 1.72 | 0.45 |
| 1:C:404:PHE:HB3 | 1:C:406:LEU:C | 2.35 | 0.45 |
| 1:D:52:ILE:HG22 | 1:D:61:LEU:HB3 | 1.97 | 0.45 |
| 1:D:97:ARG:CZ | 1:D:404:PHE:HD2 | 2.29 | 0.45 |
| 1:E:209:ASP:OD2 | 1:E:212:THR:HG23 | 2.16 | 0.45 |
| 1:F:312:TRP:CZ3 | 1:F:468:PHE:CD1 | 3.04 | 0.45 |
| 1:B:319:HIS:HE1 | 1:F:466:ARG:HH21 | 1.64 | 0.45 |
| 1:A:159:ILE:HD12 | 1:A:248:PHE:CD2 | 2.51 | 0.45 |
| 1:B:50:PHE:CE2 | 1:C:271:VAL:HG22 | 2.50 | 0.45 |
| 1:C:400:GLU:CA | 1:C:404:PHE:CZ | 2.85 | 0.45 |
| 1:C:466:ARG:HH21 | 1:D:319:HIS:HE1 | 1.62 | 0.45 |
| 1:D:109:ARG:HG3 | 1:D:307:PHE:HD2 | 1.81 | 0.45 |
| 1:D:325:TRP:CE3 | 1:D:398:ILE:HG21 | 2.50 | 0.45 |
| 1:F:420:PHE:HB3 | 1:F:430:LYS:HE3 | 1.97 | 0.45 |
| 1:A:43:LEU:HG | 1:A:44:ALA:N | 2.32 | 0.45 |
| 1:C:246:LEU:O | 1:C:246:LEU:HD12 | 2.16 | 0.45 |
| 1:C:109:ARG:HH21 | 1:C:338:ARG:HB2 | 1.81 | 0.45 |
| 1:E:246:LEU:O | 1:E:246:LEU:HD12 | 2.16 | 0.45 |
| 1:A:321:ASN:O | 1:A:323:ILE:HG12 | 2.17 | 0.45 |
| 1:B:37:ALA:HB2 | 1:B:455:PHE:HD1 | 1.81 | 0.45 |
| 1:C:298:SER:OG | 1:C:299:MET:N | 2.49 | 0.45 |
| 1:D:298:SER:OG | 1:D:299:MET:N | 2.50 | 0.45 |
| 1:E:167:GLU:CD | 1:E:233:ASP:HB2 | 2.37 | 0.45 |
| 1:E:465:GLY:O | 1:E:468:PHE:N | 2.49 | 0.45 |
| 1:F:220:VAL:HB | 1:F:224:ILE:HD11 | 1.98 | 0.45 |
| 1:F:301:THR:HG23 | 1:F:303:ASP:H | 1.82 | 0.45 |
| 1:F:65:VAL:HG13 | 1:F:71:ARG:HH22 | 1.82 | 0.45 |
| 1:A:12:TYR:O | 1:A:13:LEU:HB2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:ASP:CG | 1:A:236:LYS:H | 2.20 | 0.45 |
| 1:A:37:ALA:HB1 | 1:A:454:LYS:HB2 | 1.99 | 0.45 |
| 1:B:280:SER:O | 1:B:283:THR:OG1 | 2.28 | 0.45 |
| 1:C:348:ILE:HG22 | 1:C:359:ASN:O | 2.17 | 0.45 |
| 1:D:109:ARG:NH1 | 1:D:370:TYR:CE1 | 2.85 | 0.45 |
| 1:E:109:ARG:NH1 | 1:E:370:TYR:CE1 | 2.85 | 0.45 |
| 1:B:389:THR:O | 1:B:393:SER:N | 2.38 | 0.45 |
| 1:B:406:LEU:HA | 1:B:407:GLN:CB | 2.36 | 0.45 |
| 1:B:478:PRO:HG2 | 1:B:480:PHE:HE2 | 1.81 | 0.45 |
| 1:C:35:TYR:CD2 | 1:C:100:TRP:HH2 | 2.35 | 0.45 |
| 1:C:120:HIS:CE1 | 1:C:122:LEU:O | 2.70 | 0.45 |
| 1:C:36:HIS:HB2 | 1:C:459:LEU:HD21 | 1.98 | 0.45 |
| 1:C:459:LEU:HD23 | 1:C:459:LEU:HA | 1.66 | 0.45 |
| 1:C:53:LYS:HA | 1:C:61:LEU:N | 2.26 | 0.45 |
| 1:C:146:CYS:HG | 1:D:291:TYR:HH | 1.62 | 0.45 |
| 1:E:310:PRO:HG2 | 1:E:312:TRP:CH2 | 2.51 | 0.45 |
| 1:C:85:PHE:CZ | 1:C:378:LEU:HD21 | 2.52 | 0.45 |
| 1:D:112:PRO:HB2 | 1:E:202:ASP:OD2 | 2.17 | 0.45 |
| 1:E:155:GLN:NE2 | 1:E:305:GLN:OE1 | 2.48 | 0.45 |
| 1:F:13:LEU:HB2 | 1:F:14:PRO:HD3 | 1.98 | 0.45 |
| 1:F:381:ILE:O | 1:F:383:LEU:HG | 2.17 | 0.45 |
| 1:F:403:ASN:O | 1:F:404:PHE:HB2 | 2.17 | 0.45 |
| 1:F:9:ALA:O | 1:F:10:THR:HG23 | 2.16 | 0.45 |
| 1:B:247:PHE:O | 1:B:316:ALA:HB1 | 2.17 | 0.45 |
