



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:45 PM GMT

PDB ID : 1LVC
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 2' deoxy, 3' anthraniloyle ATP
Authors : Shen, Y.; Lee, Y.-S.; Soelaiman, S.; Bergson, P.; Lu, D.; Chen, A.; Beckingham, K.; Grabarek, Z.; Mrksich, M.; Tang, W.-J.
Deposited on : 2002-05-28
Resolution : 3.60 Å(reported)

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

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

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

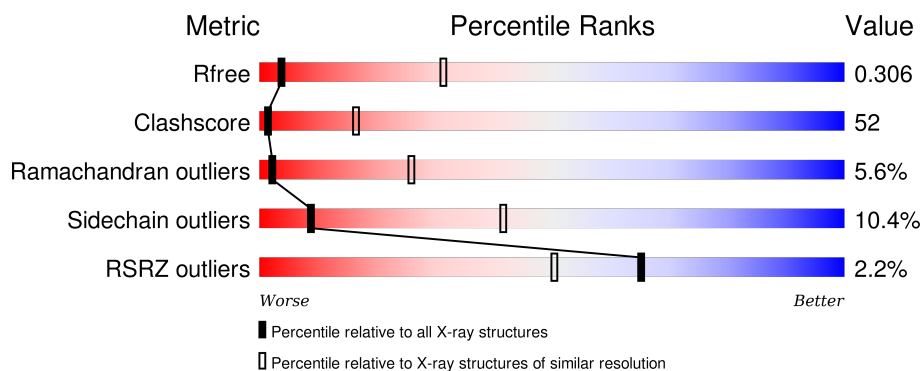
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

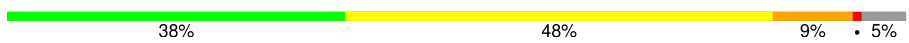

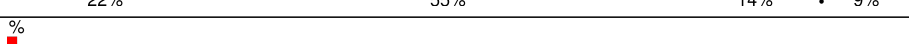
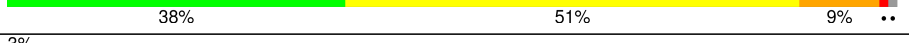
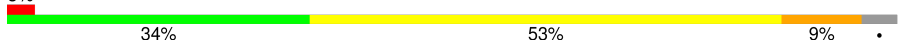
The reported resolution of this entry is 3.60 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1408 (3.80-3.40) |
| Clashscore | 102246 | 1010 (3.74-3.46) |
| Ramachandran outliers | 100387 | 1007 (3.76-3.44) |
| Sidechain outliers | 100360 | 1007 (3.76-3.44) |
| RSRZ outliers | 91569 | 1003 (3.78-3.42) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 510 |  38% 48% 9% • 5% |
| 1 | B | 510 |  3% 22% 55% 14% • 9% |
| 1 | C | 510 |  38% 51% 9% •• |
| 2 | D | 149 |  3% 34% 53% 9% • |
| 2 | E | 149 |  7% 38% 48% 9% • |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | F | 149 | <div><div></div><div>6%</div><div>36%</div><div>48%</div><div>11%</div><div></div></div> |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called calmodulin-sensitive adenylate cyclase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 485 | Total | C | N | O | S | 65 | 0 | 0 |
| | | | 3952 | 2528 | 673 | 748 | 3 | | | |
| 1 | B | 465 | Total | C | N | O | S | 113 | 0 | 0 |
| | | | 3794 | 2431 | 642 | 718 | 3 | | | |
| 1 | C | 503 | Total | C | N | O | S | 166 | 0 | 0 |
| | | | 4094 | 2616 | 696 | 779 | 3 | | | |

- Molecule 2 is a protein called calmodulin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | D | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1125 | 690 | 181 | 245 | 9 | | | |
| 2 | E | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1125 | 690 | 181 | 245 | 9 | | | |
| 2 | F | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1125 | 690 | 181 | 245 | 9 | | | |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | D | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | F | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | E | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 4 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

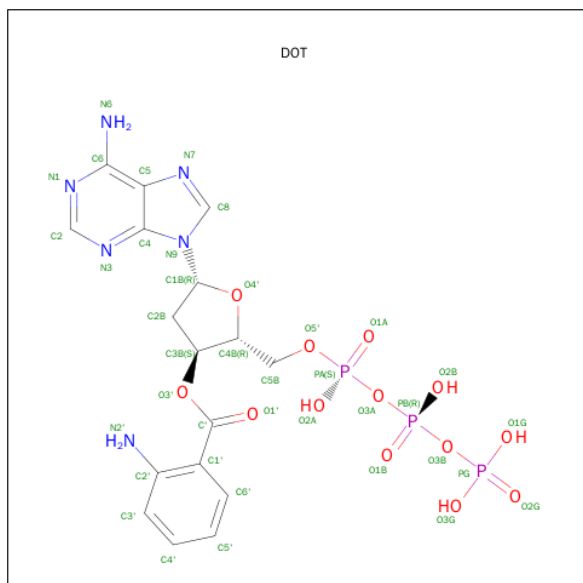
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | B | 1 | Total | Yb | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | A | 1 | Total | Yb | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | Yb | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 5 is 3'ANTHRANILOYL-2'-DEOXY-ADENOSINE-5'-TRIPHOSPHATE (three-letter code: DOT) (formula: $C_{17}H_{21}N_6O_{13}P_3$).

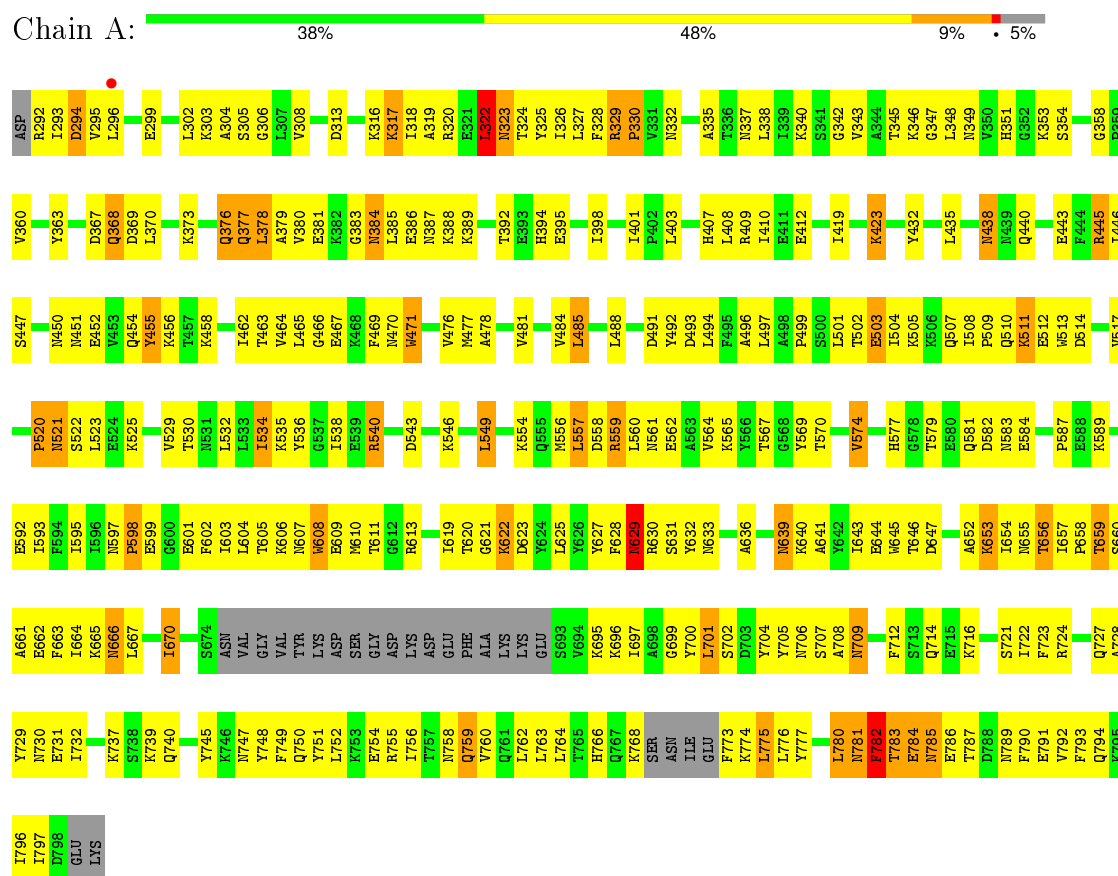


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 39 | 17 | 6 | 13 | 3 | | |
| 5 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 39 | 17 | 6 | 13 | 3 | | |

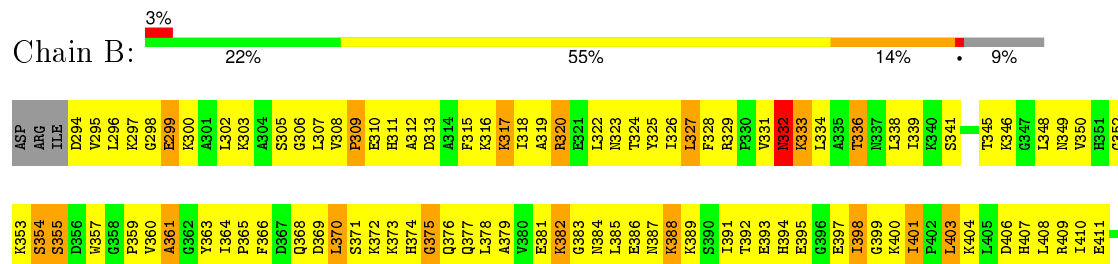
3 Residue-property plots

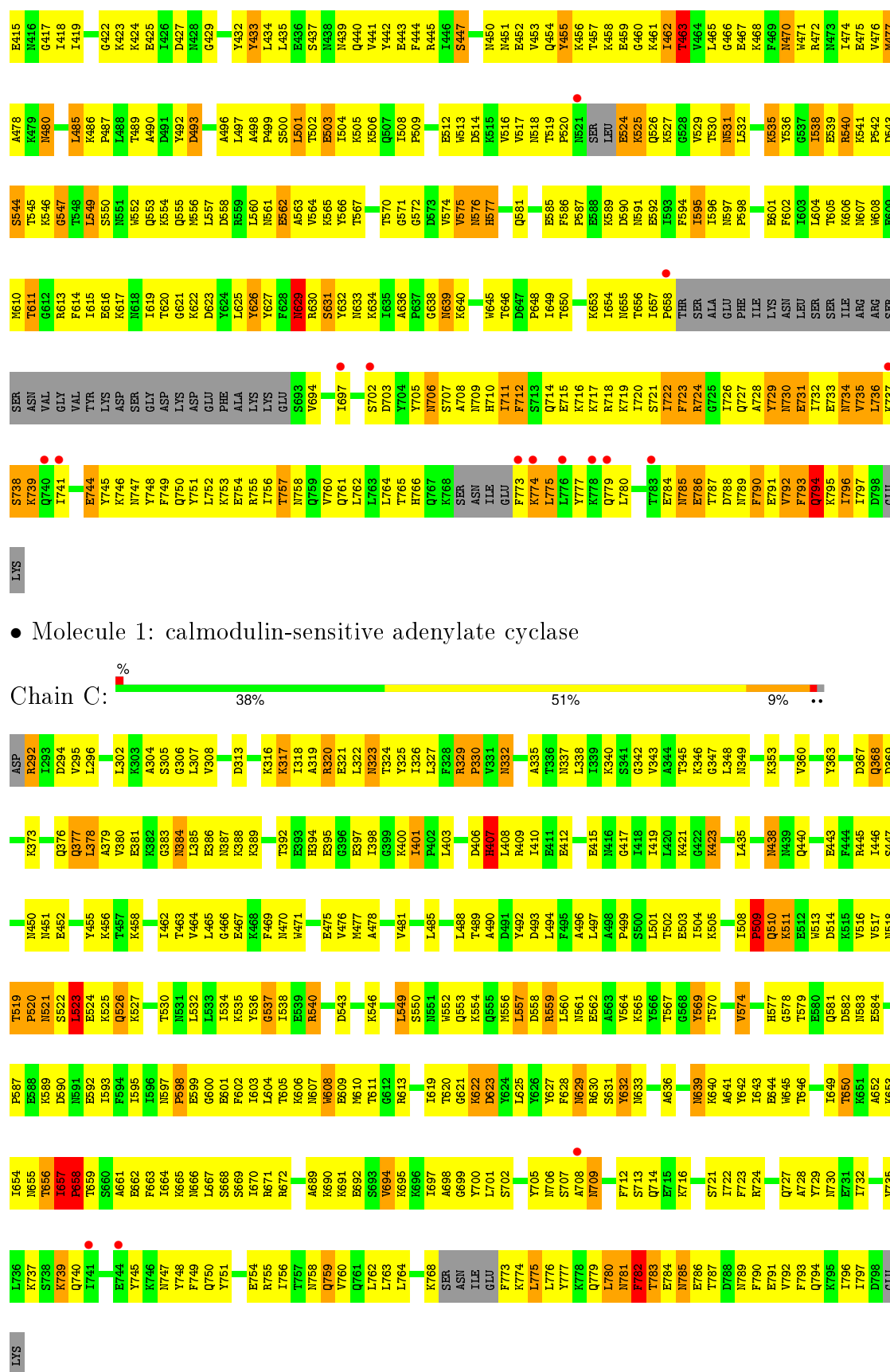
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

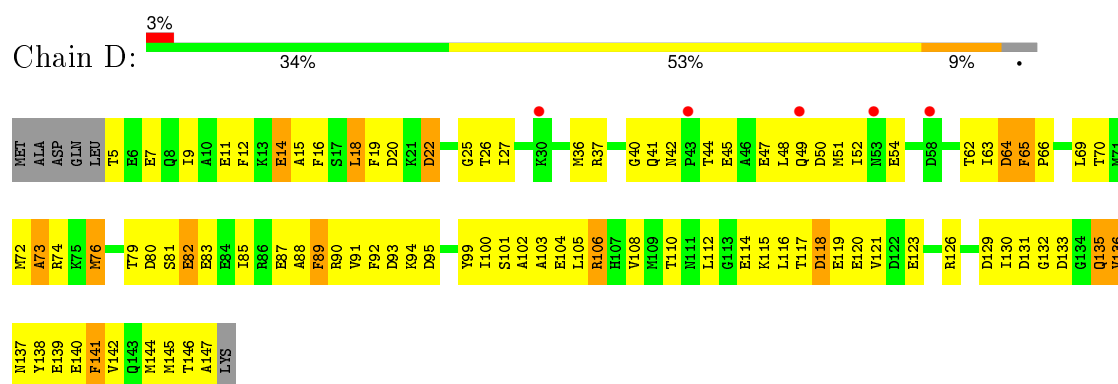
- Molecule 1: calmodulin-sensitive adenylate cyclase



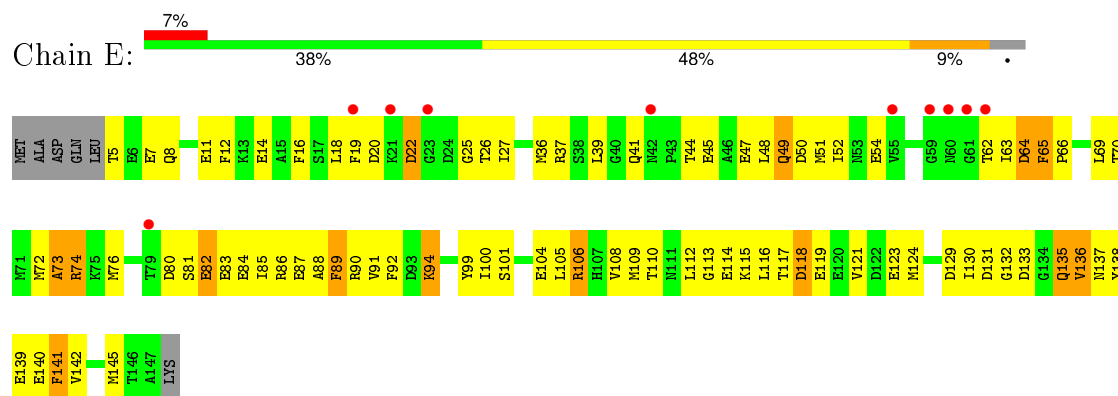
- Molecule 1: calmodulin-sensitive adenylate cyclase



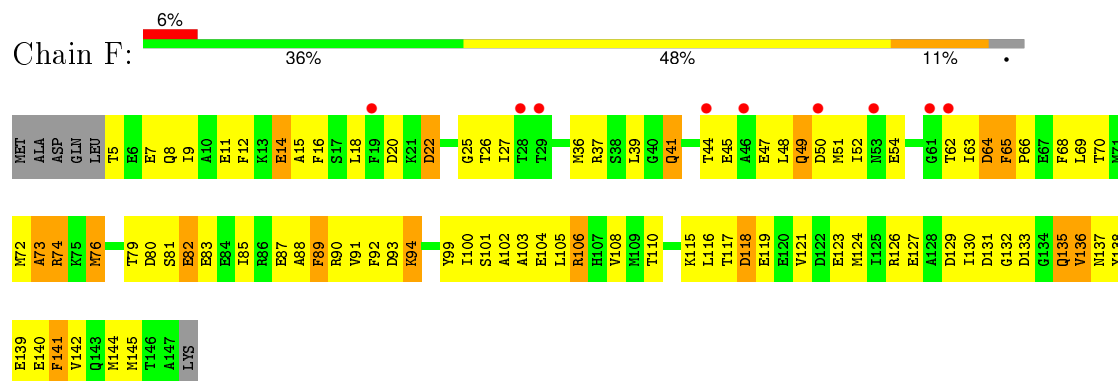




- Molecule 2: calmodulin



- Molecule 2: calmodulin



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | I 2 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 116.92Å 167.92Å 341.74Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.96 – 3.60 29.95 – 3.60 | Depositor EDS |
| % Data completeness (in resolution range) | 90.6 (29.96-3.60) 95.9 (29.95-3.60) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 7.00 (at 3.65Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.281 , 0.307 0.272 , 0.306 | Depositor DCC |
| R_{free} test set | 1889 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 98.5 | Xtriage |
| Anisotropy | 0.221 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 67.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Outliers | 0 of 38841 reflections | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 15302 | wwPDB-VP |
| Average B, all atoms (Å ²) | 81.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, YB, DOT

