



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:46 AM GMT

PDB ID : 2Y0S
Title : Crystal structure of Sulfolobus shibatae RNA polymerase in P21 space group
Authors : Wojtas, M.; Peralta, B.; Ondiviela, M.; Mogni, M.; Bell, S.D.; Abrescia, N.G.A.
Deposited on : 2010-12-07
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

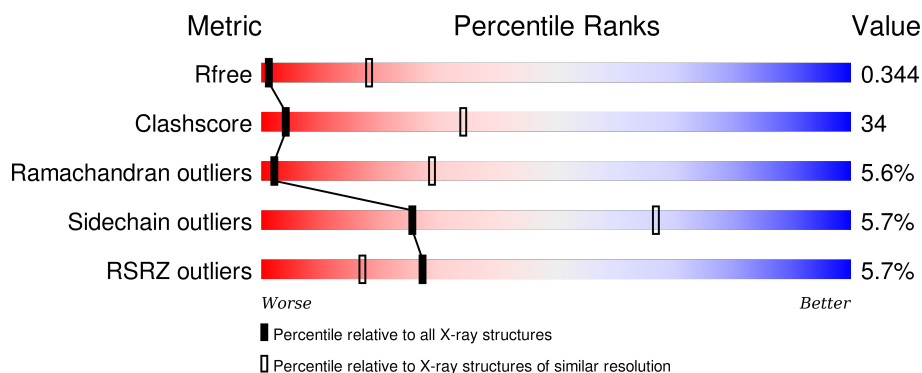
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



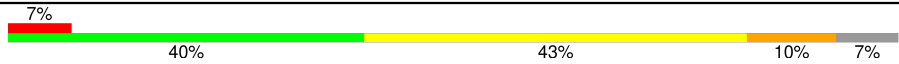

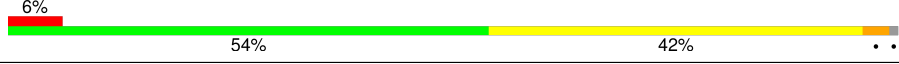
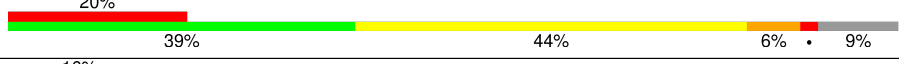
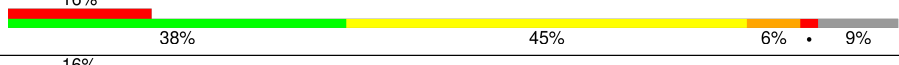
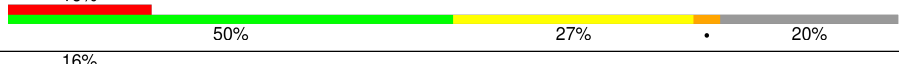
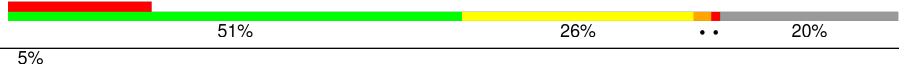
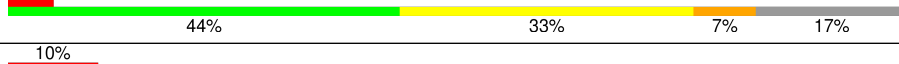
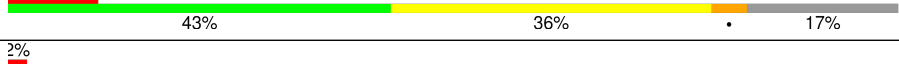


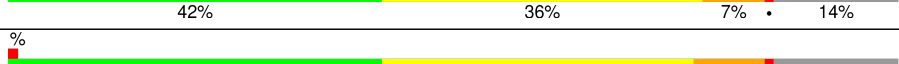


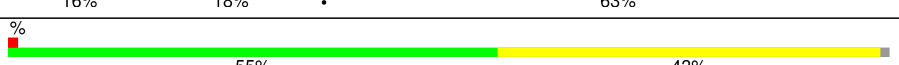
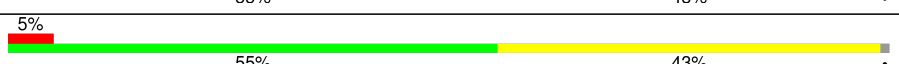
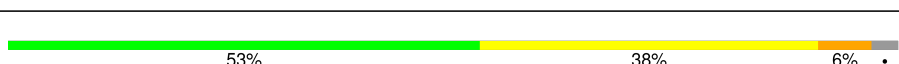

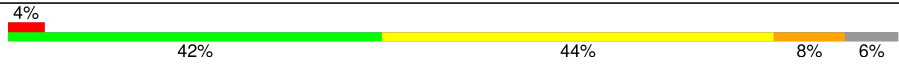


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1317 (4.10-3.50) |
| Clashscore | 102246 | 1458 (4.10-3.50) |
| Ramachandran outliers | 100387 | 1397 (4.10-3.50) |
| Sidechain outliers | 100360 | 1392 (4.10-3.50) |
| RSRZ outliers | 91569 | 1325 (4.10-3.50) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 880 | <div> <div>2%</div> <div>48% 40% 6% 6%</div> </div> |
| 1 | W | 880 | <div> <div>6%</div> <div>45% 42% 7% 6%</div> </div> |
| 2 | B | 1131 | <div> <div>4%</div> <div>43% 45% 7% . .</div> </div> |
| 2 | R | 1131 | <div> <div>4%</div> <div>43% 45% 7% . .</div> </div> |
| 3 | C | 395 | <div> <div>5%</div> <div>42% 42% 10% 7%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | Y | 395 |  |
| 4 | D | 265 |  |
| 4 | S | 265 |  |
| 5 | E | 180 |  |
| 5 | T | 180 |  |
| 6 | F | 113 |  |
| 6 | U | 113 |  |
| 7 | G | 132 |  |
| 7 | V | 132 |  |
| 8 | H | 84 |  |
| 8 | Z | 84 |  |
| 9 | I | 95 |  |
| 9 | K | 95 |  |
| 10 | J | 104 |  |
| 10 | Q | 104 |  |
| 11 | L | 92 |  |
| 11 | M | 92 |  |
| 12 | N | 66 |  |
| 12 | O | 66 |  |
| 13 | P | 48 |  |
| 13 | X | 48 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | ZN | B | 2124 | - | - | - | X |
| 16 | F3S | D | 1001 | - | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 16 | F3S | S | 1001 | - | - | X | - |

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 831 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6620 | 4211 | 1170 | 1212 | 27 | | | |
| 1 | W | 831 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6620 | 4211 | 1170 | 1212 | 27 | | | |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 1085 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8615 | 5461 | 1526 | 1599 | 29 | | | |
| 2 | R | 1085 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8615 | 5461 | 1526 | 1599 | 29 | | | |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT A’.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 368 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2845 | 1803 | 486 | 548 | 8 | | | |
| 3 | Y | 368 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2845 | 1803 | 486 | 548 | 8 | | | |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT D.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 262 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2081 | 1338 | 336 | 394 | 13 | | | |
| 4 | S | 262 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2081 | 1338 | 336 | 394 | 13 | | | |

- Molecule 5 is a protein called RNA POLYMERASE SUBUNIT 4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 164 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1297 | 833 | 219 | 240 | 5 | | | |
| 5 | T | 164 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1297 | 833 | 219 | 240 | 5 | | | |

- Molecule 6 is a protein called RNA POLYMERASE SUBUNIT 7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 90 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 701 | 439 | 114 | 145 | 3 | | | |
| 6 | U | 90 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 701 | 439 | 114 | 145 | 3 | | | |

- Molecule 7 is a protein called RNA POLYMERASE SUBUNIT 8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 878 | 558 | 147 | 169 | 4 | | | |
| 7 | V | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 878 | 558 | 147 | 169 | 4 | | | |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 8 | H | 74 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 609 | 396 | 108 | 105 | | | | |
| 8 | Z | 74 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 609 | 396 | 108 | 105 | | | | |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT K.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | I | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 419 | 117 | 116 | 1 | | | |
| 9 | K | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 419 | 117 | 116 | 1 | | | |

- Molecule 10 is a protein called RNA POLYMERASE SUBUNIT 13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | J | 39 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 332 | 210 | 54 | 67 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | Q | 39 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 332 | 210 | 54 | 67 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| J | 40 | ASN | ASP | CONFLICT | UNP B8YB65 |
| Q | 40 | ASN | ASP | CONFLICT | UNP B8YB65 |

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | L | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 707 | 454 | 114 | 137 | 2 | | | |
| 11 | M | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 707 | 454 | 114 | 137 | 2 | | | |

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT N.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | N | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 514 | 327 | 93 | 87 | 7 | | | |
| 12 | O | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 514 | 327 | 93 | 87 | 7 | | | |

- Molecule 13 is a protein called RNA POLYMERASE SUBUNIT 12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 13 | P | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 369 | 245 | 63 | 56 | 5 | | | |
| 13 | X | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 369 | 245 | 63 | 56 | 5 | | | |

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | P | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | B | 3 | Total | Zn | 0 | 0 |
| | | | 3 | 3 | | |
| 14 | W | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |

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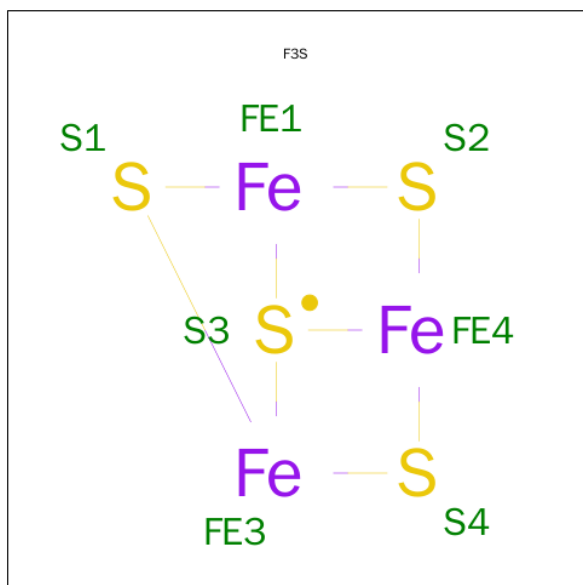
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 14 | A | 2 | Total 2 | Zn 2 | 0 | 0 |
| 14 | N | 1 | Total 1 | Zn 1 | 0 | 0 |
| 14 | X | 1 | Total 1 | Zn 1 | 0 | 0 |
| 14 | O | 1 | Total 1 | Zn 1 | 0 | 0 |
| 14 | R | 3 | Total 3 | Zn 3 | 0 | 0 |

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 15 | W | 1 | Total 1 | Mg 1 | 0 | 0 |
| 15 | A | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

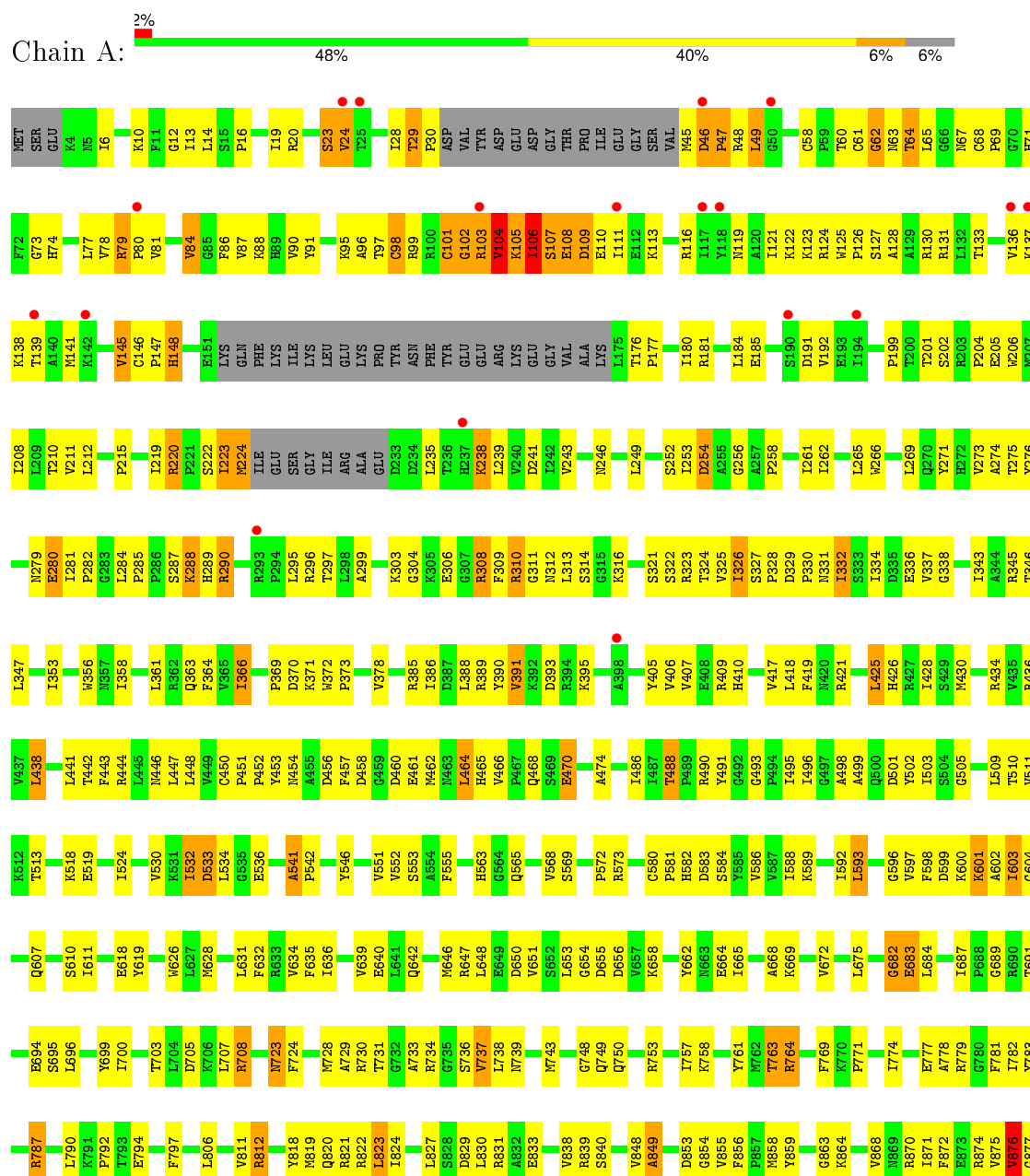


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 16 | D | 1 | Total 7 | Fe 3 | S 4 | 0 | 0 |
| 16 | S | 1 | Total 7 | Fe 3 | S 4 | 0 | 0 |

3 Residue-property plots

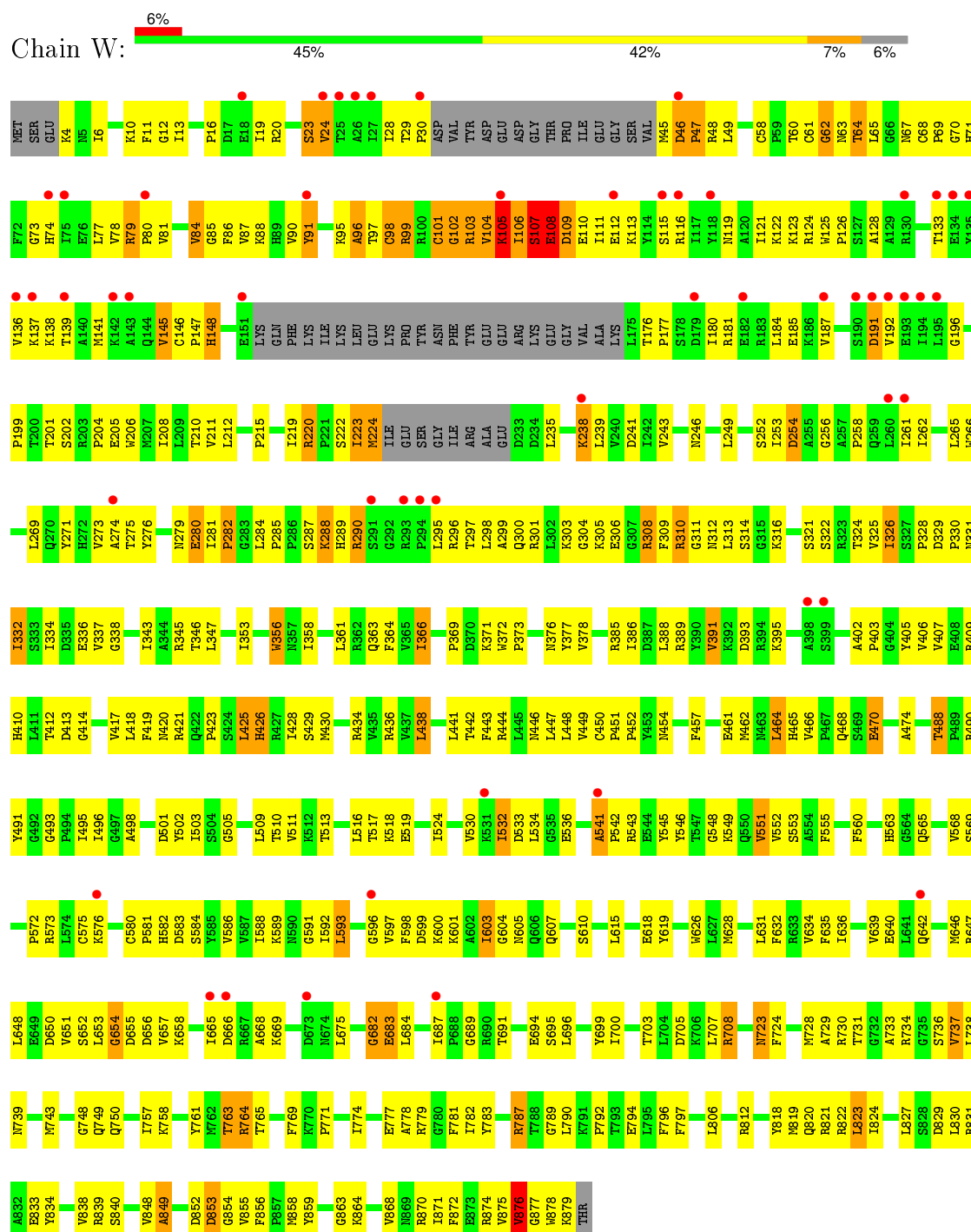
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE

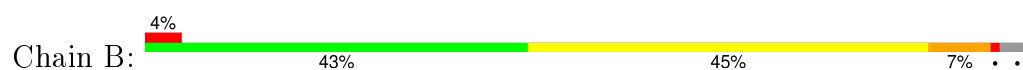




• Molecule 1: DNA-DIRECTED RNA POLYMERASE

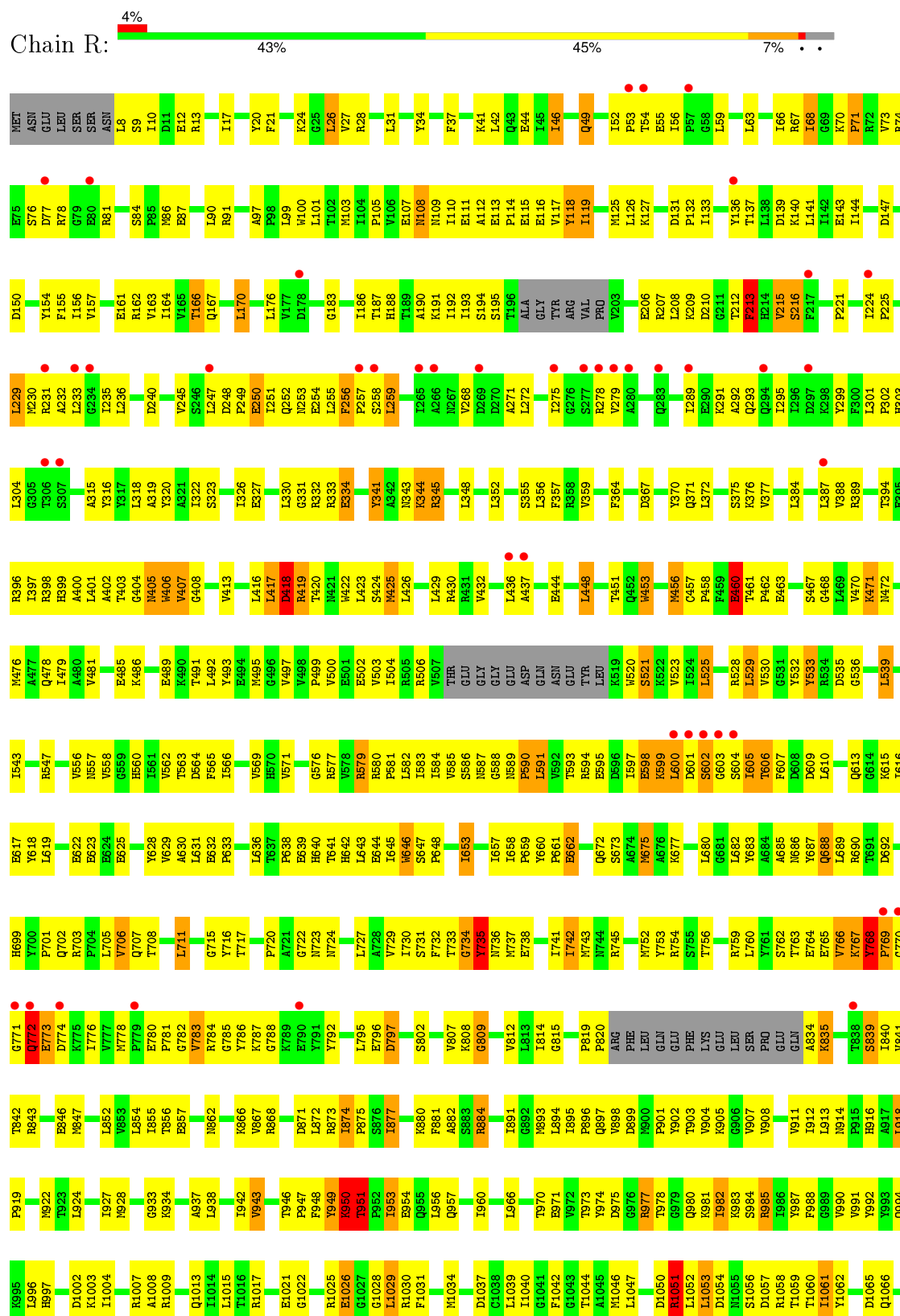


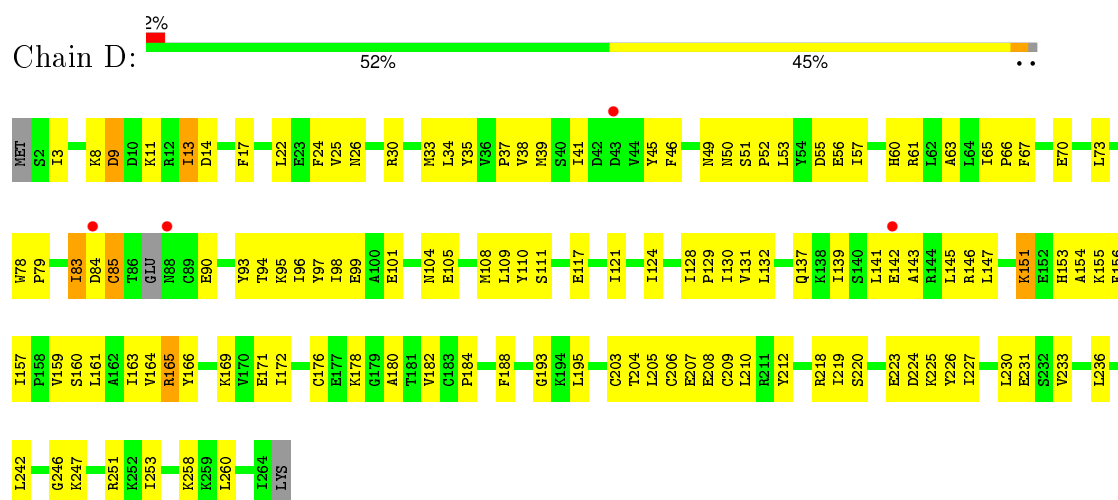
• Molecule 2: DNA-DIRECTED RNA POLYMERASE



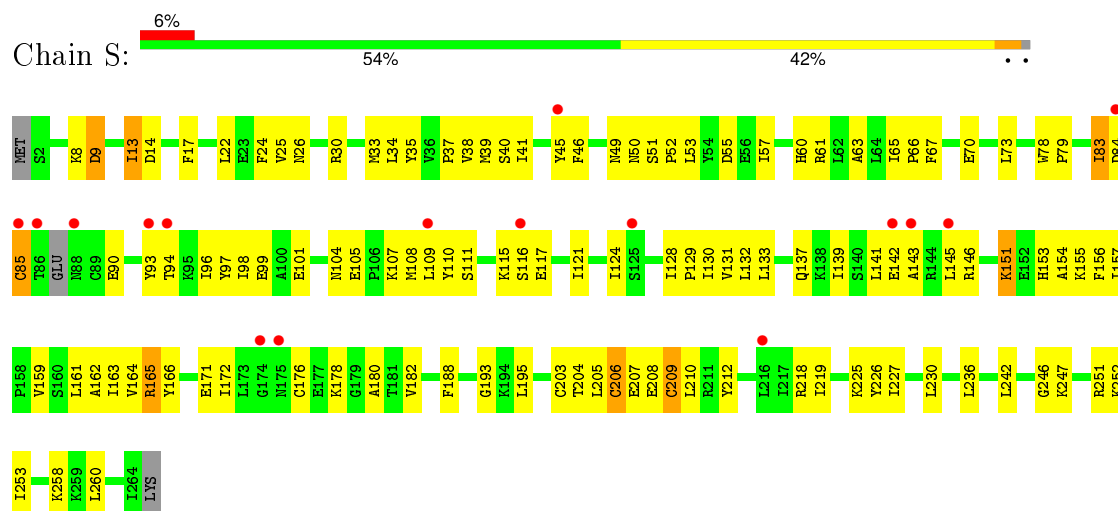


• Molecule 2: DNA-DIRECTED RNA POLYMERASE

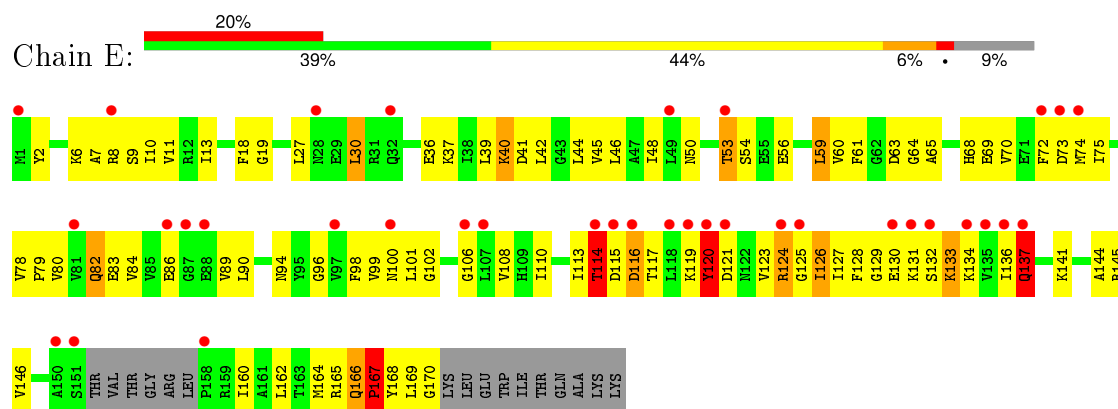




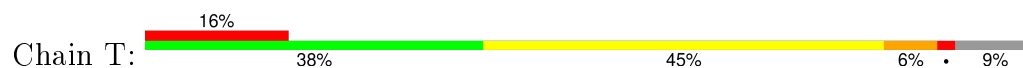
• Molecule 4: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

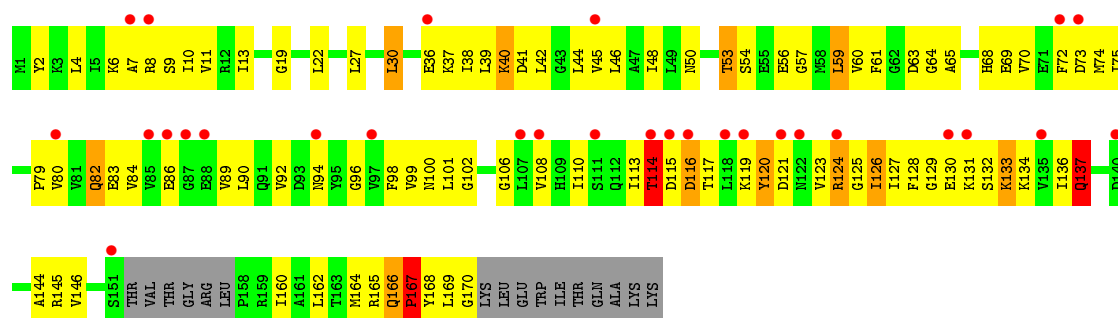


• Molecule 5: RNA POLYMERASE SUBUNIT 4

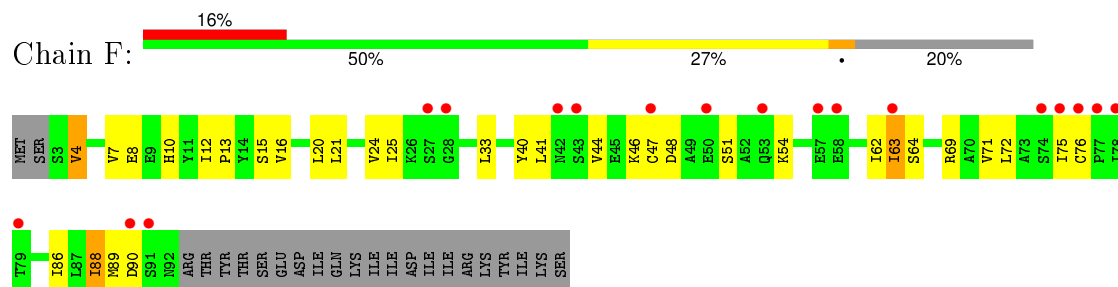


• Molecule 5: RNA POLYMERASE SUBUNIT 4

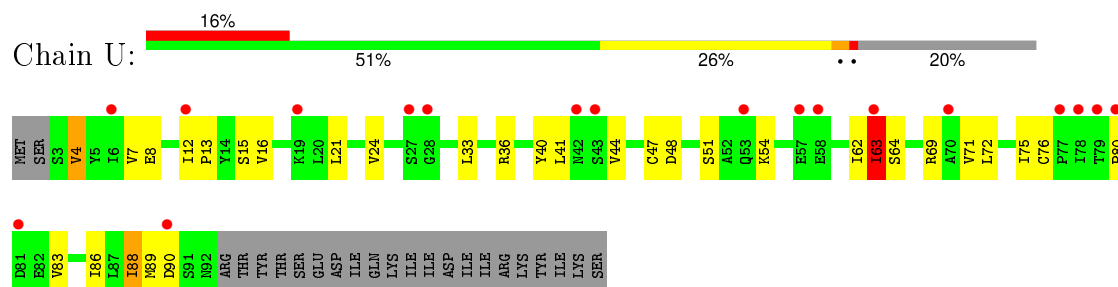




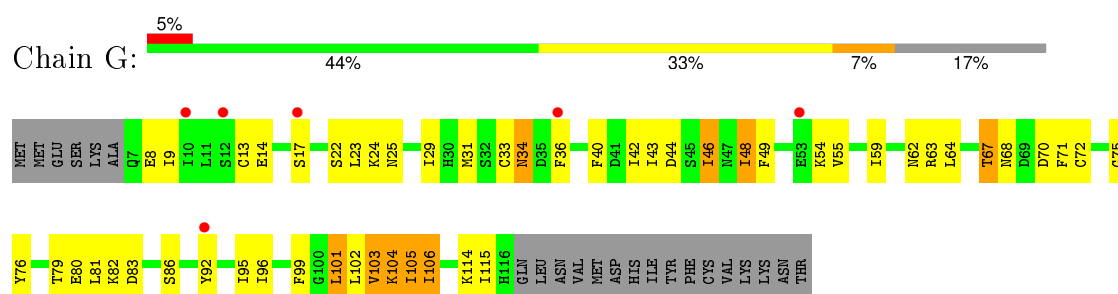
• Molecule 6: RNA POLYMERASE SUBUNIT 7



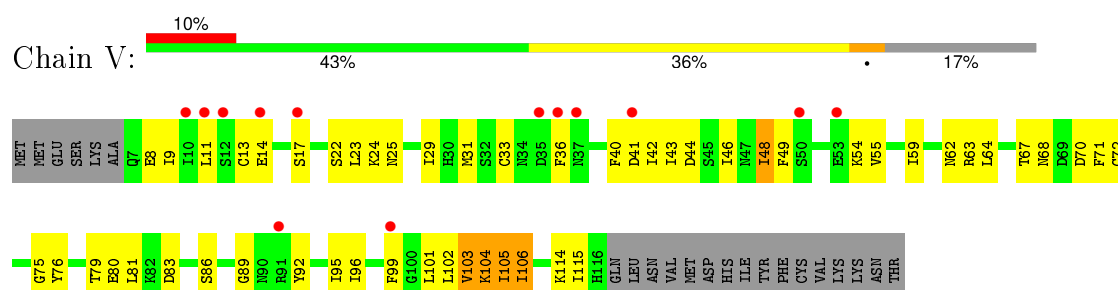
• Molecule 6: RNA POLYMERASE SUBUNIT 7



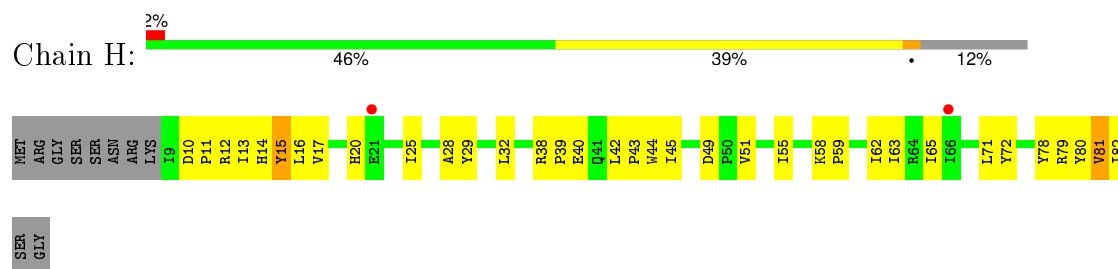
• Molecule 7: RNA POLYMERASE SUBUNIT 8



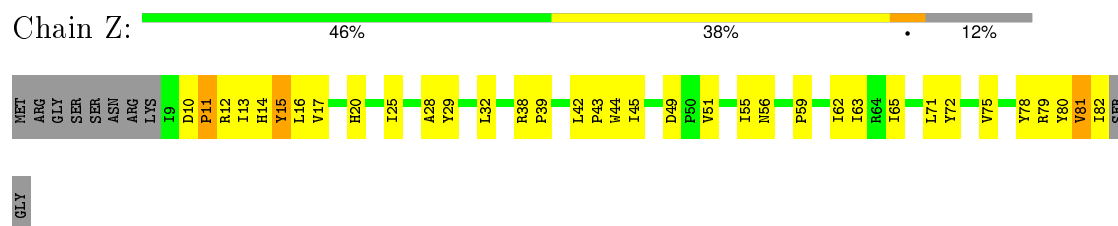
• Molecule 7: RNA POLYMERASE SUBUNIT 8



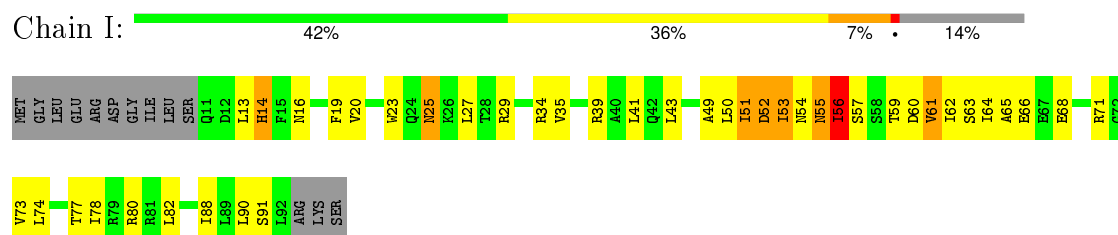
- Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H



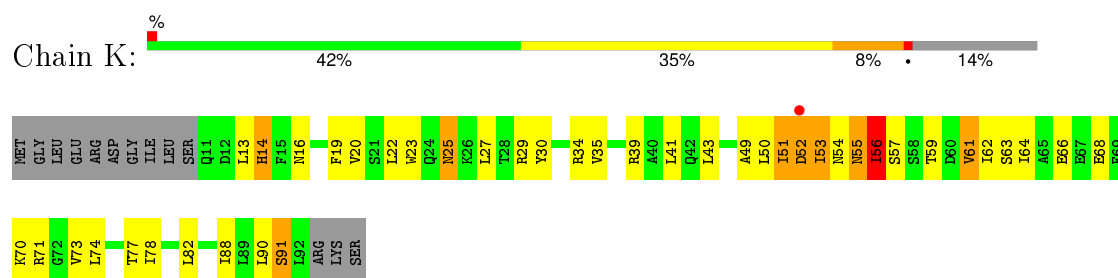
- Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H



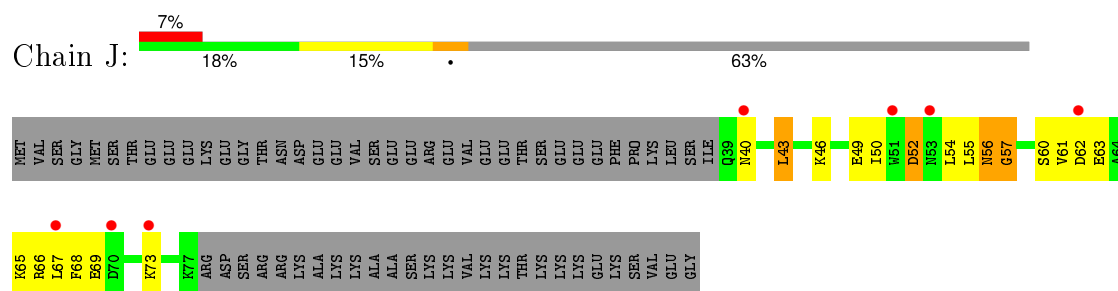
- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K



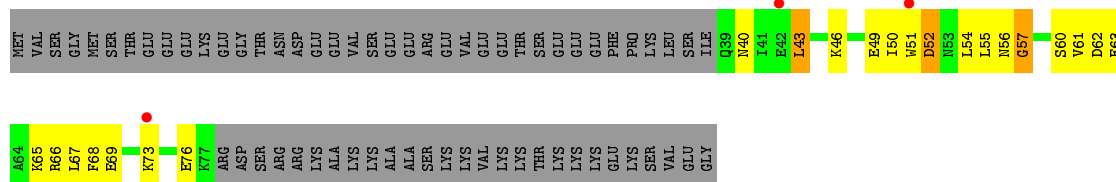
- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K



- Molecule 10: RNA POLYMERASE SUBUNIT 13



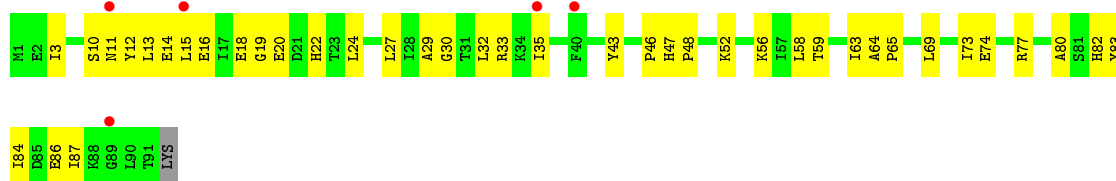
- Molecule 10: RNA POLYMERASE SUBUNIT 13



• Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L



• Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L



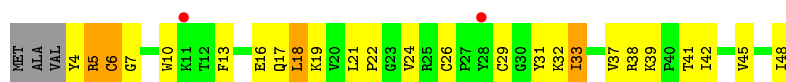
• Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N



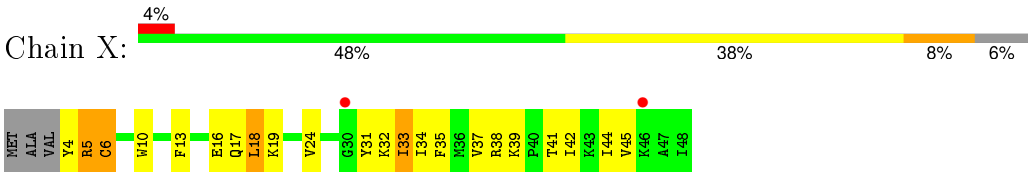
• Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N



• Molecule 13: RNA POLYMERASE SUBUNIT 12



• Molecule 13: RNA POLYMERASE SUBUNIT 12



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 129.33Å 195.91Å 212.45Å 90.00° 105.73° 90.00° | Depositor |
| Resolution (Å) | 29.86 – 3.80 47.12 – 3.79 | Depositor EDS |
| % Data completeness (in resolution range) | 99.2 (29.86-3.80) 98.6 (47.12-3.79) | Depositor EDS |
| R_{merge} | 0.20 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.94 (at 3.77Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, R_{free} | 0.300 , 0.354 0.285 , 0.344 | Depositor DCC |
| R_{free} test set | 4968 reflections (5.00%) | DCC |
| Wilson B-factor (Å ²) | 79.6 | Xtriage |
| Anisotropy | 0.414 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 96.2 | EDS |
| Estimated twinning fraction | 0.000 for h,-k,-h-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Outliers | 0 of 99994 reflections | Xtriage |
| F_o, F_c correlation | 0.84 | EDS |
| Total number of atoms | 52472 | wwPDB-VP |
| Average B, all atoms (Å ²) | 116.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6829e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, F3S, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.54 | 3/6762 (0.0%) | 0.81 | 7/9151 (0.1%) |
| 1 | W | 0.44 | 2/6762 (0.0%) | 0.62 | 4/9151 (0.0%) |
| 2 | B | 0.50 | 0/8778 | 0.81 | 1/11873 (0.0%) |
| 2 | R | 0.42 | 0/8778 | 0.60 | 0/11873 |
| 3 | C | 0.50 | 1/2869 (0.0%) | 0.80 | 0/3862 |
| 3 | Y | 0.41 | 0/2869 | 0.61 | 0/3862 |
| 4 | D | 0.39 | 0/2116 | 0.64 | 0/2859 |
| 4 | S | 0.32 | 0/2116 | 0.48 | 0/2859 |
| 5 | E | 0.40 | 0/1316 | 0.71 | 0/1775 |
| 5 | T | 0.36 | 1/1316 (0.1%) | 0.53 | 0/1775 |
| 6 | F | 0.28 | 0/709 | 0.62 | 0/961 |
| 6 | U | 0.25 | 0/709 | 0.41 | 0/961 |
| 7 | G | 0.40 | 0/890 | 0.67 | 0/1194 |
| 7 | V | 0.33 | 0/890 | 0.51 | 0/1194 |
| 8 | H | 0.53 | 0/623 | 0.77 | 0/845 |
| 8 | Z | 0.42 | 0/623 | 0.58 | 0/845 |
| 9 | I | 1.29 | 3/662 (0.5%) | 0.90 | 5/896 (0.6%) |
| 9 | K | 1.33 | 4/662 (0.6%) | 1.01 | 5/896 (0.6%) |
| 10 | J | 0.36 | 0/336 | 0.51 | 0/450 |
| 10 | Q | 0.43 | 0/336 | 0.71 | 0/450 |
| 11 | L | 0.40 | 0/717 | 0.68 | 0/968 |
| 11 | M | 0.31 | 0/717 | 0.52 | 0/968 |
| 12 | N | 0.43 | 0/524 | 0.68 | 0/706 |
| 12 | O | 0.35 | 0/524 | 0.52 | 0/706 |
| 13 | P | 0.49 | 0/378 | 0.80 | 0/507 |
| 13 | X | 0.44 | 0/378 | 0.66 | 0/507 |
| All | All | 0.49 | 14/53360 (0.0%) | 0.69 | 22/72094 (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 | A | 0 | 1 |
| 5 | E | 0 | 1 |
| 5 | T | 0 | 1 |
| 9 | I | 0 | 1 |
| 9 | K | 0 | 1 |
| All | All | 0 | 5 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 9 | I | 56 | ILE | C-N | -22.63 | 0.82 | 1.34 |
| 9 | K | 55 | ASN | C-N | 21.74 | 1.84 | 1.34 |
| 9 | K | 56 | ILE | C-N | -21.68 | 0.84 | 1.34 |
| 9 | I | 55 | ASN | C-N | 20.09 | 1.80 | 1.34 |
| 1 | A | 104 | VAL | CB-CG2 | -9.48 | 1.32 | 1.52 |
| 1 | W | 101 | CYS | CB-SG | 8.03 | 1.95 | 1.82 |
| 3 | C | 80 | GLU | CG-CD | 7.09 | 1.62 | 1.51 |
| 1 | A | 104 | VAL | CB-CG1 | -7.06 | 1.38 | 1.52 |
| 1 | A | 146 | CYS | CB-SG | -5.68 | 1.72 | 1.81 |
| 5 | T | 57 | GLY | C-N | -5.39 | 1.21 | 1.34 |
| 1 | W | 104 | VAL | CB-CG1 | -5.15 | 1.42 | 1.52 |
| 9 | I | 25 | ASN | C-N | 5.13 | 1.45 | 1.34 |
| 9 | K | 25 | ASN | C-N | 5.10 | 1.45 | 1.34 |
| 9 | K | 70 | LYS | N-CA | -5.08 | 1.36 | 1.46 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 9 | I | 55 | ASN | O-C-N | 9.91 | 138.56 | 122.70 |
| 9 | K | 55 | ASN | CA-C-N | -9.88 | 95.47 | 117.20 |
| 9 | I | 55 | ASN | CA-C-N | -9.78 | 95.68 | 117.20 |
| 9 | I | 56 | ILE | O-C-N | -9.40 | 107.66 | 122.70 |
| 9 | K | 55 | ASN | O-C-N | 9.26 | 137.52 | 122.70 |
| 1 | W | 98 | CYS | CA-CB-SG | 8.54 | 129.38 | 114.00 |
| 9 | K | 56 | ILE | O-C-N | -8.41 | 109.24 | 122.70 |
| 1 | A | 102 | GLY | N-CA-C | -7.68 | 93.91 | 113.10 |
| 9 | I | 56 | ILE | C-N-CA | 6.55 | 138.07 | 121.70 |
| 9 | K | 56 | ILE | C-N-CA | 6.40 | 137.70 | 121.70 |
| 1 | A | 456 | ASP | CB-CG-OD2 | 6.32 | 123.99 | 118.30 |
| 1 | A | 98 | CYS | CA-CB-SG | 6.29 | 125.32 | 114.00 |
| 1 | W | 105 | LYS | CD-CE-NZ | -5.97 | 97.96 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | W | 102 | GLY | N-CA-C | -5.81 | 98.58 | 113.10 |
| 2 | B | 774 | ASP | CB-CG-OD2 | 5.73 | 123.46 | 118.30 |
| 9 | I | 56 | ILE | CA-C-N | 5.61 | 129.53 | 117.20 |
| 1 | A | 106 | ILE | CG1-CB-CG2 | 5.60 | 123.73 | 111.40 |
| 1 | A | 104 | VAL | CG1-CB-CG2 | 5.53 | 119.74 | 110.90 |
| 1 | W | 104 | VAL | CG1-CB-CG2 | -5.51 | 102.09 | 110.90 |
| 1 | A | 533 | ASP | N-CA-CB | 5.20 | 119.96 | 110.60 |
| 9 | K | 91 | SER | N-CA-C | 5.08 | 124.70 | 111.00 |
| 1 | A | 460 | ASP | CB-CG-OD1 | 5.05 | 122.84 | 118.30 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 104 | VAL | Mainchain |
| 5 | E | 167 | PRO | Peptide |
| 9 | I | 56 | ILE | Mainchain |
| 9 | K | 56 | ILE | Mainchain |
| 5 | T | 167 | 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 | A | 6620 | 0 | 6690 | 471 | 0 |
| 1 | W | 6620 | 0 | 6690 | 497 | 0 |
| 2 | B | 8615 | 0 | 8753 | 693 | 0 |
| 2 | R | 8615 | 0 | 8754 | 695 | 0 |
| 3 | C | 2845 | 0 | 3004 | 244 | 0 |
| 3 | Y | 2845 | 0 | 3004 | 252 | 0 |
| 4 | D | 2081 | 0 | 2122 | 131 | 0 |
| 4 | S | 2081 | 0 | 2123 | 119 | 0 |
| 5 | E | 1297 | 0 | 1348 | 123 | 0 |
| 5 | T | 1297 | 0 | 1348 | 122 | 0 |
| 6 | F | 701 | 0 | 708 | 48 | 0 |
| 6 | U | 701 | 0 | 708 | 46 | 0 |
| 7 | G | 878 | 0 | 886 | 55 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | V | 878 | 0 | 886 | 57 | 0 |
| 8 | H | 609 | 0 | 640 | 42 | 0 |
| 8 | Z | 609 | 0 | 640 | 36 | 0 |
| 9 | I | 653 | 0 | 688 | 59 | 0 |
| 9 | K | 653 | 0 | 688 | 56 | 0 |
| 10 | J | 332 | 0 | 324 | 20 | 0 |
| 10 | Q | 332 | 0 | 324 | 29 | 0 |
| 11 | L | 707 | 0 | 739 | 36 | 0 |
| 11 | M | 707 | 0 | 739 | 32 | 0 |
| 12 | N | 514 | 0 | 528 | 32 | 0 |
| 12 | O | 514 | 0 | 528 | 36 | 0 |
| 13 | P | 369 | 0 | 396 | 45 | 0 |
| 13 | X | 369 | 0 | 396 | 49 | 0 |
| 14 | A | 2 | 0 | 0 | 0 | 0 |
| 14 | B | 3 | 0 | 0 | 0 | 0 |
| 14 | N | 1 | 0 | 0 | 0 | 0 |
| 14 | O | 1 | 0 | 0 | 0 | 0 |
| 14 | P | 1 | 0 | 0 | 0 | 0 |
| 14 | R | 3 | 0 | 0 | 0 | 0 |
| 14 | W | 2 | 0 | 0 | 0 | 0 |
| 14 | X | 1 | 0 | 0 | 0 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | W | 1 | 0 | 0 | 0 | 0 |
| 16 | D | 7 | 0 | 0 | 5 | 0 |
| 16 | S | 7 | 0 | 0 | 9 | 0 |
| All | All | 52472 | 0 | 53654 | 3571 | 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 34.