| 1:B:83:PHE:CD2 | 1:B:85:PHE:HE1 | 2.29 | 0.45 |
| 1:C:363:TYR:HE1 | 1:D:269:GLU:HG3 | 1.82 | 0.45 |
| 1:C:52:ILE:HG22 | 1:C:61:LEU:HB3 | 1.98 | 0.45 |
| 1:D:417:THR:O | 1:D:418:TYR:CG | 2.69 | 0.45 |
| 1:E:325:TRP:CE3 | 1:E:398:ILE:HG21 | 2.52 | 0.45 |
| 1:F:259:HIS:H | 1:F:294:THR:HB | 1.82 | 0.45 |
| 1:F:51:PRO:HB3 | 1:F:64:LYS:HB2 | 1.98 | 0.45 |
| 1:C:415:GLU:O | 1:C:416:ASP:HB2 | 2.16 | 0.44 |
| 1:D:117:ILE:CG1 | 1:D:118:SER:H | 2.29 | 0.44 |
| 1:D:246:LEU:HD12 | 1:D:317:GLN:NE2 | 2.32 | 0.44 |
| 1:D:51:PRO:HB3 | 1:D:64:LYS:HB2 | 1.99 | 0.44 |
| 1:E:52:ILE:HB | 1:E:62:VAL:CB | 2.45 | 0.44 |
| 1:C:210:PHE:CE2 | 1:C:220:VAL:HG11 | 2.52 | 0.44 |
| 1:E:54:LYS:HD2 | 1:E:57:ASN:HB2 | 1.99 | 0.44 |
| 1:B:203:THR:HG21 | 1:B:224:ILE:HD13 | 1.99 | 0.44 |
| 1:C:34:TYR:HE1 | 1:C:377:GLN:CG | 2.30 | 0.44 |
| 1:C:399:LEU:O | 1:C:402:TRP:N | 2.43 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:405:GLY:CA | 1:C:406:LEU:O | 2.65 | 0.44 |
| 1:D:146:CYS:SG | 1:E:291:TYR:OH | 2.59 | 0.44 |
| 1:D:258:ARG:HG2 | 1:D:259:HIS:CE1 | 2.52 | 0.44 |
| 1:D:433:PRO:HG2 | 1:D:434:PRO:HD3 | 1.99 | 0.44 |
| 1:E:216:ASN:C | 1:E:218:SER:H | 2.21 | 0.44 |
| 1:E:35:TYR:CD2 | 1:E:100:TRP:HH2 | 2.34 | 0.44 |
| 1:F:273:ASP:HA | 1:F:276:TYR:CE2 | 2.52 | 0.44 |
| 1:F:422:THR:HG23 | 1:F:430:LYS:HG3 | 1.98 | 0.44 |
| 1:F:85:PHE:HB2 | 1:F:88:THR:HG22 | 1.99 | 0.44 |
| 1:A:84:GLY:C | 1:A:85:PHE:CD2 | 2.91 | 0.44 |
| 1:B:42:LEU:O | 1:B:369:GLU:HG3 | 2.17 | 0.44 |
| 1:C:155:GLN:NE2 | 1:C:305:GLN:OE1 | 2.49 | 0.44 |
| 1:C:240:GLU:HG3 | 1:C:241:PRO:HD2 | 1.98 | 0.44 |
| 1:B:363:TYR:CE1 | 1:C:268:GLY:HA3 | 2.52 | 0.44 |
| 1:C:474:LEU:O | 1:C:474:LEU:HD12 | 2.18 | 0.44 |
| 1:D:13:LEU:HD23 | 1:D:13:LEU:HA | 1.55 | 0.44 |
| 1:E:399:LEU:HB3 | 1:E:404:PHE:HE1 | 1.72 | 0.44 |
| 1:E:474:LEU:O | 1:E:474:LEU:HD12 | 2.17 | 0.44 |
| 1:E:74:ARG:O | 1:E:75:ILE:HD13 | 2.17 | 0.44 |
| 1:E:455:PHE:CB | 1:F:13:LEU:HD11 | 2.48 | 0.44 |
| 1:F:248:PHE:CG | 1:F:249:TYR:N | 2.86 | 0.44 |
| 1:F:314:GLN:HG3 | 1:F:315:ARG:N | 2.33 | 0.44 |
| 1:F:355:TYR:HE1 | 1:F:360:PHE:CE2 | 2.35 | 0.44 |
| 1:B:85:PHE:CZ | 1:B:378:LEU:HD21 | 2.53 | 0.44 |
| 1:D:168:HIS:CE1 | 1:D:191:ILE:HB | 2.52 | 0.44 |
| 1:F:465:GLY:O | 1:F:468:PHE:N | 2.51 | 0.44 |
| 1:A:70:TYR:CE1 | 1:A:201:VAL:HG22 | 2.53 | 0.44 |
| 1:C:11:VAL:O | 1:C:12:TYR:CD1 | 2.71 | 0.44 |
| 1:A:23:SER:O | 1:A:26:GLU:HG2 | 2.18 | 0.44 |
| 1:B:314:GLN:HG3 | 1:B:315:ARG:N | 2.33 | 0.44 |
| 1:B:433:PRO:O | 1:B:435:ALA:N | 2.51 | 0.44 |
| 1:C:439:ASP:HB3 | 1:C:442:LYS:HB2 | 1.99 | 0.44 |
| 1:F:70:TYR:CE1 | 1:F:201:VAL:HG22 | 2.52 | 0.44 |
| 1:F:70:TYR:CD1 | 1:F:334:VAL:HG21 | 2.53 | 0.44 |
| 1:B:249:TYR:HE1 | 1:B:251:ARG:NH1 | 2.15 | 0.44 |