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.49 | 0/4027 | 0.82 | 13/5419 (0.2%) |
| 1 | B | 0.51 | 0/3867 | 0.78 | 9/5204 (0.2%) |
| 1 | C | 0.51 | 1/4172 (0.0%) | 0.82 | 16/5613 (0.3%) |
| 2 | D | 0.38 | 0/1137 | 0.59 | 2/1527 (0.1%) |
| 2 | E | 0.40 | 0/1137 | 0.61 | 2/1527 (0.1%) |
| 2 | F | 0.37 | 0/1137 | 0.74 | 3/1527 (0.2%) |
| All | All | 0.48 | 1/15477 (0.0%) | 0.78 | 45/20817 (0.2%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | C | 658 | PRO | CA-C | -5.34 | 1.42 | 1.52 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2 | F | 106 | ARG | NE-CZ-NH1 | -14.10 | 113.25 | 120.30 |
| 2 | F | 106 | ARG | NE-CZ-NH2 | 13.51 | 127.06 | 120.30 |
| 1 | A | 613 | ARG | NE-CZ-NH1 | -11.05 | 114.77 | 120.30 |
| 1 | C | 613 | ARG | NE-CZ-NH2 | -10.74 | 114.93 | 120.30 |
| 1 | C | 613 | ARG | NE-CZ-NH1 | 10.64 | 125.62 | 120.30 |
| 1 | A | 613 | ARG | NE-CZ-NH2 | 10.42 | 125.51 | 120.30 |
| 1 | A | 785 | ASN | CA-C-N | 9.67 | 138.46 | 117.20 |
| 1 | C | 320 | ARG | NE-CZ-NH1 | -9.11 | 115.74 | 120.30 |
| 1 | A | 320 | ARG | NE-CZ-NH1 | 9.00 | 124.80 | 120.30 |
| 1 | C | 320 | ARG | NE-CZ-NH2 | 8.95 | 124.78 | 120.30 |
| 1 | A | 320 | ARG | NE-CZ-NH2 | -8.79 | 115.91 | 120.30 |
| 1 | B | 538 | ILE | CB-CA-C | -8.57 | 94.47 | 111.60 |
| 1 | C | 509 | PRO | CA-N-CD | -8.35 | 99.81 | 111.50 |
| 1 | A | 785 | ASN | O-C-N | -7.76 | 110.28 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 632 | TYR | C-N-CA | -7.74 | 102.35 | 121.70 |
| 2 | D | 106 | ARG | NE-CZ-NH1 | 7.50 | 124.05 | 120.30 |
| 1 | B | 738 | SER | N-CA-C | -7.36 | 91.12 | 111.00 |
| 2 | E | 106 | ARG | NE-CZ-NH2 | -7.33 | 116.63 | 120.30 |
| 1 | A | 785 | ASN | C-N-CA | -7.33 | 103.38 | 121.70 |
| 2 | E | 106 | ARG | NE-CZ-NH1 | 7.29 | 123.95 | 120.30 |
| 1 | C | 785 | ASN | N-CA-C | 7.17 | 130.35 | 111.00 |
| 1 | A | 740 | GLN | N-CA-C | -6.95 | 92.25 | 111.00 |
| 2 | D | 106 | ARG | NE-CZ-NH2 | -6.70 | 116.95 | 120.30 |
| 1 | C | 783 | THR | C-N-CA | -6.65 | 105.07 | 121.70 |
| 1 | A | 322 | LEU | N-CA-C | -6.58 | 93.24 | 111.00 |
| 1 | C | 658 | PRO | CA-N-CD | -6.58 | 102.29 | 111.50 |
| 2 | F | 106 | ARG | CD-NE-CZ | 6.58 | 132.81 | 123.60 |
| 1 | C | 632 | TYR | CA-C-N | 6.50 | 131.50 | 117.20 |
| 1 | B | 470 | ASN | CA-C-N | 6.17 | 130.78 | 117.20 |
| 1 | B | 375 | GLY | C-N-CA | -6.10 | 106.46 | 121.70 |
| 1 | B | 739 | LYS | N-CA-C | 5.85 | 126.80 | 111.00 |
| 1 | A | 783 | THR | CA-C-N | 5.84 | 130.05 | 117.20 |
| 1 | C | 613 | ARG | CD-NE-CZ | 5.55 | 131.37 | 123.60 |
| 1 | C | 689 | ALA | N-CA-C | 5.50 | 125.84 | 111.00 |
| 1 | C | 632 | TYR | O-C-N | -5.47 | 113.94 | 122.70 |
| 1 | B | 470 | ASN | O-C-N | -5.47 | 113.95 | 122.70 |
| 1 | C | 784 | GLU | C-N-CA | -5.44 | 108.11 | 121.70 |
| 1 | B | 470 | ASN | C-N-CA | -5.44 | 108.11 | 121.70 |
| 1 | C | 783 | THR | CA-C-N | 5.38 | 129.04 | 117.20 |
| 1 | A | 783 | THR | C-N-CA | -5.36 | 108.29 | 121.70 |
| 1 | A | 783 | THR | N-CA-C | 5.28 | 125.25 | 111.00 |
| 1 | B | 542 | PRO | CA-N-CD | -5.22 | 104.19 | 111.50 |
| 1 | A | 782 | PHE | N-CA-C | -5.15 | 97.09 | 111.00 |
| 1 | C | 782 | PHE | N-CA-C | -5.10 | 97.23 | 111.00 |
| 1 | B | 493 | ASP | CB-CG-OD1 | 5.06 | 122.85 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3952 | 0 | 3999 | 403 | 0 |
| 1 | B | 3794 | 0 | 3828 | 500 | 0 |
| 1 | C | 4094 | 0 | 4134 | 394 | 0 |
| 2 | D | 1125 | 0 | 1049 | 113 | 0 |
| 2 | E | 1125 | 0 | 1049 | 103 | 0 |
| 2 | F | 1125 | 0 | 1049 | 109 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| 3 | E | 2 | 0 | 0 | 0 | 0 |
| 3 | F | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 39 | 0 | 17 | 8 | 0 |
| 5 | C | 39 | 0 | 17 | 5 | 0 |
| All | All | 15302 | 0 | 15142 | 1552 | 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 52.