All (3571) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 9:I:55:ASN:C | 9:I:56:ILE:N | 1.80 | 1.32 |
| 9:K:55:ASN:C | 9:K:56:ILE:N | 1.84 | 1.30 |
| 9:I:56:ILE:O | 9:I:57:SER:N | 1.67 | 1.24 |
| 9:K:56:ILE:O | 9:K:57:SER:N | 1.71 | 1.19 |
| 3:Y:168:GLN:HG2 | 3:Y:204:ASN:OD1 | 1.42 | 1.18 |
| 9:I:56:ILE:C | 9:I:57:SER:CA | 2.13 | 1.17 |
| 9:K:56:ILE:C | 9:K:57:SER:CA | 2.14 | 1.15 |
| 2:B:768:TYR:HB3 | 2:B:769:PRO:HD3 | 1.30 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:168:GLN:HG2 | 3:C:204:ASN:OD1 | 1.48 | 1.14 |
| 2:B:768:TYR:HB3 | 2:B:769:PRO:CD | 1.81 | 1.11 |
| 9:K:56:ILE:CA | 9:K:57:SER:N | 2.14 | 1.10 |
| 9:I:56:ILE:CA | 9:I:57:SER:N | 2.14 | 1.10 |
| 2:R:768:TYR:HB3 | 2:R:769:PRO:CD | 1.82 | 1.09 |
| 2:B:767:LYS:CB | 2:B:768:TYR:HA | 1.90 | 1.02 |
| 1:A:426:HIS:CE1 | 3:C:80:GLU:OE2 | 2.13 | 1.01 |
| 4:S:203:CYS:HG | 16:S:1001:F3S:FE3 | 0.70 | 1.00 |
| 2:R:768:TYR:HB3 | 2:R:769:PRO:HD3 | 1.42 | 0.99 |
| 2:B:767:LYS:HB3 | 2:B:768:TYR:HA | 1.46 | 0.98 |
| 1:W:103:ARG:HB2 | 1:W:191:ASP:OD1 | 1.62 | 0.98 |
| 3:C:244:LYS:HA | 3:C:245:LYS:HB3 | 1.46 | 0.97 |
| 1:A:426:HIS:ND1 | 3:C:80:GLU:OE2 | 1.98 | 0.97 |
| 1:W:426:HIS:CE1 | 3:Y:80:GLU:OE2 | 2.18 | 0.97 |
| 1:W:98:CYS:O | 1:W:146:CYS:SG | 2.25 | 0.95 |
| 3:Y:244:LYS:HA | 3:Y:245:LYS:HB3 | 1.50 | 0.94 |
| 2:R:31:LEU:HD23 | 2:R:125:MET:HE3 | 1.51 | 0.92 |
| 2:B:766:VAL:HG22 | 2:B:767:LYS:H | 1.34 | 0.92 |
| 1:A:99:ARG:NH1 | 1:A:147:PRO:HG2 | 1.85 | 0.91 |
| 2:R:767:LYS:HB3 | 2:R:768:TYR:CD1 | 2.03 | 0.91 |
| 2:R:767:LYS:CB | 2:R:768:TYR:HA | 1.99 | 0.91 |
| 2:B:767:LYS:HB3 | 2:B:768:TYR:CD1 | 2.06 | 0.90 |
| 2:B:767:LYS:CG | 2:B:768:TYR:HA | 2.01 | 0.90 |
| 2:B:767:LYS:HB3 | 2:B:768:TYR:CA | 2.01 | 0.90 |
| 2:B:766:VAL:HG12 | 2:B:774:ASP:OD2 | 1.71 | 0.89 |
| 2:R:31:LEU:HA | 2:R:125:MET:CE | 2.03 | 0.89 |
| 2:B:786:TYR:CE2 | 2:B:788:GLY:HA2 | 2.08 | 0.89 |
| 9:K:56:ILE:C | 9:K:57:SER:N | 0.84 | 0.89 |
| 2:B:767:LYS:HB3 | 2:B:768:TYR:CG | 2.08 | 0.88 |
| 1:W:426:HIS:ND1 | 3:Y:80:GLU:OE2 | 2.06 | 0.88 |
| 3:C:149:ILE:HD13 | 3:C:230:LYS:HB3 | 1.55 | 0.88 |
| 1:W:103:ARG:HB2 | 1:W:191:ASP:CG | 1.94 | 0.88 |
| 2:B:31:LEU:HA | 2:B:125:MET:CE | 2.04 | 0.88 |
| 2:B:953:ILE:H | 2:B:953:ILE:HD13 | 1.39 | 0.87 |
| 5:E:30:LEU:HD13 | 5:E:72:PHE:CZ | 2.10 | 0.87 |
| 9:I:56:ILE:C | 9:I:57:SER:N | 0.82 | 0.87 |
| 2:R:767:LYS:CG | 2:R:768:TYR:HA | 2.05 | 0.86 |
| 13:P:17:GLN:HG3 | 13:P:19:LYS:HG2 | 1.58 | 0.86 |
| 2:R:767:LYS:HB3 | 2:R:768:TYR:HA | 1.55 | 0.85 |
| 2:R:766:VAL:HG12 | 2:R:774:ASP:OD2 | 1.76 | 0.85 |
| 1:A:104:VAL:CG1 | 1:A:104:VAL:O | 2.21 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:767:LYS:HB3 | 2:R:768:TYR:CG | 2.12 | 0.85 |
| 2:R:786:TYR:CE2 | 2:R:788:GLY:HA2 | 2.10 | 0.85 |
| 2:R:356:LEU:HA | 2:R:407:VAL:HG21 | 1.56 | 0.84 |
| 2:B:602:SER:HB2 | 2:B:605:ILE:HG21 | 1.60 | 0.84 |
| 2:B:356:LEU:HA | 2:B:407:VAL:HG21 | 1.57 | 0.84 |
| 2:B:46:ILE:HG13 | 2:B:66:ILE:HD11 | 1.60 | 0.83 |
| 7:G:83:ASP:HB2 | 7:G:101:LEU:HG | 1.60 | 0.83 |
| 1:A:104:VAL:HG12 | 1:A:137:LYS:HA | 1.60 | 0.83 |
| 1:A:600:LYS:O | 1:A:601:LYS:HB2 | 1.77 | 0.83 |
| 1:A:586:VAL:HA | 1:A:596:GLY:HA3 | 1.60 | 0.83 |
| 2:R:646:TRP:CZ3 | 2:R:648:PRO:HB2 | 2.14 | 0.82 |
| 3:C:28:ILE:HD13 | 9:K:14:HIS:NE2 | 1.93 | 0.82 |
| 3:C:163:MET:CB | 3:C:164:SER:HA | 2.08 | 0.82 |
| 2:B:1069:TYR:HA | 2:B:1070:ILE:HB | 1.59 | 0.82 |
| 2:B:1031:PHE:CD1 | 2:B:1052:LEU:HD11 | 2.14 | 0.82 |
| 2:B:213:PHE:HB2 | 2:B:259:LEU:HD11 | 1.60 | 0.81 |
| 5:T:30:LEU:HD13 | 5:T:72:PHE:CZ | 2.16 | 0.81 |
| 7:V:83:ASP:HB2 | 7:V:101:LEU:HG | 1.63 | 0.81 |
| 2:R:767:LYS:HA | 2:R:767:LYS:CE | 2.10 | 0.81 |
| 2:R:767:LYS:HB3 | 2:R:768:TYR:CA | 2.11 | 0.81 |
| 2:R:1031:PHE:CD1 | 2:R:1052:LEU:HD11 | 2.16 | 0.81 |
| 9:I:14:HIS:CD2 | 3:Y:28:ILE:HD13 | 2.15 | 0.81 |
| 9:I:14:HIS:NE2 | 3:Y:28:ILE:HD13 | 1.96 | 0.81 |
| 3:Y:163:MET:HB2 | 3:Y:164:SER:HA | 1.62 | 0.81 |
| 1:A:103:ARG:NE | 1:A:191:ASP:OD1 | 2.14 | 0.81 |
| 3:C:163:MET:HB2 | 3:C:164:SER:HA | 1.63 | 0.81 |
| 5:E:114:THR:CB | 5:E:115:ASP:HA | 2.11 | 0.81 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:CB | 2.58 | 0.81 |
| 1:A:474:ALA:HB2 | 9:K:62:ILE:CD1 | 2.09 | 0.81 |
| 3:C:64:ILE:HG22 | 3:C:65:ALA:H | 1.46 | 0.80 |
| 2:R:26:LEU:HG | 2:R:27:VAL:HG23 | 1.64 | 0.80 |
| 2:B:113:GLU:HB3 | 2:B:114:PRO:CD | 2.10 | 0.80 |
| 2:R:856:THR:HG23 | 13:X:32:LYS:O | 1.81 | 0.80 |
| 2:B:646:TRP:CZ3 | 2:B:648:PRO:HB2 | 2.17 | 0.80 |
| 1:A:103:ARG:HB2 | 1:A:191:ASP:CG | 2.00 | 0.80 |
| 2:R:953:ILE:H | 2:R:953:ILE:HD13 | 1.45 | 0.80 |
| 1:W:600:LYS:O | 1:W:601:LYS:HB2 | 1.81 | 0.80 |
| 2:R:46:ILE:HG13 | 2:R:66:ILE:HD11 | 1.64 | 0.80 |
| 7:G:114:LYS:C | 7:G:115:ILE:HD12 | 2.03 | 0.79 |
| 2:B:31:LEU:HD23 | 2:B:125:MET:HE3 | 1.65 | 0.79 |
| 2:R:766:VAL:HG22 | 2:R:767:LYS:H | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:598:GLU:OE2 | 2:B:605:ILE:HG13 | 1.83 | 0.79 |
| 1:A:309:PHE:O | 1:A:310:ARG:HG3 | 1.82 | 0.79 |
| 3:Y:163:MET:CB | 3:Y:164:SER:HA | 2.12 | 0.79 |
| 3:Y:149:ILE:HD13 | 3:Y:230:LYS:HB3 | 1.64 | 0.79 |
| 2:B:371:GLN:HG3 | 2:B:387:LEU:HD22 | 1.64 | 0.79 |
| 1:A:258:PRO:HD2 | 1:A:261:ILE:HD12 | 1.65 | 0.79 |
| 5:T:114:THR:CB | 5:T:115:ASP:HA | 2.13 | 0.79 |
| 2:B:767:LYS:CB | 2:B:768:TYR:CD1 | 2.65 | 0.78 |
| 2:R:113:GLU:HB3 | 2:R:114:PRO:CD | 2.12 | 0.78 |
| 2:B:26:LEU:HG | 2:B:27:VAL:HG23 | 1.64 | 0.78 |
| 2:R:371:GLN:HG3 | 2:R:387:LEU:HD22 | 1.66 | 0.78 |
| 2:R:602:SER:HB2 | 2:R:605:ILE:HG21 | 1.64 | 0.78 |
| 2:R:213:PHE:HB2 | 2:R:259:LEU:HD11 | 1.63 | 0.78 |
| 1:A:104:VAL:HG12 | 1:A:104:VAL:O | 1.82 | 0.78 |
| 1:A:238:LYS:NZ | 1:A:275:THR:HG22 | 1.99 | 0.78 |
| 2:R:767:LYS:CB | 2:R:768:TYR:CD1 | 2.67 | 0.78 |
| 1:A:99:ARG:HH12 | 1:A:147:PRO:HG2 | 1.48 | 0.78 |
| 1:W:104:VAL:HG12 | 1:W:137:LYS:CG | 2.14 | 0.78 |
| 2:B:1069:TYR:CA | 2:B:1070:ILE:HB | 2.14 | 0.78 |
| 13:X:5:ARG:CD | 13:X:18:LEU:HD13 | 2.13 | 0.78 |
| 3:C:274:THR:HG22 | 3:C:276:ASN:H | 1.50 | 0.77 |
| 2:B:774:ASP:OD1 | 2:B:819:PRO:HD3 | 1.83 | 0.77 |
| 2:R:974:TYR:CE2 | 2:R:981:LYS:HB3 | 2.18 | 0.77 |
| 2:R:884:ARG:NH1 | 2:R:992:TYR:HB3 | 2.00 | 0.77 |
| 2:B:856:THR:HG23 | 13:P:32:LYS:O | 1.83 | 0.77 |
| 2:R:767:LYS:HA | 2:R:767:LYS:HE3 | 1.66 | 0.77 |
| 2:B:598:GLU:HA | 2:B:605:ILE:HD12 | 1.67 | 0.77 |
| 1:W:586:VAL:HA | 1:W:596:GLY:HA3 | 1.65 | 0.77 |
| 1:W:99:ARG:NH1 | 1:W:147:PRO:HG2 | 2.00 | 0.77 |
| 2:B:598:GLU:HA | 2:B:605:ILE:CD1 | 2.15 | 0.77 |
| 13:X:10:TRP:HB2 | 13:X:31:TYR:CE2 | 2.19 | 0.77 |
| 9:I:62:ILE:CD1 | 1:W:474:ALA:HB2 | 2.14 | 0.77 |
| 2:R:742:ILE:HG23 | 2:R:912:ILE:HB | 1.67 | 0.77 |
| 11:M:69:LEU:O | 11:M:73:ILE:HG12 | 1.85 | 0.77 |
| 13:P:10:TRP:HB2 | 13:P:31:TYR:CE2 | 2.20 | 0.77 |
| 3:Y:64:ILE:HG22 | 3:Y:65:ALA:H | 1.46 | 0.77 |
| 1:A:12:GLY:HA3 | 1:A:201:THR:HG22 | 1.66 | 0.77 |
| 2:B:46:ILE:HG13 | 2:B:66:ILE:CD1 | 2.15 | 0.76 |
| 13:X:17:GLN:HG3 | 13:X:19:LYS:HG2 | 1.67 | 0.76 |
| 11:L:69:LEU:O | 11:L:73:ILE:HG12 | 1.84 | 0.76 |
| 2:B:34:TYR:HB3 | 2:B:125:MET:HE1 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:55:ASN:CA | 9:I:56:ILE:N | 2.47 | 0.76 |
| 2:R:207:ARG:HB2 | 2:R:216:SER:HB3 | 1.66 | 0.76 |
| 2:B:974:TYR:CE2 | 2:B:981:LYS:HB3 | 2.21 | 0.76 |
| 4:D:209:CYS:SG | 4:D:219:ILE:HD11 | 2.25 | 0.76 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:HB3 | 2.16 | 0.76 |
| 3:Y:30:GLU:HG3 | 3:Y:31:ASP:N | 1.99 | 0.76 |
| 2:B:207:ARG:HB2 | 2:B:216:SER:HB3 | 1.66 | 0.76 |
| 1:W:238:LYS:NZ | 1:W:275:THR:HG22 | 2.01 | 0.75 |
| 1:A:763:THR:HG21 | 1:A:771:PRO:HB3 | 1.69 | 0.75 |
| 2:R:1069:TYR:CA | 2:R:1070:ILE:HB | 2.17 | 0.75 |
| 5:E:113:ILE:HD12 | 5:E:164:MET:SD | 2.26 | 0.75 |
| 2:B:594:ARG:NH1 | 2:B:615:LYS:HB2 | 2.01 | 0.75 |
| 9:K:55:ASN:CA | 9:K:56:ILE:N | 2.49 | 0.75 |
| 2:R:594:ARG:NH1 | 2:R:615:LYS:HB2 | 2.02 | 0.75 |
| 3:C:388:LEU:CD1 | 9:K:35:VAL:HG12 | 2.17 | 0.75 |
| 1:A:177:PRO:HD2 | 1:A:266:TRP:HZ2 | 1.52 | 0.75 |
| 2:B:605:ILE:HG12 | 2:B:606:THR:H | 1.51 | 0.75 |
| 3:C:28:ILE:HD13 | 9:K:14:HIS:CD2 | 2.21 | 0.75 |
| 4:S:207:GLU:HG2 | 4:S:210:LEU:HD12 | 1.69 | 0.75 |
| 7:G:72:CYS:HB3 | 7:G:114:LYS:HG2 | 1.68 | 0.75 |
| 1:A:106:ILE:HG22 | 1:A:107:SER:H | 1.51 | 0.75 |
| 3:C:30:GLU:HG3 | 3:C:31:ASP:N | 2.01 | 0.75 |
| 2:B:215:VAL:HG13 | 2:B:216:SER:N | 2.01 | 0.74 |
| 2:R:133:ILE:HA | 2:R:136:TYR:CD1 | 2.22 | 0.74 |
| 1:W:103:ARG:CB | 1:W:191:ASP:OD1 | 2.34 | 0.74 |
| 1:W:141:MET:HA | 1:W:148:HIS:CB | 2.17 | 0.74 |
| 8:Z:45:ILE:O | 8:Z:81:VAL:HA | 1.86 | 0.74 |
| 2:B:767:LYS:HA | 2:B:767:LYS:CE | 2.17 | 0.74 |
| 1:W:104:VAL:HG13 | 1:W:104:VAL:O | 1.87 | 0.74 |
| 12:N:40:VAL:HG11 | 12:N:46:ARG:HG3 | 1.68 | 0.74 |
| 2:R:774:ASP:OD1 | 2:R:819:PRO:HD3 | 1.88 | 0.74 |
| 1:W:820:GLN:O | 1:W:824:ILE:HB | 1.88 | 0.74 |
| 2:B:897:GLN:HG3 | 2:B:908:VAL:HG21 | 1.68 | 0.74 |
| 2:B:742:ILE:HG23 | 2:B:912:ILE:HB | 1.70 | 0.74 |
| 2:B:767:LYS:HE3 | 2:B:767:LYS:HA | 1.69 | 0.74 |
| 1:A:103:ARG:HB2 | 1:A:191:ASP:OD1 | 1.87 | 0.74 |
| 4:S:206:CYS:HG | 16:S:1001:F3S:FE4 | 1.04 | 0.74 |
| 2:R:113:GLU:HB3 | 2:R:114:PRO:HD2 | 1.70 | 0.74 |
| 1:A:141:MET:HA | 1:A:148:HIS:CB | 2.18 | 0.74 |
| 7:V:114:LYS:C | 7:V:115:ILE:HD12 | 2.08 | 0.74 |
| 9:I:35:VAL:HG12 | 3:Y:388:LEU:CD1 | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:598:GLU:HA | 2:R:605:ILE:CD1 | 2.18 | 0.73 |
| 2:B:884:ARG:NH1 | 2:B:992:TYR:HB3 | 2.03 | 0.73 |
| 2:B:31:LEU:HA | 2:B:125:MET:HE3 | 1.68 | 0.73 |
| 3:Y:274:THR:HG22 | 3:Y:276:ASN:H | 1.52 | 0.73 |
| 2:B:113:GLU:HB3 | 2:B:114:PRO:HD2 | 1.70 | 0.73 |
| 8:H:45:ILE:O | 8:H:81:VAL:HA | 1.89 | 0.73 |
| 1:W:651:VAL:HG11 | 1:W:743:MET:HB3 | 1.70 | 0.73 |
| 1:A:651:VAL:HG11 | 1:A:743:MET:HB3 | 1.70 | 0.73 |
| 1:A:769:PHE:CE2 | 1:A:778:ALA:HA | 2.23 | 0.73 |
| 5:E:136:ILE:HG22 | 5:E:137:GLN:H | 1.53 | 0.73 |
| 1:W:418:LEU:HB3 | 1:W:430:MET:HE2 | 1.70 | 0.73 |
| 2:B:157:VAL:HG21 | 2:B:402:ALA:HB2 | 1.69 | 0.73 |
| 8:H:39:PRO:HB2 | 8:H:80:TYR:CE1 | 2.23 | 0.73 |
| 3:Y:80:GLU:HB3 | 3:Y:81:PRO:HD3 | 1.70 | 0.73 |
| 2:B:190:ALA:HB3 | 2:B:208:LEU:HD12 | 1.69 | 0.73 |
| 2:R:543:ILE:HD12 | 2:R:558:VAL:HG21 | 1.71 | 0.73 |
| 8:Z:39:PRO:HB2 | 8:Z:80:TYR:CE1 | 2.24 | 0.73 |
| 1:W:854:GLY:O | 3:Y:64:ILE:HG12 | 1.88 | 0.72 |
| 2:R:46:ILE:HG13 | 2:R:66:ILE:CD1 | 2.19 | 0.72 |
| 1:A:241:ASP:OD2 | 1:A:289:HIS:CE1 | 2.43 | 0.72 |
| 1:A:426:HIS:NE2 | 3:C:80:GLU:OE1 | 2.23 | 0.72 |
| 13:X:5:ARG:O | 13:X:6:CYS:SG | 2.48 | 0.72 |
| 1:A:618:GLU:O | 1:A:619:TYR:CG | 2.43 | 0.72 |
| 2:R:1054:ASP:HA | 2:R:1058:ARG:HD2 | 1.71 | 0.72 |
| 1:W:769:PHE:CE2 | 1:W:778:ALA:HA | 2.25 | 0.72 |
| 2:R:215:VAL:HG13 | 2:R:216:SER:N | 2.03 | 0.72 |
| 2:B:133:ILE:HA | 2:B:136:TYR:CD1 | 2.24 | 0.72 |
| 2:R:563:THR:HG22 | 2:R:564:ASP:H | 1.53 | 0.72 |
| 5:E:165:ARG:C | 5:E:167:PRO:HD2 | 2.10 | 0.72 |
| 1:W:95:LYS:HB3 | 1:W:138:LYS:HG2 | 1.70 | 0.72 |
| 1:A:271:TYR:CE2 | 1:A:285:PRO:HB3 | 2.24 | 0.72 |
| 7:G:103:VAL:HG13 | 7:G:104:LYS:HD2 | 1.72 | 0.72 |
| 1:W:648:LEU:HD21 | 1:W:787:ARG:NH1 | 2.05 | 0.72 |
| 7:V:72:CYS:SG | 7:V:114:LYS:HB3 | 2.30 | 0.72 |
| 2:R:605:ILE:HG12 | 2:R:606:THR:H | 1.55 | 0.71 |
| 2:B:207:ARG:HB2 | 2:B:216:SER:CB | 2.20 | 0.71 |
| 13:P:5:ARG:CD | 13:P:18:LEU:HD13 | 2.19 | 0.71 |
| 10:Q:46:LYS:HE2 | 10:Q:50:ILE:HD11 | 1.71 | 0.71 |
| 1:W:107:SER:O | 1:W:109:ASP:N | 2.23 | 0.71 |
| 2:B:563:THR:HG22 | 2:B:564:ASP:H | 1.54 | 0.71 |
| 1:A:447:LEU:HD13 | 2:B:737:MET:SD | 2.30 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:897:GLN:HG3 | 2:R:908:VAL:HG21 | 1.72 | 0.71 |
| 2:B:194:SER:HB2 | 2:B:303:HIS:HB3 | 1.72 | 0.71 |
| 9:K:50:LEU:O | 9:K:51:ILE:O | 2.08 | 0.71 |
| 1:W:12:GLY:HA3 | 1:W:201:THR:HG22 | 1.71 | 0.71 |
| 1:A:648:LEU:HD21 | 1:A:787:ARG:NH1 | 2.05 | 0.71 |
| 1:W:258:PRO:HD2 | 1:W:261:ILE:HD12 | 1.71 | 0.71 |
| 5:T:113:ILE:HD12 | 5:T:164:MET:SD | 2.29 | 0.71 |
| 1:W:324:THR:HG21 | 1:W:441:LEU:O | 1.90 | 0.71 |
| 2:B:289:ILE:O | 2:B:293:GLN:HG3 | 1.90 | 0.71 |
| 2:B:208:LEU:HD23 | 2:B:215:VAL:HG23 | 1.72 | 0.71 |
| 1:A:105:LYS:NZ | 1:A:133:THR:HG23 | 2.05 | 0.71 |
| 2:R:207:ARG:HB2 | 2:R:216:SER:CB | 2.21 | 0.71 |
| 3:C:53:ASP:HA | 3:C:56:ILE:HG12 | 1.73 | 0.71 |
| 1:W:241:ASP:OD2 | 1:W:289:HIS:CE1 | 2.44 | 0.71 |
| 1:W:98:CYS:O | 1:W:99:ARG:HB2 | 1.89 | 0.71 |
| 3:C:30:GLU:HG3 | 3:C:31:ASP:H | 1.54 | 0.71 |
| 2:B:1017:ARG:HD3 | 2:B:1098:TYR:CD2 | 2.26 | 0.71 |
| 3:C:270:ALA:HA | 8:H:14:HIS:HB3 | 1.73 | 0.71 |
| 2:B:213:PHE:HB2 | 2:B:259:LEU:CD1 | 2.21 | 0.71 |
| 1:W:104:VAL:HG12 | 1:W:137:LYS:HG2 | 1.73 | 0.71 |
| 1:A:859:TYR:HE2 | 3:C:65:ALA:HB2 | 1.56 | 0.70 |
| 2:B:1074:ASP:HB3 | 2:B:1075:LYS:HB3 | 1.73 | 0.70 |
| 2:R:31:LEU:HA | 2:R:125:MET:HE1 | 1.73 | 0.70 |
| 2:R:208:LEU:HD23 | 2:R:215:VAL:HG23 | 1.73 | 0.70 |
| 1:A:107:SER:O | 1:A:109:ASP:N | 2.23 | 0.70 |
| 4:D:51:SER:HB2 | 4:D:52:PRO:HD2 | 1.73 | 0.70 |
| 2:R:1069:TYR:HA | 2:R:1070:ILE:HB | 1.72 | 0.70 |
| 12:O:8:PHE:CD2 | 12:O:48:MET:HE1 | 2.27 | 0.70 |
| 1:A:418:LEU:HD23 | 1:A:430:MET:HE1 | 1.74 | 0.70 |
| 1:W:426:HIS:NE2 | 3:Y:80:GLU:OE1 | 2.25 | 0.70 |
| 3:C:186:LYS:HB3 | 3:C:230:LYS:HE2 | 1.72 | 0.70 |
| 1:A:668:ALA:CB | 1:A:707:LEU:HD13 | 2.21 | 0.70 |
| 2:R:734:GLY:HA3 | 2:R:735:TYR:CG | 2.26 | 0.70 |
| 1:A:820:GLN:O | 1:A:824:ILE:HB | 1.92 | 0.70 |
| 1:W:763:THR:HG21 | 1:W:771:PRO:HB3 | 1.73 | 0.70 |
| 1:W:308:ARG:HA | 1:W:312:ASN:HB2 | 1.73 | 0.70 |
| 1:W:618:GLU:O | 1:W:619:TYR:CG | 2.44 | 0.70 |
| 1:W:271:TYR:CE2 | 1:W:285:PRO:HB3 | 2.27 | 0.70 |
| 1:W:184:LEU:HB3 | 1:W:204:PRO:HB2 | 1.73 | 0.70 |
| 7:G:103:VAL:HG22 | 7:G:104:LYS:H | 1.56 | 0.70 |
| 1:A:324:THR:HG21 | 1:A:441:LEU:O | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:856:THR:HG22 | 2:R:857:GLU:H | 1.55 | 0.69 |
| 1:A:95:LYS:HB3 | 1:A:138:LYS:HE2 | 1.72 | 0.69 |
| 1:W:589:LYS:HD3 | 1:W:877:GLY:O | 1.92 | 0.69 |
| 2:R:598:GLU:OE2 | 2:R:605:ILE:HG13 | 1.92 | 0.69 |
| 3:C:277:ILE:HG22 | 3:C:278:ARG:H | 1.55 | 0.69 |
| 1:A:103:ARG:HB2 | 1:A:191:ASP:OD2 | 1.92 | 0.69 |
| 2:R:598:GLU:HA | 2:R:605:ILE:HD12 | 1.74 | 0.69 |
| 1:A:308:ARG:HA | 1:A:312:ASN:HB2 | 1.74 | 0.69 |
| 1:A:872:PHE:CD2 | 1:A:876:VAL:HG11 | 2.27 | 0.69 |
| 3:C:231:ILE:HG23 | 3:C:232:LYS:N | 2.08 | 0.69 |
| 3:C:340:SER:HB3 | 3:C:371:GLU:HG2 | 1.74 | 0.69 |
| 1:W:177:PRO:HD2 | 1:W:266:TRP:HZ2 | 1.57 | 0.69 |
| 2:B:9:SER:HB3 | 2:B:12:GLU:HB3 | 1.74 | 0.69 |
| 2:B:768:TYR:CB | 2:B:769:PRO:CD | 2.66 | 0.69 |
| 2:B:84:SER:OG | 2:B:144:ILE:HG23 | 1.92 | 0.69 |
| 2:R:157:VAL:HG21 | 2:R:402:ALA:HB2 | 1.75 | 0.69 |
| 2:R:249:PRO:CB | 2:R:252:GLN:HB2 | 2.22 | 0.69 |
| 1:W:618:GLU:O | 1:W:619:TYR:CD2 | 2.45 | 0.69 |
| 3:C:244:LYS:HA | 3:C:245:LYS:CB | 2.16 | 0.69 |
| 1:A:184:LEU:HB3 | 1:A:204:PRO:HB2 | 1.74 | 0.69 |
| 2:B:66:ILE:HG13 | 2:B:101:LEU:HD23 | 1.74 | 0.69 |
| 2:R:658:ILE:HG12 | 2:R:672:GLN:HG2 | 1.75 | 0.69 |
| 5:T:144:ALA:HA | 5:T:169:LEU:HD23 | 1.75 | 0.69 |
| 1:A:95:LYS:HB3 | 1:A:138:LYS:HG2 | 1.75 | 0.69 |
| 1:W:668:ALA:CB | 1:W:707:LEU:HD13 | 2.22 | 0.68 |
| 2:B:787:LYS:HE3 | 2:B:841:VAL:CG2 | 2.23 | 0.68 |
| 1:W:98:CYS:C | 1:W:146:CYS:SG | 2.65 | 0.68 |
| 2:B:396:ARG:NH2 | 2:B:406:TRP:CH2 | 2.61 | 0.68 |
| 1:A:792:PRO:HG3 | 2:B:948:PHE:CE1 | 2.28 | 0.68 |
| 12:O:40:VAL:HG11 | 12:O:46:ARG:HG3 | 1.75 | 0.68 |
| 1:A:854:GLY:O | 3:C:64:ILE:HG12 | 1.93 | 0.68 |
| 2:R:212:THR:O | 2:R:213:PHE:HB2 | 1.92 | 0.68 |
| 3:C:340:SER:HA | 3:C:364:GLU:HG2 | 1.75 | 0.68 |
| 2:B:543:ILE:HD12 | 2:B:558:VAL:HG21 | 1.74 | 0.68 |
| 3:C:388:LEU:HD13 | 9:K:35:VAL:HG12 | 1.75 | 0.68 |
| 7:V:103:VAL:HG13 | 7:V:104:LYS:HD2 | 1.74 | 0.68 |
| 5:E:114:THR:OG1 | 5:E:115:ASP:HA | 1.93 | 0.68 |
| 2:R:84:SER:OG | 2:R:144:ILE:HG23 | 1.93 | 0.68 |
| 6:F:48:ASP:HB3 | 6:F:51:SER:HB2 | 1.74 | 0.68 |
| 12:N:8:PHE:CD2 | 12:N:48:MET:HE1 | 2.29 | 0.68 |
| 1:A:875:VAL:HG12 | 1:A:876:VAL:H | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:984:SER:O | 2:R:985:ARG:HB2 | 1.94 | 0.68 |
| 5:E:144:ALA:HA | 5:E:169:LEU:HD23 | 1.75 | 0.68 |
| 1:W:105:LYS:NZ | 1:W:133:THR:HG23 | 2.09 | 0.68 |
| 2:B:1017:ARG:HD3 | 2:B:1098:TYR:CE2 | 2.29 | 0.68 |
| 2:B:660:TYR:HD1 | 2:B:950:LYS:HE3 | 1.58 | 0.68 |
| 3:C:393:ILE:HG22 | 5:E:19:GLY:H | 1.57 | 0.68 |
| 1:A:311:GLY:HA2 | 2:B:1030:ARG:HH22 | 1.59 | 0.68 |
| 1:W:78:VAL:O | 1:W:79:ARG:HB2 | 1.93 | 0.68 |
| 9:I:50:LEU:O | 9:I:51:ILE:O | 2.11 | 0.67 |
| 2:B:186:ILE:HD12 | 2:B:209:LYS:HD3 | 1.76 | 0.67 |
| 2:B:252:GLN:HB3 | 2:B:326:ILE:HD12 | 1.74 | 0.67 |
| 5:E:7:ALA:HA | 6:F:7:VAL:HG13 | 1.76 | 0.67 |
| 3:Y:231:ILE:HG23 | 3:Y:232:LYS:N | 2.09 | 0.67 |
| 1:A:848:VAL:O | 1:A:849:ALA:HB3 | 1.94 | 0.67 |
| 5:T:114:THR:OG1 | 5:T:115:ASP:HA | 1.94 | 0.67 |
| 2:B:658:ILE:HG12 | 2:B:672:GLN:HG2 | 1.75 | 0.67 |
| 2:R:252:GLN:HB3 | 2:R:326:ILE:HD12 | 1.76 | 0.67 |
| 2:B:686:ASN:O | 2:B:690:ARG:HG2 | 1.93 | 0.67 |
| 1:W:848:VAL:O | 1:W:849:ALA:HB3 | 1.94 | 0.67 |
| 2:B:330:LEU:O | 2:B:332:ARG:HG2 | 1.94 | 0.67 |
| 1:W:309:PHE:O | 1:W:310:ARG:HG3 | 1.95 | 0.67 |
| 2:R:31:LEU:HA | 2:R:125:MET:HE3 | 1.76 | 0.67 |
| 1:A:474:ALA:HB2 | 9:K:62:ILE:HD12 | 1.76 | 0.67 |
| 2:R:213:PHE:HB2 | 2:R:259:LEU:CD1 | 2.24 | 0.67 |
| 1:A:330:PRO:HG3 | 2:B:734:GLY:HA2 | 1.76 | 0.67 |
| 13:X:31:TYR:CE2 | 13:X:33:ILE:HB | 2.29 | 0.67 |
| 2:R:1047:LEU:HD21 | 1:W:418:LEU:HD21 | 1.77 | 0.67 |
| 2:R:1074:ASP:HB3 | 2:R:1075:LYS:HB3 | 1.77 | 0.67 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:HG2 | 2.25 | 0.67 |
| 2:R:1017:ARG:HD3 | 2:R:1098:TYR:CD2 | 2.30 | 0.67 |
| 9:K:82:LEU:HD11 | 9:K:88:ILE:HD11 | 1.76 | 0.67 |
| 2:R:161:GLU:OE2 | 2:R:690:ARG:NH2 | 2.28 | 0.67 |
| 13:X:5:ARG:HG2 | 13:X:18:LEU:HB2 | 1.75 | 0.67 |
| 13:P:31:TYR:CE2 | 13:P:33:ILE:HB | 2.30 | 0.67 |
| 1:W:97:THR:HG23 | 1:W:102:GLY:HA2 | 1.76 | 0.67 |
| 5:E:6:LYS:O | 6:F:7:VAL:HG22 | 1.95 | 0.67 |
| 2:B:401:LEU:HG | 2:B:401:LEU:O | 1.94 | 0.67 |
| 11:L:74:GLU:HG2 | 11:L:77:ARG:NH2 | 2.09 | 0.67 |
| 5:T:30:LEU:HD22 | 5:T:72:PHE:CE2 | 2.30 | 0.67 |
| 13:X:5:ARG:HD2 | 13:X:18:LEU:HD13 | 1.75 | 0.67 |
| 2:B:584:ILE:HD11 | 2:B:617:GLU:HB2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:348:LEU:O | 2:B:352:LEU:HB2 | 1.94 | 0.67 |
| 2:R:190:ALA:HB3 | 2:R:208:LEU:HD12 | 1.76 | 0.66 |
| 1:A:792:PRO:HG3 | 2:B:948:PHE:CD1 | 2.30 | 0.66 |
| 13:X:17:GLN:CG | 13:X:19:LYS:HG2 | 2.25 | 0.66 |
| 3:C:340:SER:HA | 3:C:364:GLU:CG | 2.25 | 0.66 |
| 1:A:603:ILE:HG21 | 1:A:632:PHE:HE1 | 1.60 | 0.66 |
| 2:B:893:MET:HG3 | 2:B:894:LEU:N | 2.09 | 0.66 |
| 2:B:641:THR:HG22 | 2:B:642:HIS:CE1 | 2.31 | 0.66 |
| 1:W:603:ILE:HG21 | 1:W:632:PHE:HE1 | 1.59 | 0.66 |
| 3:C:163:MET:O | 3:C:208:ILE:HA | 1.95 | 0.66 |
| 5:E:165:ARG:C | 5:E:167:PRO:CD | 2.63 | 0.66 |
| 2:B:1054:ASP:HA | 2:B:1058:ARG:HD2 | 1.78 | 0.66 |
| 5:E:60:VAL:HG22 | 5:E:61:PHE:H | 1.60 | 0.66 |
| 1:W:123:LYS:HA | 1:W:126:PRO:CG | 2.26 | 0.66 |
| 8:H:25:ILE:HG22 | 10:Q:55:LEU:CD2 | 2.24 | 0.66 |
| 13:P:31:TYR:HE2 | 13:P:33:ILE:HB | 1.61 | 0.66 |
| 4:D:45:TYR:HB3 | 13:P:42:ILE:HD11 | 1.78 | 0.66 |
| 3:Y:168:GLN:CG | 3:Y:204:ASN:OD1 | 2.34 | 0.66 |
| 3:Y:163:MET:O | 3:Y:208:ILE:HA | 1.96 | 0.66 |
| 3:C:277:ILE:HG22 | 3:C:278:ARG:N | 2.11 | 0.66 |
| 1:W:703:THR:HG22 | 1:W:707:LEU:HD12 | 1.78 | 0.66 |
| 2:B:622:GLU:O | 2:B:625:GLU:HB3 | 1.96 | 0.66 |
| 2:R:417:LEU:HD21 | 2:R:425:MET:HG3 | 1.76 | 0.66 |
| 13:X:18:LEU:O | 13:X:18:LEU:HD12 | 1.95 | 0.66 |
| 1:W:125:TRP:N | 1:W:126:PRO:HD2 | 2.11 | 0.66 |
| 10:J:46:LYS:HE2 | 10:J:50:ILE:HD11 | 1.78 | 0.66 |
| 9:I:82:LEU:HD11 | 9:I:88:ILE:HD11 | 1.75 | 0.66 |
| 3:Y:270:ALA:HA | 8:Z:14:HIS:HB3 | 1.76 | 0.66 |
| 1:A:238:LYS:CE | 1:A:276:TYR:HA | 2.26 | 0.66 |
| 2:R:584:ILE:HD11 | 2:R:617:GLU:HB2 | 1.76 | 0.66 |
| 12:N:3:ILE:HG23 | 12:N:52:HIS:CD2 | 2.30 | 0.66 |
| 5:E:114:THR:HB | 5:E:115:ASP:CA | 2.25 | 0.66 |
| 13:P:18:LEU:HD12 | 13:P:18:LEU:O | 1.95 | 0.66 |
| 5:T:165:ARG:C | 5:T:167:PRO:HD2 | 2.15 | 0.66 |
| 2:B:322:ILE:O | 2:B:326:ILE:HG12 | 1.95 | 0.66 |
| 2:B:734:GLY:HA3 | 2:B:735:TYR:CG | 2.31 | 0.66 |
| 4:D:207:GLU:HG2 | 4:D:210:LEU:HD12 | 1.77 | 0.66 |
| 1:W:872:PHE:CD2 | 1:W:876:VAL:HG11 | 2.30 | 0.66 |
| 3:Y:244:LYS:HA | 3:Y:245:LYS:CB | 2.16 | 0.66 |
| 2:R:31:LEU:CD2 | 2:R:125:MET:HE3 | 2.25 | 0.66 |
| 3:C:147:THR:HB | 3:C:232:LYS:HB2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Y:340:SER:HA | 3:Y:364:GLU:CG | 2.26 | 0.66 |
| 3:Y:340:SER:HB3 | 3:Y:371:GLU:HG2 | 1.77 | 0.66 |
| 1:W:103:ARG:HB2 | 1:W:191:ASP:OD2 | 1.96 | 0.65 |
| 2:B:105:PRO:HD2 | 2:B:112:ALA:HB3 | 1.79 | 0.65 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:HA | 2.26 | 0.65 |
| 1:W:238:LYS:CE | 1:W:276:TYR:HA | 2.26 | 0.65 |
| 2:R:1017:ARG:HD3 | 2:R:1098:TYR:CE2 | 2.31 | 0.65 |
| 1:W:875:VAL:HG12 | 1:W:876:VAL:H | 1.61 | 0.65 |
| 1:A:304:GLY:C | 1:A:306:GLU:H | 1.98 | 0.65 |
| 3:C:327:ARG:HG3 | 3:C:334:VAL:HG23 | 1.78 | 0.65 |
| 2:B:743:MET:HE1 | 2:B:875:PRO:HB2 | 1.78 | 0.65 |
| 7:G:80:GLU:HG3 | 7:G:81:LEU:H | 1.61 | 0.65 |
| 3:C:169:LEU:HD23 | 3:C:174:LEU:CD2 | 2.26 | 0.65 |
| 2:R:743:MET:HE1 | 2:R:875:PRO:HB2 | 1.78 | 0.65 |
| 2:R:322:ILE:O | 2:R:326:ILE:HG12 | 1.95 | 0.65 |
| 2:R:815:GLY:HA2 | 2:R:839:SER:OG | 1.96 | 0.65 |
| 7:G:25:ASN:HA | 7:G:44:ASP:OD2 | 1.96 | 0.65 |
| 2:B:815:GLY:HA2 | 2:B:839:SER:OG | 1.96 | 0.65 |
| 5:E:114:THR:CB | 5:E:115:ASP:CA | 2.75 | 0.65 |
| 1:W:104:VAL:HG12 | 1:W:137:LYS:CB | 2.25 | 0.65 |
| 2:R:66:ILE:HG13 | 2:R:101:LEU:HD23 | 1.78 | 0.65 |
| 4:D:108:MET:HG2 | 4:D:110:TYR:CZ | 2.31 | 0.65 |
| 1:A:642:GLN:OE1 | 1:A:642:GLN:HA | 1.97 | 0.65 |
| 1:A:125:TRP:N | 1:A:126:PRO:HD2 | 2.12 | 0.65 |
| 4:S:51:SER:HB2 | 4:S:52:PRO:HD2 | 1.78 | 0.65 |
| 1:W:103:ARG:NE | 1:W:191:ASP:OD1 | 2.30 | 0.65 |
| 1:W:104:VAL:HG11 | 1:W:137:LYS:HB3 | 1.79 | 0.65 |
| 5:T:114:THR:CB | 5:T:115:ASP:CA | 2.75 | 0.65 |
| 5:T:114:THR:HB | 5:T:115:ASP:CA | 2.27 | 0.65 |
| 1:A:703:THR:HG22 | 1:A:707:LEU:HD12 | 1.78 | 0.65 |
| 2:R:874:ILE:HD12 | 2:R:874:ILE:H | 1.62 | 0.65 |
| 2:R:622:GLU:O | 2:R:625:GLU:HB3 | 1.96 | 0.65 |
| 1:A:78:VAL:O | 1:A:79:ARG:HB2 | 1.96 | 0.65 |
| 4:S:111:SER:HB3 | 4:S:128:ILE:HB | 1.78 | 0.65 |
| 2:B:46:ILE:HG22 | 2:B:46:ILE:O | 1.96 | 0.65 |
| 2:B:974:TYR:CE2 | 4:D:165:ARG:HA | 2.30 | 0.65 |
| 2:B:253:ASN:O | 2:B:257:PRO:HD2 | 1.96 | 0.65 |
| 7:V:80:GLU:HG3 | 7:V:81:LEU:H | 1.62 | 0.65 |
| 2:R:289:ILE:O | 2:R:293:GLN:HG3 | 1.97 | 0.65 |
| 1:A:13:ILE:HD12 | 1:A:202:SER:HB2 | 1.78 | 0.65 |
| 1:A:589:LYS:HD3 | 1:A:877:GLY:O | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:46:ILE:HG22 | 2:R:46:ILE:O | 1.95 | 0.65 |
| 3:C:169:LEU:HD23 | 3:C:174:LEU:HD21 | 1.78 | 0.65 |
| 3:Y:340:SER:HA | 3:Y:364:GLU:HG2 | 1.77 | 0.65 |
| 4:D:53:LEU:HD12 | 4:D:131:VAL:HG23 | 1.79 | 0.65 |
| 4:D:17:PHE:O | 4:D:225:LYS:HA | 1.97 | 0.65 |
| 1:W:426:HIS:CG | 3:Y:80:GLU:OE2 | 2.51 | 0.64 |
| 5:E:136:ILE:HG22 | 5:E:137:GLN:N | 2.11 | 0.64 |
| 1:A:106:ILE:HD12 | 1:A:106:ILE:H | 1.63 | 0.64 |
| 1:A:618:GLU:O | 1:A:619:TYR:CD2 | 2.50 | 0.64 |
| 2:B:212:THR:O | 2:B:213:PHE:HB2 | 1.96 | 0.64 |
| 8:H:25:ILE:HG22 | 10:Q:55:LEU:HD21 | 1.80 | 0.64 |
| 1:A:682:GLY:O | 1:A:684:LEU:N | 2.30 | 0.64 |
| 2:R:660:TYR:HD1 | 2:R:950:LYS:HE3 | 1.62 | 0.64 |
| 2:R:253:ASN:O | 2:R:257:PRO:HD2 | 1.96 | 0.64 |
| 4:S:159:VAL:HG21 | 4:S:230:LEU:HD22 | 1.78 | 0.64 |
| 4:S:45:TYR:HB3 | 13:X:42:ILE:HD11 | 1.79 | 0.64 |
| 1:W:496:ILE:HG22 | 1:W:628:MET:HE3 | 1.80 | 0.64 |
| 1:A:426:HIS:CG | 3:C:80:GLU:OE2 | 2.50 | 0.64 |
| 2:R:737:MET:SD | 1:W:447:LEU:HD13 | 2.37 | 0.64 |
| 5:E:123:VAL:HG22 | 5:E:127:ILE:HG12 | 1.80 | 0.64 |
| 13:P:5:ARG:O | 13:P:6:CYS:SG | 2.56 | 0.64 |
| 1:A:311:GLY:HA2 | 2:B:1030:ARG:NH2 | 2.13 | 0.64 |
| 2:B:405:ASN:HB2 | 2:B:413:VAL:HB | 1.79 | 0.64 |
| 2:R:641:THR:HG22 | 2:R:642:HIS:CE1 | 2.32 | 0.64 |
| 8:H:29:TYR:HE1 | 10:Q:60:SER:CB | 2.11 | 0.64 |
| 4:D:99:GLU:HA | 4:D:139:ILE:O | 1.97 | 0.64 |
| 5:E:30:LEU:HD13 | 5:E:72:PHE:CE2 | 2.33 | 0.64 |
| 1:A:474:ALA:HB2 | 9:K:62:ILE:HD11 | 1.78 | 0.64 |
| 2:R:742:ILE:CG2 | 2:R:912:ILE:HB | 2.27 | 0.64 |
| 1:A:177:PRO:HD2 | 1:A:266:TRP:CZ2 | 2.32 | 0.64 |
| 13:P:5:ARG:O | 13:P:6:CYS:CB | 2.45 | 0.64 |
| 2:B:1104:ILE:HD13 | 2:B:1116:LEU:HD11 | 1.80 | 0.64 |
| 4:S:17:PHE:O | 4:S:225:LYS:HA | 1.98 | 0.64 |
| 2:R:731:SER:HB2 | 1:W:501:ASP:OD2 | 1.98 | 0.64 |
| 5:T:7:ALA:HA | 6:U:7:VAL:HG13 | 1.80 | 0.64 |
| 1:A:108:GLU:O | 1:A:111:ILE:N | 2.30 | 0.64 |
| 1:W:418:LEU:HD23 | 1:W:430:MET:HE1 | 1.80 | 0.64 |
| 1:A:603:ILE:HG21 | 1:A:632:PHE:CE1 | 2.32 | 0.64 |
| 7:V:25:ASN:HA | 7:V:44:ASP:OD2 | 1.97 | 0.64 |
| 6:U:48:ASP:HB3 | 6:U:51:SER:HB2 | 1.79 | 0.64 |
| 9:I:56:ILE:O | 9:I:57:SER:CA | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:396:ARG:NH2 | 2:R:406:TRP:CH2 | 2.66 | 0.64 |
| 2:B:161:GLU:OE2 | 2:B:690:ARG:NH2 | 2.31 | 0.64 |
| 5:T:123:VAL:HG13 | 5:T:127:ILE:HG12 | 1.80 | 0.64 |
| 2:R:462:PRO:O | 2:R:467:SER:HA | 1.98 | 0.64 |
| 1:A:654:GLY:HA2 | 1:A:658:LYS:HE3 | 1.79 | 0.64 |
| 11:M:74:GLU:HG2 | 11:M:77:ARG:NH2 | 2.12 | 0.64 |
| 5:T:136:ILE:HG22 | 5:T:137:GLN:N | 2.12 | 0.64 |
| 2:R:686:ASN:O | 2:R:690:ARG:HG2 | 1.98 | 0.64 |
| 2:R:170:LEU:HD21 | 2:R:176:LEU:CD1 | 2.28 | 0.64 |
| 3:C:216:ILE:O | 3:C:217:ALA:CB | 2.45 | 0.64 |
| 4:S:206:CYS:SG | 16:S:1001:F3S:FE4 | 1.89 | 0.63 |
| 4:S:99:GLU:HA | 4:S:139:ILE:O | 1.98 | 0.63 |
| 1:A:309:PHE:O | 1:A:310:ARG:CG | 2.45 | 0.63 |
| 1:A:238:LYS:HZ2 | 1:A:275:THR:HG22 | 1.61 | 0.63 |
| 9:I:62:ILE:HD12 | 1:W:474:ALA:HB2 | 1.79 | 0.63 |
| 4:D:203:CYS:SG | 16:D:1001:F3S:FE3 | 1.89 | 0.63 |
| 3:Y:143:LYS:O | 3:Y:234:ILE:HG12 | 1.98 | 0.63 |
| 4:D:55:ASP:HB3 | 13:P:45:VAL:HG21 | 1.79 | 0.63 |
| 11:M:20:GLU:HG3 | 11:M:24:LEU:HD23 | 1.80 | 0.63 |
| 1:A:856:PHE:CE2 | 1:A:858:MET:HB3 | 2.33 | 0.63 |
| 2:R:212:THR:O | 2:R:259:LEU:HD11 | 1.98 | 0.63 |
| 2:R:974:TYR:CE2 | 4:S:165:ARG:HA | 2.33 | 0.63 |
| 9:K:51:ILE:O | 9:K:52:ASP:CB | 2.45 | 0.63 |
| 1:A:568:VAL:HG22 | 1:A:731:THR:HG22 | 1.79 | 0.63 |
| 2:R:583:ILE:HD12 | 2:R:591:LEU:HD21 | 1.80 | 0.63 |
| 2:R:10:ILE:HA | 2:R:13:ARG:HG2 | 1.79 | 0.63 |
| 2:R:235:ILE:HG23 | 2:R:240:ASP:HB3 | 1.80 | 0.63 |
| 1:A:505:GLY:HA3 | 1:A:639:VAL:HG22 | 1.80 | 0.63 |
| 6:F:71:VAL:HG11 | 6:F:89:MET:HE1 | 1.79 | 0.63 |
| 1:W:249:LEU:HG | 1:W:265:LEU:HB3 | 1.80 | 0.63 |
| 3:Y:216:ILE:O | 3:Y:217:ALA:CB | 2.46 | 0.63 |
| 2:R:734:GLY:HA2 | 1:W:330:PRO:HG3 | 1.79 | 0.63 |
| 12:N:3:ILE:HD13 | 12:N:15:ALA:HA | 1.79 | 0.63 |
| 3:Y:154:SER:OG | 3:Y:170:ASP:HB2 | 1.99 | 0.63 |
| 1:W:304:GLY:C | 1:W:306:GLU:H | 2.02 | 0.63 |
| 2:R:406:TRP:CG | 2:R:407:VAL:N | 2.66 | 0.63 |
| 2:B:646:TRP:CD2 | 2:B:648:PRO:HD2 | 2.34 | 0.63 |
| 1:A:252:SER:HB2 | 1:A:261:ILE:HG21 | 1.81 | 0.63 |
| 1:W:324:THR:HG22 | 1:W:325:VAL:H | 1.64 | 0.63 |
| 1:A:123:LYS:HA | 1:A:126:PRO:CG | 2.28 | 0.63 |
| 3:C:70:ILE:HA | 3:C:73:VAL:HG22 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:954:GLU:HA | 2:R:957:GLN:HB2 | 1.80 | 0.63 |
| 4:S:108:MET:HG2 | 4:S:110:TYR:CZ | 2.34 | 0.63 |
| 1:W:436:ARG:O | 1:W:438:LEU:HD22 | 1.99 | 0.63 |
| 4:S:203:CYS:SG | 16:S:1001:F3S:S1 | 2.96 | 0.63 |
| 2:R:105:PRO:HD2 | 2:R:112:ALA:HB3 | 1.80 | 0.63 |
| 1:W:95:LYS:HB3 | 1:W:138:LYS:HE2 | 1.78 | 0.63 |
| 7:V:103:VAL:HG22 | 7:V:104:LYS:H | 1.62 | 0.63 |
| 3:C:327:ARG:HG3 | 3:C:334:VAL:CG2 | 2.28 | 0.63 |
| 11:L:20:GLU:HG3 | 11:L:24:LEU:HD23 | 1.81 | 0.63 |
| 1:W:568:VAL:HG22 | 1:W:731:THR:HG22 | 1.81 | 0.63 |
| 3:C:237:ILE:HD12 | 3:C:253:THR:HB | 1.81 | 0.63 |
| 1:A:864:LYS:HE2 | 8:H:71:LEU:O | 1.98 | 0.63 |
| 2:R:401:LEU:HG | 2:R:401:LEU:O | 1.98 | 0.63 |
| 2:B:583:ILE:HD12 | 2:B:591:LEU:HD21 | 1.81 | 0.63 |
| 1:A:436:ARG:O | 1:A:438:LEU:HD22 | 1.99 | 0.63 |
| 5:T:60:VAL:HG22 | 5:T:61:PHE:H | 1.63 | 0.63 |
| 2:B:834:ALA:O | 2:B:835:LYS:HB2 | 1.98 | 0.63 |
| 2:B:406:TRP:O | 2:B:408:GLY:N | 2.31 | 0.63 |
| 2:R:330:LEU:O | 2:R:332:ARG:HG2 | 1.98 | 0.63 |
| 1:A:353:ILE:HG21 | 1:A:358:ILE:HD13 | 1.81 | 0.63 |
| 2:B:462:PRO:O | 2:B:467:SER:HA | 1.99 | 0.63 |
| 3:Y:277:ILE:HG22 | 3:Y:278:ARG:N | 2.14 | 0.63 |
| 2:B:1007:ARG:NH1 | 2:B:1028:GLY:O | 2.32 | 0.63 |
| 2:R:34:TYR:HB3 | 2:R:125:MET:HE1 | 1.80 | 0.62 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:CA | 2.76 | 0.62 |
| 13:X:5:ARG:HG2 | 13:X:18:LEU:CB | 2.29 | 0.62 |
| 2:R:86:MET:HE3 | 2:R:690:ARG:HD2 | 1.80 | 0.62 |
| 3:C:174:LEU:HB3 | 3:C:179:VAL:HG13 | 1.81 | 0.62 |
| 3:Y:174:LEU:HB3 | 3:Y:179:VAL:HG13 | 1.80 | 0.62 |
| 4:D:159:VAL:HG21 | 4:D:230:LEU:HD22 | 1.81 | 0.62 |
| 5:T:6:LYS:O | 6:U:7:VAL:HG22 | 2.00 | 0.62 |
| 1:W:104:VAL:HG13 | 1:W:137:LYS:HA | 1.79 | 0.62 |
| 9:I:35:VAL:HG12 | 3:Y:388:LEU:HD11 | 1.81 | 0.62 |
| 1:A:353:ILE:CG2 | 1:A:358:ILE:HD13 | 2.29 | 0.62 |
| 2:R:348:LEU:O | 2:R:352:LEU:HB2 | 1.98 | 0.62 |
| 2:B:320:TYR:CD1 | 2:B:529:LEU:HD12 | 2.33 | 0.62 |
| 1:W:856:PHE:CE2 | 1:W:858:MET:HB3 | 2.34 | 0.62 |
| 2:R:1069:TYR:CB | 2:R:1070:ILE:HB | 2.30 | 0.62 |
| 11:M:18:GLU:O | 11:M:18:GLU:HG2 | 1.99 | 0.62 |
| 2:B:417:LEU:HD21 | 2:B:425:MET:HG3 | 1.79 | 0.62 |
| 2:R:834:ALA:O | 2:R:835:LYS:HB2 | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:10:ILE:HA | 2:B:13:ARG:HG2 | 1.81 | 0.62 |
| 2:R:1015:LEU:HD13 | 2:R:1102:LEU:HD11 | 1.81 | 0.62 |
| 4:S:57:ILE:O | 4:S:61:ARG:HG3 | 1.99 | 0.62 |
| 5:E:165:ARG:O | 5:E:167:PRO:HD2 | 2.00 | 0.62 |
| 3:C:277:ILE:C | 3:C:279:GLU:H | 2.02 | 0.62 |
| 1:W:505:GLY:HA3 | 1:W:639:VAL:HG22 | 1.82 | 0.62 |
| 1:A:870:ARG:NH2 | 3:C:36:ILE:HD13 | 2.14 | 0.62 |
| 3:Y:70:ILE:HA | 3:Y:73:VAL:HG22 | 1.81 | 0.62 |
| 2:B:766:VAL:CG1 | 2:B:774:ASP:OD2 | 2.47 | 0.62 |
| 1:W:603:ILE:HG21 | 1:W:632:PHE:CE1 | 2.34 | 0.62 |
| 12:N:30:ASN:O | 12:N:34:VAL:HG23 | 1.99 | 0.62 |
| 13:P:17:GLN:CG | 13:P:19:LYS:HG2 | 2.29 | 0.62 |
| 3:Y:30:GLU:HG3 | 3:Y:31:ASP:H | 1.64 | 0.62 |
| 1:W:450:CYS:HB2 | 1:W:451:PRO:HD3 | 1.82 | 0.62 |
| 12:O:47:ARG:CZ | 12:O:48:MET:HE2 | 2.29 | 0.62 |
| 2:B:683:TYR:CZ | 2:B:687:TYR:HB2 | 2.34 | 0.62 |
| 2:R:1081:VAL:HG22 | 2:R:1085:HIS:HA | 1.81 | 0.62 |
| 1:W:870:ARG:CZ | 1:W:870:ARG:HB2 | 2.29 | 0.62 |
| 13:X:5:ARG:O | 13:X:6:CYS:CB | 2.48 | 0.62 |
| 2:B:874:ILE:H | 2:B:874:ILE:HD12 | 1.64 | 0.62 |
| 1:A:249:LEU:HG | 1:A:265:LEU:HB3 | 1.82 | 0.62 |
| 1:A:372:TRP:CD1 | 1:A:372:TRP:C | 2.73 | 0.62 |
| 2:R:147:ASP:HB3 | 2:R:685:ALA:HB3 | 1.82 | 0.62 |
| 1:W:104:VAL:CG1 | 1:W:137:LYS:CG | 2.78 | 0.62 |
| 2:B:742:ILE:CG2 | 2:B:912:ILE:HB | 2.29 | 0.62 |
| 2:B:984:SER:O | 2:B:985:ARG:HB2 | 2.00 | 0.62 |
| 4:S:155:LYS:HE3 | 4:S:156:PHE:CZ | 2.35 | 0.62 |
| 2:B:957:GLN:HA | 2:B:960:ILE:HD11 | 1.82 | 0.62 |
| 3:C:13:LEU:HD13 | 3:C:48:ILE:HG12 | 1.81 | 0.62 |
| 2:B:783:VAL:HG13 | 2:B:784:ARG:HB2 | 1.82 | 0.62 |
| 2:R:9:SER:HB3 | 2:R:12:GLU:HB3 | 1.80 | 0.62 |
| 5:E:89:VAL:HG23 | 5:E:98:PHE:O | 2.00 | 0.62 |
| 2:B:767:LYS:HB3 | 2:B:768:TYR:CB | 2.30 | 0.61 |
| 1:A:104:VAL:CG1 | 1:A:137:LYS:HA | 2.29 | 0.61 |
| 2:B:1069:TYR:HA | 2:B:1070:ILE:CB | 2.30 | 0.61 |
| 9:K:43:LEU:HD13 | 9:K:64:ILE:HG22 | 1.82 | 0.61 |
| 12:N:64:ARG:NH2 | 13:P:37:VAL:HG23 | 2.14 | 0.61 |
| 5:T:165:ARG:C | 5:T:167:PRO:CD | 2.68 | 0.61 |
| 3:Y:277:ILE:HG22 | 3:Y:278:ARG:H | 1.65 | 0.61 |
| 3:Y:262:LEU:HD22 | 3:Y:269:ILE:HD12 | 1.82 | 0.61 |
| 1:W:13:ILE:HD12 | 1:W:202:SER:HB2 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:84:VAL:HG13 | 1:A:274:ALA:HB1 | 1.80 | 0.61 |
| 8:H:65:ILE:HD11 | 8:H:79:ARG:HG2 | 1.81 | 0.61 |
| 12:O:3:ILE:HG23 | 12:O:52:HIS:CD2 | 2.35 | 0.61 |
| 2:B:212:THR:O | 2:B:259:LEU:HD11 | 2.00 | 0.61 |
| 12:O:64:ARG:NH2 | 13:X:37:VAL:HG23 | 2.15 | 0.61 |
| 2:R:783:VAL:HG13 | 2:R:784:ARG:HB2 | 1.83 | 0.61 |
| 3:Y:176:ASP:O | 3:Y:177:LYS:CB | 2.48 | 0.61 |
| 9:K:56:ILE:O | 9:K:57:SER:CA | 2.38 | 0.61 |
| 7:G:72:CYS:HB3 | 7:G:114:LYS:CG | 2.30 | 0.61 |
| 3:Y:147:THR:HB | 3:Y:232:LYS:HB2 | 1.82 | 0.61 |
| 6:U:71:VAL:HG11 | 6:U:89:MET:HE1 | 1.81 | 0.61 |
| 2:B:147:ASP:HB3 | 2:B:685:ALA:HB3 | 1.80 | 0.61 |
| 2:R:582:LEU:HD12 | 2:R:619:LEU:HD12 | 1.82 | 0.61 |
| 3:C:274:THR:HB | 3:C:280:ILE:HD11 | 1.82 | 0.61 |
| 1:A:141:MET:HG3 | 1:A:148:HIS:HB3 | 1.82 | 0.61 |
| 9:I:35:VAL:HG12 | 3:Y:388:LEU:HD13 | 1.81 | 0.61 |
| 7:V:102:LEU:HA | 7:V:106:ILE:HG22 | 1.83 | 0.61 |
| 1:W:642:GLN:HA | 1:W:642:GLN:OE1 | 2.00 | 0.61 |
| 10:Q:66:ARG:HG2 | 10:Q:66:ARG:HH11 | 1.66 | 0.61 |
| 3:C:297:ILE:O | 3:C:301:LEU:HD12 | 2.01 | 0.61 |
| 1:W:99:ARG:HH12 | 1:W:147:PRO:HG2 | 1.64 | 0.61 |
| 1:A:792:PRO:N | 2:B:948:PHE:HE1 | 1.98 | 0.61 |
| 2:B:981:LYS:HE2 | 4:D:205:LEU:HB2 | 1.81 | 0.61 |
| 1:A:418:LEU:HD21 | 2:B:1047:LEU:HD21 | 1.82 | 0.61 |
| 1:W:177:PRO:HD2 | 1:W:266:TRP:CZ2 | 2.36 | 0.61 |
| 2:B:191:LYS:HE2 | 2:B:193:ILE:HD11 | 1.83 | 0.61 |
| 1:W:353:ILE:CG2 | 1:W:358:ILE:HD13 | 2.30 | 0.61 |
| 4:S:209:CYS:SG | 4:S:219:ILE:HD11 | 2.40 | 0.61 |
| 2:B:356:LEU:HD12 | 2:B:407:VAL:HG21 | 1.83 | 0.61 |
| 1:A:854:GLY:O | 3:C:64:ILE:CG2 | 2.48 | 0.61 |
| 1:W:252:SER:HB2 | 1:W:261:ILE:HG21 | 1.82 | 0.61 |
| 11:L:18:GLU:O | 11:L:18:GLU:HG2 | 2.01 | 0.61 |
| 3:C:210:PHE:O | 3:C:211:ALA:HB3 | 2.01 | 0.61 |
| 3:C:143:LYS:O | 3:C:234:ILE:HG12 | 1.98 | 0.61 |
| 2:B:170:LEU:HD21 | 2:B:176:LEU:CD1 | 2.30 | 0.61 |
| 2:B:884:ARG:HB2 | 2:B:884:ARG:HH11 | 1.65 | 0.61 |
| 1:A:874:ARG:HB2 | 3:C:54:LEU:HD21 | 1.80 | 0.61 |
| 3:C:174:LEU:HD12 | 3:C:174:LEU:H | 1.65 | 0.61 |
| 2:R:1007:ARG:NH1 | 2:R:1028:GLY:C | 2.54 | 0.61 |
| 3:Y:53:ASP:HA | 3:Y:56:ILE:HG12 | 1.81 | 0.61 |
| 2:B:767:LYS:CD | 2:B:768:TYR:HA | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:R:951:THR:HG22 | 2:R:951:THR:O | 2.01 | 0.61 |
| 12:O:3:ILE:HD13 | 12:O:15:ALA:HA | 1.83 | 0.61 |
| 3:Y:327:ARG:HG3 | 3:Y:334:VAL:CG2 | 2.31 | 0.61 |
| 2:R:787:LYS:HE3 | 2:R:841:VAL:CG2 | 2.31 | 0.61 |
| 2:B:1081:VAL:HG22 | 2:B:1085:HIS:HA | 1.81 | 0.61 |
| 4:S:210:LEU:HD11 | 4:S:219:ILE:HB | 1.83 | 0.61 |
| 1:W:104:VAL:HG12 | 1:W:137:LYS:HB3 | 1.83 | 0.61 |
| 1:W:418:LEU:HD23 | 1:W:430:MET:CE | 2.31 | 0.61 |
| 3:C:174:LEU:HD12 | 3:C:174:LEU:N | 2.15 | 0.61 |
| 8:H:82:ILE:O | 8:H:82:ILE:HG22 | 2.01 | 0.61 |
| 5:E:2:TYR:HB2 | 6:F:12:ILE:O | 2.01 | 0.61 |
| 2:R:194:SER:HB2 | 2:R:303:HIS:HB3 | 1.82 | 0.61 |
| 8:Z:65:ILE:HD11 | 8:Z:79:ARG:HG2 | 1.81 | 0.61 |
| 9:I:52:ASP:O | 9:I:53:ILE:HB | 2.01 | 0.60 |
| 2:B:783:VAL:CG1 | 2:B:784:ARG:HB2 | 2.31 | 0.60 |
| 1:W:864:LYS:HE2 | 8:Z:71:LEU:O | 2.01 | 0.60 |
| 2:R:741:ILE:HD11 | 2:R:911:VAL:HG13 | 1.83 | 0.60 |
| 1:W:84:VAL:HG13 | 1:W:274:ALA:HB1 | 1.83 | 0.60 |
| 2:R:68:ILE:HG13 | 2:R:99:LEU:HD23 | 1.82 | 0.60 |
| 2:B:372:LEU:CD2 | 2:B:376:LYS:HE2 | 2.31 | 0.60 |
| 2:R:323:SER:O | 2:R:327:GLU:HB2 | 2.01 | 0.60 |
| 7:V:9:ILE:HD13 | 7:V:104:LYS:HE3 | 1.82 | 0.60 |
| 8:H:28:ALA:HB1 | 8:H:62:ILE:HD11 | 1.83 | 0.60 |
| 5:T:101:LEU:N | 5:T:101:LEU:HD12 | 2.17 | 0.60 |
| 3:Y:168:GLN:HG2 | 3:Y:204:ASN:CG | 2.21 | 0.60 |
| 1:A:736:SER:HB3 | 1:A:739:ASN:CG | 2.22 | 0.60 |
| 13:P:5:ARG:HG2 | 13:P:18:LEU:CB | 2.31 | 0.60 |
| 9:I:51:ILE:O | 9:I:52:ASP:CB | 2.49 | 0.60 |
| 2:B:1007:ARG:NH1 | 2:B:1028:GLY:C | 2.55 | 0.60 |
| 4:D:67:PHE:HB3 | 4:D:121:ILE:HG23 | 1.82 | 0.60 |
| 4:D:97:TYR:CE1 | 4:D:142:GLU:HG3 | 2.36 | 0.60 |
| 3:Y:210:PHE:O | 3:Y:211:ALA:HB3 | 2.00 | 0.60 |
| 3:C:199:ASP:HB2 | 3:C:206:LEU:HB2 | 1.81 | 0.60 |
| 3:C:340:SER:CB | 3:C:371:GLU:HG2 | 2.30 | 0.60 |
| 2:R:256:PHE:H | 2:R:257:PRO:HD2 | 1.65 | 0.60 |
| 2:B:249:PRO:CB | 2:B:252:GLN:HB2 | 2.31 | 0.60 |
| 2:B:86:MET:O | 2:B:90:LEU:HG | 2.01 | 0.60 |
| 3:Y:176:ASP:O | 3:Y:177:LYS:HB2 | 2.00 | 0.60 |
| 3:Y:305:GLY:O | 3:Y:306:LEU:HB3 | 2.00 | 0.60 |
| 1:A:238:LYS:O | 1:A:238:LYS:HG3 | 1.99 | 0.60 |
| 7:G:102:LEU:HA | 7:G:106:ILE:HG22 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:P:5:ARG:HD3 | 13:P:18:LEU:HD13 | 1.83 | 0.60 |
| 2:R:1074:ASP:HB3 | 2:R:1075:LYS:CA | 2.32 | 0.60 |
| 10:J:43:LEU:H | 10:J:43:LEU:HD12 | 1.67 | 0.60 |
| 2:R:703:ARG:HD2 | 2:R:717:THR:HG22 | 1.82 | 0.60 |
| 2:R:1104:ILE:HD13 | 2:R:1116:LEU:HD11 | 1.84 | 0.60 |
| 1:W:331:ASN:O | 1:W:332:ILE:HG12 | 2.02 | 0.60 |
| 1:A:97:THR:HG23 | 1:A:102:GLY:HA2 | 1.83 | 0.60 |
| 13:X:31:TYR:HE2 | 13:X:33:ILE:HB | 1.65 | 0.60 |
| 2:B:951:THR:HG22 | 2:B:951:THR:O | 2.02 | 0.60 |
| 1:A:848:VAL:O | 1:A:849:ALA:CB | 2.50 | 0.60 |
| 2:R:430:ARG:HH11 | 2:R:653:ILE:HG13 | 1.66 | 0.60 |
| 2:R:1008:ALA:HB2 | 1:W:346:THR:O | 2.01 | 0.60 |
| 2:R:91:ARG:HG3 | 13:X:33:ILE:HD11 | 1.83 | 0.60 |
| 2:R:208:LEU:CD2 | 2:R:215:VAL:HG23 | 2.32 | 0.60 |
| 3:C:154:SER:OG | 3:C:170:ASP:HB2 | 2.02 | 0.60 |
| 3:Y:174:LEU:N | 3:Y:174:LEU:HD12 | 2.16 | 0.60 |
| 2:B:933:GLY:HA3 | 2:B:990:VAL:HB | 1.84 | 0.60 |
| 2:B:767:LYS:HD3 | 2:B:768:TYR:HA | 1.84 | 0.60 |
| 3:C:168:GLN:CG | 3:C:204:ASN:OD1 | 2.36 | 0.60 |
| 2:R:46:ILE:HG21 | 2:R:66:ILE:HD11 | 1.83 | 0.60 |
| 11:M:47:HIS:ND1 | 11:M:48:PRO:HD2 | 2.16 | 0.60 |
| 2:R:984:SER:HB2 | 1:W:642:GLN:O | 2.01 | 0.60 |
| 5:E:123:VAL:HG13 | 5:E:127:ILE:HG12 | 1.83 | 0.60 |
| 1:W:682:GLY:O | 1:W:684:LEU:N | 2.34 | 0.60 |
| 2:B:601:ASP:O | 2:B:602:SER:CB | 2.50 | 0.60 |
| 2:R:856:THR:HG21 | 13:X:33:ILE:HD12 | 1.84 | 0.60 |
| 2:R:601:ASP:O | 2:R:602:SER:CB | 2.50 | 0.60 |
| 1:W:63:ASN:HB2 | 1:W:68:CYS:HB2 | 1.82 | 0.60 |
| 4:D:111:SER:HB3 | 4:D:128:ILE:HB | 1.83 | 0.60 |
| 10:Q:43:LEU:HD12 | 10:Q:43:LEU:H | 1.66 | 0.60 |
| 3:Y:47:GLU:HB3 | 3:Y:50:LYS:HB2 | 1.84 | 0.60 |
| 2:R:418:ASP:OD1 | 2:R:424:SER:OG | 2.19 | 0.60 |
| 3:Y:186:LYS:HB3 | 3:Y:230:LYS:HE2 | 1.84 | 0.60 |
| 1:A:141:MET:HA | 1:A:148:HIS:HB3 | 1.83 | 0.60 |
| 7:G:9:ILE:HD13 | 7:G:104:LYS:HE3 | 1.83 | 0.60 |
| 1:W:105:LYS:HZ2 | 1:W:133:THR:HG23 | 1.66 | 0.60 |
| 2:B:1046:MET:HG2 | 5:E:61:PHE:CD1 | 2.36 | 0.60 |
| 1:W:123:LYS:HA | 1:W:126:PRO:HG2 | 1.84 | 0.60 |
| 8:Z:82:ILE:HG22 | 8:Z:82:ILE:O | 2.02 | 0.60 |
| 2:R:451:THR:HG22 | 1:W:761:TYR:CD1 | 2.37 | 0.60 |
| 2:B:235:ILE:HG23 | 2:B:240:ASP:HB3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:430:ARG:HH11 | 2:B:653:ILE:HG13 | 1.67 | 0.60 |
| 2:R:320:TYR:CD1 | 2:R:529:LEU:HD12 | 2.37 | 0.60 |
| 4:S:209:CYS:SG | 16:S:1001:F3S:S2 | 2.89 | 0.59 |
| 3:C:309:ASP:OD2 | 3:C:311:ARG:HB2 | 2.01 | 0.59 |
| 5:T:164:MET:SD | 5:T:170:GLY:HA2 | 2.41 | 0.59 |
| 2:B:702:GLN:HB2 | 2:B:723:ASN:HA | 1.84 | 0.59 |
| 2:R:405:ASN:HB2 | 2:R:413:VAL:HB | 1.83 | 0.59 |
| 2:B:46:ILE:HG21 | 2:B:66:ILE:HD11 | 1.84 | 0.59 |
| 7:G:36:PHE:CD1 | 7:G:96:ILE:HD11 | 2.37 | 0.59 |
| 5:E:119:LYS:HB3 | 5:E:120:TYR:HB2 | 1.85 | 0.59 |
| 5:E:164:MET:SD | 5:E:170:GLY:HA2 | 2.42 | 0.59 |
| 13:P:5:ARG:HG2 | 13:P:18:LEU:HB2 | 1.84 | 0.59 |
| 5:T:166:GLN:N | 5:T:167:PRO:CD | 2.65 | 0.59 |
| 2:B:100:TRP:CZ3 | 2:B:118:TYR:HB2 | 2.36 | 0.59 |
| 2:R:536:GLY:HA3 | 2:R:560:HIS:CE1 | 2.37 | 0.59 |
| 5:E:36:GLU:HB3 | 6:F:33:LEU:HD22 | 1.84 | 0.59 |
| 2:R:630:ALA:HB3 | 2:R:636:LEU:CD1 | 2.32 | 0.59 |
| 1:W:58:CYS:HB3 | 1:W:62:GLY:N | 2.18 | 0.59 |
| 2:B:978:THR:HG23 | 2:B:980:GLN:HG2 | 1.84 | 0.59 |
| 2:R:683:TYR:CZ | 2:R:687:TYR:HB2 | 2.37 | 0.59 |
| 1:A:426:HIS:CD2 | 3:C:80:GLU:CD | 2.75 | 0.59 |
| 2:R:898:VAL:HG21 | 4:S:34:LEU:HD21 | 1.85 | 0.59 |
| 1:W:45:MET:O | 1:W:45:MET:HG2 | 2.01 | 0.59 |
| 2:B:954:GLU:HA | 2:B:957:GLN:HB2 | 1.85 | 0.59 |
| 2:R:520:TRP:O | 2:R:521:SER:CB | 2.51 | 0.59 |
| 9:I:41:LEU:HD23 | 5:T:64:GLY:N | 2.17 | 0.59 |
| 2:R:767:LYS:HG3 | 2:R:768:TYR:HD1 | 1.67 | 0.59 |
| 5:T:136:ILE:HG22 | 5:T:137:GLN:H | 1.64 | 0.59 |
| 1:A:109:ASP:O | 1:A:113:LYS:HG3 | 2.01 | 0.59 |
| 2:R:42:LEU:HD21 | 2:R:68:ILE:HD11 | 1.83 | 0.59 |
| 2:R:372:LEU:CD2 | 2:R:376:LYS:HE2 | 2.33 | 0.59 |
| 3:Y:297:ILE:O | 3:Y:301:LEU:HD12 | 2.02 | 0.59 |
| 3:C:168:GLN:HG2 | 3:C:204:ASN:CG | 2.22 | 0.59 |
| 1:W:109:ASP:O | 1:W:113:LYS:HG3 | 2.02 | 0.59 |
| 3:Y:169:LEU:HD23 | 3:Y:174:LEU:HD21 | 1.83 | 0.59 |
| 2:R:418:ASP:O | 2:R:418:ASP:OD1 | 2.21 | 0.59 |
| 3:Y:13:LEU:HD13 | 3:Y:48:ILE:HG12 | 1.85 | 0.59 |
| 1:W:654:GLY:HA2 | 1:W:658:LYS:HE3 | 1.84 | 0.59 |
| 1:W:378:VAL:HG13 | 1:W:386:ILE:HB | 1.85 | 0.59 |
| 2:B:166:THR:HG23 | 2:B:432:VAL:HG12 | 1.85 | 0.59 |
| 1:A:501:ASP:OD2 | 2:B:731:SER:HB2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:176:ASP:O | 3:C:177:LYS:CB | 2.50 | 0.59 |
| 3:C:80:GLU:HB3 | 3:C:81:PRO:HD3 | 1.84 | 0.59 |
| 1:W:108:GLU:O | 1:W:111:ILE:N | 2.35 | 0.59 |
| 2:B:279:VAL:HG12 | 2:B:291:LYS:HD3 | 1.83 | 0.59 |
| 4:S:97:TYR:CE1 | 4:S:142:GLU:HG3 | 2.38 | 0.59 |
| 2:R:17:ILE:HG13 | 2:R:476:MET:SD | 2.43 | 0.59 |
| 10:J:66:ARG:HD3 | 1:W:121:ILE:HG21 | 1.84 | 0.59 |
| 4:S:67:PHE:HB3 | 4:S:121:ILE:HG23 | 1.83 | 0.59 |
| 2:R:91:ARG:CG | 13:X:33:ILE:HD11 | 2.33 | 0.59 |
| 5:E:166:GLN:N | 5:E:167:PRO:CD | 2.65 | 0.59 |
| 13:P:5:ARG:HG3 | 13:P:6:CYS:H | 1.67 | 0.59 |
| 5:T:165:ARG:O | 5:T:167:PRO:HD2 | 2.01 | 0.59 |
| 12:N:47:ARG:CZ | 12:N:48:MET:HE2 | 2.32 | 0.59 |
| 2:B:834:ALA:O | 2:B:835:LYS:CB | 2.51 | 0.59 |
| 2:R:783:VAL:CG1 | 2:R:784:ARG:HB2 | 2.33 | 0.59 |
| 1:A:687:ILE:HD12 | 1:A:695:SER:HB2 | 1.83 | 0.59 |
| 5:E:64:GLY:N | 9:K:41:LEU:HD23 | 2.17 | 0.59 |
| 2:B:898:VAL:HG21 | 4:D:34:LEU:HD21 | 1.85 | 0.59 |
| 1:W:364:PHE:CE2 | 1:W:409:ARG:HD2 | 2.38 | 0.59 |
| 1:W:426:HIS:CD2 | 3:Y:80:GLU:OE1 | 2.56 | 0.59 |
| 2:B:406:TRP:CG | 2:B:407:VAL:N | 2.71 | 0.59 |
| 3:Y:274:THR:HB | 3:Y:280:ILE:HD11 | 1.85 | 0.59 |
| 2:B:256:PHE:H | 2:B:257:PRO:HD2 | 1.68 | 0.59 |
| 3:Y:169:LEU:HD23 | 3:Y:174:LEU:CD2 | 2.33 | 0.59 |
| 1:A:870:ARG:CZ | 1:A:870:ARG:HB2 | 2.32 | 0.59 |
| 2:R:1071:GLY:HA3 | 2:R:1073:TYR:HE1 | 1.67 | 0.59 |
| 2:R:186:ILE:HD12 | 2:R:209:LYS:HD3 | 1.83 | 0.59 |
| 3:C:262:LEU:HD22 | 3:C:269:ILE:HD12 | 1.84 | 0.59 |
| 2:B:68:ILE:HG13 | 2:B:99:LEU:HD23 | 1.85 | 0.59 |
| 5:T:89:VAL:HG23 | 5:T:98:PHE:O | 2.03 | 0.59 |
| 1:W:426:HIS:CD2 | 3:Y:80:GLU:CD | 2.75 | 0.59 |
| 2:R:646:TRP:CD2 | 2:R:648:PRO:HD2 | 2.37 | 0.59 |
| 5:E:136:ILE:CG2 | 5:E:137:GLN:H | 2.15 | 0.59 |
| 2:R:928:MET:CE | 2:R:953:ILE:HD12 | 2.32 | 0.59 |
| 1:W:600:LYS:HE2 | 1:W:607:GLN:OE1 | 2.03 | 0.59 |
| 1:A:821:ARG:HA | 1:A:824:ILE:HG22 | 1.84 | 0.59 |
| 4:D:161:LEU:HD12 | 4:D:163:ILE:HD13 | 1.85 | 0.59 |
| 4:D:155:LYS:HE3 | 4:D:156:PHE:CZ | 2.37 | 0.59 |
| 2:B:703:ARG:HD2 | 2:B:717:THR:HG22 | 1.84 | 0.59 |
| 1:W:822:ARG:HH22 | 3:Y:108:ILE:HG23 | 1.67 | 0.59 |
| 2:B:950:LYS:O | 2:B:951:THR:HB | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:86:MET:HE3 | 2:B:686:ASN:ND2 | 2.18 | 0.58 |
| 1:W:353:ILE:HG21 | 1:W:358:ILE:HD13 | 1.84 | 0.58 |
| 2:B:975:ASP:HB3 | 2:B:978:THR:HG22 | 1.85 | 0.58 |
| 2:R:701:PRO:HB2 | 2:R:720:PRO:HG2 | 1.85 | 0.58 |
| 3:C:286:ILE:HG12 | 8:H:49:ASP:CG | 2.24 | 0.58 |
| 2:B:557:ASN:OD1 | 2:B:577:ARG:NH1 | 2.35 | 0.58 |
| 2:B:1071:GLY:HA3 | 2:B:1073:TYR:HE1 | 1.68 | 0.58 |
| 1:W:555:PHE:HD1 | 1:W:626:TRP:CH2 | 2.21 | 0.58 |
| 2:R:1072:TRP:CZ3 | 1:W:67:ASN:OD1 | 2.56 | 0.58 |
| 1:W:104:VAL:HG11 | 1:W:137:LYS:CB | 2.33 | 0.58 |
| 2:B:157:VAL:HG11 | 2:B:401:LEU:HD23 | 1.85 | 0.58 |
| 2:R:532:TYR:O | 2:R:533:TYR:HB2 | 2.02 | 0.58 |
| 5:E:80:VAL:HG12 | 5:E:83:GLU:OE2 | 2.03 | 0.58 |
| 2:R:957:GLN:HA | 2:R:960:ILE:HD11 | 1.83 | 0.58 |
| 6:U:72:LEU:HD11 | 6:U:86:ILE:HG12 | 1.85 | 0.58 |
| 1:A:555:PHE:HD1 | 1:A:626:TRP:CH2 | 2.21 | 0.58 |
| 2:B:520:TRP:O | 2:B:521:SER:CB | 2.50 | 0.58 |
| 2:B:582:LEU:HD12 | 2:B:619:LEU:HD12 | 1.85 | 0.58 |
| 2:R:766:VAL:HG22 | 2:R:767:LYS:N | 2.18 | 0.58 |
| 5:T:30:LEU:HD13 | 5:T:72:PHE:CE2 | 2.38 | 0.58 |
| 1:W:603:ILE:HG22 | 1:W:604:GLY:H | 1.68 | 0.58 |
| 1:A:856:PHE:CD2 | 1:A:858:MET:HB3 | 2.38 | 0.58 |
| 2:R:834:ALA:O | 2:R:835:LYS:CB | 2.51 | 0.58 |
| 2:B:683:TYR:CE1 | 2:B:687:TYR:HB2 | 2.39 | 0.58 |
| 1:W:870:ARG:NH2 | 3:Y:36:ILE:HD13 | 2.17 | 0.58 |
| 2:B:703:ARG:HD2 | 2:B:717:THR:CG2 | 2.33 | 0.58 |
| 2:B:754:ARG:NH1 | 4:D:60:HIS:HD1 | 2.01 | 0.58 |
| 2:B:236:LEU:HD21 | 2:B:268:VAL:HG22 | 1.86 | 0.58 |
| 2:B:418:ASP:OD1 | 2:B:418:ASP:O | 2.22 | 0.58 |
| 1:W:553:SER:OG | 1:W:592:ILE:HA | 2.03 | 0.58 |
| 2:R:486:LYS:HA | 2:R:489:GLU:HG2 | 1.86 | 0.58 |
| 3:C:315:LEU:O | 3:C:319:VAL:HG23 | 2.04 | 0.58 |
| 2:B:187:THR:HG22 | 2:B:188:HIS:CD2 | 2.38 | 0.58 |
| 5:T:115:ASP:O | 5:T:116:ASP:CB | 2.50 | 0.58 |
| 2:B:856:THR:HG22 | 2:B:857:GLU:H | 1.68 | 0.58 |
| 4:D:253:ILE:HG13 | 11:L:73:ILE:HG23 | 1.85 | 0.58 |
| 1:A:418:LEU:HB3 | 1:A:430:MET:HE2 | 1.83 | 0.58 |
| 1:A:215:PRO:HG2 | 1:A:220:ARG:HD2 | 1.86 | 0.58 |
| 5:T:132:SER:O | 5:T:133:LYS:CB | 2.51 | 0.58 |
| 11:M:27:LEU:HD13 | 4:S:24:PHE:HA | 1.85 | 0.58 |
| 2:R:1105:GLN:HB3 | 1:W:219:ILE:HD11 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:786:TYR:CD2 | 2:B:788:GLY:HA2 | 2.38 | 0.58 |
| 2:B:394:THR:O | 2:B:397:ILE:HG22 | 2.04 | 0.58 |
| 2:R:672:GLN:NE2 | 2:R:884:ARG:HG3 | 2.18 | 0.58 |
| 11:L:47:HIS:ND1 | 11:L:48:PRO:HD2 | 2.19 | 0.58 |
| 2:R:1007:ARG:NH1 | 2:R:1028:GLY:O | 2.36 | 0.58 |
| 2:R:703:ARG:HD2 | 2:R:717:THR:CG2 | 2.34 | 0.58 |
| 2:R:653:ILE:HD12 | 2:R:653:ILE:H | 1.68 | 0.58 |
| 2:B:486:LYS:HA | 2:B:489:GLU:HG2 | 1.86 | 0.58 |
| 2:R:249:PRO:HB3 | 2:R:252:GLN:HB2 | 1.86 | 0.58 |
| 2:B:532:TYR:O | 2:B:533:TYR:HB2 | 2.04 | 0.58 |
| 2:B:17:ILE:HG13 | 2:B:476:MET:SD | 2.43 | 0.58 |
| 1:W:222:SER:C | 1:W:223:ILE:HG22 | 2.24 | 0.58 |
| 2:R:100:TRP:CZ3 | 2:R:118:TYR:HB2 | 2.39 | 0.58 |
| 1:A:45:MET:O | 1:A:45:MET:HG2 | 2.02 | 0.58 |
| 2:B:1074:ASP:HB3 | 2:B:1075:LYS:CA | 2.34 | 0.58 |
| 2:R:356:LEU:HD21 | 2:R:397:ILE:HG13 | 1.86 | 0.58 |
| 2:R:394:THR:O | 2:R:397:ILE:HG22 | 2.03 | 0.58 |
| 2:B:46:ILE:CG1 | 2:B:66:ILE:HD11 | 2.33 | 0.58 |
| 2:R:981:LYS:HE2 | 4:S:205:LEU:HB2 | 1.86 | 0.58 |
| 2:B:136:TYR:HD2 | 2:B:140:LYS:HB3 | 1.69 | 0.58 |
| 5:E:83:GLU:HA | 6:F:89:MET:HE3 | 1.86 | 0.58 |
| 2:R:9:SER:HB3 | 2:R:12:GLU:CB | 2.34 | 0.58 |
| 1:A:530:VAL:HG11 | 1:A:555:PHE:CE1 | 2.38 | 0.58 |
| 2:R:978:THR:CG2 | 2:R:980:GLN:HG2 | 2.34 | 0.58 |
| 8:Z:15:TYR:CD2 | 8:Z:16:LEU:HG | 2.39 | 0.58 |
| 2:R:364:PHE:HE1 | 2:R:388:VAL:HG13 | 1.67 | 0.58 |
| 13:X:6:CYS:CB | 13:X:37:VAL:HG12 | 2.34 | 0.58 |
| 13:X:5:ARG:HG3 | 13:X:6:CYS:H | 1.68 | 0.58 |
| 1:W:859:TYR:HE2 | 3:Y:65:ALA:HB2 | 1.68 | 0.58 |
| 4:D:210:LEU:HD11 | 4:D:219:ILE:HB | 1.86 | 0.58 |
| 2:R:950:LYS:O | 2:R:951:THR:HB | 2.03 | 0.58 |
| 5:E:102:GLY:HA2 | 6:F:40:TYR:CG | 2.39 | 0.58 |
| 1:A:665:ILE:O | 1:A:669:LYS:HG3 | 2.03 | 0.58 |
| 2:B:53:PRO:HD2 | 2:B:59:LEU:O | 2.03 | 0.58 |
| 7:V:36:PHE:CD1 | 7:V:96:ILE:HD11 | 2.39 | 0.58 |
| 4:D:203:CYS:HG | 16:D:1001:F3S:FE3 | 1.18 | 0.58 |
| 1:A:642:GLN:O | 2:B:984:SER:HB2 | 2.04 | 0.58 |
| 2:R:797:ASP:OD2 | 13:X:4:TYR:HB3 | 2.04 | 0.58 |
| 2:R:191:LYS:HE2 | 2:R:193:ILE:HD11 | 1.86 | 0.58 |
| 3:C:328:GLN:OE1 | 3:C:331:ARG:NH1 | 2.37 | 0.58 |
| 2:R:759:ARG:HG3 | 2:R:760:LEU:H | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:500:VAL:O | 2:R:504:ILE:HG12 | 2.04 | 0.58 |
| 2:B:660:TYR:CD1 | 2:B:950:LYS:HE3 | 2.38 | 0.57 |
| 3:C:231:ILE:CG2 | 3:C:232:LYS:N | 2.66 | 0.57 |
| 2:B:251:ILE:CD1 | 2:B:330:LEU:HD11 | 2.34 | 0.57 |
| 2:R:99:LEU:O | 2:R:119:ILE:HB | 2.04 | 0.57 |
| 2:B:978:THR:CG2 | 2:B:980:GLN:HG2 | 2.33 | 0.57 |
| 3:C:219:LEU:HA | 3:C:222:LEU:HD13 | 1.86 | 0.57 |
| 12:O:30:ASN:O | 12:O:34:VAL:HG23 | 2.03 | 0.57 |
| 1:W:820:GLN:OE1 | 3:Y:79:GLY:HA3 | 2.04 | 0.57 |
| 1:W:309:PHE:O | 1:W:310:ARG:CB | 2.52 | 0.57 |
| 6:F:72:LEU:HD11 | 6:F:86:ILE:HG12 | 1.85 | 0.57 |
| 1:W:874:ARG:HB2 | 3:Y:54:LEU:HD21 | 1.85 | 0.57 |
| 2:B:741:ILE:HD11 | 2:B:911:VAL:HG13 | 1.85 | 0.57 |
| 2:B:31:LEU:HA | 2:B:125:MET:HE1 | 1.84 | 0.57 |
| 1:W:326:ILE:HG13 | 1:W:457:PHE:CE1 | 2.38 | 0.57 |
| 2:B:157:VAL:HG22 | 2:B:162:ARG:HB2 | 1.86 | 0.57 |
| 1:W:848:VAL:O | 1:W:849:ALA:CB | 2.51 | 0.57 |
| 3:Y:174:LEU:HD12 | 3:Y:174:LEU:H | 1.67 | 0.57 |
| 8:H:63:ILE:HG22 | 8:H:65:ILE:HD11 | 1.86 | 0.57 |
| 3:C:176:ASP:O | 3:C:177:LYS:HG3 | 2.04 | 0.57 |
| 1:W:223:ILE:HG12 | 1:W:224:MET:N | 2.19 | 0.57 |
| 1:A:496:ILE:HG22 | 1:A:628:MET:HE3 | 1.86 | 0.57 |
| 1:A:326:ILE:HG13 | 1:A:457:PHE:CE1 | 2.39 | 0.57 |
| 1:W:534:LEU:CB | 1:W:546:TYR:CE2 | 2.88 | 0.57 |
| 2:R:333:ARG:O | 2:R:334:GLU:HB3 | 2.03 | 0.57 |
| 2:R:702:GLN:HB2 | 2:R:723:ASN:HA | 1.85 | 0.57 |
| 2:R:251:ILE:CD1 | 2:R:330:LEU:HD11 | 2.34 | 0.57 |
| 5:E:82:GLN:HB3 | 6:F:88:ILE:HB | 1.87 | 0.57 |
| 5:E:101:LEU:HD12 | 5:E:101:LEU:N | 2.19 | 0.57 |
| 1:A:553:SER:OG | 1:A:592:ILE:HA | 2.04 | 0.57 |
| 2:R:605:ILE:HG23 | 2:R:606:THR:N | 2.19 | 0.57 |
| 2:R:974:TYR:CD2 | 2:R:981:LYS:HB3 | 2.40 | 0.57 |
| 1:W:856:PHE:CD2 | 1:W:858:MET:HB3 | 2.39 | 0.57 |
| 1:A:820:GLN:OE1 | 3:C:79:GLY:HA3 | 2.05 | 0.57 |
| 3:C:292:ILE:HD13 | 3:C:292:ILE:O | 2.04 | 0.57 |
| 7:V:102:LEU:HA | 7:V:106:ILE:CG2 | 2.34 | 0.57 |
| 3:Y:327:ARG:HG3 | 3:Y:334:VAL:HG23 | 1.86 | 0.57 |
| 1:A:321:SER:HB2 | 2:B:1029:LEU:HD12 | 1.87 | 0.57 |
| 2:B:699:HIS:CE1 | 4:D:57:ILE:HD11 | 2.39 | 0.57 |
| 2:R:187:THR:HG22 | 2:R:188:HIS:CD2 | 2.40 | 0.57 |
| 7:G:48:ILE:HG22 | 7:G:49:PHE:H | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:378:VAL:HG13 | 1:A:386:ILE:HB | 1.87 | 0.57 |
| 2:B:630:ALA:HB3 | 2:B:636:LEU:CD1 | 2.33 | 0.57 |
| 3:Y:199:ASP:HB2 | 3:Y:206:LEU:HB2 | 1.86 | 0.57 |
| 3:C:388:LEU:HD11 | 9:K:35:VAL:HG12 | 1.86 | 0.57 |
| 2:B:672:GLN:NE2 | 2:B:884:ARG:HG3 | 2.20 | 0.57 |
| 7:G:102:LEU:HA | 7:G:106:ILE:CG2 | 2.34 | 0.57 |
| 1:A:458:ASP:O | 2:B:880:LYS:HE3 | 2.05 | 0.57 |
| 2:R:765:GLU:O | 2:R:766:VAL:O | 2.22 | 0.57 |
| 5:E:6:LYS:H | 6:F:8:GLU:HB2 | 1.69 | 0.57 |
| 2:R:884:ARG:HH11 | 2:R:884:ARG:HB2 | 1.70 | 0.57 |
| 1:W:859:TYR:O | 3:Y:63:LEU:HD13 | 2.04 | 0.57 |
| 1:A:141:MET:O | 1:A:141:MET:HG3 | 2.04 | 0.57 |
| 1:A:63:ASN:HB2 | 1:A:68:CYS:HB2 | 1.85 | 0.57 |
| 1:A:654:GLY:HA2 | 1:A:658:LYS:CE | 2.34 | 0.57 |
| 1:A:635:PHE:O | 1:A:639:VAL:HG23 | 2.05 | 0.57 |
| 2:B:1015:LEU:HD13 | 2:B:1102:LEU:HD11 | 1.85 | 0.57 |
| 2:B:323:SER:O | 2:B:327:GLU:HB2 | 2.03 | 0.57 |
| 5:E:9:SER:O | 5:E:70:VAL:HG12 | 2.04 | 0.57 |
| 2:R:774:ASP:OD1 | 2:R:819:PRO:CD | 2.52 | 0.57 |
| 2:B:661:PRO:HG2 | 2:B:947:PRO:HB3 | 1.87 | 0.57 |
| 2:R:927:ILE:HG21 | 1:W:648:LEU:HB2 | 1.87 | 0.57 |
| 2:R:974:TYR:CZ | 2:R:981:LYS:HB3 | 2.40 | 0.57 |
| 2:R:136:TYR:HD2 | 2:R:140:LYS:HB3 | 1.69 | 0.57 |
| 2:R:982:ILE:HD12 | 2:R:983:LYS:N | 2.20 | 0.57 |
| 2:R:451:THR:HG22 | 1:W:761:TYR:CE1 | 2.40 | 0.57 |
| 2:B:42:LEU:HD21 | 2:B:68:ILE:HD11 | 1.86 | 0.57 |
| 4:S:22:LEU:HB2 | 4:S:226:TYR:CZ | 2.40 | 0.57 |
| 3:C:305:GLY:O | 3:C:306:LEU:HB3 | 2.05 | 0.57 |
| 3:Y:219:LEU:HA | 3:Y:222:LEU:HD13 | 1.87 | 0.57 |
| 1:A:23:SER:HB2 | 1:A:74:HIS:CD2 | 2.40 | 0.57 |
| 8:H:11:PRO:O | 8:H:17:VAL:HG11 | 2.05 | 0.57 |
| 1:W:552:VAL:HG11 | 1:W:598:PHE:CE2 | 2.40 | 0.57 |
| 1:A:552:VAL:HG11 | 1:A:598:PHE:CE2 | 2.39 | 0.57 |
| 5:E:30:LEU:HD22 | 5:E:72:PHE:CE2 | 2.40 | 0.57 |
| 2:R:602:SER:HA | 2:R:605:ILE:HD12 | 1.85 | 0.57 |
| 1:W:141:MET:HA | 1:W:148:HIS:HB3 | 1.86 | 0.57 |
| 1:A:271:TYR:HE2 | 1:A:285:PRO:HB3 | 1.66 | 0.57 |
| 9:K:51:ILE:O | 9:K:52:ASP:HB2 | 2.04 | 0.57 |
| 1:A:95:LYS:CB | 1:A:138:LYS:HE2 | 2.35 | 0.57 |
| 2:B:86:MET:HE3 | 2:B:690:ARG:HD2 | 1.85 | 0.57 |
| 5:T:80:VAL:HG12 | 5:T:83:GLU:OE2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:331:ASN:O | 1:A:332:ILE:HG12 | 2.04 | 0.57 |
| 9:K:39:ARG:NE | 9:K:68:GLU:OE2 | 2.38 | 0.57 |
| 2:B:55:GLU:OE2 | 2:B:377:VAL:HG12 | 2.05 | 0.57 |
| 2:B:1069:TYR:CB | 2:B:1070:ILE:HB | 2.35 | 0.57 |
| 2:R:251:ILE:HD12 | 2:R:330:LEU:HD11 | 1.86 | 0.57 |
| 3:C:70:ILE:H | 3:C:70:ILE:HD13 | 1.68 | 0.57 |
| 2:R:683:TYR:CE1 | 2:R:687:TYR:HB2 | 2.40 | 0.57 |
| 1:W:541:ALA:HB3 | 1:W:542:PRO:CD | 2.34 | 0.57 |
| 1:A:14:LEU:HB3 | 2:B:1111:ILE:HG23 | 1.86 | 0.57 |
| 8:H:20:HIS:CE1 | 8:H:51:VAL:HG11 | 2.40 | 0.57 |
| 3:Y:231:ILE:CG2 | 3:Y:232:LYS:N | 2.68 | 0.56 |
| 2:R:978:THR:HG23 | 2:R:980:GLN:HG2 | 1.86 | 0.56 |
| 5:E:133:LYS:O | 5:E:134:LYS:HG3 | 2.05 | 0.56 |
| 2:B:364:PHE:HE1 | 2:B:388:VAL:HG13 | 1.69 | 0.56 |
| 2:B:974:TYR:CD2 | 2:B:981:LYS:HB3 | 2.40 | 0.56 |
| 8:H:59:PRO:HA | 8:H:81:VAL:HG12 | 1.87 | 0.56 |
| 2:R:975:ASP:OD1 | 2:R:977:ARG:HD3 | 2.05 | 0.56 |
| 2:R:41:LYS:HA | 2:R:44:GLU:OE1 | 2.04 | 0.56 |
| 2:R:1030:ARG:HH22 | 1:W:311:GLY:HA2 | 1.67 | 0.56 |
| 2:R:1051:ARG:NE | 2:R:1051:ARG:HA | 2.21 | 0.56 |
| 2:B:356:LEU:HD21 | 2:B:397:ILE:HG13 | 1.86 | 0.56 |
| 3:C:197:VAL:HB | 3:C:208:ILE:CG1 | 2.36 | 0.56 |
| 1:W:104:VAL:HG11 | 1:W:137:LYS:CA | 2.35 | 0.56 |
| 9:K:52:ASP:O | 9:K:53:ILE:HB | 2.05 | 0.56 |
| 2:R:249:PRO:HB2 | 2:R:252:GLN:HB2 | 1.87 | 0.56 |
| 2:R:86:MET:O | 2:R:90:LEU:HG | 2.05 | 0.56 |
| 2:B:629:VAL:HG22 | 2:B:642:HIS:HB2 | 1.86 | 0.56 |
| 2:R:661:PRO:HG2 | 2:R:947:PRO:HB3 | 1.88 | 0.56 |
| 5:T:123:VAL:HG22 | 5:T:127:ILE:HG12 | 1.87 | 0.56 |
| 8:Z:63:ILE:HG22 | 8:Z:65:ILE:HD11 | 1.86 | 0.56 |
| 4:D:60:HIS:C | 4:D:60:HIS:CD2 | 2.78 | 0.56 |
| 2:B:1112:ILE:O | 2:B:1114:PRO:HD3 | 2.05 | 0.56 |
| 4:S:53:LEU:HD12 | 4:S:131:VAL:HG23 | 1.86 | 0.56 |
| 1:W:665:ILE:O | 1:W:669:LYS:HG3 | 2.05 | 0.56 |
| 4:S:55:ASP:HB3 | 13:X:45:VAL:HG21 | 1.87 | 0.56 |
| 1:W:750:GLN:HG3 | 1:W:782:ILE:HD11 | 1.87 | 0.56 |
| 2:B:367:ASP:OD2 | 2:B:389:ARG:HD2 | 2.04 | 0.56 |
| 2:R:1004:ILE:HD12 | 1:W:441:LEU:HD22 | 1.87 | 0.56 |
| 2:B:9:SER:HB3 | 2:B:12:GLU:CB | 2.34 | 0.56 |
| 2:R:1101:LYS:HE3 | 1:W:69:PRO:HB2 | 1.87 | 0.56 |
| 3:Y:323:THR:O | 3:Y:325:VAL:N | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:898:VAL:HG22 | 4:D:33:MET:SD | 2.46 | 0.56 |
| 4:D:154:ALA:C | 4:D:156:PHE:H | 2.09 | 0.56 |
| 1:A:222:SER:C | 1:A:223:ILE:HG22 | 2.26 | 0.56 |
| 9:I:39:ARG:NE | 9:I:68:GLU:OE2 | 2.38 | 0.56 |
| 2:B:41:LYS:HA | 2:B:44:GLU:OE1 | 2.05 | 0.56 |
| 4:S:219:ILE:HD13 | 16:S:1001:F3S:S3 | 2.46 | 0.56 |
| 1:W:238:LYS:HZ2 | 1:W:275:THR:HG22 | 1.69 | 0.56 |
| 1:A:13:ILE:HG13 | 1:A:202:SER:HB3 | 1.87 | 0.56 |
| 4:S:93:TYR:HE1 | 4:S:146:ARG:HG2 | 1.70 | 0.56 |
| 3:C:69:ALA:HB2 | 3:C:381:LEU:HD13 | 1.87 | 0.56 |
| 1:A:28:ILE:HG23 | 1:A:30:PRO:HD2 | 1.87 | 0.56 |
| 2:B:155:PHE:CE1 | 2:B:164:ILE:HD12 | 2.41 | 0.56 |
| 1:W:417:VAL:HG11 | 1:W:464:LEU:CD1 | 2.36 | 0.56 |
| 2:B:249:PRO:HB3 | 2:B:252:GLN:HB2 | 1.87 | 0.56 |
| 2:B:8:LEU:HA | 2:B:633:PRO:HG3 | 1.87 | 0.56 |
| 1:A:534:LEU:CB | 1:A:546:TYR:CE1 | 2.89 | 0.56 |
| 5:E:115:ASP:O | 5:E:116:ASP:CB | 2.53 | 0.56 |
| 2:B:208:LEU:CD2 | 2:B:215:VAL:HG23 | 2.35 | 0.56 |
| 13:P:6:CYS:HB2 | 13:P:37:VAL:HG12 | 1.87 | 0.56 |
| 4:S:161:LEU:HD12 | 4:S:163:ILE:HD13 | 1.88 | 0.56 |
| 7:V:48:ILE:HG22 | 7:V:49:PHE:H | 1.71 | 0.56 |
| 3:Y:349:VAL:HG13 | 3:Y:349:VAL:O | 2.05 | 0.56 |
| 2:B:500:VAL:O | 2:B:504:ILE:HG12 | 2.05 | 0.56 |
| 8:Z:11:PRO:O | 8:Z:17:VAL:HG11 | 2.05 | 0.56 |
| 4:D:93:TYR:CD1 | 4:D:146:ARG:HB3 | 2.41 | 0.56 |
| 2:R:767:LYS:CB | 2:R:768:TYR:CA | 2.72 | 0.56 |
| 7:G:96:ILE:HD13 | 7:G:101:LEU:CD2 | 2.36 | 0.56 |
| 1:A:600:LYS:HE2 | 1:A:607:GLN:OE1 | 2.05 | 0.56 |
| 2:R:922:MET:HG2 | 1:W:743:MET:CG | 2.36 | 0.56 |
| 8:H:15:TYR:CD2 | 8:H:16:LEU:HG | 2.40 | 0.56 |
| 1:A:498:ALA:HB1 | 1:A:502:TYR:HB2 | 1.87 | 0.56 |
| 1:A:249:LEU:HD21 | 1:A:265:LEU:HB2 | 1.87 | 0.56 |
| 1:W:530:VAL:HG11 | 1:W:555:PHE:CE1 | 2.40 | 0.56 |
| 2:R:1105:GLN:CB | 1:W:219:ILE:HD11 | 2.35 | 0.56 |
| 4:D:57:ILE:O | 4:D:61:ARG:HG3 | 2.05 | 0.56 |
| 2:B:1057:ASP:N | 2:B:1057:ASP:OD1 | 2.39 | 0.56 |
| 1:A:281:ILE:N | 1:A:282:PRO:CD | 2.68 | 0.56 |
| 2:R:786:TYR:CD2 | 2:R:788:GLY:HA2 | 2.40 | 0.56 |
| 13:X:5:ARG:HD3 | 13:X:18:LEU:HD13 | 1.86 | 0.56 |
| 3:Y:64:ILE:HG22 | 3:Y:65:ALA:N | 2.19 | 0.56 |
| 13:P:6:CYS:CB | 13:P:37:VAL:HG12 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:157:VAL:HG22 | 2:R:162:ARG:HB2 | 1.88 | 0.56 |
| 1:W:336:GLU:OE2 | 1:W:436:ARG:HB2 | 2.05 | 0.56 |
| 1:A:249:LEU:CD2 | 1:A:265:LEU:HB2 | 2.36 | 0.56 |
| 2:R:809:GLY:O | 2:R:842:THR:HB | 2.06 | 0.56 |
| 1:W:326:ILE:HG13 | 1:W:457:PHE:CD1 | 2.41 | 0.56 |
| 8:Z:59:PRO:HA | 8:Z:81:VAL:HG12 | 1.88 | 0.56 |
| 5:E:132:SER:O | 5:E:133:LYS:HG3 | 2.05 | 0.56 |
| 2:R:1030:ARG:NH2 | 1:W:311:GLY:HA2 | 2.22 | 0.56 |
| 9:I:54:ASN:ND2 | 1:W:356:TRP:CE3 | 2.73 | 0.56 |
| 1:W:23:SER:HB2 | 1:W:74:HIS:CD2 | 2.41 | 0.56 |
| 8:Z:28:ALA:HB1 | 8:Z:62:ILE:HD11 | 1.86 | 0.56 |
| 5:T:22:LEU:HD21 | 3:Y:392:PRO:HG2 | 1.88 | 0.56 |
| 1:A:385:ARG:NH1 | 2:B:1009:ARG:NH2 | 2.54 | 0.56 |
| 2:B:765:GLU:O | 2:B:766:VAL:O | 2.24 | 0.55 |
| 4:S:209:CYS:SG | 16:S:1001:F3S:S3 | 3.04 | 0.55 |
| 2:B:857:GLU:HA | 2:B:862:ASN:O | 2.05 | 0.55 |
| 1:A:736:SER:HB3 | 1:A:739:ASN:OD1 | 2.05 | 0.55 |
| 1:W:324:THR:HG22 | 1:W:325:VAL:N | 2.20 | 0.55 |
| 1:A:668:ALA:HB1 | 1:A:707:LEU:HD13 | 1.88 | 0.55 |
| 3:Y:340:SER:CB | 3:Y:371:GLU:HG2 | 2.36 | 0.55 |
| 6:U:4:VAL:O | 6:U:4:VAL:HG13 | 2.06 | 0.55 |
| 3:C:389:THR:HG21 | 5:E:56:GLU:OE1 | 2.06 | 0.55 |
| 1:A:364:PHE:CE2 | 1:A:409:ARG:HD2 | 2.42 | 0.55 |
| 11:L:12:TYR:HD1 | 11:L:58:LEU:HD13 | 1.71 | 0.55 |
| 7:V:96:ILE:HD13 | 7:V:101:LEU:CD2 | 2.36 | 0.55 |
| 1:W:141:MET:HG3 | 1:W:148:HIS:HB3 | 1.87 | 0.55 |
| 7:G:8:GLU:C | 7:G:9:ILE:HG13 | 2.25 | 0.55 |
| 1:W:325:VAL:O | 1:W:442:THR:HG22 | 2.07 | 0.55 |
| 2:R:734:GLY:HA3 | 2:R:735:TYR:CD2 | 2.41 | 0.55 |
| 2:B:787:LYS:HE3 | 2:B:841:VAL:HG21 | 1.88 | 0.55 |
| 2:B:1046:MET:HG2 | 5:E:61:PHE:CE1 | 2.41 | 0.55 |
| 4:S:111:SER:HA | 4:S:130:ILE:HD11 | 1.88 | 0.55 |
| 2:R:279:VAL:HG12 | 2:R:291:LYS:HD3 | 1.87 | 0.55 |
| 3:Y:292:ILE:O | 3:Y:292:ILE:HD13 | 2.07 | 0.55 |
| 2:B:957:GLN:HA | 2:B:960:ILE:CD1 | 2.35 | 0.55 |
| 3:C:286:ILE:HG12 | 8:H:49:ASP:OD1 | 2.06 | 0.55 |
| 1:A:326:ILE:HG13 | 1:A:457:PHE:CD1 | 2.41 | 0.55 |
| 2:B:117:VAL:HG11 | 2:B:388:VAL:HG21 | 1.88 | 0.55 |
| 1:A:417:VAL:HG11 | 1:A:464:LEU:CD1 | 2.37 | 0.55 |
| 5:T:130:GLU:HG3 | 5:T:137:GLN:OE1 | 2.07 | 0.55 |
| 1:A:736:SER:O | 1:A:738:LEU:N | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:136:TYR:HB2 | 2:B:141:LEU:HD11 | 1.87 | 0.55 |
| 8:Z:44:TRP:O | 8:Z:79:ARG:HD2 | 2.06 | 0.55 |
| 1:W:853:ASP:CB | 3:Y:311:ARG:NH1 | 2.70 | 0.55 |
| 2:B:731:SER:HA | 2:B:914:ASN:ND2 | 2.22 | 0.55 |
| 5:E:132:SER:O | 5:E:133:LYS:CB | 2.54 | 0.55 |
| 3:Y:341:VAL:HG12 | 3:Y:344:ARG:NH2 | 2.21 | 0.55 |
| 3:C:29:VAL:HG12 | 3:C:61:GLU:HG3 | 1.89 | 0.55 |
| 1:A:792:PRO:CG | 2:B:948:PHE:CE1 | 2.89 | 0.55 |
| 2:R:46:ILE:CG1 | 2:R:66:ILE:HD11 | 2.36 | 0.55 |
| 2:B:17:ILE:HD12 | 2:B:476:MET:SD | 2.47 | 0.55 |
| 3:Y:315:LEU:O | 3:Y:319:VAL:HG23 | 2.05 | 0.55 |
| 2:R:236:LEU:HD21 | 2:R:268:VAL:HG22 | 1.88 | 0.55 |
| 2:R:367:ASP:OD1 | 2:R:389:ARG:HD2 | 2.07 | 0.55 |
| 2:R:107:GLU:O | 2:R:108:ASN:CB | 2.54 | 0.55 |
| 5:T:119:LYS:HB3 | 5:T:120:TYR:HB2 | 1.87 | 0.55 |
| 2:B:974:TYR:CZ | 2:B:981:LYS:HB3 | 2.41 | 0.55 |
| 2:B:982:ILE:HD12 | 2:B:983:LYS:N | 2.21 | 0.55 |
| 1:W:334:ILE:CD1 | 1:W:628:MET:HB3 | 2.36 | 0.55 |
| 1:A:859:TYR:O | 3:C:63:LEU:HD13 | 2.06 | 0.55 |
| 2:B:248:ASP:N | 2:B:249:PRO:HD3 | 2.22 | 0.55 |
| 1:A:603:ILE:HG22 | 1:A:604:GLY:H | 1.71 | 0.55 |
| 3:C:170:ASP:HB3 | 3:C:173:MET:HB2 | 1.89 | 0.55 |
| 1:A:123:LYS:HA | 1:A:126:PRO:HG2 | 1.88 | 0.55 |
| 3:C:176:ASP:O | 3:C:177:LYS:HB2 | 2.07 | 0.55 |
| 2:R:1060:THR:O | 2:R:1061:ILE:C | 2.45 | 0.55 |
| 3:C:323:THR:O | 3:C:325:VAL:N | 2.40 | 0.55 |
| 3:C:149:ILE:HA | 3:C:152:VAL:HG12 | 1.89 | 0.55 |
| 2:R:356:LEU:HD12 | 2:R:407:VAL:HG21 | 1.87 | 0.55 |
| 2:R:1031:PHE:HD2 | 1:W:465:HIS:CE1 | 2.24 | 0.55 |
| 2:R:63:LEU:HD22 | 2:R:101:LEU:HD11 | 1.89 | 0.55 |
| 1:A:105:LYS:HZ2 | 1:A:133:THR:HG23 | 1.71 | 0.55 |
| 4:D:49:ASN:OD1 | 4:D:139:ILE:CD1 | 2.55 | 0.55 |
| 3:C:70:ILE:N | 3:C:70:ILE:HD13 | 2.21 | 0.55 |
| 3:Y:104:LEU:N | 3:Y:105:PRO:CD | 2.69 | 0.55 |
| 3:C:104:LEU:N | 3:C:105:PRO:CD | 2.69 | 0.55 |
| 2:R:918:LEU:CD1 | 1:W:646:MET:HG2 | 2.37 | 0.55 |
| 10:J:55:LEU:HD21 | 8:Z:25:ILE:HG22 | 1.89 | 0.55 |
| 2:B:802:SER:OG | 13:P:39:LYS:HB2 | 2.07 | 0.55 |
| 4:S:66:PRO:HB2 | 4:S:124:ILE:HG12 | 1.89 | 0.55 |
| 2:R:768:TYR:CB | 2:R:769:PRO:CD | 2.72 | 0.55 |
| 3:Y:197:VAL:HB | 3:Y:208:ILE:CG1 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:130:GLU:HG3 | 5:E:137:GLN:OE1 | 2.06 | 0.55 |
| 9:I:62:ILE:HD11 | 1:W:474:ALA:HB2 | 1.87 | 0.55 |
| 4:D:97:TYR:CD1 | 4:D:142:GLU:HG3 | 2.41 | 0.55 |
| 1:W:654:GLY:HA2 | 1:W:658:LYS:CE | 2.37 | 0.55 |
| 1:W:121:ILE:HG23 | 8:Z:38:ARG:NH1 | 2.21 | 0.55 |
| 1:W:281:ILE:N | 1:W:282:PRO:CD | 2.69 | 0.55 |
| 2:R:1057:ASP:OD2 | 2:R:1097:SER:HB2 | 2.06 | 0.55 |
| 11:L:80:ALA:O | 11:L:84:ILE:HG12 | 2.06 | 0.55 |
| 2:B:774:ASP:OD1 | 2:B:819:PRO:CD | 2.54 | 0.55 |
| 4:D:219:ILE:HD13 | 16:D:1001:F3S:S3 | 2.47 | 0.55 |
| 1:A:124:ARG:N | 1:A:126:PRO:HD2 | 2.21 | 0.55 |
| 4:S:93:TYR:CE1 | 4:S:146:ARG:HG2 | 2.42 | 0.55 |
| 1:W:372:TRP:HB3 | 1:W:373:PRO:HD3 | 1.88 | 0.55 |
| 2:B:229:LEU:HD23 | 2:B:275:ILE:HD11 | 1.89 | 0.55 |
| 4:S:37:PRO:HG3 | 4:S:78:TRP:CE3 | 2.41 | 0.55 |
| 4:S:38:VAL:HG12 | 4:S:39:MET:N | 2.21 | 0.55 |
| 1:A:103:ARG:CB | 1:A:191:ASP:OD1 | 2.54 | 0.55 |
| 1:A:863:GLY:HA2 | 3:C:311:ARG:NH2 | 2.22 | 0.55 |
| 1:A:418:LEU:HD23 | 1:A:430:MET:CE | 2.36 | 0.55 |
| 1:W:309:PHE:O | 1:W:310:ARG:CG | 2.55 | 0.55 |
| 1:W:425:LEU:H | 1:W:425:LEU:HD12 | 1.70 | 0.55 |
| 2:B:1060:THR:O | 2:B:1061:ILE:C | 2.46 | 0.55 |
| 12:N:19:GLN:N | 12:N:20:PRO:HD2 | 2.22 | 0.55 |
| 2:R:398:ARG:HG3 | 2:R:399:HIS:N | 2.22 | 0.55 |
| 9:I:27:LEU:HD23 | 9:I:78:ILE:CD1 | 2.37 | 0.55 |
| 2:B:536:GLY:HA3 | 2:B:560:HIS:CE1 | 2.42 | 0.55 |
| 1:A:426:HIS:CE1 | 3:C:80:GLU:CD | 2.79 | 0.54 |
| 1:A:238:LYS:HE2 | 1:A:297:THR:HG22 | 1.89 | 0.54 |
| 1:W:854:GLY:O | 3:Y:64:ILE:CG2 | 2.54 | 0.54 |
| 7:V:72:CYS:HB3 | 7:V:114:LYS:HG2 | 1.89 | 0.54 |
| 1:W:763:THR:HB | 1:W:764:ARG:CD | 2.37 | 0.54 |
| 2:B:249:PRO:HB2 | 2:B:253:ASN:H | 1.72 | 0.54 |
| 1:A:655:ASP:H | 1:A:658:LYS:HD2 | 1.72 | 0.54 |
| 3:Y:277:ILE:C | 3:Y:279:GLU:H | 2.09 | 0.54 |
| 4:D:22:LEU:HB2 | 4:D:226:TYR:CZ | 2.41 | 0.54 |
| 1:W:534:LEU:HB2 | 1:W:546:TYR:CE2 | 2.41 | 0.54 |
| 1:W:372:TRP:CD1 | 1:W:372:TRP:C | 2.79 | 0.54 |
| 1:A:782:ILE:HG21 | 1:A:790:LEU:CD2 | 2.37 | 0.54 |
| 1:W:650:ASP:HB3 | 1:W:723:ASN:ND2 | 2.22 | 0.54 |
| 2:R:460:GLU:HG2 | 2:R:673:SER:HB3 | 1.88 | 0.54 |
| 2:B:603:GLY:C | 2:B:605:ILE:H | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:117:VAL:HG11 | 2:R:388:VAL:HG21 | 1.88 | 0.54 |
| 13:X:6:CYS:HB2 | 13:X:37:VAL:HG12 | 1.88 | 0.54 |
| 13:P:5:ARG:HG2 | 13:P:18:LEU:HD22 | 1.89 | 0.54 |
| 3:C:340:SER:HB3 | 3:C:371:GLU:CG | 2.37 | 0.54 |
| 2:R:1098:TYR:CE1 | 2:R:1101:LYS:HD3 | 2.43 | 0.54 |
| 2:R:948:PHE:CE1 | 1:W:792:PRO:HG3 | 2.42 | 0.54 |
| 2:R:731:SER:HA | 2:R:914:ASN:ND2 | 2.22 | 0.54 |
| 5:T:83:GLU:HA | 6:U:89:MET:HE3 | 1.88 | 0.54 |
| 2:B:1057:ASP:OD2 | 2:B:1097:SER:HB2 | 2.07 | 0.54 |
| 10:J:65:LYS:O | 10:J:68:PHE:HB3 | 2.07 | 0.54 |
| 2:R:70:LYS:HB3 | 2:R:71:PRO:HD2 | 1.89 | 0.54 |
| 1:W:86:PHE:O | 1:W:90:VAL:HG23 | 2.07 | 0.54 |
| 2:R:73:VAL:HG22 | 2:R:74:ARG:O | 2.07 | 0.54 |
| 5:E:30:LEU:CD1 | 5:E:72:PHE:CE2 | 2.91 | 0.54 |
| 1:A:106:ILE:N | 1:A:106:ILE:HD12 | 2.22 | 0.54 |
| 2:B:809:GLY:O | 2:B:842:THR:HB | 2.07 | 0.54 |
| 12:O:46:ARG:HD2 | 2:R:937:ALA:O | 2.06 | 0.54 |
| 2:B:418:ASP:OD1 | 2:B:424:SER:OG | 2.22 | 0.54 |
| 4:D:38:VAL:HG12 | 4:D:39:MET:N | 2.23 | 0.54 |
| 1:A:253:ILE:HG22 | 1:A:254:ASP:OD1 | 2.08 | 0.54 |
| 1:W:511:VAL:HA | 1:W:583:ASP:OD2 | 2.07 | 0.54 |
| 2:B:705:LEU:O | 2:B:706:VAL:HB | 2.07 | 0.54 |
| 2:R:1106:GLU:OE2 | 1:W:301:ARG:HD3 | 2.07 | 0.54 |
| 6:U:12:ILE:HG23 | 6:U:16:VAL:HG13 | 1.89 | 0.54 |
| 1:A:47:PRO:O | 1:A:48:ARG:CB | 2.55 | 0.54 |
| 9:I:61:VAL:H | 9:I:64:ILE:HD12 | 1.71 | 0.54 |
| 1:W:854:GLY:O | 3:Y:64:ILE:CG1 | 2.55 | 0.54 |
| 1:W:238:LYS:HE2 | 1:W:297:THR:HG22 | 1.88 | 0.54 |
| 2:B:251:ILE:HD12 | 2:B:330:LEU:HD11 | 1.89 | 0.54 |
| 1:A:125:TRP:O | 1:A:128:ALA:HB3 | 2.08 | 0.54 |
| 3:Y:338:LYS:HD3 | 3:Y:338:LYS:H | 1.72 | 0.54 |
| 2:R:166:THR:HG23 | 2:R:432:VAL:HG12 | 1.89 | 0.54 |
| 2:R:970:THR:HG22 | 2:R:987:TYR:HA | 1.89 | 0.54 |
| 5:T:19:GLY:H | 3:Y:393:ILE:HG22 | 1.73 | 0.54 |
| 1:A:98:CYS:SG | 1:A:145:VAL:O | 2.65 | 0.54 |
| 2:B:359:VAL:HG11 | 2:B:407:VAL:HG13 | 1.90 | 0.54 |
| 1:A:113:LYS:HG2 | 1:A:116:ARG:CZ | 2.38 | 0.54 |
| 12:O:9:THR:HB | 12:O:44:CYS:HB2 | 1.90 | 0.54 |
| 7:V:70:ASP:O | 1:W:541:ALA:HB1 | 2.08 | 0.54 |
| 3:C:133:ASP:OD2 | 3:C:136:LYS:HG2 | 2.06 | 0.54 |
| 1:A:450:CYS:HB2 | 1:A:451:PRO:HD3 | 1.87 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:767:LYS:HG3 | 2:B:768:TYR:HD1 | 1.72 | 0.54 |
| 1:A:104:VAL:O | 1:A:104:VAL:HG13 | 2.02 | 0.54 |
| 2:B:603:GLY:C | 2:B:605:ILE:N | 2.60 | 0.54 |
| 1:A:110:GLU:HA | 1:A:113:LYS:HB2 | 1.90 | 0.54 |
| 1:A:736:SER:O | 1:A:737:VAL:C | 2.46 | 0.54 |
| 1:W:324:THR:O | 1:W:461:GLU:HA | 2.08 | 0.54 |
| 2:B:1098:TYR:CE1 | 2:B:1101:LYS:HD3 | 2.43 | 0.54 |
| 7:V:8:GLU:C | 7:V:9:ILE:HG13 | 2.27 | 0.54 |
| 2:R:957:GLN:HA | 2:R:960:ILE:CD1 | 2.37 | 0.54 |
| 12:O:53:ILE:HD12 | 2:R:720:PRO:HG3 | 1.89 | 0.54 |
| 1:W:782:ILE:HG21 | 1:W:790:LEU:HD22 | 1.89 | 0.54 |
| 3:Y:12:TYR:HB2 | 3:Y:45:ARG:HH12 | 1.71 | 0.54 |
| 12:O:55:ILE:HD12 | 2:R:682:LEU:HD22 | 1.89 | 0.54 |
| 3:C:25:PRO:HD3 | 3:C:33:LYS:HD3 | 1.90 | 0.54 |
| 2:B:856:THR:HG21 | 13:P:33:ILE:HD12 | 1.89 | 0.54 |
| 4:D:53:LEU:HD12 | 4:D:131:VAL:CG2 | 2.37 | 0.54 |
| 1:W:838:VAL:HG13 | 3:Y:70:ILE:HD11 | 1.89 | 0.54 |
| 3:C:286:ILE:HD12 | 3:C:324:GLY:O | 2.08 | 0.54 |
| 4:D:93:TYR:HE1 | 4:D:146:ARG:HG2 | 1.72 | 0.54 |
| 1:A:425:LEU:HD12 | 1:A:425:LEU:H | 1.72 | 0.54 |
| 2:B:420:THR:HG21 | 2:B:677:LYS:O | 2.08 | 0.54 |
| 3:Y:69:ALA:HB2 | 3:Y:381:LEU:HD13 | 1.90 | 0.54 |
| 2:R:1050:ASP:HA | 2:R:1054:ASP:HB2 | 1.90 | 0.54 |
| 4:S:49:ASN:OD1 | 4:S:139:ILE:CD1 | 2.55 | 0.54 |
| 8:Z:43:PRO:O | 8:Z:44:TRP:HB2 | 2.07 | 0.54 |
| 2:R:628:TYR:CE2 | 2:R:640:HIS:CE1 | 2.96 | 0.54 |
| 1:W:823:LEU:HB3 | 3:Y:329:ILE:HG12 | 1.90 | 0.54 |
| 3:Y:29:VAL:HG12 | 3:Y:61:GLU:HG3 | 1.89 | 0.54 |
| 1:A:58:CYS:HB3 | 1:A:62:GLY:N | 2.23 | 0.54 |
| 1:A:110:GLU:HA | 1:A:113:LYS:HD2 | 1.90 | 0.54 |
| 10:Q:65:LYS:O | 10:Q:68:PHE:HB3 | 2.07 | 0.54 |
| 4:D:155:LYS:HE3 | 4:D:156:PHE:CE2 | 2.43 | 0.54 |
| 2:B:699:HIS:ND1 | 4:D:57:ILE:HG12 | 2.22 | 0.54 |
| 1:A:428:ILE:CG2 | 1:A:452:PRO:HB3 | 2.38 | 0.54 |
| 11:M:12:TYR:HD1 | 11:M:58:LEU:HD13 | 1.71 | 0.54 |
| 2:R:420:THR:HG21 | 2:R:677:LYS:O | 2.08 | 0.54 |
| 1:A:346:THR:O | 2:B:1008:ALA:HB2 | 2.07 | 0.54 |
| 6:F:12:ILE:HG23 | 6:F:16:VAL:HG13 | 1.90 | 0.54 |
| 3:Y:301:LEU:HD22 | 3:Y:308:VAL:CG1 | 2.37 | 0.54 |
| 1:A:223:ILE:HG12 | 1:A:224:MET:N | 2.21 | 0.54 |
| 3:C:108:ILE:O | 3:C:112:ASP:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:Y:237:ILE:HD12 | 3:Y:253:THR:HB | 1.89 | 0.54 |
| 1:A:329:ASP:O | 1:A:446:ASN:HA | 2.08 | 0.54 |
| 8:Z:20:HIS:CE1 | 8:Z:51:VAL:HG11 | 2.43 | 0.54 |
| 2:R:136:TYR:HB2 | 2:R:141:LEU:HD11 | 1.88 | 0.53 |
| 1:A:324:THR:O | 1:A:461:GLU:HA | 2.08 | 0.53 |
| 2:R:660:TYR:CD1 | 2:R:950:LYS:HE3 | 2.42 | 0.53 |
| 2:R:629:VAL:HG22 | 2:R:642:HIS:HB2 | 1.90 | 0.53 |
| 2:R:699:HIS:CE1 | 4:S:57:ILE:HG12 | 2.43 | 0.53 |
| 3:Y:309:ASP:OD2 | 3:Y:311:ARG:HB2 | 2.07 | 0.53 |
| 5:T:75:ILE:HG21 | 6:U:21:LEU:HD11 | 1.89 | 0.53 |
| 2:B:762:SER:OG | 2:B:866:LYS:HG2 | 2.08 | 0.53 |
| 1:A:299:ALA:O | 1:A:303:LYS:HB2 | 2.08 | 0.53 |
| 1:W:498:ALA:HB1 | 1:W:502:TYR:HB2 | 1.89 | 0.53 |
| 2:R:59:LEU:O | 2:R:59:LEU:HD13 | 2.08 | 0.53 |
| 1:A:601:LYS:O | 1:A:610:SER:HB2 | 2.08 | 0.53 |
| 5:T:30:LEU:CD2 | 5:T:72:PHE:CE2 | 2.91 | 0.53 |
| 2:B:857:GLU:HG3 | 13:P:24:VAL:HG11 | 1.90 | 0.53 |
| 4:D:260:LEU:HD11 | 11:L:69:LEU:HD21 | 1.89 | 0.53 |
| 1:W:428:ILE:CG2 | 1:W:452:PRO:HB3 | 2.38 | 0.53 |
| 13:P:5:ARG:O | 13:P:6:CYS:HB2 | 2.08 | 0.53 |
| 9:I:52:ASP:O | 9:I:53:ILE:CB | 2.56 | 0.53 |
| 2:B:186:ILE:CD1 | 2:B:209:LYS:HD3 | 2.38 | 0.53 |
| 2:B:249:PRO:HD2 | 2:B:253:ASN:OD1 | 2.08 | 0.53 |
| 11:L:77:ARG:NH1 | 11:L:77:ARG:HB2 | 2.23 | 0.53 |
| 3:Y:110:ILE:HD13 | 3:Y:297:ILE:HG12 | 1.89 | 0.53 |
| 5:T:132:SER:O | 5:T:133:LYS:HB2 | 2.08 | 0.53 |
| 1:W:541:ALA:HB3 | 1:W:542:PRO:HD3 | 1.90 | 0.53 |
| 2:B:230:MET:HE2 | 2:B:315:ALA:HB1 | 1.89 | 0.53 |
| 4:D:24:PHE:HA | 11:L:27:LEU:HD13 | 1.89 | 0.53 |
| 4:D:66:PRO:HB2 | 4:D:124:ILE:HG12 | 1.91 | 0.53 |
| 2:R:557:ASN:OD1 | 2:R:577:ARG:NH1 | 2.41 | 0.53 |
| 2:B:398:ARG:HG3 | 2:B:399:HIS:N | 2.23 | 0.53 |
| 2:R:768:TYR:HB3 | 2:R:769:PRO:HD2 | 1.83 | 0.53 |
| 5:T:115:ASP:O | 5:T:116:ASP:HB2 | 2.06 | 0.53 |
| 1:W:68:CYS:N | 1:W:69:PRO:HD3 | 2.23 | 0.53 |
| 2:R:1015:LEU:C | 2:R:1015:LEU:HD13 | 2.27 | 0.53 |
| 2:B:486:LYS:HG2 | 2:B:489:GLU:OE2 | 2.09 | 0.53 |
| 2:R:797:ASP:CG | 13:X:4:TYR:HB3 | 2.28 | 0.53 |
| 3:Y:328:GLN:HB3 | 3:Y:332:HIS:HB3 | 1.89 | 0.53 |
| 1:W:299:ALA:O | 1:W:303:LYS:HB2 | 2.08 | 0.53 |
| 1:A:313:LEU:HD21 | 2:B:1099:ALA:C | 2.29 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:701:PRO:HB2 | 2:B:720:PRO:HG2 | 1.88 | 0.53 |
| 1:W:145:VAL:O | 1:W:146:CYS:SG | 2.66 | 0.53 |
| 1:A:124:ARG:HD3 | 1:A:125:TRP:CZ3 | 2.42 | 0.53 |
| 2:R:808:LYS:HE3 | 2:R:847:MET:CE | 2.38 | 0.53 |
| 2:R:416:LEU:O | 2:R:418:ASP:N | 2.42 | 0.53 |
| 2:B:99:LEU:O | 2:B:119:ILE:HB | 2.09 | 0.53 |
| 5:T:133:LYS:O | 5:T:134:LYS:HG3 | 2.08 | 0.53 |
| 7:V:71:PHE:HA | 1:W:541:ALA:HB3 | 1.89 | 0.53 |
| 1:W:280:GLU:H | 1:W:282:PRO:HD2 | 1.73 | 0.53 |
| 5:T:84:VAL:HG21 | 6:U:75:ILE:HD13 | 1.90 | 0.53 |
| 3:Y:109:GLU:OE2 | 3:Y:117:PRO:HA | 2.08 | 0.53 |
| 2:B:63:LEU:HD22 | 2:B:101:LEU:HD11 | 1.91 | 0.53 |
| 1:A:792:PRO:CA | 2:B:948:PHE:CE1 | 2.92 | 0.53 |
| 1:A:68:CYS:N | 1:A:69:PRO:HD3 | 2.23 | 0.53 |
| 2:R:157:VAL:HG11 | 2:R:401:LEU:HD23 | 1.89 | 0.53 |
| 4:S:154:ALA:HA | 4:S:157:ILE:HG13 | 1.88 | 0.53 |
| 3:C:301:LEU:HD22 | 3:C:308:VAL:CG1 | 2.38 | 0.53 |
| 2:B:975:ASP:OD1 | 2:B:977:ARG:HD3 | 2.09 | 0.53 |
| 1:W:782:ILE:HG21 | 1:W:790:LEU:CD2 | 2.38 | 0.53 |
| 4:D:66:PRO:HG2 | 12:N:13:LEU:HD11 | 1.90 | 0.53 |
| 2:R:461:THR:HG21 | 2:R:468:GLY:N | 2.24 | 0.53 |
| 2:B:163:VAL:HG21 | 2:B:429:LEU:HD23 | 1.90 | 0.53 |
| 3:Y:133:ASP:OD2 | 3:Y:136:LYS:HG2 | 2.09 | 0.53 |
| 2:R:857:GLU:HA | 2:R:862:ASN:O | 2.07 | 0.53 |
| 1:W:95:LYS:CB | 1:W:138:LYS:HE2 | 2.39 | 0.53 |
| 2:R:741:ILE:HG23 | 2:R:891:ILE:HA | 1.91 | 0.53 |
| 2:B:416:LEU:O | 2:B:418:ASP:N | 2.41 | 0.53 |
| 6:U:12:ILE:HG23 | 6:U:16:VAL:CG1 | 2.39 | 0.53 |
| 4:D:37:PRO:HG3 | 4:D:78:TRP:CE3 | 2.43 | 0.53 |
| 2:R:55:GLU:OE2 | 2:R:377:VAL:HG12 | 2.09 | 0.53 |
| 3:C:12:TYR:HB2 | 3:C:45:ARG:HH12 | 1.72 | 0.53 |
| 2:B:453:TRP:CZ3 | 2:B:644:GLU:OE2 | 2.60 | 0.53 |
| 2:R:767:LYS:CD | 2:R:768:TYR:HA | 2.38 | 0.53 |
| 2:R:857:GLU:HG3 | 13:X:24:VAL:HG11 | 1.90 | 0.53 |
| 2:R:604:SER:O | 2:R:605:ILE:O | 2.27 | 0.53 |
| 2:R:258:SER:O | 2:R:259:LEU:HD22 | 2.09 | 0.53 |
| 1:W:238:LYS:O | 1:W:238:LYS:HG3 | 2.07 | 0.53 |
| 1:W:249:LEU:CD2 | 1:W:265:LEU:HB2 | 2.39 | 0.53 |
| 2:B:784:ARG:HB3 | 2:B:835:LYS:O | 2.09 | 0.53 |
| 2:R:372:LEU:HD21 | 2:R:376:LYS:HE2 | 1.91 | 0.53 |
| 1:A:448:LEU:O | 1:A:496:ILE:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:334:ILE:CD1 | 1:A:628:MET:HB3 | 2.39 | 0.53 |
| 1:A:822:ARG:HH22 | 3:C:108:ILE:HG23 | 1.74 | 0.53 |
| 1:A:450:CYS:N | 1:A:451:PRO:CD | 2.72 | 0.53 |
| 2:R:802:SER:OG | 13:X:39:LYS:HB2 | 2.09 | 0.53 |
| 2:B:1082:CYS:HB3 | 2:B:1091:LEU:HD21 | 1.91 | 0.53 |
| 3:Y:149:ILE:HA | 3:Y:152:VAL:HG12 | 1.91 | 0.53 |
| 2:R:133:ILE:HD13 | 2:R:136:TYR:CE1 | 2.43 | 0.53 |
| 2:R:525:LEU:HD22 | 2:R:571:VAL:HB | 1.91 | 0.53 |
| 1:W:110:GLU:HA | 1:W:113:LYS:HB2 | 1.90 | 0.53 |
| 1:W:113:LYS:HG2 | 1:W:116:ARG:CZ | 2.38 | 0.53 |
| 1:W:668:ALA:HB1 | 1:W:707:LEU:HD13 | 1.88 | 0.53 |
| 2:R:235:ILE:HD11 | 2:R:316:TYR:CE1 | 2.44 | 0.53 |
| 2:B:17:ILE:CD1 | 2:B:476:MET:SD | 2.97 | 0.53 |
| 2:B:20:TYR:HD2 | 2:B:607:PHE:CE2 | 2.27 | 0.53 |
| 2:B:59:LEU:O | 2:B:59:LEU:HD13 | 2.09 | 0.53 |
| 2:B:229:LEU:CD2 | 2:B:275:ILE:HD11 | 2.39 | 0.53 |
| 3:Y:237:ILE:HD11 | 3:Y:240:ALA:HB2 | 1.91 | 0.53 |
| 3:C:338:LYS:H | 3:C:338:LYS:HD3 | 1.72 | 0.53 |
| 3:C:126:LEU:HB2 | 3:C:131:LYS:HG3 | 1.90 | 0.53 |
| 7:G:72:CYS:SG | 7:G:114:LYS:HB3 | 2.49 | 0.53 |
| 5:T:114:THR:HB | 5:T:115:ASP:C | 2.29 | 0.53 |
| 2:R:598:GLU:HG3 | 2:R:605:ILE:HD11 | 1.91 | 0.53 |
| 1:A:821:ARG:HH12 | 3:C:347:PHE:HA | 1.73 | 0.53 |
| 1:W:47:PRO:O | 1:W:48:ARG:CB | 2.56 | 0.53 |
| 1:A:419:PHE:CE1 | 1:A:464:LEU:HD23 | 2.44 | 0.53 |
| 2:B:1074:ASP:HB3 | 2:B:1075:LYS:CB | 2.37 | 0.53 |
| 4:S:159:VAL:HG22 | 4:S:161:LEU:H | 1.74 | 0.53 |
| 4:D:111:SER:HA | 4:D:130:ILE:HD11 | 1.91 | 0.53 |
| 2:R:8:LEU:HA | 2:R:633:PRO:HG3 | 1.90 | 0.53 |
| 5:T:63:ASP:OD2 | 5:T:65:ALA:HB3 | 2.08 | 0.53 |
| 2:R:745:ARG:HD2 | 2:R:896:PRO:HG3 | 1.91 | 0.53 |
| 2:B:759:ARG:HG3 | 2:B:760:LEU:H | 1.73 | 0.53 |
| 1:W:363:GLN:O | 1:W:366:ILE:HG22 | 2.08 | 0.53 |
| 2:R:928:MET:HE3 | 2:R:953:ILE:HG21 | 1.90 | 0.52 |
| 2:B:934:LYS:O | 2:B:938:LEU:HG | 2.08 | 0.52 |
| 7:G:103:VAL:HG13 | 7:G:104:LYS:CD | 2.39 | 0.52 |
| 1:W:125:TRP:N | 1:W:126:PRO:CD | 2.71 | 0.52 |
| 2:B:233:LEU:HD13 | 2:B:315:ALA:HB2 | 1.91 | 0.52 |
| 4:D:8:LYS:HG2 | 4:D:9:ASP:N | 2.23 | 0.52 |
| 5:E:84:VAL:CG2 | 6:F:75:ILE:HD13 | 2.39 | 0.52 |
| 1:A:426:HIS:CD2 | 3:C:80:GLU:OE1 | 2.62 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:647:SER:N | 2:R:648:PRO:CD | 2.72 | 0.52 |
| 1:W:238:LYS:HE3 | 1:W:276:TYR:HA | 1.91 | 0.52 |
| 3:C:349:VAL:O | 3:C:349:VAL:HG13 | 2.10 | 0.52 |
| 2:B:525:LEU:O | 2:B:528:ARG:HB3 | 2.10 | 0.52 |
| 3:Y:176:ASP:O | 3:Y:177:LYS:HG3 | 2.10 | 0.52 |
| 2:B:372:LEU:HD21 | 2:B:376:LYS:HE2 | 1.91 | 0.52 |
| 2:B:235:ILE:HD11 | 2:B:316:TYR:CE1 | 2.45 | 0.52 |
| 2:B:345:ARG:NH2 | 2:B:577:ARG:HG2 | 2.24 | 0.52 |
| 1:W:534:LEU:HD22 | 1:W:534:LEU:N | 2.24 | 0.52 |
| 1:W:736:SER:O | 1:W:737:VAL:C | 2.48 | 0.52 |
| 11:M:80:ALA:O | 11:M:84:ILE:HG12 | 2.08 | 0.52 |
| 1:A:288:LYS:HA | 1:A:295:LEU:CD2 | 2.39 | 0.52 |
| 1:W:749:GLN:HA | 1:W:781:PHE:HA | 1.92 | 0.52 |
| 4:S:182:VAL:HG11 | 4:S:212:TYR:HD2 | 1.73 | 0.52 |
| 2:R:928:MET:HE1 | 2:R:953:ILE:HD12 | 1.91 | 0.52 |
| 1:A:441:LEU:HD22 | 2:B:1004:ILE:HD12 | 1.91 | 0.52 |
| 2:R:797:ASP:OD1 | 13:X:4:TYR:HB3 | 2.09 | 0.52 |
| 2:R:933:GLY:HA3 | 2:R:990:VAL:HB | 1.90 | 0.52 |
| 2:B:970:THR:HG22 | 2:B:987:TYR:HA | 1.90 | 0.52 |
| 2:R:406:TRP:O | 2:R:408:GLY:N | 2.43 | 0.52 |
| 2:B:602:SER:HA | 2:B:605:ILE:HD12 | 1.92 | 0.52 |
| 1:W:451:PRO:N | 1:W:452:PRO:CD | 2.73 | 0.52 |
| 2:B:133:ILE:HD13 | 2:B:136:TYR:CE1 | 2.44 | 0.52 |
| 1:W:271:TYR:HE2 | 1:W:285:PRO:HB3 | 1.74 | 0.52 |
| 2:R:86:MET:HE3 | 2:R:686:ASN:ND2 | 2.24 | 0.52 |
| 2:R:874:ILE:HG22 | 2:R:875:PRO:HD2 | 1.91 | 0.52 |
| 1:A:125:TRP:N | 1:A:126:PRO:CD | 2.72 | 0.52 |
| 3:C:162:SER:HA | 3:C:210:PHE:HZ | 1.75 | 0.52 |
| 2:R:107:GLU:O | 2:R:108:ASN:HB2 | 2.09 | 0.52 |
| 1:A:782:ILE:HG21 | 1:A:790:LEU:HD22 | 1.92 | 0.52 |
| 2:B:493:TYR:HD1 | 2:B:497:VAL:O | 1.92 | 0.52 |
| 2:R:705:LEU:O | 2:R:706:VAL:HB | 2.09 | 0.52 |
| 2:R:229:LEU:HD23 | 2:R:275:ILE:HD11 | 1.90 | 0.52 |
| 11:M:13:LEU:HB2 | 11:M:65:PRO:HB2 | 1.92 | 0.52 |
| 2:B:767:LYS:HD3 | 2:B:768:TYR:CA | 2.40 | 0.52 |
| 2:B:647:SER:N | 2:B:648:PRO:CD | 2.73 | 0.52 |
| 5:T:114:THR:HG21 | 5:T:117:THR:OG1 | 2.10 | 0.52 |
| 1:A:763:THR:HB | 1:A:764:ARG:CD | 2.40 | 0.52 |
| 2:R:417:LEU:CD2 | 2:R:425:MET:HG3 | 2.38 | 0.52 |
| 2:B:583:ILE:HD13 | 2:B:616:ILE:HG12 | 1.92 | 0.52 |
| 2:R:1046:MET:HG2 | 5:T:61:PHE:CD1 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:1080:TYR:HB3 | 2:R:1091:LEU:HD12 | 1.92 | 0.52 |
| 2:R:1007:ARG:HD3 | 2:R:1028:GLY:HA2 | 1.91 | 0.52 |
| 2:B:430:ARG:HD3 | 2:B:653:ILE:HG12 | 1.92 | 0.52 |
| 1:A:86:PHE:O | 1:A:90:VAL:HG23 | 2.09 | 0.52 |
| 2:B:108:ASN:O | 2:B:110:ILE:HG12 | 2.09 | 0.52 |
| 2:R:397:ILE:O | 2:R:397:ILE:HG12 | 2.10 | 0.52 |
| 9:I:62:ILE:HD12 | 1:W:474:ALA:CB | 2.39 | 0.52 |
| 1:W:141:MET:HG3 | 1:W:141:MET:O | 2.07 | 0.52 |
| 1:W:289:HIS:O | 1:W:290:ARG:HB2 | 2.09 | 0.52 |
| 2:B:752:MET:HB2 | 12:N:8:PHE:CD2 | 2.44 | 0.52 |
| 3:C:210:PHE:O | 3:C:211:ALA:CB | 2.57 | 0.52 |
| 2:R:630:ALA:HB3 | 2:R:636:LEU:HD12 | 1.91 | 0.52 |
| 1:A:534:LEU:HB3 | 1:A:546:TYR:CE1 | 2.43 | 0.52 |
| 1:A:818:TYR:CD2 | 1:A:822:ARG:NH1 | 2.78 | 0.52 |
| 3:C:11:SER:N | 3:C:45:ARG:NH2 | 2.58 | 0.52 |
| 1:W:288:LYS:HA | 1:W:295:LEU:CD2 | 2.39 | 0.52 |
| 1:A:541:ALA:HB3 | 1:A:542:PRO:HD3 | 1.92 | 0.52 |
| 11:M:16:GLU:OE2 | 11:M:52:LYS:HE2 | 2.10 | 0.52 |
| 1:A:511:VAL:HA | 1:A:583:ASP:OD2 | 2.08 | 0.52 |
| 1:A:417:VAL:HG11 | 1:A:464:LEU:HD11 | 1.91 | 0.52 |
| 5:E:114:THR:HG21 | 5:E:117:THR:OG1 | 2.09 | 0.52 |
| 13:P:10:TRP:CB | 13:P:31:TYR:CE2 | 2.93 | 0.52 |
| 2:R:215:VAL:HG12 | 2:R:224:ILE:O | 2.09 | 0.52 |
| 7:G:103:VAL:HG22 | 7:G:104:LYS:N | 2.23 | 0.52 |
| 7:V:103:VAL:HG22 | 7:V:104:LYS:N | 2.24 | 0.52 |
| 2:B:973:THR:HG21 | 2:B:988:PHE:CE1 | 2.45 | 0.52 |
| 3:Y:70:ILE:HD13 | 3:Y:70:ILE:N | 2.23 | 0.52 |
| 1:W:81:VAL:HG21 | 1:W:269:LEU:HB3 | 1.92 | 0.52 |
| 6:F:64:SER:HB2 | 6:F:69:ARG:HD3 | 1.91 | 0.52 |
| 2:B:272:LEU:HD22 | 2:B:292:ALA:O | 2.09 | 0.52 |
| 2:B:605:ILE:HG23 | 2:B:606:THR:N | 2.25 | 0.52 |
| 2:B:356:LEU:CD1 | 2:B:407:VAL:HG21 | 2.40 | 0.52 |
| 1:A:859:TYR:OH | 9:K:29:ARG:HD2 | 2.10 | 0.52 |
| 12:N:9:THR:HB | 12:N:44:CYS:HB2 | 1.90 | 0.52 |
| 2:B:558:VAL:HG22 | 2:B:571:VAL:HG22 | 1.92 | 0.52 |
| 2:B:249:PRO:HD2 | 2:B:253:ASN:CG | 2.30 | 0.52 |
| 2:R:1074:ASP:CB | 2:R:1075:LYS:HA | 2.40 | 0.52 |
| 1:W:635:PHE:O | 1:W:639:VAL:HG23 | 2.10 | 0.52 |
| 6:F:12:ILE:HG23 | 6:F:16:VAL:CG1 | 2.39 | 0.52 |
| 10:J:66:ARG:HG2 | 10:J:66:ARG:HH11 | 1.75 | 0.52 |
| 2:R:108:ASN:O | 2:R:110:ILE:HG12 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:W:736:SER:O | 1:W:738:LEU:N | 2.43 | 0.52 |
| 2:B:107:GLU:O | 2:B:108:ASN:CB | 2.57 | 0.52 |
| 4:D:182:VAL:HG11 | 4:D:212:TYR:HD2 | 1.73 | 0.52 |
| 2:R:233:LEU:HD13 | 2:R:315:ALA:HB2 | 1.92 | 0.52 |
| 2:B:333:ARG:O | 2:B:334:GLU:HB3 | 2.10 | 0.52 |
| 5:E:63:ASP:OD2 | 5:E:65:ALA:HB3 | 2.10 | 0.52 |
| 4:D:247:LYS:O | 4:D:251:ARG:HG3 | 2.09 | 0.52 |
| 2:B:461:THR:HG21 | 2:B:468:GLY:N | 2.25 | 0.52 |
| 9:I:43:LEU:HD13 | 9:I:64:ILE:HG22 | 1.90 | 0.52 |
| 3:Y:25:PRO:CG | 3:Y:33:LYS:HD3 | 2.40 | 0.52 |
| 1:A:324:THR:HG22 | 1:A:325:VAL:H | 1.74 | 0.52 |
| 2:B:330:LEU:HD22 | 2:B:332:ARG:HD3 | 1.92 | 0.52 |
| 1:W:864:LYS:HG3 | 1:W:864:LYS:O | 2.10 | 0.52 |
| 2:R:17:ILE:HD12 | 2:R:476:MET:SD | 2.50 | 0.52 |
| 1:W:223:ILE:CG1 | 1:W:224:MET:N | 2.73 | 0.52 |
| 2:R:975:ASP:HB3 | 2:R:978:THR:HG22 | 1.92 | 0.52 |
| 2:B:630:ALA:HB3 | 2:B:636:LEU:HD12 | 1.92 | 0.52 |
| 2:R:229:LEU:CD2 | 2:R:275:ILE:HD11 | 2.40 | 0.52 |
| 2:B:461:THR:CG2 | 2:B:468:GLY:N | 2.72 | 0.52 |
| 1:W:192:VAL:CG2 | 1:W:199:PRO:HB3 | 2.40 | 0.52 |
| 3:C:46:ASP:O | 3:C:47:GLU:OE1 | 2.28 | 0.52 |
| 2:R:767:LYS:HB3 | 2:R:768:TYR:CB | 2.39 | 0.52 |
| 2:B:31:LEU:HD23 | 2:B:125:MET:CE | 2.37 | 0.52 |
| 5:T:30:LEU:HD22 | 5:T:72:PHE:CZ | 2.45 | 0.52 |
| 9:K:61:VAL:H | 9:K:64:ILE:HD12 | 1.74 | 0.52 |
| 1:A:853:ASP:HB2 | 3:C:311:ARG:NH1 | 2.25 | 0.52 |
| 1:A:107:SER:O | 1:A:108:GLU:C | 2.46 | 0.52 |
| 8:H:45:ILE:HG23 | 8:H:81:VAL:HG22 | 1.92 | 0.52 |
| 1:A:69:PRO:HB2 | 2:B:1101:LYS:HE3 | 1.92 | 0.52 |
| 2:B:250:GLU:HG2 | 2:B:251:ILE:N | 2.25 | 0.52 |
| 2:R:630:ALA:CB | 2:R:636:LEU:HD12 | 2.40 | 0.52 |
| 2:B:1062:TYR:CE2 | 2:B:1093:PRO:HG3 | 2.45 | 0.52 |
| 2:R:1066:GLN:HG3 | 2:R:1089:SER:HB3 | 1.92 | 0.52 |
| 2:R:453:TRP:CZ3 | 2:R:644:GLU:OE2 | 2.63 | 0.52 |
| 6:F:41:LEU:HA | 6:F:44:VAL:HG12 | 1.90 | 0.52 |
| 2:R:1029:LEU:HD12 | 1:W:321:SER:HB2 | 1.92 | 0.52 |
| 1:A:104:VAL:HG12 | 1:A:137:LYS:CA | 2.37 | 0.51 |
| 2:B:594:ARG:CZ | 2:B:615:LYS:HG3 | 2.40 | 0.51 |
| 2:B:258:SER:O | 2:B:259:LEU:HD22 | 2.10 | 0.51 |
| 2:B:949:TYR:O | 2:B:950:LYS:HD2 | 2.10 | 0.51 |
| 1:A:309:PHE:O | 1:A:310:ARG:CB | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:51:ILE:O | 9:I:52:ASP:HB2 | 2.10 | 0.51 |
| 1:W:249:LEU:HD21 | 1:W:265:LEU:HB2 | 1.91 | 0.51 |
| 1:A:220:ARG:HG2 | 1:A:235:LEU:HD13 | 1.92 | 0.51 |
| 2:R:398:ARG:C | 2:R:400:ALA:H | 2.14 | 0.51 |
| 1:W:10:LYS:HG2 | 3:Y:363:VAL:CG1 | 2.40 | 0.51 |
| 2:B:657:ILE:HG13 | 2:B:711:LEU:CD2 | 2.40 | 0.51 |
| 5:E:128:PHE:HB3 | 5:E:137:GLN:NE2 | 2.25 | 0.51 |
| 2:R:249:PRO:HD2 | 2:R:253:ASN:CG | 2.31 | 0.51 |
| 1:W:125:TRP:O | 1:W:128:ALA:HB3 | 2.10 | 0.51 |
| 5:E:123:VAL:O | 5:E:124:ARG:O | 2.29 | 0.51 |
| 2:R:699:HIS:ND1 | 4:S:57:ILE:HG12 | 2.24 | 0.51 |
| 2:B:957:GLN:HA | 2:B:960:ILE:HG12 | 1.91 | 0.51 |
| 12:O:13:LEU:HD11 | 4:S:66:PRO:HG2 | 1.92 | 0.51 |
| 3:Y:237:ILE:HD12 | 3:Y:253:THR:CG2 | 2.40 | 0.51 |
| 2:B:1062:TYR:HE2 | 2:B:1093:PRO:HG3 | 1.74 | 0.51 |
| 1:A:541:ALA:HB3 | 7:G:71:PHE:HA | 1.92 | 0.51 |
| 2:R:877:ILE:HD12 | 2:R:877:ILE:H | 1.75 | 0.51 |
| 2:B:773:GLU:HG2 | 2:B:774:ASP:N | 2.26 | 0.51 |
| 2:B:928:MET:CE | 2:B:953:ILE:HD12 | 2.40 | 0.51 |
| 7:G:36:PHE:CE1 | 7:G:96:ILE:HD11 | 2.46 | 0.51 |
| 2:R:1039:LEU:HD22 | 2:R:1044:THR:HG21 | 1.92 | 0.51 |
| 12:O:47:ARG:HD2 | 2:R:724:ASN:O | 2.10 | 0.51 |
| 2:B:543:ILE:CD1 | 2:B:558:VAL:HG21 | 2.39 | 0.51 |
| 2:B:872:LEU:HD23 | 2:B:873:ARG:N | 2.26 | 0.51 |
| 3:C:237:ILE:HD12 | 3:C:253:THR:CG2 | 2.39 | 0.51 |
| 2:B:653:ILE:H | 2:B:653:ILE:HD12 | 1.75 | 0.51 |
| 1:A:428:ILE:HG21 | 1:A:452:PRO:HB3 | 1.93 | 0.51 |
| 5:T:84:VAL:CG2 | 6:U:75:ILE:HD13 | 2.40 | 0.51 |
| 2:R:301:LEU:N | 2:R:302:PRO:HD3 | 2.25 | 0.51 |
| 1:A:366:ILE:HG13 | 1:A:395:LYS:HG3 | 1.92 | 0.51 |
| 3:Y:126:LEU:HB2 | 3:Y:131:LYS:HG3 | 1.91 | 0.51 |
| 2:R:766:VAL:CG1 | 2:R:774:ASP:OD2 | 2.52 | 0.51 |
| 2:R:733:THR:HG23 | 2:R:734:GLY:N | 2.25 | 0.51 |
| 5:T:82:GLN:HB3 | 6:U:88:ILE:HB | 1.92 | 0.51 |
| 6:U:88:ILE:H | 6:U:88:ILE:HD13 | 1.75 | 0.51 |
| 5:T:132:SER:O | 5:T:133:LYS:HG3 | 2.11 | 0.51 |
| 1:A:534:LEU:N | 1:A:534:LEU:HD22 | 2.26 | 0.51 |
| 4:D:104:ASN:O | 4:D:105:GLU:C | 2.49 | 0.51 |
| 1:A:356:TRP:CE3 | 9:K:54:ASN:ND2 | 2.78 | 0.51 |
| 4:S:180:ALA:HA | 4:S:188:PHE:HB2 | 1.91 | 0.51 |
| 11:L:16:GLU:OE2 | 11:L:52:LYS:HE2 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:T:56:GLU:HG2 | 3:Y:391:ARG:HG2 | 1.93 | 0.51 |
| 2:R:762:SER:OG | 2:R:866:LYS:HG2 | 2.10 | 0.51 |
| 1:A:588:ILE:HG13 | 1:A:593:LEU:HA | 1.92 | 0.51 |
| 13:X:5:ARG:HG2 | 13:X:18:LEU:HD22 | 1.93 | 0.51 |
| 9:I:29:ARG:HD2 | 1:W:859:TYR:OH | 2.09 | 0.51 |
| 1:A:12:GLY:HA3 | 1:A:201:THR:CG2 | 2.40 | 0.51 |
| 2:R:1069:TYR:HA | 2:R:1070:ILE:CB | 2.38 | 0.51 |
| 8:Z:59:PRO:HA | 8:Z:81:VAL:CG1 | 2.41 | 0.51 |
| 1:W:123:LYS:HA | 1:W:126:PRO:HG3 | 1.92 | 0.51 |
| 4:D:56:GLU:HG3 | 13:P:45:VAL:HG13 | 1.91 | 0.51 |
| 2:R:1015:LEU:CD1 | 2:R:1102:LEU:HD11 | 2.40 | 0.51 |
| 4:D:154:ALA:HA | 4:D:157:ILE:HG13 | 1.93 | 0.51 |
| 5:T:84:VAL:HG13 | 6:U:75:ILE:HD11 | 1.92 | 0.51 |
| 5:E:86:GLU:O | 6:F:44:VAL:HG23 | 2.09 | 0.51 |
| 1:A:879:LYS:NZ | 3:C:44:THR:O | 2.43 | 0.51 |
| 2:R:754:ARG:NH1 | 4:S:60:HIS:HD1 | 2.09 | 0.51 |
| 4:S:60:HIS:C | 4:S:60:HIS:CD2 | 2.83 | 0.51 |
| 3:C:80:GLU:N | 3:C:81:PRO:CD | 2.73 | 0.51 |
| 2:R:708:THR:HG23 | 2:R:946:THR:HA | 1.93 | 0.51 |
| 3:C:66:PRO:HD3 | 9:K:23:TRP:CE2 | 2.45 | 0.51 |
| 2:R:539:LEU:HD12 | 2:R:569:VAL:HG11 | 1.91 | 0.51 |
| 2:B:539:LEU:HD12 | 2:B:569:VAL:HG11 | 1.93 | 0.51 |
| 8:Z:12:ARG:NH2 | 8:Z:55:ILE:HA | 2.26 | 0.51 |
| 3:Y:210:PHE:O | 3:Y:211:ALA:CB | 2.57 | 0.51 |
| 1:W:45:MET:HE2 | 1:W:46:ASP:OD1 | 2.11 | 0.51 |
| 1:W:636:ILE:O | 1:W:640:GLU:HG3 | 2.09 | 0.51 |
| 1:A:328:PRO:HB3 | 1:A:457:PHE:CE2 | 2.46 | 0.51 |
| 2:R:1056:SER:CB | 1:W:316:LYS:HD3 | 2.40 | 0.51 |
| 5:T:2:TYR:HB2 | 6:U:12:ILE:O | 2.10 | 0.51 |
| 3:Y:11:SER:N | 3:Y:45:ARG:NH2 | 2.58 | 0.51 |
| 2:R:461:THR:CG2 | 2:R:468:GLY:N | 2.74 | 0.51 |
| 2:B:247:LEU:HD11 | 2:B:503:VAL:HG12 | 1.93 | 0.51 |
| 1:W:220:ARG:HG2 | 1:W:235:LEU:HD22 | 1.91 | 0.51 |
| 12:O:19:GLN:N | 12:O:20:PRO:HD2 | 2.25 | 0.51 |
| 4:S:206:CYS:HB3 | 16:S:1001:F3S:S3 | 2.51 | 0.51 |
| 2:B:355:SER:O | 2:B:407:VAL:HG11 | 2.10 | 0.51 |
| 1:A:474:ALA:CB | 9:K:62:ILE:HD12 | 2.40 | 0.51 |
| 3:C:64:ILE:HG22 | 3:C:65:ALA:N | 2.21 | 0.51 |
| 9:I:19:PHE:HE1 | 3:Y:64:ILE:HG21 | 1.76 | 0.51 |
| 9:I:53:ILE:HG23 | 9:I:53:ILE:O | 2.11 | 0.51 |
| 2:R:1074:ASP:HB3 | 2:R:1075:LYS:CB | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:1082:CYS:HB3 | 2:R:1091:LEU:HD21 | 1.92 | 0.51 |
| 2:R:430:ARG:HD3 | 2:R:653:ILE:HG12 | 1.91 | 0.51 |
| 3:C:25:PRO:CG | 3:C:33:LYS:HD3 | 2.41 | 0.51 |
| 11:M:46:PRO:HD2 | 11:M:52:LYS:O | 2.11 | 0.51 |
| 1:A:81:VAL:HG21 | 1:A:269:LEU:HB3 | 1.91 | 0.51 |
| 1:W:421:ARG:CZ | 1:W:454:ASN:O | 2.59 | 0.51 |
| 3:Y:25:PRO:HD3 | 3:Y:33:LYS:HD3 | 1.93 | 0.51 |
| 1:A:324:THR:HG22 | 1:A:325:VAL:N | 2.26 | 0.51 |
| 1:A:13:ILE:HG13 | 1:A:202:SER:CB | 2.41 | 0.51 |
| 2:B:957:GLN:HA | 2:B:960:ILE:CG1 | 2.41 | 0.51 |
| 2:B:628:TYR:CE2 | 2:B:640:HIS:CE1 | 2.98 | 0.51 |
| 3:Y:328:GLN:OE1 | 3:Y:331:ARG:NH1 | 2.44 | 0.51 |
| 1:A:363:GLN:O | 1:A:366:ILE:HG22 | 2.10 | 0.51 |
| 12:O:62:TYR:HB3 | 2:R:689:LEU:CD1 | 2.40 | 0.51 |
| 2:R:1094:VAL:HG11 | 1:W:6:ILE:CD1 | 2.41 | 0.51 |
| 2:R:772:GLN:HG2 | 2:R:773:GLU:H | 1.76 | 0.51 |
| 2:R:356:LEU:CD1 | 2:R:407:VAL:HG21 | 2.41 | 0.51 |
| 1:A:854:GLY:O | 3:C:64:ILE:HG23 | 2.11 | 0.51 |
| 1:A:864:LYS:O | 1:A:864:LYS:HG3 | 2.10 | 0.51 |
| 2:R:856:THR:HG22 | 2:R:857:GLU:N | 2.25 | 0.51 |
| 2:R:112:ALA:O | 2:R:113:GLU:CG | 2.59 | 0.51 |
| 5:T:136:ILE:CG2 | 5:T:137:GLN:H | 2.24 | 0.51 |
| 11:M:73:ILE:HG23 | 4:S:253:ILE:HG13 | 1.92 | 0.51 |
| 2:R:732:PHE:O | 2:R:733:THR:HG22 | 2.11 | 0.51 |
| 12:O:35:LEU:HD13 | 12:O:46:ARG:CG | 2.41 | 0.51 |
| 2:R:699:HIS:CE1 | 4:S:57:ILE:HD11 | 2.46 | 0.51 |
| 2:B:1015:LEU:HD13 | 2:B:1015:LEU:C | 2.31 | 0.51 |
| 2:R:918:LEU:HD13 | 1:W:646:MET:HG2 | 1.92 | 0.51 |
| 2:R:1065:ASP:HB3 | 2:R:1089:SER:HB2 | 1.93 | 0.51 |
| 2:B:1065:ASP:HB3 | 2:B:1089:SER:HB2 | 1.93 | 0.51 |
| 2:B:843:ARG:HB2 | 2:B:846:GLU:CG | 2.41 | 0.51 |
| 3:Y:150:GLU:HG3 | 3:Y:227:LEU:HB3 | 1.92 | 0.51 |
| 1:A:600:LYS:O | 1:A:601:LYS:CB | 2.53 | 0.51 |
| 1:W:588:ILE:HG13 | 1:W:593:LEU:HA | 1.92 | 0.51 |
| 2:R:984:SER:O | 2:R:985:ARG:CB | 2.58 | 0.51 |
| 2:R:872:LEU:HD23 | 2:R:873:ARG:N | 2.25 | 0.51 |
| 1:A:119:ASN:OD1 | 1:A:126:PRO:HB3 | 2.11 | 0.51 |
| 4:D:159:VAL:HG22 | 4:D:161:LEU:H | 1.76 | 0.51 |
| 2:B:417:LEU:CD2 | 2:B:425:MET:HG3 | 2.41 | 0.51 |
| 6:U:72:LEU:HD21 | 6:U:86:ILE:CG1 | 2.41 | 0.51 |
| 3:Y:46:ASP:O | 3:Y:47:GLU:OE1 | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:97:TYR:CD1 | 4:S:142:GLU:HG3 | 2.46 | 0.51 |
| 1:A:45:MET:HE2 | 1:A:46:ASP:OD1 | 2.10 | 0.51 |
| 2:B:720:PRO:HG3 | 12:N:53:ILE:CD1 | 2.40 | 0.51 |
| 1:W:736:SER:HB3 | 1:W:739:ASN:CG | 2.31 | 0.51 |
| 2:B:877:ILE:HD12 | 2:B:877:ILE:H | 1.76 | 0.51 |
| 1:A:246:ASN:O | 1:A:246:ASN:CG | 2.50 | 0.51 |
| 1:W:246:ASN:CG | 1:W:246:ASN:O | 2.50 | 0.51 |
| 1:W:28:ILE:HG23 | 1:W:30:PRO:HD2 | 1.93 | 0.51 |
| 1:W:98:CYS:HB2 | 1:W:102:GLY:O | 2.11 | 0.50 |
| 2:B:772:GLN:HG2 | 2:B:773:GLU:H | 1.75 | 0.50 |
| 2:R:773:GLU:CG | 2:R:774:ASP:N | 2.74 | 0.50 |
| 5:E:114:THR:HB | 5:E:115:ASP:C | 2.32 | 0.50 |
| 5:E:131:LYS:HE3 | 5:E:136:ILE:HD11 | 1.93 | 0.50 |
| 2:R:974:TYR:HA | 2:R:981:LYS:HA | 1.92 | 0.50 |
| 1:W:450:CYS:N | 1:W:451:PRO:CD | 2.74 | 0.50 |
| 7:V:104:LYS:O | 7:V:105:ILE:C | 2.49 | 0.50 |
| 2:R:973:THR:HG21 | 2:R:988:PHE:CE1 | 2.46 | 0.50 |
| 1:W:124:ARG:N | 1:W:126:PRO:HD2 | 2.26 | 0.50 |
| 10:Q:49:GLU:O | 10:Q:52:ASP:HB3 | 2.11 | 0.50 |
| 7:G:80:GLU:C | 7:G:81:LEU:HD12 | 2.31 | 0.50 |
| 1:A:838:VAL:HG13 | 3:C:70:ILE:HD11 | 1.92 | 0.50 |
| 4:S:34:LEU:HD22 | 4:S:151:LYS:HB2 | 1.92 | 0.50 |
| 1:A:280:GLU:H | 1:A:282:PRO:HD2 | 1.74 | 0.50 |
| 1:A:750:GLN:HG3 | 1:A:782:ILE:HD11 | 1.94 | 0.50 |
| 1:W:737:VAL:HG23 | 1:W:738:LEU:HD23 | 1.93 | 0.50 |
| 1:W:176:THR:O | 1:W:180:ILE:HG13 | 2.11 | 0.50 |
| 1:W:185:GLU:HA | 1:W:205:GLU:OE2 | 2.11 | 0.50 |
| 3:C:330:GLY:O | 3:C:335:THR:HG22 | 2.12 | 0.50 |
| 11:L:63:ILE:HG22 | 11:L:64:ALA:O | 2.10 | 0.50 |
| 3:C:257:ASN:O | 3:C:261:VAL:HG23 | 2.11 | 0.50 |
| 5:T:9:SER:O | 5:T:70:VAL:HG12 | 2.11 | 0.50 |
| 9:K:63:SER:HA | 9:K:66:GLU:HB2 | 1.93 | 0.50 |
| 2:R:605:ILE:HG12 | 2:R:606:THR:N | 2.26 | 0.50 |
| 1:A:177:PRO:CD | 1:A:266:TRP:HZ2 | 2.22 | 0.50 |
| 8:H:12:ARG:O | 8:H:14:HIS:N | 2.44 | 0.50 |
| 2:B:12:GLU:HG3 | 2:B:595:GLU:OE1 | 2.11 | 0.50 |
| 2:R:898:VAL:HG22 | 4:S:33:MET:SD | 2.52 | 0.50 |
| 2:R:372:LEU:HD22 | 2:R:376:LYS:HG3 | 1.94 | 0.50 |
| 5:E:132:SER:O | 5:E:133:LYS:CG | 2.58 | 0.50 |
| 2:R:53:PRO:HD2 | 2:R:59:LEU:O | 2.10 | 0.50 |
| 1:W:366:ILE:HG13 | 1:W:395:LYS:HG3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:777:GLU:HG3 | 1:A:783:TYR:HE1 | 1.76 | 0.50 |
| 1:W:253:ILE:HG22 | 1:W:254:ASP:OD1 | 2.10 | 0.50 |
| 2:R:493:TYR:HD1 | 2:R:497:VAL:O | 1.95 | 0.50 |
| 1:A:488:THR:HG23 | 1:A:493:GLY:O | 2.11 | 0.50 |
| 1:A:80:PRO:HB3 | 1:A:208:ILE:HG22 | 1.93 | 0.50 |
| 2:R:767:LYS:HG3 | 2:R:768:TYR:HA | 1.92 | 0.50 |
| 3:C:197:VAL:HB | 3:C:208:ILE:HB | 1.92 | 0.50 |
| 2:R:1074:ASP:HB3 | 2:R:1075:LYS:HA | 1.93 | 0.50 |
| 3:C:70:ILE:H | 3:C:70:ILE:CD1 | 2.23 | 0.50 |
| 4:D:161:LEU:O | 4:D:230:LEU:HA | 2.12 | 0.50 |
| 2:B:230:MET:HE1 | 2:B:315:ALA:O | 2.12 | 0.50 |
| 2:B:492:LEU:HB3 | 2:B:497:VAL:HG21 | 1.93 | 0.50 |
| 1:A:541:ALA:HB3 | 1:A:542:PRO:CD | 2.40 | 0.50 |
| 3:C:150:GLU:HG3 | 3:C:227:LEU:HB3 | 1.93 | 0.50 |
| 4:D:96:ILE:HG12 | 4:D:145:LEU:HD11 | 1.93 | 0.50 |
| 1:W:687:ILE:HD12 | 1:W:695:SER:HB2 | 1.94 | 0.50 |
| 1:A:185:GLU:HA | 1:A:205:GLU:OE2 | 2.12 | 0.50 |
| 2:R:767:LYS:HD3 | 2:R:768:TYR:HA | 1.93 | 0.50 |
| 3:Y:80:GLU:CB | 3:Y:81:PRO:HD3 | 2.39 | 0.50 |
| 2:B:605:ILE:CG1 | 2:B:606:THR:H | 2.18 | 0.50 |
| 2:B:112:ALA:O | 2:B:113:GLU:CG | 2.59 | 0.50 |
| 2:R:597:ILE:HB | 2:R:603:GLY:H | 1.76 | 0.50 |
| 2:R:1044:THR:HG23 | 2:R:1044:THR:O | 2.11 | 0.50 |
| 2:B:1017:ARG:HD3 | 2:B:1098:TYR:CG | 2.47 | 0.50 |
| 8:H:29:TYR:HE1 | 10:Q:60:SER:HB2 | 1.77 | 0.50 |
| 2:B:118:TYR:C | 2:B:118:TYR:CD1 | 2.85 | 0.50 |
| 2:B:17:ILE:O | 2:B:20:TYR:HB3 | 2.11 | 0.50 |
| 2:R:230:MET:HE1 | 2:R:315:ALA:O | 2.11 | 0.50 |
| 6:U:64:SER:HB2 | 6:U:69:ARG:HD3 | 1.94 | 0.50 |
| 2:R:448:LEU:CD2 | 1:W:796:PHE:CZ | 2.94 | 0.50 |
| 1:W:110:GLU:HA | 1:W:113:LYS:HD2 | 1.93 | 0.50 |
| 11:M:48:PRO:HG2 | 2:R:735:TYR:HE2 | 1.75 | 0.50 |
| 1:W:177:PRO:CD | 1:W:266:TRP:HZ2 | 2.22 | 0.50 |
| 2:R:332:ARG:HD2 | 2:R:565:PHE:HB3 | 1.92 | 0.50 |
| 2:B:787:LYS:HE3 | 2:B:841:VAL:HG23 | 1.93 | 0.50 |
| 1:A:642:GLN:OE1 | 2:B:983:LYS:HD2 | 2.10 | 0.50 |
| 8:Z:63:ILE:HG22 | 8:Z:65:ILE:CD1 | 2.41 | 0.50 |
| 2:R:741:ILE:HD11 | 2:R:911:VAL:CG1 | 2.42 | 0.50 |
| 3:C:47:GLU:HB3 | 3:C:50:LYS:HB2 | 1.93 | 0.50 |
| 2:R:109:ASN:CG | 2:R:109:ASN:O | 2.50 | 0.50 |
| 3:C:241:ILE:O | 3:C:251:ILE:HG23 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:126:LEU:HD13 | 2:R:154:TYR:O | 2.11 | 0.50 |
| 2:B:478:GLN:HG2 | 2:B:479:ILE:N | 2.27 | 0.50 |
| 1:W:328:PRO:HB3 | 1:W:457:PHE:CE2 | 2.46 | 0.50 |
| 3:Y:197:VAL:HB | 3:Y:208:ILE:HB | 1.94 | 0.50 |
| 9:K:52:ASP:O | 9:K:53:ILE:CB | 2.59 | 0.50 |
| 3:Y:340:SER:HB3 | 3:Y:371:GLU:CG | 2.41 | 0.50 |
| 2:R:17:ILE:CD1 | 2:R:476:MET:SD | 2.99 | 0.50 |
| 2:R:486:LYS:HG2 | 2:R:489:GLU:OE2 | 2.11 | 0.50 |
| 1:A:316:LYS:HD3 | 2:B:1056:SER:CB | 2.40 | 0.50 |
| 2:R:1057:ASP:OD1 | 2:R:1057:ASP:N | 2.44 | 0.50 |
| 2:B:657:ILE:HG13 | 2:B:711:LEU:HD21 | 1.94 | 0.50 |
| 2:B:127:LYS:HE3 | 2:B:150:ASP:O | 2.12 | 0.50 |
| 11:L:14:GLU:OE1 | 11:L:56:LYS:HG2 | 2.12 | 0.50 |
| 9:I:77:THR:HG23 | 9:I:90:LEU:O | 2.12 | 0.50 |
| 2:R:843:ARG:HB2 | 2:R:846:GLU:CG | 2.41 | 0.50 |
| 2:R:1112:ILE:O | 2:R:1114:PRO:HD3 | 2.11 | 0.50 |
| 3:C:341:VAL:HG12 | 3:C:344:ARG:NH2 | 2.26 | 0.50 |
| 1:W:510:THR:O | 1:W:597:VAL:HG23 | 2.11 | 0.50 |
| 2:R:767:LYS:HA | 2:R:767:LYS:HZ2 | 1.76 | 0.50 |
| 2:B:601:ASP:O | 2:B:602:SER:HB3 | 2.12 | 0.50 |
| 2:R:543:ILE:CD1 | 2:R:558:VAL:HG21 | 2.40 | 0.50 |
| 13:P:37:VAL:HG22 | 13:P:38:ARG:N | 2.27 | 0.50 |
| 7:V:80:GLU:C | 7:V:81:LEU:HD12 | 2.32 | 0.50 |
| 7:V:24:LYS:O | 7:V:25:ASN:HB2 | 2.12 | 0.50 |
| 2:R:1062:TYR:HA | 2:R:1092:PHE:O | 2.12 | 0.50 |
| 3:C:176:ASP:O | 3:C:177:LYS:CG | 2.59 | 0.50 |
| 2:B:42:LEU:HD12 | 2:B:357:PHE:CE2 | 2.47 | 0.50 |
| 2:B:741:ILE:HG23 | 2:B:891:ILE:HA | 1.94 | 0.50 |
| 4:D:93:TYR:CE1 | 4:D:146:ARG:HG2 | 2.47 | 0.50 |
| 4:S:172:ILE:CD1 | 4:S:188:PHE:HE1 | 2.25 | 0.50 |
| 2:R:493:TYR:CD1 | 2:R:499:PRO:HD3 | 2.47 | 0.50 |
| 1:W:49:LEU:HD12 | 1:W:49:LEU:N | 2.27 | 0.50 |
| 4:D:180:ALA:HA | 4:D:188:PHE:HB2 | 1.92 | 0.50 |
| 2:B:232:ALA:HB2 | 2:B:271:ALA:HB1 | 1.94 | 0.50 |
| 2:B:953:ILE:H | 2:B:953:ILE:CD1 | 2.14 | 0.50 |
| 2:B:928:MET:HE3 | 2:B:953:ILE:HG21 | 1.92 | 0.50 |
| 3:C:66:PRO:HD3 | 9:K:23:TRP:CZ2 | 2.46 | 0.50 |
| 2:R:593:THR:HG23 | 2:R:594:ARG:N | 2.26 | 0.50 |
| 4:D:203:CYS:SG | 16:D:1001:F3S:S1 | 3.07 | 0.50 |
| 1:W:107:SER:O | 1:W:108:GLU:C | 2.48 | 0.50 |
| 2:R:732:PHE:CD2 | 2:R:733:THR:HB | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:684:LEU:HD12 | 1:A:684:LEU:H | 1.76 | 0.50 |
| 1:A:870:ARG:HH22 | 3:C:36:ILE:HD13 | 1.76 | 0.50 |
| 2:R:628:TYR:CE2 | 2:R:640:HIS:ND1 | 2.80 | 0.50 |
| 1:A:636:ILE:O | 1:A:640:GLU:HG3 | 2.11 | 0.50 |
| 2:R:20:TYR:HD2 | 2:R:607:PHE:CE2 | 2.30 | 0.50 |
| 1:W:695:SER:O | 1:W:699:TYR:CD2 | 2.65 | 0.50 |
| 1:A:819:MET:O | 1:A:819:MET:HG2 | 2.12 | 0.50 |
| 5:T:10:ILE:HG23 | 5:T:68:HIS:O | 2.12 | 0.50 |
| 4:D:84:ASP:O | 4:D:85:CYS:C | 2.49 | 0.50 |
| 2:B:597:ILE:HB | 2:B:603:GLY:H | 1.76 | 0.50 |
| 2:R:63:LEU:CD2 | 2:R:103:MET:HE2 | 2.42 | 0.50 |
| 5:T:128:PHE:HB3 | 5:T:137:GLN:NE2 | 2.26 | 0.50 |
| 3:C:348:GLU:O | 3:C:349:VAL:C | 2.50 | 0.50 |
| 3:C:393:ILE:HG22 | 5:E:19:GLY:N | 2.27 | 0.50 |
| 5:T:123:VAL:HA | 5:T:127:ILE:HA | 1.93 | 0.50 |
| 2:R:583:ILE:HD13 | 2:R:616:ILE:HG12 | 1.93 | 0.50 |
| 11:L:12:TYR:CD1 | 11:L:58:LEU:HB2 | 2.47 | 0.50 |
| 1:A:219:ILE:HD11 | 2:B:1105:GLN:HB3 | 1.94 | 0.50 |
| 10:J:60:SER:CB | 8:Z:29:TYR:HE1 | 2.24 | 0.50 |
| 2:R:1110:MET:HE2 | 1:W:298:LEU:HB3 | 1.94 | 0.50 |
| 2:B:192:ILE:O | 2:B:206:GLU:HB2 | 2.12 | 0.50 |
| 1:W:329:ASP:O | 1:W:446:ASN:HA | 2.11 | 0.50 |
| 10:Q:63:GLU:O | 10:Q:67:LEU:HB2 | 2.12 | 0.49 |
| 9:K:53:ILE:HG23 | 9:K:53:ILE:O | 2.12 | 0.49 |
| 1:A:136:VAL:HA | 1:A:139:THR:HG22 | 1.93 | 0.49 |
| 2:R:330:LEU:O | 2:R:332:ARG:N | 2.45 | 0.49 |
| 12:O:46:ARG:NH1 | 2:R:938:LEU:O | 2.45 | 0.49 |
| 2:B:732:PHE:O | 2:B:733:THR:HG22 | 2.12 | 0.49 |
| 2:R:653:ILE:CD1 | 2:R:653:ILE:H | 2.24 | 0.49 |
| 1:A:450:CYS:H | 1:A:451:PRO:CD | 2.24 | 0.49 |
| 2:B:107:GLU:O | 2:B:108:ASN:HB2 | 2.12 | 0.49 |
| 2:R:230:MET:HE2 | 2:R:315:ALA:HB1 | 1.93 | 0.49 |
| 2:B:73:VAL:HG22 | 2:B:74:ARG:O | 2.12 | 0.49 |
| 2:R:192:ILE:O | 2:R:206:GLU:HB2 | 2.11 | 0.49 |
| 5:T:36:GLU:HB3 | 6:U:33:LEU:HD22 | 1.94 | 0.49 |
| 2:R:247:LEU:HD11 | 2:R:503:VAL:HG12 | 1.93 | 0.49 |
| 1:A:863:GLY:HA2 | 3:C:311:ARG:HH22 | 1.77 | 0.49 |
| 1:A:792:PRO:HA | 2:B:948:PHE:CZ | 2.47 | 0.49 |
| 2:R:248:ASP:N | 2:R:249:PRO:HD3 | 2.26 | 0.49 |
| 2:R:250:GLU:HG2 | 2:R:251:ILE:N | 2.27 | 0.49 |
| 2:B:525:LEU:HD22 | 2:B:571:VAL:HB | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:733:THR:HG23 | 2:B:735:TYR:HB2 | 1.94 | 0.49 |
| 2:R:584:ILE:CD1 | 2:R:617:GLU:HB2 | 2.42 | 0.49 |
| 5:T:123:VAL:O | 5:T:124:ARG:O | 2.30 | 0.49 |
| 4:S:155:LYS:HE3 | 4:S:156:PHE:CE2 | 2.47 | 0.49 |
| 6:U:72:LEU:HD21 | 6:U:86:ILE:HG12 | 1.94 | 0.49 |
| 2:R:707:GLN:CD | 2:R:942:ILE:HD12 | 2.33 | 0.49 |
| 1:W:518:LYS:HA | 1:W:546:TYR:HE1 | 1.76 | 0.49 |
| 2:B:630:ALA:CB | 2:B:636:LEU:HD12 | 2.42 | 0.49 |
| 1:A:518:LYS:HA | 1:A:546:TYR:HE2 | 1.76 | 0.49 |
| 10:J:55:LEU:CD2 | 8:Z:25:ILE:HG22 | 2.42 | 0.49 |
| 2:B:1062:TYR:HA | 2:B:1092:PHE:O | 2.11 | 0.49 |
| 4:D:172:ILE:CD1 | 4:D:188:PHE:HE1 | 2.24 | 0.49 |
| 1:W:106:ILE:H | 1:W:106:ILE:HD12 | 1.75 | 0.49 |
| 2:B:1021:GLU:OE2 | 2:B:1022:GLY:N | 2.45 | 0.49 |
| 2:B:797:ASP:OD2 | 13:P:4:TYR:HB3 | 2.11 | 0.49 |
| 3:Y:257:ASN:O | 3:Y:261:VAL:HG23 | 2.12 | 0.49 |
| 1:A:238:LYS:HE3 | 1:A:276:TYR:HA | 1.94 | 0.49 |
| 1:W:428:ILE:HG21 | 1:W:452:PRO:HB3 | 1.94 | 0.49 |
| 2:B:874:ILE:HG22 | 2:B:875:PRO:HD2 | 1.94 | 0.49 |
| 3:C:237:ILE:HD11 | 3:C:240:ALA:HB2 | 1.95 | 0.49 |
| 2:B:1007:ARG:HD3 | 2:B:1028:GLY:HA2 | 1.95 | 0.49 |
| 4:D:34:LEU:HD22 | 4:D:151:LYS:HB2 | 1.95 | 0.49 |
| 2:B:707:GLN:CD | 2:B:942:ILE:HD12 | 2.33 | 0.49 |
| 3:C:328:GLN:HB3 | 3:C:332:HIS:HB3 | 1.94 | 0.49 |
| 10:J:63:GLU:O | 10:J:67:LEU:HB2 | 2.12 | 0.49 |
