



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:29 AM EDT

PDB ID : 1WZ2
Title : The crystal structure of Leucyl-tRNA synthetase and tRNA(leucine) complex
Authors : Fukunaga, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-02-21
Resolution : 3.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

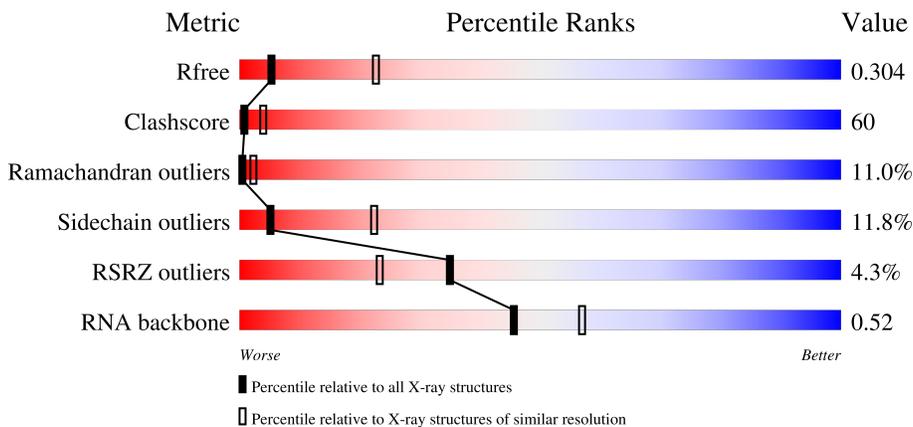
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| R_{free} | 130704 | 1335 (3.24-3.20) |
| Clashscore | 141614 | 1460 (3.24-3.20) |
| Ramachandran outliers | 138981 | 1437 (3.24-3.20) |
| Sidechain outliers | 138945 | 1436 (3.24-3.20) |
| RSRZ outliers | 127900 | 1291 (3.24-3.20) |
| RNA backbone | 3102 | 1023 (3.54-2.90) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | C | 88 | |
| 1 | D | 88 | |
| 2 | A | 967 | |
| 2 | B | 967 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19578 atoms, of which 0 are hydrogens and 0 are deuteriums.

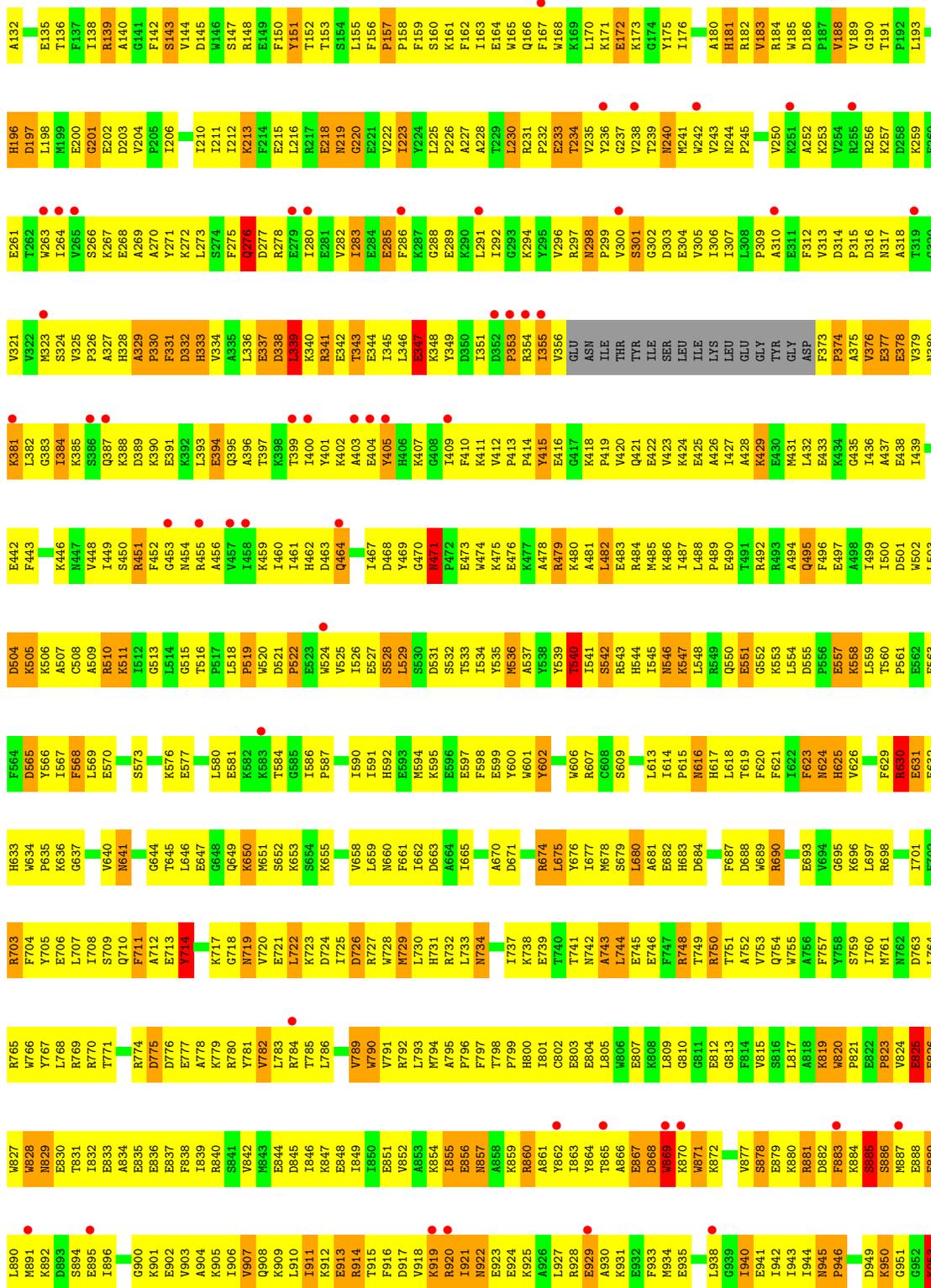
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | C | 88 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1880 | 836 | 339 | 617 | 88 | | | |
| 1 | D | 88 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1880 | 836 | 339 | 617 | 88 | | | |

- Molecule 2 is a protein called Leucyl-tRNA synthetase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | A | 948 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7909 | 5132 | 1323 | 1430 | 24 | | | |
| 2 | B | 948 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7909 | 5132 | 1323 | 1430 | 24 | | | |



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 120.55Å 231.13Å 118.18Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 14.99 – 3.21 48.69 – 3.21 | Depositor EDS |
| % Data completeness (in resolution range) | 90.7 (14.99-3.21) 90.8 (48.69-3.21) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.22 (at 3.19Å) | Xtrriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.241 , 0.305 0.243 , 0.304 | Depositor DCC |
| R_{free} test set | 5012 reflections (10.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 75.5 | Xtrriage |
| Anisotropy | 0.463 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 76.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$ | Xtrriage |
| Estimated twinning fraction | 0.046 for l,-k,h | Xtrriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 19578 | wwPDB-VP |
| Average B, all atoms (Å ²) | 84.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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 | C | 0.55 | 1/2099 (0.0%) | 0.82 | 7/3270 (0.2%) |
| 1 | D | 0.52 | 1/2099 (0.0%) | 0.81 | 3/3270 (0.1%) |
| 2 | A | 0.59 | 0/8115 | 0.76 | 6/10953 (0.1%) |
| 2 | B | 0.42 | 0/8115 | 0.67 | 2/10953 (0.0%) |
| All | All | 0.52 | 2/20428 (0.0%) | 0.74 | 18/28446 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | C | 0 | 6 |
| 1 | D | 0 | 5 |
| 2 | A | 0 | 2 |
| All | All | 0 | 13 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | C | 901 | G | OP3-P | -7.18 | 1.52 | 1.61 |
| 1 | D | 901 | G | OP3-P | -7.06 | 1.52 | 1.61 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | A | 675 | LEU | CA-CB-CG | 10.29 | 138.97 | 115.30 |
| 2 | A | 815 | VAL | CB-CA-C | -8.02 | 96.17 | 111.40 |
| 1 | C | 919 | G | N9-C1'-C2' | 7.77 | 124.10 | 114.00 |
| 1 | D | 953 | A | N9-C1'-C2' | 7.42 | 123.64 | 114.00 |
| 1 | C | 907 | G | N9-C1'-C2' | 7.18 | 123.33 | 114.00 |
| 1 | D | 920 | G | N9-C1'-C2' | 7.04 | 123.15 | 114.00 |
| 1 | C | 953 | A | N9-C1'-C2' | 6.38 | 122.30 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | C | 972 | U | N1-C1'-C2' | 5.87 | 121.63 | 114.00 |
| 1 | D | 920 | G | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 1 | C | 953 | A | C1'-O4'-C4' | -5.72 | 105.32 | 109.90 |
| 1 | C | 920 | G | N9-C1'-C2' | 5.71 | 121.43 | 114.00 |
| 2 | A | 927 | LEU | CA-CB-CG | 5.69 | 128.38 | 115.30 |
| 1 | C | 953 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 2 | B | 680 | LEU | N-CA-C | 5.50 | 125.84 | 111.00 |
| 2 | A | 680 | LEU | N-CA-C | 5.44 | 125.68 | 111.00 |
| 2 | A | 74 | VAL | N-CA-C | 5.33 | 125.39 | 111.00 |
| 2 | A | 492 | ARG | CG-CD-NE | 5.05 | 122.41 | 111.80 |
| 2 | B | 74 | VAL | N-CA-C | 5.04 | 124.61 | 111.00 |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | A | 535 | TYR | Sidechain |
| 2 | A | 767 | TYR | Sidechain |
| 1 | C | 907 | G | Sidechain |
| 1 | C | 919 | G | Sidechain |
| 1 | C | 920 | G | Sidechain |
| 1 | C | 921 | U | Sidechain |
| 1 | C | 926 | G | Sidechain |
| 1 | C | 959 | U | Sidechain |
| 1 | D | 919 | G | Sidechain |
| 1 | D | 920 | G | Sidechain |
| 1 | D | 926 | G | Sidechain |
| 1 | D | 953 | A | Sidechain |
| 1 | D | 959 | U | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 1880 | 0 | 956 | 88 | 0 |
| 1 | D | 1880 | 0 | 956 | 65 | 0 |
| 2 | A | 7909 | 0 | 7908 | 1115 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 7909 | 0 | 7908 | 1018 | 0 |
| All | All | 19578 | 0 | 17728 | 2256 | 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 60.

All (2256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:866:ALA:N | 2:A:955:LYS:HZ3 | 1.39 | 1.18 |
| 2:A:30:LYS:HB2 | 2:A:73:ASN:HD22 | 1.11 | 1.13 |
| 2:A:170:LEU:HB3 | 2:A:176:ILE:HD11 | 1.23 | 1.09 |
| 2:A:616:ASN:HD22 | 2:A:617:HIS:N | 1.51 | 1.08 |
| 2:A:68:ARG:HH22 | 2:A:143:SER:HB3 | 1.15 | 1.07 |
| 2:A:924:GLU:HB3 | 2:A:928:ARG:HH21 | 1.12 | 1.07 |
| 2:B:920:ARG:HE | 2:B:920:ARG:HA | 1.12 | 1.06 |
| 2:B:26:ASN:HB3 | 2:B:28:ARG:NH2 | 1.70 | 1.06 |
| 2:A:480:LYS:HE2 | 2:A:484:ARG:HH22 | 1.17 | 1.05 |
| 2:A:921:ILE:HD12 | 2:A:928:ARG:HH12 | 1.20 | 1.05 |
| 2:A:922:ASN:HD22 | 2:A:923:GLU:N | 1.53 | 1.05 |
| 2:B:703:ARG:HB2 | 2:B:703:ARG:HH11 | 1.18 | 1.05 |
| 2:A:724:ASP:HA | 2:A:727:ARG:HG3 | 1.33 | 1.04 |
| 2:A:771:THR:HG21 | 2:A:774:ARG:HH11 | 1.18 | 1.04 |
| 2:B:198:LEU:HB2 | 2:B:202:GLU:HG2 | 1.40 | 1.02 |
| 2:A:924:GLU:HB3 | 2:A:928:ARG:NH2 | 1.75 | 1.02 |
| 2:B:733:LEU:HD11 | 2:B:789:VAL:HG11 | 1.41 | 1.02 |
| 2:B:866:ALA:H | 2:B:955:LYS:NZ | 1.58 | 1.01 |
| 2:A:616:ASN:ND2 | 2:A:617:HIS:H | 1.57 | 1.01 |
| 2:B:558:LYS:HB3 | 2:B:584:THR:HA | 1.43 | 1.01 |
| 2:B:860:ARG:NH1 | 2:B:943:ILE:H | 1.59 | 1.01 |
| 2:B:650:LYS:HE2 | 2:B:651:MET:H | 1.22 | 1.00 |
| 2:A:529:LEU:H | 2:A:529:LEU:HD12 | 1.27 | 1.00 |
| 2:A:163:ILE:HD12 | 2:A:531:ASP:HB2 | 1.40 | 1.00 |
| 2:A:722:LEU:H | 2:A:722:LEU:HD22 | 1.22 | 1.00 |
| 2:A:87:ILE:HG13 | 2:A:88:VAL:H | 1.24 | 0.99 |
| 2:B:703:ARG:HB2 | 2:B:703:ARG:NH1 | 1.77 | 0.99 |
| 2:A:188:VAL:HG23 | 2:A:189:VAL:H | 1.28 | 0.99 |
| 1:D:904:G:H2' | 1:D:905:G:H5'' | 1.45 | 0.98 |
| 2:A:848:GLU:O | 2:A:852:VAL:HG23 | 1.63 | 0.98 |
| 2:B:227:ALA:HA | 2:B:321:VAL:HG23 | 1.45 | 0.98 |
| 2:A:567:ILE:HA | 2:A:595:LYS:HD2 | 1.44 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:916:C:H5' | 1:C:917:C:C5 | 1.99 | 0.97 |
| 2:A:227:ALA:HA | 2:A:321:VAL:HG23 | 1.46 | 0.97 |
| 2:A:426:ALA:HA | 2:A:429:LYS:HE2 | 1.45 | 0.97 |
| 2:A:690:ARG:NH1 | 2:A:693:GLU:HG3 | 1.79 | 0.96 |
| 2:A:922:ASN:HD22 | 2:A:922:ASN:C | 1.68 | 0.96 |
| 2:A:68:ARG:NH2 | 2:A:143:SER:HB3 | 1.79 | 0.96 |
| 2:A:890:LEU:HD12 | 2:A:906:ILE:HD11 | 1.48 | 0.96 |
| 1:C:986:C:H4' | 1:C:987:C:H5'' | 1.47 | 0.95 |
| 2:A:345:ILE:HG12 | 2:A:346:LEU:H | 1.29 | 0.95 |
| 2:B:88:VAL:HG21 | 2:B:513:GLY:HA2 | 1.48 | 0.95 |
| 2:A:68:ARG:HH22 | 2:A:143:SER:CB | 1.80 | 0.95 |
| 2:A:558:LYS:HB3 | 2:A:584:THR:HA | 1.48 | 0.94 |
| 2:B:860:ARG:HH11 | 2:B:943:ILE:N | 1.66 | 0.94 |
| 2:A:792:ARG:HH21 | 2:A:792:ARG:HG3 | 1.30 | 0.94 |
| 2:A:660:ASN:HB2 | 2:A:663:ASP:HB3 | 1.50 | 0.93 |
| 2:A:741:THR:HG1 | 2:A:820:TRP:HZ3 | 1.04 | 0.93 |
| 2:B:866:ALA:H | 2:B:955:LYS:HZ3 | 1.01 | 0.93 |
| 2:A:860:ARG:NH1 | 2:A:861:ALA:HA | 1.84 | 0.93 |
| 2:A:771:THR:HG21 | 2:A:774:ARG:NH1 | 1.82 | 0.93 |
| 2:B:429:LYS:O | 2:B:433:GLU:HG2 | 1.67 | 0.92 |
| 2:A:182:ARG:HD2 | 2:A:206:ILE:HG21 | 1.49 | 0.92 |
| 2:A:28:ARG:H | 2:A:28:ARG:HE | 1.01 | 0.92 |
| 2:A:139:ARG:HH11 | 2:A:139:ARG:HG3 | 1.34 | 0.92 |
| 2:A:860:ARG:NH1 | 2:A:943:ILE:H | 1.66 | 0.92 |
| 2:A:866:ALA:H | 2:A:955:LYS:HZ3 | 0.98 | 0.92 |
| 2:B:784:ARG:HH22 | 2:B:810:GLY:H | 1.15 | 0.92 |
| 2:A:770:ARG:HD2 | 2:A:933:PHE:CE2 | 2.06 | 0.91 |
| 2:B:927:LEU:HD12 | 2:B:944:ILE:HD12 | 1.50 | 0.91 |
| 2:B:82:ILE:HG21 | 2:B:126:VAL:HG13 | 1.50 | 0.91 |
| 2:A:480:LYS:HE2 | 2:A:484:ARG:NH2 | 1.84 | 0.91 |
| 2:A:866:ALA:H | 2:A:955:LYS:NZ | 1.69 | 0.91 |
| 2:B:49:LEU:H | 2:B:49:LEU:HD12 | 1.34 | 0.91 |
| 2:B:233:GLU:HA | 2:B:427:ILE:HD12 | 1.51 | 0.91 |
| 2:B:734:ASN:HD21 | 2:B:824:VAL:H | 1.12 | 0.91 |
| 2:B:355:ILE:HG22 | 2:B:356:VAL:H | 1.36 | 0.91 |
| 2:A:210:ILE:HD11 | 2:A:232:PRO:HG3 | 1.54 | 0.90 |
| 2:B:860:ARG:HH11 | 2:B:943:ILE:H | 0.99 | 0.90 |
| 2:B:26:ASN:HB3 | 2:B:28:ARG:HH22 | 1.34 | 0.90 |
| 2:B:167:PHE:HA | 2:B:170:LEU:HD12 | 1.55 | 0.89 |
| 2:B:826:GLU:C | 2:B:828:TRP:H | 1.70 | 0.89 |
| 2:A:567:ILE:HG22 | 2:A:595:LYS:HB2 | 1.51 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:49:LEU:H | 2:A:49:LEU:HD12 | 1.35 | 0.89 |
| 2:A:198:LEU:HB2 | 2:A:202:GLU:HG2 | 1.52 | 0.89 |
| 2:B:920:ARG:HA | 2:B:920:ARG:NE | 1.85 | 0.89 |
| 2:A:771:THR:CG2 | 2:A:774:ARG:HH11 | 1.86 | 0.89 |
| 2:A:496:PHE:CE1 | 2:A:614:ILE:HG12 | 2.08 | 0.89 |
| 2:A:230:LEU:H | 2:A:230:LEU:HD23 | 1.37 | 0.88 |
| 2:A:730:LEU:HB3 | 2:A:827:TRP:NE1 | 1.88 | 0.88 |
| 2:A:826:GLU:C | 2:A:828:TRP:H | 1.70 | 0.88 |
| 2:B:870:LYS:HE3 | 2:B:905:LYS:HE3 | 1.55 | 0.88 |
| 2:A:111:VAL:HG22 | 2:A:128:TYR:HE2 | 1.39 | 0.88 |
| 2:A:343:THR:HG23 | 2:A:344:GLU:H | 1.37 | 0.88 |
| 1:D:983:G:H2' | 1:D:984:C:H5'' | 1.53 | 0.88 |
| 2:B:83:THR:HG22 | 2:B:515:GLY:HA2 | 1.56 | 0.88 |
| 2:B:675:LEU:HD23 | 2:B:697:LEU:HD21 | 1.54 | 0.87 |
| 1:D:922:C:H4' | 1:D:923:A:O5' | 1.72 | 0.87 |
| 2:B:567:ILE:HG22 | 2:B:595:LYS:HB2 | 1.55 | 0.87 |
| 2:A:489:PRO:HG3 | 2:A:684:ASP:OD2 | 1.75 | 0.87 |
| 2:B:555:ASP:HB3 | 2:B:558:LYS:HG2 | 1.55 | 0.87 |
| 2:A:471:ASN:OD1 | 2:A:473:GLU:HG2 | 1.73 | 0.87 |
| 2:B:714:TYR:H | 2:B:714:TYR:HD2 | 1.21 | 0.87 |
| 2:A:219:ASN:ND2 | 2:A:220:GLY:H | 1.72 | 0.87 |
| 2:B:188:VAL:HG23 | 2:B:189:VAL:H | 1.40 | 0.87 |
| 2:A:921:ILE:HB | 2:A:928:ARG:HH22 | 1.40 | 0.87 |
| 1:C:902:C:H2' | 1:C:903:G:O4' | 1.74 | 0.86 |
| 2:A:211:ILE:HG22 | 2:A:228:ALA:HB2 | 1.57 | 0.86 |
| 2:A:482:LEU:O | 2:A:482:LEU:HD23 | 1.75 | 0.86 |
| 2:B:44:TYR:HE1 | 2:B:87:ILE:HD11 | 1.39 | 0.86 |
| 2:A:496:PHE:HE1 | 2:A:614:ILE:HG12 | 1.40 | 0.86 |
| 2:B:351:ILE:H | 2:B:351:ILE:HD12 | 1.39 | 0.86 |
| 2:A:836:GLU:O | 2:A:840:ARG:HG3 | 1.74 | 0.86 |
| 2:A:204:VAL:HG21 | 2:A:448:VAL:CG2 | 2.05 | 0.86 |
| 2:B:342:GLU:HG2 | 2:B:343:THR:H | 1.40 | 0.86 |
| 2:B:882:ASP:CG | 2:B:883:PHE:H | 1.79 | 0.85 |
| 2:A:829:ASN:OD1 | 2:A:832:ILE:HG13 | 1.77 | 0.85 |
| 2:B:587:PRO:HB2 | 2:B:590:ILE:HG12 | 1.56 | 0.85 |
| 2:B:182:ARG:HD2 | 2:B:206:ILE:HG21 | 1.59 | 0.84 |
| 2:B:413:PRO:HB2 | 2:B:414:PRO:HD3 | 1.57 | 0.84 |
| 2:A:819:LYS:H | 2:A:819:LYS:HE3 | 1.43 | 0.84 |
| 2:A:803:GLU:HA | 2:A:815:VAL:CG2 | 2.07 | 0.84 |
| 2:B:446:LYS:N | 2:B:446:LYS:HD2 | 1.92 | 0.84 |
| 1:C:928:C:H2' | 1:C:929:G:C8 | 2.13 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:703:ARG:HD2 | 2:B:707:LEU:HD11 | 1.60 | 0.84 |
| 1:C:928:C:H2' | 1:C:929:G:H8 | 1.42 | 0.83 |
| 2:A:145:ASP:OD1 | 2:A:147:SER:HB3 | 1.78 | 0.83 |
| 2:A:731:HIS:HE1 | 2:A:833:GLU:OE1 | 1.60 | 0.83 |
| 2:B:705:TYR:CE2 | 2:B:805:LEU:HD21 | 2.13 | 0.83 |
| 2:B:866:ALA:N | 2:B:955:LYS:HZ3 | 1.76 | 0.83 |
| 2:A:671:ASP:OD2 | 2:A:800:HIS:HB2 | 1.78 | 0.83 |
| 2:B:4:LEU:O | 2:B:4:LEU:HD23 | 1.79 | 0.83 |
| 2:A:966:ILE:O | 2:A:967:GLU:HB2 | 1.79 | 0.83 |
| 2:B:186:ASP:HB2 | 2:B:193:LEU:HD11 | 1.59 | 0.83 |
| 2:A:770:ARG:HD2 | 2:A:933:PHE:HE2 | 1.41 | 0.83 |
| 2:B:86:PRO:O | 2:B:90:ILE:HG12 | 1.78 | 0.83 |
| 2:A:732:ARG:HH11 | 2:A:735:LYS:HD3 | 1.45 | 0.82 |
| 2:A:28:ARG:H | 2:A:28:ARG:NE | 1.76 | 0.82 |
| 2:B:935:GLU:OE1 | 2:B:941:GLU:HA | 1.80 | 0.82 |
| 1:D:923:A:H4' | 1:D:924:A:O5' | 1.79 | 0.82 |
| 2:A:59:ILE:HG12 | 2:A:678:MET:HE1 | 1.60 | 0.82 |
| 2:A:51:VAL:O | 2:A:54:ALA:HB3 | 1.80 | 0.82 |
| 2:B:13:TRP:CE2 | 2:B:803:GLU:HB3 | 2.15 | 0.82 |
| 2:A:238:VAL:HG11 | 2:A:298:ASN:HD22 | 1.45 | 0.81 |
| 2:A:345:ILE:HG12 | 2:A:346:LEU:N | 1.94 | 0.81 |
| 2:A:384:ILE:HG22 | 2:A:385:LYS:H | 1.45 | 0.81 |
| 2:A:859:LYS:HB3 | 2:A:941:GLU:HB3 | 1.63 | 0.81 |
| 1:C:922:C:H4' | 1:C:923:A:O5' | 1.78 | 0.81 |
| 2:A:355:ILE:HG22 | 2:A:356:VAL:H | 1.45 | 0.81 |
| 2:B:230:LEU:HD23 | 2:B:230:LEU:H | 1.45 | 0.81 |
| 2:A:722:LEU:HD22 | 2:A:722:LEU:N | 1.95 | 0.81 |
| 2:B:340:LYS:NZ | 2:B:341:ARG:HH12 | 1.79 | 0.81 |
| 2:B:860:ARG:HB3 | 2:B:966:ILE:HG22 | 1.61 | 0.81 |
| 2:A:895:GLU:OE1 | 2:A:898:LYS:HD2 | 1.81 | 0.81 |
| 2:A:690:ARG:HH11 | 2:A:693:GLU:HG3 | 1.45 | 0.80 |
| 2:B:268:GLU:HG3 | 2:B:316:ASP:HA | 1.63 | 0.80 |
| 2:B:641:ASN:HA | 2:B:683:HIS:O | 1.80 | 0.80 |
| 2:B:170:LEU:HB2 | 2:B:176:ILE:HD11 | 1.62 | 0.80 |
| 2:A:660:ASN:HB2 | 2:A:663:ASP:CB | 2.10 | 0.80 |
| 2:B:186:ASP:HB3 | 2:B:191:THR:HG23 | 1.61 | 0.80 |
| 2:A:412:VAL:HG23 | 2:A:414:PRO:HD2 | 1.64 | 0.80 |
| 1:C:986:C:N3 | 2:A:506:LYS:HG2 | 1.97 | 0.80 |
| 2:B:384:ILE:HG22 | 2:B:385:LYS:H | 1.47 | 0.80 |
| 2:A:73:ASN:O | 2:A:601:TRP:HH2 | 1.64 | 0.80 |
| 2:A:39:THR:HG23 | 2:A:604:LEU:HD11 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:904:G:C2' | 1:D:905:G:H5'' | 2.11 | 0.79 |
| 2:A:931:LYS:O | 2:A:935:GLU:HG3 | 1.80 | 0.79 |
| 2:B:860:ARG:HE | 2:B:942:ILE:HA | 1.48 | 0.79 |
| 2:B:863:ILE:HB | 2:B:953:LYS:HD3 | 1.64 | 0.79 |
| 1:C:911:C:H2' | 1:C:912:C:H6 | 1.47 | 0.79 |
| 2:B:157:PRO:HB2 | 2:B:158:PRO:HD3 | 1.65 | 0.79 |
| 2:A:82:ILE:HG13 | 2:A:153:THR:HG23 | 1.63 | 0.79 |
| 2:A:170:LEU:CB | 2:A:176:ILE:HD11 | 2.11 | 0.79 |
| 2:A:732:ARG:NH1 | 2:A:735:LYS:HD3 | 1.98 | 0.79 |
| 2:A:922:ASN:ND2 | 2:A:923:GLU:N | 2.30 | 0.79 |
| 2:B:116:LEU:HD12 | 2:B:119:PHE:CD2 | 2.17 | 0.79 |
| 2:B:547:LYS:HA | 2:B:547:LYS:HE2 | 1.63 | 0.79 |
| 2:B:919:LYS:O | 2:B:922:ASN:HB2 | 1.82 | 0.79 |
| 2:A:297:ARG:HG2 | 2:A:304:GLU:HG2 | 1.63 | 0.79 |
| 2:A:487:ILE:HG22 | 2:A:489:PRO:O | 1.82 | 0.79 |
| 2:B:297:ARG:HG2 | 2:B:304:GLU:HG2 | 1.63 | 0.79 |
| 2:B:826:GLU:C | 2:B:828:TRP:N | 2.34 | 0.79 |
| 1:D:902:C:H3' | 1:D:903:G:H5'' | 1.64 | 0.79 |
| 2:A:867:GLU:H | 2:A:867:GLU:CD | 1.86 | 0.78 |
| 2:A:924:GLU:CB | 2:A:928:ARG:HH21 | 1.94 | 0.78 |
| 2:A:186:ASP:HB3 | 2:A:191:THR:HG23 | 1.65 | 0.78 |
| 2:B:343:THR:HG23 | 2:B:344:GLU:H | 1.47 | 0.78 |
| 2:B:345:ILE:HG12 | 2:B:346:LEU:H | 1.47 | 0.78 |
| 2:B:464:GLN:HA | 2:B:524:TRP:CH2 | 2.18 | 0.78 |
| 1:C:986:C:H4' | 1:C:987:C:C5' | 2.14 | 0.78 |
| 2:A:204:VAL:HG21 | 2:A:448:VAL:HG22 | 1.66 | 0.78 |
| 2:B:51:VAL:O | 2:B:54:ALA:HB3 | 1.84 | 0.78 |
| 2:B:722:LEU:H | 2:B:722:LEU:CD2 | 1.97 | 0.78 |
| 2:B:949:ASP:HB2 | 2:B:954:LYS:HE2 | 1.64 | 0.78 |
| 2:A:348:LYS:NZ | 2:A:348:LYS:HB3 | 1.99 | 0.78 |
| 2:A:871:TRP:CZ3 | 2:A:918:VAL:HG13 | 2.18 | 0.78 |
| 2:A:826:GLU:C | 2:A:828:TRP:N | 2.34 | 0.78 |
| 2:B:55:ARG:O | 2:B:59:ILE:HG13 | 1.83 | 0.78 |
| 2:B:471:ASN:ND2 | 2:B:473:GLU:HG2 | 1.99 | 0.78 |
| 2:A:87:ILE:HG13 | 2:A:88:VAL:N | 1.98 | 0.78 |
| 2:A:393:LEU:HD12 | 2:A:396:ALA:HB3 | 1.66 | 0.78 |
| 2:A:482:LEU:HD12 | 2:A:500:ILE:HD11 | 1.66 | 0.78 |
| 2:B:45:LEU:HD11 | 2:B:80:TRP:HB3 | 1.64 | 0.78 |
| 2:B:333:HIS:HA | 2:B:336:LEU:HB2 | 1.66 | 0.78 |
| 2:A:482:LEU:HD11 | 2:A:496:PHE:HB3 | 1.66 | 0.77 |
| 2:A:650:LYS:HD2 | 2:A:651:MET:H | 1.48 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:540:THR:HG23 | 2:B:541:ILE:HG23 | 1.64 | 0.77 |
| 2:B:731:HIS:CD2 | 2:B:829:ASN:H | 2.02 | 0.77 |
| 2:B:801:ILE:O | 2:B:805:LEU:HG | 1.84 | 0.77 |
| 2:A:529:LEU:H | 2:A:529:LEU:CD1 | 1.96 | 0.77 |
| 2:A:209:TYR:HE1 | 2:A:317:ASN:HD21 | 1.30 | 0.77 |
| 1:C:985:A:H61 | 2:A:504:ASP:HB2 | 1.47 | 0.77 |
| 2:A:860:ARG:HB3 | 2:A:966:ILE:HG22 | 1.64 | 0.77 |
| 2:A:871:TRP:CD1 | 2:A:959:PRO:HG3 | 2.18 | 0.77 |
| 1:C:986:C:N3 | 2:A:507:ALA:N | 2.32 | 0.77 |
| 2:A:242:TRP:HH2 | 2:A:332:ASP:HA | 1.50 | 0.77 |
| 2:B:446:LYS:HD2 | 2:B:446:LYS:H | 1.47 | 0.77 |
| 2:B:834:ALA:HA | 2:B:837:GLU:OE2 | 1.83 | 0.77 |
| 2:A:819:LYS:H | 2:A:819:LYS:CE | 1.97 | 0.77 |
| 2:A:722:LEU:H | 2:A:722:LEU:CD2 | 1.98 | 0.77 |
| 2:B:150:PHE:HD1 | 2:B:151:TYR:O | 1.68 | 0.77 |
| 2:B:866:ALA:N | 2:B:955:LYS:NZ | 2.31 | 0.77 |
| 2:A:770:ARG:NH1 | 2:A:933:PHE:HD2 | 1.81 | 0.76 |
| 2:A:919:LYS:HD2 | 2:A:960:LEU:CD1 | 2.16 | 0.76 |
| 2:B:845:ASP:O | 2:B:849:ILE:HG13 | 1.84 | 0.76 |
| 2:B:880:LYS:HG3 | 2:B:885:SER:HB2 | 1.67 | 0.76 |
| 2:A:198:LEU:HB2 | 2:A:202:GLU:CG | 2.14 | 0.76 |
| 2:B:631:GLU:HA | 2:B:634:TRP:CE2 | 2.20 | 0.76 |
| 2:A:27:ILE:N | 2:A:28:ARG:HH21 | 1.83 | 0.76 |
| 2:B:914:ARG:HH21 | 2:B:915:THR:HG23 | 1.51 | 0.76 |
| 2:A:28:ARG:HE | 2:A:28:ARG:N | 1.81 | 0.76 |
| 2:A:488:LEU:HD12 | 2:A:606:TRP:CH2 | 2.21 | 0.76 |
| 2:A:88:VAL:HG21 | 2:A:513:GLY:HA2 | 1.66 | 0.76 |
| 2:A:731:HIS:CE1 | 2:A:833:GLU:OE1 | 2.39 | 0.76 |
| 2:A:928:ARG:O | 2:A:930:ALA:N | 2.18 | 0.76 |
| 2:B:82:ILE:HG21 | 2:B:126:VAL:CG1 | 2.16 | 0.76 |
| 2:B:887:MET:SD | 2:B:906:ILE:HD12 | 2.26 | 0.76 |
| 2:B:931:LYS:O | 2:B:935:GLU:HG3 | 1.86 | 0.76 |
| 1:D:929:G:H1 | 1:D:947:U:H3 | 1.35 | 0.75 |
| 2:B:165:TRP:CD1 | 2:B:561:PRO:HA | 2.21 | 0.75 |
| 2:A:238:VAL:CG1 | 2:A:298:ASN:HD22 | 1.98 | 0.75 |
| 2:A:949:ASP:HB2 | 2:A:954:LYS:HE2 | 1.69 | 0.75 |
| 2:A:641:ASN:HA | 2:A:683:HIS:O | 1.85 | 0.75 |