All (1552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:629:ASN:ND2 | 1:B:631:SER:H | 1.14 | 1.44 |
| 1:C:456:LYS:HB2 | 1:C:470:ASN:O | 1.22 | 1.34 |
| 1:C:456:LYS:CB | 1:C:470:ASN:O | 1.84 | 1.24 |
| 1:C:659:THR:HG22 | 1:C:661:ALA:H | 1.08 | 1.14 |
| 1:A:456:LYS:HB2 | 1:A:470:ASN:O | 1.46 | 1.11 |
| 1:B:629:ASN:ND2 | 1:B:631:SER:N | 1.98 | 1.10 |
| 1:A:632:TYR:O | 1:A:643:ILE:O | 1.69 | 1.09 |
| 1:B:376:GLN:HB2 | 1:B:379:ALA:HB3 | 1.33 | 1.08 |
| 1:A:666:ASN:O | 1:A:670:ILE:HB | 1.52 | 1.07 |
| 1:B:538:ILE:HG22 | 1:B:538:ILE:O | 1.52 | 1.06 |
| 1:A:456:LYS:CB | 1:A:470:ASN:O | 2.02 | 1.06 |
| 1:B:581:GLN:NE2 | 1:B:629:ASN:H | 1.55 | 1.04 |
| 1:B:353:LYS:H | 1:B:368:GLN:NE2 | 1.55 | 1.04 |
| 1:A:705:TYR:CE2 | 2:D:139:GLU:HB3 | 1.93 | 1.04 |
| 1:C:629:ASN:ND2 | 1:C:631:SER:H | 1.56 | 1.03 |
| 1:A:759:GLN:HA | 1:A:759:GLN:HE21 | 1.21 | 1.03 |
| 1:C:510:GLN:O | 1:C:514:ASP:OD1 | 1.77 | 1.03 |
| 5:C:1999:DOT:O1' | 5:C:1999:DOT:N2' | 1.93 | 1.02 |
| 1:A:633:ASN:HD21 | 1:A:645:TRP:H | 1.09 | 1.01 |
| 1:B:348:LEU:HD21 | 1:B:577:HIS:HB3 | 1.43 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:629:ASN:ND2 | 1:A:631:SER:H | 1.57 | 1.00 |
| 1:A:605:THR:HG21 | 1:A:611:THR:HA | 1.43 | 1.00 |
| 1:C:759:GLN:HA | 1:C:759:GLN:HE21 | 1.21 | 0.99 |
| 1:C:605:THR:HG21 | 1:C:611:THR:HA | 1.44 | 0.99 |
| 1:C:664:ILE:HG21 | 2:F:15:ALA:HB2 | 1.45 | 0.99 |
| 1:A:295:VAL:HG21 | 1:A:603:ILE:HG22 | 1.44 | 0.99 |
| 1:B:629:ASN:HD22 | 1:B:631:SER:N | 1.60 | 0.98 |
| 1:B:456:LYS:HB2 | 1:B:470:ASN:O | 1.63 | 0.98 |
| 1:B:353:LYS:N | 1:B:368:GLN:HE22 | 1.62 | 0.97 |
| 1:B:657:ILE:HG12 | 1:B:658:PRO:HD2 | 1.47 | 0.96 |
| 1:C:295:VAL:HG21 | 1:C:603:ILE:HG22 | 1.45 | 0.96 |
| 5:A:999:DOT:O1' | 5:A:999:DOT:N2' | 1.92 | 0.96 |
| 1:B:777:TYR:HD1 | 1:B:780:LEU:HD12 | 1.30 | 0.95 |
| 1:B:581:GLN:HE21 | 1:B:629:ASN:H | 1.10 | 0.95 |
| 1:C:510:GLN:C | 1:C:514:ASP:OD1 | 2.05 | 0.95 |
| 1:B:456:LYS:CB | 1:B:470:ASN:O | 2.16 | 0.94 |
| 1:A:324:THR:HG21 | 1:A:556:MET:HE1 | 1.49 | 0.94 |
| 2:E:25:GLY:HA3 | 2:E:65:PHE:CE1 | 2.03 | 0.94 |
| 1:A:695:LYS:HB2 | 2:D:18:LEU:HD22 | 1.49 | 0.93 |
| 1:C:633:ASN:HD21 | 1:C:645:TRP:H | 1.15 | 0.93 |
| 1:B:538:ILE:CG2 | 1:B:538:ILE:O | 2.15 | 0.93 |
| 1:A:629:ASN:HD22 | 1:A:631:SER:H | 1.10 | 0.93 |
| 1:A:324:THR:HG21 | 1:A:556:MET:CE | 1.99 | 0.93 |
| 2:D:25:GLY:HA3 | 2:D:65:PHE:CE1 | 2.04 | 0.93 |
| 1:B:376:GLN:HB2 | 1:B:379:ALA:CB | 2.01 | 0.91 |
| 1:B:322:LEU:O | 1:B:324:THR:HG23 | 1.70 | 0.91 |
| 2:F:25:GLY:HA3 | 2:F:65:PHE:CE1 | 2.06 | 0.91 |
| 1:B:606:LYS:H | 1:B:610:MET:HE2 | 1.34 | 0.90 |
| 1:C:657:ILE:HD13 | 1:C:756:ILE:HD13 | 1.54 | 0.89 |
| 1:B:360:VAL:HG11 | 1:B:365:PRO:HG3 | 1.54 | 0.89 |
| 1:B:587:PRO:HD2 | 1:B:639:ASN:HD21 | 1.36 | 0.89 |
| 1:B:516:VAL:HA | 1:B:520:PRO:HG2 | 1.55 | 0.89 |
| 1:A:639:ASN:ND2 | 1:A:641:ALA:H | 1.70 | 0.89 |
| 1:A:559:ARG:HH11 | 1:A:559:ARG:HB3 | 1.38 | 0.89 |
| 1:A:521:ASN:ND2 | 1:A:522:SER:H | 1.69 | 0.89 |
| 1:C:705:TYR:CE2 | 2:F:139:GLU:HB3 | 2.08 | 0.88 |
| 1:B:296:LEU:HD12 | 1:B:604:LEU:HD22 | 1.55 | 0.88 |
| 1:C:659:THR:HG22 | 1:C:661:ALA:N | 1.88 | 0.88 |
| 1:B:509:PRO:HG2 | 1:B:512:GLU:HB3 | 1.55 | 0.88 |
| 1:B:518:ASN:C | 1:B:520:PRO:HD3 | 1.94 | 0.88 |
| 1:C:622:LYS:HA | 1:C:622:LYS:HE3 | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:20:ASP:OD2 | 2:E:22:ASP:HB2 | 1.74 | 0.88 |
| 1:B:514:ASP:HA | 1:B:517:VAL:HG12 | 1.56 | 0.87 |
| 1:B:709:ASN:HD21 | 1:B:720:ILE:HD11 | 1.38 | 0.87 |
| 1:B:654:ILE:HA | 1:B:755:ARG:CD | 2.04 | 0.87 |
| 2:D:20:ASP:OD2 | 2:D:22:ASP:HB2 | 1.75 | 0.87 |
| 1:B:561:ASN:O | 1:B:564:VAL:HG22 | 1.74 | 0.87 |
| 1:A:712:PHE:HD2 | 1:A:716:LYS:HG2 | 1.38 | 0.86 |
| 2:E:100:ILE:HB | 2:E:136:VAL:HG23 | 1.56 | 0.86 |
| 1:A:513:TRP:CD2 | 1:A:517:VAL:HG21 | 2.09 | 0.86 |
| 1:B:717:LYS:HD2 | 2:E:132:GLY:N | 1.91 | 0.86 |
| 1:C:657:ILE:HG13 | 1:C:759:GLN:HG2 | 1.57 | 0.86 |
| 1:A:522:SER:O | 1:A:525:LYS:HB3 | 1.76 | 0.86 |
| 1:C:639:ASN:ND2 | 1:C:641:ALA:H | 1.73 | 0.86 |
| 2:F:100:ILE:HB | 2:F:136:VAL:HG23 | 1.55 | 0.86 |
| 2:F:20:ASP:OD2 | 2:F:22:ASP:HB2 | 1.75 | 0.85 |
| 1:C:712:PHE:HD2 | 1:C:716:LYS:HG2 | 1.41 | 0.85 |
| 1:B:756:ILE:O | 1:B:760:VAL:HG23 | 1.76 | 0.85 |
| 1:C:540:ARG:NH2 | 1:C:627:TYR:CD1 | 2.45 | 0.85 |
| 1:B:779:GLN:NE2 | 1:B:796:ILE:HG13 | 1.92 | 0.84 |
| 1:A:525:LYS:O | 1:A:529:VAL:HG23 | 1.76 | 0.84 |
| 1:C:694:VAL:HG23 | 1:C:695:LYS:H | 1.41 | 0.84 |
| 1:B:391:ILE:HD12 | 1:B:399:GLY:HA2 | 1.59 | 0.84 |
| 1:C:456:LYS:HB3 | 1:C:470:ASN:O | 1.74 | 0.84 |
| 1:A:712:PHE:CD2 | 1:A:716:LYS:HG2 | 2.13 | 0.84 |
| 1:B:625:LEU:HD23 | 1:B:626:TYR:N | 1.93 | 0.83 |
| 1:B:308:VAL:HB | 1:B:311:HIS:CD2 | 2.13 | 0.83 |
| 2:D:100:ILE:HB | 2:D:136:VAL:HG23 | 1.58 | 0.83 |
| 1:B:728:ALA:HA | 1:B:731:GLU:HG3 | 1.60 | 0.83 |
| 1:B:734:ASN:C | 1:B:736:LEU:H | 1.77 | 0.83 |
| 1:B:629:ASN:HD21 | 1:B:631:SER:H | 1.22 | 0.83 |
| 1:A:747:ASN:O | 1:A:750:GLN:HG2 | 1.79 | 0.82 |
| 1:A:695:LYS:HG3 | 2:D:18:LEU:HD13 | 1.61 | 0.82 |
| 1:C:747:ASN:O | 1:C:750:GLN:HG2 | 1.79 | 0.82 |
| 2:F:36:MET:O | 2:F:41:GLN:HB2 | 1.79 | 0.82 |
| 1:B:629:ASN:HD21 | 1:B:631:SER:HB2 | 1.43 | 0.81 |
| 1:A:445:ARG:CZ | 1:A:471:TRP:NE1 | 2.43 | 0.81 |
| 1:C:510:GLN:HG3 | 1:C:510:GLN:O | 1.80 | 0.81 |
| 1:B:324:THR:HG22 | 1:B:499:PRO:HA | 1.61 | 0.81 |
| 1:B:728:ALA:HA | 1:B:731:GLU:CG | 2.10 | 0.81 |
| 1:C:712:PHE:CD2 | 1:C:716:LYS:HG2 | 2.15 | 0.81 |
| 1:A:657:ILE:HD11 | 1:A:704:TYR:CE1 | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:629:ASN:HD22 | 1:B:631:SER:H | 0.83 | 0.81 |
| 1:B:649:ILE:O | 1:B:649:ILE:HG22 | 1.80 | 0.81 |
| 1:A:445:ARG:HG3 | 1:A:471:TRP:CZ2 | 2.15 | 0.80 |
| 1:B:527:LYS:O | 1:B:531:ASN:HB2 | 1.81 | 0.80 |
| 1:A:540:ARG:NH2 | 1:A:627:TYR:CD1 | 2.49 | 0.80 |
| 1:A:445:ARG:HH22 | 1:A:456:LYS:HD3 | 1.45 | 0.80 |
| 1:C:377:GLN:HA | 1:C:380:VAL:HG12 | 1.64 | 0.80 |
| 2:E:36:MET:O | 2:E:41:GLN:HB2 | 1.81 | 0.80 |
| 1:C:633:ASN:HD21 | 1:C:645:TRP:N | 1.79 | 0.79 |
| 1:A:714:GLN:NE2 | 2:D:126:ARG:HG3 | 1.97 | 0.79 |
| 1:B:543:ASP:OD1 | 1:B:544:SER:N | 2.14 | 0.79 |
| 1:B:577:HIS:CD2 | 1:B:577:HIS:H | 1.99 | 0.79 |
| 1:B:706:ASN:ND2 | 1:B:708:ALA:HB3 | 1.97 | 0.79 |
| 1:A:445:ARG:NH2 | 1:A:456:LYS:HD3 | 1.96 | 0.79 |
| 1:A:622:LYS:HE3 | 1:A:622:LYS:HA | 1.65 | 0.79 |
| 1:B:332:ASN:C | 1:B:332:ASN:HD22 | 1.86 | 0.79 |
| 1:A:348:LEU:HD23 | 1:A:348:LEU:O | 1.82 | 0.78 |
| 1:C:629:ASN:HD22 | 1:C:631:SER:H | 1.26 | 0.78 |
| 1:C:559:ARG:HH11 | 1:C:559:ARG:HB3 | 1.45 | 0.78 |
| 1:B:654:ILE:HA | 1:B:755:ARG:HD2 | 1.64 | 0.78 |
| 1:B:550:SER:H | 1:B:553:GLN:HG3 | 1.47 | 0.78 |
| 1:A:492:TYR:CD2 | 1:A:574:VAL:HG13 | 2.19 | 0.78 |
| 1:B:391:ILE:CD1 | 1:B:399:GLY:HA2 | 2.14 | 0.78 |
| 1:C:318:ILE:HD12 | 1:C:318:ILE:H | 1.48 | 0.78 |
| 1:B:706:ASN:HD21 | 1:B:708:ALA:HB3 | 1.48 | 0.78 |
| 1:A:629:ASN:HD22 | 1:A:631:SER:N | 1.81 | 0.77 |
| 1:B:731:GLU:OE2 | 1:B:733:GLU:HB2 | 1.84 | 0.77 |
| 1:B:597:ASN:ND2 | 1:B:601:GLU:HB2 | 1.99 | 0.77 |
| 1:B:581:GLN:HE21 | 1:B:629:ASN:N | 1.82 | 0.77 |
| 1:B:779:GLN:HE22 | 1:B:796:ILE:HG13 | 1.48 | 0.77 |
| 1:B:626:TYR:CD2 | 1:B:627:TYR:N | 2.53 | 0.77 |
| 1:B:565:LYS:O | 1:B:567:THR:N | 2.18 | 0.77 |
| 1:A:445:ARG:HG3 | 1:A:471:TRP:CH2 | 2.20 | 0.77 |
| 1:B:394:HIS:O | 1:B:397:GLU:HG2 | 1.85 | 0.77 |
| 2:D:36:MET:O | 2:D:41:GLN:HB2 | 1.85 | 0.76 |
| 1:B:615:ILE:HD12 | 1:B:645:TRP:CH2 | 2.20 | 0.76 |
| 1:A:657:ILE:HD11 | 1:A:704:TYR:CZ | 2.21 | 0.76 |
| 1:C:729:TYR:HB2 | 1:C:756:ILE:HG21 | 1.65 | 0.76 |
| 1:B:709:ASN:OD1 | 1:B:717:LYS:HG3 | 1.85 | 0.76 |
| 1:A:657:ILE:CG2 | 1:A:756:ILE:HD13 | 2.16 | 0.76 |
| 1:B:712:PHE:HD1 | 1:B:712:PHE:H | 1.34 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:729:TYR:HB2 | 1:A:756:ILE:HG21 | 1.65 | 0.76 |
| 1:B:657:ILE:HG12 | 1:B:658:PRO:CD | 2.16 | 0.76 |
| 1:A:318:ILE:H | 1:A:318:ILE:HD12 | 1.47 | 0.76 |
| 1:A:492:TYR:HD2 | 1:A:574:VAL:HG13 | 1.51 | 0.76 |
| 1:A:581:GLN:HE21 | 1:A:629:ASN:H | 1.32 | 0.75 |
| 1:C:633:ASN:ND2 | 1:C:644:GLU:HA | 2.02 | 0.75 |
| 1:A:377:GLN:HA | 1:A:380:VAL:HG12 | 1.67 | 0.75 |
| 1:C:794:GLN:O | 1:C:797:ILE:HG13 | 1.85 | 0.75 |
| 1:C:492:TYR:CD2 | 1:C:574:VAL:HG13 | 2.21 | 0.75 |
| 1:C:348:LEU:O | 1:C:348:LEU:HD23 | 1.85 | 0.75 |
| 1:B:353:LYS:H | 1:B:368:GLN:HE22 | 0.81 | 0.75 |
| 1:A:794:GLN:O | 1:A:797:ILE:HG13 | 1.87 | 0.75 |
| 1:C:629:ASN:HD22 | 1:C:631:SER:N | 1.84 | 0.74 |
| 1:B:560:LEU:O | 1:B:564:VAL:HG13 | 1.87 | 0.74 |
| 1:B:463:THR:HG23 | 1:B:467:GLU:O | 1.86 | 0.74 |
| 1:B:506:LYS:NZ | 1:B:506:LYS:HB3 | 2.01 | 0.74 |
| 1:C:360:VAL:HG22 | 1:C:360:VAL:O | 1.87 | 0.74 |
| 1:C:629:ASN:ND2 | 1:C:631:SER:N | 2.34 | 0.74 |
| 1:C:632:TYR:O | 1:C:643:ILE:O | 2.05 | 0.74 |
| 1:C:493:ASP:OD2 | 1:C:577:HIS:HE1 | 1.70 | 0.74 |
| 1:B:626:TYR:HD2 | 1:B:627:TYR:N | 1.85 | 0.74 |
| 1:B:308:VAL:HB | 1:B:311:HIS:HD2 | 1.52 | 0.74 |
| 1:A:657:ILE:CG2 | 1:A:756:ILE:HA | 2.17 | 0.74 |
| 1:A:456:LYS:HB3 | 1:A:470:ASN:O | 1.85 | 0.74 |
| 1:C:722:ILE:HD13 | 1:C:764:LEU:HD23 | 1.69 | 0.74 |
| 1:C:700:TYR:HB3 | 1:C:728:ALA:HB2 | 1.67 | 0.74 |
| 1:A:759:GLN:HE21 | 1:A:759:GLN:CA | 1.97 | 0.74 |
| 1:A:493:ASP:OD2 | 1:A:577:HIS:CE1 | 2.40 | 0.74 |
| 1:A:639:ASN:C | 1:A:639:ASN:HD22 | 1.91 | 0.74 |
| 1:B:710:HIS:CE1 | 1:B:711:ILE:HG23 | 2.23 | 0.74 |
| 1:A:360:VAL:O | 1:A:360:VAL:HG22 | 1.85 | 0.74 |
| 1:A:581:GLN:NE2 | 1:A:628:PHE:HA | 2.03 | 0.73 |
| 1:B:777:TYR:CD1 | 1:B:780:LEU:HD12 | 2.20 | 0.73 |
| 1:B:747:ASN:O | 1:B:751:TYR:HB2 | 1.87 | 0.73 |
| 1:B:779:GLN:OE1 | 1:B:796:ILE:HG21 | 1.87 | 0.73 |
| 1:C:324:THR:HG21 | 1:C:556:MET:CE | 2.17 | 0.73 |
| 1:C:516:VAL:HG12 | 1:C:516:VAL:O | 1.86 | 0.73 |
| 1:B:745:TYR:HB3 | 1:B:749:PHE:HE1 | 1.51 | 0.73 |
| 1:C:759:GLN:CA | 1:C:759:GLN:HE21 | 1.97 | 0.73 |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:HD23 | 1.68 | 0.73 |
| 1:B:366:PHE:HA | 1:B:477:MET:CE | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:70:THR:O | 2:E:73:ALA:HB3 | 1.88 | 0.73 |
| 1:B:312:ALA:O | 1:B:315:PHE:HB2 | 1.87 | 0.73 |
| 1:B:650:THR:HA | 1:B:653:LYS:HB2 | 1.70 | 0.73 |
| 1:C:324:THR:HG21 | 1:C:556:MET:HE1 | 1.71 | 0.73 |
| 1:C:629:ASN:HB3 | 1:C:632:TYR:CD2 | 2.24 | 0.72 |
| 1:A:493:ASP:OD2 | 1:A:577:HIS:HE1 | 1.72 | 0.72 |
| 1:B:606:LYS:H | 1:B:610:MET:CE | 2.02 | 0.72 |
| 1:A:322:LEU:HD12 | 1:A:322:LEU:N | 2.04 | 0.72 |
| 1:B:565:LYS:C | 1:B:567:THR:H | 1.90 | 0.72 |
| 2:E:25:GLY:HA3 | 2:E:65:PHE:HE1 | 1.51 | 0.72 |
| 2:F:106:ARG:O | 2:F:110:THR:HG23 | 1.90 | 0.72 |
| 2:E:106:ARG:O | 2:E:110:THR:HG23 | 1.89 | 0.72 |
| 1:C:581:GLN:HE21 | 1:C:629:ASN:H | 1.35 | 0.72 |
| 1:C:581:GLN:NE2 | 1:C:629:ASN:H | 1.86 | 0.72 |
| 1:C:639:ASN:C | 1:C:639:ASN:HD22 | 1.91 | 0.72 |
| 2:D:44:THR:HG22 | 2:D:47:GLU:HG3 | 1.71 | 0.72 |
| 1:B:540:ARG:NH2 | 1:B:630:ARG:CZ | 2.53 | 0.71 |
| 1:C:518:ASN:O | 1:C:519:THR:HB | 1.90 | 0.71 |
| 1:B:657:ILE:CG1 | 1:B:658:PRO:HD2 | 2.19 | 0.71 |
| 1:C:523:LEU:HD21 | 2:F:127:GLU:HB3 | 1.72 | 0.71 |
| 1:C:748:TYR:O | 1:C:751:TYR:HB3 | 1.90 | 0.71 |
| 1:C:621:GLY:O | 2:F:94:LYS:HE3 | 1.90 | 0.71 |
| 2:F:81:SER:O | 2:F:83:GLU:N | 2.23 | 0.71 |
| 1:B:456:LYS:HB3 | 1:B:470:ASN:O | 1.91 | 0.71 |
| 1:B:470:ASN:OD1 | 1:B:471:TRP:N | 2.23 | 0.71 |
| 1:B:697:ILE:HD13 | 1:B:732:ILE:CD1 | 2.21 | 0.71 |
| 1:A:657:ILE:HG22 | 1:A:756:ILE:HA | 1.73 | 0.71 |
