



Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 01:42 AM EST

PDB ID : 8G9U
EMDB ID : EMD-29879
Title : Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3
for Genome Editing Applications
Authors : Hu, C.; Nam, K.H.; Ke, A.
Deposited on : 2023-02-22
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

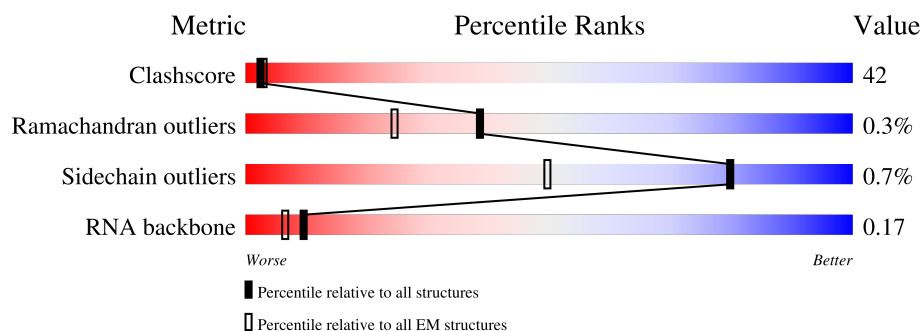
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | P | 771 | |
| 2 | A | 283 | |
| 2 | B | 283 | |
| 2 | C | 283 | |
| 2 | D | 283 | |
| 2 | E | 283 | |
| 2 | F | 283 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | M | 283 | |
| 3 | G | 124 | |
| 3 | I | 124 | |
| 3 | J | 124 | |
| 4 | H | 582 | |
| 5 | K | 43 | |
| 6 | L | 53 | |
| 7 | N | 205 | |
| 8 | O | 20 | |
| 9 | Q | 20 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11 | PO4 | P | 803 | - | - | X | - |
| 11 | PO4 | P | 804 | - | - | X | - |
| 11 | PO4 | Q | 101 | - | - | X | - |

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 33546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cas3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | P | 757 | Total | C | N | O | S | 1 | 0 |
| | | | 5855 | 3716 | 1037 | 1084 | 18 | | |

- Molecule 2 is a protein called CRISPR-associated protein, Csd2 family.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | A | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2261 | 1408 | 406 | 436 | 11 | | |
| 2 | B | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2261 | 1408 | 406 | 436 | 11 | | |
| 2 | D | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2261 | 1408 | 406 | 436 | 11 | | |
| 2 | C | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2261 | 1408 | 406 | 436 | 11 | | |
| 2 | E | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2261 | 1408 | 406 | 436 | 11 | | |
| 2 | F | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2173 | 1360 | 391 | 411 | 11 | | |
| 2 | M | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2110 | 1318 | 379 | 402 | 11 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 284 | GLY | - | expression tag | UNP D0W8X6 |
| B | 284 | GLY | - | expression tag | UNP D0W8X6 |
| D | 284 | GLY | - | expression tag | UNP D0W8X6 |
| C | 284 | GLY | - | expression tag | UNP D0W8X6 |
| E | 284 | GLY | - | expression tag | UNP D0W8X6 |
| F | 284 | GLY | - | expression tag | UNP D0W8X6 |
| M | 284 | GLY | - | expression tag | UNP D0W8X6 |

- Molecule 3 is a protein called Phage associated protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | I | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 646 | 180 | 179 | 2 | | |
| 3 | G | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 646 | 180 | 179 | 2 | | |
| 3 | J | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 646 | 180 | 179 | 2 | | |

- Molecule 4 is a protein called CRISPR-associated protein, Csd1 family.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | H | 582 | Total | C | N | O | S | 0 | 0 |
| | | | 4555 | 2889 | 800 | 849 | 17 | | |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| H | 190 | ALA | VAL | conflict | UNP D0W8X5 |
| H | 239 | ALA | ILE | conflict | UNP D0W8X5 |
| H | 242 | ILE | VAL | conflict | UNP D0W8X5 |
| H | 260 | GLY | SER | conflict | UNP D0W8X5 |
| H | 271 | THR | ALA | conflict | UNP D0W8X5 |
| H | 296 | ASN | LYS | conflict | UNP D0W8X5 |
| H | 299 | ALA | GLU | conflict | UNP D0W8X5 |
| H | 306 | ALA | THR | conflict | UNP D0W8X5 |
| H | 317 | CYS | GLN | conflict | UNP D0W8X5 |
| H | 322 | GLU | LYS | conflict | UNP D0W8X5 |
| H | 323 | ASP | GLU | conflict | UNP D0W8X5 |

- Molecule 5 is a RNA chain called crRNA (43-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5 | K | 43 | Total | C | N | O | P | 0 | 0 |
| | | | 916 | 408 | 161 | 304 | 43 | | |

- Molecule 6 is a DNA chain called Traget strand DNA (53-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6 | L | 53 | Total | C | N | O | P | 0 | 0 |
| | | | 1093 | 515 | 211 | 314 | 53 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|---------------|
| L | 7 | DA | - | expression tag | GB 1394359882 |
| L | 8 | DG | - | expression tag | GB 1394359882 |

- Molecule 7 is a protein called pre-crRNA processing endonuclease.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | N | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1674 | 1067 | 289 | 306 | 12 | | |

- Molecule 8 is a DNA chain called proximal nontarget strand DNA (5'-D(P*AP*TP*GP*A P*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 8 | O | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 414 | 198 | 87 | 109 | 20 | | |

- Molecule 9 is a DNA chain called Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*AP*TP*TP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 9 | Q | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 408 | 200 | 64 | 124 | 20 | | |

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 10 | P | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).

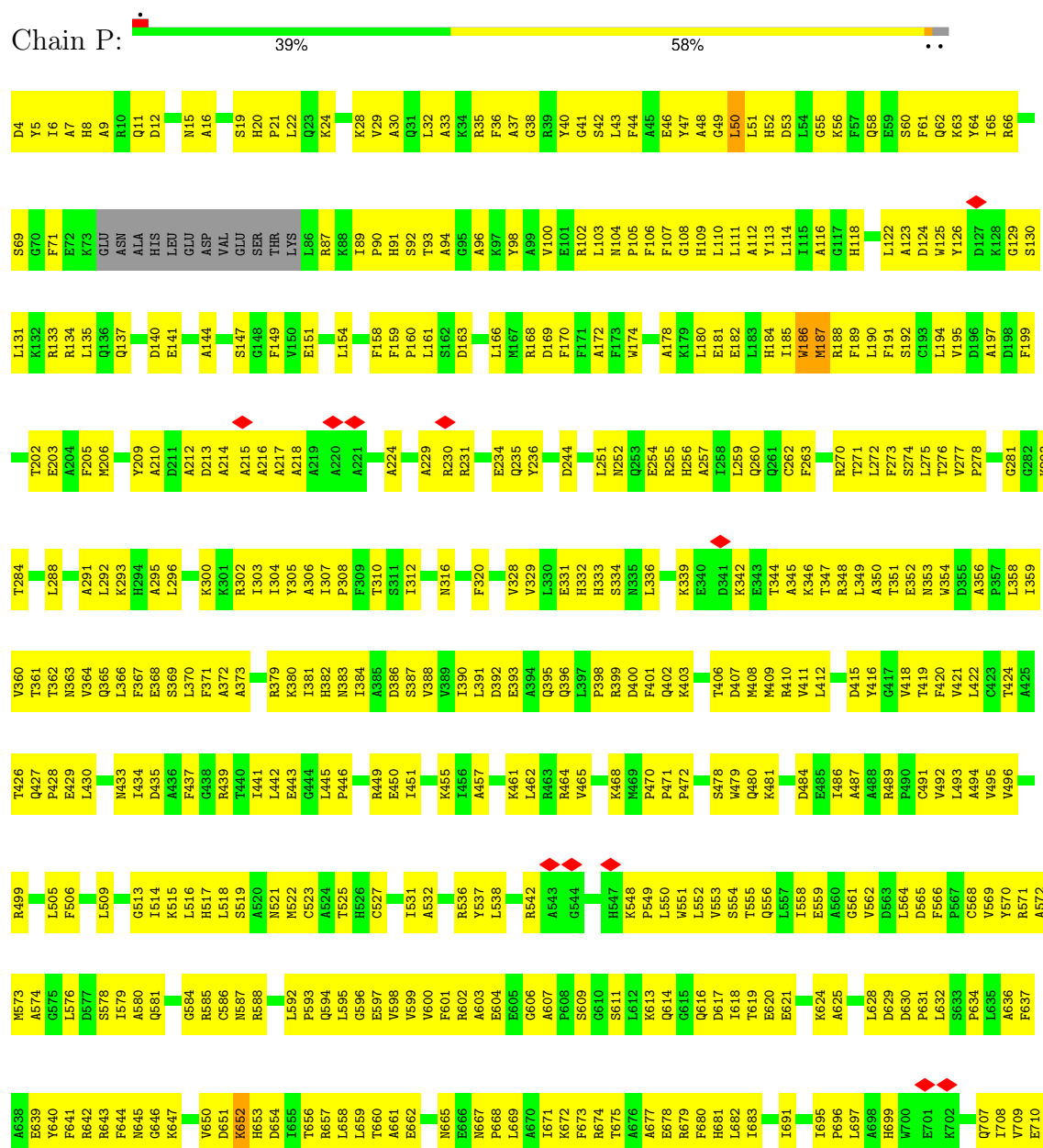


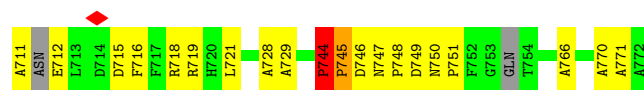
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 11 | P | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 11 | P | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 11 | O | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 11 | Q | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |

3 Residue-property plots

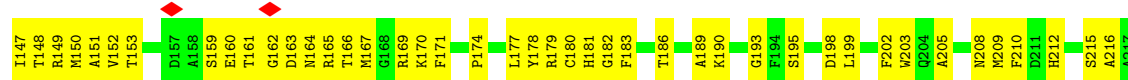
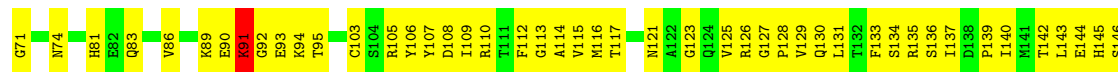
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Cas3

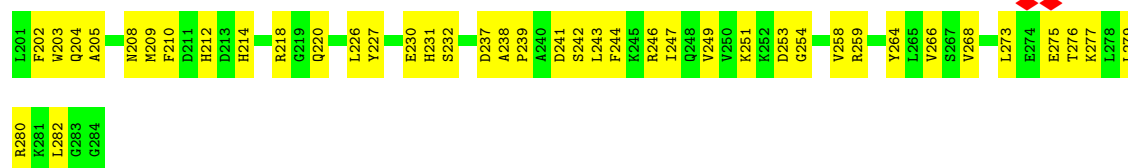
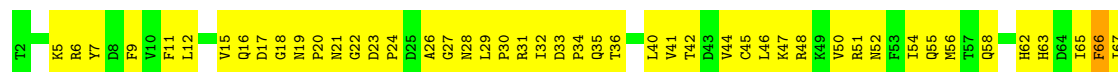




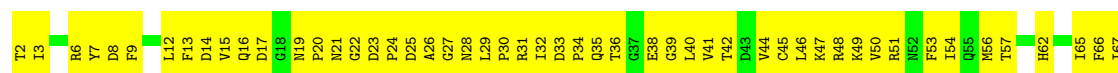
- Molecule 2: CRISPR-associated protein, Csd2 family

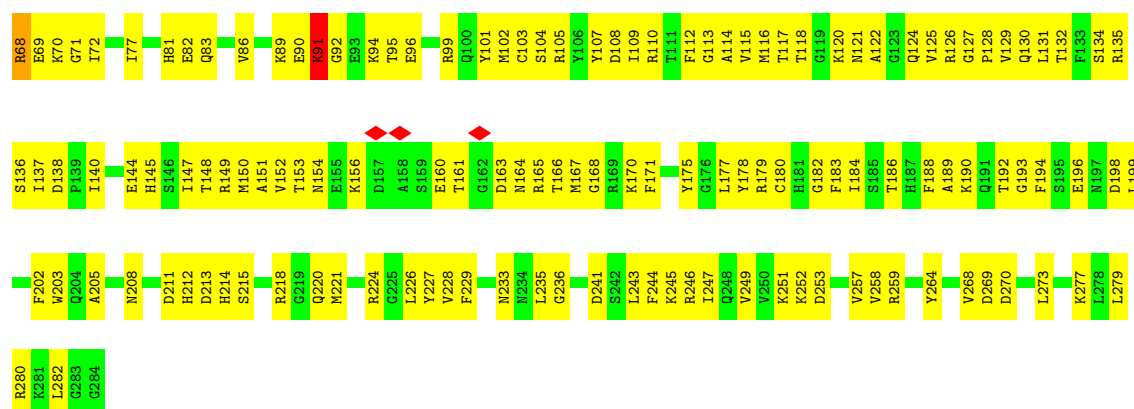


- Molecule 2: CRISPR-associated protein, Csd2 family



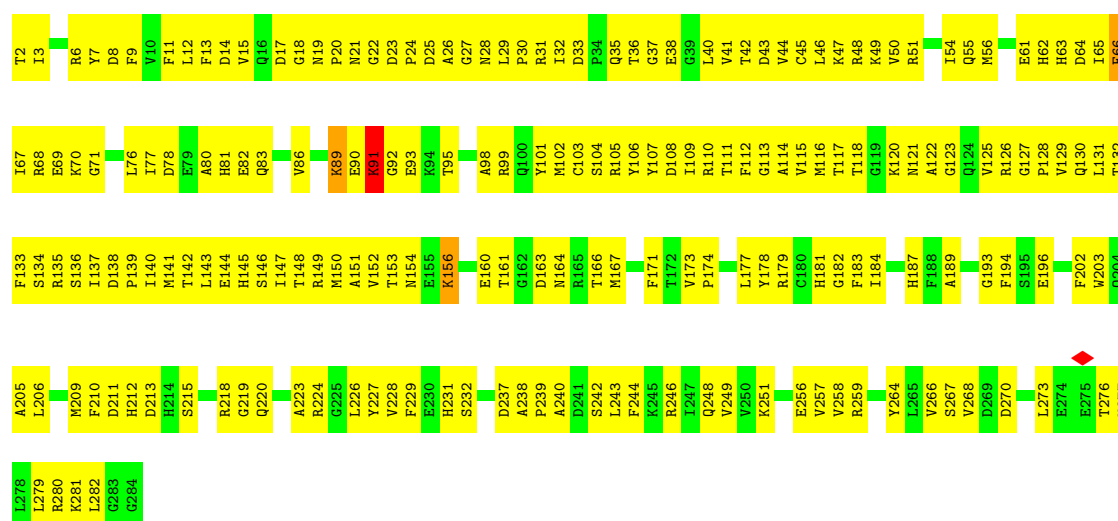
- Molecule 2: CRISPR-associated protein, Csd2 family





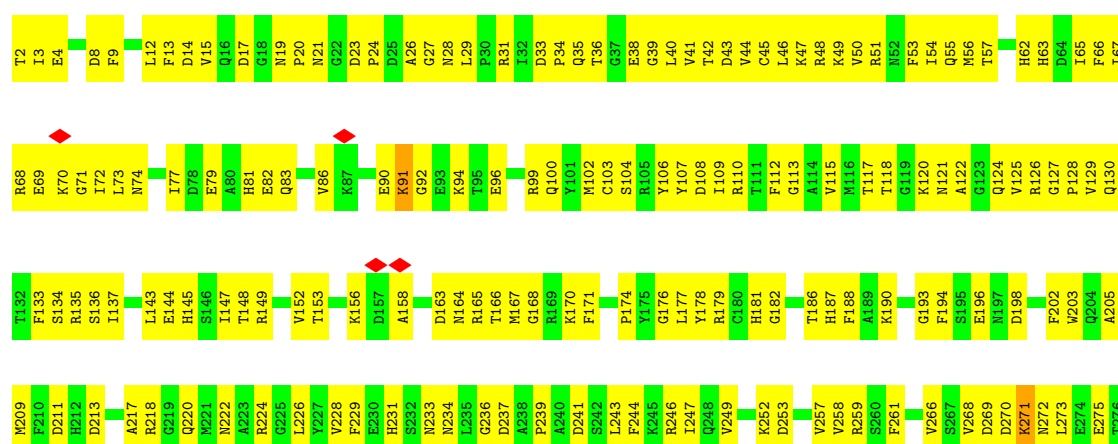
• Molecule 2: CRISPR-associated protein, Csd2 family

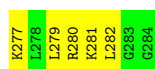
Chain C: 31% 68%



• Molecule 2: CRISPR-associated protein, Csd2 family

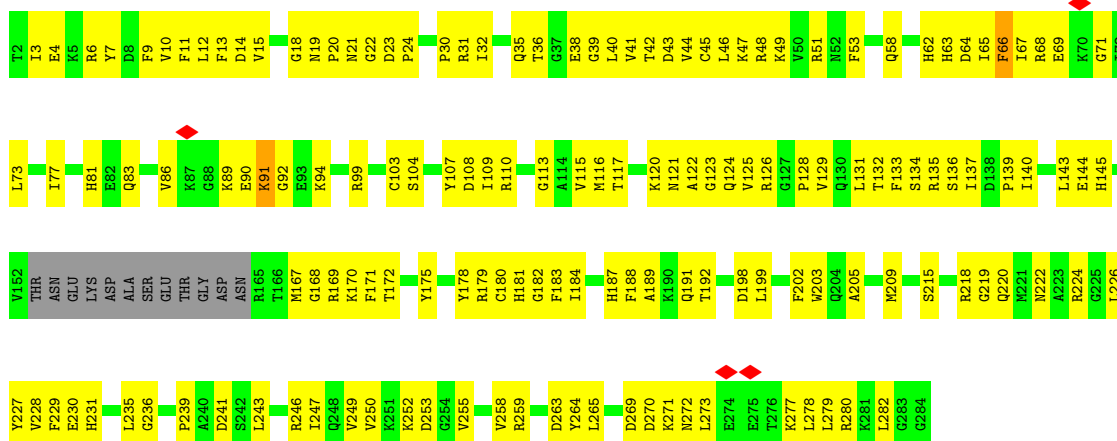
Chain E: 38% 61%





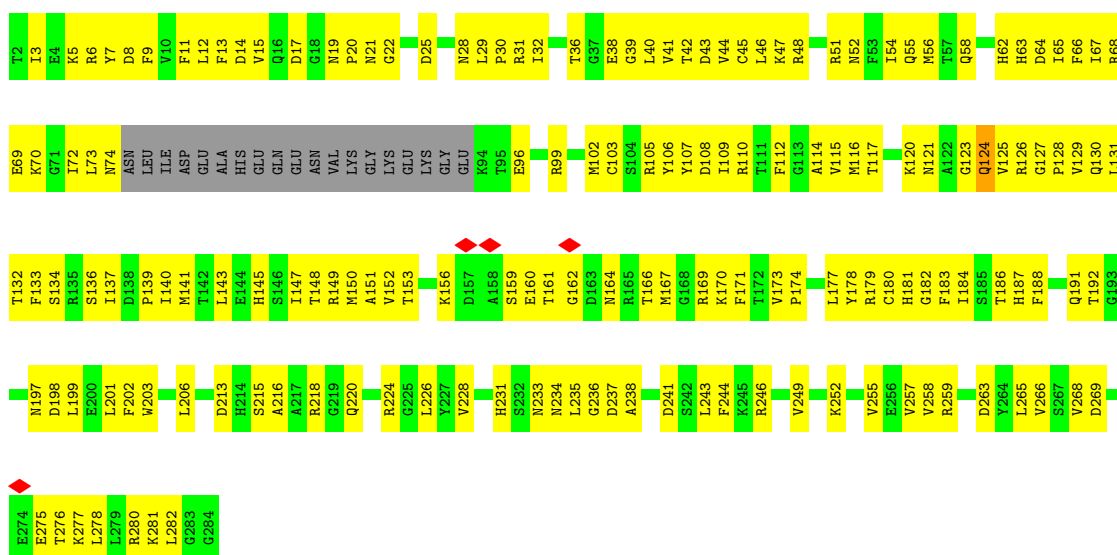
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain F: 42% 53%



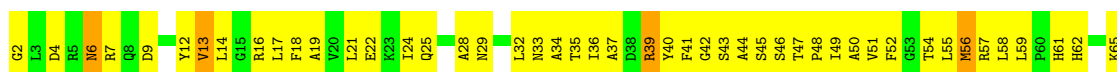
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain M: 35% 58% 7%



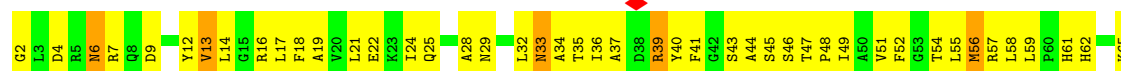
• Molecule 3: Phage associated protein

Chain I: 31% 64% 6%

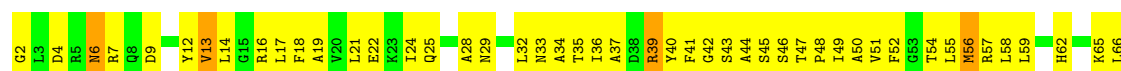




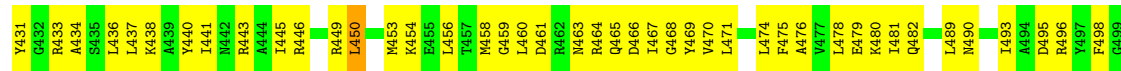
• Molecule 3: Phage associated protein

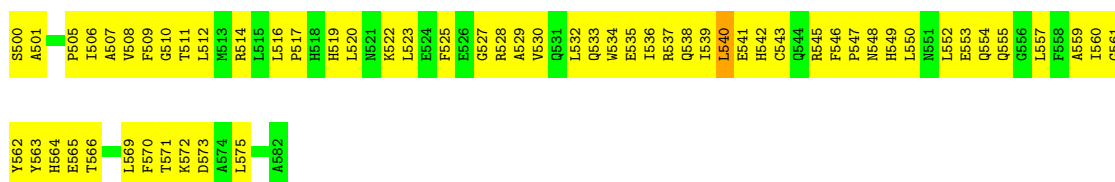


• Molecule 3: Phage associated protein

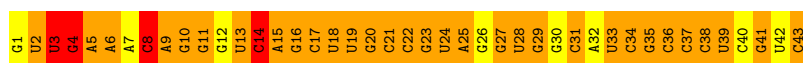


• Molecule 4: CRISPR-associated protein, Csd1 family





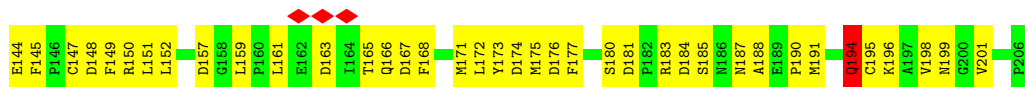
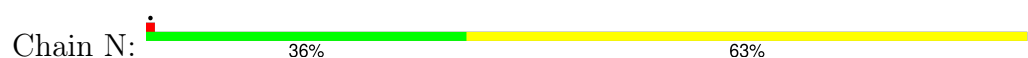
• Molecule 5: crRNA (43-MER)



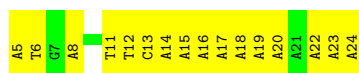
• Molecule 6: Target strand DNA (53-MER)



• Molecule 7: pre-crRNA processing endonuclease



• Molecule 8: proximal nontarget strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*A P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



• Molecule 9: Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*AP*TP*TP*TP*A)-3')