| 11:M:14:GLU:OE1 | 11:M:56:LYS:HG2 | 2.12 | 0.49 |
| 11:L:32:LEU:HD23 | 11:L:35:ILE:HD12 | 1.94 | 0.49 |
| 11:L:13:LEU:HB2 | 11:L:65:PRO:HB2 | 1.93 | 0.49 |
| 1:W:136:VAL:HA | 1:W:139:THR:HG22 | 1.94 | 0.49 |
| 2:B:579:ARG:HD3 | 2:B:618:TYR:CD2 | 2.48 | 0.49 |
| 1:W:601:LYS:O | 1:W:610:SER:HB2 | 2.12 | 0.49 |
| 3:C:174:LEU:CB | 3:C:179:VAL:HG13 | 2.42 | 0.49 |
| 2:B:973:THR:O | 2:B:982:ILE:HG13 | 2.12 | 0.49 |
| 1:A:470:GLU:HG3 | 9:K:41:LEU:HD12 | 1.94 | 0.49 |
| 2:R:345:ARG:NH2 | 2:R:577:ARG:HG2 | 2.28 | 0.49 |
| 3:Y:330:GLY:O | 3:Y:335:THR:HG22 | 2.13 | 0.49 |
| 3:C:109:GLU:OE2 | 3:C:117:PRO:HA | 2.12 | 0.49 |
| 5:T:40:LYS:O | 5:T:42:LEU:HD12 | 2.12 | 0.49 |
| 1:W:827:LEU:O | 3:Y:71:GLY:HA3 | 2.11 | 0.49 |
| 2:B:136:TYR:CB | 2:B:141:LEU:CD1 | 2.91 | 0.49 |
| 1:W:119:ASN:OD1 | 1:W:126:PRO:HB3 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:81:LEU:N | 7:G:81:LEU:HD12 | 2.27 | 0.49 |
| 2:B:1007:ARG:HH21 | 2:B:1026:GLU:C | 2.16 | 0.49 |
| 1:A:830:LEU:HD23 | 1:A:840:SER:HB3 | 1.92 | 0.49 |
| 2:R:759:ARG:HG3 | 2:R:760:LEU:N | 2.28 | 0.49 |
| 2:B:699:HIS:CE1 | 4:D:57:ILE:HG12 | 2.48 | 0.49 |
| 2:B:1091:LEU:O | 2:B:1092:PHE:CG | 2.66 | 0.49 |
| 4:S:8:LYS:HG2 | 4:S:9:ASP:N | 2.27 | 0.49 |
| 5:E:50:ASN:HB2 | 5:E:73:ASP:HB2 | 1.93 | 0.49 |
| 9:K:55:ASN:HA | 9:K:56:ILE:N | 2.28 | 0.49 |
| 2:R:767:LYS:NZ | 2:R:767:LYS:HA | 2.27 | 0.49 |
| 1:W:426:HIS:CE1 | 3:Y:80:GLU:CD | 2.86 | 0.49 |
| 13:X:5:ARG:CZ | 13:X:6:CYS:O | 2.61 | 0.49 |
| 2:R:973:THR:O | 2:R:982:ILE:HG13 | 2.11 | 0.49 |
| 2:B:776:ILE:HG23 | 2:B:815:GLY:O | 2.13 | 0.49 |
| 1:A:13:ILE:CD1 | 1:A:202:SER:HB2 | 2.42 | 0.49 |
| 1:A:505:GLY:HA3 | 1:A:639:VAL:CG2 | 2.43 | 0.49 |
| 1:W:13:ILE:CD1 | 1:W:202:SER:HB2 | 2.43 | 0.49 |
| 1:W:879:LYS:NZ | 3:Y:44:THR:O | 2.45 | 0.49 |
| 10:J:66:ARG:CD | 1:W:121:ILE:HG21 | 2.43 | 0.49 |
| 1:W:830:LEU:HD23 | 1:W:840:SER:HB3 | 1.93 | 0.49 |
| 5:T:84:VAL:CG1 | 6:U:75:ILE:CD1 | 2.90 | 0.49 |
| 4:D:171:GLU:HB2 | 4:D:218:ARG:HB3 | 1.93 | 0.49 |
| 2:R:163:VAL:HG21 | 2:R:429:LEU:HD23 | 1.93 | 0.49 |
| 2:R:856:THR:HG23 | 13:X:32:LYS:C | 2.33 | 0.49 |
| 9:I:62:ILE:O | 9:I:66:GLU:HG3 | 2.13 | 0.49 |
| 3:C:277:ILE:CG2 | 3:C:278:ARG:H | 2.22 | 0.49 |
| 12:O:43:TYR:HB3 | 2:R:938:LEU:HD23 | 1.94 | 0.49 |
| 7:V:102:LEU:O | 7:V:103:VAL:C | 2.51 | 0.49 |
| 7:V:103:VAL:HG13 | 7:V:104:LYS:CD | 2.41 | 0.49 |
| 2:B:1050:ASP:HA | 2:B:1054:ASP:HB2 | 1.94 | 0.49 |
| 1:A:304:GLY:C | 1:A:306:GLU:N | 2.65 | 0.49 |
| 10:Q:62:ASP:O | 10:Q:66:ARG:HB3 | 2.13 | 0.49 |
| 3:Y:211:ALA:O | 3:Y:212:ASN:HB2 | 2.13 | 0.49 |
| 1:A:235:LEU:O | 1:A:239:LEU:HB2 | 2.12 | 0.49 |
| 3:Y:347:PHE:O | 3:Y:348:GLU:HB3 | 2.12 | 0.49 |
| 8:Z:62:ILE:HG13 | 8:Z:62:ILE:O | 2.11 | 0.49 |
| 5:E:84:VAL:HG13 | 6:F:75:ILE:HD11 | 1.94 | 0.49 |
| 5:T:36:GLU:CG | 6:U:33:LEU:HD22 | 2.42 | 0.49 |
| 5:E:40:LYS:O | 5:E:42:LEU:HD12 | 2.13 | 0.49 |
| 2:B:502:GLU:O | 2:B:506:ARG:HB2 | 2.12 | 0.49 |
| 3:C:284:PHE:HB3 | 3:C:288:ALA:HB1 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:W:98:CYS:O | 1:W:99:ARG:CB | 2.59 | 0.49 |
| 2:R:359:VAL:HG11 | 2:R:407:VAL:HG13 | 1.93 | 0.49 |
| 13:X:10:TRP:CB | 13:X:31:TYR:CE2 | 2.93 | 0.49 |
| 2:R:364:PHE:CE1 | 2:R:388:VAL:HG13 | 2.47 | 0.49 |
| 2:R:659:PRO:HG3 | 2:R:884:ARG:NH2 | 2.28 | 0.49 |
| 4:D:209:CYS:SG | 4:D:219:ILE:CD1 | 2.99 | 0.49 |
| 3:Y:258:LEU:HD11 | 3:Y:272:VAL:HG11 | 1.94 | 0.49 |
| 9:K:49:ALA:O | 9:K:50:LEU:C | 2.50 | 0.49 |
| 2:B:1074:ASP:HB3 | 2:B:1075:LYS:HA | 1.95 | 0.49 |
| 2:R:934:LYS:O | 2:R:938:LEU:HG | 2.13 | 0.49 |
| 2:B:584:ILE:CD1 | 2:B:617:GLU:HB2 | 2.42 | 0.49 |
| 12:N:5:ILE:HA | 12:N:15:ALA:HB2 | 1.94 | 0.49 |
| 11:M:77:ARG:HB2 | 11:M:77:ARG:NH1 | 2.28 | 0.49 |
| 6:F:72:LEU:HD21 | 6:F:86:ILE:CG1 | 2.43 | 0.49 |
| 2:R:404:GLY:O | 2:R:405:ASN:O | 2.31 | 0.49 |
| 5:T:132:SER:O | 5:T:133:LYS:CG | 2.60 | 0.49 |
| 4:S:93:TYR:CD1 | 4:S:146:ARG:HB3 | 2.46 | 0.49 |
| 1:A:534:LEU:HB2 | 1:A:546:TYR:CE1 | 2.48 | 0.49 |
| 3:C:127:THR:H | 3:C:268:ASP:HB2 | 1.77 | 0.49 |
| 6:F:4:VAL:HG13 | 6:F:4:VAL:O | 2.12 | 0.49 |
| 5:E:94:ASN:HA | 5:E:121:ASP:OD2 | 2.13 | 0.49 |
| 9:I:34:ARG:HB2 | 3:Y:386:VAL:HG11 | 1.95 | 0.49 |
| 2:B:604:SER:O | 2:B:605:ILE:O | 2.31 | 0.49 |
| 7:G:36:PHE:CE1 | 7:G:96:ILE:HG12 | 2.48 | 0.49 |
| 5:E:115:ASP:O | 5:E:116:ASP:HB2 | 2.13 | 0.49 |
| 5:E:168:TYR:C | 5:E:169:LEU:HD12 | 2.33 | 0.49 |
| 2:B:659:PRO:HG3 | 2:B:884:ARG:NH2 | 2.28 | 0.49 |
| 8:H:59:PRO:HA | 8:H:81:VAL:CG1 | 2.43 | 0.49 |
| 2:B:1074:ASP:CB | 2:B:1075:LYS:HA | 2.43 | 0.49 |
| 2:B:532:TYR:O | 2:B:533:TYR:CB | 2.60 | 0.49 |
| 3:Y:232:LYS:HE3 | 3:Y:232:LYS:HA | 1.95 | 0.49 |
| 1:A:123:LYS:HA | 1:A:126:PRO:HG3 | 1.93 | 0.49 |
| 2:B:1111:ILE:HG22 | 2:B:1111:ILE:O | 2.12 | 0.49 |
| 1:W:220:ARG:HG2 | 1:W:235:LEU:HD13 | 1.95 | 0.49 |
| 1:W:235:LEU:O | 1:W:239:LEU:HB2 | 2.13 | 0.49 |
| 2:R:272:LEU:HD22 | 2:R:292:ALA:O | 2.13 | 0.49 |
| 3:Y:102:LEU:HD11 | 3:Y:118:SER:HB3 | 1.95 | 0.49 |
| 1:A:761:TYR:CD1 | 2:B:451:THR:HG22 | 2.48 | 0.49 |
| 8:H:12:ARG:NH2 | 8:H:55:ILE:HA | 2.27 | 0.49 |
| 1:A:95:LYS:HD3 | 1:A:138:LYS:HD3 | 1.95 | 0.49 |
| 2:B:84:SER:HG | 2:B:144:ILE:HG23 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:732:PHE:CD2 | 2:B:733:THR:HB | 2.48 | 0.49 |
| 8:Z:12:ARG:O | 8:Z:14:HIS:N | 2.45 | 0.49 |
| 3:Y:170:ASP:HB3 | 3:Y:173:MET:HB2 | 1.95 | 0.49 |
| 2:R:957:GLN:HA | 2:R:960:ILE:HG12 | 1.94 | 0.49 |
| 1:A:328:PRO:HD3 | 1:A:457:PHE:CG | 2.47 | 0.49 |
| 2:B:1056:SER:CB | 2:B:1057:ASP:OD1 | 2.60 | 0.49 |
| 5:T:94:ASN:HA | 5:T:121:ASP:OD2 | 2.13 | 0.49 |
| 5:T:121:ASP:OD1 | 5:T:129:GLY:HA3 | 2.13 | 0.49 |
| 2:B:599:LYS:O | 2:B:600:LEU:C | 2.50 | 0.49 |
| 1:A:421:ARG:HD3 | 1:A:453:TYR:O | 2.13 | 0.49 |
| 1:W:80:PRO:HB3 | 1:W:208:ILE:HG22 | 1.95 | 0.49 |
| 2:B:808:LYS:HE3 | 2:B:847:MET:CE | 2.43 | 0.49 |
| 2:B:772:GLN:O | 2:B:773:GLU:HB2 | 2.13 | 0.48 |
| 2:B:598:GLU:HA | 2:B:605:ILE:HD11 | 1.91 | 0.48 |
| 2:R:601:ASP:O | 2:R:602:SER:HB3 | 2.12 | 0.48 |
| 1:A:763:THR:HB | 1:A:764:ARG:HD3 | 1.94 | 0.48 |
| 7:V:8:GLU:HG2 | 7:V:9:ILE:H | 1.78 | 0.48 |
| 9:I:51:ILE:O | 9:I:52:ASP:CG | 2.51 | 0.48 |
| 1:W:334:ILE:HD12 | 1:W:628:MET:CB | 2.43 | 0.48 |
| 8:H:44:TRP:O | 8:H:79:ARG:HD2 | 2.13 | 0.48 |
| 3:C:211:ALA:O | 3:C:212:ASN:HB2 | 2.13 | 0.48 |
| 1:A:695:SER:O | 1:A:699:TYR:CD2 | 2.66 | 0.48 |
| 4:D:246:GLY:HA3 | 11:L:84:ILE:CD1 | 2.43 | 0.48 |
| 9:K:77:THR:HG23 | 9:K:90:LEU:O | 2.13 | 0.48 |
| 1:W:758:LYS:HA | 1:W:779:ARG:HH11 | 1.78 | 0.48 |
| 5:E:10:ILE:HG23 | 5:E:68:HIS:O | 2.13 | 0.48 |
| 2:B:766:VAL:HG22 | 2:B:767:LYS:N | 2.15 | 0.48 |
| 1:A:465:HIS:CE1 | 2:B:1031:PHE:HD2 | 2.30 | 0.48 |
| 1:A:853:ASP:CB | 3:C:311:ARG:NH1 | 2.76 | 0.48 |
| 2:B:734:GLY:HA3 | 2:B:735:TYR:CD2 | 2.48 | 0.48 |
| 1:A:687:ILE:HD12 | 1:A:695:SER:CB | 2.44 | 0.48 |
| 1:A:45:MET:O | 1:A:45:MET:CG | 2.61 | 0.48 |
| 2:B:155:PHE:HE1 | 2:B:164:ILE:HD12 | 1.78 | 0.48 |
| 3:C:127:THR:N | 3:C:268:ASP:HB2 | 2.27 | 0.48 |
| 4:S:182:VAL:HG11 | 4:S:212:TYR:CD2 | 2.48 | 0.48 |
| 12:O:61:HIS:O | 12:O:62:TYR:CG | 2.66 | 0.48 |
| 4:S:13:ILE:HD13 | 4:S:14:ASP:N | 2.27 | 0.48 |
| 1:A:192:VAL:CG2 | 1:A:199:PRO:HB3 | 2.43 | 0.48 |
| 2:B:631:LEU:O | 2:B:632:GLU:OE1 | 2.31 | 0.48 |
| 2:R:767:LYS:HD3 | 2:R:768:TYR:CA | 2.43 | 0.48 |
| 4:D:260:LEU:HD11 | 11:L:69:LEU:CD2 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:558:VAL:HG22 | 2:R:571:VAL:HG22 | 1.94 | 0.48 |
| 2:R:983:LYS:HD2 | 1:W:642:GLN:OE1 | 2.13 | 0.48 |
| 8:H:62:ILE:O | 8:H:62:ILE:HG13 | 2.12 | 0.48 |
| 2:B:1040:ILE:HG23 | 3:C:381:LEU:HD11 | 1.95 | 0.48 |
| 1:A:782:ILE:HG23 | 1:A:794:GLU:CD | 2.34 | 0.48 |
| 2:B:1066:GLN:HG3 | 2:B:1089:SER:HB3 | 1.94 | 0.48 |
| 1:W:647:ARG:HE | 1:W:724:PHE:HE1 | 1.61 | 0.48 |
| 1:A:823:LEU:HB3 | 3:C:329:ILE:HG12 | 1.95 | 0.48 |
| 5:E:30:LEU:CD2 | 5:E:72:PHE:CE2 | 2.96 | 0.48 |
| 5:T:30:LEU:CD1 | 5:T:72:PHE:CE2 | 2.96 | 0.48 |
| 1:W:417:VAL:HG11 | 1:W:464:LEU:HD11 | 1.95 | 0.48 |
| 5:E:116:ASP:O | 5:E:117:THR:HG23 | 2.14 | 0.48 |
| 5:E:119:LYS:HG2 | 5:E:120:TYR:CD2 | 2.48 | 0.48 |
| 2:R:66:ILE:HG22 | 2:R:67:ARG:N | 2.29 | 0.48 |
| 13:X:5:ARG:NH1 | 13:X:6:CYS:O | 2.46 | 0.48 |
| 1:A:648:LEU:HB2 | 2:B:927:ILE:HG21 | 1.94 | 0.48 |
| 3:C:147:THR:HB | 3:C:232:LYS:CB | 2.41 | 0.48 |
| 1:A:6:ILE:HD13 | 2:B:1116:LEU:HD23 | 1.95 | 0.48 |
| 1:W:818:TYR:CD2 | 1:W:822:ARG:NH1 | 2.81 | 0.48 |
| 3:C:133:ASP:O | 3:C:249:TYR:CD2 | 2.66 | 0.48 |
| 2:R:301:LEU:HB3 | 2:R:304:LEU:HD12 | 1.94 | 0.48 |
| 5:E:121:ASP:OD1 | 5:E:129:GLY:HA3 | 2.13 | 0.48 |
| 2:B:301:LEU:N | 2:B:302:PRO:HD3 | 2.29 | 0.48 |
| 1:A:647:ARG:HE | 1:A:724:PHE:HE1 | 1.60 | 0.48 |
| 6:F:62:ILE:HG22 | 6:F:63:ILE:H | 1.78 | 0.48 |
| 2:B:745:ARG:HD2 | 2:B:896:PRO:HG3 | 1.96 | 0.48 |
| 3:C:186:LYS:CB | 3:C:230:LYS:HE2 | 2.40 | 0.48 |
| 2:B:356:LEU:HD12 | 2:B:407:VAL:CG2 | 2.43 | 0.48 |
| 1:A:338:GLY:HA3 | 1:A:444:ARG:HB2 | 1.95 | 0.48 |
| 5:T:6:LYS:HA | 5:T:72:PHE:O | 2.13 | 0.48 |
| 5:T:116:ASP:O | 5:T:117:THR:HG23 | 2.14 | 0.48 |
| 2:R:594:ARG:CZ | 2:R:615:LYS:HG3 | 2.43 | 0.48 |
| 2:R:672:GLN:HG2 | 2:R:884:ARG:O | 2.14 | 0.48 |
| 2:B:215:VAL:HG12 | 2:B:224:ILE:O | 2.12 | 0.48 |
| 2:B:908:VAL:O | 12:N:9:THR:HG23 | 2.14 | 0.48 |
| 1:A:289:HIS:O | 1:A:290:ARG:HB2 | 2.13 | 0.48 |
| 2:R:249:PRO:HB2 | 2:R:253:ASN:H | 1.79 | 0.48 |
| 1:W:124:ARG:HD3 | 1:W:125:TRP:CZ3 | 2.48 | 0.48 |
| 2:R:957:GLN:HA | 2:R:960:ILE:CG1 | 2.44 | 0.48 |
| 2:R:784:ARG:HB3 | 2:R:835:LYS:O | 2.13 | 0.48 |
| 1:W:13:ILE:CG1 | 1:W:202:SER:HB2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:Y:133:ASP:O | 3:Y:249:TYR:CD2 | 2.66 | 0.48 |
| 5:T:10:ILE:HG22 | 5:T:11:VAL:N | 2.29 | 0.48 |
| 2:B:502:GLU:O | 2:B:506:ARG:N | 2.46 | 0.48 |
| 1:W:819:MET:HG2 | 1:W:819:MET:O | 2.13 | 0.48 |
| 4:S:84:ASP:O | 4:S:85:CYS:C | 2.51 | 0.48 |
| 4:S:171:GLU:HB2 | 4:S:218:ARG:HB3 | 1.96 | 0.48 |
| 5:E:30:LEU:HD13 | 5:E:72:PHE:HZ | 1.70 | 0.48 |
| 1:A:859:TYR:CE2 | 3:C:65:ALA:HB2 | 2.43 | 0.48 |
| 13:X:5:ARG:HG3 | 13:X:6:CYS:N | 2.27 | 0.48 |
| 1:A:736:SER:HB3 | 1:A:739:ASN:ND2 | 2.28 | 0.48 |
| 7:G:104:LYS:O | 7:G:105:ILE:C | 2.52 | 0.48 |
| 2:R:734:GLY:HA3 | 2:R:735:TYR:CB | 2.44 | 0.48 |
| 2:B:735:TYR:HE2 | 11:L:48:PRO:HG2 | 1.77 | 0.48 |
| 3:Y:162:SER:HA | 3:Y:210:PHE:HZ | 1.78 | 0.48 |
| 2:R:703:ARG:NH2 | 2:R:942:ILE:HG21 | 2.29 | 0.48 |
| 12:O:53:ILE:CD1 | 2:R:720:PRO:HG3 | 2.44 | 0.48 |
| 1:A:73:GLY:O | 1:A:74:HIS:ND1 | 2.47 | 0.48 |
| 1:A:223:ILE:CG1 | 1:A:224:MET:N | 2.76 | 0.48 |
| 4:S:38:VAL:CG1 | 4:S:39:MET:N | 2.76 | 0.48 |
| 9:I:27:LEU:HD23 | 9:I:78:ILE:HD11 | 1.95 | 0.48 |
| 4:S:96:ILE:HG12 | 4:S:145:LEU:HD11 | 1.95 | 0.48 |
| 3:C:160:ILE:O | 3:C:161:ALA:C | 2.52 | 0.48 |
| 2:R:422:TRP:HZ3 | 2:R:715:GLY:HA3 | 1.78 | 0.48 |
| 2:R:502:GLU:O | 2:R:506:ARG:HB2 | 2.13 | 0.48 |
| 1:W:337:VAL:O | 1:W:337:VAL:HG13 | 2.14 | 0.48 |
| 1:W:419:PHE:CE1 | 1:W:464:LEU:HD23 | 2.49 | 0.48 |
| 5:E:114:THR:CG2 | 5:E:131:LYS:HD3 | 2.44 | 0.48 |
| 13:X:37:VAL:HG22 | 13:X:38:ARG:N | 2.28 | 0.48 |
| 2:B:157:VAL:CG1 | 2:B:401:LEU:HD23 | 2.43 | 0.48 |
| 1:W:763:THR:HB | 1:W:764:ARG:HD3 | 1.96 | 0.48 |
| 1:A:325:VAL:O | 1:A:442:THR:HG22 | 2.14 | 0.48 |
| 3:C:237:ILE:HD12 | 3:C:253:THR:CB | 2.43 | 0.48 |
| 11:M:18:GLU:O | 11:M:18:GLU:CG | 2.60 | 0.48 |
| 1:W:121:ILE:HD12 | 8:Z:38:ARG:NH1 | 2.29 | 0.48 |
| 1:A:29:THR:HG23 | 1:A:243:VAL:HB | 1.95 | 0.48 |
| 1:W:215:PRO:HG2 | 1:W:220:ARG:HD2 | 1.94 | 0.48 |
| 2:R:502:GLU:O | 2:R:506:ARG:N | 2.47 | 0.48 |
| 2:B:1044:THR:O | 2:B:1044:THR:HG23 | 2.13 | 0.48 |
| 11:M:32:LEU:HD23 | 11:M:35:ILE:HD12 | 1.96 | 0.48 |
| 3:Y:286:ILE:HD12 | 3:Y:324:GLY:O | 2.12 | 0.48 |
| 11:M:63:ILE:HG22 | 11:M:64:ALA:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:359:VAL:HG11 | 2:B:407:VAL:HG22 | 1.94 | 0.48 |
| 1:A:763:THR:CG2 | 1:A:771:PRO:HB3 | 2.43 | 0.48 |
| 2:R:733:THR:HG23 | 2:R:735:TYR:HB2 | 1.96 | 0.48 |
| 6:F:51:SER:HA | 6:F:54:LYS:HD2 | 1.95 | 0.48 |
| 2:R:417:LEU:CG | 2:R:425:MET:HG3 | 2.43 | 0.48 |
| 4:D:129:PRO:HD2 | 12:N:15:ALA:HB1 | 1.96 | 0.48 |
| 4:D:161:LEU:CD1 | 4:D:163:ILE:HD13 | 2.43 | 0.48 |
| 4:S:153:HIS:O | 4:S:154:ALA:HB3 | 2.13 | 0.48 |
| 1:W:58:CYS:HB3 | 1:W:62:GLY:H | 1.79 | 0.48 |
| 1:W:655:ASP:H | 1:W:658:LYS:HD2 | 1.78 | 0.48 |
| 11:M:22:HIS:ND1 | 2:R:977:ARG:HB2 | 2.29 | 0.48 |
| 4:S:53:LEU:HD12 | 4:S:131:VAL:CG2 | 2.43 | 0.48 |
| 3:C:386:VAL:HG11 | 9:K:34:ARG:HB2 | 1.95 | 0.48 |
| 2:B:103:MET:SD | 2:B:384:LEU:HD13 | 2.54 | 0.48 |
| 2:R:103:MET:SD | 2:R:384:LEU:HD13 | 2.54 | 0.48 |
| 1:A:739:ASN:HB2 | 2:B:922:MET:SD | 2.54 | 0.48 |
| 2:R:1017:ARG:HD3 | 2:R:1098:TYR:CZ | 2.49 | 0.48 |
| 1:W:334:ILE:HD12 | 1:W:628:MET:HB3 | 1.95 | 0.48 |
| 1:A:640:GLU:OE1 | 2:B:977:ARG:NH1 | 2.46 | 0.48 |
| 2:R:980:GLN:HA | 4:S:22:LEU:HD21 | 1.94 | 0.48 |
| 4:D:38:VAL:CG1 | 4:D:39:MET:N | 2.77 | 0.48 |
| 2:B:493:TYR:CD1 | 2:B:499:PRO:HD3 | 2.49 | 0.48 |
| 2:R:843:ARG:HB2 | 2:R:846:GLU:CD | 2.34 | 0.48 |
| 5:E:40:LYS:O | 5:E:41:ASP:CG | 2.52 | 0.48 |
| 3:Y:281:GLU:OE1 | 3:Y:326:VAL:HG12 | 2.14 | 0.48 |
| 6:F:47:CYS:HB3 | 6:F:76:CYS:SG | 2.54 | 0.48 |
| 6:U:41:LEU:HA | 6:U:44:VAL:HG12 | 1.96 | 0.48 |
| 1:A:490:ARG:HD2 | 1:A:491:TYR:HD1 | 1.78 | 0.48 |
| 1:A:104:VAL:HG12 | 1:A:137:LYS:HG2 | 1.96 | 0.48 |
| 1:A:792:PRO:HA | 2:B:948:PHE:CE1 | 2.48 | 0.48 |
| 2:R:927:ILE:CG2 | 1:W:648:LEU:HB2 | 2.44 | 0.48 |
| 5:T:136:ILE:CG2 | 5:T:137:GLN:N | 2.76 | 0.48 |
| 2:R:598:GLU:HA | 2:R:605:ILE:HD11 | 1.92 | 0.48 |
| 12:O:9:THR:HG23 | 2:R:908:VAL:O | 2.13 | 0.48 |
| 9:K:51:ILE:O | 9:K:52:ASP:CG | 2.51 | 0.48 |
| 2:B:330:LEU:O | 2:B:332:ARG:N | 2.46 | 0.48 |
| 2:B:893:MET:CG | 2:B:894:LEU:N | 2.76 | 0.48 |
| 2:R:873:ARG:HH22 | 2:R:1002:ASP:CG | 2.17 | 0.48 |
| 2:B:984:SER:O | 2:B:985:ARG:CB | 2.61 | 0.48 |
| 5:E:83:GLU:O | 5:E:145:ARG:HA | 2.14 | 0.48 |
| 1:W:874:ARG:HG3 | 3:Y:53:ASP:OD2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:182:VAL:HG11 | 4:D:212:TYR:CD2 | 2.49 | 0.48 |
| 1:W:488:THR:HG23 | 1:W:493:GLY:O | 2.14 | 0.48 |
| 5:E:45:VAL:HG21 | 5:E:74:MET:SD | 2.54 | 0.48 |
| 5:T:59:LEU:HD12 | 3:Y:390:MET:HB2 | 1.96 | 0.48 |
| 2:B:115:GLU:O | 2:B:117:VAL:HG23 | 2.14 | 0.47 |
| 5:E:128:PHE:HB3 | 5:E:137:GLN:CD | 2.35 | 0.47 |
| 2:R:599:LYS:O | 2:R:600:LEU:C | 2.52 | 0.47 |
| 11:M:69:LEU:HD21 | 4:S:260:LEU:HD11 | 1.95 | 0.47 |
| 1:W:854:GLY:O | 3:Y:64:ILE:HG23 | 2.13 | 0.47 |
| 12:N:35:LEU:HD13 | 12:N:46:ARG:CG | 2.44 | 0.47 |
| 7:V:81:LEU:HD12 | 7:V:81:LEU:N | 2.29 | 0.47 |
| 2:R:808:LYS:HE3 | 2:R:847:MET:HE2 | 1.95 | 0.47 |
| 2:B:1061:ILE:HD12 | 2:B:1061:ILE:H | 1.78 | 0.47 |
| 1:A:510:THR:O | 1:A:597:VAL:HG23 | 2.14 | 0.47 |
| 1:A:532:ILE:HG13 | 1:A:533:ASP:O | 2.14 | 0.47 |
| 2:R:221:PRO:O | 2:R:278:ARG:HD2 | 2.14 | 0.47 |
| 2:B:295:ILE:O | 2:B:299:TYR:HB2 | 2.14 | 0.47 |
| 2:R:34:TYR:HB3 | 2:R:125:MET:CE | 2.43 | 0.47 |
| 2:B:593:THR:HG23 | 2:B:594:ARG:N | 2.29 | 0.47 |
| 2:B:364:PHE:CE1 | 2:B:388:VAL:HG13 | 2.48 | 0.47 |
| 1:A:792:PRO:N | 2:B:948:PHE:CE1 | 2.80 | 0.47 |
| 1:W:586:VAL:CG1 | 1:W:588:ILE:HD12 | 2.43 | 0.47 |
| 7:V:72:CYS:HB3 | 7:V:114:LYS:CG | 2.44 | 0.47 |
| 1:A:743:MET:CG | 2:B:922:MET:HG2 | 2.44 | 0.47 |
| 2:R:583:ILE:HG23 | 2:R:591:LEU:HD21 | 1.96 | 0.47 |
| 1:A:336:GLU:HA | 1:A:434:ARG:O | 2.14 | 0.47 |
| 3:Y:110:ILE:HD12 | 3:Y:296:GLU:HB3 | 1.97 | 0.47 |
| 2:R:186:ILE:CD1 | 2:R:209:LYS:HD3 | 2.43 | 0.47 |
| 1:W:818:TYR:O | 1:W:822:ARG:HG3 | 2.14 | 0.47 |
| 2:R:1061:ILE:HD12 | 2:R:1061:ILE:H | 1.78 | 0.47 |
| 2:B:843:ARG:HB2 | 2:B:846:GLU:CD | 2.35 | 0.47 |
| 2:R:448:LEU:HD21 | 1:W:796:PHE:CZ | 2.48 | 0.47 |
| 3:Y:160:ILE:O | 3:Y:161:ALA:C | 2.53 | 0.47 |
| 10:J:73:LYS:CE | 1:W:115:SER:HB3 | 2.44 | 0.47 |
| 2:R:852:LEU:HB3 | 2:R:868:ARG:HG2 | 1.96 | 0.47 |
| 1:A:729:ALA:O | 1:A:730:ARG:HB2 | 2.14 | 0.47 |
| 2:B:736:ASN:HA | 2:B:740:SER:HB3 | 1.95 | 0.47 |
| 1:A:569:SER:HB2 | 1:A:584:SER:HG | 1.79 | 0.47 |
| 1:A:586:VAL:CG1 | 1:A:588:ILE:HD12 | 2.43 | 0.47 |
| 7:V:36:PHE:CE1 | 7:V:96:ILE:HD11 | 2.49 | 0.47 |
| 13:X:24:VAL:O | 13:X:24:VAL:HG22 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:884:ARG:HH12 | 2:R:992:TYR:HB3 | 1.79 | 0.47 |
| 1:A:121:ILE:HG21 | 10:Q:66:ARG:HD3 | 1.96 | 0.47 |
| 1:W:304:GLY:C | 1:W:306:GLU:N | 2.68 | 0.47 |
| 3:Y:70:ILE:HD13 | 3:Y:70:ILE:H | 1.79 | 0.47 |
| 2:R:12:GLU:HG3 | 2:R:595:GLU:OE1 | 2.13 | 0.47 |
| 1:W:534:LEU:HB3 | 1:W:546:TYR:CE2 | 2.49 | 0.47 |
| 1:A:28:ILE:CG2 | 1:A:29:THR:N | 2.77 | 0.47 |
| 5:E:84:VAL:CG1 | 6:F:75:ILE:CD1 | 2.92 | 0.47 |
| 1:W:29:THR:HB | 1:W:30:PRO:HD3 | 1.97 | 0.47 |
| 1:A:758:LYS:HA | 1:A:779:ARG:HH11 | 1.80 | 0.47 |
| 2:R:1040:ILE:CG2 | 3:Y:72:ILE:HG13 | 2.45 | 0.47 |
| 2:R:245:VAL:HA | 2:R:319:ALA:HB1 | 1.96 | 0.47 |
| 2:R:245:VAL:HG22 | 2:R:319:ALA:HB1 | 1.95 | 0.47 |
| 2:B:109:ASN:CG | 2:B:109:ASN:O | 2.52 | 0.47 |
| 1:A:426:HIS:CG | 3:C:80:GLU:CD | 2.88 | 0.47 |
| 3:C:64:ILE:HG21 | 9:K:19:PHE:HE1 | 1.78 | 0.47 |
| 8:Z:45:ILE:HG23 | 8:Z:81:VAL:HG22 | 1.96 | 0.47 |
| 2:B:332:ARG:HD2 | 2:B:565:PHE:HB3 | 1.97 | 0.47 |
| 12:N:3:ILE:HD13 | 12:N:15:ALA:CA | 2.43 | 0.47 |
| 4:S:154:ALA:C | 4:S:156:PHE:H | 2.16 | 0.47 |
| 12:O:5:ILE:O | 12:O:6:ARG:HB2 | 2.14 | 0.47 |
| 2:B:699:HIS:HD1 | 4:D:57:ILE:HG12 | 1.78 | 0.47 |
| 2:B:301:LEU:HB3 | 2:B:304:LEU:HD12 | 1.95 | 0.47 |
| 5:E:53:THR:O | 5:E:54:SER:C | 2.52 | 0.47 |
| 2:B:245:VAL:HG22 | 2:B:319:ALA:HB1 | 1.95 | 0.47 |
| 2:R:586:SER:O | 2:R:587:ASN:HB2 | 2.14 | 0.47 |
| 2:R:766:VAL:HG13 | 2:R:767:LYS:N | 2.30 | 0.47 |
| 1:A:490:ARG:HH21 | 3:C:80:GLU:HG2 | 1.80 | 0.47 |
| 2:B:605:ILE:HG12 | 2:B:606:THR:N | 2.24 | 0.47 |
| 2:R:603:GLY:C | 2:R:605:ILE:N | 2.66 | 0.47 |
| 1:W:95:LYS:O | 1:W:138:LYS:HG2 | 2.14 | 0.47 |
| 8:H:12:ARG:HH22 | 8:H:55:ILE:HD12 | 1.79 | 0.47 |
| 2:R:249:PRO:HD2 | 2:R:253:ASN:OD1 | 2.14 | 0.47 |
| 2:B:330:LEU:O | 2:B:332:ARG:CG | 2.62 | 0.47 |
| 2:R:1017:ARG:HD3 | 2:R:1098:TYR:CG | 2.48 | 0.47 |
| 2:R:1062:TYR:HE2 | 2:R:1093:PRO:HG3 | 1.80 | 0.47 |
| 1:A:565:GLN:HB3 | 1:A:569:SER:HB3 | 1.96 | 0.47 |
| 2:B:370:TYR:O | 2:B:370:TYR:CG | 2.68 | 0.47 |
| 2:B:70:LYS:HB3 | 2:B:71:PRO:HD2 | 1.96 | 0.47 |
| 2:B:126:LEU:HD13 | 2:B:154:TYR:O | 2.14 | 0.47 |
| 3:Y:192:LYS:O | 3:Y:194:GLY:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:K:71:ARG:HB3 | 9:K:73:VAL:HG22 | 1.96 | 0.47 |
| 5:T:8:ARG:NE | 5:T:69:GLU:OE2 | 2.48 | 0.47 |
| 1:A:10:LYS:HG2 | 3:C:363:VAL:CG1 | 2.45 | 0.47 |
| 2:R:356:LEU:O | 2:R:359:VAL:HG12 | 2.14 | 0.47 |
| 1:A:338:GLY:HA3 | 1:A:444:ARG:CG | 2.45 | 0.47 |
| 2:R:63:LEU:HD23 | 2:R:103:MET:HG2 | 1.96 | 0.47 |
| 5:T:119:LYS:HG2 | 5:T:120:TYR:CD2 | 2.49 | 0.47 |
| 1:W:821:ARG:HA | 1:W:824:ILE:HG22 | 1.96 | 0.47 |
| 1:A:651:VAL:CG1 | 1:A:743:MET:HB3 | 2.43 | 0.47 |
| 2:B:1082:CYS:HB2 | 2:B:1083:PRO:HD2 | 1.97 | 0.47 |
| 3:C:303:GLU:C | 3:C:303:GLU:OE1 | 2.52 | 0.47 |
| 2:R:657:ILE:HG13 | 2:R:711:LEU:CD2 | 2.44 | 0.47 |
| 11:L:11:ASN:HB3 | 11:L:59:THR:HG23 | 1.96 | 0.47 |
| 3:Y:80:GLU:N | 3:Y:81:PRO:CD | 2.78 | 0.47 |
| 2:B:396:ARG:NH2 | 2:B:406:TRP:CZ2 | 2.83 | 0.47 |
| 2:R:647:SER:HB2 | 2:R:648:PRO:HD3 | 1.97 | 0.47 |
| 7:V:33:CYS:HB3 | 7:V:36:PHE:O | 2.14 | 0.47 |
| 1:A:103:ARG:CG | 1:A:191:ASP:OD1 | 2.63 | 0.47 |
| 5:T:114:THR:CG2 | 5:T:131:LYS:HD3 | 2.45 | 0.47 |
| 2:R:371:GLN:HG2 | 2:R:387:LEU:O | 2.14 | 0.47 |
| 3:Y:33:LYS:HG3 | 3:Y:34:ASN:N | 2.30 | 0.47 |
| 2:R:525:LEU:O | 2:R:528:ARG:HB3 | 2.13 | 0.47 |
| 2:B:136:TYR:HB3 | 2:B:141:LEU:CD1 | 2.44 | 0.47 |
| 2:R:157:VAL:CG1 | 2:R:401:LEU:HD23 | 2.44 | 0.47 |
| 3:Y:147:THR:HB | 3:Y:232:LYS:CB | 2.45 | 0.47 |
| 2:B:330:LEU:HD22 | 2:B:332:ARG:HH11 | 1.79 | 0.47 |
| 7:V:24:LYS:O | 1:W:513:THR:HG21 | 2.15 | 0.47 |
| 2:R:1046:MET:HG2 | 5:T:61:PHE:CE1 | 2.50 | 0.47 |
| 1:W:505:GLY:HA3 | 1:W:639:VAL:CG2 | 2.44 | 0.47 |
| 5:T:83:GLU:O | 5:T:145:ARG:HA | 2.14 | 0.47 |
| 2:B:372:LEU:CD2 | 2:B:376:LYS:CE | 2.92 | 0.47 |
| 2:B:520:TRP:O | 2:B:521:SER:HB3 | 2.14 | 0.47 |
| 2:B:1015:LEU:CD1 | 2:B:1102:LEU:HD11 | 2.45 | 0.47 |
| 1:W:782:ILE:HG23 | 1:W:794:GLU:CD | 2.35 | 0.47 |
| 1:A:316:LYS:HD3 | 2:B:1056:SER:HB3 | 1.97 | 0.47 |
| 2:R:1056:SER:CB | 2:R:1057:ASP:OD1 | 2.62 | 0.47 |
| 2:R:457:CYS:SG | 2:R:460:GLU:HB2 | 2.54 | 0.47 |
| 2:R:73:VAL:O | 2:R:73:VAL:HG13 | 2.15 | 0.47 |
| 2:R:126:LEU:HD21 | 2:R:156:ILE:HD11 | 1.97 | 0.47 |
| 2:R:370:TYR:O | 2:R:370:TYR:CG | 2.68 | 0.47 |
| 3:Y:241:ILE:O | 3:Y:251:ILE:HG23 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:K:27:LEU:HD23 | 9:K:78:ILE:CD1 | 2.44 | 0.47 |
| 9:I:23:TRP:CE2 | 3:Y:66:PRO:HD3 | 2.50 | 0.47 |
| 2:R:1111:ILE:HG22 | 2:R:1111:ILE:O | 2.15 | 0.47 |
| 2:R:1099:ALA:C | 1:W:313:LEU:HD21 | 2.35 | 0.47 |
| 7:V:31:MET:HE2 | 7:V:55:VAL:HG11 | 1.97 | 0.47 |
| 2:R:1009:ARG:NH2 | 1:W:385:ARG:NH1 | 2.62 | 0.47 |
| 5:E:6:LYS:HA | 5:E:72:PHE:O | 2.14 | 0.47 |
| 5:T:30:LEU:HD22 | 5:T:72:PHE:CD2 | 2.49 | 0.47 |
| 1:W:855:VAL:HG13 | 3:Y:63:LEU:O | 2.15 | 0.47 |
| 2:R:1069:TYR:HB2 | 2:R:1070:ILE:HB | 1.97 | 0.47 |
| 1:A:141:MET:CA | 1:A:148:HIS:HB3 | 2.45 | 0.47 |
| 1:A:241:ASP:OD2 | 1:A:289:HIS:NE2 | 2.48 | 0.47 |
| 2:R:730:ILE:CG2 | 2:R:732:PHE:HB2 | 2.45 | 0.47 |
| 3:C:277:ILE:CG2 | 3:C:278:ARG:N | 2.77 | 0.47 |
| 2:B:1053:LEU:HD23 | 2:B:1054:ASP:OD1 | 2.15 | 0.47 |
| 6:F:88:ILE:HD13 | 6:F:88:ILE:H | 1.79 | 0.47 |
| 3:Y:215:SER:O | 3:Y:216:ILE:HB | 2.15 | 0.47 |
| 3:Y:277:ILE:HG13 | 3:Y:292:ILE:HD12 | 1.97 | 0.47 |
| 2:B:372:LEU:HD23 | 2:B:376:LYS:HG2 | 1.97 | 0.47 |
| 9:I:41:LEU:HD12 | 1:W:470:GLU:HG3 | 1.96 | 0.47 |
| 10:J:62:ASP:O | 10:J:66:ARG:HB3 | 2.14 | 0.47 |
| 2:R:977:ARG:NH1 | 1:W:640:GLU:OE1 | 2.48 | 0.47 |
| 1:W:73:GLY:O | 1:W:74:HIS:ND1 | 2.48 | 0.47 |
| 2:R:166:THR:CG2 | 2:R:432:VAL:HG12 | 2.45 | 0.47 |
| 1:A:749:GLN:HA | 1:A:781:PHE:HA | 1.97 | 0.47 |
| 2:R:778:MET:HE1 | 2:R:795:LEU:HB2 | 1.96 | 0.47 |
| 3:Y:372:ASN:ND2 | 3:Y:380:LYS:HE3 | 2.29 | 0.47 |
| 2:R:585:VAL:HG13 | 2:R:589:ASN:H | 1.79 | 0.47 |
| 7:G:33:CYS:HB3 | 7:G:36:PHE:O | 2.15 | 0.47 |
| 2:B:708:THR:HG23 | 2:B:946:THR:HA | 1.97 | 0.47 |
| 2:R:609:ASP:O | 2:R:613:GLN:HB2 | 2.14 | 0.47 |
| 1:W:141:MET:HA | 1:W:148:HIS:HB2 | 1.96 | 0.47 |
| 1:W:95:LYS:HB3 | 1:W:138:LYS:CG | 2.43 | 0.47 |
| 2:R:330:LEU:HD22 | 2:R:332:ARG:HD3 | 1.96 | 0.47 |
| 5:E:60:VAL:HG22 | 5:E:61:PHE:N | 2.29 | 0.47 |
| 2:B:583:ILE:HG23 | 2:B:591:LEU:HD21 | 1.97 | 0.47 |
| 2:B:956:LEU:O | 2:B:960:ILE:HG12 | 2.15 | 0.47 |
| 3:Y:176:ASP:O | 3:Y:177:LYS:CG | 2.62 | 0.47 |
| 2:R:787:LYS:HE3 | 2:R:841:VAL:HG23 | 1.97 | 0.47 |
| 6:F:12:ILE:CG2 | 6:F:16:VAL:HG13 | 2.44 | 0.47 |
| 1:W:853:ASP:HB2 | 3:Y:311:ARG:NH1 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:863:GLY:HA2 | 3:Y:311:ARG:NH2 | 2.30 | 0.47 |
| 2:B:166:THR:CG2 | 2:B:432:VAL:HG12 | 2.44 | 0.47 |
| 1:A:829:ASP:O | 1:A:840:SER:HA | 2.15 | 0.47 |
| 1:A:326:ILE:HG21 | 1:A:462:MET:SD | 2.55 | 0.47 |
| 1:A:23:SER:O | 1:A:24:VAL:HG13 | 2.15 | 0.47 |
| 3:Y:328:GLN:HG2 | 3:Y:330:GLY:H | 1.80 | 0.47 |
| 13:P:4:TYR:CD1 | 13:P:4:TYR:O | 2.67 | 0.47 |
| 2:R:657:ILE:HG13 | 2:R:711:LEU:HD21 | 1.96 | 0.47 |
| 2:B:422:TRP:HZ3 | 2:B:715:GLY:HA3 | 1.80 | 0.47 |
| 2:R:928:MET:HG2 | 1:W:648:LEU:HD11 | 1.96 | 0.47 |
| 2:R:532:TYR:O | 2:R:533:TYR:CB | 2.62 | 0.47 |
| 13:P:37:VAL:HG22 | 13:P:38:ARG:H | 1.80 | 0.47 |
| 2:B:724:ASN:O | 12:N:47:ARG:HD2 | 2.15 | 0.47 |
| 1:A:336:GLU:OE2 | 1:A:436:ARG:HB2 | 2.15 | 0.47 |
| 2:R:1062:TYR:CE2 | 2:R:1093:PRO:HG3 | 2.50 | 0.47 |
| 12:O:5:ILE:HA | 12:O:15:ALA:HB2 | 1.97 | 0.47 |
| 2:R:787:LYS:HE3 | 2:R:841:VAL:HG21 | 1.97 | 0.47 |
| 3:Y:330:GLY:C | 3:Y:335:THR:HG22 | 2.34 | 0.47 |
| 2:R:492:LEU:HB3 | 2:R:497:VAL:HG21 | 1.97 | 0.47 |
| 2:B:232:ALA:HB2 | 2:B:271:ALA:CB | 2.45 | 0.47 |
| 4:S:41:ILE:HB | 4:S:63:ALA:HA | 1.97 | 0.47 |
| 1:W:774:ILE:HG22 | 1:W:774:ILE:O | 2.15 | 0.47 |
| 2:R:893:MET:HG3 | 2:R:894:LEU:N | 2.30 | 0.47 |
| 1:A:49:LEU:HD12 | 1:A:49:LEU:N | 2.30 | 0.47 |
| 3:C:167:LEU:N | 3:C:167:LEU:HD12 | 2.30 | 0.47 |
| 3:C:390:MET:HB2 | 5:E:59:LEU:HD12 | 1.96 | 0.47 |
| 3:C:192:LYS:O | 3:C:194:GLY:N | 2.48 | 0.47 |
| 1:W:419:PHE:HZ | 1:W:443:PHE:HB3 | 1.80 | 0.46 |
| 2:B:371:GLN:HG2 | 2:B:387:LEU:O | 2.15 | 0.46 |
| 1:W:238:LYS:HE2 | 1:W:297:THR:CG2 | 2.45 | 0.46 |
| 1:W:451:PRO:HB2 | 1:W:495:ILE:O | 2.15 | 0.46 |
| 7:G:8:GLU:HG2 | 7:G:9:ILE:H | 1.80 | 0.46 |
| 2:B:404:GLY:O | 2:B:405:ASN:O | 2.32 | 0.46 |
| 6:F:71:VAL:HG11 | 6:F:89:MET:CE | 2.43 | 0.46 |
| 11:L:18:GLU:O | 11:L:18:GLU:CG | 2.62 | 0.46 |
| 2:R:430:ARG:NH1 | 2:R:653:ILE:HG13 | 2.30 | 0.46 |
| 2:B:430:ARG:HH11 | 2:B:653:ILE:CG1 | 2.28 | 0.46 |
| 2:B:1062:TYR:CE2 | 2:B:1080:TYR:HE1 | 2.33 | 0.46 |
| 3:Y:127:THR:N | 3:Y:268:ASP:HB2 | 2.30 | 0.46 |
| 11:L:46:PRO:HD2 | 11:L:52:LYS:O | 2.15 | 0.46 |
| 2:B:665:GLN:HG2 | 2:B:667:PRO:HD2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:THR:O | 1:A:180:ILE:HG13 | 2.15 | 0.46 |
| 2:R:580:ARG:HA | 2:R:581:PRO:HD3 | 1.78 | 0.46 |
| 1:A:573:ARG:HA | 1:A:582:HIS:CD2 | 2.50 | 0.46 |
| 2:R:1082:CYS:HB2 | 2:R:1083:PRO:HD2 | 1.96 | 0.46 |
| 1:A:321:SER:OG | 2:B:1029:LEU:HB2 | 2.16 | 0.46 |
| 5:E:132:SER:O | 5:E:133:LYS:HB2 | 2.16 | 0.46 |
| 1:A:67:ASN:OD1 | 2:B:1072:TRP:CZ3 | 2.68 | 0.46 |
| 11:M:11:ASN:HB3 | 11:M:59:THR:HG23 | 1.96 | 0.46 |
| 6:U:47:CYS:HB3 | 6:U:76:CYS:SG | 2.55 | 0.46 |
| 2:B:396:ARG:O | 2:B:396:ARG:HG2 | 2.14 | 0.46 |
| 2:R:1091:LEU:O | 2:R:1092:PHE:CG | 2.68 | 0.46 |
| 1:W:13:ILE:HG13 | 1:W:202:SER:CB | 2.46 | 0.46 |
| 5:T:83:GLU:HA | 6:U:89:MET:CE | 2.44 | 0.46 |
| 2:R:42:LEU:HD12 | 2:R:357:PHE:CE2 | 2.51 | 0.46 |
| 1:A:29:THR:HB | 1:A:30:PRO:HD3 | 1.97 | 0.46 |
| 5:E:84:VAL:HG21 | 6:F:75:ILE:HD13 | 1.95 | 0.46 |
| 5:T:40:LYS:O | 5:T:41:ASP:CG | 2.53 | 0.46 |
| 9:K:90:LEU:HA | 9:K:90:LEU:HD23 | 1.61 | 0.46 |
| 2:R:562:VAL:O | 2:R:566:ILE:O | 2.33 | 0.46 |
| 2:R:662:GLU:O | 1:W:789:GLY:HA2 | 2.15 | 0.46 |
| 1:A:646:MET:HG2 | 2:B:918:LEU:CD1 | 2.45 | 0.46 |
| 5:E:90:LEU:HD13 | 5:E:100:ASN:OD1 | 2.15 | 0.46 |
| 2:R:767:LYS:HD3 | 2:R:768:TYR:O | 2.15 | 0.46 |
| 2:B:103:MET:O | 2:B:114:PRO:O | 2.34 | 0.46 |
| 9:K:13:LEU:O | 9:K:14:HIS:C | 2.53 | 0.46 |
| 2:R:928:MET:HG2 | 1:W:648:LEU:CD1 | 2.45 | 0.46 |
| 1:W:105:LYS:HE2 | 1:W:108:GLU:OE1 | 2.15 | 0.46 |
| 3:C:277:ILE:HG13 | 3:C:292:ILE:HD12 | 1.97 | 0.46 |
| 1:A:513:THR:HG21 | 7:G:24:LYS:O | 2.15 | 0.46 |
| 2:R:948:PHE:HE1 | 1:W:792:PRO:N | 2.13 | 0.46 |
| 5:E:123:VAL:HG22 | 5:E:127:ILE:HG23 | 1.98 | 0.46 |
| 3:Y:174:LEU:CB | 3:Y:179:VAL:HG13 | 2.44 | 0.46 |
| 2:R:476:MET:HE1 | 2:R:645:ILE:HD12 | 1.98 | 0.46 |
| 2:B:476:MET:HE1 | 2:B:645:ILE:HD12 | 1.96 | 0.46 |
| 1:A:334:ILE:HD12 | 1:A:628:MET:CB | 2.45 | 0.46 |
| 2:B:399:HIS:O | 2:B:403:THR:HG21 | 2.16 | 0.46 |
| 3:Y:331:ARG:H | 3:Y:331:ARG:HD3 | 1.80 | 0.46 |
| 11:M:84:ILE:CD1 | 4:S:246:GLY:HA3 | 2.45 | 0.46 |
| 2:B:491:THR:HG22 | 2:B:495:MET:HE2 | 1.98 | 0.46 |
| 1:W:729:ALA:O | 1:W:730:ARG:HB2 | 2.16 | 0.46 |
| 2:B:131:ASP:OD1 | 2:B:132:PRO:HD2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:T:90:LEU:HD13 | 5:T:100:ASN:OD1 | 2.15 | 0.46 |
| 1:A:104:VAL:HG11 | 1:A:137:LYS:O | 2.15 | 0.46 |
| 13:P:5:ARG:CZ | 13:P:6:CYS:O | 2.63 | 0.46 |
| 5:T:167:PRO:C | 5:T:169:LEU:H | 2.19 | 0.46 |
| 1:A:498:ALA:H | 1:A:604:GLY:H | 1.62 | 0.46 |
| 5:E:82:GLN:H | 5:E:146:VAL:HG13 | 1.80 | 0.46 |
| 2:B:417:LEU:CG | 2:B:425:MET:HG3 | 2.46 | 0.46 |
| 1:W:45:MET:O | 1:W:45:MET:CG | 2.60 | 0.46 |
| 1:A:331:ASN:O | 1:A:332:ILE:CG1 | 2.63 | 0.46 |
| 2:B:720:PRO:HG3 | 12:N:53:ILE:HD12 | 1.98 | 0.46 |
| 3:Y:286:ILE:HG12 | 8:Z:49:ASP:CG | 2.36 | 0.46 |
| 9:K:27:LEU:CD2 | 9:K:78:ILE:HD11 | 2.46 | 0.46 |
| 1:A:748:GLY:HA2 | 1:A:781:PHE:CE1 | 2.51 | 0.46 |
| 3:C:102:LEU:HD11 | 3:C:118:SER:HB3 | 1.97 | 0.46 |
| 2:B:460:GLU:HG2 | 2:B:673:SER:HB3 | 1.96 | 0.46 |
| 2:B:772:GLN:HG2 | 2:B:773:GLU:N | 2.31 | 0.46 |
| 1:A:337:VAL:HG21 | 1:A:419:PHE:CE1 | 2.51 | 0.46 |
| 1:W:600:LYS:O | 1:W:601:LYS:CB | 2.56 | 0.46 |
| 2:B:27:VAL:O | 2:B:29:GLN:N | 2.40 | 0.46 |
| 2:R:539:LEU:O | 2:R:543:ILE:HG13 | 2.15 | 0.46 |
| 2:B:533:TYR:CE2 | 2:B:539:LEU:HB2 | 2.51 | 0.46 |
| 4:S:161:LEU:O | 4:S:230:LEU:HA | 2.16 | 0.46 |
| 1:A:220:ARG:HG2 | 1:A:235:LEU:HD22 | 1.97 | 0.46 |
| 2:R:163:VAL:O | 2:R:163:VAL:HG13 | 2.16 | 0.46 |
| 4:S:83:ILE:HD12 | 4:S:84:ASP:N | 2.30 | 0.46 |
| 3:Y:286:ILE:HG12 | 8:Z:49:ASP:OD1 | 2.16 | 0.46 |
| 2:R:232:ALA:HB2 | 2:R:271:ALA:CB | 2.46 | 0.46 |
| 1:A:145:VAL:O | 1:A:145:VAL:HG13 | 2.15 | 0.46 |
| 2:B:585:VAL:HG13 | 2:B:589:ASN:H | 1.80 | 0.46 |
| 2:B:356:LEU:CA | 2:B:407:VAL:HG21 | 2.38 | 0.46 |
| 2:B:63:LEU:CD2 | 2:B:103:MET:HE2 | 2.46 | 0.46 |
| 2:R:646:TRP:CZ2 | 2:R:946:THR:HG21 | 2.51 | 0.46 |
| 2:B:646:TRP:CZ2 | 2:B:946:THR:HG21 | 2.50 | 0.46 |
| 1:W:141:MET:CA | 1:W:148:HIS:HB3 | 2.46 | 0.46 |
| 2:B:730:ILE:CG2 | 2:B:732:PHE:HB2 | 2.46 | 0.46 |
| 3:C:215:SER:O | 3:C:216:ILE:HB | 2.15 | 0.46 |
| 1:A:856:PHE:CE2 | 1:A:858:MET:CB | 2.98 | 0.46 |
| 1:A:353:ILE:HD13 | 1:A:405:TYR:HB2 | 1.97 | 0.46 |
| 2:B:430:ARG:NH1 | 2:B:653:ILE:HG13 | 2.30 | 0.46 |
| 2:B:245:VAL:HA | 2:B:319:ALA:HB1 | 1.97 | 0.46 |
| 2:B:463:GLU:OE1 | 2:B:463:GLU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:833:GLU:HG3 | 1:W:839:ARG:CD | 2.45 | 0.46 |
| 5:T:44:LEU:O | 5:T:46:LEU:HD12 | 2.16 | 0.46 |
| 3:Y:30:GLU:O | 3:Y:33:LYS:HG2 | 2.16 | 0.46 |
| 2:B:672:GLN:HG2 | 2:B:884:ARG:O | 2.16 | 0.46 |
| 1:W:262:ILE:O | 1:W:266:TRP:HB3 | 2.16 | 0.46 |
| 9:I:49:ALA:O | 9:I:50:LEU:C | 2.54 | 0.46 |
| 2:R:467:SER:OG | 1:W:806:LEU:HB3 | 2.16 | 0.46 |
| 2:B:582:LEU:HD12 | 2:B:619:LEU:CD1 | 2.45 | 0.46 |
| 2:R:118:TYR:C | 2:R:118:TYR:CD1 | 2.89 | 0.46 |
| 2:R:71:PRO:HA | 2:R:97:ALA:HB2 | 1.98 | 0.46 |
| 1:A:451:PRO:N | 1:A:452:PRO:CD | 2.79 | 0.46 |
| 3:Y:133:ASP:O | 3:Y:249:TYR:CE2 | 2.69 | 0.46 |
| 3:C:372:ASN:ND2 | 3:C:380:LYS:HE3 | 2.31 | 0.46 |
| 1:A:181:ARG:NH1 | 1:A:210:THR:OG1 | 2.49 | 0.46 |
| 5:T:119:LYS:O | 5:T:131:LYS:HA | 2.16 | 0.46 |
| 2:R:732:PHE:C | 2:R:733:THR:HG22 | 2.36 | 0.46 |
| 3:C:340:SER:HB3 | 3:C:371:GLU:OE2 | 2.16 | 0.46 |
| 2:R:162:ARG:HG2 | 2:R:402:ALA:HA | 1.98 | 0.46 |
| 2:R:904:VAL:O | 4:S:163:ILE:HG12 | 2.15 | 0.46 |
| 2:B:872:LEU:HD23 | 2:B:873:ARG:H | 1.81 | 0.46 |
| 2:R:947:PRO:HB2 | 2:R:948:PHE:CD2 | 2.51 | 0.46 |
| 4:S:17:PHE:CD2 | 4:S:25:VAL:HG22 | 2.51 | 0.46 |
| 5:T:123:VAL:HG22 | 5:T:127:ILE:HG23 | 1.98 | 0.46 |
| 1:A:249:LEU:HG | 1:A:265:LEU:CB | 2.46 | 0.46 |
| 3:Y:104:LEU:CD1 | 3:Y:108:ILE:HD11 | 2.45 | 0.46 |
| 3:Y:108:ILE:O | 3:Y:112:ASP:HB2 | 2.16 | 0.46 |
| 1:W:830:LEU:HD13 | 3:Y:315:LEU:HD21 | 1.97 | 0.46 |
| 3:C:33:LYS:HG3 | 3:C:34:ASN:N | 2.30 | 0.46 |
| 1:A:58:CYS:HB3 | 1:A:62:GLY:H | 1.80 | 0.46 |
| 2:R:232:ALA:HB2 | 2:R:271:ALA:HB1 | 1.98 | 0.46 |
| 2:B:763:THR:HG22 | 2:B:764:GLU:O | 2.16 | 0.46 |
| 2:R:396:ARG:O | 2:R:396:ARG:HG2 | 2.16 | 0.46 |
| 2:R:646:TRP:CH2 | 2:R:648:PRO:HB2 | 2.50 | 0.46 |
| 2:B:660:TYR:N | 2:B:661:PRO:CD | 2.79 | 0.46 |
| 2:B:938:LEU:HD23 | 12:N:43:TYR:HB3 | 1.98 | 0.46 |
| 1:W:124:ARG:NH2 | 3:Y:323:THR:HG21 | 2.31 | 0.46 |
| 4:D:53:LEU:CD1 | 4:D:131:VAL:HG23 | 2.44 | 0.46 |
| 2:B:1007:ARG:CZ | 2:B:1028:GLY:N | 2.78 | 0.46 |
| 8:H:28:ALA:CB | 8:H:62:ILE:HD11 | 2.46 | 0.46 |
| 1:W:331:ASN:O | 1:W:332:ILE:CG1 | 2.64 | 0.46 |
| 2:B:741:ILE:HD11 | 2:B:911:VAL:CG1 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:759:ARG:HG3 | 2:B:760:LEU:N | 2.30 | 0.46 |
| 2:B:666:SER:N | 2:B:667:PRO:HD2 | 2.31 | 0.46 |
| 2:B:254:GLU:O | 2:B:254:GLU:HG2 | 2.16 | 0.46 |
| 4:S:50:ASN:ND2 | 4:S:137:GLN:HG2 | 2.30 | 0.46 |
| 2:B:221:PRO:O | 2:B:278:ARG:HD2 | 2.15 | 0.46 |
| 2:R:63:LEU:HD22 | 2:R:103:MET:HE2 | 1.96 | 0.45 |
| 5:T:167:PRO:HA | 5:T:169:LEU:HD13 | 1.98 | 0.45 |
| 2:R:686:ASN:C | 2:R:688:GLN:N | 2.68 | 0.45 |
| 4:D:108:MET:SD | 4:D:132:LEU:HD23 | 2.55 | 0.45 |
| 4:S:153:HIS:CG | 4:S:153:HIS:O | 2.69 | 0.45 |
| 12:O:3:ILE:HG12 | 12:O:18:TRP:CB | 2.46 | 0.45 |
| 2:R:1007:ARG:HH21 | 2:R:1026:GLU:C | 2.19 | 0.45 |
| 1:W:81:VAL:HG11 | 1:W:269:LEU:O | 2.17 | 0.45 |
| 5:T:56:GLU:OE1 | 3:Y:389:THR:HG21 | 2.16 | 0.45 |
| 2:R:493:TYR:OH | 2:R:530:VAL:HG13 | 2.15 | 0.45 |
| 5:E:8:ARG:NE | 5:E:69:GLU:OE2 | 2.49 | 0.45 |
| 1:W:777:GLU:CD | 1:W:777:GLU:H | 2.19 | 0.45 |
| 1:W:361:LEU:HD23 | 1:W:407:VAL:HB | 1.98 | 0.45 |
| 2:R:1021:GLU:OE2 | 2:R:1022:GLY:N | 2.49 | 0.45 |
| 3:Y:81:PRO:O | 3:Y:83:THR:N | 2.49 | 0.45 |
| 2:B:112:ALA:O | 2:B:113:GLU:HG3 | 2.16 | 0.45 |
| 7:V:36:PHE:CE1 | 7:V:96:ILE:HG12 | 2.51 | 0.45 |
| 5:T:128:PHE:HB3 | 5:T:137:GLN:CD | 2.37 | 0.45 |
| 10:Q:61:VAL:C | 10:Q:63:GLU:N | 2.70 | 0.45 |
| 1:A:105:LYS:HD3 | 1:A:136:VAL:HG11 | 1.97 | 0.45 |
| 2:B:1017:ARG:HD3 | 2:B:1098:TYR:CZ | 2.51 | 0.45 |
| 3:C:277:ILE:C | 3:C:279:GLU:N | 2.67 | 0.45 |
| 12:N:3:ILE:HG12 | 12:N:18:TRP:CB | 2.46 | 0.45 |
| 6:F:86:ILE:HG23 | 6:F:89:MET:SD | 2.56 | 0.45 |
| 3:Y:151:ASN:O | 3:Y:173:MET:HG3 | 2.17 | 0.45 |
| 1:W:505:GLY:CA | 1:W:639:VAL:HG22 | 2.46 | 0.45 |
| 2:R:582:LEU:HD12 | 2:R:619:LEU:CD1 | 2.46 | 0.45 |
| 3:C:107:LEU:O | 3:C:110:ILE:HG22 | 2.15 | 0.45 |
| 3:C:110:ILE:HD13 | 3:C:297:ILE:HG12 | 1.97 | 0.45 |
| 2:R:1007:ARG:CZ | 2:R:1028:GLY:N | 2.80 | 0.45 |
| 2:R:430:ARG:HH11 | 2:R:653:ILE:CG1 | 2.29 | 0.45 |
| 1:A:687:ILE:HG13 | 1:A:699:TYR:OH | 2.16 | 0.45 |
| 6:U:12:ILE:CG2 | 6:U:16:VAL:HG13 | 2.45 | 0.45 |
| 2:R:589:ASN:HA | 2:R:590:PRO:HD3 | 1.73 | 0.45 |
| 7:G:76:TYR:CD1 | 7:G:76:TYR:N | 2.84 | 0.45 |
| 7:V:75:GLY:HA3 | 7:V:86:SER:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:580:CYS:HA | 1:A:581:PRO:HD3 | 1.75 | 0.45 |
| 2:B:594:ARG:NH1 | 2:B:615:LYS:CB | 2.76 | 0.45 |
| 2:B:609:ASP:O | 2:B:613:GLN:HB2 | 2.16 | 0.45 |
| 2:B:397:ILE:O | 2:B:397:ILE:HG12 | 2.16 | 0.45 |
| 2:B:396:ARG:NH2 | 2:B:406:TRP:CZ3 | 2.85 | 0.45 |
| 2:R:213:PHE:HB2 | 2:R:259:LEU:CG | 2.46 | 0.45 |
| 3:C:258:LEU:HD11 | 3:C:272:VAL:HG11 | 1.98 | 0.45 |
| 2:R:1003:LYS:O | 2:R:1004:ILE:C | 2.54 | 0.45 |
| 2:R:752:MET:HG2 | 2:R:753:TYR:CD2 | 2.51 | 0.45 |
| 3:C:292:ILE:HB | 8:H:16:LEU:HD13 | 1.98 | 0.45 |
| 2:R:903:THR:HA | 2:R:973:THR:HG22 | 1.97 | 0.45 |
| 2:R:982:ILE:CD1 | 2:R:984:SER:H | 2.29 | 0.45 |
| 1:W:872:PHE:CZ | 1:W:876:VAL:HG21 | 2.51 | 0.45 |
| 1:W:336:GLU:HA | 1:W:434:ARG:O | 2.16 | 0.45 |
| 1:W:13:ILE:HG13 | 1:W:202:SER:HB3 | 1.98 | 0.45 |
| 1:W:682:GLY:O | 1:W:683:GLU:C | 2.55 | 0.45 |
| 2:R:520:TRP:O | 2:R:521:SER:HB3 | 2.16 | 0.45 |
| 3:C:133:ASP:O | 3:C:249:TYR:CE2 | 2.69 | 0.45 |
| 1:A:451:PRO:HB2 | 1:A:495:ILE:O | 2.16 | 0.45 |
| 2:R:895:ILE:HG23 | 2:R:899:ASP:HB2 | 1.98 | 0.45 |
| 1:W:599:ASP:N | 1:W:599:ASP:OD1 | 2.49 | 0.45 |
| 1:A:361:LEU:HD23 | 1:A:407:VAL:HB | 1.96 | 0.45 |
| 1:A:519:GLU:HG2 | 11:L:33:ARG:HD2 | 1.99 | 0.45 |
| 2:B:1064:CYS:HB3 | 2:B:1068:GLY:H | 1.81 | 0.45 |
| 11:M:33:ARG:HD2 | 1:W:519:GLU:HG2 | 1.98 | 0.45 |
| 3:Y:284:PHE:HB3 | 3:Y:288:ALA:HB1 | 1.98 | 0.45 |
| 7:G:29:ILE:CD1 | 7:G:42:ILE:HG13 | 2.46 | 0.45 |
| 2:R:127:LYS:HE3 | 2:R:150:ASP:O | 2.16 | 0.45 |
| 7:G:67:THR:HG22 | 7:G:68:ASN:H | 1.81 | 0.45 |
| 2:B:974:TYR:HA | 2:B:981:LYS:HA | 1.98 | 0.45 |
| 2:R:136:TYR:CB | 2:R:141:LEU:CD1 | 2.94 | 0.45 |
| 2:R:1042:PHE:HE2 | 1:W:430:MET:O | 1.99 | 0.45 |
| 1:W:12:GLY:HA3 | 1:W:201:THR:CG2 | 2.44 | 0.45 |
| 1:A:874:ARG:HG3 | 3:C:53:ASP:OD2 | 2.16 | 0.45 |
| 4:D:56:GLU:HG3 | 13:P:45:VAL:CG1 | 2.45 | 0.45 |
| 3:Y:216:ILE:O | 3:Y:217:ALA:HB2 | 2.17 | 0.45 |
| 2:R:841:VAL:HG12 | 2:R:842:THR:O | 2.16 | 0.45 |
| 10:Q:40:ASN:HA | 10:Q:43:LEU:CD1 | 2.46 | 0.45 |
| 2:R:476:MET:HE1 | 2:R:645:ILE:HB | 1.97 | 0.45 |
| 3:Y:112:ASP:O | 3:Y:114:LYS:N | 2.49 | 0.45 |
| 2:R:345:ARG:HG3 | 2:R:576:GLY:HA3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:493:TYR:OH | 2:B:530:VAL:HG13 | 2.16 | 0.45 |
| 2:B:1039:LEU:HD22 | 2:B:1044:THR:HG21 | 1.98 | 0.45 |
| 2:B:126:LEU:HD21 | 2:B:156:ILE:HD11 | 1.98 | 0.45 |
| 2:B:918:LEU:H | 2:B:919:PRO:HD2 | 1.82 | 0.45 |
| 1:A:406:VAL:O | 1:A:406:VAL:HG12 | 2.16 | 0.45 |
| 3:Y:394:LEU:O | 3:Y:395:ARG:C | 2.54 | 0.45 |
| 3:C:201:SER:HB2 | 3:C:204:ASN:HB2 | 1.99 | 0.45 |
| 2:B:46:ILE:CB | 2:B:66:ILE:HD11 | 2.47 | 0.45 |
| 1:W:328:PRO:HD3 | 1:W:457:PHE:CG | 2.51 | 0.45 |
| 1:W:417:VAL:HG13 | 1:W:465:HIS:O | 2.17 | 0.45 |
| 2:B:194:SER:CB | 2:B:303:HIS:HB3 | 2.44 | 0.45 |
| 5:E:145:ARG:HD3 | 6:F:88:ILE:HG21 | 1.98 | 0.45 |
| 4:S:108:MET:SD | 4:S:132:LEU:HD23 | 2.56 | 0.45 |
| 5:E:44:LEU:O | 5:E:46:LEU:HD12 | 2.16 | 0.45 |
| 2:B:476:MET:HE1 | 2:B:645:ILE:HB | 1.97 | 0.45 |
| 3:Y:290:ARG:CB | 3:Y:321:THR:HG21 | 2.47 | 0.45 |
| 3:C:394:LEU:O | 3:C:395:ARG:C | 2.54 | 0.45 |
| 7:V:62:ASN:O | 7:V:63:ARG:HB2 | 2.17 | 0.45 |
| 1:W:490:ARG:HD2 | 1:W:491:TYR:HD1 | 1.80 | 0.45 |
| 3:C:281:GLU:OE1 | 3:C:326:VAL:HG12 | 2.16 | 0.45 |
| 2:R:854:LEU:HA | 13:X:35:PHE:HA | 1.99 | 0.45 |
| 7:G:75:GLY:HA3 | 7:G:86:SER:O | 2.17 | 0.45 |
| 3:C:28:ILE:HD13 | 9:K:14:HIS:CE1 | 2.51 | 0.45 |
| 3:Y:258:LEU:HD22 | 3:Y:280:ILE:HD13 | 1.98 | 0.45 |
| 2:B:137:THR:HG22 | 2:B:140:LYS:HD2 | 1.99 | 0.45 |
| 7:G:102:LEU:O | 7:G:103:VAL:C | 2.55 | 0.45 |
| 2:R:419:ARG:NH1 | 2:R:690:ARG:HH12 | 2.14 | 0.45 |
| 1:A:13:ILE:CG1 | 1:A:202:SER:HB2 | 2.47 | 0.45 |
| 2:R:1059:THR:CG2 | 2:R:1061:ILE:HD12 | 2.46 | 0.45 |
| 4:D:60:HIS:HD2 | 4:D:60:HIS:O | 2.00 | 0.45 |
| 3:Y:348:GLU:O | 3:Y:349:VAL:C | 2.54 | 0.45 |
| 1:W:23:SER:O | 1:W:24:VAL:HG13 | 2.16 | 0.45 |
| 2:B:399:HIS:O | 2:B:403:THR:CG2 | 2.65 | 0.45 |
| 5:E:13:ILE:HD12 | 5:E:68:HIS:CD2 | 2.51 | 0.45 |
| 1:W:777:GLU:HG3 | 1:W:783:TYR:HE1 | 1.81 | 0.45 |
| 10:J:49:GLU:O | 10:J:52:ASP:HB3 | 2.17 | 0.45 |
| 1:W:196:GLY:O | 3:Y:360:ARG:HD3 | 2.16 | 0.45 |
| 2:R:355:SER:O | 2:R:407:VAL:HG11 | 2.16 | 0.45 |
| 2:R:722:GLY:O | 2:R:992:TYR:CE1 | 2.70 | 0.45 |
| 2:R:330:LEU:HD22 | 2:R:332:ARG:HH11 | 1.82 | 0.45 |
| 2:R:904:VAL:O | 4:S:163:ILE:HG21 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:870:ARG:HD2 | 3:C:57:LYS:HB3 | 1.99 | 0.45 |
| 2:R:1062:TYR:CE2 | 2:R:1080:TYR:HE1 | 2.34 | 0.45 |
| 8:H:63:ILE:HG22 | 8:H:65:ILE:CD1 | 2.46 | 0.45 |
| 5:T:145:ARG:HD3 | 6:U:88:ILE:HD12 | 1.98 | 0.45 |
| 3:C:110:ILE:HD12 | 3:C:296:GLU:HB3 | 1.98 | 0.45 |
| 4:D:153:HIS:CG | 4:D:153:HIS:O | 2.70 | 0.45 |
| 1:W:28:ILE:CG2 | 1:W:29:THR:N | 2.80 | 0.45 |
| 1:A:421:ARG:CZ | 1:A:454:ASN:O | 2.64 | 0.45 |
| 5:E:10:ILE:HG22 | 5:E:11:VAL:N | 2.32 | 0.45 |
| 5:T:100:ASN:HD21 | 6:U:36:ARG:NH1 | 2.14 | 0.45 |
| 4:S:35:TYR:CE1 | 4:S:252:LYS:HE3 | 2.51 | 0.45 |
| 1:A:728:MET:HG3 | 1:A:733:ALA:O | 2.17 | 0.45 |
| 1:A:426:HIS:NE2 | 3:C:80:GLU:CD | 2.70 | 0.45 |
| 2:B:31:LEU:CD2 | 2:B:125:MET:HE3 | 2.43 | 0.45 |
| 5:E:115:ASP:O | 5:E:116:ASP:CG | 2.55 | 0.45 |
| 2:B:91:ARG:CG | 13:P:33:ILE:HD11 | 2.47 | 0.45 |
| 12:O:8:PHE:CD2 | 2:R:752:MET:HB2 | 2.51 | 0.45 |
| 2:R:948:PHE:CD1 | 1:W:792:PRO:HG3 | 2.52 | 0.45 |
| 3:Y:277:ILE:CG2 | 3:Y:278:ARG:H | 2.30 | 0.45 |
| 12:O:3:ILE:HG12 | 12:O:18:TRP:HB2 | 1.99 | 0.45 |
| 12:O:3:ILE:HD13 | 12:O:15:ALA:CA | 2.47 | 0.45 |
| 4:S:33:MET:HE3 | 4:S:162:ALA:HB3 | 1.99 | 0.45 |
| 2:R:500:VAL:HG12 | 2:R:504:ILE:HG12 | 1.99 | 0.45 |
| 1:A:327:SER:HB2 | 1:A:328:PRO:HD2 | 1.99 | 0.45 |
| 6:U:13:PRO:HG2 | 6:U:16:VAL:HG12 | 1.98 | 0.45 |
| 3:Y:11:SER:HB2 | 3:Y:14:GLU:HB2 | 1.99 | 0.45 |
| 2:R:295:ILE:O | 2:R:299:TYR:HB2 | 2.16 | 0.45 |
| 3:Y:127:THR:H | 3:Y:268:ASP:HB2 | 1.82 | 0.45 |
| 4:D:96:ILE:HD11 | 4:D:143:ALA:HB3 | 1.98 | 0.45 |
| 2:R:1110:MET:CE | 1:W:298:LEU:HB3 | 2.47 | 0.45 |
| 9:K:27:LEU:CD2 | 9:K:78:ILE:CD1 | 2.94 | 0.45 |
| 2:B:75:GLU:N | 2:B:79:GLY:O | 2.50 | 0.45 |
| 4:D:35:TYR:HE2 | 11:L:23:THR:HG21 | 1.82 | 0.45 |
| 2:B:680:LEU:HD21 | 2:B:997:HIS:HB3 | 1.98 | 0.45 |
| 5:E:75:ILE:HG21 | 6:F:21:LEU:HD11 | 1.97 | 0.45 |
| 7:G:62:ASN:O | 7:G:63:ARG:HB2 | 2.16 | 0.45 |
| 1:W:426:HIS:CG | 3:Y:80:GLU:CD | 2.91 | 0.45 |
| 2:B:63:LEU:HD22 | 2:B:103:MET:HE2 | 1.99 | 0.45 |
| 1:A:792:PRO:CD | 2:B:948:PHE:CE1 | 3.00 | 0.45 |
| 2:R:101:LEU:CD1 | 2:R:103:MET:HE2 | 2.47 | 0.45 |
| 3:Y:149:ILE:HG12 | 3:Y:230:LYS:HD3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:594:ARG:O | 2:R:597:ILE:HG12 | 2.17 | 0.45 |
| 9:I:61:VAL:O | 9:I:62:ILE:C | 2.55 | 0.45 |
| 13:X:17:GLN:HG3 | 13:X:19:LYS:H | 1.82 | 0.45 |
| 1:A:116:ARG:HA | 1:A:130:ARG:NH2 | 2.31 | 0.45 |
| 2:B:884:ARG:HH12 | 2:B:992:TYR:HB3 | 1.80 | 0.45 |
| 5:T:168:TYR:C | 5:T:169:LEU:HD12 | 2.36 | 0.45 |
| 3:C:289:ALA:HA | 3:C:292:ILE:HG22 | 1.99 | 0.45 |
| 2:R:251:ILE:O | 2:R:255:LEU:HD12 | 2.17 | 0.45 |
| 2:B:732:PHE:C | 2:B:733:THR:HG22 | 2.37 | 0.45 |
| 1:A:502:TYR:O | 1:A:503:ILE:C | 2.54 | 0.45 |
| 1:W:879:LYS:NZ | 3:Y:44:THR:HG22 | 2.32 | 0.45 |
| 1:A:486:ILE:HG12 | 1:A:496:ILE:HD12 | 1.99 | 0.45 |
| 1:W:829:ASP:O | 1:W:840:SER:HA | 2.16 | 0.45 |
| 11:M:12:TYR:CD1 | 11:M:58:LEU:HB2 | 2.52 | 0.45 |
| 1:A:81:VAL:HG11 | 1:A:269:LEU:O | 2.17 | 0.45 |
| 4:D:83:ILE:HD12 | 4:D:84:ASP:N | 2.31 | 0.45 |
| 6:F:15:SER:HB3 | 6:F:47:CYS:SG | 2.57 | 0.45 |
| 1:W:406:VAL:HG12 | 1:W:406:VAL:O | 2.16 | 0.45 |
| 2:B:852:LEU:HB3 | 2:B:868:ARG:HG2 | 1.98 | 0.45 |
| 2:B:689:LEU:CD1 | 12:N:62:TYR:HB3 | 2.47 | 0.45 |
| 2:R:131:ASP:OD1 | 2:R:132:PRO:HD2 | 2.17 | 0.45 |
| 1:A:60:THR:HG21 | 1:A:71:HIS:CG | 2.52 | 0.45 |
| 3:Y:244:LYS:CA | 3:Y:245:LYS:CB | 2.93 | 0.45 |
| 2:B:594:ARG:O | 2:B:597:ILE:HG12 | 2.17 | 0.45 |
| 5:T:131:LYS:HE3 | 5:T:136:ILE:HD11 | 1.99 | 0.45 |
| 13:P:6:CYS:HA | 13:P:16:GLU:O | 2.16 | 0.45 |
| 13:P:5:ARG:HD2 | 13:P:18:LEU:HD13 | 1.95 | 0.45 |
| 2:R:903:THR:HG22 | 2:R:904:VAL:H | 1.82 | 0.45 |
| 2:B:872:LEU:HD22 | 2:B:874:ILE:HG13 | 1.99 | 0.45 |
| 5:E:36:GLU:CG | 6:F:33:LEU:HD22 | 2.47 | 0.45 |
| 1:A:687:ILE:CD1 | 1:A:695:SER:HB2 | 2.46 | 0.45 |
| 2:B:398:ARG:C | 2:B:400:ALA:H | 2.19 | 0.45 |
| 1:A:20:ARG:NE | 1:A:211:VAL:HG21 | 2.31 | 0.45 |
| 1:W:871:ILE:CD1 | 3:Y:39:LYS:O | 2.65 | 0.45 |
| 2:R:966:LEU:CD2 | 4:S:208:GLU:HG3 | 2.47 | 0.45 |
| 3:C:80:GLU:CB | 3:C:81:PRO:HD3 | 2.46 | 0.44 |
| 3:C:28:ILE:CD1 | 9:K:14:HIS:CD2 | 2.97 | 0.44 |
| 1:A:419:PHE:HZ | 1:A:443:PHE:HB3 | 1.82 | 0.44 |
| 2:B:733:THR:HG23 | 2:B:734:GLY:N | 2.32 | 0.44 |
| 4:D:128:ILE:HG21 | 12:N:5:ILE:HD12 | 1.99 | 0.44 |
| 8:H:40:GLU:OE2 | 10:Q:66:ARG:NH1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:660:TYR:N | 2:R:661:PRO:CD | 2.80 | 0.44 |
| 2:B:236:LEU:HD21 | 2:B:268:VAL:CG2 | 2.47 | 0.44 |
| 5:E:84:VAL:HG13 | 6:F:75:ILE:CD1 | 2.46 | 0.44 |
| 4:D:223:GLU:OE1 | 4:D:223:GLU:HA | 2.17 | 0.44 |
| 1:A:345:ARG:HA | 1:A:410:HIS:ND1 | 2.32 | 0.44 |
| 2:B:767:LYS:HD3 | 2:B:768:TYR:O | 2.17 | 0.44 |
| 2:B:605:ILE:O | 2:B:609:ASP:HB2 | 2.17 | 0.44 |
| 2:B:91:ARG:HG3 | 13:P:33:ILE:HD11 | 1.99 | 0.44 |
| 1:W:420:ASN:HB2 | 1:W:430:MET:HG3 | 1.99 | 0.44 |
| 6:U:86:ILE:HG23 | 6:U:89:MET:SD | 2.57 | 0.44 |
| 3:C:331:ARG:HD3 | 3:C:331:ARG:H | 1.83 | 0.44 |
| 2:B:1080:TYR:HB3 | 2:B:1091:LEU:HD12 | 1.98 | 0.44 |
| 3:Y:129:GLU:HB3 | 3:Y:130:TYR:CD2 | 2.51 | 0.44 |
| 3:C:330:GLY:C | 3:C:335:THR:HG22 | 2.37 | 0.44 |
| 3:Y:167:LEU:HD12 | 3:Y:167:LEU:N | 2.32 | 0.44 |
| 10:Q:69:GLU:CD | 10:Q:73:LYS:HE3 | 2.37 | 0.44 |
| 1:W:580:CYS:HA | 1:W:581:PRO:HD3 | 1.80 | 0.44 |
| 13:P:26:CYS:HB3 | 13:P:29:CYS:HB2 | 1.65 | 0.44 |
| 1:W:97:THR:CG2 | 1:W:102:GLY:HA2 | 2.43 | 0.44 |
| 1:W:326:ILE:HG21 | 1:W:462:MET:HG3 | 2.00 | 0.44 |
| 9:I:43:LEU:HD12 | 9:I:65:ALA:HB2 | 2.00 | 0.44 |
| 2:B:981:LYS:HG2 | 4:D:166:TYR:CE2 | 2.52 | 0.44 |
| 5:E:167:PRO:C | 5:E:169:LEU:H | 2.21 | 0.44 |
| 12:N:40:VAL:O | 12:N:40:VAL:HG12 | 2.15 | 0.44 |
| 7:V:104:LYS:O | 7:V:106:ILE:N | 2.50 | 0.44 |
| 2:B:873:ARG:HH22 | 2:B:1002:ASP:CG | 2.20 | 0.44 |
| 2:B:903:THR:HA | 2:B:973:THR:HG22 | 2.00 | 0.44 |
| 2:R:463:GLU:OE1 | 2:R:463:GLU:N | 2.50 | 0.44 |
| 4:D:50:ASN:ND2 | 4:D:137:GLN:HG2 | 2.32 | 0.44 |
| 1:A:343:ILE:HG22 | 1:A:347:LEU:HD12 | 2.00 | 0.44 |
| 5:E:79:PRO:HB3 | 5:E:160:ILE:HD11 | 2.00 | 0.44 |
| 1:A:774:ILE:HG22 | 1:A:774:ILE:O | 2.17 | 0.44 |
| 1:W:145:VAL:HG13 | 1:W:145:VAL:O | 2.18 | 0.44 |
| 2:R:396:ARG:NH2 | 2:R:406:TRP:CZ2 | 2.86 | 0.44 |
| 2:B:259:LEU:HD13 | 2:B:259:LEU:HA | 1.64 | 0.44 |
| 3:Y:28:ILE:HG13 | 3:Y:28:ILE:H | 1.53 | 0.44 |
| 2:R:605:ILE:O | 2:R:609:ASP:HB2 | 2.18 | 0.44 |
| 2:B:937:ALA:O | 12:N:46:ARG:HD2 | 2.16 | 0.44 |
| 2:R:732:PHE:O | 2:R:733:THR:CG2 | 2.66 | 0.44 |
| 3:Y:340:SER:HB3 | 3:Y:371:GLU:OE2 | 2.17 | 0.44 |
| 2:B:982:ILE:CD1 | 2:B:984:SER:H | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:R:1082:CYS:HB2 | 2:R:1083:PRO:CD | 2.47 | 0.44 |
| 2:B:1082:CYS:HB2 | 2:B:1083:PRO:CD | 2.47 | 0.44 |
| 4:S:96:ILE:HD11 | 4:S:143:ALA:HB3 | 1.99 | 0.44 |
| 1:A:691:THR:HB | 1:A:694:GLU:CB | 2.48 | 0.44 |
| 1:W:516:LEU:CD2 | 1:W:524:ILE:HD12 | 2.47 | 0.44 |
| 4:S:26:ASN:O | 4:S:30:ARG:HG3 | 2.18 | 0.44 |
| 9:K:56:ILE:N | 9:K:57:SER:N | 2.63 | 0.44 |
| 9:K:59:THR:HB | 9:K:63:SER:OG | 2.17 | 0.44 |
| 2:B:947:PRO:O | 2:B:948:PHE:CD2 | 2.70 | 0.44 |
| 2:R:259:LEU:HA | 2:R:259:LEU:HD13 | 1.67 | 0.44 |
| 5:E:165:ARG:C | 5:E:167:PRO:HD3 | 2.37 | 0.44 |
| 1:W:428:ILE:C | 1:W:430:MET:H | 2.21 | 0.44 |
| 1:W:95:LYS:HD3 | 1:W:138:LYS:HD3 | 1.98 | 0.44 |
| 7:G:8:GLU:OE2 | 7:G:64:LEU:HD22 | 2.18 | 0.44 |
| 2:B:291:LYS:C | 2:B:293:GLN:H | 2.21 | 0.44 |
| 3:C:232:LYS:HA | 3:C:232:LYS:HE3 | 1.99 | 0.44 |
| 2:B:780:GLU:O | 2:B:782:GLY:N | 2.50 | 0.44 |
| 2:R:167:GLN:HG2 | 2:R:352:LEU:HD21 | 1.99 | 0.44 |
| 3:Y:70:ILE:H | 3:Y:70:ILE:CD1 | 2.29 | 0.44 |
| 2:B:1061:ILE:HG13 | 2:B:1072:TRP:HE1 | 1.83 | 0.44 |
| 2:R:457:CYS:HA | 2:R:458:PRO:HD3 | 1.80 | 0.44 |
| 4:D:26:ASN:O | 4:D:30:ARG:HG3 | 2.17 | 0.44 |
| 3:C:120:PRO:HB2 | 3:C:256:SER:HB3 | 1.99 | 0.44 |
| 2:B:213:PHE:HB2 | 2:B:259:LEU:CG | 2.48 | 0.44 |
| 2:R:101:LEU:HD13 | 2:R:103:MET:HG3 | 1.99 | 0.44 |
| 2:B:884:ARG:HB2 | 2:B:884:ARG:NH1 | 2.30 | 0.44 |
| 8:H:12:ARG:NH2 | 8:H:55:ILE:HD12 | 2.33 | 0.44 |
| 2:B:539:LEU:O | 2:B:543:ILE:HG13 | 2.18 | 0.44 |
| 3:C:393:ILE:HG13 | 3:C:393:ILE:O | 2.16 | 0.44 |
| 3:Y:182:ASP:HB2 | 3:Y:232:LYS:HZ2 | 1.83 | 0.44 |
| 4:D:108:MET:CG | 4:D:110:TYR:CE2 | 3.00 | 0.44 |
| 4:S:40:SER:OG | 4:S:156:PHE:CE1 | 2.66 | 0.44 |
| 6:F:13:PRO:HG2 | 6:F:16:VAL:HG12 | 2.00 | 0.44 |
| 4:D:153:HIS:HE2 | 13:P:48:ILE:HG23 | 1.82 | 0.44 |
| 1:A:334:ILE:HD12 | 1:A:628:MET:HB3 | 1.98 | 0.44 |
| 2:B:628:TYR:CE2 | 2:B:640:HIS:ND1 | 2.85 | 0.44 |
| 2:R:895:ILE:HA | 2:R:896:PRO:HD3 | 1.83 | 0.44 |
| 1:W:181:ARG:NH1 | 1:W:210:THR:OG1 | 2.51 | 0.44 |
| 2:R:680:LEU:HD21 | 2:R:997:HIS:HB3 | 2.00 | 0.44 |
| 13:P:24:VAL:O | 13:P:24:VAL:HG22 | 2.18 | 0.44 |
| 13:P:33:ILE:CD1 | 13:P:33:ILE:N | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:207:ARG:HB2 | 2:R:216:SER:HB2 | 1.98 | 0.44 |
| 1:W:241:ASP:OD2 | 1:W:289:HIS:NE2 | 2.50 | 0.44 |
| 2:B:1003:LYS:HA | 2:B:1003:LYS:HD2 | 1.70 | 0.44 |
| 3:C:292:ILE:HD13 | 3:C:292:ILE:C | 2.37 | 0.44 |
| 12:O:40:VAL:O | 12:O:40:VAL:HG12 | 2.15 | 0.44 |
| 7:V:8:GLU:OE2 | 7:V:64:LEU:HD22 | 2.18 | 0.44 |
| 7:V:25:ASN:O | 7:V:43:ILE:HA | 2.17 | 0.44 |
| 2:R:1081:VAL:C | 2:R:1091:LEU:HD11 | 2.38 | 0.44 |
| 5:T:80:VAL:HG12 | 5:T:83:GLU:CD | 2.38 | 0.44 |
| 3:Y:219:LEU:HD12 | 3:Y:219:LEU:N | 2.33 | 0.44 |
| 3:C:25:PRO:CD | 3:C:33:LYS:HD3 | 2.48 | 0.44 |
| 2:R:299:TYR:O | 2:R:302:PRO:HD3 | 2.17 | 0.44 |
| 1:W:77:LEU:N | 1:W:77:LEU:HD22 | 2.33 | 0.44 |
| 1:W:728:MET:HG3 | 1:W:733:ALA:O | 2.17 | 0.44 |
| 1:W:16:PRO:CD | 1:W:206:TRP:CD1 | 3.01 | 0.44 |
| 1:A:672:VAL:HG13 | 1:A:700:ILE:HG12 | 2.00 | 0.44 |
| 4:S:104:ASN:O | 4:S:105:GLU:C | 2.55 | 0.44 |
| 12:O:1:MET:O | 12:O:2:MET:HB2 | 2.17 | 0.44 |
| 2:B:767:LYS:HA | 2:B:767:LYS:HZ2 | 1.83 | 0.44 |
| 2:B:646:TRP:CH2 | 2:B:648:PRO:HB2 | 2.53 | 0.44 |
| 2:B:947:PRO:C | 2:B:948:PHE:CD2 | 2.91 | 0.44 |
| 3:Y:25:PRO:HG3 | 3:Y:33:LYS:HD3 | 2.00 | 0.44 |
| 2:B:162:ARG:HG2 | 2:B:402:ALA:HA | 2.00 | 0.44 |
| 11:M:48:PRO:HG2 | 2:R:735:TYR:CE2 | 2.52 | 0.44 |
| 2:B:841:VAL:HG12 | 2:B:842:THR:O | 2.17 | 0.44 |
| 2:R:872:LEU:HD22 | 2:R:874:ILE:HG13 | 2.00 | 0.44 |
| 1:A:121:ILE:HG21 | 10:Q:66:ARG:CD | 2.48 | 0.44 |
| 5:E:123:VAL:HA | 5:E:127:ILE:HA | 2.00 | 0.44 |
| 5:E:145:ARG:HD3 | 6:F:88:ILE:HD12 | 2.00 | 0.44 |
| 1:A:84:VAL:O | 1:A:87:VAL:HG12 | 2.18 | 0.44 |
| 6:U:71:VAL:HG11 | 6:U:89:MET:CE | 2.46 | 0.44 |
| 1:W:353:ILE:HD13 | 1:W:405:TYR:HB2 | 1.99 | 0.44 |
| 1:W:84:VAL:O | 1:W:87:VAL:HG12 | 2.18 | 0.44 |
| 3:Y:47:GLU:CB | 3:Y:50:LYS:HB2 | 2.47 | 0.44 |
| 2:R:630:ALA:HB2 | 2:R:640:HIS:CG | 2.53 | 0.44 |
| 1:W:509:LEU:HD23 | 1:W:552:VAL:CG2 | 2.48 | 0.44 |
| 1:A:818:TYR:O | 1:A:822:ARG:HG3 | 2.17 | 0.44 |
| 3:Y:129:GLU:HB3 | 3:Y:130:TYR:CE2 | 2.53 | 0.44 |
| 2:B:808:LYS:HE3 | 2:B:847:MET:HE1 | 2.00 | 0.44 |
| 1:W:369:PRO:CG | 1:W:389:ARG:HD2 | 2.48 | 0.44 |
| 7:G:22:SER:O | 7:G:23:LEU:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:345:ARG:HA | 1:W:410:HIS:ND1 | 2.33 | 0.44 |
| 2:R:597:ILE:HD12 | 2:R:605:ILE:N | 2.32 | 0.44 |
| 1:A:872:PHE:CZ | 1:A:876:VAL:HG21 | 2.52 | 0.44 |
| 1:W:78:VAL:HG13 | 1:W:78:VAL:O | 2.18 | 0.44 |
| 7:G:25:ASN:O | 7:G:43:ILE:HA | 2.18 | 0.44 |
| 3:Y:234:ILE:HG22 | 3:Y:235:LYS:N | 2.33 | 0.44 |
| 2:B:783:VAL:HA | 2:B:784:ARG:HA | 1.72 | 0.44 |
| 2:R:8:LEU:O | 2:R:9:SER:HB3 | 2.18 | 0.44 |
| 2:R:17:ILE:O | 2:R:20:TYR:HB3 | 2.17 | 0.44 |
| 1:W:723:ASN:HD22 | 1:W:723:ASN:C | 2.21 | 0.44 |
| 1:W:29:THR:HG23 | 1:W:243:VAL:HB | 1.99 | 0.44 |
| 7:V:76:TYR:CD1 | 7:V:76:TYR:N | 2.85 | 0.44 |
| 2:B:697:LEU:C | 2:B:697:LEU:HD13 | 2.38 | 0.44 |
| 1:W:852:ASP:CG | 8:Z:75:VAL:HG21 | 2.39 | 0.44 |
| 1:A:599:ASP:H | 1:A:602:ALA:HB3 | 1.83 | 0.44 |
| 3:C:244:LYS:CA | 3:C:245:LYS:CB | 2.93 | 0.43 |
| 7:G:96:ILE:HD13 | 7:G:101:LEU:HD22 | 1.99 | 0.43 |
| 9:I:14:HIS:CE1 | 3:Y:28:ILE:HD13 | 2.53 | 0.43 |
| 1:A:238:LYS:HE2 | 1:A:297:THR:CG2 | 2.47 | 0.43 |
| 3:C:258:LEU:HD22 | 3:C:280:ILE:HD13 | 2.00 | 0.43 |
| 3:Y:34:ASN:O | 3:Y:37:SER:HB3 | 2.18 | 0.43 |
| 2:R:137:THR:HG22 | 2:R:140:LYS:HD2 | 2.00 | 0.43 |
| 2:R:330:LEU:O | 2:R:332:ARG:CG | 2.65 | 0.43 |
| 11:L:77:ARG:HH11 | 11:L:77:ARG:HB2 | 1.83 | 0.43 |
| 1:W:249:LEU:HG | 1:W:265:LEU:CB | 2.45 | 0.43 |
| 1:A:371:LYS:HD3 | 1:A:372:TRP:N | 2.33 | 0.43 |
| 5:T:145:ARG:HD3 | 6:U:88:ILE:HG21 | 1.98 | 0.43 |
| 1:A:29:THR:OG1 | 1:A:243:VAL:HG12 | 2.18 | 0.43 |
| 2:R:460:GLU:OE1 | 2:R:472:ASN:ND2 | 2.51 | 0.43 |
| 2:B:493:TYR:CE1 | 2:B:499:PRO:HD3 | 2.52 | 0.43 |
| 4:D:41:ILE:HB | 4:D:63:ALA:HA | 2.00 | 0.43 |
| 7:V:75:GLY:C | 7:V:76:TYR:CD1 | 2.91 | 0.43 |
| 1:A:871:ILE:CD1 | 3:C:39:LYS:O | 2.66 | 0.43 |
| 4:D:73:LEU:HD11 | 4:D:236:LEU:HD21 | 1.99 | 0.43 |
| 2:B:28:ARG:HD2 | 2:B:32:ASP:OD2 | 2.18 | 0.43 |
| 8:H:32:LEU:HD21 | 8:H:42:LEU:HD11 | 2.00 | 0.43 |
| 7:V:29:ILE:CD1 | 7:V:42:ILE:HG13 | 2.48 | 0.43 |
| 5:T:102:GLY:HA2 | 6:U:40:TYR:CG | 2.53 | 0.43 |
| 1:A:855:VAL:HB | 3:C:311:ARG:NH1 | 2.33 | 0.43 |
| 1:A:853:ASP:HA | 8:H:72:TYR:HB2 | 1.99 | 0.43 |
| 2:R:103:MET:O | 2:R:114:PRO:O | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:46:ILE:CB | 2:R:66:ILE:HD11 | 2.46 | 0.43 |
| 1:A:461:GLU:OE2 | 2:B:1003:LYS:HG3 | 2.17 | 0.43 |
| 12:N:8:PHE:CG | 12:N:48:MET:HE1 | 2.54 | 0.43 |
| 2:B:252:GLN:O | 2:B:256:PHE:CD2 | 2.71 | 0.43 |
| 3:Y:170:ASP:O | 3:Y:174:LEU:HD12 | 2.18 | 0.43 |
| 2:B:904:VAL:O | 4:D:163:ILE:HG12 | 2.18 | 0.43 |
| 1:W:870:ARG:HD2 | 3:Y:57:LYS:HB3 | 1.99 | 0.43 |
| 2:R:372:LEU:CD2 | 2:R:376:LYS:CE | 2.96 | 0.43 |
| 2:B:17:ILE:CG1 | 2:B:476:MET:SD | 3.06 | 0.43 |
| 3:C:219:LEU:O | 3:C:222:LEU:HB2 | 2.18 | 0.43 |
| 6:U:21:LEU:O | 6:U:24:VAL:HG12 | 2.18 | 0.43 |
| 2:R:493:TYR:CE1 | 2:R:499:PRO:HD3 | 2.52 | 0.43 |
| 1:A:10:LYS:HA | 3:C:363:VAL:HG22 | 2.00 | 0.43 |
| 7:V:41:ASP:O | 7:V:42:ILE:HD13 | 2.18 | 0.43 |
| 3:Y:310:MET:HE3 | 3:Y:314:LEU:HD21 | 2.00 | 0.43 |
| 4:D:98:ILE:HD13 | 4:D:141:LEU:HD11 | 2.00 | 0.43 |
| 1:A:650:ASP:HB3 | 1:A:723:ASN:ND2 | 2.33 | 0.43 |
| 2:R:1120:ASP:HA | 1:W:4:LYS:HE2 | 1.99 | 0.43 |
| 2:R:814:ILE:HD11 | 2:R:867:VAL:HG23 | 1.99 | 0.43 |
| 12:N:1:MET:HA | 12:N:56:ILE:HB | 1.99 | 0.43 |
| 1:A:98:CYS:HB3 | 1:A:101:CYS:HB2 | 1.86 | 0.43 |
| 2:B:946:THR:O | 2:B:947:PRO:C | 2.57 | 0.43 |
| 1:W:856:PHE:CE2 | 1:W:858:MET:CB | 3.01 | 0.43 |
| 2:R:1034:MET:O | 2:R:1037:ASP:HB2 | 2.19 | 0.43 |
| 2:R:1037:ASP:OD2 | 1:W:824:ILE:HD13 | 2.19 | 0.43 |
| 4:D:108:MET:CG | 4:D:110:TYR:CZ | 3.01 | 0.43 |
| 4:S:65:ILE:HG23 | 4:S:128:ILE:HD12 | 2.00 | 0.43 |
| 2:R:194:SER:CB | 2:R:303:HIS:HB3 | 2.48 | 0.43 |
| 10:J:40:ASN:HA | 10:J:43:LEU:CD1 | 2.48 | 0.43 |
| 3:C:286:ILE:HG23 | 3:C:324:GLY:O | 2.18 | 0.43 |
| 2:B:1056:SER:HB3 | 2:B:1057:ASP:OD1 | 2.18 | 0.43 |
| 4:D:8:LYS:HG3 | 4:D:13:ILE:CG1 | 2.48 | 0.43 |
| 1:W:736:SER:HB3 | 1:W:739:ASN:ND2 | 2.33 | 0.43 |
| 9:I:90:LEU:HA | 9:I:90:LEU:HD23 | 1.71 | 0.43 |
| 2:B:555:GLU:HG2 | 2:B:579:ARG:HH12 | 1.83 | 0.43 |
| 1:W:20:ARG:NE | 1:W:211:VAL:HG21 | 2.33 | 0.43 |
| 11:L:29:ALA:HB2 | 11:L:43:TYR:HB3 | 1.99 | 0.43 |
| 2:R:675:MET:HG3 | 2:R:996:LEU:HD21 | 1.99 | 0.43 |
| 5:T:53:THR:O | 5:T:54:SER:C | 2.55 | 0.43 |
| 7:V:96:ILE:HD13 | 7:V:101:LEU:HD21 | 2.00 | 0.43 |
| 9:I:13:LEU:O | 9:I:14:HIS:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:136:TYR:HB2 | 2:R:141:LEU:CD1 | 2.48 | 0.43 |
| 2:R:533:TYR:CE2 | 2:R:539:LEU:HD23 | 2.53 | 0.43 |
| 1:A:139:THR:O | 1:A:139:THR:HG23 | 2.18 | 0.43 |
| 8:H:25:ILE:HG22 | 10:Q:55:LEU:HD22 | 1.99 | 0.43 |
| 2:B:873:ARG:HB3 | 2:B:999:MET:CE | 2.48 | 0.43 |
| 5:T:60:VAL:HG22 | 5:T:61:PHE:N | 2.32 | 0.43 |
| 8:H:28:ALA:HB1 | 8:H:62:ILE:CD1 | 2.48 | 0.43 |
| 4:D:153:HIS:O | 4:D:154:ALA:HB3 | 2.18 | 0.43 |
| 11:M:27:LEU:CD1 | 4:S:24:PHE:HA | 2.48 | 0.43 |
| 1:A:19:ILE:O | 1:A:74:HIS:NE2 | 2.52 | 0.43 |
| 3:C:34:ASN:O | 3:C:37:SER:HB3 | 2.18 | 0.43 |
| 5:T:84:VAL:CG2 | 6:U:75:ILE:CD1 | 2.97 | 0.43 |
| 3:C:129:GLU:HB3 | 3:C:130:TYR:CD2 | 2.54 | 0.43 |
| 2:B:586:SER:O | 2:B:587:ASN:HB2 | 2.17 | 0.43 |
| 1:W:575:CYS:SG | 1:W:584:SER:HB3 | 2.58 | 0.43 |
| 11:M:29:ALA:HB2 | 11:M:43:TYR:HB3 | 2.00 | 0.43 |
| 3:Y:213:ILE:O | 3:Y:214:ASP:CG | 2.57 | 0.43 |
| 7:V:22:SER:O | 7:V:23:LEU:C | 2.57 | 0.43 |
| 2:R:765:GLU:HB3 | 2:R:774:ASP:O | 2.19 | 0.43 |
| 5:T:70:VAL:CG1 | 5:T:72:PHE:CE2 | 3.01 | 0.43 |
| 1:A:859:TYR:HB2 | 3:C:63:LEU:HB3 | 2.00 | 0.43 |
| 5:T:136:ILE:O | 5:T:137:GLN:CB | 2.66 | 0.43 |
| 1:A:95:LYS:HB3 | 1:A:138:LYS:CE | 2.45 | 0.43 |
| 3:C:170:ASP:O | 3:C:174:LEU:HD12 | 2.18 | 0.43 |
| 1:A:122:LYS:NZ | 10:Q:66:ARG:HG3 | 2.34 | 0.43 |
| 3:C:216:ILE:O | 3:C:217:ALA:HB3 | 2.17 | 0.43 |
| 1:A:353:ILE:HG23 | 1:A:358:ILE:HD13 | 1.99 | 0.43 |
| 4:D:153:HIS:ND1 | 4:D:155:LYS:HG2 | 2.33 | 0.43 |
| 1:A:378:VAL:CG1 | 1:A:386:ILE:HB | 2.49 | 0.43 |
| 3:Y:393:ILE:O | 3:Y:393:ILE:HG13 | 2.16 | 0.43 |
| 2:R:52:ILE:N | 2:R:53:PRO:HD3 | 2.33 | 0.43 |
| 4:S:98:ILE:HD13 | 4:S:141:LEU:HD11 | 2.00 | 0.43 |
| 1:A:757:ILE:CD1 | 1:A:797:PHE:HD1 | 2.31 | 0.43 |
| 2:B:1103:LEU:O | 2:B:1107:LEU:HG | 2.18 | 0.43 |
| 7:V:67:THR:HG22 | 7:V:68:ASN:H | 1.83 | 0.43 |
| 3:C:213:ILE:O | 3:C:214:ASP:CG | 2.57 | 0.43 |
| 7:G:14:GLU:OE2 | 7:G:54:LYS:HE2 | 2.19 | 0.43 |
| 2:B:814:ILE:HD11 | 2:B:867:VAL:HG23 | 2.01 | 0.43 |
| 1:A:827:LEU:O | 3:C:71:GLY:HA3 | 2.19 | 0.43 |
| 4:D:219:ILE:CD1 | 16:D:1001:F3S:S3 | 3.07 | 0.43 |
| 3:Y:24:LEU:N | 3:Y:25:PRO:HD2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Y:146:TYR:HE2 | 3:Y:231:ILE:HD11 | 1.83 | 0.43 |
| 8:Z:12:ARG:HH22 | 8:Z:55:ILE:HD12 | 1.83 | 0.43 |
| 1:A:119:ASN:OD1 | 1:A:126:PRO:CB | 2.67 | 0.43 |
| 2:R:638:PRO:HG2 | 2:R:640:HIS:NE2 | 2.33 | 0.43 |
| 2:B:980:GLN:HA | 4:D:22:LEU:HD21 | 1.99 | 0.43 |
| 1:W:541:ALA:CB | 1:W:542:PRO:CD | 2.97 | 0.43 |
| 5:T:4:LEU:HB2 | 6:U:12:ILE:HD11 | 1.99 | 0.43 |
| 4:D:41:ILE:HD13 | 4:D:145:LEU:HG | 2.01 | 0.43 |
| 4:S:8:LYS:HA | 4:S:13:ILE:HA | 2.01 | 0.43 |
| 4:S:41:ILE:HD13 | 4:S:145:LEU:HG | 2.00 | 0.43 |
| 5:E:75:ILE:CD1 | 6:F:20:LEU:HB3 | 2.48 | 0.43 |
| 1:W:631:LEU:O | 1:W:634:VAL:HB | 2.19 | 0.43 |
| 7:V:89:GLY:HA2 | 1:W:549:LYS:HE2 | 2.01 | 0.43 |
| 1:W:565:GLN:HB3 | 1:W:569:SER:HB3 | 2.01 | 0.43 |
| 1:A:16:PRO:CD | 1:A:206:TRP:CD1 | 3.02 | 0.43 |
| 2:R:359:VAL:HG11 | 2:R:407:VAL:HG22 | 2.00 | 0.43 |
| 2:B:113:GLU:CB | 2:B:114:PRO:CD | 2.89 | 0.43 |
| 2:R:856:THR:CG2 | 2:R:857:GLU:H | 2.21 | 0.43 |
| 1:W:648:LEU:HD21 | 1:W:787:ARG:HH11 | 1.81 | 0.43 |
| 5:E:164:MET:O | 5:E:167:PRO:HD3 | 2.19 | 0.43 |
| 2:R:922:MET:HG2 | 1:W:743:MET:HG3 | 2.00 | 0.43 |
| 2:B:485:GLU:OE1 | 2:B:528:ARG:NH1 | 2.52 | 0.43 |
| 7:V:8:GLU:O | 7:V:9:ILE:HG13 | 2.19 | 0.43 |
| 4:S:108:MET:CG | 4:S:110:TYR:CE2 | 3.01 | 0.43 |
| 1:W:378:VAL:CG1 | 1:W:386:ILE:HB | 2.49 | 0.43 |
| 3:C:222:LEU:O | 3:C:226:ILE:HG13 | 2.19 | 0.43 |
| 3:C:112:ASP:O | 3:C:114:LYS:N | 2.51 | 0.43 |
| 2:B:163:VAL:HG21 | 2:B:429:LEU:CD2 | 2.49 | 0.43 |
| 2:R:448:LEU:HD22 | 1:W:796:PHE:CZ | 2.54 | 0.43 |
| 10:J:61:VAL:C | 10:J:63:GLU:N | 2.72 | 0.43 |
| 3:Y:284:PHE:O | 3:Y:288:ALA:HB2 | 2.19 | 0.43 |
| 2:R:254:GLU:HG2 | 2:R:254:GLU:O | 2.19 | 0.43 |
| 5:E:39:LEU:N | 5:E:39:LEU:HD12 | 2.34 | 0.43 |
| 5:T:79:PRO:HB3 | 5:T:160:ILE:HD11 | 2.01 | 0.43 |
| 2:B:547:ARG:NH1 | 2:B:556:VAL:O | 2.52 | 0.43 |
| 4:S:206:CYS:SG | 4:S:207:GLU:N | 2.91 | 0.43 |
| 3:Y:186:LYS:CB | 3:Y:230:LYS:HE2 | 2.46 | 0.43 |
| 2:R:903:THR:HG21 | 2:R:971:GLU:OE1 | 2.19 | 0.43 |
| 4:S:161:LEU:CD1 | 4:S:163:ILE:HD13 | 2.48 | 0.43 |
| 1:W:309:PHE:O | 1:W:310:ARG:HB2 | 2.18 | 0.43 |
| 4:D:65:ILE:HG23 | 4:D:128:ILE:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:904:VAL:O | 4:D:163:ILE:HG21 | 2.19 | 0.43 |
| 2:R:703:ARG:HH22 | 2:R:942:ILE:HG21 | 1.84 | 0.43 |
| 2:R:17:ILE:CG1 | 2:R:476:MET:SD | 3.07 | 0.43 |
| 2:R:1061:ILE:HA | 2:R:1072:TRP:NE1 | 2.34 | 0.43 |
| 1:A:631:LEU:O | 1:A:634:VAL:HB | 2.19 | 0.43 |
| 3:Y:344:ARG:HB3 | 3:Y:353:HIS:ND1 | 2.34 | 0.43 |
| 3:C:104:LEU:CD1 | 3:C:108:ILE:HD11 | 2.49 | 0.43 |
| 2:R:729:VAL:HG23 | 2:R:987:TYR:CD1 | 2.54 | 0.43 |
| 3:Y:237:ILE:HD12 | 3:Y:253:THR:HG21 | 2.00 | 0.43 |
| 1:W:376:ASN:HB2 | 1:W:377:TYR:CD1 | 2.53 | 0.43 |
| 1:A:753:ARG:NH2 | 2:B:447:ASP:OD2 | 2.52 | 0.43 |
| 1:W:426:HIS:NE2 | 3:Y:80:GLU:CD | 2.72 | 0.43 |
| 3:C:28:ILE:H | 3:C:28:ILE:HG13 | 1.51 | 0.43 |
| 1:A:417:VAL:HG13 | 1:A:465:HIS:O | 2.18 | 0.43 |
| 2:R:208:LEU:HD23 | 2:R:215:VAL:CG2 | 2.46 | 0.43 |
| 1:W:122:LYS:O | 1:W:126:PRO:HG3 | 2.18 | 0.43 |
| 2:R:948:PHE:CE1 | 1:W:792:PRO:CG | 3.02 | 0.43 |
| 3:C:216:ILE:O | 3:C:217:ALA:HB2 | 2.19 | 0.43 |
| 4:S:22:LEU:HD13 | 4:S:226:TYR:CD1 | 2.54 | 0.43 |
| 2:B:699:HIS:CE1 | 4:D:57:ILE:CD1 | 3.01 | 0.43 |
| 2:B:638:PRO:HG2 | 2:B:640:HIS:NE2 | 2.34 | 0.43 |
| 3:Y:127:THR:OG1 | 3:Y:129:GLU:O | 2.35 | 0.43 |
| 12:O:1:MET:HA | 12:O:56:ILE:HB | 2.01 | 0.43 |
| 7:G:82:LYS:HD3 | 7:G:95:ILE:HG12 | 2.01 | 0.43 |
| 2:B:139:ASP:O | 2:B:143:GLU:HG3 | 2.18 | 0.43 |
| 2:R:547:ARG:NH1 | 2:R:556:VAL:O | 2.51 | 0.43 |
| 1:W:64:THR:O | 1:W:65:LEU:HB2 | 2.19 | 0.43 |
| 9:I:16:ASN:O | 9:I:20:VAL:HG23 | 2.18 | 0.43 |
| 9:I:55:ASN:HA | 9:I:56:ILE:N | 2.30 | 0.43 |
| 1:W:103:ARG:CG | 1:W:191:ASP:OD1 | 2.67 | 0.43 |
| 3:C:149:ILE:O | 3:C:153:VAL:HG12 | 2.19 | 0.43 |
| 1:W:337:VAL:HG21 | 1:W:419:PHE:CE1 | 2.53 | 0.43 |
| 2:B:949:TYR:O | 2:B:951:THR:N | 2.52 | 0.43 |
| 2:R:598:GLU:O | 2:R:599:LYS:C | 2.57 | 0.43 |
| 12:O:64:ARG:O | 12:O:64:ARG:CG | 2.67 | 0.43 |
| 7:G:8:GLU:O | 7:G:9:ILE:HG13 | 2.19 | 0.43 |
| 1:A:563:HIS:CD2 | 1:A:872:PHE:CE2 | 3.07 | 0.43 |
| 1:A:184:LEU:HD22 | 1:A:204:PRO:HB2 | 2.01 | 0.43 |
| 2:B:533:TYR:CE2 | 2:B:539:LEU:HD23 | 2.54 | 0.43 |
| 8:Z:12:ARG:NH2 | 8:Z:55:ILE:HD12 | 2.34 | 0.43 |
| 5:E:124:ARG:O | 5:E:126:ILE:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:F:72:LEU:HD21 | 6:F:86:ILE:HG12 | 2.01 | 0.43 |
| 4:S:108:MET:CG | 4:S:110:TYR:CZ | 3.02 | 0.43 |
| 1:A:372:TRP:HB3 | 1:A:373:PRO:HD3 | 2.01 | 0.43 |
| 2:R:619:LEU:HD22 | 2:R:623:GLU:HG2 | 2.01 | 0.43 |
| 2:R:1105:GLN:HE22 | 1:W:70:GLY:HA2 | 1.84 | 0.43 |
| 2:B:500:VAL:HG12 | 2:B:504:ILE:HG12 | 2.01 | 0.43 |
| 10:J:55:LEU:O | 10:J:56:ASN:CB | 2.67 | 0.43 |
| 2:R:398:ARG:HD2 | 2:R:399:HIS:CE1 | 2.54 | 0.43 |
| 2:R:399:HIS:O | 2:R:403:THR:HG21 | 2.19 | 0.43 |
| 4:D:39:MET:HE2 | 4:D:39:MET:HB2 | 1.89 | 0.43 |
| 3:C:11:SER:HB2 | 3:C:14:GLU:HB2 | 2.01 | 0.43 |
| 1:W:192:VAL:HG21 | 1:W:199:PRO:HB3 | 2.00 | 0.43 |
| 1:A:219:ILE:O | 1:A:219:ILE:HG22 | 2.19 | 0.43 |
| 2:R:341:TYR:CD1 | 2:R:344:LYS:HB3 | 2.54 | 0.43 |
| 1:W:412:THR:O | 1:W:414:GLY:N | 2.52 | 0.43 |
| 1:A:390:TYR:O | 1:A:391:VAL:C | 2.58 | 0.43 |
| 1:W:757:ILE:CD1 | 1:W:797:PHE:HD1 | 2.32 | 0.43 |
| 2:B:562:VAL:O | 2:B:566:ILE:O | 2.37 | 0.43 |
| 4:S:219:ILE:CD1 | 16:S:1001:F3S:S3 | 3.07 | 0.42 |
| 2:B:947:PRO:O | 2:B:948:PHE:HD2 | 2.01 | 0.42 |
| 13:X:37:VAL:HG22 | 13:X:38:ARG:H | 1.83 | 0.42 |
| 11:M:69:LEU:CD2 | 4:S:260:LEU:HD11 | 2.48 | 0.42 |
| 2:B:162:ARG:HG2 | 2:B:401:LEU:O | 2.18 | 0.42 |
| 3:C:146:TYR:HE2 | 3:C:231:ILE:HD11 | 1.84 | 0.42 |
| 1:A:682:GLY:O | 1:A:683:GLU:C | 2.57 | 0.42 |
| 1:A:683:GLU:OE1 | 1:A:683:GLU:N | 2.52 | 0.42 |
| 1:W:870:ARG:CZ | 1:W:870:ARG:CB | 2.96 | 0.42 |
| 12:O:15:ALA:HB1 | 4:S:129:PRO:HD2 | 2.01 | 0.42 |
| 2:B:173:ASN:N | 2:B:193:ILE:O | 2.49 | 0.42 |
| 2:R:37:PHE:CZ | 2:R:42:LEU:HD13 | 2.53 | 0.42 |
| 3:Y:237:ILE:HD12 | 3:Y:253:THR:CB | 2.48 | 0.42 |
| 1:W:736:SER:HB3 | 1:W:739:ASN:OD1 | 2.18 | 0.42 |
| 1:A:646:MET:HG2 | 2:B:918:LEU:HD13 | 2.01 | 0.42 |
| 10:Q:73:LYS:HA | 10:Q:76:GLU:OE2 | 2.19 | 0.42 |
| 2:R:675:MET:HG2 | 2:R:882:ALA:CB | 2.49 | 0.42 |
| 13:P:17:GLN:HG3 | 13:P:19:LYS:H | 1.84 | 0.42 |
| 2:B:605:ILE:CG1 | 2:B:606:THR:N | 2.81 | 0.42 |
| 3:C:163:MET:SD | 3:C:206:LEU:CD2 | 3.07 | 0.42 |
| 2:R:87:GLU:HG2 | 13:X:31:TYR:OH | 2.19 | 0.42 |
| 2:R:115:GLU:O | 2:R:117:VAL:HG23 | 2.19 | 0.42 |
| 2:R:956:LEU:O | 2:R:960:ILE:HG12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:353:ILE:HG23 | 1:W:358:ILE:HD13 | 1.99 | 0.42 |
| 2:B:703:ARG:NH2 | 2:B:942:ILE:HG21 | 2.33 | 0.42 |
| 2:R:918:LEU:H | 2:R:919:PRO:HD2 | 1.84 | 0.42 |
| 5:T:84:VAL:HG13 | 6:U:75:ILE:CD1 | 2.49 | 0.42 |
| 4:D:13:ILE:HD13 | 4:D:14:ASP:N | 2.34 | 0.42 |
| 9:I:34:ARG:CB | 3:Y:386:VAL:HG11 | 2.49 | 0.42 |
| 6:U:15:SER:HB3 | 6:U:47:CYS:SG | 2.59 | 0.42 |
| 2:B:678:GLN:HG2 | 2:B:997:HIS:NE2 | 2.34 | 0.42 |
| 2:B:1051:ARG:NE | 2:B:1051:ARG:HA | 2.33 | 0.42 |
| 4:S:73:LEU:HD11 | 4:S:236:LEU:HD21 | 2.02 | 0.42 |
| 2:B:756:THR:HG23 | 2:B:871:ASP:O | 2.18 | 0.42 |
| 1:A:212:LEU:CD1 | 1:A:273:VAL:HG13 | 2.50 | 0.42 |
| 1:A:369:PRO:CG | 1:A:389:ARG:HD2 | 2.48 | 0.42 |
| 1:W:85:GLY:HA3 | 3:Y:355:LEU:HD22 | 2.01 | 0.42 |
| 2:R:763:THR:HG22 | 2:R:764:GLU:O | 2.19 | 0.42 |
| 1:A:833:GLU:HG3 | 1:A:839:ARG:CD | 2.49 | 0.42 |
| 1:A:77:LEU:HD22 | 1:A:77:LEU:N | 2.33 | 0.42 |
| 3:Y:201:SER:HB2 | 3:Y:204:ASN:HB2 | 2.00 | 0.42 |
| 2:B:767:LYS:HA | 2:B:767:LYS:NZ | 2.34 | 0.42 |
| 2:B:774:ASP:OD1 | 2:B:818:SER:HA | 2.19 | 0.42 |
| 2:R:603:GLY:C | 2:R:605:ILE:H | 2.22 | 0.42 |
| 2:B:856:THR:CG2 | 2:B:857:GLU:H | 2.29 | 0.42 |
| 9:I:59:THR:O | 9:I:60:ASP:CG | 2.57 | 0.42 |
| 1:W:856:PHE:HB3 | 1:W:859:TYR:CD2 | 2.53 | 0.42 |
| 1:W:450:CYS:H | 1:W:451:PRO:CD | 2.33 | 0.42 |
| 13:P:6:CYS:HB3 | 13:P:7:GLY:H | 1.67 | 0.42 |
| 1:A:95:LYS:O | 1:A:138:LYS:HG2 | 2.19 | 0.42 |
| 2:R:162:ARG:HG2 | 2:R:401:LEU:O | 2.19 | 0.42 |
| 2:B:249:PRO:HB2 | 2:B:252:GLN:HB2 | 2.01 | 0.42 |
| 4:D:154:ALA:C | 4:D:156:PHE:N | 2.72 | 0.42 |
| 2:B:636:LEU:HD13 | 2:B:643:LEU:HD12 | 2.01 | 0.42 |
| 3:Y:219:LEU:O | 3:Y:222:LEU:HB2 | 2.19 | 0.42 |
| 2:R:1096:VAL:CG1 | 2:R:1097:SER:N | 2.82 | 0.42 |
| 9:I:27:LEU:CD2 | 9:I:78:ILE:CD1 | 2.97 | 0.42 |
| 1:W:81:VAL:CG2 | 1:W:269:LEU:HB3 | 2.49 | 0.42 |
| 2:B:333:ARG:NH1 | 2:B:333:ARG:HB3 | 2.35 | 0.42 |
| 12:O:61:HIS:O | 12:O:62:TYR:CD2 | 2.72 | 0.42 |
| 1:A:185:GLU:HG3 | 1:A:205:GLU:HG2 | 2.01 | 0.42 |
| 10:J:57:GLY:C | 10:J:61:VAL:CG1 | 2.88 | 0.42 |
| 5:T:40:LYS:O | 5:T:41:ASP:OD1 | 2.37 | 0.42 |
| 4:D:101:GLU:HB2 | 4:D:137:GLN:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:127:SER:O | 1:A:131:ARG:HG3 | 2.19 | 0.42 |
| 1:W:212:LEU:CD1 | 1:W:273:VAL:HG13 | 2.50 | 0.42 |
| 2:R:155:PHE:CE1 | 2:R:164:ILE:HD12 | 2.54 | 0.42 |
| 4:D:3:ILE:HD12 | 11:L:86:GLU:OE1 | 2.20 | 0.42 |
| 4:S:247:LYS:O | 4:S:251:ARG:HG3 | 2.19 | 0.42 |
| 2:R:478:GLN:HG2 | 2:R:479:ILE:N | 2.34 | 0.42 |
| 5:T:45:VAL:HG21 | 5:T:74:MET:SD | 2.59 | 0.42 |
| 1:A:64:THR:O | 1:A:65:LEU:HB2 | 2.19 | 0.42 |
| 1:A:101:CYS:HB2 | 1:A:102:GLY:H | 1.67 | 0.42 |
| 9:K:61:VAL:O | 9:K:62:ILE:C | 2.52 | 0.42 |
| 3:C:63:LEU:HA | 3:C:63:LEU:HD23 | 1.89 | 0.42 |
| 13:X:24:VAL:HG13 | 13:X:24:VAL:O | 2.19 | 0.42 |
| 4:D:205:LEU:O | 4:D:207:GLU:N | 2.52 | 0.42 |
| 9:I:35:VAL:CG1 | 3:Y:388:LEU:HD11 | 2.49 | 0.42 |
| 1:W:450:CYS:C | 1:W:452:PRO:HD2 | 2.39 | 0.42 |
| 2:B:1046:MET:CG | 5:E:61:PHE:HD1 | 2.32 | 0.42 |
| 8:H:29:TYR:HE1 | 10:Q:60:SER:HB3 | 1.84 | 0.42 |
| 2:R:736:ASN:OD1 | 2:R:914:ASN:HB2 | 2.19 | 0.42 |
| 5:T:123:VAL:O | 5:T:123:VAL:HG12 | 2.18 | 0.42 |
| 3:Y:277:ILE:C | 3:Y:279:GLU:N | 2.71 | 0.42 |
| 2:R:1025:ARG:O | 2:R:1026:GLU:C | 2.57 | 0.42 |
| 2:B:1059:THR:CG2 | 2:B:1061:ILE:HD12 | 2.50 | 0.42 |
| 9:I:27:LEU:CD2 | 9:I:78:ILE:HD11 | 2.48 | 0.42 |
| 5:T:37:LYS:O | 5:T:44:LEU:HA | 2.19 | 0.42 |
| 2:R:854:LEU:HD12 | 13:X:35:PHE:CE1 | 2.54 | 0.42 |
| 4:D:70:GLU:OE1 | 4:D:70:GLU:HA | 2.20 | 0.42 |
| 2:B:217:PHE:HA | 2:B:218:PRO:HD3 | 1.96 | 0.42 |
| 9:K:16:ASN:O | 9:K:20:VAL:HG23 | 2.20 | 0.42 |
| 2:B:769:PRO:O | 2:B:770:GLY:O | 2.37 | 0.42 |
| 4:S:206:CYS:O | 4:S:207:GLU:HB2 | 2.20 | 0.42 |
| 2:B:928:MET:HE1 | 2:B:953:ILE:HD12 | 2.00 | 0.42 |
| 3:Y:163:MET:SD | 3:Y:206:LEU:CD2 | 3.08 | 0.42 |
| 2:R:101:LEU:CD1 | 2:R:103:MET:HG3 | 2.49 | 0.42 |
| 3:C:289:ALA:O | 3:C:293:ILE:HG12 | 2.20 | 0.42 |
| 2:B:249:PRO:HB2 | 2:B:253:ASN:N | 2.34 | 0.42 |
| 2:R:291:LYS:C | 2:R:293:GLN:H | 2.22 | 0.42 |
| 1:W:448:LEU:O | 1:W:496:ILE:HG23 | 2.18 | 0.42 |
| 5:E:83:GLU:HA | 6:F:89:MET:CE | 2.48 | 0.42 |
| 8:Z:65:ILE:HD12 | 8:Z:78:TYR:HA | 2.01 | 0.42 |
| 4:S:33:MET:CE | 4:S:162:ALA:HB3 | 2.49 | 0.42 |
| 5:E:99:VAL:O | 5:E:101:LEU:HD12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:S:46:PHE:CG | 4:S:55:ASP:OD2 | 2.73 | 0.42 |
| 1:W:19:ILE:O | 1:W:74:HIS:NE2 | 2.52 | 0.42 |
| 1:A:488:THR:CG2 | 1:A:493:GLY:O | 2.68 | 0.42 |
| 1:W:687:ILE:CD1 | 1:W:695:SER:HB2 | 2.49 | 0.42 |
| 1:W:488:THR:CG2 | 1:W:493:GLY:O | 2.67 | 0.42 |
| 1:A:696:LEU:HD13 | 1:A:700:ILE:HD12 | 2.01 | 0.42 |
| 1:W:573:ARG:HA | 1:W:582:HIS:CD2 | 2.53 | 0.42 |
| 2:B:93:LEU:HD11 | 2:B:859:ALA:H | 1.85 | 0.42 |
| 11:M:3:ILE:CG2 | 11:M:15:LEU:HD11 | 2.50 | 0.42 |
| 1:W:691:THR:HB | 1:W:694:GLU:CB | 2.50 | 0.42 |
| 7:G:36:PHE:CE1 | 7:G:96:ILE:CG1 | 3.03 | 0.42 |
| 5:T:115:ASP:O | 5:T:116:ASP:CG | 2.58 | 0.42 |
| 2:B:525:LEU:CD2 | 2:B:571:VAL:HB | 2.50 | 0.42 |
| 1:A:121:ILE:HG23 | 8:H:38:ARG:NH1 | 2.35 | 0.42 |
| 2:R:949:TYR:C | 2:R:950:LYS:HG3 | 2.39 | 0.42 |
| 5:E:80:VAL:HG12 | 5:E:83:GLU:CD | 2.40 | 0.42 |
| 2:R:782:GLY:O | 2:R:783:VAL:C | 2.58 | 0.42 |
| 3:Y:327:ARG:HG3 | 3:Y:334:VAL:HG22 | 1.99 | 0.42 |
| 3:Y:311:ARG:NH2 | 8:Z:71:LEU:HD22 | 2.35 | 0.42 |
| 3:Y:107:LEU:O | 3:Y:110:ILE:HG22 | 2.19 | 0.42 |
| 4:D:153:HIS:NE2 | 13:P:48:ILE:HG23 | 2.34 | 0.42 |
| 2:B:1061:ILE:HA | 2:B:1072:TRP:NE1 | 2.35 | 0.42 |
| 1:A:450:CYS:H | 1:A:451:PRO:HD2 | 1.83 | 0.42 |
| 3:Y:127:THR:O | 3:Y:131:LYS:HD2 | 2.20 | 0.42 |
| 1:W:687:ILE:HD12 | 1:W:695:SER:CB | 2.49 | 0.42 |
| 6:F:4:VAL:HG22 | 6:F:4:VAL:O | 2.18 | 0.42 |
| 2:B:895:ILE:HG23 | 2:B:899:ASP:HB2 | 2.02 | 0.42 |
| 1:A:572:PRO:HD2 | 1:A:730:ARG:HH12 | 1.85 | 0.42 |
| 1:A:831:ARG:CZ | 3:C:385:MET:HG3 | 2.49 | 0.42 |
| 2:R:579:ARG:HD3 | 2:R:618:TYR:CD2 | 2.55 | 0.42 |
| 11:L:83:TYR:CZ | 11:L:87:ILE:HD11 | 2.55 | 0.42 |
| 8:H:58:LYS:NZ | 10:Q:51:TRP:CH2 | 2.88 | 0.42 |
| 1:W:417:VAL:CG1 | 1:W:464:LEU:HD13 | 2.49 | 0.42 |
| 1:W:326:ILE:HG21 | 1:W:462:MET:SD | 2.60 | 0.42 |
| 3:Y:24:LEU:HD11 | 3:Y:55:ALA:HB1 | 2.02 | 0.42 |
| 2:B:938:LEU:O | 12:N:46:ARG:NH1 | 2.52 | 0.42 |
| 2:R:1039:LEU:HD22 | 2:R:1044:THR:CG2 | 2.49 | 0.42 |
| 2:R:734:GLY:CA | 2:R:735:TYR:CB | 2.97 | 0.42 |
| 1:W:668:ALA:HB2 | 1:W:707:LEU:HD13 | 2.01 | 0.42 |
| 2:B:86:MET:HE3 | 2:B:686:ASN:HD22 | 1.84 | 0.42 |
| 2:R:622:GLU:O | 2:R:625:GLU:CB | 2.64 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:6:ILE:CD1 | 2:B:1094:VAL:HG11 | 2.49 | 0.42 |
| 1:A:505:GLY:CA | 1:A:639:VAL:HG22 | 2.47 | 0.42 |
| 4:D:22:LEU:HD13 | 4:D:226:TYR:CD1 | 2.55 | 0.42 |
| 1:W:224:MET:HE3 | 1:W:224:MET:HA | 2.02 | 0.42 |
| 1:A:45:MET:CE | 1:A:46:ASP:OD1 | 2.67 | 0.42 |
| 2:B:630:ALA:HB2 | 2:B:640:HIS:CG | 2.54 | 0.42 |
| 8:Z:28:ALA:CB | 8:Z:62:ILE:HD11 | 2.49 | 0.42 |
| 1:A:818:TYR:HD2 | 1:A:822:ARG:NH1 | 2.17 | 0.42 |
| 1:W:371:LYS:HD3 | 1:W:372:TRP:N | 2.35 | 0.42 |
| 4:S:37:PRO:HG3 | 4:S:78:TRP:CZ3 | 2.54 | 0.42 |
| 3:C:129:GLU:HB3 | 3:C:130:TYR:CE2 | 2.55 | 0.42 |
| 2:B:126:LEU:HD22 | 2:B:154:TYR:CE2 | 2.55 | 0.42 |
| 9:I:23:TRP:CZ2 | 3:Y:66:PRO:HD3 | 2.55 | 0.42 |
| 7:V:31:MET:CE | 7:V:55:VAL:HG11 | 2.50 | 0.42 |
| 2:B:457:CYS:SG | 2:B:460:GLU:HB2 | 2.60 | 0.42 |
| 1:A:388:LEU:HA | 1:A:391:VAL:HG22 | 2.02 | 0.42 |
| 1:A:833:GLU:HG3 | 1:A:839:ARG:HD2 | 2.01 | 0.42 |
| 8:H:58:LYS:H | 8:H:58:LYS:HG3 | 1.61 | 0.42 |
| 1:W:657:VAL:HG12 | 1:W:657:VAL:O | 2.19 | 0.42 |
| 6:U:62:ILE:HG22 | 6:U:63:ILE:H | 1.84 | 0.42 |
| 1:W:560:PHE:CZ | 1:W:615:LEU:HG | 2.55 | 0.42 |
| 2:R:855:ILE:O | 13:X:34:ILE:CG2 | 2.68 | 0.42 |
| 7:V:40:PHE:HA | 7:V:92:TYR:CD1 | 2.54 | 0.42 |
| 4:S:164:VAL:HA | 4:S:227:ILE:O | 2.18 | 0.42 |
| 1:W:705:ASP:O | 1:W:708:ARG:HG3 | 2.18 | 0.42 |
| 2:R:772:GLN:HG2 | 2:R:773:GLU:N | 2.35 | 0.42 |
| 2:R:356:LEU:HD12 | 2:R:407:VAL:CG2 | 2.48 | 0.42 |
| 2:B:589:ASN:HA | 2:B:590:PRO:HD3 | 1.70 | 0.42 |
| 2:B:101:LEU:CD1 | 2:B:103:MET:HE2 | 2.50 | 0.42 |
| 7:V:95:ILE:C | 7:V:96:ILE:HD12 | 2.40 | 0.42 |
| 5:T:92:VAL:HG11 | 5:T:137:GLN:HA | 2.02 | 0.42 |
| 9:I:63:SER:HA | 9:I:66:GLU:HB2 | 2.01 | 0.42 |
| 4:D:203:CYS:SG | 4:D:204:THR:N | 2.93 | 0.42 |
| 1:A:262:ILE:O | 1:A:266:TRP:HB3 | 2.20 | 0.42 |
| 2:R:252:GLN:O | 2:R:256:PHE:CD2 | 2.73 | 0.42 |
| 1:W:119:ASN:OD1 | 1:W:126:PRO:CB | 2.67 | 0.42 |
| 3:Y:277:ILE:CG2 | 3:Y:278:ARG:N | 2.80 | 0.42 |
| 1:W:853:ASP:HA | 8:Z:72:TYR:HB2 | 2.01 | 0.42 |
| 2:B:345:ARG:HG3 | 2:B:576:GLY:HA3 | 2.01 | 0.42 |
| 4:D:37:PRO:HG3 | 4:D:78:TRP:CZ3 | 2.54 | 0.42 |
| 5:T:13:ILE:HD12 | 5:T:68:HIS:CD2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:139:ASP:O | 2:R:143:GLU:HG3 | 2.19 | 0.42 |
| 1:W:543:ARG:HB2 | 1:W:545:TYR:CE2 | 2.55 | 0.42 |
| 2:B:423:LEU:HB2 | 2:B:716:TYR:HD1 | 1.85 | 0.42 |
| 1:A:811:VAL:O | 1:A:812:ARG:HB2 | 2.20 | 0.42 |
| 1:W:831:ARG:CZ | 3:Y:385:MET:HG3 | 2.50 | 0.42 |
| 3:C:171:ASN:CG | 3:C:172:GLU:H | 2.23 | 0.42 |
| 5:E:136:ILE:CG2 | 5:E:137:GLN:N | 2.75 | 0.42 |
| 3:C:65:ALA:HA | 3:C:66:PRO:HD3 | 1.85 | 0.42 |
| 3:Y:25:PRO:CD | 3:Y:33:LYS:HD3 | 2.50 | 0.42 |
| 1:A:141:MET:O | 1:A:141:MET:CG | 2.67 | 0.42 |
| 2:B:157:VAL:CG2 | 2:B:402:ALA:HB2 | 2.45 | 0.42 |
| 2:R:252:GLN:HA | 2:R:255:LEU:HD12 | 2.02 | 0.42 |
| 10:Q:66:ARG:C | 10:Q:68:PHE:H | 2.23 | 0.42 |
| 3:Y:174:LEU:HB3 | 3:Y:179:VAL:CG1 | 2.47 | 0.42 |
| 2:R:820:PRO:HD3 | 2:R:835:LYS:HA | 2.01 | 0.42 |
| 3:C:301:LEU:HD22 | 3:C:308:VAL:HG12 | 2.02 | 0.42 |
| 5:T:99:VAL:O | 5:T:101:LEU:HD12 | 2.20 | 0.42 |
| 10:Q:40:ASN:HA | 10:Q:43:LEU:HD11 | 2.01 | 0.42 |
| 2:R:492:LEU:HD13 | 2:R:523:VAL:HG11 | 2.02 | 0.42 |
| 11:L:82:HIS:NE2 | 11:L:86:GLU:OE2 | 2.52 | 0.42 |
| 2:B:1100:PHE:CZ | 3:C:375:ILE:HD13 | 2.55 | 0.42 |
| 5:T:96:GLY:HA2 | 5:T:110:ILE:CD1 | 2.50 | 0.42 |
| 8:Z:32:LEU:HD21 | 8:Z:42:LEU:HD11 | 2.02 | 0.42 |
| 5:E:141:LYS:HE3 | 6:F:46:LYS:HZ3 | 1.85 | 0.42 |
| 1:W:102:GLY:O | 1:W:103:ARG:C | 2.58 | 0.42 |
| 2:B:767:LYS:HG3 | 2:B:768:TYR:HA | 1.97 | 0.42 |
| 5:E:167:PRO:HA | 5:E:169:LEU:N | 2.34 | 0.42 |
| 1:W:108:GLU:O | 1:W:109:ASP:C | 2.57 | 0.42 |
| 2:R:690:ARG:HB3 | 2:R:692:ASP:OD1 | 2.19 | 0.42 |
| 2:B:622:GLU:O | 2:B:625:GLU:CB | 2.66 | 0.42 |
| 4:S:65:ILE:HG23 | 4:S:128:ILE:CD1 | 2.49 | 0.42 |
| 2:B:405:ASN:HB3 | 2:B:413:VAL:CG2 | 2.50 | 0.42 |
| 8:H:43:PRO:O | 8:H:44:TRP:HB2 | 2.20 | 0.42 |
| 1:W:684:LEU:H | 1:W:684:LEU:HD12 | 1.84 | 0.42 |
| 2:R:630:ALA:HB3 | 2:R:636:LEU:HD13 | 2.01 | 0.42 |
| 2:R:636:LEU:HD13 | 2:R:643:LEU:HD12 | 2.02 | 0.42 |
| 4:S:53:LEU:CD1 | 4:S:131:VAL:HG23 | 2.50 | 0.42 |
| 4:D:146:ARG:HD2 | 4:D:147:LEU:O | 2.20 | 0.42 |
| 2:B:231:ARG:C | 2:B:233:LEU:H | 2.23 | 0.42 |
| 1:A:541:ALA:HB1 | 7:G:70:ASP:O | 2.20 | 0.42 |
| 1:W:29:THR:OG1 | 1:W:243:VAL:HG12 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:R:126:LEU:HD22 | 2:R:154:TYR:CE2 | 2.55 | 0.42 |
| 3:Y:281:GLU:CD | 3:Y:326:VAL:HG12 | 2.39 | 0.42 |
| 9:K:22:LEU:HA | 9:K:22:LEU:HD23 | 1.82 | 0.42 |
| 9:I:80:ARG:HG2 | 1:W:834:TYR:CE1 | 2.54 | 0.42 |
| 11:M:83:TYR:CZ | 11:M:87:ILE:HD11 | 2.55 | 0.42 |
| 9:I:56:ILE:N | 9:I:57:SER:N | 2.66 | 0.41 |
| 5:E:30:LEU:HD22 | 5:E:72:PHE:CZ | 2.55 | 0.41 |
| 2:B:359:VAL:CG1 | 2:B:407:VAL:HG13 | 2.49 | 0.41 |
| 3:C:311:ARG:NH2 | 8:H:71:LEU:HD22 | 2.35 | 0.41 |
| 1:W:652:SER:HA | 1:W:787:ARG:HG3 | 2.02 | 0.41 |
| 2:R:1053:LEU:HD23 | 2:R:1054:ASP:OD1 | 2.20 | 0.41 |
| 12:O:8:PHE:HE2 | 2:R:723:ASN:ND2 | 2.17 | 0.41 |
| 1:W:618:GLU:HG3 | 1:W:619:TYR:CE2 | 2.55 | 0.41 |
| 1:A:563:HIS:CD2 | 1:A:872:PHE:HE2 | 2.37 | 0.41 |
| 2:B:735:TYR:CE2 | 11:L:48:PRO:HG2 | 2.55 | 0.41 |
| 3:C:151:ASN:O | 3:C:173:MET:HG3 | 2.20 | 0.41 |
| 2:R:776:ILE:HG23 | 2:R:815:GLY:O | 2.20 | 0.41 |
| 2:R:947:PRO:C | 2:R:948:PHE:CD2 | 2.93 | 0.41 |
| 2:B:425:MET:HB3 | 2:B:425:MET:HE2 | 1.77 | 0.41 |
| 2:B:40:ASN:O | 2:B:44:GLU:HG3 | 2.20 | 0.41 |
| 6:U:4:VAL:O | 6:U:4:VAL:HG22 | 2.20 | 0.41 |
| 1:W:748:GLY:HA2 | 1:W:781:PHE:CE2 | 2.55 | 0.41 |
| 2:B:930:GLY:HA3 | 2:B:987:TYR:OH | 2.20 | 0.41 |
| 5:E:40:LYS:O | 5:E:41:ASP:OD1 | 2.38 | 0.41 |
| 2:B:222:GLY:HA3 | 2:B:278:ARG:NH1 | 2.35 | 0.41 |
| 11:M:30:GLY:HA2 | 11:M:33:ARG:NH1 | 2.35 | 0.41 |
| 7:G:34:ASN:N | 7:G:34:ASN:OD1 | 2.53 | 0.41 |
| 2:R:81:ARG:HD3 | 2:R:81:ARG:HA | 1.87 | 0.41 |
| 2:R:880:LYS:C | 2:R:881:PHE:CD1 | 2.94 | 0.41 |
| 1:W:343:ILE:HG22 | 1:W:347:LEU:HD12 | 2.01 | 0.41 |
| 1:A:705:ASP:O | 1:A:708:ARG:HG3 | 2.20 | 0.41 |
| 4:S:176:CYS:O | 4:S:195:LEU:HD11 | 2.19 | 0.41 |
| 2:R:756:THR:HG23 | 2:R:871:ASP:O | 2.20 | 0.41 |
| 2:B:765:GLU:OE2 | 2:B:863:LYS:HB3 | 2.19 | 0.41 |
| 2:B:947:PRO:HB2 | 2:B:948:PHE:CD2 | 2.55 | 0.41 |
| 2:R:101:LEU:HD12 | 2:R:103:MET:HE2 | 2.01 | 0.41 |
| 13:X:6:CYS:HA | 13:X:16:GLU:O | 2.19 | 0.41 |
| 1:A:737:VAL:HG23 | 1:A:738:LEU:HD23 | 2.01 | 0.41 |
| 8:H:39:PRO:HG3 | 10:Q:67:LEU:HD11 | 2.03 | 0.41 |
| 5:T:113:ILE:HG13 | 5:T:164:MET:HB2 | 2.02 | 0.41 |
| 2:B:1053:LEU:CD1 | 3:C:376:GLY:HA3 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:5:ILE:O | 12:N:6:ARG:HB2 | 2.20 | 0.41 |
| 3:C:174:LEU:HB3 | 3:C:179:VAL:CG1 | 2.46 | 0.41 |
| 3:Y:108:ILE:HA | 3:Y:111:VAL:HG12 | 2.02 | 0.41 |
| 13:X:4:TYR:CD1 | 13:X:4:TYR:O | 2.73 | 0.41 |
| 2:B:1112:ILE:O | 2:B:1114:PRO:CD | 2.68 | 0.41 |
| 3:C:127:THR:OG1 | 3:C:129:GLU:O | 2.39 | 0.41 |
| 2:R:1065:ASP:OD2 | 2:R:1118:LEU:HD13 | 2.20 | 0.41 |
| 2:R:1029:LEU:HD11 | 1:W:322:SER:C | 2.41 | 0.41 |
| 2:B:843:ARG:HB2 | 2:B:846:GLU:HB2 | 2.01 | 0.41 |
| 10:J:60:SER:HB2 | 8:Z:29:TYR:HE1 | 1.84 | 0.41 |
| 2:B:808:LYS:NZ | 2:B:847:MET:CE | 2.83 | 0.41 |
| 1:A:823:LEU:HD13 | 3:C:75:ALA:HB1 | 2.02 | 0.41 |
| 11:L:15:LEU:HD12 | 11:L:15:LEU:HA | 1.93 | 0.41 |
| 2:B:22:LYS:O | 2:B:22:LYS:HG2 | 2.20 | 0.41 |
| 4:S:70:GLU:HA | 4:S:70:GLU:OE1 | 2.19 | 0.41 |
| 1:W:696:LEU:HD22 | 1:W:696:LEU:O | 2.21 | 0.41 |
| 2:R:786:TYR:CE1 | 2:R:792:TYR:CE2 | 3.08 | 0.41 |
| 2:B:598:GLU:HG3 | 2:B:605:ILE:HD11 | 2.02 | 0.41 |
| 1:A:338:GLY:O | 1:A:443:PHE:HA | 2.20 | 0.41 |
| 2:R:1052:LEU:N | 2:R:1052:LEU:HD12 | 2.36 | 0.41 |
| 9:K:62:ILE:O | 9:K:66:GLU:HG3 | 2.20 | 0.41 |
| 2:R:115:GLU:HG2 | 2:R:384:LEU:HD12 | 2.01 | 0.41 |
| 2:R:981:LYS:HG2 | 4:S:166:TYR:CE2 | 2.56 | 0.41 |
| 2:B:207:ARG:HB2 | 2:B:216:SER:HB2 | 1.96 | 0.41 |
| 1:W:651:VAL:CG1 | 1:W:743:MET:HB3 | 2.44 | 0.41 |
| 12:O:8:PHE:CG | 12:O:48:MET:HE1 | 2.55 | 0.41 |
| 2:B:807:VAL:HG12 | 2:B:842:THR:HG21 | 2.01 | 0.41 |
| 7:G:25:ASN:HA | 7:G:44:ASP:CG | 2.40 | 0.41 |
| 7:G:24:LYS:O | 7:G:25:ASN:HB2 | 2.20 | 0.41 |
| 1:A:78:VAL:HG13 | 1:A:78:VAL:O | 2.20 | 0.41 |
| 2:R:176:LEU:CD2 | 2:R:343:ASN:OD1 | 2.68 | 0.41 |
| 1:A:856:PHE:HE2 | 1:A:858:MET:HB3 | 1.81 | 0.41 |
| 2:R:780:GLU:O | 2:R:782:GLY:N | 2.53 | 0.41 |
| 1:W:870:ARG:HH22 | 3:Y:36:ILE:HD13 | 1.82 | 0.41 |
| 2:R:808:LYS:O | 2:R:809:GLY:C | 2.59 | 0.41 |
| 5:E:36:GLU:CB | 6:F:33:LEU:HD22 | 2.50 | 0.41 |
| 1:A:45:MET:O | 1:A:45:MET:CE | 2.68 | 0.41 |
| 1:W:517:THR:HG22 | 1:W:518:LYS:N | 2.35 | 0.41 |
| 1:A:23:SER:CB | 1:A:74:HIS:NE2 | 2.83 | 0.41 |
| 2:R:453:TRP:HZ3 | 2:R:644:GLU:OE2 | 2.03 | 0.41 |
| 1:W:139:THR:HG23 | 1:W:139:THR:O | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:T:39:LEU:O | 5:T:40:LYS:C | 2.58 | 0.41 |
| 1:W:757:ILE:HG22 | 1:W:765:THR:HG21 | 2.02 | 0.41 |
| 2:B:778:MET:HE1 | 2:B:795:LEU:HB2 | 2.02 | 0.41 |
| 4:D:169:LYS:HD2 | 4:D:220:SER:OG | 2.20 | 0.41 |
| 1:A:466:VAL:HG12 | 1:A:468:GLN:NE2 | 2.36 | 0.41 |
| 5:E:96:GLY:HA2 | 5:E:110:ILE:CD1 | 2.51 | 0.41 |
| 1:W:338:GLY:HA3 | 1:W:444:ARG:CG | 2.51 | 0.41 |
| 2:R:767:LYS:HG3 | 2:R:768:TYR:CD1 | 2.51 | 0.41 |
| 2:B:594:ARG:NH1 | 2:B:615:LYS:CG | 2.83 | 0.41 |
| 2:B:647:SER:HB2 | 2:B:648:PRO:HD3 | 2.02 | 0.41 |
| 9:I:62:ILE:HA | 9:I:62:ILE:HD13 | 1.84 | 0.41 |
| 2:R:485:GLU:OE1 | 2:R:528:ARG:NH1 | 2.54 | 0.41 |
| 7:V:103:VAL:HG13 | 7:V:104:LYS:N | 2.34 | 0.41 |
| 2:B:209:LYS:O | 2:B:210:ASP:HB3 | 2.20 | 0.41 |
| 3:C:320:MET:HG2 | 3:C:327:ARG:O | 2.21 | 0.41 |
| 1:A:124:ARG:C | 1:A:126:PRO:HD2 | 2.40 | 0.41 |
| 7:V:25:ASN:HA | 7:V:44:ASP:CG | 2.41 | 0.41 |
| 4:D:46:PHE:CG | 4:D:55:ASP:OD2 | 2.73 | 0.41 |
| 1:W:863:GLY:HA2 | 3:Y:311:ARG:HH22 | 1.85 | 0.41 |
| 1:W:879:LYS:NZ | 3:Y:46:ASP:HB3 | 2.35 | 0.41 |
| 5:E:37:LYS:O | 5:E:44:LEU:HA | 2.19 | 0.41 |
| 1:W:45:MET:CE | 1:W:46:ASP:OD1 | 2.67 | 0.41 |
| 2:B:108:ASN:C | 2:B:110:ILE:N | 2.72 | 0.41 |
| 1:A:269:LEU:HA | 1:A:269:LEU:HD23 | 1.93 | 0.41 |
| 1:A:81:VAL:CG2 | 1:A:269:LEU:HB3 | 2.49 | 0.41 |
| 2:B:1042:PHE:C | 2:B:1044:THR:H | 2.23 | 0.41 |
| 7:G:29:ILE:HD12 | 7:G:42:ILE:HG13 | 2.01 | 0.41 |
| 5:E:78:VAL:HA | 5:E:79:PRO:HD3 | 1.92 | 0.41 |
| 3:C:193:LEU:O | 3:C:195:GLU:N | 2.53 | 0.41 |
| 2:R:423:LEU:HB2 | 2:R:716:TYR:HD1 | 1.85 | 0.41 |
| 2:R:792:TYR:CE1 | 2:R:812:VAL:HG21 | 2.55 | 0.41 |
| 2:B:590:PRO:O | 2:B:615:LYS:HD2 | 2.20 | 0.41 |
| 2:B:115:GLU:HG2 | 2:B:384:LEU:HD12 | 2.02 | 0.41 |
| 7:G:115:ILE:N | 7:G:115:ILE:HD12 | 2.34 | 0.41 |
| 3:Y:62:GLY:O | 3:Y:63:LEU:HG | 2.20 | 0.41 |
| 1:A:499:ALA:HB3 | 2:B:737:MET:CE | 2.50 | 0.41 |
| 2:R:1004:ILE:CD1 | 1:W:441:LEU:HD22 | 2.50 | 0.41 |
| 2:B:732:PHE:O | 2:B:733:THR:CG2 | 2.69 | 0.41 |
| 3:C:327:ARG:HG3 | 3:C:334:VAL:HG22 | 2.02 | 0.41 |
| 4:D:49:ASN:OD1 | 4:D:139:ILE:HD11 | 2.20 | 0.41 |
| 2:B:1007:ARG:CZ | 2:B:1028:GLY:H | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:783:VAL:HG11 | 2:R:834:ALA:N | 2.36 | 0.41 |
| 1:W:13:ILE:HG12 | 3:Y:358:ALA:HB1 | 2.02 | 0.41 |
| 1:W:219:ILE:O | 1:W:219:ILE:HG22 | 2.19 | 0.41 |
| 2:B:630:ALA:HB3 | 2:B:636:LEU:HD13 | 2.02 | 0.41 |
| 1:A:509:LEU:HD23 | 1:A:552:VAL:CG2 | 2.49 | 0.41 |
| 2:B:163:VAL:HG13 | 2:B:163:VAL:O | 2.20 | 0.41 |
| 4:D:8:LYS:HG3 | 4:D:13:ILE:HG12 | 2.03 | 0.41 |
| 4:S:13:ILE:HG21 | 4:S:242:LEU:HD11 | 2.02 | 0.41 |
| 1:W:569:SER:HA | 1:W:573:ARG:O | 2.21 | 0.41 |
| 4:S:176:CYS:HB3 | 4:S:195:LEU:HD11 | 2.02 | 0.41 |
| 4:S:94:THR:O | 4:S:94:THR:HG23 | 2.20 | 0.41 |
| 2:B:675:MET:HG2 | 2:B:882:ALA:CB | 2.51 | 0.41 |
| 4:D:176:CYS:O | 4:D:195:LEU:HD11 | 2.20 | 0.41 |
| 2:R:727:LEU:HD22 | 2:R:991:VAL:HG21 | 2.03 | 0.41 |
| 2:R:456:MET:HG2 | 2:R:471:LYS:HD2 | 2.01 | 0.41 |
| 7:G:31:MET:HE2 | 7:G:55:VAL:HG11 | 2.03 | 0.41 |
| 4:D:160:SER:HB3 | 4:D:233:VAL:HG12 | 2.02 | 0.41 |
| 5:T:6:LYS:H | 6:U:8:GLU:HB2 | 1.86 | 0.41 |
| 3:C:347:PHE:O | 3:C:348:GLU:HB3 | 2.20 | 0.41 |
| 2:R:872:LEU:HD23 | 2:R:873:ARG:H | 1.84 | 0.41 |
| 2:R:17:ILE:HG12 | 2:R:21:PHE:CE2 | 2.56 | 0.41 |
| 5:T:98:PHE:HA | 5:T:106:GLY:O | 2.20 | 0.41 |
| 2:B:1096:VAL:CG1 | 2:B:1097:SER:N | 2.84 | 0.41 |
| 2:R:918:LEU:HD12 | 1:W:646:MET:HG2 | 2.02 | 0.41 |
| 4:D:13:ILE:HG21 | 4:D:242:LEU:HD11 | 2.03 | 0.41 |
| 2:R:231:ARG:C | 2:R:233:LEU:H | 2.24 | 0.41 |
| 2:B:73:VAL:O | 2:B:73:VAL:HG13 | 2.20 | 0.41 |
| 1:A:761:TYR:CE1 | 2:B:451:THR:HG22 | 2.56 | 0.41 |
| 2:B:71:PRO:HA | 2:B:97:ALA:HB2 | 2.02 | 0.41 |
| 1:W:831:ARG:HA | 3:Y:68:GLU:O | 2.20 | 0.41 |
| 1:A:675:LEU:O | 1:A:675:LEU:HD23 | 2.20 | 0.41 |
| 9:I:71:ARG:HB3 | 9:I:73:VAL:HG22 | 2.02 | 0.41 |
| 2:B:792:TYR:CE1 | 2:B:812:VAL:HG21 | 2.55 | 0.41 |
| 1:W:60:THR:HG21 | 1:W:71:HIS:CG | 2.56 | 0.41 |
| 4:S:107:LYS:O | 4:S:133:LEU:HB2 | 2.20 | 0.41 |
| 6:F:8:GLU:OE1 | 6:F:10:HIS:ND1 | 2.54 | 0.41 |
| 5:E:119:LYS:O | 5:E:131:LYS:HA | 2.20 | 0.41 |
| 1:A:855:VAL:HG13 | 3:C:63:LEU:O | 2.20 | 0.41 |
| 9:I:59:THR:HB | 9:I:63:SER:OG | 2.21 | 0.41 |
| 10:Q:57:GLY:C | 10:Q:61:VAL:CG1 | 2.89 | 0.41 |
| 2:B:734:GLY:HA3 | 2:B:735:TYR:CB | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:Q:54:LEU:C | 10:Q:55:LEU:HD12 | 2.41 | 0.41 |
| 4:D:65:ILE:HG23 | 4:D:128:ILE:CD1 | 2.51 | 0.41 |
| 1:A:122:LYS:O | 1:A:126:PRO:HG3 | 2.20 | 0.41 |
| 4:D:17:PHE:CD2 | 4:D:25:VAL:HG22 | 2.54 | 0.41 |
| 5:T:124:ARG:O | 5:T:126:ILE:N | 2.54 | 0.41 |
| 2:B:653:ILE:CD1 | 2:B:653:ILE:H | 2.28 | 0.41 |
| 5:E:36:GLU:O | 5:E:37:LYS:HG3 | 2.20 | 0.41 |
| 1:W:46:ASP:H | 1:W:47:PRO:CD | 2.34 | 0.41 |
| 1:A:323:ARG:HB2 | 2:B:1029:LEU:HD21 | 2.02 | 0.41 |
| 2:B:1059:THR:HB | 2:B:1061:ILE:HD12 | 2.03 | 0.41 |
| 10:J:69:GLU:CD | 10:J:73:LYS:HE3 | 2.41 | 0.41 |
| 3:C:120:PRO:HB2 | 3:C:256:SER:CB | 2.51 | 0.41 |
| 1:A:370:ASP:OD1 | 1:A:389:ARG:NH1 | 2.51 | 0.41 |
| 5:T:50:ASN:HB2 | 5:T:73:ASP:HB2 | 2.03 | 0.41 |
| 4:D:94:THR:O | 4:D:94:THR:HG23 | 2.21 | 0.41 |
| 2:B:682:LEU:HD22 | 12:N:55:ILE:HD12 | 2.02 | 0.41 |
| 9:K:62:ILE:HD13 | 9:K:62:ILE:HA | 1.78 | 0.41 |
| 1:W:856:PHE:HE2 | 1:W:858:MET:HB3 | 1.83 | 0.41 |
| 3:Y:32:LEU:O | 3:Y:33:LYS:C | 2.59 | 0.41 |
| 2:B:161:GLU:OE1 | 2:B:419:ARG:NH1 | 2.54 | 0.41 |
| 3:Y:340:SER:HA | 3:Y:364:GLU:HG3 | 2.02 | 0.41 |
| 4:S:154:ALA:C | 4:S:156:PHE:N | 2.74 | 0.41 |
| 5:T:82:GLN:H | 5:T:146:VAL:HG13 | 1.85 | 0.41 |
| 2:R:807:VAL:HG12 | 2:R:842:THR:HG21 | 2.03 | 0.41 |
| 1:W:45:MET:O | 1:W:45:MET:CE | 2.68 | 0.41 |
| 1:A:555:PHE:CD2 | 1:A:631:LEU:HD13 | 2.56 | 0.41 |
| 2:R:236:LEU:HD21 | 2:R:268:VAL:CG2 | 2.50 | 0.41 |
| 3:C:25:PRO:HG3 | 3:C:33:LYS:HD3 | 2.02 | 0.41 |
| 2:R:843:ARG:HB2 | 2:R:846:GLU:HB2 | 2.03 | 0.41 |
| 3:Y:102:LEU:HD21 | 3:Y:119:THR:OG1 | 2.19 | 0.41 |
| 5:T:86:GLU:O | 6:U:44:VAL:HG23 | 2.21 | 0.41 |
| 7:V:13:CYS:O | 7:V:55:VAL:HG12 | 2.21 | 0.41 |
| 1:W:833:GLU:HG3 | 1:W:839:ARG:HD2 | 2.02 | 0.41 |
| 6:F:21:LEU:O | 6:F:24:VAL:HG12 | 2.20 | 0.41 |
| 7:G:13:CYS:O | 7:G:55:VAL:HG12 | 2.20 | 0.41 |
| 7:G:46:ILE:HA | 7:G:46:ILE:HD12 | 1.92 | 0.41 |
| 4:D:11:LYS:O | 4:D:231:GLU:HA | 2.20 | 0.41 |
| 13:P:21:LEU:HD22 | 13:P:22:PRO:HA | 2.02 | 0.41 |
| 1:W:146:CYS:HA | 1:W:147:PRO:HD3 | 1.92 | 0.41 |
| 2:B:773:GLU:CG | 2:B:774:ASP:N | 2.82 | 0.41 |
| 2:B:212:THR:O | 2:B:213:PHE:CB | 2.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:W:326:ILE:HG21 | 1:W:462:MET:CG | 2.50 | 0.41 |
| 2:R:66:ILE:CG2 | 2:R:67:ARG:N | 2.83 | 0.41 |
| 2:R:902:TYR:CZ | 2:R:974:TYR:HB2 | 2.56 | 0.41 |
| 1:A:108:GLU:O | 1:A:109:ASP:C | 2.58 | 0.41 |
| 1:A:141:MET:HA | 1:A:148:HIS:HB2 | 2.02 | 0.41 |
| 2:B:136:TYR:HB2 | 2:B:141:LEU:CD1 | 2.51 | 0.41 |
| 7:G:9:ILE:HB | 7:G:59:ILE:O | 2.21 | 0.41 |
| 5:T:164:MET:O | 5:T:167:PRO:HD3 | 2.20 | 0.41 |
| 2:R:732:PHE:CG | 2:R:733:THR:N | 2.89 | 0.41 |
| 1:W:271:TYR:CZ | 1:W:285:PRO:HB3 | 2.56 | 0.41 |
| 2:B:9:SER:HB3 | 2:B:12:GLU:OE1 | 2.21 | 0.41 |
| 4:D:129:PRO:HG2 | 12:N:3:ILE:HD11 | 2.01 | 0.41 |
| 3:C:122:MET:HB2 | 3:C:253:THR:OG1 | 2.21 | 0.41 |
| 2:B:782:GLY:O | 2:B:783:VAL:C | 2.59 | 0.41 |
| 5:T:82:GLN:OE1 | 6:U:88:ILE:HB | 2.21 | 0.41 |
| 3:C:234:ILE:HG22 | 3:C:235:LYS:N | 2.35 | 0.41 |
| 2:R:1007:ARG:CZ | 2:R:1028:GLY:H | 2.33 | 0.41 |
| 1:A:830:LEU:HD13 | 3:C:315:LEU:HD21 | 2.03 | 0.41 |
| 1:A:47:PRO:O | 1:A:48:ARG:HB2 | 2.20 | 0.41 |
| 3:C:127:THR:O | 3:C:131:LYS:HD2 | 2.21 | 0.41 |
| 5:E:84:VAL:CG2 | 6:F:75:ILE:CD1 | 2.99 | 0.41 |
| 1:A:542:PRO:HD3 | 7:G:70:ASP:O | 2.21 | 0.41 |
| 2:B:1065:ASP:OD2 | 2:B:1118:LEU:HD13 | 2.20 | 0.41 |
| 3:C:284:PHE:HB3 | 3:C:288:ALA:CB | 2.51 | 0.41 |
| 6:F:62:ILE:HG22 | 6:F:63:ILE:N | 2.36 | 0.41 |
| 1:A:696:LEU:O | 1:A:696:LEU:HD22 | 2.20 | 0.41 |
| 11:L:86:GLU:O | 11:L:90:LEU:HB2 | 2.21 | 0.41 |
| 5:E:141:LYS:HE3 | 6:F:46:LYS:NZ | 2.35 | 0.41 |
| 2:B:675:MET:HG3 | 2:B:996:LEU:HD21 | 2.02 | 0.41 |
| 2:B:966:LEU:CD2 | 4:D:184:PRO:HG3 | 2.51 | 0.41 |
| 2:B:966:LEU:CD2 | 4:D:208:GLU:HG3 | 2.51 | 0.41 |
| 11:M:82:HIS:NE2 | 11:M:86:GLU:OE2 | 2.54 | 0.41 |
| 4:D:164:VAL:HA | 4:D:227:ILE:O | 2.21 | 0.41 |
| 1:W:548:GLY:O | 1:W:551:VAL:HG13 | 2.21 | 0.41 |
| 1:W:466:VAL:HG12 | 1:W:468:GLN:NE2 | 2.35 | 0.41 |
| 7:G:40:PHE:HA | 7:G:92:TYR:CD1 | 2.56 | 0.41 |
| 5:E:108:VAL:HB | 5:E:162:LEU:HB2 | 2.03 | 0.41 |
| 5:E:30:LEU:HD22 | 5:E:72:PHE:CD2 | 2.56 | 0.41 |
| 2:B:356:LEU:O | 2:B:359:VAL:HG12 | 2.21 | 0.41 |
| 7:V:96:ILE:HD13 | 7:V:101:LEU:HD22 | 2.01 | 0.41 |
| 3:Y:149:ILE:O | 3:Y:153:VAL:HG12 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:275:THR:HG23 | 1:A:279:ASN:OD1 | 2.21 | 0.41 |
| 2:R:332:ARG:HD2 | 2:R:565:PHE:CD1 | 2.56 | 0.41 |
| 2:R:949:TYR:O | 2:R:950:LYS:HD2 | 2.21 | 0.41 |
| 5:E:123:VAL:HG13 | 5:E:127:ILE:CG1 | 2.49 | 0.41 |
| 3:Y:216:ILE:O | 3:Y:217:ALA:HB3 | 2.21 | 0.41 |
| 2:R:808:LYS:NZ | 2:R:847:MET:CE | 2.84 | 0.41 |
| 3:Y:104:LEU:HD13 | 3:Y:108:ILE:CD1 | 2.51 | 0.41 |
| 2:B:619:LEU:HD22 | 2:B:623:GLU:HG2 | 2.02 | 0.41 |
| 2:B:476:MET:CE | 2:B:645:ILE:HD12 | 2.50 | 0.41 |
| 1:A:662:TYR:HA | 1:A:665:ILE:HG12 | 2.03 | 0.41 |
| 4:D:37:PRO:CG | 4:D:78:TRP:CZ3 | 3.04 | 0.41 |
| 1:A:532:ILE:HG13 | 1:A:533:ASP:N | 2.35 | 0.41 |
| 1:W:675:LEU:HD23 | 1:W:675:LEU:O | 2.20 | 0.41 |
| 3:C:103:GLY:O | 3:C:106:ARG:HB3 | 2.21 | 0.41 |
| 1:W:402:ALA:HB1 | 1:W:403:PRO:HD2 | 2.03 | 0.41 |
| 2:R:491:THR:HG22 | 2:R:495:MET:HE2 | 2.03 | 0.41 |
| 2:R:76:SER:HA | 2:R:77:ASP:HA | 1.83 | 0.41 |
| 2:B:597:ILE:CD1 | 2:B:605:ILE:HA | 2.51 | 0.40 |
| 2:R:928:MET:HE3 | 2:R:953:ILE:HD12 | 2.02 | 0.40 |
| 2:R:112:ALA:O | 2:R:113:GLU:HG3 | 2.20 | 0.40 |
| 7:G:114:LYS:O | 7:G:115:ILE:HD12 | 2.20 | 0.40 |
| 2:R:224:ILE:HG23 | 2:R:225:PRO:HD2 | 2.03 | 0.40 |
| 3:C:388:LEU:HD11 | 9:K:35:VAL:CG1 | 2.51 | 0.40 |
| 13:P:5:ARG:HG3 | 13:P:6:CYS:N | 2.34 | 0.40 |
| 1:W:109:ASP:O | 1:W:112:GLU:C | 2.59 | 0.40 |
| 2:R:734:GLY:H | 2:R:735:TYR:HD2 | 1.69 | 0.40 |
| 10:Q:52:ASP:O | 10:Q:55:LEU:HB2 | 2.21 | 0.40 |
| 2:R:947:PRO:HB2 | 2:R:948:PHE:CE2 | 2.56 | 0.40 |
| 4:S:45:TYR:CE2 | 13:X:44:ILE:HG23 | 2.55 | 0.40 |
| 2:R:914:ASN:OD1 | 2:R:916:HIS:HB2 | 2.21 | 0.40 |
| 6:U:51:SER:HA | 6:U:54:LYS:HD2 | 2.02 | 0.40 |
| 1:W:503:ILE:HG21 | 1:W:731:THR:O | 2.21 | 0.40 |
| 3:C:145:GLU:HG3 | 3:C:240:ALA:HB3 | 2.02 | 0.40 |
| 5:E:98:PHE:HA | 5:E:106:GLY:O | 2.21 | 0.40 |
| 2:B:372:LEU:HD22 | 2:B:376:LYS:HG3 | 2.04 | 0.40 |
| 4:D:224:ASP:HA | 4:D:226:TYR:CZ | 2.55 | 0.40 |
| 1:W:47:PRO:O | 1:W:48:ARG:HB2 | 2.21 | 0.40 |
| 1:A:322:SER:C | 2:B:1029:LEU:HD11 | 2.42 | 0.40 |
| 1:W:666:ASP:HA | 1:W:669:LYS:HD2 | 2.03 | 0.40 |
| 2:B:1040:ILE:HD11 | 3:C:373:ILE:CD1 | 2.51 | 0.40 |
| 10:J:54:LEU:C | 10:J:55:LEU:HD12 | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Y:237:ILE:HA | 3:Y:255:GLY:HA3 | 2.03 | 0.40 |
| 4:D:24:PHE:HA | 11:L:27:LEU:CD1 | 2.50 | 0.40 |
| 1:A:777:GLU:H | 1:A:777:GLU:CD | 2.24 | 0.40 |
| 4:S:83:ILE:CD1 | 4:S:84:ASP:H | 2.34 | 0.40 |
| 1:W:572:PRO:HD2 | 1:W:730:ARG:HH12 | 1.86 | 0.40 |
| 1:W:575:CYS:O | 1:W:576:LYS:HB2 | 2.22 | 0.40 |
| 2:R:855:ILE:O | 13:X:34:ILE:HG23 | 2.21 | 0.40 |
| 3:C:265:LYS:H | 3:C:265:LYS:HD2 | 1.84 | 0.40 |
| 3:C:383:THR:HA | 9:K:30:TYR:HB3 | 2.03 | 0.40 |
| 3:Y:369:VAL:HG12 | 3:Y:379:ILE:HG22 | 2.04 | 0.40 |
| 1:W:279:ASN:HB3 | 1:W:300:GLN:OE1 | 2.22 | 0.40 |
| 7:V:14:GLU:OE2 | 7:V:54:LYS:HE2 | 2.20 | 0.40 |
| 2:R:767:LYS:CG | 2:R:768:TYR:CD1 | 3.04 | 0.40 |
| 1:A:98:CYS:O | 1:A:99:ARG:HB2 | 2.21 | 0.40 |
| 2:B:101:LEU:HD12 | 2:B:103:MET:HE2 | 2.03 | 0.40 |
| 2:B:46:ILE:CG2 | 2:B:66:ILE:HD11 | 2.50 | 0.40 |
| 1:W:419:PHE:CE2 | 1:W:462:MET:HE1 | 2.56 | 0.40 |
| 1:A:855:VAL:HB | 3:C:311:ARG:HH12 | 1.86 | 0.40 |
| 13:X:33:ILE:N | 13:X:33:ILE:CD1 | 2.83 | 0.40 |
| 2:B:647:SER:O | 2:B:650:ILE:HG12 | 2.21 | 0.40 |
| 3:Y:63:LEU:HD23 | 3:Y:63:LEU:HA | 1.96 | 0.40 |
| 4:D:253:ILE:HG13 | 11:L:73:ILE:CG2 | 2.49 | 0.40 |
| 2:B:974:TYR:CZ | 4:D:165:ARG:HA | 2.56 | 0.40 |
| 2:R:525:LEU:CD2 | 2:R:571:VAL:HB | 2.52 | 0.40 |
| 1:A:648:LEU:HD21 | 1:A:787:ARG:HH11 | 1.82 | 0.40 |
| 1:A:668:ALA:HB2 | 1:A:707:LEU:HD13 | 2.00 | 0.40 |
| 3:C:232:LYS:HB3 | 3:C:232:LYS:HE2 | 1.79 | 0.40 |
| 7:V:9:ILE:HB | 7:V:59:ILE:O | 2.21 | 0.40 |
| 1:W:876:VAL:C | 1:W:878:TRP:N | 2.75 | 0.40 |
| 2:B:902:TYR:HD1 | 2:B:903:THR:O | 2.05 | 0.40 |
| 5:T:123:VAL:O | 5:T:123:VAL:CG1 | 2.69 | 0.40 |
| 1:A:806:LEU:HB3 | 2:B:467:SER:OG | 2.22 | 0.40 |
| 6:U:71:VAL:HG13 | 6:U:72:LEU:HD12 | 2.03 | 0.40 |
| 2:B:41:LYS:O | 2:B:43:GLN:N | 2.53 | 0.40 |
| 2:B:1057:ASP:O | 2:B:1097:SER:HA | 2.21 | 0.40 |
| 2:R:796:GLU:OE2 | 13:X:39:LYS:HE2 | 2.21 | 0.40 |
| 2:B:333:ARG:HH11 | 2:B:333:ARG:HB3 | 1.86 | 0.40 |
| 3:Y:284:PHE:HB3 | 3:Y:288:ALA:CB | 2.52 | 0.40 |
| 1:W:11:PHE:HB2 | 3:Y:362:ASP:O | 2.21 | 0.40 |
| 6:U:80:PRO:O | 6:U:83:VAL:HG12 | 2.21 | 0.40 |
| 3:C:392:PRO:HB3 | 5:E:18:PHE:CD1 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:203:CYS:SG | 4:S:204:THR:N | 2.94 | 0.40 |
| 2:B:31:LEU:CD2 | 2:B:125:MET:CE | 2.98 | 0.40 |
| 2:B:25:GLY:O | 2:B:27:VAL:N | 2.54 | 0.40 |
| 3:Y:322:ARG:O | 3:Y:323:THR:CB | 2.69 | 0.40 |
| 6:F:71:VAL:HG13 | 6:F:72:LEU:HD12 | 2.04 | 0.40 |
| 3:C:70:ILE:N | 3:C:70:ILE:CD1 | 2.84 | 0.40 |
| 2:R:784:ARG:HD3 | 2:R:785:GLY:H | 1.85 | 0.40 |
| 2:R:9:SER:HB3 | 2:R:12:GLU:OE1 | 2.21 | 0.40 |
| 3:Y:262:LEU:CD2 | 3:Y:269:ILE:HD12 | 2.51 | 0.40 |
| 8:H:65:ILE:HD12 | 8:H:78:TYR:HA | 2.03 | 0.40 |
| 4:D:95:LYS:HD3 | 4:D:142:GLU:OE2 | 2.22 | 0.40 |
| 2:B:977:ARG:HB2 | 11:L:22:HIS:ND1 | 2.35 | 0.40 |
| 1:W:591:GLY:O | 1:W:592:ILE:HD13 | 2.21 | 0.40 |
| 2:R:759:ARG:CG | 2:R:760:LEU:N | 2.83 | 0.40 |
| 2:R:399:HIS:O | 2:R:403:THR:CG2 | 2.69 | 0.40 |
| 1:A:879:LYS:NZ | 3:C:44:THR:HG22 | 2.36 | 0.40 |
| 1:A:192:VAL:HG21 | 1:A:199:PRO:HB3 | 2.03 | 0.40 |
| 3:Y:286:ILE:HG23 | 3:Y:324:GLY:O | 2.21 | 0.40 |
| 4:S:101:GLU:HB2 | 4:S:137:GLN:O | 2.21 | 0.40 |
| 2:B:800:VAL:HG22 | 2:B:814:ILE:HG23 | 2.03 | 0.40 |
| 2:B:308:ALA:C | 2:B:310:ASP:H | 2.24 | 0.40 |
| 2:R:631:LEU:O | 2:R:632:GLU:OE1 | 2.37 | 0.40 |
| 1:W:388:LEU:HA | 1:W:391:VAL:HG22 | 2.04 | 0.40 |
| 2:B:535:ASP:OD2 | 2:B:538:GLU:OE2 | 2.39 | 0.40 |
| 1:W:532:ILE:HG13 | 1:W:533:ASP:O | 2.22 | 0.40 |
| 4:S:115:LYS:O | 4:S:116:SER:HB2 | 2.21 | 0.40 |
| 5:T:108:VAL:HB | 5:T:162:LEU:HB2 | 2.02 | 0.40 |
| 3:Y:81:PRO:HA | 3:Y:84:GLN:OE1 | 2.21 | 0.40 |
| 2:B:597:ILE:HB | 2:B:603:GLY:HA3 | 2.03 | 0.40 |
| 7:G:96:ILE:HD13 | 7:G:101:LEU:HD21 | 2.03 | 0.40 |
| 7:V:11:LEU:HD23 | 7:V:33:CYS:SG | 2.62 | 0.40 |
| 5:E:167:PRO:HA | 5:E:169:LEU:HD13 | 2.02 | 0.40 |
| 1:A:141:MET:HA | 1:A:148:HIS:CG | 2.55 | 0.40 |
| 2:B:1074:ASP:CB | 2:B:1075:LYS:CA | 2.98 | 0.40 |
| 1:A:664:GLU:OE2 | 1:A:707:LEU:HD22 | 2.22 | 0.40 |
| 1:W:184:LEU:HD22 | 1:W:204:PRO:HB2 | 2.03 | 0.40 |
| 1:W:563:HIS:CD2 | 1:W:872:PHE:HE2 | 2.39 | 0.40 |
| 2:R:947:PRO:O | 2:R:948:PHE:CD2 | 2.75 | 0.40 |
| 2:R:176:LEU:HD21 | 2:R:343:ASN:OD1 | 2.21 | 0.40 |
| 3:Y:292:ILE:C | 3:Y:292:ILE:HD13 | 2.40 | 0.40 |
| 2:R:699:HIS:CE1 | 4:S:57:ILE:CD1 | 3.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:942:ILE:O | 2:R:943:VAL:HB | 2.21 | 0.40 |
| 1:A:524:ILE:CG2 | 1:A:634:VAL:HG13 | 2.52 | 0.40 |
| 1:W:552:VAL:CG1 | 1:W:598:PHE:CE2 | 3.05 | 0.40 |
| 1:A:598:PHE:CE1 | 1:A:611:ILE:CD1 | 3.05 | 0.40 |
| 1:A:552:VAL:CG1 | 1:A:598:PHE:CE2 | 3.04 | 0.40 |
| 7:V:70:ASP:O | 1:W:541:ALA:CB | 2.69 | 0.40 |
| 9:I:27:LEU:N | 9:I:27:LEU:HD12 | 2.37 | 0.40 |
| 2:B:895:ILE:HA | 2:B:896:PRO:HD3 | 1.86 | 0.40 |
| 1:W:524:ILE:CG2 | 1:W:634:VAL:HG13 | 2.51 | 0.40 |
| 3:Y:303:GLU:C | 3:Y:303:GLU:OE1 | 2.59 | 0.40 |
| 5:T:70:VAL:HG13 | 5:T:72:PHE:CE2 | 2.57 | 0.40 |
| 2:B:367:ASP:O | 2:B:371:GLN:N | 2.55 | 0.40 |
| 5:E:167:PRO:CA | 5:E:169:LEU:H | 2.34 | 0.40 |
| 7:V:72:CYS:HA | 7:V:114:LYS:HA | 2.02 | 0.40 |
| 2:R:1042:PHE:C | 2:R:1044:THR:H | 2.24 | 0.40 |
| 10:Q:61:VAL:C | 10:Q:63:GLU:H | 2.24 | 0.40 |
| 1:W:91:TYR:CE1 | 1:W:95:LYS:HD2 | 2.56 | 0.40 |
| 1:W:95:LYS:O | 1:W:96:ALA:HB2 | 2.22 | 0.40 |
| 1:A:648:LEU:HB2 | 2:B:927:ILE:CG2 | 2.52 | 0.40 |
| 12:O:35:LEU:HD13 | 12:O:46:ARG:HD3 | 2.03 | 0.40 |
| 2:B:690:ARG:HB3 | 2:B:692:ASP:OD1 | 2.21 | 0.40 |
| 2:R:1074:ASP:CB | 2:R:1075:LYS:CA | 2.96 | 0.40 |
| 1:A:503:ILE:HG21 | 1:A:731:THR:O | 2.21 | 0.40 |
| 12:N:3:ILE:HG12 | 12:N:18:TRP:HB2 | 2.03 | 0.40 |
| 1:W:563:HIS:CD2 | 1:W:872:PHE:CE2 | 3.10 | 0.40 |
| 2:R:873:ARG:NH2 | 2:R:1002:ASP:OD2 | 2.54 | 0.40 |
| 2:R:170:LEU:HD21 | 2:R:176:LEU:HD12 | 2.00 | 0.40 |
| 3:Y:170:ASP:O | 3:Y:174:LEU:CD1 | 2.70 | 0.40 |
| 3:Y:70:ILE:CD1 | 3:Y:70:ILE:N | 2.84 | 0.40 |
| 2:R:808:LYS:HE3 | 2:R:847:MET:HE1 | 2.04 | 0.40 |
| 5:T:101:LEU:CD1 | 5:T:101:LEU:N | 2.85 | 0.40 |
| 1:W:366:ILE:HD13 | 1:W:366:ILE:O | 2.22 | 0.40 |
| 2:B:492:LEU:HD13 | 2:B:523:VAL:HG11 | 2.03 | 0.40 |
| 1:W:10:LYS:HG2 | 3:Y:363:VAL:HG13 | 2.03 | 0.40 |
| 1:W:696:LEU:HD13 | 1:W:700:ILE:HD12 | 2.04 | 0.40 |
| 1:W:187:VAL:HG23 | 1:W:187:VAL:O | 2.21 | 0.40 |
| 2:R:1103:LEU:O | 2:R:1107:LEU:HG | 2.21 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1 | A | 823/880 (94%) | 669 (81%) | 120 (15%) | 34 (4%) | 3 | 37 |
| 1 | W | 823/880 (94%) | 672 (82%) | 111 (14%) | 40 (5%) | 3 | 32 |
| 2 | B | 1077/1131 (95%) | 887 (82%) | 118 (11%) | 72 (7%) | 1 | 25 |
| 2 | R | 1077/1131 (95%) | 881 (82%) | 122 (11%) | 74 (7%) | 1 | 23 |
| 3 | C | 364/395 (92%) | 278 (76%) | 63 (17%) | 23 (6%) | 2 | 26 |
| 3 | Y | 364/395 (92%) | 282 (78%) | 54 (15%) | 28 (8%) | 1 | 20 |
| 4 | D | 258/265 (97%) | 219 (85%) | 31 (12%) | 8 (3%) | 5 | 45 |
| 4 | S | 258/265 (97%) | 220 (85%) | 30 (12%) | 8 (3%) | 5 | 45 |
| 5 | E | 160/180 (89%) | 127 (79%) | 21 (13%) | 12 (8%) | 1 | 20 |
| 5 | T | 160/180 (89%) | 125 (78%) | 24 (15%) | 11 (7%) | 1 | 23 |
| 6 | F | 88/113 (78%) | 75 (85%) | 11 (12%) | 2 (2%) | 8 | 51 |
| 6 | U | 88/113 (78%) | 77 (88%) | 9 (10%) | 2 (2%) | 8 | 51 |
| 7 | G | 108/132 (82%) | 89 (82%) | 15 (14%) | 4 (4%) | 4 | 40 |
| 7 | V | 108/132 (82%) | 88 (82%) | 16 (15%) | 4 (4%) | 4 | 40 |
| 8 | H | 72/84 (86%) | 59 (82%) | 9 (12%) | 4 (6%) | 2 | 29 |
| 8 | Z | 72/84 (86%) | 59 (82%) | 7 (10%) | 6 (8%) | 1 | 18 |
| 9 | I | 80/95 (84%) | 64 (80%) | 9 (11%) | 7 (9%) | 1 | 16 |
| 9 | K | 80/95 (84%) | 64 (80%) | 9 (11%) | 7 (9%) | 1 | 16 |
| 10 | J | 37/104 (36%) | 27 (73%) | 8 (22%) | 2 (5%) | 2 | 30 |
| 10 | Q | 37/104 (36%) | 27 (73%) | 8 (22%) | 2 (5%) | 2 | 30 |
| 11 | L | 89/92 (97%) | 78 (88%) | 9 (10%) | 2 (2%) | 8 | 52 |
| 11 | M | 89/92 (97%) | 79 (89%) | 8 (9%) | 2 (2%) | 8 | 52 |
| 12 | N | 62/66 (94%) | 50 (81%) | 10 (16%) | 2 (3%) | 5 | 44 |
| 12 | O | 62/66 (94%) | 50 (81%) | 9 (14%) | 3 (5%) | 3 | 32 |
| 13 | P | 43/48 (90%) | 33 (77%) | 7 (16%) | 3 (7%) | 1 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 13 | X | 43/48 (90%) | 33 (77%) | 7 (16%) | 3 (7%) | 1 | 23 |
| All | All | 6522/7170 (91%) | 5312 (81%) | 845 (13%) | 365 (6%) | 2 | 29 |

