



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:28 pm BST

PDB ID : 2D6F
Title : Crystal structure of Glu-tRNA(Gln) amidotransferase in the complex with tRNA(Gln)
Authors : Nureki, O.
Deposited on : 2005-11-13
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

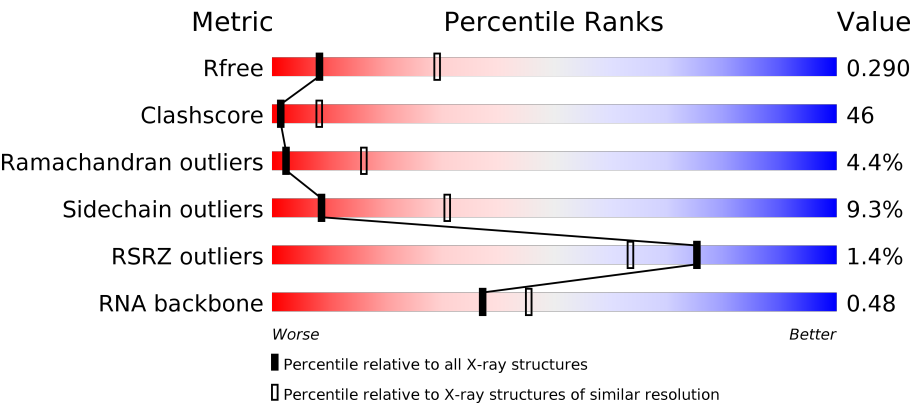
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1665 (3.20-3.12) |
| Clashscore | 141614 | 1804 (3.20-3.12) |
| Ramachandran outliers | 138981 | 1770 (3.20-3.12) |
| Sidechain outliers | 138945 | 1769 (3.20-3.12) |
| RSRZ outliers | 127900 | 1616 (3.20-3.12) |
| RNA backbone | 3102 | 1073 (3.50-2.82) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | E | 74 | <div><div>7%</div><div>18%</div><div>58%</div><div>22%</div><div>.</div></div> |
| 1 | F | 74 | <div><div>5%</div><div>27%</div><div>47%</div><div>24%</div><div>.</div></div> |
| 2 | A | 435 | <div><div>%</div><div>37%</div><div>51%</div><div>9%</div><div>.</div></div> |
| 2 | B | 435 | <div><div>37%</div><div>51%</div><div>9%</div><div>.</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 3 | C | 619 | <div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>26%</div><div>47%</div><div>6%</div><div>22%</div></div></div> |
| 3 | D | 619 | <div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>30%</div><div>46%</div><div>8%</div><div>16%</div></div></div> |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1 | E | 72 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1539 | 684 | 272 | 511 | 72 | | | |
| 1 | F | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1579 | 702 | 278 | 525 | 74 | | | |

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit D.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | A | 424 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3268 | 2028 | 575 | 641 | 24 | | | |
| 2 | B | 424 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3274 | 2032 | 575 | 643 | 24 | | | |

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 485 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3847 | 2390 | 690 | 752 | 15 | | | |
| 3 | D | 522 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4127 | 2563 | 741 | 808 | 15 | | | |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | D | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

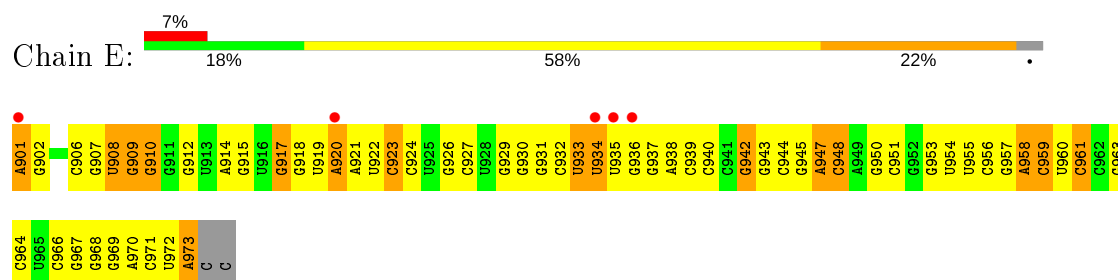
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5 | E | 16 | Total 16 | O 16 | 0 | 0 |
| 5 | F | 24 | Total 24 | O 24 | 0 | 0 |
| 5 | A | 31 | Total 31 | O 31 | 0 | 0 |
| 5 | B | 24 | Total 24 | O 24 | 0 | 0 |
| 5 | C | 36 | Total 36 | O 36 | 0 | 0 |
| 5 | D | 49 | Total 49 | O 49 | 0 | 0 |

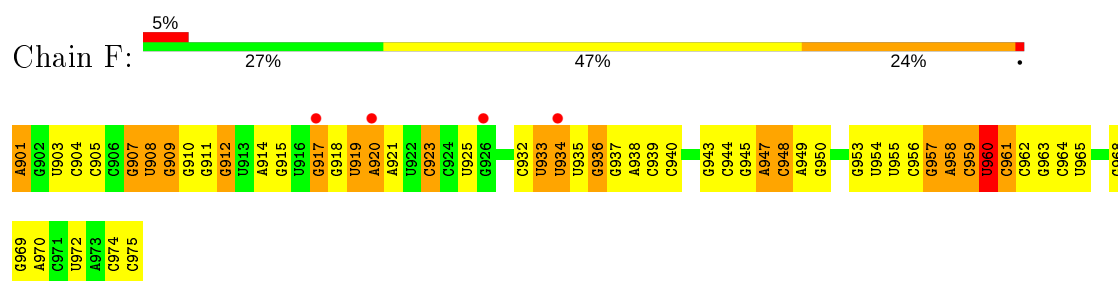
3 Residue-property plots

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

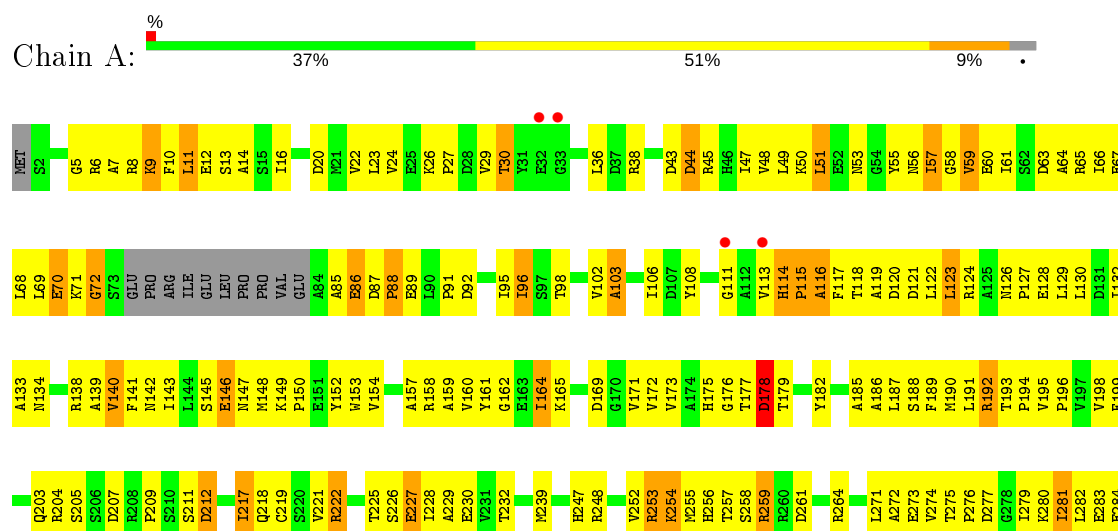
• Molecule 1: tRNA

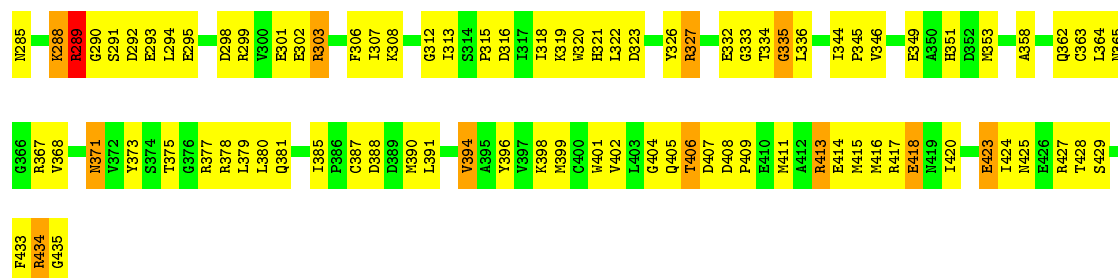


• Molecule 1: tRNA

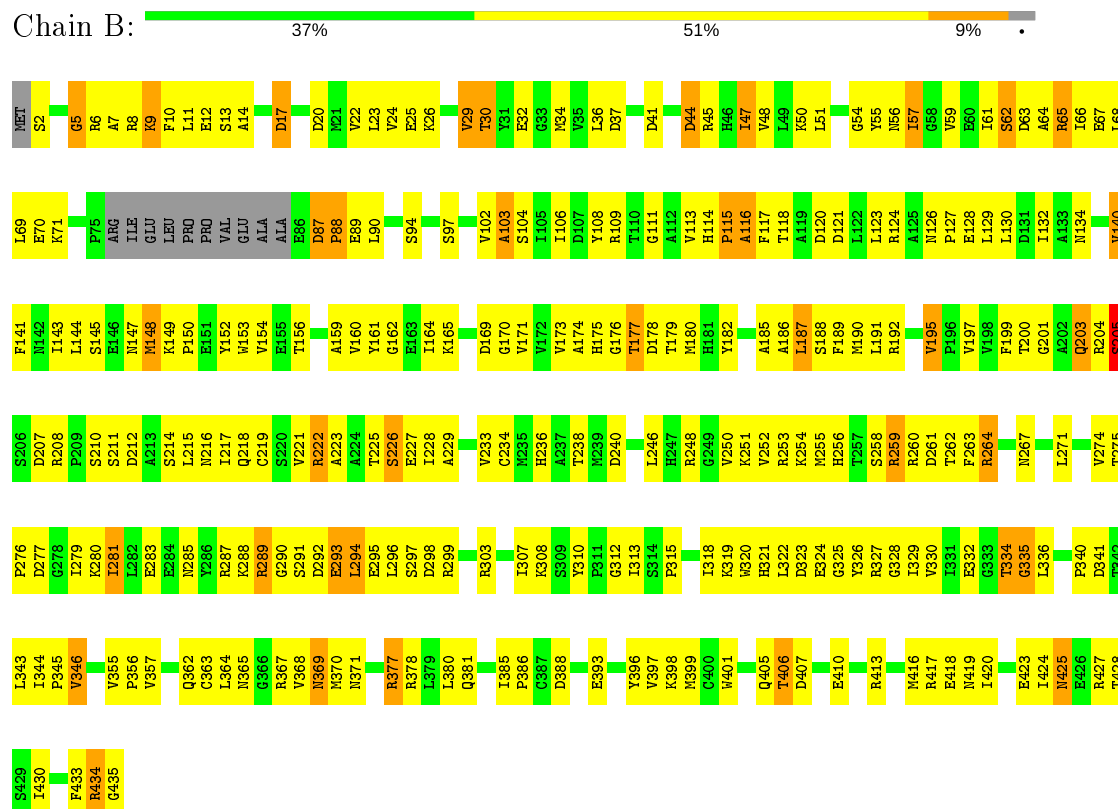


• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D

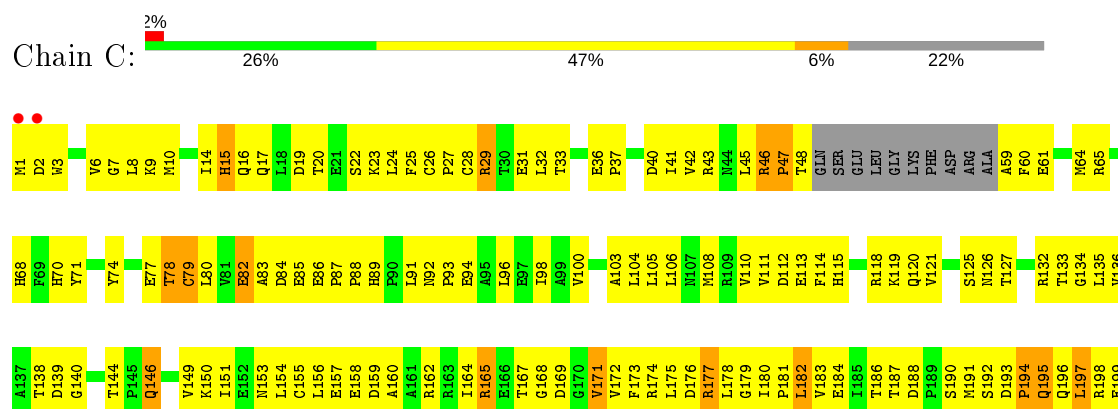


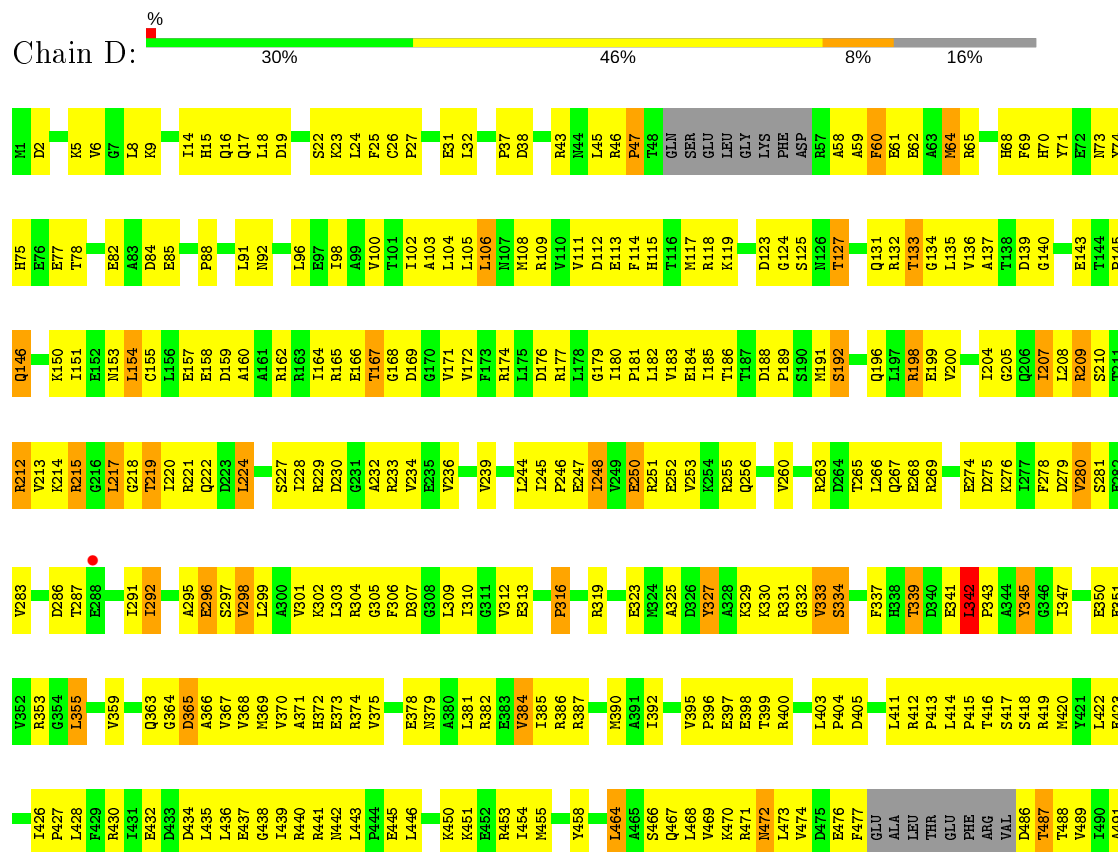
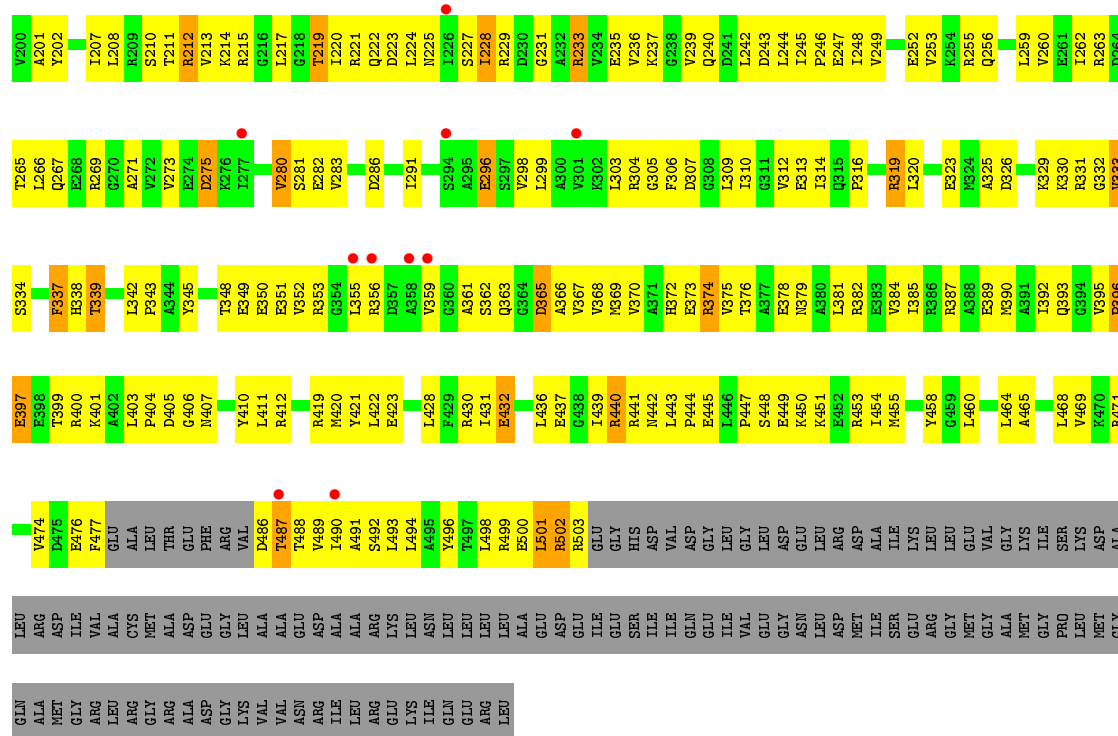


- Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E





| | | |
|------|-----|-----|
| S492 | ARG | ARG |
| L493 | LYS | LYS |
| L494 | LEU | LEU |
| A495 | ASN | ASN |
| Y496 | LEU | ILE |
| T497 | LEU | LEU |
| L498 | LEU | GLN |
| R499 | LEU | ARG |
| E500 | ALA | LEU |
| L501 | GLU | ALA |
| R502 | ASP | GLU |
| R503 | GLU | ASP |
| E504 | ILE | GLY |
| G505 | GLU | LYS |
| H506 | SER | VAL |
| D507 | ILE | ASN |
| V508 | ILE | LEU |
| D509 | GLN | ASP |
| G510 | GLU | MET |
| L511 | ILE | ILE |
| G512 | VAL | ILE |
| L513 | GLU | GLU |
| D514 | GLY | GLY |
| E515 | ASN | ALA |
| L516 | LEU | MET |
| R517 | ASP | GLY |
| D518 | MET | PRO |
| A519 | ILE | LEU |
| I520 | SER | MET |
| R521 | GLU | GLY |
| L522 | ARG | GLN |
| L523 | GLY | ALA |
| E524 | MET | MET |
| V525 | GLY | ARG |
| G526 | ALA | LEU |
| K527 | MET | GLY |
| I528 | GLY | LEU |
| S529 | PRO | ARG |
| R530 | LEU | GLY |
| D531 | MET | ARG |
| A532 | GLY | ALA |
| L533 | GLN | ASP |
| R534 | ALA | GLY |
| D535 | MET | LYS |
| D536 | GLY | VAL |
| V537 | ARG | VAL |
| A538 | LEU | ALA |
| CYS | ARG | ASN |
| MET | GLY | GLU |
| ALA | ARG | ASP |
| ASP | ALA | ILE |
| GLU | ASP | LEU |
| GLY | GLY | ALA |
| LEU | LYS | GLU |
| ALA | VAL | ASP |
| ALA | VAL | ILE |
| GLU | ASN | LEU |
| ASP | ARG | |
| ALA | ILE | |
| LEU | LEU | |

ARG

GLU

LYS

ILE

GLN

GLU

ARG

LEU

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 118.81Å 140.71Å 186.04Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 46.52 – 3.15 70.35 – 3.15 | Depositor EDS |
| % Data completeness (in resolution range) | 98.8 (46.52-3.15) 98.9 (70.35-3.15) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.01 (at 3.13Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.230 , 0.292 0.228 , 0.290 | Depositor DCC |
| R_{free} test set | 2728 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 60.0 | Xtriage |
| Anisotropy | 0.215 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.24 , 55.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 17816 | wwPDB-VP |
| Average B, all atoms (Å ²) | 62.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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 | E | 0.37 | 1/1718 (0.1%) | 0.69 | 0/2676 |
| 1 | F | 0.40 | 1/1762 (0.1%) | 0.72 | 0/2744 |
| 2 | A | 0.44 | 0/3323 | 0.71 | 1/4501 (0.0%) |
| 2 | B | 0.45 | 0/3330 | 0.71 | 0/4511 |
| 3 | C | 0.36 | 0/3898 | 0.64 | 0/5265 |
| 3 | D | 0.44 | 0/4179 | 0.68 | 0/5642 |
| All | All | 0.42 | 2/18210 (0.0%) | 0.69 | 1/25339 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | F | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | E | 901 | A | OP3-P | -7.11 | 1.52 | 1.61 |
| 1 | F | 901 | A | OP3-P | -6.87 | 1.52 | 1.61 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | A | 192 | ARG | N-CA-C | -5.15 | 97.09 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | F | 960 | U | Sidechain |

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 | E | 1539 | 0 | 777 | 77 | 0 |
| 1 | F | 1579 | 0 | 799 | 68 | 0 |
| 2 | A | 3268 | 0 | 3217 | 332 | 0 |
| 2 | B | 3274 | 0 | 3220 | 318 | 0 |
| 3 | C | 3847 | 0 | 3861 | 425 | 1 |
| 3 | D | 4127 | 0 | 4152 | 399 | 1 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 31 | 0 | 0 | 11 | 0 |
| 5 | B | 24 | 0 | 0 | 5 | 0 |
| 5 | C | 36 | 0 | 0 | 9 | 0 |
| 5 | D | 49 | 0 | 0 | 14 | 0 |
| 5 | E | 16 | 0 | 0 | 2 | 0 |
| 5 | F | 24 | 0 | 0 | 6 | 0 |
| All | All | 17816 | 0 | 16026 | 1543 | 1 |

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 46.