| 1:B:332:ASN:ND2 | 1:B:334:LEU:H | 1.87 | 0.71 |
| 1:B:526:GLN:H | 1:B:526:GLN:CD | 1.94 | 0.71 |
| 1:B:530:THR:HG22 | 2:E:92:PHE:CZ | 2.25 | 0.71 |
| 1:A:351:HIS:CD2 | 5:A:999:DOT:H3B | 2.26 | 0.71 |
| 1:C:401:ILE:HD13 | 1:C:478:ALA:HB2 | 1.73 | 0.71 |
| 2:E:44:THR:HG22 | 2:E:47:GLU:HG3 | 1.72 | 0.71 |
| 1:A:581:GLN:NE2 | 1:A:629:ASN:H | 1.88 | 0.71 |
| 2:E:81:SER:O | 2:E:83:GLU:N | 2.24 | 0.71 |
| 1:B:777:TYR:HD1 | 1:B:780:LEU:CD1 | 2.02 | 0.71 |
| 1:C:318:ILE:HG23 | 1:C:322:LEU:HD13 | 1.73 | 0.71 |
| 1:C:759:GLN:HA | 1:C:759:GLN:NE2 | 2.01 | 0.70 |
| 1:A:445:ARG:HH12 | 1:A:456:LYS:HB3 | 1.56 | 0.70 |
| 1:A:513:TRP:O | 1:A:517:VAL:HG23 | 1.91 | 0.70 |
| 2:E:65:PHE:HB2 | 2:E:66:PRO:HD3 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:65:PHE:HB2 | 2:F:66:PRO:HD3 | 1.74 | 0.70 |
| 1:B:540:ARG:NH1 | 2:E:87:GLU:OE1 | 2.24 | 0.70 |
| 2:D:25:GLY:HA3 | 2:D:65:PHE:HE1 | 1.54 | 0.70 |
| 1:B:363:TYR:O | 1:B:365:PRO:HD3 | 1.92 | 0.70 |
| 1:C:723:PHE:HB2 | 1:C:793:PHE:CE2 | 2.26 | 0.70 |
| 2:D:106:ARG:O | 2:D:110:THR:HG23 | 1.92 | 0.70 |
| 1:C:633:ASN:HD22 | 1:C:644:GLU:HA | 1.57 | 0.70 |
| 1:A:633:ASN:ND2 | 1:A:645:TRP:H | 1.87 | 0.70 |
| 2:D:25:GLY:O | 2:D:64:ASP:HA | 1.92 | 0.70 |
| 2:D:70:THR:O | 2:D:73:ALA:HB3 | 1.92 | 0.70 |
| 1:C:540:ARG:HB3 | 1:C:549:LEU:C | 2.12 | 0.70 |
| 2:D:65:PHE:HB2 | 2:D:66:PRO:HD3 | 1.73 | 0.69 |
| 1:C:446:ILE:HG12 | 1:C:447:SER:N | 2.07 | 0.69 |
| 2:E:89:PHE:CD2 | 2:E:89:PHE:C | 2.65 | 0.69 |
| 2:F:44:THR:HG22 | 2:F:47:GLU:HG3 | 1.74 | 0.69 |
| 1:B:540:ARG:NH2 | 1:B:630:ARG:NH2 | 2.40 | 0.69 |
| 1:B:727:GLN:HG3 | 1:B:786:GLU:CD | 2.13 | 0.69 |
| 1:A:445:ARG:HH22 | 1:A:456:LYS:CD | 2.06 | 0.69 |
| 1:B:385:LEU:HA | 1:B:388:LYS:HD3 | 1.74 | 0.69 |
| 1:B:585:GLU:O | 1:B:638:GLY:HA3 | 1.93 | 0.69 |
| 1:B:349:ASN:OD1 | 1:B:350:VAL:HG23 | 1.93 | 0.69 |
| 1:B:376:GLN:CB | 1:B:379:ALA:HB3 | 2.17 | 0.69 |
| 2:F:25:GLY:HA3 | 2:F:65:PHE:HE1 | 1.55 | 0.69 |
| 1:A:782:PHE:H | 1:A:782:PHE:HD1 | 1.39 | 0.69 |
| 1:C:782:PHE:HD1 | 1:C:782:PHE:H | 1.39 | 0.69 |
| 1:A:723:PHE:HB2 | 1:A:793:PHE:CE2 | 2.27 | 0.69 |
| 1:C:367:ASP:O | 1:C:369:ASP:N | 2.26 | 0.69 |
| 1:B:478:ALA:HB1 | 1:B:486:LYS:O | 1.92 | 0.69 |
| 1:C:492:TYR:HD2 | 1:C:574:VAL:HG13 | 1.54 | 0.69 |
| 2:D:133:ASP:OD1 | 2:D:135:GLN:HG3 | 1.93 | 0.69 |
| 2:D:89:PHE:CD2 | 2:D:89:PHE:C | 2.66 | 0.68 |
| 2:F:89:PHE:CD2 | 2:F:89:PHE:C | 2.66 | 0.68 |
| 1:C:501:LEU:O | 1:C:504:ILE:HG22 | 1.93 | 0.68 |
| 1:B:653:LYS:O | 1:B:755:ARG:HD3 | 1.93 | 0.68 |
| 1:A:477:MET:O | 1:A:488:LEU:HD12 | 1.93 | 0.68 |
| 1:A:657:ILE:HG22 | 1:A:756:ILE:HD13 | 1.75 | 0.68 |
| 1:B:525:LYS:HB2 | 1:B:526:GLN:NE2 | 2.07 | 0.68 |
| 2:D:48:LEU:O | 2:D:52:ILE:HG22 | 1.92 | 0.68 |
| 2:F:25:GLY:O | 2:F:64:ASP:HA | 1.93 | 0.68 |
| 1:C:657:ILE:HD13 | 1:C:756:ILE:CD1 | 2.23 | 0.68 |
| 1:A:759:GLN:HA | 1:A:759:GLN:NE2 | 2.01 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:136:VAL:HA | 2:D:140:GLU:OE1 | 1.92 | 0.68 |
| 1:A:748:TYR:O | 1:A:751:TYR:HB3 | 1.94 | 0.68 |
| 1:A:782:PHE:N | 1:A:782:PHE:CD1 | 2.61 | 0.68 |
| 1:C:793:PHE:O | 1:C:796:ILE:HG12 | 1.94 | 0.68 |
| 1:C:782:PHE:N | 1:C:782:PHE:CD1 | 2.62 | 0.68 |
| 2:F:70:THR:O | 2:F:73:ALA:HB3 | 1.93 | 0.68 |
| 1:B:454:GLN:HB3 | 1:B:472:ARG:O | 1.93 | 0.68 |
| 1:C:508:ILE:HD13 | 1:C:532:LEU:HB3 | 1.75 | 0.68 |
| 1:B:748:TYR:O | 1:B:752:LEU:HG | 1.92 | 0.68 |
| 1:B:432:TYR:CD2 | 1:B:447:SER:HA | 2.28 | 0.68 |
| 1:C:445:ARG:NH1 | 1:C:471:TRP:CD1 | 2.62 | 0.68 |
| 1:B:720:ILE:HD12 | 1:B:721:SER:N | 2.08 | 0.68 |
| 1:C:665:LYS:HE2 | 2:F:11:GLU:OE2 | 1.92 | 0.68 |
| 1:C:514:ASP:HA | 1:C:517:VAL:HG12 | 1.76 | 0.68 |
| 1:A:501:LEU:O | 1:A:504:ILE:HG22 | 1.94 | 0.68 |
| 1:A:446:ILE:HG12 | 1:A:447:SER:N | 2.09 | 0.68 |
| 1:C:690:LYS:HG2 | 1:C:691:LYS:O | 1.94 | 0.68 |
| 1:C:463:THR:HG22 | 1:C:465:LEU:H | 1.59 | 0.68 |
| 1:B:615:ILE:HD13 | 1:B:626:TYR:CE1 | 2.28 | 0.67 |
| 1:B:596:ILE:HG12 | 1:B:602:PHE:CE2 | 2.29 | 0.67 |
| 2:F:48:LEU:O | 2:F:52:ILE:HG22 | 1.95 | 0.67 |
| 2:F:136:VAL:HA | 2:F:140:GLU:OE1 | 1.95 | 0.67 |
| 1:B:462:ILE:HD11 | 1:B:466:GLY:HA2 | 1.76 | 0.67 |
| 1:C:313:ASP:HA | 1:C:316:LYS:HE2 | 1.77 | 0.67 |
| 1:A:313:ASP:HA | 1:A:316:LYS:HE2 | 1.77 | 0.67 |
| 1:A:388:LYS:O | 1:A:392:THR:HG23 | 1.95 | 0.67 |
| 1:A:367:ASP:O | 1:A:369:ASP:N | 2.28 | 0.67 |
| 1:B:760:VAL:O | 1:B:764:LEU:HG | 1.95 | 0.67 |
| 1:B:747:ASN:O | 1:B:751:TYR:CB | 2.43 | 0.67 |
| 1:C:712:PHE:HB3 | 1:C:716:LYS:HG2 | 1.75 | 0.67 |
| 1:B:734:ASN:O | 1:B:736:LEU:N | 2.28 | 0.67 |
| 1:B:366:PHE:HA | 1:B:477:MET:HE3 | 1.77 | 0.67 |
| 1:B:734:ASN:C | 1:B:736:LEU:N | 2.48 | 0.67 |
| 1:B:388:LYS:O | 1:B:392:THR:HG23 | 1.94 | 0.67 |
| 1:B:432:TYR:HE2 | 1:B:447:SER:HB2 | 1.59 | 0.66 |
| 1:A:793:PHE:O | 1:A:796:ILE:HG12 | 1.94 | 0.66 |
| 1:C:561:ASN:O | 1:C:565:LYS:HG3 | 1.96 | 0.66 |
| 2:E:48:LEU:O | 2:E:52:ILE:HG22 | 1.95 | 0.66 |
| 1:A:295:VAL:HG21 | 1:A:603:ILE:CG2 | 2.22 | 0.66 |
| 2:E:25:GLY:O | 2:E:64:ASP:HA | 1.94 | 0.66 |
| 1:B:746:LYS:O | 1:B:750:GLN:N | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:654:ILE:O | 1:C:755:ARG:HG2 | 1.95 | 0.66 |
| 1:A:463:THR:HG22 | 1:A:465:LEU:N | 2.10 | 0.66 |
| 1:A:295:VAL:CG2 | 1:A:603:ILE:HG22 | 2.22 | 0.66 |
| 1:A:561:ASN:O | 1:A:565:LYS:HG3 | 1.96 | 0.66 |
| 1:C:758:ASN:O | 1:C:762:LEU:HB2 | 1.95 | 0.66 |
| 1:A:540:ARG:HB3 | 1:A:549:LEU:C | 2.16 | 0.66 |
| 1:A:700:TYR:HD1 | 1:A:728:ALA:HA | 1.58 | 0.66 |
| 1:C:463:THR:HG22 | 1:C:465:LEU:N | 2.10 | 0.66 |
| 1:A:337:ASN:HB3 | 1:A:412:GLU:OE2 | 1.95 | 0.66 |
| 2:D:101:SER:OG | 2:D:104:GLU:HG3 | 1.96 | 0.66 |
| 1:A:670:ILE:HD12 | 1:A:745:TYR:CE1 | 2.31 | 0.66 |
| 1:B:324:THR:CG2 | 1:B:499:PRO:HA | 2.26 | 0.66 |
| 2:D:81:SER:O | 2:D:83:GLU:N | 2.29 | 0.66 |
| 1:B:616:GLU:HA | 1:B:620:THR:HG22 | 1.78 | 0.66 |
| 1:A:705:TYR:HE2 | 2:D:139:GLU:HB3 | 1.58 | 0.65 |
| 1:C:705:TYR:HE2 | 2:F:139:GLU:HB3 | 1.55 | 0.65 |
| 1:B:792:VAL:O | 1:B:792:VAL:HG12 | 1.96 | 0.65 |
| 1:C:388:LYS:O | 1:C:392:THR:HG23 | 1.96 | 0.65 |
| 1:C:302:LEU:C | 1:C:302:LEU:HD23 | 2.16 | 0.65 |
| 1:B:562:GLU:HA | 1:B:565:LYS:HG3 | 1.77 | 0.65 |
| 1:C:540:ARG:NH2 | 1:C:627:TYR:CE1 | 2.65 | 0.65 |
| 2:E:115:LYS:O | 2:E:116:LEU:HD23 | 1.95 | 0.65 |
| 2:E:101:SER:OG | 2:E:104:GLU:HG3 | 1.97 | 0.65 |
| 1:A:758:ASN:O | 1:A:762:LEU:HB2 | 1.96 | 0.65 |
| 1:A:639:ASN:HD22 | 1:A:641:ALA:H | 1.45 | 0.65 |
| 1:A:521:ASN:ND2 | 1:A:522:SER:N | 2.44 | 0.65 |
| 1:B:513:TRP:HH2 | 2:E:113:GLY:HA3 | 1.61 | 0.65 |
| 1:A:377:GLN:O | 1:A:379:ALA:N | 2.29 | 0.65 |
| 1:A:302:LEU:C | 1:A:302:LEU:HD23 | 2.17 | 0.65 |
| 2:F:81:SER:O | 2:F:82:GLU:C | 2.35 | 0.65 |
| 1:A:401:ILE:HD13 | 1:A:478:ALA:HB2 | 1.78 | 0.65 |
| 1:B:577:HIS:N | 1:B:577:HIS:CD2 | 2.65 | 0.65 |
| 1:B:629:ASN:HD21 | 1:B:631:SER:N | 1.84 | 0.65 |
| 1:A:633:ASN:HD21 | 1:A:645:TRP:N | 1.88 | 0.65 |
| 1:B:722:ILE:HD13 | 1:B:764:LEU:HD21 | 1.78 | 0.65 |
| 2:E:92:PHE:CE2 | 2:E:108:VAL:HG11 | 2.32 | 0.65 |
| 2:E:81:SER:O | 2:E:82:GLU:C | 2.35 | 0.65 |
| 1:A:659:THR:OG1 | 1:A:660:SER:N | 2.31 | 0.65 |
| 1:A:481:VAL:HG23 | 1:A:481:VAL:O | 1.97 | 0.65 |
| 1:C:295:VAL:HG21 | 1:C:603:ILE:CG2 | 2.24 | 0.64 |
| 1:C:337:ASN:HB3 | 1:C:412:GLU:OE2 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:513:TRP:CE3 | 1:A:517:VAL:HG21 | 2.32 | 0.64 |
| 1:B:306:GLY:O | 1:B:336:THR:HB | 1.96 | 0.64 |
| 1:A:656:THR:O | 1:A:755:ARG:HD2 | 1.97 | 0.64 |
| 1:C:692:GLU:O | 1:C:735:VAL:HG22 | 1.96 | 0.64 |
| 1:C:530:THR:HG21 | 2:F:145:MET:CE | 2.27 | 0.64 |
| 1:B:615:ILE:HD12 | 1:B:645:TRP:HH2 | 1.60 | 0.64 |
| 2:F:140:GLU:O | 2:F:142:VAL:N | 2.30 | 0.64 |
| 2:E:92:PHE:CD2 | 2:E:108:VAL:HG21 | 2.32 | 0.64 |
| 1:C:353:LYS:HG3 | 1:C:373:LYS:HD3 | 1.78 | 0.64 |
| 1:C:463:THR:HB | 1:C:467:GLU:H | 1.63 | 0.64 |
| 1:C:349:ASN:HD21 | 1:C:398:ILE:HG13 | 1.62 | 0.64 |
| 1:A:445:ARG:NH2 | 1:A:471:TRP:NE1 | 2.45 | 0.64 |
| 1:B:654:ILE:HA | 1:B:755:ARG:CG | 2.26 | 0.64 |
| 1:B:377:GLN:HG2 | 1:B:378:LEU:HD22 | 1.80 | 0.64 |
| 1:C:522:SER:O | 1:C:525:LYS:N | 2.30 | 0.64 |
| 1:B:332:ASN:C | 1:B:332:ASN:ND2 | 2.49 | 0.64 |
| 1:A:663:PHE:CE1 | 1:A:752:LEU:HD11 | 2.32 | 0.64 |
| 1:A:353:LYS:HG3 | 1:A:373:LYS:HD3 | 1.78 | 0.64 |
| 1:A:658:PRO:O | 1:A:701:LEU:HD13 | 1.98 | 0.64 |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:HB2 | 1.62 | 0.64 |
| 1:B:697:ILE:HD13 | 1:B:732:ILE:HD13 | 1.80 | 0.63 |
| 2:E:136:VAL:HA | 2:E:140:GLU:OE1 | 1.98 | 0.63 |
| 1:A:463:THR:HG22 | 1:A:465:LEU:H | 1.61 | 0.63 |
| 1:A:696:LYS:HA | 1:A:696:LYS:HE2 | 1.80 | 0.63 |
| 1:A:633:ASN:HD22 | 1:A:644:GLU:HA | 1.63 | 0.63 |
| 1:C:349:ASN:ND2 | 1:C:398:ILE:HG13 | 2.13 | 0.63 |
| 2:E:5:THR:OG1 | 2:E:8:GLN:HB2 | 1.98 | 0.63 |
| 1:A:445:ARG:NH2 | 1:A:471:TRP:HE1 | 1.95 | 0.63 |
| 1:B:712:PHE:CD1 | 1:B:712:PHE:N | 2.66 | 0.63 |
| 1:B:619:ILE:C | 1:B:621:GLY:H | 2.00 | 0.63 |
| 1:B:722:ILE:HD13 | 1:B:764:LEU:CD2 | 2.29 | 0.63 |
| 1:B:728:ALA:CA | 1:B:731:GLU:HG3 | 2.28 | 0.63 |
| 1:B:712:PHE:HD1 | 1:B:712:PHE:N | 1.97 | 0.63 |
| 1:C:622:LYS:O | 1:C:623:ASP:HB2 | 1.97 | 0.63 |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:CD2 | 2.28 | 0.63 |
| 1:B:360:VAL:CG1 | 1:B:365:PRO:HG3 | 2.28 | 0.63 |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:CD1 | 2.34 | 0.63 |
| 1:B:407:HIS:H | 1:B:407:HIS:CD2 | 2.16 | 0.63 |
| 1:B:320:ARG:HG3 | 1:B:320:ARG:HH21 | 1.64 | 0.63 |
| 1:B:432:TYR:HD2 | 1:B:447:SER:HA | 1.61 | 0.63 |
| 1:A:653:LYS:O | 1:A:755:ARG:HD3 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:656:THR:O | 1:B:705:TYR:HE1 | 1.80 | 0.63 |
| 1:A:349:ASN:HD21 | 1:A:398:ILE:HG13 | 1.62 | 0.63 |
| 1:C:508:ILE:HG12 | 1:C:536:TYR:CD2 | 2.34 | 0.63 |
| 1:C:653:LYS:O | 1:C:656:THR:HG23 | 1.99 | 0.63 |
| 1:A:697:ILE:N | 1:A:697:ILE:HD12 | 2.14 | 0.63 |
| 2:D:99:TYR:CD2 | 2:D:137:ASN:HB3 | 2.34 | 0.62 |
| 2:F:115:LYS:O | 2:F:116:LEU:HD23 | 1.99 | 0.62 |
| 1:A:385:LEU:HD13 | 1:A:385:LEU:O | 1.99 | 0.62 |
| 1:C:722:ILE:HD13 | 1:C:764:LEU:CD2 | 2.29 | 0.62 |
| 1:C:722:ILE:HG23 | 1:C:760:VAL:HG13 | 1.81 | 0.62 |
| 1:B:424:LYS:HE2 | 1:B:433:TYR:OH | 1.98 | 0.62 |
| 1:C:327:LEU:HG | 1:C:595:ILE:HG23 | 1.81 | 0.62 |
| 2:D:115:LYS:O | 2:D:116:LEU:HD23 | 1.99 | 0.62 |
| 1:B:376:GLN:CB | 1:B:379:ALA:CB | 2.77 | 0.62 |
| 1:C:581:GLN:NE2 | 1:C:628:PHE:HA | 2.14 | 0.62 |
| 1:B:777:TYR:CD1 | 1:B:780:LEU:HB2 | 2.34 | 0.62 |
| 1:C:324:THR:HG23 | 1:C:324:THR:O | 1.99 | 0.62 |
| 1:B:525:LYS:O | 1:B:529:VAL:HG22 | 1.99 | 0.62 |
| 2:E:133:ASP:OD1 | 2:E:135:GLN:HG3 | 2.00 | 0.62 |
| 2:F:133:ASP:OD1 | 2:F:135:GLN:HG3 | 1.99 | 0.62 |
| 1:A:318:ILE:N | 1:A:318:ILE:HD12 | 2.14 | 0.62 |
| 2:E:140:GLU:O | 2:E:142:VAL:N | 2.31 | 0.62 |
| 1:B:649:ILE:O | 1:B:649:ILE:CG2 | 2.48 | 0.62 |
| 1:B:310:GLU:CD | 1:B:310:GLU:H | 2.03 | 0.62 |
| 1:B:333:LYS:O | 1:B:336:THR:HG22 | 1.99 | 0.62 |
| 1:C:602:PHE:O | 1:C:603:ILE:HD13 | 1.99 | 0.62 |
| 1:C:700:TYR:CE1 | 1:C:727:GLN:HG2 | 2.35 | 0.62 |
| 2:D:81:SER:O | 2:D:82:GLU:C | 2.37 | 0.62 |
| 1:C:319:ALA:O | 1:C:598:PRO:HA | 1.99 | 0.62 |
| 1:B:633:ASN:O | 1:B:634:LYS:HG3 | 2.00 | 0.62 |
| 1:B:445:ARG:HB3 | 1:B:471:TRP:CZ3 | 2.35 | 0.62 |
| 1:B:361:ALA:O | 1:B:409:ARG:NH2 | 2.30 | 0.62 |
| 2:F:99:TYR:CD2 | 2:F:137:ASN:HB3 | 2.35 | 0.62 |
| 1:A:630:ARG:HE | 2:D:87:GLU:CD | 2.03 | 0.62 |
| 1:B:419:ILE:HD12 | 1:B:435:LEU:HD22 | 1.81 | 0.62 |