All (365) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 23 | SER |
| 1 | A | 103 | ARG |
| 1 | A | 108 | GLU |
| 1 | A | 683 | GLU |
| 1 | A | 737 | VAL |
| 2 | B | 28 | ARG |
| 2 | B | 108 | ASN |
| 2 | B | 213 | PHE |
| 2 | B | 331 | GLY |
| 2 | B | 405 | ASN |
| 2 | B | 460 | GLU |
| 2 | B | 521 | SER |
| 2 | B | 590 | PRO |
| 2 | B | 591 | LEU |
| 2 | B | 600 | LEU |
| 2 | B | 602 | SER |
| 2 | B | 605 | ILE |
| 2 | B | 735 | TYR |
| 2 | B | 766 | VAL |
| 2 | B | 768 | TYR |
| 2 | B | 770 | GLY |
| 2 | B | 835 | LYS |
| 2 | B | 950 | LYS |
| 2 | B | 1061 | ILE |
| 2 | B | 1070 | ILE |
| 3 | C | 162 | SER |
| 3 | C | 177 | LYS |
| 3 | C | 192 | LYS |
| 3 | C | 193 | LEU |
| 3 | C | 217 | ALA |
| 3 | C | 236 | GLY |
| 3 | C | 324 | GLY |
| 4 | D | 90 | GLU |
| 5 | E | 114 | THR |
| 5 | E | 116 | ASP |
| 5 | E | 124 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | E | 126 | ILE |
| 5 | E | 133 | LYS |
| 5 | E | 167 | PRO |
| 7 | G | 17 | SER |
| 7 | G | 105 | ILE |
| 8 | H | 13 | ILE |
| 9 | I | 51 | ILE |
| 9 | I | 52 | ASP |
| 9 | I | 53 | ILE |
| 9 | I | 56 | ILE |
| 10 | J | 56 | ASN |
| 9 | K | 51 | ILE |
| 9 | K | 52 | ASP |
| 9 | K | 53 | ILE |
| 9 | K | 56 | ILE |
| 13 | P | 6 | CYS |
| 10 | Q | 56 | ASN |
| 2 | R | 108 | ASN |
| 2 | R | 213 | PHE |
| 2 | R | 405 | ASN |
| 2 | R | 460 | GLU |
| 2 | R | 521 | SER |
| 2 | R | 533 | TYR |
| 2 | R | 590 | PRO |
| 2 | R | 591 | LEU |
| 2 | R | 600 | LEU |
| 2 | R | 602 | SER |
| 2 | R | 605 | ILE |
| 2 | R | 735 | TYR |
| 2 | R | 766 | VAL |
| 2 | R | 768 | TYR |
| 2 | R | 835 | LYS |
| 2 | R | 950 | LYS |
| 2 | R | 1026 | GLU |
| 2 | R | 1061 | ILE |
| 2 | R | 1070 | ILE |
| 4 | S | 90 | GLU |
| 5 | T | 114 | THR |
| 5 | T | 116 | ASP |
| 5 | T | 124 | ARG |
| 5 | T | 126 | ILE |
| 5 | T | 133 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | T | 167 | PRO |
| 7 | V | 17 | SER |
| 7 | V | 105 | ILE |
| 1 | W | 23 | SER |
| 1 | W | 103 | ARG |
| 1 | W | 108 | GLU |
| 1 | W | 683 | GLU |
| 1 | W | 737 | VAL |
| 13 | X | 6 | CYS |
| 3 | Y | 177 | LYS |
| 3 | Y | 192 | LYS |
| 3 | Y | 193 | LEU |
| 3 | Y | 217 | ALA |
| 3 | Y | 324 | GLY |
| 8 | Z | 13 | ILE |
| 1 | A | 96 | ALA |
| 1 | A | 280 | GLU |
| 1 | A | 310 | ARG |
| 1 | A | 332 | ILE |
| 1 | A | 391 | VAL |
| 1 | A | 734 | ARG |
| 1 | A | 812 | ARG |
| 1 | A | 876 | VAL |
| 2 | B | 24 | LYS |
| 2 | B | 46 | ILE |
| 2 | B | 418 | ASP |
| 2 | B | 533 | TYR |
| 2 | B | 598 | GLU |
| 2 | B | 599 | LYS |
| 2 | B | 771 | GLY |
| 2 | B | 772 | GLN |
| 2 | B | 797 | ASP |
| 2 | B | 809 | GLY |
| 2 | B | 877 | ILE |
| 2 | B | 1026 | GLU |
| 2 | B | 1072 | TRP |
| 3 | C | 12 | TYR |
| 3 | C | 194 | GLY |
| 3 | C | 245 | LYS |
| 3 | C | 365 | GLU |
| 4 | D | 206 | CYS |
| 5 | E | 125 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | E | 137 | GLN |
| 7 | G | 103 | VAL |
| 9 | I | 14 | HIS |
| 9 | I | 61 | VAL |
| 9 | K | 61 | VAL |
| 13 | P | 5 | ARG |
| 2 | R | 24 | LYS |
| 2 | R | 49 | GLN |
| 2 | R | 331 | GLY |
| 2 | R | 418 | ASP |
| 2 | R | 598 | GLU |
| 2 | R | 599 | LYS |
| 2 | R | 770 | GLY |
| 2 | R | 771 | GLY |
| 2 | R | 797 | ASP |
| 2 | R | 809 | GLY |
| 2 | R | 877 | ILE |
| 2 | R | 943 | VAL |
| 2 | R | 1029 | LEU |
| 2 | R | 1072 | TRP |
| 4 | S | 117 | GLU |
| 5 | T | 137 | GLN |
| 7 | V | 99 | PHE |
| 7 | V | 103 | VAL |
| 1 | W | 96 | ALA |
| 1 | W | 256 | GLY |
| 1 | W | 308 | ARG |
| 1 | W | 310 | ARG |
| 1 | W | 332 | ILE |
| 1 | W | 391 | VAL |
| 1 | W | 605 | ASN |
| 1 | W | 734 | ARG |
| 1 | W | 812 | ARG |
| 1 | W | 876 | VAL |
| 13 | X | 13 | PHE |
| 3 | Y | 12 | TYR |
| 3 | Y | 82 | GLY |
| 3 | Y | 162 | SER |
| 3 | Y | 194 | GLY |
| 3 | Y | 245 | LYS |
| 3 | Y | 349 | VAL |
| 1 | A | 109 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 148 | HIS |
| 1 | A | 290 | ARG |
| 1 | A | 532 | ILE |
| 1 | A | 536 | GLU |
| 1 | A | 849 | ALA |
| 2 | B | 49 | GLN |
| 2 | B | 116 | GLU |
| 2 | B | 250 | GLU |
| 2 | B | 256 | PHE |
| 2 | B | 375 | SER |
| 2 | B | 407 | VAL |
| 2 | B | 417 | LEU |
| 2 | B | 606 | THR |
| 2 | B | 734 | GLY |
| 2 | B | 918 | LEU |
| 2 | B | 943 | VAL |
| 2 | B | 982 | ILE |
| 2 | B | 985 | ARG |
| 2 | B | 1029 | LEU |
| 3 | C | 53 | ASP |
| 3 | C | 113 | ALA |
| 3 | C | 114 | LYS |
| 3 | C | 171 | ASN |
| 3 | C | 211 | ALA |
| 4 | D | 83 | ILE |
| 4 | D | 85 | CYS |
| 4 | D | 117 | GLU |
| 5 | E | 40 | LYS |
| 7 | G | 99 | PHE |
| 10 | J | 57 | GLY |
| 9 | K | 14 | HIS |
| 9 | K | 91 | SER |
| 11 | L | 19 | GLY |
| 11 | M | 19 | GLY |
| 13 | P | 13 | PHE |
| 10 | Q | 57 | GLY |
| 2 | R | 26 | LEU |
| 2 | R | 28 | ARG |
| 2 | R | 250 | GLU |
| 2 | R | 256 | PHE |
| 2 | R | 375 | SER |
| 2 | R | 406 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 417 | LEU |
| 2 | R | 453 | TRP |
| 2 | R | 772 | GLN |
| 2 | R | 918 | LEU |
| 2 | R | 985 | ARG |
| 4 | S | 83 | ILE |
| 4 | S | 85 | CYS |
| 4 | S | 206 | CYS |
| 5 | T | 40 | LYS |
| 5 | T | 82 | GLN |
| 1 | W | 107 | SER |
| 1 | W | 109 | ASP |
| 1 | W | 148 | HIS |
| 1 | W | 280 | GLU |
| 1 | W | 290 | ARG |
| 1 | W | 393 | ASP |
| 1 | W | 541 | ALA |
| 1 | W | 682 | GLY |
| 1 | W | 849 | ALA |
| 13 | X | 5 | ARG |
| 3 | Y | 53 | ASP |
| 3 | Y | 114 | LYS |
| 3 | Y | 127 | THR |
| 3 | Y | 170 | ASP |
| 3 | Y | 201 | SER |
| 3 | Y | 365 | GLU |
| 8 | Z | 15 | TYR |
| 1 | A | 79 | ARG |
| 1 | A | 256 | GLY |
| 1 | A | 308 | ARG |
| 1 | A | 393 | ASP |
| 1 | A | 541 | ALA |
| 1 | A | 601 | LYS |
| 2 | B | 26 | LEU |
| 2 | B | 437 | ALA |
| 2 | B | 453 | TRP |
| 2 | B | 738 | GLU |
| 2 | B | 781 | PRO |
| 2 | B | 949 | TYR |
| 2 | B | 951 | THR |
| 3 | C | 161 | ALA |
| 3 | C | 170 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | C | 201 | SER |
| 3 | C | 216 | ILE |
| 3 | C | 234 | ILE |
| 4 | D | 193 | GLY |
| 5 | E | 82 | GLN |
| 8 | H | 15 | TYR |
| 8 | H | 81 | VAL |
| 9 | I | 91 | SER |
| 12 | N | 41 | LYS |
| 12 | O | 41 | LYS |
| 2 | R | 116 | GLU |
| 2 | R | 210 | ASP |
| 2 | R | 437 | ALA |
| 2 | R | 535 | ASP |
| 2 | R | 606 | THR |
| 2 | R | 734 | GLY |
| 2 | R | 738 | GLU |
| 2 | R | 839 | SER |
| 2 | R | 949 | TYR |
| 2 | R | 951 | THR |
| 2 | R | 982 | ILE |
| 2 | R | 1053 | LEU |
| 2 | R | 1073 | TYR |
| 5 | T | 125 | GLY |
| 1 | W | 46 | ASP |
| 1 | W | 79 | ARG |
| 1 | W | 287 | SER |
| 1 | W | 413 | ASP |
| 1 | W | 536 | GLU |
| 3 | Y | 113 | ALA |
| 3 | Y | 171 | ASN |
| 3 | Y | 216 | ILE |
| 3 | Y | 234 | ILE |
| 8 | Z | 81 | VAL |
| 1 | A | 46 | ASP |
| 1 | A | 47 | PRO |
| 1 | A | 287 | SER |
| 1 | A | 682 | GLY |
| 2 | B | 71 | PRO |
| 2 | B | 74 | ARG |
| 2 | B | 183 | GLY |
| 2 | B | 210 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 334 | GLU |
| 2 | B | 535 | ASP |
| 2 | B | 706 | VAL |
| 2 | B | 839 | SER |
| 2 | B | 907 | VAL |
| 2 | B | 1044 | THR |
| 3 | C | 44 | THR |
| 3 | C | 349 | VAL |
| 4 | D | 9 | ASP |
| 4 | D | 79 | PRO |
| 5 | E | 120 | TYR |
| 11 | L | 10 | SER |
| 11 | M | 10 | SER |
| 12 | N | 6 | ARG |
| 12 | O | 6 | ARG |
| 2 | R | 78 | ARG |
| 2 | R | 334 | GLU |
| 2 | R | 706 | VAL |
| 2 | R | 1051 | ARG |
| 2 | R | 1079 | LYS |
| 4 | S | 9 | ASP |
| 4 | S | 193 | GLY |
| 1 | W | 62 | GLY |
| 1 | W | 305 | LYS |
| 1 | W | 429 | SER |
| 1 | W | 656 | ASP |
| 3 | Y | 30 | GLU |
| 3 | Y | 161 | ALA |
| 3 | Y | 196 | PHE |
| 3 | Y | 306 | LEU |
| 8 | Z | 10 | ASP |
| 8 | Z | 56 | ASN |
| 1 | A | 62 | GLY |
| 1 | A | 656 | ASP |
| 2 | B | 56 | ILE |
| 2 | B | 438 | ARG |
| 2 | B | 1079 | LYS |
| 5 | E | 166 | GLN |
| 8 | H | 10 | ASP |
| 12 | O | 63 | THR |
| 2 | R | 56 | ILE |
| 2 | R | 183 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | R | 407 | VAL |
| 2 | R | 781 | PRO |
| 2 | R | 783 | VAL |
| 2 | R | 907 | VAL |
| 5 | T | 166 | GLN |
| 6 | U | 4 | VAL |
| 3 | Y | 132 | HIS |
| 3 | Y | 146 | TYR |
| 3 | Y | 210 | PHE |
| 1 | A | 145 | VAL |
| 2 | R | 46 | ILE |
| 2 | R | 1114 | PRO |
| 4 | S | 79 | PRO |
| 1 | W | 282 | PRO |
| 1 | W | 689 | GLY |
| 1 | A | 689 | GLY |
| 2 | B | 769 | PRO |
| 1 | W | 47 | PRO |
| 1 | W | 145 | VAL |
| 1 | W | 532 | ILE |
| 1 | W | 654 | GLY |
| 1 | A | 29 | THR |
| 2 | B | 588 | GLY |
| 2 | B | 901 | PRO |
| 2 | B | 1114 | PRO |
| 6 | F | 25 | ILE |
| 2 | R | 71 | PRO |
| 2 | R | 588 | GLY |
| 2 | B | 783 | VAL |
| 6 | F | 4 | VAL |
| 2 | R | 769 | PRO |
| 2 | R | 901 | PRO |
| 6 | U | 63 | ILE |
| 8 | Z | 11 | PRO |
| 1 | W | 449 | VAL |