All (1543) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:133:THR:HG23 | 3:D:157:GLU:HB3 | 1.26 | 1.10 |
| 2:A:301:GLU:HG3 | 2:A:303:ARG:NH1 | 1.67 | 1.10 |
| 2:B:238:THR:HG23 | 2:B:240:ASP:H | 1.12 | 1.08 |
| 3:D:43:ARG:HH11 | 3:D:43:ARG:HG2 | 1.19 | 1.06 |
| 3:C:233:ARG:HG3 | 3:C:397:GLU:HB3 | 1.37 | 1.06 |
| 2:A:178:ASP:OD2 | 2:B:334:THR:HB | 1.53 | 1.05 |
| 2:B:315:PRO:HB3 | 2:B:346:VAL:HG21 | 1.40 | 1.04 |
| 1:F:958:A:H4' | 1:F:959:C:OP1 | 1.56 | 1.03 |
| 2:A:264:ARG:HH21 | 2:B:435:GLY:HA2 | 1.24 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:450:LYS:HD2 | 3:C:474:VAL:HG11 | 1.38 | 1.02 |
| 3:D:305:GLY:H | 3:D:365:ASP:HB3 | 1.23 | 1.01 |
| 3:C:259:LEU:HD23 | 3:C:262:ILE:HD12 | 1.43 | 1.01 |
| 2:A:435:GLY:HA2 | 2:B:264:ARG:HH21 | 1.26 | 0.99 |
| 3:D:454:ILE:HD12 | 3:D:474:VAL:HG13 | 1.45 | 0.98 |
| 1:E:958:A:H4' | 1:E:959:C:OP1 | 1.64 | 0.97 |
| 1:E:919:U:H5'' | 1:E:920:A:H5'' | 1.43 | 0.96 |
| 2:A:275:THR:HG22 | 2:A:277:ASP:H | 1.27 | 0.96 |
| 2:B:26:LYS:HB2 | 2:B:29:VAL:HG23 | 1.47 | 0.95 |
| 3:C:165:ARG:HB2 | 3:C:165:ARG:HH11 | 1.30 | 0.95 |
| 2:A:23:LEU:HB2 | 2:A:69:LEU:HD11 | 1.46 | 0.94 |
| 3:C:68:HIS:NE2 | 3:C:70:HIS:HE1 | 1.63 | 0.94 |
| 3:D:275:ASP:HA | 3:D:385:ILE:HD13 | 1.47 | 0.94 |
| 3:D:146:GLN:HG3 | 3:D:196:GLN:HB2 | 1.50 | 0.94 |
| 2:A:256:HIS:HD2 | 2:A:259:ARG:H | 1.05 | 0.93 |
| 3:D:291:ILE:HD12 | 3:D:291:ILE:H | 1.32 | 0.93 |
| 3:C:195:GLN:HE22 | 3:C:198:ARG:HH21 | 1.14 | 0.93 |
| 3:D:224:LEU:HD11 | 3:D:239:VAL:HG21 | 1.52 | 0.92 |
| 3:D:164:ILE:HG22 | 3:D:165:ARG:HG3 | 1.51 | 0.92 |
| 3:C:16:GLN:HE21 | 3:C:16:GLN:HA | 1.32 | 0.91 |
| 3:C:454:ILE:HD11 | 3:C:474:VAL:HG13 | 1.53 | 0.90 |
| 2:A:336:LEU:O | 2:A:368:VAL:HG13 | 1.71 | 0.90 |
| 2:B:385:ILE:HG23 | 2:B:413:ARG:HH11 | 1.33 | 0.90 |
| 1:E:917:G:H2' | 1:E:957:G:H22 | 1.36 | 0.90 |
| 1:F:917:G:H2' | 1:F:957:G:H22 | 1.36 | 0.89 |
| 3:C:191:MET:HG3 | 3:C:197:LEU:HD12 | 1.54 | 0.89 |
| 1:F:969:G:H2' | 1:F:970:A:H8 | 1.35 | 0.89 |
| 2:A:256:HIS:CD2 | 2:A:259:ARG:H | 1.91 | 0.88 |
| 3:D:70:HIS:CE1 | 3:D:169:ASP:OD2 | 2.26 | 0.88 |
| 2:B:186:ALA:HB1 | 2:B:190:MET:HE2 | 1.57 | 0.87 |
| 2:A:301:GLU:HG3 | 2:A:303:ARG:HH12 | 1.38 | 0.87 |
| 2:B:118:THR:HG22 | 2:B:120:ASP:H | 1.39 | 0.87 |
| 3:C:133:THR:HG23 | 3:C:157:GLU:HB3 | 1.54 | 0.87 |
| 3:C:9:LYS:HB2 | 3:C:227:SER:HB3 | 1.55 | 0.87 |
| 2:B:275:THR:HG22 | 2:B:277:ASP:H | 1.38 | 0.86 |
| 3:C:305:GLY:H | 3:C:365:ASP:HB3 | 1.38 | 0.86 |
| 3:D:305:GLY:N | 3:D:365:ASP:HB3 | 1.89 | 0.86 |
| 1:F:917:G:H2' | 1:F:957:G:N2 | 1.90 | 0.86 |
| 2:A:113:VAL:HG11 | 2:A:207:ASP:HB3 | 1.58 | 0.86 |
| 3:D:256:GLN:O | 3:D:260:VAL:HG23 | 1.75 | 0.86 |
| 2:A:303:ARG:HH11 | 2:A:303:ARG:H | 1.24 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:140:VAL:HG23 | 2:A:141:PHE:H | 1.41 | 0.85 |
| 2:A:160:VAL:O | 2:A:164:ILE:HG22 | 1.76 | 0.85 |
| 2:A:385:ILE:HD12 | 2:A:413:ARG:HB2 | 1.58 | 0.85 |
| 2:B:238:THR:HG23 | 2:B:240:ASP:N | 1.91 | 0.85 |
| 1:F:918:G:O2' | 1:F:919:U:H5' | 1.75 | 0.85 |
| 2:B:25:GLU:HG2 | 2:B:65:ARG:HB3 | 1.59 | 0.84 |
| 2:A:8:ARG:HH12 | 2:A:9:LYS:HZ1 | 1.24 | 0.84 |
| 2:B:132:ILE:HG12 | 2:B:222:ARG:HH12 | 1.42 | 0.84 |
| 2:A:299:ARG:HH11 | 2:A:299:ARG:HG3 | 1.41 | 0.84 |
| 2:B:140:VAL:HG12 | 2:B:141:PHE:HD2 | 1.41 | 0.84 |
| 2:B:106:ILE:HD11 | 2:B:207:ASP:HB2 | 1.59 | 0.84 |
| 2:B:344:ILE:HB | 2:B:345:PRO:HD3 | 1.58 | 0.84 |
| 2:B:106:ILE:HG12 | 2:B:113:VAL:HG22 | 1.60 | 0.84 |
| 1:F:960:U:H5" | 1:F:961:C:OP2 | 1.78 | 0.83 |
| 2:A:303:ARG:HH11 | 2:A:303:ARG:HG2 | 1.44 | 0.83 |
| 1:F:958:A:O2' | 1:F:959:C:H5' | 1.78 | 0.83 |
| 2:A:264:ARG:HH21 | 2:B:435:GLY:CA | 1.91 | 0.83 |
| 3:D:70:HIS:HE1 | 3:D:169:ASP:OD2 | 1.62 | 0.83 |
| 3:C:195:GLN:NE2 | 3:C:198:ARG:HH21 | 1.76 | 0.82 |
| 2:B:200:THR:HG22 | 2:B:201:GLY:N | 1.94 | 0.82 |
| 3:C:437:GLU:HA | 3:C:440:ARG:HB3 | 1.61 | 0.82 |
| 3:C:500:GLU:O | 3:C:503:ARG:HB3 | 1.79 | 0.82 |
| 3:D:125:SER:HB2 | 3:D:160:ALA:HB1 | 1.61 | 0.82 |
| 3:C:309:LEU:HA | 3:C:312:VAL:HG23 | 1.62 | 0.82 |
| 1:F:921:A:N1 | 1:F:948:C:H1' | 1.95 | 0.82 |
| 1:E:947:A:H2' | 1:E:948:C:H5' | 1.60 | 0.81 |
| 3:C:493:LEU:O | 3:C:498:LEU:HG | 1.79 | 0.81 |
| 2:A:315:PRO:HB3 | 2:A:346:VAL:HG21 | 1.63 | 0.81 |
| 2:A:371:ASN:HD22 | 2:A:371:ASN:N | 1.78 | 0.81 |
| 2:B:299:ARG:HB2 | 2:B:405:GLN:HE22 | 1.44 | 0.81 |
| 3:D:146:GLN:HG3 | 3:D:196:GLN:CB | 2.10 | 0.81 |
| 3:C:70:HIS:CE1 | 3:C:169:ASP:OD2 | 2.33 | 0.81 |
| 3:C:368:VAL:HG11 | 3:C:384:VAL:HG21 | 1.63 | 0.80 |
| 3:D:84:ASP:HB2 | 3:D:127:THR:HG23 | 1.63 | 0.80 |
| 3:D:111:VAL:HG12 | 3:D:113:GLU:H | 1.47 | 0.80 |
| 3:D:522:LEU:HD23 | 3:D:522:LEU:O | 1.81 | 0.80 |
| 2:A:303:ARG:NH1 | 2:A:303:ARG:H | 1.79 | 0.80 |
| 2:A:222:ARG:HH11 | 2:A:222:ARG:HG2 | 1.47 | 0.80 |
| 2:B:51:LEU:HD11 | 2:B:57:ILE:HD12 | 1.63 | 0.80 |
| 3:C:356:ARG:NH2 | 3:C:363:GLN:HA | 1.97 | 0.80 |
| 2:A:264:ARG:NH2 | 2:B:435:GLY:HA2 | 1.95 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:43:ARG:NH1 | 3:D:43:ARG:HG2 | 1.93 | 0.80 |
| 3:C:454:ILE:HD11 | 3:C:474:VAL:CG1 | 2.13 | 0.79 |
| 3:C:165:ARG:CB | 3:C:165:ARG:HH11 | 1.95 | 0.79 |
| 3:D:466:SER:O | 3:D:470:LYS:HG3 | 1.82 | 0.79 |
| 2:A:319:LYS:HE3 | 2:A:323:ASP:OD2 | 1.82 | 0.79 |
| 2:A:193:THR:HG22 | 2:A:195:VAL:H | 1.47 | 0.79 |
| 1:E:947:A:C2' | 1:E:948:C:H5' | 2.13 | 0.79 |
| 2:A:435:GLY:HA2 | 2:B:264:ARG:NH2 | 1.97 | 0.79 |
| 3:C:167:THR:HG22 | 3:C:168:GLY:H | 1.45 | 0.79 |
| 3:C:125:SER:HB2 | 3:C:160:ALA:HB1 | 1.65 | 0.78 |
| 3:C:105:LEU:HD21 | 3:C:443:LEU:HB3 | 1.63 | 0.78 |
| 3:C:331:ARG:HH21 | 3:C:376:THR:HA | 1.48 | 0.78 |
| 3:D:296:GLU:HB3 | 3:D:373:GLU:HA | 1.64 | 0.78 |
| 2:A:303:ARG:HG2 | 2:A:303:ARG:NH1 | 1.98 | 0.78 |
| 3:C:471:ARG:HD3 | 3:C:499:ARG:NH2 | 1.99 | 0.78 |
| 2:A:118:THR:HG22 | 2:A:120:ASP:H | 1.48 | 0.78 |
| 2:B:29:VAL:HG13 | 3:D:109:ARG:HG3 | 1.66 | 0.78 |
| 3:C:401:LYS:HB3 | 3:C:411:LEU:HD11 | 1.64 | 0.77 |
| 3:D:19:ASP:HA | 3:D:214:LYS:HE2 | 1.66 | 0.77 |
| 3:D:368:VAL:HG11 | 3:D:384:VAL:HG21 | 1.67 | 0.77 |
| 2:A:399:MET:HA | 2:A:416:MET:HE3 | 1.66 | 0.77 |
| 3:D:342:LEU:HD13 | 3:D:342:LEU:O | 1.85 | 0.77 |
| 2:A:9:LYS:HA | 2:A:9:LYS:HE3 | 1.65 | 0.77 |
| 2:A:391:LEU:HB2 | 2:A:394:VAL:HG12 | 1.63 | 0.77 |
| 3:C:356:ARG:HH21 | 3:C:363:GLN:HA | 1.50 | 0.77 |
| 3:D:167:THR:HG22 | 3:D:169:ASP:H | 1.50 | 0.77 |
| 3:C:65:ARG:HG3 | 3:C:65:ARG:HH11 | 1.50 | 0.76 |
| 2:B:177:THR:HG22 | 2:B:263:PHE:HE2 | 1.51 | 0.76 |
| 1:E:931:G:H1 | 1:E:939:C:H42 | 1.34 | 0.76 |
| 2:B:203:GLN:HA | 2:B:203:GLN:HE21 | 1.50 | 0.76 |
| 3:C:68:HIS:NE2 | 3:C:70:HIS:CE1 | 2.51 | 0.76 |
| 3:C:108:MET:HG2 | 3:C:140:GLY:HA3 | 1.68 | 0.76 |
| 3:C:445:GLU:OE2 | 3:C:450:LYS:HA | 1.85 | 0.76 |
| 3:D:59:ALA:C | 3:D:61:GLU:H | 1.88 | 0.76 |
| 3:C:16:GLN:NE2 | 3:C:16:GLN:HA | 2.00 | 0.76 |
| 3:C:1:MET:CE | 3:C:6:VAL:HG21 | 2.15 | 0.75 |
| 2:B:315:PRO:HB3 | 2:B:346:VAL:CG2 | 2.16 | 0.75 |
| 3:D:105:LEU:HD21 | 3:D:443:LEU:HB3 | 1.68 | 0.75 |
| 3:D:228:ILE:HD11 | 3:D:253:VAL:HG13 | 1.68 | 0.75 |
| 3:C:114:PHE:CZ | 3:C:134:GLY:HA3 | 2.20 | 0.75 |
| 1:F:948:C:H5" | 1:F:949:A:H5" | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:20:THR:HG22 | 3:C:94:GLU:HG2 | 1.68 | 0.75 |
| 3:C:146:GLN:HG3 | 3:C:196:GLN:HB2 | 1.69 | 0.75 |
| 1:F:918:G:H3' | 5:F:48:HOH:O | 1.85 | 0.75 |
| 3:C:164:ILE:HG22 | 3:C:165:ARG:HD2 | 1.68 | 0.75 |
| 3:D:15:HIS:CE1 | 3:D:184:GLU:HG2 | 2.22 | 0.75 |
| 3:D:301:VAL:HG11 | 3:D:385:ILE:HD11 | 1.67 | 0.75 |
| 3:C:19:ASP:HA | 3:C:214:LYS:NZ | 2.01 | 0.74 |
| 1:F:907:G:H5'' | 1:F:908:U:OP2 | 1.86 | 0.74 |
| 3:D:105:LEU:HD23 | 3:D:443:LEU:HD13 | 1.67 | 0.74 |
| 1:E:932:C:H3' | 1:E:933:U:H5'' | 1.69 | 0.74 |
| 2:A:145:SER:HB2 | 2:A:176:GLY:HA3 | 1.70 | 0.74 |
| 2:B:369:ASN:HD21 | 2:B:371:ASN:HB2 | 1.53 | 0.74 |
| 2:A:344:ILE:HB | 2:A:345:PRO:HD3 | 1.69 | 0.74 |
| 3:D:132:ARG:HG3 | 3:D:158:GLU:OE2 | 1.88 | 0.74 |
| 2:B:145:SER:HB2 | 2:B:176:GLY:HA3 | 1.69 | 0.74 |
| 1:F:911:G:N2 | 1:F:925:U:H1' | 2.03 | 0.74 |
| 2:A:147:ASN:ND2 | 2:B:341:ASP:H | 1.85 | 0.74 |
| 3:C:110:VAL:HG21 | 3:C:436:LEU:HD11 | 1.70 | 0.74 |
| 2:A:301:GLU:OE2 | 2:A:327:ARG:HG3 | 1.88 | 0.73 |
| 2:A:6:ARG:HB2 | 2:A:44:ASP:OD2 | 1.87 | 0.73 |
| 3:C:319:ARG:N | 3:C:319:ARG:HD2 | 2.03 | 0.73 |
| 3:D:232:ALA:HB3 | 3:D:395:VAL:HG12 | 1.71 | 0.73 |
| 1:F:969:G:H2' | 1:F:970:A:C8 | 2.22 | 0.73 |
| 3:D:476:GLU:OE2 | 3:D:476:GLU:N | 2.22 | 0.73 |
| 3:C:164:ILE:HG22 | 3:C:165:ARG:CD | 2.19 | 0.73 |
| 3:C:331:ARG:NH2 | 3:C:379:ASN:HD22 | 1.87 | 0.73 |
| 2:A:177:THR:HG21 | 2:A:203:GLN:HE21 | 1.54 | 0.72 |
| 3:C:228:ILE:N | 3:C:228:ILE:HD12 | 2.04 | 0.72 |
| 2:B:11:LEU:HD13 | 2:B:47:ILE:CD1 | 2.19 | 0.72 |
| 3:C:10:MET:HB2 | 3:C:191:MET:HB2 | 1.69 | 0.72 |
| 3:C:266:LEU:HD13 | 3:C:392:ILE:HD13 | 1.70 | 0.72 |
| 2:A:140:VAL:HG11 | 2:A:159:ALA:HB1 | 1.70 | 0.72 |
| 2:A:264:ARG:HE | 2:B:435:GLY:C | 1.92 | 0.72 |
| 3:D:18:LEU:HB2 | 3:D:181:PRO:HB2 | 1.71 | 0.72 |
| 2:A:140:VAL:HG23 | 2:A:141:PHE:N | 2.05 | 0.72 |
| 2:B:200:THR:HG22 | 2:B:201:GLY:H | 1.54 | 0.72 |
| 3:D:250:GLU:HG3 | 3:D:251:ARG:N | 2.04 | 0.72 |
| 2:B:170:GLY:HA2 | 2:B:195:VAL:HG13 | 1.70 | 0.72 |
| 2:A:257:THR:HG21 | 2:B:367:ARG:O | 1.90 | 0.72 |
| 3:D:32:LEU:HD13 | 3:D:162:ARG:CZ | 2.20 | 0.72 |
| 2:A:119:ALA:O | 2:A:123:LEU:HD22 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:1:MET:HE1 | 3:C:253:VAL:HG11 | 1.72 | 0.71 |
| 2:A:222:ARG:HG2 | 2:A:222:ARG:NH1 | 2.04 | 0.71 |
| 3:D:191:MET:O | 3:D:192:SER:HB3 | 1.88 | 0.71 |
| 1:E:917:G:H2' | 1:E:957:G:N2 | 2.05 | 0.71 |
| 2:A:204:ARG:HH22 | 2:A:258:SER:HB2 | 1.54 | 0.71 |
| 2:B:36:LEU:HD11 | 2:B:50:LYS:HB2 | 1.73 | 0.71 |
| 3:C:381:LEU:O | 3:C:384:VAL:HG12 | 1.90 | 0.71 |
| 2:A:315:PRO:HB3 | 2:A:346:VAL:CG2 | 2.20 | 0.71 |
| 3:D:301:VAL:HG23 | 3:D:381:LEU:HD22 | 1.72 | 0.71 |
| 1:F:934:U:H1' | 5:F:157:HOH:O | 1.90 | 0.71 |
| 2:A:308:LYS:HA | 2:A:332:GLU:HB3 | 1.73 | 0.71 |
| 2:B:318:ILE:HG13 | 2:B:343:LEU:CD1 | 2.21 | 0.71 |
| 3:D:533:LEU:HA | 3:D:536:ILE:HD12 | 1.71 | 0.71 |
| 3:C:155:CYS:O | 3:C:183:VAL:HA | 1.90 | 0.71 |
| 2:A:123:LEU:HG | 2:A:130:LEU:HD21 | 1.73 | 0.71 |
| 2:B:205:SER:O | 2:B:211:SER:HB2 | 1.90 | 0.71 |
| 2:B:222:ARG:HG2 | 2:B:222:ARG:HH11 | 1.56 | 0.71 |
| 2:B:123:LEU:HD21 | 2:B:130:LEU:HD21 | 1.73 | 0.70 |
| 3:C:498:LEU:O | 3:C:501:LEU:HB3 | 1.91 | 0.70 |
| 3:D:234:VAL:HG11 | 3:D:400:ARG:HD2 | 1.72 | 0.70 |
| 3:C:98:ILE:HG23 | 3:C:211:THR:HG21 | 1.72 | 0.70 |
| 3:D:319:ARG:HG3 | 3:D:319:ARG:HH11 | 1.53 | 0.70 |
| 2:B:320:TRP:O | 2:B:324:GLU:HG2 | 1.92 | 0.70 |
| 3:C:342:LEU:HD13 | 3:C:342:LEU:O | 1.91 | 0.70 |
| 2:B:335:GLY:O | 2:B:336:LEU:HB2 | 1.90 | 0.70 |
| 2:B:385:ILE:HG23 | 2:B:413:ARG:NH1 | 2.05 | 0.70 |
| 3:D:437:GLU:C | 3:D:439:ILE:H | 1.94 | 0.70 |
| 2:B:217:ILE:HG23 | 2:B:218:GLN:N | 2.07 | 0.70 |
| 2:B:434:ARG:HB3 | 2:B:434:ARG:NH1 | 2.06 | 0.70 |
| 3:C:228:ILE:HB | 3:C:231:GLY:HA3 | 1.73 | 0.70 |
| 3:C:305:GLY:N | 3:C:365:ASP:HB3 | 2.05 | 0.70 |
| 2:A:193:THR:CG2 | 2:A:194:PRO:HD2 | 2.22 | 0.70 |
| 2:A:164:ILE:HD13 | 2:A:195:VAL:HG22 | 1.72 | 0.70 |
| 2:A:333:GLY:O | 2:A:362:GLN:HG3 | 1.91 | 0.70 |
| 3:D:342:LEU:N | 3:D:343:PRO:HD3 | 2.07 | 0.70 |
| 1:E:901:A:H3' | 5:E:109:HOH:O | 1.91 | 0.70 |
| 3:C:349:GLU:OE2 | 3:C:352:VAL:HG21 | 1.92 | 0.69 |
| 3:C:275:ASP:HA | 3:C:385:ILE:HD13 | 1.72 | 0.69 |
| 3:D:403:LEU:HB3 | 3:D:404:PRO:CD | 2.22 | 0.69 |
| 2:B:256:HIS:HD2 | 2:B:259:ARG:H | 1.39 | 0.69 |
| 3:D:174:ARG:HG2 | 3:D:176:ASP:OD1 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:518:ASP:HA | 3:D:521:LYS:HG2 | 1.74 | 0.69 |
| 3:D:6:VAL:HG12 | 3:D:228:ILE:HG23 | 1.74 | 0.69 |
| 2:A:381:GLN:OE1 | 2:B:41:ASP:HA | 1.92 | 0.69 |
| 3:C:19:ASP:HA | 3:C:214:LYS:HZ3 | 1.55 | 0.69 |
| 3:C:256:GLN:O | 3:C:260:VAL:HG23 | 1.92 | 0.69 |
| 2:B:11:LEU:HD13 | 2:B:47:ILE:HD11 | 1.72 | 0.69 |
| 3:C:9:LYS:HB2 | 3:C:227:SER:CB | 2.23 | 0.69 |
| 1:E:960:U:H5'' | 1:E:961:C:OP2 | 1.93 | 0.69 |
| 2:B:417:ARG:HB3 | 2:B:417:ARG:NH1 | 2.08 | 0.69 |
| 3:C:219:THR:HG22 | 3:C:220:ILE:HG13 | 1.75 | 0.69 |
| 3:D:329:LYS:HE2 | 3:D:334:SER:O | 1.92 | 0.69 |
| 3:C:149:VAL:HG21 | 3:C:191:MET:HE3 | 1.73 | 0.69 |
| 2:B:260:ARG:HD2 | 3:D:85:GLU:OE2 | 1.92 | 0.69 |
| 3:D:339:THR:HB | 3:D:366:ALA:HB1 | 1.75 | 0.69 |
| 3:D:523:LEU:HB2 | 3:D:524:GLU:OE2 | 1.92 | 0.69 |
| 3:D:331:ARG:HA | 3:D:331:ARG:HE | 1.58 | 0.69 |
| 3:C:19:ASP:HB2 | 3:C:214:LYS:HG2 | 1.75 | 0.69 |
| 3:D:18:LEU:O | 3:D:19:ASP:HB3 | 1.93 | 0.69 |
| 3:C:167:THR:HG22 | 3:C:168:GLY:N | 2.07 | 0.68 |
| 2:A:145:SER:OG | 2:A:179:THR:HG22 | 1.94 | 0.68 |
| 2:A:228:ILE:HD11 | 2:A:281:ILE:HG12 | 1.74 | 0.68 |
| 2:A:303:ARG:HH11 | 2:A:303:ARG:CG | 2.06 | 0.68 |
| 3:C:184:GLU:HB3 | 5:C:902:HOH:O | 1.93 | 0.68 |
| 3:C:191:MET:HG3 | 3:C:197:LEU:CD1 | 2.23 | 0.68 |
| 3:D:169:ASP:OD2 | 5:D:1906:HOH:O | 2.10 | 0.68 |
| 3:C:422:LEU:HD12 | 3:C:422:LEU:N | 2.08 | 0.68 |
| 3:D:309:LEU:HA | 3:D:312:VAL:HG23 | 1.76 | 0.68 |
| 3:C:43:ARG:HH11 | 3:C:43:ARG:HG2 | 1.59 | 0.68 |
| 2:A:205:SER:O | 2:A:211:SER:HB2 | 1.94 | 0.67 |
| 2:A:402:VAL:HG22 | 2:A:415:MET:HE2 | 1.76 | 0.67 |
| 1:F:968:G:O2' | 1:F:969:G:H5' | 1.94 | 0.67 |
| 3:C:59:ALA:C | 3:C:61:GLU:H | 1.98 | 0.67 |
| 3:D:477:PHE:HZ | 3:D:487:THR:HG23 | 1.60 | 0.67 |
| 2:B:154:VAL:HG13 | 2:B:298:ASP:HB2 | 1.76 | 0.67 |
| 3:C:1:MET:HE3 | 3:C:6:VAL:HG21 | 1.75 | 0.67 |
| 3:C:225:ASN:ND2 | 3:C:235:GLU:HB3 | 2.09 | 0.67 |
| 3:D:98:ILE:HD11 | 3:D:212:ARG:NH1 | 2.08 | 0.67 |
| 3:D:472:ASN:O | 3:D:473:LEU:HD23 | 1.94 | 0.67 |
| 1:F:954:U:H2' | 1:F:955:U:H5' | 1.76 | 0.67 |
| 3:D:266:LEU:HD13 | 3:D:392:ILE:HD13 | 1.77 | 0.67 |
| 3:C:1:MET:HE1 | 3:C:253:VAL:CG1 | 2.25 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:244:LEU:HD12 | 3:D:247:GLU:HB3 | 1.77 | 0.67 |
| 3:D:520:ILE:O | 3:D:523:LEU:HD13 | 1.95 | 0.67 |
| 2:A:68:LEU:HD21 | 2:A:71:LYS:HG2 | 1.77 | 0.67 |
| 3:D:304:ARG:HA | 3:D:365:ASP:HB3 | 1.75 | 0.66 |
| 3:C:162:ARG:HA | 3:C:177:ARG:HH21 | 1.60 | 0.66 |
| 3:C:492:SER:O | 3:C:496:TYR:HB2 | 1.95 | 0.66 |
| 3:C:439:ILE:O | 3:C:442:ASN:N | 2.28 | 0.66 |
| 3:C:7:GLY:HA3 | 3:C:229:ARG:HB2 | 1.76 | 0.66 |
| 2:A:303:ARG:HH11 | 2:A:303:ARG:N | 1.93 | 0.66 |
| 2:B:140:VAL:HG12 | 2:B:141:PHE:CD2 | 2.29 | 0.66 |
| 3:D:115:HIS:CE1 | 3:D:428:LEU:HD13 | 2.31 | 0.66 |
| 3:D:210:SER:OG | 3:D:446:LEU:HA | 1.95 | 0.66 |
| 3:C:304:ARG:HA | 3:C:365:ASP:HB3 | 1.77 | 0.66 |
| 3:C:390:MET:SD | 3:C:396:PRO:HG3 | 2.34 | 0.66 |
| 3:D:244:LEU:O | 3:D:248:ILE:HG23 | 1.96 | 0.66 |
| 1:E:932:C:H2' | 1:E:933:U:H4' | 1.77 | 0.66 |
| 2:B:251:LYS:HE3 | 2:B:425:ASN:HD22 | 1.60 | 0.66 |
| 3:D:280:VAL:HG11 | 3:D:355:LEU:HD23 | 1.76 | 0.66 |
| 2:B:108:TYR:CD2 | 3:D:419:ARG:HB3 | 2.31 | 0.66 |
| 3:D:451:LYS:O | 3:D:454:ILE:HG22 | 1.95 | 0.66 |
| 2:B:200:THR:CG2 | 2:B:201:GLY:N | 2.59 | 0.65 |
| 2:A:29:VAL:HG12 | 2:A:30:THR:H | 1.60 | 0.65 |
| 3:C:422:LEU:H | 3:C:422:LEU:HD12 | 1.60 | 0.65 |
| 3:D:291:ILE:CD1 | 3:D:291:ILE:H | 2.09 | 0.65 |
| 2:A:9:LYS:HA | 2:A:9:LYS:CE | 2.27 | 0.65 |
| 3:D:486:ASP:N | 5:D:1902:HOH:O | 2.28 | 0.65 |
| 2:B:68:LEU:HD21 | 2:B:71:LYS:HG2 | 1.78 | 0.65 |
| 1:F:912:G:H1 | 1:F:923:C:H42 | 1.44 | 0.65 |
| 2:B:169:ASP:O | 2:B:195:VAL:HG22 | 1.97 | 0.65 |
| 3:C:184:GLU:OE1 | 5:C:905:HOH:O | 2.14 | 0.65 |
| 3:D:65:ARG:HB3 | 3:D:65:ARG:NH1 | 2.12 | 0.65 |
| 2:B:10:PHE:HE2 | 2:B:66:ILE:HD11 | 1.61 | 0.65 |
| 3:C:16:GLN:HE22 | 3:C:220:ILE:HG12 | 1.61 | 0.65 |
| 3:D:331:ARG:HA | 3:D:331:ARG:NE | 2.12 | 0.65 |
| 1:E:909:G:H5' | 1:E:910:G:OP2 | 1.97 | 0.65 |
| 1:F:920:A:H61 | 1:F:959:C:H5 | 1.45 | 0.65 |
| 3:C:303:LEU:HB3 | 3:C:306:PHE:CD1 | 2.31 | 0.64 |
| 3:D:292:ILE:HG23 | 3:D:371:ALA:HB2 | 1.79 | 0.64 |
| 3:C:224:LEU:HD23 | 3:C:236:VAL:HB | 1.78 | 0.64 |
| 2:A:50:LYS:CD | 2:A:56:ASN:HD21 | 2.10 | 0.64 |
| 3:C:115:HIS:CD2 | 3:C:428:LEU:HD22 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:104:LEU:HD13 | 3:C:440:ARG:HA | 1.79 | 0.64 |
| 3:C:501:LEU:HD23 | 3:C:502:ARG:N | 2.11 | 0.64 |
| 2:A:435:GLY:CA | 2:B:264:ARG:HE | 2.09 | 0.64 |
| 2:B:256:HIS:CD2 | 2:B:259:ARG:H | 2.15 | 0.64 |
| 2:B:274:VAL:HG22 | 2:B:279:ILE:HG23 | 1.77 | 0.64 |
| 3:C:448:SER:HA | 3:C:451:LYS:HD2 | 1.80 | 0.64 |
| 3:D:96:LEU:O | 3:D:100:VAL:HG23 | 1.97 | 0.64 |
| 2:A:164:ILE:HD13 | 2:A:195:VAL:CG2 | 2.27 | 0.64 |
| 2:A:8:ARG:NH2 | 2:A:9:LYS:HZ2 | 1.95 | 0.64 |
| 2:B:45:ARG:HH22 | 3:D:430:ARG:CZ | 2.10 | 0.64 |
| 2:B:66:ILE:HG22 | 2:B:67:GLU:H | 1.63 | 0.64 |
| 3:C:111:VAL:HG23 | 3:C:136:VAL:O | 1.97 | 0.64 |
| 3:C:330:LYS:O | 3:C:331:ARG:HB3 | 1.98 | 0.64 |
| 3:D:378:GLU:O | 3:D:382:ARG:HG3 | 1.97 | 0.64 |
| 2:A:149:LYS:HG2 | 2:A:152:TYR:CD1 | 2.33 | 0.64 |
| 2:B:200:THR:CG2 | 2:B:201:GLY:H | 2.10 | 0.64 |
| 3:D:445:GLU:HG3 | 3:D:450:LYS:HG2 | 1.79 | 0.64 |
| 2:A:435:GLY:C | 2:B:264:ARG:HE | 2.00 | 0.63 |
| 2:A:177:THR:HB | 2:A:254:LYS:NZ | 2.13 | 0.63 |
| 2:A:68:LEU:HD12 | 2:A:69:LEU:H | 1.64 | 0.63 |
| 2:A:96:ILE:HG13 | 2:A:140:VAL:HG13 | 1.81 | 0.63 |
| 2:B:208:ARG:HD3 | 5:D:1907:HOH:O | 1.97 | 0.63 |
| 2:A:108:TYR:CD2 | 3:C:419:ARG:HB2 | 2.32 | 0.63 |
| 3:D:82:GLU:O | 3:D:127:THR:HG21 | 1.98 | 0.63 |
| 2:A:273:GLU:HB3 | 2:A:280:LYS:HB3 | 1.79 | 0.63 |
| 3:C:14:ILE:HG12 | 3:C:222:GLN:HG2 | 1.78 | 0.63 |
| 3:C:32:LEU:HD21 | 3:C:177:ARG:HG3 | 1.80 | 0.63 |
| 3:D:167:THR:CG2 | 3:D:168:GLY:N | 2.62 | 0.63 |
| 3:D:184:GLU:OE1 | 5:D:1901:HOH:O | 2.15 | 0.63 |
| 1:E:939:C:O2' | 1:E:940:C:H5' | 1.97 | 0.63 |
| 2:A:289:ARG:HG3 | 2:A:289:ARG:HH11 | 1.64 | 0.63 |
| 2:A:280:LYS:O | 2:A:280:LYS:HG2 | 1.97 | 0.63 |
| 2:B:192:ARG:HG3 | 2:B:295:GLU:HB2 | 1.79 | 0.63 |
| 3:C:211:THR:O | 3:C:213:VAL:HG23 | 1.99 | 0.63 |
| 2:A:8:ARG:NH1 | 2:A:9:LYS:HZ1 | 1.94 | 0.63 |
| 2:A:192:ARG:HG3 | 2:A:295:GLU:HB2 | 1.81 | 0.62 |
| 2:B:175:HIS:CD2 | 2:B:180:MET:HA | 2.34 | 0.62 |
| 3:C:223:ASP:OD1 | 3:C:237:LYS:HD3 | 1.99 | 0.62 |
| 3:D:514:ASP:OD2 | 3:D:535:ASP:HA | 1.99 | 0.62 |
| 1:E:953:G:H21 | 3:C:496:TYR:HE2 | 1.46 | 0.62 |
| 2:B:132:ILE:HG12 | 2:B:222:ARG:NH1 | 2.11 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:963:G:H5' | 3:D:471:ARG:HH22 | 1.63 | 0.62 |
| 2:A:301:GLU:OE2 | 2:A:303:ARG:CZ | 2.48 | 0.62 |
| 2:B:222:ARG:HG3 | 2:B:275:THR:O | 2.00 | 0.62 |
| 2:B:417:ARG:HB3 | 2:B:417:ARG:HH11 | 1.64 | 0.62 |
| 2:B:228:ILE:HD11 | 2:B:281:ILE:HD13 | 1.80 | 0.62 |
| 3:C:381:LEU:O | 3:C:385:ILE:HG13 | 1.99 | 0.62 |
| 3:C:263:ARG:HD3 | 3:C:393:GLN:O | 2.00 | 0.62 |
| 2:A:44:ASP:O | 2:A:45:ARG:HB2 | 1.99 | 0.62 |
| 3:D:516:LEU:O | 3:D:520:ILE:HG13 | 1.99 | 0.62 |
| 3:C:320:LEU:CD1 | 3:C:387:ARG:HH21 | 2.12 | 0.62 |
| 1:E:908:U:H3 | 1:E:914:A:H62 | 1.44 | 0.62 |
| 2:A:147:ASN:HD22 | 2:B:340:PRO:HA | 1.62 | 0.62 |
| 2:B:177:THR:HB | 2:B:254:LYS:NZ | 2.14 | 0.62 |
| 1:E:918:G:O2' | 1:E:919:U:H5' | 1.99 | 0.62 |
| 1:E:933:U:O5' | 1:E:934:U:H5'' | 2.00 | 0.62 |
| 1:F:933:U:H3 | 1:F:936:G:H5'' | 1.63 | 0.62 |
| 1:F:939:C:O2' | 1:F:940:C:H5' | 2.00 | 0.62 |
| 2:A:129:LEU:HD23 | 2:A:132:ILE:HD12 | 1.81 | 0.62 |
| 2:B:385:ILE:HD13 | 2:B:413:ARG:HA | 1.81 | 0.62 |
| 3:D:381:LEU:HA | 3:D:384:VAL:CG1 | 2.30 | 0.62 |
| 3:D:62:GLU:HA | 3:D:65:ARG:NH1 | 2.14 | 0.62 |
| 2:A:175:HIS:HD2 | 2:A:176:GLY:O | 1.83 | 0.62 |
| 2:B:388:ASP:OD1 | 2:B:424:ILE:HD13 | 2.00 | 0.62 |
| 3:C:471:ARG:NH2 | 3:C:499:ARG:HB2 | 2.14 | 0.62 |
| 3:D:136:VAL:HG22 | 3:D:154:LEU:O | 2.00 | 0.61 |
| 3:D:224:LEU:HD12 | 3:D:236:VAL:HB | 1.81 | 0.61 |
| 3:D:466:SER:OG | 3:D:470:LYS:HE3 | 2.00 | 0.61 |
| 3:D:102:ILE:O | 3:D:106:LEU:HD12 | 2.00 | 0.61 |
| 2:A:86:GLU:HG2 | 2:A:86:GLU:O | 2.00 | 0.61 |
| 3:C:267:GLN:HA | 5:C:920:HOH:O | 2.00 | 0.61 |
| 3:D:111:VAL:HG12 | 3:D:113:GLU:N | 2.14 | 0.61 |
| 3:D:62:GLU:HA | 3:D:65:ARG:HH12 | 1.65 | 0.61 |
| 3:C:223:ASP:OD1 | 3:C:237:LYS:HA | 2.01 | 0.61 |
| 2:A:29:VAL:HG12 | 2:A:30:THR:N | 2.16 | 0.61 |
| 3:C:16:GLN:HE21 | 3:C:16:GLN:CA | 2.02 | 0.61 |
| 3:C:162:ARG:CA | 3:C:177:ARG:HH21 | 2.12 | 0.61 |
| 3:C:331:ARG:NH2 | 3:C:379:ASN:ND2 | 2.48 | 0.61 |
| 3:D:145:PRO:HD2 | 3:D:146:GLN:HE21 | 1.64 | 0.61 |
| 2:A:161:TYR:CD1 | 2:A:294:LEU:HD21 | 2.35 | 0.61 |
| 2:B:204:ARG:NH2 | 2:B:258:SER:O | 2.32 | 0.61 |
| 3:C:319:ARG:HH11 | 3:C:319:ARG:HG3 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:15:HIS:NE2 | 3:D:184:GLU:HG2 | 2.16 | 0.61 |
| 3:D:330:LYS:O | 3:D:331:ARG:HB3 | 2.00 | 0.61 |
| 3:D:432:GLU:HG3 | 3:D:435:LEU:HG | 1.82 | 0.61 |
| 1:E:955:U:H2' | 1:E:957:G:OP2 | 1.98 | 0.61 |
| 2:B:222:ARG:HG2 | 2:B:222:ARG:NH1 | 2.12 | 0.61 |
| 3:C:215:ARG:HD3 | 5:C:922:HOH:O | 2.00 | 0.61 |
| 3:C:245:ILE:HB | 3:C:246:PRO:HD3 | 1.81 | 0.61 |
| 3:C:319:ARG:HD2 | 3:C:319:ARG:H | 1.63 | 0.61 |
| 3:C:339:THR:HB | 3:C:366:ALA:HB1 | 1.81 | 0.61 |
| 3:C:105:LEU:CD2 | 3:C:443:LEU:HB3 | 2.30 | 0.61 |
| 2:B:177:THR:HG22 | 2:B:263:PHE:CE2 | 2.35 | 0.61 |
| 3:C:65:ARG:HG3 | 3:C:65:ARG:NH1 | 2.13 | 0.61 |
| 3:D:15:HIS:HE1 | 5:D:1901:HOH:O | 1.83 | 0.61 |
| 3:D:517:ARG:HH21 | 3:D:521:LYS:NZ | 1.97 | 0.61 |
| 1:E:926:G:H2' | 1:E:927:C:C6 | 2.36 | 0.61 |
| 3:D:278:PHE:CD1 | 3:D:359:VAL:HG23 | 2.36 | 0.61 |
| 2:A:239:MET:O | 3:C:43:ARG:NH1 | 2.32 | 0.61 |
| 2:A:36:LEU:HD11 | 2:A:50:LYS:HB2 | 1.83 | 0.61 |
| 2:A:427:ARG:NH2 | 2:A:429:SER:HB2 | 2.15 | 0.61 |
| 2:A:427:ARG:NH2 | 3:D:75:HIS:O | 2.33 | 0.61 |
| 2:B:308:LYS:HA | 2:B:332:GLU:HB3 | 1.81 | 0.61 |
| 3:C:191:MET:O | 3:C:192:SER:HB3 | 2.00 | 0.61 |
| 3:C:208:LEU:O | 3:C:213:VAL:HG21 | 1.99 | 0.61 |
| 3:C:355:LEU:O | 3:C:359:VAL:HG12 | 2.00 | 0.61 |
| 2:A:182:TYR:O | 2:A:185:ALA:HB3 | 2.01 | 0.60 |
| 3:C:296:GLU:HB2 | 3:C:373:GLU:HA | 1.83 | 0.60 |
| 3:C:248:ILE:HG22 | 3:C:406:GLY:HA2 | 1.82 | 0.60 |
| 3:C:265:THR:O | 3:C:269:ARG:HG2 | 2.02 | 0.60 |
| 3:D:469:VAL:HG22 | 3:D:474:VAL:HG21 | 1.83 | 0.60 |
| 2:B:124:ARG:HH11 | 2:B:124:ARG:HG3 | 1.65 | 0.60 |
| 2:B:165:LYS:HE2 | 2:B:294:LEU:HD23 | 1.82 | 0.60 |
| 3:C:98:ILE:HD11 | 3:C:212:ARG:HB2 | 1.82 | 0.60 |
| 3:D:14:ILE:HG12 | 3:D:222:GLN:HG2 | 1.83 | 0.60 |
| 2:A:158:ARG:HG3 | 2:A:158:ARG:HH11 | 1.66 | 0.60 |
| 2:A:164:ILE:HG13 | 2:A:294:LEU:HD22 | 1.83 | 0.60 |
| 2:A:320:TRP:CD1 | 2:B:320:TRP:CD1 | 2.90 | 0.60 |
| 3:C:430:ARG:NH1 | 3:C:430:ARG:HB3 | 2.16 | 0.60 |
| 3:C:437:GLU:HA | 3:C:440:ARG:CB | 2.32 | 0.60 |
| 3:D:397:GLU:HB3 | 3:D:414:LEU:HD22 | 1.82 | 0.60 |
| 2:A:256:HIS:HD2 | 2:A:259:ARG:N | 1.89 | 0.60 |
| 2:B:200:THR:CG2 | 2:B:216:ASN:HB3 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:LEU:N | 2:B:36:LEU:HD12 | 2.17 | 0.60 |
| 3:C:136:VAL:CG1 | 3:C:154:LEU:HD22 | 2.31 | 0.60 |
| 2:B:36:LEU:HD13 | 2:B:48:VAL:HG12 | 1.83 | 0.60 |
| 3:D:299:LEU:HD11 | 3:D:374:ARG:HD3 | 1.83 | 0.60 |
| 2:A:175:HIS:CD2 | 2:A:176:GLY:N | 2.70 | 0.60 |
| 2:A:256:HIS:CD2 | 2:A:258:SER:H | 2.20 | 0.60 |
| 2:A:222:ARG:HG3 | 2:A:275:THR:O | 2.02 | 0.60 |
| 2:A:95:ILE:HG22 | 2:A:117:PHE:CE2 | 2.37 | 0.60 |
| 3:D:19:ASP:HA | 3:D:214:LYS:CE | 2.31 | 0.60 |
| 3:D:45:LEU:HD23 | 3:D:69:PHE:CE1 | 2.37 | 0.60 |
| 2:A:399:MET:HA | 2:A:416:MET:CE | 2.31 | 0.59 |
| 3:D:468:LEU:HD21 | 3:D:477:PHE:HB2 | 1.83 | 0.59 |
| 3:C:325:ALA:O | 3:C:329:LYS:HG3 | 2.02 | 0.59 |
| 1:E:943:G:O2' | 1:E:944:C:H5' | 2.02 | 0.59 |
| 2:B:287:ARG:HD2 | 2:B:292:ASP:OD2 | 2.03 | 0.59 |
| 2:B:26:LYS:CB | 2:B:29:VAL:HG23 | 2.26 | 0.59 |
| 3:C:350:GLU:HA | 3:C:353:ARG:HD3 | 1.84 | 0.59 |
| 3:D:280:VAL:HG11 | 3:D:355:LEU:CD2 | 2.32 | 0.59 |
| 2:A:371:ASN:N | 2:A:371:ASN:ND2 | 2.49 | 0.59 |
| 3:C:233:ARG:O | 3:C:397:GLU:HA | 2.02 | 0.59 |
| 2:B:195:VAL:HG22 | 2:B:289:ARG:HH12 | 1.68 | 0.59 |
| 2:B:9:LYS:HZ2 | 2:B:9:LYS:HA | 1.67 | 0.59 |
| 3:C:307:ASP:O | 3:C:309:LEU:HD12 | 2.03 | 0.59 |
| 3:C:323:GLU:O | 3:C:326:ASP:HB2 | 2.02 | 0.59 |
| 2:B:108:TYR:CE2 | 3:D:419:ARG:HB3 | 2.37 | 0.59 |
| 1:E:972:U:H2' | 1:E:973:A:C8 | 2.37 | 0.59 |
| 3:C:195:GLN:HE22 | 3:C:198:ARG:NH2 | 1.92 | 0.59 |
| 2:A:169:ASP:O | 2:A:195:VAL:HB | 2.02 | 0.59 |
| 2:A:434:ARG:HB2 | 5:B:446:HOH:O | 2.03 | 0.59 |
| 2:B:222:ARG:O | 2:B:225:THR:HB | 2.03 | 0.59 |
| 3:C:489:VAL:HA | 3:C:492:SER:OG | 2.02 | 0.59 |
| 2:B:45:ARG:HH22 | 3:D:430:ARG:NH2 | 2.00 | 0.59 |
| 2:A:192:ARG:CG | 2:A:295:GLU:HB2 | 2.33 | 0.59 |
| 3:D:374:ARG:HD2 | 3:D:378:GLU:OE2 | 2.03 | 0.59 |
| 2:A:161:TYR:HD1 | 2:A:294:LEU:HD21 | 1.67 | 0.59 |
| 3:C:378:GLU:O | 3:C:382:ARG:HG3 | 2.03 | 0.59 |
| 3:C:120:GLN:HE21 | 3:C:419:ARG:HD2 | 1.67 | 0.59 |
| 3:C:437:GLU:HB3 | 3:C:441:ARG:NH2 | 2.18 | 0.59 |
| 2:B:141:PHE:HZ | 2:B:156:THR:HG1 | 1.51 | 0.59 |
| 3:C:374:ARG:HH22 | 3:C:378:GLU:CB | 2.15 | 0.59 |
| 1:F:964:C:H2' | 1:F:965:U:O4' | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:274:VAL:HG12 | 2:B:275:THR:N | 2.18 | 0.58 |
| 3:C:499:ARG:O | 3:C:502:ARG:HG3 | 2.03 | 0.58 |
| 3:D:154:LEU:HD22 | 3:D:185:ILE:HG12 | 1.84 | 0.58 |
| 1:E:931:G:H1 | 1:E:939:C:N4 | 2.00 | 0.58 |
| 3:D:247:GLU:OE2 | 3:D:251:ARG:HG3 | 2.04 | 0.58 |
| 3:D:274:GLU:HB3 | 3:D:276:LYS:HG3 | 1.85 | 0.58 |
| 3:D:8:LEU:O | 3:D:9:LYS:HD3 | 2.02 | 0.58 |
| 3:C:120:GLN:NE2 | 3:C:419:ARG:HD2 | 2.17 | 0.58 |
| 3:C:342:LEU:CD1 | 3:C:352:VAL:HG22 | 2.34 | 0.58 |
| 3:D:205:GLY:O | 3:D:209:ARG:HG2 | 2.02 | 0.58 |
| 3:D:323:GLU:CD | 3:D:400:ARG:HH22 | 2.07 | 0.58 |
| 1:E:909:G:O2' | 1:E:945:G:O2' | 2.17 | 0.58 |
| 1:E:967:G:H2' | 1:E:968:G:H8 | 1.69 | 0.58 |
| 2:B:111:GLY:HA3 | 5:B:455:HOH:O | 2.03 | 0.58 |
| 3:D:275:ASP:HA | 3:D:385:ILE:CD1 | 2.28 | 0.58 |
| 1:F:974:C:O2 | 3:D:412:ARG:NH2 | 2.37 | 0.58 |
| 2:A:299:ARG:HG3 | 2:A:299:ARG:NH1 | 2.16 | 0.58 |
| 3:C:448:SER:HA | 3:C:451:LYS:CE | 2.34 | 0.58 |
| 3:C:77:GLU:H | 3:C:77:GLU:CD | 2.06 | 0.58 |
| 3:D:143:GLU:HB3 | 5:D:1948:HOH:O | 2.02 | 0.58 |
| 2:B:56:ASN:HD22 | 2:B:56:ASN:N | 2.00 | 0.58 |
| 2:A:435:GLY:HA2 | 2:B:264:ARG:HE | 1.67 | 0.58 |
| 3:C:331:ARG:NE | 3:C:379:ASN:HB2 | 2.18 | 0.58 |
| 3:C:496:TYR:O | 3:C:499:ARG:HB3 | 2.04 | 0.58 |
| 1:E:914:A:H2' | 1:E:915:G:O4' | 2.04 | 0.58 |
| 2:A:177:THR:HB | 2:A:254:LYS:HZ2 | 1.69 | 0.58 |
| 3:D:19:ASP:HB2 | 3:D:214:LYS:HD3 | 1.84 | 0.58 |
| 3:D:454:ILE:CD1 | 3:D:474:VAL:HG13 | 2.29 | 0.58 |
| 2:A:98:THR:HG21 | 2:A:148:MET:HE1 | 1.86 | 0.58 |
| 2:B:149:LYS:HZ3 | 2:B:152:TYR:HE1 | 1.51 | 0.58 |
| 3:D:212:ARG:CB | 3:D:212:ARG:HH11 | 2.16 | 0.58 |
| 3:D:386:ARG:O | 3:D:390:MET:HG3 | 2.03 | 0.58 |
| 1:E:932:C:H2' | 1:E:933:U:C4' | 2.34 | 0.58 |
| 1:F:919:U:H5'' | 1:F:920:A:O5' | 2.04 | 0.58 |
| 2:B:170:GLY:HA2 | 2:B:195:VAL:CG1 | 2.34 | 0.57 |
| 3:C:202:TYR:HB2 | 3:C:242:LEU:HD21 | 1.85 | 0.57 |
| 3:D:16:GLN:HG2 | 3:D:208:LEU:HD13 | 1.86 | 0.57 |
| 2:B:264:ARG:HH11 | 2:B:264:ARG:HG2 | 1.69 | 0.57 |
| 3:D:68:HIS:HE1 | 3:D:169:ASP:OD2 | 1.86 | 0.57 |
| 2:B:144:LEU:HB2 | 2:B:147:ASN:ND2 | 2.19 | 0.57 |
| 2:B:186:ALA:HB1 | 2:B:190:MET:CE | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:178:LEU:HD23 | 3:C:179:GLY:N | 2.20 | 0.57 |
| 3:D:133:THR:HG23 | 3:D:157:GLU:CB | 2.18 | 0.57 |
| 3:C:349:GLU:O | 3:C:353:ARG:HG2 | 2.04 | 0.57 |
| 3:D:111:VAL:HG12 | 3:D:112:ASP:N | 2.19 | 0.57 |
| 3:D:32:LEU:HD13 | 3:D:162:ARG:NH1 | 2.19 | 0.57 |
| 1:E:926:G:H2' | 1:E:927:C:H6 | 1.68 | 0.57 |
| 2:A:193:THR:HG22 | 2:A:194:PRO:HD2 | 1.84 | 0.57 |
| 2:A:336:LEU:HB2 | 5:A:459:HOH:O | 2.04 | 0.57 |
| 2:B:385:ILE:HD11 | 2:B:413:ARG:HB2 | 1.86 | 0.57 |
| 3:C:219:THR:HG22 | 3:C:220:ILE:N | 2.18 | 0.57 |
| 1:F:962:C:O3' | 3:D:499:ARG:HD3 | 2.04 | 0.57 |
| 2:A:138:ARG:HH12 | 2:A:140:VAL:HG12 | 1.69 | 0.57 |