| 2:B:767:TYR:HE2 | 2:B:783:LEU:HD11 | 1.49 | 0.75 |
| 2:B:678:MET:HB3 | 2:B:749:THR:HB | 1.68 | 0.75 |
| 2:A:492:ARG:HH11 | 2:A:492:ARG:CG | 1.99 | 0.75 |
| 2:A:17:TRP:CH2 | 2:A:800:HIS:HD2 | 2.04 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:957:ALA:HB2 | 2:A:963:ALA:HB2 | 1.67 | 0.75 |
| 2:B:846:ILE:HG12 | 2:B:964:ILE:CD1 | 2.16 | 0.75 |
| 2:A:139:ARG:HG3 | 2:A:139:ARG:NH1 | 1.95 | 0.74 |
| 2:A:624:ASN:HD22 | 2:A:624:ASN:H | 1.35 | 0.74 |
| 2:B:211:ILE:HG22 | 2:B:228:ALA:HB2 | 1.68 | 0.74 |
| 2:A:213:LYS:HD2 | 2:A:435:GLY:O | 1.87 | 0.74 |
| 2:B:631:GLU:HA | 2:B:634:TRP:NE1 | 2.01 | 0.74 |
| 2:A:551:GLU:O | 2:A:553:LYS:HG2 | 1.86 | 0.74 |
| 2:B:89:GLY:O | 2:B:93:ARG:HG3 | 1.87 | 0.74 |
| 2:B:681:ALA:HA | 2:B:750:ARG:HG3 | 1.68 | 0.74 |
| 2:A:755:TRP:O | 2:A:759:SER:HB3 | 1.87 | 0.74 |
| 2:A:645:THR:HG22 | 2:A:650:LYS:HA | 1.68 | 0.74 |
| 1:C:908:U:H5' | 1:C:961:C:OP2 | 1.88 | 0.74 |
| 1:D:902:C:C3' | 1:D:903:G:H5'' | 2.17 | 0.74 |
| 2:A:354:ARG:HD2 | 2:A:376:VAL:CG1 | 2.17 | 0.74 |
| 2:A:432:LEU:HD11 | 2:A:439:ILE:HG13 | 1.70 | 0.74 |
| 2:B:836:GLU:O | 2:B:840:ARG:HG3 | 1.87 | 0.74 |
| 2:A:30:LYS:HB2 | 2:A:73:ASN:ND2 | 1.96 | 0.73 |
| 2:A:230:LEU:H | 2:A:230:LEU:CD2 | 2.01 | 0.73 |
| 2:A:882:ASP:CG | 2:A:883:PHE:H | 1.92 | 0.73 |
| 2:B:26:ASN:CB | 2:B:28:ARG:HH22 | 2.01 | 0.73 |
| 2:B:928:ARG:O | 2:B:930:ALA:N | 2.21 | 0.73 |
| 2:A:566:TYR:HA | 2:A:570:GLU:HB2 | 1.70 | 0.73 |
| 2:A:766:TRP:CH2 | 2:A:770:ARG:HD3 | 2.23 | 0.73 |
| 2:B:703:ARG:HH11 | 2:B:703:ARG:CB | 2.00 | 0.73 |
| 2:B:859:LYS:HB3 | 2:B:941:GLU:HB3 | 1.69 | 0.73 |
| 2:A:345:ILE:HG23 | 2:A:346:LEU:HD13 | 1.71 | 0.73 |
| 2:B:198:LEU:CB | 2:B:202:GLU:HG2 | 2.19 | 0.73 |
| 2:B:544:HIS:O | 2:B:548:LEU:HG | 1.87 | 0.73 |
| 2:B:857:ASN:ND2 | 2:B:967:GLU:HG2 | 2.03 | 0.73 |
| 2:B:867:GLU:H | 2:B:867:GLU:CD | 1.92 | 0.73 |
| 2:B:957:ALA:HB2 | 2:B:963:ALA:HB2 | 1.67 | 0.73 |
| 1:C:982:C:H2' | 1:C:983:G:C8 | 2.24 | 0.73 |
| 2:A:413:PRO:HB2 | 2:A:414:PRO:HD3 | 1.70 | 0.73 |
| 2:A:537:ALA:O | 2:A:540:THR:HG22 | 1.88 | 0.73 |
| 2:A:691:ARG:O | 2:A:694:VAL:HG12 | 1.88 | 0.73 |
| 2:A:42:PHE:CD1 | 2:A:81:HIS:HB2 | 2.24 | 0.73 |
| 2:A:233:GLU:HB3 | 2:A:423:VAL:HG23 | 1.68 | 0.73 |
| 2:A:792:ARG:HG3 | 2:A:792:ARG:NH2 | 2.04 | 0.73 |
| 2:A:832:ILE:HA | 2:A:835:GLU:HG3 | 1.71 | 0.73 |
| 2:A:17:TRP:CH2 | 2:A:800:HIS:CD2 | 2.76 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:373:PHE:CD1 | 2:A:374:PRO:HD3 | 2.24 | 0.73 |
| 2:A:250:VAL:HG12 | 2:A:285:GLU:HA | 1.70 | 0.72 |
| 2:A:342:GLU:HG2 | 2:A:343:THR:H | 1.54 | 0.72 |
| 2:A:558:LYS:HD2 | 2:A:583:LYS:O | 1.89 | 0.72 |
| 2:A:860:ARG:NH2 | 2:A:862:TYR:HB3 | 2.04 | 0.72 |
| 2:B:734:ASN:HD21 | 2:B:824:VAL:N | 1.86 | 0.72 |
| 2:B:803:GLU:OE2 | 2:B:815:VAL:N | 2.23 | 0.72 |
| 2:B:925:LYS:HA | 2:B:928:ARG:HG2 | 1.68 | 0.72 |
| 2:A:771:THR:HG22 | 2:A:774:ARG:HD3 | 1.70 | 0.72 |
| 2:B:695:GLY:O | 2:B:698:ARG:HB3 | 1.90 | 0.72 |
| 2:B:848:GLU:O | 2:B:852:VAL:HG23 | 1.89 | 0.72 |
| 2:A:488:LEU:HD12 | 2:A:606:TRP:CZ3 | 2.24 | 0.72 |
| 2:A:239:THR:CG2 | 2:A:326:PRO:HD2 | 2.20 | 0.72 |
| 2:B:757:PHE:HD1 | 2:B:794:MET:SD | 2.12 | 0.72 |
| 2:B:480:LYS:HA | 2:B:483:GLU:OE1 | 1.89 | 0.72 |
| 2:B:167:PHE:HA | 2:B:170:LEU:CD1 | 2.19 | 0.72 |
| 2:B:467:ILE:HG13 | 2:B:508:CYS:SG | 2.30 | 0.72 |
| 2:A:863:ILE:HB | 2:A:953:LYS:HD3 | 1.70 | 0.71 |
| 2:A:119:PHE:CD1 | 2:A:125:ILE:HG12 | 2.24 | 0.71 |
| 2:A:342:GLU:HG2 | 2:A:343:THR:N | 2.04 | 0.71 |
| 2:A:690:ARG:HD3 | 2:A:693:GLU:OE2 | 1.89 | 0.71 |
| 2:B:32:LYS:HG2 | 2:B:600:TYR:CD1 | 2.25 | 0.71 |
| 2:A:860:ARG:HH22 | 2:A:862:TYR:N | 1.87 | 0.71 |
| 2:A:922:ASN:C | 2:A:922:ASN:ND2 | 2.34 | 0.71 |
| 2:B:22:ILE:HG13 | 2:B:817:LEU:HD21 | 1.73 | 0.71 |
| 2:B:784:ARG:NH2 | 2:B:810:GLY:H | 1.88 | 0.71 |
| 2:B:957:ALA:HB2 | 2:B:963:ALA:CB | 2.21 | 0.71 |
| 2:A:219:ASN:HD22 | 2:A:220:GLY:H | 1.37 | 0.71 |
| 2:A:731:HIS:CD2 | 2:A:829:ASN:H | 2.08 | 0.71 |
| 2:A:770:ARG:NH1 | 2:A:933:PHE:CD2 | 2.59 | 0.71 |
| 2:A:957:ALA:HB2 | 2:A:963:ALA:CB | 2.20 | 0.71 |
| 2:A:67:LYS:HD3 | 2:A:70:GLN:HE21 | 1.54 | 0.71 |
| 2:A:734:ASN:OD1 | 2:A:823:PRO:HA | 1.91 | 0.71 |
| 2:B:30:LYS:HE3 | 2:B:71:GLY:O | 1.90 | 0.71 |
| 2:B:890:LEU:HD12 | 2:B:906:ILE:HD11 | 1.73 | 0.71 |
| 2:A:730:LEU:HB3 | 2:A:827:TRP:HE1 | 1.54 | 0.70 |
| 2:A:198:LEU:HD22 | 2:A:202:GLU:HA | 1.73 | 0.70 |
| 2:A:631:GLU:HA | 2:A:634:TRP:CE2 | 2.26 | 0.70 |
| 2:B:282:VAL:HG12 | 2:B:283:ILE:N | 2.07 | 0.70 |
| 2:A:276:GLN:HA | 2:A:460:ILE:HD13 | 1.71 | 0.70 |
| 2:A:419:PRO:HG2 | 2:A:422:GLU:HG3 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:857:ASN:O | 2:A:940:ILE:HD11 | 1.90 | 0.70 |
| 2:B:471:ASN:HD21 | 2:B:473:GLU:HG2 | 1.55 | 0.70 |
| 2:B:826:GLU:O | 2:B:827:TRP:HB3 | 1.91 | 0.70 |
| 1:C:970:A:H4' | 1:C:971:A:OP1 | 1.91 | 0.70 |
| 2:A:824:VAL:HG11 | 2:A:827:TRP:HE3 | 1.56 | 0.70 |
| 2:B:487:ILE:HG22 | 2:B:489:PRO:O | 1.91 | 0.70 |
| 2:A:613:LEU:O | 2:A:618:LEU:HB2 | 1.91 | 0.70 |
| 2:A:140:ALA:HB2 | 2:A:665:ILE:HD11 | 1.72 | 0.70 |
| 2:A:204:VAL:HG21 | 2:A:448:VAL:HG21 | 1.74 | 0.70 |
| 2:A:333:HIS:HA | 2:A:336:LEU:HB2 | 1.73 | 0.70 |
| 2:A:795:ALA:HB3 | 2:A:796:PRO:HD3 | 1.72 | 0.70 |
| 2:A:826:GLU:O | 2:A:827:TRP:HB3 | 1.90 | 0.70 |
| 2:A:12:LYS:NZ | 2:A:16:ARG:HH12 | 1.90 | 0.70 |
| 2:B:803:GLU:OE2 | 2:B:815:VAL:HG12 | 1.91 | 0.70 |
| 2:A:866:ALA:N | 2:A:955:LYS:NZ | 2.27 | 0.69 |
| 2:A:919:LYS:O | 2:A:922:ASN:HB2 | 1.92 | 0.69 |
| 2:B:297:ARG:HB3 | 2:B:297:ARG:NH2 | 2.07 | 0.69 |
| 2:B:927:LEU:CD1 | 2:B:944:ILE:HD12 | 2.23 | 0.69 |
| 1:C:920:G:H5'' | 1:C:921:U:H5 | 1.57 | 0.69 |
| 2:A:339:LEU:HD22 | 2:A:340:LYS:N | 2.08 | 0.69 |
| 2:A:374:PRO:HG2 | 2:A:379:VAL:HG21 | 1.74 | 0.69 |
| 2:B:95:LYS:C | 2:B:97:ARG:H | 1.96 | 0.69 |
| 2:B:660:ASN:HB2 | 2:B:663:ASP:CB | 2.22 | 0.69 |
| 2:B:690:ARG:HB3 | 2:B:690:ARG:NH1 | 2.06 | 0.69 |
| 2:A:22:ILE:HG23 | 2:A:23:PHE:CD1 | 2.27 | 0.69 |
| 2:A:165:TRP:HD1 | 2:A:561:PRO:HA | 1.58 | 0.69 |
| 2:B:741:THR:HG1 | 2:B:820:TRP:HZ3 | 1.41 | 0.69 |
| 1:C:923:A:H4' | 1:C:924:A:O5' | 1.91 | 0.69 |
| 2:A:91:ALA:O | 2:A:94:ILE:HG13 | 1.91 | 0.69 |
| 2:B:400:ILE:HD12 | 2:B:401:TYR:N | 2.06 | 0.69 |
| 2:B:770:ARG:HD2 | 2:B:933:PHE:CE2 | 2.27 | 0.69 |
| 2:A:577:GLU:OE2 | 2:A:592:HIS:HB2 | 1.92 | 0.69 |
| 2:B:7:LYS:HB2 | 2:B:7:LYS:NZ | 2.07 | 0.69 |
| 2:B:675:LEU:CD2 | 2:B:697:LEU:HD21 | 2.22 | 0.69 |
| 2:B:675:LEU:HD22 | 2:B:701:ILE:HD11 | 1.74 | 0.69 |
| 2:A:163:ILE:CD1 | 2:A:531:ASP:HB2 | 2.22 | 0.69 |
| 2:A:449:ILE:N | 2:A:449:ILE:HD12 | 2.08 | 0.69 |
| 2:A:863:ILE:HG22 | 2:A:953:LYS:HG2 | 1.74 | 0.69 |
| 2:B:35:LYS:HB2 | 2:B:601:TRP:CZ3 | 2.28 | 0.69 |
| 2:A:45:LEU:HD11 | 2:A:80:TRP:HB3 | 1.75 | 0.69 |
| 2:A:221:GLU:OE2 | 2:A:221:GLU:HA | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:10:GLU:O | 2:A:14:GLN:HG3 | 1.93 | 0.69 |
| 2:A:480:LYS:CE | 2:A:484:ARG:HH22 | 1.99 | 0.68 |
| 2:B:920:ARG:C | 2:B:922:ASN:H | 1.97 | 0.68 |
| 2:A:730:LEU:HB3 | 2:A:827:TRP:CD1 | 2.28 | 0.68 |
| 2:B:341:ARG:HD3 | 2:B:341:ARG:N | 2.07 | 0.68 |
| 2:A:95:LYS:C | 2:A:97:ARG:H | 1.96 | 0.68 |
| 2:A:920:ARG:C | 2:A:922:ASN:H | 1.96 | 0.68 |
| 2:B:14:GLN:O | 2:B:18:LEU:HB2 | 1.93 | 0.68 |
| 2:B:566:TYR:HA | 2:B:570:GLU:HB3 | 1.75 | 0.68 |
| 2:B:882:ASP:CG | 2:B:883:PHE:N | 2.47 | 0.68 |
| 2:A:30:LYS:CB | 2:A:73:ASN:HD22 | 1.98 | 0.68 |
| 2:A:62:VAL:HG21 | 2:A:678:MET:HE3 | 1.75 | 0.68 |
| 2:A:198:LEU:CB | 2:A:202:GLU:HG2 | 2.23 | 0.68 |
| 2:A:239:THR:HG23 | 2:A:326:PRO:HD2 | 1.74 | 0.68 |
| 2:B:65:ARG:HA | 2:B:68:ARG:NH1 | 2.08 | 0.68 |
| 2:B:650:LYS:HE2 | 2:B:651:MET:N | 2.03 | 0.68 |
| 2:B:871:TRP:NE1 | 2:B:959:PRO:HB3 | 2.09 | 0.68 |
| 2:A:629:PHE:O | 2:A:631:GLU:N | 2.25 | 0.68 |
| 2:B:116:LEU:HD12 | 2:B:119:PHE:HD2 | 1.59 | 0.68 |
| 2:B:276:GLN:O | 2:B:460:ILE:HD12 | 1.92 | 0.68 |
| 2:B:767:TYR:CE2 | 2:B:783:LEU:HD11 | 2.27 | 0.68 |
| 2:A:717:LYS:O | 2:A:717:LYS:HD3 | 1.94 | 0.68 |
| 2:B:28:ARG:HH11 | 2:B:28:ARG:HG3 | 1.59 | 0.68 |
| 2:B:678:MET:HE3 | 2:B:749:THR:HG21 | 1.74 | 0.68 |
| 2:A:82:ILE:HG21 | 2:A:126:VAL:HG13 | 1.74 | 0.68 |
| 2:A:652:SER:OG | 2:A:655:LYS:HB2 | 1.94 | 0.68 |
| 2:A:722:LEU:N | 2:A:722:LEU:CD2 | 2.55 | 0.68 |
| 2:B:770:ARG:HA | 2:B:933:PHE:HE2 | 1.58 | 0.68 |
| 2:B:26:ASN:HB2 | 2:B:29:ASP:OD2 | 1.93 | 0.68 |
| 2:B:198:LEU:H | 2:B:198:LEU:HD12 | 1.59 | 0.68 |
| 2:B:734:ASN:ND2 | 2:B:823:PRO:HA | 2.07 | 0.68 |
| 1:C:929:G:H1 | 1:C:947:U:H3 | 1.42 | 0.68 |
| 1:C:988:A:H5'' | 2:A:528:SER:OG | 1.94 | 0.68 |
| 2:A:803:GLU:CD | 2:A:815:VAL:HG23 | 2.14 | 0.68 |
| 2:B:237:GLY:O | 2:B:325:VAL:HG13 | 1.94 | 0.68 |
| 2:B:300:VAL:HG13 | 2:B:301:SER:H | 1.59 | 0.68 |
| 2:A:75:LEU:C | 2:A:75:LEU:HD12 | 2.14 | 0.67 |
| 2:B:185:TRP:CZ2 | 2:B:190:GLY:HA2 | 2.29 | 0.67 |
| 2:B:345:ILE:HG12 | 2:B:346:LEU:N | 2.09 | 0.67 |
| 1:D:920:G:H5'' | 1:D:921:U:H5 | 1.59 | 0.67 |
| 2:B:92:GLU:O | 2:B:95:LYS:HB3 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:555:ASP:HB3 | 2:B:558:LYS:CG | 2.24 | 0.67 |
| 2:A:423:VAL:C | 2:A:425:GLU:H | 1.95 | 0.67 |
| 2:B:795:ALA:HB3 | 2:B:796:PRO:HD3 | 1.77 | 0.67 |
| 2:A:919:LYS:H | 2:A:919:LYS:CE | 2.07 | 0.67 |
| 2:B:26:ASN:CB | 2:B:28:ARG:NH2 | 2.55 | 0.67 |
| 1:D:977:G:H2' | 1:D:978:C:C6 | 2.30 | 0.67 |
| 2:A:404:GLU:O | 2:A:420:VAL:HG21 | 1.95 | 0.67 |
| 2:A:872:LYS:O | 2:A:876:VAL:HG23 | 1.94 | 0.67 |
| 2:B:423:VAL:C | 2:B:425:GLU:H | 1.97 | 0.67 |
| 2:A:242:TRP:CH2 | 2:A:332:ASP:HA | 2.29 | 0.67 |
| 2:B:614:ILE:N | 2:B:615:PRO:HD2 | 2.09 | 0.67 |
| 2:A:139:ARG:NH2 | 2:A:666:GLU:OE1 | 2.27 | 0.67 |
| 2:A:870:LYS:HE2 | 2:A:905:LYS:HE3 | 1.77 | 0.67 |
| 1:C:916:C:OP1 | 1:C:916:C:H4' | 1.93 | 0.66 |
| 2:A:428:ALA:O | 2:A:432:LEU:HD23 | 1.95 | 0.66 |
| 2:A:891:MET:SD | 2:A:897:ARG:HG3 | 2.35 | 0.66 |
| 2:B:57:TYR:O | 2:B:60:PRO:HG2 | 1.95 | 0.66 |
| 2:B:741:THR:OG1 | 2:B:820:TRP:HZ3 | 1.78 | 0.66 |
| 2:A:529:LEU:HD12 | 2:A:529:LEU:N | 2.06 | 0.66 |
| 2:A:536:MET:SD | 2:A:607:ARG:NH1 | 2.69 | 0.66 |
| 2:A:682:GLU:OE1 | 2:A:748:ARG:HB3 | 1.95 | 0.66 |
| 2:A:717:LYS:HD3 | 2:A:717:LYS:C | 2.15 | 0.66 |
| 2:B:136:THR:HG22 | 2:B:661:PHE:HD2 | 1.60 | 0.66 |
| 2:B:326:PRO:HA | 2:B:332:ASP:HB2 | 1.77 | 0.66 |
| 2:A:266:SER:HB2 | 2:A:269:ALA:HB2 | 1.78 | 0.66 |
| 2:A:488:LEU:HD22 | 2:A:683:HIS:CE1 | 2.31 | 0.66 |
| 2:B:935:GLU:HG2 | 2:B:942:ILE:HD13 | 1.78 | 0.66 |
| 2:A:703:ARG:HG3 | 2:A:707:LEU:HD12 | 1.78 | 0.66 |
| 2:B:871:TRP:CZ3 | 2:B:918:VAL:HG13 | 2.30 | 0.66 |
| 2:B:793:LEU:CD2 | 2:B:821:PRO:HG2 | 2.25 | 0.66 |
| 2:B:921:ILE:HB | 2:B:928:ARG:NH2 | 2.09 | 0.66 |
| 2:A:188:VAL:HG23 | 2:A:189:VAL:N | 2.06 | 0.66 |
| 2:A:434:LYS:HB3 | 2:A:436:ILE:HG12 | 1.77 | 0.66 |
| 2:A:921:ILE:HD12 | 2:A:928:ARG:NH1 | 2.03 | 0.66 |
| 2:B:171:LYS:HG2 | 2:B:176:ILE:HD12 | 1.78 | 0.66 |
| 2:B:459:LYS:NZ | 2:B:461:ILE:HD13 | 2.11 | 0.66 |
| 2:B:690:ARG:HB3 | 2:B:690:ARG:CZ | 2.25 | 0.66 |
| 2:A:198:LEU:HB2 | 2:A:202:GLU:CD | 2.15 | 0.66 |
| 2:A:947:THR:HG23 | 2:A:948:GLU:N | 2.11 | 0.66 |
| 2:B:256:ARG:HG3 | 2:B:257:LYS:H | 1.61 | 0.66 |
| 2:A:784:ARG:HH22 | 2:A:810:GLY:H | 1.45 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:139:ARG:HG3 | 2:B:139:ARG:HH11 | 1.60 | 0.65 |
| 1:D:983:G:C2' | 1:D:984:C:H5'' | 2.25 | 0.65 |
| 2:A:860:ARG:NH1 | 2:A:943:ILE:N | 2.41 | 0.65 |
| 2:B:197:ASP:HB3 | 2:B:451:ARG:HB2 | 1.78 | 0.65 |
| 2:B:650:LYS:CE | 2:B:651:MET:H | 2.05 | 0.65 |
| 2:A:83:THR:HG23 | 2:A:152:THR:HB | 1.78 | 0.65 |
| 2:B:198:LEU:HB2 | 2:B:202:GLU:CG | 2.20 | 0.65 |
| 2:B:537:ALA:HB2 | 2:B:602:TYR:CZ | 2.31 | 0.65 |
| 2:A:354:ARG:HD2 | 2:A:376:VAL:HG12 | 1.78 | 0.65 |
| 2:A:914:ARG:NH2 | 2:A:915:THR:HG23 | 2.11 | 0.65 |
| 2:A:82:ILE:HG21 | 2:A:126:VAL:CG1 | 2.26 | 0.65 |
| 2:A:730:LEU:HD22 | 2:A:827:TRP:CZ2 | 2.31 | 0.65 |
| 2:A:210:ILE:CD1 | 2:A:232:PRO:HG3 | 2.24 | 0.65 |
| 2:A:297:ARG:HG2 | 2:A:304:GLU:CG | 2.25 | 0.65 |
| 1:C:967:U:H2' | 1:C:969:G:N7 | 2.11 | 0.65 |
| 2:A:86:PRO:O | 2:A:90:ILE:HG13 | 1.95 | 0.65 |
| 2:A:109:TYR:OH | 2:A:653:LYS:HE2 | 1.96 | 0.65 |
| 2:A:590:ILE:O | 2:A:594:MET:HG3 | 1.97 | 0.65 |
| 2:A:647:GLU:OE2 | 2:A:690:ARG:HA | 1.97 | 0.65 |
| 2:A:767:TYR:HE2 | 2:A:783:LEU:CD1 | 2.09 | 0.65 |
| 2:A:914:ARG:HH21 | 2:A:915:THR:HG23 | 1.62 | 0.65 |
| 2:B:50:HIS:CE1 | 2:B:52:GLY:HA3 | 2.31 | 0.65 |
| 2:B:616:ASN:ND2 | 2:B:617:HIS:H | 1.93 | 0.65 |
| 2:A:233:GLU:HA | 2:A:427:ILE:HD12 | 1.77 | 0.65 |
| 2:A:4:LEU:O | 2:A:4:LEU:HD23 | 1.97 | 0.65 |
| 2:B:87:ILE:HD13 | 2:B:126:VAL:CG2 | 2.27 | 0.65 |
| 2:B:540:THR:CG2 | 2:B:541:ILE:HG23 | 2.25 | 0.65 |
| 2:B:909:LYS:NZ | 2:B:914:ARG:O | 2.29 | 0.65 |
| 2:A:197:ASP:HB3 | 2:A:451:ARG:HB2 | 1.78 | 0.64 |
| 2:A:650:LYS:HD2 | 2:A:651:MET:N | 2.11 | 0.64 |
| 2:B:39:THR:HG22 | 2:B:40:VAL:H | 1.60 | 0.64 |
| 2:B:300:VAL:HG13 | 2:B:301:SER:N | 2.12 | 0.64 |
| 2:B:924:GLU:O | 2:B:928:ARG:N | 2.28 | 0.64 |
| 2:B:924:GLU:HB3 | 2:B:928:ARG:HH21 | 1.62 | 0.64 |
| 2:B:922:ASN:HD22 | 2:B:923:GLU:N | 1.96 | 0.64 |
| 2:A:345:ILE:CG1 | 2:A:346:LEU:H | 2.06 | 0.64 |
| 2:B:27:ILE:HG13 | 2:B:28:ARG:N | 2.13 | 0.64 |
| 2:B:198:LEU:HD22 | 2:B:202:GLU:HA | 1.78 | 0.64 |
| 2:B:724:ASP:HA | 2:B:727:ARG:HG3 | 1.79 | 0.64 |
| 2:B:880:LYS:CG | 2:B:885:SER:HB2 | 2.28 | 0.64 |
| 2:A:139:ARG:HH11 | 2:A:139:ARG:CG | 2.09 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:467:ILE:HG13 | 2:A:508:CYS:HB3 | 1.80 | 0.64 |
| 2:B:33:GLU:CD | 2:B:33:GLU:H | 2.00 | 0.64 |
| 2:B:563:PHE:CD1 | 2:B:584:THR:HG21 | 2.33 | 0.64 |
| 2:B:632:GLU:HG3 | 2:B:633:HIS:ND1 | 2.13 | 0.64 |
| 2:B:958:MET:CE | 2:B:959:PRO:HD2 | 2.27 | 0.64 |
| 2:A:313:VAL:HG12 | 2:A:322:VAL:HG21 | 1.78 | 0.64 |
| 2:A:890:LEU:CD1 | 2:A:906:ILE:HD11 | 2.27 | 0.64 |
| 2:B:289:GLU:O | 2:B:292:ILE:HB | 1.98 | 0.64 |
| 2:B:570:GLU:OE1 | 2:B:576:LYS:HE2 | 1.98 | 0.64 |
| 2:B:729:MET:HE3 | 2:B:763:ASP:O | 1.97 | 0.64 |
| 1:C:920:G:H5'' | 1:C:921:U:C5 | 2.33 | 0.64 |
| 1:D:977:G:H2' | 1:D:978:C:H6 | 1.62 | 0.64 |
| 2:A:492:ARG:HH11 | 2:A:492:ARG:HG2 | 1.63 | 0.64 |
| 2:A:871:TRP:HH2 | 2:A:919:LYS:HE3 | 1.61 | 0.64 |
| 2:B:660:ASN:HB2 | 2:B:663:ASP:HB3 | 1.80 | 0.64 |
| 1:D:943:C:H2' | 1:D:944:C:C6 | 2.33 | 0.64 |
| 2:A:212:ILE:HD13 | 2:A:235:VAL:CG1 | 2.27 | 0.64 |
| 2:A:475:LYS:NZ | 2:A:503:LEU:O | 2.31 | 0.64 |
| 2:B:860:ARG:HB3 | 2:B:966:ILE:HA | 1.78 | 0.64 |
| 2:A:136:THR:HG23 | 2:A:662:ILE:HB | 1.80 | 0.64 |
| 2:B:864:TYR:HH | 2:B:871:TRP:HZ2 | 1.45 | 0.64 |
| 2:A:49:LEU:HD12 | 2:A:49:LEU:N | 2.10 | 0.63 |
| 2:A:92:GLU:O | 2:A:95:LYS:HB3 | 1.99 | 0.63 |
| 2:B:73:ASN:O | 2:B:601:TRP:HH2 | 1.81 | 0.63 |
| 2:A:342:GLU:CG | 2:A:343:THR:H | 2.11 | 0.63 |
| 2:A:924:GLU:O | 2:A:928:ARG:N | 2.28 | 0.63 |
| 2:B:373:PHE:N | 2:B:374:PRO:HD2 | 2.14 | 0.63 |
| 2:B:213:LYS:HD2 | 2:B:435:GLY:O | 1.99 | 0.63 |
| 2:B:256:ARG:HH11 | 2:B:278:ARG:HG3 | 1.63 | 0.63 |
| 2:A:272:LYS:HE3 | 2:A:442:GLU:OE1 | 1.98 | 0.63 |
| 2:A:343:THR:HG23 | 2:A:344:GLU:N | 2.12 | 0.63 |
| 2:A:924:GLU:CD | 2:A:927:LEU:HD13 | 2.19 | 0.63 |
| 2:B:755:TRP:O | 2:B:759:SER:HB3 | 1.99 | 0.63 |
| 2:A:616:ASN:ND2 | 2:A:617:HIS:N | 2.24 | 0.63 |
| 2:B:10:GLU:O | 2:B:14:GLN:HG3 | 1.97 | 0.63 |
| 2:A:85:SER:H | 2:A:86:PRO:CD | 2.12 | 0.63 |
| 2:A:724:ASP:HA | 2:A:727:ARG:CG | 2.19 | 0.63 |
| 2:B:139:ARG:HG3 | 2:B:139:ARG:NH1 | 2.13 | 0.63 |
| 2:B:681:ALA:CA | 2:B:750:ARG:HG3 | 2.28 | 0.63 |
| 2:B:428:ALA:O | 2:B:432:LEU:HD23 | 1.98 | 0.63 |
| 2:B:87:ILE:HD13 | 2:B:126:VAL:HG22 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:495:GLN:HE21 | 2:B:614:ILE:HG21 | 1.63 | 0.63 |
| 2:A:282:VAL:HG12 | 2:A:283:ILE:H | 1.64 | 0.63 |
| 2:A:631:GLU:HA | 2:A:634:TRP:NE1 | 2.14 | 0.63 |
| 2:A:728:TRP:HE3 | 2:A:729:MET:N | 1.97 | 0.63 |
| 2:A:924:GLU:O | 2:A:927:LEU:HB3 | 1.99 | 0.63 |
| 2:B:45:LEU:HD11 | 2:B:80:TRP:CB | 2.29 | 0.63 |
| 2:B:826:GLU:CD | 2:B:826:GLU:N | 2.52 | 0.63 |
| 2:A:268:GLU:OE1 | 2:A:268:GLU:N | 2.26 | 0.62 |
| 2:A:544:HIS:H | 2:A:544:HIS:CD2 | 2.15 | 0.62 |
| 2:B:332:ASP:O | 2:B:333:HIS:HB2 | 1.99 | 0.62 |
| 2:B:894:SER:C | 2:B:896:ILE:H | 2.03 | 0.62 |
| 1:C:918:U:H5'' | 1:C:919:G:OP1 | 1.98 | 0.62 |
| 2:A:180:ALA:O | 2:A:181:HIS:HB2 | 1.99 | 0.62 |
| 2:B:26:ASN:HB2 | 2:B:29:ASP:CG | 2.19 | 0.62 |
| 2:B:216:LEU:HD11 | 2:B:294:LYS:HB3 | 1.80 | 0.62 |
| 2:B:764:LEU:HD13 | 2:B:786:LEU:HD13 | 1.80 | 0.62 |
| 2:A:235:VAL:HB | 2:A:300:VAL:HG11 | 1.79 | 0.62 |
| 2:B:51:VAL:HG11 | 2:B:689:TRP:CE3 | 2.33 | 0.62 |
| 2:A:41:ALA:HA | 2:A:607:ARG:NH2 | 2.15 | 0.62 |
| 2:A:126:VAL:HG12 | 2:A:126:VAL:O | 1.99 | 0.62 |
| 2:A:724:ASP:CA | 2:A:727:ARG:HG3 | 2.20 | 0.62 |
| 2:A:730:LEU:CB | 2:A:827:TRP:HE1 | 2.12 | 0.62 |
| 1:C:911:C:H2' | 1:C:912:C:C6 | 2.33 | 0.62 |
| 2:A:733:LEU:O | 2:A:737:ILE:HG13 | 1.99 | 0.62 |
| 2:A:94:ILE:HD12 | 2:A:95:LYS:N | 2.14 | 0.62 |
| 2:A:168:TRP:CH2 | 2:A:520:TRP:HB3 | 2.34 | 0.62 |
| 2:A:306:ILE:HG12 | 2:A:307:ILE:N | 2.14 | 0.62 |
| 2:A:540:THR:OG1 | 2:A:598:PHE:HA | 2.00 | 0.62 |
| 2:A:894:SER:C | 2:A:896:ILE:H | 2.02 | 0.62 |
| 2:A:7:LYS:HB2 | 2:A:7:LYS:NZ | 2.15 | 0.62 |
| 2:B:181:HIS:ND1 | 2:B:464:GLN:HG2 | 2.14 | 0.62 |
| 2:B:218:GLU:CD | 2:B:219:ASN:HD22 | 2.03 | 0.62 |
| 2:B:531:ASP:OD2 | 2:B:532:SER:N | 2.32 | 0.62 |
| 2:A:213:LYS:HB2 | 2:A:224:TYR:CD2 | 2.35 | 0.62 |
| 2:A:933:PHE:CD1 | 2:A:933:PHE:C | 2.72 | 0.62 |
| 2:B:68:ARG:NH2 | 2:B:143:SER:HB3 | 2.14 | 0.62 |
| 2:B:85:SER:H | 2:B:86:PRO:HD3 | 1.64 | 0.62 |
| 2:B:126:VAL:O | 2:B:126:VAL:HG12 | 1.99 | 0.62 |
| 2:B:212:ILE:HD13 | 2:B:235:VAL:HG12 | 1.82 | 0.62 |
| 2:B:277:ASP:O | 2:B:278:ARG:HG3 | 1.99 | 0.62 |