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 723/766 (94%) | 683 (94%) | 40 (6%) | 27 | 68 |
| 1 | W | 723/766 (94%) | 678 (94%) | 45 (6%) | 23 | 64 |
| 2 | B | 937/975 (96%) | 880 (94%) | 57 (6%) | 23 | 65 |
| 2 | R | 937/975 (96%) | 871 (93%) | 66 (7%) | 19 | 60 |
| 3 | C | 316/341 (93%) | 290 (92%) | 26 (8%) | 14 | 53 |
| 3 | Y | 316/341 (93%) | 294 (93%) | 22 (7%) | 19 | 60 |
| 4 | D | 233/238 (98%) | 227 (97%) | 6 (3%) | 54 | 82 |
| 4 | S | 233/238 (98%) | 226 (97%) | 7 (3%) | 48 | 80 |
| 5 | E | 144/158 (91%) | 136 (94%) | 8 (6%) | 26 | 67 |
| 5 | T | 144/158 (91%) | 135 (94%) | 9 (6%) | 22 | 63 |
| 6 | F | 84/107 (78%) | 81 (96%) | 3 (4%) | 42 | 77 |
| 6 | U | 84/107 (78%) | 81 (96%) | 3 (4%) | 42 | 77 |
| 7 | G | 104/125 (83%) | 96 (92%) | 8 (8%) | 16 | 56 |
| 7 | V | 104/125 (83%) | 99 (95%) | 5 (5%) | 31 | 71 |
| 8 | H | 67/75 (89%) | 67 (100%) | 0 | 100 | 100 |
| 8 | Z | 67/75 (89%) | 67 (100%) | 0 | 100 | 100 |
| 9 | I | 72/83 (87%) | 70 (97%) | 2 (3%) | 51 | 81 |
| 9 | K | 72/83 (87%) | 70 (97%) | 2 (3%) | 51 | 81 |
| 10 | J | 37/96 (38%) | 35 (95%) | 2 (5%) | 27 | 68 |
| 10 | Q | 37/96 (38%) | 35 (95%) | 2 (5%) | 27 | 68 |
| 11 | L | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 11 | M | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 12 | N | 58/60 (97%) | 53 (91%) | 5 (9%) | 13 | 51 |
| 12 | O | 58/60 (97%) | 54 (93%) | 4 (7%) | 19 | 60 |
| 13 | P | 41/43 (95%) | 38 (93%) | 3 (7%) | 17 | 58 |
| 13 | X | 41/43 (95%) | 38 (93%) | 3 (7%) | 17 | 58 |
| All | All | 5790/6294 (92%) | 5462 (94%) | 328 (6%) | 25 | 67 |