| 1:B:519:THR:N | 1:B:520:PRO:HD3 | 2.15 | 0.61 |
| 1:B:723:PHE:O | 1:B:727:GLN:N | 2.30 | 0.61 |
| 1:C:525:LYS:HB2 | 2:F:124:MET:CE | 2.30 | 0.61 |
| 2:F:65:PHE:O | 2:F:69:LEU:HG | 2.00 | 0.61 |
| 1:B:514:ASP:HA | 1:B:517:VAL:CG1 | 2.29 | 0.61 |
| 1:A:622:LYS:O | 1:A:623:ASP:HB2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:653:LYS:O | 1:B:653:LYS:HG3 | 1.99 | 0.61 |
| 1:B:649:ILE:CD1 | 2:E:86:ARG:HG3 | 2.29 | 0.61 |
| 1:C:481:VAL:HG23 | 1:C:481:VAL:O | 2.00 | 0.61 |
| 1:A:605:THR:CG2 | 1:A:611:THR:HA | 2.25 | 0.61 |
| 1:A:712:PHE:HB3 | 1:A:716:LYS:HG2 | 1.81 | 0.61 |
| 1:C:543:ASP:OD2 | 1:C:546:LYS:HG3 | 1.99 | 0.61 |
| 1:B:639:ASN:H | 1:B:639:ASN:ND2 | 1.98 | 0.61 |
| 1:B:722:ILE:HG22 | 1:B:726:ILE:HD12 | 1.81 | 0.61 |
| 1:C:377:GLN:O | 1:C:379:ALA:N | 2.33 | 0.61 |
| 2:E:99:TYR:CD2 | 2:E:137:ASN:HB3 | 2.36 | 0.61 |
| 1:B:501:LEU:HB2 | 1:B:623:ASP:O | 2.01 | 0.61 |
| 1:B:508:ILE:HG21 | 1:B:532:LEU:HD22 | 1.83 | 0.61 |
| 1:C:653:LYS:O | 1:C:755:ARG:HD3 | 2.01 | 0.61 |
| 1:C:649:ILE:HD13 | 2:F:90:ARG:HE | 1.66 | 0.61 |
| 1:C:385:LEU:HD13 | 1:C:385:LEU:O | 2.01 | 0.61 |
| 1:C:663:PHE:HD2 | 1:C:664:ILE:HD12 | 1.66 | 0.61 |
| 1:C:657:ILE:HG22 | 1:C:658:PRO:N | 2.16 | 0.61 |
| 2:F:63:ILE:N | 2:F:63:ILE:HD12 | 2.16 | 0.61 |
| 1:A:792:VAL:HG12 | 1:A:796:ILE:HD11 | 1.83 | 0.61 |
| 1:A:349:ASN:ND2 | 1:A:398:ILE:HG13 | 2.16 | 0.61 |
| 1:C:776:LEU:HD12 | 1:C:776:LEU:N | 2.15 | 0.61 |
| 1:B:535:LYS:C | 1:B:536:TYR:HD2 | 2.03 | 0.60 |
| 1:C:535:LYS:HE2 | 1:C:536:TYR:CZ | 2.36 | 0.60 |
| 1:B:339:ILE:HG12 | 1:B:489:THR:HG21 | 1.83 | 0.60 |
| 1:C:659:THR:HB | 1:C:662:GLU:HG3 | 1.82 | 0.60 |
| 1:B:459:GLU:O | 1:B:461:LYS:N | 2.27 | 0.60 |
| 1:B:565:LYS:C | 1:B:567:THR:N | 2.55 | 0.60 |
| 1:C:368:GLN:HB2 | 1:C:384:ASN:OD1 | 2.02 | 0.60 |
| 2:F:130:ILE:O | 2:F:130:ILE:HG22 | 2.01 | 0.60 |
| 1:C:324:THR:CG2 | 1:C:324:THR:O | 2.50 | 0.60 |
| 1:A:408:LEU:C | 1:A:408:LEU:HD23 | 2.20 | 0.60 |
| 1:C:438:ASN:C | 1:C:438:ASN:HD22 | 2.05 | 0.60 |
| 1:A:299:GLU:HG3 | 1:A:303:LYS:NZ | 2.16 | 0.60 |
| 1:A:445:ARG:CZ | 1:A:471:TRP:CD1 | 2.83 | 0.60 |
| 1:B:516:VAL:CA | 1:B:520:PRO:HG2 | 2.28 | 0.60 |
| 1:B:319:ALA:HB2 | 1:B:326:ILE:HD12 | 1.83 | 0.60 |
| 1:B:346:LYS:NZ | 1:B:352:GLY:O | 2.34 | 0.60 |
| 1:A:538:ILE:HD11 | 2:D:91:VAL:HG21 | 1.83 | 0.60 |
| 2:F:7:GLU:O | 2:F:11:GLU:HG3 | 2.02 | 0.60 |
| 1:A:776:LEU:HD12 | 1:A:776:LEU:N | 2.17 | 0.60 |
| 1:A:462:ILE:HD11 | 1:A:466:GLY:HA2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:615:ILE:HD12 | 1:B:645:TRP:CZ2 | 2.37 | 0.59 |
| 1:A:587:PRO:HB2 | 1:A:643:ILE:HD12 | 1.83 | 0.59 |
| 1:B:318:ILE:HD12 | 1:B:319:ALA:N | 2.18 | 0.59 |
| 1:A:540:ARG:HD3 | 1:A:582:ASP:OD1 | 2.01 | 0.59 |
| 1:B:498:ALA:CB | 1:B:619:ILE:HD13 | 2.32 | 0.59 |
| 2:E:7:GLU:O | 2:E:11:GLU:HG3 | 2.01 | 0.59 |
| 1:A:589:LYS:HE2 | 1:A:643:ILE:HG23 | 1.85 | 0.59 |
| 1:C:639:ASN:HD22 | 1:C:641:ALA:H | 1.51 | 0.59 |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:HD1 | 1.67 | 0.59 |
| 1:B:432:TYR:CE2 | 1:B:447:SER:HB2 | 2.37 | 0.59 |
| 1:B:369:ASP:OD2 | 1:B:442:TYR:OH | 2.19 | 0.59 |
| 1:C:655:ASN:HD22 | 1:C:655:ASN:N | 1.97 | 0.59 |
| 1:A:787:THR:O | 1:A:791:GLU:HG2 | 2.02 | 0.59 |
| 1:A:670:ILE:HG23 | 1:A:745:TYR:CE1 | 2.38 | 0.59 |
| 1:C:605:THR:CG2 | 1:C:611:THR:HA | 2.27 | 0.59 |
| 1:C:740:GLN:H | 1:C:740:GLN:CD | 2.05 | 0.59 |
| 1:C:583:ASN:ND2 | 5:C:1999:DOT:H1' | 2.18 | 0.59 |
| 1:C:587:PRO:HB2 | 1:C:643:ILE:HD12 | 1.83 | 0.59 |
| 1:A:695:LYS:CB | 2:D:18:LEU:HD22 | 2.30 | 0.59 |
| 1:B:554:LYS:O | 1:B:557:LEU:N | 2.35 | 0.59 |
| 1:B:540:ARG:HH22 | 1:B:630:ARG:CZ | 2.15 | 0.59 |
| 1:A:432:TYR:CE1 | 1:A:471:TRP:HZ3 | 2.20 | 0.59 |
| 1:C:639:ASN:HD22 | 1:C:640:LYS:N | 2.00 | 0.59 |
| 1:B:629:ASN:HD21 | 1:B:631:SER:CB | 2.14 | 0.59 |
| 1:A:592:GLU:HB3 | 1:A:604:LEU:HD21 | 1.85 | 0.59 |
| 1:B:752:LEU:O | 1:B:756:ILE:HG13 | 2.02 | 0.59 |
| 1:B:540:ARG:HD2 | 1:B:627:TYR:CE1 | 2.38 | 0.59 |
| 1:B:322:LEU:HA | 1:B:503:GLU:OE1 | 2.02 | 0.59 |
| 1:B:733:GLU:O | 1:B:735:VAL:N | 2.35 | 0.59 |
| 1:B:546:LYS:N | 1:B:546:LYS:HD2 | 2.18 | 0.59 |
| 1:A:722:ILE:HG23 | 1:A:760:VAL:HG13 | 1.83 | 0.59 |
| 5:C:1999:DOT:O1' | 5:C:1999:DOT:H2'1 | 2.01 | 0.58 |
| 1:A:697:ILE:H | 1:A:697:ILE:HD12 | 1.67 | 0.58 |
| 1:A:438:ASN:HD22 | 1:A:438:ASN:C | 2.05 | 0.58 |
| 1:B:606:LYS:N | 1:B:610:MET:CE | 2.65 | 0.58 |
| 1:C:698:ALA:O | 1:C:701:LEU:HB2 | 2.02 | 0.58 |
| 1:C:792:VAL:HG12 | 1:C:796:ILE:HD11 | 1.84 | 0.58 |
| 1:C:295:VAL:HG23 | 1:C:604:LEU:O | 2.02 | 0.58 |
| 1:B:605:THR:HG22 | 1:B:606:LYS:N | 2.18 | 0.58 |
| 1:C:477:MET:O | 1:C:488:LEU:HD12 | 2.03 | 0.58 |
| 1:C:320:ARG:HG3 | 1:C:598:PRO:O | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:363:TYR:HD1 | 1:C:403:LEU:HD11 | 1.68 | 0.58 |
| 2:D:65:PHE:O | 2:D:69:LEU:HG | 2.04 | 0.58 |
| 1:A:621:GLY:O | 2:D:94:LYS:HE3 | 2.03 | 0.58 |
| 1:C:294:ASP:O | 1:C:610:MET:HE1 | 2.04 | 0.58 |
| 1:B:761:GLN:OE1 | 1:B:765:THR:HG23 | 2.04 | 0.58 |
| 1:C:659:THR:O | 1:C:701:LEU:HD13 | 2.04 | 0.58 |
| 1:A:454:GLN:OE1 | 1:A:471:TRP:CE3 | 2.56 | 0.58 |
| 2:D:63:ILE:N | 2:D:63:ILE:HD12 | 2.19 | 0.58 |
| 1:B:728:ALA:HA | 1:B:731:GLU:HG2 | 1.86 | 0.58 |
| 1:C:318:ILE:N | 1:C:318:ILE:HD12 | 2.17 | 0.58 |
| 1:C:664:ILE:CG2 | 2:F:15:ALA:HB2 | 2.24 | 0.58 |
| 1:C:519:THR:O | 1:C:525:LYS:HE2 | 2.04 | 0.58 |
| 1:C:326:ILE:C | 1:C:327:LEU:HD12 | 2.24 | 0.58 |
| 1:B:621:GLY:O | 2:E:94:LYS:HE3 | 2.04 | 0.58 |
| 1:A:322:LEU:HD12 | 1:A:322:LEU:H | 1.68 | 0.58 |
| 2:D:140:GLU:O | 2:D:142:VAL:N | 2.37 | 0.58 |
| 1:B:761:GLN:HA | 1:B:761:GLN:OE1 | 2.03 | 0.58 |
| 1:C:450:ASN:O | 1:C:451:ASN:HB2 | 2.04 | 0.58 |
| 2:F:5:THR:O | 2:F:9:ILE:HG13 | 2.03 | 0.58 |
| 1:C:558:ASP:O | 1:C:562:GLU:HG3 | 2.03 | 0.58 |
| 1:B:354:SER:O | 1:B:371:SER:HB2 | 2.04 | 0.57 |
| 1:C:304:ALA:HB3 | 1:C:604:LEU:HD13 | 1.86 | 0.57 |
| 1:C:584:GLU:OE1 | 1:C:630:ARG:HG3 | 2.04 | 0.57 |
| 2:D:133:ASP:OD1 | 2:D:135:GLN:O | 2.22 | 0.57 |
| 1:B:550:SER:N | 1:B:553:GLN:HG3 | 2.19 | 0.57 |
| 1:C:324:THR:OG1 | 1:C:499:PRO:HA | 2.04 | 0.57 |
| 1:C:697:ILE:HD11 | 1:C:735:VAL:HG21 | 1.85 | 0.57 |
| 1:C:408:LEU:C | 1:C:408:LEU:HD23 | 2.25 | 0.57 |
| 1:C:302:LEU:HD12 | 1:C:602:PHE:HE1 | 1.69 | 0.57 |
| 1:A:295:VAL:HG23 | 1:A:604:LEU:O | 2.04 | 0.57 |
| 1:A:540:ARG:NH1 | 1:A:630:ARG:HH21 | 2.03 | 0.57 |
| 2:F:131:ASP:OD1 | 2:F:133:ASP:OD2 | 2.22 | 0.57 |
| 1:B:307:LEU:HD21 | 1:B:328:PHE:CD1 | 2.40 | 0.57 |
| 1:A:790:PHE:O | 1:A:793:PHE:HB3 | 2.05 | 0.57 |
| 1:C:462:ILE:HD11 | 1:C:466:GLY:HA2 | 1.85 | 0.57 |
| 1:B:657:ILE:CG1 | 1:B:658:PRO:CD | 2.81 | 0.57 |
| 1:B:586:PHE:N | 1:B:587:PRO:HD3 | 2.20 | 0.57 |
| 2:E:65:PHE:O | 2:E:69:LEU:HG | 2.05 | 0.57 |
| 1:B:605:THR:HG21 | 1:B:611:THR:OG1 | 2.03 | 0.57 |
| 1:A:583:ASN:ND2 | 5:A:999:DOT:H1' | 2.19 | 0.57 |
| 1:B:513:TRP:CH2 | 2:E:113:GLY:HA3 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:450:ASN:OD1 | 1:C:452:GLU:HG3 | 2.05 | 0.57 |
| 1:C:787:THR:O | 1:C:791:GLU:HG2 | 2.05 | 0.57 |
| 1:C:714:GLN:NE2 | 2:F:126:ARG:HG2 | 2.20 | 0.57 |
| 2:F:137:ASN:OD1 | 2:F:139:GLU:HB2 | 2.05 | 0.56 |
| 1:A:574:VAL:O | 1:A:574:VAL:HG13 | 2.05 | 0.56 |
| 1:C:324:THR:OG1 | 1:C:499:PRO:CA | 2.53 | 0.56 |
| 1:C:363:TYR:CD1 | 1:C:403:LEU:HD11 | 2.40 | 0.56 |
| 2:F:92:PHE:CD2 | 2:F:108:VAL:HG21 | 2.40 | 0.56 |
| 1:C:712:PHE:CD2 | 1:C:716:LYS:HE2 | 2.39 | 0.56 |
| 1:A:505:LYS:HD3 | 2:D:112:LEU:O | 2.05 | 0.56 |
| 1:C:518:ASN:O | 1:C:519:THR:CB | 2.54 | 0.56 |
| 1:B:385:LEU:CD2 | 1:B:389:LYS:HE2 | 2.36 | 0.56 |
| 1:C:606:LYS:O | 1:C:607:ASN:HB3 | 2.05 | 0.56 |
| 1:B:307:LEU:HD21 | 1:B:328:PHE:CE1 | 2.40 | 0.56 |
| 1:A:781:ASN:ND2 | 1:A:783:THR:OG1 | 2.38 | 0.56 |
| 1:B:773:PHE:C | 1:B:775:LEU:H | 2.08 | 0.56 |
| 1:B:509:PRO:HD2 | 1:B:536:TYR:HE1 | 1.69 | 0.56 |
| 1:B:562:GLU:O | 1:B:564:VAL:N | 2.38 | 0.56 |
| 1:A:712:PHE:CD2 | 1:A:716:LYS:HE2 | 2.41 | 0.56 |
| 1:C:377:GLN:O | 1:C:378:LEU:C | 2.42 | 0.56 |
| 1:B:331:VAL:O | 1:B:332:ASN:C | 2.44 | 0.56 |
| 1:B:597:ASN:HB2 | 1:B:598:PRO:HD2 | 1.87 | 0.56 |
| 1:B:526:GLN:HE21 | 2:E:124:MET:HE2 | 1.67 | 0.56 |
| 2:E:133:ASP:OD1 | 2:E:135:GLN:O | 2.23 | 0.56 |
| 1:B:327:LEU:HG | 1:B:595:ILE:HG23 | 1.88 | 0.56 |
| 1:C:295:VAL:HG22 | 1:C:296:LEU:N | 2.19 | 0.56 |
| 1:A:318:ILE:H | 1:A:318:ILE:CD1 | 2.17 | 0.56 |
| 1:A:378:LEU:HD22 | 1:B:378:LEU:HD11 | 1.87 | 0.56 |
| 1:A:581:GLN:HE21 | 1:A:629:ASN:N | 2.03 | 0.56 |
| 1:C:639:ASN:ND2 | 1:C:641:ALA:N | 2.50 | 0.56 |
| 1:A:318:ILE:HG23 | 1:A:322:LEU:HD13 | 1.86 | 0.56 |
| 1:A:509:PRO:HD3 | 1:A:536:TYR:HE1 | 1.70 | 0.56 |
| 1:B:554:LYS:O | 1:B:555:GLN:C | 2.43 | 0.56 |
| 2:E:63:ILE:HD12 | 2:E:63:ILE:N | 2.20 | 0.56 |
| 1:B:751:TYR:O | 1:B:754:GLU:N | 2.39 | 0.56 |
| 1:A:385:LEU:CD1 | 1:A:389:LYS:HD2 | 2.36 | 0.56 |
| 1:B:506:LYS:HZ3 | 1:B:506:LYS:HB3 | 1.68 | 0.56 |
| 1:C:607:ASN:HD21 | 1:C:609:GLU:HB2 | 1.71 | 0.56 |
| 1:B:308:VAL:O | 1:B:311:HIS:HB2 | 2.06 | 0.56 |
| 1:A:377:GLN:O | 1:A:378:LEU:C | 2.44 | 0.56 |
| 1:B:324:THR:HG22 | 1:B:499:PRO:CA | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:513:TRP:CE2 | 1:A:517:VAL:HG21 | 2.41 | 0.56 |
| 1:B:720:ILE:HD12 | 1:B:720:ILE:C | 2.26 | 0.56 |
| 1:B:332:ASN:ND2 | 1:B:334:LEU:N | 2.53 | 0.56 |
| 1:A:308:VAL:HG23 | 1:A:492:TYR:OH | 2.06 | 0.56 |
| 2:E:130:ILE:HG22 | 2:E:130:ILE:O | 2.06 | 0.56 |
| 1:C:603:ILE:HG22 | 1:C:604:LEU:H | 1.70 | 0.55 |
| 1:C:523:LEU:CD2 | 2:F:127:GLU:HB3 | 2.36 | 0.55 |
| 1:C:697:ILE:HD13 | 1:C:732:ILE:HG12 | 1.88 | 0.55 |
| 2:D:7:GLU:O | 2:D:11:GLU:HG3 | 2.05 | 0.55 |
| 1:B:733:GLU:C | 1:B:735:VAL:H | 2.10 | 0.55 |
| 2:D:92:PHE:CE2 | 2:D:108:VAL:HG11 | 2.41 | 0.55 |
| 1:B:400:LYS:HD2 | 1:B:475:GLU:OE2 | 2.05 | 0.55 |
| 1:B:454:GLN:CB | 1:B:472:ARG:O | 2.54 | 0.55 |
| 2:F:117:THR:C | 2:F:119:GLU:H | 2.08 | 0.55 |
| 1:B:654:ILE:HA | 1:B:755:ARG:HG2 | 1.87 | 0.55 |
| 1:A:368:GLN:HB2 | 1:A:384:ASN:OD1 | 2.07 | 0.55 |
| 1:B:616:GLU:HG3 | 1:B:617:LYS:N | 2.20 | 0.55 |
| 1:A:450:ASN:O | 1:A:451:ASN:HB2 | 2.06 | 0.55 |
| 1:B:536:TYR:CD2 | 1:B:536:TYR:N | 2.73 | 0.55 |
| 1:A:322:LEU:HB3 | 1:A:503:GLU:OE2 | 2.05 | 0.55 |
| 1:A:540:ARG:NH1 | 1:A:630:ARG:NH2 | 2.54 | 0.55 |
| 1:C:652:ALA:O | 1:C:656:THR:HG22 | 2.07 | 0.55 |
| 1:C:527:LYS:NZ | 2:F:145:MET:O | 2.39 | 0.55 |
| 1:C:775:LEU:HB2 | 1:C:776:LEU:HD12 | 1.87 | 0.55 |
| 1:A:293:ILE:HG13 | 1:A:293:ILE:O | 2.06 | 0.55 |
| 1:A:632:TYR:C | 1:A:643:ILE:O | 2.42 | 0.55 |
| 1:A:581:GLN:HE21 | 1:A:628:PHE:HA | 1.70 | 0.55 |
| 1:A:639:ASN:HD22 | 1:A:640:LYS:N | 2.05 | 0.55 |
| 1:A:521:ASN:CG | 1:A:522:SER:N | 2.60 | 0.55 |
| 1:B:529:VAL:HG23 | 1:B:530:THR:H | 1.71 | 0.55 |
| 1:A:463:THR:HB | 1:A:467:GLU:H | 1.70 | 0.55 |
| 1:C:667:LEU:HA | 1:C:670:ILE:HG22 | 1.88 | 0.55 |
| 1:C:589:LYS:HE2 | 1:C:643:ILE:HG23 | 1.87 | 0.55 |
| 2:E:105:LEU:HD23 | 2:E:105:LEU:O | 2.06 | 0.55 |
| 1:C:534:ILE:HA | 1:C:538:ILE:HB | 1.88 | 0.55 |
| 1:A:670:ILE:HG23 | 1:A:745:TYR:CZ | 2.41 | 0.55 |
| 1:A:602:PHE:O | 1:A:603:ILE:HD13 | 2.07 | 0.55 |
| 1:C:540:ARG:HD3 | 1:C:582:ASP:OD1 | 2.07 | 0.55 |
| 1:C:694:VAL:HG23 | 1:C:695:LYS:N | 2.15 | 0.55 |
| 1:B:549:LEU:HD23 | 1:B:549:LEU:N | 2.22 | 0.55 |
| 1:C:706:ASN:O | 1:C:709:ASN:HB2 | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:20:ASP:C | 2:D:22:ASP:H | 2.11 | 0.55 |
| 1:A:517:VAL:C | 1:A:525:LYS:HZ1 | 2.09 | 0.55 |