| 2:A:391:LEU:HB2 | 2:A:394:VAL:CG1 | 2.33 | 0.57 |
| 3:C:228:ILE:HG12 | 3:C:256:GLN:HG2 | 1.87 | 0.57 |
| 3:C:369:MET:HG2 | 3:C:370:VAL:N | 2.20 | 0.57 |
| 2:A:378:ARG:NH1 | 2:A:378:ARG:O | 2.38 | 0.57 |
| 2:B:179:THR:HG23 | 2:B:182:TYR:HB2 | 1.87 | 0.57 |
| 2:B:248:ARG:HB2 | 2:B:271:LEU:HD11 | 1.87 | 0.57 |
| 3:C:71:TYR:CD2 | 3:C:127:THR:HG22 | 2.40 | 0.57 |
| 3:C:211:THR:HG22 | 3:C:212:ARG:H | 1.69 | 0.57 |
| 3:C:348:THR:OG1 | 3:C:351:GLU:HG3 | 2.05 | 0.57 |
| 3:D:155:CYS:O | 3:D:183:VAL:HA | 2.04 | 0.57 |
| 3:D:228:ILE:CD1 | 3:D:253:VAL:HG13 | 2.34 | 0.57 |
| 1:E:950:G:O2' | 1:E:951:C:H5' | 2.04 | 0.57 |
| 3:C:132:ARG:NH1 | 3:C:158:GLU:OE2 | 2.37 | 0.57 |
| 3:C:201:ALA:HB3 | 3:C:242:LEU:HD13 | 1.86 | 0.57 |
| 3:C:332:GLY:O | 3:C:333:VAL:HB | 2.04 | 0.57 |
| 3:C:211:THR:HG22 | 3:C:212:ARG:N | 2.20 | 0.56 |
| 3:D:59:ALA:C | 3:D:61:GLU:N | 2.57 | 0.56 |
| 2:A:318:ILE:HB | 2:A:346:VAL:HG11 | 1.87 | 0.56 |
| 2:B:124:ARG:HH11 | 2:B:124:ARG:CG | 2.18 | 0.56 |
| 3:D:332:GLY:O | 3:D:333:VAL:HG23 | 2.05 | 0.56 |
| 3:C:194:PRO:HG3 | 3:C:249:VAL:HG11 | 1.86 | 0.56 |
| 3:C:299:LEU:HB2 | 3:C:381:LEU:CD1 | 2.35 | 0.56 |
| 3:D:464:LEU:HD22 | 3:D:491:ALA:HB1 | 1.86 | 0.56 |
| 2:A:9:LYS:CA | 2:A:9:LYS:HE3 | 2.35 | 0.56 |
| 3:C:16:GLN:HB3 | 3:C:183:VAL:CG2 | 2.35 | 0.56 |
| 3:D:104:LEU:HD11 | 3:D:436:LEU:HD11 | 1.87 | 0.56 |
| 1:F:901:A:H2' | 5:F:137:HOH:O | 2.05 | 0.56 |
| 1:F:954:U:C2' | 1:F:955:U:H5' | 2.35 | 0.56 |
| 2:B:401:TRP:O | 2:B:405:GLN:HG2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:195:GLN:NE2 | 3:C:198:ARG:NH2 | 2.51 | 0.56 |
| 3:C:471:ARG:HH11 | 3:C:499:ARG:CZ | 2.17 | 0.56 |
| 3:D:331:ARG:HG2 | 3:D:379:ASN:HB3 | 1.87 | 0.56 |
| 1:E:929:G:H2' | 1:E:929:G:N3 | 2.20 | 0.56 |
| 2:A:55:TYR:OH | 3:C:133:THR:HG21 | 2.06 | 0.56 |
| 3:D:32:LEU:HD21 | 3:D:177:ARG:HB2 | 1.87 | 0.56 |
| 3:D:437:GLU:C | 3:D:439:ILE:N | 2.59 | 0.56 |
| 3:D:337:PHE:CE2 | 3:D:345:TYR:CD2 | 2.94 | 0.56 |
| 2:A:68:LEU:HD11 | 2:A:70:GLU:C | 2.26 | 0.56 |
| 3:C:448:SER:HA | 3:C:451:LYS:CD | 2.36 | 0.56 |
| 1:E:908:U:H3 | 1:E:914:A:N6 | 2.04 | 0.56 |
| 2:B:217:ILE:CG2 | 2:B:218:GLN:N | 2.69 | 0.56 |
| 3:C:489:VAL:HA | 3:C:492:SER:HG | 1.70 | 0.56 |
| 3:D:451:LYS:O | 3:D:455:MET:HG3 | 2.06 | 0.56 |
| 2:A:299:ARG:HA | 5:A:465:HOH:O | 2.05 | 0.56 |
| 2:B:5:GLY:O | 2:B:8:ARG:HG2 | 2.06 | 0.56 |
| 3:C:174:ARG:HG2 | 3:C:176:ASP:OD1 | 2.05 | 0.56 |
| 2:A:363:CYS:O | 2:A:364:LEU:HB2 | 2.06 | 0.55 |
| 3:D:6:VAL:HG11 | 3:D:228:ILE:HD13 | 1.88 | 0.55 |
| 3:D:58:ALA:HA | 5:D:1905:HOH:O | 2.04 | 0.55 |
| 2:A:12:GLU:C | 2:A:14:ALA:H | 2.09 | 0.55 |
| 2:B:149:LYS:HB2 | 2:B:150:PRO:HD2 | 1.88 | 0.55 |
| 2:B:275:THR:HG23 | 2:B:276:PRO:HD2 | 1.88 | 0.55 |
| 2:B:318:ILE:HG13 | 2:B:343:LEU:HD12 | 1.88 | 0.55 |
| 3:D:281:SER:HA | 3:D:298:VAL:HG13 | 1.87 | 0.55 |
| 2:A:114:HIS:O | 2:A:115:PRO:O | 2.24 | 0.55 |
| 2:A:8:ARG:NH1 | 2:A:9:LYS:NZ | 2.54 | 0.55 |
| 3:D:403:LEU:HB3 | 3:D:404:PRO:HD2 | 1.88 | 0.55 |
| 3:D:526:GLY:HA3 | 3:D:534:ARG:NH1 | 2.21 | 0.55 |
| 2:A:281:ILE:HG22 | 2:A:281:ILE:O | 2.06 | 0.55 |
| 2:B:434:ARG:HB3 | 2:B:434:ARG:CZ | 2.36 | 0.55 |
| 3:C:23:LYS:HG3 | 3:C:28:CYS:O | 2.06 | 0.55 |
| 3:C:291:ILE:HD12 | 3:C:291:ILE:H | 1.72 | 0.55 |
| 3:C:74:TYR:CB | 3:C:77:GLU:HG2 | 2.35 | 0.55 |
| 2:A:427:ARG:HB3 | 3:D:27:PRO:HG2 | 1.88 | 0.55 |
| 2:A:132:ILE:HG12 | 2:A:222:ARG:HH12 | 1.70 | 0.55 |
| 2:A:51:LEU:HD11 | 2:A:57:ILE:HG21 | 1.88 | 0.55 |
| 2:B:192:ARG:CG | 2:B:295:GLU:HB2 | 2.36 | 0.55 |
| 3:C:374:ARG:HH22 | 3:C:378:GLU:HB2 | 1.72 | 0.55 |
| 1:E:907:G:H1' | 1:E:967:G:N2 | 2.21 | 0.55 |
| 2:A:113:VAL:HG11 | 2:A:207:ASP:CB | 2.33 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:331:ARG:HE | 3:D:331:ARG:CA | 2.18 | 0.55 |
| 3:D:342:LEU:N | 3:D:343:PRO:CD | 2.69 | 0.55 |
| 3:D:59:ALA:O | 3:D:61:GLU:N | 2.30 | 0.55 |
| 3:D:68:HIS:CE1 | 3:D:169:ASP:OD2 | 2.60 | 0.55 |
| 2:A:189:PHE:CE2 | 2:A:423:GLU:HG2 | 2.42 | 0.55 |
| 2:A:50:LYS:HD2 | 2:A:56:ASN:HD21 | 1.72 | 0.55 |
| 3:D:108:MET:CE | 3:D:151:ILE:HG22 | 2.37 | 0.55 |
| 3:D:531:ASP:O | 3:D:533:LEU:N | 2.28 | 0.55 |
| 3:D:98:ILE:HD11 | 3:D:212:ARG:HH12 | 1.69 | 0.55 |
| 1:E:958:A:C4' | 1:E:959:C:OP1 | 2.49 | 0.55 |
| 3:C:309:LEU:HA | 3:C:312:VAL:CG2 | 2.34 | 0.55 |
| 3:D:477:PHE:CZ | 3:D:487:THR:HG23 | 2.39 | 0.55 |
| 3:D:510:GLY:O | 3:D:513:LEU:HB3 | 2.06 | 0.55 |
| 2:A:95:ILE:HG22 | 2:A:117:PHE:HE2 | 1.71 | 0.55 |
| 2:B:7:ALA:HA | 2:B:61:ILE:CD1 | 2.37 | 0.55 |
| 3:C:494:LEU:HA | 3:C:498:LEU:HD12 | 1.89 | 0.55 |
| 3:D:486:ASP:O | 3:D:488:THR:N | 2.40 | 0.55 |
| 2:A:204:ARG:NH2 | 2:A:258:SER:HB2 | 2.22 | 0.54 |
| 3:D:119:LYS:NZ | 3:D:131:GLN:OE1 | 2.40 | 0.54 |
| 3:D:224:LEU:HD21 | 3:D:245:ILE:HG12 | 1.88 | 0.54 |
| 2:A:387:CYS:HB3 | 2:A:390:MET:HE3 | 1.90 | 0.54 |
| 3:D:319:ARG:HG3 | 3:D:319:ARG:NH1 | 2.21 | 0.54 |
| 3:D:418:SER:HA | 5:D:1945:HOH:O | 2.06 | 0.54 |
| 1:F:963:G:C4' | 3:D:467:GLN:HE22 | 2.20 | 0.54 |
| 2:A:102:VAL:O | 2:A:103:ALA:HB2 | 2.07 | 0.54 |
| 2:A:146:GLU:OE1 | 2:A:146:GLU:N | 2.38 | 0.54 |
| 3:D:119:LYS:HA | 3:D:420:MET:HB3 | 1.89 | 0.54 |
| 3:D:303:LEU:HD12 | 3:D:310:ILE:HD11 | 1.90 | 0.54 |
| 2:B:9:LYS:HA | 2:B:9:LYS:NZ | 2.22 | 0.54 |
| 3:C:136:VAL:HG11 | 3:C:154:LEU:HD22 | 1.90 | 0.54 |
| 3:C:164:ILE:O | 3:C:165:ARG:HG3 | 2.07 | 0.54 |
| 3:C:16:GLN:NE2 | 3:C:220:ILE:HG12 | 2.21 | 0.54 |
| 2:A:187:LEU:HD12 | 2:A:191:LEU:HD12 | 1.89 | 0.54 |
| 2:B:369:ASN:C | 2:B:369:ASN:HD22 | 2.10 | 0.54 |
| 3:C:136:VAL:HG12 | 3:C:154:LEU:O | 2.07 | 0.54 |
| 3:C:8:LEU:HD12 | 3:C:227:SER:O | 2.07 | 0.54 |
| 3:C:198:ARG:HG3 | 3:C:242:LEU:CD1 | 2.38 | 0.54 |
| 1:F:912:G:H1 | 1:F:923:C:N4 | 2.06 | 0.54 |
| 2:A:172:VAL:HG22 | 2:A:198:VAL:CG2 | 2.37 | 0.54 |
| 2:A:132:ILE:HG23 | 2:A:222:ARG:NH1 | 2.22 | 0.54 |
| 2:A:335:GLY:O | 2:A:336:LEU:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:167:THR:HG23 | 3:D:168:GLY:N | 2.23 | 0.54 |
| 3:D:304:ARG:HA | 3:D:365:ASP:CB | 2.38 | 0.54 |
| 3:D:301:VAL:CG2 | 3:D:381:LEU:HD22 | 2.38 | 0.54 |
| 3:C:374:ARG:HG2 | 3:C:374:ARG:HH11 | 1.71 | 0.54 |
| 3:C:80:LEU:HD22 | 3:C:85:GLU:HB2 | 1.89 | 0.54 |
| 3:D:265:THR:O | 3:D:269:ARG:HG2 | 2.08 | 0.54 |
| 3:D:458:TYR:O | 3:D:487:THR:HG21 | 2.07 | 0.54 |
| 3:D:64:MET:HG2 | 3:D:65:ARG:N | 2.22 | 0.54 |
| 2:A:257:THR:HG23 | 2:B:336:LEU:HA | 1.89 | 0.54 |
| 3:C:375:VAL:O | 3:C:379:ASN:ND2 | 2.41 | 0.54 |
| 3:D:337:PHE:HB2 | 3:D:369:MET:HG2 | 1.89 | 0.54 |
| 1:E:932:C:C3' | 1:E:933:U:H5'' | 2.37 | 0.54 |
| 3:C:118:ARG:HG3 | 3:C:423:GLU:HB2 | 1.90 | 0.54 |
| 2:A:61:ILE:HA | 2:A:64:ALA:HB2 | 1.88 | 0.53 |
| 3:C:291:ILE:H | 3:C:291:ILE:CD1 | 2.21 | 0.53 |
| 3:C:33:THR:O | 3:C:162:ARG:NH2 | 2.42 | 0.53 |
| 3:D:287:THR:HG22 | 5:D:1925:HOH:O | 2.06 | 0.53 |
| 3:D:341:GLU:C | 3:D:343:PRO:HD3 | 2.28 | 0.53 |
| 3:D:45:LEU:HD23 | 3:D:69:PHE:CD1 | 2.42 | 0.53 |
| 1:F:903:U:H2' | 1:F:904:C:O4' | 2.07 | 0.53 |
| 2:A:175:HIS:CD2 | 2:A:176:GLY:H | 2.25 | 0.53 |
| 2:A:158:ARG:NE | 2:A:298:ASP:OD2 | 2.37 | 0.53 |
| 2:A:49:LEU:HD12 | 2:A:59:VAL:HG11 | 1.89 | 0.53 |
| 2:A:68:LEU:HD11 | 2:A:70:GLU:O | 2.07 | 0.53 |
| 2:A:8:ARG:HH22 | 2:A:9:LYS:HZ2 | 1.56 | 0.53 |
| 2:B:150:PRO:HA | 2:B:153:TRP:CE3 | 2.43 | 0.53 |
| 3:C:111:VAL:O | 3:C:431:ILE:HD12 | 2.08 | 0.53 |
| 3:C:59:ALA:O | 3:C:61:GLU:N | 2.32 | 0.53 |
| 3:D:157:GLU:OE2 | 3:D:184:GLU:OE1 | 2.26 | 0.53 |
| 1:E:910:G:H3' | 1:E:910:G:OP2 | 2.09 | 0.53 |
| 2:A:275:THR:HG23 | 2:A:276:PRO:HD2 | 1.89 | 0.53 |
| 2:B:195:VAL:HG22 | 2:B:289:ARG:NH1 | 2.22 | 0.53 |
| 2:B:293:GLU:O | 2:B:295:GLU:HG3 | 2.09 | 0.53 |
| 3:C:3:TRP:HZ3 | 3:C:253:VAL:HG11 | 1.72 | 0.53 |
| 1:F:958:A:C4' | 1:F:959:C:OP1 | 2.45 | 0.53 |
| 2:B:214:SER:O | 2:B:217:ILE:HG22 | 2.08 | 0.53 |
| 2:B:271:LEU:HD22 | 2:B:283:GLU:HG2 | 1.91 | 0.53 |
| 3:D:119:LYS:HD2 | 3:D:418:SER:HB3 | 1.91 | 0.53 |
| 3:D:200:VAL:O | 3:D:204:ILE:HG13 | 2.09 | 0.53 |
| 3:D:365:ASP:OD2 | 3:D:365:ASP:N | 2.40 | 0.53 |
| 3:D:486:ASP:HB3 | 3:D:489:VAL:CG2 | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:142:ASN:C | 2:A:143:ILE:HG13 | 2.28 | 0.53 |
| 2:A:157:ALA:HA | 2:A:187:LEU:CD1 | 2.39 | 0.53 |
| 2:A:194:PRO:O | 2:A:289:ARG:HD3 | 2.08 | 0.53 |
| 2:A:47:ILE:HD12 | 2:A:61:ILE:HG21 | 1.90 | 0.53 |
| 2:B:102:VAL:O | 2:B:103:ALA:HB2 | 2.09 | 0.53 |
| 2:A:365:ASN:HB2 | 2:B:255:MET:O | 2.08 | 0.53 |
| 2:B:380:LEU:HD21 | 2:B:386:PRO:CG | 2.38 | 0.53 |
| 1:E:937:G:H2' | 1:E:938:A:O4' | 2.09 | 0.53 |
| 2:A:8:ARG:HH12 | 2:A:9:LYS:NZ | 2.01 | 0.53 |
| 2:B:205:SER:HB2 | 2:B:207:ASP:OD1 | 2.09 | 0.53 |
| 3:C:10:MET:O | 3:C:191:MET:HG2 | 2.07 | 0.53 |
| 3:C:299:LEU:HB2 | 3:C:381:LEU:HD12 | 1.90 | 0.53 |
| 3:C:121:VAL:HB | 3:C:126:ASN:HD21 | 1.74 | 0.53 |
| 3:C:146:GLN:HG3 | 3:C:196:GLN:CB | 2.39 | 0.53 |
| 3:C:162:ARG:HA | 3:C:177:ARG:NH2 | 2.23 | 0.53 |
| 3:C:15:HIS:ND1 | 3:C:184:GLU:HG2 | 2.23 | 0.53 |
| 1:E:922:U:H2' | 1:E:923:C:N1 | 2.23 | 0.53 |
| 2:B:123:LEU:CD2 | 2:B:130:LEU:HD21 | 2.38 | 0.53 |
| 2:B:203:GLN:HA | 2:B:203:GLN:NE2 | 2.22 | 0.53 |
| 3:C:259:LEU:CD2 | 3:C:262:ILE:HD12 | 2.29 | 0.53 |
| 3:D:488:THR:HG23 | 5:D:1921:HOH:O | 2.07 | 0.53 |
| 3:D:515:GLU:HA | 3:D:518:ASP:OD1 | 2.09 | 0.53 |
| 2:B:66:ILE:HG22 | 2:B:67:GLU:N | 2.24 | 0.53 |
| 3:D:15:HIS:CE1 | 3:D:184:GLU:CG | 2.91 | 0.53 |
| 2:A:158:ARG:HG3 | 2:A:158:ARG:NH1 | 2.25 | 0.52 |
| 2:A:193:THR:HG23 | 2:A:194:PRO:HD2 | 1.91 | 0.52 |
| 2:A:232:THR:HG22 | 2:A:248:ARG:HA | 1.90 | 0.52 |
| 2:B:23:LEU:HB2 | 2:B:69:LEU:HD11 | 1.91 | 0.52 |
| 3:C:121:VAL:O | 3:C:121:VAL:HG12 | 2.09 | 0.52 |
| 3:C:201:ALA:HB3 | 3:C:242:LEU:CD1 | 2.38 | 0.52 |
| 3:C:306:PHE:CZ | 3:C:392:ILE:HD11 | 2.43 | 0.52 |
| 3:C:342:LEU:HD13 | 3:C:352:VAL:HG22 | 1.90 | 0.52 |
| 1:E:922:U:H2' | 1:E:923:C:C6 | 2.44 | 0.52 |
| 2:A:198:VAL:HG12 | 2:A:232:THR:OG1 | 2.09 | 0.52 |
| 2:B:140:VAL:HG11 | 2:B:159:ALA:HB2 | 1.92 | 0.52 |
| 3:D:15:HIS:CE1 | 3:D:184:GLU:OE1 | 2.62 | 0.52 |
| 2:A:12:GLU:O | 2:A:14:ALA:N | 2.42 | 0.52 |
| 2:B:204:ARG:O | 2:B:205:SER:C | 2.48 | 0.52 |
| 3:D:307:ASP:HB3 | 3:D:364:GLY:O | 2.09 | 0.52 |
| 2:A:154:VAL:HG13 | 2:A:298:ASP:HB2 | 1.91 | 0.52 |
| 3:C:228:ILE:CG1 | 3:C:256:GLN:HG2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:441:ARG:O | 3:C:442:ASN:ND2 | 2.42 | 0.52 |
| 3:D:177:ARG:HG3 | 3:D:180:ILE:HD12 | 1.91 | 0.52 |
| 3:D:468:LEU:HD21 | 3:D:477:PHE:CB | 2.39 | 0.52 |
| 3:D:503:ARG:O | 3:D:504:GLU:HG3 | 2.08 | 0.52 |
| 1:E:930:G:O2' | 1:E:931:G:H5' | 2.09 | 0.52 |
| 2:A:247:HIS:HB3 | 2:A:252:VAL:HG22 | 1.91 | 0.52 |
| 2:B:325:GLY:O | 2:B:327:ARG:NH1 | 2.43 | 0.52 |
| 3:D:224:LEU:CD1 | 3:D:248:ILE:HD11 | 2.38 | 0.52 |
| 3:D:381:LEU:HD23 | 3:D:384:VAL:HG11 | 1.92 | 0.52 |
| 3:D:105:LEU:CD2 | 3:D:443:LEU:HB3 | 2.38 | 0.52 |
| 2:A:95:ILE:HD13 | 2:A:217:ILE:HD11 | 1.92 | 0.52 |
| 3:C:183:VAL:HG23 | 3:C:183:VAL:O | 2.10 | 0.52 |
| 3:C:454:ILE:CD1 | 3:C:474:VAL:HG13 | 2.34 | 0.52 |
| 3:D:32:LEU:HD22 | 3:D:176:ASP:CG | 2.30 | 0.52 |
| 2:A:229:ALA:HB3 | 2:A:288:LYS:O | 2.09 | 0.52 |
| 2:A:344:ILE:HD13 | 2:A:379:LEU:HD23 | 1.91 | 0.52 |
| 2:B:10:PHE:CB | 2:B:61:ILE:HD12 | 2.40 | 0.52 |
| 3:C:74:TYR:CG | 3:C:77:GLU:HG2 | 2.45 | 0.52 |
| 3:D:162:ARG:HB3 | 3:D:177:ARG:HH21 | 1.75 | 0.52 |
| 3:D:263:ARG:O | 3:D:267:GLN:HG3 | 2.08 | 0.52 |
| 3:D:62:GLU:CG | 3:D:65:ARG:HH12 | 2.22 | 0.52 |
| 2:B:204:ARG:HB2 | 2:B:211:SER:HA | 1.92 | 0.52 |
| 3:C:313:GLU:HG3 | 3:C:319:ARG:NH1 | 2.25 | 0.52 |
| 3:D:191:MET:O | 3:D:192:SER:CB | 2.55 | 0.52 |
| 3:D:68:HIS:CE1 | 5:D:1906:HOH:O | 2.63 | 0.52 |
| 1:F:914:A:H2' | 1:F:915:G:O4' | 2.10 | 0.52 |
| 2:B:410:GLU:CD | 2:B:410:GLU:H | 2.13 | 0.52 |
| 3:C:355:LEU:HD22 | 3:C:367:VAL:HG11 | 1.90 | 0.52 |
| 3:D:22:SER:OG | 3:D:27:PRO:HA | 2.10 | 0.52 |
| 3:D:440:ARG:HA | 3:D:443:LEU:HD21 | 1.92 | 0.52 |
| 3:D:531:ASP:C | 3:D:533:LEU:H | 2.12 | 0.52 |
| 3:D:65:ARG:HB3 | 3:D:65:ARG:HH11 | 1.72 | 0.52 |
| 2:B:161:TYR:CE1 | 2:B:294:LEU:HG | 2.45 | 0.52 |
| 3:C:471:ARG:NH1 | 3:C:499:ARG:NE | 2.57 | 0.52 |
| 3:D:292:ILE:HG23 | 3:D:371:ALA:CB | 2.40 | 0.52 |
| 1:F:962:C:OP1 | 3:D:503:ARG:NH1 | 2.43 | 0.52 |
| 2:A:299:ARG:HH11 | 2:A:299:ARG:CG | 2.18 | 0.51 |
| 3:C:10:MET:HE2 | 3:C:197:LEU:HD22 | 1.92 | 0.51 |
| 3:C:118:ARG:HE | 3:C:423:GLU:CD | 2.14 | 0.51 |
| 3:D:416:THR:HG22 | 3:D:417:SER:N | 2.25 | 0.51 |
| 3:C:22:SER:HB2 | 3:C:27:PRO:HA | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:196:PRO:HG3 | 2:A:228:ILE:O | 2.10 | 0.51 |
| 1:F:949:A:OP1 | 1:F:959:C:H1' | 2.10 | 0.51 |
| 2:A:221:VAL:O | 2:A:225:THR:HG23 | 2.10 | 0.51 |
| 3:D:114:PHE:CZ | 3:D:134:GLY:HA3 | 2.45 | 0.51 |
| 3:D:43:ARG:CG | 3:D:43:ARG:NH1 | 2.62 | 0.51 |
| 1:F:932:C:H2' | 1:F:933:U:H4' | 1.91 | 0.51 |
| 2:B:175:HIS:HD2 | 2:B:176:GLY:O | 1.94 | 0.51 |
| 3:C:146:GLN:CD | 3:C:146:GLN:N | 2.64 | 0.51 |
| 3:C:355:LEU:CD2 | 3:C:367:VAL:HG11 | 2.39 | 0.51 |
| 2:B:274:VAL:CG1 | 2:B:275:THR:N | 2.74 | 0.51 |
| 2:B:87:ASP:OD1 | 2:B:90:LEU:HD23 | 2.10 | 0.51 |
| 2:B:418:GLU:O | 2:B:420:ILE:HG13 | 2.11 | 0.51 |
| 3:D:88:PRO:HG3 | 3:D:132:ARG:NH2 | 2.26 | 0.51 |
| 2:A:283:GLU:OE1 | 2:A:285:ASN:N | 2.42 | 0.51 |
| 2:A:68:LEU:HD12 | 2:A:69:LEU:N | 2.26 | 0.51 |
| 2:B:321:HIS:O | 2:B:326:TYR:HB2 | 2.10 | 0.51 |
| 3:C:262:ILE:HG23 | 3:C:309:LEU:HD23 | 1.92 | 0.51 |
| 1:F:911:G:C2 | 1:F:925:U:H1' | 2.45 | 0.51 |
| 2:A:367:ARG:NH2 | 2:A:428:THR:HG23 | 2.25 | 0.51 |
| 2:B:363:CYS:O | 2:B:364:LEU:HB2 | 2.11 | 0.51 |
| 3:C:319:ARG:NH1 | 3:C:319:ARG:HG3 | 2.23 | 0.51 |
| 3:D:177:ARG:HA | 3:D:180:ILE:CD1 | 2.41 | 0.51 |
| 3:C:29:ARG:NH1 | 3:C:29:ARG:HB2 | 2.26 | 0.51 |
| 3:C:59:ALA:C | 3:C:61:GLU:N | 2.63 | 0.51 |
| 3:D:278:PHE:HD1 | 3:D:359:VAL:HA | 1.75 | 0.51 |
| 1:E:917:G:C2' | 1:E:957:G:H22 | 2.18 | 0.51 |
| 2:A:283:GLU:CD | 2:A:285:ASN:H | 2.13 | 0.50 |
| 2:A:362:GLN:NE2 | 5:A:447:HOH:O | 2.43 | 0.50 |
| 2:A:68:LEU:CD1 | 2:A:70:GLU:H | 2.24 | 0.50 |
| 2:B:344:ILE:HB | 2:B:345:PRO:CD | 2.35 | 0.50 |
| 3:C:138:THR:HG22 | 3:C:153:ASN:OD1 | 2.11 | 0.50 |
| 3:D:106:LEU:HB2 | 3:D:108:MET:HG3 | 1.92 | 0.50 |
| 1:F:960:U:OP2 | 1:F:960:U:H6 | 1.94 | 0.50 |
| 2:A:162:GLY:O | 2:A:165:LYS:N | 2.41 | 0.50 |
| 2:B:161:TYR:O | 2:B:164:ILE:HG22 | 2.11 | 0.50 |
| 2:B:189:PHE:CE2 | 2:B:398:LYS:HG3 | 2.46 | 0.50 |
| 3:C:167:THR:CG2 | 3:C:168:GLY:H | 2.22 | 0.50 |
| 3:C:228:ILE:N | 3:C:228:ILE:CD1 | 2.73 | 0.50 |
| 1:F:960:U:C5' | 1:F:961:C:OP2 | 2.56 | 0.50 |
| 2:A:124:ARG:HG3 | 2:A:124:ARG:HH11 | 1.76 | 0.50 |
| 2:B:149:LYS:HB2 | 2:B:150:PRO:CD | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:88:PRO:O | 2:B:89:GLU:HB3 | 2.11 | 0.50 |
| 3:C:111:VAL:HG12 | 3:C:113:GLU:H | 1.75 | 0.50 |
| 2:B:430:ILE:HD11 | 3:C:41:ILE:HD11 | 1.94 | 0.50 |
| 3:D:278:PHE:HE1 | 3:D:359:VAL:O | 1.94 | 0.50 |
| 2:B:260:ARG:NH2 | 3:D:84:ASP:OD2 | 2.44 | 0.50 |
| 2:A:274:VAL:HG12 | 2:A:275:THR:N | 2.26 | 0.50 |
| 2:B:417:ARG:HH11 | 2:B:417:ARG:CB | 2.24 | 0.50 |
| 3:C:489:VAL:HG23 | 3:C:490:ILE:N | 2.26 | 0.50 |
| 3:D:108:MET:HE1 | 3:D:151:ILE:HG22 | 1.92 | 0.50 |
| 1:E:926:G:H2' | 1:E:927:C:O4' | 2.11 | 0.50 |
| 1:E:958:A:H1' | 1:E:960:U:H5 | 1.77 | 0.50 |
| 2:A:259:ARG:NH1 | 2:A:261:ASP:OD1 | 2.45 | 0.50 |
| 2:A:27:PRO:HD2 | 2:A:63:ASP:OD2 | 2.11 | 0.50 |
| 2:B:281:ILE:HG22 | 2:B:283:GLU:O | 2.11 | 0.50 |
| 2:B:29:VAL:HG13 | 3:D:109:ARG:CG | 2.39 | 0.50 |
| 3:C:31:GLU:OE2 | 3:C:32:LEU:O | 2.30 | 0.50 |
| 2:A:150:PRO:HA | 2:A:153:TRP:CD2 | 2.46 | 0.50 |
| 2:B:219:CYS:O | 2:B:274:VAL:HG11 | 2.11 | 0.50 |
| 3:C:343:PRO:HA | 3:C:349:GLU:OE2 | 2.11 | 0.50 |
| 3:D:108:MET:HG2 | 3:D:140:GLY:HA3 | 1.92 | 0.50 |
| 3:D:278:PHE:CD1 | 3:D:359:VAL:HA | 2.47 | 0.50 |
| 3:C:291:ILE:HD12 | 3:C:291:ILE:N | 2.27 | 0.50 |
| 2:B:8:ARG:HG3 | 2:B:9:LYS:N | 2.26 | 0.50 |
| 3:C:501:LEU:C | 3:C:503:ARG:H | 2.15 | 0.50 |
| 3:D:111:VAL:CG1 | 3:D:112:ASP:N | 2.75 | 0.50 |
| 3:C:16:GLN:OE1 | 3:C:213:VAL:CG1 | 2.60 | 0.50 |
| 3:D:176:ASP:N | 3:D:176:ASP:OD1 | 2.45 | 0.50 |
| 3:D:207:ILE:HG22 | 3:D:208:LEU:N | 2.26 | 0.50 |
| 1:E:906:C:O2' | 1:E:907:G:H5' | 2.12 | 0.50 |
| 1:E:960:U:O5' | 1:E:960:U:H6 | 1.95 | 0.50 |
| 1:F:957:G:H2' | 1:F:957:G:N3 | 2.26 | 0.50 |
| 2:A:248:ARG:CZ | 2:A:271:LEU:HD21 | 2.42 | 0.49 |
| 2:B:17:ASP:OD2 | 2:B:71:LYS:NZ | 2.41 | 0.49 |
| 3:C:20:THR:CG2 | 3:C:94:GLU:HG2 | 2.40 | 0.49 |
| 3:C:98:ILE:HD13 | 3:C:212:ARG:O | 2.12 | 0.49 |
| 3:D:108:MET:HB3 | 3:D:137:ALA:HB1 | 1.93 | 0.49 |
| 3:D:499:ARG:CB | 3:D:499:ARG:HH11 | 2.25 | 0.49 |
| 2:B:90:LEU:O | 2:B:134:ASN:ND2 | 2.45 | 0.49 |
| 3:D:523:LEU:C | 3:D:524:GLU:HG3 | 2.32 | 0.49 |
| 2:A:87:ASP:HB3 | 5:A:446:HOH:O | 2.12 | 0.49 |
| 2:B:140:VAL:HG11 | 2:B:159:ALA:CB | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:222:ARG:NH2 | 2:B:277:ASP:O | 2.45 | 0.49 |
| 2:B:44:ASP:O | 2:B:45:ARG:HB2 | 2.11 | 0.49 |
| 2:B:54:GLY:O | 3:D:117:MET:HE2 | 2.12 | 0.49 |
| 3:C:71:TYR:CE2 | 3:C:127:THR:HG22 | 2.48 | 0.49 |
| 3:C:339:THR:O | 3:C:343:PRO:HD3 | 2.12 | 0.49 |
| 3:C:471:ARG:HH22 | 3:C:499:ARG:HB2 | 1.78 | 0.49 |
| 3:C:471:ARG:NH1 | 3:C:499:ARG:CZ | 2.75 | 0.49 |
| 2:B:428:THR:HG21 | 3:C:80:LEU:HD12 | 1.95 | 0.49 |
| 3:D:43:ARG:HD2 | 3:D:71:TYR:CE1 | 2.48 | 0.49 |
| 3:D:68:HIS:HE1 | 5:D:1906:HOH:O | 1.96 | 0.49 |
| 1:E:914:A:C2 | 1:E:915:G:H1' | 2.48 | 0.49 |
| 2:A:111:GLY:O | 3:C:421:TYR:HB2 | 2.13 | 0.49 |
| 2:A:11:LEU:HG | 2:A:47:ILE:HD13 | 1.93 | 0.49 |
| 3:C:165:ARG:CB | 3:C:165:ARG:NH1 | 2.72 | 0.49 |
| 3:C:207:ILE:O | 3:C:210:SER:OG | 2.20 | 0.49 |
| 3:C:46:ARG:HH11 | 3:C:46:ARG:HG3 | 1.77 | 0.49 |
| 2:B:55:TYR:HA | 3:D:117:MET:HE2 | 1.94 | 0.49 |
| 3:D:313:GLU:OE2 | 3:D:316:PRO:HA | 2.13 | 0.49 |
| 3:D:118:ARG:HG3 | 3:D:423:GLU:HB2 | 1.94 | 0.49 |
| 1:E:918:G:H5' | 1:E:920:A:C2 | 2.47 | 0.49 |
| 2:B:212:ASP:HB2 | 2:B:236:HIS:CE1 | 2.47 | 0.49 |
| 2:B:393:GLU:O | 2:B:397:VAL:HG23 | 2.12 | 0.49 |
| 3:C:100:VAL:O | 3:C:103:ALA:HB3 | 2.12 | 0.49 |
| 3:D:347:ILE:HG22 | 3:D:351:GLU:HB2 | 1.95 | 0.49 |
| 1:E:948:C:N3 | 1:E:959:C:N4 | 2.60 | 0.49 |
| 2:A:115:PRO:O | 2:A:116:ALA:HB2 | 2.13 | 0.49 |
| 2:A:116:ALA:HB1 | 2:A:121:ASP:OD2 | 2.12 | 0.49 |
| 2:A:264:ARG:NE | 2:B:435:GLY:C | 2.64 | 0.49 |
| 2:B:12:GLU:C | 2:B:14:ALA:H | 2.16 | 0.49 |
| 3:D:454:ILE:O | 3:D:458:TYR:HD1 | 1.95 | 0.49 |
| 2:A:186:ALA:HB1 | 2:A:190:MET:HE3 | 1.94 | 0.49 |
| 2:A:193:THR:HG22 | 2:A:194:PRO:CD | 2.43 | 0.49 |
| 3:C:1:MET:HE2 | 3:C:6:VAL:HG21 | 1.94 | 0.49 |
| 3:D:108:MET:SD | 3:D:154:LEU:HB2 | 2.53 | 0.49 |
| 3:D:417:SER:N | 5:D:1909:HOH:O | 2.44 | 0.49 |
| 3:D:502:ARG:HD2 | 3:D:507:ASP:OD1 | 2.12 | 0.49 |
| 1:F:963:G:O4' | 3:D:467:GLN:NE2 | 2.39 | 0.49 |
| 2:B:160:VAL:O | 2:B:164:ILE:HG22 | 2.13 | 0.49 |
| 3:D:207:ILE:O | 3:D:210:SER:HB2 | 2.12 | 0.49 |
| 3:D:17:GLN:O | 3:D:213:VAL:HG13 | 2.13 | 0.49 |
| 3:D:303:LEU:HB3 | 3:D:306:PHE:CD1 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:325:ALA:O | 3:D:329:LYS:HG3 | 2.13 | 0.49 |
| 3:D:62:GLU:HG2 | 3:D:65:ARG:HH12 | 1.78 | 0.49 |
| 2:A:164:ILE:HD12 | 2:A:164:ILE:O | 2.12 | 0.49 |
| 2:A:306:PHE:HB3 | 2:B:310:TYR:CE2 | 2.47 | 0.49 |
| 2:A:435:GLY:HA2 | 2:B:264:ARG:NE | 2.28 | 0.49 |
| 3:C:146:GLN:CD | 3:C:146:GLN:H | 2.15 | 0.49 |
| 3:C:201:ALA:CB | 3:C:242:LEU:HD13 | 2.42 | 0.49 |
| 3:D:252:GLU:OE2 | 3:D:255:ARG:NH2 | 2.46 | 0.49 |
| 3:C:159:ASP:OD2 | 3:C:177:ARG:HD2 | 2.13 | 0.48 |
| 3:C:271:ALA:HB1 | 3:C:304:ARG:O | 2.13 | 0.48 |
| 3:C:79:CYS:H | 3:C:82:GLU:HG3 | 1.78 | 0.48 |
| 3:D:274:GLU:OE1 | 3:D:276:LYS:HE2 | 2.12 | 0.48 |
| 3:D:493:LEU:HD12 | 3:D:497:THR:HB | 1.94 | 0.48 |
| 1:E:954:U:H2' | 1:E:955:U:H5' | 1.95 | 0.48 |
| 1:F:921:A:H61 | 1:F:947:A:H2' | 1.78 | 0.48 |
| 2:B:22:VAL:HB | 2:B:66:ILE:CG2 | 2.43 | 0.48 |
| 3:C:16:GLN:NE2 | 3:C:16:GLN:CA | 2.67 | 0.48 |
| 3:C:256:GLN:OE1 | 3:C:395:VAL:HG11 | 2.12 | 0.48 |
| 3:C:365:ASP:N | 3:C:365:ASP:OD2 | 2.34 | 0.48 |
| 3:D:219:THR:HG22 | 3:D:220:ILE:N | 2.28 | 0.48 |
| 3:D:309:LEU:HA | 3:D:312:VAL:CG2 | 2.44 | 0.48 |
| 3:D:46:ARG:O | 3:D:47:PRO:O | 2.31 | 0.48 |
| 3:D:494:LEU:HD22 | 3:D:498:LEU:HD11 | 1.94 | 0.48 |
| 3:D:6:VAL:HG12 | 3:D:228:ILE:CG2 | 2.43 | 0.48 |
| 1:E:912:G:N2 | 1:E:924:C:N3 | 2.61 | 0.48 |
| 1:E:947:A:C3' | 1:E:948:C:H5' | 2.43 | 0.48 |
| 1:E:957:G:H2' | 1:E:957:G:N3 | 2.27 | 0.48 |
| 1:E:920:A:N6 | 1:E:959:C:H5 | 2.10 | 0.48 |
| 2:A:253:ARG:HG3 | 2:A:391:LEU:HD13 | 1.94 | 0.48 |
| 2:B:143:ILE:CG2 | 2:B:148:MET:HE3 | 2.43 | 0.48 |
| 2:B:418:GLU:HG2 | 2:B:420:ILE:HG13 | 1.95 | 0.48 |
| 3:C:486:ASP:O | 3:C:488:THR:N | 2.46 | 0.48 |
| 3:D:167:THR:HG23 | 3:D:168:GLY:H | 1.78 | 0.48 |
| 3:D:227:SER:HB2 | 3:D:233:ARG:HD3 | 1.94 | 0.48 |
| 2:B:55:TYR:CE2 | 3:D:420:MET:HE1 | 2.49 | 0.48 |
| 3:D:91:LEU:HD22 | 3:D:114:PHE:CD2 | 2.49 | 0.48 |
| 1:E:966:C:H2' | 1:E:967:G:H8 | 1.79 | 0.48 |
| 1:F:918:G:H5' | 5:F:107:HOH:O | 2.13 | 0.48 |
| 2:A:248:ARG:HB2 | 2:A:271:LEU:HD11 | 1.94 | 0.48 |
| 2:B:161:TYR:CB | 2:B:296:LEU:HD22 | 2.43 | 0.48 |
| 2:B:200:THR:HG21 | 2:B:216:ASN:HB3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:319:ARG:HD3 | 5:C:936:HOH:O | 2.13 | 0.48 |
| 3:D:135:LEU:HD11 | 3:D:153:ASN:OD1 | 2.14 | 0.48 |
| 3:D:396:PRO:O | 3:D:398:GLU:HG2 | 2.13 | 0.48 |
| 2:A:319:LYS:O | 2:A:322:LEU:N | 2.46 | 0.48 |
| 3:C:96:LEU:O | 3:C:100:VAL:HG23 | 2.14 | 0.48 |
| 3:D:224:LEU:HD11 | 3:D:248:ILE:HD11 | 1.95 | 0.48 |
| 3:D:104:LEU:HD11 | 3:D:436:LEU:CD1 | 2.43 | 0.48 |
| 3:D:486:ASP:CG | 3:D:486:ASP:O | 2.52 | 0.48 |
| 3:D:62:GLU:HA | 3:D:65:ARG:NH2 | 2.28 | 0.48 |
| 2:A:193:THR:CG2 | 2:A:195:VAL:O | 2.62 | 0.48 |
| 2:A:7:ALA:HA | 2:A:61:ILE:HD11 | 1.95 | 0.48 |
| 2:B:115:PRO:O | 2:B:116:ALA:HB2 | 2.13 | 0.48 |
| 2:A:48:VAL:HG22 | 3:C:115:HIS:HE1 | 1.79 | 0.48 |
| 3:C:299:LEU:HD11 | 3:C:374:ARG:NH1 | 2.28 | 0.48 |
| 3:C:331:ARG:HH21 | 3:C:379:ASN:HD22 | 1.60 | 0.48 |
| 3:C:437:GLU:HB3 | 3:C:441:ARG:CZ | 2.44 | 0.48 |
| 3:C:445:GLU:OE1 | 3:C:453:ARG:NH1 | 2.47 | 0.48 |
| 3:D:370:VAL:HG21 | 3:D:381:LEU:HG | 1.96 | 0.48 |
| 3:C:331:ARG:NH2 | 3:C:376:THR:HA | 2.23 | 0.48 |
| 1:E:918:G:C1' | 1:E:957:G:N2 | 2.77 | 0.48 |
| 2:A:299:ARG:HB2 | 2:A:405:GLN:HE22 | 1.79 | 0.48 |
| 2:B:143:ILE:HD11 | 2:B:152:TYR:CE2 | 2.49 | 0.48 |
| 2:B:165:LYS:HE2 | 2:B:294:LEU:CD2 | 2.44 | 0.48 |
| 2:B:328:GLY:HA3 | 2:B:399:MET:CE | 2.43 | 0.48 |
| 2:B:330:VAL:HG21 | 2:B:396:TYR:HA | 1.94 | 0.48 |
| 3:C:291:ILE:HG21 | 3:C:337:PHE:HZ | 1.79 | 0.48 |
| 3:C:42:VAL:HG22 | 3:C:70:HIS:CD2 | 2.49 | 0.48 |
| 1:F:953:G:O2' | 1:F:954:U:H5' | 2.14 | 0.48 |
| 2:A:301:GLU:OE2 | 2:A:303:ARG:NH2 | 2.47 | 0.47 |
| 2:B:336:LEU:O | 2:B:368:VAL:HG13 | 2.14 | 0.47 |
| 2:B:428:THR:CG2 | 3:C:80:LEU:HD12 | 2.44 | 0.47 |
| 3:C:46:ARG:HH11 | 3:C:46:ARG:CG | 2.27 | 0.47 |
| 3:D:25:PHE:CE2 | 3:D:426:ILE:HD13 | 2.49 | 0.47 |
| 1:E:931:G:H2' | 1:E:932:C:O4' | 2.14 | 0.47 |
| 2:A:264:ARG:HE | 2:B:435:GLY:CA | 2.28 | 0.47 |
| 3:C:281:SER:HA | 3:C:298:VAL:CG1 | 2.44 | 0.47 |
| 3:C:468:LEU:HD11 | 3:C:491:ALA:HB1 | 1.95 | 0.47 |
| 3:D:355:LEU:O | 3:D:359:VAL:HG12 | 2.15 | 0.47 |
| 2:A:102:VAL:O | 2:A:102:VAL:HG23 | 2.14 | 0.47 |
| 2:A:157:ALA:HA | 2:A:187:LEU:HD11 | 1.95 | 0.47 |
| 3:C:106:LEU:HD13 | 3:C:151:ILE:HD13 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:303:LEU:HB3 | 3:C:306:PHE:CG | 2.48 | 0.47 |
| 3:C:437:GLU:C | 3:C:439:ILE:H | 2.18 | 0.47 |
| 3:D:159:ASP:HB2 | 3:D:182:LEU:HD13 | 1.95 | 0.47 |
| 3:D:486:ASP:OD2 | 3:D:486:ASP:O | 2.32 | 0.47 |
| 1:F:921:A:N1 | 1:F:948:C:C1' | 2.75 | 0.47 |
| 3:D:437:GLU:O | 3:D:439:ILE:N | 2.47 | 0.47 |
| 2:B:114:HIS:O | 2:B:115:PRO:O | 2.33 | 0.47 |
| 2:B:12:GLU:O | 2:B:14:ALA:N | 2.47 | 0.47 |
| 2:B:320:TRP:CZ2 | 2:B:324:GLU:HG3 | 2.49 | 0.47 |
| 3:C:111:VAL:HG12 | 3:C:112:ASP:N | 2.28 | 0.47 |
| 3:C:156:LEU:HA | 3:C:182:LEU:O | 2.14 | 0.47 |
| 3:C:337:PHE:N | 3:C:337:PHE:CD1 | 2.82 | 0.47 |
| 3:D:493:LEU:HG | 3:D:493:LEU:O | 2.14 | 0.47 |
| 3:D:62:GLU:CA | 3:D:65:ARG:HH12 | 2.26 | 0.47 |
| 2:B:11:LEU:HD13 | 2:B:47:ILE:HD13 | 1.93 | 0.47 |
| 2:B:124:ARG:NH1 | 2:B:124:ARG:CG | 2.76 | 0.47 |
| 2:B:150:PRO:HA | 2:B:153:TRP:CD2 | 2.49 | 0.47 |
| 2:B:327:ARG:O | 2:B:356:PRO:HD2 | 2.14 | 0.47 |
| 3:C:98:ILE:CD1 | 3:C:212:ARG:HB2 | 2.44 | 0.47 |
| 3:D:2:ASP:HB3 | 3:D:5:LYS:CG | 2.45 | 0.47 |
| 3:D:454:ILE:HD12 | 3:D:474:VAL:CG1 | 2.32 | 0.47 |
| 2:A:161:TYR:CD1 | 2:A:294:LEU:HD11 | 2.49 | 0.47 |
| 3:C:193:ASP:OD2 | 3:C:196:GLN:HB2 | 2.15 | 0.47 |
| 3:D:105:LEU:HD23 | 3:D:443:LEU:CD1 | 2.41 | 0.47 |
| 1:E:930:G:H2' | 1:E:931:G:C8 | 2.50 | 0.47 |
| 2:A:106:ILE:HG12 | 2:A:113:VAL:HG22 | 1.97 | 0.47 |
| 2:B:128:GLU:HG2 | 2:B:218:GLN:HE22 | 1.80 | 0.47 |
| 2:B:320:TRP:CE2 | 2:B:324:GLU:HG3 | 2.50 | 0.47 |
| 2:B:50:LYS:NZ | 2:B:56:ASN:HD21 | 2.12 | 0.47 |
| 2:B:56:ASN:N | 2:B:56:ASN:ND2 | 2.63 | 0.47 |
| 2:B:87:ASP:O | 2:B:87:ASP:OD1 | 2.32 | 0.47 |
| 3:C:32:LEU:HD13 | 3:C:162:ARG:CZ | 2.44 | 0.47 |
| 1:F:954:U:H5'' | 3:D:488:THR:HG22 | 1.97 | 0.47 |
| 1:F:954:U:H4' | 3:D:492:SER:HB3 | 1.97 | 0.47 |
| 1:E:908:U:OP2 | 1:E:908:U:H6 | 1.97 | 0.47 |
| 1:E:921:A:OP2 | 1:E:921:A:H8 | 1.97 | 0.47 |
| 2:A:435:GLY:HA2 | 2:B:264:ARG:CZ | 2.45 | 0.47 |
| 2:B:104:SER:HA | 2:B:116:ALA:HB3 | 1.97 | 0.47 |
| 2:B:25:GLU:OE1 | 2:B:65:ARG:HG2 | 2.15 | 0.47 |
| 2:A:307:ILE:HD13 | 2:A:318:ILE:HD13 | 1.97 | 0.47 |
| 2:A:388:ASP:HB2 | 2:A:424:ILE:HG23 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:147:ASN:ND2 | 2:B:340:PRO:HA | 2.29 | 0.47 |
| 3:D:171:VAL:HG12 | 3:D:172:VAL:N | 2.30 | 0.47 |
| 3:D:220:ILE:HG12 | 3:D:221:ARG:H | 1.80 | 0.47 |
| 3:D:228:ILE:HG22 | 3:D:229:ARG:O | 2.15 | 0.47 |
| 3:D:423:GLU:HG2 | 3:D:426:ILE:HD12 | 1.95 | 0.47 |
| 3:D:468:LEU:HD12 | 3:D:473:LEU:HB2 | 1.96 | 0.47 |
| 3:C:171:VAL:CG2 | 3:C:172:VAL:N | 2.78 | 0.46 |
| 3:C:280:VAL:HG11 | 3:C:355:LEU:HG | 1.97 | 0.46 |
| 3:C:355:LEU:O | 3:C:355:LEU:HD23 | 2.15 | 0.46 |
| 2:B:57:ILE:CD1 | 3:D:135:LEU:HD23 | 2.45 | 0.46 |
| 3:D:426:ILE:HA | 3:D:427:PRO:HD3 | 1.76 | 0.46 |
| 3:D:43:ARG:HD2 | 3:D:71:TYR:HE1 | 1.80 | 0.46 |
| 2:A:175:HIS:CD2 | 2:A:176:GLY:O | 2.68 | 0.46 |
| 2:A:189:PHE:CE1 | 2:A:398:LYS:HG3 | 2.49 | 0.46 |
| 2:B:299:ARG:HB2 | 2:B:405:GLN:NE2 | 2.21 | 0.46 |
| 3:C:19:ASP:HA | 3:C:214:LYS:HZ2 | 1.80 | 0.46 |
| 3:C:20:THR:HG22 | 3:C:94:GLU:CG | 2.41 | 0.46 |
| 3:C:220:ILE:HG22 | 3:C:221:ARG:N | 2.30 | 0.46 |
| 3:C:3:TRP:CZ3 | 3:C:253:VAL:HG21 | 2.50 | 0.46 |
| 3:D:145:PRO:HB2 | 3:D:146:GLN:NE2 | 2.30 | 0.46 |
| 3:D:331:ARG:NE | 3:D:331:ARG:CA | 2.78 | 0.46 |
| 3:D:526:GLY:HA3 | 3:D:534:ARG:HH12 | 1.80 | 0.46 |
| 1:E:906:C:C2' | 1:E:907:G:H5' | 2.45 | 0.46 |
| 2:A:212:ASP:OD1 | 2:A:212:ASP:N | 2.39 | 0.46 |
| 2:A:351:HIS:HB2 | 5:A:457:HOH:O | 2.14 | 0.46 |
| 2:B:118:THR:HB | 2:B:121:ASP:OD2 | 2.15 | 0.46 |
| 2:B:293:GLU:HG3 | 2:B:293:GLU:O | 2.16 | 0.46 |
| 3:C:313:GLU:HG3 | 3:C:319:ARG:HH12 | 1.80 | 0.46 |
| 3:C:24:LEU:O | 3:C:92:ASN:HB2 | 2.15 | 0.46 |
| 1:E:907:G:H5'' | 1:E:908:U:OP2 | 2.15 | 0.46 |
| 2:A:363:CYS:O | 2:A:364:LEU:CB | 2.63 | 0.46 |
| 2:A:189:PHE:CZ | 2:A:398:LYS:HG3 | 2.51 | 0.46 |
| 2:B:143:ILE:HG21 | 2:B:148:MET:HE3 | 1.97 | 0.46 |
| 2:B:369:ASN:C | 2:B:369:ASN:ND2 | 2.67 | 0.46 |
| 3:C:361:ALA:N | 5:C:917:HOH:O | 2.48 | 0.46 |
| 3:D:115:HIS:NE2 | 3:D:428:LEU:HD13 | 2.30 | 0.46 |
| 3:D:125:SER:CB | 3:D:160:ALA:HB1 | 2.38 | 0.46 |
| 3:D:73:ASN:HD22 | 3:D:73:ASN:N | 2.13 | 0.46 |
| 2:A:408:ASP:HB3 | 2:A:411:MET:HB3 | 1.98 | 0.46 |
| 2:B:111:GLY:C | 3:D:422:LEU:HD12 | 2.36 | 0.46 |