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 307088 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 67000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.947 | Depositor |
| Minimum map value | -0.276 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.026 | Depositor |
| Recommended contour level | 0.111 | Depositor |
| Map size (Å) | 381.30002, 381.30002, 381.30002 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.271, 1.271, 1.271 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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 | P | 0.38 | 1/5983 (0.0%) | 0.56 | 2/8111 (0.0%) |
| 2 | A | 0.63 | 0/2303 | 0.69 | 2/3101 (0.1%) |
| 2 | B | 0.61 | 0/2303 | 0.65 | 0/3101 |
| 2 | C | 0.61 | 0/2303 | 0.63 | 0/3101 |
| 2 | D | 0.62 | 0/2303 | 0.65 | 0/3101 |
| 2 | E | 0.55 | 0/2303 | 0.62 | 0/3101 |
| 2 | F | 0.40 | 0/2214 | 0.56 | 0/2979 |
| 2 | M | 0.58 | 0/2150 | 0.61 | 0/2896 |
| 3 | G | 0.58 | 0/1030 | 0.67 | 1/1392 (0.1%) |
| 3 | I | 0.58 | 0/1030 | 0.67 | 1/1392 (0.1%) |
| 3 | J | 0.58 | 0/1030 | 0.67 | 1/1392 (0.1%) |
| 4 | H | 0.53 | 0/4644 | 0.64 | 2/6277 (0.0%) |
| 5 | K | 1.20 | 0/1022 | 1.17 | 9/1591 (0.6%) |
| 6 | L | 1.26 | 1/1228 (0.1%) | 0.91 | 0/1894 |
| 7 | N | 0.51 | 0/1712 | 0.64 | 1/2307 (0.0%) |
| 8 | O | 0.78 | 0/468 | 0.83 | 0/719 |
| 9 | Q | 0.78 | 0/455 | 1.04 | 0/700 |
| All | All | 0.61 | 2/34481 (0.0%) | 0.68 | 19/47155 (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 | P | 0 | 4 |
| 2 | A | 0 | 2 |
| 2 | B | 0 | 2 |
| 2 | C | 0 | 2 |
| 2 | D | 0 | 1 |
| 2 | E | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | F | 0 | 1 |
| 2 | M | 0 | 1 |
| 3 | G | 0 | 1 |
| 3 | I | 0 | 1 |
| 3 | J | 0 | 1 |
| 4 | H | 0 | 5 |
| 7 | N | 0 | 1 |
| All | All | 0 | 23 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | P | 186 | TRP | CB-CG | -5.91 | 1.39 | 1.50 |
| 6 | L | 46 | DT | C3'-O3' | -5.64 | 1.36 | 1.44 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | A | 22 | GLY | C-N-CA | -7.91 | 101.94 | 121.70 |
| 5 | K | 14 | C | N1-C2-O2 | 7.54 | 123.42 | 118.90 |
| 2 | A | 23 | ASP | CB-CG-OD2 | 7.07 | 124.66 | 118.30 |
| 5 | K | 28 | U | O5'-P-OP2 | -7.00 | 99.40 | 105.70 |
| 5 | K | 8 | C | N1-C2-O2 | 6.99 | 123.09 | 118.90 |
| 5 | K | 14 | C | N3-C2-O2 | -6.74 | 117.18 | 121.90 |
| 5 | K | 8 | C | N3-C2-O2 | -6.47 | 117.37 | 121.90 |
| 4 | H | 540 | LEU | CB-CG-CD1 | -6.21 | 100.44 | 111.00 |
| 5 | K | 3 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 5 | K | 3 | U | C2-N1-C1' | 6.08 | 125.00 | 117.70 |
| 1 | P | 187 | MET | CG-SD-CE | -5.92 | 90.72 | 100.20 |
| 5 | K | 4 | G | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 4 | H | 207 | LEU | CB-CG-CD1 | -5.72 | 101.28 | 111.00 |
| 7 | N | 195 | CYS | N-CA-C | -5.62 | 95.83 | 111.00 |
| 5 | K | 3 | U | N1-C2-O2 | 5.61 | 126.72 | 122.80 |
| 1 | P | 50 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 3 | J | 95 | LEU | CB-CG-CD2 | -5.08 | 102.37 | 111.00 |
| 3 | I | 95 | LEU | CB-CG-CD2 | -5.08 | 102.37 | 111.00 |
| 3 | G | 95 | LEU | CB-CG-CD2 | -5.07 | 102.38 | 111.00 |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | A | 22 | GLY | Peptide |
| 2 | A | 26 | ALA | Peptide |
| 2 | B | 66 | PHE | Peptide |
| 2 | B | 89 | LYS | Peptide |
| 2 | C | 66 | PHE | Peptide |
| 2 | C | 89 | LYS | Peptide |
| 2 | D | 66 | PHE | Peptide |
| 2 | E | 66 | PHE | Peptide |
| 2 | F | 66 | PHE | Peptide |
| 3 | G | 56 | MET | Peptide |
| 4 | H | 158 | SER | Peptide |
| 4 | H | 209 | ASN | Peptide |
| 4 | H | 228 | ALA | Peptide |
| 4 | H | 450 | LEU | Peptide |
| 4 | H | 8 | GLN | Peptide |
| 3 | I | 56 | MET | Peptide |
| 3 | J | 56 | MET | Peptide |
| 2 | M | 124 | GLN | Peptide |
| 7 | N | 194 | GLN | Peptide |
| 1 | P | 606 | GLY | Peptide |
| 1 | P | 652 | LYS | Peptide |
| 1 | P | 654 | ASP | Peptide |
| 1 | P | 744 | PRO | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | P | 5855 | 0 | 5783 | 460 | 0 |
| 2 | A | 2261 | 0 | 2193 | 229 | 0 |
| 2 | B | 2261 | 0 | 2193 | 228 | 0 |
| 2 | C | 2261 | 0 | 2193 | 233 | 0 |
| 2 | D | 2261 | 0 | 2193 | 227 | 0 |
| 2 | E | 2261 | 0 | 2193 | 212 | 0 |
| 2 | F | 2173 | 0 | 2120 | 161 | 0 |
| 2 | M | 2110 | 0 | 2050 | 220 | 0 |
| 3 | G | 1007 | 0 | 992 | 112 | 0 |
| 3 | I | 1007 | 0 | 992 | 126 | 0 |
| 3 | J | 1007 | 0 | 992 | 138 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | H | 4555 | 0 | 4558 | 418 | 0 |
| 5 | K | 916 | 0 | 464 | 172 | 0 |
| 6 | L | 1093 | 0 | 592 | 96 | 0 |
| 7 | N | 1674 | 0 | 1663 | 173 | 0 |
| 8 | O | 414 | 0 | 224 | 24 | 0 |
| 9 | Q | 408 | 0 | 233 | 20 | 0 |
| 10 | P | 2 | 0 | 0 | 0 | 0 |
| 11 | O | 5 | 0 | 0 | 1 | 0 |
| 11 | P | 10 | 0 | 0 | 14 | 0 |
| 11 | Q | 5 | 0 | 0 | 2 | 0 |
| All | All | 33546 | 0 | 31628 | 2726 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:56:LYS:HZ3 | 11:P:804:PO4:P | 1.75 | 1.08 |
| 4:H:370:PRO:HB2 | 11:Q:101:PO4:O2 | 1.52 | 1.08 |
| 1:P:56:LYS:NZ | 11:P:804:PO4:O1 | 1.94 | 0.99 |
| 1:P:180:LEU:HD21 | 4:H:289:ILE:HG23 | 1.46 | 0.96 |
| 2:C:126:ARG:HH21 | 5:K:14:C:H41 | 1.13 | 0.95 |
| 2:E:51:ARG:NE | 2:E:108:ASP:OD1 | 1.99 | 0.94 |
| 2:E:205:ALA:O | 2:E:209:MET:HB3 | 1.67 | 0.94 |
| 1:P:69:SER:OG | 11:P:803:PO4:O4 | 1.83 | 0.93 |
| 3:I:113:PHE:HB2 | 3:J:80:ARG:HH12 | 1.32 | 0.93 |
| 1:P:56:LYS:NZ | 11:P:804:PO4:P | 2.40 | 0.93 |
| 1:P:56:LYS:NZ | 11:P:804:PO4:O4 | 2.01 | 0.93 |
| 3:I:80:ARG:HH12 | 3:G:113:PHE:HB2 | 1.35 | 0.91 |
| 2:F:205:ALA:O | 2:F:209:MET:HB3 | 1.70 | 0.90 |
| 4:H:422:ARG:NH1 | 6:L:36:DA:OP1 | 2.04 | 0.90 |
| 4:H:67:LEU:H | 4:H:79:ASN:HD21 | 1.16 | 0.88 |
| 2:A:15:VAL:HG11 | 2:A:20:PRO:HG3 | 1.55 | 0.88 |
| 4:H:385:VAL:HG11 | 4:H:389:LYS:HA | 1.55 | 0.88 |
| 2:B:129:VAL:HG22 | 2:B:184:ILE:HG12 | 1.55 | 0.88 |
| 4:H:231:SER:HB3 | 7:N:20:LYS:HE3 | 1.56 | 0.88 |
| 2:B:205:ALA:O | 2:B:209:MET:HB3 | 1.75 | 0.87 |
| 1:P:65:ILE:HD11 | 11:P:803:PO4:O1 | 1.73 | 0.87 |
| 5:K:27:G:N2 | 6:L:28:DC:O2 | 2.08 | 0.87 |
| 2:E:15:VAL:HG11 | 2:E:20:PRO:HG3 | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:45:CYS:SG | 2:E:49:LYS:NZ | 2.48 | 0.87 |
| 2:D:68:ARG:HD3 | 2:D:69:GLU:H | 1.40 | 0.86 |
| 3:J:33:ASN:HD21 | 6:L:26:DC:H3' | 1.38 | 0.86 |
| 2:D:110:ARG:NE | 2:D:198:ASP:OD2 | 2.08 | 0.85 |
| 2:E:246:ARG:HE | 2:E:273:LEU:HD23 | 1.39 | 0.85 |
| 5:K:15:A:N6 | 6:L:40:DT:O4 | 2.09 | 0.85 |
| 2:F:24:PRO:HB3 | 2:F:31:ARG:HG3 | 1.56 | 0.85 |
| 2:D:15:VAL:HG11 | 2:D:20:PRO:HG3 | 1.58 | 0.85 |
| 2:D:21:ASN:ND2 | 5:K:33:U:OP1 | 2.10 | 0.85 |
| 2:C:205:ALA:O | 2:C:209:MET:HB3 | 1.74 | 0.85 |
| 2:B:68:ARG:HG3 | 2:B:69:GLU:H | 1.38 | 0.85 |
| 2:C:32:ILE:HD12 | 3:J:95:LEU:HD21 | 1.58 | 0.85 |
| 2:D:257:VAL:HG21 | 2:E:35:GLN:HB3 | 1.58 | 0.84 |
| 4:H:540:LEU:HD23 | 3:J:106:TYR:HB2 | 1.59 | 0.84 |
| 2:M:69:GLU:HG3 | 2:M:72:ILE:HD12 | 1.59 | 0.84 |
| 4:H:370:PRO:CB | 11:Q:101:PO4:O2 | 2.26 | 0.83 |
| 3:J:34:ALA:O | 3:J:39:ARG:NH2 | 2.12 | 0.83 |
| 2:B:149:ARG:NH2 | 2:B:153:THR:OG1 | 2.11 | 0.83 |
| 3:I:7:ARG:HG2 | 3:I:12:TYR:HD2 | 1.44 | 0.83 |
| 3:G:34:ALA:O | 3:G:39:ARG:NH2 | 2.12 | 0.83 |
| 3:G:7:ARG:HG2 | 3:G:12:TYR:HD2 | 1.44 | 0.82 |
| 2:F:48:ARG:HA | 2:F:51:ARG:HD2 | 1.61 | 0.82 |
| 2:C:218:ARG:NH1 | 5:K:23:G:OP1 | 2.12 | 0.82 |
| 3:J:7:ARG:HG2 | 3:J:12:TYR:HD2 | 1.44 | 0.82 |
| 2:C:62:HIS:O | 2:C:110:ARG:NH1 | 2.13 | 0.81 |
| 3:I:14:LEU:HD11 | 3:I:90:PRO:HD2 | 1.61 | 0.81 |
| 3:I:34:ALA:O | 3:I:39:ARG:NH2 | 2.12 | 0.81 |
| 2:M:149:ARG:HH21 | 2:M:166:THR:HG21 | 1.45 | 0.81 |
| 3:G:14:LEU:HD11 | 3:G:90:PRO:HD2 | 1.61 | 0.81 |
| 3:J:14:LEU:HD11 | 3:J:90:PRO:HD2 | 1.61 | 0.81 |
| 2:A:149:ARG:HH21 | 6:L:24:DG:H21 | 1.25 | 0.81 |
| 1:P:744:PRO:O | 1:P:746:ASP:N | 2.13 | 0.81 |
| 2:F:68:ARG:HD3 | 2:F:69:GLU:H | 1.46 | 0.81 |
| 1:P:493:LEU:HB3 | 1:P:569:VAL:HG22 | 1.62 | 0.81 |
| 2:B:22:GLY:N | 5:K:16:G:OP2 | 2.14 | 0.81 |
| 2:D:19:ASN:ND2 | 2:D:28:ASN:O | 2.10 | 0.80 |
| 2:B:179:ARG:NH1 | 2:B:244:PHE:O | 2.15 | 0.80 |
| 2:D:149:ARG:NH2 | 2:D:153:THR:OG1 | 2.14 | 0.80 |
| 2:E:258:VAL:O | 2:E:259:ARG:NH2 | 2.13 | 0.80 |
| 5:K:4:G:OP2 | 7:N:36:ASN:ND2 | 2.15 | 0.80 |
| 1:P:48:ALA:HB1 | 1:P:194:LEU:HD21 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:206:MET:CE | 11:P:803:PO4:O2 | 2.29 | 0.80 |
| 4:H:228:ALA:HB2 | 7:N:73:LYS:HG2 | 1.62 | 0.79 |
| 4:H:514:ARG:HH22 | 3:J:46:SER:HB3 | 1.45 | 0.79 |
| 2:A:21:ASN:HD22 | 2:A:42:THR:H | 1.28 | 0.79 |
| 1:P:4:ASP:OD1 | 1:P:66:ARG:NH2 | 2.15 | 0.79 |
| 2:D:51:ARG:NH2 | 5:K:31:C:OP1 | 2.14 | 0.79 |
| 3:J:54:THR:HA | 3:J:57:ARG:HD3 | 1.63 | 0.79 |
| 1:P:468:LYS:HB3 | 1:P:599:VAL:HG22 | 1.65 | 0.79 |
| 3:I:54:THR:HA | 3:I:57:ARG:HD3 | 1.64 | 0.79 |
| 4:H:422:ARG:HB2 | 4:H:433:ARG:HD3 | 1.63 | 0.79 |
| 1:P:206:MET:HE1 | 11:P:803:PO4:O2 | 1.83 | 0.78 |
| 2:A:51:ARG:NH2 | 5:K:25:A:OP1 | 2.15 | 0.78 |
| 2:C:15:VAL:HG11 | 2:C:20:PRO:HG3 | 1.63 | 0.78 |
| 2:C:68:ARG:HE | 2:C:69:GLU:H | 1.30 | 0.78 |
| 4:H:404:ALA:O | 4:H:443:ARG:NH2 | 2.16 | 0.78 |
| 4:H:397:LEU:O | 4:H:400:GLN:N | 2.13 | 0.78 |
| 3:G:54:THR:HA | 3:G:57:ARG:HD3 | 1.63 | 0.78 |
| 3:G:119:LYS:O | 3:G:123:ASN:ND2 | 2.17 | 0.78 |
| 4:H:168:LEU:HB2 | 4:H:171:GLN:HG2 | 1.65 | 0.78 |
| 4:H:416:LEU:O | 4:H:420:LEU:HB2 | 1.84 | 0.78 |
| 2:M:179:ARG:NH1 | 2:M:244:PHE:O | 2.17 | 0.78 |
| 2:A:27:GLY:HA2 | 3:J:40:TYR:CD1 | 2.19 | 0.78 |
| 3:G:94:ASN:O | 3:G:98:GLN:N | 2.17 | 0.78 |
| 2:B:187:HIS:NE2 | 2:M:72:ILE:O | 2.15 | 0.77 |
| 3:I:107:HIS:NE2 | 3:J:83:LEU:O | 2.17 | 0.77 |
| 4:H:69:ARG:NH1 | 4:H:79:ASN:OD1 | 2.17 | 0.77 |
| 2:M:126:ARG:O | 7:N:143:ARG:NH2 | 2.18 | 0.77 |
| 4:H:511:THR:HA | 4:H:514:ARG:HE | 1.48 | 0.77 |
| 3:I:83:LEU:O | 3:G:107:HIS:NE2 | 2.18 | 0.77 |
| 2:M:117:THR:N | 7:N:74:MET:O | 2.17 | 0.77 |
| 7:N:37:ILE:HG23 | 7:N:138:PRO:HB3 | 1.67 | 0.77 |
| 3:I:119:LYS:O | 3:I:123:ASN:ND2 | 2.17 | 0.77 |
| 3:J:94:ASN:O | 3:J:98:GLN:N | 2.17 | 0.77 |
| 4:H:6:LEU:HD23 | 4:H:9:TYR:HE1 | 1.49 | 0.77 |
| 2:D:243:LEU:HD21 | 2:D:277:LYS:HE3 | 1.67 | 0.76 |
| 2:C:55:GLN:HB2 | 2:C:65:ILE:HG13 | 1.66 | 0.76 |
| 3:J:119:LYS:O | 3:J:123:ASN:ND2 | 2.17 | 0.76 |
| 2:A:62:HIS:O | 2:A:110:ARG:NH1 | 2.19 | 0.76 |
| 2:C:127:GLY:O | 2:C:130:GLN:NE2 | 2.17 | 0.76 |
| 6:L:36:DA:H2'' | 6:L:37:DA:H5' | 1.67 | 0.76 |
| 1:P:184:HIS:HD2 | 1:P:188:ARG:HH22 | 1.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:353:ASN:O | 1:P:383:ASN:ND2 | 2.19 | 0.76 |
| 3:I:94:ASN:O | 3:I:98:GLN:N | 2.17 | 0.76 |
| 1:P:643:ARG:HG2 | 4:H:165:ALA:HB1 | 1.68 | 0.76 |
| 2:C:8:ASP:OD2 | 2:C:231:HIS:NE2 | 2.19 | 0.76 |
| 2:M:67:ILE:HD11 | 7:N:74:MET:SD | 2.26 | 0.75 |
| 7:N:138:PRO:HB2 | 7:N:147:CYS:HB2 | 1.67 | 0.75 |
| 1:P:53:ASP:OD1 | 1:P:118:HIS:NE2 | 2.18 | 0.75 |
| 1:P:609:SER:HA | 1:P:613:LYS:HE2 | 1.68 | 0.75 |
| 2:D:136:SER:HA | 2:D:178:TYR:HA | 1.69 | 0.75 |
| 1:P:295:ALA:HB2 | 1:P:303:ILE:HD11 | 1.67 | 0.75 |
| 2:B:74:ASN:ND2 | 2:B:118:THR:OG1 | 2.20 | 0.75 |
| 2:B:91:LYS:HA | 2:B:94:LYS:HB3 | 1.67 | 0.75 |
| 2:D:27:GLY:HA2 | 3:I:39:ARG:HG3 | 1.68 | 0.75 |
| 4:H:381:LEU:HD13 | 4:H:398:ILE:HG22 | 1.68 | 0.75 |
| 4:H:385:VAL:HG12 | 4:H:392:ASN:HB2 | 1.69 | 0.75 |
| 1:P:212:ALA:HA | 1:P:217:ALA:HB3 | 1.68 | 0.74 |
| 2:C:152:VAL:HG12 | 2:C:166:THR:HG23 | 1.69 | 0.74 |
| 3:G:22:GLU:OE1 | 3:G:105:TYR:OH | 2.04 | 0.74 |
| 1:P:209:TYR:HB3 | 1:P:216:ALA:HB1 | 1.67 | 0.74 |
| 2:A:150:MET:SD | 2:D:48:ARG:HD3 | 2.27 | 0.74 |
| 2:F:255:VAL:HG11 | 2:F:263:ASP:HB3 | 1.69 | 0.74 |
| 2:C:136:SER:HA | 2:C:178:TYR:HA | 1.69 | 0.74 |
| 2:D:51:ARG:NH1 | 2:D:108:ASP:OD2 | 2.21 | 0.74 |
| 6:L:19:DG:H2'' | 6:L:20:DC:H5' | 1.69 | 0.74 |
| 2:A:150:MET:HE2 | 2:D:68:ARG:HG2 | 1.70 | 0.74 |
| 2:A:160:GLU:HG3 | 2:A:161:THR:H | 1.53 | 0.74 |
| 2:A:41:VAL:HB | 2:A:134:SER:HB2 | 1.69 | 0.74 |
| 2:A:270:ASP:HB3 | 2:A:279:LEU:HD23 | 1.70 | 0.74 |
| 4:H:506:ILE:HG12 | 4:H:548:ASN:HA | 1.70 | 0.74 |
| 3:J:6:ASN:HA | 3:J:85:HIS:CE1 | 2.23 | 0.74 |
| 2:B:156:LYS:HE2 | 6:L:37:DA:H5'' | 1.69 | 0.74 |
| 1:P:6:ILE:N | 1:P:62:GLN:OE1 | 2.20 | 0.73 |
| 3:G:58:LEU:HG | 3:G:62:HIS:CE1 | 2.23 | 0.73 |
| 1:P:410:ARG:NH1 | 1:P:443:GLU:O | 2.21 | 0.73 |
| 3:I:33:ASN:HD21 | 6:L:20:DC:H3' | 1.54 | 0.73 |
| 3:I:58:LEU:HG | 3:I:62:HIS:CE1 | 2.23 | 0.73 |
| 2:E:156:LYS:HG3 | 2:E:158:ALA:H | 1.52 | 0.73 |
| 1:P:531:ILE:HG23 | 1:P:564:LEU:HD21 | 1.70 | 0.73 |
| 2:E:117:THR:OG1 | 6:L:20:DC:O2 | 2.04 | 0.73 |
| 3:I:6:ASN:HA | 3:I:85:HIS:CE1 | 2.23 | 0.73 |
| 1:P:114:LEU:HD23 | 1:P:194:LEU:HD13 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:37:DA:H2'' | 6:L:38:DG:H5' | 1.71 | 0.73 |
| 3:G:6:ASN:HA | 3:G:85:HIS:CE1 | 2.23 | 0.73 |
| 1:P:472:PRO:O | 1:P:624:LYS:NZ | 2.19 | 0.73 |
| 2:C:27:GLY:HA2 | 4:H:496:ARG:HG2 | 1.70 | 0.73 |
| 1:P:429:GLU:O | 1:P:645:ASN:ND2 | 2.20 | 0.73 |
| 4:H:445:ILE:HD13 | 4:H:450:LEU:HB3 | 1.70 | 0.73 |
| 2:M:41:VAL:HB | 2:M:134:SER:HB2 | 1.70 | 0.73 |
| 2:D:241:ASP:OD2 | 2:D:245:LYS:NZ | 2.22 | 0.73 |
| 2:M:235:LEU:HB3 | 7:N:133:GLN:HB3 | 1.68 | 0.73 |
| 1:P:331:GLU:OE1 | 1:P:365:GLN:NE2 | 2.21 | 0.72 |
| 2:B:51:ARG:HH22 | 5:K:13:U:P | 2.11 | 0.72 |
| 3:J:58:LEU:HG | 3:J:62:HIS:CE1 | 2.23 | 0.72 |
| 2:A:130:GLN:NE2 | 5:K:24:U:OP1 | 2.22 | 0.72 |
| 2:D:160:GLU:HG3 | 2:D:161:THR:H | 1.54 | 0.72 |
| 2:B:132:THR:HG21 | 2:M:220:GLN:HB2 | 1.69 | 0.72 |
| 3:I:17:LEU:HD21 | 3:I:56:MET:HE1 | 1.70 | 0.72 |
| 2:B:133:PHE:HB2 | 2:M:17:ASP:HB3 | 1.71 | 0.72 |
| 3:J:32:LEU:HD11 | 6:L:24:DG:H5'' | 1.71 | 0.72 |
| 2:A:179:ARG:NH1 | 2:A:244:PHE:O | 2.23 | 0.72 |
| 2:D:273:LEU:HD21 | 2:D:279:LEU:HB2 | 1.71 | 0.72 |
| 2:M:213:ASP:HB3 | 2:M:218:ARG:HH12 | 1.54 | 0.72 |
| 2:M:114:ALA:N | 2:M:125:VAL:O | 2.19 | 0.72 |
| 2:B:51:ARG:NE | 2:B:108:ASP:OD1 | 2.23 | 0.72 |
| 2:C:129:VAL:HG22 | 2:C:184:ILE:HD12 | 1.70 | 0.72 |
| 3:G:17:LEU:HD21 | 3:G:56:MET:HE1 | 1.71 | 0.72 |
| 1:P:401:PHE:HE2 | 1:P:680:PHE:HA | 1.55 | 0.72 |
| 3:I:22:GLU:OE1 | 3:I:105:TYR:OH | 2.04 | 0.72 |
| 4:H:20:ILE:HG13 | 4:H:256:THR:HG21 | 1.72 | 0.72 |
| 2:B:35:GLN:NE2 | 4:H:449:ARG:O | 2.20 | 0.71 |
| 2:E:68:ARG:HD3 | 2:E:69:GLU:H | 1.55 | 0.71 |
| 3:J:17:LEU:HD21 | 3:J:56:MET:HE1 | 1.70 | 0.71 |
| 2:M:66:PHE:CE2 | 7:N:74:MET:HB3 | 2.24 | 0.71 |
| 2:B:179:ARG:NH1 | 2:B:247:ILE:O | 2.22 | 0.71 |
| 2:A:22:GLY:N | 5:K:28:U:OP2 | 2.23 | 0.71 |
| 2:D:28:ASN:OD1 | 5:K:33:U:O2' | 2.06 | 0.71 |
| 2:M:7:TYR:HB2 | 2:M:184:ILE:HB | 1.72 | 0.71 |
| 4:H:522:LYS:NZ | 6:L:28:DC:OP1 | 2.22 | 0.71 |
| 2:D:179:ARG:NH1 | 2:D:244:PHE:O | 2.23 | 0.71 |
| 2:E:28:ASN:OD1 | 5:K:39:U:O2' | 2.08 | 0.71 |
| 7:N:7:ILE:HD12 | 7:N:147:CYS:HB3 | 1.71 | 0.71 |
| 2:A:23:ASP:OD1 | 2:A:30:PRO:HA | 1.88 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:51:ARG:HE | 2:C:108:ASP:CG | 1.94 | 0.71 |
| 2:E:27:GLY:HA2 | 3:G:39:ARG:HG3 | 1.72 | 0.71 |
| 2:E:257:VAL:HG21 | 2:F:35:GLN:HB3 | 1.72 | 0.71 |
| 2:F:51:ARG:NH2 | 5:K:43:C:OP1 | 2.24 | 0.71 |
| 4:H:23:GLU:O | 4:H:183:ASN:ND2 | 2.20 | 0.71 |
| 5:K:12:G:OP2 | 2:M:215:SER:OG | 2.07 | 0.71 |
| 2:D:125:VAL:O | 5:K:29:G:O2' | 2.08 | 0.71 |
| 6:L:24:DG:H2'' | 6:L:25:DC:H5' | 1.73 | 0.71 |
| 2:B:160:GLU:HG3 | 2:B:161:THR:HG23 | 1.72 | 0.71 |
| 2:F:269:ASP:OD2 | 2:F:271:LYS:NZ | 2.23 | 0.71 |
| 2:A:163:ASP:OD2 | 2:A:165:ARG:NE | 2.23 | 0.71 |
| 2:B:51:ARG:NH2 | 5:K:13:U:OP1 | 2.18 | 0.70 |
| 2:E:68:ARG:NH2 | 2:E:69:GLU:OE1 | 2.24 | 0.70 |
| 1:P:284:THR:OG1 | 1:P:316:ASN:OD1 | 2.06 | 0.70 |
| 2:D:14:ASP:OD2 | 2:D:224:ARG:NE | 2.17 | 0.70 |
| 2:A:143:LEU:HG | 2:A:174:PRO:HG3 | 1.73 | 0.70 |
| 7:N:67:ARG:NE | 7:N:69:GLU:OE2 | 2.22 | 0.70 |
| 3:I:80:ARG:NH2 | 9:Q:11:DT:O2 | 2.25 | 0.70 |
| 1:P:607:ALA:HB1 | 1:P:613:LYS:HA | 1.74 | 0.70 |
| 4:H:124:VAL:HA | 4:H:127:VAL:HG12 | 1.73 | 0.70 |
| 1:P:399:ARG:HA | 1:P:402:GLN:HB2 | 1.74 | 0.70 |
| 2:E:57:THR:HG22 | 2:F:235:LEU:HD11 | 1.72 | 0.70 |
| 7:N:198:VAL:HG23 | 7:N:199:ASN:H | 1.56 | 0.70 |
| 4:H:12:ARG:NH2 | 4:H:275:GLY:O | 2.25 | 0.70 |
| 4:H:397:LEU:O | 4:H:399:ALA:N | 2.25 | 0.70 |
| 7:N:68:ASN:ND2 | 7:N:89:GLN:OE1 | 2.25 | 0.70 |
| 2:A:51:ARG:NH1 | 2:A:108:ASP:OD2 | 2.24 | 0.70 |
| 2:B:169:ARG:NH1 | 4:H:424:LYS:O | 2.24 | 0.70 |
| 3:G:32:LEU:HD23 | 3:G:35:THR:HG22 | 1.74 | 0.70 |
| 2:D:2:THR:HG21 | 2:D:190:LYS:HA | 1.72 | 0.69 |
| 4:H:266:ILE:HG22 | 4:H:406:LEU:HD13 | 1.74 | 0.69 |
| 2:B:28:ASN:OD1 | 5:K:15:A:O2' | 2.08 | 0.69 |
| 4:H:220:PRO:HB2 | 4:H:223:SER:HB3 | 1.73 | 0.69 |
| 7:N:35:ARG:NE | 7:N:174:ASP:OD2 | 2.25 | 0.69 |
| 2:C:113:GLY:HA3 | 5:K:18:U:H5'' | 1.75 | 0.69 |
| 4:H:429:ILE:HD13 | 4:H:559:ALA:HA | 1.74 | 0.69 |
| 4:H:510:GLY:O | 4:H:514:ARG:NE | 2.25 | 0.69 |
| 3:J:32:LEU:HD23 | 3:J:35:THR:HG22 | 1.74 | 0.69 |
| 1:P:398:PRO:HG2 | 1:P:682:LEU:HG | 1.74 | 0.69 |
| 2:E:19:ASN:ND2 | 2:E:28:ASN:O | 2.26 | 0.69 |
| 2:M:121:ASN:HB2 | 2:M:124:GLN:HG2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:39:GLY:N | 2:E:136:SER:OG | 2.24 | 0.69 |
| 3:I:32:LEU:HD23 | 3:I:35:THR:HG22 | 1.74 | 0.69 |
| 3:J:43:SER:O | 3:J:47:THR:N | 2.23 | 0.69 |
| 4:H:206:ARG:HG2 | 4:H:207:LEU:HD23 | 1.73 | 0.69 |
| 3:J:6:ASN:HA | 3:J:85:HIS:HE1 | 1.58 | 0.69 |
| 1:P:558:ILE:HD12 | 1:P:564:LEU:HD11 | 1.74 | 0.68 |
| 2:B:80:ALA:HB2 | 2:B:102:MET:SD | 2.33 | 0.68 |
| 2:C:77:ILE:HG23 | 2:C:122:ALA:HB2 | 1.76 | 0.68 |
| 2:F:64:ASP:O | 2:F:107:TYR:N | 2.25 | 0.68 |
| 3:J:51:VAL:O | 3:J:54:THR:N | 2.27 | 0.68 |
| 1:P:33:ALA:HA | 1:P:36:PHE:HB2 | 1.75 | 0.68 |
| 1:P:295:ALA:HA | 1:P:300:LYS:HB2 | 1.74 | 0.68 |
| 2:D:117:THR:OG1 | 6:L:26:DC:O2 | 2.10 | 0.68 |
| 2:F:21:ASN:HD22 | 2:F:42:THR:H | 1.40 | 0.68 |
| 2:M:258:VAL:O | 2:M:259:ARG:NH2 | 2.25 | 0.68 |
| 1:P:187:MET:HE1 | 1:P:669:LEU:HD11 | 1.76 | 0.68 |
| 1:P:291:ALA:HB1 | 1:P:303:ILE:HD12 | 1.74 | 0.68 |
| 1:P:628:LEU:HB3 | 1:P:631:PRO:HG3 | 1.76 | 0.68 |
| 2:B:259:ARG:NH1 | 2:C:35:GLN:HE21 | 1.91 | 0.68 |
| 2:F:7:TYR:HB2 | 2:F:184:ILE:HD13 | 1.76 | 0.68 |
| 4:H:527:GLY:HA3 | 9:Q:-1:DA:H2'' | 1.74 | 0.68 |
| 7:N:194:GLN:HG3 | 7:N:201:VAL:HG21 | 1.75 | 0.68 |
| 1:P:168:ARG:O | 1:P:172:ALA:N | 2.23 | 0.68 |
| 2:B:126:ARG:O | 2:B:130:GLN:NE2 | 2.27 | 0.68 |
| 2:B:204:GLN:O | 2:B:208:ASN:ND2 | 2.27 | 0.68 |
| 2:B:26:ALA:HB1 | 2:B:29:LEU:HD12 | 1.75 | 0.68 |
| 2:D:27:GLY:HA3 | 3:I:40:TYR:HE1 | 1.57 | 0.68 |
| 3:I:6:ASN:HA | 3:I:85:HIS:HE1 | 1.58 | 0.68 |
| 4:H:69:ARG:HG2 | 4:H:77:VAL:HB | 1.76 | 0.68 |
| 2:M:109:ILE:HG23 | 2:M:114:ALA:HB2 | 1.74 | 0.68 |
| 3:G:6:ASN:HA | 3:G:85:HIS:HE1 | 1.58 | 0.68 |
| 2:M:43:ASP:HB2 | 2:M:131:LEU:HB3 | 1.75 | 0.68 |
| 1:P:536:ARG:HB3 | 1:P:721:LEU:HD21 | 1.75 | 0.68 |
| 2:A:220:GLN:HB2 | 2:D:132:THR:HG21 | 1.76 | 0.68 |
| 3:I:51:VAL:O | 3:I:54:THR:N | 2.27 | 0.68 |
| 3:J:59:LEU:HD21 | 3:J:79:ILE:HD13 | 1.76 | 0.68 |
| 2:B:24:PRO:HG2 | 2:M:167:MET:HE1 | 1.75 | 0.68 |
| 2:B:31:ARG:O | 2:B:40:LEU:N | 2.26 | 0.68 |
| 2:B:220:GLN:HB2 | 2:C:132:THR:HG21 | 1.74 | 0.68 |
| 3:J:93:LEU:HD22 | 3:J:97:GLN:HB3 | 1.75 | 0.68 |
| 2:A:224:ARG:NH1 | 2:D:241:ASP:OD2 | 2.22 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:259:ARG:NH2 | 2:D:35:GLN:OE1 | 2.27 | 0.67 |
| 7:N:140:LEU:HG | 7:N:147:CYS:SG | 2.35 | 0.67 |
| 1:P:536:ARG:HD3 | 1:P:716:PHE:HB3 | 1.77 | 0.67 |
| 2:B:77:ILE:HG23 | 2:B:122:ALA:HB2 | 1.75 | 0.67 |
| 3:G:51:VAL:O | 3:G:54:THR:N | 2.27 | 0.67 |
| 1:P:94:ALA:HB2 | 1:P:141:GLU:HG2 | 1.74 | 0.67 |
| 1:P:278:PRO:HD2 | 1:P:462:LEU:HD23 | 1.75 | 0.67 |
| 1:P:486:ILE:HD11 | 1:P:509:LEU:HD21 | 1.77 | 0.67 |
| 3:I:93:LEU:HD22 | 3:I:97:GLN:HB3 | 1.75 | 0.67 |
| 4:H:51:LEU:HD23 | 4:H:56:LYS:HD2 | 1.77 | 0.67 |
| 2:C:251:LYS:NZ | 2:C:256:GLU:O | 2.27 | 0.67 |
| 4:H:490:ASN:N | 6:L:31:DA:OP1 | 2.22 | 0.67 |
| 6:L:13:DG:H2'' | 6:L:14:DC:H5' | 1.76 | 0.67 |
| 4:H:134:ALA:H | 4:H:137:LYS:HZ3 | 1.42 | 0.67 |
| 2:B:125:VAL:O | 5:K:11:G:O2' | 2.11 | 0.67 |
| 7:N:63:THR:HG23 | 7:N:96:LYS:HB2 | 1.75 | 0.67 |
| 1:P:521:ASN:HB3 | 1:P:771:ALA:H | 1.60 | 0.67 |
| 1:P:542:ARG:NH2 | 1:P:565:ASP:OD2 | 2.28 | 0.67 |
| 3:G:93:LEU:HD22 | 3:G:97:GLN:HB3 | 1.75 | 0.67 |
| 3:J:77:TRP:HD1 | 3:J:80:ARG:HH21 | 1.43 | 0.67 |
| 1:P:412:LEU:HA | 1:P:416:TYR:HD2 | 1.60 | 0.67 |
| 2:B:109:ILE:HG23 | 2:B:125:VAL:HG21 | 1.75 | 0.67 |
| 3:G:43:SER:O | 3:G:47:THR:N | 2.23 | 0.67 |
| 3:G:59:LEU:HD21 | 3:G:79:ILE:HD13 | 1.76 | 0.67 |
| 4:H:67:LEU:N | 4:H:79:ASN:HD21 | 1.92 | 0.67 |
| 2:E:33:ASP:OD2 | 2:E:135:ARG:NH1 | 2.28 | 0.66 |
| 4:H:69:ARG:NH1 | 4:H:83:ASP:OD1 | 2.28 | 0.66 |
| 4:H:108:THR:HA | 4:H:131:LEU:HD23 | 1.78 | 0.66 |
| 4:H:383:ASN:HB3 | 4:H:433:ARG:HG3 | 1.76 | 0.66 |
| 3:J:33:ASN:N | 6:L:25:DC:OP1 | 2.27 | 0.66 |
| 2:M:268:VAL:HG21 | 2:M:281:LYS:HE3 | 1.77 | 0.66 |
| 2:E:9:PHE:CZ | 2:E:182:GLY:HA3 | 2.30 | 0.66 |
| 3:I:46:SER:HB3 | 3:J:57:ARG:NH2 | 2.10 | 0.66 |
| 1:P:494:ALA:HA | 1:P:570:TYR:O | 1.96 | 0.66 |
| 2:B:152:VAL:HA | 2:B:166:THR:HG23 | 1.78 | 0.66 |
| 3:I:59:LEU:HD21 | 3:I:79:ILE:HD13 | 1.76 | 0.66 |
| 4:H:245:GLN:NE2 | 4:H:249:GLU:OE2 | 2.27 | 0.66 |
| 2:D:96:GLU:OE1 | 2:D:99:ARG:NH1 | 2.28 | 0.66 |
| 2:C:148:THR:HA | 2:C:167:MET:HA | 1.76 | 0.66 |
| 3:G:77:TRP:HD1 | 3:G:80:ARG:HH21 | 1.43 | 0.66 |
| 1:P:302:ARG:HD2 | 1:P:383:ASN:HB3 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:571:ARG:HH22 | 1:P:574:ALA:HB3 | 1.59 | 0.66 |
| 3:G:58:LEU:HG | 3:G:62:HIS:HE1 | 1.61 | 0.66 |
| 2:C:45:CYS:SG | 2:C:49:LYS:NZ | 2.68 | 0.66 |
| 4:H:9:TYR:CZ | 4:H:253:ALA:HB1 | 2.31 | 0.66 |
| 2:M:6:ARG:NH1 | 2:M:8:ASP:OD2 | 2.28 | 0.66 |
| 2:A:24:PRO:C | 2:A:26:ALA:H | 1.98 | 0.66 |
| 1:P:328:VAL:HG22 | 1:P:358:LEU:HD23 | 1.78 | 0.66 |
| 2:A:183:PHE:HZ | 2:C:220:GLN:HG3 | 1.59 | 0.66 |
| 2:F:68:ARG:HD3 | 2:F:69:GLU:N | 2.11 | 0.66 |
| 2:F:258:VAL:HG13 | 2:F:263:ASP:HB2 | 1.77 | 0.66 |
| 4:H:454:LYS:HE2 | 4:H:464:ARG:HD2 | 1.77 | 0.66 |
| 7:N:167:ASP:HB2 | 7:N:196:LYS:HG3 | 1.77 | 0.66 |
| 2:B:169:ARG:NH2 | 2:C:25:ASP:OD2 | 2.29 | 0.65 |
| 3:I:58:LEU:HG | 3:I:62:HIS:HE1 | 1.61 | 0.65 |
| 2:B:161:THR:O | 2:C:70:LYS:NZ | 2.27 | 0.65 |
| 2:D:147:ILE:HD13 | 2:D:170:LYS:HB2 | 1.79 | 0.65 |
| 3:I:77:TRP:HD1 | 3:I:80:ARG:HH21 | 1.43 | 0.65 |
| 7:N:6:GLU:HA | 7:N:101:ARG:HA | 1.77 | 0.65 |
| 2:B:33:ASP:OD2 | 2:B:135:ARG:NH1 | 2.28 | 0.65 |
| 2:M:170:LYS:HZ3 | 2:M:216:ALA:HB1 | 1.62 | 0.65 |
| 2:B:259:ARG:HH12 | 2:C:35:GLN:HE21 | 1.42 | 0.65 |
| 2:D:6:ARG:HH11 | 2:D:236:GLY:HA3 | 1.61 | 0.65 |
| 2:E:149:ARG:NH2 | 2:E:153:THR:OG1 | 2.29 | 0.65 |
| 2:D:161:THR:HG22 | 2:F:91:LYS:HB2 | 1.79 | 0.65 |
| 2:E:168:GLY:HA3 | 6:L:12:DG:C5 | 2.32 | 0.65 |
| 2:M:69:GLU:HB2 | 2:M:72:ILE:HB | 1.78 | 0.65 |
| 7:N:69:GLU:HG3 | 7:N:90:ARG:HD3 | 1.79 | 0.65 |
| 2:A:17:ASP:OD2 | 2:D:135:ARG:NH1 | 2.30 | 0.65 |
| 4:H:49:ARG:O | 4:H:50:GLU:HG3 | 1.96 | 0.65 |
| 1:P:665:ASN:ND2 | 4:H:279:THR:OG1 | 2.28 | 0.65 |
| 2:D:47:LYS:O | 2:D:51:ARG:HG2 | 1.97 | 0.65 |
| 2:M:121:ASN:HA | 7:N:184:ASP:OD1 | 1.97 | 0.65 |
| 4:H:392:ASN:O | 4:H:394:PRO:HD3 | 1.97 | 0.65 |
| 2:C:153:THR:OG1 | 6:L:31:DA:H4' | 1.97 | 0.65 |
| 2:M:19:ASN:ND2 | 2:M:28:ASN:O | 2.30 | 0.65 |
| 2:C:104:SER:O | 2:C:110:ARG:NH1 | 2.27 | 0.65 |
| 4:H:196:LEU:HB3 | 4:H:242:ILE:HG12 | 1.78 | 0.65 |
| 2:M:55:GLN:NE2 | 2:M:68:ARG:HB2 | 2.12 | 0.65 |
| 4:H:214:VAL:HG21 | 4:H:337:ILE:HD13 | 1.80 | 0.64 |
| 2:M:55:GLN:HE22 | 2:M:68:ARG:HB2 | 1.62 | 0.64 |
| 1:P:272:LEU:HD21 | 1:P:445:LEU:HD22 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:339:LYS:O | 1:P:344:THR:OG1 | 2.13 | 0.64 |
| 2:B:9:PHE:CZ | 2:B:182:GLY:HA3 | 2.31 | 0.64 |
| 2:D:151:ALA:HB1 | 2:E:71:GLY:O | 1.97 | 0.64 |
| 2:E:224:ARG:NH2 | 2:F:241:ASP:OD2 | 2.30 | 0.64 |
| 2:M:54:ILE:HB | 2:M:65:ILE:HD11 | 1.79 | 0.64 |
| 3:G:77:TRP:HA | 3:G:80:ARG:HE | 1.63 | 0.64 |
| 4:H:262:ASN:ND2 | 4:H:273:CYS:O | 2.21 | 0.64 |
| 2:M:21:ASN:HB2 | 2:M:41:VAL:HG13 | 1.78 | 0.64 |
| 1:P:561:GLY:H | 1:P:585:ARG:HH21 | 1.46 | 0.64 |
| 2:F:229:PHE:HE1 | 2:F:279:LEU:HD22 | 1.63 | 0.64 |
| 2:A:210:PHE:HB3 | 2:A:221:MET:O | 1.98 | 0.64 |
| 3:I:102:ALA:HB1 | 3:J:56:MET:SD | 2.37 | 0.64 |
| 4:H:236:GLN:O | 4:H:236:GLN:HG2 | 1.98 | 0.64 |
| 3:J:77:TRP:HA | 3:J:80:ARG:HE | 1.63 | 0.64 |
| 1:P:332:HIS:O | 1:P:333:HIS:ND1 | 2.30 | 0.64 |
| 2:B:21:ASN:OD1 | 2:B:31:ARG:NE | 2.28 | 0.64 |
| 2:B:156:LYS:HG3 | 2:B:158:ALA:H | 1.63 | 0.64 |
| 2:E:31:ARG:O | 2:E:40:LEU:N | 2.24 | 0.64 |
| 4:H:464:ARG:NH2 | 4:H:466:ASP:OD2 | 2.31 | 0.64 |
| 1:P:369:SER:HA | 1:P:372:ALA:HB2 | 1.79 | 0.63 |
| 3:J:58:LEU:HG | 3:J:62:HIS:HE1 | 1.61 | 0.63 |
| 2:A:149:ARG:NH1 | 2:A:151:ALA:O | 2.31 | 0.63 |
| 2:D:68:ARG:CD | 2:D:69:GLU:H | 2.11 | 0.63 |
| 4:H:194:ILE:HD13 | 4:H:201:ALA:HA | 1.80 | 0.63 |
| 7:N:30:THR:HG22 | 7:N:32:SER:H | 1.62 | 0.63 |
| 1:P:48:ALA:HB3 | 1:P:194:LEU:HD11 | 1.79 | 0.63 |
| 1:P:657:ARG:HH22 | 4:H:296:ASN:HB3 | 1.62 | 0.63 |
| 2:B:117:THR:OG1 | 6:L:44:DC:O2 | 2.12 | 0.63 |
| 2:C:32:ILE:HG22 | 2:C:140:ILE:HD11 | 1.79 | 0.63 |
| 1:P:56:LYS:HG3 | 1:P:61:PHE:CE2 | 2.33 | 0.63 |
| 3:I:77:TRP:HA | 3:I:80:ARG:HE | 1.63 | 0.63 |
| 3:I:80:ARG:HG2 | 3:G:106:TYR:HD1 | 1.62 | 0.63 |
| 3:J:80:ARG:NH2 | 9:Q:6:DT:O2 | 2.31 | 0.63 |
| 5:K:3:U:OP1 | 2:M:121:ASN:ND2 | 2.29 | 0.63 |
| 2:M:255:VAL:HG11 | 2:M:263:ASP:HB3 | 1.81 | 0.63 |
| 1:P:652:LYS:HG3 | 1:P:653:HIS:H | 1.62 | 0.63 |
| 2:C:49:LYS:HB2 | 2:C:209:MET:CE | 2.29 | 0.63 |
| 2:F:137:ILE:HG13 | 2:F:249:VAL:HG13 | 1.81 | 0.63 |
| 1:P:480:GLN:NE2 | 1:P:484:ASP:OD1 | 2.31 | 0.63 |
| 2:C:126:ARG:NH2 | 5:K:14:C:H41 | 1.91 | 0.63 |
| 2:E:40:LEU:HD23 | 2:E:133:PHE:HD2 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:11:PHE:HB3 | 2:F:180:CYS:HB3 | 1.79 | 0.63 |
| 3:G:45:SER:O | 3:G:98:GLN:NE2 | 2.32 | 0.63 |
| 3:J:45:SER:O | 3:J:98:GLN:NE2 | 2.32 | 0.63 |
| 2:B:35:GLN:NE2 | 2:M:141:MET:SD | 2.63 | 0.63 |
| 2:C:148:THR:N | 5:K:27:G:OP2 | 2.31 | 0.63 |
| 2:E:83:GLN:O | 2:E:86:VAL:HG23 | 1.99 | 0.63 |
| 2:F:230:GLU:HB2 | 2:F:278:LEU:HB2 | 1.81 | 0.63 |
| 3:I:43:SER:O | 3:I:47:THR:N | 2.23 | 0.63 |
| 4:H:178:TYR:O | 4:H:182:ALA:N | 2.31 | 0.63 |
| 1:P:110:LEU:HG | 1:P:187:MET:HE1 | 1.81 | 0.62 |
| 2:C:33:ASP:OD2 | 2:C:135:ARG:NE | 2.32 | 0.62 |
| 2:F:258:VAL:O | 2:F:259:ARG:NH2 | 2.28 | 0.62 |
| 4:H:85:TYR:HD2 | 4:H:155:CYS:HB3 | 1.64 | 0.62 |
| 4:H:525:PHE:HB3 | 9:Q:-1:DA:H1' | 1.81 | 0.62 |
| 1:P:98:TYR:CZ | 1:P:102:ARG:HD3 | 2.34 | 0.62 |
| 2:F:179:ARG:NH2 | 2:F:247:ILE:O | 2.32 | 0.62 |
| 4:H:214:VAL:HG11 | 4:H:337:ILE:HG23 | 1.81 | 0.62 |
| 1:P:538:LEU:O | 1:P:542:ARG:HG2 | 1.99 | 0.62 |
| 5:K:13:U:H1' | 2:M:149:ARG:HB2 | 1.81 | 0.62 |
| 2:B:127:GLY:O | 2:B:130:GLN:NE2 | 2.31 | 0.62 |
| 2:D:82:GLU:HA | 2:D:86:VAL:HG12 | 1.81 | 0.62 |
| 2:D:95:THR:HG21 | 2:C:161:THR:HB | 1.81 | 0.62 |
| 4:H:229:PHE:CE1 | 7:N:90:ARG:HD2 | 2.34 | 0.62 |
| 2:B:5:LYS:O | 2:B:186:THR:OG1 | 2.17 | 0.62 |
| 2:C:144:GLU:HG2 | 2:C:171:PHE:HD1 | 1.63 | 0.62 |
| 4:H:34:ILE:HB | 4:H:159:PHE:H | 1.62 | 0.62 |
| 4:H:123:GLY:HA2 | 4:H:161:LEU:HD13 | 1.79 | 0.62 |
| 4:H:514:ARG:HD2 | 3:J:45:SER:CB | 2.29 | 0.62 |
| 2:E:152:VAL:H | 2:E:164:ASN:HB3 | 1.65 | 0.62 |
| 2:F:110:ARG:NE | 2:F:198:ASP:OD2 | 2.32 | 0.62 |
| 3:I:46:SER:HB3 | 3:J:57:ARG:HH21 | 1.65 | 0.62 |
| 7:N:171:MET:HG3 | 7:N:194:GLN:HE22 | 1.64 | 0.62 |
| 1:P:331:GLU:H | 1:P:361:THR:HG22 | 1.62 | 0.62 |
| 2:B:17:ASP:OD1 | 2:C:135:ARG:NH1 | 2.28 | 0.62 |
| 2:C:9:PHE:CZ | 2:C:182:GLY:HA3 | 2.35 | 0.62 |
| 2:E:170:LYS:NZ | 2:F:43:ASP:OD1 | 2.33 | 0.62 |
| 2:E:275:GLU:OE2 | 2:E:277:LYS:NZ | 2.33 | 0.62 |
| 3:I:45:SER:O | 3:I:98:GLN:NE2 | 2.32 | 0.62 |
| 4:H:208:HIS:HE1 | 4:H:242:ILE:HD12 | 1.65 | 0.62 |
| 4:H:42:PHE:HZ | 4:H:45:LEU:HB2 | 1.64 | 0.62 |
| 2:C:80:ALA:HB2 | 2:C:102:MET:SD | 2.40 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:154:ASN:O | 2:C:156:LYS:N | 2.29 | 0.62 |
| 2:E:148:THR:HA | 2:E:167:MET:HB2 | 1.79 | 0.62 |
| 2:E:96:GLU:OE2 | 2:E:99:ARG:NH1 | 2.31 | 0.62 |
| 1:P:244:ASP:HA | 1:P:252:ASN:HD21 | 1.65 | 0.61 |
| 2:A:128:PRO:HG3 | 2:A:189:ALA:HA | 1.82 | 0.61 |
| 2:D:56:MET:HG2 | 2:E:187:HIS:CG | 2.35 | 0.61 |
| 4:H:429:ILE:HD12 | 4:H:562:TYR:CD2 | 2.35 | 0.61 |
| 1:P:65:ILE:HD11 | 11:P:803:PO4:P | 2.39 | 0.61 |
| 1:P:393:GLU:OE1 | 1:P:396:GLN:NE2 | 2.33 | 0.61 |
| 1:P:525:THR:OG1 | 1:P:747:ASN:OD1 | 2.12 | 0.61 |
| 2:A:136:SER:HA | 2:A:178:TYR:HA | 1.80 | 0.61 |
| 2:C:42:THR:HG22 | 2:C:133:PHE:CZ | 2.35 | 0.61 |
| 4:H:6:LEU:HD23 | 4:H:9:TYR:CE1 | 2.34 | 0.61 |
| 4:H:541:GLU:HG3 | 3:J:2:GLY:HA3 | 1.82 | 0.61 |
| 2:M:21:ASN:HD22 | 2:M:42:THR:H | 1.49 | 0.61 |
| 1:P:465:VAL:HG21 | 1:P:586:CYS:HB3 | 1.82 | 0.61 |
| 2:B:21:ASN:HD22 | 2:B:45:CYS:HB2 | 1.65 | 0.61 |
| 2:F:115:VAL:HG22 | 5:K:41:G:C4 | 2.36 | 0.61 |
| 1:P:625:ALA:HB1 | 4:H:162:VAL:HG11 | 1.82 | 0.61 |
| 2:A:21:ASN:ND2 | 2:A:42:THR:H | 1.99 | 0.61 |
| 2:A:91:LYS:HB2 | 2:B:161:THR:HG22 | 1.82 | 0.61 |
| 3:I:12:TYR:OH | 3:I:107:HIS:ND1 | 2.32 | 0.61 |
| 7:N:8:SER:O | 7:N:148:ASP:N | 2.33 | 0.61 |
| 7:N:69:GLU:HG3 | 7:N:90:ARG:HB2 | 1.82 | 0.61 |
| 2:D:51:ARG:HH22 | 5:K:31:C:H5" | 1.63 | 0.61 |
| 2:F:42:THR:HG23 | 2:F:133:PHE:CZ | 2.36 | 0.61 |
| 4:H:363:MET:HB3 | 4:H:431:TYR:CE2 | 2.35 | 0.61 |
| 4:H:468:GLY:HA3 | 4:H:554:GLN:HB3 | 1.82 | 0.61 |
| 2:M:114:ALA:HA | 7:N:74:MET:CE | 2.30 | 0.61 |
| 2:A:130:GLN:HE21 | 2:C:215:SER:HA | 1.64 | 0.61 |
| 2:C:23:ASP:OD1 | 2:C:31:ARG:NH1 | 2.33 | 0.61 |
| 1:P:437:PHE:CD2 | 4:H:176:ARG:HD2 | 2.35 | 0.61 |
| 2:B:42:THR:HG22 | 2:B:133:PHE:CE2 | 2.36 | 0.61 |
| 2:D:65:ILE:HB | 2:D:67:ILE:HG22 | 1.82 | 0.61 |
| 2:E:149:ARG:NH2 | 2:E:166:THR:OG1 | 2.33 | 0.61 |
| 3:J:22:GLU:OE1 | 3:J:105:TYR:OH | 2.04 | 0.61 |
| 2:M:130:GLN:HB2 | 7:N:143:ARG:HH11 | 1.65 | 0.61 |
| 7:N:20:LYS:O | 7:N:90:ARG:NH2 | 2.28 | 0.61 |
| 4:H:514:ARG:HD2 | 3:J:45:SER:HB3 | 1.83 | 0.61 |
| 1:P:41:GLY:HA3 | 1:P:190:LEU:HD21 | 1.83 | 0.61 |
| 2:B:174:PRO:HB2 | 2:B:259:ARG:HH22 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:259:ARG:HD2 | 2:C:36:THR:HB | 1.82 | 0.61 |
| 2:C:19:ASN:ND2 | 2:C:28:ASN:O | 2.25 | 0.61 |
| 4:H:188:ASP:HA | 4:H:203:PRO:HG3 | 1.82 | 0.61 |
| 1:P:306:ALA:HB3 | 1:P:391:LEU:HD23 | 1.81 | 0.61 |
| 2:B:144:GLU:HG3 | 2:B:171:PHE:CD1 | 2.36 | 0.61 |
| 2:D:44:VAL:HG11 | 5:K:31:C:H2' | 1.82 | 0.61 |
| 2:F:3:ILE:HG21 | 2:F:199:LEU:HD13 | 1.83 | 0.61 |
| 4:H:33:ILE:HG13 | 4:H:158:SER:O | 2.01 | 0.61 |
| 2:M:132:THR:HB | 2:M:181:HIS:H | 1.64 | 0.61 |
| 7:N:10:ASP:O | 7:N:97:ASP:N | 2.30 | 0.61 |
| 2:A:91:LYS:HA | 2:A:94:LYS:HB3 | 1.82 | 0.60 |
| 2:E:68:ARG:HD3 | 2:E:69:GLU:N | 2.16 | 0.60 |
| 4:H:83:ASP:O | 4:H:156:ASN:ND2 | 2.30 | 0.60 |
| 1:P:93:THR:HG22 | 1:P:134:ARG:HH21 | 1.67 | 0.60 |
| 1:P:306:ALA:HB1 | 1:P:363:ASN:HB3 | 1.83 | 0.60 |
| 1:P:426:THR:OG1 | 1:P:427:GLN:N | 2.29 | 0.60 |
| 4:H:70:SER:HA | 8:O:13:DC:H1' | 1.83 | 0.60 |
| 4:H:228:ALA:HB2 | 7:N:73:LYS:CG | 2.30 | 0.60 |
| 7:N:83:ILE:HD12 | 7:N:87:ARG:NH1 | 2.16 | 0.60 |
| 7:N:175:MET:HB3 | 7:N:187:ASN:HD22 | 1.66 | 0.60 |
| 1:P:44:PHE:CE2 | 1:P:110:LEU:HD22 | 2.36 | 0.60 |
| 1:P:556:GLN:O | 1:P:559:GLU:HB2 | 2.02 | 0.60 |
| 2:A:31:ARG:O | 2:A:40:LEU:N | 2.21 | 0.60 |
| 2:A:167:MET:H | 6:L:22:DA:H2'' | 1.67 | 0.60 |
| 2:D:167:MET:HG3 | 6:L:16:DA:H2' | 1.82 | 0.60 |
| 2:E:156:LYS:NZ | 6:L:11:DG:OP1 | 2.27 | 0.60 |
| 3:G:24:ILE:HG23 | 3:G:66:LEU:HD11 | 1.84 | 0.60 |
| 4:H:31:PRO:HB3 | 4:H:57:VAL:HB | 1.82 | 0.60 |
| 4:H:441:ILE:O | 4:H:445:ILE:HG12 | 2.01 | 0.60 |
| 2:M:44:VAL:HA | 2:M:47:LYS:HB2 | 1.82 | 0.60 |
| 1:P:110:LEU:HG | 1:P:187:MET:CE | 2.32 | 0.60 |
| 2:B:161:THR:OG1 | 2:B:162:GLY:N | 2.34 | 0.60 |
| 2:D:9:PHE:CZ | 2:D:182:GLY:HA3 | 2.36 | 0.60 |
| 3:J:2:GLY:O | 3:J:107:HIS:ND1 | 2.35 | 0.60 |
| 2:A:103:CYS:O | 2:A:110:ARG:HG3 | 2.02 | 0.60 |
| 2:A:183:PHE:CZ | 2:C:220:GLN:HG3 | 2.36 | 0.60 |
| 4:H:52:LYS:HE2 | 4:H:53:VAL:HG22 | 1.82 | 0.60 |
| 4:H:411:LEU:HB3 | 4:H:415:LEU:HD12 | 1.82 | 0.60 |
| 1:P:100:VAL:HG11 | 1:P:135:LEU:HD13 | 1.84 | 0.60 |
| 1:P:305:TYR:CE2 | 1:P:307:ILE:HD11 | 2.36 | 0.60 |
| 2:A:152:VAL:HG12 | 2:A:164:ASN:HB3 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:243:LEU:HD21 | 2:A:277:LYS:HG2 | 1.83 | 0.60 |
| 2:B:73:LEU:HB2 | 2:M:153:THR:HA | 1.83 | 0.60 |
| 2:C:65:ILE:HB | 2:C:67:ILE:HG22 | 1.83 | 0.60 |
| 2:C:98:ALA:O | 2:C:102:MET:HG2 | 2.02 | 0.60 |
| 2:F:47:LYS:HG3 | 2:F:131:LEU:HD12 | 1.82 | 0.60 |
| 4:H:6:LEU:HD13 | 4:H:254:LEU:HD21 | 1.82 | 0.60 |
| 4:H:9:TYR:HH | 4:H:257:LEU:HD13 | 1.66 | 0.60 |
| 4:H:208:HIS:CE1 | 4:H:242:ILE:HB | 2.36 | 0.60 |
| 4:H:411:LEU:HD13 | 4:H:443:ARG:HD2 | 1.83 | 0.60 |
| 2:M:64:ASP:OD2 | 2:M:105:ARG:NH1 | 2.22 | 0.60 |
| 1:P:336:LEU:HD13 | 1:P:348:ARG:HH21 | 1.65 | 0.60 |
| 1:P:370:LEU:HG | 1:P:408:MET:SD | 2.42 | 0.60 |
| 1:P:617:ASP:OD1 | 4:H:44:GLN:NE2 | 2.29 | 0.60 |
| 2:A:45:CYS:SG | 2:A:49:LYS:NZ | 2.70 | 0.60 |
| 2:C:64:ASP:HB2 | 2:C:106:TYR:HD1 | 1.66 | 0.60 |
| 2:M:52:ASN:O | 2:M:56:MET:HG3 | 2.01 | 0.60 |
| 2:E:21:ASN:HD22 | 2:E:45:CYS:HB2 | 1.66 | 0.60 |
| 2:F:103:CYS:O | 2:F:110:ARG:HG3 | 2.01 | 0.60 |
| 3:G:48:PRO:O | 3:G:52:PHE:HB2 | 2.02 | 0.60 |
| 2:B:164:ASN:HB2 | 2:C:69:GLU:O | 2.02 | 0.60 |
| 2:D:19:ASN:H | 2:D:218:ARG:HA | 1.67 | 0.60 |
| 2:D:144:GLU:HA | 2:D:171:PHE:HD1 | 1.67 | 0.60 |
| 2:E:3:ILE:HG23 | 2:E:186:THR:HG22 | 1.82 | 0.60 |
| 2:E:4:GLU:O | 2:E:234:ASN:ND2 | 2.33 | 0.60 |
| 2:F:131:LEU:HB3 | 2:F:180:CYS:SG | 2.42 | 0.60 |
| 3:I:2:GLY:O | 3:I:107:HIS:ND1 | 2.35 | 0.60 |
| 4:H:256:THR:O | 4:H:260:GLY:N | 2.34 | 0.60 |
| 2:M:174:PRO:HB2 | 2:M:259:ARG:CZ | 2.32 | 0.60 |
| 7:N:176:ASP:N | 7:N:188:ALA:O | 2.25 | 0.60 |
| 1:P:199:PHE:HA | 1:P:202:THR:HG22 | 1.82 | 0.60 |
| 2:A:24:PRO:O | 2:C:146:SER:HB3 | 2.02 | 0.60 |
| 2:A:27:GLY:N | 3:J:39:ARG:O | 2.21 | 0.60 |
| 5:K:4:G:OP2 | 7:N:139:TYR:OH | 2.20 | 0.60 |
| 1:P:342:LYS:HD2 | 1:P:346:LYS:HB2 | 1.82 | 0.59 |
| 3:G:2:GLY:O | 3:G:107:HIS:ND1 | 2.35 | 0.59 |
| 3:J:48:PRO:O | 3:J:52:PHE:HB2 | 2.02 | 0.59 |
| 2:M:145:HIS:HB2 | 2:M:170:LYS:O | 2.02 | 0.59 |
| 2:A:39:GLY:N | 2:A:136:SER:OG | 2.35 | 0.59 |
| 2:B:48:ARG:HD3 | 2:M:150:MET:SD | 2.41 | 0.59 |
| 2:E:129:VAL:HG11 | 2:E:202:PHE:CZ | 2.37 | 0.59 |
| 3:I:24:ILE:HG23 | 3:I:66:LEU:HD11 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:48:PRO:O | 3:I:52:PHE:HB2 | 2.02 | 0.59 |
| 3:J:24:ILE:HG23 | 3:J:66:LEU:HD11 | 1.84 | 0.59 |
| 1:P:114:LEU:HB3 | 1:P:194:LEU:HD22 | 1.84 | 0.59 |
| 1:P:124:ASP:OD1 | 1:P:673:PHE:N | 2.35 | 0.59 |
| 1:P:464:ARG:HB3 | 1:P:587:ASN:HD22 | 1.67 | 0.59 |
| 1:P:537:TYR:HB3 | 1:P:550:LEU:HD11 | 1.83 | 0.59 |
| 1:P:629:ASP:OD1 | 1:P:630:ASP:N | 2.35 | 0.59 |
| 2:A:205:ALA:O | 2:A:209:MET:HB3 | 2.03 | 0.59 |
| 2:B:21:ASN:ND2 | 2:B:45:CYS:HB2 | 2.17 | 0.59 |
| 2:D:90:GLU:O | 2:D:92:GLY:N | 2.35 | 0.59 |
| 2:E:270:ASP:HA | 2:E:273:LEU:HD21 | 1.84 | 0.59 |
| 3:J:12:TYR:CE1 | 3:J:104:GLY:HA2 | 2.38 | 0.59 |
| 2:M:252:LYS:HG2 | 2:M:265:LEU:HG | 1.83 | 0.59 |
| 4:H:67:LEU:H | 4:H:79:ASN:ND2 | 1.95 | 0.59 |
| 4:H:393:LEU:HD22 | 6:L:41:DG:C6 | 2.37 | 0.59 |
| 9:Q:-4:DT:H2'' | 9:Q:-3:DA:H5' | 1.84 | 0.59 |
| 2:B:147:ILE:HD13 | 2:B:170:LYS:HB2 | 1.85 | 0.59 |
| 2:D:77:ILE:HG23 | 2:D:122:ALA:HB2 | 1.85 | 0.59 |
| 4:H:470:VAL:HG23 | 4:H:471:LEU:HD12 | 1.83 | 0.59 |
| 6:L:50:DG:N2 | 8:O:11:DT:O2 | 2.34 | 0.59 |
| 2:A:90:GLU:O | 2:A:92:GLY:N | 2.36 | 0.59 |
| 2:E:91:LYS:HA | 2:E:94:LYS:HB3 | 1.84 | 0.59 |
| 1:P:114:LEU:HD21 | 1:P:190:LEU:HB3 | 1.82 | 0.59 |
| 1:P:133:ARG:NH1 | 1:P:137:GLN:OE1 | 2.36 | 0.59 |
| 1:P:304:ILE:O | 1:P:390:ILE:N | 2.32 | 0.59 |
| 2:E:42:THR:HG22 | 2:E:133:PHE:CE2 | 2.38 | 0.59 |
| 2:E:126:ARG:HG3 | 5:K:35:G:H5' | 1.84 | 0.59 |
| 3:J:12:TYR:OH | 3:J:107:HIS:ND1 | 2.32 | 0.59 |
| 2:M:36:THR:HG23 | 2:M:38:GLU:H | 1.67 | 0.59 |
| 2:C:270:ASP:HB3 | 2:C:279:LEU:HD23 | 1.85 | 0.59 |
| 2:E:165:ARG:HH12 | 6:L:9:DG:N2 | 2.00 | 0.59 |
| 3:G:12:TYR:OH | 3:G:107:HIS:ND1 | 2.32 | 0.59 |
| 4:H:6:LEU:HD22 | 4:H:254:LEU:HD22 | 1.83 | 0.59 |
| 6:L:9:DG:N7 | 6:L:10:DA:N6 | 2.51 | 0.59 |
| 2:B:148:THR:N | 5:K:21:C:OP2 | 2.28 | 0.59 |
| 2:D:203:TRP:HE1 | 2:D:280:ARG:HH12 | 1.51 | 0.59 |
| 2:D:229:PHE:CE2 | 2:D:279:LEU:HD12 | 2.38 | 0.59 |
| 2:D:247:ILE:HD11 | 2:D:279:LEU:HD11 | 1.85 | 0.59 |
| 2:M:9:PHE:CE2 | 2:M:182:GLY:HA3 | 2.37 | 0.59 |
| 2:M:102:MET:HE2 | 7:N:76:GLU:HA | 1.85 | 0.59 |
| 1:P:395:GLN:NE2 | 1:P:581:GLN:OE1 | 2.35 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:143:LEU:HD21 | 2:E:174:PRO:HG3 | 1.84 | 0.58 |
| 2:B:220:GLN:HG3 | 2:C:183:PHE:HZ | 1.68 | 0.58 |
| 2:C:152:VAL:HG13 | 2:C:164:ASN:HB3 | 1.85 | 0.58 |
| 2:E:51:ARG:NH2 | 5:K:37:C:OP1 | 2.35 | 0.58 |
| 2:A:164:ASN:HB2 | 2:D:69:GLU:O | 2.03 | 0.58 |
| 2:B:17:ASP:HB3 | 2:C:133:PHE:HB2 | 1.85 | 0.58 |
| 2:B:99:ARG:HH21 | 2:B:125:VAL:HG12 | 1.68 | 0.58 |
| 2:B:100:GLN:NE2 | 2:B:191:GLN:O | 2.26 | 0.58 |
| 2:C:32:ILE:HD12 | 3:J:95:LEU:CD2 | 2.33 | 0.58 |
| 2:C:68:ARG:HG3 | 2:C:69:GLU:HG2 | 1.85 | 0.58 |
| 2:F:116:MET:HB3 | 2:F:122:ALA:HB3 | 1.85 | 0.58 |
| 4:H:209:ASN:H | 4:H:251:THR:HG21 | 1.67 | 0.58 |
| 4:H:401:ILE:HD12 | 4:H:415:LEU:HD11 | 1.85 | 0.58 |
| 4:H:464:ARG:O | 4:H:466:ASP:N | 2.37 | 0.58 |
| 4:H:523:LEU:HD12 | 4:H:529:ALA:HA | 1.84 | 0.58 |
| 5:K:12:G:H21 | 2:M:149:ARG:HH12 | 1.51 | 0.58 |
| 2:D:34:PRO:HB3 | 3:I:47:THR:HG23 | 1.84 | 0.58 |
| 2:F:14:ASP:OD1 | 2:F:222:ASN:N | 2.35 | 0.58 |
| 2:F:134:SER:OG | 2:F:178:TYR:HB3 | 2.04 | 0.58 |
| 3:I:80:ARG:HG2 | 3:G:106:TYR:CD1 | 2.39 | 0.58 |
| 4:H:225:ASN:ND2 | 6:L:49:DA:H2' | 2.18 | 0.58 |
| 7:N:5:LEU:HD22 | 7:N:38:LEU:HD21 | 1.84 | 0.58 |
| 2:A:47:LYS:HG2 | 2:A:112:PHE:CD1 | 2.38 | 0.58 |
| 2:F:19:ASN:HB3 | 2:F:22:GLY:HA3 | 1.85 | 0.58 |
| 2:F:91:LYS:HA | 2:F:94:LYS:HB3 | 1.84 | 0.58 |
| 4:H:511:THR:HG22 | 4:H:514:ARG:HH11 | 1.68 | 0.58 |
| 3:J:33:ASN:ND2 | 6:L:26:DC:H5'' | 2.19 | 0.58 |
| 2:M:237:ASP:OD2 | 2:M:276:THR:OG1 | 2.13 | 0.58 |
| 7:N:47:ILE:HG13 | 7:N:106:PHE:CD2 | 2.38 | 0.58 |
| 1:P:364:VAL:HG11 | 1:P:683:ILE:HG13 | 1.85 | 0.58 |
| 1:P:571:ARG:NH2 | 1:P:574:ALA:HB3 | 2.18 | 0.58 |
| 1:P:744:PRO:HB2 | 1:P:745:PRO:CD | 2.34 | 0.58 |
| 2:A:215:SER:OG | 5:K:30:G:OP2 | 2.12 | 0.58 |
| 2:B:169:ARG:HH22 | 2:C:25:ASP:CG | 2.06 | 0.58 |
| 2:D:134:SER:OG | 2:D:178:TYR:HB3 | 2.03 | 0.58 |
| 2:C:95:THR:HG21 | 2:M:162:GLY:HA2 | 1.85 | 0.58 |
| 3:J:115:LYS:HA | 9:Q:2:DA:H5'' | 1.85 | 0.58 |
| 2:A:30:PRO:O | 2:A:32:ILE:HG23 | 2.03 | 0.58 |
| 3:I:17:LEU:HB2 | 3:I:82:ILE:HG21 | 1.86 | 0.58 |
| 3:G:12:TYR:CE1 | 3:G:104:GLY:HA2 | 2.38 | 0.58 |
| 4:H:514:ARG:HG2 | 3:J:42:GLY:HA2 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:426:THR:O | 1:P:427:GLN:HG2 | 2.04 | 0.58 |
| 5:K:16:G:N7 | 5:K:17:C:N4 | 2.51 | 0.58 |
| 2:M:110:ARG:NE | 2:M:198:ASP:OD2 | 2.35 | 0.58 |
| 2:B:21:ASN:HD21 | 5:K:15:A:P | 2.27 | 0.58 |
| 2:B:58:GLN:HG2 | 2:B:63:HIS:CG | 2.39 | 0.58 |
| 2:D:83:GLN:O | 2:D:86:VAL:HG13 | 2.03 | 0.58 |
| 2:C:83:GLN:O | 2:C:86:VAL:HG13 | 2.03 | 0.58 |
| 2:C:91:LYS:HB2 | 2:M:161:THR:HG22 | 1.84 | 0.58 |
| 2:F:62:HIS:O | 2:F:110:ARG:NH1 | 2.37 | 0.58 |
| 4:H:35:VAL:HA | 4:H:160:ARG:O | 2.03 | 0.58 |
| 4:H:83:ASP:HB3 | 4:H:87:TYR:HB2 | 1.86 | 0.58 |
| 2:A:66:PHE:CZ | 2:A:109:ILE:HD11 | 2.39 | 0.58 |
| 2:F:38:GLU:HA | 2:F:139:PRO:HA | 1.85 | 0.58 |
| 3:I:12:TYR:CE1 | 3:I:104:GLY:HA2 | 2.38 | 0.58 |
| 1:P:573:MET:HB2 | 1:P:602:ARG:HA | 1.86 | 0.57 |
| 1:P:672:LYS:HB3 | 1:P:675:THR:HB | 1.86 | 0.57 |
| 1:P:745:PRO:O | 1:P:748:PRO:HD3 | 2.04 | 0.57 |
| 2:A:32:ILE:HD12 | 3:I:95:LEU:HD21 | 1.86 | 0.57 |
| 2:A:249:VAL:HG13 | 2:A:266:VAL:HG22 | 1.85 | 0.57 |
| 2:C:25:ASP:HB3 | 4:H:500:SER:HB2 | 1.85 | 0.57 |
| 2:C:131:LEU:HD11 | 2:C:202:PHE:HZ | 1.69 | 0.57 |
| 2:F:22:GLY:HA2 | 2:F:30:PRO:HA | 1.85 | 0.57 |
| 2:F:134:SER:HG | 2:F:178:TYR:HB3 | 1.69 | 0.57 |
| 4:H:48:THR:HG21 | 4:H:61:PHE:HZ | 1.69 | 0.57 |
| 2:M:114:ALA:HA | 7:N:74:MET:HE3 | 1.86 | 0.57 |
| 1:P:662:GLU:O | 4:H:300:HIS:NE2 | 2.37 | 0.57 |
| 2:B:227:TYR:HB3 | 2:B:279:LEU:HD11 | 1.86 | 0.57 |
| 4:H:170:CYS:HA | 4:H:175:VAL:HG11 | 1.86 | 0.57 |
| 1:P:170:PHE:HA | 1:P:186:TRP:HH2 | 1.68 | 0.57 |
| 1:P:514:ILE:HG23 | 1:P:548:LYS:HD3 | 1.85 | 0.57 |
| 2:B:62:HIS:HA | 2:B:105:ARG:HA | 1.87 | 0.57 |
| 2:E:233:ASN:OD1 | 2:E:234:ASN:N | 2.37 | 0.57 |
| 2:F:63:HIS:HA | 2:F:107:TYR:HB2 | 1.86 | 0.57 |
| 4:H:42:PHE:CD1 | 4:H:140:VAL:HG22 | 2.40 | 0.57 |
| 7:N:142:CYS:HB3 | 7:N:144:GLU:OE1 | 2.05 | 0.57 |
| 1:P:407:ASP:HA | 1:P:410:ARG:NH1 | 2.19 | 0.57 |
| 1:P:570:TYR:CD1 | 1:P:599:VAL:HB | 2.40 | 0.57 |
| 1:P:628:LEU:HD22 | 1:P:631:PRO:HB3 | 1.85 | 0.57 |
| 2:B:7:TYR:HB2 | 2:B:184:ILE:HB | 1.85 | 0.57 |
| 2:B:68:ARG:CG | 2:B:69:GLU:H | 2.13 | 0.57 |
| 2:C:20:PRO:HD2 | 2:C:30:PRO:HB3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:143:LEU:CD2 | 2:E:174:PRO:HG3 | 2.35 | 0.57 |
| 5:K:32:A:H2' | 5:K:33:U:H4' | 1.86 | 0.57 |
| 5:K:38:C:N4 | 5:K:40:C:O2' | 2.37 | 0.57 |
| 2:B:109:ILE:HD13 | 2:B:116:MET:HE3 | 1.87 | 0.57 |
| 2:E:47:LYS:HG2 | 2:E:112:PHE:CE1 | 2.39 | 0.57 |
| 2:F:246:ARG:HH22 | 2:F:272:ASN:H | 1.53 | 0.57 |
| 4:H:545:ARG:NE | 3:J:96:GLU:OE2 | 2.34 | 0.57 |
| 5:K:8:C:H1' | 5:K:10:G:OP1 | 2.03 | 0.57 |
| 2:M:215:SER:OG | 2:M:216:ALA:N | 2.37 | 0.57 |
| 1:P:122:LEU:N | 1:P:373:ALA:O | 2.33 | 0.57 |
| 1:P:390:ILE:HG23 | 1:P:421:VAL:HB | 1.84 | 0.57 |
| 2:D:68:ARG:HD3 | 2:D:69:GLU:N | 2.14 | 0.57 |
| 2:D:258:VAL:O | 2:D:259:ARG:NH2 | 2.36 | 0.57 |
| 2:C:51:ARG:NH2 | 2:C:108:ASP:OD1 | 2.37 | 0.57 |
| 3:I:42:GLY:HA2 | 3:J:57:ARG:HG3 | 1.86 | 0.57 |
| 1:P:412:LEU:HA | 1:P:416:TYR:CD2 | 2.40 | 0.57 |
| 2:B:241:ASP:OD2 | 2:M:224:ARG:NH2 | 2.37 | 0.57 |
| 2:D:20:PRO:HD2 | 2:D:30:PRO:HB3 | 1.87 | 0.57 |
| 2:D:129:VAL:HG11 | 2:D:202:PHE:CZ | 2.40 | 0.57 |
| 2:F:81:HIS:NE2 | 2:F:120:LYS:O | 2.38 | 0.57 |
| 3:I:19:ALA:HB2 | 3:I:105:TYR:HA | 1.86 | 0.57 |
| 3:I:115:LYS:HA | 9:Q:7:DT:H5'' | 1.87 | 0.57 |
| 2:A:167:MET:HE1 | 6:L:22:DA:C2 | 2.39 | 0.57 |
| 2:A:179:ARG:NH1 | 2:A:247:ILE:O | 2.38 | 0.57 |
| 2:B:142:THR:O | 4:H:549:HIS:NE2 | 2.38 | 0.57 |
| 2:D:149:ARG:HB2 | 5:K:37:C:H1' | 1.85 | 0.57 |
| 2:E:77:ILE:HG23 | 2:E:122:ALA:HB2 | 1.86 | 0.57 |
| 4:H:81:LEU:HB2 | 4:H:170:CYS:HB3 | 1.86 | 0.57 |
| 2:A:117:THR:OG1 | 6:L:32:DC:O2 | 2.22 | 0.57 |
| 2:C:21:ASN:ND2 | 2:C:45:CYS:SG | 2.77 | 0.57 |
| 2:C:41:VAL:HB | 2:C:134:SER:HB2 | 1.87 | 0.57 |
| 2:M:152:VAL:HG22 | 2:M:164:ASN:HB3 | 1.87 | 0.57 |
| 1:P:189:PHE:CD2 | 1:P:190:LEU:HD12 | 2.40 | 0.57 |
| 2:D:134:SER:HB2 | 2:D:180:CYS:HB2 | 1.86 | 0.57 |
| 2:C:47:LYS:HG2 | 2:C:112:PHE:CD1 | 2.40 | 0.57 |
| 2:E:17:ASP:HB3 | 2:F:133:PHE:HB2 | 1.87 | 0.57 |
| 4:H:361:LEU:HD21 | 4:H:380:LEU:HD22 | 1.87 | 0.57 |
| 3:J:17:LEU:HB2 | 3:J:82:ILE:HG21 | 1.86 | 0.57 |
| 1:P:744:PRO:HB2 | 1:P:745:PRO:HD3 | 1.86 | 0.56 |
| 2:A:29:LEU:HD13 | 3:J:54:THR:HG21 | 1.87 | 0.56 |
| 2:A:146:SER:O | 2:D:31:ARG:NH2 | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:12:LEU:HD12 | 2:C:227:TYR:HE2 | 1.69 | 0.56 |
| 3:G:19:ALA:HB2 | 3:G:105:TYR:HA | 1.86 | 0.56 |
| 1:P:584:GLY:O | 1:P:588:ARG:NH2 | 2.37 | 0.56 |
| 2:A:2:THR:HG22 | 2:A:193:GLY:HA2 | 1.87 | 0.56 |
| 2:A:55:GLN:HB2 | 2:A:65:ILE:HG13 | 1.87 | 0.56 |
| 2:A:148:THR:O | 5:K:31:C:O2' | 2.19 | 0.56 |
| 2:A:169:ARG:NH2 | 2:D:25:ASP:OD2 | 2.34 | 0.56 |
| 2:D:31:ARG:O | 2:D:40:LEU:N | 2.27 | 0.56 |
| 2:E:21:ASN:ND2 | 2:E:45:CYS:HB2 | 2.20 | 0.56 |
| 2:F:77:ILE:HG23 | 2:F:122:ALA:HB2 | 1.86 | 0.56 |
| 2:F:243:LEU:HD21 | 2:F:277:LYS:HZ3 | 1.70 | 0.56 |
| 4:H:88:VAL:HG13 | 4:H:159:PHE:CZ | 2.40 | 0.56 |
| 4:H:501:ALA:HB2 | 4:H:508:VAL:HG11 | 1.87 | 0.56 |
| 3:J:19:ALA:HB2 | 3:J:105:TYR:HA | 1.86 | 0.56 |
| 2:M:160:GLU:HG3 | 2:M:161:THR:HG23 | 1.86 | 0.56 |
| 1:P:8:HIS:HD2 | 1:P:20:HIS:HD1 | 1.53 | 0.56 |
| 1:P:65:ILE:CD1 | 11:P:803:PO4:O1 | 2.50 | 0.56 |
| 1:P:486:ILE:HG22 | 1:P:570:TYR:CD2 | 2.40 | 0.56 |
| 2:A:74:ASN:HD22 | 2:C:154:ASN:HB3 | 1.70 | 0.56 |
| 2:D:29:LEU:HD21 | 3:I:54:THR:HG21 | 1.88 | 0.56 |
| 2:D:144:GLU:OE1 | 3:I:57:ARG:NH2 | 2.39 | 0.56 |
| 2:C:9:PHE:HB3 | 2:C:228:VAL:HG22 | 1.86 | 0.56 |
| 2:C:64:ASP:HB2 | 2:C:106:TYR:CD1 | 2.39 | 0.56 |
| 2:E:271:LYS:HD2 | 2:E:272:ASN:HB2 | 1.86 | 0.56 |
| 1:P:11:GLN:NE2 | 1:P:15:ASN:HA | 2.21 | 0.56 |
| 2:A:151:ALA:HB1 | 2:D:71:GLY:O | 2.05 | 0.56 |
| 2:B:15:VAL:HG11 | 2:B:20:PRO:HG3 | 1.85 | 0.56 |
| 2:D:152:VAL:HG22 | 2:D:164:ASN:HB3 | 1.86 | 0.56 |
| 2:D:168:GLY:HA3 | 6:L:18:DG:C6 | 2.41 | 0.56 |
| 2:C:90:GLU:O | 2:C:92:GLY:N | 2.37 | 0.56 |
| 2:F:83:GLN:O | 2:F:86:VAL:HG23 | 2.05 | 0.56 |
| 6:L:40:DT:H2'' | 6:L:41:DG:H5' | 1.87 | 0.56 |
| 1:P:51:LEU:HD11 | 1:P:161:LEU:HD21 | 1.87 | 0.56 |
| 2:B:32:ILE:HD11 | 4:H:552:LEU:HD22 | 1.87 | 0.56 |
| 4:H:572:LYS:NZ | 4:H:573:ASP:OD1 | 2.35 | 0.56 |
| 1:P:215:ALA:HA | 1:P:218:ALA:HB3 | 1.87 | 0.56 |
| 1:P:561:GLY:H | 1:P:585:ARG:NH2 | 2.02 | 0.56 |
| 2:A:51:ARG:NH1 | 5:K:25:A:H5'' | 2.20 | 0.56 |
| 2:A:152:VAL:HA | 2:A:166:THR:OG1 | 2.06 | 0.56 |
| 3:I:56:MET:SD | 3:G:102:ALA:HB1 | 2.45 | 0.56 |
| 4:H:87:TYR:HD2 | 4:H:107:PHE:HB2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:66:PHE:HB2 | 2:M:106:TYR:CD1 | 2.39 | 0.56 |
| 1:P:43:LEU:HG | 1:P:169:ASP:OD2 | 2.05 | 0.56 |
| 2:A:13:PHE:CE1 | 2:A:46:LEU:HD11 | 2.40 | 0.56 |
| 2:B:12:LEU:HD12 | 2:B:227:TYR:HE2 | 1.69 | 0.56 |
| 2:B:27:GLY:N | 4:H:421:ARG:HD3 | 2.21 | 0.56 |
| 4:H:319:PRO:HG2 | 4:H:348:ALA:HA | 1.88 | 0.56 |
| 4:H:476:ALA:HB3 | 4:H:565:GLU:HB3 | 1.88 | 0.56 |
| 2:M:15:VAL:HG11 | 2:M:20:PRO:HG3 | 1.86 | 0.56 |
| 1:P:170:PHE:CZ | 1:P:178:ALA:HB2 | 2.41 | 0.56 |
| 1:P:406:THR:HA | 1:P:409:MET:HG2 | 1.88 | 0.56 |
| 2:B:83:GLN:O | 2:B:86:VAL:HG13 | 2.06 | 0.56 |
| 2:D:47:LYS:HG2 | 2:D:112:PHE:CE1 | 2.41 | 0.56 |
| 1:P:12:ASP:N | 1:P:16:ALA:O | 2.37 | 0.56 |
| 1:P:305:TYR:HB3 | 1:P:360:VAL:HG22 | 1.87 | 0.56 |
| 2:A:144:GLU:HG2 | 2:A:171:PHE:HD2 | 1.71 | 0.56 |
| 2:B:103:CYS:SG | 2:B:125:VAL:HG11 | 2.46 | 0.56 |
| 2:F:31:ARG:O | 2:F:40:LEU:N | 2.32 | 0.56 |
| 4:H:205:ALA:HB2 | 4:H:244:GLU:HA | 1.88 | 0.56 |
| 2:M:12:LEU:HD21 | 2:M:249:VAL:HG21 | 1.88 | 0.56 |
| 2:A:22:GLY:HA3 | 5:K:27:G:O2' | 2.06 | 0.56 |
| 3:I:40:TYR:HD2 | 3:I:55:LEU:HD21 | 1.71 | 0.56 |
| 3:G:39:ARG:HG2 | 3:G:40:TYR:CD1 | 2.41 | 0.56 |
| 4:H:84:HIS:NE2 | 4:H:154:GLY:HA2 | 2.21 | 0.56 |
| 4:H:265:ARG:HH21 | 8:O:17:DA:H1' | 1.69 | 0.56 |
| 4:H:380:LEU:HG | 4:H:436:LEU:HD22 | 1.87 | 0.56 |
| 4:H:467:ILE:O | 4:H:471:LEU:HD13 | 2.06 | 0.56 |
| 1:P:673:PHE:O | 1:P:677:ALA:N | 2.39 | 0.55 |
| 2:A:113:GLY:HA2 | 2:A:125:VAL:HG12 | 1.87 | 0.55 |
| 2:D:50:VAL:O | 2:D:54:ILE:HG12 | 2.07 | 0.55 |
| 2:E:34:PRO:HB3 | 3:G:47:THR:HG23 | 1.87 | 0.55 |
| 3:I:77:TRP:HD1 | 3:I:80:ARG:NH2 | 2.04 | 0.55 |
| 3:G:17:LEU:HB2 | 3:G:82:ILE:HG21 | 1.86 | 0.55 |
| 6:L:47:DG:H2'' | 6:L:48:DA:C8 | 2.40 | 0.55 |
| 2:M:129:VAL:HG22 | 2:M:184:ILE:HG13 | 1.88 | 0.55 |
| 7:N:14:PHE:CE1 | 7:N:29:ILE:HG13 | 2.41 | 0.55 |
| 7:N:128:ARG:O | 7:N:133:GLN:N | 2.38 | 0.55 |
| 4:H:79:ASN:N | 4:H:83:ASP:OD2 | 2.40 | 0.55 |
| 5:K:8:C:H5' | 2:M:48:ARG:HB2 | 1.88 | 0.55 |
| 7:N:50:LYS:HE3 | 7:N:52:LEU:HD21 | 1.88 | 0.55 |
| 2:B:82:GLU:HA | 2:B:86:VAL:HG12 | 1.88 | 0.55 |
| 3:I:24:ILE:HG22 | 3:I:62:HIS:HB3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:36:DA:C2' | 6:L:37:DA:H5' | 2.36 | 0.55 |
| 1:P:274:SER:HB2 | 1:P:422:LEU:HD12 | 1.88 | 0.55 |
| 2:D:20:PRO:HG2 | 2:D:178:TYR:OH | 2.06 | 0.55 |
| 2:D:153:THR:HB | 6:L:19:DG:H4' | 1.88 | 0.55 |
| 4:H:48:THR:O | 4:H:59:ARG:N | 2.40 | 0.55 |
| 4:H:275:GLY:HA2 | 4:H:325:PHE:HD1 | 1.70 | 0.55 |
| 4:H:415:LEU:O | 4:H:419:ALA:N | 2.31 | 0.55 |
| 3:J:24:ILE:HG22 | 3:J:62:HIS:HB3 | 1.89 | 0.55 |
| 1:P:184:HIS:CD2 | 1:P:188:ARG:HH22 | 2.19 | 0.55 |
| 1:P:187:MET:O | 1:P:191:PHE:HB2 | 2.07 | 0.55 |
| 1:P:402:GLN:HE21 | 1:P:430:LEU:HA | 1.71 | 0.55 |
| 1:P:696:PRO:HD2 | 1:P:729:ALA:HB3 | 1.87 | 0.55 |
| 2:C:30:PRO:O | 2:C:32:ILE:HG23 | 2.07 | 0.55 |
| 2:M:249:VAL:HG13 | 2:M:266:VAL:HG22 | 1.88 | 0.55 |
| 1:P:195:VAL:HG12 | 1:P:379:ARG:HG2 | 1.88 | 0.55 |
| 1:P:395:GLN:HB2 | 1:P:641:PHE:CZ | 2.40 | 0.55 |
| 2:D:34:PRO:HA | 3:I:49:ILE:HD11 | 1.89 | 0.55 |
| 2:D:224:ARG:NH2 | 2:E:241:ASP:OD2 | 2.32 | 0.55 |
| 3:G:24:ILE:HG22 | 3:G:62:HIS:HB3 | 1.89 | 0.55 |
| 4:H:425:ALA:O | 6:L:35:DC:H2' | 2.06 | 0.55 |
| 7:N:181:ASP:OD1 | 7:N:185:SER:OG | 2.22 | 0.55 |
| 1:P:187:MET:HG3 | 1:P:671:ILE:HD12 | 1.89 | 0.55 |
| 1:P:348:ARG:HA | 1:P:351:THR:HG22 | 1.89 | 0.55 |
| 1:P:695:ILE:HB | 1:P:728:ALA:HA | 1.88 | 0.55 |
| 2:A:29:LEU:HD23 | 2:A:29:LEU:H | 1.72 | 0.55 |
| 2:B:126:ARG:HG2 | 2:B:188:PHE:CZ | 2.42 | 0.55 |
| 2:E:63:HIS:HA | 2:E:107:TYR:HB2 | 1.87 | 0.55 |
| 2:F:20:PRO:HD2 | 2:F:30:PRO:HB3 | 1.88 | 0.55 |
| 3:G:39:ARG:HH12 | 6:L:12:DG:H2' | 1.72 | 0.55 |
| 3:G:77:TRP:HD1 | 3:G:80:ARG:NH2 | 2.04 | 0.55 |
| 5:K:3:U:H4' | 5:K:4:G:N2 | 2.21 | 0.55 |
| 2:M:21:ASN:ND2 | 2:M:42:THR:OG1 | 2.40 | 0.55 |
| 2:A:148:THR:HG22 | 2:A:167:MET:SD | 2.47 | 0.55 |
| 2:B:124:GLN:NE2 | 5:K:11:G:N3 | 2.55 | 0.55 |
| 2:D:113:GLY:HA2 | 2:D:125:VAL:HG12 | 1.88 | 0.55 |
| 2:C:36:THR:HG23 | 2:C:38:GLU:H | 1.70 | 0.55 |
| 3:I:39:ARG:HG2 | 3:I:40:TYR:CD1 | 2.41 | 0.55 |
| 3:J:77:TRP:HD1 | 3:J:80:ARG:NH2 | 2.04 | 0.55 |
| 5:K:14:C:H5' | 2:M:148:THR:O | 2.07 | 0.55 |
| 2:M:161:THR:OG1 | 2:M:162:GLY:N | 2.39 | 0.55 |
| 1:P:42:SER:OG | 1:P:169:ASP:OD2 | 2.23 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:491:CYS:N | 1:P:550:LEU:O | 2.39 | 0.55 |
| 2:A:26:ALA:HB1 | 3:J:42:GLY:HA3 | 1.89 | 0.55 |
| 2:A:149:ARG:HH21 | 6:L:24:DG:N2 | 1.99 | 0.55 |
| 3:G:40:TYR:HD2 | 3:G:55:LEU:HD21 | 1.71 | 0.55 |
| 3:J:39:ARG:HG2 | 3:J:40:TYR:CD1 | 2.41 | 0.55 |
| 1:P:100:VAL:HA | 1:P:108:GLY:HA3 | 1.87 | 0.55 |
| 2:A:27:GLY:HA2 | 3:J:40:TYR:HD1 | 1.68 | 0.55 |
| 2:A:42:THR:HG22 | 2:A:133:PHE:CE2 | 2.42 | 0.55 |
| 2:A:210:PHE:CD1 | 2:A:221:MET:HE3 | 2.42 | 0.55 |
| 2:E:148:THR:HA | 2:E:167:MET:CB | 2.37 | 0.55 |
| 2:F:9:PHE:HB3 | 2:F:228:VAL:HG12 | 1.89 | 0.55 |
| 5:K:7:A:H61 | 7:N:23:ARG:HH21 | 1.53 | 0.55 |
| 2:M:99:ARG:HE | 2:M:125:VAL:HG22 | 1.71 | 0.55 |
| 1:P:276:THR:HG21 | 1:P:450:GLU:HG2 | 1.88 | 0.54 |
| 2:A:35:GLN:NE2 | 2:C:257:VAL:HG12 | 2.22 | 0.54 |
| 2:A:137:ILE:HG12 | 2:A:177:LEU:O | 2.06 | 0.54 |
| 2:B:90:GLU:O | 2:B:92:GLY:N | 2.39 | 0.54 |
| 2:B:174:PRO:HB2 | 2:B:259:ARG:NH2 | 2.22 | 0.54 |
| 2:B:183:PHE:HZ | 2:M:220:GLN:HG3 | 1.72 | 0.54 |
| 2:E:34:PRO:HB2 | 3:G:92:HIS:HB2 | 1.87 | 0.54 |
| 2:E:82:GLU:HA | 2:E:86:VAL:HG22 | 1.88 | 0.54 |
| 4:H:134:ALA:H | 4:H:137:LYS:NZ | 2.05 | 0.54 |
| 4:H:247:MET:HA | 4:H:250:TYR:CE1 | 2.42 | 0.54 |
| 4:H:426:GLU:OE2 | 4:H:433:ARG:NH1 | 2.40 | 0.54 |
| 2:M:62:HIS:HA | 2:M:105:ARG:HA | 1.89 | 0.54 |
| 7:N:6:GLU:HB2 | 7:N:152:LEU:HG | 1.89 | 0.54 |
| 7:N:163:ASP:O | 7:N:165:THR:HG23 | 2.06 | 0.54 |
| 2:D:36:THR:HG23 | 2:D:38:GLU:H | 1.72 | 0.54 |
| 4:H:107:PHE:HE2 | 4:H:159:PHE:HE2 | 1.54 | 0.54 |
| 4:H:195:CYS:SG | 4:H:202:ALA:HB3 | 2.47 | 0.54 |
| 1:P:90:PRO:HA | 8:O:24:DA:H4' | 1.88 | 0.54 |
| 2:C:23:ASP:HB3 | 2:C:26:ALA:HB3 | 1.90 | 0.54 |
| 2:E:144:GLU:OE1 | 3:G:57:ARG:HG2 | 2.07 | 0.54 |
| 2:F:137:ILE:HD11 | 2:F:179:ARG:HG3 | 1.88 | 0.54 |
| 4:H:84:HIS:HA | 4:H:155:CYS:O | 2.08 | 0.54 |
| 1:P:401:PHE:CE2 | 1:P:680:PHE:HA | 2.40 | 0.54 |
| 2:A:44:VAL:HG12 | 5:K:25:A:OP2 | 2.07 | 0.54 |
| 2:E:237:ASP:HB2 | 2:E:277:LYS:HE3 | 1.89 | 0.54 |
| 2:F:220:GLN:NE2 | 2:F:222:ASN:OD1 | 2.32 | 0.54 |
| 2:M:110:ARG:HA | 2:M:192:THR:HB | 1.90 | 0.54 |
| 1:P:305:TYR:HD2 | 1:P:360:VAL:HG13 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:252:LYS:HG2 | 2:A:265:LEU:HG | 1.90 | 0.54 |
| 2:A:258:VAL:HG11 | 2:A:264:TYR:CZ | 2.42 | 0.54 |
| 2:D:20:PRO:HB3 | 2:D:221:MET:HE3 | 1.88 | 0.54 |
| 2:C:51:ARG:HH22 | 5:K:19:U:P | 2.31 | 0.54 |
| 2:C:179:ARG:NH1 | 2:C:244:PHE:O | 2.41 | 0.54 |
| 2:E:35:GLN:HA | 3:G:91:ASN:HB3 | 1.90 | 0.54 |
| 3:G:32:LEU:HD11 | 6:L:12:DG:H5'' | 1.90 | 0.54 |
| 2:M:213:ASP:HB3 | 2:M:218:ARG:NH1 | 2.21 | 0.54 |
| 2:A:161:THR:HG22 | 2:E:91:LYS:HB2 | 1.89 | 0.54 |
| 2:D:113:GLY:HA3 | 5:K:30:G:H5'' | 1.90 | 0.54 |
| 2:C:69:GLU:HG3 | 2:C:70:LYS:H | 1.70 | 0.54 |
| 2:C:150:MET:HE2 | 5:K:26:G:C4 | 2.42 | 0.54 |
| 2:C:203:TRP:HE1 | 2:C:280:ARG:HH11 | 1.54 | 0.54 |
| 2:E:55:GLN:HB2 | 2:E:65:ILE:HG13 | 1.88 | 0.54 |
| 3:I:21:LEU:HD13 | 3:I:55:LEU:HB3 | 1.90 | 0.54 |
| 4:H:80:LEU:HD11 | 4:H:114:LEU:HD12 | 1.88 | 0.54 |
| 4:H:331:SER:OG | 4:H:340:ARG:NE | 2.38 | 0.54 |
| 5:K:9:A:O2' | 5:K:10:G:O5' | 2.26 | 0.54 |
| 2:A:83:GLN:O | 2:A:86:VAL:HG23 | 2.07 | 0.54 |
| 2:B:32:ILE:HG22 | 2:B:140:ILE:HD11 | 1.88 | 0.54 |
| 3:I:24:ILE:CD1 | 3:I:79:ILE:HD11 | 2.38 | 0.54 |
| 3:G:17:LEU:HD22 | 3:G:83:LEU:HD21 | 1.90 | 0.54 |
| 3:J:24:ILE:CD1 | 3:J:79:ILE:HD11 | 2.38 | 0.54 |
| 2:M:114:ALA:O | 2:M:125:VAL:N | 2.29 | 0.54 |
| 2:B:114:ALA:N | 2:B:125:VAL:HG23 | 2.23 | 0.54 |
| 2:C:141:MET:HB3 | 3:J:92:HIS:CD2 | 2.43 | 0.54 |
| 3:G:25:GLN:HG3 | 3:G:62:HIS:NE2 | 2.23 | 0.54 |
| 3:G:37:ALA:HA | 3:G:41:PHE:HB2 | 1.90 | 0.54 |
| 3:G:46:SER:HA | 3:G:98:GLN:OE1 | 2.08 | 0.54 |
| 4:H:441:ILE:HD12 | 4:H:560:ILE:HD12 | 1.89 | 0.54 |
| 4:H:534:TRP:O | 4:H:538:GLN:HG2 | 2.08 | 0.54 |
| 2:C:33:ASP:O | 2:C:37:GLY:N | 2.41 | 0.54 |
| 2:E:163:ASP:HA | 2:F:69:GLU:HG3 | 1.88 | 0.54 |
| 3:I:17:LEU:HD22 | 3:I:83:LEU:HD21 | 1.90 | 0.54 |
| 3:I:25:GLN:HG3 | 3:I:62:HIS:NE2 | 2.23 | 0.54 |
| 3:I:46:SER:HA | 3:I:98:GLN:OE1 | 2.08 | 0.54 |
| 3:G:24:ILE:CD1 | 3:G:79:ILE:HD11 | 2.38 | 0.54 |
| 3:G:119:LYS:HD2 | 9:Q:14:DA:H3' | 1.89 | 0.54 |
| 4:H:563:TYR:HA | 4:H:566:THR:HG22 | 1.90 | 0.54 |
| 3:J:37:ALA:HA | 3:J:41:PHE:HB2 | 1.90 | 0.54 |
| 1:P:113:TYR:OH | 1:P:125:TRP:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:380:LYS:O | 1:P:383:ASN:N | 2.39 | 0.54 |
| 2:B:5:LYS:NZ | 2:B:232:SER:O | 2.23 | 0.54 |
| 2:E:56:MET:HG3 | 2:F:187:HIS:HB2 | 1.90 | 0.54 |
| 2:E:153:THR:HA | 2:F:73:LEU:HB2 | 1.88 | 0.54 |
| 2:F:10:VAL:HG22 | 2:F:181:HIS:CD2 | 2.42 | 0.54 |
| 4:H:214:VAL:HG22 | 4:H:330:LEU:HD13 | 1.90 | 0.54 |
| 4:H:364:VAL:CG1 | 4:H:459:GLY:HA2 | 2.38 | 0.54 |
| 4:H:533:GLN:HA | 4:H:536:ILE:HG22 | 1.90 | 0.54 |
| 3:J:25:GLN:HG3 | 3:J:62:HIS:NE2 | 2.23 | 0.54 |
| 8:O:11:DT:H2" | 8:O:12:DT:H5" | 1.90 | 0.54 |
| 1:P:410:ARG:HG3 | 1:P:446:PRO:HD3 | 1.89 | 0.53 |
| 2:B:253:ASP:OD1 | 2:B:254:GLY:N | 2.41 | 0.53 |
| 2:C:42:THR:HB | 2:C:44:VAL:HG22 | 1.90 | 0.53 |
| 4:H:64:PRO:HG3 | 4:H:179:VAL:HG21 | 1.90 | 0.53 |
| 3:J:46:SER:HA | 3:J:98:GLN:OE1 | 2.08 | 0.53 |
| 2:M:160:GLU:HG3 | 2:M:161:THR:H | 1.73 | 0.53 |
| 2:C:69:GLU:O | 2:C:71:GLY:N | 2.36 | 0.53 |
| 2:C:113:GLY:CA | 5:K:18:U:H5" | 2.37 | 0.53 |
| 2:M:63:HIS:HA | 2:M:107:TYR:HB2 | 1.90 | 0.53 |
| 7:N:13:CYS:HG | 7:N:15:THR:HG1 | 1.55 | 0.53 |
| 1:P:576:LEU:HD11 | 1:P:628:LEU:HD21 | 1.90 | 0.53 |
| 1:P:668:PRO:HB3 | 4:H:285:LEU:HD21 | 1.90 | 0.53 |
| 2:A:74:ASN:ND2 | 6:L:32:DC:OP1 | 2.41 | 0.53 |
| 2:B:41:VAL:HB | 2:B:134:SER:OG | 2.07 | 0.53 |
| 2:B:160:GLU:HG3 | 2:B:161:THR:H | 1.73 | 0.53 |
| 2:F:280:ARG:HH22 | 2:F:282:LEU:HD21 | 1.73 | 0.53 |
| 4:H:344:GLU:OE1 | 7:N:166:GLN:NE2 | 2.40 | 0.53 |
| 4:H:478:LEU:HD23 | 4:H:516:LEU:HD13 | 1.90 | 0.53 |
| 5:K:9:A:OP1 | 2:M:21:ASN:ND2 | 2.39 | 0.53 |
| 1:P:320:PHE:HB3 | 1:P:328:VAL:HG21 | 1.91 | 0.53 |
| 2:E:213:ASP:HB3 | 2:E:218:ARG:NH1 | 2.24 | 0.53 |
| 2:E:252:LYS:HG2 | 2:E:253:ASP:H | 1.71 | 0.53 |
| 3:G:21:LEU:HD13 | 3:G:55:LEU:HB3 | 1.90 | 0.53 |
| 7:N:101:ARG:HH22 | 7:N:157:ASP:N | 2.06 | 0.53 |
| 1:P:50:LEU:HD23 | 1:P:159:PHE:HD1 | 1.73 | 0.53 |
| 1:P:174:TRP:CE3 | 1:P:178:ALA:HA | 2.43 | 0.53 |
| 1:P:400:ASP:O | 1:P:652:LYS:N | 2.40 | 0.53 |
| 2:A:29:LEU:HD13 | 3:J:54:THR:CG2 | 2.38 | 0.53 |
| 2:B:50:VAL:O | 2:B:54:ILE:HG12 | 2.07 | 0.53 |
| 2:D:150:MET:SD | 2:E:48:ARG:HD3 | 2.49 | 0.53 |
| 2:E:53:PHE:CD2 | 2:E:205:ALA:HA | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:81:HIS:NE2 | 2:E:120:LYS:O | 2.41 | 0.53 |
| 2:E:90:GLU:O | 2:E:92:GLY:N | 2.41 | 0.53 |
| 2:F:229:PHE:CG | 2:F:243:LEU:HD12 | 2.44 | 0.53 |
| 3:I:33:ASN:ND2 | 6:L:20:DC:H3' | 2.23 | 0.53 |
| 4:H:453:MET:HE3 | 4:H:557:LEU:HD11 | 1.91 | 0.53 |
| 6:L:8:DG:H2'' | 6:L:9:DG:H5'' | 1.91 | 0.53 |
| 2:M:133:PHE:CZ | 7:N:67:ARG:HD3 | 2.44 | 0.53 |
| 2:M:149:ARG:NH2 | 2:M:166:THR:HG21 | 2.20 | 0.53 |
| 7:N:55:GLU:HB3 | 7:N:101:ARG:HG3 | 1.89 | 0.53 |
| 1:P:44:PHE:HE1 | 1:P:166:LEU:HD21 | 1.74 | 0.53 |
| 1:P:187:MET:HB2 | 1:P:673:PHE:CZ | 2.43 | 0.53 |
| 2:D:21:ASN:OD1 | 2:D:42:THR:OG1 | 2.20 | 0.53 |
| 2:F:20:PRO:HB2 | 2:F:41:VAL:HG22 | 1.91 | 0.53 |
| 4:H:7:THR:HG23 | 4:H:249:GLU:OE1 | 2.09 | 0.53 |
| 4:H:51:LEU:HB3 | 4:H:56:LYS:HG2 | 1.89 | 0.53 |
| 4:H:291:GLY:N | 4:H:292:GLY:HA2 | 2.24 | 0.53 |
| 7:N:34:ALA:HB1 | 7:N:102:ILE:HG12 | 1.90 | 0.53 |
| 8:O:5:DA:H2'' | 8:O:6:DT:C5 | 2.44 | 0.53 |
| 1:P:707:GLN:HE22 | 1:P:711:ALA:HA | 1.73 | 0.53 |
| 2:A:259:ARG:NH2 | 2:D:33:ASP:OD2 | 2.34 | 0.53 |
| 2:B:174:PRO:HG3 | 2:C:35:GLN:HE22 | 1.74 | 0.53 |
| 2:D:104:SER:O | 2:D:110:ARG:NH2 | 2.42 | 0.53 |
| 2:F:9:PHE:CZ | 2:F:182:GLY:HA3 | 2.44 | 0.53 |
| 3:I:95:LEU:O | 3:I:98:GLN:HB2 | 2.09 | 0.53 |
| 3:G:115:LYS:HA | 9:Q:12:DT:H5'' | 1.89 | 0.53 |
| 4:H:196:LEU:HA | 7:N:191:MET:SD | 2.48 | 0.53 |
| 4:H:229:PHE:CD2 | 7:N:21:VAL:HG12 | 2.44 | 0.53 |
| 7:N:32:SER:HB3 | 7:N:174:ASP:HA | 1.90 | 0.53 |
| 1:P:652:LYS:HG3 | 1:P:653:HIS:N | 2.22 | 0.53 |
| 2:A:268:VAL:HG11 | 2:A:281:LYS:HE3 | 1.90 | 0.53 |
| 2:E:21:ASN:ND2 | 2:E:42:THR:OG1 | 2.41 | 0.53 |
| 2:E:147:ILE:O | 2:E:167:MET:HB2 | 2.08 | 0.53 |
| 4:H:3:LEU:HD21 | 4:H:221:PHE:HE2 | 1.73 | 0.53 |
| 9:Q:-3:DA:H2'' | 9:Q:-2:DT:H5' | 1.90 | 0.53 |
| 1:P:96:ALA:HB1 | 1:P:112:ALA:HB1 | 1.89 | 0.53 |
| 1:P:188:ARG:HG2 | 1:P:381:ILE:HD13 | 1.91 | 0.53 |
| 2:A:238:ALA:HB3 | 2:A:243:LEU:HD11 | 1.91 | 0.53 |
| 2:E:34:PRO:HG2 | 3:G:92:HIS:CD2 | 2.44 | 0.53 |
| 4:H:69:ARG:NH2 | 8:O:14:DA:OP2 | 2.40 | 0.53 |
| 3:J:95:LEU:O | 3:J:98:GLN:HB2 | 2.09 | 0.53 |
| 5:K:6:A:O3' | 2:M:51:ARG:NH2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:36:PHE:HA | 1:P:382:HIS:HE1 | 1.74 | 0.53 |
| 1:P:113:TYR:HA | 1:P:131:LEU:HD11 | 1.91 | 0.53 |
| 2:A:142:THR:HG22 | 2:A:144:GLU:HG3 | 1.91 | 0.53 |
| 2:A:181:HIS:HB3 | 2:A:244:PHE:CE2 | 2.43 | 0.53 |
| 2:F:227:TYR:HB2 | 2:F:247:ILE:HD11 | 1.91 | 0.53 |
| 3:G:95:LEU:O | 3:G:98:GLN:HB2 | 2.09 | 0.53 |
| 4:H:224:VAL:HG13 | 4:H:229:PHE:HB2 | 1.91 | 0.53 |
| 2:M:66:PHE:HD1 | 2:M:106:TYR:CZ | 2.26 | 0.53 |
| 1:P:291:ALA:O | 1:P:295:ALA:N | 2.41 | 0.52 |
| 2:A:24:PRO:HG2 | 2:A:26:ALA:O | 2.10 | 0.52 |
| 2:A:42:THR:HG21 | 2:C:147:ILE:HG22 | 1.90 | 0.52 |
| 2:B:56:MET:HE3 | 2:C:187:HIS:HB2 | 1.90 | 0.52 |
| 2:F:68:ARG:CD | 2:F:69:GLU:H | 2.19 | 0.52 |
| 1:P:495:VAL:HB | 1:P:571:ARG:HG2 | 1.91 | 0.52 |
| 1:P:658:LEU:HD13 | 1:P:675:THR:HG22 | 1.90 | 0.52 |
| 2:A:23:ASP:HB3 | 2:A:29:LEU:O | 2.09 | 0.52 |
| 2:A:218:ARG:HH11 | 2:A:221:MET:HE1 | 1.74 | 0.52 |
| 2:B:68:ARG:HG3 | 2:B:69:GLU:N | 2.16 | 0.52 |
| 2:D:189:ALA:O | 2:D:193:GLY:N | 2.41 | 0.52 |
| 2:E:36:THR:HG23 | 2:E:38:GLU:H | 1.73 | 0.52 |
| 2:E:246:ARG:HH12 | 2:E:272:ASN:HB3 | 1.73 | 0.52 |
| 3:G:16:ARG:NE | 3:G:108:GLU:OE1 | 2.41 | 0.52 |
| 3:J:17:LEU:HD22 | 3:J:83:LEU:HD21 | 1.89 | 0.52 |
| 3:J:40:TYR:HD2 | 3:J:55:LEU:HD21 | 1.71 | 0.52 |
| 8:O:24:DA:H2' | 11:O:101:PO4:O1 | 2.08 | 0.52 |
| 1:P:30:ALA:HB1 | 1:P:46:GLU:HB2 | 1.92 | 0.52 |
| 1:P:180:LEU:HD11 | 4:H:289:ILE:HD12 | 1.91 | 0.52 |
| 2:A:21:ASN:O | 2:A:23:ASP:HA | 2.09 | 0.52 |
| 2:A:31:ARG:HB3 | 2:A:40:LEU:O | 2.09 | 0.52 |
| 2:B:128:PRO:HG3 | 2:B:189:ALA:HA | 1.91 | 0.52 |
| 2:D:23:ASP:HB3 | 2:D:26:ALA:HB3 | 1.92 | 0.52 |
| 2:D:103:CYS:HB3 | 2:D:192:THR:O | 2.09 | 0.52 |
| 2:C:49:LYS:HB2 | 2:C:209:MET:HE2 | 1.91 | 0.52 |
| 2:E:103:CYS:O | 2:E:110:ARG:HG2 | 2.09 | 0.52 |
| 2:E:280:ARG:NH2 | 2:E:282:LEU:HD11 | 2.23 | 0.52 |
| 3:I:12:TYR:HE1 | 3:I:104:GLY:HA2 | 1.75 | 0.52 |
| 3:I:33:ASN:HD21 | 6:L:20:DC:C3' | 2.19 | 0.52 |
| 3:I:48:PRO:HG2 | 3:I:93:LEU:HG | 1.92 | 0.52 |
| 4:H:141:MET:HG3 | 4:H:146:TRP:CZ2 | 2.44 | 0.52 |
| 4:H:429:ILE:HD11 | 4:H:498:PHE:CZ | 2.45 | 0.52 |
| 2:M:99:ARG:NH1 | 2:M:125:VAL:HG13 | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:187:HIS:HB3 | 7:N:135:PHE:CE2 | 2.44 | 0.52 |
| 2:B:35:GLN:HB3 | 2:M:257:VAL:HG11 | 1.90 | 0.52 |
| 2:B:181:HIS:HB3 | 2:B:244:PHE:CE2 | 2.45 | 0.52 |
| 2:C:117:THR:HG21 | 6:L:38:DG:H21 | 1.73 | 0.52 |
| 2:M:143:LEU:HG | 2:M:174:PRO:HG3 | 1.90 | 0.52 |
| 1:P:47:TYR:HE1 | 1:P:160:PRO:HG2 | 1.73 | 0.52 |
| 1:P:64:TYR:HB2 | 1:P:89:ILE:HD12 | 1.90 | 0.52 |
| 2:A:216:ALA:HB2 | 2:D:47:LYS:HZ2 | 1.74 | 0.52 |
| 2:B:147:ILE:HG22 | 2:C:42:THR:HG21 | 1.91 | 0.52 |
| 2:F:89:LYS:O | 2:F:94:LYS:N | 2.42 | 0.52 |
| 4:H:393:LEU:O | 4:H:395:SER:N | 2.42 | 0.52 |
| 3:J:16:ARG:NE | 3:J:108:GLU:OE1 | 2.42 | 0.52 |
| 5:K:1:G:C2 | 7:N:43:TRP:HB3 | 2.44 | 0.52 |
| 2:M:203:TRP:CE3 | 2:M:226:LEU:HD21 | 2.44 | 0.52 |
| 1:P:47:TYR:CD2 | 1:P:166:LEU:HD12 | 2.44 | 0.52 |
| 1:P:106:PHE:CE1 | 1:P:669:LEU:HD12 | 2.44 | 0.52 |
| 1:P:368:GLU:OE1 | 1:P:681:HIS:HA | 2.10 | 0.52 |
| 2:D:179:ARG:NH2 | 2:D:247:ILE:O | 2.40 | 0.52 |
| 2:C:231:HIS:CE1 | 2:C:243:LEU:HD11 | 2.45 | 0.52 |
| 2:F:124:GLN:HB3 | 5:K:41:G:H1' | 1.91 | 0.52 |
| 3:G:48:PRO:HG2 | 3:G:93:LEU:HG | 1.92 | 0.52 |
| 4:H:85:TYR:CD2 | 4:H:155:CYS:HB3 | 2.43 | 0.52 |
| 4:H:101:ASP:O | 4:H:105:ALA:N | 2.42 | 0.52 |
| 4:H:108:THR:O | 4:H:112:ASN:ND2 | 2.30 | 0.52 |
| 3:J:21:LEU:HD13 | 3:J:55:LEU:HB3 | 1.90 | 0.52 |
| 1:P:271:THR:O | 1:P:419:THR:HA | 2.08 | 0.52 |
| 2:E:48:ARG:HA | 2:E:51:ARG:HD2 | 1.92 | 0.52 |
| 2:E:224:ARG:HD2 | 2:E:261:PHE:CD2 | 2.45 | 0.52 |
| 2:F:131:LEU:HD21 | 2:F:202:PHE:HZ | 1.75 | 0.52 |
| 3:I:37:ALA:HA | 3:I:41:PHE:HB2 | 1.90 | 0.52 |
| 4:H:530:VAL:HG13 | 9:Q:1:DT:C4 | 2.45 | 0.52 |
| 2:M:70:LYS:O | 2:M:74:ASN:ND2 | 2.42 | 0.52 |
| 7:N:30:THR:HG23 | 7:N:172:LEU:O | 2.09 | 0.52 |
| 1:P:517:HIS:CE1 | 1:P:770:ALA:HB2 | 2.45 | 0.52 |
| 1:P:639:GLU:OE1 | 1:P:642:ARG:NH1 | 2.25 | 0.52 |
| 1:P:658:LEU:HD21 | 1:P:679:ARG:NH2 | 2.25 | 0.52 |
| 2:C:106:TYR:HD2 | 2:C:109:ILE:HD12 | 1.75 | 0.52 |
| 2:C:268:VAL:HG11 | 2:C:281:LYS:HE2 | 1.90 | 0.52 |
| 2:E:54:ILE:HB | 2:E:65:ILE:HD11 | 1.91 | 0.52 |
| 2:E:179:ARG:NH1 | 2:E:244:PHE:O | 2.43 | 0.52 |
| 4:H:456:LEU:HD22 | 4:H:464:ARG:HH11 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:11:PHE:HB3 | 2:M:180:CYS:HB3 | 1.90 | 0.52 |
| 2:M:136:SER:HA | 2:M:178:TYR:HA | 1.91 | 0.52 |
| 7:N:51:VAL:HG13 | 7:N:102:ILE:HG23 | 1.91 | 0.52 |
| 1:P:236:TYR:HE2 | 1:P:263:PHE:HZ | 1.56 | 0.52 |
| 1:P:391:LEU:HD11 | 1:P:420:PHE:HD2 | 1.75 | 0.52 |
| 2:B:156:LYS:H | 2:B:159:SER:HB3 | 1.75 | 0.52 |
| 2:D:19:ASN:N | 2:D:218:ARG:HA | 2.24 | 0.52 |
| 3:I:7:ARG:HG2 | 3:I:12:TYR:CD2 | 2.34 | 0.52 |
| 4:H:225:ASN:ND2 | 6:L:49:DA:H8 | 2.08 | 0.52 |
| 3:J:12:TYR:HE1 | 3:J:104:GLY:HA2 | 1.75 | 0.52 |
| 3:J:22:GLU:OE1 | 3:J:37:ALA:HB2 | 2.10 | 0.52 |
| 1:P:252:ASN:HA | 1:P:255:ARG:HB2 | 1.92 | 0.52 |
| 1:P:527:CYS:O | 1:P:531:ILE:HD12 | 2.10 | 0.52 |
| 1:P:715:ASP:HA | 1:P:718:ARG:HH11 | 1.75 | 0.52 |
| 2:A:32:ILE:CD1 | 3:I:95:LEU:HD21 | 2.40 | 0.52 |
| 2:A:149:ARG:NH2 | 2:A:153:THR:OG1 | 2.42 | 0.52 |
| 2:B:102:MET:HG3 | 2:B:106:TYR:CD1 | 2.44 | 0.52 |
| 2:C:29:LEU:HD22 | 4:H:511:THR:HG21 | 1.92 | 0.52 |
| 2:C:51:ARG:NH2 | 5:K:19:U:OP1 | 2.41 | 0.52 |
| 2:F:273:LEU:HD11 | 2:F:279:LEU:HB2 | 1.90 | 0.52 |
| 4:H:302:ASP:HA | 4:H:305:LYS:HB2 | 1.93 | 0.52 |
| 7:N:68:ASN:HB3 | 7:N:87:ARG:NE | 2.25 | 0.52 |
| 1:P:329:VAL:HG22 | 1:P:351:THR:HB | 1.92 | 0.51 |
| 2:A:32:ILE:HD11 | 3:J:50:ALA:HB2 | 1.92 | 0.51 |
| 2:B:144:GLU:HG3 | 2:B:171:PHE:CE1 | 2.45 | 0.51 |
| 2:D:32:ILE:CD1 | 3:G:95:LEU:HD21 | 2.40 | 0.51 |
| 2:C:91:LYS:HD3 | 2:M:161:THR:HG22 | 1.91 | 0.51 |
| 2:E:34:PRO:HG3 | 3:G:47:THR:OG1 | 2.09 | 0.51 |
| 2:F:126:ARG:HG3 | 5:K:41:G:H5" | 1.92 | 0.51 |
| 1:P:387:SER:O | 1:P:418:VAL:HA | 2.10 | 0.51 |
| 1:P:402:GLN:HG2 | 1:P:442:LEU:HD11 | 1.92 | 0.51 |
| 2:C:205:ALA:O | 2:C:209:MET:CB | 2.53 | 0.51 |
| 2:F:128:PRO:HD3 | 2:F:192:THR:HG21 | 1.92 | 0.51 |
| 4:H:263:ARG:NH1 | 8:O:18:DA:OP1 | 2.43 | 0.51 |
| 1:P:581:GLN:O | 1:P:585:ARG:NH1 | 2.43 | 0.51 |
| 2:B:23:ASP:N | 2:B:29:LEU:O | 2.34 | 0.51 |
| 4:H:214:VAL:HG13 | 4:H:330:LEU:HD13 | 1.92 | 0.51 |
| 4:H:364:VAL:HG13 | 4:H:458:MET:O | 2.11 | 0.51 |
| 2:M:55:GLN:HE21 | 2:M:73:LEU:HB3 | 1.75 | 0.51 |
| 7:N:39:MET:HG2 | 7:N:43:TRP:CD1 | 2.46 | 0.51 |
| 1:P:307:ILE:HG21 | 1:P:312:ILE:HB | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:429:GLU:HG2 | 1:P:642:ARG:HG3 | 1.91 | 0.51 |
| 1:P:646:GLY:O | 4:H:59:ARG:NH1 | 2.44 | 0.51 |
| 2:A:21:ASN:ND2 | 2:A:42:THR:OG1 | 2.43 | 0.51 |
| 2:A:144:GLU:HG2 | 2:A:171:PHE:CD2 | 2.45 | 0.51 |
| 2:B:148:THR:HA | 2:B:167:MET:HA | 1.91 | 0.51 |
| 2:F:89:LYS:HB3 | 2:F:94:LYS:HA | 1.92 | 0.51 |
| 3:I:106:TYR:HD1 | 3:J:80:ARG:HG2 | 1.75 | 0.51 |
| 3:G:12:TYR:HE1 | 3:G:104:GLY:HA2 | 1.75 | 0.51 |
| 4:H:212:LYS:HB2 | 4:H:218:PRO:HB3 | 1.92 | 0.51 |
| 1:P:40:TYR:OH | 1:P:386:ASP:OD1 | 2.29 | 0.51 |
| 1:P:457:ALA:O | 1:P:461:LYS:N | 2.37 | 0.51 |
| 2:D:16:GLN:HB3 | 2:D:220:GLN:HB3 | 1.92 | 0.51 |
| 2:C:38:GLU:HA | 2:C:139:PRO:HA | 1.92 | 0.51 |
| 3:I:52:PHE:HA | 3:I:55:LEU:HB2 | 1.93 | 0.51 |
| 4:H:328:LEU:HB2 | 4:H:342:TRP:HZ3 | 1.75 | 0.51 |
| 2:M:238:ALA:HB2 | 2:M:277:LYS:CE | 2.40 | 0.51 |
| 1:P:48:ALA:HB2 | 1:P:111:LEU:CD1 | 2.39 | 0.51 |
| 1:P:366:LEU:O | 1:P:370:LEU:N | 2.30 | 0.51 |
| 1:P:455:LYS:HE3 | 1:P:634:PRO:HB2 | 1.93 | 0.51 |
| 2:C:2:THR:HG22 | 2:C:193:GLY:HA2 | 1.93 | 0.51 |
| 2:F:128:PRO:HG3 | 2:F:189:ALA:HA | 1.93 | 0.51 |
| 2:F:187:HIS:O | 2:F:191:GLN:NE2 | 2.43 | 0.51 |
| 2:F:253:ASP:N | 2:F:253:ASP:OD1 | 2.42 | 0.51 |
| 3:I:29:ASN:HB3 | 3:I:65:LYS:HE3 | 1.93 | 0.51 |
| 3:I:71:ARG:HH22 | 3:I:118:LEU:HD23 | 1.76 | 0.51 |
| 3:G:29:ASN:HB3 | 3:G:65:LYS:HE3 | 1.93 | 0.51 |
| 4:H:537:ARG:NH2 | 3:J:110:GLN:OE1 | 2.40 | 0.51 |
| 3:J:71:ARG:HH22 | 3:J:118:LEU:HD23 | 1.76 | 0.51 |
| 1:P:178:ALA:N | 4:H:288:MET:O | 2.32 | 0.51 |
| 1:P:263:PHE:CD2 | 1:P:293:LYS:HD2 | 2.46 | 0.51 |
| 1:P:310:THR:HG21 | 1:P:334:SER:HB3 | 1.93 | 0.51 |
| 2:D:152:VAL:H | 2:D:164:ASN:HB3 | 1.75 | 0.51 |
| 2:E:125:VAL:O | 5:K:35:G:O2' | 2.23 | 0.51 |
| 2:F:32:ILE:HG22 | 2:F:140:ILE:HD11 | 1.93 | 0.51 |
| 4:H:81:LEU:HD13 | 4:H:169:VAL:HG12 | 1.93 | 0.51 |
| 2:M:48:ARG:NH2 | 2:M:67:ILE:O | 2.42 | 0.51 |
| 2:A:71:GLY:O | 2:C:151:ALA:HB1 | 2.10 | 0.51 |
| 2:D:32:ILE:HD12 | 3:G:95:LEU:HD21 | 1.92 | 0.51 |
| 2:D:48:ARG:HA | 2:D:51:ARG:HG2 | 1.92 | 0.51 |
| 2:D:188:PHE:O | 2:D:192:THR:HG23 | 2.11 | 0.51 |
| 2:E:220:GLN:HG3 | 2:F:183:PHE:HZ | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:22:GLU:OE1 | 3:I:37:ALA:HB2 | 2.10 | 0.51 |
| 3:J:48:PRO:HG2 | 3:J:93:LEU:HG | 1.92 | 0.51 |
| 5:K:27:G:N1 | 6:L:28:DC:N3 | 2.40 | 0.51 |
| 1:P:571:ARG:HH12 | 1:P:574:ALA:HB3 | 1.76 | 0.51 |
| 2:B:66:PHE:CD1 | 2:B:109:ILE:HD11 | 2.46 | 0.51 |
| 2:F:227:TYR:HB2 | 2:F:247:ILE:CD1 | 2.40 | 0.51 |
| 3:J:33:ASN:ND2 | 6:L:26:DC:H3' | 2.18 | 0.51 |
| 6:L:52:DT:H3 | 8:O:8:DA:H61 | 1.59 | 0.51 |
| 7:N:5:LEU:HD11 | 7:N:41:ILE:HD12 | 1.93 | 0.51 |
| 7:N:66:ARG:HA | 7:N:91:ALA:HA | 1.93 | 0.51 |
| 7:N:83:ILE:HG13 | 7:N:84:GLU:N | 2.25 | 0.51 |
| 1:P:229:ALA:HB1 | 1:P:296:LEU:HD11 | 1.92 | 0.51 |
| 2:B:71:GLY:O | 2:M:151:ALA:HB1 | 2.11 | 0.51 |
| 3:J:29:ASN:HB3 | 3:J:65:LYS:HE3 | 1.93 | 0.51 |
| 1:P:7:ALA:HB2 | 1:P:22:LEU:HA | 1.93 | 0.50 |
| 1:P:122:LEU:O | 1:P:674:ARG:HG3 | 2.10 | 0.50 |
| 1:P:661:ALA:HA | 1:P:671:ILE:HG12 | 1.92 | 0.50 |
| 2:A:144:GLU:HA | 2:A:171:PHE:HA | 1.94 | 0.50 |
| 2:B:35:GLN:HG2 | 2:M:141:MET:SD | 2.50 | 0.50 |
| 2:B:145:HIS:HE1 | 2:C:40:LEU:HD13 | 1.76 | 0.50 |
| 2:D:177:LEU:HD23 | 2:D:249:VAL:HG11 | 1.93 | 0.50 |
| 3:G:52:PHE:HA | 3:G:55:LEU:HB2 | 1.92 | 0.50 |
| 7:N:13:CYS:HB2 | 7:N:94:LEU:CD2 | 2.41 | 0.50 |
| 7:N:150:ARG:HE | 7:N:152:LEU:HD21 | 1.76 | 0.50 |
| 1:P:147:SER:O | 1:P:151:GLU:HB2 | 2.11 | 0.50 |
| 1:P:647:LYS:HZ1 | 4:H:160:ARG:CZ | 2.24 | 0.50 |
| 2:A:14:ASP:OD2 | 2:A:224:ARG:NE | 2.42 | 0.50 |
| 2:B:16:GLN:HB3 | 2:B:220:GLN:HB3 | 1.93 | 0.50 |
| 2:B:33:ASP:OD2 | 2:M:259:ARG:NE | 2.36 | 0.50 |
| 2:B:196:GLU:O | 2:B:200:GLU:HG2 | 2.10 | 0.50 |
| 2:D:89:LYS:HB3 | 2:D:94:LYS:HA | 1.92 | 0.50 |
| 2:C:68:ARG:NE | 2:C:69:GLU:H | 2.01 | 0.50 |
| 2:F:65:ILE:HB | 2:F:67:ILE:HG22 | 1.93 | 0.50 |
| 4:H:130:PHE:O | 4:H:137:LYS:NZ | 2.38 | 0.50 |
| 3:J:7:ARG:HG2 | 3:J:12:TYR:CD2 | 2.34 | 0.50 |
| 5:K:38:C:N4 | 5:K:40:C:HO2' | 2.09 | 0.50 |
| 2:A:49:LYS:HB2 | 2:A:209:MET:SD | 2.51 | 0.50 |
| 2:D:9:PHE:HB3 | 2:D:228:VAL:HG22 | 1.94 | 0.50 |
| 2:D:31:ARG:NE | 2:D:42:THR:OG1 | 2.45 | 0.50 |
| 2:D:130:GLN:NE2 | 5:K:30:G:OP1 | 2.45 | 0.50 |
| 2:D:184:ILE:HD13 | 2:D:199:LEU:HD11 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:257:VAL:HG21 | 2:E:35:GLN:CB | 2.34 | 0.50 |
| 2:F:188:PHE:HA | 2:F:191:GLN:NE2 | 2.26 | 0.50 |
| 4:H:4:HIS:O | 4:H:8:GLN:HB2 | 2.11 | 0.50 |
| 4:H:29:GLU:HG2 | 4:H:57:VAL:O | 2.11 | 0.50 |
| 4:H:420:LEU:HD21 | 4:H:555:GLN:HB2 | 1.92 | 0.50 |
| 3:J:77:TRP:O | 3:J:81:GLN:HG2 | 2.11 | 0.50 |
| 5:K:17:C:C2' | 5:K:18:U:H5' | 2.41 | 0.50 |
| 6:L:48:DA:H1' | 6:L:49:DA:H5' | 1.92 | 0.50 |
| 2:M:149:ARG:NH2 | 2:M:153:THR:HG23 | 2.26 | 0.50 |
| 2:M:188:PHE:HA | 2:M:191:GLN:OE1 | 2.11 | 0.50 |
| 2:E:14:ASP:HA | 2:E:176:GLY:O | 2.12 | 0.50 |
| 4:H:152:VAL:HG23 | 4:H:155:CYS:HB2 | 1.93 | 0.50 |
| 4:H:324:LYS:HB3 | 4:H:344:GLU:O | 2.12 | 0.50 |
| 4:H:397:LEU:HD13 | 4:H:401:ILE:HD11 | 1.93 | 0.50 |
| 4:H:467:ILE:HG13 | 4:H:547:PRO:HD3 | 1.93 | 0.50 |
| 3:J:52:PHE:HA | 3:J:55:LEU:HB2 | 1.92 | 0.50 |
| 5:K:7:A:C5 | 7:N:69:GLU:OE1 | 2.65 | 0.50 |
| 5:K:21:C:H1' | 5:K:22:C:O4' | 2.12 | 0.50 |
| 2:M:54:ILE:HG21 | 2:M:107:TYR:CD2 | 2.46 | 0.50 |
| 8:O:22:DA:C8 | 8:O:23:DA:H2' | 2.46 | 0.50 |
| 2:B:26:ALA:CB | 4:H:417:GLN:HB3 | 2.42 | 0.50 |
| 2:D:7:TYR:HB2 | 2:D:184:ILE:HD12 | 1.94 | 0.50 |
| 4:H:554:GLN:HG3 | 4:H:557:LEU:HD12 | 1.93 | 0.50 |
| 2:M:58:GLN:HG3 | 2:M:63:HIS:HB3 | 1.94 | 0.50 |
| 7:N:18:GLU:HG2 | 7:N:19:LEU:H | 1.75 | 0.50 |
| 7:N:194:GLN:HG3 | 7:N:201:VAL:CG2 | 2.40 | 0.50 |
| 2:A:130:GLN:NE2 | 2:C:215:SER:HA | 2.26 | 0.50 |
| 2:B:145:HIS:CE1 | 2:C:40:LEU:HD13 | 2.47 | 0.50 |
| 2:D:13:PHE:HA | 2:D:224:ARG:H | 1.77 | 0.50 |
| 1:P:37:ALA:HB1 | 1:P:41:GLY:H | 1.77 | 0.50 |
| 1:P:305:TYR:HD1 | 1:P:390:ILE:HB | 1.77 | 0.50 |
| 1:P:556:GLN:HA | 1:P:559:GLU:HG3 | 1.93 | 0.50 |
| 2:C:144:GLU:HA | 2:C:171:PHE:HA | 1.92 | 0.50 |
| 2:C:246:ARG:HD3 | 2:C:273:LEU:HD23 | 1.92 | 0.50 |
| 2:E:243:LEU:HA | 2:E:246:ARG:HD2 | 1.94 | 0.50 |
| 2:M:186:THR:HG21 | 2:M:234:ASN:HA | 1.92 | 0.50 |
| 7:N:56:ILE:H | 7:N:56:ILE:HD12 | 1.76 | 0.50 |
| 7:N:68:ASN:HB3 | 7:N:87:ARG:CZ | 2.40 | 0.50 |
| 7:N:98:VAL:HB | 7:N:100:TYR:CE2 | 2.47 | 0.50 |
| 1:P:276:THR:HG22 | 1:P:427:GLN:OE1 | 2.12 | 0.50 |
| 1:P:515:LYS:HB3 | 1:P:551:TRP:HE1 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:65:ILE:O | 2:A:66:PHE:HB2 | 2.12 | 0.50 |
| 2:B:42:THR:HG22 | 2:B:133:PHE:HE2 | 1.76 | 0.50 |
| 2:B:126:ARG:HD3 | 5:K:11:G:H5'' | 1.94 | 0.50 |
| 2:E:203:TRP:HB3 | 2:E:282:LEU:HD22 | 1.94 | 0.50 |
| 2:F:11:PHE:CD1 | 2:F:226:LEU:HD12 | 2.46 | 0.50 |
| 3:I:16:ARG:NE | 3:I:108:GLU:OE1 | 2.42 | 0.50 |
| 4:H:28:LYS:HG2 | 4:H:82:TRP:CZ3 | 2.47 | 0.50 |
| 4:H:360:ASP:CG | 4:H:446:ARG:HH22 | 2.15 | 0.50 |
| 2:M:64:ASP:O | 2:M:107:TYR:N | 2.43 | 0.50 |
| 1:P:44:PHE:HD1 | 1:P:166:LEU:HG | 1.77 | 0.50 |
| 1:P:187:MET:HB2 | 1:P:673:PHE:HZ | 1.76 | 0.50 |
| 1:P:354:TRP:CE2 | 1:P:380:LYS:HD2 | 2.46 | 0.50 |
| 1:P:402:GLN:HE22 | 1:P:645:ASN:HD22 | 1.60 | 0.50 |
| 2:B:231:HIS:CD2 | 2:B:277:LYS:NZ | 2.80 | 0.50 |
| 2:D:91:LYS:HD2 | 2:D:92:GLY:N | 2.26 | 0.50 |
| 2:F:13:PHE:HE1 | 2:F:134:SER:HG | 1.60 | 0.50 |
| 3:I:77:TRP:O | 3:I:81:GLN:HG2 | 2.11 | 0.50 |
| 4:H:196:LEU:CD2 | 7:N:18:GLU:HB3 | 2.42 | 0.50 |
| 4:H:210:ALA:HB1 | 4:H:218:PRO:HB2 | 1.92 | 0.50 |
| 5:K:8:C:H4' | 2:M:45:CYS:HA | 1.94 | 0.50 |
| 1:P:64:TYR:HE1 | 1:P:87:ARG:H | 1.58 | 0.49 |
| 1:P:106:PHE:HB2 | 4:H:285:LEU:HD13 | 1.94 | 0.49 |
| 1:P:230:ARG:NH2 | 1:P:234:GLU:HG3 | 2.27 | 0.49 |
| 1:P:618:ILE:HG12 | 1:P:647:LYS:HE3 | 1.93 | 0.49 |
| 2:A:20:PRO:HG2 | 2:A:178:TYR:OH | 2.12 | 0.49 |
| 2:A:23:ASP:O | 2:A:31:ARG:NE | 2.45 | 0.49 |
| 2:A:40:LEU:HD13 | 2:C:145:HIS:CE1 | 2.47 | 0.49 |
| 2:A:170:LYS:HZ2 | 2:D:44:VAL:HG13 | 1.77 | 0.49 |
| 2:A:246:ARG:HH22 | 2:A:273:LEU:H | 1.60 | 0.49 |
| 2:D:8:ASP:O | 2:D:229:PHE:HD1 | 1.95 | 0.49 |
| 2:C:137:ILE:HG12 | 2:C:177:LEU:O | 2.11 | 0.49 |
| 2:E:41:VAL:HB | 2:E:134:SER:HB2 | 1.94 | 0.49 |
| 3:I:58:LEU:HD11 | 6:L:17:DG:O3' | 2.11 | 0.49 |
| 3:G:22:GLU:OE1 | 3:G:37:ALA:HB2 | 2.10 | 0.49 |
| 3:G:77:TRP:O | 3:G:81:GLN:HG2 | 2.11 | 0.49 |
| 4:H:136:GLU:HA | 4:H:139:LYS:HD3 | 1.94 | 0.49 |
| 1:P:107:PHE:HE1 | 1:P:170:PHE:CD2 | 2.30 | 0.49 |
| 2:C:22:GLY:O | 2:C:24:PRO:HD3 | 2.13 | 0.49 |
| 2:C:228:VAL:HG21 | 2:C:282:LEU:HD12 | 1.94 | 0.49 |
| 2:E:44:VAL:HG12 | 5:K:37:C:OP2 | 2.13 | 0.49 |
| 2:E:45:CYS:SG | 5:K:38:C:O2' | 2.70 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:104:SER:O | 2:F:110:ARG:NH2 | 2.45 | 0.49 |
| 2:F:117:THR:HB | 2:F:121:ASN:HD22 | 1.77 | 0.49 |
| 4:H:69:ARG:HD2 | 4:H:87:TYR:OH | 2.12 | 0.49 |
| 4:H:107:PHE:CE2 | 4:H:159:PHE:HE2 | 2.29 | 0.49 |
| 4:H:208:HIS:CE1 | 4:H:242:ILE:HD12 | 2.44 | 0.49 |
| 2:M:102:MET:CE | 7:N:76:GLU:HA | 2.41 | 0.49 |
| 2:M:278:LEU:HD13 | 2:M:280:ARG:NH1 | 2.26 | 0.49 |
| 7:N:42:LEU:HD23 | 7:N:125:PHE:HB2 | 1.94 | 0.49 |
| 1:P:288:LEU:HD21 | 1:P:292:LEU:HD12 | 1.94 | 0.49 |
| 1:P:428:PRO:HB2 | 1:P:430:LEU:HG | 1.94 | 0.49 |
| 2:A:152:VAL:HG11 | 2:A:159:SER:HB3 | 1.94 | 0.49 |
| 2:A:170:LYS:NZ | 2:A:216:ALA:HB1 | 2.28 | 0.49 |
| 2:B:151:ALA:HB2 | 2:C:67:ILE:O | 2.12 | 0.49 |
| 2:D:280:ARG:NH2 | 2:D:282:LEU:HD11 | 2.26 | 0.49 |
| 2:C:232:SER:HB3 | 2:C:276:THR:O | 2.12 | 0.49 |
| 2:C:249:VAL:HG13 | 2:C:266:VAL:HG22 | 1.94 | 0.49 |
| 2:E:69:GLU:HG2 | 2:E:70:LYS:HE2 | 1.94 | 0.49 |
| 2:E:130:GLN:O | 2:E:182:GLY:HA2 | 2.12 | 0.49 |
| 2:E:179:ARG:NH2 | 2:E:247:ILE:O | 2.46 | 0.49 |
| 2:E:249:VAL:HG22 | 2:E:266:VAL:HG22 | 1.92 | 0.49 |
| 4:H:265:ARG:HG2 | 4:H:270:THR:HG22 | 1.94 | 0.49 |
| 4:H:265:ARG:NH2 | 8:O:17:DA:H1' | 2.27 | 0.49 |
| 7:N:18:GLU:HG2 | 7:N:19:LEU:N | 2.28 | 0.49 |
| 7:N:29:ILE:HG23 | 7:N:54:ILE:HG12 | 1.93 | 0.49 |
| 1:P:154:LEU:HD12 | 1:P:158:PHE:CD2 | 2.48 | 0.49 |
| 1:P:434:ILE:O | 1:P:441:ILE:HB | 2.12 | 0.49 |
| 1:P:594:GLN:HG2 | 1:P:595:LEU:N | 2.27 | 0.49 |
| 2:A:160:GLU:CG | 2:A:161:THR:H | 2.25 | 0.49 |
| 2:C:102:MET:HB3 | 2:C:109:ILE:HD13 | 1.94 | 0.49 |
| 2:C:131:LEU:HD11 | 2:C:202:PHE:CZ | 2.46 | 0.49 |
| 2:F:167:MET:HB2 | 2:F:169:ARG:HH22 | 1.78 | 0.49 |
| 5:K:5:A:H1' | 2:M:124:GLN:CB | 2.42 | 0.49 |
| 6:L:9:DG:H2' | 6:L:10:DA:C4 | 2.48 | 0.49 |
| 2:M:65:ILE:O | 2:M:108:ASP:HB3 | 2.12 | 0.49 |
| 1:P:104:ASN:HB2 | 1:P:163:ASP:OD2 | 2.12 | 0.49 |
| 1:P:364:VAL:O | 1:P:368:GLU:HB2 | 2.12 | 0.49 |
| 1:P:571:ARG:HD2 | 1:P:579:ILE:HD13 | 1.94 | 0.49 |
| 2:D:62:HIS:O | 2:D:110:ARG:NH1 | 2.46 | 0.49 |
| 2:D:211:ASP:OD2 | 2:E:239:PRO:HA | 2.12 | 0.49 |
| 2:C:128:PRO:HG2 | 2:C:194:PHE:CB | 2.43 | 0.49 |
| 2:C:215:SER:HB2 | 2:C:218:ARG:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:229:PHE:HB3 | 2:C:277:LYS:CE | 2.42 | 0.49 |
| 2:E:229:PHE:HZ | 2:E:247:ILE:HG12 | 1.78 | 0.49 |
| 4:H:467:ILE:HD11 | 4:H:545:ARG:O | 2.13 | 0.49 |
| 7:N:48:ARG:HB2 | 7:N:109:THR:HG22 | 1.95 | 0.49 |
| 2:A:69:GLU:O | 2:C:164:ASN:HB2 | 2.12 | 0.49 |
| 2:A:170:LYS:HZ3 | 2:A:216:ALA:HB1 | 1.78 | 0.49 |
| 2:B:24:PRO:HG3 | 5:K:15:A:H2' | 1.95 | 0.49 |
| 2:D:56:MET:SD | 2:D:212:HIS:HB3 | 2.52 | 0.49 |
| 2:E:13:PHE:O | 2:E:177:LEU:HD12 | 2.12 | 0.49 |
| 3:G:71:ARG:HH22 | 3:G:118:LEU:HD23 | 1.76 | 0.49 |
| 4:H:48:THR:HG21 | 4:H:61:PHE:CZ | 2.47 | 0.49 |
| 4:H:164:GLU:HB3 | 4:H:167:ASP:HB2 | 1.95 | 0.49 |
| 1:P:44:PHE:HE2 | 1:P:110:LEU:HD22 | 1.76 | 0.49 |
| 1:P:47:TYR:CE1 | 1:P:160:PRO:HG2 | 2.48 | 0.49 |
| 2:D:152:VAL:HG12 | 2:D:166:THR:HG23 | 1.94 | 0.49 |
| 2:D:153:THR:HA | 2:E:73:LEU:HB2 | 1.93 | 0.49 |
| 2:F:126:ARG:HA | 5:K:41:G:O3' | 2.13 | 0.49 |