All (328) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 24 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 49 | LEU |
| 1 | A | 61 | CYS |
| 1 | A | 64 | THR |
| 1 | A | 84 | VAL |
| 1 | A | 88 | LYS |
| 1 | A | 91 | TYR |
| 1 | A | 101 | CYS |
| 1 | A | 104 | VAL |
| 1 | A | 105 | LYS |
| 1 | A | 106 | ILE |
| 1 | A | 107 | SER |
| 1 | A | 220 | ARG |
| 1 | A | 223 | ILE |
| 1 | A | 224 | MET |
| 1 | A | 238 | LYS |
| 1 | A | 254 | ASP |
| 1 | A | 284 | LEU |
| 1 | A | 288 | LYS |
| 1 | A | 296 | ARG |
| 1 | A | 314 | SER |
| 1 | A | 326 | ILE |
| 1 | A | 366 | ILE |
| 1 | A | 425 | LEU |
| 1 | A | 438 | LEU |
| 1 | A | 464 | LEU |
| 1 | A | 470 | GLU |
| 1 | A | 488 | THR |
| 1 | A | 551 | VAL |
| 1 | A | 593 | LEU |
| 1 | A | 603 | ILE |
| 1 | A | 653 | LEU |
| 1 | A | 708 | ARG |
| 1 | A | 723 | ASN |
| 1 | A | 763 | THR |
| 1 | A | 764 | ARG |
| 1 | A | 787 | ARG |
| 1 | A | 823 | LEU |
| 1 | A | 868 | VAL |
| 1 | A | 876 | VAL |
| 2 | B | 54 | THR |
| 2 | B | 104 | ILE |
| 2 | B | 111 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 118 | TYR |
| 2 | B | 119 | ILE |
| 2 | B | 166 | THR |
| 2 | B | 170 | LEU |
| 2 | B | 195 | SER |
| 2 | B | 203 | VAL |
| 2 | B | 213 | PHE |
| 2 | B | 215 | VAL |
| 2 | B | 216 | SER |
| 2 | B | 259 | LEU |
| 2 | B | 318 | LEU |
| 2 | B | 344 | LYS |
| 2 | B | 345 | ARG |
| 2 | B | 346 | LEU |
| 2 | B | 418 | ASP |
| 2 | B | 419 | ARG |
| 2 | B | 426 | LEU |
| 2 | B | 436 | LEU |
| 2 | B | 444 | GLU |
| 2 | B | 448 | LEU |
| 2 | B | 456 | MET |
| 2 | B | 470 | VAL |
| 2 | B | 471 | LYS |
| 2 | B | 481 | VAL |
| 2 | B | 525 | LEU |
| 2 | B | 529 | LEU |
| 2 | B | 563 | THR |
| 2 | B | 579 | ARG |
| 2 | B | 591 | LEU |
| 2 | B | 610 | LEU |
| 2 | B | 653 | ILE |
| 2 | B | 662 | GLU |
| 2 | B | 675 | MET |
| 2 | B | 688 | GLN |
| 2 | B | 711 | LEU |
| 2 | B | 735 | TYR |
| 2 | B | 742 | ILE |
| 2 | B | 767 | LYS |
| 2 | B | 874 | ILE |
| 2 | B | 884 | ARG |
| 2 | B | 905 | LYS |
| 2 | B | 913 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 924 | LEU |
| 2 | B | 950 | LYS |
| 2 | B | 951 | THR |
| 2 | B | 953 | ILE |
| 2 | B | 977 | ARG |
| 2 | B | 994 | GLN |
| 2 | B | 1013 | GLN |
| 2 | B | 1051 | ARG |
| 2 | B | 1070 | ILE |
| 2 | B | 1079 | LYS |
| 2 | B | 1081 | VAL |
| 2 | B | 1118 | LEU |
| 3 | C | 47 | GLU |
| 3 | C | 49 | ASP |
| 3 | C | 52 | PHE |
| 3 | C | 64 | ILE |
| 3 | C | 70 | ILE |
| 3 | C | 107 | LEU |
| 3 | C | 111 | VAL |
| 3 | C | 119 | THR |
| 3 | C | 164 | SER |
| 3 | C | 174 | LEU |
| 3 | C | 180 | THR |
| 3 | C | 231 | ILE |
| 3 | C | 232 | LYS |
| 3 | C | 237 | ILE |
| 3 | C | 238 | LYS |
| 3 | C | 278 | ARG |
| 3 | C | 292 | ILE |
| 3 | C | 311 | ARG |
| 3 | C | 315 | LEU |
| 3 | C | 327 | ARG |
| 3 | C | 331 | ARG |
| 3 | C | 338 | LYS |
| 3 | C | 365 | GLU |
| 3 | C | 369 | VAL |
| 3 | C | 380 | LYS |
| 3 | C | 389 | THR |
| 4 | D | 13 | ILE |
| 4 | D | 109 | LEU |
| 4 | D | 151 | LYS |
| 4 | D | 165 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 178 | LYS |
| 4 | D | 258 | LYS |
| 5 | E | 27 | LEU |
| 5 | E | 30 | LEU |
| 5 | E | 48 | ILE |
| 5 | E | 53 | THR |
| 5 | E | 59 | LEU |
| 5 | E | 114 | THR |
| 5 | E | 120 | TYR |
| 5 | E | 137 | GLN |
| 6 | F | 63 | ILE |
| 6 | F | 88 | ILE |
| 6 | F | 90 | ASP |
| 7 | G | 34 | ASN |
| 7 | G | 46 | ILE |
| 7 | G | 48 | ILE |
| 7 | G | 67 | THR |
| 7 | G | 79 | THR |
| 7 | G | 101 | LEU |
| 7 | G | 104 | LYS |
| 7 | G | 106 | ILE |
| 9 | I | 25 | ASN |
| 9 | I | 74 | LEU |
| 10 | J | 43 | LEU |
| 10 | J | 52 | ASP |
| 9 | K | 25 | ASN |
| 9 | K | 74 | LEU |
| 12 | N | 3 | ILE |
| 12 | N | 5 | ILE |
| 12 | N | 40 | VAL |
| 12 | N | 45 | CYS |
| 12 | N | 63 | THR |
| 12 | O | 3 | ILE |
| 12 | O | 5 | ILE |
| 12 | O | 7 | CYS |
| 12 | O | 40 | VAL |
| 13 | P | 18 | LEU |
| 13 | P | 33 | ILE |
| 13 | P | 41 | THR |
| 10 | Q | 43 | LEU |
| 10 | Q | 52 | ASP |
| 2 | R | 49 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 54 | THR |
| 2 | R | 68 | ILE |
| 2 | R | 111 | GLU |
| 2 | R | 118 | TYR |
| 2 | R | 119 | ILE |
| 2 | R | 166 | THR |
| 2 | R | 170 | LEU |
| 2 | R | 195 | SER |
| 2 | R | 213 | PHE |
| 2 | R | 215 | VAL |
| 2 | R | 216 | SER |
| 2 | R | 229 | LEU |
| 2 | R | 259 | LEU |
| 2 | R | 318 | LEU |
| 2 | R | 341 | TYR |
| 2 | R | 344 | LYS |
| 2 | R | 345 | ARG |
| 2 | R | 418 | ASP |
| 2 | R | 419 | ARG |
| 2 | R | 425 | MET |
| 2 | R | 426 | LEU |
| 2 | R | 436 | LEU |
| 2 | R | 444 | GLU |
| 2 | R | 448 | LEU |
| 2 | R | 456 | MET |
| 2 | R | 460 | GLU |
| 2 | R | 470 | VAL |
| 2 | R | 471 | LYS |
| 2 | R | 481 | VAL |
| 2 | R | 525 | LEU |
| 2 | R | 529 | LEU |
| 2 | R | 539 | LEU |
| 2 | R | 579 | ARG |
| 2 | R | 610 | LEU |
| 2 | R | 639 | GLU |
| 2 | R | 646 | TRP |
| 2 | R | 653 | ILE |
| 2 | R | 662 | GLU |
| 2 | R | 675 | MET |
| 2 | R | 688 | GLN |
| 2 | R | 711 | LEU |
| 2 | R | 735 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | R | 742 | ILE |
| 2 | R | 767 | LYS |
| 2 | R | 768 | TYR |
| 2 | R | 772 | GLN |
| 2 | R | 773 | GLU |
| 2 | R | 840 | ILE |
| 2 | R | 874 | ILE |
| 2 | R | 884 | ARG |
| 2 | R | 905 | LYS |
| 2 | R | 913 | LEU |
| 2 | R | 924 | LEU |
| 2 | R | 950 | LYS |
| 2 | R | 951 | THR |
| 2 | R | 953 | ILE |
| 2 | R | 977 | ARG |
| 2 | R | 994 | GLN |
| 2 | R | 1013 | GLN |
| 2 | R | 1051 | ARG |
| 2 | R | 1070 | ILE |
| 2 | R | 1079 | LYS |
| 2 | R | 1081 | VAL |
| 2 | R | 1118 | LEU |
| 2 | R | 1121 | ARG |
| 4 | S | 13 | ILE |
| 4 | S | 109 | LEU |
| 4 | S | 151 | LYS |
| 4 | S | 165 | ARG |
| 4 | S | 178 | LYS |
| 4 | S | 209 | CYS |
| 4 | S | 258 | LYS |
| 5 | T | 27 | LEU |
| 5 | T | 30 | LEU |
| 5 | T | 38 | ILE |
| 5 | T | 48 | ILE |
| 5 | T | 53 | THR |
| 5 | T | 59 | LEU |
| 5 | T | 114 | THR |
| 5 | T | 120 | TYR |
| 5 | T | 137 | GLN |
| 6 | U | 63 | ILE |
| 6 | U | 88 | ILE |
| 6 | U | 90 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | V | 46 | ILE |
| 7 | V | 48 | ILE |
| 7 | V | 79 | THR |
| 7 | V | 104 | LYS |
| 7 | V | 106 | ILE |
| 1 | W | 24 | VAL |
| 1 | W | 61 | CYS |
| 1 | W | 64 | THR |
| 1 | W | 84 | VAL |
| 1 | W | 88 | LYS |
| 1 | W | 91 | TYR |
| 1 | W | 99 | ARG |
| 1 | W | 101 | CYS |
| 1 | W | 105 | LYS |
| 1 | W | 106 | ILE |
| 1 | W | 107 | SER |
| 1 | W | 108 | GLU |
| 1 | W | 191 | ASP |
| 1 | W | 220 | ARG |
| 1 | W | 223 | ILE |
| 1 | W | 224 | MET |
| 1 | W | 238 | LYS |
| 1 | W | 254 | ASP |
| 1 | W | 284 | LEU |
| 1 | W | 288 | LYS |
| 1 | W | 296 | ARG |
| 1 | W | 314 | SER |
| 1 | W | 326 | ILE |
| 1 | W | 356 | TRP |
| 1 | W | 366 | ILE |
| 1 | W | 423 | PRO |
| 1 | W | 425 | LEU |
| 1 | W | 426 | HIS |
| 1 | W | 438 | LEU |
| 1 | W | 464 | LEU |
| 1 | W | 470 | GLU |
| 1 | W | 488 | THR |
| 1 | W | 551 | VAL |
| 1 | W | 593 | LEU |
| 1 | W | 603 | ILE |
| 1 | W | 653 | LEU |
| 1 | W | 708 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | W | 723 | ASN |
| 1 | W | 763 | THR |
| 1 | W | 764 | ARG |
| 1 | W | 787 | ARG |
| 1 | W | 823 | LEU |
| 1 | W | 853 | ASP |
| 1 | W | 868 | VAL |
| 1 | W | 876 | VAL |
| 13 | X | 18 | LEU |
| 13 | X | 33 | ILE |
| 13 | X | 41 | THR |
| 3 | Y | 47 | GLU |
| 3 | Y | 49 | ASP |
| 3 | Y | 52 | PHE |
| 3 | Y | 70 | ILE |
| 3 | Y | 78 | VAL |
| 3 | Y | 119 | THR |
| 3 | Y | 174 | LEU |
| 3 | Y | 231 | ILE |
| 3 | Y | 232 | LYS |
| 3 | Y | 237 | ILE |
| 3 | Y | 238 | LYS |
| 3 | Y | 278 | ARG |
| 3 | Y | 292 | ILE |
| 3 | Y | 311 | ARG |
| 3 | Y | 315 | LEU |
| 3 | Y | 327 | ARG |
| 3 | Y | 331 | ARG |
| 3 | Y | 338 | LYS |
| 3 | Y | 365 | GLU |
| 3 | Y | 369 | VAL |
| 3 | Y | 380 | LYS |
| 3 | Y | 389 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 897 | GLN |
| 2 | R | 897 | GLN |
| 5 | T | 100 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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 | $\# Z > 2$ |
| 16 | F3S | D | 1001 | 4 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 16 | F3S | S | 1001 | 4 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 16 | F3S | D | 1001 | 4 | - | 0/0/24/24 | 0/0/3/3 |
| 16 | F3S | S | 1001 | 4 | - | 0/0/24/24 | 0/0/3/3 |