| 3:D:70:HIS:HB2 | 3:D:172:VAL:HG22 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:274:VAL:CG1 | 2:A:275:THR:N | 2.79 | 0.46 |
| 2:A:281:ILE:HG22 | 2:A:284:GLU:OE2 | 2.15 | 0.46 |
| 2:B:203:GLN:O | 2:B:204:ARG:NH1 | 2.49 | 0.46 |
| 3:C:19:ASP:HB2 | 3:C:214:LYS:CG | 2.45 | 0.46 |
| 3:C:233:ARG:HG3 | 3:C:397:GLU:CB | 2.26 | 0.46 |
| 3:C:198:ARG:HG3 | 3:C:242:LEU:HD11 | 1.97 | 0.46 |
| 2:B:111:GLY:HA3 | 3:D:422:LEU:HD12 | 1.98 | 0.46 |
| 3:D:532:ALA:O | 3:D:533:LEU:HG | 2.16 | 0.46 |
| 2:A:91:PRO:O | 2:A:133:ALA:HB1 | 2.16 | 0.46 |
| 2:A:47:ILE:CD1 | 2:A:61:ILE:HG21 | 2.46 | 0.46 |
| 2:B:161:TYR:HB2 | 2:B:296:LEU:HD22 | 1.98 | 0.46 |
| 2:B:61:ILE:O | 2:B:62:SER:C | 2.54 | 0.46 |
| 1:F:959:C:O2 | 1:F:959:C:H2' | 2.16 | 0.46 |
| 2:A:205:SER:CB | 2:A:207:ASP:OD1 | 2.64 | 0.46 |
| 2:B:23:LEU:HD12 | 2:B:32:GLU:CG | 2.46 | 0.46 |
| 2:B:253:ARG:NH1 | 2:B:393:GLU:OE1 | 2.48 | 0.46 |
| 2:B:369:ASN:ND2 | 2:B:371:ASN:HB2 | 2.27 | 0.46 |
| 3:C:451:LYS:CB | 5:C:915:HOH:O | 2.63 | 0.46 |
| 3:C:74:TYR:H | 3:C:78:THR:HB | 1.81 | 0.46 |
| 3:D:146:GLN:HG3 | 3:D:196:GLN:CA | 2.45 | 0.46 |
| 1:F:943:G:O2' | 1:F:944:C:H5' | 2.15 | 0.46 |
| 2:A:434:ARG:HG2 | 2:A:434:ARG:H | 1.56 | 0.46 |
| 2:B:10:PHE:C | 2:B:10:PHE:CD2 | 2.89 | 0.46 |
| 2:B:171:VAL:O | 2:B:197:VAL:HA | 2.15 | 0.46 |
| 3:C:16:GLN:HB3 | 3:C:183:VAL:HG22 | 1.98 | 0.46 |
| 3:C:1:MET:HG2 | 3:C:1:MET:O | 2.16 | 0.46 |
| 3:D:501:LEU:HD21 | 3:D:536:ILE:CD1 | 2.46 | 0.46 |
| 3:D:59:ALA:O | 3:D:62:GLU:N | 2.41 | 0.46 |
| 2:A:255:MET:O | 2:B:365:ASN:HB2 | 2.16 | 0.46 |
| 2:B:20:ASP:HB3 | 2:B:68:LEU:CD1 | 2.46 | 0.46 |
| 3:D:280:VAL:HG13 | 3:D:283:VAL:HG21 | 1.97 | 0.46 |
| 3:D:302:LYS:NZ | 3:D:304:ARG:HE | 2.14 | 0.46 |
| 3:D:518:ASP:HA | 3:D:521:LYS:CG | 2.43 | 0.46 |
| 1:E:970:A:H2' | 1:E:971:C:C6 | 2.51 | 0.46 |
| 2:A:218:GLN:HG3 | 2:A:276:PRO:HG3 | 1.97 | 0.45 |
| 2:A:387:CYS:HB3 | 2:A:390:MET:CE | 2.45 | 0.45 |
| 2:A:358:ALA:HB1 | 2:A:387:CYS:SG | 2.56 | 0.45 |
| 2:A:88:PRO:HA | 5:A:453:HOH:O | 2.16 | 0.45 |
| 3:C:8:LEU:HA | 3:C:227:SER:O | 2.15 | 0.45 |
| 3:D:145:PRO:HD2 | 3:D:146:GLN:NE2 | 2.31 | 0.45 |
| 3:D:213:VAL:HG12 | 3:D:214:LYS:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:62:GLU:HA | 3:D:65:ARG:CZ | 2.45 | 0.45 |
| 1:F:918:G:HO2' | 1:F:919:U:H5' | 1.80 | 0.45 |
| 1:F:954:U:H2' | 1:F:955:U:C5' | 2.43 | 0.45 |
| 2:B:256:HIS:HD2 | 2:B:258:SER:H | 1.64 | 0.45 |
| 2:B:303:ARG:NH1 | 2:B:324:GLU:O | 2.49 | 0.45 |
| 2:B:419:ASN:ND2 | 2:B:424:ILE:O | 2.49 | 0.45 |
| 3:C:228:ILE:HD13 | 3:C:256:GLN:CD | 2.36 | 0.45 |
| 3:C:310:ILE:HG22 | 3:C:338:HIS:CD2 | 2.51 | 0.45 |
| 3:D:19:ASP:CA | 3:D:214:LYS:HE2 | 2.43 | 0.45 |
| 1:E:950:G:H2' | 1:E:951:C:H6 | 1.82 | 0.45 |
| 1:F:950:G:N2 | 1:F:965:U:C2 | 2.83 | 0.45 |
| 2:A:346:VAL:HG23 | 5:A:439:HOH:O | 2.16 | 0.45 |
| 2:B:175:HIS:CD2 | 2:B:176:GLY:O | 2.69 | 0.45 |
| 3:C:135:LEU:CD1 | 3:C:153:ASN:HB3 | 2.45 | 0.45 |
| 3:C:228:ILE:HG12 | 3:C:256:GLN:CG | 2.46 | 0.45 |
| 3:C:359:VAL:HG22 | 3:C:359:VAL:O | 2.17 | 0.45 |
| 3:D:58:ALA:HB3 | 5:D:1917:HOH:O | 2.16 | 0.45 |
| 2:A:349:GLU:O | 2:A:353:MET:HG3 | 2.15 | 0.45 |
| 2:A:362:GLN:O | 2:A:364:LEU:HG | 2.17 | 0.45 |
| 2:B:262:THR:HG23 | 2:B:263:PHE:CD2 | 2.51 | 0.45 |
| 2:B:45:ARG:NH2 | 3:D:430:ARG:CZ | 2.78 | 0.45 |
| 3:D:164:ILE:CG2 | 3:D:165:ARG:HG3 | 2.33 | 0.45 |
| 3:D:198:ARG:HG3 | 3:D:199:GLU:N | 2.32 | 0.45 |
| 3:D:234:VAL:CG1 | 3:D:400:ARG:HD2 | 2.44 | 0.45 |
| 3:D:468:LEU:CD1 | 3:D:473:LEU:HB2 | 2.46 | 0.45 |
| 1:E:960:U:H3' | 5:E:146:HOH:O | 2.16 | 0.45 |
| 2:A:66:ILE:HG22 | 2:A:67:GLU:H | 1.81 | 0.45 |
| 3:C:17:GLN:HB3 | 3:C:214:LYS:HG3 | 1.99 | 0.45 |
| 3:C:144:THR:HB | 3:C:199:GLU:HG2 | 1.99 | 0.45 |
| 3:C:372:HIS:CD2 | 3:C:373:GLU:H | 2.34 | 0.45 |
| 3:C:273:VAL:HB | 3:C:389:GLU:OE1 | 2.16 | 0.45 |
| 3:C:80:LEU:HD22 | 3:C:85:GLU:CB | 2.45 | 0.45 |
| 3:C:98:ILE:HG23 | 3:C:211:THR:CG2 | 2.43 | 0.45 |
| 3:D:160:ALA:O | 3:D:177:ARG:HG2 | 2.17 | 0.45 |
| 3:D:298:VAL:C | 3:D:299:LEU:HD23 | 2.37 | 0.45 |
| 3:D:331:ARG:O | 3:D:331:ARG:HG3 | 2.15 | 0.45 |
| 3:D:441:ARG:C | 3:D:442:ASN:OD1 | 2.55 | 0.45 |
| 2:A:367:ARG:HG3 | 2:A:367:ARG:HH11 | 1.81 | 0.45 |
| 2:B:423:GLU:HG2 | 2:B:424:ILE:HG13 | 1.97 | 0.45 |
| 3:C:111:VAL:HG23 | 3:C:136:VAL:C | 2.36 | 0.45 |
| 3:C:498:LEU:O | 3:C:501:LEU:HD22 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:520:ILE:O | 3:D:522:LEU:N | 2.47 | 0.45 |
| 2:B:128:GLU:CD | 2:B:128:GLU:H | 2.20 | 0.45 |
| 2:B:371:ASN:O | 2:B:377:ARG:HD3 | 2.17 | 0.45 |
| 2:B:393:GLU:CD | 2:B:393:GLU:H | 2.20 | 0.45 |
| 2:B:61:ILE:O | 2:B:63:ASP:N | 2.49 | 0.45 |
| 3:C:135:LEU:HD21 | 3:C:138:THR:CG2 | 2.46 | 0.45 |
| 3:C:262:ILE:HD11 | 3:C:314:ILE:HG22 | 1.99 | 0.45 |
| 3:C:29:ARG:HB2 | 3:C:29:ARG:HH11 | 1.80 | 0.45 |
| 3:D:132:ARG:HG3 | 3:D:132:ARG:NH1 | 2.32 | 0.45 |
| 3:D:341:GLU:C | 3:D:343:PRO:CD | 2.85 | 0.45 |
| 3:D:501:LEU:C | 3:D:503:ARG:H | 2.20 | 0.45 |
| 1:E:958:A:H1' | 1:E:960:U:C5 | 2.52 | 0.45 |
| 2:A:161:TYR:HD1 | 2:A:294:LEU:HD11 | 1.82 | 0.45 |
| 2:A:7:ALA:O | 2:A:11:LEU:HB2 | 2.17 | 0.45 |
| 2:A:88:PRO:O | 2:A:89:GLU:CB | 2.65 | 0.45 |
| 3:C:342:LEU:HD12 | 3:C:352:VAL:HG13 | 1.99 | 0.45 |
| 3:C:374:ARG:HH12 | 3:C:378:GLU:HB2 | 1.81 | 0.45 |
| 1:F:963:G:OP1 | 3:D:499:ARG:HD3 | 2.17 | 0.45 |
| 2:A:141:PHE:HD1 | 2:A:143:ILE:HD12 | 1.82 | 0.45 |
| 2:A:319:LYS:O | 2:A:320:TRP:C | 2.55 | 0.45 |
| 2:A:378:ARG:NH1 | 2:A:378:ARG:HG3 | 2.32 | 0.45 |
| 2:B:6:ARG:HB2 | 2:B:44:ASP:OD2 | 2.17 | 0.45 |
| 3:C:454:ILE:O | 3:C:458:TYR:HB2 | 2.17 | 0.45 |
| 3:C:494:LEU:HD23 | 3:C:498:LEU:HD11 | 1.98 | 0.45 |
| 1:E:930:G:H2' | 1:E:931:G:H8 | 1.82 | 0.45 |
| 2:A:49:LEU:CD1 | 2:A:59:VAL:HG11 | 2.47 | 0.45 |
| 2:A:256:HIS:HA | 2:B:365:ASN:O | 2.17 | 0.45 |
| 3:C:105:LEU:HD23 | 3:C:443:LEU:HD13 | 1.99 | 0.45 |
| 3:D:18:LEU:HD22 | 3:D:98:ILE:HG21 | 1.99 | 0.45 |
| 3:D:38:ASP:OD2 | 3:D:75:HIS:N | 2.35 | 0.45 |
| 2:B:10:PHE:CZ | 2:B:64:ALA:HB3 | 2.52 | 0.44 |
| 2:B:385:ILE:CG2 | 2:B:417:ARG:HD3 | 2.47 | 0.44 |
| 2:B:89:GLU:HA | 2:B:89:GLU:OE1 | 2.18 | 0.44 |
| 3:C:26:CYS:SG | 3:C:27:PRO:CD | 3.06 | 0.44 |
| 3:C:451:LYS:O | 3:C:455:MET:HG3 | 2.17 | 0.44 |
| 3:D:68:HIS:CE1 | 3:D:169:ASP:OD1 | 2.70 | 0.44 |
| 1:F:908:U:O2' | 1:F:947:A:H2' | 2.17 | 0.44 |
| 1:F:920:A:C6 | 1:F:948:C:N3 | 2.86 | 0.44 |
| 2:A:289:ARG:HB3 | 2:A:290:GLY:H | 1.61 | 0.44 |
| 2:A:413:ARG:HG3 | 2:A:414:GLU:N | 2.30 | 0.44 |
| 2:A:88:PRO:O | 2:A:89:GLU:HB3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:164:ILE:CD1 | 3:C:174:ARG:HB2 | 2.47 | 0.44 |
| 3:C:187:THR:O | 3:C:188:ASP:C | 2.56 | 0.44 |
| 2:A:147:ASN:ND2 | 2:B:341:ASP:N | 2.58 | 0.44 |
| 2:A:92:ASP:OD1 | 2:A:134:ASN:HB2 | 2.17 | 0.44 |
| 3:C:177:ARG:HG2 | 3:C:180:ILE:HD12 | 1.99 | 0.44 |
| 3:C:191:MET:O | 3:C:192:SER:CB | 2.64 | 0.44 |
| 3:D:46:ARG:HA | 3:D:47:PRO:HD3 | 1.80 | 0.44 |
| 2:A:160:VAL:HG13 | 2:A:171:VAL:HG11 | 1.99 | 0.44 |
| 2:A:275:THR:HG22 | 2:A:277:ASP:N | 2.11 | 0.44 |
| 2:A:38:ARG:HD3 | 2:A:48:VAL:HG23 | 1.99 | 0.44 |
| 2:B:275:THR:HG23 | 2:B:276:PRO:CD | 2.48 | 0.44 |
| 3:C:460:LEU:HD22 | 3:C:464:LEU:HD13 | 1.99 | 0.44 |
| 3:C:450:LYS:CD | 3:C:474:VAL:HG11 | 2.28 | 0.44 |
| 3:C:77:GLU:N | 3:C:77:GLU:CD | 2.71 | 0.44 |
| 3:D:399:THR:HG22 | 3:D:411:LEU:HD12 | 2.00 | 0.44 |
| 2:B:217:ILE:CG2 | 2:B:218:GLN:H | 2.31 | 0.44 |
| 2:B:307:ILE:HD13 | 2:B:318:ILE:HD13 | 2.00 | 0.44 |
| 2:B:87:ASP:OD2 | 2:B:90:LEU:HD23 | 2.16 | 0.44 |
| 3:C:454:ILE:CG2 | 3:C:460:LEU:HD12 | 2.47 | 0.44 |
| 2:A:336:LEU:HD23 | 2:A:336:LEU:HA | 1.77 | 0.44 |
| 2:A:402:VAL:C | 2:A:404:GLY:H | 2.20 | 0.44 |
| 2:B:406:THR:OG1 | 2:B:407:ASP:N | 2.51 | 0.44 |
| 3:C:242:LEU:HD12 | 3:C:245:ILE:HD12 | 1.98 | 0.44 |
| 3:C:477:PHE:HE1 | 3:C:487:THR:HA | 1.82 | 0.44 |
| 2:A:146:GLU:CD | 2:A:146:GLU:H | 2.20 | 0.44 |
| 2:A:149:LYS:HG2 | 2:A:152:TYR:CE1 | 2.52 | 0.44 |
| 2:A:280:LYS:O | 2:A:281:ILE:C | 2.55 | 0.44 |
| 2:A:417:ARG:HH11 | 2:A:417:ARG:HG2 | 1.83 | 0.44 |
| 2:A:50:LYS:HG3 | 2:A:56:ASN:ND2 | 2.32 | 0.44 |
| 3:C:132:ARG:NH2 | 5:C:935:HOH:O | 2.51 | 0.44 |
| 3:D:16:GLN:CG | 3:D:208:LEU:HD13 | 2.47 | 0.44 |
| 3:D:297:SER:OG | 3:D:374:ARG:HB2 | 2.17 | 0.44 |
| 3:D:520:ILE:C | 3:D:522:LEU:H | 2.20 | 0.44 |
| 1:E:942:G:C2 | 1:E:943:G:C8 | 3.06 | 0.44 |
| 2:A:141:PHE:CD1 | 2:A:143:ILE:HD12 | 2.52 | 0.44 |
| 2:A:98:THR:CG2 | 2:A:148:MET:HE1 | 2.48 | 0.44 |
| 2:A:68:LEU:HD22 | 2:A:71:LYS:HE2 | 1.99 | 0.44 |
| 3:C:119:LYS:O | 3:C:121:VAL:HG23 | 2.17 | 0.44 |
| 3:C:342:LEU:N | 3:C:343:PRO:CD | 2.81 | 0.44 |
| 3:C:46:ARG:O | 3:C:47:PRO:O | 2.36 | 0.44 |
| 3:C:8:LEU:HD21 | 3:C:10:MET:SD | 2.57 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:962:C:H1' | 3:D:496:TYR:CD1 | 2.53 | 0.44 |
| 2:A:334:THR:O | 2:A:335:GLY:C | 2.56 | 0.44 |
| 2:A:38:ARG:HH11 | 2:A:38:ARG:HG2 | 1.83 | 0.44 |
| 3:C:16:GLN:OE1 | 3:C:213:VAL:HG12 | 2.17 | 0.44 |
| 3:C:471:ARG:HH12 | 3:C:499:ARG:HA | 1.82 | 0.44 |
| 3:D:299:LEU:HB2 | 3:D:381:LEU:HD12 | 1.99 | 0.44 |
| 3:D:43:ARG:CG | 3:D:43:ARG:HH11 | 2.00 | 0.44 |
| 1:F:955:U:H3' | 5:F:35:HOH:O | 2.18 | 0.44 |
| 2:B:130:LEU:HD23 | 2:B:130:LEU:HA | 1.79 | 0.43 |
| 2:B:212:ASP:N | 2:B:212:ASP:OD1 | 2.36 | 0.43 |
| 2:B:217:ILE:HG23 | 2:B:218:GLN:H | 1.81 | 0.43 |
| 2:B:9:LYS:HB2 | 2:B:9:LYS:HZ3 | 1.83 | 0.43 |
| 3:C:486:ASP:C | 3:C:487:THR:HG1 | 2.21 | 0.43 |
| 3:D:104:LEU:HA | 3:D:104:LEU:HD23 | 1.86 | 0.43 |
| 3:D:305:GLY:H | 3:D:365:ASP:CB | 2.12 | 0.43 |
| 3:D:494:LEU:HD21 | 3:D:515:GLU:OE1 | 2.17 | 0.43 |
| 2:A:138:ARG:HG2 | 2:A:139:ALA:H | 1.83 | 0.43 |
| 2:A:175:HIS:HD2 | 2:A:176:GLY:N | 2.13 | 0.43 |
| 2:A:185:ALA:O | 2:A:188:SER:HB2 | 2.18 | 0.43 |
| 2:A:264:ARG:NH1 | 2:B:433:PHE:HE2 | 2.16 | 0.43 |
| 2:A:272:ALA:HA | 2:A:282:LEU:HG | 2.00 | 0.43 |
| 2:A:407:ASP:O | 2:A:409:PRO:HD3 | 2.17 | 0.43 |
| 2:A:53:ASN:OD1 | 2:A:55:TYR:HB2 | 2.18 | 0.43 |
| 2:A:60:GLU:HB3 | 3:C:112:ASP:OD1 | 2.18 | 0.43 |
| 2:B:161:TYR:C | 2:B:164:ILE:HG22 | 2.38 | 0.43 |
| 2:B:215:LEU:O | 2:B:219:CYS:HB2 | 2.17 | 0.43 |
| 2:B:308:LYS:HE3 | 2:B:362:GLN:HE21 | 1.83 | 0.43 |
| 3:C:144:THR:OG1 | 3:C:196:GLN:HG3 | 2.19 | 0.43 |
| 3:C:245:ILE:O | 3:C:249:VAL:HG23 | 2.18 | 0.43 |
| 3:C:307:ASP:HA | 3:C:366:ALA:HB2 | 1.99 | 0.43 |
| 3:C:374:ARG:NH2 | 3:C:378:GLU:HB2 | 2.34 | 0.43 |
| 3:C:82:GLU:H | 3:C:82:GLU:HG2 | 1.30 | 0.43 |
| 3:D:280:VAL:HG12 | 3:D:280:VAL:O | 2.18 | 0.43 |
| 3:D:375:VAL:O | 3:D:379:ASN:ND2 | 2.51 | 0.43 |
| 3:D:512:GLY:O | 3:D:516:LEU:HB2 | 2.18 | 0.43 |
| 3:D:517:ARG:HH21 | 3:D:521:LYS:HZ3 | 1.62 | 0.43 |
| 1:E:901:A:H1' | 3:C:240:GLN:HB3 | 1.99 | 0.43 |
| 2:A:140:VAL:CG2 | 2:A:141:PHE:H | 2.22 | 0.43 |
| 2:A:16:ILE:HG21 | 2:A:22:VAL:HG11 | 1.99 | 0.43 |
| 2:A:217:ILE:CG2 | 2:A:218:GLN:N | 2.80 | 0.43 |
| 2:B:238:THR:CG2 | 2:B:240:ASP:HB2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:385:ILE:HG12 | 2:B:413:ARG:HD3 | 1.99 | 0.43 |
| 3:C:332:GLY:O | 3:C:333:VAL:CB | 2.66 | 0.43 |
| 3:C:445:GLU:OE2 | 3:C:450:LYS:CA | 2.62 | 0.43 |
| 3:D:337:PHE:HE2 | 3:D:345:TYR:CD2 | 2.35 | 0.43 |
| 2:A:128:GLU:OE2 | 3:C:46:ARG:NH2 | 2.49 | 0.43 |
| 2:A:398:LYS:NZ | 2:A:418:GLU:O | 2.52 | 0.43 |
| 2:A:66:ILE:O | 2:A:67:GLU:HG3 | 2.18 | 0.43 |
| 2:B:64:ALA:O | 2:B:65:ARG:HB2 | 2.18 | 0.43 |
| 3:C:113:GLU:CD | 3:C:428:LEU:HD13 | 2.39 | 0.43 |
| 3:C:87:PRO:HA | 3:C:88:PRO:HD3 | 1.78 | 0.43 |
| 3:D:527:LYS:O | 3:D:528:ILE:C | 2.56 | 0.43 |
| 1:E:956:C:C2 | 1:E:957:G:C8 | 3.06 | 0.43 |
| 2:A:256:HIS:CD2 | 2:A:259:ARG:HB2 | 2.54 | 0.43 |
| 2:A:204:ARG:NH2 | 2:A:258:SER:O | 2.50 | 0.43 |
| 2:B:378:ARG:O | 2:B:381:GLN:HB3 | 2.17 | 0.43 |
| 3:C:15:HIS:N | 3:C:15:HIS:CD2 | 2.87 | 0.43 |
| 3:C:342:LEU:HD13 | 3:C:342:LEU:C | 2.38 | 0.43 |
| 3:C:410:TYR:O | 3:C:411:LEU:HD23 | 2.18 | 0.43 |
| 2:B:208:ARG:NH2 | 3:D:118:ARG:HH22 | 2.16 | 0.43 |
| 3:D:69:PHE:CE2 | 3:D:124:GLY:HA3 | 2.53 | 0.43 |
| 3:D:162:ARG:HH21 | 3:D:174:ARG:HD2 | 1.82 | 0.43 |
| 3:D:502:ARG:CZ | 3:D:508:VAL:HG22 | 2.48 | 0.43 |
| 2:B:259:ARG:NH1 | 2:B:261:ASP:OD2 | 2.51 | 0.43 |
| 3:C:28:CYS:SG | 3:C:79:CYS:HB3 | 2.59 | 0.43 |
| 3:D:517:ARG:HH21 | 3:D:521:LYS:HZ2 | 1.64 | 0.43 |
| 2:A:126:ASN:N | 2:A:127:PRO:HD3 | 2.34 | 0.43 |
| 2:A:344:ILE:CB | 2:A:345:PRO:HD3 | 2.45 | 0.43 |
| 2:A:365:ASN:ND2 | 2:A:433:PHE:HE1 | 2.17 | 0.43 |
| 2:A:58:GLY:HA3 | 3:C:113:GLU:HB3 | 2.01 | 0.43 |
| 2:B:102:VAL:HG21 | 2:B:217:ILE:HD13 | 1.99 | 0.43 |
| 2:B:259:ARG:HB3 | 2:B:261:ASP:OD1 | 2.19 | 0.43 |
| 3:C:159:ASP:HA | 3:C:182:LEU:HD22 | 2.01 | 0.43 |
| 3:C:36:GLU:OE1 | 3:C:37:PRO:HD2 | 2.19 | 0.43 |
| 3:C:451:LYS:HB3 | 5:C:915:HOH:O | 2.19 | 0.43 |
| 3:D:212:ARG:HH11 | 3:D:212:ARG:HB3 | 1.83 | 0.43 |
| 3:D:62:GLU:HA | 3:D:65:ARG:HH22 | 1.82 | 0.43 |
| 1:E:909:G:O2' | 1:E:945:G:C2' | 2.67 | 0.43 |
| 2:A:205:SER:HB2 | 2:A:207:ASP:OD1 | 2.19 | 0.43 |
| 2:A:209:PRO:HB2 | 3:C:45:LEU:HD12 | 2.00 | 0.43 |
| 2:A:222:ARG:HH11 | 2:A:222:ARG:CG | 2.22 | 0.43 |
| 2:A:307:ILE:CD1 | 2:A:318:ILE:HD13 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:256:HIS:CD2 | 2:B:259:ARG:HB2 | 2.53 | 0.43 |
| 2:B:385:ILE:CD1 | 2:B:413:ARG:HA | 2.49 | 0.43 |
| 3:C:400:ARG:HG2 | 3:C:410:TYR:HA | 2.01 | 0.43 |
| 3:D:37:PRO:HA | 3:D:74:TYR:CE2 | 2.54 | 0.43 |
| 2:B:10:PHE:HE2 | 2:B:66:ILE:CD1 | 2.31 | 0.43 |
| 3:C:244:LEU:HD12 | 3:C:247:GLU:HB3 | 2.01 | 0.43 |
| 3:C:283:VAL:O | 3:C:283:VAL:HG12 | 2.18 | 0.43 |
| 3:D:502:ARG:C | 3:D:503:ARG:HG3 | 2.39 | 0.43 |
| 2:A:406:THR:OG1 | 2:A:407:ASP:N | 2.51 | 0.43 |
| 2:B:129:LEU:HD22 | 2:B:221:VAL:HG21 | 2.01 | 0.43 |
| 2:B:188:SER:HA | 5:B:449:HOH:O | 2.19 | 0.43 |
| 2:B:173:VAL:HB | 2:B:199:PHE:CD1 | 2.54 | 0.43 |
| 2:B:226:SER:OG | 2:B:227:GLU:N | 2.51 | 0.43 |
| 2:B:399:MET:N | 2:B:416:MET:HE1 | 2.34 | 0.43 |
| 2:B:88:PRO:C | 2:B:90:LEU:H | 2.21 | 0.43 |
| 3:C:348:THR:O | 3:C:352:VAL:HG23 | 2.18 | 0.43 |
| 3:C:374:ARG:NH1 | 3:C:374:ARG:HG2 | 2.33 | 0.43 |
| 3:C:430:ARG:HH11 | 3:C:430:ARG:HB3 | 1.83 | 0.43 |
| 3:C:447:PRO:O | 3:C:451:LYS:HG3 | 2.18 | 0.43 |
| 3:D:77:GLU:N | 3:D:77:GLU:OE2 | 2.46 | 0.43 |
| 1:F:901:A:H61 | 1:F:972:U:H3 | 1.66 | 0.43 |
| 1:F:909:G:O2' | 1:F:945:G:C2' | 2.67 | 0.43 |
| 2:A:187:LEU:HG | 2:A:199:PHE:HZ | 1.84 | 0.42 |
| 2:A:380:LEU:HD23 | 2:A:380:LEU:HA | 1.87 | 0.42 |
| 1:F:907:G:C6 | 1:F:949:A:N6 | 2.88 | 0.42 |
| 2:A:20:ASP:OD1 | 2:A:72:GLY:N | 2.49 | 0.42 |
| 2:A:87:ASP:CB | 5:A:446:HOH:O | 2.66 | 0.42 |
| 2:B:335:GLY:O | 2:B:336:LEU:CB | 2.64 | 0.42 |
| 3:C:14:ILE:CD1 | 3:C:222:GLN:HE21 | 2.32 | 0.42 |
| 3:C:439:ILE:O | 3:C:441:ARG:N | 2.52 | 0.42 |
| 3:C:465:ALA:O | 3:C:469:VAL:HG23 | 2.19 | 0.42 |
| 2:B:55:TYR:HE2 | 3:D:133:THR:HB | 1.83 | 0.42 |
| 3:D:224:LEU:CD1 | 3:D:239:VAL:HG21 | 2.35 | 0.42 |
| 2:A:332:GLU:CD | 5:A:450:HOH:O | 2.57 | 0.42 |
| 2:A:24:VAL:HG21 | 2:A:49:LEU:HD11 | 2.01 | 0.42 |
| 2:B:321:HIS:O | 2:B:326:TYR:HD1 | 2.02 | 0.42 |
| 3:C:240:GLN:HG2 | 3:C:240:GLN:H | 1.55 | 0.42 |
| 3:C:331:ARG:O | 3:C:331:ARG:HG3 | 2.19 | 0.42 |
| 3:C:331:ARG:HE | 3:C:379:ASN:HB2 | 1.83 | 0.42 |
| 3:D:229:ARG:O | 3:D:230:ASP:OD1 | 2.38 | 0.42 |
| 2:A:49:LEU:HD12 | 2:A:59:VAL:CG1 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:187:LEU:CD1 | 2:B:191:LEU:HD22 | 2.50 | 0.42 |
| 2:B:97:SER:HA | 2:B:174:ALA:HB3 | 2.00 | 0.42 |
| 3:C:14:ILE:HD13 | 3:C:222:GLN:HE21 | 1.85 | 0.42 |
| 3:C:252:GLU:OE2 | 3:C:255:ARG:NH2 | 2.53 | 0.42 |
| 3:D:103:ALA:HB1 | 3:D:137:ALA:CB | 2.50 | 0.42 |
| 3:D:108:MET:SD | 3:D:154:LEU:HD23 | 2.58 | 0.42 |
| 3:D:188:ASP:HA | 3:D:189:PRO:HD3 | 1.83 | 0.42 |
| 3:D:414:LEU:HG | 3:D:415:PRO:HD2 | 2.02 | 0.42 |
| 1:E:939:C:H2' | 1:E:940:C:H6 | 1.84 | 0.42 |
| 1:F:975:C:H5' | 5:F:60:HOH:O | 2.18 | 0.42 |
| 2:A:367:ARG:HH21 | 2:A:428:THR:HG23 | 1.84 | 0.42 |
| 2:A:50:LYS:CG | 2:A:56:ASN:ND2 | 2.83 | 0.42 |
| 2:B:126:ASN:N | 2:B:127:PRO:HD3 | 2.34 | 0.42 |
| 2:B:177:THR:HB | 2:B:254:LYS:CE | 2.50 | 0.42 |
| 2:B:180:MET:CE | 2:B:233:VAL:HG13 | 2.49 | 0.42 |
| 2:B:367:ARG:HG3 | 2:B:367:ARG:HH11 | 1.85 | 0.42 |
| 2:B:34:MET:O | 2:B:36:LEU:HD12 | 2.19 | 0.42 |
| 3:C:339:THR:CB | 3:C:366:ALA:HB1 | 2.49 | 0.42 |
| 3:C:420:MET:HE3 | 3:C:420:MET:HB2 | 1.97 | 0.42 |
| 3:D:23:LYS:HD3 | 3:D:179:GLY:HA3 | 2.02 | 0.42 |
| 3:D:339:THR:CB | 3:D:366:ALA:HB1 | 2.47 | 0.42 |
| 1:F:959:C:C5 | 1:F:960:U:C4 | 3.07 | 0.42 |
| 2:A:139:ALA:O | 2:A:140:VAL:C | 2.58 | 0.42 |
| 2:A:378:ARG:HH11 | 2:A:378:ARG:HG3 | 1.85 | 0.42 |
| 2:B:251:LYS:NZ | 2:B:267:ASN:HB2 | 2.34 | 0.42 |
| 2:B:263:PHE:HB2 | 5:B:437:HOH:O | 2.18 | 0.42 |
| 2:B:290:GLY:O | 2:B:292:ASP:N | 2.53 | 0.42 |
| 2:B:318:ILE:O | 2:B:321:HIS:HB2 | 2.18 | 0.42 |
| 3:C:171:VAL:HG22 | 3:C:173:PHE:CE2 | 2.55 | 0.42 |
| 3:C:164:ILE:HD11 | 3:C:174:ARG:HB2 | 2.02 | 0.42 |
| 3:C:228:ILE:CB | 3:C:256:GLN:HG2 | 2.50 | 0.42 |
| 3:C:362:SER:HB2 | 3:C:365:ASP:OD2 | 2.19 | 0.42 |
| 3:C:430:ARG:CB | 3:C:430:ARG:CZ | 2.96 | 0.42 |
| 3:D:6:VAL:CG1 | 3:D:228:ILE:HD13 | 2.50 | 0.42 |
| 3:D:24:LEU:HD11 | 3:D:91:LEU:HD12 | 2.01 | 0.42 |
| 3:D:327:TYR:CE1 | 3:D:387:ARG:HD3 | 2.55 | 0.42 |
| 2:B:319:LYS:O | 2:B:322:LEU:N | 2.52 | 0.42 |
| 3:C:16:GLN:CG | 3:C:213:VAL:HG11 | 2.50 | 0.42 |
| 3:C:349:GLU:HA | 3:C:352:VAL:HB | 2.02 | 0.42 |
| 3:C:374:ARG:HH22 | 3:C:378:GLU:CD | 2.22 | 0.42 |
| 3:D:299:LEU:HD21 | 3:D:374:ARG:HE | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:332:GLY:O | 3:D:333:VAL:CB | 2.68 | 0.42 |
| 3:D:471:ARG:HG2 | 3:D:471:ARG:HH11 | 1.84 | 0.42 |
| 3:D:6:VAL:O | 3:D:6:VAL:HG12 | 2.20 | 0.42 |
| 2:A:148:MET:HE3 | 2:A:175:HIS:CE1 | 2.54 | 0.42 |
| 2:A:293:GLU:HA | 2:A:293:GLU:OE1 | 2.19 | 0.42 |
| 2:A:391:LEU:CB | 2:A:394:VAL:HG12 | 2.44 | 0.42 |
| 2:B:114:HIS:HA | 2:B:115:PRO:HD3 | 1.95 | 0.42 |
| 2:B:234:CYS:HB2 | 2:B:246:LEU:HD12 | 2.02 | 0.42 |
| 3:C:171:VAL:HG23 | 3:C:172:VAL:N | 2.34 | 0.42 |
| 3:C:291:ILE:HG21 | 3:C:337:PHE:CZ | 2.55 | 0.42 |
| 3:C:403:LEU:HB3 | 3:C:404:PRO:CD | 2.50 | 0.42 |
| 5:A:463:HOH:O | 3:C:64:MET:HE1 | 2.19 | 0.42 |
| 3:C:25:PHE:CE2 | 3:C:91:LEU:HD12 | 2.55 | 0.42 |
| 3:C:9:LYS:O | 3:C:227:SER:HB3 | 2.20 | 0.42 |
| 3:D:132:ARG:HH11 | 3:D:132:ARG:HG3 | 1.83 | 0.42 |
| 3:D:177:ARG:HA | 3:D:180:ILE:HD11 | 2.02 | 0.42 |
| 3:D:342:LEU:HA | 3:D:342:LEU:HD22 | 1.85 | 0.42 |
| 2:A:122:LEU:O | 2:A:126:ASN:N | 2.53 | 0.42 |
| 2:A:427:ARG:HH22 | 2:A:429:SER:HB2 | 1.81 | 0.42 |
| 2:A:8:ARG:HH22 | 2:A:9:LYS:NZ | 2.18 | 0.42 |
| 2:B:204:ARG:O | 2:B:205:SER:O | 2.38 | 0.42 |
| 2:B:312:GLY:O | 2:B:313:ILE:C | 2.57 | 0.42 |
| 2:B:356:PRO:HB2 | 2:B:399:MET:HE1 | 2.01 | 0.42 |
| 3:C:91:LEU:O | 3:C:93:PRO:HD3 | 2.20 | 0.42 |
| 3:D:217:LEU:HA | 3:D:217:LEU:HD23 | 1.84 | 0.42 |
| 3:D:372:HIS:CD2 | 3:D:373:GLU:H | 2.38 | 0.42 |
| 3:D:469:VAL:CG2 | 3:D:474:VAL:HG21 | 2.48 | 0.42 |
| 1:F:932:C:H3' | 1:F:933:U:H5'' | 2.00 | 0.42 |
| 1:F:956:C:C4 | 1:F:957:G:N7 | 2.88 | 0.42 |
| 2:A:189:PHE:HE2 | 2:A:423:GLU:HG2 | 1.81 | 0.42 |
| 2:A:272:ALA:HB2 | 2:A:281:ILE:HA | 2.01 | 0.42 |
| 2:A:385:ILE:CD1 | 2:A:413:ARG:HB2 | 2.37 | 0.42 |
| 2:B:156:THR:HG22 | 2:B:187:LEU:HD21 | 2.01 | 0.42 |
| 2:B:256:HIS:CD2 | 2:B:258:SER:H | 2.38 | 0.42 |
| 2:B:329:ILE:HB | 2:B:357:VAL:HG22 | 2.01 | 0.42 |
| 3:C:422:LEU:CD1 | 3:C:422:LEU:N | 2.79 | 0.42 |
| 3:C:498:LEU:C | 3:C:501:LEU:HB3 | 2.40 | 0.42 |
| 3:D:162:ARG:HB3 | 3:D:177:ARG:NH2 | 2.33 | 0.42 |
| 3:D:523:LEU:N | 3:D:523:LEU:HD12 | 2.35 | 0.42 |
| 2:A:306:PHE:HB2 | 2:A:396:TYR:CD1 | 2.55 | 0.41 |
| 2:B:10:PHE:CD1 | 2:B:61:ILE:HB | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:228:ILE:HD12 | 2:B:246:LEU:HD23 | 2.02 | 0.41 |
| 3:C:214:LYS:O | 3:C:219:THR:HG21 | 2.20 | 0.41 |
| 3:C:323:GLU:OE1 | 3:C:400:ARG:NH2 | 2.53 | 0.41 |
| 3:C:42:VAL:HG22 | 3:C:70:HIS:NE2 | 2.35 | 0.41 |
| 3:D:164:ILE:HD13 | 3:D:174:ARG:HB2 | 2.02 | 0.41 |
| 3:D:269:ARG:HD2 | 3:D:305:GLY:O | 2.20 | 0.41 |
| 2:B:111:GLY:O | 3:D:422:LEU:HD12 | 2.20 | 0.41 |
| 1:E:963:G:O2' | 1:E:964:C:H5' | 2.20 | 0.41 |
| 2:A:96:ILE:HG22 | 2:A:173:VAL:HG13 | 2.02 | 0.41 |
| 2:A:227:GLU:HA | 2:A:227:GLU:OE1 | 2.20 | 0.41 |
| 2:B:89:GLU:C | 2:B:90:LEU:HD22 | 2.40 | 0.41 |
| 3:C:108:MET:HG2 | 3:C:140:GLY:CA | 2.46 | 0.41 |
| 3:C:342:LEU:O | 3:C:342:LEU:HD22 | 2.20 | 0.41 |
| 3:C:422:LEU:H | 3:C:422:LEU:CD1 | 2.29 | 0.41 |
| 2:A:148:MET:CB | 2:A:179:THR:HG21 | 2.50 | 0.41 |
| 2:A:289:ARG:HG3 | 2:A:289:ARG:NH1 | 2.32 | 0.41 |
| 2:B:223:ALA:C | 2:B:225:THR:N | 2.74 | 0.41 |
| 3:C:16:GLN:CG | 3:C:213:VAL:CG1 | 2.98 | 0.41 |
| 3:C:3:TRP:CE3 | 3:C:3:TRP:HA | 2.55 | 0.41 |
| 3:D:150:LYS:C | 3:D:151:ILE:HD12 | 2.40 | 0.41 |
| 3:D:215:ARG:N | 3:D:215:ARG:HD3 | 2.36 | 0.41 |
| 3:D:350:GLU:O | 3:D:353:ARG:HG2 | 2.20 | 0.41 |
| 3:D:487:THR:C | 3:D:489:VAL:N | 2.72 | 0.41 |
| 2:A:401:TRP:CZ3 | 2:A:420:ILE:HD13 | 2.55 | 0.41 |
| 2:B:370:MET:O | 2:B:380:LEU:HD12 | 2.19 | 0.41 |
| 3:C:430:ARG:NH2 | 3:C:432:GLU:OE2 | 2.48 | 0.41 |
| 3:D:227:SER:O | 3:D:228:ILE:HG13 | 2.20 | 0.41 |
| 2:B:229:ALA:HB3 | 2:B:288:LYS:O | 2.20 | 0.41 |
| 2:B:319:LYS:HD2 | 2:B:323:ASP:OD1 | 2.20 | 0.41 |
| 3:C:83:ALA:O | 3:C:84:ASP:CB | 2.69 | 0.41 |
| 3:D:292:ILE:O | 3:D:295:ALA:HB3 | 2.20 | 0.41 |
| 3:D:342:LEU:HD11 | 3:D:347:ILE:HD12 | 2.02 | 0.41 |
| 3:D:487:THR:C | 3:D:489:VAL:H | 2.24 | 0.41 |
| 3:D:523:LEU:CD1 | 3:D:523:LEU:N | 2.83 | 0.41 |
| 2:A:138:ARG:NH1 | 2:A:140:VAL:HG12 | 2.35 | 0.41 |
| 2:A:193:THR:HG21 | 2:A:195:VAL:O | 2.20 | 0.41 |
| 2:A:283:GLU:OE1 | 2:A:285:ASN:O | 2.38 | 0.41 |
| 2:A:299:ARG:NH1 | 2:A:299:ARG:CG | 2.79 | 0.41 |
| 2:A:373:TYR:C | 2:A:377:ARG:NH1 | 2.73 | 0.41 |
| 2:B:145:SER:HB2 | 2:B:176:GLY:CA | 2.44 | 0.41 |
| 2:B:179:THR:O | 2:B:179:THR:CG2 | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:55:TYR:OH | 3:D:133:THR:HG21 | 2.21 | 0.41 |
| 3:C:127:THR:CG2 | 3:C:175:LEU:HD21 | 2.50 | 0.41 |
| 3:C:180:ILE:HA | 3:C:181:PRO:HD3 | 1.92 | 0.41 |
| 3:C:225:ASN:HD22 | 3:C:235:GLU:HB3 | 1.82 | 0.41 |
| 3:C:471:ARG:CZ | 3:C:499:ARG:HB2 | 2.51 | 0.41 |
| 3:D:24:LEU:O | 3:D:92:ASN:HB2 | 2.20 | 0.41 |
| 3:D:304:ARG:CA | 3:D:365:ASP:HB3 | 2.49 | 0.41 |
| 3:D:506:HIS:O | 3:D:506:HIS:CG | 2.73 | 0.41 |
| 1:F:914:A:C2' | 1:F:915:G:H5' | 2.51 | 0.41 |
| 3:C:105:LEU:HD11 | 3:C:444:PRO:HD2 | 2.03 | 0.41 |
| 2:A:55:TYR:HD2 | 3:C:135:LEU:HB2 | 1.85 | 0.41 |
| 3:C:15:HIS:HD2 | 3:C:221:ARG:O | 2.03 | 0.41 |
| 3:C:10:MET:HB3 | 3:C:197:LEU:HD13 | 2.03 | 0.41 |
| 3:C:405:ASP:OD2 | 3:C:407:ASN:ND2 | 2.53 | 0.41 |
| 3:D:16:GLN:O | 3:D:182:LEU:HA | 2.19 | 0.41 |
| 1:E:966:C:H2' | 1:E:967:G:C8 | 2.55 | 0.41 |
| 1:F:907:G:N1 | 1:F:949:A:C6 | 2.89 | 0.41 |
| 1:F:963:G:O2' | 1:F:964:C:H5' | 2.21 | 0.41 |
| 2:A:124:ARG:HG3 | 2:A:124:ARG:NH1 | 2.34 | 0.41 |
| 2:A:102:VAL:HG21 | 2:A:217:ILE:HG12 | 2.02 | 0.41 |
| 3:C:120:GLN:HB3 | 3:C:419:ARG:HG3 | 2.03 | 0.41 |
| 3:C:157:GLU:OE2 | 3:C:184:GLU:OE1 | 2.39 | 0.41 |
| 3:C:255:ARG:HB3 | 3:C:255:ARG:HE | 1.71 | 0.41 |
| 3:C:403:LEU:HB3 | 3:C:404:PRO:HD2 | 2.03 | 0.41 |
| 3:C:120:GLN:CB | 3:C:419:ARG:HG3 | 2.51 | 0.41 |
| 3:C:47:PRO:O | 3:C:48:THR:OG1 | 2.27 | 0.41 |
| 2:B:57:ILE:HD11 | 3:D:135:LEU:HD23 | 2.02 | 0.41 |
| 1:E:926:G:O2' | 1:E:927:C:H5' | 2.20 | 0.41 |
| 2:A:118:THR:C | 2:A:120:ASP:N | 2.73 | 0.41 |
| 2:A:204:ARG:O | 2:A:205:SER:C | 2.59 | 0.41 |
| 2:A:219:CYS:O | 2:A:274:VAL:HG11 | 2.21 | 0.41 |
| 2:B:182:TYR:O | 2:B:185:ALA:HB3 | 2.20 | 0.41 |
| 2:B:280:LYS:O | 2:B:281:ILE:C | 2.59 | 0.41 |
| 2:A:108:TYR:HD2 | 3:C:420:MET:N | 2.19 | 0.41 |
| 3:D:9:LYS:O | 3:D:227:SER:HB3 | 2.21 | 0.41 |
| 1:E:931:G:N2 | 1:E:940:C:C2 | 2.89 | 0.41 |
| 1:F:940:C:H6 | 1:F:940:C:O5' | 2.03 | 0.41 |
| 2:A:321:HIS:O | 2:A:326:TYR:HB2 | 2.21 | 0.41 |
| 2:A:36:LEU:HB2 | 2:A:48:VAL:CG1 | 2.51 | 0.41 |
| 2:A:98:THR:CG2 | 2:A:98:THR:O | 2.69 | 0.41 |
| 2:B:2:SER:N | 2:B:37:ASP:OD2 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:239:VAL:O | 3:C:239:VAL:HG12 | 2.21 | 0.41 |
| 3:C:46:ARG:NH1 | 3:C:46:ARG:CG | 2.83 | 0.41 |
| 3:D:291:ILE:HD12 | 3:D:291:ILE:N | 2.15 | 0.41 |
| 2:A:345:PRO:HB2 | 5:A:439:HOH:O | 2.19 | 0.41 |
| 2:A:7:ALA:H | 2:A:44:ASP:HB2 | 1.86 | 0.41 |
| 2:B:327:ARG:O | 2:B:355:VAL:HG13 | 2.21 | 0.41 |
| 3:C:149:VAL:CG2 | 3:C:191:MET:HE3 | 2.46 | 0.41 |
| 3:C:198:ARG:HD2 | 3:C:243:ASP:HA | 2.02 | 0.41 |
| 3:C:227:SER:C | 3:C:228:ILE:HD12 | 2.41 | 0.41 |
| 3:D:245:ILE:N | 3:D:246:PRO:CD | 2.83 | 0.41 |
| 3:D:274:GLU:C | 3:D:276:LYS:H | 2.25 | 0.41 |
| 3:D:279:ASP:O | 3:D:281:SER:N | 2.50 | 0.41 |
| 3:D:302:LYS:HZ1 | 3:D:304:ARG:HE | 1.67 | 0.41 |
| 3:D:337:PHE:HE2 | 3:D:345:TYR:HD2 | 1.69 | 0.41 |
| 1:E:968:G:O2' | 1:E:969:G:H5' | 2.21 | 0.41 |
| 2:A:312:GLY:O | 2:A:313:ILE:C | 2.56 | 0.40 |
| 2:B:210:SER:O | 2:B:211:SER:C | 2.59 | 0.40 |
| 3:C:399:THR:O | 3:C:411:LEU:HB2 | 2.21 | 0.40 |
| 3:C:445:GLU:HB2 | 3:C:449:GLU:HB2 | 2.02 | 0.40 |
| 3:C:490:ILE:O | 3:C:494:LEU:HG | 2.20 | 0.40 |
| 3:D:359:VAL:HG22 | 3:D:359:VAL:O | 2.21 | 0.40 |
| 3:D:535:ASP:O | 3:D:538:ALA:N | 2.54 | 0.40 |
| 2:A:118:THR:O | 2:A:120:ASP:N | 2.55 | 0.40 |
| 2:A:161:TYR:O | 2:A:164:ILE:HG23 | 2.21 | 0.40 |
| 2:B:162:GLY:O | 2:B:165:LYS:N | 2.53 | 0.40 |
| 2:B:234:CYS:HB2 | 2:B:246:LEU:CD1 | 2.52 | 0.40 |
| 2:B:24:VAL:O | 2:B:30:THR:HA | 2.22 | 0.40 |
| 3:C:135:LEU:HD11 | 3:C:153:ASN:HB3 | 2.02 | 0.40 |
| 3:C:223:ASP:CG | 3:C:237:LYS:HD3 | 2.42 | 0.40 |
| 3:C:237:LYS:NZ | 3:C:412:ARG:HH22 | 2.20 | 0.40 |
| 3:C:439:ILE:O | 3:C:440:ARG:C | 2.59 | 0.40 |
| 1:E:967:G:H2' | 1:E:968:G:C8 | 2.52 | 0.40 |
| 2:A:279:ILE:HG12 | 2:A:281:ILE:H | 1.87 | 0.40 |
| 2:B:109:ARG:HD2 | 2:B:109:ARG:HA | 1.88 | 0.40 |
| 2:B:161:TYR:O | 2:B:164:ILE:CG2 | 2.70 | 0.40 |
| 3:C:164:ILE:CG2 | 3:C:165:ARG:HD2 | 2.44 | 0.40 |
| 3:C:197:LEU:HD22 | 3:C:224:LEU:HD12 | 2.03 | 0.40 |
| 3:C:249:VAL:O | 3:C:253:VAL:HG23 | 2.21 | 0.40 |
| 1:E:918:G:O5' | 1:E:918:G:H8 | 2.03 | 0.40 |
| 2:A:160:VAL:O | 2:A:161:TYR:C | 2.60 | 0.40 |
| 2:A:148:MET:CE | 2:A:175:HIS:CE1 | 3.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:26:LYS:HB3 | 2:A:27:PRO:HD2 | 2.04 | 0.40 |
| 2:B:370:MET:SD | 2:B:386:PRO:HG3 | 2.61 | 0.40 |
| 2:B:380:LEU:HD21 | 2:B:386:PRO:HG3 | 2.02 | 0.40 |
| 3:C:47:PRO:O | 3:C:48:THR:CB | 2.68 | 0.40 |
| 3:D:102:ILE:HD13 | 3:D:208:LEU:CD2 | 2.51 | 0.40 |
| 3:D:15:HIS:CD2 | 3:D:184:GLU:HG2 | 2.56 | 0.40 |
| 3:D:370:VAL:CG2 | 3:D:381:LEU:HG | 2.51 | 0.40 |
| 3:D:491:ALA:C | 3:D:493:LEU:H | 2.25 | 0.40 |
| 1:E:902:G:C2 | 1:E:972:U:C2 | 3.09 | 0.40 |
| 1:F:937:G:C4 | 1:F:938:A:C8 | 3.08 | 0.40 |
| 2:A:264:ARG:NH1 | 2:B:433:PHE:CE2 | 2.89 | 0.40 |
| 2:B:140:VAL:CG1 | 2:B:141:PHE:HD2 | 2.20 | 0.40 |
| 2:B:223:ALA:C | 2:B:225:THR:H | 2.25 | 0.40 |
| 2:B:254:LYS:HB3 | 5:B:440:HOH:O | 2.22 | 0.40 |
| 3:C:273:VAL:CG1 | 3:C:385:ILE:HG23 | 2.51 | 0.40 |
| 3:C:469:VAL:HG22 | 3:C:474:VAL:HG21 | 2.03 | 0.40 |
| 3:D:499:ARG:CG | 3:D:499:ARG:HH11 | 2.34 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 3:C:169:ASP:OD2 | 3:D:268:GLU:OE1[4_556] | 2.08 | 0.12 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | A | 420/435 (97%) | 349 (83%) | 50 (12%) | 21 (5%) | 2 | 14 |
| 2 | B | 420/435 (97%) | 337 (80%) | 65 (16%) | 18 (4%) | 2 | 17 |
| 3 | C | 479/619 (77%) | 411 (86%) | 52 (11%) | 16 (3%) | 4 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 3 | D | 516/619 (83%) | 436 (84%) | 55 (11%) | 25 (5%) | 2 | 15 |
| All | All | 1835/2108 (87%) | 1533 (84%) | 222 (12%) | 80 (4%) | 2 | 16 |