| 1:B:73:PHE:CD1 | 1:B:447:TRP:CD1 | 3.06 | 0.44 |
| 1:C:50:PHE:HE2 | 1:D:271:VAL:HG22 | 1.82 | 0.44 |
| 1:D:70:TYR:HE1 | 1:D:201:VAL:HG22 | 1.82 | 0.44 |
| 1:E:106:GLU:OE1 | 1:E:310:PRO:HA | 2.18 | 0.44 |
| 1:E:313:LEU:HD23 | 1:E:313:LEU:HA | 1.71 | 0.44 |
| 1:E:366:HIS:NE2 | 1:E:368:GLU:OE2 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:TYR:HE1 | 1:E:377:GLN:CG | 2.31 | 0.44 |
| 1:E:409:PRO:O | 1:E:411:GLY:N | 2.50 | 0.44 |
| 1:E:73:PHE:HZ | 1:E:370:TYR:CD2 | 2.36 | 0.44 |
| 1:F:11:VAL:HG12 | 1:F:13:LEU:H | 1.82 | 0.44 |
| 1:A:98:LEU:HA | 1:A:379:CYS:O | 2.17 | 0.44 |
| 1:B:115:VAL:HG12 | 1:B:116:GLY:O | 2.17 | 0.44 |
| 1:C:248:PHE:CG | 1:C:249:TYR:N | 2.85 | 0.44 |
| 1:C:409:PRO:C | 1:C:411:GLY:N | 2.70 | 0.44 |
| 1:B:273:ASP:HA | 1:B:276:TYR:CE2 | 2.53 | 0.43 |
| 1:B:366:HIS:CE1 | 1:B:368:GLU:OE2 | 2.71 | 0.43 |
| 1:D:248:PHE:CG | 1:D:249:TYR:N | 2.85 | 0.43 |
| 1:B:366:HIS:HE1 | 1:B:368:GLU:OE2 | 2.01 | 0.43 |
| 1:C:408:PRO:N | 1:C:410:PRO:HD2 | 2.33 | 0.43 |
| 1:D:120:HIS:ND1 | 1:D:122:LEU:N | 2.61 | 0.43 |
| 1:E:171:LYS:HB2 | 1:E:213:LEU:HD11 | 2.00 | 0.43 |
| 1:E:421:VAL:HG12 | 1:E:423:SER:H | 1.83 | 0.43 |
| 1:F:120:HIS:CE1 | 1:F:122:LEU:O | 2.70 | 0.43 |
| 1:B:80:PRO:HD3 | 1:B:100:TRP:HE1 | 1.83 | 0.43 |
| 1:B:80:PRO:HD3 | 1:B:100:TRP:NE1 | 2.33 | 0.43 |
| 1:B:81:ASN:OD1 | 1:B:98:LEU:N | 2.51 | 0.43 |
| 1:C:259:HIS:C | 1:C:260:LEU:HD12 | 2.38 | 0.43 |
| 1:D:106:GLU:OE1 | 1:D:310:PRO:HA | 2.19 | 0.43 |
| 1:E:120:HIS:CE1 | 1:E:122:LEU:O | 2.71 | 0.43 |
| 1:D:365:ARG:NH2 | 1:E:185:CYS:SG | 2.91 | 0.43 |
| 1:E:248:PHE:CG | 1:E:249:TYR:N | 2.87 | 0.43 |
| 1:D:466:ARG:NH2 | 1:E:319:HIS:CE1 | 2.85 | 0.43 |
| 1:F:97:ARG:HG3 | 1:F:402:TRP:CZ3 | 2.53 | 0.43 |
| 1:A:49:TYR:HB3 | 1:A:222:LEU:HD22 | 2.00 | 0.43 |
| 1:C:344:LEU:HD22 | 1:D:213:LEU:HD23 | 2.00 | 0.43 |
| 1:D:259:HIS:C | 1:D:260:LEU:HD12 | 2.39 | 0.43 |
| 1:F:298:SER:OG | 1:F:299:MET:N | 2.50 | 0.43 |
| 1:B:256:PHE:HB3 | 1:F:299:MET:HA | 2.00 | 0.43 |
| 1:F:73:PHE:HZ | 1:F:370:TYR:CD2 | 2.36 | 0.43 |
| 1:F:385:ALA:HA | 1:F:388:MET:CE | 2.48 | 0.43 |
| 1:A:209:ASP:O | 1:A:213:LEU:HB2 | 2.18 | 0.43 |
| 1:A:76:HIS:HB3 | 1:A:452:LYS:HE3 | 2.00 | 0.43 |
| 1:B:35:TYR:HD2 | 1:B:100:TRP:HH2 | 1.66 | 0.43 |
| 1:B:52:ILE:O | 1:B:61:LEU:N | 2.52 | 0.43 |
| 1:C:423:SER:C | 1:C:425:ALA:H | 2.20 | 0.43 |
| 1:D:192:ASN:CG | 1:D:236:LYS:HE2 | 2.39 | 0.43 |
| 1:E:404:PHE:CE2 | 1:E:406:LEU:HD12 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:65:VAL:HA | 1:C:69:GLN:OE1 | 2.18 | 0.43 |
| 1:D:210:PHE:CE2 | 1:D:224:ILE:HD12 | 2.46 | 0.43 |
| 1:D:244:ASP:OD1 | 1:D:320:ASN:ND2 | 2.43 | 0.43 |
| 1:A:255:MET:HG2 | 1:A:256:PHE:N | 2.34 | 0.43 |
| 1:B:246:LEU:HD12 | 1:B:317:GLN:NE2 | 2.34 | 0.43 |