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.

2 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 16 | D | 1001 | F3S | 5 | 0 |
| 16 | S | 1001 | F3S | 9 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 831/880 (94%) | 0.08 | 18 (2%) 65 50 | 28, 92, 200, 308 | 0 |
| 1 | W | 831/880 (94%) | 0.29 | 54 (6%) 22 13 | 46, 106, 212, 378 | 0 |
| 2 | B | 1085/1131 (95%) | 0.11 | 46 (4%) 40 26 | 29, 88, 181, 293 | 0 |
| 2 | R | 1085/1131 (95%) | 0.15 | 47 (4%) 39 25 | 55, 93, 190, 334 | 0 |
| 3 | C | 368/395 (93%) | 0.38 | 20 (5%) 29 19 | 33, 108, 214, 329 | 0 |
| 3 | Y | 368/395 (93%) | 0.46 | 26 (7%) 19 11 | 56, 115, 224, 338 | 0 |
| 4 | D | 262/265 (98%) | 0.14 | 4 (1%) 76 62 | 59, 116, 219, 298 | 0 |
| 4 | S | 262/265 (98%) | 0.39 | 16 (6%) 25 15 | 77, 134, 209, 265 | 0 |
| 5 | E | 164/180 (91%) | 1.25 | 36 (21%) 1 1 | 70, 166, 254, 302 | 0 |
| 5 | T | 164/180 (91%) | 1.17 | 29 (17%) 2 2 | 72, 164, 255, 300 | 0 |
| 6 | F | 90/113 (79%) | 0.98 | 18 (20%) 1 1 | 98, 188, 257, 327 | 0 |
| 6 | U | 90/113 (79%) | 0.94 | 18 (20%) 1 1 | 128, 184, 276, 323 | 0 |
| 7 | G | 110/132 (83%) | 0.48 | 6 (5%) 29 19 | 66, 132, 226, 301 | 0 |
| 7 | V | 110/132 (83%) | 0.75 | 13 (11%) 6 5 | 75, 145, 228, 295 | 0 |
| 8 | H | 74/84 (88%) | 0.05 | 2 (2%) 58 42 | 53, 82, 153, 205 | 0 |
| 8 | Z | 74/84 (88%) | 0.01 | 0 100 100 | 83, 99, 171, 205 | 0 |
| 9 | I | 82/95 (86%) | 0.09 | 0 100 100 | 57, 91, 160, 195 | 0 |
| 9 | K | 82/95 (86%) | 0.06 | 1 (1%) 81 67 | 35, 84, 181, 219 | 0 |
| 10 | J | 39/104 (37%) | 0.91 | 7 (17%) 2 2 | 130, 183, 243, 268 | 0 |
| 10 | Q | 39/104 (37%) | 0.68 | 3 (7%) 16 10 | 112, 162, 213, 265 | 0 |
| 11 | L | 91/92 (98%) | 0.02 | 1 (1%) 82 69 | 65, 99, 194, 250 | 0 |
| 11 | M | 91/92 (98%) | 0.29 | 5 (5%) 29 19 | 95, 121, 175, 247 | 0 |
| 12 | N | 64/66 (96%) | 0.01 | 0 100 100 | 59, 103, 177, 205 | 0 |
| 12 | O | 64/66 (96%) | -0.15 | 0 100 100 | 91, 112, 168, 192 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | P | 45/48 (93%) | 0.33 | 2 (4%) 38 25 | 71, 93, 189, 275 | 0 |
| 13 | X | 45/48 (93%) | 0.31 | 2 (4%) 38 25 | 85, 105, 197, 249 | 0 |
| All | All | 6610/7170 (92%) | 0.28 | 374 (5%) 27 17 | 28, 105, 217, 378 | 0 |