All (80) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 13 | SER |
| 2 | A | 115 | PRO |
| 2 | A | 140 | VAL |
| 2 | A | 281 | ILE |
| 2 | B | 44 | ASP |
| 2 | B | 115 | PRO |
| 2 | B | 140 | VAL |
| 2 | B | 226 | SER |
| 2 | B | 291 | SER |
| 3 | C | 47 | PRO |
| 3 | C | 217 | LEU |
| 3 | C | 333 | VAL |
| 3 | D | 47 | PRO |
| 3 | D | 219 | THR |
| 3 | D | 296 | GLU |
| 3 | D | 333 | VAL |
| 3 | D | 532 | ALA |
| 2 | A | 5 | GLY |
| 2 | A | 44 | ASP |
| 2 | A | 65 | ARG |
| 2 | A | 103 | ALA |
| 2 | A | 116 | ALA |
| 2 | A | 178 | ASP |
| 2 | A | 288 | LYS |
| 2 | A | 289 | ARG |
| 2 | A | 291 | SER |
| 2 | A | 335 | GLY |
| 2 | B | 13 | SER |
| 2 | B | 65 | ARG |
| 2 | B | 116 | ALA |
| 2 | B | 205 | SER |
| 2 | B | 281 | ILE |
| 2 | B | 289 | ARG |
| 2 | B | 335 | GLY |
| 3 | C | 296 | GLU |
| 3 | C | 316 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 487 | THR |
| 3 | D | 217 | LEU |
| 3 | D | 316 | PRO |
| 3 | D | 528 | ILE |
| 2 | A | 70 | GLU |
| 2 | A | 85 | ALA |
| 2 | A | 226 | SER |
| 2 | B | 5 | GLY |
| 2 | B | 62 | SER |
| 2 | B | 294 | LEU |
| 3 | C | 60 | PHE |
| 3 | C | 440 | ARG |
| 3 | D | 60 | PHE |
| 3 | D | 192 | SER |
| 3 | D | 280 | VAL |
| 3 | D | 339 | THR |
| 3 | D | 507 | ASP |
| 3 | D | 513 | LEU |
| 3 | D | 521 | LYS |
| 2 | A | 51 | LEU |
| 2 | A | 86 | GLU |
| 3 | C | 219 | THR |
| 3 | C | 339 | THR |
| 3 | C | 432 | GLU |
| 3 | D | 139 | ASP |
| 3 | D | 334 | SER |
| 3 | D | 487 | THR |
| 2 | B | 70 | GLU |
| 2 | B | 103 | ALA |
| 3 | C | 2 | ASP |
| 3 | C | 212 | ARG |
| 3 | C | 334 | SER |
| 3 | D | 413 | PRO |
| 3 | D | 508 | VAL |
| 3 | D | 525 | VAL |
| 3 | D | 533 | LEU |
| 2 | A | 72 | GLY |
| 2 | A | 88 | PRO |
| 3 | C | 396 | PRO |
| 2 | B | 88 | PRO |
| 3 | C | 280 | VAL |
| 3 | D | 342 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 438 | GLY |
| 3 | D | 218 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2 | A | 356/367 (97%) | 320 (90%) | 36 (10%) | 7 | 27 |
| 2 | B | 358/367 (98%) | 325 (91%) | 33 (9%) | 9 | 31 |
| 3 | C | 423/529 (80%) | 388 (92%) | 35 (8%) | 11 | 37 |
| 3 | D | 452/529 (85%) | 408 (90%) | 44 (10%) | 8 | 29 |
| All | All | 1589/1792 (89%) | 1441 (91%) | 148 (9%) | 9 | 31 |