| 1:B:77:LEU:HD22 | 1:B:455:PHE:HZ | 1.82 | 0.43 |
| 1:B:70:TYR:HD2 | 1:B:199:ASP:HB2 | 1.83 | 0.43 |
| 1:F:109:ARG:NH1 | 1:F:370:TYR:CE1 | 2.86 | 0.43 |
| 1:B:162:LYS:HG2 | 1:B:244:ASP:HB3 | 2.01 | 0.43 |
| 1:C:365:ARG:NH2 | 1:D:185:CYS:SG | 2.92 | 0.43 |
| 1:D:240:GLU:HG3 | 1:D:241:PRO:HD2 | 2.01 | 0.43 |
| 1:F:52:ILE:HG22 | 1:F:61:LEU:HB3 | 2.00 | 0.43 |
| 1:A:118:SER:O | 1:A:148:SER:HB2 | 2.18 | 0.43 |
| 1:A:314:GLN:HG3 | 1:A:315:ARG:H | 1.84 | 0.43 |
| 1:A:459:LEU:O | 1:A:461:GLN:N | 2.52 | 0.43 |
| 1:D:280:SER:O | 1:D:283:THR:OG1 | 2.28 | 0.43 |
| 1:E:246:LEU:HD12 | 1:E:317:GLN:NE2 | 2.33 | 0.43 |
| 1:A:108:GLY:H | 1:A:371:ASP:HB3 | 1.84 | 0.43 |
| 1:C:247:PHE:CE1 | 1:C:313:LEU:HD13 | 2.51 | 0.43 |
| 1:C:34:TYR:CE1 | 1:C:377:GLN:HG3 | 2.54 | 0.43 |
| 1:E:120:HIS:CE1 | 1:E:122:LEU:H | 2.36 | 0.43 |
| 1:E:399:LEU:HD22 | 1:E:404:PHE:HE1 | 1.83 | 0.43 |
| 1:E:83:PHE:HD2 | 1:E:85:PHE:CE1 | 2.37 | 0.43 |
| 1:E:85:PHE:HB2 | 1:E:88:THR:HG22 | 2.01 | 0.43 |
| 1:F:384:THR:O | 1:F:388:MET:HG3 | 2.19 | 0.43 |
| 1:A:216:ASN:OD1 | 1:A:218:SER:HB2 | 2.19 | 0.42 |
| 1:A:109:ARG:NH1 | 1:A:369:GLU:O | 2.51 | 0.42 |
| 1:A:197:ASP:CB | 1:A:446:PHE:HA | 2.47 | 0.42 |
| 1:B:78:PRO:HD3 | 1:B:452:LYS:HG2 | 2.01 | 0.42 |
| 1:D:30:ARG:HD3 | 1:D:379:CYS:SG | 2.58 | 0.42 |
| 1:E:11:VAL:HG12 | 1:E:12:TYR:N | 2.34 | 0.42 |
| 1:E:357:ASN:HB3 | 1:F:265:GLY:HA2 | 2.00 | 0.42 |
| 1:B:24:THR:HG21 | 1:B:320:ASN:HA | 2.02 | 0.42 |
| 1:C:153:GLN:CD | 1:C:300:VAL:HG12 | 2.40 | 0.42 |
| 1:C:399:LEU:CB | 1:C:404:PHE:CE1 | 3.00 | 0.42 |
| 1:C:404:PHE:HB3 | 1:C:407:GLN:CA | 2.47 | 0.42 |
| 1:C:408:PRO:C | 1:C:410:PRO:HD2 | 2.39 | 0.42 |
| 1:E:407:GLN:HB2 | 1:E:408:PRO:HD3 | 2.02 | 0.42 |
| 1:F:259:HIS:C | 1:F:260:LEU:HD12 | 2.39 | 0.42 |
| 1:F:414:LEU:HA | 1:F:414:LEU:HD23 | 1.73 | 0.42 |
| 1:A:240:GLU:HG2 | 1:A:242:TYR:H | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:280:SER:O | 1:A:283:THR:OG1 | 2.23 | 0.42 |
| 1:A:306:ILE:HG22 | 1:A:311:TYR:OH | 2.19 | 0.42 |
| 1:B:117:ILE:HG13 | 1:B:118:SER:N | 2.34 | 0.42 |
| 1:B:109:ARG:CD | 1:B:370:TYR:HD1 | 2.31 | 0.42 |
| 1:B:436:PRO:O | 1:B:438:GLU:HG3 | 2.18 | 0.42 |
| 1:C:321:ASN:O | 1:C:323:ILE:HG12 | 2.20 | 0.42 |
| 1:C:395:ASN:HB3 | 1:C:398:ILE:HD12 | 2.01 | 0.42 |
| 1:D:44:ALA:HB3 | 1:D:368:GLU:HB2 | 2.01 | 0.42 |
| 1:F:383:LEU:HD23 | 1:F:387:VAL:HG11 | 2.01 | 0.42 |
| 1:A:258:ARG:HG2 | 1:A:259:HIS:CE1 | 2.54 | 0.42 |
| 1:A:86:PRO:O | 1:F:88:THR:OG1 | 2.25 | 0.42 |
| 1:B:70:TYR:CE1 | 1:B:201:VAL:HG22 | 2.55 | 0.42 |
| 1:B:50:PHE:HA | 1:B:64:LYS:HD2 | 2.01 | 0.42 |
| 1:B:52:ILE:HG22 | 1:B:61:LEU:HB3 | 2.01 | 0.42 |
| 1:C:276:TYR:CZ | 1:C:286:LEU:HD21 | 2.55 | 0.42 |