| 1:P:69:SER:HG | 11:P:803:PO4:P | 2.27 | 0.49 |
| 1:P:708:ILE:HG23 | 1:P:709:VAL:HG13 | 1.95 | 0.49 |
| 2:A:42:THR:HG22 | 2:A:133:PHE:CZ | 2.48 | 0.49 |
| 2:A:68:ARG:HG3 | 2:C:150:MET:SD | 2.53 | 0.49 |
| 2:A:145:HIS:CE1 | 2:D:40:LEU:HD13 | 2.48 | 0.49 |
| 2:D:149:ARG:NH2 | 2:D:166:THR:OG1 | 2.41 | 0.49 |
| 2:E:231:HIS:HD1 | 2:E:236:GLY:HA2 | 1.78 | 0.49 |
| 3:I:95:LEU:HA | 3:I:98:GLN:HB2 | 1.95 | 0.49 |
| 3:I:110:GLN:O | 3:I:114:THR:HG23 | 2.13 | 0.49 |
| 4:H:83:ASP:HB3 | 4:H:87:TYR:CB | 2.42 | 0.49 |
| 5:K:3:U:C5 | 7:N:184:ASP:HB3 | 2.47 | 0.49 |
| 2:M:48:ARG:NH2 | 2:M:67:ILE:HG22 | 2.28 | 0.49 |
| 2:M:246:ARG:HD3 | 2:M:269:ASP:O | 2.12 | 0.49 |
| 1:P:581:GLN:NE2 | 1:P:585:ARG:HH22 | 2.11 | 0.49 |
| 1:P:745:PRO:C | 1:P:748:PRO:HD3 | 2.33 | 0.49 |
| 2:A:6:ARG:NH1 | 2:A:8:ASP:OD2 | 2.46 | 0.49 |
| 2:C:17:ASP:O | 2:C:219:GLY:HA3 | 2.12 | 0.49 |
| 2:E:27:GLY:HA3 | 3:G:40:TYR:HE1 | 1.78 | 0.49 |
| 2:F:126:ARG:HD3 | 2:F:188:PHE:CE1 | 2.47 | 0.49 |
| 4:H:396:ASP:HB2 | 2:M:169:ARG:NH1 | 2.27 | 0.49 |
| 5:K:1:G:N2 | 7:N:39:MET:O | 2.41 | 0.49 |
| 5:K:14:C:O2' | 5:K:16:G:OP1 | 2.30 | 0.49 |
| 1:P:28:LYS:NZ | 1:P:210:ALA:O | 2.40 | 0.49 |
| 1:P:32:LEU:HD23 | 1:P:197:ALA:HA | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:36:THR:HG23 | 2:C:259:ARG:HG3 | 1.95 | 0.49 |
| 2:A:74:ASN:HB2 | 2:C:154:ASN:HA | 1.94 | 0.49 |
| 2:B:114:ALA:H | 2:B:125:VAL:HG23 | 1.77 | 0.49 |
| 2:E:51:ARG:HH22 | 5:K:37:C:P | 2.35 | 0.49 |
| 2:F:30:PRO:O | 2:F:32:ILE:HG23 | 2.13 | 0.49 |
| 3:I:98:GLN:NE2 | 3:J:57:ARG:NH2 | 2.60 | 0.49 |
| 6:L:43:DC:H3' | 6:L:44:DC:H5'' | 1.94 | 0.49 |
| 2:M:11:PHE:CG | 2:M:206:LEU:HD23 | 2.47 | 0.49 |
| 1:P:98:TYR:OH | 1:P:102:ARG:NH2 | 2.40 | 0.48 |
| 2:D:138:ASP:OD2 | 2:D:251:LYS:HG3 | 2.12 | 0.48 |
| 2:E:220:GLN:OE1 | 2:F:181:HIS:ND1 | 2.41 | 0.48 |
| 4:H:32:PHE:CG | 4:H:149:CYS:HB3 | 2.48 | 0.48 |
| 4:H:168:LEU:H | 4:H:171:GLN:HG3 | 1.78 | 0.48 |
| 4:H:224:VAL:O | 4:H:236:GLN:HA | 2.13 | 0.48 |
| 4:H:227:SER:HB2 | 7:N:72:THR:HA | 1.94 | 0.48 |
| 4:H:422:ARG:NH2 | 4:H:426:GLU:OE1 | 2.44 | 0.48 |
| 5:K:6:A:H5'' | 2:M:112:PHE:O | 2.13 | 0.48 |
| 5:K:12:G:H21 | 2:M:149:ARG:NH1 | 2.11 | 0.48 |
| 2:M:54:ILE:HG13 | 2:M:107:TYR:CE2 | 2.48 | 0.48 |
| 2:M:228:VAL:HG21 | 2:M:282:LEU:HD12 | 1.95 | 0.48 |
| 1:P:518:LEU:HD11 | 1:P:527:CYS:SG | 2.52 | 0.48 |
| 2:A:174:PRO:HB2 | 2:A:259:ARG:NH1 | 2.28 | 0.48 |
| 2:B:26:ALA:HB2 | 4:H:417:GLN:HB3 | 1.95 | 0.48 |
| 2:B:54:ILE:HG13 | 2:B:107:TYR:CE2 | 2.48 | 0.48 |
| 2:C:154:ASN:N | 2:C:154:ASN:OD1 | 2.45 | 0.48 |
| 2:F:250:VAL:O | 2:F:265:LEU:HD23 | 2.13 | 0.48 |
| 3:I:19:ALA:HB3 | 3:I:108:GLU:HB3 | 1.95 | 0.48 |
| 3:I:110:GLN:HA | 3:J:80:ARG:NH1 | 2.27 | 0.48 |
| 3:G:94:ASN:HB3 | 3:G:97:GLN:HG2 | 1.95 | 0.48 |
| 4:H:245:GLN:O | 4:H:249:GLU:HG3 | 2.13 | 0.48 |
| 4:H:445:ILE:HD11 | 4:H:453:MET:HB2 | 1.94 | 0.48 |
| 4:H:514:ARG:CG | 3:J:42:GLY:HA2 | 2.43 | 0.48 |
| 3:J:110:GLN:O | 3:J:114:THR:HG23 | 2.13 | 0.48 |
| 6:L:9:DG:H2' | 6:L:10:DA:C5 | 2.47 | 0.48 |
| 2:M:134:SER:OG | 2:M:180:CYS:HB2 | 2.13 | 0.48 |
| 1:P:181:GLU:HA | 1:P:660:THR:HA | 1.93 | 0.48 |
| 1:P:254:GLU:HA | 1:P:257:ALA:HB3 | 1.96 | 0.48 |
| 1:P:558:ILE:HG22 | 1:P:585:ARG:HG3 | 1.95 | 0.48 |
| 2:B:107:TYR:HD1 | 2:B:110:ARG:HH11 | 1.60 | 0.48 |
| 2:B:134:SER:HB3 | 2:B:180:CYS:HB2 | 1.95 | 0.48 |
| 2:D:165:ARG:HB2 | 6:L:16:DA:H1' | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:68:ARG:HG3 | 2:C:69:GLU:H | 1.78 | 0.48 |
| 2:E:13:PHE:HA | 2:E:224:ARG:H | 1.79 | 0.48 |
| 2:E:115:VAL:HG22 | 5:K:35:G:C4 | 2.48 | 0.48 |
| 2:E:268:VAL:HG21 | 2:E:281:LYS:HE3 | 1.94 | 0.48 |
| 2:F:134:SER:HB2 | 2:F:180:CYS:HB2 | 1.95 | 0.48 |
| 3:G:71:ARG:NH2 | 3:G:118:LEU:HD23 | 2.29 | 0.48 |
| 4:H:34:ILE:O | 4:H:160:ARG:N | 2.33 | 0.48 |
| 4:H:474:LEU:HD12 | 4:H:536:ILE:HG13 | 1.95 | 0.48 |
| 2:M:25:ASP:OD1 | 7:N:66:ARG:HG3 | 2.13 | 0.48 |
| 2:M:203:TRP:HE3 | 2:M:226:LEU:HD21 | 1.78 | 0.48 |
| 7:N:4:ILE:HG22 | 7:N:4:ILE:O | 2.14 | 0.48 |
| 7:N:16:ARG:HG2 | 7:N:26:TYR:CD1 | 2.49 | 0.48 |
| 1:P:126:TYR:CD2 | 4:H:302:ASP:HB2 | 2.49 | 0.48 |
| 1:P:329:VAL:HG23 | 1:P:347:THR:HG22 | 1.94 | 0.48 |
| 1:P:678:GLU:O | 1:P:681:HIS:NE2 | 2.46 | 0.48 |
| 2:D:48:ARG:HG2 | 5:K:32:A:O4' | 2.14 | 0.48 |
| 2:C:44:VAL:HG12 | 5:K:19:U:OP2 | 2.13 | 0.48 |
| 2:F:10:VAL:HG22 | 2:F:181:HIS:HD2 | 1.78 | 0.48 |
| 2:F:99:ARG:NH2 | 2:F:191:GLN:O | 2.37 | 0.48 |
| 2:F:129:VAL:HG22 | 2:F:184:ILE:CG1 | 2.43 | 0.48 |
| 2:F:169:ARG:HB3 | 2:F:171:PHE:CE1 | 2.49 | 0.48 |
| 4:H:3:LEU:HD21 | 4:H:221:PHE:CE2 | 2.47 | 0.48 |
| 1:P:231:ARG:HH12 | 1:P:292:LEU:HD13 | 1.78 | 0.48 |
| 1:P:564:LEU:HD13 | 1:P:566:PHE:HE1 | 1.78 | 0.48 |
| 1:P:613:LYS:HE3 | 4:H:47:ASP:OD2 | 2.13 | 0.48 |
| 1:P:643:ARG:HB3 | 1:P:647:LYS:HE3 | 1.95 | 0.48 |
| 2:B:54:ILE:HG13 | 2:B:107:TYR:CD2 | 2.48 | 0.48 |
| 2:D:13:PHE:CZ | 2:D:46:LEU:HD21 | 2.49 | 0.48 |
| 2:C:76:LEU:HD23 | 2:C:106:TYR:CZ | 2.48 | 0.48 |
| 2:E:13:PHE:CE1 | 2:E:46:LEU:HD11 | 2.48 | 0.48 |
| 2:F:43:ASP:HB3 | 2:F:132:THR:C | 2.34 | 0.48 |
| 2:F:51:ARG:NH2 | 5:K:43:C:H5'' | 2.29 | 0.48 |
| 2:F:62:HIS:HA | 2:F:104:SER:O | 2.14 | 0.48 |
| 3:G:25:GLN:OE1 | 3:G:36:ILE:N | 2.42 | 0.48 |
| 4:H:273:CYS:SG | 4:H:301:ILE:HB | 2.54 | 0.48 |
| 4:H:301:ILE:HG13 | 4:H:305:LYS:HD3 | 1.96 | 0.48 |
| 4:H:482:GLN:HG3 | 4:H:519:HIS:CE1 | 2.48 | 0.48 |
| 2:M:149:ARG:HE | 2:M:166:THR:CG2 | 2.24 | 0.48 |
| 1:P:125:TRP:NE1 | 1:P:667:ASN:OD1 | 2.31 | 0.48 |
| 1:P:669:LEU:O | 1:P:669:LEU:HD23 | 2.14 | 0.48 |
| 2:A:68:ARG:HG2 | 2:A:69:GLU:H | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:195:SER:H | 2:A:198:ASP:HB2 | 1.79 | 0.48 |
| 2:B:51:ARG:HE | 2:B:108:ASP:CG | 2.17 | 0.48 |
| 2:E:3:ILE:HD12 | 2:E:196:GLU:HG3 | 1.95 | 0.48 |
| 3:G:7:ARG:HG2 | 3:G:12:TYR:CD2 | 2.34 | 0.48 |
| 4:H:287:SER:OG | 4:H:288:MET:SD | 2.71 | 0.48 |
| 3:J:95:LEU:HA | 3:J:98:GLN:HB2 | 1.95 | 0.48 |
| 7:N:35:ARG:NH1 | 7:N:174:ASP:OD1 | 2.43 | 0.48 |
| 7:N:171:MET:HG3 | 7:N:194:GLN:NE2 | 2.26 | 0.48 |
| 8:O:16:DA:H1' | 8:O:17:DA:H5' | 1.95 | 0.48 |
| 1:P:96:ALA:O | 1:P:100:VAL:HG13 | 2.13 | 0.48 |
| 2:B:56:MET:SD | 2:B:212:HIS:HB3 | 2.54 | 0.48 |
| 2:B:246:ARG:HD3 | 2:B:273:LEU:HD23 | 1.96 | 0.48 |
| 2:D:77:ILE:HA | 2:D:102:MET:CE | 2.43 | 0.48 |
| 2:D:273:LEU:HB2 | 2:D:277:LYS:HE2 | 1.95 | 0.48 |
| 2:E:69:GLU:O | 2:E:71:GLY:N | 2.43 | 0.48 |
| 3:G:110:GLN:O | 3:G:114:THR:HG23 | 2.13 | 0.48 |
| 7:N:128:ARG:HG2 | 7:N:133:GLN:HB2 | 1.96 | 0.48 |
| 1:P:189:PHE:HD2 | 1:P:190:LEU:HD12 | 1.79 | 0.48 |
| 1:P:424:THR:HG21 | 1:P:428:PRO:HD3 | 1.95 | 0.48 |
| 1:P:651:ASP:OD2 | 1:P:656:THR:HG22 | 2.14 | 0.48 |
| 2:A:134:SER:HB3 | 2:A:178:TYR:HB3 | 1.95 | 0.48 |
| 2:B:47:LYS:HD3 | 5:K:13:U:OP1 | 2.14 | 0.48 |
| 2:B:109:ILE:HD13 | 2:B:116:MET:CE | 2.43 | 0.48 |
| 2:D:68:ARG:NH2 | 2:D:69:GLU:HB2 | 2.28 | 0.48 |
| 2:D:116:MET:C | 2:D:118:THR:H | 2.17 | 0.48 |
| 2:D:270:ASP:OD1 | 2:D:270:ASP:N | 2.38 | 0.48 |
| 2:F:13:PHE:CZ | 2:F:46:LEU:HD21 | 2.48 | 0.48 |
| 2:F:270:ASP:HA | 2:F:273:LEU:HD21 | 1.96 | 0.48 |
| 4:H:3:LEU:HA | 4:H:6:LEU:HD12 | 1.95 | 0.48 |
| 4:H:85:TYR:HE1 | 4:H:93:GLY:H | 1.62 | 0.48 |
| 4:H:471:LEU:HD23 | 4:H:505:PRO:HB3 | 1.95 | 0.48 |
| 2:M:102:MET:HG3 | 2:M:116:MET:SD | 2.53 | 0.48 |
| 2:M:128:PRO:HG2 | 2:M:194:PHE:CD2 | 2.49 | 0.48 |
| 1:P:576:LEU:HA | 1:P:579:ILE:HB | 1.96 | 0.48 |
| 2:B:18:GLY:O | 2:B:20:PRO:HD3 | 2.14 | 0.48 |
| 2:B:146:SER:HB2 | 2:B:169:ARG:NH2 | 2.29 | 0.48 |
| 2:E:144:GLU:HG2 | 2:E:171:PHE:HE1 | 1.78 | 0.48 |
| 2:E:156:LYS:HZ2 | 2:E:158:ALA:HB3 | 1.79 | 0.48 |
| 2:F:243:LEU:HD11 | 2:F:277:LYS:CD | 2.43 | 0.48 |
| 3:G:49:ILE:HD13 | 3:G:91:ASN:OD1 | 2.14 | 0.48 |
| 4:H:40:GLY:HA2 | 4:H:130:PHE:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:127:VAL:HA | 4:H:130:PHE:HB3 | 1.96 | 0.48 |
| 4:H:392:ASN:HB3 | 4:H:398:ILE:HG23 | 1.96 | 0.48 |
| 4:H:482:GLN:HG3 | 4:H:519:HIS:NE2 | 2.29 | 0.48 |
| 5:K:13:U:C4 | 2:M:147:ILE:HD11 | 2.49 | 0.48 |
| 6:L:39:DC:H2'' | 6:L:40:DT:H5' | 1.95 | 0.48 |
| 2:M:20:PRO:HD2 | 2:M:30:PRO:HB3 | 1.95 | 0.48 |
| 2:M:96:GLU:OE2 | 2:M:99:ARG:NH2 | 2.47 | 0.48 |
| 2:M:140:ILE:HB | 2:M:173:VAL:HG13 | 1.95 | 0.48 |
| 7:N:7:ILE:HD11 | 7:N:37:ILE:HG21 | 1.95 | 0.48 |
| 9:Q:-1:DA:OP2 | 9:Q:-1:DA:H8 | 1.96 | 0.48 |
| 1:P:21:PRO:HG2 | 1:P:24:LYS:NZ | 2.29 | 0.48 |
| 1:P:30:ALA:CB | 1:P:50:LEU:HD12 | 2.44 | 0.48 |
| 1:P:170:PHE:HZ | 1:P:178:ALA:HB2 | 1.77 | 0.48 |
| 1:P:184:HIS:CG | 1:P:659:LEU:HB3 | 2.49 | 0.48 |
| 2:B:89:LYS:O | 2:B:94:LYS:N | 2.47 | 0.48 |
| 2:F:83:GLN:O | 2:F:86:VAL:N | 2.46 | 0.48 |
| 2:F:215:SER:HB3 | 2:F:218:ARG:HB2 | 1.95 | 0.48 |
| 3:G:95:LEU:HA | 3:G:98:GLN:HB2 | 1.95 | 0.48 |
| 4:H:42:PHE:HB2 | 4:H:130:PHE:HE1 | 1.79 | 0.48 |
| 4:H:240:PHE:HB3 | 7:N:17:SER:C | 2.34 | 0.48 |
| 3:J:71:ARG:NH2 | 3:J:118:LEU:HD23 | 2.29 | 0.48 |
| 1:P:506:PHE:CD1 | 1:P:517:HIS:HB2 | 2.49 | 0.47 |
| 2:A:91:LYS:HD2 | 2:A:92:GLY:N | 2.29 | 0.47 |
| 2:B:51:ARG:CZ | 2:B:108:ASP:OD1 | 2.62 | 0.47 |
| 2:D:31:ARG:HB2 | 2:D:40:LEU:O | 2.14 | 0.47 |
| 3:I:71:ARG:NH2 | 3:I:118:LEU:HD23 | 2.28 | 0.47 |
| 6:L:23:DT:H5' | 6:L:23:DT:O2 | 2.14 | 0.47 |
| 2:M:13:PHE:O | 2:M:177:LEU:HD12 | 2.14 | 0.47 |
| 7:N:8:SER:HA | 7:N:99:ALA:HA | 1.96 | 0.47 |
| 1:P:487:ALA:HA | 1:P:551:TRP:CZ3 | 2.49 | 0.47 |
| 2:A:21:ASN:HD22 | 2:A:42:THR:N | 2.04 | 0.47 |
| 2:B:77:ILE:HG23 | 2:B:122:ALA:CB | 2.44 | 0.47 |
| 2:B:102:MET:CE | 2:B:122:ALA:HB1 | 2.44 | 0.47 |
| 2:B:152:VAL:HB | 2:B:164:ASN:HB3 | 1.96 | 0.47 |
| 2:D:137:ILE:HG12 | 2:D:177:LEU:O | 2.14 | 0.47 |
| 2:E:143:LEU:HG | 2:E:145:HIS:CE1 | 2.49 | 0.47 |
| 2:F:45:CYS:O | 2:F:49:LYS:HG2 | 2.13 | 0.47 |
| 1:P:354:TRP:CD2 | 1:P:359:ILE:HG12 | 2.50 | 0.47 |
| 1:P:518:LEU:HA | 1:P:522:MET:SD | 2.54 | 0.47 |
| 1:P:580:ALA:HB2 | 1:P:637:PHE:CZ | 2.49 | 0.47 |
| 2:A:34:PRO:HB3 | 3:J:47:THR:HG23 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:199:LEU:HD21 | 2:A:203:TRP:HE1 | 1.79 | 0.47 |
| 2:C:115:VAL:HG22 | 5:K:17:C:C2 | 2.50 | 0.47 |
| 2:E:246:ARG:NE | 2:E:273:LEU:HD23 | 2.18 | 0.47 |
| 2:F:40:LEU:HD21 | 2:F:135:ARG:NH1 | 2.29 | 0.47 |
| 3:I:7:ARG:CG | 3:I:12:TYR:HD2 | 2.22 | 0.47 |
| 3:J:44:ALA:HB2 | 3:J:51:VAL:HG21 | 1.96 | 0.47 |
| 5:K:7:A:OP1 | 2:M:47:LYS:HD3 | 2.15 | 0.47 |
| 2:M:233:ASN:OD1 | 2:M:237:ASP:HB3 | 2.14 | 0.47 |
| 7:N:168:PHE:HB2 | 7:N:194:GLN:NE2 | 2.30 | 0.47 |
| 8:O:19:DA:H1' | 8:O:20:DA:C4 | 2.49 | 0.47 |
| 1:P:69:SER:OG | 11:P:803:PO4:P | 2.71 | 0.47 |
| 1:P:123:ALA:HB1 | 1:P:129:GLY:O | 2.14 | 0.47 |
| 2:A:129:VAL:HG11 | 2:A:202:PHE:CZ | 2.49 | 0.47 |
| 3:I:25:GLN:OE1 | 3:I:36:ILE:N | 2.42 | 0.47 |
| 3:I:49:ILE:HD13 | 3:I:91:ASN:OD1 | 2.14 | 0.47 |
| 3:G:19:ALA:HB3 | 3:G:108:GLU:HB3 | 1.95 | 0.47 |
| 1:P:381:ILE:H | 1:P:381:ILE:HD12 | 1.78 | 0.47 |
| 1:P:518:LEU:HD23 | 1:P:558:ILE:HG12 | 1.96 | 0.47 |
| 2:C:81:HIS:NE2 | 2:C:120:LYS:O | 2.47 | 0.47 |
| 2:E:65:ILE:HB | 2:E:67:ILE:HG22 | 1.96 | 0.47 |
| 2:E:79:GLU:HA | 2:E:82:GLU:HG2 | 1.96 | 0.47 |
| 2:F:42:THR:HG23 | 2:F:133:PHE:CE2 | 2.50 | 0.47 |
| 4:H:361:LEU:HD11 | 4:H:380:LEU:HD21 | 1.96 | 0.47 |
| 4:H:431:TYR:HB2 | 4:H:563:TYR:OH | 2.15 | 0.47 |
| 4:H:490:ASN:HD21 | 6:L:32:DC:H3' | 1.78 | 0.47 |
| 6:L:23:DT:O2 | 6:L:23:DT:H2' | 2.14 | 0.47 |
| 2:M:6:ARG:HD3 | 2:M:236:GLY:HA3 | 1.96 | 0.47 |
| 2:M:42:THR:HG21 | 7:N:67:ARG:HG2 | 1.96 | 0.47 |
| 1:P:186:TRP:HD1 | 1:P:416:TYR:HH | 1.61 | 0.47 |
| 2:A:174:PRO:HB2 | 2:A:259:ARG:HH12 | 1.79 | 0.47 |
| 2:D:91:LYS:HA | 2:D:94:LYS:HB3 | 1.96 | 0.47 |
| 2:D:112:PHE:HE1 | 2:D:131:LEU:HD13 | 1.80 | 0.47 |
| 2:D:121:ASN:ND2 | 2:C:163:ASP:OD2 | 2.46 | 0.47 |
| 2:C:11:PHE:HE1 | 2:C:223:ALA:HB1 | 1.80 | 0.47 |
| 2:C:32:ILE:HD11 | 4:H:507:ALA:HA | 1.97 | 0.47 |
| 2:C:68:ARG:HG3 | 2:C:69:GLU:N | 2.30 | 0.47 |
| 2:C:258:VAL:HG11 | 2:C:264:TYR:CZ | 2.49 | 0.47 |
| 3:I:44:ALA:HB2 | 3:I:51:VAL:HG21 | 1.96 | 0.47 |
| 4:H:31:PRO:HB2 | 4:H:32:PHE:CD2 | 2.50 | 0.47 |
| 4:H:37:ASP:HA | 4:H:162:VAL:HG12 | 1.96 | 0.47 |
| 4:H:535:GLU:OE2 | 4:H:569:LEU:HD21 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:19:ALA:HB3 | 3:J:108:GLU:HB3 | 1.95 | 0.47 |
| 5:K:3:U:O2 | 7:N:35:ARG:NH1 | 2.42 | 0.47 |
| 2:M:6:ARG:NH2 | 2:M:236:GLY:HA3 | 2.30 | 0.47 |
| 2:M:103:CYS:SG | 2:M:125:VAL:HG11 | 2.54 | 0.47 |
| 2:M:133:PHE:HZ | 7:N:67:ARG:HD3 | 1.79 | 0.47 |
| 1:P:55:GLY:O | 1:P:58:GLN:HB2 | 2.14 | 0.47 |
| 1:P:345:ALA:H | 1:P:348:ARG:HB3 | 1.80 | 0.47 |
| 1:P:399:ARG:NH2 | 1:P:614:GLN:OE1 | 2.33 | 0.47 |
| 2:A:135:ARG:NE | 2:C:17:ASP:OD2 | 2.36 | 0.47 |
| 2:A:143:LEU:HD21 | 2:D:34:PRO:HG2 | 1.97 | 0.47 |
| 2:A:147:ILE:HD11 | 5:K:31:C:C4 | 2.50 | 0.47 |
| 2:A:218:ARG:HD3 | 2:A:221:MET:HE2 | 1.96 | 0.47 |
| 2:B:17:ASP:CG | 2:C:135:ARG:HH22 | 2.18 | 0.47 |
| 2:D:22:GLY:HA3 | 2:D:28:ASN:OD1 | 2.15 | 0.47 |
| 2:D:102:MET:HG3 | 2:D:116:MET:SD | 2.55 | 0.47 |
| 2:D:246:ARG:NE | 2:D:269:ASP:O | 2.36 | 0.47 |
| 2:C:33:ASP:N | 2:C:38:GLU:O | 2.38 | 0.47 |
| 2:C:142:THR:HG22 | 2:C:144:GLU:HG3 | 1.97 | 0.47 |
| 3:G:7:ARG:CG | 3:G:12:TYR:HD2 | 2.22 | 0.47 |
| 3:G:48:PRO:CG | 3:G:93:LEU:HG | 2.45 | 0.47 |
| 4:H:24:GLY:HA2 | 4:H:183:ASN:HD22 | 1.78 | 0.47 |
| 4:H:127:VAL:O | 4:H:131:LEU:N | 2.45 | 0.47 |
| 4:H:437:LEU:C | 4:H:560:ILE:HD11 | 2.35 | 0.47 |
| 4:H:474:LEU:HD23 | 4:H:509:PHE:CD1 | 2.50 | 0.47 |
| 3:J:88:ARG:NH2 | 3:J:90:PRO:HA | 2.30 | 0.47 |
| 5:K:5:A:HI' | 2:M:124:GLN:HB3 | 1.97 | 0.47 |
| 2:A:109:ILE:HD13 | 2:A:116:MET:SD | 2.54 | 0.47 |
| 2:D:243:LEU:HD23 | 2:D:246:ARG:HD2 | 1.97 | 0.47 |
| 2:E:40:LEU:HD23 | 2:E:133:PHE:CD2 | 2.47 | 0.47 |
| 2:F:58:GLN:HE21 | 2:F:63:HIS:CD2 | 2.32 | 0.47 |
| 4:H:42:PHE:HB2 | 4:H:130:PHE:CE1 | 2.50 | 0.47 |
| 3:J:48:PRO:CG | 3:J:93:LEU:HG | 2.45 | 0.47 |
| 3:J:49:ILE:HD13 | 3:J:91:ASN:OD1 | 2.14 | 0.47 |
| 2:M:48:ARG:HH22 | 2:M:67:ILE:HG22 | 1.79 | 0.47 |
| 2:M:120:LYS:HE3 | 7:N:183:ARG:HB2 | 1.97 | 0.47 |
| 1:P:224:ALA:HB3 | 1:P:350:ALA:HB2 | 1.97 | 0.47 |
| 2:A:144:GLU:OE1 | 3:J:54:THR:HG22 | 2.15 | 0.47 |
| 2:B:126:ARG:CD | 5:K:11:G:H5'' | 2.45 | 0.47 |
| 2:B:149:ARG:NH2 | 2:B:153:THR:HG1 | 2.12 | 0.47 |
| 2:D:126:ARG:HG3 | 5:K:29:G:H5'' | 1.96 | 0.47 |
| 2:D:129:VAL:HG13 | 2:D:184:ILE:HG12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:149:ARG:HG2 | 2:C:151:ALA:H | 1.80 | 0.47 |
| 2:E:229:PHE:CE2 | 2:E:279:LEU:HD11 | 2.49 | 0.47 |
| 3:G:88:ARG:NH2 | 3:G:90:PRO:HA | 2.30 | 0.47 |
| 4:H:328:LEU:HB2 | 4:H:342:TRP:CZ3 | 2.49 | 0.47 |
| 5:K:17:C:H2' | 5:K:18:U:H5' | 1.97 | 0.47 |
| 2:M:40:LEU:HD12 | 2:M:133:PHE:HB3 | 1.97 | 0.47 |
| 7:N:7:ILE:HD13 | 7:N:149:PHE:HB3 | 1.96 | 0.47 |
| 7:N:198:VAL:HG23 | 7:N:199:ASN:N | 2.28 | 0.47 |
| 2:D:91:LYS:HD3 | 2:C:160:GLU:O | 2.15 | 0.47 |
| 3:I:48:PRO:CG | 3:I:93:LEU:HG | 2.45 | 0.47 |
| 3:G:33:ASN:N | 6:L:13:DG:OP2 | 2.43 | 0.47 |
| 4:H:461:ASP:O | 4:H:463:ASN:N | 2.43 | 0.47 |
| 3:J:94:ASN:HB3 | 3:J:97:GLN:HG2 | 1.95 | 0.47 |
| 5:K:3:U:C6 | 7:N:184:ASP:HB3 | 2.50 | 0.47 |
| 1:P:30:ALA:HB1 | 1:P:50:LEU:HD12 | 1.97 | 0.46 |
| 1:P:32:LEU:HD13 | 1:P:213:ASP:HB3 | 1.98 | 0.46 |
| 1:P:256:HIS:O | 1:P:260:GLN:HB2 | 2.15 | 0.46 |
| 1:P:306:ALA:HA | 1:P:361:THR:O | 2.15 | 0.46 |
| 1:P:492:VAL:HG22 | 1:P:568:CYS:SG | 2.54 | 0.46 |
| 2:A:69:GLU:O | 2:A:71:GLY:N | 2.47 | 0.46 |
| 2:A:215:SER:HB3 | 2:A:218:ARG:HG2 | 1.98 | 0.46 |
| 2:B:47:LYS:O | 2:B:51:ARG:HG3 | 2.14 | 0.46 |
| 2:B:143:LEU:HA | 2:B:143:LEU:HD23 | 1.66 | 0.46 |
| 2:B:148:THR:O | 5:K:20:G:H5'' | 2.15 | 0.46 |
| 2:D:131:LEU:HD11 | 2:D:202:PHE:HZ | 1.79 | 0.46 |
| 2:E:246:ARG:HB3 | 2:E:269:ASP:HB2 | 1.97 | 0.46 |
| 3:I:94:ASN:HB3 | 3:I:97:GLN:HG2 | 1.96 | 0.46 |
| 3:G:44:ALA:HB2 | 3:G:51:VAL:HG21 | 1.96 | 0.46 |
| 4:H:393:LEU:HB2 | 4:H:397:LEU:HD23 | 1.97 | 0.46 |
| 4:H:395:SER:OG | 2:M:169:ARG:NH1 | 2.47 | 0.46 |
| 4:H:411:LEU:HD23 | 4:H:415:LEU:CD1 | 2.45 | 0.46 |
| 4:H:420:LEU:O | 4:H:424:LYS:HG2 | 2.15 | 0.46 |
| 7:N:36:ASN:ND2 | 7:N:139:TYR:OH | 2.38 | 0.46 |
| 1:P:20:HIS:HB2 | 1:P:205:PHE:CD2 | 2.51 | 0.46 |
| 1:P:103:LEU:CD2 | 1:P:166:LEU:HD13 | 2.46 | 0.46 |
| 1:P:104:ASN:OD1 | 1:P:105:PRO:HD2 | 2.15 | 0.46 |
| 1:P:199:PHE:CE1 | 1:P:203:GLU:HG3 | 2.50 | 0.46 |
| 1:P:270:ARG:HB2 | 1:P:273:PHE:CZ | 2.51 | 0.46 |
| 2:A:23:ASP:HB2 | 2:A:28:ASN:HA | 1.97 | 0.46 |
| 2:A:252:LYS:HE2 | 2:A:262:ASP:O | 2.14 | 0.46 |
| 2:B:5:LYS:HD3 | 2:B:231:HIS:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:183:PHE:CZ | 2:M:220:GLN:HG3 | 2.49 | 0.46 |
| 2:E:229:PHE:CZ | 2:E:279:LEU:HD11 | 2.50 | 0.46 |
| 2:F:129:VAL:HG22 | 2:F:184:ILE:HG12 | 1.97 | 0.46 |
| 3:I:112:LEU:HD23 | 3:I:112:LEU:HA | 1.66 | 0.46 |
| 3:G:21:LEU:HD21 | 3:G:59:LEU:HD22 | 1.98 | 0.46 |
| 4:H:173:LYS:HD2 | 4:H:173:LYS:O | 2.15 | 0.46 |
| 4:H:226:LEU:HD23 | 4:H:226:LEU:HA | 1.84 | 0.46 |
| 5:K:8:C:O2' | 7:N:68:ASN:OD1 | 2.33 | 0.46 |
| 6:L:20:DC:H2'' | 6:L:21:DG:C8 | 2.50 | 0.46 |
| 7:N:180:SER:HB3 | 7:N:184:ASP:HA | 1.96 | 0.46 |
| 1:P:9:ALA:HB1 | 1:P:71:PHE:HB2 | 1.97 | 0.46 |
| 1:P:36:PHE:CD1 | 1:P:382:HIS:CE1 | 3.04 | 0.46 |
| 1:P:536:ARG:HG2 | 1:P:721:LEU:HD11 | 1.97 | 0.46 |
| 2:A:269:ASP:OD1 | 2:A:269:ASP:N | 2.46 | 0.46 |
| 2:B:35:GLN:HG3 | 2:M:257:VAL:HG21 | 1.98 | 0.46 |
| 2:B:72:ILE:H | 2:B:72:ILE:HD12 | 1.81 | 0.46 |
| 2:B:126:ARG:HG2 | 2:B:188:PHE:CE1 | 2.50 | 0.46 |
| 2:B:218:ARG:NH2 | 5:K:16:G:H5' | 2.30 | 0.46 |
| 2:D:259:ARG:NH1 | 2:E:35:GLN:HB2 | 2.31 | 0.46 |
| 2:C:179:ARG:NH1 | 2:C:181:HIS:HE1 | 2.14 | 0.46 |
| 2:E:149:ARG:HB2 | 5:K:43:C:H1' | 1.96 | 0.46 |
| 2:E:153:THR:HB | 6:L:13:DG:H4' | 1.98 | 0.46 |
| 4:H:224:VAL:HG22 | 7:N:21:VAL:HG13 | 1.96 | 0.46 |
| 4:H:269:VAL:O | 4:H:269:VAL:HG13 | 2.16 | 0.46 |
| 5:K:14:C:C2' | 5:K:15:A:H4' | 2.46 | 0.46 |
| 5:K:26:G:H2' | 5:K:27:G:H4' | 1.97 | 0.46 |
| 2:M:48:ARG:O | 2:M:48:ARG:HD3 | 2.15 | 0.46 |
| 7:N:62:TRP:CE3 | 7:N:93:MET:HG2 | 2.50 | 0.46 |
| 1:P:133:ARG:NH1 | 4:H:316:TYR:O | 2.49 | 0.46 |
| 2:A:149:ARG:NH2 | 6:L:24:DG:H21 | 2.04 | 0.46 |
| 2:A:246:ARG:HH12 | 2:A:273:LEU:N | 2.12 | 0.46 |
| 2:B:249:VAL:HG13 | 2:B:266:VAL:HG22 | 1.97 | 0.46 |
| 2:D:81:HIS:NE2 | 2:D:120:LYS:O | 2.49 | 0.46 |
| 2:C:82:GLU:HA | 2:C:86:VAL:HG12 | 1.96 | 0.46 |
| 2:F:39:GLY:N | 2:F:136:SER:OG | 2.46 | 0.46 |
| 3:I:108:GLU:O | 3:I:112:LEU:HG | 2.16 | 0.46 |
| 4:H:83:ASP:HB2 | 4:H:107:PHE:CE1 | 2.50 | 0.46 |
| 5:K:8:C:O2' | 7:N:68:ASN:HB2 | 2.15 | 0.46 |
| 2:M:275:GLU:OE2 | 2:M:277:LYS:NZ | 2.26 | 0.46 |
| 7:N:26:TYR:O | 7:N:95:LEU:HD11 | 2.15 | 0.46 |
| 1:P:44:PHE:HD2 | 1:P:190:LEU:CD2 | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:441:ILE:H | 1:P:441:ILE:HD12 | 1.80 | 0.46 |
| 2:A:95:THR:HG21 | 2:B:162:GLY:HA2 | 1.97 | 0.46 |
| 2:B:99:ARG:HB2 | 2:B:123:GLY:HA3 | 1.98 | 0.46 |
| 2:B:232:SER:N | 2:B:237:ASP:OD2 | 2.35 | 0.46 |
| 2:D:54:ILE:HG13 | 2:D:107:TYR:CE2 | 2.51 | 0.46 |
| 2:D:148:THR:O | 5:K:38:C:H5'' | 2.15 | 0.46 |
| 2:E:21:ASN:ND2 | 2:E:42:THR:H | 2.14 | 0.46 |
| 2:F:19:ASN:HB3 | 2:F:22:GLY:H | 1.80 | 0.46 |
| 3:I:88:ARG:NH2 | 3:I:90:PRO:HA | 2.30 | 0.46 |
| 4:H:30:ILE:HG23 | 4:H:156:ASN:O | 2.14 | 0.46 |
| 4:H:490:ASN:ND2 | 6:L:32:DC:H3' | 2.31 | 0.46 |
| 4:H:540:LEU:HA | 4:H:540:LEU:HD12 | 1.71 | 0.46 |
| 3:J:108:GLU:O | 3:J:112:LEU:HG | 2.16 | 0.46 |
| 7:N:57:LEU:HB2 | 7:N:99:ALA:HB3 | 1.97 | 0.46 |
| 1:P:331:GLU:N | 1:P:361:THR:HG22 | 2.29 | 0.46 |
| 1:P:611:SER:HB2 | 1:P:644:PHE:HZ | 1.80 | 0.46 |
| 2:B:128:PRO:O | 2:B:184:ILE:HA | 2.15 | 0.46 |
| 2:B:136:SER:HA | 2:B:178:TYR:HA | 1.98 | 0.46 |
| 2:E:62:HIS:HA | 2:E:104:SER:O | 2.16 | 0.46 |
| 2:E:102:MET:O | 2:E:106:TYR:HB2 | 2.15 | 0.46 |
| 2:E:127:GLY:O | 2:E:130:GLN:NE2 | 2.37 | 0.46 |
| 3:I:106:TYR:CD1 | 3:J:80:ARG:HG2 | 2.51 | 0.46 |
| 4:H:481:ILE:HG22 | 4:H:519:HIS:HB3 | 1.97 | 0.46 |
| 3:J:21:LEU:HD21 | 3:J:59:LEU:HD22 | 1.98 | 0.46 |
| 2:M:12:LEU:HD21 | 2:M:249:VAL:CG2 | 2.46 | 0.46 |
| 7:N:57:LEU:HD11 | 7:N:101:ARG:HB3 | 1.96 | 0.46 |
| 1:P:126:TYR:O | 1:P:130:SER:HB3 | 2.15 | 0.46 |
| 1:P:203:GLU:HA | 1:P:206:MET:HB2 | 1.96 | 0.46 |
| 1:P:307:ILE:CD1 | 1:P:392:ASP:HB3 | 2.46 | 0.46 |
| 2:A:151:ALA:HB2 | 2:D:67:ILE:O | 2.16 | 0.46 |
| 2:B:20:PRO:HD2 | 2:B:30:PRO:HB3 | 1.98 | 0.46 |
| 2:B:44:VAL:HG12 | 5:K:13:U:OP2 | 2.16 | 0.46 |
| 2:B:110:ARG:NE | 2:B:198:ASP:OD2 | 2.49 | 0.46 |
| 2:D:44:VAL:HG12 | 5:K:31:C:OP2 | 2.16 | 0.46 |
| 2:D:109:ILE:HG12 | 2:D:114:ALA:HB2 | 1.97 | 0.46 |
| 2:D:243:LEU:HD21 | 2:D:277:LYS:CE | 2.42 | 0.46 |
| 2:C:61:GLU:CD | 2:C:62:HIS:HD1 | 2.19 | 0.46 |
| 2:C:63:HIS:HA | 2:C:107:TYR:HB2 | 1.96 | 0.46 |
| 2:C:89:LYS:HA | 2:C:89:LYS:HD2 | 1.73 | 0.46 |
| 2:E:99:ARG:NH1 | 2:E:100:GLN:OE1 | 2.48 | 0.46 |
| 2:E:144:GLU:HA | 2:E:171:PHE:HD1 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:113:GLY:HA3 | 5:K:42:U:H5'' | 1.98 | 0.46 |
| 4:H:407:ASN:HB2 | 4:H:409:ARG:HG2 | 1.98 | 0.46 |
| 4:H:482:GLN:CD | 4:H:493:ILE:HG23 | 2.36 | 0.46 |
| 2:A:45:CYS:O | 2:A:49:LYS:HG2 | 2.15 | 0.46 |
| 2:D:144:GLU:HA | 2:D:171:PHE:CD1 | 2.49 | 0.46 |
| 2:D:154:ASN:OD1 | 2:E:74:ASN:ND2 | 2.44 | 0.46 |
| 2:C:68:ARG:HH22 | 5:K:20:G:H1 | 1.63 | 0.46 |
| 2:C:99:ARG:CG | 2:C:123:GLY:HA3 | 2.46 | 0.46 |
| 3:I:57:ARG:NH2 | 3:G:46:SER:HB3 | 2.30 | 0.46 |
| 4:H:376:PRO:O | 4:H:380:LEU:N | 2.45 | 0.46 |
| 3:J:93:LEU:HA | 3:J:93:LEU:HD23 | 1.79 | 0.46 |
| 2:M:238:ALA:HB2 | 2:M:277:LYS:HE3 | 1.97 | 0.46 |
| 1:P:44:PHE:CE1 | 1:P:166:LEU:HD21 | 2.50 | 0.46 |
| 2:F:38:GLU:OE1 | 2:F:135:ARG:NH2 | 2.48 | 0.46 |
| 1:P:320:PHE:CD2 | 1:P:358:LEU:HD21 | 2.50 | 0.46 |
| 1:P:464:ARG:HD3 | 1:P:587:ASN:ND2 | 2.31 | 0.46 |
| 1:P:499:ARG:HH11 | 1:P:521:ASN:HA | 1.80 | 0.46 |
| 1:P:580:ALA:HB2 | 1:P:637:PHE:CE1 | 2.51 | 0.46 |
| 1:P:592:LEU:HG | 1:P:593:PRO:HD2 | 1.98 | 0.46 |
| 2:A:39:GLY:O | 2:A:135:ARG:HA | 2.16 | 0.46 |
| 2:A:106:TYR:HB2 | 2:A:109:ILE:HD12 | 1.98 | 0.46 |
| 2:A:161:THR:O | 2:D:70:LYS:NZ | 2.35 | 0.46 |
| 2:B:20:PRO:HB2 | 2:B:41:VAL:HG22 | 1.98 | 0.46 |
| 2:D:39:GLY:N | 2:D:136:SER:OG | 2.48 | 0.46 |
| 2:E:110:ARG:HD3 | 2:E:198:ASP:OD2 | 2.16 | 0.46 |
| 2:E:118:THR:HA | 6:L:20:DC:H5'' | 1.97 | 0.46 |
| 2:E:280:ARG:HH12 | 2:E:282:LEU:HD21 | 1.81 | 0.46 |
| 4:H:39:GLN:HG2 | 4:H:41:ASN:ND2 | 2.30 | 0.46 |
| 4:H:219:ALA:HB1 | 4:H:335:ALA:O | 2.16 | 0.46 |
| 6:L:7:DA:H2'' | 6:L:8:DG:H5' | 1.96 | 0.46 |
| 1:P:412:LEU:C | 1:P:418:VAL:HG22 | 2.37 | 0.45 |
| 1:P:519:SER:HA | 1:P:555:THR:OG1 | 2.15 | 0.45 |
| 2:A:89:LYS:HA | 2:A:89:LYS:HD2 | 1.74 | 0.45 |
| 2:D:164:ASN:HB2 | 2:E:69:GLU:O | 2.16 | 0.45 |
| 2:C:6:ARG:HH12 | 2:C:240:ALA:HB2 | 1.81 | 0.45 |
| 3:I:61:HIS:HB3 | 6:L:17:DG:C5 | 2.51 | 0.45 |
| 4:H:54:LYS:HD2 | 8:O:17:DA:OP2 | 2.16 | 0.45 |
| 4:H:539:ILE:HD11 | 4:H:565:GLU:CD | 2.37 | 0.45 |
| 5:K:36:C:O2' | 5:K:37:C:OP2 | 2.29 | 0.45 |
| 2:M:105:ARG:HG3 | 2:M:106:TYR:CD2 | 2.51 | 0.45 |
| 1:P:489:ARG:HG3 | 1:P:492:VAL:CG2 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:16:GLN:N | 2:A:220:GLN:O | 2.46 | 0.45 |
| 2:A:89:LYS:O | 2:A:93:GLU:HG2 | 2.15 | 0.45 |
| 2:B:89:LYS:O | 2:B:93:GLU:HG2 | 2.16 | 0.45 |
| 2:B:105:ARG:HD3 | 2:B:106:TYR:CE1 | 2.50 | 0.45 |
| 2:B:243:LEU:O | 2:B:246:ARG:HB3 | 2.16 | 0.45 |
| 2:D:53:PHE:CD2 | 2:D:205:ALA:HA | 2.51 | 0.45 |
| 2:D:101:TYR:OH | 2:D:105:ARG:HD2 | 2.16 | 0.45 |
| 2:C:109:ILE:CG2 | 2:C:116:MET:HE1 | 2.46 | 0.45 |
| 2:C:243:LEU:CD1 | 2:C:277:LYS:HE3 | 2.46 | 0.45 |
| 2:E:33:ASP:HB2 | 2:E:40:LEU:HD11 | 1.99 | 0.45 |
| 2:F:273:LEU:HB2 | 2:F:277:LYS:HD2 | 1.97 | 0.45 |
| 4:H:168:LEU:HB2 | 4:H:171:GLN:CG | 2.43 | 0.45 |
| 6:L:44:DC:H2'' | 6:L:45:DC:H5' | 1.98 | 0.45 |
| 2:M:129:VAL:HG11 | 2:M:202:PHE:CE1 | 2.50 | 0.45 |
| 1:P:48:ALA:CB | 1:P:194:LEU:HD21 | 2.41 | 0.45 |
| 1:P:206:MET:HE2 | 11:P:803:PO4:O2 | 2.13 | 0.45 |
| 1:P:275:LEU:HB2 | 1:P:451:ILE:HD11 | 1.99 | 0.45 |
| 1:P:275:LEU:HG | 1:P:277:VAL:HG12 | 1.98 | 0.45 |
| 1:P:381:ILE:HA | 1:P:384:ILE:HD13 | 1.99 | 0.45 |
| 1:P:415:ASP:N | 1:P:415:ASP:OD1 | 2.48 | 0.45 |
| 1:P:571:ARG:NH1 | 1:P:574:ALA:HB3 | 2.31 | 0.45 |
| 2:A:6:ARG:NH1 | 2:A:231:HIS:HE1 | 2.14 | 0.45 |
| 2:D:229:PHE:CD2 | 2:D:243:LEU:HD22 | 2.52 | 0.45 |
| 2:D:280:ARG:HH21 | 2:D:282:LEU:HD11 | 1.81 | 0.45 |
| 2:C:31:ARG:HB2 | 2:C:40:LEU:O | 2.16 | 0.45 |
| 2:C:47:LYS:HD3 | 5:K:19:U:OP1 | 2.15 | 0.45 |
| 2:C:101:TYR:O | 2:C:104:SER:N | 2.50 | 0.45 |
| 2:E:2:THR:HG22 | 2:E:193:GLY:HA2 | 1.98 | 0.45 |
| 2:E:34:PRO:HG2 | 3:G:92:HIS:HD2 | 1.81 | 0.45 |
| 2:E:50:VAL:O | 2:E:54:ILE:HG12 | 2.16 | 0.45 |
| 2:F:258:VAL:HG11 | 2:F:264:TYR:CE2 | 2.51 | 0.45 |
| 3:G:61:HIS:CD2 | 6:L:11:DG:C2 | 3.04 | 0.45 |
| 4:H:31:PRO:HG2 | 4:H:155:CYS:SG | 2.56 | 0.45 |
| 4:H:69:ARG:HG2 | 4:H:77:VAL:CB | 2.45 | 0.45 |
| 3:J:120:ASN:O | 3:J:123:ASN:N | 2.48 | 0.45 |
| 2:M:15:VAL:CG1 | 2:M:20:PRO:HG3 | 2.46 | 0.45 |
| 2:M:47:LYS:HB3 | 2:M:51:ARG:HH12 | 1.82 | 0.45 |
| 2:M:70:LYS:N | 7:N:84:GLU:OE2 | 2.49 | 0.45 |
| 2:M:131:LEU:HD12 | 2:M:131:LEU:HA | 1.85 | 0.45 |
| 1:P:140:ASP:OD1 | 1:P:141:GLU:N | 2.49 | 0.45 |
| 1:P:412:LEU:HB3 | 1:P:418:VAL:HG21 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:523:CYS:O | 1:P:527:CYS:N | 2.36 | 0.45 |
| 2:A:34:PRO:HA | 3:J:49:ILE:HD11 | 1.98 | 0.45 |
| 2:B:17:ASP:CB | 2:C:133:PHE:HB2 | 2.46 | 0.45 |
| 2:B:247:ILE:HD12 | 2:B:268:VAL:HG12 | 1.97 | 0.45 |
| 2:D:224:ARG:HD3 | 2:D:224:ARG:HA | 1.71 | 0.45 |
| 2:C:42:THR:OG1 | 5:K:21:C:OP1 | 2.16 | 0.45 |
| 2:C:138:ASP:HB2 | 2:C:264:TYR:OH | 2.17 | 0.45 |
| 2:C:149:ARG:NH2 | 2:C:166:THR:OG1 | 2.46 | 0.45 |
| 2:E:72:ILE:H | 2:E:72:ILE:HD12 | 1.80 | 0.45 |
| 2:E:247:ILE:HD12 | 2:E:268:VAL:HG12 | 1.97 | 0.45 |
| 3:G:108:GLU:O | 3:G:112:LEU:HG | 2.16 | 0.45 |
| 4:H:1:MET:HE1 | 7:N:27:PRO:HG3 | 1.98 | 0.45 |
| 4:H:196:LEU:N | 4:H:241:PRO:O | 2.46 | 0.45 |
| 4:H:207:LEU:HA | 4:H:207:LEU:HD13 | 1.77 | 0.45 |
| 4:H:363:MET:HE2 | 4:H:434:ALA:HB1 | 1.99 | 0.45 |
| 4:H:478:LEU:HD13 | 4:H:512:LEU:HB3 | 1.98 | 0.45 |
| 4:H:517:PRO:HB3 | 3:J:37:ALA:HB1 | 1.99 | 0.45 |
| 5:K:9:A:OP1 | 2:M:42:THR:OG1 | 2.33 | 0.45 |
| 2:M:7:TYR:O | 2:M:184:ILE:N | 2.49 | 0.45 |
| 2:M:116:MET:O | 2:M:123:GLY:HA2 | 2.16 | 0.45 |
| 1:P:46:GLU:O | 1:P:50:LEU:N | 2.35 | 0.45 |
| 1:P:403:LYS:HA | 1:P:442:LEU:HD12 | 1.99 | 0.45 |
| 2:A:131:LEU:HD23 | 2:A:180:CYS:SG | 2.57 | 0.45 |
| 2:C:117:THR:O | 2:C:121:ASN:ND2 | 2.50 | 0.45 |
| 2:C:125:VAL:O | 5:K:17:C:O2' | 2.33 | 0.45 |
| 2:E:24:PRO:HD3 | 5:K:39:U:H5' | 1.99 | 0.45 |
| 2:F:6:ARG:HH11 | 2:F:236:GLY:HA3 | 1.81 | 0.45 |
| 4:H:32:PHE:CD1 | 4:H:47:ASP:HB3 | 2.52 | 0.45 |
| 4:H:66:GLY:HA2 | 4:H:79:ASN:ND2 | 2.31 | 0.45 |
| 4:H:514:ARG:O | 4:H:517:PRO:HD2 | 2.16 | 0.45 |
| 2:M:156:LYS:HB3 | 2:M:159:SER:HB3 | 1.97 | 0.45 |
| 1:P:11:GLN:HE21 | 1:P:15:ASN:HA | 1.81 | 0.45 |
| 2:B:154:ASN:HD22 | 6:L:38:DG:P | 2.40 | 0.45 |
| 2:D:163:ASP:HA | 2:E:69:GLU:HG3 | 1.99 | 0.45 |
| 2:E:9:PHE:HB3 | 2:E:228:VAL:HG22 | 1.98 | 0.45 |
| 2:F:12:LEU:HA | 2:F:178:TYR:O | 2.17 | 0.45 |
| 3:I:120:ASN:O | 3:I:123:ASN:N | 2.48 | 0.45 |
| 5:K:7:A:C4 | 7:N:69:GLU:OE1 | 2.69 | 0.45 |
| 5:K:9:A:H1' | 5:K:10:G:O4' | 2.17 | 0.45 |
| 7:N:36:ASN:HB2 | 7:N:139:TYR:CE1 | 2.52 | 0.45 |
| 1:P:329:VAL:HG11 | 1:P:356:ALA:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:658:LEU:HD22 | 1:P:672:LYS:HE3 | 1.98 | 0.45 |
| 2:A:17:ASP:O | 2:A:219:GLY:HA3 | 2.17 | 0.45 |
| 2:A:50:VAL:O | 2:A:54:ILE:HG12 | 2.16 | 0.45 |
| 2:C:181:HIS:HB3 | 2:C:244:PHE:CE2 | 2.52 | 0.45 |
| 2:E:8:ASP:O | 2:E:229:PHE:HD1 | 1.99 | 0.45 |
| 2:F:15:VAL:O | 2:F:175:TYR:HA | 2.17 | 0.45 |
| 3:I:58:LEU:HD11 | 6:L:18:DG:P | 2.56 | 0.45 |
| 4:H:429:ILE:CD1 | 4:H:559:ALA:HA | 2.46 | 0.45 |
| 4:H:466:ASP:O | 4:H:470:VAL:HG22 | 2.16 | 0.45 |
| 5:K:6:A:C4 | 2:M:115:VAL:HG11 | 2.52 | 0.45 |
| 2:M:213:ASP:O | 2:M:218:ARG:NH1 | 2.50 | 0.45 |
| 1:P:532:ALA:HB1 | 1:P:712:GLU:HA | 1.98 | 0.45 |
| 2:B:231:HIS:CD2 | 2:B:277:LYS:HZ2 | 2.35 | 0.45 |
| 2:D:247:ILE:HD12 | 2:D:268:VAL:HG12 | 1.99 | 0.45 |
| 2:E:42:THR:HG22 | 2:E:133:PHE:CZ | 2.51 | 0.45 |
| 2:F:109:ILE:O | 2:F:125:VAL:HG11 | 2.17 | 0.45 |
| 3:I:21:LEU:HD21 | 3:I:59:LEU:HD22 | 1.98 | 0.45 |
| 3:I:29:ASN:ND2 | 3:I:32:LEU:HD13 | 2.32 | 0.45 |
| 3:J:29:ASN:ND2 | 3:J:32:LEU:HD13 | 2.32 | 0.45 |
| 1:P:7:ALA:O | 1:P:56:LYS:HD3 | 2.17 | 0.45 |
| 2:A:54:ILE:HG13 | 2:A:107:TYR:CE2 | 2.51 | 0.45 |
| 2:A:70:LYS:NZ | 2:D:96:GLU:HB2 | 2.32 | 0.45 |
| 2:A:126:ARG:NH2 | 2:C:213:ASP:OD1 | 2.50 | 0.45 |
| 2:A:130:GLN:OE1 | 2:A:130:GLN:HA | 2.17 | 0.45 |
| 2:A:208:ASN:O | 2:A:212:HIS:ND1 | 2.47 | 0.45 |
| 2:A:256:GLU:HG3 | 2:A:257:VAL:HG22 | 1.99 | 0.45 |
| 2:B:46:LEU:HB3 | 2:B:209:MET:HE1 | 1.99 | 0.45 |
| 2:D:126:ARG:HH21 | 5:K:26:G:H21 | 1.65 | 0.45 |
| 2:C:3:ILE:HG22 | 2:C:196:GLU:HG3 | 1.99 | 0.45 |
| 2:C:31:ARG:NE | 2:C:42:THR:HG23 | 2.32 | 0.45 |
| 2:E:68:ARG:HD3 | 2:E:69:GLU:HB3 | 1.97 | 0.45 |
| 2:E:211:ASP:OD2 | 2:F:239:PRO:HA | 2.17 | 0.45 |
| 4:H:45:LEU:O | 4:H:145:ASN:ND2 | 2.46 | 0.45 |
| 2:M:3:ILE:O | 2:M:186:THR:OG1 | 2.33 | 0.45 |
| 2:M:259:ARG:HA | 2:M:259:ARG:HD3 | 1.69 | 0.45 |
| 7:N:24:VAL:HA | 7:N:93:MET:HB3 | 1.98 | 0.45 |
| 7:N:55:GLU:HB3 | 7:N:101:ARG:CG | 2.46 | 0.45 |
| 7:N:161:LEU:HB3 | 7:N:165:THR:OG1 | 2.17 | 0.45 |
| 7:N:180:SER:CB | 7:N:184:ASP:HA | 2.47 | 0.45 |
| 1:P:5:TYR:HD2 | 1:P:62:GLN:HG3 | 1.82 | 0.45 |
| 1:P:277:VAL:HG11 | 1:P:283:LYS:HA | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:9:PHE:CZ | 2:A:182:GLY:HA3 | 2.52 | 0.45 |
| 2:A:95:THR:HG22 | 2:A:121:ASN:O | 2.17 | 0.45 |
| 2:A:109:ILE:HG12 | 2:A:114:ALA:HB2 | 1.99 | 0.45 |
| 2:A:163:ASP:HA | 2:D:69:GLU:HG3 | 1.99 | 0.45 |
| 2:D:215:SER:HB3 | 2:D:218:ARG:HG2 | 1.99 | 0.45 |
| 2:C:47:LYS:HG2 | 2:C:112:PHE:CE1 | 2.52 | 0.45 |
| 2:F:144:GLU:HA | 2:F:171:PHE:CD1 | 2.52 | 0.45 |
| 2:F:258:VAL:HG11 | 2:F:264:TYR:CD2 | 2.52 | 0.45 |
| 3:I:98:GLN:HE21 | 3:J:57:ARG:NH1 | 2.15 | 0.45 |
| 4:H:535:GLU:HB3 | 4:H:575:LEU:HD11 | 1.99 | 0.45 |
| 5:K:9:A:C2 | 6:L:46:DT:H72 | 2.53 | 0.45 |
| 2:M:21:ASN:O | 2:M:31:ARG:HG3 | 2.16 | 0.45 |
| 2:M:102:MET:HE2 | 7:N:76:GLU:OE1 | 2.17 | 0.45 |
| 1:P:354:TRP:CG | 1:P:359:ILE:HG12 | 2.52 | 0.44 |
| 1:P:620:GLU:O | 1:P:624:LYS:HG3 | 2.17 | 0.44 |
| 2:B:95:THR:HG23 | 2:B:123:GLY:H | 1.82 | 0.44 |
| 2:D:99:ARG:HD3 | 2:D:125:VAL:HG22 | 1.98 | 0.44 |
| 2:E:54:ILE:HG13 | 2:E:107:TYR:CE2 | 2.51 | 0.44 |
| 2:E:259:ARG:NH1 | 2:F:35:GLN:HB2 | 2.32 | 0.44 |
| 4:H:141:MET:HG3 | 4:H:146:TRP:CE2 | 2.52 | 0.44 |
| 4:H:290:ASN:C | 4:H:292:GLY:HA2 | 2.36 | 0.44 |
| 4:H:429:ILE:HD11 | 4:H:498:PHE:CE2 | 2.52 | 0.44 |
| 4:H:479:GLU:OE1 | 4:H:562:TYR:OH | 2.09 | 0.44 |
| 2:M:114:ALA:HB3 | 2:M:125:VAL:HB | 1.98 | 0.44 |
| 1:P:56:LYS:HG3 | 1:P:61:PHE:HE2 | 1.80 | 0.44 |
| 1:P:102:ARG:NH1 | 1:P:160:PRO:O | 2.51 | 0.44 |
| 1:P:601:PHE:CE1 | 1:P:603:ALA:HB2 | 2.52 | 0.44 |
| 1:P:707:GLN:NE2 | 1:P:711:ALA:HA | 2.33 | 0.44 |
| 2:B:110:ARG:O | 2:B:128:PRO:HD2 | 2.17 | 0.44 |
| 2:D:53:PHE:CZ | 2:D:57:THR:HG21 | 2.52 | 0.44 |
| 3:I:55:LEU:HA | 3:I:55:LEU:HD23 | 1.72 | 0.44 |
| 3:G:120:ASN:O | 3:G:123:ASN:N | 2.48 | 0.44 |
| 4:H:281:LEU:HD22 | 4:H:293:GLY:HA3 | 1.98 | 0.44 |
| 4:H:375:MET:HE3 | 4:H:379:ARG:NH2 | 2.32 | 0.44 |
| 2:M:68:ARG:HD2 | 7:N:82:TYR:CE1 | 2.52 | 0.44 |
| 7:N:129:ALA:HB1 | 7:N:151:LEU:HB2 | 1.98 | 0.44 |
| 7:N:129:ALA:CB | 7:N:151:LEU:HB2 | 2.47 | 0.44 |
| 7:N:177:PHE:CD1 | 7:N:184:ASP:HB2 | 2.51 | 0.44 |
| 1:P:275:LEU:HA | 1:P:451:ILE:HG12 | 1.98 | 0.44 |
| 1:P:275:LEU:HD13 | 1:P:451:ILE:HD11 | 1.98 | 0.44 |
| 1:P:618:ILE:O | 1:P:621:GLU:HG2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:8:ASP:O | 2:A:229:PHE:HD2 | 2.01 | 0.44 |
| 2:A:51:ARG:HH21 | 2:A:112:PHE:HB2 | 1.82 | 0.44 |
| 2:A:62:HIS:HA | 2:A:105:ARG:HA | 1.98 | 0.44 |
| 2:A:167:MET:HG2 | 6:L:23:DT:C6 | 2.53 | 0.44 |
| 2:C:13:PHE:CE1 | 2:C:46:LEU:HD11 | 2.52 | 0.44 |
| 2:C:64:ASP:OD2 | 2:C:105:ARG:NH1 | 2.51 | 0.44 |
| 2:C:91:LYS:HD2 | 2:C:92:GLY:N | 2.32 | 0.44 |
| 2:C:148:THR:O | 5:K:25:A:O2' | 2.27 | 0.44 |
| 2:F:113:GLY:HA2 | 2:F:125:VAL:HG12 | 1.99 | 0.44 |
| 2:F:203:TRP:HB3 | 2:F:282:LEU:HD22 | 1.98 | 0.44 |
| 4:H:32:PHE:HD2 | 4:H:155:CYS:SG | 2.41 | 0.44 |
| 4:H:481:ILE:HG12 | 4:H:532:LEU:HD13 | 2.00 | 0.44 |
| 5:K:7:A:N1 | 7:N:90:ARG:NH1 | 2.65 | 0.44 |
| 6:L:48:DA:C6 | 6:L:49:DA:C6 | 3.06 | 0.44 |
| 2:M:47:LYS:HG2 | 2:M:112:PHE:CE1 | 2.52 | 0.44 |
| 7:N:23:ARG:O | 7:N:93:MET:N | 2.48 | 0.44 |
| 7:N:40:ALA:HB1 | 7:N:136:HIS:O | 2.17 | 0.44 |
| 1:P:109:HIS:CD2 | 1:P:668:PRO:HG2 | 2.52 | 0.44 |
| 1:P:169:ASP:HA | 1:P:172:ALA:HB3 | 1.98 | 0.44 |
| 1:P:562:VAL:HG23 | 1:P:564:LEU:HG | 1.98 | 0.44 |
| 2:A:229:PHE:CE1 | 2:A:279:LEU:HD13 | 2.53 | 0.44 |
| 2:B:19:ASN:N | 2:B:218:ARG:HA | 2.33 | 0.44 |
| 2:B:150:MET:SD | 2:C:48:ARG:HD3 | 2.57 | 0.44 |
| 2:B:205:ALA:O | 2:B:209:MET:CB | 2.57 | 0.44 |
| 2:D:72:ILE:H | 2:D:72:ILE:HD12 | 1.81 | 0.44 |
| 2:E:20:PRO:HB2 | 2:E:41:VAL:HG22 | 1.98 | 0.44 |
| 2:E:128:PRO:HG2 | 2:E:194:PHE:CB | 2.47 | 0.44 |
| 3:I:109:THR:O | 3:I:113:PHE:HD2 | 2.01 | 0.44 |
| 3:G:58:LEU:HD12 | 6:L:11:DG:H2' | 1.99 | 0.44 |
| 4:H:420:LEU:CD2 | 4:H:555:GLN:HB2 | 2.47 | 0.44 |
| 3:J:109:THR:O | 3:J:113:PHE:HD2 | 2.01 | 0.44 |
| 5:K:7:A:N3 | 7:N:69:GLU:HB3 | 2.33 | 0.44 |
| 2:M:9:PHE:CZ | 2:M:182:GLY:HA3 | 2.53 | 0.44 |
| 2:M:187:HIS:CD2 | 7:N:135:PHE:HA | 2.52 | 0.44 |
| 2:A:41:VAL:N | 2:A:134:SER:O | 2.47 | 0.44 |
| 2:A:105:ARG:HD3 | 2:A:106:TYR:CE1 | 2.52 | 0.44 |
| 2:A:160:GLU:HG3 | 2:A:161:THR:N | 2.25 | 0.44 |
| 2:B:280:ARG:NH2 | 2:B:282:LEU:HD11 | 2.32 | 0.44 |
| 2:D:186:THR:O | 2:D:190:LYS:HG2 | 2.17 | 0.44 |
| 2:C:103:CYS:O | 2:C:110:ARG:HB2 | 2.17 | 0.44 |
| 2:E:9:PHE:CE1 | 2:E:182:GLY:HA3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:220:GLN:HE21 | 2:E:222:ASN:HD21 | 1.65 | 0.44 |
| 3:I:18:PHE:HZ | 3:I:36:ILE:O | 2.00 | 0.44 |
| 4:H:208:HIS:HE1 | 4:H:242:ILE:HB | 1.78 | 0.44 |
| 4:H:385:VAL:CG1 | 4:H:392:ASN:HB2 | 2.43 | 0.44 |
| 4:H:450:LEU:HD11 | 4:H:553:GLU:HB3 | 1.99 | 0.44 |
| 4:H:450:LEU:HG | 4:H:453:MET:SD | 2.57 | 0.44 |
| 5:K:2:U:H2' | 7:N:43:TRP:CH2 | 2.52 | 0.44 |
| 1:P:51:LEU:HD11 | 1:P:161:LEU:HD11 | 2.00 | 0.44 |
| 1:P:304:ILE:HG12 | 1:P:359:ILE:CG2 | 2.47 | 0.44 |
| 1:P:516:LEU:O | 1:P:553:VAL:N | 2.50 | 0.44 |
| 1:P:749:ASP:OD1 | 1:P:751:PRO:HD3 | 2.17 | 0.44 |
| 2:A:23:ASP:CG | 2:A:30:PRO:HA | 2.38 | 0.44 |
| 2:B:114:ALA:O | 2:B:116:MET:HG3 | 2.18 | 0.44 |
| 2:B:131:LEU:HD11 | 2:B:202:PHE:HZ | 1.82 | 0.44 |
| 2:D:13:PHE:O | 2:D:177:LEU:HD12 | 2.18 | 0.44 |
| 2:C:18:GLY:HA3 | 2:C:218:ARG:O | 2.18 | 0.44 |
| 2:E:137:ILE:HD11 | 2:E:179:ARG:HB2 | 2.00 | 0.44 |
| 2:E:145:HIS:CD2 | 2:F:31:ARG:HD3 | 2.52 | 0.44 |
| 3:G:109:THR:O | 3:G:113:PHE:HD2 | 2.01 | 0.44 |
| 4:H:121:ASP:HB3 | 4:H:124:VAL:HG22 | 1.99 | 0.44 |
| 4:H:362:GLN:O | 4:H:438:LYS:HD2 | 2.18 | 0.44 |
| 5:K:3:U:H2' | 7:N:39:MET:HE1 | 2.00 | 0.44 |
| 2:M:31:ARG:NH2 | 7:N:66:ARG:O | 2.33 | 0.44 |
| 8:O:23:DA:H8 | 8:O:24:DA:C2 | 2.36 | 0.44 |
| 1:P:40:TYR:HD2 | 1:P:189:PHE:CZ | 2.36 | 0.44 |
| 1:P:363:ASN:HA | 1:P:366:LEU:HB3 | 1.99 | 0.44 |
| 1:P:691:ILE:HA | 1:P:748:PRO:HA | 1.99 | 0.44 |
| 2:D:129:VAL:HG22 | 2:D:184:ILE:HG12 | 1.99 | 0.44 |
| 2:E:113:GLY:HA3 | 5:K:36:C:H5'' | 1.98 | 0.44 |
| 3:G:18:PHE:HZ | 3:G:36:ILE:O | 2.00 | 0.44 |
| 4:H:396:ASP:C | 4:H:397:LEU:HD22 | 2.38 | 0.44 |
| 4:H:543:CYS:O | 3:J:107:HIS:NE2 | 2.49 | 0.44 |
| 5:K:8:C:H6 | 2:M:48:ARG:HG2 | 1.83 | 0.44 |
| 2:M:6:ARG:NH1 | 2:M:231:HIS:HE1 | 2.16 | 0.44 |
| 7:N:15:THR:HG21 | 7:N:23:ARG:HG2 | 1.99 | 0.44 |
| 7:N:83:ILE:HD12 | 7:N:87:ARG:HH12 | 1.79 | 0.44 |
| 1:P:185:ILE:HG23 | 1:P:408:MET:HE2 | 1.99 | 0.44 |
| 2:A:81:HIS:ND1 | 2:A:94:LYS:HE2 | 2.32 | 0.44 |
| 2:B:6:ARG:NH1 | 2:B:231:HIS:HE1 | 2.15 | 0.44 |
| 2:D:140:ILE:O | 2:D:140:ILE:HG13 | 2.18 | 0.44 |
| 2:C:259:ARG:HD3 | 2:C:259:ARG:HA | 1.79 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:211:ASP:O | 2:F:6:ARG:NH2 | 2.50 | 0.44 |
| 2:E:218:ARG:NH2 | 5:K:38:C:H6 | 2.15 | 0.44 |
| 2:F:252:LYS:HA | 2:F:265:LEU:HD22 | 1.99 | 0.44 |
| 3:I:99:GLY:HA3 | 3:J:89:PHE:HD2 | 1.82 | 0.44 |
| 3:G:93:LEU:HD23 | 3:G:93:LEU:HA | 1.79 | 0.44 |
| 4:H:10:TYR:CD1 | 4:H:249:GLU:HG2 | 2.53 | 0.44 |
| 4:H:360:ASP:O | 4:H:438:LYS:HD3 | 2.17 | 0.44 |
| 4:H:461:ASP:OD1 | 4:H:463:ASN:HB2 | 2.17 | 0.44 |
| 3:J:55:LEU:HA | 3:J:55:LEU:HD23 | 1.72 | 0.44 |
| 2:M:5:LYS:O | 2:M:186:THR:HB | 2.18 | 0.44 |
| 2:M:183:PHE:CD2 | 7:N:137:GLN:HG2 | 2.52 | 0.44 |
| 1:P:281:GLY:HA3 | 1:P:462:LEU:HD21 | 1.99 | 0.44 |
| 1:P:442:LEU:HD22 | 1:P:650:VAL:HG21 | 2.00 | 0.44 |
| 2:A:210:PHE:CE1 | 2:A:221:MET:HE3 | 2.53 | 0.44 |
| 2:B:52:ASN:O | 2:B:56:MET:HG3 | 2.17 | 0.44 |
| 2:B:129:VAL:HG11 | 2:B:202:PHE:CZ | 2.53 | 0.44 |
| 2:B:214:HIS:O | 2:C:126:ARG:NH1 | 2.51 | 0.44 |
| 2:B:227:TYR:OH | 2:B:266:VAL:HG11 | 2.18 | 0.44 |
| 2:D:3:ILE:HG22 | 2:D:196:GLU:HA | 1.99 | 0.44 |
| 2:D:12:LEU:HD12 | 2:D:227:TYR:HE1 | 1.82 | 0.44 |
| 2:D:124:GLN:HG3 | 5:K:29:G:H1' | 1.98 | 0.44 |
| 4:H:97:GLN:C | 4:H:99:GLN:H | 2.21 | 0.44 |
| 4:H:262:ASN:HA | 4:H:301:ILE:HD12 | 1.99 | 0.44 |
| 3:J:4:ASP:HB3 | 3:J:7:ARG:HB2 | 1.99 | 0.44 |
| 3:J:28:ALA:HB1 | 3:J:65:LYS:HB3 | 2.00 | 0.44 |
| 2:M:197:ASN:O | 2:M:201:LEU:HD23 | 2.17 | 0.44 |
| 1:P:55:GLY:C | 1:P:91:HIS:HB2 | 2.38 | 0.43 |
| 1:P:308:PRO:HD2 | 1:P:393:GLU:HB3 | 2.00 | 0.43 |
| 1:P:766:ALA:HA | 1:P:771:ALA:HA | 1.99 | 0.43 |
| 2:A:47:LYS:HD3 | 5:K:25:A:OP1 | 2.18 | 0.43 |
| 2:D:115:VAL:HG22 | 5:K:29:G:C4 | 2.53 | 0.43 |
| 2:C:239:PRO:HG2 | 2:C:242:SER:HB3 | 1.99 | 0.43 |
| 2:E:68:ARG:CD | 2:E:69:GLU:H | 2.25 | 0.43 |
| 2:F:42:THR:CG2 | 2:F:44:VAL:HG22 | 2.47 | 0.43 |
| 4:H:357:TRP:HA | 4:H:443:ARG:NH1 | 2.33 | 0.43 |
| 4:H:481:ILE:HD13 | 4:H:520:LEU:HD21 | 1.99 | 0.43 |
| 4:H:550:LEU:HA | 4:H:550:LEU:HD23 | 1.65 | 0.43 |
| 5:K:32:A:O2' | 5:K:33:U:OP1 | 2.36 | 0.43 |
| 2:M:241:ASP:OD2 | 7:N:148:ASP:HB3 | 2.18 | 0.43 |
| 7:N:29:ILE:HD13 | 7:N:102:ILE:HD11 | 2.00 | 0.43 |
| 7:N:108:MET:HE2 | 7:N:118:TYR:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:35:ARG:HH12 | 1:P:213:ASP:CB | 2.31 | 0.43 |
| 1:P:568:CYS:HA | 1:P:597:GLU:O | 2.18 | 0.43 |
| 2:A:21:ASN:HB2 | 2:A:41:VAL:HG22 | 2.00 | 0.43 |
| 2:A:273:LEU:HB2 | 2:A:277:LYS:HB2 | 2.00 | 0.43 |
| 2:B:124:GLN:HG3 | 5:K:11:G:H1' | 1.99 | 0.43 |
| 2:B:151:ALA:HB1 | 2:C:71:GLY:O | 2.18 | 0.43 |
| 2:C:129:VAL:HG11 | 2:C:202:PHE:CZ | 2.53 | 0.43 |
| 2:E:23:ASP:N | 2:E:29:LEU:O | 2.44 | 0.43 |
| 2:E:102:MET:HB3 | 2:E:109:ILE:HD12 | 2.01 | 0.43 |
| 2:E:124:GLN:HG3 | 5:K:35:G:H1' | 2.00 | 0.43 |
| 2:F:90:GLU:O | 2:F:92:GLY:N | 2.51 | 0.43 |
| 3:I:28:ALA:HB1 | 3:I:65:LYS:HB3 | 2.00 | 0.43 |
| 3:I:83:LEU:HD23 | 3:I:83:LEU:HA | 1.76 | 0.43 |
| 4:H:357:TRP:O | 4:H:361:LEU:HB2 | 2.17 | 0.43 |
| 4:H:404:ALA:HA | 4:H:409:ARG:HB2 | 2.00 | 0.43 |
| 4:H:512:LEU:HA | 4:H:512:LEU:HD23 | 1.78 | 0.43 |
| 3:J:18:PHE:HZ | 3:J:36:ILE:O | 2.00 | 0.43 |
| 1:P:6:ILE:HD12 | 1:P:19:SER:OG | 2.18 | 0.43 |
| 1:P:465:VAL:HG22 | 1:P:596:GLY:HA3 | 2.00 | 0.43 |
| 2:A:110:ARG:NH2 | 2:A:198:ASP:OD2 | 2.51 | 0.43 |
| 2:A:258:VAL:O | 2:A:259:ARG:NE | 2.46 | 0.43 |
| 2:D:23:ASP:N | 2:D:29:LEU:O | 2.47 | 0.43 |
| 2:E:27:GLY:O | 5:K:39:U:H5 | 2.01 | 0.43 |
| 2:F:229:PHE:CE1 | 2:F:279:LEU:HD22 | 2.48 | 0.43 |
| 3:G:29:ASN:ND2 | 3:G:32:LEU:HD13 | 2.32 | 0.43 |
| 4:H:82:TRP:O | 4:H:82:TRP:CG | 2.72 | 0.43 |
| 4:H:571:THR:HG22 | 4:H:572:LYS:H | 1.84 | 0.43 |
| 2:M:39:GLY:H | 2:M:136:SER:HB3 | 1.83 | 0.43 |
| 1:P:251:LEU:O | 1:P:252:ASN:HB3 | 2.19 | 0.43 |
| 1:P:570:TYR:HA | 1:P:599:VAL:O | 2.18 | 0.43 |
| 2:A:144:GLU:CD | 3:J:54:THR:HG22 | 2.39 | 0.43 |
| 2:B:107:TYR:HD1 | 2:B:110:ARG:NH1 | 2.16 | 0.43 |
| 2:B:115:VAL:HG22 | 5:K:11:G:C4 | 2.53 | 0.43 |
| 2:D:7:TYR:HE2 | 2:D:280:ARG:HH11 | 1.61 | 0.43 |
| 2:D:156:LYS:HZ2 | 6:L:17:DG:P | 2.39 | 0.43 |
| 2:E:144:GLU:HG2 | 2:E:171:PHE:CE1 | 2.53 | 0.43 |
| 2:E:273:LEU:C | 2:E:275:GLU:H | 2.22 | 0.43 |
| 2:F:167:MET:HG3 | 2:F:168:GLY:N | 2.33 | 0.43 |
| 3:G:28:ALA:HB1 | 3:G:65:LYS:HB3 | 2.00 | 0.43 |
| 3:G:41:PHE:HE2 | 3:G:105:TYR:CG | 2.36 | 0.43 |
| 3:G:119:LYS:HD3 | 9:Q:14:DA:OP1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:206:ARG:HG3 | 4:H:236:GLN:O | 2.19 | 0.43 |
| 4:H:221:PHE:CE2 | 7:N:19:LEU:HD21 | 2.54 | 0.43 |
| 4:H:396:ASP:OD2 | 4:H:414:SER:OG | 2.26 | 0.43 |
| 2:M:9:PHE:HE1 | 2:M:11:PHE:HB2 | 1.83 | 0.43 |
| 7:N:168:PHE:HB2 | 7:N:194:GLN:HE21 | 1.83 | 0.43 |
| 1:P:125:TRP:HE1 | 1:P:667:ASN:CG | 2.19 | 0.43 |
| 1:P:144:ALA:O | 1:P:147:SER:OG | 2.37 | 0.43 |
| 1:P:288:LEU:HD12 | 1:P:320:PHE:CE2 | 2.53 | 0.43 |
| 1:P:479:TRP:NE1 | 1:P:604:GLU:HB2 | 2.33 | 0.43 |
| 2:A:140:ILE:O | 2:A:140:ILE:HG13 | 2.18 | 0.43 |
| 2:A:227:TYR:HB3 | 2:A:279:LEU:HD11 | 2.00 | 0.43 |
| 2:B:132:THR:HG23 | 2:B:181:HIS:O | 2.18 | 0.43 |
| 2:B:239:PRO:HG2 | 2:B:242:SER:HB3 | 2.00 | 0.43 |
| 2:D:15:VAL:O | 2:D:175:TYR:HA | 2.18 | 0.43 |
| 2:D:128:PRO:HG3 | 2:D:189:ALA:HA | 2.00 | 0.43 |
| 2:C:134:SER:HB3 | 2:C:178:TYR:HB3 | 2.01 | 0.43 |
| 2:E:205:ALA:O | 2:E:209:MET:CB | 2.54 | 0.43 |
| 3:I:21:LEU:HD23 | 3:I:59:LEU:HD13 | 2.01 | 0.43 |
| 3:G:39:ARG:HH12 | 6:L:12:DG:C2' | 2.31 | 0.43 |
| 4:H:9:TYR:HB2 | 4:H:297:PRO:HB3 | 2.00 | 0.43 |
| 4:H:64:PRO:HD3 | 4:H:170:CYS:HB2 | 2.01 | 0.43 |
| 4:H:466:ASP:HB2 | 4:H:469:TYR:HB3 | 2.00 | 0.43 |
| 3:J:112:LEU:HD23 | 3:J:112:LEU:HA | 1.66 | 0.43 |
| 2:M:21:ASN:HD22 | 2:M:42:THR:N | 2.16 | 0.43 |
| 1:P:569:VAL:O | 1:P:598:VAL:HA | 2.18 | 0.43 |
| 2:A:54:ILE:HG23 | 2:A:58:GLN:HG2 | 2.01 | 0.43 |
| 2:C:109:ILE:HG12 | 2:C:114:ALA:CB | 2.48 | 0.43 |
| 2:E:164:ASN:ND2 | 2:F:69:GLU:O | 2.35 | 0.43 |
| 2:F:18:GLY:HA3 | 2:F:219:GLY:HA3 | 1.99 | 0.43 |
| 2:F:126:ARG:HD3 | 2:F:188:PHE:CZ | 2.53 | 0.43 |
| 3:G:76:GLN:O | 3:G:80:ARG:HG3 | 2.18 | 0.43 |
| 3:G:97:GLN:OE1 | 3:G:97:GLN:HA | 2.19 | 0.43 |
| 4:H:6:LEU:HA | 4:H:9:TYR:CE1 | 2.54 | 0.43 |
| 4:H:133:SER:H | 4:H:137:LYS:HZ1 | 1.66 | 0.43 |
| 4:H:266:ILE:HG13 | 4:H:341:PHE:CE2 | 2.54 | 0.43 |
| 4:H:440:TYR:CD2 | 4:H:440:TYR:C | 2.91 | 0.43 |
| 2:M:184:ILE:HG21 | 2:M:199:LEU:HD12 | 2.01 | 0.43 |
| 1:P:92:SER:HB2 | 1:P:116:ALA:HA | 2.00 | 0.43 |
| 1:P:224:ALA:H | 1:P:346:LYS:HE2 | 1.84 | 0.43 |
| 1:P:332:HIS:C | 1:P:334:SER:H | 2.22 | 0.43 |
| 1:P:554:SER:OG | 1:P:555:THR:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:6:ARG:NH2 | 2:C:211:ASP:O | 2.51 | 0.43 |
| 2:B:63:HIS:HA | 2:B:107:TYR:HB2 | 1.99 | 0.43 |
| 2:E:112:PHE:HE1 | 2:E:131:LEU:HD13 | 1.84 | 0.43 |
| 2:E:130:GLN:NE2 | 5:K:36:C:OP1 | 2.51 | 0.43 |
| 2:F:39:GLY:O | 2:F:135:ARG:HA | 2.19 | 0.43 |
| 2:F:227:TYR:HB3 | 2:F:279:LEU:HD11 | 2.00 | 0.43 |
| 2:F:269:ASP:OD1 | 2:F:269:ASP:N | 2.45 | 0.43 |
| 3:I:97:GLN:OE1 | 3:I:97:GLN:HA | 2.19 | 0.43 |
| 3:G:7:ARG:NE | 3:G:9:ASP:OD2 | 2.52 | 0.43 |
| 3:G:39:ARG:NH1 | 6:L:12:DG:H2' | 2.33 | 0.43 |
| 3:G:68:PHE:CD1 | 9:Q:14:DA:N7 | 2.87 | 0.43 |
| 2:M:243:LEU:O | 2:M:246:ARG:HB2 | 2.18 | 0.43 |
| 7:N:38:LEU:O | 7:N:49:TRP:NE1 | 2.52 | 0.43 |
| 7:N:45:PRO:O | 7:N:111:GLU:HG2 | 2.17 | 0.43 |
| 8:O:12:DT:H2' | 8:O:13:DC:O4' | 2.18 | 0.43 |
| 1:P:8:HIS:CD2 | 1:P:20:HIS:HD1 | 2.34 | 0.43 |
| 1:P:38:GLY:O | 1:P:42:SER:HB3 | 2.19 | 0.43 |
| 1:P:424:THR:CG2 | 1:P:428:PRO:HD3 | 2.49 | 0.43 |
| 1:P:505:LEU:HD12 | 1:P:505:LEU:HA | 1.89 | 0.43 |
| 2:B:42:THR:HA | 2:B:133:PHE:CD2 | 2.54 | 0.43 |
| 2:B:118:THR:HG21 | 2:M:153:THR:HG21 | 2.01 | 0.43 |
| 2:D:47:LYS:HG2 | 2:D:112:PHE:CD1 | 2.54 | 0.43 |
| 2:C:61:GLU:O | 2:C:62:HIS:HB2 | 2.19 | 0.43 |
| 2:C:90:GLU:HB3 | 2:C:93:GLU:OE2 | 2.17 | 0.43 |
| 2:C:106:TYR:CD2 | 2:C:109:ILE:HD12 | 2.52 | 0.43 |
| 2:C:128:PRO:HG3 | 2:C:189:ALA:HA | 2.01 | 0.43 |
| 2:E:224:ARG:HD3 | 2:E:224:ARG:HA | 1.72 | 0.43 |
| 2:F:7:TYR:HA | 2:F:229:PHE:O | 2.18 | 0.43 |
| 2:F:21:ASN:O | 2:F:23:ASP:N | 2.47 | 0.43 |
| 2:F:103:CYS:O | 2:F:110:ARG:NH2 | 2.51 | 0.43 |
| 2:F:110:ARG:HE | 2:F:198:ASP:CG | 2.21 | 0.43 |
| 4:H:208:HIS:HD1 | 4:H:250:TYR:HH | 0.55 | 0.43 |
| 3:J:76:GLN:O | 3:J:80:ARG:HG3 | 2.18 | 0.43 |
| 7:N:142:CYS:HB2 | 7:N:145:PHE:CD2 | 2.54 | 0.43 |
| 1:P:306:ALA:HB2 | 1:P:366:LEU:HD13 | 2.00 | 0.43 |
| 1:P:455:LYS:HG2 | 1:P:634:PRO:HG2 | 2.01 | 0.43 |
| 2:A:26:ALA:HB1 | 3:J:42:GLY:CA | 2.49 | 0.43 |
| 2:B:238:ALA:HB3 | 2:B:243:LEU:HD21 | 2.01 | 0.43 |
| 2:D:47:LYS:HD3 | 5:K:31:C:OP1 | 2.19 | 0.43 |
| 2:C:149:ARG:HB2 | 5:K:25:A:H1' | 2.01 | 0.43 |
| 2:E:53:PHE:O | 2:E:57:THR:HG23 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:229:PHE:CD1 | 2:F:243:LEU:HD12 | 2.54 | 0.43 |
| 3:I:7:ARG:NE | 3:I:9:ASP:OD2 | 2.52 | 0.43 |
| 4:H:108:THR:HG22 | 4:H:131:LEU:HG | 2.01 | 0.43 |
| 4:H:225:ASN:O | 4:H:226:LEU:HG | 2.19 | 0.43 |
| 4:H:281:LEU:CD2 | 4:H:293:GLY:HA3 | 2.48 | 0.43 |
| 4:H:557:LEU:O | 4:H:561:GLY:N | 2.27 | 0.43 |
| 2:M:15:VAL:HG12 | 2:M:178:TYR:HE1 | 1.84 | 0.43 |
| 2:A:130:GLN:HE22 | 5:K:24:U:P | 2.41 | 0.43 |
| 2:B:35:GLN:HB3 | 2:M:257:VAL:HG21 | 2.01 | 0.43 |
| 2:C:140:ILE:HB | 2:C:173:VAL:HG13 | 2.00 | 0.43 |
| 2:C:248:GLN:HG2 | 2:C:267:SER:HB2 | 2.00 | 0.43 |
| 2:F:14:ASP:OD2 | 2:F:224:ARG:NE | 2.50 | 0.43 |
| 3:I:4:ASP:HB3 | 3:I:7:ARG:HB2 | 1.99 | 0.43 |
| 3:I:41:PHE:HE2 | 3:I:105:TYR:CG | 2.36 | 0.43 |
| 3:G:4:ASP:HB3 | 3:G:7:ARG:HB2 | 1.99 | 0.43 |
| 3:G:14:LEU:HD11 | 3:G:90:PRO:CD | 2.42 | 0.43 |
| 4:H:226:LEU:HB2 | 4:H:229:PHE:CD2 | 2.53 | 0.43 |
| 4:H:335:ALA:HB3 | 6:L:47:DG:H1' | 2.00 | 0.43 |
| 5:K:7:A:C2 | 7:N:69:GLU:HB3 | 2.53 | 0.43 |
| 6:L:35:DC:H2" | 6:L:36:DA:OP2 | 2.19 | 0.43 |
| 2:M:55:GLN:HB2 | 2:M:65:ILE:HG13 | 2.01 | 0.43 |
| 2:M:66:PHE:HE2 | 7:N:74:MET:HB3 | 1.81 | 0.43 |
| 7:N:117:ASN:HB3 | 7:N:120:LYS:HB2 | 2.01 | 0.43 |
| 1:P:104:ASN:HB3 | 1:P:107:PHE:HB2 | 2.01 | 0.42 |
| 1:P:274:SER:HA | 1:P:422:LEU:H | 1.82 | 0.42 |
| 1:P:486:ILE:HD11 | 1:P:509:LEU:HD11 | 2.01 | 0.42 |
| 1:P:576:LEU:HB2 | 1:P:640:TYR:CG | 2.54 | 0.42 |
| 1:P:699:HIS:CE1 | 1:P:707:GLN:HG3 | 2.54 | 0.42 |
| 1:P:715:ASP:O | 1:P:719:ARG:HG2 | 2.19 | 0.42 |
| 2:A:116:MET:HB2 | 2:A:123:GLY:O | 2.19 | 0.42 |
| 2:B:152:VAL:HG11 | 2:B:159:SER:HB2 | 2.01 | 0.42 |
| 2:B:273:LEU:C | 2:B:275:GLU:H | 2.22 | 0.42 |
| 2:D:203:TRP:CE3 | 2:D:226:LEU:HD21 | 2.54 | 0.42 |
| 2:E:117:THR:HA | 2:E:121:ASN:OD1 | 2.19 | 0.42 |
| 3:I:9:ASP:O | 3:I:13:VAL:HG13 | 2.19 | 0.42 |
| 3:G:83:LEU:HD23 | 3:G:83:LEU:HA | 1.76 | 0.42 |
| 4:H:32:PHE:CD2 | 4:H:155:CYS:SG | 3.12 | 0.42 |
| 4:H:69:ARG:HB3 | 4:H:74:SER:OG | 2.19 | 0.42 |
| 4:H:460:LEU:HA | 4:H:564:HIS:HB3 | 2.01 | 0.42 |
| 3:J:41:PHE:HE2 | 3:J:105:TYR:CG | 2.36 | 0.42 |
| 5:K:5:A:C8 | 5:K:6:A:N7 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:29:ILE:HD11 | 7:N:37:ILE:HD12 | 2.01 | 0.42 |
| 7:N:32:SER:N | 7:N:173:TYR:O | 2.52 | 0.42 |
| 1:P:367:PHE:O | 1:P:371:PHE:N | 2.50 | 0.42 |
| 1:P:665:ASN:OD1 | 4:H:282:GLU:N | 2.51 | 0.42 |
| 2:A:48:ARG:HA | 2:A:48:ARG:HD2 | 1.80 | 0.42 |
| 2:A:133:PHE:HB2 | 2:C:17:ASP:HB3 | 2.00 | 0.42 |
| 2:B:126:ARG:HG2 | 2:B:188:PHE:CE2 | 2.54 | 0.42 |
| 2:D:49:LYS:HA | 2:D:213:ASP:OD2 | 2.19 | 0.42 |
| 2:D:116:MET:HB3 | 2:D:122:ALA:HB3 | 2.01 | 0.42 |
| 2:D:150:MET:HE3 | 2:E:68:ARG:HG2 | 2.01 | 0.42 |
| 2:C:140:ILE:O | 2:C:140:ILE:HG13 | 2.19 | 0.42 |
| 2:F:53:PHE:CD2 | 2:F:205:ALA:HA | 2.54 | 0.42 |
| 3:I:33:ASN:HB3 | 6:L:19:DG:OP2 | 2.18 | 0.42 |
| 4:H:6:LEU:HD13 | 4:H:254:LEU:CD2 | 2.49 | 0.42 |
| 4:H:131:LEU:HD11 | 4:H:159:PHE:CZ | 2.55 | 0.42 |
| 4:H:160:ARG:HB2 | 4:H:168:LEU:HD13 | 2.00 | 0.42 |
| 4:H:208:HIS:ND1 | 4:H:250:TYR:OH | 2.10 | 0.42 |
| 4:H:357:TRP:HZ3 | 4:H:411:LEU:HD11 | 1.84 | 0.42 |
| 4:H:474:LEU:HD13 | 4:H:540:LEU:HD13 | 2.00 | 0.42 |
| 3:J:7:ARG:CG | 3:J:12:TYR:HD2 | 2.22 | 0.42 |
| 9:Q:-3:DA:H5' | 9:Q:-3:DA:C8 | 2.55 | 0.42 |
| 1:P:149:PHE:CE1 | 1:P:154:LEU:HB3 | 2.54 | 0.42 |
| 1:P:509:LEU:HD13 | 1:P:551:TRP:CD1 | 2.55 | 0.42 |
| 2:A:19:ASN:OD1 | 2:A:23:ASP:OD1 | 2.37 | 0.42 |
| 2:B:34:PRO:HG2 | 4:H:413:VAL:HG21 | 2.01 | 0.42 |
| 2:B:160:GLU:CG | 2:B:161:THR:H | 2.32 | 0.42 |
| 2:D:130:GLN:O | 2:D:182:GLY:HA2 | 2.19 | 0.42 |
| 2:D:168:GLY:HA3 | 6:L:18:DG:C5 | 2.53 | 0.42 |
| 2:C:68:ARG:CG | 2:C:69:GLU:H | 2.32 | 0.42 |
| 2:C:95:THR:O | 2:C:99:ARG:HG3 | 2.19 | 0.42 |
| 2:C:111:THR:HG23 | 2:C:129:VAL:HG21 | 2.00 | 0.42 |
| 2:F:215:SER:HB3 | 2:F:218:ARG:HD3 | 2.01 | 0.42 |
| 4:H:133:SER:H | 4:H:137:LYS:NZ | 2.16 | 0.42 |
| 4:H:262:ASN:HD21 | 4:H:298:ASP:HB3 | 1.84 | 0.42 |
| 4:H:396:ASP:O | 4:H:397:LEU:HD22 | 2.19 | 0.42 |
| 2:M:38:GLU:HA | 2:M:139:PRO:HA | 2.01 | 0.42 |
| 2:M:68:ARG:HD2 | 7:N:82:TYR:CZ | 2.53 | 0.42 |
| 2:M:99:ARG:HH11 | 2:M:125:VAL:HG13 | 1.84 | 0.42 |
| 7:N:83:ILE:O | 7:N:87:ARG:N | 2.52 | 0.42 |
| 7:N:101:ARG:HG3 | 7:N:101:ARG:O | 2.19 | 0.42 |
| 1:P:594:GLN:OE1 | 1:P:594:GLN:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:203:TRP:HB3 | 2:A:282:LEU:HD22 | 2.01 | 0.42 |
| 2:D:44:VAL:CG1 | 5:K:31:C:H2' | 2.48 | 0.42 |
| 2:D:152:VAL:HA | 2:D:166:THR:HG23 | 2.01 | 0.42 |
| 2:C:174:PRO:HB2 | 2:C:259:ARG:CZ | 2.49 | 0.42 |
| 2:E:2:THR:HG21 | 2:E:190:LYS:HA | 2.01 | 0.42 |
| 2:E:19:ASN:N | 2:E:217:ALA:O | 2.33 | 0.42 |
| 3:I:52:PHE:HB3 | 3:I:89:PHE:CE2 | 2.54 | 0.42 |
| 3:I:58:LEU:HD12 | 6:L:17:DG:H2'' | 2.00 | 0.42 |
| 4:H:69:ARG:NH2 | 8:O:14:DA:P | 2.92 | 0.42 |
| 3:J:25:GLN:OE1 | 3:J:36:ILE:N | 2.42 | 0.42 |
| 3:J:97:GLN:OE1 | 3:J:97:GLN:HA | 2.19 | 0.42 |
| 7:N:108:MET:CE | 7:N:118:TYR:HA | 2.50 | 0.42 |
| 1:P:29:VAL:HG11 | 1:P:52:HIS:ND1 | 2.34 | 0.42 |
| 1:P:40:TYR:HD2 | 1:P:189:PHE:CE2 | 2.36 | 0.42 |
| 1:P:336:LEU:HA | 1:P:336:LEU:HD23 | 1.87 | 0.42 |
| 1:P:437:PHE:CE1 | 4:H:62:LEU:HD22 | 2.54 | 0.42 |
| 1:P:696:PRO:O | 1:P:697:LEU:HG | 2.20 | 0.42 |
| 2:A:24:PRO:HD2 | 2:A:27:GLY:O | 2.18 | 0.42 |
| 2:A:66:PHE:CE2 | 2:A:109:ILE:HD11 | 2.54 | 0.42 |
| 2:D:149:ARG:HH22 | 2:D:153:THR:HG1 | 1.57 | 0.42 |
| 2:D:273:LEU:HD11 | 2:D:279:LEU:H | 1.84 | 0.42 |
| 2:C:6:ARG:O | 2:C:231:HIS:HD2 | 2.03 | 0.42 |
| 2:E:26:ALA:O | 2:E:29:LEU:N | 2.42 | 0.42 |
| 4:H:52:LYS:NZ | 8:O:18:DA:H3' | 2.34 | 0.42 |
| 4:H:146:TRP:CD1 | 4:H:149:CYS:SG | 3.13 | 0.42 |
| 4:H:182:ALA:O | 4:H:186:GLN:HG2 | 2.19 | 0.42 |
| 4:H:217:LYS:HE2 | 8:O:14:DA:O4' | 2.19 | 0.42 |
| 3:J:7:ARG:NE | 3:J:9:ASP:OD2 | 2.52 | 0.42 |
| 5:K:4:G:H3' | 7:N:139:TYR:CE2 | 2.53 | 0.42 |
| 2:M:151:ALA:O | 2:M:166:THR:HG22 | 2.20 | 0.42 |
| 1:P:513:GLY:HA2 | 1:P:549:PRO:HD2 | 2.00 | 0.42 |
| 1:P:559:GLU:OE1 | 1:P:578:SER:HB3 | 2.19 | 0.42 |
| 2:A:83:GLN:O | 2:A:86:VAL:N | 2.52 | 0.42 |
| 2:B:5:LYS:HG3 | 2:B:230:GLU:OE2 | 2.20 | 0.42 |
| 2:B:11:PHE:CZ | 2:B:210:PHE:HE2 | 2.38 | 0.42 |
| 2:B:153:THR:HB | 6:L:37:DA:H4' | 2.02 | 0.42 |
| 2:D:34:PRO:HB3 | 3:I:91:ASN:O | 2.20 | 0.42 |
| 2:D:233:ASN:HB2 | 2:D:235:LEU:O | 2.19 | 0.42 |
| 2:C:12:LEU:CD2 | 2:C:249:VAL:HG21 | 2.49 | 0.42 |
| 2:C:232:SER:N | 2:C:237:ASP:OD2 | 2.33 | 0.42 |
| 2:E:39:GLY:C | 2:E:178:TYR:HE1 | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:43:ASP:HB3 | 2:E:47:LYS:HE3 | 2.01 | 0.42 |
| 2:E:65:ILE:HD13 | 2:E:65:ILE:HA | 1.74 | 0.42 |
| 2:E:77:ILE:HG23 | 2:E:122:ALA:CB | 2.49 | 0.42 |
| 2:E:168:GLY:HA3 | 6:L:12:DG:C6 | 2.54 | 0.42 |
| 2:F:7:TYR:CE2 | 2:F:230:GLU:HG2 | 2.55 | 0.42 |
| 3:I:76:GLN:O | 3:I:80:ARG:HG3 | 2.18 | 0.42 |
| 4:H:32:PHE:HD2 | 4:H:155:CYS:HG | 1.59 | 0.42 |
| 4:H:471:LEU:HD21 | 4:H:546:PHE:HD1 | 1.84 | 0.42 |
| 3:J:9:ASP:O | 3:J:13:VAL:HG13 | 2.19 | 0.42 |
| 2:M:152:VAL:HG13 | 2:M:164:ASN:HB3 | 2.02 | 0.42 |
| 2:M:166:THR:HG23 | 2:M:166:THR:O | 2.19 | 0.42 |
| 1:P:478:SER:HB3 | 1:P:481:LYS:HB2 | 2.00 | 0.42 |
| 1:P:491:CYS:HA | 1:P:550:LEU:HD22 | 2.01 | 0.42 |
| 1:P:570:TYR:CE1 | 1:P:599:VAL:HB | 2.55 | 0.42 |
| 2:B:203:TRP:HA | 2:B:203:TRP:CE3 | 2.55 | 0.42 |
| 2:D:44:VAL:HA | 2:D:47:LYS:HB2 | 2.00 | 0.42 |
| 2:D:51:ARG:HH11 | 2:D:51:ARG:HG3 | 1.85 | 0.42 |
| 2:C:238:ALA:HB3 | 2:C:243:LEU:HD21 | 2.01 | 0.42 |
| 2:F:19:ASN:HB3 | 2:F:22:GLY:CA | 2.48 | 0.42 |
| 2:F:188:PHE:HA | 2:F:191:GLN:HE21 | 1.82 | 0.42 |
| 3:G:9:ASP:O | 3:G:13:VAL:HG13 | 2.19 | 0.42 |
| 3:G:21:LEU:HD23 | 3:G:59:LEU:HD13 | 2.01 | 0.42 |
| 4:H:127:VAL:HG21 | 4:H:159:PHE:CD2 | 2.55 | 0.42 |
| 3:J:74:GLN:HG3 | 9:Q:4:DT:H5" | 2.02 | 0.42 |
| 5:K:7:A:P | 2:M:51:ARG:HH22 | 2.42 | 0.42 |
| 7:N:176:ASP:HB2 | 7:N:190:PRO:HD3 | 2.00 | 0.42 |
| 1:P:46:GLU:O | 1:P:49:GLY:N | 2.53 | 0.42 |
| 1:P:122:LEU:O | 1:P:373:ALA:HB1 | 2.20 | 0.42 |
| 1:P:496:VAL:HA | 1:P:572:ALA:HB2 | 2.01 | 0.42 |
| 1:P:624:LYS:HB2 | 4:H:43:ILE:HG23 | 2.02 | 0.42 |
| 2:A:131:LEU:HD11 | 2:A:202:PHE:CZ | 2.55 | 0.42 |
| 2:D:126:ARG:HA | 5:K:29:G:O3' | 2.19 | 0.42 |
| 2:C:43:ASP:OD1 | 2:C:44:VAL:N | 2.53 | 0.42 |
| 2:C:48:ARG:NH1 | 5:K:20:G:OP1 | 2.43 | 0.42 |
| 2:C:229:PHE:HB3 | 2:C:277:LYS:HE2 | 2.01 | 0.42 |
| 2:F:231:HIS:HE2 | 2:F:243:LEU:HG | 1.85 | 0.42 |
| 3:I:25:GLN:CD | 3:I:36:ILE:HG23 | 2.40 | 0.42 |
| 3:G:52:PHE:HB3 | 3:G:89:PHE:CE2 | 2.55 | 0.42 |
| 3:G:62:HIS:O | 3:G:66:LEU:HG | 2.20 | 0.42 |
| 4:H:84:HIS:CD2 | 4:H:154:GLY:HA2 | 2.54 | 0.42 |
| 4:H:196:LEU:HD21 | 7:N:18:GLU:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:234:LYS:HD3 | 4:H:234:LYS:HA | 1.80 | 0.42 |
| 4:H:431:TYR:HB2 | 4:H:563:TYR:CZ | 2.54 | 0.42 |
| 4:H:454:LYS:O | 4:H:464:ARG:NH1 | 2.53 | 0.42 |
| 4:H:469:TYR:HB2 | 4:H:557:LEU:HD13 | 2.01 | 0.42 |
| 4:H:570:PHE:HB3 | 9:Q:-4:DT:C2 | 2.54 | 0.42 |
| 3:J:45:SER:C | 3:J:98:GLN:HE22 | 2.23 | 0.42 |
| 3:J:78:GLU:OE1 | 3:J:112:LEU:HD21 | 2.20 | 0.42 |
| 7:N:69:GLU:CG | 7:N:90:ARG:HB2 | 2.48 | 0.42 |
| 7:N:83:ILE:HG13 | 7:N:84:GLU:H | 1.84 | 0.42 |
| 1:P:449:ARG:NE | 1:P:449:ARG:HA | 2.35 | 0.42 |
| 2:A:161:THR:OG1 | 2:A:162:GLY:N | 2.53 | 0.42 |
| 2:A:165:ARG:HH21 | 2:E:124:GLN:HE22 | 1.66 | 0.42 |
| 2:B:55:GLN:HG3 | 2:B:65:ILE:HG13 | 2.02 | 0.42 |
| 2:D:24:PRO:CG | 5:K:33:U:H5'' | 2.49 | 0.42 |
| 2:D:156:LYS:NZ | 6:L:17:DG:OP1 | 2.38 | 0.42 |
| 2:D:243:LEU:HD23 | 2:D:243:LEU:HA | 1.77 | 0.42 |
| 2:E:181:HIS:HB3 | 2:E:244:PHE:CE2 | 2.55 | 0.42 |
| 2:F:243:LEU:HA | 2:F:246:ARG:HG3 | 2.01 | 0.42 |
| 3:G:78:GLU:OE1 | 3:G:112:LEU:HD21 | 2.20 | 0.42 |
| 4:H:118:LEU:HD12 | 4:H:178:TYR:HB2 | 2.01 | 0.42 |
| 4:H:308:TYR:HD1 | 4:H:406:LEU:HD22 | 1.85 | 0.42 |
| 4:H:334:SER:HB3 | 6:L:47:DG:H5' | 2.01 | 0.42 |
| 5:K:6:A:C5 | 2:M:115:VAL:HG11 | 2.54 | 0.42 |
| 6:L:40:DT:H6 | 6:L:40:DT:H2' | 1.60 | 0.42 |
| 2:M:9:PHE:CE1 | 2:M:11:PHE:HB2 | 2.55 | 0.42 |
| 2:M:54:ILE:HG21 | 2:M:107:TYR:CG | 2.55 | 0.42 |
| 7:N:19:LEU:O | 7:N:23:ARG:HA | 2.20 | 0.42 |
| 7:N:23:ARG:O | 7:N:92:SER:HA | 2.19 | 0.42 |
| 7:N:43:TRP:HA | 7:N:47:ILE:HG21 | 2.02 | 0.42 |
| 1:P:263:PHE:HD2 | 1:P:293:LYS:HD2 | 1.83 | 0.42 |
| 1:P:305:TYR:CD1 | 1:P:390:ILE:HB | 2.54 | 0.42 |
| 1:P:365:GLN:HG2 | 1:P:365:GLN:O | 2.20 | 0.42 |
| 2:B:74:ASN:HA | 2:B:77:ILE:HB | 2.01 | 0.42 |
| 2:B:145:HIS:CD2 | 2:C:133:PHE:CE2 | 3.08 | 0.42 |
| 2:D:102:MET:HB3 | 2:D:109:ILE:HD12 | 2.02 | 0.42 |
| 3:G:25:GLN:CD | 3:G:36:ILE:HG23 | 2.40 | 0.42 |
| 4:H:537:ARG:HD2 | 3:J:109:THR:CG2 | 2.50 | 0.42 |
| 5:K:8:C:OP1 | 7:N:87:ARG:NH1 | 2.51 | 0.42 |
| 2:M:13:PHE:CZ | 2:M:46:LEU:HD21 | 2.55 | 0.42 |
| 2:M:42:THR:HG22 | 2:M:133:PHE:CE2 | 2.55 | 0.42 |
| 2:M:147:ILE:HD13 | 2:M:170:LYS:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:44:LYS:C | 7:N:46:ALA:H | 2.23 | 0.42 |
| 7:N:48:ARG:HB2 | 7:N:109:THR:CG2 | 2.50 | 0.42 |
| 1:P:44:PHE:CZ | 1:P:110:LEU:HD22 | 2.54 | 0.41 |
| 1:P:251:LEU:HD21 | 1:P:464:ARG:HH22 | 1.85 | 0.41 |
| 2:B:68:ARG:NH2 | 2:B:69:GLU:HB2 | 2.35 | 0.41 |
| 2:B:277:LYS:HE2 | 2:B:277:LYS:HB2 | 1.83 | 0.41 |
| 2:D:128:PRO:HG2 | 2:D:194:PHE:CB | 2.50 | 0.41 |
| 2:C:8:ASP:HB3 | 2:C:244:PHE:CZ | 2.55 | 0.41 |
| 2:E:31:ARG:HB2 | 2:E:40:LEU:O | 2.20 | 0.41 |
| 2:E:259:ARG:HG3 | 2:F:36:THR:HG21 | 2.02 | 0.41 |
| 2:F:69:GLU:C | 2:F:71:GLY:H | 2.23 | 0.41 |
| 2:F:116:MET:HB2 | 2:F:123:GLY:O | 2.20 | 0.41 |
| 2:F:145:HIS:HB2 | 2:F:170:LYS:O | 2.20 | 0.41 |
| 4:H:12:ARG:HB2 | 4:H:297:PRO:HG3 | 2.02 | 0.41 |
| 4:H:345:THR:HB | 4:H:349:ALA:HB3 | 2.02 | 0.41 |
| 4:H:427:GLN:HB3 | 4:H:495:ASP:HA | 2.01 | 0.41 |
| 4:H:465:GLN:HA | 4:H:542:HIS:HB3 | 2.02 | 0.41 |
| 4:H:523:LEU:HB2 | 4:H:529:ALA:HB2 | 2.01 | 0.41 |
| 3:J:21:LEU:HD23 | 3:J:59:LEU:HD13 | 2.01 | 0.41 |
| 3:J:52:PHE:HB3 | 3:J:89:PHE:CE2 | 2.55 | 0.41 |
| 7:N:175:MET:HA | 7:N:190:PRO:HD2 | 2.02 | 0.41 |
| 1:P:29:VAL:HG21 | 1:P:52:HIS:CE1 | 2.54 | 0.41 |
| 1:P:56:LYS:HG3 | 1:P:61:PHE:CD2 | 2.55 | 0.41 |
| 1:P:126:TYR:CE1 | 4:H:303:ALA:HB2 | 2.55 | 0.41 |
| 1:P:352:GLU:CD | 1:P:379:ARG:HH22 | 2.23 | 0.41 |
| 2:B:102:MET:HE1 | 2:B:122:ALA:HB1 | 2.02 | 0.41 |
| 2:C:12:LEU:HD21 | 2:C:249:VAL:HG21 | 2.01 | 0.41 |
| 2:C:76:LEU:HD23 | 2:C:106:TYR:CE2 | 2.55 | 0.41 |
| 2:C:118:THR:HA | 6:L:38:DG:H5' | 2.01 | 0.41 |
| 2:C:181:HIS:CE1 | 2:C:244:PHE:HB3 | 2.55 | 0.41 |
| 2:E:12:LEU:HA | 2:E:178:TYR:O | 2.20 | 0.41 |
| 2:E:21:ASN:OD1 | 2:E:31:ARG:NE | 2.51 | 0.41 |
| 2:F:280:ARG:NH2 | 2:F:282:LEU:HD11 | 2.36 | 0.41 |
| 3:I:78:GLU:OE1 | 3:I:112:LEU:HD21 | 2.20 | 0.41 |
| 4:H:13:LYS:HB2 | 4:H:297:PRO:HG2 | 2.01 | 0.41 |
| 4:H:95:LYS:CE | 8:O:15:DA:H61 | 2.33 | 0.41 |
| 4:H:131:LEU:HD11 | 4:H:159:PHE:HZ | 1.84 | 0.41 |
| 4:H:480:LYS:NZ | 4:H:528:ARG:HH11 | 2.18 | 0.41 |
| 3:J:51:VAL:HG23 | 3:J:52:PHE:N | 2.35 | 0.41 |
| 3:J:62:HIS:O | 3:J:66:LEU:HG | 2.20 | 0.41 |
| 5:K:10:G:C5 | 5:K:11:G:C6 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:42:U:H3 | 6:L:13:DG:H1 | 1.68 | 0.41 |
| 2:M:47:LYS:HE3 | 2:M:131:LEU:HB2 | 2.02 | 0.41 |
| 1:P:102:ARG:HE | 1:P:102:ARG:HB3 | 1.55 | 0.41 |
| 1:P:116:ALA:O | 1:P:134:ARG:NH2 | 2.44 | 0.41 |
| 1:P:349:LEU:HD23 | 1:P:349:LEU:HA | 1.89 | 0.41 |
| 2:A:131:LEU:HD11 | 2:A:202:PHE:HZ | 1.85 | 0.41 |
| 2:A:148:THR:HA | 2:A:167:MET:HA | 2.02 | 0.41 |
| 2:B:276:THR:HG22 | 2:B:276:THR:O | 2.20 | 0.41 |
| 2:D:17:ASP:OD2 | 2:E:135:ARG:HD3 | 2.21 | 0.41 |
| 2:D:21:ASN:ND2 | 2:D:45:CYS:HB2 | 2.35 | 0.41 |
| 2:C:21:ASN:OD1 | 2:C:31:ARG:NE | 2.42 | 0.41 |
| 2:C:256:GLU:HG3 | 2:C:257:VAL:H | 1.85 | 0.41 |
| 4:H:24:GLY:HA2 | 4:H:183:ASN:ND2 | 2.35 | 0.41 |
| 4:H:84:HIS:HB3 | 4:H:87:TYR:HB2 | 2.02 | 0.41 |
| 4:H:196:LEU:HD21 | 7:N:18:GLU:OE1 | 2.20 | 0.41 |
| 4:H:540:LEU:HD11 | 3:J:103:ILE:CD1 | 2.50 | 0.41 |
| 5:K:26:G:O2' | 5:K:28:U:OP1 | 2.17 | 0.41 |
| 5:K:33:U:H1' | 5:K:34:C:O4' | 2.20 | 0.41 |
| 1:P:202:THR:HG23 | 1:P:203:GLU:HG2 | 2.03 | 0.41 |
| 1:P:433:ASN:OD1 | 1:P:443:GLU:HG2 | 2.20 | 0.41 |
| 1:P:499:ARG:NH2 | 1:P:750:ASN:O | 2.53 | 0.41 |
| 1:P:695:ILE:O | 1:P:695:ILE:HG13 | 2.20 | 0.41 |
| 2:A:15:VAL:O | 2:A:15:VAL:HG13 | 2.20 | 0.41 |
| 2:A:28:ASN:O | 2:A:171:PHE:CD1 | 2.73 | 0.41 |
| 2:A:34:PRO:HG3 | 3:J:47:THR:HG23 | 2.02 | 0.41 |
| 2:A:113:GLY:N | 2:A:127:GLY:HA3 | 2.35 | 0.41 |
| 2:A:181:HIS:CE1 | 2:A:244:PHE:HB3 | 2.56 | 0.41 |
| 2:A:241:ASP:OD2 | 2:A:245:LYS:HE3 | 2.20 | 0.41 |
| 2:B:15:VAL:CG1 | 2:B:20:PRO:HG3 | 2.50 | 0.41 |
| 2:B:103:CYS:HB3 | 2:B:192:THR:O | 2.19 | 0.41 |
| 2:D:62:HIS:O | 2:D:110:ARG:NH2 | 2.53 | 0.41 |
| 2:D:203:TRP:CE3 | 2:D:203:TRP:HA | 2.55 | 0.41 |
| 2:E:186:THR:OG1 | 2:E:234:ASN:HB3 | 2.20 | 0.41 |
| 2:E:229:PHE:CD2 | 2:E:279:LEU:HD21 | 2.55 | 0.41 |
| 2:F:4:GLU:OE1 | 2:F:4:GLU:N | 2.53 | 0.41 |
| 3:I:12:TYR:HH | 3:I:107:HIS:CG | 2.31 | 0.41 |
| 4:H:31:PRO:HA | 4:H:58:GLY:CA | 2.50 | 0.41 |
| 4:H:569:LEU:HA | 4:H:569:LEU:HD23 | 1.55 | 0.41 |
| 3:J:25:GLN:CD | 3:J:36:ILE:HG23 | 2.40 | 0.41 |
| 5:K:8:C:C5' | 2:M:48:ARG:HB2 | 2.49 | 0.41 |
| 5:K:14:C:O2 | 5:K:14:C:H2' | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:11:DG:H5' | 6:L:12:DG:H5' | 2.02 | 0.41 |
| 2:M:22:GLY:HA3 | 2:M:28:ASN:OD1 | 2.20 | 0.41 |
| 2:M:47:LYS:HG2 | 2:M:112:PHE:CD1 | 2.55 | 0.41 |
| 1:P:259:LEU:HA | 1:P:262:CYS:HB2 | 2.02 | 0.41 |
| 1:P:344:THR:C | 1:P:346:LYS:H | 2.23 | 0.41 |
| 1:P:412:LEU:O | 1:P:418:VAL:HG22 | 2.21 | 0.41 |
| 1:P:435:ASP:OD1 | 1:P:435:ASP:N | 2.39 | 0.41 |
| 1:P:470:PRO:HD3 | 1:P:600:VAL:HB | 2.01 | 0.41 |
| 1:P:516:LEU:O | 1:P:552:LEU:HD12 | 2.20 | 0.41 |
| 1:P:566:PHE:O | 1:P:586:CYS:HA | 2.21 | 0.41 |
| 1:P:707:GLN:NE2 | 1:P:710:GLU:O | 2.53 | 0.41 |
| 2:A:47:LYS:HD3 | 5:K:25:A:P | 2.60 | 0.41 |
| 2:A:153:THR:HB | 6:L:25:DC:H4' | 2.02 | 0.41 |
| 2:B:65:ILE:O | 2:B:65:ILE:HG22 | 2.19 | 0.41 |
| 2:D:41:VAL:HG23 | 2:D:178:TYR:CE2 | 2.55 | 0.41 |
| 2:D:145:HIS:HB2 | 2:D:170:LYS:O | 2.21 | 0.41 |
| 2:D:183:PHE:CE1 | 2:D:244:PHE:CE2 | 3.08 | 0.41 |
| 2:E:147:ILE:O | 2:E:147:ILE:HG13 | 2.19 | 0.41 |
| 3:I:51:VAL:HG23 | 3:I:52:PHE:N | 2.35 | 0.41 |
| 4:H:78:SER:HA | 4:H:87:TYR:CE2 | 2.56 | 0.41 |
| 4:H:217:LYS:HE3 | 8:O:13:DC:C2 | 2.55 | 0.41 |
| 2:M:160:GLU:CG | 2:M:161:THR:H | 2.33 | 0.41 |
| 1:P:60:SER:HB3 | 1:P:89:ILE:HD13 | 2.03 | 0.41 |
| 1:P:270:ARG:O | 1:P:272:LEU:N | 2.53 | 0.41 |
| 2:A:115:VAL:HG13 | 5:K:23:G:C2 | 2.55 | 0.41 |
| 2:B:21:ASN:HB2 | 2:B:41:VAL:HG13 | 2.02 | 0.41 |
| 2:B:203:TRP:CE3 | 2:B:226:LEU:HD21 | 2.55 | 0.41 |
| 2:D:56:MET:HE2 | 2:E:187:HIS:HB2 | 2.03 | 0.41 |
| 2:D:163:ASP:OD1 | 2:E:69:GLU:HB2 | 2.21 | 0.41 |
| 2:D:208:ASN:O | 2:D:212:HIS:ND1 | 2.54 | 0.41 |
| 2:D:280:ARG:HH22 | 2:D:282:LEU:HD21 | 1.86 | 0.41 |
| 2:C:7:TYR:HB2 | 2:C:184:ILE:CG1 | 2.51 | 0.41 |
| 2:C:46:LEU:HB2 | 2:C:131:LEU:HD22 | 2.02 | 0.41 |
| 2:C:50:VAL:HG13 | 2:C:205:ALA:HB1 | 2.03 | 0.41 |
| 2:C:137:ILE:HB | 2:C:264:TYR:CE1 | 2.55 | 0.41 |
| 2:C:206:LEU:O | 2:C:209:MET:HG2 | 2.20 | 0.41 |
| 2:C:258:VAL:HG21 | 2:C:264:TYR:CE2 | 2.55 | 0.41 |
| 2:E:259:ARG:HH11 | 2:F:35:GLN:HB2 | 1.84 | 0.41 |
| 3:I:113:PHE:HB2 | 3:J:80:ARG:NH1 | 2.16 | 0.41 |
| 4:H:206:ARG:HG2 | 4:H:207:LEU:CD2 | 2.46 | 0.41 |
| 6:L:9:DG:C8 | 6:L:10:DA:N6 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:39:GLY:N | 2:M:136:SER:HB3 | 2.36 | 0.41 |
| 2:M:137:ILE:HG12 | 2:M:177:LEU:O | 2.20 | 0.41 |
| 1:P:93:THR:HG22 | 1:P:134:ARG:NH2 | 2.34 | 0.41 |
| 1:P:195:VAL:HG12 | 1:P:379:ARG:CG | 2.50 | 0.41 |
| 2:A:23:ASP:CB | 2:A:24:PRO:HD3 | 2.51 | 0.41 |
| 2:A:186:THR:O | 2:A:190:LYS:HG3 | 2.20 | 0.41 |
| 2:B:36:THR:HG21 | 2:M:259:ARG:HG3 | 2.02 | 0.41 |
| 2:B:73:LEU:N | 2:M:152:VAL:O | 2.44 | 0.41 |
| 2:B:138:ASP:OD2 | 2:B:251:LYS:HB3 | 2.20 | 0.41 |
| 2:D:113:GLY:CA | 5:K:30:G:H5'' | 2.50 | 0.41 |
| 2:D:258:VAL:HG11 | 2:D:264:TYR:CE2 | 2.55 | 0.41 |
| 2:C:143:LEU:HD23 | 2:C:143:LEU:HA | 1.61 | 0.41 |
| 2:E:54:ILE:HG21 | 2:E:107:TYR:CD2 | 2.55 | 0.41 |
| 2:E:259:ARG:HD3 | 2:E:259:ARG:HA | 1.86 | 0.41 |
| 3:I:22:GLU:N | 3:I:36:ILE:HD11 | 2.36 | 0.41 |
| 4:H:248:PHE:CE1 | 4:H:252:THR:HG21 | 2.55 | 0.41 |
| 4:H:384:LEU:HD21 | 4:H:436:LEU:HD23 | 2.02 | 0.41 |
| 4:H:441:ILE:HG23 | 4:H:450:LEU:CD2 | 2.51 | 0.41 |
| 2:M:29:LEU:HB3 | 2:M:171:PHE:CE2 | 2.55 | 0.41 |
| 2:M:166:THR:O | 2:M:167:MET:C | 2.59 | 0.41 |
| 1:P:182:GLU:OE1 | 1:P:411:VAL:HG11 | 2.20 | 0.41 |
| 1:P:329:VAL:HG13 | 1:P:359:ILE:CD1 | 2.50 | 0.41 |
| 1:P:333:HIS:HD1 | 1:P:362:THR:HG1 | 1.66 | 0.41 |
| 1:P:573:MET:HE1 | 1:P:619:THR:HG22 | 2.02 | 0.41 |
| 1:P:616:GLN:O | 1:P:620:GLU:HG3 | 2.21 | 0.41 |
| 1:P:628:LEU:HD23 | 1:P:636:ALA:HB1 | 2.03 | 0.41 |
| 1:P:647:LYS:HD3 | 4:H:46:GLU:OE2 | 2.21 | 0.41 |
| 2:A:34:PRO:HG3 | 3:J:47:THR:CG2 | 2.50 | 0.41 |
| 2:A:134:SER:HA | 2:A:179:ARG:O | 2.20 | 0.41 |
| 2:B:147:ILE:HD11 | 5:K:19:U:C4 | 2.56 | 0.41 |
| 2:B:243:LEU:HD21 | 2:B:277:LYS:HE3 | 2.02 | 0.41 |
| 2:D:109:ILE:HD13 | 2:D:116:MET:SD | 2.61 | 0.41 |
| 2:C:11:PHE:CZ | 2:C:210:PHE:HE2 | 2.38 | 0.41 |
| 2:C:43:ASP:OD1 | 2:C:44:VAL:HG13 | 2.20 | 0.41 |
| 2:C:66:PHE:N | 2:C:67:ILE:HG23 | 2.36 | 0.41 |
| 2:E:44:VAL:HG11 | 5:K:37:C:H2' | 2.02 | 0.41 |
| 2:E:51:ARG:HH12 | 5:K:37:C:P | 2.44 | 0.41 |
| 2:F:51:ARG:NH2 | 2:F:108:ASP:OD2 | 2.54 | 0.41 |
| 2:F:89:LYS:HD3 | 2:F:89:LYS:HA | 1.93 | 0.41 |
| 3:I:93:LEU:HA | 3:I:93:LEU:HD23 | 1.79 | 0.41 |
| 3:G:51:VAL:HG23 | 3:G:52:PHE:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:478:LEU:HD21 | 4:H:516:LEU:HD22 | 2.02 | 0.41 |
| 3:J:49:ILE:HG13 | 3:J:50:ALA:N | 2.36 | 0.41 |
| 1:P:47:TYR:HD2 | 1:P:166:LEU:HD12 | 1.84 | 0.41 |
| 1:P:93:THR:HG22 | 1:P:134:ARG:HE | 1.86 | 0.41 |
| 1:P:272:LEU:HD21 | 1:P:445:LEU:HB3 | 2.03 | 0.41 |
| 1:P:274:SER:OG | 1:P:422:LEU:HB2 | 2.21 | 0.41 |
| 1:P:471:PRO:HA | 1:P:472:PRO:HD3 | 1.96 | 0.41 |
| 1:P:493:LEU:HD13 | 1:P:552:LEU:HD23 | 2.03 | 0.41 |
| 2:A:134:SER:OG | 2:A:180:CYS:HB2 | 2.21 | 0.41 |
| 2:A:166:THR:O | 2:A:167:MET:C | 2.59 | 0.41 |
| 2:B:18:GLY:HA3 | 2:B:218:ARG:C | 2.41 | 0.41 |
| 2:B:48:ARG:HD2 | 5:K:14:C:P | 2.61 | 0.41 |
| 2:B:137:ILE:HD11 | 2:B:179:ARG:HB2 | 2.02 | 0.41 |
| 2:B:144:GLU:HG3 | 2:B:171:PHE:HD1 | 1.81 | 0.41 |
| 2:B:149:ARG:NE | 2:B:166:THR:OG1 | 2.51 | 0.41 |
| 2:D:27:GLY:CA | 3:I:40:TYR:HE1 | 2.29 | 0.41 |
| 2:D:128:PRO:HG2 | 2:D:194:PHE:CD2 | 2.55 | 0.41 |
| 2:D:129:VAL:HG22 | 2:D:184:ILE:HG23 | 2.02 | 0.41 |
| 2:D:252:LYS:HG2 | 2:D:253:ASP:H | 1.86 | 0.41 |
| 2:C:78:ASP:O | 2:C:82:GLU:HG2 | 2.20 | 0.41 |
| 2:C:109:ILE:HG12 | 2:C:114:ALA:HB3 | 2.02 | 0.41 |
| 2:E:203:TRP:CE3 | 2:E:226:LEU:HD21 | 2.55 | 0.41 |
| 2:E:218:ARG:NH1 | 2:F:126:ARG:HH22 | 2.18 | 0.41 |
| 2:F:66:PHE:CD1 | 2:F:109:ILE:HD11 | 2.56 | 0.41 |
| 3:I:49:ILE:HG13 | 3:I:50:ALA:N | 2.36 | 0.41 |
| 3:I:62:HIS:O | 3:I:66:LEU:HG | 2.20 | 0.41 |
| 3:G:76:GLN:HA | 3:G:79:ILE:HD12 | 2.03 | 0.41 |
| 4:H:112:ASN:O | 4:H:116:GLN:HG2 | 2.20 | 0.41 |
| 4:H:214:VAL:CG2 | 4:H:330:LEU:HD13 | 2.50 | 0.41 |
| 4:H:269:VAL:HG23 | 4:H:331:SER:HB3 | 2.02 | 0.41 |
| 4:H:424:LYS:O | 4:H:427:GLN:NE2 | 2.54 | 0.41 |
| 4:H:441:ILE:HD12 | 4:H:560:ILE:CD1 | 2.50 | 0.41 |
| 4:H:482:GLN:HG2 | 4:H:489:LEU:HD11 | 2.02 | 0.41 |
| 4:H:537:ARG:HD2 | 3:J:109:THR:HG22 | 2.03 | 0.41 |
| 4:H:554:GLN:HA | 4:H:557:LEU:HB2 | 2.03 | 0.41 |
| 3:J:14:LEU:HD11 | 3:J:90:PRO:CD | 2.42 | 0.41 |
| 3:J:40:TYR:HD2 | 3:J:55:LEU:CD2 | 2.34 | 0.41 |
| 5:K:39:U:C2 | 5:K:40:C:C2 | 3.08 | 0.41 |
| 2:M:32:ILE:HG22 | 2:M:140:ILE:HD11 | 2.03 | 0.41 |
| 2:M:69:GLU:OE2 | 7:N:83:ILE:HD11 | 2.21 | 0.41 |
| 2:M:127:GLY:HA2 | 2:M:192:THR:HG21 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:40:ALA:HB1 | 7:N:136:HIS:HB3 | 2.02 | 0.41 |
| 7:N:65:ILE:HG13 | 7:N:94:LEU:HD12 | 2.03 | 0.41 |
| 9:Q:11:DT:H6 | 9:Q:11:DT:H2' | 1.72 | 0.41 |
| 1:P:106:PHE:HB2 | 4:H:285:LEU:CD1 | 2.51 | 0.41 |
| 1:P:186:TRP:HD1 | 1:P:416:TYR:OH | 2.03 | 0.41 |
| 1:P:192:SER:CB | 1:P:382:HIS:H | 2.33 | 0.41 |
| 1:P:395:GLN:N | 1:P:428:PRO:HG3 | 2.36 | 0.41 |
| 1:P:464:ARG:HD3 | 1:P:587:ASN:HD22 | 1.86 | 0.41 |
| 1:P:632:LEU:HA | 1:P:637:PHE:CE2 | 2.56 | 0.41 |
| 2:A:51:ARG:NH2 | 2:A:112:PHE:HB2 | 2.36 | 0.41 |
| 2:A:137:ILE:HD11 | 2:A:179:ARG:HB2 | 2.03 | 0.41 |
| 2:B:50:VAL:HG21 | 2:B:202:PHE:CE1 | 2.56 | 0.41 |
| 2:C:102:MET:HG3 | 2:C:116:MET:SD | 2.61 | 0.41 |
| 2:C:107:TYR:OH | 2:C:202:PHE:HB2 | 2.21 | 0.41 |
| 2:E:40:LEU:HA | 2:E:134:SER:O | 2.21 | 0.41 |
| 4:H:263:ARG:NH2 | 8:O:17:DA:H4' | 2.36 | 0.41 |
| 5:K:2:U:H6 | 7:N:43:TRP:CH2 | 2.39 | 0.41 |
| 6:L:26:DC:H2' | 6:L:27:DA:C8 | 2.56 | 0.41 |
| 2:M:67:ILE:HG23 | 2:M:67:ILE:HD12 | 1.60 | 0.41 |
| 2:M:141:MET:O | 2:M:174:PRO:HD3 | 2.21 | 0.41 |
| 2:M:236:GLY:O | 7:N:133:GLN:HG2 | 2.20 | 0.41 |
| 7:N:36:ASN:HA | 7:N:39:MET:HE2 | 2.03 | 0.41 |
| 1:P:202:THR:O | 1:P:206:MET:N | 2.49 | 0.40 |
| 1:P:231:ARG:HG3 | 1:P:235:GLN:NE2 | 2.36 | 0.40 |
| 2:A:143:LEU:HD21 | 2:D:34:PRO:CG | 2.51 | 0.40 |
| 2:A:218:ARG:HD3 | 2:A:221:MET:CE | 2.52 | 0.40 |
| 2:D:128:PRO:HG2 | 2:D:194:PHE:CG | 2.57 | 0.40 |
| 2:D:214:HIS:O | 2:E:126:ARG:NH1 | 2.46 | 0.40 |
| 2:C:14:ASP:CG | 2:C:224:ARG:HE | 2.23 | 0.40 |
| 2:C:54:ILE:HG13 | 2:C:107:TYR:CE1 | 2.57 | 0.40 |
| 2:C:203:TRP:CE3 | 2:C:226:LEU:HD21 | 2.57 | 0.40 |
| 2:E:137:ILE:HG13 | 2:E:249:VAL:CG1 | 2.51 | 0.40 |
| 2:E:177:LEU:HD12 | 2:E:177:LEU:HA | 1.83 | 0.40 |
| 2:F:9:PHE:CB | 2:F:228:VAL:HG12 | 2.50 | 0.40 |
| 2:F:20:PRO:HB2 | 2:F:41:VAL:CG2 | 2.51 | 0.40 |
| 2:F:143:LEU:HB2 | 2:F:172:THR:HG23 | 2.03 | 0.40 |
| 3:I:14:LEU:HD11 | 3:I:90:PRO:CD | 2.42 | 0.40 |
| 3:G:40:TYR:HD2 | 3:G:55:LEU:CD2 | 2.34 | 0.40 |
| 4:H:33:ILE:HD13 | 4:H:160:ARG:NH2 | 2.35 | 0.40 |
| 4:H:234:LYS:HB3 | 4:H:239:ALA:N | 2.35 | 0.40 |
| 4:H:398:ILE:HG13 | 4:H:399:ALA:N | 2.35 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:14:ASP:OD2 | 2:M:224:ARG:NE | 2.44 | 0.40 |
| 1:P:129:GLY:HA3 | 1:P:674:ARG:NH2 | 2.36 | 0.40 |
| 1:P:213:ASP:OD1 | 1:P:214:ALA:N | 2.53 | 0.40 |
| 1:P:302:ARG:CD | 1:P:383:ASN:HB3 | 2.47 | 0.40 |
| 1:P:303:ILE:CD1 | 1:P:388:VAL:HB | 2.52 | 0.40 |
| 1:P:515:LYS:HA | 1:P:551:TRP:CD1 | 2.56 | 0.40 |
| 2:B:44:VAL:HG21 | 2:M:147:ILE:HB | 2.02 | 0.40 |
| 2:B:258:VAL:HG21 | 2:B:264:TYR:OH | 2.21 | 0.40 |
| 2:D:31:ARG:HH21 | 5:K:33:U:P | 2.43 | 0.40 |
| 2:D:113:GLY:N | 2:D:127:GLY:HA3 | 2.37 | 0.40 |
| 2:D:129:VAL:HG11 | 2:D:202:PHE:CE2 | 2.56 | 0.40 |
| 2:C:105:ARG:HB3 | 2:C:106:TYR:CD1 | 2.56 | 0.40 |
| 3:I:12:TYR:HB2 | 3:I:100:LEU:HD22 | 2.03 | 0.40 |
| 3:G:12:TYR:HB2 | 3:G:100:LEU:HD22 | 2.03 | 0.40 |
| 4:H:39:GLN:HG2 | 4:H:41:ASN:HD21 | 1.86 | 0.40 |
| 4:H:51:LEU:HD12 | 4:H:51:LEU:HA | 1.75 | 0.40 |
| 4:H:234:LYS:O | 4:H:238:PHE:HB2 | 2.21 | 0.40 |
| 4:H:313:ASN:OD1 | 8:O:20:DA:H4' | 2.21 | 0.40 |
| 4:H:475:PHE:CE1 | 4:H:512:LEU:HD11 | 2.57 | 0.40 |
| 5:K:13:U:C5 | 2:M:147:ILE:HD11 | 2.57 | 0.40 |
| 7:N:47:ILE:HG13 | 7:N:106:PHE:CG | 2.57 | 0.40 |
| 1:P:63:LYS:HB3 | 1:P:63:LYS:HE2 | 1.93 | 0.40 |
| 1:P:106:PHE:CE2 | 1:P:110:LEU:HD12 | 2.57 | 0.40 |
| 1:P:244:ASP:HA | 1:P:252:ASN:ND2 | 2.32 | 0.40 |
| 1:P:332:HIS:HB2 | 1:P:336:LEU:H | 1.87 | 0.40 |
| 2:A:22:GLY:HA3 | 5:K:27:G:C2' | 2.51 | 0.40 |
| 2:A:25:ASP:HB3 | 2:C:167:MET:HE1 | 2.03 | 0.40 |
| 2:D:127:GLY:HA2 | 2:D:128:PRO:HD3 | 1.87 | 0.40 |
| 2:D:147:ILE:HA | 2:E:31:ARG:HH22 | 1.85 | 0.40 |
| 2:C:56:MET:CE | 2:C:212:HIS:HB3 | 2.51 | 0.40 |
| 2:E:113:GLY:CA | 5:K:36:C:H5'' | 2.51 | 0.40 |
| 2:E:213:ASP:HB3 | 2:E:218:ARG:HH12 | 1.86 | 0.40 |
| 2:F:19:ASN:HB3 | 2:F:22:GLY:N | 2.36 | 0.40 |
| 4:H:12:ARG:O | 4:H:16:SER:N | 2.53 | 0.40 |
| 4:H:257:LEU:HB3 | 4:H:272:VAL:HB | 2.02 | 0.40 |
| 4:H:274:TRP:HA | 4:H:301:ILE:HG22 | 2.02 | 0.40 |
| 4:H:514:ARG:HH21 | 3:J:45:SER:HB3 | 1.87 | 0.40 |
| 2:M:282:LEU:HA | 2:M:282:LEU:HD23 | 1.90 | 0.40 |
| 7:N:16:ARG:HG3 | 7:N:24:VAL:O | 2.20 | 0.40 |
| 9:Q:2:DA:H2' | 9:Q:3:DA:C8 | 2.56 | 0.40 |
| 1:P:125:TRP:CE3 | 1:P:131:LEU:HB2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:300:LYS:HD2 | 1:P:387:SER:O | 2.21 | 0.40 |
| 1:P:331:GLU:HB3 | 1:P:365:GLN:HE22 | 1.86 | 0.40 |
| 1:P:395:GLN:HA | 1:P:428:PRO:HG3 | 2.03 | 0.40 |
| 1:P:426:THR:HB | 1:P:637:PHE:CG | 2.57 | 0.40 |
| 1:P:486:ILE:HG22 | 1:P:570:TYR:HD2 | 1.84 | 0.40 |
| 2:B:67:ILE:HB | 2:B:68:ARG:H | 1.66 | 0.40 |
| 2:B:87:LYS:HE3 | 2:B:87:LYS:HB3 | 1.93 | 0.40 |
| 2:B:144:GLU:OE1 | 4:H:424:LYS:HD2 | 2.22 | 0.40 |
| 2:B:149:ARG:HB2 | 5:K:19:U:H1' | 2.04 | 0.40 |
| 2:D:54:ILE:HG13 | 2:D:107:TYR:CD2 | 2.57 | 0.40 |
| 2:D:259:ARG:HD3 | 2:D:259:ARG:HA | 1.71 | 0.40 |
| 2:C:76:LEU:HD12 | 2:C:76:LEU:H | 1.86 | 0.40 |
| 2:E:113:GLY:C | 5:K:36:C:H5'' | 2.41 | 0.40 |
| 2:E:126:ARG:HD2 | 2:E:188:PHE:CG | 2.56 | 0.40 |
| 4:H:465:GLN:OE1 | 4:H:542:HIS:ND1 | 2.54 | 0.40 |
| 3:J:12:TYR:HB2 | 3:J:100:LEU:HD22 | 2.03 | 0.40 |
| 5:K:3:U:O2 | 7:N:39:MET:HE1 | 2.22 | 0.40 |
| 6:L:19:DG:OP2 | 6:L:19:DG:H2' | 2.21 | 0.40 |
| 2:M:115:VAL:HA | 2:M:124:GLN:HA | 2.03 | 0.40 |
| 1:P:65:ILE:CD1 | 11:P:803:PO4:P | 3.09 | 0.40 |
| 1:P:412:LEU:HA | 1:P:416:TYR:HB2 | 2.04 | 0.40 |
| 2:A:38:GLU:HA | 2:A:139:PRO:HA | 2.03 | 0.40 |
| 2:A:128:PRO:HG3 | 2:A:189:ALA:CA | 2.50 | 0.40 |
| 2:B:15:VAL:O | 2:B:175:TYR:HA | 2.21 | 0.40 |
| 2:B:259:ARG:NH2 | 2:C:33:ASP:OD1 | 2.54 | 0.40 |
| 2:C:40:LEU:HA | 2:C:134:SER:O | 2.22 | 0.40 |
| 2:C:109:ILE:HG21 | 2:C:116:MET:HE1 | 2.04 | 0.40 |
| 2:E:273:LEU:C | 2:E:275:GLU:N | 2.75 | 0.40 |
| 3:I:73:VAL:HG13 | 9:Q:11:DT:C4 | 2.57 | 0.40 |
| 3:G:96:GLU:HG3 | 3:G:100:LEU:HD12 | 2.04 | 0.40 |
| 4:H:333:ASN:HB2 | 4:H:338:VAL:HG23 | 2.04 | 0.40 |
| 4:H:508:VAL:CG1 | 4:H:512:LEU:HG | 2.51 | 0.40 |
| 4:H:516:LEU:CD2 | 4:H:536:ILE:HD13 | 2.51 | 0.40 |
| 5:K:17:C:N4 | 5:K:18:U:O4 | 2.54 | 0.40 |
| 5:K:18:U:O2' | 5:K:19:U:OP2 | 2.30 | 0.40 |
| 2:M:6:ARG:HH11 | 2:M:231:HIS:HE1 | 1.69 | 0.40 |
| 2:M:238:ALA:HB2 | 2:M:277:LYS:HE2 | 2.03 | 0.40 |
| 7:N:57:LEU:HA | 7:N:159:LEU:HA | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1 | P | 752/771 (98%) | 627 (83%) | 123 (16%) | 2 (0%) | 37 | 70 |
| 2 | A | 281/283 (99%) | 223 (79%) | 55 (20%) | 3 (1%) | 12 | 44 |
| 2 | B | 281/283 (99%) | 223 (79%) | 56 (20%) | 2 (1%) | 19 | 54 |
| 2 | C | 281/283 (99%) | 233 (83%) | 47 (17%) | 1 (0%) | 30 | 66 |
| 2 | D | 281/283 (99%) | 229 (82%) | 51 (18%) | 1 (0%) | 30 | 66 |
| 2 | E | 281/283 (99%) | 231 (82%) | 49 (17%) | 1 (0%) | 30 | 66 |
| 2 | F | 267/283 (94%) | 218 (82%) | 48 (18%) | 1 (0%) | 30 | 66 |
| 2 | M | 260/283 (92%) | 214 (82%) | 46 (18%) | 0 | 100 | 100 |
| 3 | G | 122/124 (98%) | 114 (93%) | 8 (7%) | 0 | 100 | 100 |
| 3 | I | 122/124 (98%) | 114 (93%) | 8 (7%) | 0 | 100 | 100 |
| 3 | J | 122/124 (98%) | 114 (93%) | 8 (7%) | 0 | 100 | 100 |
| 4 | H | 580/582 (100%) | 477 (82%) | 102 (18%) | 1 (0%) | 44 | 77 |
| 7 | N | 203/205 (99%) | 163 (80%) | 39 (19%) | 1 (0%) | 25 | 61 |
| All | All | 3833/3911 (98%) | 3180 (83%) | 640 (17%) | 13 (0%) | 38 | 70 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 745 | PRO |
| 2 | A | 91 | LYS |
| 2 | D | 91 | LYS |
| 2 | C | 91 | LYS |
| 2 | E | 91 | LYS |
| 2 | B | 91 | LYS |
| 2 | F | 91 | LYS |
| 4 | H | 398 | ILE |
| 2 | A | 68 | ARG |
| 7 | N | 194 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 23 | ASP |
| 2 | B | 68 | ARG |
| 1 | P | 744 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | P | 588/601 (98%) | 587 (100%) | 1 (0%) | 92 | 97 |
| 2 | A | 245/245 (100%) | 244 (100%) | 1 (0%) | 89 | 95 |
| 2 | B | 245/245 (100%) | 245 (100%) | 0 | 100 | 100 |
| 2 | C | 245/245 (100%) | 243 (99%) | 2 (1%) | 79 | 90 |
| 2 | D | 245/245 (100%) | 243 (99%) | 2 (1%) | 79 | 90 |
| 2 | E | 245/245 (100%) | 244 (100%) | 1 (0%) | 89 | 95 |
| 2 | F | 235/245 (96%) | 235 (100%) | 0 | 100 | 100 |
| 2 | M | 229/245 (94%) | 229 (100%) | 0 | 100 | 100 |
| 3 | G | 104/104 (100%) | 98 (94%) | 6 (6%) | 17 | 48 |
| 3 | I | 104/104 (100%) | 99 (95%) | 5 (5%) | 21 | 55 |
| 3 | J | 104/104 (100%) | 99 (95%) | 5 (5%) | 21 | 55 |
| 4 | H | 475/475 (100%) | 475 (100%) | 0 | 100 | 100 |
| 7 | N | 182/182 (100%) | 182 (100%) | 0 | 100 | 100 |
| All | All | 3246/3285 (99%) | 3223 (99%) | 23 (1%) | 80 | 91 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 439 | ARG |
| 2 | A | 91 | LYS |
| 2 | D | 68 | ARG |
| 2 | D | 91 | LYS |
| 2 | C | 91 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 156 | LYS |
| 2 | E | 271 | LYS |
| 3 | I | 6 | ASN |
| 3 | I | 13 | VAL |
| 3 | I | 39 | ARG |
| 3 | I | 97 | GLN |
| 3 | I | 100 | LEU |
| 3 | G | 6 | ASN |
| 3 | G | 13 | VAL |
| 3 | G | 33 | ASN |
| 3 | G | 39 | ARG |
| 3 | G | 97 | GLN |
| 3 | G | 100 | LEU |
| 3 | J | 6 | ASN |
| 3 | J | 13 | VAL |
| 3 | J | 39 | ARG |
| 3 | J | 97 | GLN |
| 3 | J | 100 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 8 | HIS |
| 1 | P | 184 | HIS |
| 1 | P | 252 | ASN |
| 1 | P | 382 | HIS |
| 1 | P | 402 | GLN |
| 1 | P | 427 | GLN |
| 1 | P | 501 | HIS |
| 1 | P | 517 | HIS |
| 1 | P | 587 | ASN |
| 1 | P | 707 | GLN |
| 2 | A | 21 | ASN |
| 2 | A | 130 | GLN |
| 2 | B | 74 | ASN |
| 2 | B | 124 | GLN |
| 2 | B | 181 | HIS |
| 2 | B | 231 | HIS |
| 2 | D | 181 | HIS |
| 2 | D | 222 | ASN |
| 2 | C | 145 | HIS |
| 2 | C | 181 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 181 | HIS |
| 2 | E | 222 | ASN |
| 2 | F | 21 | ASN |
| 2 | F | 58 | GLN |
| 3 | I | 33 | ASN |
| 3 | I | 85 | HIS |
| 3 | G | 85 | HIS |
| 4 | H | 79 | ASN |
| 4 | H | 225 | ASN |
| 4 | H | 236 | GLN |
| 4 | H | 490 | ASN |
| 4 | H | 544 | GLN |
| 3 | J | 33 | ASN |
| 3 | J | 85 | HIS |
| 2 | M | 21 | ASN |
| 2 | M | 220 | GLN |
| 7 | N | 68 | ASN |
| 7 | N | 89 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 5 | K | 42/43 (97%) | 33 (78%) | 3 (7%) |