All (148) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 9 | LYS |
| 2 | A | 10 | PHE |
| 2 | A | 11 | LEU |
| 2 | A | 30 | THR |
| 2 | A | 43 | ASP |
| 2 | A | 57 | ILE |
| 2 | A | 59 | VAL |
| 2 | A | 96 | ILE |
| 2 | A | 114 | HIS |
| 2 | A | 123 | LEU |
| 2 | A | 146 | GLU |
| 2 | A | 164 | ILE |
| 2 | A | 178 | ASP |
| 2 | A | 212 | ASP |
| 2 | A | 217 | ILE |
| 2 | A | 222 | ARG |
| 2 | A | 227 | GLU |
| 2 | A | 230 | GLU |
| 2 | A | 253 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 254 | LYS |
| 2 | A | 259 | ARG |
| 2 | A | 289 | ARG |
| 2 | A | 292 | ASP |
| 2 | A | 302 | GLU |
| 2 | A | 303 | ARG |
| 2 | A | 316 | ASP |
| 2 | A | 327 | ARG |
| 2 | A | 371 | ASN |
| 2 | A | 375 | THR |
| 2 | A | 394 | VAL |
| 2 | A | 406 | THR |
| 2 | A | 413 | ARG |
| 2 | A | 418 | GLU |
| 2 | A | 423 | GLU |
| 2 | A | 425 | ASN |
| 2 | A | 434 | ARG |
| 2 | B | 9 | LYS |
| 2 | B | 17 | ASP |
| 2 | B | 29 | VAL |
| 2 | B | 30 | THR |
| 2 | B | 47 | ILE |
| 2 | B | 57 | ILE |
| 2 | B | 59 | VAL |
| 2 | B | 87 | ASP |
| 2 | B | 94 | SER |
| 2 | B | 117 | PHE |
| 2 | B | 148 | MET |
| 2 | B | 177 | THR |
| 2 | B | 178 | ASP |
| 2 | B | 187 | LEU |
| 2 | B | 195 | VAL |
| 2 | B | 203 | GLN |
| 2 | B | 205 | SER |
| 2 | B | 222 | ARG |
| 2 | B | 250 | VAL |
| 2 | B | 252 | VAL |
| 2 | B | 259 | ARG |
| 2 | B | 264 | ARG |
| 2 | B | 285 | ASN |
| 2 | B | 293 | GLU |
| 2 | B | 297 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 334 | THR |
| 2 | B | 346 | VAL |
| 2 | B | 369 | ASN |
| 2 | B | 377 | ARG |
| 2 | B | 406 | THR |
| 2 | B | 425 | ASN |
| 2 | B | 427 | ARG |
| 2 | B | 434 | ARG |
| 3 | C | 15 | HIS |
| 3 | C | 29 | ARG |
| 3 | C | 40 | ASP |
| 3 | C | 46 | ARG |
| 3 | C | 78 | THR |
| 3 | C | 79 | CYS |
| 3 | C | 82 | GLU |
| 3 | C | 86 | GLU |
| 3 | C | 89 | HIS |
| 3 | C | 139 | ASP |
| 3 | C | 146 | GLN |
| 3 | C | 150 | LYS |
| 3 | C | 165 | ARG |
| 3 | C | 171 | VAL |
| 3 | C | 177 | ARG |
| 3 | C | 182 | LEU |
| 3 | C | 186 | THR |
| 3 | C | 190 | SER |
| 3 | C | 194 | PRO |
| 3 | C | 195 | GLN |
| 3 | C | 197 | LEU |
| 3 | C | 228 | ILE |
| 3 | C | 233 | ARG |
| 3 | C | 275 | ASP |
| 3 | C | 282 | GLU |
| 3 | C | 286 | ASP |
| 3 | C | 319 | ARG |
| 3 | C | 337 | PHE |
| 3 | C | 345 | TYR |
| 3 | C | 365 | ASP |
| 3 | C | 374 | ARG |
| 3 | C | 397 | GLU |
| 3 | C | 476 | GLU |
| 3 | C | 501 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 502 | ARG |
| 3 | D | 26 | CYS |
| 3 | D | 31 | GLU |
| 3 | D | 60 | PHE |
| 3 | D | 64 | MET |
| 3 | D | 78 | THR |
| 3 | D | 106 | LEU |
| 3 | D | 123 | ASP |
| 3 | D | 127 | THR |
| 3 | D | 133 | THR |
| 3 | D | 146 | GLN |
| 3 | D | 154 | LEU |
| 3 | D | 166 | GLU |
| 3 | D | 167 | THR |
| 3 | D | 186 | THR |
| 3 | D | 198 | ARG |
| 3 | D | 207 | ILE |
| 3 | D | 209 | ARG |
| 3 | D | 212 | ARG |
| 3 | D | 215 | ARG |
| 3 | D | 224 | LEU |
| 3 | D | 248 | ILE |
| 3 | D | 250 | GLU |
| 3 | D | 286 | ASP |
| 3 | D | 292 | ILE |
| 3 | D | 298 | VAL |
| 3 | D | 327 | TYR |
| 3 | D | 342 | LEU |
| 3 | D | 345 | TYR |
| 3 | D | 355 | LEU |
| 3 | D | 363 | GLN |
| 3 | D | 365 | ASP |
| 3 | D | 367 | VAL |
| 3 | D | 384 | VAL |
| 3 | D | 405 | ASP |
| 3 | D | 434 | ASP |
| 3 | D | 453 | ARG |
| 3 | D | 464 | LEU |
| 3 | D | 472 | ASN |
| 3 | D | 499 | ARG |
| 3 | D | 502 | ARG |
| 3 | D | 504 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 518 | ASP |
| 3 | D | 524 | GLU |
| 3 | D | 529 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 4 | GLN |
| 2 | A | 56 | ASN |
| 2 | A | 147 | ASN |
| 2 | A | 175 | HIS |
| 2 | A | 203 | GLN |
| 2 | A | 218 | GLN |
| 2 | A | 256 | HIS |
| 2 | A | 338 | HIS |
| 2 | A | 362 | GLN |
| 2 | A | 371 | ASN |
| 2 | A | 405 | GLN |
| 2 | B | 46 | HIS |
| 2 | B | 56 | ASN |
| 2 | B | 134 | ASN |
| 2 | B | 175 | HIS |
| 2 | B | 203 | GLN |
| 2 | B | 218 | GLN |
| 2 | B | 256 | HIS |
| 2 | B | 285 | ASN |
| 2 | B | 362 | GLN |
| 2 | B | 369 | ASN |
| 2 | B | 405 | GLN |
| 2 | B | 425 | ASN |
| 3 | C | 70 | HIS |
| 3 | C | 73 | ASN |
| 3 | C | 115 | HIS |
| 3 | C | 126 | ASN |
| 3 | C | 131 | GLN |
| 3 | C | 146 | GLN |
| 3 | C | 195 | GLN |
| 3 | C | 222 | GLN |
| 3 | C | 225 | ASN |
| 3 | C | 267 | GLN |
| 3 | C | 372 | HIS |
| 3 | C | 379 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 442 | ASN |
| 3 | D | 15 | HIS |
| 3 | D | 39 | HIS |
| 3 | D | 68 | HIS |
| 3 | D | 70 | HIS |
| 3 | D | 73 | ASN |
| 3 | D | 115 | HIS |
| 3 | D | 146 | GLN |
| 3 | D | 203 | GLN |
| 3 | D | 222 | GLN |
| 3 | D | 267 | GLN |
| 3 | D | 372 | HIS |
| 3 | D | 379 | ASN |
| 3 | D | 393 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1 | E | 71/74 (95%) | 16 (22%) | 1 (1%) |
| 1 | F | 73/74 (98%) | 19 (26%) | 4 (5%) |
| All | All | 144/148 (97%) | 35 (24%) | 5 (3%) |