| 1:C:914:A:H1' | 1:C:925:A:C6 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:186:ASP:HB2 | 2:A:193:LEU:HD11 | 1.82 | 0.62 |
| 2:A:702:GLU:O | 2:A:706:GLU:HG3 | 2.00 | 0.62 |
| 2:B:234:THR:HG22 | 2:B:325:VAL:HG11 | 1.80 | 0.62 |
| 2:A:709:SER:O | 2:A:712:ALA:HB3 | 1.99 | 0.62 |
| 2:A:776:ASP:OD2 | 2:A:778:ALA:HB3 | 1.99 | 0.62 |
| 2:A:860:ARG:HH11 | 2:A:943:ILE:H | 1.48 | 0.62 |
| 2:B:140:ALA:O | 2:B:674:ARG:NH1 | 2.31 | 0.62 |
| 2:B:709:SER:O | 2:B:712:ALA:HB3 | 2.00 | 0.62 |
| 1:D:970:A:H2' | 1:D:972:U:OP2 | 2.00 | 0.61 |
| 2:A:906:ILE:O | 2:A:910:LEU:HB2 | 2.00 | 0.61 |
| 2:B:49:LEU:HD12 | 2:B:49:LEU:N | 2.13 | 0.61 |
| 2:B:793:LEU:HD21 | 2:B:821:PRO:HG2 | 1.81 | 0.61 |
| 2:A:297:ARG:NH2 | 2:A:297:ARG:CB | 2.63 | 0.61 |
| 2:B:745:GLU:HA | 2:B:745:GLU:OE2 | 1.99 | 0.61 |
| 1:C:986:C:C2 | 2:A:507:ALA:HB3 | 2.36 | 0.61 |
| 2:A:11:GLU:O | 2:A:15:LYS:HG3 | 2.00 | 0.61 |
| 2:A:102:ILE:HD12 | 2:A:103:TRP:N | 2.15 | 0.61 |
| 2:B:44:TYR:CE1 | 2:B:87:ILE:HD11 | 2.30 | 0.61 |
| 2:B:264:ILE:HG21 | 2:B:291:LEU:HD21 | 1.81 | 0.61 |
| 2:A:326:PRO:HA | 2:A:332:ASP:HB2 | 1.81 | 0.61 |
| 2:A:803:GLU:HA | 2:A:815:VAL:HG23 | 1.82 | 0.61 |
| 2:B:44:TYR:OH | 2:B:87:ILE:HG13 | 2.00 | 0.61 |
| 2:B:401:TYR:O | 2:B:405:TYR:HB2 | 2.00 | 0.61 |
| 2:B:920:ARG:HE | 2:B:920:ARG:CA | 2.01 | 0.61 |
| 2:A:82:ILE:H | 2:A:152:THR:HG1 | 1.45 | 0.61 |
| 2:A:864:TYR:CZ | 2:A:922:ASN:OD1 | 2.53 | 0.61 |
| 2:B:91:ALA:O | 2:B:94:ILE:HG13 | 1.99 | 0.61 |
| 2:B:345:ILE:CG1 | 2:B:346:LEU:H | 2.13 | 0.61 |
| 2:B:723:LYS:HG3 | 2:B:724:ASP:H | 1.66 | 0.61 |
| 2:A:26:ASN:O | 2:A:29:ASP:HB2 | 2.01 | 0.61 |
| 2:A:297:ARG:NH2 | 2:A:297:ARG:HB3 | 2.15 | 0.61 |
| 2:A:857:ASN:ND2 | 2:A:967:GLU:HG2 | 2.16 | 0.61 |
| 2:A:924:GLU:OE2 | 2:A:927:LEU:HD13 | 2.01 | 0.61 |
| 2:B:879:GLU:O | 2:B:880:LYS:HD2 | 2.00 | 0.61 |
| 2:A:618:LEU:O | 2:A:621:PHE:HB3 | 2.00 | 0.61 |
| 2:B:277:ASP:OD1 | 2:B:462:HIS:NE2 | 2.33 | 0.61 |
| 2:B:890:LEU:CD1 | 2:B:906:ILE:HD11 | 2.31 | 0.61 |
| 2:A:893:ASP:OD1 | 2:A:894:SER:O | 2.19 | 0.61 |
| 2:A:919:LYS:HD2 | 2:A:960:LEU:HD11 | 1.82 | 0.61 |
| 2:B:145:ASP:OD1 | 2:B:147:SER:HB3 | 1.99 | 0.61 |
| 2:B:914:ARG:NE | 2:B:915:THR:O | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:28:ARG:NH1 | 2:B:28:ARG:H | 1.98 | 0.61 |
| 1:D:970:A:H4' | 1:D:971:A:OP1 | 2.01 | 0.61 |
| 2:A:866:ALA:CA | 2:A:955:LYS:HZ3 | 2.11 | 0.61 |
| 2:B:770:ARG:HA | 2:B:933:PHE:CE2 | 2.35 | 0.61 |
| 2:A:94:ILE:HD11 | 2:A:120:GLU:N | 2.15 | 0.60 |
| 2:A:492:ARG:HD2 | 2:A:614:ILE:CD1 | 2.30 | 0.60 |
| 2:A:123:ILE:O | 2:A:127:LYS:HB2 | 2.00 | 0.60 |
| 2:A:241:MET:HB2 | 2:A:307:ILE:HA | 1.81 | 0.60 |
| 2:A:567:ILE:O | 2:A:568:PHE:CG | 2.54 | 0.60 |
| 2:A:803:GLU:OE2 | 2:A:814:PHE:HB3 | 2.01 | 0.60 |
| 2:B:448:VAL:HG12 | 2:B:456:ALA:HB3 | 1.82 | 0.60 |
| 2:B:730:LEU:HB3 | 2:B:827:TRP:NE1 | 2.16 | 0.60 |
| 2:A:45:LEU:HD11 | 2:A:80:TRP:CB | 2.31 | 0.60 |
| 2:A:427:ILE:O | 2:A:431:MET:HG3 | 2.00 | 0.60 |
| 2:A:860:ARG:NE | 2:A:860:ARG:O | 2.35 | 0.60 |
| 2:A:381:LYS:HB3 | 2:A:382:LEU:HD12 | 1.83 | 0.60 |
| 2:A:594:MET:O | 2:A:597:GLU:HB2 | 2.01 | 0.60 |
| 2:B:748:ARG:HB3 | 2:B:748:ARG:HH11 | 1.67 | 0.60 |
| 2:A:210:ILE:HG22 | 2:A:439:ILE:HG12 | 1.83 | 0.60 |
| 2:A:234:THR:HG22 | 2:A:325:VAL:HG11 | 1.83 | 0.60 |
| 2:A:461:ILE:CG2 | 2:A:464:GLN:HB2 | 2.32 | 0.60 |
| 2:B:166:GLN:O | 2:B:170:LEU:HG | 2.01 | 0.60 |
| 2:B:186:ASP:HB3 | 2:B:191:THR:CG2 | 2.32 | 0.60 |
| 1:C:976:C:O2' | 1:C:977:G:H5' | 2.01 | 0.60 |
| 1:C:953:A:H5' | 1:C:954:G:OP1 | 2.02 | 0.60 |
| 2:A:12:LYS:HZ3 | 2:A:16:ARG:HH12 | 1.50 | 0.60 |
| 2:A:266:SER:HB2 | 2:A:269:ALA:CB | 2.32 | 0.60 |
| 2:A:919:LYS:H | 2:A:919:LYS:HE3 | 1.66 | 0.60 |
| 2:A:919:LYS:NZ | 2:A:960:LEU:HD11 | 2.16 | 0.60 |
| 2:B:32:LYS:HG2 | 2:B:600:TYR:HD1 | 1.65 | 0.60 |
| 2:B:85:SER:H | 2:B:86:PRO:CD | 2.14 | 0.60 |
| 2:B:266:SER:HB3 | 2:B:269:ALA:HB2 | 1.83 | 0.60 |
| 1:D:979:C:H2' | 1:D:980:C:C6 | 2.37 | 0.60 |
| 2:A:412:VAL:CG2 | 2:A:414:PRO:HD2 | 2.32 | 0.60 |
| 2:B:781:TYR:CE2 | 2:B:785:THR:HG21 | 2.37 | 0.60 |
| 2:B:781:TYR:O | 2:B:785:THR:HG23 | 2.02 | 0.60 |
| 2:A:560:THR:HB | 2:A:561:PRO:HD2 | 1.84 | 0.60 |
| 2:A:767:TYR:CZ | 2:A:782:VAL:HG11 | 2.37 | 0.60 |
| 2:B:79:ALA:HB1 | 2:B:150:PHE:O | 2.01 | 0.60 |
| 2:B:282:VAL:HG12 | 2:B:283:ILE:H | 1.66 | 0.60 |
| 2:A:857:ASN:OD1 | 2:A:967:GLU:HA | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:725:ILE:HG21 | 2:B:771:THR:CG2 | 2.31 | 0.59 |
| 2:A:17:TRP:HH2 | 2:A:800:HIS:CD2 | 2.20 | 0.59 |
| 2:A:297:ARG:HH21 | 2:A:297:ARG:HB2 | 1.67 | 0.59 |
| 2:A:354:ARG:HD2 | 2:A:376:VAL:HG13 | 1.82 | 0.59 |
| 2:A:915:THR:OG1 | 2:A:916:PHE:N | 2.31 | 0.59 |
| 2:B:540:THR:OG1 | 2:B:598:PHE:HA | 2.01 | 0.59 |
| 2:B:569:LEU:HA | 2:B:630:ARG:HD3 | 1.85 | 0.59 |
| 2:B:746:GLU:HB2 | 2:B:748:ARG:HD2 | 1.84 | 0.59 |
| 2:A:678:MET:HB3 | 2:A:749:THR:HB | 1.84 | 0.59 |
| 2:A:895:GLU:OE1 | 2:A:898:LYS:CD | 2.50 | 0.59 |
| 2:A:960:LEU:N | 2:A:960:LEU:HD22 | 2.17 | 0.59 |
| 2:A:711:PHE:HA | 2:A:714:TYR:CD2 | 2.38 | 0.59 |
| 2:A:914:ARG:NE | 2:A:915:THR:O | 2.35 | 0.59 |
| 2:B:339:LEU:HD22 | 2:B:340:LYS:N | 2.17 | 0.59 |
| 2:B:475:LYS:HG2 | 2:B:479:ARG:NH2 | 2.18 | 0.59 |
| 2:B:935:GLU:OE1 | 2:B:942:ILE:N | 2.34 | 0.59 |
| 2:A:75:LEU:HD23 | 2:A:601:TRP:CD2 | 2.37 | 0.59 |
| 2:A:79:ALA:HB1 | 2:A:150:PHE:O | 2.01 | 0.59 |
| 2:A:182:ARG:O | 2:A:183:VAL:HB | 2.02 | 0.59 |
| 2:A:824:VAL:HG11 | 2:A:827:TRP:CE3 | 2.37 | 0.59 |
| 2:A:860:ARG:CB | 2:A:966:ILE:HG22 | 2.33 | 0.59 |
| 2:B:100:LYS:HE2 | 2:B:104:ILE:HD11 | 1.83 | 0.59 |
| 2:B:241:MET:HB2 | 2:B:307:ILE:HA | 1.84 | 0.59 |
| 2:B:711:PHE:CD1 | 2:B:783:LEU:HB3 | 2.38 | 0.59 |
| 1:C:986:C:C2 | 2:A:506:LYS:HG2 | 2.37 | 0.59 |
| 2:A:152:THR:HG22 | 2:A:159:PHE:HE1 | 1.67 | 0.59 |
| 2:A:560:THR:O | 2:A:563:PHE:HB3 | 2.03 | 0.59 |
| 2:A:819:LYS:N | 2:A:819:LYS:HD2 | 2.17 | 0.59 |
| 2:A:921:ILE:HB | 2:A:928:ARG:NH2 | 2.16 | 0.59 |
| 2:B:112:PRO:O | 2:B:114:GLU:N | 2.36 | 0.59 |
| 2:B:594:MET:O | 2:B:597:GLU:HB2 | 2.02 | 0.59 |
| 2:B:618:LEU:O | 2:B:621:PHE:HB3 | 2.03 | 0.59 |
| 1:D:916:C:O2' | 1:D:972:U:H4' | 2.03 | 0.59 |
| 2:A:242:TRP:CE3 | 2:A:324:SER:HB2 | 2.38 | 0.59 |
| 2:A:401:TYR:O | 2:A:405:TYR:HB2 | 2.03 | 0.59 |
| 2:B:94:ILE:HD12 | 2:B:95:LYS:N | 2.18 | 0.59 |
| 2:A:231:ARG:HB3 | 2:A:233:GLU:OE2 | 2.02 | 0.59 |
| 2:B:227:ALA:CA | 2:B:321:VAL:HG23 | 2.26 | 0.59 |
| 2:B:233:GLU:HB3 | 2:B:423:VAL:HG23 | 1.84 | 0.59 |
| 2:B:250:VAL:O | 2:B:264:ILE:HA | 2.02 | 0.59 |
| 2:A:211:ILE:CG2 | 2:A:228:ALA:HB2 | 2.30 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:297:ARG:CB | 2:A:297:ARG:HH21 | 2.16 | 0.59 |
| 2:B:50:HIS:H | 2:B:53:HIS:CD2 | 2.21 | 0.59 |
| 2:B:404:GLU:HA | 2:B:407:LYS:O | 2.03 | 0.59 |
| 2:B:921:ILE:HD12 | 2:B:928:ARG:HH22 | 1.68 | 0.59 |
| 2:B:943:ILE:HG22 | 2:B:946:PRO:HG3 | 1.84 | 0.59 |
| 2:B:966:ILE:O | 2:B:967:GLU:HB2 | 2.03 | 0.59 |
| 2:A:66:PHE:CD1 | 2:A:744:LEU:HD12 | 2.37 | 0.58 |
| 2:A:250:VAL:O | 2:A:264:ILE:HA | 2.04 | 0.58 |
| 2:A:378:GLU:HA | 2:A:378:GLU:OE2 | 2.02 | 0.58 |
| 2:A:393:LEU:HG | 2:A:397:THR:OG1 | 2.03 | 0.58 |
| 2:A:547:LYS:O | 2:A:550:GLN:HB3 | 2.03 | 0.58 |
| 2:A:847:LYS:O | 2:A:851:GLU:HG3 | 2.03 | 0.58 |
| 2:A:882:ASP:CG | 2:A:883:PHE:N | 2.56 | 0.58 |
| 2:B:355:ILE:HG22 | 2:B:356:VAL:N | 2.12 | 0.58 |
| 2:B:641:ASN:C | 2:B:641:ASN:HD22 | 2.06 | 0.58 |
| 2:B:722:LEU:H | 2:B:722:LEU:HD23 | 1.68 | 0.58 |
| 1:D:904:G:C3' | 1:D:905:G:H5'' | 2.33 | 0.58 |
| 2:A:75:LEU:HD12 | 2:A:77:PRO:HD3 | 1.85 | 0.58 |
| 2:A:966:ILE:O | 2:A:967:GLU:CB | 2.50 | 0.58 |
| 2:B:49:LEU:H | 2:B:49:LEU:CD1 | 2.12 | 0.58 |
| 2:B:105:TYR:O | 2:B:111:VAL:HG23 | 2.03 | 0.58 |
| 2:A:216:LEU:HG | 2:A:216:LEU:O | 2.03 | 0.58 |
| 2:A:263:TRP:HH2 | 2:A:438:GLU:OE1 | 1.86 | 0.58 |
| 2:A:819:LYS:N | 2:A:819:LYS:CD | 2.66 | 0.58 |
| 2:A:860:ARG:HH22 | 2:A:862:TYR:HB3 | 1.68 | 0.58 |
| 2:A:860:ARG:HH11 | 2:A:943:ILE:N | 2.01 | 0.58 |
| 2:A:920:ARG:O | 2:A:922:ASN:N | 2.36 | 0.58 |
| 2:B:733:LEU:HD13 | 2:B:737:ILE:HG13 | 1.85 | 0.58 |
| 2:B:857:ASN:O | 2:B:940:ILE:HD11 | 2.03 | 0.58 |
| 2:A:27:ILE:H | 2:A:28:ARG:NH2 | 2.01 | 0.58 |
| 2:A:235:VAL:HA | 2:A:323:MET:HE3 | 1.85 | 0.58 |
| 2:A:541:ILE:HB | 2:A:594:MET:HE2 | 1.86 | 0.58 |
| 2:A:729:MET:SD | 2:A:764:LEU:HA | 2.44 | 0.58 |
| 2:B:901:LYS:O | 2:B:901:LYS:HD3 | 2.03 | 0.58 |
| 2:A:410:PHE:O | 2:A:416:GLU:HB3 | 2.03 | 0.58 |
| 2:A:944:ILE:HG22 | 2:A:945:ASN:N | 2.18 | 0.58 |
| 2:B:180:ALA:O | 2:B:181:HIS:HB2 | 2.04 | 0.58 |
| 2:B:429:LYS:HB3 | 2:B:429:LYS:NZ | 2.19 | 0.58 |
| 2:B:660:ASN:HB2 | 2:B:663:ASP:HB2 | 1.86 | 0.58 |
| 2:B:60:PRO:HB2 | 2:B:76:PHE:CE1 | 2.39 | 0.58 |
| 2:B:342:GLU:HG2 | 2:B:343:THR:N | 2.15 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:804:GLU:O | 2:B:807:GLU:HB3 | 2.03 | 0.58 |
| 2:B:50:HIS:HE1 | 2:B:52:GLY:HA3 | 1.68 | 0.58 |
| 2:B:238:VAL:HA | 2:B:325:VAL:HG22 | 1.85 | 0.58 |
| 2:A:239:THR:O | 2:A:240:ASN:HB3 | 2.03 | 0.58 |
| 2:A:566:TYR:O | 2:A:595:LYS:HD2 | 2.04 | 0.58 |
| 2:A:710:GLN:O | 2:A:712:ALA:N | 2.37 | 0.58 |
| 2:B:495:GLN:O | 2:B:499:ILE:HG12 | 2.04 | 0.58 |
| 2:B:652:SER:OG | 2:B:655:LYS:HB2 | 2.04 | 0.58 |
| 2:B:682:GLU:OE1 | 2:B:748:ARG:HB3 | 2.03 | 0.58 |
| 2:B:713:GLU:HA | 2:B:713:GLU:OE2 | 2.04 | 0.58 |
| 2:A:167:PHE:O | 2:A:170:LEU:HB2 | 2.04 | 0.58 |
| 2:A:482:LEU:HD23 | 2:A:482:LEU:C | 2.24 | 0.58 |
| 2:A:862:TYR:C | 2:A:862:TYR:CD2 | 2.77 | 0.58 |
| 2:B:211:ILE:HG12 | 2:B:438:GLU:O | 2.03 | 0.58 |
| 2:B:377:GLU:OE2 | 2:B:380:ASN:HB2 | 2.04 | 0.58 |
| 2:B:410:PHE:O | 2:B:416:GLU:HB3 | 2.04 | 0.58 |
| 2:B:835:GLU:OE1 | 2:B:921:ILE:HG13 | 2.03 | 0.58 |
| 1:C:937:C:O5' | 1:C:937:C:H6 | 1.87 | 0.57 |
| 2:A:860:ARG:NE | 2:A:860:ARG:C | 2.57 | 0.57 |
| 2:A:871:TRP:HZ3 | 2:A:918:VAL:HG22 | 1.69 | 0.57 |
| 2:B:467:ILE:HG13 | 2:B:508:CYS:HB3 | 1.85 | 0.57 |
| 2:B:860:ARG:CZ | 2:B:860:ARG:O | 2.52 | 0.57 |
| 2:A:112:PRO:O | 2:A:114:GLU:N | 2.37 | 0.57 |
| 2:A:355:ILE:HG23 | 2:A:412:VAL:CG1 | 2.34 | 0.57 |
| 2:B:459:LYS:HZ3 | 2:B:461:ILE:HD13 | 1.70 | 0.57 |
| 2:B:629:PHE:O | 2:B:631:GLU:N | 2.29 | 0.57 |
| 2:A:145:ASP:OD1 | 2:A:145:ASP:C | 2.43 | 0.57 |
| 2:A:404:GLU:HA | 2:A:407:LYS:O | 2.05 | 0.57 |
| 2:A:614:ILE:N | 2:A:615:PRO:HD2 | 2.19 | 0.57 |
| 2:A:646:LEU:O | 2:A:647:GLU:HB2 | 2.04 | 0.57 |
| 2:B:563:PHE:CE1 | 2:B:584:THR:HG21 | 2.39 | 0.57 |
| 2:B:727:ARG:HG2 | 2:B:727:ARG:HH11 | 1.69 | 0.57 |
| 2:B:831:THR:O | 2:B:835:GLU:HG3 | 2.05 | 0.57 |
| 1:D:943:C:H2' | 1:D:944:C:H6 | 1.66 | 0.57 |
| 2:A:42:PHE:O | 2:A:42:PHE:HD1 | 1.87 | 0.57 |
| 2:B:784:ARG:O | 2:B:784:ARG:HD3 | 2.05 | 0.57 |
| 2:A:348:LYS:HB3 | 2:A:348:LYS:HZ3 | 1.70 | 0.57 |
| 2:A:541:ILE:HB | 2:A:594:MET:CE | 2.34 | 0.57 |
| 2:B:631:GLU:HA | 2:B:634:TRP:CD1 | 2.40 | 0.57 |
| 2:A:757:PHE:HD1 | 2:A:794:MET:SD | 2.27 | 0.57 |
| 2:A:860:ARG:CB | 2:A:966:ILE:HA | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:116:LEU:HD12 | 2:B:119:PHE:CE2 | 2.40 | 0.57 |
| 2:B:541:ILE:O | 2:B:545:ILE:HG12 | 2.05 | 0.57 |
| 2:B:793:LEU:CD2 | 2:B:821:PRO:CG | 2.82 | 0.57 |
| 2:A:331:PHE:O | 2:A:334:VAL:HG23 | 2.04 | 0.57 |
| 2:A:559:LEU:HD22 | 2:A:563:PHE:CE2 | 2.40 | 0.57 |
| 2:A:770:ARG:HD2 | 2:A:933:PHE:CD2 | 2.39 | 0.57 |
| 2:B:32:LYS:O | 2:B:35:LYS:HG3 | 2.04 | 0.57 |
| 2:B:410:PHE:CE2 | 2:B:423:VAL:HG11 | 2.40 | 0.57 |
| 2:B:846:ILE:HG12 | 2:B:964:ILE:HD13 | 1.86 | 0.57 |
| 1:D:928:C:OP1 | 2:B:696:LYS:HE3 | 2.04 | 0.57 |
| 2:A:233:GLU:HA | 2:A:427:ILE:CD1 | 2.34 | 0.57 |
| 2:A:253:LYS:HD3 | 2:A:260:GLU:OE1 | 2.04 | 0.57 |
| 2:A:551:GLU:O | 2:A:553:LYS:N | 2.37 | 0.57 |
| 2:A:804:GLU:O | 2:A:807:GLU:HB3 | 2.05 | 0.57 |
| 2:B:242:TRP:CH2 | 2:B:332:ASP:HA | 2.40 | 0.57 |
| 2:B:624:ASN:HD22 | 2:B:624:ASN:H | 1.51 | 0.57 |
| 2:B:697:LEU:O | 2:B:701:ILE:HG12 | 2.05 | 0.57 |
| 2:B:928:ARG:C | 2:B:930:ALA:H | 2.09 | 0.57 |
| 2:A:171:LYS:HE2 | 2:A:520:TRP:CE2 | 2.40 | 0.57 |
| 2:A:745:GLU:HA | 2:A:745:GLU:OE2 | 2.05 | 0.57 |
| 2:B:151:TYR:CD1 | 2:B:156:PHE:HB2 | 2.40 | 0.57 |
| 2:A:83:THR:HG22 | 2:A:153:THR:HG22 | 1.87 | 0.56 |
| 2:A:256:ARG:HH11 | 2:A:278:ARG:HD3 | 1.70 | 0.56 |
| 2:A:920:ARG:C | 2:A:922:ASN:N | 2.58 | 0.56 |
| 2:B:239:THR:O | 2:B:240:ASN:HB3 | 2.04 | 0.56 |
| 2:B:662:ILE:HG23 | 2:B:663:ASP:H | 1.70 | 0.56 |
| 2:A:840:ARG:O | 2:A:844:GLU:HG3 | 2.04 | 0.56 |
| 2:B:57:TYR:C | 2:B:60:PRO:HD2 | 2.26 | 0.56 |
| 2:B:161:LYS:HD2 | 2:B:559:LEU:O | 2.05 | 0.56 |
| 2:B:212:ILE:HD13 | 2:B:235:VAL:CG1 | 2.35 | 0.56 |
| 2:B:705:TYR:CD2 | 2:B:805:LEU:HD21 | 2.40 | 0.56 |
| 2:B:870:LYS:HE2 | 2:B:957:ALA:O | 2.05 | 0.56 |
| 2:A:93:ARG:HG2 | 2:A:451:ARG:NH2 | 2.21 | 0.56 |
| 2:A:196:HIS:CD2 | 2:A:197:ASP:H | 2.22 | 0.56 |
| 2:A:864:TYR:HD2 | 2:A:962:PRO:HB3 | 1.70 | 0.56 |
| 2:A:877:VAL:HG22 | 2:A:906:ILE:HG23 | 1.85 | 0.56 |
| 2:B:95:LYS:C | 2:B:97:ARG:N | 2.58 | 0.56 |
| 2:B:135:GLU:O | 2:B:138:ILE:HG22 | 2.06 | 0.56 |
| 2:B:389:ASP:O | 2:B:390:LYS:HD3 | 2.05 | 0.56 |
| 2:B:432:LEU:HD11 | 2:B:439:ILE:HG13 | 1.87 | 0.56 |
| 2:B:609:SER:O | 2:B:640:VAL:HA | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:867:GLU:CD | 2:B:867:GLU:N | 2.57 | 0.56 |
| 2:B:918:VAL:HG11 | 2:B:920:ARG:HD2 | 1.87 | 0.56 |
| 2:A:93:ARG:HD3 | 2:A:451:ARG:NH2 | 2.20 | 0.56 |
| 2:A:481:ALA:O | 2:A:484:ARG:N | 2.34 | 0.56 |
| 2:B:44:TYR:HE1 | 2:B:87:ILE:CD1 | 2.16 | 0.56 |
| 2:B:165:TRP:HD1 | 2:B:561:PRO:HA | 1.70 | 0.56 |
| 2:B:725:ILE:HD13 | 2:B:770:ARG:NH2 | 2.21 | 0.56 |
| 2:B:743:ALA:HB2 | 2:B:751:THR:HG22 | 1.87 | 0.56 |
| 2:B:884:LYS:O | 2:B:887:MET:N | 2.38 | 0.56 |
| 2:A:325:VAL:N | 2:A:332:ASP:OD2 | 2.39 | 0.56 |
| 2:A:662:ILE:HG23 | 2:A:663:ASP:N | 2.19 | 0.56 |
| 2:A:928:ARG:C | 2:A:930:ALA:H | 2.08 | 0.56 |
| 2:B:53:HIS:O | 2:B:57:TYR:HD2 | 1.89 | 0.56 |
| 2:B:852:VAL:O | 2:B:852:VAL:HG12 | 2.06 | 0.56 |
| 2:B:920:ARG:O | 2:B:922:ASN:N | 2.37 | 0.56 |
| 1:D:979:C:H2' | 1:D:980:C:H6 | 1.71 | 0.56 |
| 2:A:16:ARG:CG | 2:A:16:ARG:HH11 | 2.19 | 0.56 |
| 2:A:45:LEU:HD21 | 2:A:80:TRP:HB3 | 1.87 | 0.56 |
| 2:A:384:ILE:HG22 | 2:A:385:LYS:N | 2.18 | 0.56 |
| 2:A:825:GLU:HG2 | 2:A:826:GLU:HG2 | 1.87 | 0.56 |
| 2:B:98:ASP:O | 2:B:102:ILE:HG23 | 2.06 | 0.56 |
| 2:B:236:TYR:CE2 | 2:B:414:PRO:HG2 | 2.41 | 0.56 |
| 2:B:272:LYS:HE2 | 2:B:442:GLU:OE1 | 2.05 | 0.56 |
| 2:B:708:ILE:HB | 2:B:805:LEU:HD13 | 1.87 | 0.56 |
| 2:B:742:ASN:HD22 | 2:B:742:ASN:N | 2.03 | 0.56 |
| 2:A:27:ILE:N | 2:A:28:ARG:NH2 | 2.53 | 0.56 |
| 2:A:95:LYS:C | 2:A:97:ARG:N | 2.58 | 0.56 |
| 2:A:771:THR:CG2 | 2:A:774:ARG:HD3 | 2.35 | 0.56 |
| 2:A:831:THR:O | 2:A:835:GLU:HG3 | 2.06 | 0.56 |
| 2:A:884:LYS:O | 2:A:887:MET:N | 2.38 | 0.56 |
| 2:B:374:PRO:HG3 | 2:B:379:VAL:HG21 | 1.88 | 0.56 |
| 2:B:475:LYS:HG2 | 2:B:475:LYS:O | 2.06 | 0.56 |
| 2:B:779:LYS:O | 2:B:783:LEU:HD13 | 2.04 | 0.56 |
| 2:B:797:PHE:CD2 | 2:B:797:PHE:N | 2.73 | 0.56 |
| 2:A:355:ILE:HD12 | 2:A:412:VAL:HG11 | 1.88 | 0.56 |
| 2:A:706:GLU:O | 2:A:709:SER:HB2 | 2.06 | 0.56 |
| 2:A:953:LYS:NZ | 2:A:953:LYS:HB3 | 2.19 | 0.56 |
| 2:A:67:LYS:CE | 2:A:70:GLN:NE2 | 2.69 | 0.56 |
| 2:A:212:ILE:HD13 | 2:A:235:VAL:HG12 | 1.88 | 0.56 |
| 2:A:690:ARG:HH12 | 2:A:693:GLU:HG3 | 1.70 | 0.56 |
| 2:A:860:ARG:HH22 | 2:A:862:TYR:CB | 2.18 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:767:TYR:HE2 | 2:B:783:LEU:CD1 | 2.19 | 0.56 |
| 1:C:905:G:H2' | 1:C:906:G:O4' | 2.06 | 0.56 |
| 2:A:82:ILE:HG13 | 2:A:153:THR:CG2 | 2.33 | 0.56 |
| 2:A:708:ILE:HD12 | 2:A:791:VAL:HG23 | 1.87 | 0.56 |
| 2:A:866:ALA:HB3 | 2:A:955:LYS:NZ | 2.21 | 0.56 |
| 2:B:551:GLU:O | 2:B:553:LYS:N | 2.39 | 0.56 |
| 2:B:744:LEU:HD23 | 2:B:752:ALA:HB2 | 1.87 | 0.56 |
| 2:B:935:GLU:CD | 2:B:942:ILE:H | 2.09 | 0.56 |
| 2:A:468:ASP:C | 2:A:470:GLY:H | 2.08 | 0.55 |
| 2:A:675:LEU:HD12 | 2:A:697:LEU:HD21 | 1.88 | 0.55 |
| 2:A:728:TRP:O | 2:A:731:HIS:N | 2.38 | 0.55 |
| 2:A:863:ILE:HG13 | 2:A:945:ASN:OD1 | 2.05 | 0.55 |
| 2:B:613:LEU:O | 2:B:618:LEU:HB2 | 2.06 | 0.55 |
| 2:B:746:GLU:O | 2:B:748:ARG:HG3 | 2.06 | 0.55 |
| 2:B:868:ASP:O | 2:B:870:LYS:N | 2.39 | 0.55 |
| 2:A:112:PRO:HG2 | 2:A:115:ILE:HD12 | 1.87 | 0.55 |
| 2:A:331:PHE:HD1 | 2:A:334:VAL:HG21 | 1.72 | 0.55 |
| 2:B:167:PHE:O | 2:B:170:LEU:HB2 | 2.06 | 0.55 |
| 2:B:727:ARG:HG2 | 2:B:727:ARG:NH1 | 2.21 | 0.55 |
| 1:C:920:G:H4' | 1:C:920:G:OP1 | 2.06 | 0.55 |
| 2:A:198:LEU:H | 2:A:198:LEU:HD12 | 1.70 | 0.55 |
| 2:A:631:GLU:HA | 2:A:634:TRP:CD1 | 2.42 | 0.55 |
| 2:A:933:PHE:C | 2:A:933:PHE:HD1 | 2.08 | 0.55 |
| 2:B:468:ASP:C | 2:B:470:GLY:H | 2.09 | 0.55 |
| 2:B:555:ASP:OD2 | 2:B:558:LYS:HE2 | 2.07 | 0.55 |
| 2:B:636:LYS:HZ2 | 2:B:636:LYS:HB3 | 1.71 | 0.55 |
| 2:B:920:ARG:C | 2:B:922:ASN:N | 2.60 | 0.55 |
| 1:D:980:C:O2' | 1:D:981:C:H5' | 2.06 | 0.55 |
| 2:A:84:GLY:O | 2:A:513:GLY:HA3 | 2.07 | 0.55 |
| 2:A:349:TYR:H | 2:A:349:TYR:HD1 | 1.55 | 0.55 |
| 2:A:644:GLY:O | 2:A:650:LYS:NZ | 2.38 | 0.55 |
| 2:A:767:TYR:HE2 | 2:A:783:LEU:HD13 | 1.70 | 0.55 |
| 2:A:859:LYS:CB | 2:A:941:GLU:HB3 | 2.33 | 0.55 |
| 2:A:868:ASP:O | 2:A:870:LYS:N | 2.40 | 0.55 |
| 2:B:878:SER:CB | 2:B:915:THR:HG22 | 2.36 | 0.55 |
| 2:A:297:ARG:HG2 | 2:A:304:GLU:CD | 2.27 | 0.55 |
| 2:A:488:LEU:HA | 2:A:489:PRO:C | 2.27 | 0.55 |
| 2:B:314:ASP:HB3 | 2:B:317:ASN:HB3 | 1.88 | 0.55 |
| 2:B:835:GLU:O | 2:B:838:PHE:HB3 | 2.07 | 0.55 |
| 2:B:847:LYS:O | 2:B:851:GLU:HG3 | 2.06 | 0.55 |
| 2:A:142:PHE:C | 2:A:144:VAL:H | 2.11 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:884:LYS:O | 2:A:886:SER:N | 2.40 | 0.55 |
| 2:B:142:PHE:C | 2:B:144:VAL:H | 2.10 | 0.55 |