| 1:D:314:GLN:HG3 | 1:D:315:ARG:N | 2.35 | 0.42 |
| 1:D:356:LYS:HA | 1:E:141:VAL:HG13 | 2.01 | 0.42 |
| 1:D:408:PRO:N | 1:D:409:PRO:CD | 2.82 | 0.42 |
| 1:D:57:ASN:CG | 1:D:59:LYS:H | 2.21 | 0.42 |
| 1:F:335:ASP:OD1 | 1:F:337:THR:N | 2.43 | 0.42 |
| 1:C:30:ARG:HB3 | 1:C:377:GLN:NE2 | 2.34 | 0.42 |
| 1:D:466:ARG:NH1 | 1:E:317:GLN:O | 2.52 | 0.42 |
| 1:E:280:SER:N | 1:E:283:THR:OG1 | 2.41 | 0.42 |
| 1:A:124:ASN:HD22 | 1:A:219:GLU:CD | 2.23 | 0.42 |
| 1:A:119:GLY:CA | 1:A:148:SER:HA | 2.50 | 0.42 |
| 1:A:153:GLN:NE2 | 1:A:300:VAL:HG12 | 2.35 | 0.42 |
| 1:A:220:VAL:HG23 | 1:A:225:CYS:HB2 | 2.02 | 0.42 |
| 1:C:109:ARG:NE | 1:C:338:ARG:HD2 | 2.34 | 0.42 |
| 1:A:72:VAL:HB | 1:A:446:PHE:HB2 | 2.00 | 0.42 |
| 1:B:312:TRP:HH2 | 1:B:468:PHE:HD1 | 1.57 | 0.42 |
| 1:D:299:MET:HA | 1:E:256:PHE:HB3 | 2.01 | 0.42 |
| 1:A:121:PRO:HA | 1:A:146:CYS:SG | 2.60 | 0.42 |
| 1:A:169:TRP:CD2 | 1:A:190:LEU:HD13 | 2.55 | 0.42 |
| 1:A:390:TYR:O | 1:A:393:SER:HB2 | 2.20 | 0.42 |
| 1:B:418:TYR:HB3 | 1:B:419:ARG:CG | 2.50 | 0.42 |
| 1:C:216:ASN:ND2 | 1:C:219:GLU:OE2 | 2.50 | 0.42 |
| 1:C:240:GLU:CG | 1:C:241:PRO:HD2 | 2.50 | 0.42 |
| 1:D:115:VAL:HG12 | 1:D:116:GLY:O | 2.20 | 0.42 |
| 1:F:169:TRP:O | 1:F:208:MET:HA | 2.20 | 0.42 |
| 1:F:301:THR:HG23 | 1:F:303:ASP:N | 2.35 | 0.42 |
| 1:A:53:LYS:CB | 1:A:60:ILE:HA | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:41:ARG:NH2 | 1:C:167:GLU:OE1 | 2.52 | 0.42 |
| 1:C:167:GLU:CD | 1:C:233:ASP:HB2 | 2.39 | 0.42 |
| 1:D:466:ARG:HH21 | 1:E:319:HIS:HE1 | 1.63 | 0.42 |
| 1:E:375:ILE:HG23 | 1:E:375:ILE:HD12 | 1.85 | 0.42 |
| 1:B:109:ARG:HH21 | 1:B:338:ARG:HB2 | 1.84 | 0.42 |
| 1:B:120:HIS:ND1 | 1:B:122:LEU:N | 2.64 | 0.42 |
| 1:B:54:LYS:HD2 | 1:B:57:ASN:HB2 | 2.01 | 0.42 |
| 1:E:153:GLN:CD | 1:E:300:VAL:HG12 | 2.40 | 0.42 |
| 1:E:97:ARG:HG3 | 1:E:402:TRP:CZ3 | 2.55 | 0.42 |
| 1:A:117:ILE:CG1 | 1:A:118:SER:H | 2.24 | 0.41 |
| 1:A:216:ASN:C | 1:A:218:SER:H | 2.23 | 0.41 |
| 1:A:21:VAL:HG12 | 1:A:22:VAL:O | 2.20 | 0.41 |
| 1:B:146:CYS:HG | 1:C:291:TYR:HH | 1.67 | 0.41 |
| 1:E:387:VAL:O | 1:E:391:ILE:HD12 | 2.20 | 0.41 |
| 1:E:451:LEU:O | 1:E:453:GLU:N | 2.53 | 0.41 |
| 1:F:306:ILE:HD12 | 1:F:306:ILE:HG23 | 1.88 | 0.41 |
| 1:B:312:TRP:CZ3 | 1:B:468:PHE:CD1 | 3.04 | 0.41 |
| 1:C:276:TYR:CE1 | 1:C:278:LYS:HD2 | 2.55 | 0.41 |
| 1:C:426:ILE:HG22 | 1:C:427:ALA:N | 2.35 | 0.41 |
| 1:D:276:TYR:CZ | 1:D:286:LEU:HD21 | 2.55 | 0.41 |
| 1:D:36:HIS:CG | 1:D:37:ALA:N | 2.88 | 0.41 |
| 1:E:112:PRO:HB3 | 1:F:231:TYR:CG | 2.55 | 0.41 |
| 1:F:276:TYR:CZ | 1:F:286:LEU:HD21 | 2.55 | 0.41 |
| 1:B:248:PHE:CG | 1:B:249:TYR:N | 2.88 | 0.41 |
| 1:B:431:HIS:O | 1:B:433:PRO:HD2 | 2.20 | 0.41 |
| 1:B:345:CYS:SG | 1:C:215:ALA:N | 2.93 | 0.41 |