All (35) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 908 | U |
| 1 | E | 909 | G |
| 1 | E | 910 | G |
| 1 | E | 917 | G |
| 1 | E | 920 | A |
| 1 | E | 923 | C |
| 1 | E | 933 | U |
| 1 | E | 934 | U |
| 1 | E | 935 | U |
| 1 | E | 936 | G |
| 1 | E | 942 | G |
| 1 | E | 947 | A |
| 1 | E | 948 | C |
| 1 | E | 959 | C |
| 1 | E | 961 | C |
| 1 | E | 973 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 905 | C |
| 1 | F | 908 | U |
| 1 | F | 909 | G |
| 1 | F | 910 | G |
| 1 | F | 912 | G |
| 1 | F | 917 | G |
| 1 | F | 919 | U |
| 1 | F | 920 | A |
| 1 | F | 923 | C |
| 1 | F | 933 | U |
| 1 | F | 934 | U |
| 1 | F | 935 | U |
| 1 | F | 936 | G |
| 1 | F | 947 | A |
| 1 | F | 948 | C |
| 1 | F | 957 | G |
| 1 | F | 959 | C |
| 1 | F | 960 | U |
| 1 | F | 961 | C |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 958 | A |
| 1 | F | 907 | G |
| 1 | F | 909 | G |
| 1 | F | 958 | A |
| 1 | F | 960 | U |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | E | 72/74 (97%) | 0.29 | 5 (6%) 16 9 | 83, 122, 174, 192 | 0 |
| 1 | F | 74/74 (100%) | 0.33 | 4 (5%) 25 13 | 55, 88, 139, 152 | 0 |
| 2 | A | 424/435 (97%) | -0.48 | 4 (0%) 84 75 | 7, 33, 81, 113 | 0 |
| 2 | B | 424/435 (97%) | -0.49 | 0 100 100 | 12, 36, 68, 93 | 0 |
| 3 | C | 485/619 (78%) | -0.07 | 12 (2%) 57 42 | 23, 76, 133, 143 | 0 |
| 3 | D | 522/619 (84%) | -0.43 | 4 (0%) 86 78 | 9, 41, 102, 122 | 0 |
| All | All | 2001/2256 (88%) | -0.31 | 29 (1%) 75 63 | 7, 46, 127, 192 | 0 |