| 2:B:235:VAL:HB | 2:B:300:VAL:HG11 | 1.88 | 0.55 |
| 2:B:860:ARG:CZ | 2:B:860:ARG:C | 2.75 | 0.55 |
| 2:B:884:LYS:HG2 | 2:B:888:GLU:OE1 | 2.07 | 0.55 |
| 2:A:66:PHE:CE2 | 2:A:70:GLN:NE2 | 2.69 | 0.55 |
| 2:A:469:TYR:HB3 | 2:A:503:LEU:HD23 | 1.89 | 0.55 |
| 2:A:567:ILE:HA | 2:A:595:LYS:CD | 2.28 | 0.55 |
| 2:B:508:CYS:O | 2:B:509:ALA:HB2 | 2.06 | 0.55 |
| 2:A:555:ASP:OD2 | 2:A:558:LYS:HG2 | 2.07 | 0.55 |
| 2:A:733:LEU:HD11 | 2:A:789:VAL:HG21 | 1.89 | 0.55 |
| 2:B:489:PRO:HG3 | 2:B:684:ASP:OD2 | 2.06 | 0.55 |
| 2:B:537:ALA:O | 2:B:540:THR:HG22 | 2.07 | 0.55 |
| 2:A:58:THR:O | 2:A:62:VAL:HG23 | 2.07 | 0.54 |
| 2:A:342:GLU:CG | 2:A:343:THR:N | 2.68 | 0.54 |
| 2:A:714:TYR:CD1 | 2:A:780:ARG:HG2 | 2.42 | 0.54 |
| 2:A:766:TRP:CH2 | 2:A:836:GLU:OE1 | 2.60 | 0.54 |
| 2:B:84:GLY:O | 2:B:513:GLY:HA3 | 2.07 | 0.54 |
| 2:B:139:ARG:HH11 | 2:B:139:ARG:CG | 2.19 | 0.54 |
| 2:B:471:ASN:CG | 2:B:473:GLU:HG2 | 2.28 | 0.54 |
| 2:B:864:TYR:HD2 | 2:B:962:PRO:HB3 | 1.72 | 0.54 |
| 1:D:933:G:O2' | 1:D:934:A:H5' | 2.07 | 0.54 |
| 2:A:152:THR:HG22 | 2:A:159:PHE:CE1 | 2.43 | 0.54 |
| 2:B:136:THR:HG22 | 2:B:661:PHE:CD2 | 2.41 | 0.54 |
| 2:B:219:ASN:OD1 | 2:B:220:GLY:N | 2.41 | 0.54 |
| 2:A:388:LYS:HD3 | 2:A:389:ASP:N | 2.21 | 0.54 |
| 2:A:480:LYS:CE | 2:A:484:ARG:NH2 | 2.64 | 0.54 |
| 2:A:784:ARG:CZ | 2:A:809:LEU:HD23 | 2.37 | 0.54 |
| 2:B:432:LEU:HD13 | 2:B:437:ALA:O | 2.06 | 0.54 |
| 1:C:986:C:C5 | 2:A:181:HIS:NE2 | 2.72 | 0.54 |
| 2:A:27:ILE:H | 2:A:28:ARG:HH21 | 1.54 | 0.54 |
| 2:A:49:LEU:H | 2:A:49:LEU:CD1 | 2.13 | 0.54 |
| 2:A:75:LEU:HD12 | 2:A:76:PHE:N | 2.22 | 0.54 |
| 2:A:922:ASN:HD22 | 2:A:923:GLU:CA | 2.18 | 0.54 |
| 2:B:536:MET:N | 2:B:536:MET:SD | 2.81 | 0.54 |
| 2:B:728:TRP:O | 2:B:731:HIS:N | 2.38 | 0.54 |
| 2:B:753:VAL:HG23 | 2:B:797:PHE:CE1 | 2.42 | 0.54 |
| 2:A:67:LYS:HE2 | 2:A:70:GLN:NE2 | 2.23 | 0.54 |
| 2:A:282:VAL:HG12 | 2:A:283:ILE:N | 2.22 | 0.54 |
| 2:A:623:PHE:O | 2:A:626:VAL:HG22 | 2.08 | 0.54 |
| 2:A:964:ILE:HD12 | 2:A:965:PHE:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:173:LYS:HB3 | 2:B:175:TYR:CE2 | 2.43 | 0.54 |
| 2:B:298:ASN:HD22 | 2:B:299:PRO:HD2 | 1.71 | 0.54 |
| 2:B:730:LEU:HD22 | 2:B:827:TRP:CZ2 | 2.42 | 0.54 |
| 2:A:98:ASP:O | 2:A:102:ILE:HG23 | 2.07 | 0.54 |
| 2:A:343:THR:HG23 | 2:A:344:GLU:HG2 | 1.89 | 0.54 |
| 2:A:377:GLU:O | 2:A:378:GLU:HB2 | 2.07 | 0.54 |
| 2:A:734:ASN:OD1 | 2:A:823:PRO:CA | 2.56 | 0.54 |
| 2:B:206:ILE:O | 2:B:206:ILE:HG22 | 2.08 | 0.54 |
| 2:B:275:PHE:O | 2:B:277:ASP:N | 2.39 | 0.54 |
| 2:B:567:ILE:O | 2:B:568:PHE:CG | 2.60 | 0.54 |
| 2:B:729:MET:HG3 | 2:B:729:MET:O | 2.07 | 0.54 |
| 2:B:757:PHE:CD1 | 2:B:794:MET:SD | 2.99 | 0.54 |
| 1:D:914:A:H4' | 2:B:750:ARG:HH22 | 1.72 | 0.54 |
| 1:D:960:C:O2' | 1:D:961:C:OP2 | 2.16 | 0.54 |
| 2:A:51:VAL:HG23 | 2:A:52:GLY:N | 2.23 | 0.54 |
| 2:A:75:LEU:HD23 | 2:A:601:TRP:CG | 2.42 | 0.54 |
| 2:A:560:THR:HB | 2:A:561:PRO:CD | 2.38 | 0.54 |
| 2:A:724:ASP:HB2 | 2:A:929:GLU:OE2 | 2.07 | 0.54 |
| 2:B:48:HIS:HB2 | 2:B:109:TYR:HD1 | 1.73 | 0.54 |
| 2:B:50:HIS:ND1 | 2:B:52:GLY:N | 2.56 | 0.54 |
| 2:B:213:LYS:NZ | 2:B:213:LYS:HB3 | 2.21 | 0.54 |
| 2:B:226:PRO:HG3 | 2:B:263:TRP:CE3 | 2.43 | 0.54 |
| 2:B:343:THR:HG23 | 2:B:344:GLU:N | 2.21 | 0.54 |
| 2:B:413:PRO:CB | 2:B:414:PRO:HD3 | 2.33 | 0.54 |
| 2:A:67:LYS:CD | 2:A:70:GLN:HE21 | 2.18 | 0.54 |
| 2:B:45:LEU:HD13 | 2:B:130:MET:CB | 2.38 | 0.54 |
| 2:B:347:GLU:OE1 | 2:B:348:LYS:N | 2.39 | 0.54 |
| 2:B:467:ILE:HG13 | 2:B:508:CYS:CB | 2.37 | 0.54 |
| 2:B:475:LYS:HA | 2:B:623:PHE:HE1 | 1.72 | 0.54 |
| 2:A:388:LYS:HD3 | 2:A:389:ASP:HB2 | 1.89 | 0.54 |
| 2:A:860:ARG:NH2 | 2:A:862:TYR:N | 2.56 | 0.54 |
| 2:A:923:GLU:N | 2:A:923:GLU:CD | 2.61 | 0.54 |
| 2:B:51:VAL:HG23 | 2:B:659:LEU:HB3 | 1.89 | 0.54 |
| 2:B:188:VAL:HG23 | 2:B:189:VAL:N | 2.16 | 0.54 |
| 2:B:393:LEU:HD12 | 2:B:396:ALA:HB3 | 1.88 | 0.54 |
| 2:B:776:ASP:OD2 | 2:B:778:ALA:HB3 | 2.08 | 0.54 |
| 2:B:838:PHE:O | 2:B:842:VAL:HG23 | 2.07 | 0.54 |
| 1:C:955:G:OP1 | 2:A:961:LYS:NZ | 2.39 | 0.54 |
| 2:A:62:VAL:HG21 | 2:A:678:MET:CE | 2.38 | 0.54 |
| 2:A:150:PHE:HD1 | 2:A:151:TYR:O | 1.91 | 0.54 |
| 2:A:420:VAL:HG12 | 2:A:424:LYS:NZ | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:420:VAL:C | 2:A:422:GLU:H | 2.12 | 0.54 |
| 2:A:495:GLN:HG2 | 2:A:614:ILE:HG21 | 1.90 | 0.54 |
| 2:A:609:SER:O | 2:A:640:VAL:HA | 2.08 | 0.54 |
| 2:A:824:VAL:CG1 | 2:A:827:TRP:HE3 | 2.20 | 0.54 |
| 2:A:867:GLU:CD | 2:A:867:GLU:N | 2.58 | 0.54 |
| 2:B:243:VAL:HG12 | 2:B:321:VAL:HG12 | 1.90 | 0.54 |
| 1:C:985:A:H2' | 1:C:986:C:C4 | 2.43 | 0.53 |
| 2:A:15:LYS:NZ | 2:A:15:LYS:HB3 | 2.23 | 0.53 |
| 2:A:216:LEU:HB2 | 2:A:296:VAL:HG12 | 1.91 | 0.53 |
| 2:A:508:CYS:O | 2:A:509:ALA:HB2 | 2.07 | 0.53 |
| 2:A:953:LYS:HB3 | 2:A:953:LYS:HZ3 | 1.72 | 0.53 |
| 2:B:55:ARG:HD2 | 2:B:687:PHE:CE1 | 2.44 | 0.53 |
| 2:B:710:GLN:O | 2:B:712:ALA:N | 2.41 | 0.53 |
| 2:B:871:TRP:CD1 | 2:B:959:PRO:HB3 | 2.42 | 0.53 |
| 2:A:12:LYS:NZ | 2:A:16:ARG:NH1 | 2.55 | 0.53 |
| 2:A:193:LEU:HG | 2:A:197:ASP:HB2 | 1.90 | 0.53 |
| 2:B:616:ASN:HA | 2:B:620:PHE:CE1 | 2.44 | 0.53 |
| 2:B:725:ILE:HD13 | 2:B:770:ARG:HH21 | 1.72 | 0.53 |
| 2:B:733:LEU:CD1 | 2:B:789:VAL:HG11 | 2.28 | 0.53 |
| 2:A:233:GLU:HB3 | 2:A:423:VAL:CG2 | 2.36 | 0.53 |
| 2:A:263:TRP:CH2 | 2:A:438:GLU:OE1 | 2.62 | 0.53 |
| 2:A:555:ASP:OD2 | 2:A:558:LYS:HE2 | 2.09 | 0.53 |
| 2:A:730:LEU:O | 2:A:827:TRP:NE1 | 2.42 | 0.53 |
| 2:B:66:PHE:CG | 2:B:744:LEU:HD12 | 2.43 | 0.53 |
| 2:B:182:ARG:O | 2:B:183:VAL:HB | 2.07 | 0.53 |
| 2:B:235:VAL:HG23 | 2:B:236:TYR:N | 2.23 | 0.53 |
| 2:B:240:ASN:HA | 2:B:305:VAL:HB | 1.90 | 0.53 |
| 2:B:729:MET:HE2 | 2:B:729:MET:HA | 1.90 | 0.53 |
| 2:B:855:ILE:O | 2:B:856:GLU:HB2 | 2.07 | 0.53 |
| 2:A:39:THR:HG23 | 2:A:604:LEU:CD1 | 2.36 | 0.53 |
| 2:A:826:GLU:O | 2:A:828:TRP:N | 2.40 | 0.53 |
| 2:A:860:ARG:HB3 | 2:A:966:ILE:HA | 1.90 | 0.53 |
| 2:B:42:PHE:O | 2:B:42:PHE:HD1 | 1.91 | 0.53 |
| 2:B:166:GLN:NE2 | 2:B:534:ILE:HG12 | 2.23 | 0.53 |
| 2:B:475:LYS:O | 2:B:479:ARG:NH1 | 2.41 | 0.53 |
| 2:B:966:ILE:O | 2:B:967:GLU:CB | 2.57 | 0.53 |
| 2:A:242:TRP:CD1 | 2:A:310:ALA:HB2 | 2.44 | 0.53 |
| 2:A:336:LEU:O | 2:A:338:ASP:N | 2.42 | 0.53 |
| 2:A:459:LYS:HG2 | 2:A:460:ILE:N | 2.22 | 0.53 |
| 2:A:923:GLU:CD | 2:A:923:GLU:H | 2.11 | 0.53 |
| 2:B:461:ILE:CG2 | 2:B:464:GLN:HB2 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:256:ARG:NH1 | 2:A:278:ARG:HD3 | 2.24 | 0.53 |
| 2:A:733:LEU:HD11 | 2:A:789:VAL:CB | 2.38 | 0.53 |
| 2:A:884:LYS:NZ | 2:A:884:LYS:HB2 | 2.23 | 0.53 |
| 2:B:253:LYS:NZ | 2:B:283:ILE:HD11 | 2.23 | 0.53 |
| 2:B:340:LYS:HZ2 | 2:B:341:ARG:HH12 | 1.55 | 0.53 |
| 2:B:488:LEU:HA | 2:B:489:PRO:C | 2.29 | 0.53 |
| 2:B:681:ALA:N | 2:B:750:ARG:HG3 | 2.23 | 0.53 |
| 2:B:797:PHE:H | 2:B:797:PHE:HD2 | 1.56 | 0.53 |
| 2:B:39:THR:HG22 | 2:B:40:VAL:N | 2.23 | 0.53 |
| 2:B:79:ALA:HB2 | 2:B:539:TYR:HE2 | 1.73 | 0.53 |
| 2:B:336:LEU:O | 2:B:338:ASP:N | 2.42 | 0.53 |
| 2:B:620:PHE:N | 2:B:620:PHE:CD1 | 2.76 | 0.53 |
| 1:C:985:A:H2' | 1:C:986:C:C5 | 2.44 | 0.53 |
| 2:A:173:LYS:HD3 | 2:A:175:TYR:CE2 | 2.44 | 0.53 |
| 2:A:198:LEU:HD13 | 2:A:202:GLU:OE1 | 2.09 | 0.53 |
| 2:A:887:MET:HE2 | 2:A:891:MET:HG2 | 1.90 | 0.53 |
| 2:B:66:PHE:CE2 | 2:B:744:LEU:HB3 | 2.44 | 0.53 |
| 2:B:171:LYS:HD2 | 2:B:520:TRP:CZ3 | 2.44 | 0.53 |
| 2:B:384:ILE:HG22 | 2:B:385:LYS:N | 2.20 | 0.53 |
| 2:B:395:GLN:HG3 | 2:B:396:ALA:N | 2.24 | 0.53 |
| 2:B:860:ARG:NE | 2:B:942:ILE:HA | 2.20 | 0.53 |
| 2:B:884:LYS:O | 2:B:886:SER:N | 2.41 | 0.53 |
| 2:A:51:VAL:HG13 | 2:A:659:LEU:HB3 | 1.90 | 0.53 |
| 2:A:235:VAL:HA | 2:A:323:MET:CE | 2.38 | 0.53 |
| 2:A:676:TYR:HB2 | 2:A:697:LEU:HD23 | 1.91 | 0.53 |
| 2:A:751:THR:O | 2:A:752:ALA:C | 2.48 | 0.53 |
| 2:B:44:TYR:CD1 | 2:B:44:TYR:C | 2.82 | 0.53 |
| 2:B:751:THR:O | 2:B:752:ALA:C | 2.47 | 0.53 |
| 2:B:860:ARG:HA | 2:B:966:ILE:HA | 1.90 | 0.53 |
| 1:C:988:A:C5' | 2:A:528:SER:OG | 2.57 | 0.53 |
| 1:D:902:C:C2' | 1:D:903:G:H5'' | 2.38 | 0.53 |
| 2:A:150:PHE:CE2 | 2:A:538:TYR:HD2 | 2.27 | 0.53 |
| 2:B:54:ALA:HB1 | 2:B:661:PHE:CE1 | 2.44 | 0.53 |
| 2:A:17:TRP:CZ3 | 2:A:800:HIS:CD2 | 2.97 | 0.52 |
| 2:A:136:THR:CG2 | 2:A:662:ILE:HB | 2.39 | 0.52 |
| 2:B:687:PHE:C | 2:B:687:PHE:CD2 | 2.82 | 0.52 |
| 2:A:241:MET:HG3 | 2:A:296:VAL:HG21 | 1.90 | 0.52 |
| 2:A:528:SER:OG | 2:A:529:LEU:HD12 | 2.09 | 0.52 |
| 2:A:716:VAL:O | 2:A:716:VAL:HG12 | 2.09 | 0.52 |
| 2:A:766:TRP:CZ3 | 2:A:836:GLU:OE1 | 2.63 | 0.52 |
| 2:A:801:ILE:O | 2:A:805:LEU:HG | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:733:LEU:O | 2:B:737:ILE:HG13 | 2.09 | 0.52 |
| 2:B:761:MET:SD | 2:B:790:TRP:HH2 | 2.32 | 0.52 |
| 2:B:781:TYR:CZ | 2:B:785:THR:HG21 | 2.44 | 0.52 |
| 2:A:662:ILE:HG23 | 2:A:663:ASP:H | 1.74 | 0.52 |
| 2:A:826:GLU:OE2 | 2:A:826:GLU:N | 2.42 | 0.52 |
| 2:B:703:ARG:HD2 | 2:B:707:LEU:CD1 | 2.37 | 0.52 |
| 2:B:782:VAL:HG12 | 2:B:783:LEU:HD12 | 1.91 | 0.52 |
| 1:D:988:A:C8 | 2:B:529:LEU:HD21 | 2.44 | 0.52 |
| 2:A:188:VAL:CG2 | 2:A:189:VAL:H | 2.07 | 0.52 |
| 2:B:82:ILE:HG13 | 2:B:153:THR:HG23 | 1.91 | 0.52 |
| 2:B:83:THR:HG23 | 2:B:152:THR:HB | 1.91 | 0.52 |
| 2:B:297:ARG:NH2 | 2:B:297:ARG:CB | 2.72 | 0.52 |
| 2:B:420:VAL:C | 2:B:422:GLU:H | 2.12 | 0.52 |
| 2:B:486:LYS:H | 2:B:637:GLY:HA2 | 1.74 | 0.52 |
| 2:B:624:ASN:HD22 | 2:B:624:ASN:N | 2.08 | 0.52 |
| 2:B:625:HIS:CD2 | 2:B:635:PRO:HD3 | 2.44 | 0.52 |
| 2:B:720:VAL:HG12 | 2:B:777:GLU:HG2 | 1.91 | 0.52 |
| 2:A:292:ILE:HD13 | 2:A:307:ILE:HG22 | 1.91 | 0.52 |
| 2:A:482:LEU:CD1 | 2:A:500:ILE:HD11 | 2.38 | 0.52 |
| 2:B:223:ILE:HD11 | 2:B:264:ILE:HG13 | 1.92 | 0.52 |
| 2:B:661:PHE:CE2 | 2:B:665:ILE:HD11 | 2.44 | 0.52 |
| 2:B:722:LEU:H | 2:B:722:LEU:HD22 | 1.71 | 0.52 |
| 2:B:723:LYS:HG3 | 2:B:724:ASP:N | 2.24 | 0.52 |
| 2:A:14:GLN:O | 2:A:18:LEU:HB2 | 2.08 | 0.52 |
| 2:A:234:THR:O | 2:A:325:VAL:HG21 | 2.10 | 0.52 |
| 2:A:752:ALA:O | 2:A:755:TRP:N | 2.43 | 0.52 |
| 2:A:860:ARG:O | 2:A:860:ARG:CZ | 2.58 | 0.52 |
| 2:B:100:LYS:O | 2:B:104:ILE:HG13 | 2.10 | 0.52 |
| 2:B:356:VAL:HG21 | 2:B:411:LYS:HB2 | 1.91 | 0.52 |
| 2:B:764:LEU:O | 2:B:768:LEU:HG | 2.08 | 0.52 |
| 2:A:342:GLU:N | 2:A:342:GLU:OE2 | 2.41 | 0.52 |
| 2:A:355:ILE:HG22 | 2:A:356:VAL:N | 2.21 | 0.52 |
| 2:B:803:GLU:HG2 | 2:B:815:VAL:HG12 | 1.92 | 0.52 |
| 2:A:323:MET:HG3 | 2:A:323:MET:O | 2.08 | 0.52 |
| 2:B:671:ASP:OD1 | 2:B:799:PRO:HD2 | 2.10 | 0.52 |
| 2:B:826:GLU:O | 2:B:828:TRP:N | 2.42 | 0.52 |
| 2:A:37:TYR:HD2 | 2:A:38:ILE:H | 1.58 | 0.52 |
| 2:B:241:MET:HG3 | 2:B:296:VAL:HG21 | 1.91 | 0.52 |
| 2:B:345:ILE:CG1 | 2:B:346:LEU:N | 2.73 | 0.52 |
| 2:B:676:TYR:O | 2:B:679:SER:HB3 | 2.10 | 0.52 |
| 2:A:480:LYS:HG2 | 2:A:484:ARG:NH2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:GLU:CD | 2:B:147:SER:HB2 | 2.30 | 0.52 |
| 2:B:232:PRO:HD2 | 2:B:424:LYS:HG3 | 1.92 | 0.52 |
| 2:B:233:GLU:OE2 | 2:B:234:THR:N | 2.42 | 0.52 |
| 2:B:433:GLU:HA | 2:B:433:GLU:OE2 | 2.10 | 0.52 |
| 2:B:558:LYS:O | 2:B:584:THR:HG22 | 2.10 | 0.52 |
| 2:A:177:VAL:HG23 | 2:A:466:PHE:HB2 | 1.92 | 0.51 |
| 2:A:864:TYR:CG | 2:A:865:THR:N | 2.77 | 0.51 |
| 2:B:44:TYR:C | 2:B:44:TYR:HD1 | 2.14 | 0.51 |
| 2:B:266:SER:HB3 | 2:B:269:ALA:CB | 2.41 | 0.51 |
| 2:B:956:GLN:O | 2:B:956:GLN:HG2 | 2.09 | 0.51 |
| 2:A:44:TYR:OH | 2:A:87:ILE:HG12 | 2.09 | 0.51 |
| 2:A:326:PRO:HA | 2:A:332:ASP:CB | 2.40 | 0.51 |
| 2:A:373:PHE:HD1 | 2:A:374:PRO:HD3 | 1.68 | 0.51 |
| 2:A:486:LYS:H | 2:A:637:GLY:HA2 | 1.75 | 0.51 |
| 2:A:496:PHE:HE1 | 2:A:614:ILE:CG1 | 2.18 | 0.51 |
| 2:A:860:ARG:CZ | 2:A:861:ALA:HA | 2.39 | 0.51 |
| 2:B:35:LYS:HB2 | 2:B:601:TRP:HZ3 | 1.75 | 0.51 |
| 2:B:273:LEU:HA | 2:B:276:GLN:HG3 | 1.92 | 0.51 |
| 2:B:834:ALA:O | 2:B:837:GLU:OE2 | 2.29 | 0.51 |
| 2:B:915:THR:O | 2:B:916:PHE:HD2 | 1.93 | 0.51 |
| 2:A:36:PHE:O | 2:A:36:PHE:CD2 | 2.64 | 0.51 |
| 2:A:65:ARG:O | 2:A:68:ARG:N | 2.44 | 0.51 |
| 2:A:555:ASP:HB3 | 2:A:558:LYS:HG2 | 1.93 | 0.51 |
| 2:A:672:VAL:HG21 | 2:A:698:ARG:HG3 | 1.93 | 0.51 |
| 2:A:789:VAL:O | 2:A:790:TRP:C | 2.49 | 0.51 |
| 2:B:427:ILE:HG22 | 2:B:431:MET:SD | 2.50 | 0.51 |
| 2:B:679:SER:O | 2:B:750:ARG:HG2 | 2.10 | 0.51 |
| 2:B:863:ILE:HG22 | 2:B:953:LYS:HG2 | 1.92 | 0.51 |
| 2:A:102:ILE:HD12 | 2:A:102:ILE:C | 2.30 | 0.51 |
| 2:A:148:ARG:NH1 | 2:A:597:GLU:OE1 | 2.43 | 0.51 |
| 2:B:62:VAL:HG21 | 2:B:678:MET:CE | 2.39 | 0.51 |
| 2:B:235:VAL:HG23 | 2:B:236:TYR:H | 1.76 | 0.51 |
| 2:A:488:LEU:HD22 | 2:A:683:HIS:HE1 | 1.75 | 0.51 |
| 2:A:722:LEU:HD23 | 2:A:722:LEU:O | 2.10 | 0.51 |
| 2:B:789:VAL:O | 2:B:790:TRP:C | 2.49 | 0.51 |
| 2:B:913:GLU:O | 2:B:914:ARG:O | 2.29 | 0.51 |
| 2:B:946:PRO:HG2 | 2:B:953:LYS:HE2 | 1.92 | 0.51 |
| 2:A:53:HIS:O | 2:A:57:TYR:HD2 | 1.93 | 0.51 |
| 2:A:268:GLU:O | 2:A:271:TYR:HB3 | 2.11 | 0.51 |
| 2:A:306:ILE:CG1 | 2:A:307:ILE:N | 2.74 | 0.51 |
| 2:A:423:VAL:C | 2:A:425:GLU:N | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:630:ARG:O | 2:A:632:GLU:N | 2.38 | 0.51 |
| 2:B:44:TYR:OH | 2:B:86:PRO:HD2 | 2.11 | 0.51 |
| 2:B:67:LYS:HE3 | 2:B:72:TYR:CE1 | 2.45 | 0.51 |
| 2:B:297:ARG:CB | 2:B:297:ARG:HH21 | 2.24 | 0.51 |
| 2:B:391:GLU:HG3 | 2:B:394:GLU:HB2 | 1.93 | 0.51 |
| 2:B:678:MET:CE | 2:B:749:THR:HG21 | 2.40 | 0.51 |
| 2:B:717:LYS:O | 2:B:717:LYS:HD3 | 2.11 | 0.51 |
| 2:A:480:LYS:HA | 2:A:483:GLU:OE1 | 2.11 | 0.51 |
| 2:A:803:GLU:OE1 | 2:A:815:VAL:HG23 | 2.11 | 0.51 |
| 2:B:547:LYS:O | 2:B:550:GLN:HB3 | 2.10 | 0.51 |
| 2:B:636:LYS:HB3 | 2:B:636:LYS:NZ | 2.25 | 0.51 |
| 2:B:870:LYS:O | 2:B:872:LYS:N | 2.43 | 0.51 |
| 1:C:916:C:O2' | 1:C:972:U:H1' | 2.10 | 0.51 |
| 1:D:961:C:O2 | 1:D:961:C:H2' | 2.10 | 0.51 |
| 2:A:51:VAL:O | 2:A:54:ALA:CB | 2.56 | 0.51 |
| 2:A:268:GLU:H | 2:A:268:GLU:CD | 2.12 | 0.51 |
| 2:A:860:ARG:CZ | 2:A:861:ALA:CA | 2.89 | 0.51 |
| 2:A:913:GLU:O | 2:A:914:ARG:O | 2.29 | 0.51 |
| 2:B:45:LEU:HD13 | 2:B:130:MET:HA | 1.92 | 0.51 |
| 2:B:793:LEU:HD23 | 2:B:821:PRO:HG3 | 1.93 | 0.51 |
| 1:C:949:C:C2 | 1:C:957:G:N2 | 2.79 | 0.51 |
| 2:A:93:ARG:HG3 | 2:A:93:ARG:HH11 | 1.74 | 0.51 |
| 2:A:95:LYS:O | 2:A:97:ARG:N | 2.44 | 0.51 |
| 2:A:112:PRO:CG | 2:A:115:ILE:HD12 | 2.41 | 0.51 |
| 2:A:168:TRP:NE1 | 2:A:519:PRO:HB2 | 2.25 | 0.51 |
| 2:A:239:THR:HG21 | 2:A:326:PRO:HD2 | 1.92 | 0.51 |
| 2:A:690:ARG:HH11 | 2:A:693:GLU:CG | 2.20 | 0.51 |
| 2:A:838:PHE:HE2 | 2:A:922:ASN:ND2 | 2.09 | 0.51 |
| 2:B:630:ARG:O | 2:B:632:GLU:N | 2.41 | 0.51 |
| 2:B:742:ASN:O | 2:B:743:ALA:C | 2.49 | 0.51 |
| 2:A:819:LYS:H | 2:A:819:LYS:CD | 2.24 | 0.51 |
| 2:A:871:TRP:NE1 | 2:A:959:PRO:HB3 | 2.26 | 0.51 |
| 2:A:873:VAL:CG1 | 2:A:906:ILE:HG12 | 2.40 | 0.51 |
| 2:B:200:GLU:HG2 | 2:B:201:GLY:N | 2.26 | 0.51 |
| 2:B:860:ARG:CB | 2:B:966:ILE:HA | 2.41 | 0.51 |
| 1:D:902:C:H2' | 1:D:903:G:H5'' | 1.92 | 0.50 |
| 2:A:332:ASP:O | 2:A:333:HIS:HB2 | 2.11 | 0.50 |
| 2:A:490:GLU:OE1 | 2:A:493:ARG:HB2 | 2.11 | 0.50 |
| 2:A:751:THR:O | 2:A:754:GLN:N | 2.43 | 0.50 |
| 2:A:919:LYS:HD2 | 2:A:960:LEU:HD13 | 1.93 | 0.50 |
| 2:B:915:THR:OG1 | 2:B:916:PHE:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:217:ARG:HH21 | 2:A:222:VAL:CG1 | 2.24 | 0.50 |
| 2:A:269:ALA:O | 2:A:273:LEU:HD12 | 2.10 | 0.50 |
| 2:A:880:LYS:HG3 | 2:A:886:SER:HA | 1.92 | 0.50 |
| 2:A:950:LYS:H | 2:A:953:LYS:NZ | 2.10 | 0.50 |
| 2:B:51:VAL:CG2 | 2:B:659:LEU:HB3 | 2.41 | 0.50 |
| 2:B:160:SER:O | 2:B:164:GLU:HG3 | 2.11 | 0.50 |
| 2:B:743:ALA:HB2 | 2:B:751:THR:CG2 | 2.41 | 0.50 |
| 2:A:135:GLU:O | 2:A:138:ILE:HG22 | 2.11 | 0.50 |
| 2:A:676:TYR:HA | 2:A:697:LEU:CD2 | 2.41 | 0.50 |
| 2:A:793:LEU:HD23 | 2:A:821:PRO:CG | 2.41 | 0.50 |
| 2:B:51:VAL:CG2 | 2:B:659:LEU:HD23 | 2.40 | 0.50 |
| 2:B:51:VAL:HG21 | 2:B:659:LEU:HD23 | 1.92 | 0.50 |
| 2:B:148:ARG:HB3 | 2:B:542:SER:HB3 | 1.93 | 0.50 |
| 2:B:210:ILE:C | 2:B:210:ILE:HD12 | 2.31 | 0.50 |
| 2:B:540:THR:HG21 | 2:B:598:PHE:HD1 | 1.76 | 0.50 |
| 2:B:730:LEU:HB3 | 2:B:827:TRP:CD1 | 2.46 | 0.50 |
| 1:C:941:A:O3' | 2:A:699:LYS:NZ | 2.32 | 0.50 |
| 2:A:41:ALA:HA | 2:A:607:ARG:HH22 | 1.75 | 0.50 |
| 2:A:172:GLU:OE1 | 2:A:172:GLU:N | 2.45 | 0.50 |
| 2:A:240:ASN:O | 2:A:324:SER:HB3 | 2.11 | 0.50 |
| 2:A:275:PHE:O | 2:A:277:ASP:N | 2.39 | 0.50 |
| 2:A:871:TRP:CD2 | 2:A:920:ARG:NH2 | 2.78 | 0.50 |
| 2:A:884:LYS:HG3 | 2:A:888:GLU:HG3 | 1.93 | 0.50 |
| 2:B:94:ILE:HD11 | 2:B:120:GLU:N | 2.27 | 0.50 |
| 2:B:242:TRP:HH2 | 2:B:332:ASP:HA | 1.75 | 0.50 |
| 2:B:395:GLN:O | 2:B:399:THR:HG23 | 2.10 | 0.50 |
| 2:B:910:LEU:C | 2:B:910:LEU:HD13 | 2.32 | 0.50 |
| 2:A:235:VAL:HG23 | 2:A:236:TYR:N | 2.26 | 0.50 |
| 2:A:354:ARG:HE | 2:A:375:ALA:C | 2.13 | 0.50 |
| 2:A:381:LYS:NZ | 2:A:381:LYS:C | 2.64 | 0.50 |
| 2:B:495:GLN:HG2 | 2:B:614:ILE:HG21 | 1.92 | 0.50 |
| 2:B:782:VAL:HG12 | 2:B:783:LEU:N | 2.26 | 0.50 |
| 2:A:61:ASP:OD1 | 2:A:143:SER:N | 2.25 | 0.50 |
| 2:A:72:TYR:O | 2:A:74:VAL:HG23 | 2.11 | 0.50 |
| 2:A:413:PRO:CB | 2:A:414:PRO:HD3 | 2.42 | 0.50 |
| 2:B:244:ASN:HB2 | 2:B:313:VAL:HG23 | 1.94 | 0.50 |
| 2:B:327:ALA:HB2 | 2:B:353:PRO:O | 2.12 | 0.50 |
| 2:A:98:ASP:OD2 | 2:A:99:PRO:HD2 | 2.11 | 0.50 |
| 2:A:231:ARG:HB3 | 2:A:233:GLU:CD | 2.32 | 0.50 |
| 2:A:235:VAL:HG11 | 2:A:431:MET:CE | 2.42 | 0.50 |
| 2:A:389:ASP:O | 2:A:390:LYS:HD3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:781:TYR:O | 2:A:785:THR:HG23 | 2.12 | 0.50 |
| 2:A:817:LEU:N | 2:A:817:LEU:HD23 | 2.27 | 0.50 |
| 2:A:862:TYR:OH | 2:A:926:ALA:HB1 | 2.11 | 0.50 |
| 2:A:863:ILE:CB | 2:A:953:LYS:HD3 | 2.41 | 0.50 |
| 2:B:196:HIS:CD2 | 2:B:197:ASP:H | 2.30 | 0.50 |
| 2:B:482:LEU:HD11 | 2:B:496:PHE:HB3 | 1.94 | 0.50 |
| 2:B:587:PRO:HB2 | 2:B:590:ILE:CG1 | 2.35 | 0.50 |