| 1:C:314:GLN:HG3 | 1:C:315:ARG:N | 2.35 | 0.41 |
| 1:C:81:ASN:ND2 | 1:C:98:LEU:O | 2.52 | 0.41 |
| 1:D:426:ILE:HD13 | 1:D:426:ILE:HG21 | 1.69 | 0.41 |
| 1:E:247:PHE:CE1 | 1:E:313:LEU:HD13 | 2.56 | 0.41 |
| 1:A:324:CYS:HB3 | 1:A:328:GLN:O | 2.20 | 0.41 |
| 1:A:35:TYR:HE1 | 1:A:457:ALA:HA | 1.85 | 0.41 |
| 1:C:397:THR:HA | 1:C:400:GLU:CG | 2.50 | 0.41 |
| 1:D:114:GLY:HA2 | 1:E:255:MET:HE1 | 2.01 | 0.41 |
| 1:D:219:GLU:OE1 | 1:D:263:ARG:CZ | 2.67 | 0.41 |
| 1:C:117:ILE:CD1 | 1:D:260:LEU:HG | 2.49 | 0.41 |
| 1:D:77:LEU:HD22 | 1:D:455:PHE:CZ | 2.55 | 0.41 |
| 1:F:312:TRP:CH2 | 1:F:468:PHE:CD1 | 2.99 | 0.41 |
| 1:F:384:THR:H | 1:F:387:VAL:HB | 1.86 | 0.41 |
| 1:A:312:TRP:CD2 | 1:A:471:GLN:OE1 | 2.73 | 0.41 |
| 1:A:36:HIS:ND1 | 1:A:462:PHE:HD2 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:ARG:NH1 | 1:B:370:TYR:CD1 | 2.88 | 0.41 |
| 1:B:43:LEU:HD11 | 1:C:169:TRP:CZ2 | 2.55 | 0.41 |
| 1:C:45:VAL:HG12 | 1:C:46:GLY:N | 2.36 | 0.41 |
| 1:E:152:LYS:HD3 | 1:E:202:ASP:OD1 | 2.19 | 0.41 |
| 1:F:174:PRO:HA | 1:F:187:PRO:HG3 | 2.02 | 0.41 |
| 1:F:389:THR:O | 1:F:393:SER:N | 2.39 | 0.41 |
| 1:A:372:LEU:HD22 | 1:A:374:PHE:HZ | 1.85 | 0.41 |
| 1:A:407:GLN:HB3 | 1:A:408:PRO:CD | 2.48 | 0.41 |
| 1:A:51:PRO:HB3 | 1:A:63:PRO:HA | 2.01 | 0.41 |
| 1:B:291:TYR:HH | 1:F:146:CYS:HG | 1.49 | 0.41 |
| 1:D:312:TRP:CZ3 | 1:D:468:PHE:CD1 | 3.08 | 0.41 |
| 1:F:246:LEU:HD12 | 1:F:317:GLN:NE2 | 2.35 | 0.41 |
| 1:B:185:CYS:SG | 1:F:365:ARG:NH2 | 2.94 | 0.41 |
| 1:F:459:LEU:HA | 1:F:459:LEU:HD23 | 1.85 | 0.41 |
| 1:F:81:ASN:OD1 | 1:F:98:LEU:HB2 | 2.21 | 0.41 |
| 1:B:120:HIS:CE1 | 1:B:122:LEU:O | 2.73 | 0.41 |
| 1:B:416:ASP:O | 1:B:418:TYR:N | 2.54 | 0.41 |
| 1:C:120:HIS:ND1 | 1:C:122:LEU:N | 2.64 | 0.41 |
| 1:C:423:SER:OG | 1:C:425:ALA:HB3 | 2.20 | 0.41 |
| 1:D:97:ARG:NH2 | 1:D:404:PHE:H | 2.19 | 0.41 |
| 1:D:439:ASP:OD1 | 1:D:441:LEU:N | 2.50 | 0.41 |
| 1:D:65:VAL:HA | 1:D:69:GLN:OE1 | 2.20 | 0.41 |
| 1:F:258:ARG:HG2 | 1:F:259:HIS:CE1 | 2.56 | 0.41 |
| 1:A:463:PRO:HA | 1:A:466:ARG:HH11 | 1.85 | 0.41 |
| 1:A:97:ARG:HD3 | 1:A:97:ARG:HA | 1.92 | 0.41 |
| 1:B:109:ARG:HE | 1:B:338:ARG:HD2 | 1.85 | 0.41 |
| 1:B:90:PHE:CE1 | 1:B:91:TYR:HD2 | 2.39 | 0.41 |
| 1:E:34:TYR:CE1 | 1:E:377:GLN:HG3 | 2.55 | 0.41 |
| 1:A:210:PHE:CD2 | 1:A:220:VAL:HG21 | 2.56 | 0.41 |
| 1:A:278:LYS:HA | 1:A:278:LYS:HD2 | 1.83 | 0.41 |
| 1:B:255:MET:CE | 1:F:114:GLY:HA2 | 2.50 | 0.41 |
| 1:D:209:ASP:OD2 | 1:D:212:THR:HG23 | 2.21 | 0.41 |
| 1:D:240:GLU:CG | 1:D:241:PRO:HD2 | 2.51 | 0.41 |
| 1:E:317:GLN:OE1 | 1:E:317:GLN:N | 2.40 | 0.41 |
| 1:B:246:LEU:O | 1:B:246:LEU:HD12 | 2.20 | 0.41 |
| 1:B:77:LEU:O | 1:B:327:ASN:HB3 | 2.21 | 0.41 |