All (374) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | E | 119 | LYS | 8.1 |
| 5 | T | 119 | LYS | 7.4 |
| 5 | E | 87 | GLY | 6.8 |
| 1 | W | 24 | VAL | 6.7 |
| 3 | Y | 212 | ASN | 6.4 |
| 7 | G | 17 | SER | 5.7 |
| 1 | W | 25 | THR | 5.7 |
| 5 | T | 87 | GLY | 5.6 |
| 3 | Y | 224 | ASP | 5.6 |
| 2 | R | 279 | VAL | 5.3 |
| 3 | Y | 234 | ILE | 5.3 |
| 1 | W | 191 | ASP | 5.3 |
| 3 | C | 234 | ILE | 5.2 |
| 1 | W | 105 | LYS | 5.1 |
| 5 | T | 88 | GLU | 5.0 |
| 5 | T | 107 | LEU | 4.8 |
| 2 | R | 234 | GLY | 4.8 |
| 5 | T | 121 | ASP | 4.7 |
| 1 | W | 118 | TYR | 4.7 |
| 5 | E | 130 | GLU | 4.7 |
| 2 | B | 838 | THR | 4.5 |
| 3 | Y | 229 | THR | 4.4 |
| 5 | E | 116 | ASP | 4.4 |
| 1 | A | 117 | ILE | 4.3 |
| 1 | W | 194 | ILE | 4.3 |
| 4 | S | 86 | THR | 4.3 |
| 7 | V | 17 | SER | 4.3 |
| 5 | E | 88 | GLU | 4.3 |
| 1 | W | 291 | SER | 4.3 |
| 5 | E | 131 | LYS | 4.3 |
| 5 | E | 151 | SER | 4.2 |
| 5 | T | 72 | PHE | 4.2 |
| 1 | W | 115 | SER | 4.2 |
| 5 | T | 73 | ASP | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | W | 293 | ARG | 4.1 |
| 5 | E | 86 | GLU | 4.1 |
| 2 | R | 1072 | TRP | 4.1 |
| 5 | E | 118 | LEU | 4.0 |
| 2 | B | 771 | GLY | 4.0 |
| 2 | R | 771 | GLY | 4.0 |
| 2 | R | 257 | PRO | 4.0 |
| 2 | B | 772 | GLN | 4.0 |
| 5 | T | 8 | ARG | 4.0 |
| 1 | W | 75 | ILE | 3.9 |
| 2 | R | 779 | PRO | 3.8 |
| 5 | E | 124 | ARG | 3.8 |
| 3 | C | 229 | THR | 3.8 |
| 5 | E | 121 | ASP | 3.8 |
| 3 | Y | 189 | ASN | 3.7 |
| 5 | E | 135 | VAL | 3.7 |
| 11 | M | 11 | ASN | 3.7 |
| 6 | F | 43 | SER | 3.7 |
| 2 | B | 283 | GLN | 3.7 |
| 5 | T | 131 | LYS | 3.7 |
| 3 | Y | 214 | ASP | 3.7 |
| 1 | W | 26 | ALA | 3.7 |
| 3 | C | 189 | ASN | 3.7 |
| 6 | F | 78 | ILE | 3.7 |
| 1 | W | 46 | ASP | 3.6 |
| 5 | T | 130 | GLU | 3.6 |
| 5 | E | 74 | MET | 3.6 |
| 3 | Y | 211 | ALA | 3.6 |
| 2 | B | 279 | VAL | 3.6 |
| 6 | F | 74 | SER | 3.6 |
| 1 | W | 192 | VAL | 3.6 |
| 1 | A | 118 | TYR | 3.6 |
| 5 | T | 122 | ASN | 3.5 |
| 1 | W | 142 | LYS | 3.5 |
| 2 | R | 278 | ARG | 3.5 |
| 2 | B | 770 | GLY | 3.5 |
| 6 | U | 58 | GLU | 3.5 |
| 4 | S | 143 | ALA | 3.5 |
| 2 | R | 838 | THR | 3.4 |
| 1 | A | 139 | THR | 3.4 |
| 7 | V | 53 | GLU | 3.4 |
| 13 | P | 11 | LYS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 57 | GLU | 3.4 |
| 2 | R | 231 | ARG | 3.4 |
| 3 | Y | 194 | GLY | 3.4 |
| 3 | C | 213 | ILE | 3.4 |
| 5 | E | 125 | GLY | 3.3 |
| 1 | W | 30 | PRO | 3.3 |
| 2 | B | 224 | ILE | 3.3 |
| 2 | R | 224 | ILE | 3.3 |
| 3 | Y | 249 | TYR | 3.3 |
| 2 | R | 437 | ALA | 3.3 |
| 5 | T | 124 | ARG | 3.2 |
| 6 | F | 75 | ILE | 3.2 |
| 6 | U | 27 | SER | 3.2 |
| 6 | F | 77 | PRO | 3.2 |
| 2 | R | 283 | GLN | 3.2 |
| 2 | R | 603 | GLY | 3.2 |
| 5 | T | 118 | LEU | 3.2 |
| 2 | B | 55 | GLU | 3.2 |
| 6 | U | 81 | ASP | 3.2 |
| 1 | W | 134 | GLU | 3.2 |
| 7 | V | 14 | GLU | 3.2 |
| 2 | R | 770 | GLY | 3.2 |
| 4 | S | 94 | THR | 3.2 |
| 4 | D | 84 | ASP | 3.2 |
| 3 | C | 194 | GLY | 3.2 |
| 2 | B | 604 | SER | 3.1 |
| 7 | V | 12 | SER | 3.1 |
| 2 | R | 280 | ALA | 3.1 |
| 2 | R | 772 | GLN | 3.1 |
| 5 | E | 134 | LYS | 3.1 |
| 3 | Y | 192 | LYS | 3.1 |
| 2 | R | 275 | ILE | 3.1 |
| 3 | Y | 213 | ILE | 3.1 |
| 1 | A | 80 | PRO | 3.1 |
| 2 | B | 437 | ALA | 3.1 |
| 1 | W | 135 | TYR | 3.1 |
| 1 | W | 190 | SER | 3.1 |
| 2 | B | 1072 | TRP | 3.0 |
| 2 | R | 774 | ASP | 3.0 |
| 11 | L | 11 | ASN | 3.0 |
| 1 | A | 24 | VAL | 3.0 |
| 2 | R | 217 | PHE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | W | 143 | ALA | 3.0 |
| 6 | U | 42 | ASN | 3.0 |
| 1 | W | 195 | LEU | 3.0 |
| 1 | W | 398 | ALA | 3.0 |
| 2 | B | 54 | THR | 3.0 |
| 3 | Y | 244 | LYS | 3.0 |
| 4 | S | 142 | GLU | 3.0 |
| 5 | T | 114 | THR | 3.0 |
| 1 | W | 399 | SER | 3.0 |
| 1 | W | 139 | THR | 2.9 |
| 1 | A | 190 | SER | 2.9 |
| 7 | V | 99 | PHE | 2.9 |
| 2 | B | 790 | GLU | 2.9 |
| 2 | B | 769 | PRO | 2.9 |
| 1 | W | 187 | VAL | 2.9 |
| 5 | E | 28 | ASN | 2.9 |
| 6 | F | 28 | GLY | 2.9 |
| 13 | X | 30 | GLY | 2.9 |
| 1 | A | 25 | THR | 2.9 |
| 1 | W | 74 | HIS | 2.9 |
| 1 | W | 238 | LYS | 2.9 |
| 2 | R | 54 | THR | 2.9 |
| 2 | R | 604 | SER | 2.9 |
| 10 | J | 51 | TRP | 2.9 |
| 2 | B | 217 | PHE | 2.8 |
| 4 | D | 43 | ASP | 2.8 |
| 2 | B | 278 | ARG | 2.8 |
| 5 | T | 135 | VAL | 2.8 |
| 6 | F | 27 | SER | 2.8 |
| 6 | U | 90 | ASP | 2.8 |
| 2 | B | 387 | LEU | 2.8 |
| 3 | Y | 262 | LEU | 2.8 |
| 6 | F | 58 | GLU | 2.8 |
| 2 | B | 280 | ALA | 2.8 |
| 5 | E | 1 | MET | 2.8 |
| 1 | W | 274 | ALA | 2.8 |
| 3 | C | 254 | ASP | 2.8 |
| 2 | R | 53 | PRO | 2.8 |
| 4 | S | 174 | GLY | 2.8 |
| 3 | C | 212 | ASN | 2.7 |
| 6 | U | 63 | ILE | 2.7 |
| 6 | U | 78 | ILE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | V | 10 | ILE | 2.7 |
| 2 | R | 307 | SER | 2.7 |
| 2 | R | 790 | GLU | 2.7 |
| 4 | S | 145 | LEU | 2.7 |
| 2 | B | 287 | ASN | 2.7 |
| 1 | W | 665 | ILE | 2.7 |
| 2 | B | 257 | PRO | 2.7 |
| 1 | W | 531 | LYS | 2.7 |
| 6 | U | 77 | PRO | 2.7 |
| 5 | T | 108 | VAL | 2.7 |
| 6 | F | 91 | SER | 2.7 |
| 9 | K | 52 | ASP | 2.7 |
| 7 | V | 36 | PHE | 2.7 |
| 6 | U | 12 | ILE | 2.6 |
| 5 | E | 158 | PRO | 2.6 |
| 5 | T | 116 | ASP | 2.6 |
| 7 | V | 35 | ASP | 2.6 |
| 5 | E | 8 | ARG | 2.6 |
| 6 | U | 43 | SER | 2.6 |
| 2 | R | 269 | ASP | 2.6 |
| 5 | E | 97 | VAL | 2.6 |
| 2 | B | 234 | GLY | 2.6 |
| 5 | E | 115 | ASP | 2.6 |
| 4 | D | 88 | ASN | 2.6 |
| 5 | E | 106 | GLY | 2.6 |
| 2 | R | 602 | SER | 2.6 |
| 5 | E | 72 | PHE | 2.6 |
| 5 | E | 136 | ILE | 2.6 |
| 1 | W | 151 | GLU | 2.6 |
| 3 | Y | 349 | VAL | 2.6 |
| 6 | F | 50 | GLU | 2.6 |
| 2 | B | 189 | THR | 2.6 |
| 2 | R | 178 | ASP | 2.6 |
| 3 | Y | 256 | SER | 2.6 |
| 5 | T | 7 | ALA | 2.6 |
| 5 | E | 120 | TYR | 2.6 |
| 1 | W | 91 | TYR | 2.5 |
| 5 | E | 137 | GLN | 2.5 |
| 2 | R | 258 | SER | 2.5 |
| 4 | S | 85 | CYS | 2.5 |
| 10 | J | 73 | LYS | 2.5 |
| 3 | C | 190 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | S | 116 | SER | 2.5 |
| 1 | A | 194 | ILE | 2.5 |
| 2 | R | 294 | GLN | 2.5 |
| 3 | C | 214 | ASP | 2.5 |
| 11 | M | 89 | GLY | 2.5 |
| 3 | C | 256 | SER | 2.5 |
| 1 | W | 130 | ARG | 2.5 |
| 7 | G | 12 | SER | 2.5 |
| 7 | V | 11 | LEU | 2.5 |
| 10 | Q | 42 | GLU | 2.5 |
| 1 | W | 182 | GLU | 2.5 |
| 3 | C | 177 | LYS | 2.5 |
| 2 | R | 277 | SER | 2.5 |
| 2 | R | 1076 | ASN | 2.4 |
| 2 | B | 306 | THR | 2.4 |
| 1 | A | 137 | LYS | 2.4 |
| 1 | W | 596 | GLY | 2.4 |
| 2 | R | 306 | THR | 2.4 |
| 5 | T | 86 | GLU | 2.4 |
| 6 | F | 53 | GLN | 2.4 |
| 2 | B | 57 | PRO | 2.4 |
| 11 | M | 15 | LEU | 2.4 |
| 3 | Y | 167 | LEU | 2.4 |
| 1 | W | 27 | ILE | 2.4 |
| 11 | M | 40 | PHE | 2.4 |
| 2 | R | 436 | LEU | 2.4 |
| 2 | R | 265 | ILE | 2.4 |
| 13 | P | 28 | TYR | 2.4 |
| 5 | T | 97 | VAL | 2.4 |
| 10 | Q | 51 | TRP | 2.4 |
| 1 | W | 80 | PRO | 2.4 |
| 2 | R | 769 | PRO | 2.4 |
| 2 | B | 774 | ASP | 2.4 |
| 2 | R | 266 | ALA | 2.4 |
| 2 | R | 600 | LEU | 2.4 |
| 2 | R | 57 | PRO | 2.4 |
| 5 | T | 80 | VAL | 2.4 |
| 10 | J | 70 | ASP | 2.4 |
| 1 | A | 103 | ARG | 2.4 |
| 5 | T | 140 | ASP | 2.4 |
| 3 | Y | 267 | VAL | 2.4 |
| 5 | E | 150 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 142 | LYS | 2.3 |
| 5 | E | 81 | VAL | 2.3 |
| 5 | E | 114 | THR | 2.3 |
| 5 | T | 111 | SER | 2.3 |
| 3 | C | 332 | HIS | 2.3 |
| 5 | E | 73 | ASP | 2.3 |
| 8 | H | 66 | ILE | 2.3 |
| 7 | V | 50 | SER | 2.3 |
| 3 | Y | 190 | ARG | 2.3 |
| 2 | B | 779 | PRO | 2.3 |
| 3 | C | 131 | LYS | 2.3 |
| 1 | A | 50 | GLY | 2.3 |
| 1 | A | 136 | VAL | 2.3 |
| 1 | A | 237 | HIS | 2.3 |
| 5 | T | 151 | SER | 2.3 |
| 1 | W | 18 | GLU | 2.3 |
| 3 | C | 27 | LYS | 2.3 |
| 2 | R | 247 | LEU | 2.3 |
| 6 | U | 80 | PRO | 2.3 |
| 6 | F | 79 | THR | 2.3 |
| 3 | C | 178 | GLY | 2.3 |
| 2 | B | 286 | GLU | 2.3 |
| 3 | Y | 168 | GLN | 2.3 |
| 3 | Y | 254 | ASP | 2.3 |
| 1 | W | 136 | VAL | 2.3 |
| 6 | F | 63 | ILE | 2.3 |
| 2 | B | 1076 | ASN | 2.3 |
| 3 | Y | 193 | LEU | 2.3 |
| 4 | S | 45 | TYR | 2.3 |
| 2 | B | 289 | ILE | 2.3 |
| 7 | G | 53 | GLU | 2.3 |
| 1 | W | 261 | ILE | 2.3 |
| 2 | B | 814 | ILE | 2.3 |
| 5 | E | 107 | LEU | 2.3 |
| 6 | U | 79 | THR | 2.3 |
| 4 | S | 88 | ASN | 2.2 |
| 6 | F | 76 | CYS | 2.2 |
| 2 | R | 297 | ASP | 2.2 |
| 10 | J | 40 | ASN | 2.2 |
| 1 | W | 260 | LEU | 2.2 |
| 2 | R | 136 | TYR | 2.2 |
| 6 | F | 47 | CYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | G | 92 | TYR | 2.2 |
| 2 | B | 785 | GLY | 2.2 |
| 7 | G | 36 | PHE | 2.2 |
| 2 | B | 817 | VAL | 2.2 |
| 2 | B | 773 | GLU | 2.2 |
| 13 | X | 46 | LYS | 2.2 |
| 3 | Y | 159 | ASP | 2.2 |
| 7 | G | 10 | ILE | 2.2 |
| 1 | W | 112 | GLU | 2.2 |
| 10 | J | 67 | LEU | 2.2 |
| 1 | W | 576 | LYS | 2.2 |
| 2 | B | 266 | ALA | 2.2 |
| 4 | S | 84 | ASP | 2.2 |
| 2 | B | 837 | ASP | 2.2 |
| 2 | R | 80 | GLU | 2.2 |
| 4 | D | 142 | GLU | 2.2 |
| 3 | Y | 124 | ILE | 2.2 |
| 2 | R | 289 | ILE | 2.2 |
| 1 | W | 179 | ASP | 2.2 |
| 1 | W | 666 | ASP | 2.2 |
| 3 | C | 183 | ASP | 2.2 |
| 1 | A | 293 | ARG | 2.2 |
| 1 | A | 398 | ALA | 2.2 |
| 1 | W | 133 | THR | 2.2 |
| 6 | F | 42 | ASN | 2.2 |
| 3 | C | 241 | ILE | 2.2 |
| 3 | Y | 198 | ILE | 2.2 |
| 1 | W | 642 | GLN | 2.2 |
| 1 | W | 294 | PRO | 2.2 |
| 6 | U | 53 | GLN | 2.2 |
| 5 | T | 45 | VAL | 2.1 |
| 6 | F | 90 | ASP | 2.1 |
| 6 | U | 28 | GLY | 2.1 |
| 1 | A | 46 | ASP | 2.1 |
| 5 | T | 36 | GLU | 2.1 |
| 7 | V | 37 | ASN | 2.1 |
| 10 | J | 53 | ASN | 2.1 |
| 2 | B | 436 | LEU | 2.1 |
| 3 | Y | 39 | LYS | 2.1 |
| 2 | B | 818 | SER | 2.1 |
| 6 | U | 70 | ALA | 2.1 |
| 10 | J | 62 | ASP | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | R | 233 | LEU | 2.1 |
| 6 | U | 19 | LYS | 2.1 |
| 3 | C | 337 | GLU | 2.1 |
| 1 | W | 541 | ALA | 2.1 |
| 1 | W | 673 | ASP | 2.1 |
| 2 | B | 1065 | ASP | 2.1 |
| 1 | W | 116 | ARG | 2.1 |
| 5 | T | 85 | VAL | 2.1 |
| 1 | W | 137 | LYS | 2.1 |
| 2 | B | 22 | LYS | 2.1 |
| 2 | R | 387 | LEU | 2.1 |
| 4 | S | 216 | LEU | 2.1 |
| 5 | E | 53 | THR | 2.1 |
| 1 | W | 295 | LEU | 2.1 |
| 2 | B | 840 | ILE | 2.1 |
| 2 | R | 601 | ASP | 2.1 |
| 6 | U | 6 | ILE | 2.1 |
| 4 | S | 109 | LEU | 2.1 |
| 2 | B | 248 | ASP | 2.1 |
| 2 | B | 1079 | LYS | 2.1 |
| 3 | C | 244 | LYS | 2.1 |
| 5 | T | 115 | ASP | 2.1 |
| 3 | Y | 158 | ILE | 2.0 |
| 4 | S | 93 | TYR | 2.0 |
| 10 | Q | 73 | LYS | 2.0 |
| 5 | E | 100 | ASN | 2.0 |
| 4 | S | 175 | ASN | 2.0 |
| 1 | W | 193 | GLU | 2.0 |
| 2 | B | 959 | GLU | 2.0 |
| 5 | E | 32 | GLN | 2.0 |
| 8 | H | 21 | GLU | 2.0 |
| 2 | B | 531 | GLY | 2.0 |
| 11 | M | 35 | ILE | 2.0 |
| 5 | E | 132 | SER | 2.0 |
| 2 | B | 601 | ASP | 2.0 |
| 3 | C | 365 | GLU | 2.0 |
| 4 | S | 125 | SER | 2.0 |
| 6 | U | 57 | GLU | 2.0 |
| 7 | V | 41 | ASP | 2.0 |
| 5 | E | 49 | LEU | 2.0 |
| 1 | A | 111 | ILE | 2.0 |
| 1 | W | 687 | ILE | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 605 | ILE | 2.0 |
| 2 | R | 77 | ASP | 2.0 |
| 5 | T | 94 | ASN | 2.0 |
| 7 | V | 91 | ARG | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 14 | ZN | B | 2124 | 1/1 | 0.10 | 0.46 | 2.00 | 246,246,246,246 | 0 |
| 16 | F3S | D | 1001 | 7/7 | 0.83 | 0.33 | 1.10 | 232,235,241,245 | 0 |
| 16 | F3S | S | 1001 | 7/7 | 0.86 | 0.36 | 1.09 | 247,251,257,260 | 0 |
| 14 | ZN | W | 1881 | 1/1 | 0.91 | 0.22 | -0.57 | 246,246,246,246 | 0 |
| 14 | ZN | A | 1880 | 1/1 | 0.91 | 0.14 | -0.87 | 246,246,246,246 | 0 |
| 14 | ZN | B | 2123 | 1/1 | 0.91 | 0.25 | -0.89 | 246,246,246,246 | 0 |
| 14 | ZN | R | 2123 | 1/1 | 0.88 | 0.22 | -0.90 | 246,246,246,246 | 0 |
| 14 | ZN | P | 1049 | 1/1 | 0.97 | 0.10 | -1.07 | 142,142,142,142 | 0 |
| 14 | ZN | X | 1049 | 1/1 | 0.95 | 0.13 | -1.15 | 157,157,157,157 | 0 |
| 14 | ZN | O | 1065 | 1/1 | 0.97 | 0.14 | -1.31 | 165,165,165,165 | 0 |
| 14 | ZN | A | 1881 | 1/1 | 0.95 | 0.06 | -1.33 | 246,246,246,246 | 0 |
| 14 | ZN | N | 1065 | 1/1 | 0.98 | 0.13 | -1.37 | 130,130,130,130 | 0 |
| 14 | ZN | W | 1880 | 1/1 | 0.89 | 0.07 | -1.93 | 246,246,246,246 | 0 |
| 15 | MG | A | 1882 | 1/1 | 0.78 | 0.25 | - | 246,246,246,246 | 0 |
| 14 | ZN | R | 2124 | 1/1 | 0.39 | 0.48 | - | 246,246,246,246 | 0 |
| 14 | ZN | B | 2125 | 1/1 | 0.17 | 0.63 | - | 246,246,246,246 | 0 |
| 14 | ZN | R | 2125 | 1/1 | 0.48 | 1.06 | - | 246,246,246,246 | 0 |
| 15 | MG | W | 1882 | 1/1 | 0.70 | 0.45 | - | 246,246,246,246 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.