| 2:A:235:VAL:HG23 | 2:A:236:TYR:H | 1.76 | 0.50 |
| 2:A:300:VAL:HG13 | 2:A:301:SER:N | 2.27 | 0.50 |
| 2:A:425:GLU:O | 2:A:429:LYS:HD3 | 2.11 | 0.50 |
| 2:A:569:LEU:N | 2:A:569:LEU:HD12 | 2.26 | 0.50 |
| 2:A:860:ARG:HA | 2:A:966:ILE:HA | 1.93 | 0.50 |
| 2:A:931:LYS:HE2 | 2:A:942:ILE:HG22 | 1.92 | 0.50 |
| 2:A:947:THR:HG23 | 2:A:948:GLU:H | 1.77 | 0.50 |
| 1:C:909:U:H5'' | 1:C:910:G:OP2 | 2.12 | 0.50 |
| 2:A:232:PRO:HD2 | 2:A:424:LYS:HG3 | 1.93 | 0.50 |
| 2:A:252:ALA:HB2 | 2:A:282:VAL:HA | 1.94 | 0.50 |
| 2:A:292:ILE:HG13 | 2:A:309:PRO:HB3 | 1.94 | 0.50 |
| 2:A:382:LEU:C | 2:A:384:ILE:H | 2.15 | 0.50 |
| 2:A:474:TRP:NE1 | 2:A:627:ALA:HB2 | 2.27 | 0.50 |
| 2:A:855:ILE:HG23 | 2:A:855:ILE:O | 2.10 | 0.50 |
| 2:B:866:ALA:HB3 | 2:B:869:TRP:CD1 | 2.47 | 0.50 |
| 1:C:916:C:C5' | 1:C:917:C:C5 | 2.86 | 0.49 |
| 2:A:79:ALA:HB2 | 2:A:539:TYR:HE2 | 1.76 | 0.49 |
| 2:A:85:SER:H | 2:A:86:PRO:HD3 | 1.78 | 0.49 |
| 2:A:393:LEU:C | 2:A:395:GLN:H | 2.15 | 0.49 |
| 2:A:568:PHE:HD1 | 2:A:598:PHE:CE2 | 2.30 | 0.49 |
| 2:B:49:LEU:HA | 2:B:53:HIS:HD2 | 1.77 | 0.49 |
| 2:B:268:GLU:OE2 | 2:B:315:PRO:HB2 | 2.11 | 0.49 |
| 2:B:330:PRO:CD | 2:B:400:ILE:HG12 | 2.42 | 0.49 |
| 2:B:871:TRP:CE3 | 2:B:920:ARG:NH1 | 2.80 | 0.49 |
| 2:B:921:ILE:HD12 | 2:B:928:ARG:NH2 | 2.27 | 0.49 |
| 2:A:45:LEU:HD13 | 2:A:130:MET:HB2 | 1.94 | 0.49 |
| 2:A:142:PHE:O | 2:A:144:VAL:N | 2.45 | 0.49 |
| 2:A:870:LYS:O | 2:A:872:LYS:N | 2.44 | 0.49 |
| 2:A:924:GLU:OE1 | 2:A:927:LEU:HD22 | 2.13 | 0.49 |
| 2:B:175:TYR:CE1 | 2:B:474:TRP:HB2 | 2.47 | 0.49 |
| 2:B:185:TRP:CD1 | 2:B:186:ASP:N | 2.81 | 0.49 |
| 2:B:587:PRO:O | 2:B:591:ILE:HG12 | 2.12 | 0.49 |
| 2:B:966:ILE:O | 2:B:966:ILE:HG13 | 2.12 | 0.49 |
| 2:A:41:ALA:HB2 | 2:A:607:ARG:HH21 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:111:VAL:HG22 | 2:A:128:TYR:CE2 | 2.31 | 0.49 |
| 2:A:697:LEU:O | 2:A:701:ILE:HG12 | 2.12 | 0.49 |
| 2:A:878:SER:CB | 2:A:915:THR:HG22 | 2.42 | 0.49 |
| 2:B:196:HIS:HD2 | 2:B:197:ASP:H | 1.58 | 0.49 |
| 2:B:282:VAL:CG1 | 2:B:283:ILE:N | 2.72 | 0.49 |
| 2:B:662:ILE:HG23 | 2:B:663:ASP:N | 2.25 | 0.49 |
| 2:A:616:ASN:HB2 | 2:A:620:PHE:CE2 | 2.47 | 0.49 |
| 2:A:717:LYS:HD2 | 2:A:777:GLU:OE2 | 2.12 | 0.49 |
| 2:A:894:SER:C | 2:A:896:ILE:N | 2.65 | 0.49 |
| 2:B:42:PHE:O | 2:B:42:PHE:CD1 | 2.65 | 0.49 |
| 2:B:95:LYS:O | 2:B:97:ARG:N | 2.45 | 0.49 |
| 2:B:297:ARG:HB3 | 2:B:297:ARG:CZ | 2.41 | 0.49 |
| 2:B:354:ARG:HD2 | 2:B:376:VAL:HG12 | 1.95 | 0.49 |
| 2:B:455:ARG:HG2 | 2:B:455:ARG:HH11 | 1.78 | 0.49 |
| 2:B:746:GLU:OE1 | 2:B:748:ARG:HD2 | 2.13 | 0.49 |
| 2:B:846:ILE:HD12 | 2:B:938:LEU:HD21 | 1.94 | 0.49 |
| 2:B:907:VAL:O | 2:B:910:LEU:HB3 | 2.12 | 0.49 |
| 1:C:958:U:H6 | 1:C:958:U:H3' | 1.78 | 0.49 |
| 2:A:467:ILE:HG21 | 2:A:469:TYR:CZ | 2.47 | 0.49 |
| 2:A:691:ARG:HH11 | 2:A:691:ARG:CG | 2.26 | 0.49 |
| 2:B:185:TRP:HZ2 | 2:B:190:GLY:HA2 | 1.75 | 0.49 |
| 2:B:273:LEU:HB3 | 2:B:280:ILE:HD11 | 1.94 | 0.49 |
| 2:B:423:VAL:C | 2:B:425:GLU:N | 2.66 | 0.49 |
| 2:A:218:GLU:HG3 | 2:A:219:ASN:N | 2.28 | 0.49 |
| 2:B:79:ALA:O | 2:B:80:TRP:CE3 | 2.65 | 0.49 |
| 2:B:488:LEU:HD12 | 2:B:606:TRP:CZ3 | 2.46 | 0.49 |
| 2:B:724:ASP:HB2 | 2:B:929:GLU:OE2 | 2.11 | 0.49 |
| 2:B:741:THR:HA | 2:B:820:TRP:CH2 | 2.47 | 0.49 |
| 2:A:66:PHE:CZ | 2:A:70:GLN:OE1 | 2.66 | 0.49 |
| 2:A:214:PHE:CE2 | 2:A:298:ASN:HA | 2.48 | 0.49 |
| 2:A:240:ASN:HA | 2:A:305:VAL:HB | 1.93 | 0.49 |
| 2:A:730:LEU:HD22 | 2:A:827:TRP:HZ2 | 1.78 | 0.49 |
| 2:A:947:THR:CG2 | 2:A:948:GLU:N | 2.75 | 0.49 |
| 2:B:298:ASN:HD22 | 2:B:299:PRO:CD | 2.25 | 0.49 |
| 2:B:889:GLU:HG3 | 2:B:889:GLU:O | 2.11 | 0.49 |
| 1:C:910:G:C6 | 1:C:911:C:N4 | 2.81 | 0.49 |
| 1:C:941:A:H2' | 1:C:942:U:C6 | 2.48 | 0.49 |
| 2:A:184:ARG:NH1 | 2:A:195:ASP:OD2 | 2.46 | 0.49 |
| 2:A:184:ARG:NH2 | 2:A:202:GLU:O | 2.45 | 0.49 |
| 2:A:691:ARG:NH1 | 2:A:691:ARG:HG2 | 2.26 | 0.49 |
| 2:A:871:TRP:CZ3 | 2:A:918:VAL:HA | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:22:ILE:CG1 | 2:B:817:LEU:HD21 | 2.42 | 0.49 |
| 2:B:151:TYR:CE1 | 2:B:156:PHE:HD1 | 2.30 | 0.49 |
| 2:B:163:ILE:O | 2:B:166:GLN:HB3 | 2.13 | 0.49 |
| 2:B:393:LEU:C | 2:B:395:GLN:H | 2.16 | 0.49 |
| 2:B:474:TRP:CZ2 | 2:B:623:PHE:HB3 | 2.47 | 0.49 |
| 1:D:935:C:H5' | 1:D:936:U:H5'' | 1.95 | 0.49 |
| 2:A:227:ALA:CA | 2:A:321:VAL:HG23 | 2.31 | 0.49 |
| 2:A:826:GLU:N | 2:A:826:GLU:CD | 2.63 | 0.49 |
| 2:B:172:GLU:OE1 | 2:B:172:GLU:N | 2.46 | 0.49 |
| 2:B:212:ILE:HD13 | 2:B:431:MET:HE1 | 1.94 | 0.49 |
| 2:B:213:LYS:HB3 | 2:B:213:LYS:HZ2 | 1.77 | 0.49 |
| 2:B:540:THR:HG21 | 2:B:598:PHE:HB2 | 1.93 | 0.49 |
| 2:B:751:THR:O | 2:B:754:GLN:N | 2.45 | 0.49 |
| 2:B:860:ARG:HH22 | 2:B:861:ALA:C | 2.16 | 0.49 |
| 2:B:922:ASN:O | 2:B:925:LYS:N | 2.44 | 0.49 |
| 2:A:196:HIS:CD2 | 2:A:197:ASP:N | 2.81 | 0.49 |
| 2:A:237:GLY:C | 2:A:325:VAL:HG22 | 2.33 | 0.49 |
| 2:A:311:GLU:HG2 | 2:A:389:ASP:OD2 | 2.12 | 0.49 |
| 2:A:840:ARG:O | 2:A:843:MET:HB2 | 2.12 | 0.49 |
| 2:B:37:TYR:HD2 | 2:B:38:ILE:H | 1.60 | 0.49 |
| 2:B:45:LEU:HD13 | 2:B:130:MET:HB2 | 1.95 | 0.49 |
| 2:B:760:ILE:HD12 | 2:B:790:TRP:CD1 | 2.48 | 0.49 |
| 2:B:868:ASP:O | 2:B:869:TRP:C | 2.52 | 0.49 |
| 2:A:355:ILE:HD12 | 2:A:412:VAL:CG1 | 2.43 | 0.48 |
| 2:A:570:GLU:O | 2:A:595:LYS:HE2 | 2.13 | 0.48 |
| 2:A:782:VAL:HG12 | 2:A:783:LEU:N | 2.28 | 0.48 |
| 2:A:836:GLU:HA | 2:A:839:ILE:HD11 | 1.94 | 0.48 |
| 2:B:65:ARG:O | 2:B:68:ARG:N | 2.46 | 0.48 |
| 2:B:166:GLN:CG | 2:B:534:ILE:HD11 | 2.43 | 0.48 |
| 2:B:256:ARG:CZ | 2:B:277:ASP:OD2 | 2.61 | 0.48 |
| 2:B:676:TYR:CZ | 2:B:680:LEU:HD11 | 2.48 | 0.48 |
| 2:B:728:TRP:C | 2:B:730:LEU:N | 2.67 | 0.48 |
| 2:B:834:ALA:O | 2:B:837:GLU:CD | 2.52 | 0.48 |
| 1:D:953:A:O2' | 2:B:849:ILE:HG23 | 2.12 | 0.48 |
| 2:A:65:ARG:HG2 | 2:A:143:SER:OG | 2.13 | 0.48 |
| 2:A:165:TRP:CD1 | 2:A:561:PRO:HA | 2.44 | 0.48 |
| 2:A:880:LYS:HG3 | 2:A:886:SER:HB3 | 1.95 | 0.48 |
| 2:A:933:PHE:HD1 | 2:A:933:PHE:O | 1.95 | 0.48 |
| 2:B:67:LYS:HD2 | 2:B:70:GLN:NE2 | 2.28 | 0.48 |
| 2:B:282:VAL:CG1 | 2:B:283:ILE:H | 2.25 | 0.48 |
| 2:B:375:ALA:O | 2:B:377:GLU:N | 2.40 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:389:ASP:C | 2:B:390:LYS:HD3 | 2.33 | 0.48 |
| 2:A:126:VAL:CG1 | 2:A:126:VAL:O | 2.60 | 0.48 |
| 2:A:242:TRP:HZ3 | 2:A:332:ASP:CG | 2.17 | 0.48 |
| 2:A:289:GLU:O | 2:A:292:ILE:HB | 2.13 | 0.48 |
| 2:A:388:LYS:CD | 2:A:389:ASP:HB2 | 2.42 | 0.48 |
| 2:A:467:ILE:HG13 | 2:A:508:CYS:CB | 2.43 | 0.48 |
| 2:A:488:LEU:CD1 | 2:A:606:TRP:CH2 | 2.92 | 0.48 |
| 2:A:931:LYS:HE2 | 2:A:942:ILE:O | 2.13 | 0.48 |
| 2:B:35:LYS:HD2 | 2:B:35:LYS:C | 2.34 | 0.48 |
| 2:B:275:PHE:C | 2:B:277:ASP:H | 2.17 | 0.48 |
| 2:B:382:LEU:C | 2:B:384:ILE:H | 2.16 | 0.48 |
| 2:B:496:PHE:CE1 | 2:B:614:ILE:HG23 | 2.49 | 0.48 |
| 2:B:614:ILE:N | 2:B:615:PRO:CD | 2.75 | 0.48 |
| 2:B:741:THR:O | 2:B:745:GLU:HG2 | 2.13 | 0.48 |
| 1:C:954:G:N2 | 2:A:961:LYS:HG3 | 2.29 | 0.48 |
| 2:A:42:PHE:CD1 | 2:A:42:PHE:O | 2.66 | 0.48 |
| 2:A:170:LEU:O | 2:A:176:ILE:HG12 | 2.13 | 0.48 |
| 2:A:227:ALA:HA | 2:A:321:VAL:O | 2.12 | 0.48 |
| 2:A:256:ARG:HG3 | 2:A:257:LYS:H | 1.78 | 0.48 |
| 2:A:501:ASP:O | 2:A:503:LEU:N | 2.39 | 0.48 |
| 2:A:725:ILE:CD1 | 2:A:770:ARG:HE | 2.26 | 0.48 |
| 2:A:784:ARG:HH22 | 2:A:810:GLY:N | 2.11 | 0.48 |
| 2:A:871:TRP:C | 2:A:875:GLU:OE2 | 2.52 | 0.48 |
| 2:B:42:PHE:CD1 | 2:B:81:HIS:HB2 | 2.49 | 0.48 |
| 2:B:79:ALA:N | 2:B:539:TYR:OH | 2.46 | 0.48 |
| 2:B:256:ARG:HG3 | 2:B:257:LYS:N | 2.28 | 0.48 |
| 2:B:340:LYS:HB3 | 2:B:341:ARG:HH11 | 1.77 | 0.48 |
| 2:B:351:ILE:H | 2:B:351:ILE:CD1 | 2.16 | 0.48 |
| 2:B:429:LYS:O | 2:B:433:GLU:CG | 2.52 | 0.48 |
| 2:B:505:LYS:H | 2:B:505:LYS:HD2 | 1.78 | 0.48 |
| 2:B:601:TRP:HA | 2:B:601:TRP:CE3 | 2.48 | 0.48 |
| 2:B:677:ILE:HG22 | 2:B:678:MET:N | 2.28 | 0.48 |
| 2:B:775:ASP:C | 2:B:775:ASP:OD1 | 2.51 | 0.48 |
| 1:C:916:C:H2' | 1:C:972:U:O3' | 2.12 | 0.48 |
| 2:A:631:GLU:C | 2:A:633:HIS:H | 2.16 | 0.48 |
| 2:A:725:ILE:HD13 | 2:A:770:ARG:HE | 1.78 | 0.48 |
| 2:A:742:ASN:O | 2:A:743:ALA:C | 2.51 | 0.48 |
| 2:A:855:ILE:HG13 | 2:A:856:GLU:HG2 | 1.95 | 0.48 |
| 2:A:964:ILE:HD11 | 2:A:966:ILE:HG23 | 1.96 | 0.48 |
| 2:B:37:TYR:CD2 | 2:B:38:ILE:N | 2.82 | 0.48 |
| 2:B:327:ALA:HB1 | 2:B:354:ARG:CB | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:500:ILE:HG23 | 2:B:623:PHE:CZ | 2.49 | 0.48 |
| 2:B:501:ASP:O | 2:B:503:LEU:N | 2.41 | 0.48 |
| 2:B:752:ALA:O | 2:B:755:TRP:N | 2.46 | 0.48 |
| 2:B:894:SER:C | 2:B:896:ILE:N | 2.66 | 0.48 |
| 1:D:917:C:H6 | 1:D:917:C:O5' | 1.96 | 0.48 |
| 2:A:41:ALA:CA | 2:A:607:ARG:NH2 | 2.77 | 0.48 |
| 2:A:162:PHE:HA | 2:A:564:PHE:CE2 | 2.49 | 0.48 |
| 2:A:198:LEU:HD22 | 2:A:202:GLU:CA | 2.43 | 0.48 |
| 2:A:705:TYR:CD2 | 2:A:805:LEU:HD11 | 2.48 | 0.48 |
| 2:B:126:VAL:CG1 | 2:B:126:VAL:O | 2.61 | 0.48 |
| 2:B:354:ARG:HD2 | 2:B:376:VAL:CG1 | 2.42 | 0.48 |
| 2:B:377:GLU:O | 2:B:378:GLU:HB2 | 2.13 | 0.48 |
| 2:B:464:GLN:NE2 | 2:B:507:ALA:HB1 | 2.28 | 0.48 |
| 2:B:732:ARG:HB3 | 2:B:732:ARG:HH11 | 1.77 | 0.48 |
| 2:A:449:ILE:N | 2:A:449:ILE:CD1 | 2.75 | 0.48 |
| 2:A:892:LYS:O | 2:A:892:LYS:HG2 | 2.13 | 0.48 |
| 2:B:471:ASN:ND2 | 2:B:471:ASN:C | 2.66 | 0.48 |
| 1:C:920:G:H1' | 1:C:969:G:H21 | 1.78 | 0.48 |
| 1:D:958:U:O5' | 1:D:958:U:H6 | 1.97 | 0.48 |
| 2:A:860:ARG:C | 2:A:860:ARG:CZ | 2.82 | 0.48 |
| 2:A:868:ASP:O | 2:A:869:TRP:C | 2.52 | 0.48 |
| 2:B:48:HIS:HB2 | 2:B:109:TYR:CD1 | 2.48 | 0.48 |
| 2:B:171:LYS:CG | 2:B:176:ILE:HD12 | 2.42 | 0.48 |
| 2:B:345:ILE:O | 2:B:346:LEU:HB2 | 2.13 | 0.48 |
| 2:B:356:VAL:HB | 2:B:409:ILE:O | 2.14 | 0.48 |
| 2:B:423:VAL:HA | 2:B:426:ALA:HB3 | 1.95 | 0.48 |
| 2:B:623:PHE:O | 2:B:624:ASN:C | 2.52 | 0.48 |
| 1:C:941:A:H4' | 2:A:699:LYS:NZ | 2.29 | 0.48 |
| 1:D:970:A:O2' | 1:D:971:A:O5' | 2.32 | 0.48 |
| 2:A:792:ARG:HH21 | 2:A:792:ARG:CG | 2.15 | 0.48 |
| 2:A:860:ARG:NH2 | 2:A:861:ALA:C | 2.67 | 0.48 |
| 2:B:53:HIS:O | 2:B:57:TYR:CD2 | 2.67 | 0.48 |
| 2:B:112:PRO:O | 2:B:113:GLU:C | 2.52 | 0.48 |
| 2:B:198:LEU:HD23 | 2:B:448:VAL:HG13 | 1.95 | 0.48 |
| 2:B:420:VAL:HG12 | 2:B:424:LYS:NZ | 2.28 | 0.48 |
| 2:B:560:THR:HB | 2:B:561:PRO:HD2 | 1.95 | 0.48 |
| 2:B:732:ARG:HB3 | 2:B:732:ARG:NH1 | 2.29 | 0.48 |
| 2:B:894:SER:O | 2:B:896:ILE:N | 2.47 | 0.48 |
| 2:A:953:LYS:NZ | 2:A:953:LYS:CB | 2.76 | 0.48 |
| 2:A:956:GLN:O | 2:A:956:GLN:HG2 | 2.14 | 0.48 |
| 2:B:710:GLN:O | 2:B:713:GLU:HG2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:55:ARG:O | 2:A:59:ILE:HG13 | 2.14 | 0.47 |
| 2:A:188:VAL:HG23 | 2:A:190:GLY:H | 1.79 | 0.47 |
| 2:A:419:PRO:O | 2:A:422:GLU:HB2 | 2.14 | 0.47 |
| 2:A:846:ILE:O | 2:A:850:ILE:HG13 | 2.14 | 0.47 |
| 2:A:877:VAL:C | 2:A:879:GLU:H | 2.16 | 0.47 |
| 2:B:276:GLN:O | 2:B:277:ASP:HB3 | 2.14 | 0.47 |
| 2:B:568:PHE:C | 2:B:569:LEU:HD12 | 2.34 | 0.47 |
| 2:B:793:LEU:HD23 | 2:B:821:PRO:CG | 2.44 | 0.47 |
| 1:C:958:U:H3' | 1:C:958:U:C6 | 2.49 | 0.47 |
| 1:D:984:C:H6 | 1:D:984:C:H5' | 1.79 | 0.47 |
| 2:A:279:GLU:OE1 | 2:A:281:GLU:OE1 | 2.32 | 0.47 |
| 2:A:671:ASP:OD1 | 2:A:799:PRO:HD2 | 2.13 | 0.47 |
| 2:A:717:LYS:HD2 | 2:A:718:GLY:O | 2.14 | 0.47 |
| 2:A:770:ARG:CD | 2:A:933:PHE:HE2 | 2.19 | 0.47 |
| 2:A:827:TRP:O | 2:A:827:TRP:HD1 | 1.95 | 0.47 |
| 2:B:233:GLU:HA | 2:B:427:ILE:CD1 | 2.33 | 0.47 |
| 2:B:646:LEU:HD12 | 2:B:689:TRP:HB3 | 1.96 | 0.47 |
| 2:B:704:PHE:HE1 | 2:B:790:TRP:CD2 | 2.31 | 0.47 |
| 1:C:986:C:H5 | 2:A:181:HIS:HE2 | 1.56 | 0.47 |
| 2:A:42:PHE:CE1 | 2:A:81:HIS:HB2 | 2.48 | 0.47 |
| 2:A:112:PRO:O | 2:A:113:GLU:C | 2.53 | 0.47 |
| 2:A:375:ALA:O | 2:A:377:GLU:N | 2.40 | 0.47 |
| 2:A:714:TYR:HD1 | 2:A:780:ARG:CG | 2.27 | 0.47 |
| 2:A:746:GLU:O | 2:A:748:ARG:HG3 | 2.14 | 0.47 |
| 2:A:767:TYR:CE2 | 2:A:782:VAL:HG11 | 2.49 | 0.47 |
| 2:A:854:LYS:HE2 | 2:A:967:GLU:CD | 2.34 | 0.47 |
| 2:B:68:ARG:HB2 | 2:B:74:VAL:HG11 | 1.96 | 0.47 |
| 2:B:340:LYS:CB | 2:B:341:ARG:HH11 | 2.28 | 0.47 |
| 2:B:701:ILE:O | 2:B:704:PHE:HB3 | 2.13 | 0.47 |
| 1:C:922:C:H4' | 1:C:923:A:C5' | 2.44 | 0.47 |
| 2:A:37:TYR:HD2 | 2:A:38:ILE:N | 2.12 | 0.47 |
| 2:A:53:HIS:O | 2:A:57:TYR:CD2 | 2.67 | 0.47 |
| 2:A:145:ASP:OD1 | 2:A:145:ASP:O | 2.32 | 0.47 |
| 2:A:238:VAL:HA | 2:A:325:VAL:HG22 | 1.96 | 0.47 |
| 2:A:568:PHE:HB2 | 2:A:569:LEU:HD12 | 1.96 | 0.47 |
| 2:A:695:GLY:O | 2:A:698:ARG:HB3 | 2.15 | 0.47 |
| 2:B:326:PRO:HA | 2:B:332:ASP:CB | 2.44 | 0.47 |
| 2:B:725:ILE:CD1 | 2:B:770:ARG:HE | 2.27 | 0.47 |
| 2:B:734:ASN:HD21 | 2:B:823:PRO:HA | 1.75 | 0.47 |
| 2:A:198:LEU:CD2 | 2:A:202:GLU:HA | 2.44 | 0.47 |
| 2:A:609:SER:OG | 2:A:610:GLY:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:710:GLN:C | 2:A:712:ALA:N | 2.68 | 0.47 |
| 2:A:964:ILE:CD1 | 2:A:966:ILE:HG23 | 2.45 | 0.47 |
| 2:B:400:ILE:HD12 | 2:B:400:ILE:C | 2.34 | 0.47 |
| 2:B:729:MET:HE3 | 2:B:763:ASP:C | 2.35 | 0.47 |
| 2:A:12:LYS:HZ2 | 2:A:16:ARG:NH1 | 2.12 | 0.47 |
| 2:A:267:LYS:O | 2:A:270:ALA:HB3 | 2.14 | 0.47 |
| 2:A:546:ASN:O | 2:A:550:GLN:HB2 | 2.14 | 0.47 |
| 2:A:871:TRP:CH2 | 2:A:919:LYS:HE3 | 2.47 | 0.47 |
| 2:A:922:ASN:O | 2:A:925:LYS:N | 2.47 | 0.47 |
| 2:A:942:ILE:C | 2:A:943:ILE:HG13 | 2.35 | 0.47 |
| 2:A:944:ILE:HG22 | 2:A:945:ASN:H | 1.78 | 0.47 |
| 2:B:45:LEU:HD13 | 2:B:130:MET:CA | 2.45 | 0.47 |
| 2:B:58:THR:HG22 | 2:B:678:MET:HE1 | 1.96 | 0.47 |
| 2:B:85:SER:N | 2:B:86:PRO:CD | 2.77 | 0.47 |
| 2:B:277:ASP:O | 2:B:277:ASP:CG | 2.50 | 0.47 |
| 2:B:830:GLU:HG3 | 2:B:831:THR:N | 2.29 | 0.47 |
| 2:A:75:LEU:CD1 | 2:A:77:PRO:HD3 | 2.44 | 0.47 |
| 2:A:99:PRO:O | 2:A:102:ILE:HG13 | 2.14 | 0.47 |
| 2:A:318:ALA:HA | 2:A:440:MET:SD | 2.55 | 0.47 |
| 2:A:518:LEU:HD12 | 2:A:524:TRP:CB | 2.44 | 0.47 |
| 2:A:835:GLU:O | 2:A:838:PHE:HB3 | 2.15 | 0.47 |
| 2:A:866:ALA:HB3 | 2:A:955:LYS:HZ1 | 1.78 | 0.47 |
| 2:A:877:VAL:CG2 | 2:A:906:ILE:HG23 | 2.45 | 0.47 |
| 2:A:894:SER:O | 2:A:896:ILE:N | 2.47 | 0.47 |
| 2:B:83:THR:CG2 | 2:B:153:THR:HG22 | 2.44 | 0.47 |
| 2:B:150:PHE:CD1 | 2:B:151:TYR:O | 2.58 | 0.47 |
| 2:B:212:ILE:CD1 | 2:B:235:VAL:CG1 | 2.93 | 0.47 |
| 2:B:216:LEU:CD1 | 2:B:294:LYS:HB3 | 2.43 | 0.47 |
| 2:B:256:ARG:CG | 2:B:257:LYS:H | 2.23 | 0.47 |
| 2:B:393:LEU:HG | 2:B:397:THR:OG1 | 2.14 | 0.47 |
| 2:B:395:GLN:HG3 | 2:B:396:ALA:H | 1.80 | 0.47 |
| 2:B:540:THR:HG21 | 2:B:598:PHE:CD1 | 2.50 | 0.47 |
| 2:B:554:LEU:HD12 | 2:B:586:ILE:HD11 | 1.97 | 0.47 |
| 2:B:860:ARG:NH1 | 2:B:861:ALA:HA | 2.30 | 0.47 |
| 2:B:862:TYR:HB3 | 2:B:964:ILE:HB | 1.95 | 0.47 |
| 2:B:864:TYR:CG | 2:B:865:THR:N | 2.82 | 0.47 |
| 2:B:951:GLY:HA3 | 2:B:965:PHE:CE1 | 2.49 | 0.47 |
| 1:C:919:G:C6 | 1:C:969:G:C6 | 3.03 | 0.47 |
| 1:C:957:G:O2' | 1:C:958:U:H5' | 2.15 | 0.47 |
| 2:A:241:MET:HG3 | 2:A:296:VAL:CG2 | 2.45 | 0.47 |
| 2:A:348:LYS:HB3 | 2:A:348:LYS:HZ2 | 1.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:423:VAL:HA | 2:A:426:ALA:HB3 | 1.96 | 0.47 |
| 2:A:558:LYS:HB3 | 2:A:584:THR:CA | 2.34 | 0.47 |
| 2:A:728:TRP:C | 2:A:730:LEU:N | 2.68 | 0.47 |
| 2:A:767:TYR:HE2 | 2:A:783:LEU:HD11 | 1.79 | 0.47 |
| 2:A:830:GLU:HG3 | 2:A:831:THR:N | 2.30 | 0.47 |
| 2:B:135:GLU:HA | 2:B:138:ILE:HG22 | 1.97 | 0.47 |
| 2:B:238:VAL:HG13 | 2:B:238:VAL:O | 2.15 | 0.47 |
| 2:B:519:PRO:HG2 | 2:B:520:TRP:CE3 | 2.49 | 0.47 |
| 2:B:690:ARG:HB2 | 2:B:693:GLU:HG3 | 1.97 | 0.47 |
| 1:D:914:A:H2' | 1:D:915:G:O4' | 2.15 | 0.47 |
| 2:A:16:ARG:CG | 2:A:16:ARG:NH1 | 2.77 | 0.47 |
| 2:A:59:ILE:HB | 2:A:60:PRO:CD | 2.45 | 0.47 |
| 2:A:210:ILE:HG22 | 2:A:439:ILE:HG23 | 1.97 | 0.47 |
| 2:A:314:ASP:HB3 | 2:A:317:ASN:HB3 | 1.95 | 0.47 |
| 2:A:327:ALA:HB2 | 2:A:353:PRO:O | 2.15 | 0.47 |
| 2:A:461:ILE:HG21 | 2:A:464:GLN:HB2 | 1.97 | 0.47 |
| 2:A:747:PHE:N | 2:A:747:PHE:CD1 | 2.83 | 0.47 |
| 2:A:825:GLU:OE2 | 2:A:825:GLU:O | 2.33 | 0.47 |
| 2:A:860:ARG:NH1 | 2:A:860:ARG:O | 2.47 | 0.47 |
| 2:A:880:LYS:HG3 | 2:A:886:SER:CA | 2.45 | 0.47 |
| 2:B:402:LYS:O | 2:B:405:TYR:HB3 | 2.15 | 0.47 |
| 2:B:793:LEU:HD21 | 2:B:821:PRO:CG | 2.43 | 0.47 |
| 2:B:958:MET:HE1 | 2:B:959:PRO:HD2 | 1.95 | 0.47 |
| 2:A:93:ARG:O | 2:A:98:ASP:HB2 | 2.15 | 0.47 |
| 2:A:168:TRP:CE2 | 2:A:519:PRO:HB2 | 2.49 | 0.47 |
| 2:A:215:GLU:O | 2:A:296:VAL:HA | 2.15 | 0.47 |
| 2:A:354:ARG:HH11 | 2:A:354:ARG:HG3 | 1.80 | 0.47 |
| 2:A:544:HIS:H | 2:A:544:HIS:HD2 | 1.59 | 0.47 |
| 2:A:576:LYS:O | 2:A:580:LEU:HD13 | 2.15 | 0.47 |
| 2:A:800:HIS:O | 2:A:802:CYS:N | 2.48 | 0.47 |
| 2:B:63:ILE:O | 2:B:67:LYS:HG2 | 2.15 | 0.47 |
| 2:B:167:PHE:HA | 2:B:170:LEU:CG | 2.44 | 0.47 |
| 2:B:521:ASP:N | 2:B:522:PRO:HD3 | 2.30 | 0.47 |
| 1:D:980:C:H2' | 1:D:981:C:H6 | 1.79 | 0.46 |
| 2:A:75:LEU:HD23 | 2:A:601:TRP:CE2 | 2.50 | 0.46 |
| 2:A:243:VAL:HG22 | 2:A:292:ILE:HD11 | 1.95 | 0.46 |
| 2:A:275:PHE:C | 2:A:277:ASP:H | 2.18 | 0.46 |
| 2:A:331:PHE:CD1 | 2:A:334:VAL:HG21 | 2.51 | 0.46 |
| 2:A:587:PRO:O | 2:A:591:ILE:HG12 | 2.15 | 0.46 |
| 2:B:164:GLU:O | 2:B:165:TRP:C | 2.54 | 0.46 |
| 2:B:259:LYS:HE2 | 2:B:261:GLU:OE1 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:482:LEU:CD1 | 2:B:496:PHE:HB3 | 2.45 | 0.46 |
| 1:D:953:A:C2 | 2:B:966:ILE:HG12 | 2.50 | 0.46 |
| 2:A:196:HIS:HD2 | 2:A:197:ASP:H | 1.64 | 0.46 |
| 2:A:213:LYS:NZ | 2:A:213:LYS:HB3 | 2.30 | 0.46 |
| 2:A:238:VAL:HG11 | 2:A:298:ASN:HB2 | 1.97 | 0.46 |
| 2:A:268:GLU:HG3 | 2:A:316:ASP:HA | 1.97 | 0.46 |
| 2:A:381:LYS:HZ2 | 2:A:382:LEU:HD12 | 1.80 | 0.46 |
| 2:A:457:VAL:HG23 | 2:A:458:ILE:N | 2.31 | 0.46 |
| 2:A:544:HIS:O | 2:A:547:LYS:HB3 | 2.14 | 0.46 |
| 2:A:626:VAL:HG12 | 2:A:634:TRP:CE2 | 2.50 | 0.46 |
| 2:A:772:GLU:OE1 | 2:A:936:LYS:HE3 | 2.15 | 0.46 |
| 2:B:45:LEU:CD1 | 2:B:80:TRP:HB3 | 2.40 | 0.46 |
| 2:B:495:GLN:HE21 | 2:B:614:ILE:CG2 | 2.27 | 0.46 |