All (33) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | K | 2 | U |
| 5 | K | 3 | U |
| 5 | K | 4 | G |
| 5 | K | 5 | A |
| 5 | K | 6 | A |
| 5 | K | 8 | C |
| 5 | K | 9 | A |
| 5 | K | 10 | G |
| 5 | K | 11 | G |
| 5 | K | 13 | U |
| 5 | K | 15 | A |
| 5 | K | 16 | G |
| 5 | K | 17 | C |
| 5 | K | 18 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | K | 19 | U |
| 5 | K | 20 | G |
| 5 | K | 21 | C |
| 5 | K | 22 | C |
| 5 | K | 23 | G |
| 5 | K | 24 | U |
| 5 | K | 25 | A |
| 5 | K | 27 | G |
| 5 | K | 29 | G |
| 5 | K | 31 | C |
| 5 | K | 33 | U |
| 5 | K | 34 | C |
| 5 | K | 35 | G |
| 5 | K | 36 | C |
| 5 | K | 37 | C |
| 5 | K | 38 | C |
| 5 | K | 39 | U |
| 5 | K | 41 | G |
| 5 | K | 43 | C |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | K | 4 | G |
| 5 | K | 9 | A |
| 5 | K | 14 | C |

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 11 | PO4 | Q | 101 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.46 | 0 |
| 11 | PO4 | P | 804 | 10 | 4,4,4 | 1.27 | 0 | 6,6,6 | 0.31 | 0 |
| 11 | PO4 | P | 803 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.44 | 0 |
| 11 | PO4 | O | 101 | - | 4,4,4 | 0.89 | 0 | 6,6,6 | 0.46 | 0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