| 1:B:400:LYS:NZ | 1:B:475:GLU:OE2 | 2.35 | 0.55 |
| 1:B:616:GLU:CG | 1:B:617:LYS:N | 2.68 | 0.55 |
| 1:A:327:LEU:HG | 1:A:595:ILE:HG23 | 1.89 | 0.55 |
| 1:A:494:LEU:HD23 | 1:A:497:LEU:HG | 1.89 | 0.55 |
| 1:C:667:LEU:HB2 | 2:F:14:GLU:OE2 | 2.07 | 0.55 |
| 1:C:295:VAL:CG2 | 1:C:603:ILE:HG22 | 2.27 | 0.55 |
| 1:A:540:ARG:HH12 | 1:A:630:ARG:NH2 | 2.05 | 0.55 |
| 1:B:332:ASN:HD22 | 1:B:333:LYS:N | 2.04 | 0.55 |
| 1:B:557:LEU:HD11 | 1:B:575:VAL:HG12 | 1.89 | 0.55 |
| 1:B:427:ASP:C | 1:B:429:GLY:H | 2.11 | 0.55 |
| 1:B:445:ARG:HB2 | 1:B:471:TRP:CH2 | 2.42 | 0.54 |
| 1:B:726:ILE:HA | 1:B:729:TYR:HB2 | 1.88 | 0.54 |
| 1:B:527:LYS:O | 1:B:527:LYS:HG2 | 2.07 | 0.54 |
| 1:B:616:GLU:O | 1:B:621:GLY:HA3 | 2.07 | 0.54 |
| 2:E:117:THR:C | 2:E:119:GLU:H | 2.09 | 0.54 |
| 2:D:130:ILE:HG22 | 2:D:130:ILE:O | 2.06 | 0.54 |
| 1:C:629:ASN:HB3 | 1:C:632:TYR:CE2 | 2.42 | 0.54 |
| 1:B:775:LEU:HD22 | 1:B:775:LEU:H | 1.72 | 0.54 |
| 2:F:100:ILE:HB | 2:F:136:VAL:CG2 | 2.33 | 0.54 |
| 1:A:664:ILE:HD13 | 2:D:15:ALA:HB2 | 1.88 | 0.54 |
| 1:C:669:SER:HA | 1:C:672:ARG:HG2 | 1.90 | 0.54 |
| 2:E:20:ASP:C | 2:E:22:ASP:H | 2.10 | 0.54 |
| 1:C:790:PHE:O | 1:C:793:PHE:HB3 | 2.07 | 0.54 |
| 2:D:44:THR:CG2 | 2:D:47:GLU:HG3 | 2.37 | 0.54 |
| 2:E:87:GLU:O | 2:E:91:VAL:HG23 | 2.08 | 0.54 |
| 1:C:661:ALA:C | 1:C:663:PHE:H | 2.11 | 0.54 |
| 1:A:445:ARG:NE | 1:A:471:TRP:CE2 | 2.75 | 0.54 |
| 1:A:295:VAL:HG22 | 1:A:296:LEU:N | 2.23 | 0.54 |
| 1:A:768:LYS:HG2 | 1:A:768:LYS:O | 2.08 | 0.54 |
| 1:A:663:PHE:HE1 | 1:A:752:LEU:HD11 | 1.73 | 0.54 |
| 1:A:456:LYS:HD3 | 1:A:471:TRP:CD1 | 2.43 | 0.54 |
| 1:C:631:SER:O | 1:C:632:TYR:C | 2.44 | 0.54 |
| 1:A:603:ILE:HG22 | 1:A:604:LEU:H | 1.72 | 0.54 |
| 1:B:753:LYS:O | 1:B:757:THR:OG1 | 2.23 | 0.54 |
| 1:C:318:ILE:CD1 | 1:C:318:ILE:H | 2.18 | 0.54 |
| 1:B:530:THR:HG22 | 2:E:92:PHE:HZ | 1.70 | 0.54 |
| 1:A:700:TYR:CE1 | 1:A:731:GLU:HG2 | 2.42 | 0.54 |
| 1:A:583:ASN:O | 1:A:629:ASN:OD1 | 2.25 | 0.54 |
| 1:A:408:LEU:O | 1:A:408:LEU:HD23 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:324:THR:HG21 | 1:A:556:MET:HE3 | 1.85 | 0.54 |
| 1:B:592:GLU:HG2 | 1:B:605:THR:O | 2.08 | 0.54 |
| 2:E:137:ASN:OD1 | 2:E:139:GLU:HB2 | 2.08 | 0.54 |
| 1:C:462:ILE:CD1 | 1:C:466:GLY:HA2 | 2.38 | 0.54 |
| 1:A:706:ASN:O | 1:A:709:ASN:HB2 | 2.08 | 0.54 |
| 1:B:606:LYS:N | 1:B:610:MET:HE2 | 2.11 | 0.54 |
| 1:C:494:LEU:HD23 | 1:C:497:LEU:HG | 1.90 | 0.54 |
| 1:B:415:GLU:C | 1:B:417:GLY:N | 2.61 | 0.54 |
| 1:B:785:ASN:HD22 | 1:B:787:THR:HG22 | 1.73 | 0.54 |
| 1:A:387:ASN:CB | 1:A:477:MET:HE1 | 2.38 | 0.54 |
| 1:C:521:ASN:O | 1:C:524:GLU:HB2 | 2.08 | 0.54 |
| 1:C:505:LYS:HE3 | 1:C:513:TRP:CG | 2.43 | 0.54 |
| 1:B:774:LYS:HG3 | 1:B:774:LYS:O | 2.08 | 0.54 |
| 1:B:732:ILE:HG22 | 1:B:732:ILE:O | 2.07 | 0.54 |
| 1:C:385:LEU:CD1 | 1:C:389:LYS:HD2 | 2.37 | 0.54 |
| 1:A:652:ALA:O | 1:A:653:LYS:C | 2.46 | 0.54 |
| 1:A:775:LEU:HB2 | 1:A:776:LEU:HD12 | 1.89 | 0.53 |
| 1:B:761:GLN:O | 1:B:765:THR:N | 2.38 | 0.53 |
| 1:B:727:GLN:HG3 | 1:B:786:GLU:OE2 | 2.08 | 0.53 |
| 1:B:654:ILE:HG13 | 1:B:654:ILE:O | 2.08 | 0.53 |
| 1:A:462:ILE:CD1 | 1:A:466:GLY:HA2 | 2.38 | 0.53 |
| 1:A:450:ASN:OD1 | 1:A:452:GLU:HG3 | 2.08 | 0.53 |
| 2:D:117:THR:C | 2:D:119:GLU:H | 2.11 | 0.53 |
| 1:A:324:THR:OG1 | 1:A:499:PRO:HB3 | 2.08 | 0.53 |
| 1:A:639:ASN:ND2 | 1:A:641:ALA:N | 2.50 | 0.53 |
| 1:B:721:SER:O | 1:B:723:PHE:N | 2.41 | 0.53 |
| 1:B:654:ILE:HG22 | 1:B:755:ARG:HG2 | 1.90 | 0.53 |
| 1:A:764:LEU:O | 1:A:768:LYS:N | 2.40 | 0.53 |
| 1:C:327:LEU:N | 1:C:327:LEU:HD12 | 2.22 | 0.53 |
| 1:A:665:LYS:HG3 | 2:D:11:GLU:OE1 | 2.08 | 0.53 |
| 1:B:502:THR:O | 1:B:505:LYS:HG2 | 2.08 | 0.53 |
| 1:B:581:GLN:NE2 | 1:B:629:ASN:N | 2.39 | 0.53 |
| 1:C:581:GLN:HE21 | 1:C:629:ASN:N | 2.05 | 0.53 |
| 2:F:44:THR:CG2 | 2:F:47:GLU:HG3 | 2.38 | 0.53 |
| 1:C:707:SER:C | 1:C:709:ASN:H | 2.12 | 0.53 |
| 2:D:137:ASN:OD1 | 2:D:139:GLU:HB2 | 2.08 | 0.53 |
| 1:A:540:ARG:HH12 | 1:A:630:ARG:HH21 | 1.57 | 0.53 |
| 1:B:381:GLU:HG2 | 1:B:465:LEU:HD11 | 1.90 | 0.53 |
| 1:B:443:GLU:OE1 | 1:B:456:LYS:HE2 | 2.09 | 0.53 |
| 2:F:62:THR:C | 2:F:63:ILE:HD12 | 2.29 | 0.53 |
| 1:B:732:ILE:O | 1:B:735:VAL:HG12 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:654:ILE:O | 1:B:655:ASN:ND2 | 2.40 | 0.53 |
| 2:F:92:PHE:CE2 | 2:F:108:VAL:HG11 | 2.43 | 0.53 |
| 1:C:317:LYS:HB3 | 1:C:318:ILE:HD12 | 1.91 | 0.53 |
| 1:A:383:GLY:O | 1:A:386:GLU:HB2 | 2.08 | 0.53 |
| 2:F:27:ILE:CG1 | 2:F:63:ILE:HB | 2.39 | 0.53 |
| 2:F:101:SER:OG | 2:F:104:GLU:HG3 | 2.09 | 0.53 |
| 2:F:105:LEU:O | 2:F:105:LEU:HD23 | 2.08 | 0.53 |
| 1:A:445:ARG:HH22 | 1:A:456:LYS:CG | 2.21 | 0.53 |
| 1:A:509:PRO:O | 1:A:511:LYS:N | 2.40 | 0.53 |
| 1:A:697:ILE:HD11 | 1:A:731:GLU:O | 2.09 | 0.53 |
| 2:D:105:LEU:HD23 | 2:D:105:LEU:O | 2.08 | 0.53 |
| 1:A:523:LEU:C | 1:A:525:LYS:N | 2.62 | 0.53 |
| 1:B:793:PHE:HA | 1:B:796:ILE:HG12 | 1.91 | 0.53 |
| 1:B:574:VAL:O | 1:B:575:VAL:HG23 | 2.09 | 0.53 |
| 1:A:319:ALA:O | 1:A:598:PRO:HA | 2.09 | 0.53 |
| 1:B:596:ILE:HG12 | 1:B:602:PHE:CD2 | 2.44 | 0.53 |
| 1:A:385:LEU:HD13 | 1:A:385:LEU:C | 2.29 | 0.53 |
| 1:C:384:ASN:N | 1:C:384:ASN:OD1 | 2.42 | 0.53 |
| 1:A:440:GLN:H | 1:A:440:GLN:CD | 2.13 | 0.53 |
| 1:B:629:ASN:HD22 | 1:B:629:ASN:C | 2.11 | 0.52 |
| 1:A:535:LYS:HZ3 | 1:A:536:TYR:HE2 | 1.57 | 0.52 |
| 1:A:534:ILE:HG22 | 1:A:535:LYS:N | 2.24 | 0.52 |
| 1:C:338:LEU:O | 1:C:343:VAL:HG23 | 2.09 | 0.52 |
| 1:A:324:THR:O | 1:A:324:THR:HG23 | 2.07 | 0.52 |
| 1:B:296:LEU:HB2 | 1:B:604:LEU:HB3 | 1.92 | 0.52 |
| 1:C:574:VAL:O | 1:C:574:VAL:HG13 | 2.09 | 0.52 |
| 1:A:360:VAL:CG2 | 1:A:360:VAL:O | 2.57 | 0.52 |
| 2:E:44:THR:CG2 | 2:E:47:GLU:HG3 | 2.37 | 0.52 |
| 1:A:707:SER:C | 1:A:709:ASN:H | 2.12 | 0.52 |
| 1:A:338:LEU:O | 1:A:343:VAL:HG23 | 2.10 | 0.52 |
| 2:E:72:MET:C | 2:E:74:ARG:H | 2.12 | 0.52 |
| 1:C:669:SER:C | 1:C:671:ARG:H | 2.13 | 0.52 |
| 2:F:89:PHE:C | 2:F:89:PHE:HD2 | 2.13 | 0.52 |
| 1:A:523:LEU:C | 1:A:525:LYS:H | 2.13 | 0.52 |
| 1:B:391:ILE:HD13 | 1:B:398:ILE:HG22 | 1.90 | 0.52 |
| 1:B:557:LEU:CD1 | 1:B:575:VAL:HG12 | 2.40 | 0.52 |
| 1:B:415:GLU:C | 1:B:417:GLY:H | 2.11 | 0.52 |
| 1:B:714:GLN:OE1 | 1:B:718:ARG:NH2 | 2.42 | 0.52 |
| 1:C:509:PRO:HD2 | 1:C:536:TYR:CZ | 2.45 | 0.52 |
| 1:A:540:ARG:NH2 | 1:A:627:TYR:CE1 | 2.77 | 0.52 |
| 2:E:37:ARG:HG2 | 2:E:41:GLN:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:308:VAL:HG23 | 1:C:492:TYR:OH | 2.10 | 0.52 |
| 1:C:781:ASN:ND2 | 1:C:783:THR:OG1 | 2.42 | 0.52 |
| 1:B:744:GLU:OE1 | 1:B:744:GLU:HA | 2.08 | 0.52 |
| 1:A:633:ASN:ND2 | 1:A:644:GLU:HA | 2.25 | 0.52 |
| 1:B:309:PRO:O | 1:B:312:ALA:N | 2.42 | 0.52 |
| 1:B:540:ARG:HD2 | 1:B:627:TYR:CZ | 2.44 | 0.52 |
| 1:B:423:LYS:HB3 | 1:B:434:LEU:CD2 | 2.39 | 0.52 |
| 2:F:20:ASP:C | 2:F:22:ASP:H | 2.11 | 0.52 |
| 2:F:65:PHE:CD1 | 2:F:65:PHE:N | 2.77 | 0.52 |
| 1:B:516:VAL:O | 1:B:520:PRO:HD2 | 2.10 | 0.52 |
| 1:A:636:ALA:O | 1:A:640:LYS:HA | 2.10 | 0.52 |
| 1:B:728:ALA:C | 1:B:730:ASN:H | 2.13 | 0.52 |
| 1:B:785:ASN:ND2 | 1:B:787:THR:CG2 | 2.73 | 0.52 |
| 1:B:311:HIS:ND1 | 1:B:564:VAL:HB | 2.24 | 0.52 |
| 1:C:636:ALA:O | 1:C:640:LYS:HA | 2.10 | 0.52 |
| 2:D:92:PHE:CD2 | 2:D:108:VAL:HG21 | 2.44 | 0.52 |
| 1:B:306:GLY:O | 1:B:336:THR:CB | 2.57 | 0.52 |
| 2:E:85:ILE:O | 2:E:88:ALA:HB3 | 2.10 | 0.52 |
| 2:F:72:MET:C | 2:F:74:ARG:H | 2.14 | 0.52 |
| 1:B:298:GLY:O | 1:B:300:LYS:N | 2.43 | 0.52 |
| 1:B:509:PRO:CD | 1:B:536:TYR:HE1 | 2.21 | 0.52 |
| 1:B:748:TYR:O | 1:B:752:LEU:CG | 2.58 | 0.52 |
| 1:C:530:THR:HG21 | 2:F:145:MET:HE1 | 1.92 | 0.52 |
| 1:A:299:GLU:HG3 | 1:A:303:LYS:HZ2 | 1.74 | 0.52 |
| 1:B:536:TYR:N | 1:B:536:TYR:HD2 | 2.09 | 0.51 |
| 1:B:749:PHE:O | 1:B:752:LEU:HB2 | 2.11 | 0.51 |
| 1:C:292:ARG:NE | 1:C:292:ARG:HA | 2.25 | 0.51 |
| 1:C:657:ILE:CG1 | 1:C:759:GLN:HG2 | 2.37 | 0.51 |
| 1:A:384:ASN:O | 1:A:385:LEU:C | 2.48 | 0.51 |
| 2:E:36:MET:C | 2:E:41:GLN:HB2 | 2.31 | 0.51 |
| 2:D:37:ARG:HG2 | 2:D:41:GLN:O | 2.11 | 0.51 |
| 2:E:89:PHE:HD2 | 2:E:89:PHE:C | 2.11 | 0.51 |
| 2:E:131:ASP:OD1 | 2:E:133:ASP:OD2 | 2.27 | 0.51 |
| 1:B:540:ARG:NH1 | 1:B:627:TYR:CD1 | 2.79 | 0.51 |
| 1:A:517:VAL:HA | 1:A:525:LYS:NZ | 2.25 | 0.51 |
| 1:A:509:PRO:HD3 | 1:A:536:TYR:CE1 | 2.44 | 0.51 |
| 1:B:525:LYS:NZ | 2:E:114:GLU:OE2 | 2.43 | 0.51 |
| 1:B:785:ASN:O | 1:B:786:GLU:C | 2.48 | 0.51 |
| 1:C:346:LYS:O | 1:C:346:LYS:HG3 | 2.10 | 0.51 |
| 1:C:666:ASN:O | 1:C:670:ILE:HG22 | 2.10 | 0.51 |
| 2:F:140:GLU:C | 2:F:142:VAL:N | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:ILE:HG23 | 1:A:322:LEU:CD1 | 2.41 | 0.51 |
| 1:B:389:LYS:HG2 | 1:B:393:GLU:OE2 | 2.11 | 0.51 |
| 1:C:440:GLN:CD | 1:C:440:GLN:H | 2.14 | 0.51 |
| 1:A:607:ASN:O | 1:A:610:MET:N | 2.43 | 0.51 |
| 1:C:657:ILE:HG23 | 1:C:658:PRO:HD2 | 1.91 | 0.51 |
| 1:A:324:THR:CG2 | 1:A:324:THR:O | 2.58 | 0.51 |
| 2:E:27:ILE:CG1 | 2:E:63:ILE:HB | 2.40 | 0.51 |
| 1:B:513:TRP:O | 1:B:517:VAL:HG12 | 2.10 | 0.51 |
| 1:B:730:ASN:HA | 1:B:733:GLU:HB3 | 1.93 | 0.51 |
| 1:B:787:THR:HG23 | 1:B:788:ASP:N | 2.25 | 0.51 |
| 1:A:384:ASN:O | 1:A:387:ASN:N | 2.44 | 0.51 |
| 1:A:607:ASN:HD21 | 1:A:609:GLU:HB2 | 1.75 | 0.51 |
| 1:A:394:HIS:O | 1:A:395:GLU:C | 2.49 | 0.51 |
| 1:C:510:GLN:CG | 1:C:510:GLN:O | 2.57 | 0.51 |
| 1:C:608:TRP:O | 1:C:609:GLU:C | 2.47 | 0.51 |
| 1:B:355:SER:HB2 | 1:B:371:SER:HA | 1.91 | 0.51 |
| 1:B:327:LEU:CG | 1:B:595:ILE:HG23 | 2.40 | 0.51 |
| 1:A:606:LYS:O | 1:A:607:ASN:HB3 | 2.11 | 0.51 |
| 1:A:558:ASP:O | 1:A:562:GLU:HG3 | 2.11 | 0.51 |
| 1:C:774:LYS:O | 1:C:777:TYR:N | 2.38 | 0.51 |
| 1:A:445:ARG:NE | 1:A:471:TRP:NE1 | 2.59 | 0.51 |
| 1:A:705:TYR:CE2 | 2:D:139:GLU:CB | 2.81 | 0.51 |
| 1:B:717:LYS:CD | 2:E:132:GLY:N | 2.70 | 0.51 |
| 2:F:37:ARG:HG2 | 2:F:41:GLN:O | 2.10 | 0.51 |
| 1:A:697:ILE:O | 1:A:701:LEU:HG | 2.10 | 0.51 |
| 1:C:383:GLY:O | 1:C:386:GLU:HB2 | 2.10 | 0.51 |
| 1:A:419:ILE:O | 1:A:419:ILE:HG13 | 2.11 | 0.51 |
| 1:C:628:PHE:CD1 | 1:C:628:PHE:C | 2.84 | 0.51 |
| 2:E:44:THR:HG23 | 2:E:47:GLU:H | 1.76 | 0.51 |
| 1:A:652:ALA:O | 1:A:654:ILE:N | 2.44 | 0.51 |
| 2:D:44:THR:HG23 | 2:D:47:GLU:H | 1.75 | 0.51 |
| 1:B:508:ILE:HA | 1:B:536:TYR:HD1 | 1.75 | 0.50 |
| 1:B:298:GLY:O | 1:B:299:GLU:C | 2.48 | 0.50 |
| 1:B:309:PRO:O | 1:B:310:GLU:C | 2.50 | 0.50 |
| 1:C:639:ASN:C | 1:C:639:ASN:ND2 | 2.59 | 0.50 |
| 1:A:502:THR:O | 1:A:505:LYS:N | 2.44 | 0.50 |
| 1:B:622:LYS:O | 1:B:623:ASP:HB2 | 2.12 | 0.50 |
| 1:B:722:ILE:O | 1:B:726:ILE:HG13 | 2.11 | 0.50 |
| 2:F:44:THR:HG23 | 2:F:47:GLU:H | 1.76 | 0.50 |
| 1:B:300:LYS:HA | 1:B:303:LYS:NZ | 2.25 | 0.50 |
| 1:B:576:ASN:N | 1:B:576:ASN:OD1 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:667:LEU:HA | 1:A:670:ILE:CG2 | 2.41 | 0.50 |
| 2:E:65:PHE:N | 2:E:65:PHE:CD1 | 2.75 | 0.50 |
| 2:D:27:ILE:CG1 | 2:D:63:ILE:HB | 2.42 | 0.50 |
| 1:A:774:LYS:O | 1:A:777:TYR:N | 2.39 | 0.50 |
| 1:B:616:GLU:HA | 1:B:620:THR:CG2 | 2.40 | 0.50 |
| 1:A:494:LEU:HB3 | 1:A:579:THR:HG22 | 1.93 | 0.50 |
| 1:C:668:SER:HA | 2:F:14:GLU:HG3 | 1.94 | 0.50 |
| 1:B:746:LYS:CG | 1:B:750:GLN:HB2 | 2.41 | 0.50 |
| 1:C:540:ARG:HB3 | 1:C:549:LEU:O | 2.11 | 0.50 |
| 2:F:36:MET:C | 2:F:41:GLN:HB2 | 2.31 | 0.50 |
| 1:B:649:ILE:HD12 | 2:E:86:ARG:HG3 | 1.92 | 0.50 |
| 1:A:697:ILE:H | 1:A:697:ILE:CD1 | 2.25 | 0.50 |
| 2:E:117:THR:C | 2:E:119:GLU:N | 2.64 | 0.50 |
| 1:C:409:ARG:O | 1:C:410:ILE:C | 2.49 | 0.50 |