| 2:B:558:LYS:HG3 | 2:B:584:THR:O | 2.14 | 0.46 |
| 2:B:698:ARG:HH11 | 2:B:698:ARG:HG3 | 1.80 | 0.46 |
| 2:B:733:LEU:CD1 | 2:B:737:ILE:HD11 | 2.45 | 0.46 |
| 2:B:766:TRP:HH2 | 2:B:836:GLU:OE1 | 1.97 | 0.46 |
| 2:B:860:ARG:CB | 2:B:966:ILE:HG22 | 2.40 | 0.46 |
| 2:A:42:PHE:CE1 | 2:A:81:HIS:CG | 3.04 | 0.46 |
| 2:A:150:PHE:CD1 | 2:A:150:PHE:C | 2.88 | 0.46 |
| 2:A:164:GLU:O | 2:A:165:TRP:C | 2.53 | 0.46 |
| 2:A:768:LEU:O | 2:A:769:ARG:C | 2.53 | 0.46 |
| 2:B:67:LYS:O | 2:B:72:TYR:HD1 | 1.99 | 0.46 |
| 2:B:418:LYS:HB3 | 2:B:419:PRO:HD2 | 1.97 | 0.46 |
| 2:B:436:ILE:HG22 | 2:B:436:ILE:O | 2.16 | 0.46 |
| 2:B:546:ASN:O | 2:B:550:GLN:HB2 | 2.15 | 0.46 |
| 2:B:616:ASN:HD22 | 2:B:617:HIS:H | 1.60 | 0.46 |
| 2:B:829:ASN:OD1 | 2:B:832:ILE:HG13 | 2.16 | 0.46 |
| 2:B:834:ALA:CA | 2:B:837:GLU:OE2 | 2.60 | 0.46 |
| 2:B:933:PHE:CD1 | 2:B:933:PHE:C | 2.89 | 0.46 |
| 2:A:204:VAL:HG23 | 2:A:204:VAL:O | 2.16 | 0.46 |
| 2:A:297:ARG:HB3 | 2:A:297:ARG:CZ | 2.45 | 0.46 |
| 2:A:355:ILE:HG23 | 2:A:412:VAL:HG11 | 1.97 | 0.46 |
| 2:A:412:VAL:HG23 | 2:A:414:PRO:CD | 2.39 | 0.46 |
| 2:A:717:LYS:NZ | 2:A:719:ASN:HB2 | 2.29 | 0.46 |
| 2:A:933:PHE:HE1 | 2:A:937:GLU:HB2 | 1.81 | 0.46 |
| 2:B:418:LYS:HG3 | 2:B:422:GLU:OE2 | 2.16 | 0.46 |
| 2:A:210:ILE:HD11 | 2:A:232:PRO:CG | 2.37 | 0.46 |
| 2:A:393:LEU:C | 2:A:395:GLN:N | 2.69 | 0.46 |
| 2:A:455:ARG:HD3 | 2:A:456:ALA:N | 2.30 | 0.46 |
| 2:A:728:TRP:CE3 | 2:A:729:MET:N | 2.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:809:LEU:O | 2:A:810:GLY:C | 2.54 | 0.46 |
| 2:A:918:VAL:HG11 | 2:A:920:ARG:HD2 | 1.97 | 0.46 |
| 1:C:956:G:O2' | 1:C:957:G:H5' | 2.16 | 0.46 |
| 2:A:50:HIS:H | 2:A:53:HIS:CD2 | 2.34 | 0.46 |
| 2:A:327:ALA:HB1 | 2:A:354:ARG:CB | 2.46 | 0.46 |
| 2:A:860:ARG:NH1 | 2:A:861:ALA:CA | 2.69 | 0.46 |
| 2:A:911:ILE:O | 2:A:911:ILE:HG13 | 2.15 | 0.46 |
| 2:B:204:VAL:HG11 | 2:B:443:PHE:HB3 | 1.97 | 0.46 |
| 2:B:238:VAL:HB | 2:B:323:MET:HE1 | 1.96 | 0.46 |
| 2:B:722:LEU:HG | 2:B:727:ARG:NH1 | 2.31 | 0.46 |
| 1:D:954:G:O6 | 2:B:963:ALA:HA | 2.16 | 0.46 |
| 2:A:356:VAL:HB | 2:A:409:ILE:O | 2.16 | 0.46 |
| 2:A:678:MET:N | 2:A:678:MET:SD | 2.88 | 0.46 |
| 2:A:872:LYS:HA | 2:A:875:GLU:OE2 | 2.15 | 0.46 |
| 2:B:734:ASN:ND2 | 2:B:824:VAL:H | 1.94 | 0.46 |
| 2:B:789:VAL:O | 2:B:791:VAL:N | 2.49 | 0.46 |
| 2:B:789:VAL:O | 2:B:792:ARG:N | 2.49 | 0.46 |
| 2:A:93:ARG:HG2 | 2:A:451:ARG:HH21 | 1.80 | 0.46 |
| 2:A:183:VAL:HG13 | 2:A:184:ARG:O | 2.16 | 0.46 |
| 2:A:424:LYS:NZ | 2:A:424:LYS:HB2 | 2.31 | 0.46 |
| 2:A:806:TRP:CB | 2:A:815:VAL:HG22 | 2.45 | 0.46 |
| 2:A:863:ILE:HG22 | 2:A:953:LYS:CG | 2.44 | 0.46 |
| 2:B:65:ARG:O | 2:B:68:ARG:HB3 | 2.16 | 0.46 |
| 2:B:459:LYS:HZ2 | 2:B:461:ILE:CD1 | 2.29 | 0.46 |
| 2:B:557:GLU:O | 2:B:559:LEU:N | 2.49 | 0.46 |
| 2:B:631:GLU:C | 2:B:633:HIS:H | 2.17 | 0.46 |
| 2:B:717:LYS:HD3 | 2:B:717:LYS:C | 2.36 | 0.46 |
| 2:B:722:LEU:HD23 | 2:B:722:LEU:N | 2.30 | 0.46 |
| 2:B:824:VAL:O | 2:B:825:GLU:C | 2.53 | 0.46 |
| 2:B:839:ILE:C | 2:B:839:ILE:HD12 | 2.36 | 0.46 |
| 2:B:877:VAL:C | 2:B:879:GLU:H | 2.18 | 0.46 |
| 2:B:918:VAL:CG1 | 2:B:920:ARG:HD2 | 2.46 | 0.46 |
| 2:A:64:ALA:O | 2:A:68:ARG:HB2 | 2.16 | 0.46 |
| 2:A:232:PRO:HG2 | 2:A:428:ALA:HB2 | 1.98 | 0.46 |
| 2:A:731:HIS:HD2 | 2:A:828:TRP:HA | 1.80 | 0.46 |
| 2:B:328:HIS:O | 2:B:329:ALA:C | 2.53 | 0.46 |
| 2:B:476:GLU:OE1 | 2:B:476:GLU:HA | 2.16 | 0.46 |
| 2:B:710:GLN:C | 2:B:712:ALA:N | 2.69 | 0.46 |
| 2:A:159:PHE:O | 2:A:162:PHE:HB3 | 2.16 | 0.46 |
| 2:A:173:LYS:HB3 | 2:A:175:TYR:CE2 | 2.51 | 0.46 |
| 2:A:230:LEU:CD2 | 2:A:230:LEU:N | 2.76 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:382:LEU:HD12 | 2:A:382:LEU:N | 2.31 | 0.46 |
| 2:A:395:GLN:HG3 | 2:A:396:ALA:H | 1.81 | 0.46 |
| 2:A:489:PRO:HD3 | 2:A:683:HIS:HB3 | 1.98 | 0.46 |
| 2:A:624:ASN:HD22 | 2:A:624:ASN:N | 2.07 | 0.46 |
| 2:A:660:ASN:HB2 | 2:A:663:ASP:HB2 | 1.94 | 0.46 |
| 2:B:70:GLN:HB3 | 2:B:72:TYR:CD1 | 2.51 | 0.46 |
| 2:B:234:THR:O | 2:B:325:VAL:HG21 | 2.16 | 0.46 |
| 2:B:516:THR:O | 2:B:526:ILE:HG13 | 2.15 | 0.46 |
| 2:B:641:ASN:C | 2:B:641:ASN:ND2 | 2.69 | 0.46 |
| 1:C:949:C:C2 | 1:C:957:G:C2 | 3.04 | 0.45 |
| 2:A:183:VAL:O | 2:A:184:ARG:C | 2.54 | 0.45 |
| 2:A:297:ARG:O | 2:A:299:PRO:HD3 | 2.16 | 0.45 |
| 2:A:393:LEU:O | 2:A:395:GLN:N | 2.49 | 0.45 |
| 2:A:545:ILE:HG12 | 2:A:594:MET:HE3 | 1.98 | 0.45 |
| 2:A:903:VAL:HG12 | 2:A:906:ILE:HG13 | 1.97 | 0.45 |
| 2:B:231:ARG:HB3 | 2:B:233:GLU:OE2 | 2.17 | 0.45 |
| 2:B:882:ASP:O | 2:B:883:PHE:HB3 | 2.15 | 0.45 |
| 2:A:51:VAL:CG2 | 2:A:52:GLY:N | 2.79 | 0.45 |
| 2:A:741:THR:O | 2:A:745:GLU:HG2 | 2.17 | 0.45 |
| 2:A:855:ILE:O | 2:A:856:GLU:HB2 | 2.15 | 0.45 |
| 2:B:292:ILE:HG13 | 2:B:309:PRO:HB3 | 1.98 | 0.45 |
| 2:B:505:LYS:HD2 | 2:B:505:LYS:N | 2.30 | 0.45 |
| 2:B:914:ARG:HE | 2:B:915:THR:N | 2.13 | 0.45 |
| 1:D:919:G:H1' | 1:D:970:A:C2 | 2.52 | 0.45 |
| 2:A:23:PHE:CD2 | 2:A:143:SER:HA | 2.51 | 0.45 |
| 2:A:166:GLN:HB2 | 2:A:534:ILE:HD11 | 1.97 | 0.45 |
| 2:A:186:ASP:HB3 | 2:A:191:THR:CG2 | 2.41 | 0.45 |
| 2:A:328:HIS:O | 2:A:329:ALA:C | 2.54 | 0.45 |
| 2:A:950:LYS:HG2 | 2:A:953:LYS:HZ1 | 1.82 | 0.45 |
| 2:B:9:ILE:HD13 | 2:B:804:GLU:HG2 | 1.97 | 0.45 |
| 2:B:535:TYR:CE1 | 2:B:536:MET:SD | 3.10 | 0.45 |
| 2:B:928:ARG:C | 2:B:930:ALA:N | 2.69 | 0.45 |
| 1:C:918:U:H2' | 1:C:918:U:O2 | 2.15 | 0.45 |
| 1:D:905:G:H5' | 1:D:905:G:H8 | 1.82 | 0.45 |
| 2:A:61:ASP:OD2 | 2:A:674:ARG:NH2 | 2.45 | 0.45 |
| 2:A:155:LEU:C | 2:A:157:PRO:HD3 | 2.37 | 0.45 |
| 2:A:211:ILE:HG21 | 2:A:319:THR:CG2 | 2.46 | 0.45 |
| 2:A:464:GLN:NE2 | 2:A:465:TRP:O | 2.49 | 0.45 |
| 2:A:742:ASN:O | 2:A:744:LEU:N | 2.50 | 0.45 |
| 2:B:136:THR:CG2 | 2:B:661:PHE:HD2 | 2.26 | 0.45 |
| 2:B:412:VAL:H | 2:B:416:GLU:HG2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:485:MET:SD | 2:B:635:PRO:HB2 | 2.57 | 0.45 |
| 2:A:17:TRP:CZ2 | 2:A:803:GLU:HG3 | 2.52 | 0.45 |
| 2:B:266:SER:O | 2:B:269:ALA:HB3 | 2.16 | 0.45 |
| 2:B:306:ILE:HG12 | 2:B:307:ILE:N | 2.31 | 0.45 |
| 2:B:411:LYS:HA | 2:B:416:GLU:CD | 2.37 | 0.45 |
| 2:B:676:TYR:HA | 2:B:697:LEU:CD2 | 2.46 | 0.45 |
| 2:B:729:MET:HA | 2:B:729:MET:CE | 2.47 | 0.45 |
| 2:B:953:LYS:HB3 | 2:B:953:LYS:NZ | 2.30 | 0.45 |
| 1:D:944:C:H2' | 1:D:945:C:H6 | 1.81 | 0.45 |
| 2:A:294:LYS:N | 2:A:294:LYS:HD2 | 2.32 | 0.45 |
| 2:A:377:GLU:CD | 2:A:377:GLU:C | 2.75 | 0.45 |
| 2:A:544:HIS:CD2 | 2:A:544:HIS:N | 2.85 | 0.45 |
| 2:A:582:LYS:H | 2:A:582:LYS:HD2 | 1.81 | 0.45 |
| 2:A:713:GLU:O | 2:A:714:TYR:C | 2.53 | 0.45 |
| 2:A:838:PHE:HE2 | 2:A:922:ASN:HD21 | 1.63 | 0.45 |
| 2:B:142:PHE:O | 2:B:144:VAL:N | 2.49 | 0.45 |
| 2:B:231:ARG:HB3 | 2:B:233:GLU:CD | 2.37 | 0.45 |
| 2:B:342:GLU:N | 2:B:342:GLU:OE2 | 2.50 | 0.45 |
| 2:B:393:LEU:C | 2:B:395:GLN:N | 2.70 | 0.45 |
| 2:B:393:LEU:CD1 | 2:B:396:ALA:HB3 | 2.46 | 0.45 |
| 2:B:711:PHE:HE1 | 2:B:783:LEU:HD23 | 1.82 | 0.45 |
| 2:B:713:GLU:OE2 | 2:B:713:GLU:CA | 2.65 | 0.45 |
| 1:C:960:C:H4' | 1:C:961:C:OP2 | 2.17 | 0.45 |
| 2:A:80:TRP:CD1 | 2:A:130:MET:HG3 | 2.51 | 0.45 |
| 2:A:557:GLU:O | 2:A:559:LEU:N | 2.49 | 0.45 |
| 2:B:55:ARG:HD2 | 2:B:687:PHE:CD1 | 2.51 | 0.45 |
| 2:B:83:THR:HG22 | 2:B:153:THR:HG22 | 1.97 | 0.45 |
| 2:B:123:ILE:HD11 | 2:B:155:LEU:CD1 | 2.47 | 0.45 |
| 2:B:232:PRO:HG2 | 2:B:428:ALA:HB2 | 1.99 | 0.45 |
| 2:B:252:ALA:HB2 | 2:B:282:VAL:HA | 1.99 | 0.45 |
| 2:B:730:LEU:HD23 | 2:B:730:LEU:HA | 1.84 | 0.45 |
| 2:B:742:ASN:O | 2:B:745:GLU:N | 2.50 | 0.45 |
| 2:B:921:ILE:HB | 2:B:928:ARG:HH22 | 1.77 | 0.45 |
| 2:A:93:ARG:HG3 | 2:A:93:ARG:NH1 | 2.32 | 0.45 |
| 2:A:112:PRO:HB2 | 2:A:115:ILE:HG13 | 1.99 | 0.45 |
| 2:A:210:ILE:O | 2:A:210:ILE:HG13 | 2.16 | 0.45 |
| 2:A:211:ILE:HG21 | 2:A:319:THR:HG21 | 1.99 | 0.45 |
| 2:A:211:ILE:HA | 2:A:227:ALA:O | 2.17 | 0.45 |
| 2:A:218:GLU:OE2 | 2:A:294:LYS:HE2 | 2.16 | 0.45 |
| 2:A:277:ASP:HB2 | 2:A:460:ILE:HB | 1.99 | 0.45 |
| 2:A:341:ARG:HG2 | 2:A:341:ARG:HH11 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:426:ALA:HA | 2:A:429:LYS:CE | 2.31 | 0.45 |
| 2:A:717:LYS:C | 2:A:717:LYS:CD | 2.83 | 0.45 |
| 2:B:51:VAL:O | 2:B:54:ALA:CB | 2.62 | 0.45 |
| 2:B:54:ALA:CB | 2:B:661:PHE:CD1 | 3.00 | 0.45 |
| 1:C:916:C:H5' | 1:C:917:C:H5 | 1.66 | 0.45 |
| 1:C:939:A:H4' | 1:C:939:A:OP1 | 2.16 | 0.45 |
| 1:D:921:U:OP2 | 1:D:922:C:H3' | 2.17 | 0.45 |
| 2:A:61:ASP:OD2 | 2:A:674:ARG:NH1 | 2.48 | 0.45 |
| 2:A:266:SER:O | 2:A:269:ALA:HB3 | 2.17 | 0.45 |
| 2:A:482:LEU:C | 2:A:482:LEU:CD2 | 2.85 | 0.45 |
| 2:A:831:THR:O | 2:A:835:GLU:CG | 2.65 | 0.45 |
| 2:A:840:ARG:HE | 2:A:840:ARG:HB3 | 1.60 | 0.45 |
| 2:B:7:LYS:HB2 | 2:B:7:LYS:HZ3 | 1.81 | 0.45 |
| 2:B:227:ALA:HA | 2:B:321:VAL:O | 2.15 | 0.45 |
| 2:B:245:PRO:O | 2:B:288:GLY:HA3 | 2.17 | 0.45 |
| 2:B:387:GLN:HE21 | 2:B:387:GLN:HA | 1.82 | 0.45 |
| 2:B:387:GLN:HG3 | 2:B:388:LYS:N | 2.32 | 0.45 |
| 2:B:731:HIS:HE1 | 2:B:833:GLU:OE1 | 2.00 | 0.45 |
| 2:B:766:TRP:HZ3 | 2:B:836:GLU:CG | 2.30 | 0.45 |
| 2:B:950:LYS:H | 2:B:953:LYS:NZ | 2.15 | 0.45 |
| 2:A:250:VAL:HG12 | 2:A:285:GLU:HG3 | 1.99 | 0.45 |
| 2:A:463:ASP:O | 2:A:464:GLN:C | 2.55 | 0.45 |
| 2:A:568:PHE:CB | 2:A:569:LEU:HD12 | 2.46 | 0.45 |
| 2:A:728:TRP:HE3 | 2:A:729:MET:CA | 2.29 | 0.45 |
| 2:B:28:ARG:HG3 | 2:B:28:ARG:NH1 | 2.30 | 0.45 |
| 2:B:682:GLU:OE1 | 2:B:748:ARG:NH1 | 2.49 | 0.45 |
| 2:B:713:GLU:O | 2:B:714:TYR:C | 2.55 | 0.45 |
| 2:B:890:LEU:O | 2:B:892:LYS:N | 2.50 | 0.45 |
| 2:B:911:ILE:O | 2:B:911:ILE:HG13 | 2.16 | 0.45 |
| 1:D:960:C:H4' | 1:D:961:C:H5'' | 1.98 | 0.44 |
| 2:A:94:ILE:HD11 | 2:A:120:GLU:CA | 2.46 | 0.44 |
| 2:A:518:LEU:HD12 | 2:A:524:TRP:HB3 | 1.98 | 0.44 |
| 2:A:553:LYS:NZ | 2:A:553:LYS:HB3 | 2.32 | 0.44 |
| 2:A:800:HIS:C | 2:A:802:CYS:N | 2.70 | 0.44 |
| 2:A:800:HIS:C | 2:A:802:CYS:H | 2.21 | 0.44 |
| 2:A:902:GLU:C | 2:A:904:ALA:H | 2.21 | 0.44 |
| 2:A:916:PHE:HB3 | 2:A:917:ASP:H | 1.67 | 0.44 |
| 2:B:373:PHE:N | 2:B:374:PRO:CD | 2.80 | 0.44 |
| 2:B:860:ARG:HB3 | 2:B:966:ILE:CG2 | 2.40 | 0.44 |
| 2:A:26:ASN:C | 2:A:28:ARG:HH21 | 2.20 | 0.44 |
| 2:A:67:LYS:HE2 | 2:A:70:GLN:HE22 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:42:PHE:CD1 | 2:B:42:PHE:N | 2.85 | 0.44 |
| 2:B:215:GLU:O | 2:B:296:VAL:HA | 2.17 | 0.44 |
| 2:B:429:LYS:HB3 | 2:B:429:LYS:HZ2 | 1.82 | 0.44 |
| 2:B:511:LYS:HE3 | 2:B:524:TRP:CE2 | 2.51 | 0.44 |
| 2:B:714:TYR:CD2 | 2:B:714:TYR:N | 2.73 | 0.44 |
| 2:A:31:PRO:HD2 | 2:A:34:LYS:HG3 | 1.98 | 0.44 |
| 2:A:69:MET:HB3 | 2:A:818:ALA:O | 2.17 | 0.44 |
| 2:A:85:SER:N | 2:A:86:PRO:CD | 2.77 | 0.44 |
| 2:A:119:PHE:C | 2:A:121:ASP:N | 2.69 | 0.44 |
| 2:A:482:LEU:O | 2:A:493:ARG:NH1 | 2.50 | 0.44 |
| 2:A:768:LEU:O | 2:A:770:ARG:N | 2.49 | 0.44 |
| 2:B:57:TYR:O | 2:B:60:PRO:CG | 2.62 | 0.44 |
| 2:B:170:LEU:CB | 2:B:176:ILE:HD11 | 2.41 | 0.44 |
| 2:B:211:ILE:O | 2:B:211:ILE:HG13 | 2.16 | 0.44 |
| 2:B:234:THR:HA | 2:B:355:ILE:CD1 | 2.47 | 0.44 |
| 2:B:476:GLU:HA | 2:B:479:ARG:NH1 | 2.32 | 0.44 |
| 2:B:809:LEU:O | 2:B:810:GLY:C | 2.56 | 0.44 |
| 2:B:860:ARG:NH1 | 2:B:860:ARG:O | 2.50 | 0.44 |
| 2:B:902:GLU:C | 2:B:904:ALA:H | 2.21 | 0.44 |
| 2:A:234:THR:HB | 2:A:325:VAL:HG21 | 1.99 | 0.44 |
| 2:A:400:ILE:C | 2:A:400:ILE:HD12 | 2.37 | 0.44 |
| 2:A:432:LEU:HD11 | 2:A:439:ILE:CG1 | 2.45 | 0.44 |
| 2:A:730:LEU:CA | 2:A:827:TRP:HE1 | 2.30 | 0.44 |
| 2:A:766:TRP:O | 2:A:770:ARG:N | 2.47 | 0.44 |
| 2:B:150:PHE:CD1 | 2:B:150:PHE:C | 2.90 | 0.44 |
| 2:B:186:ASP:OD2 | 2:B:188:VAL:HG13 | 2.18 | 0.44 |
| 2:B:518:LEU:HD22 | 2:B:520:TRP:CZ2 | 2.52 | 0.44 |
| 2:B:742:ASN:N | 2:B:742:ASN:ND2 | 2.65 | 0.44 |
| 2:A:703:ARG:HG2 | 2:A:761:MET:CE | 2.48 | 0.44 |
| 2:A:872:LYS:HA | 2:A:872:LYS:HZ2 | 1.83 | 0.44 |
| 2:A:878:SER:HB2 | 2:A:914:ARG:HB2 | 1.99 | 0.44 |
| 2:A:933:PHE:CE1 | 2:A:937:GLU:HB2 | 2.51 | 0.44 |
| 2:B:340:LYS:HG2 | 2:B:341:ARG:NH1 | 2.32 | 0.44 |
| 2:B:490:GLU:C | 2:B:492:ARG:H | 2.21 | 0.44 |
| 2:B:679:SER:HA | 2:B:753:VAL:HG11 | 2.00 | 0.44 |
| 2:B:718:GLY:O | 2:B:720:VAL:HG13 | 2.18 | 0.44 |
| 2:B:750:ARG:HE | 2:B:750:ARG:HB3 | 1.50 | 0.44 |
| 2:B:783:LEU:HD12 | 2:B:783:LEU:N | 2.33 | 0.44 |
| 2:B:846:ILE:HG12 | 2:B:964:ILE:HD12 | 1.94 | 0.44 |
| 2:B:866:ALA:H | 2:B:955:LYS:HZ1 | 1.57 | 0.44 |
| 1:D:902:C:H2' | 1:D:903:G:C4' | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:972:U:H5'' | 1:D:973:C:OP2 | 2.18 | 0.44 |
| 2:A:518:LEU:HD22 | 2:A:520:TRP:CZ2 | 2.53 | 0.44 |
| 2:A:789:VAL:O | 2:A:791:VAL:N | 2.50 | 0.44 |
| 2:B:216:LEU:O | 2:B:216:LEU:HG | 2.17 | 0.44 |
| 2:B:330:PRO:HD3 | 2:B:400:ILE:HG12 | 2.00 | 0.44 |
| 2:B:393:LEU:O | 2:B:395:GLN:N | 2.51 | 0.44 |
| 2:B:725:ILE:HG21 | 2:B:771:THR:HG21 | 1.99 | 0.44 |
| 2:B:768:LEU:O | 2:B:769:ARG:C | 2.55 | 0.44 |
| 1:C:957:G:C2 | 1:C:958:U:C2 | 3.06 | 0.44 |
| 2:A:50:HIS:CE1 | 2:A:53:HIS:CE1 | 3.06 | 0.44 |
| 2:A:244:ASN:HB2 | 2:A:313:VAL:HG23 | 1.99 | 0.44 |
| 2:A:862:TYR:HB2 | 2:A:964:ILE:HA | 1.99 | 0.44 |
| 2:B:218:GLU:CD | 2:B:219:ASN:ND2 | 2.70 | 0.44 |
| 2:B:261:GLU:HB2 | 2:B:263:TRP:HE1 | 1.81 | 0.44 |
| 2:B:339:LEU:HD13 | 2:B:339:LEU:N | 2.33 | 0.44 |
| 2:B:449:ILE:HG23 | 2:B:454:ASN:O | 2.18 | 0.44 |
| 2:B:908:GLN:HE22 | 2:B:958:MET:HG3 | 1.83 | 0.44 |
| 1:D:937:C:O2 | 1:D:937:C:H2' | 2.18 | 0.44 |
| 2:A:863:ILE:CG2 | 2:A:953:LYS:HD3 | 2.48 | 0.44 |
| 2:B:75:LEU:HD22 | 2:B:601:TRP:CD1 | 2.53 | 0.44 |
| 2:B:104:ILE:HG21 | 2:B:653:LYS:HD3 | 1.99 | 0.44 |
| 2:B:168:TRP:NE1 | 2:B:519:PRO:HB2 | 2.33 | 0.44 |
| 2:B:250:VAL:HG12 | 2:B:285:GLU:HG3 | 2.00 | 0.44 |
| 2:B:463:ASP:O | 2:B:464:GLN:C | 2.56 | 0.44 |
| 2:B:729:MET:HE2 | 2:B:729:MET:HB2 | 1.78 | 0.44 |
| 1:D:953:A:H1' | 2:B:849:ILE:CG2 | 2.48 | 0.44 |
| 2:A:243:VAL:HG23 | 2:A:244:ASN:N | 2.33 | 0.44 |
| 2:A:803:GLU:HA | 2:A:815:VAL:HG21 | 1.98 | 0.44 |
| 2:B:58:THR:HA | 2:B:142:PHE:HE1 | 1.83 | 0.44 |
| 2:B:79:ALA:HB2 | 2:B:539:TYR:CE2 | 2.51 | 0.44 |
| 2:B:331:PHE:O | 2:B:334:VAL:HG23 | 2.17 | 0.44 |
| 2:B:739:GLU:HB3 | 2:B:755:TRP:CD1 | 2.53 | 0.44 |
| 1:C:937:C:H2' | 1:C:938:A:O4' | 2.18 | 0.43 |
| 1:C:941:A:H4' | 2:A:699:LYS:HZ1 | 1.82 | 0.43 |
| 1:C:958:U:C6 | 1:C:958:U:C3' | 3.01 | 0.43 |
| 1:C:972:U:H5' | 1:C:973:C:OP2 | 2.18 | 0.43 |
| 1:D:923:A:HO2' | 1:D:924:A:P | 2.40 | 0.43 |
| 2:A:49:LEU:HD22 | 2:A:137:PHE:HE1 | 1.83 | 0.43 |
| 2:A:238:VAL:HG13 | 2:A:238:VAL:O | 2.16 | 0.43 |
| 2:A:245:PRO:O | 2:A:288:GLY:HA3 | 2.18 | 0.43 |
| 2:A:636:LYS:HB3 | 2:A:636:LYS:NZ | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:703:ARG:HG3 | 2:A:707:LEU:CD1 | 2.47 | 0.43 |
| 2:A:767:TYR:CE2 | 2:A:783:LEU:HD11 | 2.52 | 0.43 |
| 2:A:824:VAL:CG1 | 2:A:827:TRP:CE3 | 3.00 | 0.43 |
| 2:A:966:ILE:O | 2:A:966:ILE:HG13 | 2.17 | 0.43 |
| 2:B:57:TYR:O | 2:B:60:PRO:HD2 | 2.17 | 0.43 |
| 2:B:267:LYS:O | 2:B:270:ALA:HB3 | 2.18 | 0.43 |
| 2:B:459:LYS:HZ2 | 2:B:461:ILE:HD13 | 1.82 | 0.43 |
| 2:B:711:PHE:CE1 | 2:B:783:LEU:HD23 | 2.53 | 0.43 |
| 2:B:724:ASP:OD2 | 2:B:928:ARG:HD3 | 2.18 | 0.43 |
| 2:B:738:LYS:NZ | 2:B:738:LYS:HB3 | 2.33 | 0.43 |
| 2:A:81:HIS:HD2 | 2:A:152:THR:HG21 | 1.83 | 0.43 |
| 2:A:83:THR:O | 2:A:528:SER:HB3 | 2.17 | 0.43 |
| 2:A:381:LYS:HB3 | 2:A:381:LYS:HZ2 | 1.83 | 0.43 |
| 2:A:420:VAL:HG12 | 2:A:424:LYS:HZ1 | 1.82 | 0.43 |
| 2:A:675:LEU:CD1 | 2:A:697:LEU:HD21 | 2.48 | 0.43 |
| 2:A:677:ILE:HD11 | 2:A:689:TRP:HZ3 | 1.83 | 0.43 |
| 2:A:701:ILE:O | 2:A:704:PHE:HB3 | 2.16 | 0.43 |
| 2:A:890:LEU:O | 2:A:892:LYS:N | 2.51 | 0.43 |
| 2:A:921:ILE:O | 2:A:924:GLU:HB3 | 2.17 | 0.43 |
| 2:B:331:PHE:HD1 | 2:B:334:VAL:HG21 | 1.83 | 0.43 |
| 2:B:355:ILE:HG23 | 2:B:412:VAL:CG1 | 2.49 | 0.43 |
| 2:B:742:ASN:O | 2:B:744:LEU:N | 2.51 | 0.43 |
| 2:A:58:THR:HG22 | 2:A:62:VAL:CG2 | 2.49 | 0.43 |
| 2:A:75:LEU:C | 2:A:75:LEU:CD1 | 2.84 | 0.43 |
| 2:A:166:GLN:NE2 | 2:A:534:ILE:HG12 | 2.33 | 0.43 |
| 2:A:244:ASN:HD22 | 2:A:313:VAL:HG23 | 1.82 | 0.43 |
| 2:A:490:GLU:C | 2:A:492:ARG:H | 2.22 | 0.43 |
| 2:A:824:VAL:HB | 2:A:827:TRP:CE3 | 2.53 | 0.43 |
| 2:B:188:VAL:HG23 | 2:B:190:GLY:H | 1.84 | 0.43 |
| 2:B:339:LEU:HD22 | 2:B:340:LYS:HG3 | 2.00 | 0.43 |
| 2:B:449:ILE:HG22 | 2:B:450:SER:N | 2.33 | 0.43 |
| 2:B:618:LEU:HD23 | 2:B:618:LEU:HA | 1.88 | 0.43 |
| 2:B:911:ILE:O | 2:B:912:LYS:HG3 | 2.18 | 0.43 |
| 1:C:985:A:H61 | 2:A:504:ASP:CB | 2.24 | 0.43 |
| 1:D:917:C:C2 | 1:D:918:U:C5 | 3.06 | 0.43 |
| 2:A:919:LYS:H | 2:A:919:LYS:HE2 | 1.82 | 0.43 |
| 2:B:163:ILE:HD13 | 2:B:163:ILE:HA | 1.92 | 0.43 |
| 2:B:210:ILE:HG22 | 2:B:439:ILE:HG12 | 1.99 | 0.43 |
| 2:B:373:PHE:N | 2:B:373:PHE:CD1 | 2.86 | 0.43 |
| 2:B:412:VAL:HG23 | 2:B:414:PRO:HD2 | 2.00 | 0.43 |
| 2:B:577:GLU:OE1 | 2:B:592:HIS:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:644:GLY:HA2 | 2:B:687:PHE:O | 2.18 | 0.43 |
| 2:B:860:ARG:HH12 | 2:B:861:ALA:HA | 1.83 | 0.43 |
| 2:B:877:VAL:HG22 | 2:B:906:ILE:HG23 | 2.01 | 0.43 |
| 1:C:988:A:N7 | 2:A:529:LEU:HD21 | 2.33 | 0.43 |
| 2:A:446:LYS:H | 2:A:446:LYS:HD2 | 1.84 | 0.43 |
| 2:A:460:ILE:N | 2:A:460:ILE:HD12 | 2.33 | 0.43 |
| 2:A:623:PHE:O | 2:A:624:ASN:C | 2.56 | 0.43 |
| 2:A:884:LYS:C | 2:A:886:SER:N | 2.72 | 0.43 |
| 2:B:119:PHE:C | 2:B:121:ASP:N | 2.70 | 0.43 |
| 2:B:310:ALA:HB1 | 2:B:312:PHE:CE1 | 2.53 | 0.43 |
| 1:C:964:G:O2' | 1:C:965:G:H5' | 2.18 | 0.43 |
| 2:A:27:ILE:HG12 | 2:A:28:ARG:CZ | 2.49 | 0.43 |
| 2:A:45:LEU:CD1 | 2:A:80:TRP:HB3 | 2.47 | 0.43 |
| 2:A:183:VAL:O | 2:A:183:VAL:CG1 | 2.65 | 0.43 |
| 2:A:330:PRO:CD | 2:A:400:ILE:HG12 | 2.48 | 0.43 |
| 2:A:508:CYS:O | 2:A:508:CYS:SG | 2.77 | 0.43 |
| 2:B:62:VAL:HG21 | 2:B:678:MET:HE2 | 1.98 | 0.43 |
| 2:B:114:GLU:OE1 | 2:B:114:GLU:HA | 2.18 | 0.43 |