| 1:B:409:PRO:HA | 1:B:410:PRO:HD3 | 1.86 | 0.41 |
| 1:C:112:PRO:HB3 | 1:D:231:TYR:CD1 | 2.56 | 0.41 |
| 1:B:360:PHE:CE2 | 1:C:216:ASN:HA | 2.56 | 0.41 |
| 1:D:77:LEU:HD22 | 1:D:455:PHE:HZ | 1.86 | 0.41 |
| 1:D:82:LYS:O | 1:E:12:TYR:CE2 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:ILE:O | 1:E:239:SER:N | 2.50 | 0.41 |
| 1:E:71:ARG:HG3 | 1:E:370:TYR:CE2 | 2.56 | 0.41 |
| 1:F:399:LEU:HA | 1:F:399:LEU:HD23 | 1.90 | 0.41 |
| 1:A:77:LEU:O | 1:A:327:ASN:HB3 | 2.22 | 0.41 |
| 1:A:406:LEU:HD12 | 1:A:406:LEU:O | 2.20 | 0.41 |
| 1:A:474:LEU:HD13 | 1:A:478:PRO:HD2 | 2.02 | 0.41 |
| 1:B:417:THR:HB | 1:B:426:ILE:HG12 | 2.03 | 0.41 |
| 1:D:54:LYS:HD2 | 1:D:57:ASN:HB2 | 2.03 | 0.41 |
| 1:E:123:LEU:H | 1:E:145:GLU:H | 1.69 | 0.41 |
| 1:E:478:PRO:HG2 | 1:E:480:PHE:HD2 | 1.86 | 0.41 |
| 1:B:290:ASN:ND2 | 1:F:362:GLU:HB3 | 2.36 | 0.41 |
| 1:F:473:GLY:O | 1:F:474:LEU:HG | 2.21 | 0.41 |
| 1:A:306:ILE:HG23 | 1:A:306:ILE:HD12 | 1.87 | 0.40 |
| 1:A:314:GLN:HG3 | 1:A:315:ARG:N | 2.37 | 0.40 |
| 1:A:77:LEU:HD22 | 1:A:455:PHE:HZ | 1.85 | 0.40 |
| 1:A:420:PHE:HZ | 1:B:236:LYS:HZ3 | 1.65 | 0.40 |
| 1:C:123:LEU:H | 1:C:145:GLU:N | 2.17 | 0.40 |
| 1:C:36:HIS:NE2 | 1:C:373:GLN:HB3 | 2.36 | 0.40 |
| 1:D:74:ARG:O | 1:D:75:ILE:HD13 | 2.21 | 0.40 |
| 1:E:66:SER:HA | 1:E:366:HIS:CD2 | 2.55 | 0.40 |
| 1:F:70:TYR:HD2 | 1:F:199:ASP:HB2 | 1.86 | 0.40 |
| 1:F:90:PHE:HD1 | 1:F:380:LYS:NZ | 2.19 | 0.40 |
| 1:A:70:TYR:CZ | 1:A:201:VAL:HA | 2.55 | 0.40 |
| 1:A:274:ASP:OD1 | 1:A:274:ASP:N | 2.53 | 0.40 |
| 1:A:321:ASN:O | 1:A:323:ILE:N | 2.54 | 0.40 |
| 1:A:113:LEU:HD11 | 1:A:338:ARG:NH2 | 2.37 | 0.40 |
| 1:A:397:THR:O | 1:A:400:GLU:HB2 | 2.20 | 0.40 |
| 1:A:474:LEU:HB2 | 1:A:477:LYS:HG2 | 2.04 | 0.40 |
| 1:B:220:VAL:HB | 1:B:224:ILE:HD11 | 2.02 | 0.40 |
| 1:B:324:CYS:HB3 | 1:B:328:GLN:O | 2.21 | 0.40 |
| 1:B:43:LEU:CD2 | 1:C:190:LEU:HB2 | 2.49 | 0.40 |
| 1:C:455:PHE:HB2 | 1:D:13:LEU:CD1 | 2.48 | 0.40 |
| 1:D:35:TYR:CD2 | 1:D:100:TRP:HH2 | 2.36 | 0.40 |
| 1:E:146:CYS:SG | 1:F:291:TYR:OH | 2.73 | 0.40 |
| 1:E:78:PRO:HD2 | 1:E:455:PHE:HZ | 1.86 | 0.40 |
| 1:F:14:PRO:HA | 1:F:15:PRO:HA | 1.33 | 0.40 |
| 1:F:210:PHE:CE2 | 1:F:220:VAL:HG11 | 2.57 | 0.40 |
| 1:F:153:GLN:CD | 1:F:300:VAL:HG12 | 2.41 | 0.40 |
| 1:A:23:SER:O | 1:A:25:ASP:N | 2.54 | 0.40 |
| 1:A:79:ASP:OD2 | 1:A:82:LYS:HD3 | 2.21 | 0.40 |
| 1:B:319:HIS:CE1 | 1:F:466:ARG:NH2 | 2.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:105:VAL:HG21 | 1:C:159:ILE:HD13 | 2.03 | 0.40 |
| 1:F:36:HIS:CG | 1:F:37:ALA:N | 2.89 | 0.40 |
| 1:A:467:LYS:O | 1:A:471:GLN:N | 2.32 | 0.40 |
| 1:B:341:ASN:OD1 | 1:B:366:HIS:HD2 | 2.05 | 0.40 |
| 1:C:170:GLY:O | 1:C:189:GLU:N | 2.54 | 0.40 |
| 1:C:276:TYR:HE1 | 1:C:278:LYS:HD2 | 1.87 | 0.40 |