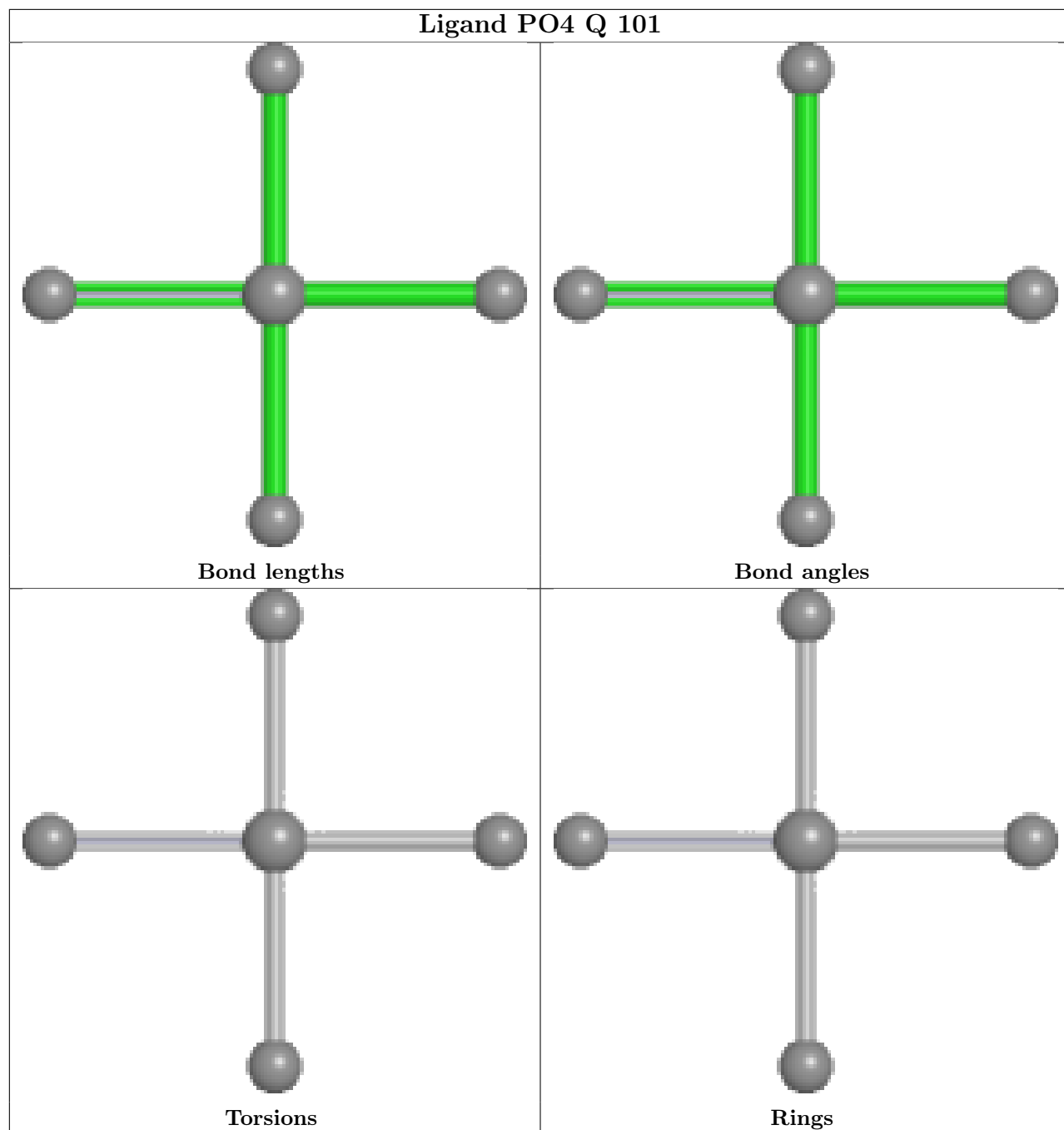
There are no torsion outliers.