| 2:B:171:LYS:HD2 | 2:B:520:TRP:CE3 | 2.54 | 0.43 |
| 2:B:198:LEU:H | 2:B:198:LEU:CD1 | 2.29 | 0.43 |
| 2:B:340:LYS:CE | 2:B:341:ARG:HH12 | 2.32 | 0.43 |
| 2:B:401:TYR:OH | 2:B:424:LYS:HE3 | 2.19 | 0.43 |
| 1:C:955:G:P | 2:A:961:LYS:HZ3 | 2.40 | 0.43 |
| 2:A:138:ILE:HD12 | 2:A:138:ILE:HA | 1.87 | 0.43 |
| 2:A:273:LEU:HD21 | 2:A:440:MET:HG3 | 2.00 | 0.43 |
| 2:A:703:ARG:O | 2:A:707:LEU:HD12 | 2.18 | 0.43 |
| 2:A:728:TRP:O | 2:A:730:LEU:N | 2.51 | 0.43 |
| 2:A:960:LEU:N | 2:A:960:LEU:CD2 | 2.81 | 0.43 |
| 2:B:45:LEU:HD11 | 2:B:130:MET:HG3 | 2.00 | 0.43 |
| 2:B:183:VAL:O | 2:B:184:ARG:C | 2.57 | 0.43 |
| 2:B:211:ILE:HA | 2:B:227:ALA:O | 2.19 | 0.43 |
| 2:B:546:ASN:HD22 | 2:B:546:ASN:HA | 1.59 | 0.43 |
| 2:B:573:SER:HB2 | 2:B:576:LYS:HG2 | 2.00 | 0.43 |
| 2:B:922:ASN:ND2 | 2:B:923:GLU:N | 2.63 | 0.43 |
| 2:B:923:GLU:HB2 | 2:B:945:ASN:HD21 | 1.84 | 0.43 |
| 1:C:986:C:O3' | 2:A:510:ARG:HD2 | 2.19 | 0.43 |
| 1:D:976:C:O2' | 1:D:977:G:H5' | 2.18 | 0.43 |
| 2:A:36:PHE:O | 2:A:38:ILE:HG22 | 2.18 | 0.43 |
| 2:A:94:ILE:HD12 | 2:A:94:ILE:C | 2.39 | 0.43 |
| 2:A:128:TYR:O | 2:A:128:TYR:CD1 | 2.71 | 0.43 |
| 2:A:198:LEU:HD22 | 2:A:202:GLU:CB | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:742:ASN:O | 2:A:745:GLU:N | 2.52 | 0.43 |
| 2:B:173:LYS:HD2 | 2:B:175:TYR:CE2 | 2.54 | 0.43 |
| 2:B:218:GLU:O | 2:B:219:ASN:C | 2.56 | 0.43 |
| 2:B:337:GLU:HG2 | 2:B:337:GLU:O | 2.18 | 0.43 |
| 2:B:379:VAL:O | 2:B:383:GLY:HA3 | 2.19 | 0.43 |
| 2:B:481:ALA:O | 2:B:484:ARG:N | 2.34 | 0.43 |
| 1:D:969:G:O2' | 1:D:970:A:H5' | 2.18 | 0.43 |
| 2:A:37:TYR:CE2 | 2:A:39:THR:CG2 | 3.01 | 0.43 |
| 2:A:182:ARG:O | 2:A:183:VAL:CB | 2.66 | 0.43 |
| 2:A:246:ASN:OD1 | 2:A:247:ALA:N | 2.52 | 0.43 |
| 2:A:380:ASN:O | 2:A:384:ILE:HG13 | 2.19 | 0.43 |
| 2:A:566:TYR:OH | 2:A:572:PHE:HD1 | 2.01 | 0.43 |
| 2:B:25:PRO:HD2 | 2:B:145:ASP:OD2 | 2.19 | 0.43 |
| 2:B:33:GLU:OE2 | 2:B:33:GLU:N | 2.39 | 0.43 |
| 2:B:273:LEU:CB | 2:B:280:ILE:HD11 | 2.49 | 0.43 |
| 2:B:343:THR:HG23 | 2:B:344:GLU:HG2 | 2.00 | 0.43 |
| 2:B:539:TYR:HA | 2:B:542:SER:HB2 | 2.01 | 0.43 |
| 2:B:646:LEU:O | 2:B:647:GLU:HB2 | 2.19 | 0.43 |
| 2:B:728:TRP:HZ3 | 2:B:729:MET:CE | 2.32 | 0.43 |
| 2:B:803:GLU:CG | 2:B:815:VAL:HG12 | 2.49 | 0.43 |
| 2:B:864:TYR:OH | 2:B:871:TRP:HZ2 | 2.02 | 0.43 |
| 2:B:953:LYS:O | 2:B:954:LYS:C | 2.57 | 0.43 |
| 2:A:214:PHE:HA | 2:A:299:PRO:CG | 2.49 | 0.43 |
| 2:A:231:ARG:O | 2:A:234:THR:OG1 | 2.36 | 0.43 |
| 2:A:511:LYS:HE2 | 2:A:524:TRP:CE2 | 2.53 | 0.43 |
| 2:A:544:HIS:HE1 | 2:A:593:GLU:OE2 | 2.01 | 0.43 |
| 2:B:98:ASP:OD2 | 2:B:99:PRO:HD2 | 2.19 | 0.43 |
| 2:B:231:ARG:O | 2:B:234:THR:OG1 | 2.37 | 0.43 |
| 2:B:471:ASN:OD1 | 2:B:473:GLU:HG2 | 2.18 | 0.43 |
| 2:B:560:THR:O | 2:B:563:PHE:HB3 | 2.19 | 0.43 |
| 1:C:941:A:H2' | 1:C:942:U:H6 | 1.84 | 0.42 |
| 1:C:964:G:N2 | 1:C:975:C:C2 | 2.86 | 0.42 |
| 1:D:920:G:H5'' | 1:D:921:U:C5 | 2.48 | 0.42 |
| 2:A:184:ARG:HD3 | 2:A:198:LEU:HD21 | 2.01 | 0.42 |
| 2:A:198:LEU:HD23 | 2:A:448:VAL:HG13 | 2.01 | 0.42 |
| 2:A:232:PRO:O | 2:A:427:ILE:HG21 | 2.19 | 0.42 |
| 2:A:311:GLU:OE2 | 2:A:335:ALA:HB2 | 2.19 | 0.42 |
| 2:A:384:ILE:CG2 | 2:A:385:LYS:H | 2.19 | 0.42 |
| 2:A:470:GLY:O | 2:A:471:ASN:C | 2.57 | 0.42 |
| 2:A:475:LYS:HE3 | 2:A:500:ILE:O | 2.19 | 0.42 |
| 2:A:521:ASP:N | 2:A:522:PRO:HD3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:884:LYS:HB2 | 2:A:884:LYS:HZ3 | 1.82 | 0.42 |
| 2:B:22:ILE:HD12 | 2:B:22:ILE:HA | 1.82 | 0.42 |
| 2:B:223:ILE:HG23 | 2:B:223:ILE:O | 2.19 | 0.42 |
| 2:B:373:PHE:HB2 | 2:B:374:PRO:HD3 | 2.02 | 0.42 |
| 2:B:374:PRO:HG3 | 2:B:379:VAL:CG2 | 2.49 | 0.42 |
| 2:B:614:ILE:HA | 2:B:618:LEU:HB2 | 2.01 | 0.42 |
| 2:B:680:LEU:C | 2:B:750:ARG:HG3 | 2.39 | 0.42 |
| 2:B:698:ARG:O | 2:B:701:ILE:HB | 2.18 | 0.42 |
| 2:B:737:ILE:HG22 | 2:B:823:PRO:HD3 | 2.00 | 0.42 |
| 2:B:840:ARG:O | 2:B:844:GLU:HG3 | 2.18 | 0.42 |
| 1:C:958:U:H2' | 1:C:959:U:O5' | 2.19 | 0.42 |
| 1:D:916:C:O2' | 1:D:972:U:O3' | 2.36 | 0.42 |
| 1:D:958:U:H2' | 1:D:959:U:O5' | 2.19 | 0.42 |
| 2:A:314:ASP:HA | 2:A:315:PRO:HD3 | 1.89 | 0.42 |
| 2:A:675:LEU:CD1 | 2:A:697:LEU:HD11 | 2.48 | 0.42 |
| 2:A:714:TYR:CD2 | 2:A:714:TYR:N | 2.88 | 0.42 |
| 2:A:786:LEU:C | 2:A:786:LEU:HD23 | 2.40 | 0.42 |
| 2:A:854:LYS:HG3 | 2:A:855:ILE:H | 1.83 | 0.42 |
| 2:A:890:LEU:C | 2:A:892:LYS:N | 2.72 | 0.42 |
| 2:A:959:PRO:C | 2:A:960:LEU:CD2 | 2.87 | 0.42 |
| 2:B:54:ALA:HB2 | 2:B:661:PHE:CD1 | 2.54 | 0.42 |
| 2:B:355:ILE:CG2 | 2:B:410:PHE:CE1 | 3.02 | 0.42 |
| 2:B:706:GLU:O | 2:B:709:SER:HB2 | 2.19 | 0.42 |
| 2:B:872:LYS:HD3 | 2:B:872:LYS:HA | 1.88 | 0.42 |
| 1:C:960:C:C2 | 1:C:971:A:H1' | 2.54 | 0.42 |
| 2:A:244:ASN:ND2 | 2:A:313:VAL:HG23 | 2.34 | 0.42 |
| 2:A:469:TYR:CE2 | 2:A:620:PHE:CD1 | 3.07 | 0.42 |
| 2:A:774:ARG:HG2 | 2:A:775:ASP:N | 2.34 | 0.42 |
| 2:B:159:PHE:O | 2:B:162:PHE:HB3 | 2.19 | 0.42 |
| 2:B:165:TRP:HZ2 | 2:B:565:ASP:OD2 | 2.02 | 0.42 |
| 2:B:827:TRP:O | 2:B:827:TRP:HD1 | 2.02 | 0.42 |
| 2:B:884:LYS:O | 2:B:885:SER:C | 2.57 | 0.42 |
| 1:D:953:A:HO2' | 1:D:954:G:H8 | 1.62 | 0.42 |
| 2:A:218:GLU:O | 2:A:219:ASN:C | 2.57 | 0.42 |
| 2:A:373:PHE:N | 2:A:374:PRO:CD | 2.83 | 0.42 |
| 2:A:572:PHE:HE1 | 2:A:595:LYS:HB3 | 1.85 | 0.42 |
| 2:A:614:ILE:HA | 2:A:618:LEU:HB2 | 2.02 | 0.42 |
| 2:A:691:ARG:CG | 2:A:691:ARG:NH1 | 2.80 | 0.42 |
| 2:A:860:ARG:NH2 | 2:A:862:TYR:CB | 2.77 | 0.42 |
| 2:B:388:LYS:H | 2:B:390:LYS:HE2 | 1.84 | 0.42 |
| 2:B:720:VAL:CG1 | 2:B:777:GLU:HG2 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:985:A:O3' | 1:C:986:C:C6 | 2.72 | 0.42 |
| 2:A:160:SER:HB3 | 2:A:516:THR:HG23 | 2.01 | 0.42 |
| 2:A:191:THR:HA | 2:A:192:PRO:HD3 | 1.88 | 0.42 |
| 2:A:195:ASP:C | 2:A:202:GLU:OE1 | 2.57 | 0.42 |
| 2:A:724:ASP:C | 2:A:726:ASP:N | 2.73 | 0.42 |
| 2:A:733:LEU:HD11 | 2:A:789:VAL:CG2 | 2.48 | 0.42 |
| 2:B:225:LEU:HD12 | 2:B:264:ILE:O | 2.20 | 0.42 |
| 2:B:800:HIS:O | 2:B:802:CYS:N | 2.53 | 0.42 |
| 2:B:819:LYS:HD2 | 2:B:819:LYS:N | 2.34 | 0.42 |
| 1:C:982:C:O5' | 1:C:982:C:H6 | 2.02 | 0.42 |
| 1:D:922:C:H4' | 1:D:923:A:C5' | 2.46 | 0.42 |
| 2:A:37:TYR:OH | 2:A:536:MET:O | 2.30 | 0.42 |
| 2:A:211:ILE:HG12 | 2:A:438:GLU:O | 2.20 | 0.42 |
| 2:A:256:ARG:NH1 | 2:A:278:ARG:NH1 | 2.68 | 0.42 |
| 2:A:911:ILE:HG13 | 2:A:912:LYS:HG3 | 2.02 | 0.42 |
| 2:B:581:GLU:HG3 | 2:B:586:ILE:O | 2.20 | 0.42 |
| 2:B:616:ASN:O | 2:B:619:THR:N | 2.52 | 0.42 |
| 1:D:922:C:H5'' | 1:D:923:A:OP1 | 2.20 | 0.42 |
| 2:A:83:THR:HA | 2:A:153:THR:HG22 | 2.02 | 0.42 |
| 2:A:145:ASP:OD1 | 2:A:147:SER:N | 2.52 | 0.42 |
| 2:A:276:GLN:HE21 | 2:A:276:GLN:HB3 | 1.62 | 0.42 |
| 2:A:379:VAL:O | 2:A:383:GLY:HA3 | 2.19 | 0.42 |
| 2:A:730:LEU:HD23 | 2:A:730:LEU:HA | 1.90 | 0.42 |
| 2:A:767:TYR:OH | 2:A:782:VAL:HG21 | 2.19 | 0.42 |
| 2:A:947:THR:CG2 | 2:A:948:GLU:H | 2.33 | 0.42 |
| 2:B:176:ILE:HD13 | 2:B:520:TRP:CH2 | 2.55 | 0.42 |
| 2:B:469:TYR:HB2 | 2:B:504:ASP:O | 2.20 | 0.42 |
| 2:B:470:GLY:O | 2:B:471:ASN:C | 2.58 | 0.42 |
| 2:B:645:THR:OG1 | 2:B:688:ASP:OD1 | 2.28 | 0.42 |
| 2:B:721:GLU:HA | 2:B:721:GLU:OE2 | 2.19 | 0.42 |
| 2:B:728:TRP:O | 2:B:730:LEU:N | 2.53 | 0.42 |
| 2:B:764:LEU:HD13 | 2:B:786:LEU:CD1 | 2.48 | 0.42 |
| 2:B:766:TRP:O | 2:B:770:ARG:N | 2.45 | 0.42 |
| 2:B:890:LEU:C | 2:B:892:LYS:N | 2.71 | 0.42 |
| 2:A:544:HIS:HE1 | 2:A:593:GLU:CD | 2.23 | 0.42 |
| 2:A:560:THR:O | 2:A:563:PHE:N | 2.52 | 0.42 |
| 2:A:711:PHE:N | 2:A:711:PHE:CD1 | 2.88 | 0.42 |
| 2:A:931:LYS:NZ | 2:A:935:GLU:OE2 | 2.42 | 0.42 |
| 2:B:129:PHE:HA | 2:B:132:ALA:HB3 | 2.01 | 0.42 |
| 2:B:478:ALA:HB2 | 2:B:623:PHE:CD1 | 2.55 | 0.42 |
| 2:B:661:PHE:O | 2:B:665:ILE:HG13 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:775:ASP:OD1 | 2:B:775:ASP:O | 2.38 | 0.42 |
| 2:B:921:ILE:HD12 | 2:B:928:ARG:HH12 | 1.85 | 0.42 |
| 1:C:927:G:C6 | 1:C:928:C:C4 | 3.08 | 0.42 |
| 1:C:953:A:C5' | 1:C:954:G:OP1 | 2.68 | 0.42 |
| 2:A:12:LYS:HZ1 | 2:A:16:ARG:HH22 | 1.67 | 0.42 |
| 2:A:67:LYS:HA | 2:A:70:GLN:HB2 | 2.01 | 0.42 |
| 2:A:181:HIS:ND1 | 2:A:182:ARG:O | 2.52 | 0.42 |
| 2:A:519:PRO:HG2 | 2:A:520:TRP:CE3 | 2.55 | 0.42 |
| 2:B:147:SER:OG | 2:B:543:ARG:HG3 | 2.20 | 0.42 |
| 2:B:152:THR:HG22 | 2:B:159:PHE:CE1 | 2.55 | 0.42 |
| 2:B:277:ASP:OD2 | 2:B:462:HIS:CE1 | 2.73 | 0.42 |
| 2:B:317:ASN:O | 2:B:318:ALA:HB3 | 2.20 | 0.42 |
| 2:B:576:LYS:O | 2:B:580:LEU:HD13 | 2.20 | 0.42 |
| 2:B:714:TYR:CD1 | 2:B:780:ARG:HD3 | 2.55 | 0.42 |
| 2:B:725:ILE:CD1 | 2:B:770:ARG:NE | 2.82 | 0.42 |
| 2:B:871:TRP:CD2 | 2:B:920:ARG:NH2 | 2.80 | 0.42 |
| 1:D:923:A:O2' | 1:D:924:A:OP2 | 2.30 | 0.42 |
| 2:A:290:LYS:HE3 | 2:A:290:LYS:HB3 | 1.95 | 0.42 |
| 2:A:347:GLU:CD | 2:A:347:GLU:C | 2.78 | 0.42 |
| 2:A:402:LYS:O | 2:A:403:ALA:C | 2.58 | 0.42 |
| 2:A:418:LYS:HB3 | 2:A:422:GLU:OE2 | 2.20 | 0.42 |
| 2:A:434:LYS:HB3 | 2:A:436:ILE:CG1 | 2.46 | 0.42 |
| 2:A:708:ILE:HD12 | 2:A:791:VAL:CG2 | 2.49 | 0.42 |
| 2:A:887:MET:CE | 2:A:891:MET:HG2 | 2.49 | 0.42 |
| 2:A:924:GLU:HA | 2:A:927:LEU:HB3 | 2.02 | 0.42 |
| 2:B:32:LYS:HA | 2:B:600:TYR:CE1 | 2.55 | 0.42 |
| 2:B:567:ILE:HG21 | 2:B:594:MET:HE3 | 2.01 | 0.42 |
| 2:B:734:ASN:HD22 | 2:B:734:ASN:HA | 1.51 | 0.42 |
| 2:B:800:HIS:C | 2:B:802:CYS:N | 2.72 | 0.42 |
| 1:C:923:A:O2' | 1:C:924:A:OP2 | 2.34 | 0.41 |
| 1:C:926:G:O2' | 1:C:927:G:H5' | 2.20 | 0.41 |
| 1:D:903:G:H2' | 1:D:904:G:O4' | 2.20 | 0.41 |
| 1:D:953:A:N1 | 2:B:966:ILE:HG12 | 2.35 | 0.41 |
| 2:A:87:ILE:O | 2:A:90:ILE:HB | 2.20 | 0.41 |
| 2:A:123:ILE:HD11 | 2:A:155:LEU:HD11 | 2.02 | 0.41 |
| 2:A:235:VAL:HG11 | 2:A:431:MET:HE3 | 2.02 | 0.41 |
| 2:B:325:VAL:N | 2:B:332:ASP:OD2 | 2.51 | 0.41 |
| 2:B:553:LYS:HE3 | 2:B:553:LYS:HB3 | 1.80 | 0.41 |
| 2:B:671:ASP:HB3 | 2:B:798:THR:HG22 | 2.02 | 0.41 |
| 1:C:976:C:C2' | 1:C:977:G:H5' | 2.50 | 0.41 |
| 2:A:711:PHE:O | 2:A:784:ARG:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:824:VAL:O | 2:A:825:GLU:C | 2.57 | 0.41 |
| 2:B:412:VAL:O | 2:B:416:GLU:OE1 | 2.37 | 0.41 |
| 2:B:677:ILE:HD13 | 2:B:677:ILE:HA | 1.85 | 0.41 |
| 2:B:728:TRP:HE3 | 2:B:729:MET:N | 2.18 | 0.41 |
| 2:B:768:LEU:O | 2:B:770:ARG:N | 2.52 | 0.41 |
| 2:B:803:GLU:CD | 2:B:815:VAL:HG12 | 2.41 | 0.41 |
| 2:B:824:VAL:HG12 | 2:B:825:GLU:N | 2.35 | 0.41 |
| 2:B:825:GLU:O | 2:B:825:GLU:CG | 2.68 | 0.41 |
| 1:C:970:A:O2' | 1:C:971:A:O5' | 2.38 | 0.41 |
| 1:D:988:A:N7 | 2:B:529:LEU:HD21 | 2.36 | 0.41 |
| 2:A:9:ILE:HD13 | 2:A:804:GLU:HG2 | 2.02 | 0.41 |
| 2:A:236:TYR:CE2 | 2:A:414:PRO:HG2 | 2.55 | 0.41 |
| 2:A:250:VAL:CG1 | 2:A:285:GLU:HG3 | 2.50 | 0.41 |
| 2:A:264:ILE:O | 2:A:264:ILE:HG22 | 2.18 | 0.41 |
| 2:A:341:ARG:HD3 | 2:A:341:ARG:N | 2.36 | 0.41 |
| 2:A:691:ARG:O | 2:A:694:VAL:CG1 | 2.64 | 0.41 |
| 2:A:871:TRP:CE3 | 2:A:920:ARG:NH2 | 2.88 | 0.41 |
| 2:B:263:TRP:N | 2:B:263:TRP:CD1 | 2.88 | 0.41 |
| 2:B:264:ILE:HG23 | 2:B:286:PHE:CE2 | 2.55 | 0.41 |
| 2:B:289:GLU:OE2 | 2:B:289:GLU:N | 2.53 | 0.41 |
| 2:B:934:MET:O | 2:B:938:LEU:HD13 | 2.21 | 0.41 |
| 2:A:12:LYS:NZ | 2:A:16:ARG:HH2 | 2.18 | 0.41 |
| 2:A:148:ARG:HB3 | 2:A:542:SER:HB3 | 2.02 | 0.41 |
| 2:A:459:LYS:CG | 2:A:460:ILE:N | 2.83 | 0.41 |
| 2:A:499:ILE:HG12 | 2:A:615:PRO:HA | 2.02 | 0.41 |
| 2:A:710:GLN:O | 2:A:711:PHE:C | 2.57 | 0.41 |
| 2:A:909:LYS:NZ | 2:A:913:GLU:O | 2.52 | 0.41 |
| 2:B:173:LYS:HD2 | 2:B:175:TYR:HE2 | 1.85 | 0.41 |
| 2:B:212:ILE:CD1 | 2:B:235:VAL:HG12 | 2.47 | 0.41 |
| 2:B:510:ARG:HA | 2:B:510:ARG:HE | 1.84 | 0.41 |
| 2:B:730:LEU:O | 2:B:827:TRP:NE1 | 2.53 | 0.41 |
| 2:B:847:LYS:HE3 | 2:B:847:LYS:HB2 | 1.89 | 0.41 |
| 1:C:987:C:H5 | 2:A:506:LYS:NZ | 2.18 | 0.41 |
| 2:A:16:ARG:NH1 | 2:A:16:ARG:HG3 | 2.36 | 0.41 |
| 2:A:45:LEU:HD13 | 2:A:130:MET:CB | 2.51 | 0.41 |
| 2:A:61:ASP:O | 2:A:64:ALA:N | 2.53 | 0.41 |
| 2:A:317:ASN:O | 2:A:318:ALA:HB3 | 2.21 | 0.41 |
| 2:A:395:GLN:HG3 | 2:A:396:ALA:N | 2.34 | 0.41 |
| 2:A:410:PHE:CZ | 2:A:412:VAL:HG21 | 2.54 | 0.41 |
| 2:A:574:GLU:HA | 2:A:577:GLU:OE1 | 2.20 | 0.41 |
| 2:A:767:TYR:OH | 2:A:782:VAL:HG11 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:182:ARG:O | 2:B:183:VAL:CB | 2.69 | 0.41 |
| 2:B:506:LYS:HE3 | 2:B:527:GLU:OE1 | 2.21 | 0.41 |
| 2:B:570:GLU:OE1 | 2:B:576:LYS:HG3 | 2.20 | 0.41 |
| 2:B:774:ARG:CG | 2:B:775:ASP:N | 2.84 | 0.41 |
| 1:C:960:C:H2' | 1:C:971:A:H1' | 2.03 | 0.41 |
| 1:D:902:C:H2' | 1:D:903:G:C5' | 2.51 | 0.41 |
| 2:A:540:THR:HG21 | 2:A:598:PHE:CD1 | 2.55 | 0.41 |
| 2:A:544:HIS:CE1 | 2:A:593:GLU:OE2 | 2.73 | 0.41 |
| 2:A:711:PHE:HA | 2:A:714:TYR:CE2 | 2.56 | 0.41 |
| 2:B:196:HIS:CD2 | 2:B:197:ASP:N | 2.89 | 0.41 |
| 2:B:241:MET:HG3 | 2:B:296:VAL:CG2 | 2.51 | 0.41 |
| 2:B:725:ILE:HD13 | 2:B:770:ARG:NE | 2.36 | 0.41 |
| 2:B:884:LYS:C | 2:B:886:SER:N | 2.73 | 0.41 |
| 1:C:920:G:OP1 | 1:C:920:G:C4' | 2.68 | 0.41 |
| 2:A:7:LYS:HB2 | 2:A:7:LYS:HZ3 | 1.85 | 0.41 |
| 2:A:412:VAL:H | 2:A:416:GLU:HG2 | 1.86 | 0.41 |
| 2:A:612:ASP:OD1 | 2:A:613:LEU:HD23 | 2.21 | 0.41 |
| 2:A:614:ILE:N | 2:A:615:PRO:CD | 2.83 | 0.41 |
| 2:A:950:LYS:H | 2:A:953:LYS:HZ3 | 1.68 | 0.41 |
| 2:B:136:THR:HG23 | 2:B:662:ILE:HB | 2.02 | 0.41 |
| 2:B:856:GLU:O | 2:B:857:ASN:O | 2.38 | 0.41 |
| 2:B:863:ILE:HG13 | 2:B:945:ASN:HA | 2.03 | 0.41 |
| 2:B:880:LYS:O | 2:B:881:ARG:C | 2.59 | 0.41 |
| 1:D:944:C:OP1 | 2:B:765:ARG:HD3 | 2.20 | 0.41 |
| 2:A:116:LEU:C | 2:A:116:LEU:HD23 | 2.41 | 0.41 |
| 2:A:181:HIS:HD2 | 2:A:466:PHE:CE1 | 2.38 | 0.41 |
| 2:A:382:LEU:C | 2:A:384:ILE:N | 2.74 | 0.41 |
| 2:A:405:TYR:HE2 | 2:A:424:LYS:HZ3 | 1.68 | 0.41 |
| 2:A:626:VAL:HG12 | 2:A:634:TRP:CD2 | 2.56 | 0.41 |
| 2:A:676:TYR:O | 2:A:679:SER:HB3 | 2.21 | 0.41 |
| 2:A:793:LEU:HD23 | 2:A:821:PRO:HG3 | 2.03 | 0.41 |
| 2:A:884:LYS:O | 2:A:885:SER:C | 2.58 | 0.41 |
| 2:B:65:ARG:HA | 2:B:68:ARG:HH11 | 1.81 | 0.41 |
| 2:B:276:GLN:HE21 | 2:B:460:ILE:HD11 | 1.86 | 0.41 |
| 2:B:471:ASN:C | 2:B:471:ASN:HD22 | 2.23 | 0.41 |
| 2:B:623:PHE:O | 2:B:626:VAL:HG22 | 2.21 | 0.41 |
| 2:B:860:ARG:HH21 | 2:B:860:ARG:HB2 | 1.86 | 0.41 |
| 1:C:914:A:H1' | 1:C:925:A:N1 | 2.36 | 0.41 |
| 1:C:958:U:C2' | 1:C:959:U:O5' | 2.68 | 0.41 |
| 1:D:925:A:H2' | 1:D:926:G:O4' | 2.21 | 0.41 |
| 2:A:112:PRO:HD2 | 2:A:115:ILE:HD12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:175:TYR:CE1 | 2:A:474:TRP:HB2 | 2.56 | 0.41 |
| 2:A:293:GLY:O | 2:A:295:TYR:CD1 | 2.74 | 0.41 |
| 2:A:406:HIS:ND1 | 2:A:421:GLN:OE1 | 2.54 | 0.41 |
| 2:A:467:ILE:CG1 | 2:A:508:CYS:HB3 | 2.50 | 0.41 |
| 2:A:644:GLY:HA2 | 2:A:687:PHE:O | 2.20 | 0.41 |
| 2:A:714:TYR:CE1 | 2:A:780:ARG:HG2 | 2.56 | 0.41 |
| 2:A:831:THR:O | 2:A:834:ALA:HB3 | 2.21 | 0.41 |
| 2:A:872:LYS:O | 2:A:876:VAL:CG2 | 2.65 | 0.41 |
| 2:A:872:LYS:HA | 2:A:875:GLU:CD | 2.41 | 0.41 |
| 2:A:882:ASP:C | 2:A:883:PHE:HD1 | 2.24 | 0.41 |
| 2:B:560:THR:HB | 2:B:561:PRO:CD | 2.51 | 0.41 |
| 2:B:652:SER:HG | 2:B:655:LYS:HB2 | 1.85 | 0.41 |
| 2:B:725:ILE:HB | 2:B:929:GLU:OE1 | 2.20 | 0.41 |
| 2:B:749:THR:O | 2:B:750:ARG:C | 2.57 | 0.41 |
| 2:B:846:ILE:HD12 | 2:B:938:LEU:CD2 | 2.51 | 0.41 |
| 2:B:849:ILE:HD12 | 2:B:964:ILE:CD1 | 2.51 | 0.41 |
| 2:B:944:ILE:HG22 | 2:B:945:ASN:N | 2.36 | 0.41 |
| 2:B:964:ILE:HG13 | 2:B:965:PHE:N | 2.34 | 0.41 |
| 2:A:135:GLU:O | 2:A:139:ARG:HB2 | 2.21 | 0.41 |
| 2:A:168:TRP:CZ3 | 2:A:520:TRP:CE3 | 3.09 | 0.41 |
| 2:A:173:LYS:CB | 2:A:175:TYR:CE2 | 3.04 | 0.41 |
| 2:A:232:PRO:O | 2:A:235:VAL:HG22 | 2.21 | 0.41 |
| 2:A:252:ALA:HB1 | 2:A:281:GLU:O | 2.21 | 0.41 |
| 2:B:412:VAL:O | 2:B:413:PRO:C | 2.60 | 0.41 |
| 2:B:488:LEU:HA | 2:B:488:LEU:HD23 | 1.81 | 0.41 |
| 2:B:771:THR:HB | 2:B:774:ARG:HD3 | 2.03 | 0.41 |
| 2:B:786:LEU:HD23 | 2:B:786:LEU:C | 2.41 | 0.41 |
| 2:B:846:ILE:HA | 2:B:849:ILE:HD12 | 2.03 | 0.41 |
| 2:B:870:LYS:HE3 | 2:B:905:LYS:CE | 2.40 | 0.41 |
| 1:C:980:C:H2' | 1:C:981:C:H6 | 1.86 | 0.40 |
| 1:C:986:C:C2 | 2:A:507:ALA:N | 2.89 | 0.40 |
| 2:A:9:ILE:O | 2:A:12:LYS:HB3 | 2.22 | 0.40 |
| 2:A:345:ILE:O | 2:A:346:LEU:HB2 | 2.20 | 0.40 |
| 2:A:581:GLU:HG3 | 2:A:586:ILE:O | 2.21 | 0.40 |
| 2:B:152:THR:HG22 | 2:B:159:PHE:CZ | 2.56 | 0.40 |
| 2:B:155:LEU:C | 2:B:157:PRO:HD3 | 2.42 | 0.40 |
| 2:B:240:ASN:O | 2:B:324:SER:HB3 | 2.21 | 0.40 |
| 2:B:334:VAL:HG13 | 2:B:388:LYS:O | 2.20 | 0.40 |
| 2:B:381:LYS:HD2 | 2:B:381:LYS:C | 2.40 | 0.40 |
| 2:B:482:LEU:HD23 | 2:B:482:LEU:C | 2.41 | 0.40 |
| 2:B:704:PHE:HD1 | 2:B:790:TRP:CH2 | 2.39 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:914:ARG:HH21 | 2:B:915:THR:CG2 | 2.27 | 0.40 |
| 2:B:914:ARG:CZ | 2:B:915:THR:O | 2.69 | 0.40 |
| 2:B:914:ARG:NH2 | 2:B:915:THR:HG23 | 2.29 | 0.40 |
| 2:B:949:ASP:HB2 | 2:B:954:LYS:CE | 2.45 | 0.40 |
| 2:A:9:ILE:O | 2:A:10:GLU:C | 2.60 | 0.40 |
| 2:A:232:PRO:CG | 2:A:428:ALA:HB2 | 2.51 | 0.40 |
| 2:A:339:LEU:N | 2:A:339:LEU:HD13 | 2.36 | 0.40 |
| 2:A:646:LEU:O | 2:A:647:GLU:CB | 2.69 | 0.40 |
| 2:A:713:GLU:O | 2:A:714:TYR:O | 2.40 | 0.40 |
| 2:A:733:LEU:HD11 | 2:A:789:VAL:HB | 2.02 | 0.40 |
| 2:A:803:GLU:HA | 2:A:803:GLU:OE1 | 2.20 | 0.40 |
| 2:A:824:VAL:CG1 | 2:A:825:GLU:N | 2.84 | 0.40 |
| 2:A:914:ARG:HH21 | 2:A:915:THR:C | 2.25 | 0.40 |
| 2:B:497:GLU:O | 2:B:500:ILE:N | 2.54 | 0.40 |
| 2:A:50:HIS:H | 2:A:53:HIS:HD2 | 1.68 | 0.40 |
| 2:A:173:LYS:HD3 | 2:A:175:TYR:HE2 | 1.86 | 0.40 |
| 2:A:441:TYR:O | 2:A:442:GLU:OE2 | 2.40 | 0.40 |
| 2:A:959:PRO:O | 2:A:960:LEU:HB2 | 2.20 | 0.40 |
| 2:B:13:TRP:CZ2 | 2:B:803:GLU:HB3 | 2.53 | 0.40 |
| 2:B:186:ASP:CB | 2:B:193:LEU:HD11 | 2.42 | 0.40 |
| 2:B:216:LEU:HB2 | 2:B:296:VAL:HG12 | 2.04 | 0.40 |
| 2:B:337:GLU:O | 2:B:339:LEU:HD12 | 2.21 | 0.40 |
| 2:B:461:ILE:HB | 2:B:464:GLN:HB2 | 2.03 | 0.40 |
| 2:B:597:GLU:O | 2:B:600:TYR:N | 2.53 | 0.40 |
| 2:B:783:LEU:CD1 | 2:B:783:LEU:N | 2.84 | 0.40 |