| 1:B:625:LEU:C | 1:B:625:LEU:HD23 | 2.32 | 0.50 |
| 1:A:377:GLN:C | 1:A:379:ALA:N | 2.64 | 0.50 |
| 1:B:404:LYS:HG3 | 1:B:452:GLU:HA | 1.93 | 0.50 |
| 1:A:324:THR:HA | 1:A:499:PRO:HA | 1.94 | 0.50 |
| 2:D:72:MET:C | 2:D:74:ARG:H | 2.13 | 0.50 |
| 2:D:140:GLU:C | 2:D:142:VAL:N | 2.65 | 0.50 |
| 1:C:385:LEU:HD13 | 1:C:385:LEU:C | 2.31 | 0.50 |
| 2:F:5:THR:N | 2:F:8:GLN:HB2 | 2.27 | 0.50 |
| 2:F:117:THR:C | 2:F:119:GLU:N | 2.64 | 0.50 |
| 1:A:346:LYS:O | 1:A:346:LYS:HG3 | 2.12 | 0.50 |
| 1:B:453:VAL:CG1 | 1:B:474:ILE:HD12 | 2.42 | 0.50 |
| 2:E:100:ILE:HB | 2:E:136:VAL:CG2 | 2.37 | 0.49 |
| 1:C:360:VAL:CG2 | 1:C:360:VAL:O | 2.57 | 0.49 |
| 1:C:387:ASN:CB | 1:C:477:MET:HE1 | 2.42 | 0.49 |
| 1:C:650:THR:C | 1:C:652:ALA:N | 2.63 | 0.49 |
| 1:C:400:LYS:HD2 | 1:C:475:GLU:OE1 | 2.12 | 0.49 |
| 1:A:348:LEU:HD12 | 1:A:577:HIS:CB | 2.42 | 0.49 |
| 1:C:592:GLU:HB3 | 1:C:604:LEU:HD21 | 1.93 | 0.49 |
| 1:B:489:THR:HG23 | 1:B:490:ALA:O | 2.12 | 0.49 |
| 1:C:363:TYR:CD1 | 1:C:403:LEU:CD1 | 2.95 | 0.49 |
| 1:C:739:LYS:HE2 | 1:C:739:LYS:HA | 1.94 | 0.49 |
| 1:C:318:ILE:CG2 | 1:C:322:LEU:HD13 | 2.42 | 0.49 |
| 1:A:722:ILE:HG21 | 1:A:764:LEU:HD21 | 1.94 | 0.49 |
| 2:D:117:THR:C | 2:D:119:GLU:N | 2.65 | 0.49 |
| 1:C:602:PHE:C | 1:C:603:ILE:HD13 | 2.33 | 0.49 |
| 2:E:37:ARG:HA | 2:E:41:GLN:O | 2.12 | 0.49 |
| 1:A:780:LEU:HD12 | 1:A:780:LEU:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:530:THR:OG1 | 2:E:145:MET:SD | 2.70 | 0.49 |
| 1:C:320:ARG:HH21 | 1:C:600:GLY:HA3 | 1.77 | 0.49 |
| 1:C:655:ASN:ND2 | 1:C:655:ASN:N | 2.60 | 0.49 |
| 1:C:340:LYS:C | 1:C:342:GLY:H | 2.15 | 0.49 |
| 2:D:42:ASN:ND2 | 2:D:147:ALA:HB2 | 2.27 | 0.49 |
| 1:B:773:PHE:O | 1:B:775:LEU:N | 2.46 | 0.49 |
| 1:B:605:THR:CG2 | 1:B:606:LYS:N | 2.76 | 0.49 |
| 1:B:709:ASN:O | 1:B:709:ASN:OD1 | 2.30 | 0.49 |
| 1:B:709:ASN:ND2 | 1:B:720:ILE:HD11 | 2.19 | 0.49 |
| 1:B:315:PHE:CE2 | 1:B:560:LEU:HD23 | 2.47 | 0.49 |
| 1:C:525:LYS:HB2 | 2:F:124:MET:HE3 | 1.94 | 0.49 |
| 1:B:524:GLU:O | 1:B:525:LYS:C | 2.51 | 0.49 |
| 1:A:597:ASN:OD1 | 1:A:601:GLU:HB2 | 2.13 | 0.49 |
| 1:C:381:GLU:C | 1:C:383:GLY:N | 2.66 | 0.49 |
| 1:B:629:ASN:ND2 | 1:B:631:SER:HB2 | 2.21 | 0.49 |
| 1:C:540:ARG:HH12 | 1:C:630:ARG:NH2 | 2.10 | 0.49 |
| 1:C:322:LEU:O | 1:C:323:ASN:C | 2.50 | 0.49 |
| 1:C:502:THR:O | 1:C:505:LYS:N | 2.45 | 0.49 |
| 1:A:325:TYR:CE1 | 1:A:619:ILE:HG12 | 2.47 | 0.49 |
| 1:A:608:TRP:O | 1:A:609:GLU:C | 2.50 | 0.49 |
| 1:C:581:GLN:HE21 | 1:C:628:PHE:HA | 1.77 | 0.49 |
| 1:A:629:ASN:ND2 | 1:A:631:SER:N | 2.41 | 0.49 |
| 1:B:587:PRO:CD | 1:B:639:ASN:HD21 | 2.18 | 0.49 |
| 1:B:639:ASN:ND2 | 1:B:639:ASN:N | 2.58 | 0.49 |
| 1:B:655:ASN:H | 1:B:755:ARG:HD2 | 1.78 | 0.49 |
| 1:C:561:ASN:O | 1:C:564:VAL:HG22 | 2.12 | 0.49 |
| 1:C:325:TYR:CE2 | 1:C:598:PRO:HD2 | 2.48 | 0.49 |
| 2:F:117:THR:O | 2:F:119:GLU:N | 2.46 | 0.49 |
| 1:A:557:LEU:O | 1:A:560:LEU:HB2 | 2.11 | 0.49 |
| 1:C:305:SER:OG | 1:C:306:GLY:N | 2.45 | 0.49 |
| 2:F:140:GLU:C | 2:F:142:VAL:H | 2.16 | 0.49 |
| 1:C:607:ASN:O | 1:C:610:MET:N | 2.44 | 0.49 |
| 2:E:117:THR:O | 2:E:119:GLU:N | 2.46 | 0.49 |
| 1:C:335:ALA:O | 1:C:338:LEU:HB2 | 2.12 | 0.49 |
| 1:C:557:LEU:O | 1:C:560:LEU:HB2 | 2.12 | 0.49 |
| 1:C:670:ILE:O | 1:C:745:TYR:HE1 | 1.95 | 0.49 |
| 2:D:62:THR:C | 2:D:63:ILE:HD12 | 2.33 | 0.49 |
| 1:B:294:ASP:O | 1:B:606:LYS:HE3 | 2.12 | 0.49 |
| 1:B:338:LEU:O | 1:B:339:ILE:C | 2.50 | 0.49 |
| 1:A:639:ASN:C | 1:A:639:ASN:ND2 | 2.60 | 0.49 |
| 1:B:795:LYS:O | 1:B:797:ILE:HG12 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:36:MET:C | 2:D:41:GLN:HB2 | 2.33 | 0.49 |
| 1:A:326:ILE:C | 1:A:327:LEU:HD12 | 2.33 | 0.49 |
| 1:A:602:PHE:C | 1:A:603:ILE:HD13 | 2.34 | 0.48 |
| 2:D:65:PHE:CD1 | 2:D:65:PHE:N | 2.78 | 0.48 |
| 1:C:318:ILE:HG23 | 1:C:322:LEU:CD1 | 2.41 | 0.48 |
| 1:A:700:TYR:HE1 | 1:A:731:GLU:HG2 | 1.77 | 0.48 |
| 1:C:438:ASN:ND2 | 1:C:438:ASN:C | 2.66 | 0.48 |
| 1:C:780:LEU:HD12 | 1:C:780:LEU:O | 2.12 | 0.48 |
| 1:A:403:LEU:HD13 | 1:A:476:VAL:HG21 | 1.93 | 0.48 |
| 1:B:315:PHE:O | 1:B:316:LYS:C | 2.51 | 0.48 |
| 2:E:140:GLU:C | 2:E:142:VAL:N | 2.64 | 0.48 |
| 1:C:401:ILE:HD13 | 1:C:478:ALA:CB | 2.42 | 0.48 |
| 1:A:438:ASN:ND2 | 1:A:438:ASN:C | 2.66 | 0.48 |
| 1:B:722:ILE:HG23 | 1:B:760:VAL:HG13 | 1.95 | 0.48 |
| 1:B:315:PHE:HA | 1:B:318:ILE:HD11 | 1.95 | 0.48 |
| 1:A:325:TYR:CE2 | 1:A:598:PRO:HD2 | 2.49 | 0.48 |
| 1:A:432:TYR:CD1 | 1:A:471:TRP:CZ3 | 3.01 | 0.48 |
| 2:E:50:ASP:OD1 | 2:E:51:MET:N | 2.47 | 0.48 |
| 1:B:359:PRO:HG2 | 1:B:444:PHE:CD2 | 2.49 | 0.48 |
| 1:A:587:PRO:HB2 | 1:A:643:ILE:CD1 | 2.44 | 0.48 |
| 2:D:89:PHE:C | 2:D:89:PHE:HD2 | 2.14 | 0.48 |
| 1:A:304:ALA:HB3 | 1:A:604:LEU:HD13 | 1.95 | 0.48 |
| 1:B:717:LYS:HD2 | 2:E:132:GLY:CA | 2.43 | 0.48 |
| 1:C:667:LEU:O | 1:C:671:ARG:HB2 | 2.14 | 0.48 |
| 1:B:423:LYS:O | 1:B:434:LEU:CD2 | 2.62 | 0.48 |
| 1:B:331:VAL:O | 1:B:331:VAL:HG12 | 2.13 | 0.48 |
| 1:C:583:ASN:ND2 | 5:C:1999:DOT:C1B | 2.77 | 0.48 |
| 1:B:338:LEU:HD11 | 1:B:409:ARG:NE | 2.28 | 0.48 |
| 1:A:508:ILE:HG21 | 1:A:532:LEU:HD13 | 1.96 | 0.48 |
| 1:B:626:TYR:CD2 | 1:B:626:TYR:C | 2.87 | 0.48 |
| 1:A:604:LEU:C | 1:A:604:LEU:HD23 | 2.33 | 0.48 |
| 1:B:535:LYS:HB3 | 1:B:536:TYR:CD2 | 2.48 | 0.48 |
| 1:B:746:LYS:HG3 | 1:B:750:GLN:HB2 | 1.95 | 0.48 |
| 2:D:100:ILE:HB | 2:D:136:VAL:CG2 | 2.37 | 0.48 |
| 1:A:401:ILE:HD13 | 1:A:478:ALA:CB | 2.44 | 0.48 |
| 1:C:419:ILE:HG13 | 1:C:419:ILE:O | 2.12 | 0.48 |
| 1:A:543:ASP:OD2 | 1:A:546:LYS:HG3 | 2.13 | 0.48 |
| 1:B:737:LYS:C | 1:B:738:SER:O | 2.47 | 0.48 |
| 2:E:140:GLU:C | 2:E:142:VAL:H | 2.17 | 0.48 |
| 1:A:477:MET:C | 1:A:488:LEU:HD12 | 2.34 | 0.48 |
| 1:C:377:GLN:C | 1:C:379:ALA:N | 2.66 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:543:ASP:HB3 | 1:B:546:LYS:O | 2.14 | 0.48 |
| 1:B:333:LYS:O | 1:B:336:THR:CG2 | 2.61 | 0.48 |
| 2:D:117:THR:O | 2:D:119:GLU:N | 2.46 | 0.48 |
| 1:A:423:LYS:NZ | 1:A:423:LYS:HB3 | 2.28 | 0.48 |
| 1:C:394:HIS:O | 1:C:395:GLU:C | 2.53 | 0.48 |
| 1:C:304:ALA:HB3 | 1:C:604:LEU:CD1 | 2.43 | 0.48 |
| 2:E:65:PHE:HD1 | 2:E:65:PHE:H | 1.56 | 0.48 |
| 1:A:540:ARG:NH2 | 2:D:87:GLU:OE1 | 2.45 | 0.48 |
| 1:B:400:LYS:HA | 1:B:476:VAL:O | 2.14 | 0.48 |
| 1:B:526:GLN:HE21 | 2:E:124:MET:CE | 2.27 | 0.48 |
| 1:B:529:VAL:HG23 | 1:B:530:THR:N | 2.28 | 0.48 |
| 1:B:619:ILE:C | 1:B:621:GLY:N | 2.67 | 0.48 |
| 1:A:652:ALA:O | 1:A:655:ASN:N | 2.38 | 0.48 |
| 1:B:726:ILE:O | 1:B:729:TYR:CB | 2.62 | 0.47 |
| 1:A:559:ARG:NH1 | 1:A:559:ARG:HB3 | 2.19 | 0.47 |
| 1:B:720:ILE:O | 1:B:724:ARG:HG2 | 2.14 | 0.47 |
| 1:B:497:LEU:HD13 | 1:B:556:MET:HG2 | 1.96 | 0.47 |
| 1:C:527:LYS:HZ3 | 2:F:145:MET:HA | 1.79 | 0.47 |
| 1:C:403:LEU:CD1 | 1:C:476:VAL:HG21 | 2.44 | 0.47 |
| 1:A:493:ASP:OD2 | 5:A:999:DOT:O1A | 2.33 | 0.47 |
| 1:A:583:ASN:HD21 | 5:A:999:DOT:H1' | 1.79 | 0.47 |
| 1:A:462:ILE:HD11 | 1:A:466:GLY:CA | 2.43 | 0.47 |
| 2:F:45:GLU:O | 2:F:49:GLN:HG2 | 2.15 | 0.47 |
| 1:A:657:ILE:HG21 | 1:A:756:ILE:HD13 | 1.92 | 0.47 |
| 1:A:561:ASN:O | 1:A:564:VAL:HG22 | 2.14 | 0.47 |
| 1:B:574:VAL:C | 1:B:575:VAL:HG23 | 2.35 | 0.47 |
| 1:A:789:ASN:N | 1:A:789:ASN:HD22 | 2.11 | 0.47 |
| 1:C:445:ARG:NH1 | 1:C:471:TRP:NE1 | 2.61 | 0.47 |
| 1:B:773:PHE:HE1 | 1:B:777:TYR:HB2 | 1.78 | 0.47 |
| 1:B:587:PRO:HD2 | 1:B:639:ASN:ND2 | 2.18 | 0.47 |
| 1:B:735:VAL:HG22 | 1:B:735:VAL:O | 2.15 | 0.47 |
| 1:A:317:LYS:HB3 | 1:A:318:ILE:HD12 | 1.97 | 0.47 |
| 1:A:419:ILE:HD12 | 1:A:435:LEU:HD22 | 1.97 | 0.47 |
| 1:A:340:LYS:C | 1:A:342:GLY:H | 2.18 | 0.47 |
| 1:B:615:ILE:HD13 | 1:B:626:TYR:CZ | 2.50 | 0.47 |
| 1:A:628:PHE:HD1 | 1:A:629:ASN:O | 1.98 | 0.47 |
| 1:B:456:LYS:HG3 | 1:B:457:THR:O | 2.14 | 0.47 |
| 1:B:785:ASN:ND2 | 1:B:787:THR:HG22 | 2.29 | 0.47 |
| 1:B:313:ASP:C | 1:B:315:PHE:N | 2.68 | 0.47 |
| 1:A:504:ILE:CG2 | 1:A:505:LYS:N | 2.77 | 0.47 |
| 1:A:534:ILE:HA | 1:A:538:ILE:HB | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:538:ILE:CD1 | 2:D:88:ALA:HA | 2.45 | 0.47 |
| 1:C:699:GLY:O | 1:C:702:SER:N | 2.46 | 0.47 |
| 2:D:22:ASP:HB3 | 2:D:26:THR:OG1 | 2.15 | 0.47 |
| 1:B:514:ASP:CA | 1:B:517:VAL:HG12 | 2.38 | 0.47 |
| 1:B:750:GLN:O | 1:B:753:LYS:HB3 | 2.15 | 0.47 |
| 1:B:785:ASN:HD22 | 1:B:787:THR:CG2 | 2.27 | 0.47 |
| 1:C:540:ARG:NH1 | 1:C:630:ARG:NH2 | 2.63 | 0.47 |
| 2:D:140:GLU:C | 2:D:142:VAL:H | 2.18 | 0.47 |
| 1:C:408:LEU:O | 1:C:408:LEU:HD23 | 2.14 | 0.47 |
| 1:A:370:LEU:HD11 | 1:A:455:TYR:CE1 | 2.49 | 0.47 |
| 1:B:357:TRP:CZ2 | 1:B:370:LEU:HA | 2.49 | 0.47 |
| 2:D:45:GLU:O | 2:D:49:GLN:HG2 | 2.15 | 0.47 |
| 1:C:789:ASN:HD22 | 1:C:789:ASN:N | 2.12 | 0.47 |
| 2:E:62:THR:C | 2:E:63:ILE:HD12 | 2.35 | 0.47 |
| 1:B:338:LEU:O | 1:B:341:SER:N | 2.47 | 0.47 |
| 1:B:721:SER:C | 1:B:723:PHE:N | 2.68 | 0.47 |
| 1:B:733:GLU:C | 1:B:735:VAL:N | 2.68 | 0.47 |
| 2:F:37:ARG:HA | 2:F:41:GLN:O | 2.15 | 0.47 |
| 1:B:377:GLN:HG3 | 1:B:465:LEU:HD23 | 1.97 | 0.47 |
| 1:C:349:ASN:HD21 | 1:C:398:ILE:CG1 | 2.27 | 0.47 |
| 1:B:574:VAL:O | 1:B:575:VAL:CG2 | 2.63 | 0.47 |
| 2:D:5:THR:O | 2:D:9:ILE:HG13 | 2.15 | 0.47 |
| 1:C:657:ILE:CG2 | 1:C:658:PRO:N | 2.78 | 0.47 |
| 1:C:583:ASN:O | 1:C:629:ASN:OD1 | 2.32 | 0.47 |
| 1:B:498:ALA:HB3 | 1:B:619:ILE:HD13 | 1.95 | 0.47 |
| 1:C:363:TYR:HD1 | 1:C:403:LEU:CD1 | 2.27 | 0.47 |
| 1:A:443:GLU:HB2 | 1:A:458:LYS:HG2 | 1.97 | 0.47 |
| 1:A:329:ARG:O | 1:A:330:PRO:O | 2.33 | 0.47 |
| 1:B:327:LEU:HA | 1:B:594:PHE:O | 2.14 | 0.47 |
| 1:B:328:PHE:HB2 | 1:B:594:PHE:HB3 | 1.97 | 0.47 |
| 1:C:629:ASN:HD21 | 1:C:631:SER:H | 1.52 | 0.46 |
| 1:C:597:ASN:OD1 | 1:C:601:GLU:HB2 | 2.14 | 0.46 |
| 1:C:517:VAL:HG22 | 1:C:517:VAL:O | 2.13 | 0.46 |
| 1:C:722:ILE:HG21 | 1:C:764:LEU:HD21 | 1.97 | 0.46 |
| 1:B:758:ASN:HA | 1:B:761:GLN:HB2 | 1.97 | 0.46 |
| 1:B:327:LEU:HD13 | 1:B:496:ALA:HB3 | 1.96 | 0.46 |
| 1:A:327:LEU:HB2 | 1:A:496:ALA:O | 2.14 | 0.46 |
| 1:C:658:PRO:HB2 | 1:C:701:LEU:CD1 | 2.44 | 0.46 |
| 1:A:628:PHE:C | 1:A:628:PHE:CD1 | 2.88 | 0.46 |
| 1:C:302:LEU:HD12 | 1:C:602:PHE:CE1 | 2.48 | 0.46 |
| 2:D:37:ARG:HA | 2:D:41:GLN:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:384:ASN:O | 1:C:385:LEU:C | 2.51 | 0.46 |
| 1:A:299:GLU:CG | 1:A:303:LYS:NZ | 2.79 | 0.46 |
| 1:C:419:ILE:HD12 | 1:C:435:LEU:HD22 | 1.97 | 0.46 |
| 1:B:470:ASN:CG | 1:B:471:TRP:N | 2.69 | 0.46 |
| 2:E:22:ASP:HB3 | 2:E:26:THR:OG1 | 2.15 | 0.46 |
| 1:A:722:ILE:HG12 | 1:A:763:LEU:HB2 | 1.98 | 0.46 |
| 1:B:476:VAL:HG12 | 1:B:477:MET:N | 2.30 | 0.46 |
| 1:A:700:TYR:HD1 | 1:A:728:ALA:CA | 2.28 | 0.46 |
| 1:B:418:ILE:HG22 | 1:B:419:ILE:HG23 | 1.96 | 0.46 |
| 1:B:480:ASN:HA | 1:B:485:LEU:HD12 | 1.97 | 0.46 |
| 1:B:450:ASN:O | 1:B:451:ASN:HB2 | 2.15 | 0.46 |
| 1:C:663:PHE:O | 1:C:667:LEU:HG | 2.16 | 0.46 |
| 1:B:368:GLN:H | 1:B:384:ASN:ND2 | 2.13 | 0.46 |
| 1:B:327:LEU:HD23 | 1:B:595:ILE:HG23 | 1.98 | 0.46 |
| 1:C:462:ILE:HD11 | 1:C:466:GLY:CA | 2.45 | 0.46 |
| 1:C:381:GLU:C | 1:C:383:GLY:H | 2.19 | 0.46 |
| 2:D:42:ASN:HD21 | 2:D:147:ALA:HB2 | 1.80 | 0.46 |
| 1:B:324:THR:CB | 1:B:499:PRO:HA | 2.46 | 0.46 |
| 1:B:509:PRO:HD2 | 1:B:536:TYR:CE1 | 2.51 | 0.46 |
| 1:A:657:ILE:HD11 | 1:A:704:TYR:CD1 | 2.50 | 0.46 |
| 2:D:87:GLU:O | 2:D:91:VAL:HG23 | 2.15 | 0.46 |
| 1:A:345:THR:HB | 1:A:491:ASP:HA | 1.97 | 0.46 |
| 1:C:325:TYR:CD2 | 1:C:597:ASN:HA | 2.51 | 0.46 |
| 1:B:501:LEU:HA | 1:B:504:ILE:HG12 | 1.98 | 0.46 |