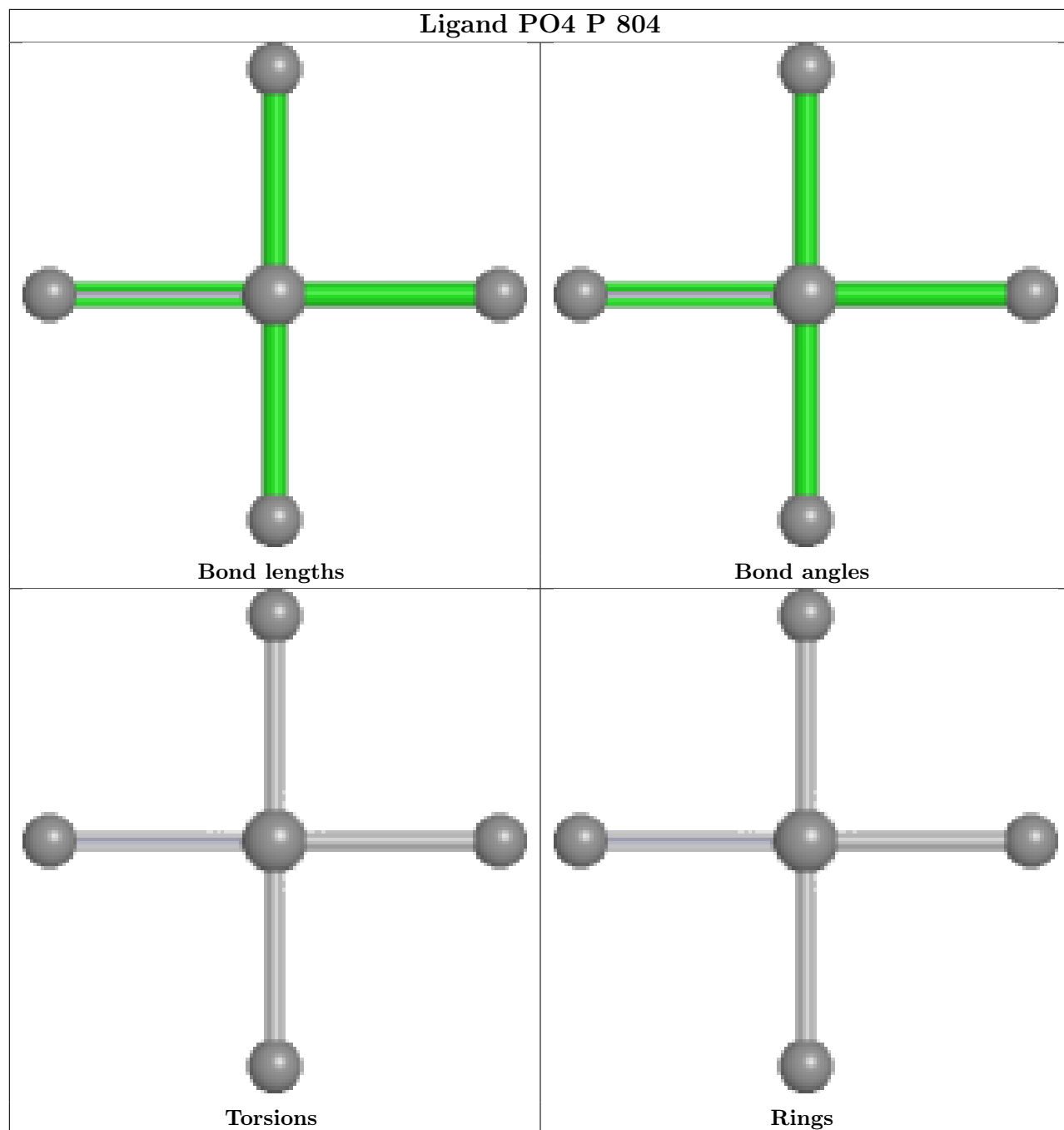
There are no ring outliers.