| 2:B:871:TRP:HZ3 | 2:B:918:VAL:HA | 1.87 | 0.40 |
| 2:B:915:THR:O | 2:B:916:PHE:CD2 | 2.74 | 0.40 |
| 2:A:14:GLN:HG3 | 2:A:14:GLN:H | 1.61 | 0.40 |
| 2:A:77:PRO:HG3 | 2:A:539:TYR:CD1 | 2.56 | 0.40 |
| 2:A:217:ARG:HE | 2:A:217:ARG:HB3 | 1.62 | 0.40 |
| 2:A:497:GLU:O | 2:A:500:ILE:N | 2.54 | 0.40 |
| 2:A:518:LEU:C | 2:A:520:TRP:H | 2.24 | 0.40 |
| 2:A:918:VAL:HG11 | 2:A:920:ARG:NH1 | 2.37 | 0.40 |
| 2:A:953:LYS:O | 2:A:954:LYS:C | 2.59 | 0.40 |
| 2:B:48:HIS:NE2 | 2:B:132:ALA:HB1 | 2.36 | 0.40 |
| 2:B:70:GLN:HB3 | 2:B:72:TYR:CE1 | 2.56 | 0.40 |
| 2:B:349:TYR:O | 2:B:349:TYR:CG | 2.74 | 0.40 |
| 2:B:555:ASP:OD2 | 2:B:557:GLU:HB2 | 2.22 | 0.40 |
| 2:B:718:GLY:O | 2:B:719:ASN:C | 2.60 | 0.40 |
| 2:B:849:ILE:HD12 | 2:B:964:ILE:HD11 | 2.04 | 0.40 |
| 2:A:96:ASN:N | 2:A:96:ASN:ND2 | 2.70 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:A:330:PRO:HD3 | 2:A:400:ILE:HG12 | 2.04 | 0.40 |
| 2:A:559:LEU:HA | 2:A:563:PHE:CD2 | 2.57 | 0.40 |
| 2:A:867:GLU:N | 2:A:867:GLU:OE1 | 2.38 | 0.40 |
| 2:B:44:TYR:O | 2:B:46:SER:N | 2.54 | 0.40 |
| 2:B:525:VAL:O | 2:B:525:VAL:HG13 | 2.22 | 0.40 |
| 2:B:646:LEU:O | 2:B:647:GLU:CB | 2.69 | 0.40 |
| 2:B:724:ASP:C | 2:B:726:ASP:N | 2.75 | 0.40 |
| 2:B:780:ARG:O | 2:B:781:TYR:C | 2.59 | 0.40 |
| 2:B:919:LYS:NZ | 2:B:960:LEU:HD11 | 2.36 | 0.40 |
| 2:B:921:ILE:O | 2:B:924:GLU:CB | 2.69 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-----------|-------------------|
| 2 | A | 944/967 (98%) | 630 (67%) | 211 (22%) | 103 (11%) | 0 2 |
| 2 | B | 944/967 (98%) | 632 (67%) | 208 (22%) | 104 (11%) | 0 2 |
| All | All | 1888/1934 (98%) | 1262 (67%) | 419 (22%) | 207 (11%) | 0 2 |

All (207) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 74 | VAL |
| 2 | A | 110 | LYS |
| 2 | A | 143 | SER |
| 2 | A | 183 | VAL |
| 2 | A | 188 | VAL |
| 2 | A | 276 | GLN |
| 2 | A | 333 | HIS |
| 2 | A | 347 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 377 | GLU |
| 2 | A | 378 | GLU |
| 2 | A | 552 | GLY |
| 2 | A | 630 | ARG |
| 2 | A | 714 | TYR |
| 2 | A | 854 | LYS |
| 2 | A | 867 | GLU |
| 2 | A | 871 | TRP |
| 2 | A | 883 | PHE |
| 2 | A | 913 | GLU |
| 2 | A | 914 | ARG |
| 2 | A | 929 | GLU |
| 2 | A | 953 | LYS |
| 2 | B | 45 | LEU |
| 2 | B | 74 | VAL |
| 2 | B | 110 | LYS |
| 2 | B | 183 | VAL |
| 2 | B | 188 | VAL |
| 2 | B | 276 | GLN |
| 2 | B | 333 | HIS |
| 2 | B | 347 | GLU |
| 2 | B | 377 | GLU |
| 2 | B | 378 | GLU |
| 2 | B | 552 | GLY |
| 2 | B | 630 | ARG |
| 2 | B | 714 | TYR |
| 2 | B | 854 | LYS |
| 2 | B | 867 | GLU |
| 2 | B | 871 | TRP |
| 2 | B | 883 | PHE |
| 2 | B | 913 | GLU |
| 2 | B | 914 | ARG |
| 2 | B | 929 | GLU |
| 2 | B | 953 | LYS |
| 2 | A | 45 | LEU |
| 2 | A | 113 | GLU |
| 2 | A | 181 | HIS |
| 2 | A | 201 | GLY |
| 2 | A | 219 | ASN |
| 2 | A | 301 | SER |
| 2 | A | 343 | THR |
| 2 | A | 374 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 376 | VAL |
| 2 | A | 415 | TYR |
| 2 | A | 464 | GLN |
| 2 | A | 494 | ALA |
| 2 | A | 502 | TRP |
| 2 | A | 528 | SER |
| 2 | A | 529 | LEU |
| 2 | A | 568 | PHE |
| 2 | A | 616 | ASN |
| 2 | A | 711 | PHE |
| 2 | A | 782 | VAL |
| 2 | A | 857 | ASN |
| 2 | A | 868 | ASP |
| 2 | A | 869 | TRP |
| 2 | A | 885 | SER |
| 2 | A | 900 | GLY |
| 2 | A | 921 | ILE |
| 2 | A | 922 | ASN |
| 2 | A | 950 | LYS |
| 2 | A | 954 | LYS |
| 2 | A | 955 | LYS |
| 2 | B | 113 | GLU |
| 2 | B | 143 | SER |
| 2 | B | 181 | HIS |
| 2 | B | 201 | GLY |
| 2 | B | 219 | ASN |
| 2 | B | 301 | SER |
| 2 | B | 343 | THR |
| 2 | B | 374 | PRO |
| 2 | B | 376 | VAL |
| 2 | B | 415 | TYR |
| 2 | B | 464 | GLN |
| 2 | B | 502 | TRP |
| 2 | B | 528 | SER |
| 2 | B | 529 | LEU |
| 2 | B | 568 | PHE |
| 2 | B | 616 | ASN |
| 2 | B | 782 | VAL |
| 2 | B | 857 | ASN |
| 2 | B | 868 | ASP |
| 2 | B | 869 | TRP |
| 2 | B | 885 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 900 | GLY |
| 2 | B | 921 | ILE |
| 2 | B | 922 | ASN |
| 2 | B | 950 | LYS |
| 2 | B | 954 | LYS |
| 2 | B | 955 | LYS |
| 2 | A | 73 | ASN |
| 2 | A | 223 | ILE |
| 2 | A | 240 | ASN |
| 2 | A | 453 | GLY |
| 2 | A | 482 | LEU |
| 2 | A | 558 | LYS |
| 2 | A | 631 | GLU |
| 2 | A | 775 | ASP |
| 2 | A | 825 | GLU |
| 2 | A | 895 | GLU |
| 2 | A | 911 | ILE |
| 2 | B | 73 | ASN |
| 2 | B | 96 | ASN |
| 2 | B | 220 | GLY |
| 2 | B | 223 | ILE |
| 2 | B | 240 | ASN |
| 2 | B | 453 | GLY |
| 2 | B | 494 | ALA |
| 2 | B | 558 | LYS |
| 2 | B | 631 | GLU |
| 2 | B | 711 | PHE |
| 2 | B | 775 | ASP |
| 2 | B | 825 | GLU |
| 2 | B | 891 | MET |
| 2 | B | 895 | GLU |
| 2 | B | 911 | ILE |
| 2 | A | 85 | SER |
| 2 | A | 96 | ASN |
| 2 | A | 117 | TRP |
| 2 | A | 220 | GLY |
| 2 | A | 283 | ILE |
| 2 | A | 421 | GLN |
| 2 | A | 542 | SER |
| 2 | A | 623 | PHE |
| 2 | A | 670 | ALA |
| 2 | A | 719 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 856 | GLU |
| 2 | A | 881 | ARG |
| 2 | A | 891 | MET |
| 2 | A | 903 | VAL |
| 2 | A | 907 | VAL |
| 2 | B | 85 | SER |
| 2 | B | 117 | TRP |
| 2 | B | 421 | GLN |
| 2 | B | 482 | LEU |
| 2 | B | 623 | PHE |
| 2 | B | 670 | ALA |
| 2 | B | 719 | ASN |
| 2 | B | 790 | TRP |
| 2 | B | 856 | GLU |
| 2 | B | 881 | ARG |
| 2 | B | 903 | VAL |
| 2 | B | 907 | VAL |
| 2 | A | 157 | PRO |
| 2 | A | 337 | GLU |
| 2 | A | 339 | LEU |
| 2 | A | 394 | GLU |
| 2 | A | 452 | PHE |
| 2 | A | 519 | PRO |
| 2 | A | 790 | TRP |
| 2 | A | 878 | SER |
| 2 | A | 898 | LYS |
| 2 | B | 157 | PRO |
| 2 | B | 283 | ILE |
| 2 | B | 339 | LEU |
| 2 | B | 403 | ALA |
| 2 | B | 452 | PHE |
| 2 | B | 519 | PRO |
| 2 | B | 540 | THR |
| 2 | B | 542 | SER |
| 2 | B | 743 | ALA |
| 2 | B | 878 | SER |
| 2 | A | 303 | ASP |
| 2 | A | 403 | ALA |
| 2 | A | 743 | ALA |
| 2 | A | 813 | GLY |
| 2 | B | 337 | GLU |
| 2 | B | 394 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 495 | GLN |
| 2 | A | 945 | ASN |
| 2 | A | 946 | PRO |
| 2 | B | 945 | ASN |
| 2 | B | 946 | PRO |
| 2 | A | 88 | VAL |
| 2 | A | 471 | ASN |
| 2 | A | 522 | PRO |
| 2 | A | 823 | PRO |
| 2 | B | 471 | ASN |
| 2 | B | 522 | PRO |
| 2 | B | 789 | VAL |
| 2 | A | 302 | GLY |
| 2 | A | 353 | PRO |
| 2 | A | 355 | ILE |
| 2 | A | 384 | ILE |
| 2 | B | 222 | VAL |
| 2 | B | 302 | GLY |
| 2 | B | 353 | PRO |
| 2 | B | 355 | ILE |
| 2 | B | 384 | ILE |
| 2 | A | 115 | ILE |
| 2 | A | 222 | VAL |
| 2 | A | 329 | ALA |
| 2 | A | 330 | PRO |
| 2 | B | 88 | VAL |
| 2 | B | 115 | ILE |
| 2 | B | 329 | ALA |
| 2 | B | 330 | PRO |
| 2 | B | 813 | GLY |
| 2 | B | 823 | PRO |

5.3.2 Protein sidechains [i](#)

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.

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2 | A | 841/857 (98%) | 731 (87%) | 110 (13%) | 4 | 18 |
| 2 | B | 841/857 (98%) | 752 (89%) | 89 (11%) | 6 | 27 |
| All | All | 1682/1714 (98%) | 1483 (88%) | 199 (12%) | 5 | 22 |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 16 | ARG |
| 2 | A | 28 | ARG |
| 2 | A | 29 | ASP |
| 2 | A | 35 | LYS |
| 2 | A | 37 | TYR |
| 2 | A | 38 | ILE |
| 2 | A | 42 | PHE |
| 2 | A | 70 | GLN |
| 2 | A | 75 | LEU |
| 2 | A | 77 | PRO |
| 2 | A | 107 | ASP |
| 2 | A | 124 | ASN |
| 2 | A | 135 | GLU |
| 2 | A | 138 | ILE |
| 2 | A | 139 | ARG |
| 2 | A | 157 | PRO |
| 2 | A | 172 | GLU |
| 2 | A | 173 | LYS |
| 2 | A | 183 | VAL |
| 2 | A | 196 | HIS |
| 2 | A | 203 | ASP |
| 2 | A | 213 | LYS |
| 2 | A | 217 | ARG |
| 2 | A | 230 | LEU |
| 2 | A | 233 | GLU |
| 2 | A | 234 | THR |
| 2 | A | 239 | THR |
| 2 | A | 246 | ASN |
| 2 | A | 276 | GLN |
| 2 | A | 278 | ARG |
| 2 | A | 289 | GLU |
| 2 | A | 294 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 317 | ASN |
| 2 | A | 331 | PHE |
| 2 | A | 339 | LEU |
| 2 | A | 341 | ARG |
| 2 | A | 347 | GLU |
| 2 | A | 349 | TYR |
| 2 | A | 373 | PHE |
| 2 | A | 381 | LYS |
| 2 | A | 433 | GLU |
| 2 | A | 446 | LYS |
| 2 | A | 455 | ARG |
| 2 | A | 463 | ASP |
| 2 | A | 492 | ARG |
| 2 | A | 527 | GLU |
| 2 | A | 529 | LEU |
| 2 | A | 531 | ASP |
| 2 | A | 536 | MET |
| 2 | A | 540 | THR |
| 2 | A | 551 | GLU |
| 2 | A | 562 | GLU |
| 2 | A | 569 | LEU |
| 2 | A | 590 | ILE |
| 2 | A | 602 | TYR |
| 2 | A | 616 | ASN |
| 2 | A | 624 | ASN |
| 2 | A | 625 | HIS |
| 2 | A | 636 | LYS |
| 2 | A | 640 | VAL |
| 2 | A | 645 | THR |
| 2 | A | 649 | GLN |
| 2 | A | 658 | VAL |
| 2 | A | 678 | MET |
| 2 | A | 679 | SER |
| 2 | A | 685 | SER |
| 2 | A | 691 | ARG |
| 2 | A | 700 | GLN |
| 2 | A | 703 | ARG |
| 2 | A | 707 | LEU |
| 2 | A | 720 | VAL |
| 2 | A | 722 | LEU |
| 2 | A | 727 | ARG |
| 2 | A | 732 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 733 | LEU |
| 2 | A | 744 | LEU |
| 2 | A | 747 | PHE |
| 2 | A | 771 | THR |
| 2 | A | 776 | ASP |
| 2 | A | 784 | ARG |
| 2 | A | 792 | ARG |
| 2 | A | 809 | LEU |
| 2 | A | 815 | VAL |
| 2 | A | 817 | LEU |
| 2 | A | 819 | LYS |
| 2 | A | 820 | TRP |
| 2 | A | 823 | PRO |
| 2 | A | 825 | GLU |
| 2 | A | 826 | GLU |
| 2 | A | 828 | TRP |
| 2 | A | 829 | ASN |
| 2 | A | 852 | VAL |
| 2 | A | 860 | ARG |
| 2 | A | 862 | TYR |
| 2 | A | 869 | TRP |
| 2 | A | 872 | LYS |
| 2 | A | 879 | GLU |
| 2 | A | 881 | ARG |
| 2 | A | 884 | LYS |
| 2 | A | 910 | LEU |
| 2 | A | 916 | PHE |
| 2 | A | 917 | ASP |
| 2 | A | 919 | LYS |
| 2 | A | 922 | ASN |
| 2 | A | 923 | GLU |
| 2 | A | 932 | GLU |
| 2 | A | 933 | PHE |
| 2 | A | 942 | ILE |
| 2 | A | 953 | LYS |
| 2 | A | 964 | ILE |
| 2 | B | 7 | LYS |
| 2 | B | 18 | LEU |
| 2 | B | 42 | PHE |
| 2 | B | 44 | TYR |
| 2 | B | 70 | GLN |
| 2 | B | 97 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 139 | ARG |
| 2 | B | 151 | TYR |
| 2 | B | 172 | GLU |
| 2 | B | 196 | HIS |
| 2 | B | 197 | ASP |
| 2 | B | 203 | ASP |
| 2 | B | 213 | LYS |
| 2 | B | 218 | GLU |
| 2 | B | 230 | LEU |
| 2 | B | 233 | GLU |
| 2 | B | 234 | THR |
| 2 | B | 271 | TYR |
| 2 | B | 276 | GLN |
| 2 | B | 285 | GLU |
| 2 | B | 298 | ASN |
| 2 | B | 303 | ASP |
| 2 | B | 331 | PHE |
| 2 | B | 332 | ASP |
| 2 | B | 338 | ASP |
| 2 | B | 339 | LEU |
| 2 | B | 341 | ARG |
| 2 | B | 347 | GLU |
| 2 | B | 381 | LYS |
| 2 | B | 405 | TYR |
| 2 | B | 415 | TYR |
| 2 | B | 429 | LYS |
| 2 | B | 451 | ARG |
| 2 | B | 471 | ASN |
| 2 | B | 479 | ARG |
| 2 | B | 504 | ASP |
| 2 | B | 505 | LYS |
| 2 | B | 510 | ARG |
| 2 | B | 511 | LYS |
| 2 | B | 528 | SER |
| 2 | B | 533 | THR |
| 2 | B | 536 | MET |
| 2 | B | 540 | THR |
| 2 | B | 546 | ASN |
| 2 | B | 547 | LYS |
| 2 | B | 551 | GLU |
| 2 | B | 557 | GLU |
| 2 | B | 565 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 599 | GLU |
| 2 | B | 602 | TYR |
| 2 | B | 607 | ARG |
| 2 | B | 624 | ASN |
| 2 | B | 625 | HIS |
| 2 | B | 630 | ARG |
| 2 | B | 641 | ASN |
| 2 | B | 649 | GLN |
| 2 | B | 650 | LYS |
| 2 | B | 658 | VAL |
| 2 | B | 674 | ARG |
| 2 | B | 675 | LEU |
| 2 | B | 690 | ARG |
| 2 | B | 703 | ARG |
| 2 | B | 714 | TYR |
| 2 | B | 722 | LEU |
| 2 | B | 726 | ASP |
| 2 | B | 729 | MET |
| 2 | B | 734 | ASN |
| 2 | B | 744 | LEU |
| 2 | B | 748 | ARG |
| 2 | B | 750 | ARG |
| 2 | B | 812 | GLU |
| 2 | B | 819 | LYS |
| 2 | B | 820 | TRP |
| 2 | B | 825 | GLU |
| 2 | B | 826 | GLU |
| 2 | B | 828 | TRP |
| 2 | B | 829 | ASN |
| 2 | B | 855 | ILE |
| 2 | B | 860 | ARG |
| 2 | B | 869 | TRP |
| 2 | B | 885 | SER |
| 2 | B | 886 | SER |
| 2 | B | 889 | GLU |
| 2 | B | 917 | ASP |
| 2 | B | 919 | LYS |
| 2 | B | 920 | ARG |
| 2 | B | 940 | ILE |
| 2 | B | 953 | LYS |
| 2 | B | 964 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 5 | ASN |
| 2 | A | 53 | HIS |
| 2 | A | 70 | GLN |
| 2 | A | 73 | ASN |
| 2 | A | 81 | HIS |
| 2 | A | 96 | ASN |
| 2 | A | 124 | ASN |
| 2 | A | 166 | GLN |
| 2 | A | 196 | HIS |
| 2 | A | 219 | ASN |
| 2 | A | 276 | GLN |
| 2 | A | 317 | ASN |
| 2 | A | 421 | GLN |
| 2 | A | 447 | ASN |
| 2 | A | 464 | GLN |
| 2 | A | 544 | HIS |
| 2 | A | 546 | ASN |
| 2 | A | 616 | ASN |
| 2 | A | 624 | ASN |
| 2 | A | 625 | HIS |
| 2 | A | 683 | HIS |
| 2 | A | 731 | HIS |
| 2 | A | 742 | ASN |
| 2 | A | 800 | HIS |
| 2 | A | 922 | ASN |
| 2 | B | 53 | HIS |
| 2 | B | 70 | GLN |
| 2 | B | 73 | ASN |
| 2 | B | 124 | ASN |
| 2 | B | 166 | GLN |
| 2 | B | 196 | HIS |
| 2 | B | 276 | GLN |
| 2 | B | 298 | ASN |
| 2 | B | 317 | ASN |
| 2 | B | 387 | GLN |
| 2 | B | 421 | GLN |
| 2 | B | 447 | ASN |
| 2 | B | 471 | ASN |
| 2 | B | 495 | GLN |
| 2 | B | 546 | ASN |
| 2 | B | 616 | ASN |
| 2 | B | 731 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 734 | ASN |
| 2 | B | 742 | ASN |
| 2 | B | 908 | GLN |
| 2 | B | 922 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1 | C | 87/88 (98%) | 24 (27%) | 7 (8%) |
| 1 | D | 87/88 (98%) | 22 (25%) | 8 (9%) |
| All | All | 174/176 (98%) | 46 (26%) | 15 (8%) |

All (46) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 907 | G |
| 1 | C | 908 | U |
| 1 | C | 910 | G |
| 1 | C | 916 | C |
| 1 | C | 917 | C |
| 1 | C | 918 | U |
| 1 | C | 919 | G |
| 1 | C | 920 | G |
| 1 | C | 921 | U |
| 1 | C | 922 | C |
| 1 | C | 923 | A |
| 1 | C | 924 | A |
| 1 | C | 936 | U |
| 1 | C | 937 | C |
| 1 | C | 952 | U |
| 1 | C | 953 | A |
| 1 | C | 954 | G |
| 1 | C | 961 | C |
| 1 | C | 968 | C |
| 1 | C | 971 | A |
| 1 | C | 972 | U |
| 1 | C | 983 | G |
| 1 | C | 987 | C |
| 1 | C | 988 | A |
| 1 | D | 903 | G |
| 1 | D | 905 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 908 | U |
| 1 | D | 909 | U |
| 1 | D | 910 | G |
| 1 | D | 917 | C |
| 1 | D | 918 | U |
| 1 | D | 919 | G |
| 1 | D | 920 | G |
| 1 | D | 921 | U |
| 1 | D | 923 | A |
| 1 | D | 924 | A |
| 1 | D | 936 | U |
| 1 | D | 952 | U |
| 1 | D | 961 | C |
| 1 | D | 971 | A |
| 1 | D | 972 | U |
| 1 | D | 973 | C |
| 1 | D | 984 | C |
| 1 | D | 985 | A |
| 1 | D | 987 | C |
| 1 | D | 988 | A |

All (15) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 907 | G |
| 1 | C | 922 | C |
| 1 | C | 923 | A |
| 1 | C | 953 | A |
| 1 | C | 960 | C |
| 1 | C | 970 | A |
| 1 | C | 972 | U |
| 1 | D | 907 | G |
| 1 | D | 920 | G |
| 1 | D | 922 | C |
| 1 | D | 923 | A |
| 1 | D | 953 | A |
| 1 | D | 960 | C |
| 1 | D | 970 | A |
| 1 | D | 972 | U |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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 | C | 88/88 (100%) | 0.20 | 4 (4%) 33 21 | 53, 78, 126, 149 | 0 |
| 1 | D | 88/88 (100%) | 0.41 | 7 (7%) 12 7 | 53, 91, 146, 150 | 0 |
| 2 | A | 948/967 (98%) | -0.09 | 26 (2%) 54 40 | 8, 59, 131, 150 | 0 |
| 2 | B | 948/967 (98%) | 0.26 | 53 (5%) 24 14 | 48, 102, 149, 150 | 0 |
| All | All | 2072/2110 (98%) | 0.10 | 90 (4%) 35 23 | 8, 82, 143, 150 | 0 |

All (90) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | A | 407 | LYS | 5.3 |
| 1 | D | 936 | U | 5.3 |
| 2 | B | 524 | TRP | 5.1 |
| 1 | D | 939 | A | 4.9 |
| 2 | B | 236 | TYR | 4.9 |
| 2 | B | 386 | SER | 4.7 |
| 2 | B | 862 | TYR | 4.6 |
| 2 | A | 456 | ALA | 4.1 |
| 2 | B | 403 | ALA | 3.9 |
| 2 | B | 920 | ARG | 3.8 |
| 2 | A | 457 | VAL | 3.8 |
| 2 | B | 895 | GLU | 3.7 |
| 2 | A | 406 | HIS | 3.6 |
| 2 | B | 891 | MET | 3.6 |
| 2 | B | 869 | TRP | 3.6 |
| 2 | B | 265 | VAL | 3.6 |
| 2 | A | 869 | TRP | 3.5 |
| 2 | A | 455 | ARG | 3.5 |
| 2 | B | 583 | LYS | 3.4 |
| 1 | D | 909 | U | 3.4 |
| 2 | B | 457 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | B | 291 | LEU | 3.2 |
| 2 | B | 167 | PHE | 3.2 |
| 1 | D | 988 | A | 3.2 |
| 2 | B | 310 | ALA | 3.2 |
| 2 | B | 405 | TYR | 3.2 |
| 2 | A | 915 | THR | 3.1 |
| 2 | B | 887 | MET | 3.1 |
| 2 | A | 586 | ILE | 3.1 |
| 1 | D | 986 | C | 3.0 |
| 2 | B | 280 | ILE | 3.0 |
| 2 | B | 255 | ARG | 2.9 |
| 2 | B | 784 | ARG | 2.9 |
| 2 | A | 291 | LEU | 2.9 |
| 2 | A | 404 | GLU | 2.9 |
| 2 | A | 450 | SER | 2.8 |
| 2 | B | 300 | VAL | 2.8 |
| 2 | B | 387 | GLN | 2.8 |
| 2 | B | 929 | GLU | 2.8 |
| 2 | B | 938 | LEU | 2.7 |
| 2 | B | 966 | ILE | 2.7 |
| 2 | B | 263 | TRP | 2.7 |
| 1 | D | 907 | G | 2.6 |
| 2 | B | 264 | ILE | 2.6 |
| 2 | B | 399 | THR | 2.6 |
| 2 | B | 883 | PHE | 2.6 |
| 2 | B | 238 | VAL | 2.6 |
| 2 | A | 447 | ASN | 2.6 |
| 2 | A | 191 | THR | 2.5 |
| 2 | B | 865 | THR | 2.5 |
| 2 | A | 448 | VAL | 2.5 |
| 2 | A | 917 | ASP | 2.5 |
| 2 | B | 455 | ARG | 2.5 |
| 2 | B | 381 | LYS | 2.5 |
| 1 | C | 987 | C | 2.4 |
| 2 | B | 355 | ILE | 2.4 |
| 2 | A | 862 | TYR | 2.4 |
| 2 | B | 242 | TRP | 2.4 |
| 1 | C | 986 | C | 2.3 |
| 2 | B | 870 | LYS | 2.3 |
| 2 | A | 868 | ASP | 2.3 |
| 2 | A | 449 | ILE | 2.3 |
| 2 | A | 502 | TRP | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 453 | GLY | 2.3 |
| 2 | B | 919 | LYS | 2.3 |
| 2 | B | 353 | PRO | 2.3 |
| 2 | B | 400 | ILE | 2.3 |
| 2 | B | 964 | ILE | 2.2 |
| 2 | B | 279 | GLU | 2.2 |
| 2 | A | 584 | THR | 2.2 |
| 2 | B | 286 | PHE | 2.2 |
| 2 | B | 323 | MET | 2.2 |
| 1 | D | 940 | G | 2.2 |
| 2 | B | 404 | GLU | 2.2 |
| 2 | B | 352 | ASP | 2.1 |
| 2 | B | 251 | LYS | 2.1 |
| 2 | B | 409 | ILE | 2.1 |
| 2 | B | 458 | ILE | 2.1 |
| 2 | B | 354 | ARG | 2.1 |
| 2 | B | 967 | GLU | 2.1 |
| 1 | C | 939 | A | 2.1 |
| 2 | B | 319 | THR | 2.1 |
| 2 | A | 190 | GLY | 2.1 |
| 2 | A | 195 | ASP | 2.1 |
| 2 | A | 452 | PHE | 2.0 |
| 1 | C | 988 | A | 2.0 |
| 2 | A | 206 | ILE | 2.0 |
| 2 | A | 194 | GLY | 2.0 |
| 2 | B | 464 | GLN | 2.0 |
| 2 | A | 890 | LEU | 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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.