All (29) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 935 | U | 13.7 |
| 3 | D | 511 | LEU | 8.4 |
| 1 | E | 934 | U | 6.5 |
| 3 | C | 359 | VAL | 6.4 |
| 1 | E | 936 | G | 5.3 |
| 3 | C | 355 | LEU | 3.8 |
| 1 | E | 920 | A | 3.7 |
| 3 | C | 1 | MET | 3.6 |
| 2 | A | 113 | VAL | 3.1 |
| 3 | C | 490 | ILE | 2.7 |
| 1 | F | 920 | A | 2.7 |
| 1 | F | 917 | G | 2.7 |
| 3 | C | 277 | ILE | 2.5 |
| 2 | A | 33 | GLY | 2.5 |
| 2 | A | 32 | GLU | 2.5 |
| 3 | C | 2 | ASP | 2.5 |
| 3 | C | 294 | SER | 2.4 |
| 2 | A | 111 | GLY | 2.3 |
| 3 | D | 507 | ASP | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | C | 487 | THR | 2.2 |
| 3 | C | 226 | ILE | 2.2 |
| 3 | C | 301 | VAL | 2.2 |
| 3 | D | 535 | ASP | 2.2 |
| 3 | D | 288 | GLU | 2.2 |
| 3 | C | 358 | ALA | 2.1 |
| 1 | F | 926 | G | 2.1 |
| 3 | C | 356 | ARG | 2.1 |
| 1 | F | 934 | U | 2.1 |
| 1 | E | 901 | A | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4 | ZN | D | 1900 | 1/1 | 1.00 | 0.13 | 35,35,35,35 | 0 |
| 4 | ZN | C | 900 | 1/1 | 1.00 | 0.14 | 41,41,41,41 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.