| 1:C:375:ILE:HG23 | 1:C:375:ILE:HD12 | 1.90 | 0.40 |
| 1:E:169:TRP:O | 1:E:208:MET:HA | 2.21 | 0.40 |
| 1:F:249:TYR:HE1 | 1:F:251:ARG:HH11 | 1.67 | 0.40 |
| 1:F:71:ARG:HG3 | 1:F:370:TYR:CZ | 2.57 | 0.40 |
| 1:A:111:GLN:HB2 | 1:A:338:ARG:HG2 | 2.04 | 0.40 |
| 1:A:344:LEU:HD12 | 1:A:363:TYR:HB2 | 2.04 | 0.40 |
| 1:B:18:VAL:HG11 | 1:F:480:PHE:CE1 | 2.51 | 0.40 |
| 1:C:254:GLN:OE1 | 1:C:298:SER:HB3 | 2.22 | 0.40 |
| 1:C:306:ILE:HG23 | 1:C:306:ILE:HD12 | 1.88 | 0.40 |
| 1:D:306:ILE:HG23 | 1:D:306:ILE:HD12 | 1.84 | 0.40 |
| 1:D:384:THR:H | 1:D:387:VAL:HB | 1.86 | 0.40 |
| 1:E:220:VAL:HB | 1:E:224:ILE:HD11 | 2.03 | 0.40 |
| 1:E:24:THR:HG21 | 1:E:320:ASN:HA | 2.03 | 0.40 |
| 1:F:366:HIS:CE1 | 1:F:367:GLY:O | 2.75 | 0.40 |
| 1:F:51:PRO:CB | 1:F:64:LYS:HB2 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 472/483 (98%) | 431 (91%) | 38 (8%) | 3 (1%) | 30 | 74 |
| 1 | B | 461/483 (95%) | 430 (93%) | 28 (6%) | 3 (1%) | 26 | 71 |
| 1 | C | 470/483 (97%) | 431 (92%) | 33 (7%) | 6 (1%) | 15 | 60 |
| 1 | D | 469/483 (97%) | 430 (92%) | 35 (8%) | 4 (1%) | 21 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | E | 480/483 (99%) | 441 (92%) | 35 (7%) | 4 (1%) | 24 | 70 |
| 1 | F | 471/483 (98%) | 440 (93%) | 25 (5%) | 6 (1%) | 15 | 60 |
| All | All | 2823/2898 (97%) | 2603 (92%) | 194 (7%) | 26 (1%) | 26 | 67 |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 408 | PRO |
| 1 | A | 117 | ILE |
| 1 | C | 406 | LEU |
| 1 | D | 117 | ILE |
| 1 | F | 422 | THR |
| 1 | F | 423 | SER |
| 1 | C | 409 | PRO |
| 1 | E | 424 | GLN |
| 1 | F | 403 | ASN |
| 1 | F | 410 | PRO |
| 1 | B | 410 | PRO |
| 1 | C | 14 | PRO |
| 1 | D | 478 | PRO |
| 1 | E | 117 | ILE |
| 1 | A | 394 | MET |
| 1 | E | 409 | PRO |
| 1 | F | 117 | ILE |
| 1 | D | 20 | LYS |
| 1 | E | 436 | PRO |
| 1 | A | 434 | PRO |
| 1 | B | 235 | ILE |
| 1 | B | 387 | VAL |
| 1 | C | 407 | GLN |
| 1 | F | 235 | ILE |
| 1 | C | 387 | VAL |
| 1 | D | 387 | VAL |

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 | 412/420 (98%) | 411 (100%) | 1 (0%) | 95 | 97 |
| 1 | B | 402/420 (96%) | 402 (100%) | 0 | 100 | 100 |
| 1 | C | 410/420 (98%) | 410 (100%) | 0 | 100 | 100 |
| 1 | D | 410/420 (98%) | 410 (100%) | 0 | 100 | 100 |
| 1 | E | 419/420 (100%) | 419 (100%) | 0 | 100 | 100 |
| 1 | F | 411/420 (98%) | 411 (100%) | 0 | 100 | 100 |
| All | All | 2464/2520 (98%) | 2463 (100%) | 1 (0%) | 100 | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 406 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | D | 1 |
| 1 | C | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | C | 46:GLY | C | 47:HIS | N | 1.14 |
| 1 | D | 435:ALA | C | 436:PRO | N | 1.14 |