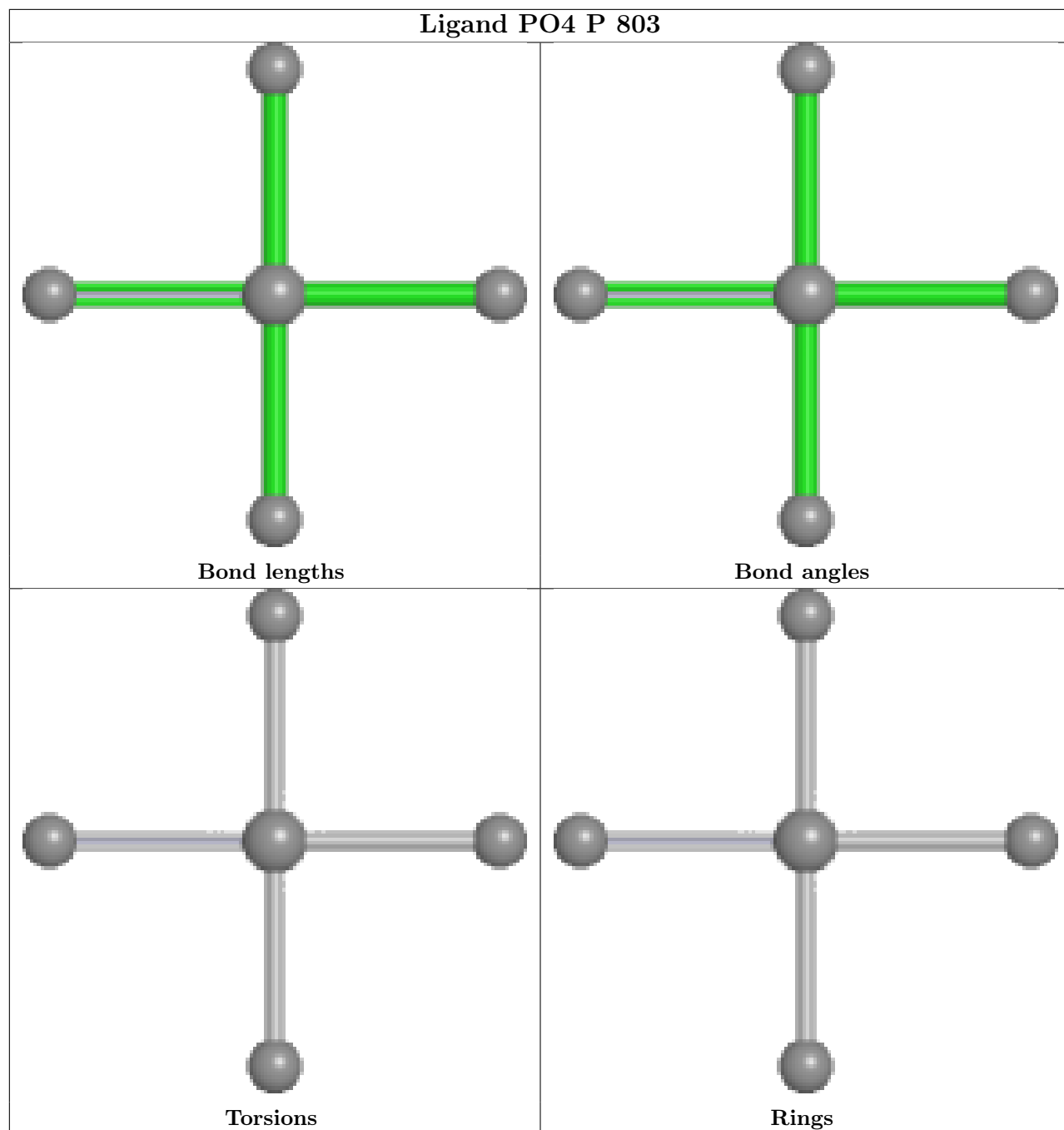
4 monomers are involved in 17 short contacts:

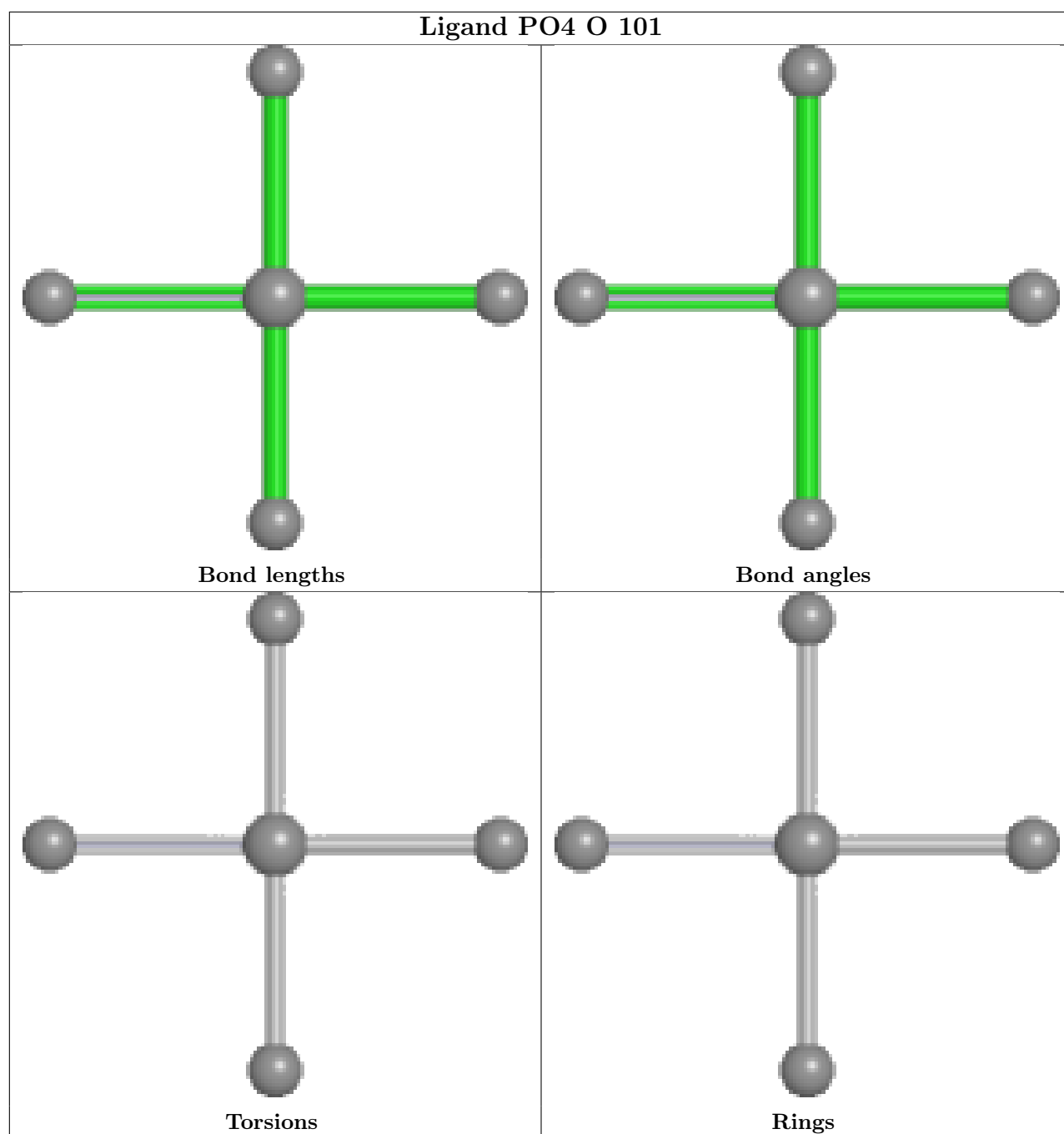
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11 | Q | 101 | PO4 | 2 | 0 |
| 11 | P | 804 | PO4 | 4 | 0 |
| 11 | P | 803 | PO4 | 10 | 0 |
| 11 | O | 101 | PO4 | 1 | 0 |

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | P | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | P | 759:LEU | C | 760:ALA | N | 6.63 |

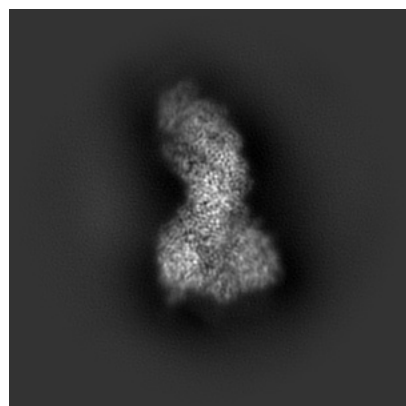
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29879. These allow visual inspection of the internal detail of the map and identification of artifacts.

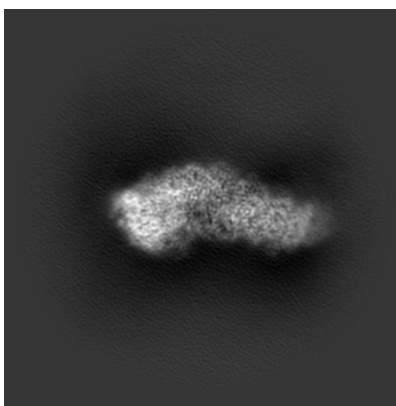
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

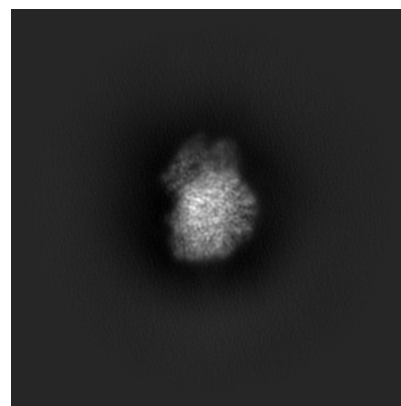
6.1.1 Primary map



X

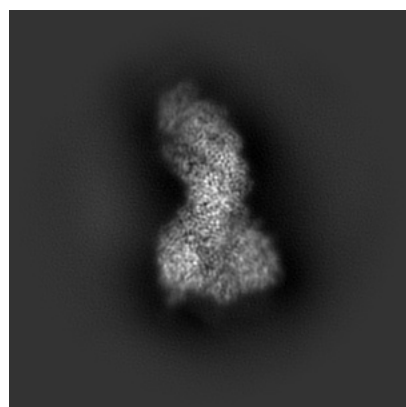


Y

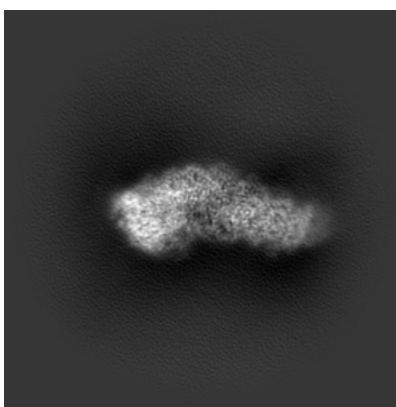


Z

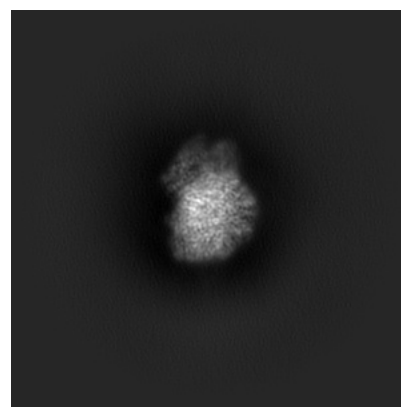
6.1.2 Raw map



X



Y

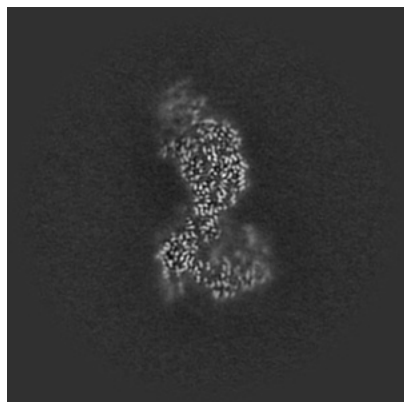


Z

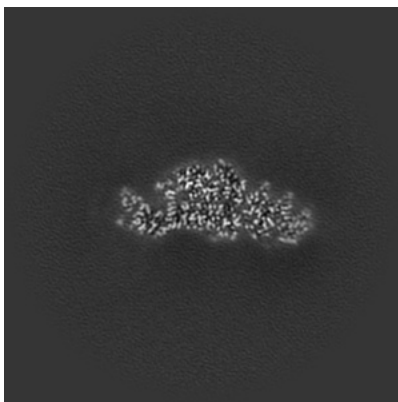
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

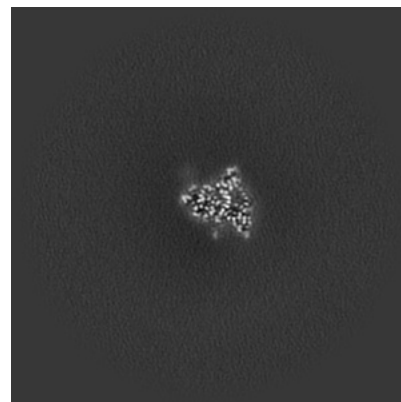
6.2.1 Primary map



X Index: 150

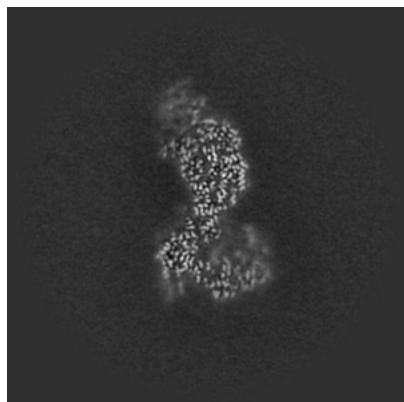


Y Index: 150

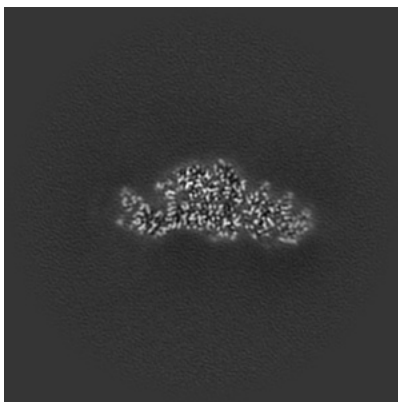


Z Index: 150

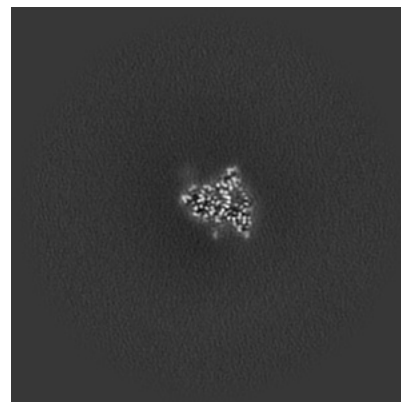
6.2.2 Raw map



X Index: 150



Y Index: 150

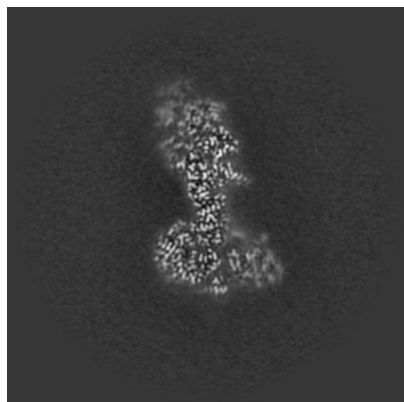


Z Index: 150

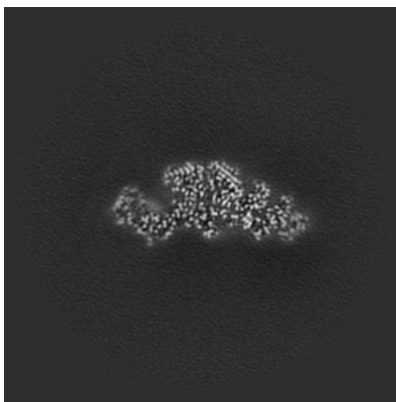
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

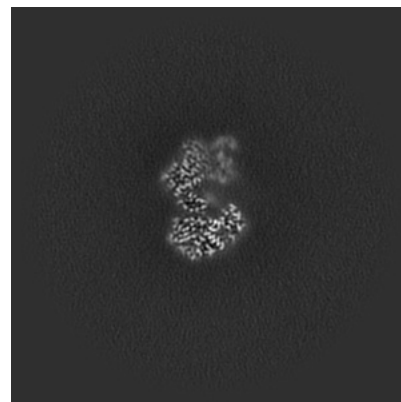
6.3.1 Primary map



X Index: 141

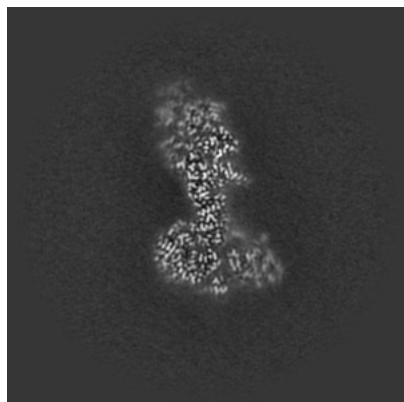


Y Index: 155

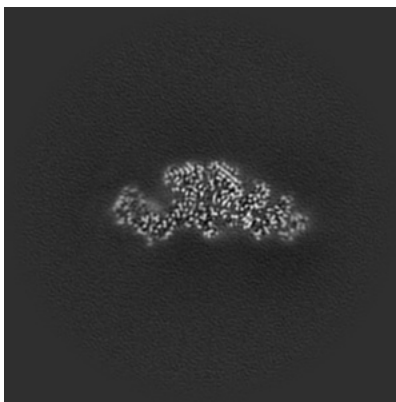


Z Index: 115

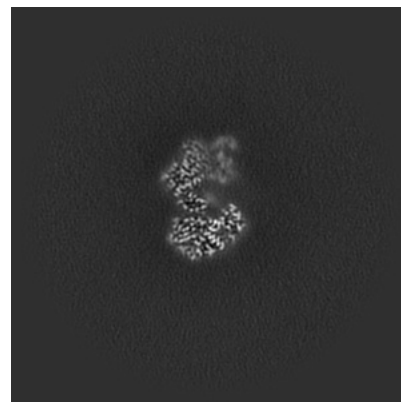
6.3.2 Raw map



X Index: 141



Y Index: 155

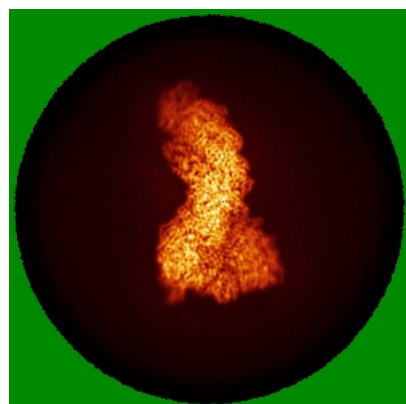


Z Index: 115

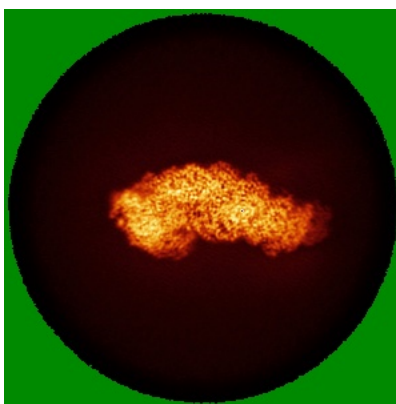
The images above show the largest variance slices of the map in three orthogonal directions.

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

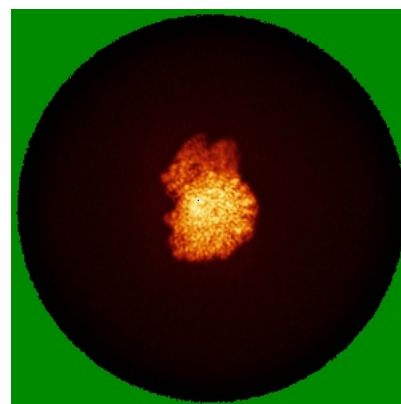
6.4.1 Primary map



X

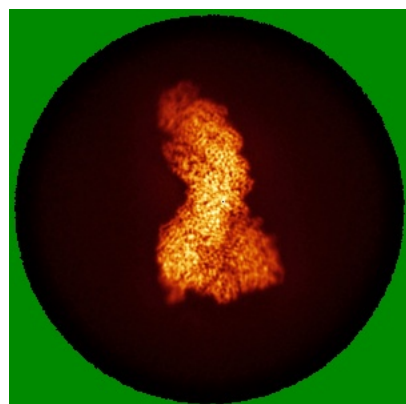


Y

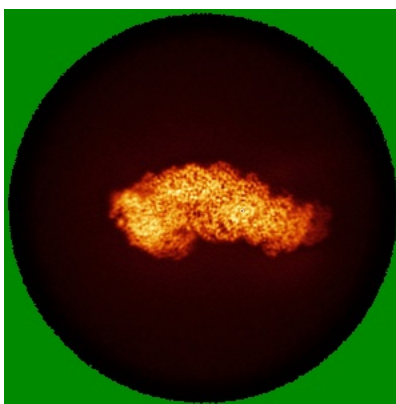


Z

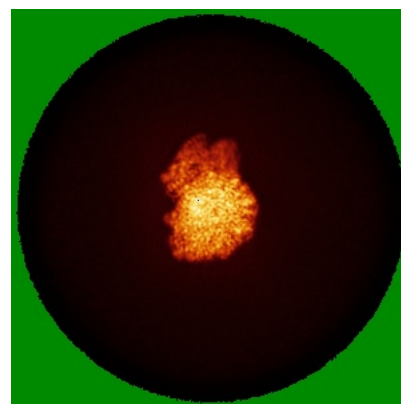
6.4.2 Raw map



X



Y



Z

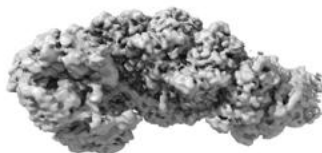
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



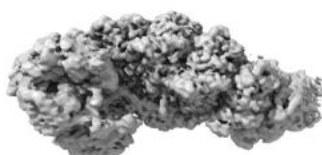
Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

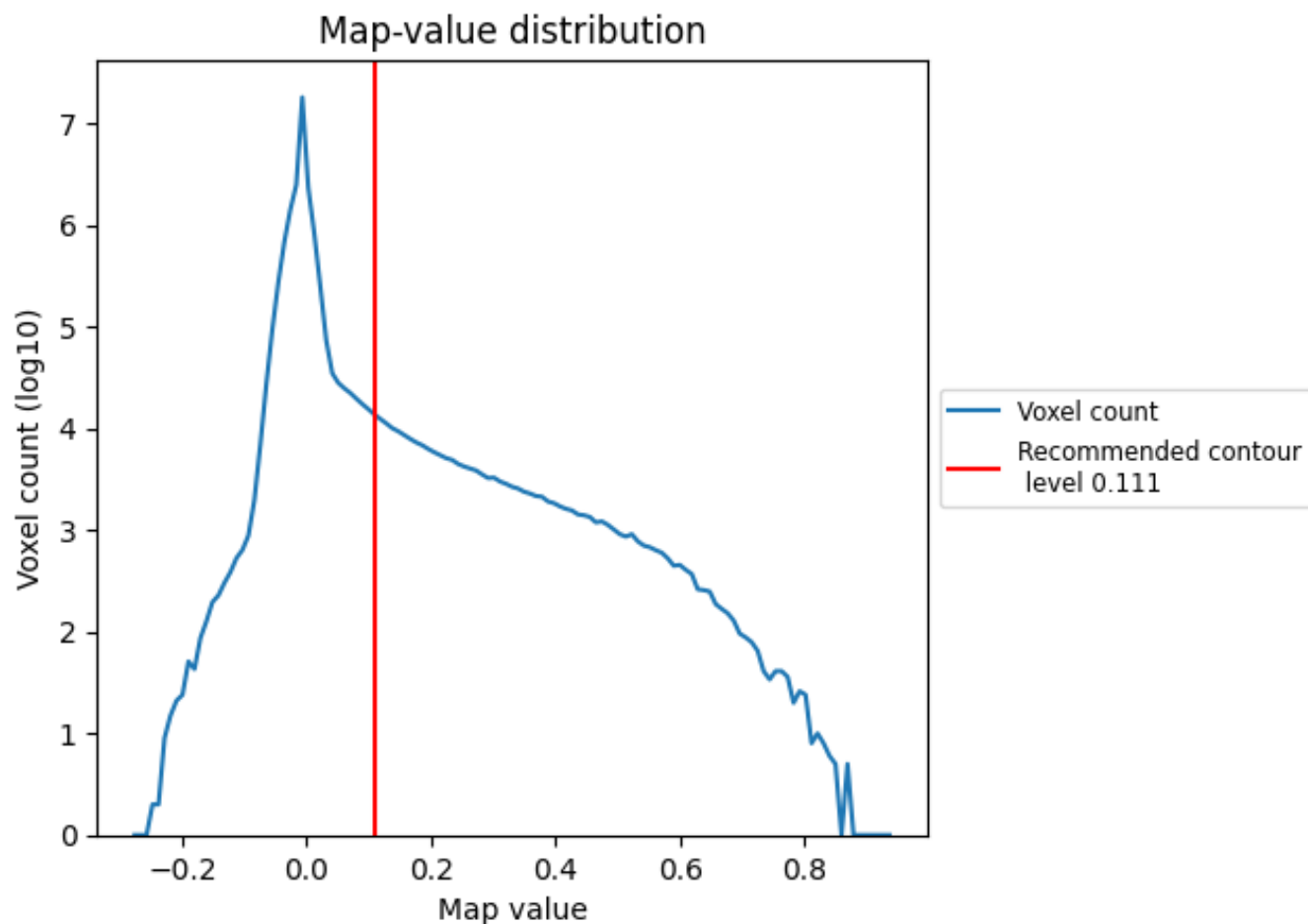
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

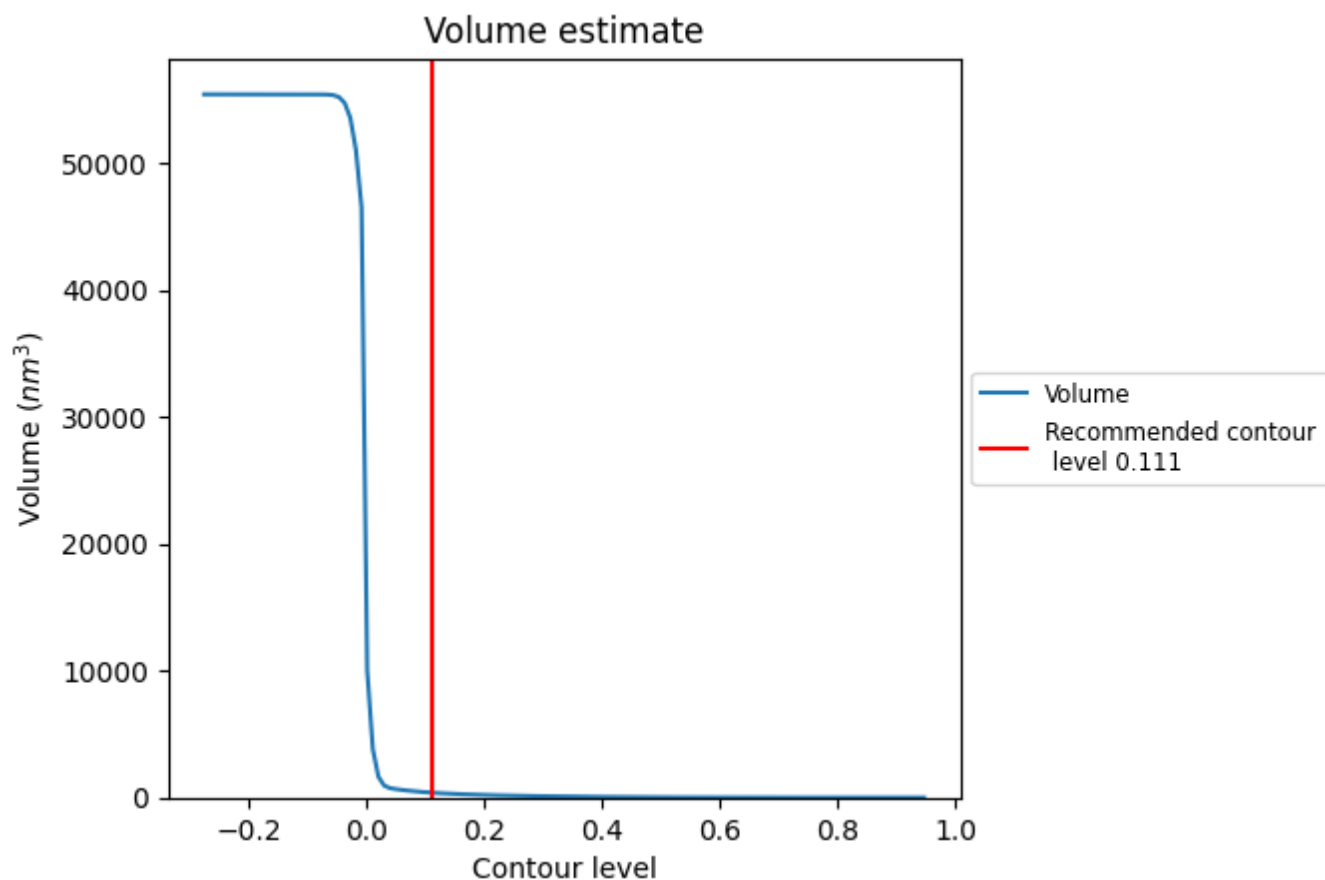
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

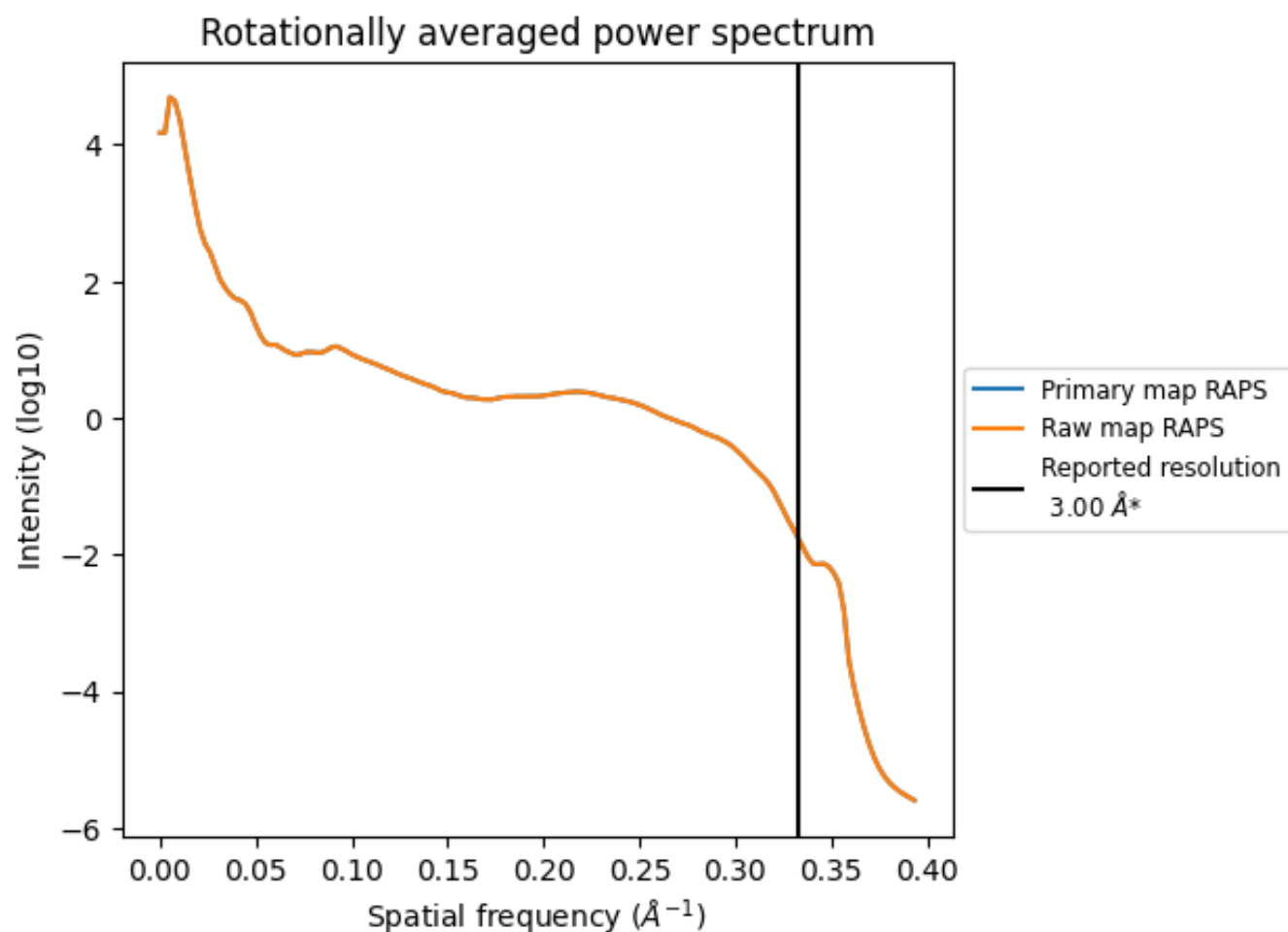
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

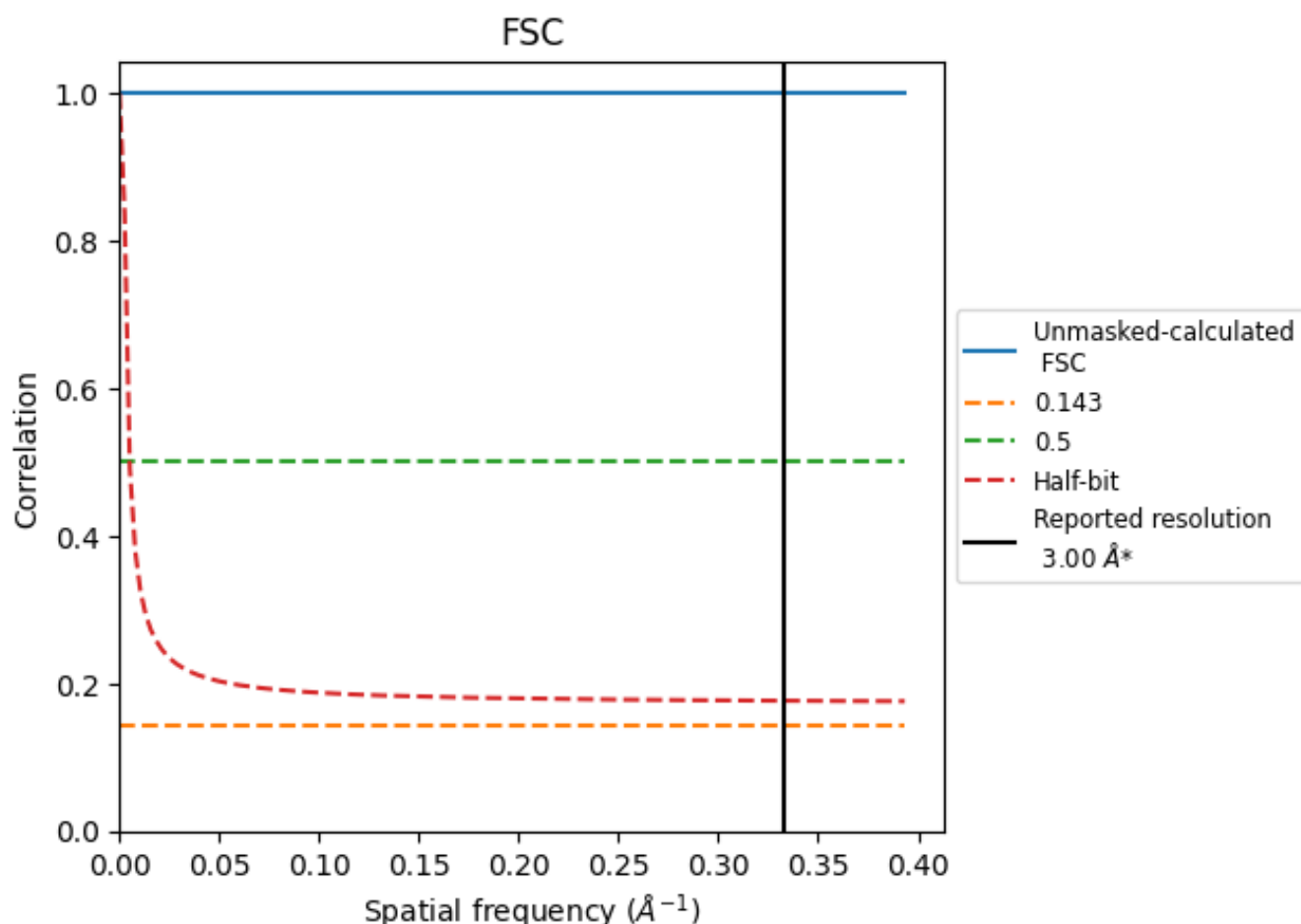


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

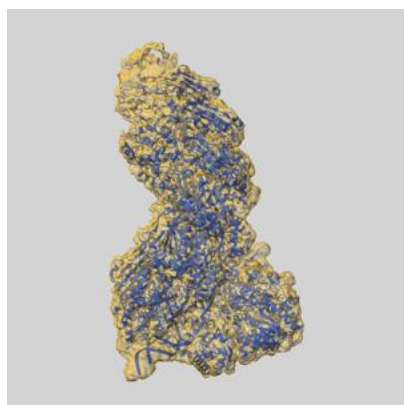
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-----|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.00 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

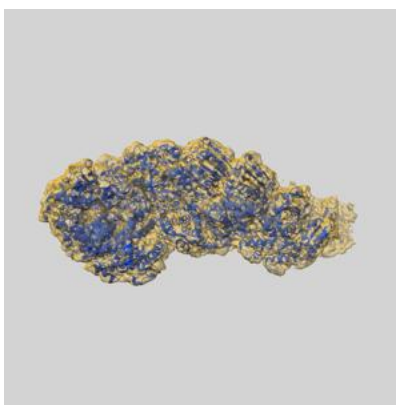
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29879 and PDB model 8G9U. Per-residue inclusion information can be found in section [3](#) on page [8](#).

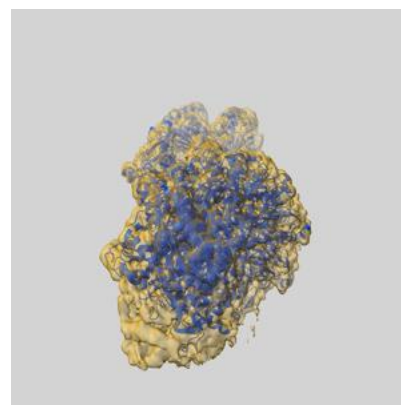
9.1 Map-model overlay [i](#)



X



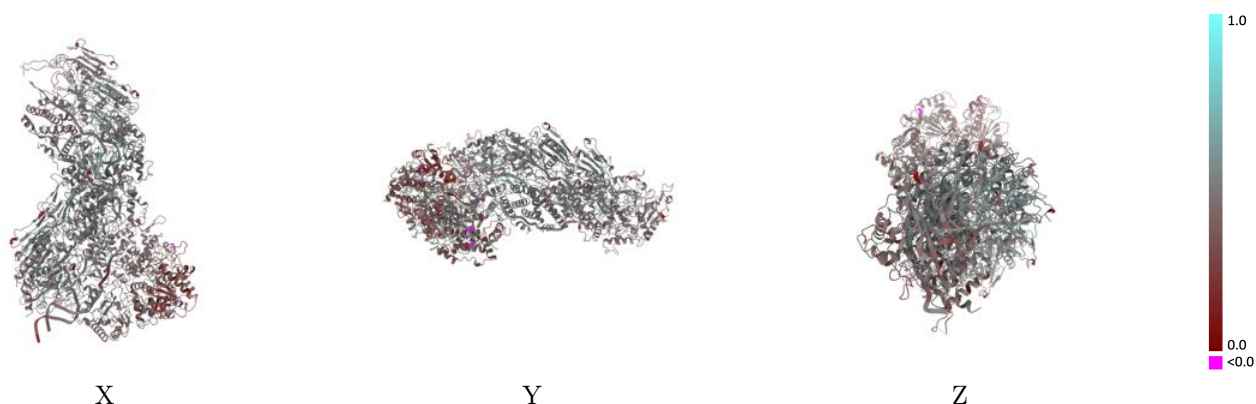
Y



Z

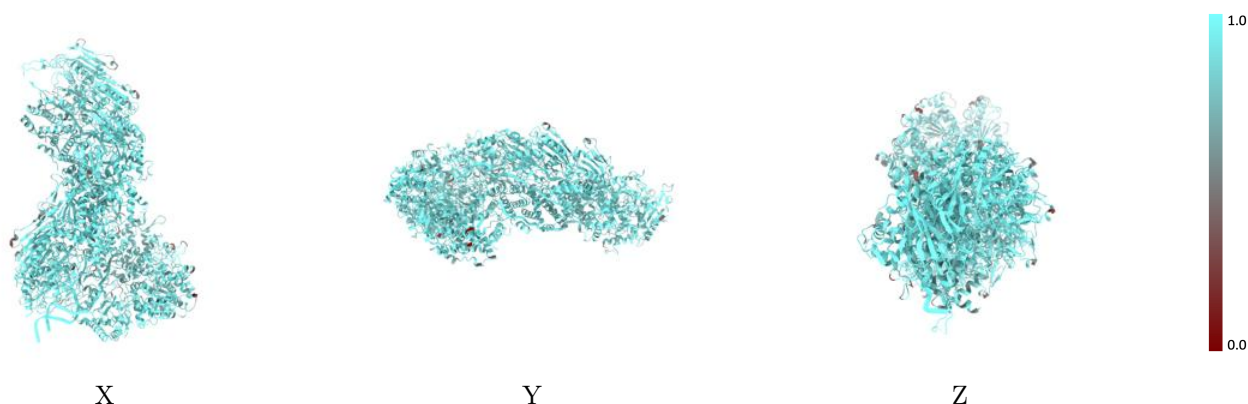
The images above show the 3D surface view of the map at the recommended contour level 0.111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



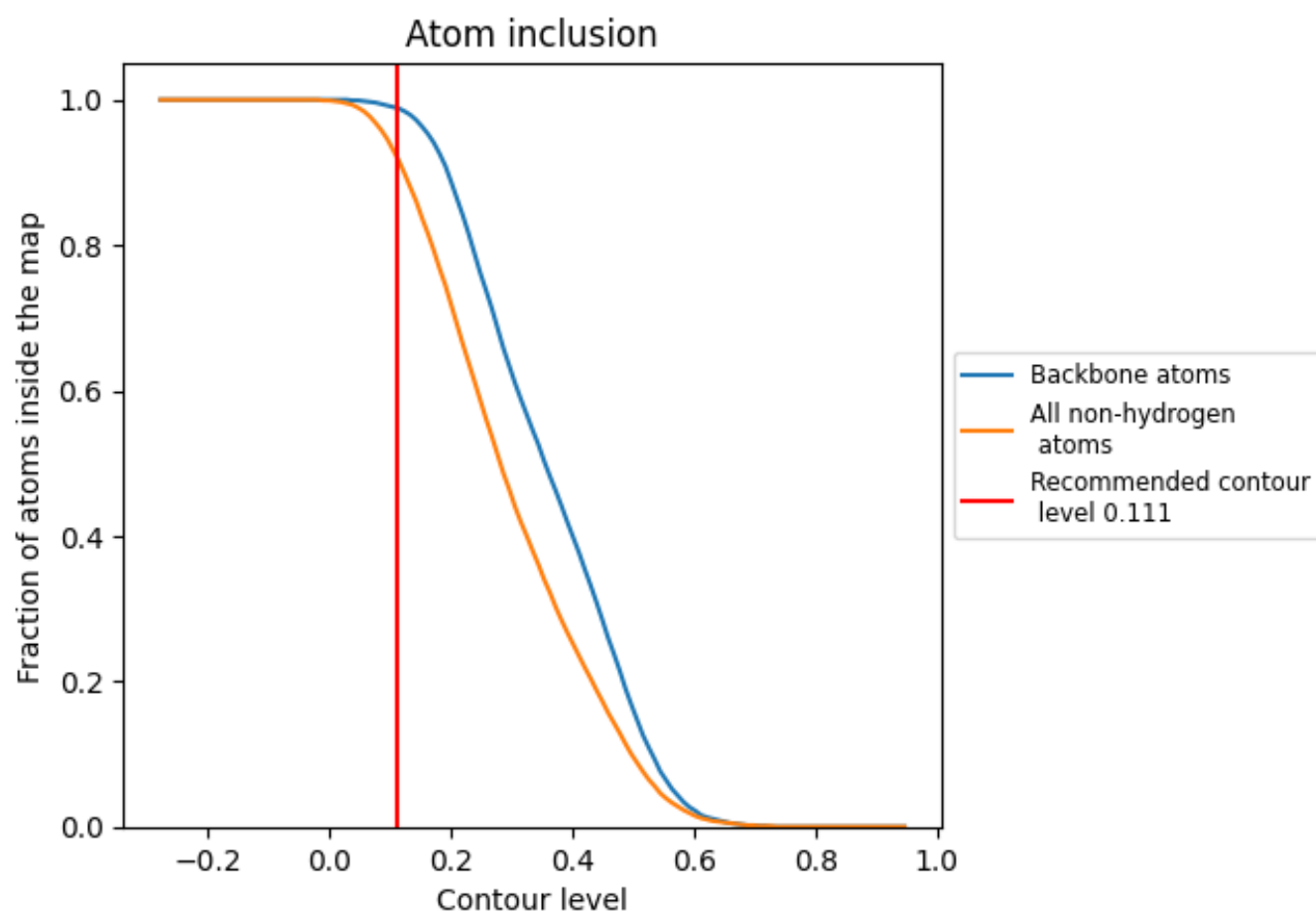
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.111).





































9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.111) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9230 |  0.4400 |
| A |  0.9470 |  0.4750 |
| B |  0.9280 |  0.4660 |
| C |  0.9490 |  0.4800 |
| D |  0.9320 |  0.4710 |
| E |  0.9180 |  0.4500 |
| F |  0.9050 |  0.4000 |
| G |  0.8340 |  0.4130 |
| H |  0.9250 |  0.4580 |
| I |  0.9340 |  0.4510 |
| J |  0.9500 |  0.4620 |
| K |  0.9960 |  0.4920 |
| L |  0.9950 |  0.4760 |
| M |  0.9210 |  0.4580 |
| N |  0.9220 |  0.4530 |
| O |  0.9760 |  0.3930 |
| P |  0.8840 |  0.3630 |
| Q |  0.9400 |  0.4630 |