| 1:B:346:LYS:HD3 | 1:B:364:ILE:CD1 | 2.46 | 0.46 |
| 1:B:368:GLN:H | 1:B:384:ASN:HD21 | 1.64 | 0.46 |
| 1:A:324:THR:OG1 | 1:A:499:PRO:CA | 2.64 | 0.46 |
| 1:B:332:ASN:HD21 | 1:B:334:LEU:H | 1.62 | 0.46 |
| 1:A:663:PHE:CE1 | 1:A:752:LEU:CD1 | 2.98 | 0.46 |
| 1:B:622:LYS:O | 1:B:623:ASP:CB | 2.64 | 0.46 |
| 1:C:340:LYS:C | 1:C:342:GLY:N | 2.68 | 0.46 |
| 1:C:593:ILE:O | 1:C:604:LEU:HA | 2.15 | 0.46 |
| 1:B:423:LYS:HB3 | 1:B:434:LEU:HD22 | 1.97 | 0.46 |
| 2:F:65:PHE:H | 2:F:65:PHE:HD1 | 1.58 | 0.46 |
| 1:B:791:GLU:C | 1:B:793:PHE:H | 2.19 | 0.46 |
| 1:B:350:VAL:HG22 | 1:B:398:ILE:HG13 | 1.98 | 0.46 |
| 1:C:385:LEU:HD11 | 1:C:389:LYS:HD2 | 1.97 | 0.46 |
| 1:C:650:THR:C | 1:C:652:ALA:H | 2.19 | 0.46 |
| 1:B:613:ARG:O | 1:B:616:GLU:HG2 | 2.15 | 0.46 |
| 1:B:745:TYR:HB3 | 1:B:749:PHE:CE1 | 2.41 | 0.46 |
| 1:C:504:ILE:CG2 | 1:C:505:LYS:N | 2.78 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:463:THR:CG2 | 1:A:465:LEU:H | 2.28 | 0.46 |
| 1:A:349:ASN:HD21 | 1:A:398:ILE:CG1 | 2.28 | 0.46 |
| 1:A:789:ASN:ND2 | 1:A:789:ASN:N | 2.63 | 0.46 |
| 2:F:50:ASP:OD1 | 2:F:51:MET:N | 2.48 | 0.46 |
| 1:A:292:ARG:HH11 | 1:A:292:ARG:HG3 | 1.79 | 0.46 |
| 2:D:50:ASP:OD1 | 2:D:51:MET:N | 2.48 | 0.46 |
| 2:F:22:ASP:HB3 | 2:F:26:THR:OG1 | 2.16 | 0.46 |
| 1:B:315:PHE:O | 1:B:318:ILE:CD1 | 2.64 | 0.46 |
| 2:D:118:ASP:N | 2:D:118:ASP:OD2 | 2.48 | 0.46 |
| 1:C:583:ASN:HD21 | 5:C:1999:DOT:H1' | 1.79 | 0.45 |
| 1:B:777:TYR:HA | 1:B:780:LEU:HD12 | 1.97 | 0.45 |
| 2:F:87:GLU:O | 2:F:91:VAL:HG23 | 2.15 | 0.45 |
| 1:A:714:GLN:HE22 | 2:D:126:ARG:HG3 | 1.75 | 0.45 |
| 1:C:463:THR:CG2 | 1:C:465:LEU:H | 2.28 | 0.45 |
| 2:F:76:MET:HE2 | 2:F:79:THR:HG23 | 1.98 | 0.45 |
| 1:A:432:TYR:CD1 | 1:A:471:TRP:HZ3 | 2.33 | 0.45 |
| 2:E:89:PHE:HE1 | 2:E:138:TYR:N | 2.14 | 0.45 |
| 1:A:697:ILE:N | 1:A:697:ILE:CD1 | 2.80 | 0.45 |
| 1:A:654:ILE:O | 1:A:654:ILE:HG13 | 2.14 | 0.45 |
| 1:A:655:ASN:OD1 | 1:A:758:ASN:HB3 | 2.16 | 0.45 |
| 1:B:549:LEU:CD2 | 1:B:549:LEU:N | 2.79 | 0.45 |
| 1:C:403:LEU:HD13 | 1:C:476:VAL:HG21 | 1.97 | 0.45 |
| 2:E:12:PHE:O | 2:E:16:PHE:HB2 | 2.16 | 0.45 |
| 1:B:408:LEU:O | 1:B:411:GLU:HB3 | 2.16 | 0.45 |
| 2:F:99:TYR:HD2 | 2:F:137:ASN:HB3 | 1.79 | 0.45 |
| 2:E:129:ASP:OD1 | 2:E:132:GLY:N | 2.44 | 0.45 |
| 1:C:639:ASN:HD21 | 1:C:641:ALA:CB | 2.29 | 0.45 |
| 1:B:744:GLU:HG2 | 1:C:397:GLU:HG2 | 1.99 | 0.45 |
| 1:A:456:LYS:HD3 | 1:A:471:TRP:HD1 | 1.81 | 0.45 |
| 1:A:625:LEU:HA | 1:A:625:LEU:HD12 | 1.64 | 0.45 |
| 1:B:717:LYS:HE3 | 1:B:717:LYS:HB3 | 1.67 | 0.45 |
| 1:B:716:LYS:O | 1:B:720:ILE:HG23 | 2.17 | 0.45 |
| 1:B:787:THR:HG23 | 1:B:788:ASP:H | 1.81 | 0.45 |
| 2:F:92:PHE:O | 2:F:94:LYS:N | 2.38 | 0.45 |
| 1:C:322:LEU:N | 1:C:322:LEU:HD12 | 2.31 | 0.45 |
| 1:B:302:LEU:HD13 | 1:B:594:PHE:CZ | 2.52 | 0.45 |
| 2:E:105:LEU:O | 2:E:109:MET:HG2 | 2.16 | 0.45 |
| 1:A:327:LEU:N | 1:A:327:LEU:HD12 | 2.32 | 0.45 |
| 2:D:12:PHE:O | 2:D:16:PHE:HB2 | 2.16 | 0.45 |
| 1:C:423:LYS:HB3 | 1:C:423:LYS:NZ | 2.32 | 0.45 |
| 2:E:45:GLU:O | 2:E:49:GLN:HG2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:790:PHE:O | 1:B:794:GLN:HB2 | 2.17 | 0.45 |
| 1:B:581:GLN:O | 1:B:629:ASN:HA | 2.15 | 0.45 |
| 2:F:89:PHE:CE1 | 2:F:138:TYR:N | 2.85 | 0.45 |
| 1:B:723:PHE:O | 1:B:726:ILE:N | 2.49 | 0.45 |
| 1:B:308:VAL:HG23 | 1:B:492:TYR:OH | 2.16 | 0.45 |
| 1:C:522:SER:O | 1:C:524:GLU:N | 2.49 | 0.45 |
| 1:B:387:ASN:C | 1:B:389:LYS:N | 2.69 | 0.45 |
| 1:B:703:ASP:O | 1:B:705:TYR:O | 2.35 | 0.45 |
| 1:A:607:ASN:O | 1:A:608:TRP:C | 2.54 | 0.45 |
| 1:C:789:ASN:ND2 | 1:C:789:ASN:N | 2.63 | 0.45 |
| 2:F:144:MET:SD | 2:F:144:MET:C | 2.95 | 0.45 |
| 1:C:669:SER:C | 1:C:671:ARG:N | 2.70 | 0.45 |
| 1:A:535:LYS:NZ | 1:A:536:TYR:HE2 | 2.14 | 0.45 |
| 1:B:462:ILE:HG12 | 1:B:463:THR:O | 2.17 | 0.45 |
| 2:E:89:PHE:HD2 | 2:E:90:ARG:N | 2.14 | 0.45 |
| 1:B:589:LYS:HA | 1:B:608:TRP:CZ3 | 2.51 | 0.45 |
| 1:A:530:THR:HG21 | 2:D:145:MET:HE1 | 1.99 | 0.45 |
| 1:B:455:TYR:H | 1:B:455:TYR:HD2 | 1.64 | 0.45 |
| 1:A:513:TRP:CD2 | 1:A:517:VAL:CG2 | 2.92 | 0.45 |
| 1:C:721:SER:O | 1:C:724:ARG:N | 2.50 | 0.45 |
| 2:E:89:PHE:CE1 | 2:E:138:TYR:N | 2.85 | 0.45 |
| 1:A:367:ASP:C | 1:A:369:ASP:H | 2.20 | 0.45 |
| 1:A:325:TYR:CD2 | 1:A:597:ASN:HA | 2.52 | 0.45 |
| 1:B:636:ALA:O | 1:B:640:LYS:HA | 2.17 | 0.45 |
| 1:C:658:PRO:HB2 | 1:C:701:LEU:HD13 | 1.98 | 0.45 |
| 1:A:667:LEU:HA | 1:A:670:ILE:HG21 | 1.99 | 0.45 |
| 1:A:663:PHE:HE1 | 1:A:752:LEU:CD1 | 2.30 | 0.45 |
| 1:C:776:LEU:CD1 | 1:C:776:LEU:N | 2.79 | 0.45 |
| 2:F:130:ILE:CG2 | 2:F:130:ILE:O | 2.65 | 0.45 |
| 1:A:335:ALA:O | 1:A:338:LEU:HB2 | 2.16 | 0.45 |
| 1:B:408:LEU:O | 1:B:411:GLU:N | 2.48 | 0.45 |
| 1:C:537:GLY:HA2 | 1:C:552:TRP:NE1 | 2.31 | 0.45 |
| 1:B:629:ASN:C | 1:B:629:ASN:ND2 | 2.70 | 0.45 |
| 1:C:659:THR:HB | 1:C:662:GLU:H | 1.82 | 0.45 |
| 1:A:581:GLN:O | 1:A:629:ASN:HA | 2.17 | 0.45 |
| 1:A:695:LYS:CG | 2:D:18:LEU:HD13 | 2.39 | 0.45 |
| 1:A:520:PRO:O | 1:A:521:ASN:O | 2.36 | 0.45 |
| 1:B:786:GLU:O | 1:B:789:ASN:N | 2.44 | 0.45 |
| 1:B:312:ALA:HB1 | 1:B:602:PHE:CZ | 2.52 | 0.45 |
| 1:B:422:GLY:O | 1:B:433:TYR:CD2 | 2.70 | 0.45 |
| 1:A:340:LYS:C | 1:A:342:GLY:N | 2.67 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:329:ARG:O | 1:C:330:PRO:O | 2.35 | 0.45 |
| 2:F:121:VAL:C | 2:F:123:GLU:N | 2.70 | 0.45 |
| 1:A:409:ARG:O | 1:A:410:ILE:C | 2.54 | 0.45 |
| 1:B:540:ARG:CZ | 1:B:627:TYR:CE1 | 3.00 | 0.44 |
| 1:A:667:LEU:O | 1:A:670:ILE:HG22 | 2.16 | 0.44 |
| 2:D:138:TYR:O | 2:D:139:GLU:C | 2.55 | 0.44 |
| 1:B:508:ILE:HA | 1:B:536:TYR:CD1 | 2.52 | 0.44 |
| 1:B:793:PHE:C | 1:B:795:LYS:H | 2.20 | 0.44 |
| 1:C:768:LYS:HD2 | 1:C:797:ILE:O | 2.17 | 0.44 |
| 1:A:722:ILE:CG1 | 1:A:763:LEU:HB2 | 2.47 | 0.44 |
| 1:C:478:ALA:HA | 1:C:488:LEU:HD12 | 1.99 | 0.44 |
| 1:C:776:LEU:H | 1:C:776:LEU:HD12 | 1.80 | 0.44 |
| 1:B:345:THR:HG21 | 1:B:574:VAL:HG23 | 1.99 | 0.44 |
| 1:A:323:ASN:O | 1:A:323:ASN:ND2 | 2.50 | 0.44 |
| 1:B:517:VAL:O | 1:B:517:VAL:HG22 | 2.17 | 0.44 |
| 2:F:100:ILE:HD12 | 2:F:141:PHE:CD1 | 2.52 | 0.44 |
| 1:C:722:ILE:CG1 | 1:C:763:LEU:HB2 | 2.47 | 0.44 |
| 1:C:522:SER:C | 1:C:524:GLU:N | 2.71 | 0.44 |
| 1:C:776:LEU:H | 1:C:776:LEU:CD1 | 2.31 | 0.44 |
| 1:A:305:SER:OG | 1:A:306:GLY:N | 2.50 | 0.44 |
| 1:C:663:PHE:CD2 | 1:C:664:ILE:HD12 | 2.49 | 0.44 |
| 1:A:445:ARG:N | 1:A:445:ARG:HD2 | 2.32 | 0.44 |
| 1:B:732:ILE:O | 1:B:735:VAL:HB | 2.17 | 0.44 |
| 1:B:550:SER:H | 1:B:553:GLN:CG | 2.24 | 0.44 |
| 1:A:509:PRO:HG2 | 1:A:512:GLU:HB2 | 2.00 | 0.44 |
| 1:A:584:GLU:OE1 | 1:A:630:ARG:HG3 | 2.17 | 0.44 |
| 1:B:348:LEU:HD22 | 1:B:348:LEU:N | 2.32 | 0.44 |
| 2:D:26:THR:HA | 2:D:63:ILE:O | 2.17 | 0.44 |
| 1:B:391:ILE:CD1 | 1:B:399:GLY:CA | 2.90 | 0.44 |
| 1:A:760:VAL:HG11 | 1:A:773:PHE:HE1 | 1.83 | 0.44 |
| 2:E:99:TYR:HD2 | 2:E:137:ASN:HB3 | 1.82 | 0.44 |
| 2:E:99:TYR:CE2 | 2:E:137:ASN:HB3 | 2.52 | 0.44 |
| 1:B:478:ALA:HB2 | 1:B:487:PRO:HA | 1.99 | 0.44 |
| 1:C:527:LYS:NZ | 2:F:145:MET:HA | 2.31 | 0.44 |
| 1:A:667:LEU:HB3 | 2:D:14:GLU:OE2 | 2.17 | 0.44 |
| 1:B:353:LYS:N | 1:B:368:GLN:NE2 | 2.40 | 0.44 |
| 1:B:773:PHE:C | 1:B:775:LEU:N | 2.71 | 0.44 |
| 1:A:639:ASN:HD21 | 1:A:641:ALA:CB | 2.30 | 0.44 |
| 1:B:728:ALA:C | 1:B:731:GLU:HG3 | 2.37 | 0.44 |
| 2:E:100:ILE:HD12 | 2:E:141:PHE:CD1 | 2.52 | 0.44 |
| 2:E:105:LEU:HD23 | 2:E:109:MET:HG2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:42:ASN:ND2 | 2:D:147:ALA:CB | 2.81 | 0.44 |
| 1:C:625:LEU:HD12 | 1:C:625:LEU:HA | 1.66 | 0.44 |
| 2:F:89:PHE:HE1 | 2:F:138:TYR:N | 2.16 | 0.44 |
| 1:C:712:PHE:HB3 | 1:C:716:LYS:CG | 2.44 | 0.44 |
| 1:A:721:SER:O | 1:A:722:ILE:C | 2.55 | 0.44 |
| 1:A:700:TYR:CE1 | 1:A:727:GLN:O | 2.71 | 0.44 |
| 1:C:327:LEU:HB2 | 1:C:496:ALA:O | 2.18 | 0.44 |
| 1:C:400:LYS:CE | 1:C:475:GLU:OE1 | 2.66 | 0.44 |
| 2:D:146:THR:HG22 | 2:D:147:ALA:N | 2.31 | 0.44 |
| 1:B:562:GLU:C | 1:B:564:VAL:N | 2.70 | 0.44 |
| 2:D:145:MET:O | 2:D:145:MET:HG3 | 2.18 | 0.44 |
| 2:D:121:VAL:C | 2:D:123:GLU:N | 2.71 | 0.44 |
| 2:D:141:PHE:CD2 | 2:D:141:PHE:O | 2.70 | 0.44 |
| 2:D:19:PHE:CD2 | 2:D:19:PHE:C | 2.89 | 0.44 |
| 2:D:65:PHE:HB2 | 2:D:66:PRO:CD | 2.46 | 0.44 |
| 1:B:489:THR:HG23 | 1:B:490:ALA:N | 2.31 | 0.44 |
| 1:C:749:PHE:C | 1:C:751:TYR:N | 2.71 | 0.44 |
| 1:B:403:LEU:HD23 | 1:B:453:VAL:HB | 1.99 | 0.44 |
| 1:C:384:ASN:O | 1:C:387:ASN:N | 2.51 | 0.44 |
| 1:C:659:THR:HB | 1:C:662:GLU:CG | 2.47 | 0.44 |
| 1:A:499:PRO:HD2 | 1:A:625:LEU:HB3 | 1.99 | 0.44 |
| 2:D:65:PHE:H | 2:D:65:PHE:HD1 | 1.59 | 0.44 |
| 1:B:606:LYS:HG3 | 1:B:610:MET:HE1 | 2.00 | 0.44 |
| 1:B:562:GLU:C | 1:B:564:VAL:H | 2.22 | 0.44 |
| 2:F:141:PHE:CD2 | 2:F:141:PHE:O | 2.70 | 0.44 |
| 1:B:649:ILE:HD12 | 2:E:86:ARG:CG | 2.48 | 0.44 |
| 1:C:700:TYR:HD1 | 1:C:728:ALA:HA | 1.82 | 0.44 |
| 2:D:131:ASP:OD1 | 2:D:133:ASP:OD2 | 2.35 | 0.44 |
| 1:A:299:GLU:CG | 1:A:303:LYS:HZ2 | 2.31 | 0.44 |
| 1:A:776:LEU:H | 1:A:776:LEU:HD12 | 1.81 | 0.44 |
| 1:A:597:ASN:HB2 | 1:A:598:PRO:HD2 | 1.99 | 0.44 |
| 2:F:121:VAL:C | 2:F:123:GLU:H | 2.22 | 0.44 |
| 1:C:550:SER:OG | 1:C:553:GLN:HB2 | 2.17 | 0.44 |
| 2:D:99:TYR:CE2 | 2:D:137:ASN:HB3 | 2.53 | 0.43 |
| 1:B:773:PHE:O | 1:B:773:PHE:CD1 | 2.71 | 0.43 |
| 2:E:26:THR:HA | 2:E:63:ILE:O | 2.18 | 0.43 |
| 2:D:26:THR:HG22 | 2:D:64:ASP:OD1 | 2.18 | 0.43 |
| 1:B:727:GLN:O | 1:B:730:ASN:O | 2.35 | 0.43 |
| 1:A:385:LEU:HD11 | 1:A:389:LYS:HD2 | 1.99 | 0.43 |
| 1:C:712:PHE:HD2 | 1:C:716:LYS:HE2 | 1.81 | 0.43 |
| 1:A:768:LYS:CG | 1:A:768:LYS:O | 2.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:325:TYR:CE1 | 1:C:619:ILE:HG12 | 2.53 | 0.43 |
| 2:E:26:THR:HG22 | 2:E:64:ASP:OD1 | 2.19 | 0.43 |
| 1:A:322:LEU:HA | 1:A:503:GLU:OE2 | 2.18 | 0.43 |
| 1:C:597:ASN:HB2 | 1:C:598:PRO:HD2 | 2.00 | 0.43 |
| 1:C:332:ASN:O | 1:C:335:ALA:N | 2.39 | 0.43 |
| 1:A:294:ASP:O | 1:A:610:MET:HE1 | 2.18 | 0.43 |
| 1:B:607:ASN:OD1 | 1:B:610:MET:CB | 2.66 | 0.43 |
| 1:B:639:ASN:HD22 | 1:B:639:ASN:N | 2.16 | 0.43 |
| 1:B:721:SER:O | 1:B:722:ILE:C | 2.56 | 0.43 |
| 1:B:553:GLN:O | 1:B:556:MET:HB3 | 2.18 | 0.43 |
| 1:A:384:ASN:N | 1:A:384:ASN:OD1 | 2.49 | 0.43 |
| 1:A:793:PHE:O | 1:A:794:GLN:C | 2.56 | 0.43 |
| 1:C:527:LYS:HZ1 | 2:F:145:MET:C | 2.22 | 0.43 |
| 1:A:381:GLU:C | 1:A:383:GLY:N | 2.71 | 0.43 |
| 2:D:129:ASP:OD1 | 2:D:132:GLY:N | 2.47 | 0.43 |
| 2:E:19:PHE:C | 2:E:19:PHE:CD2 | 2.91 | 0.43 |
| 2:F:12:PHE:O | 2:F:16:PHE:HB2 | 2.18 | 0.43 |
| 2:D:137:ASN:O | 2:D:138:TYR:C | 2.56 | 0.43 |
| 2:F:26:THR:HG22 | 2:F:64:ASP:OD1 | 2.19 | 0.43 |
| 2:F:99:TYR:CE2 | 2:F:137:ASN:HB3 | 2.54 | 0.43 |
| 1:C:630:ARG:HE | 2:F:87:GLU:CD | 2.21 | 0.43 |
| 1:C:519:THR:OG1 | 1:C:520:PRO:HD2 | 2.18 | 0.43 |
| 1:C:367:ASP:C | 1:C:369:ASP:H | 2.22 | 0.43 |
| 1:A:514:ASP:HA | 1:A:517:VAL:HB | 2.01 | 0.43 |
| 1:B:508:ILE:HG22 | 1:B:509:PRO:HD2 | 2.01 | 0.43 |
| 1:A:345:THR:HG21 | 1:A:574:VAL:CG2 | 2.49 | 0.43 |
| 1:C:721:SER:O | 1:C:722:ILE:C | 2.55 | 0.43 |
| 1:B:549:LEU:HD11 | 1:B:554:LYS:HG2 | 1.99 | 0.43 |
| 1:B:437:SER:C | 1:B:439:ASN:H | 2.21 | 0.43 |
| 1:B:383:GLY:O | 1:B:386:GLU:HB2 | 2.19 | 0.43 |
| 2:D:144:MET:C | 2:D:144:MET:SD | 2.97 | 0.43 |
| 1:B:607:ASN:O | 1:B:610:MET:N | 2.52 | 0.43 |
| 1:B:747:ASN:O | 1:B:751:TYR:HB3 | 2.17 | 0.43 |
| 1:B:326:ILE:HG23 | 1:B:497:LEU:HD21 | 2.00 | 0.43 |
| 1:A:504:ILE:O | 1:A:505:LYS:C | 2.55 | 0.43 |
| 1:B:441:VAL:HA | 1:B:461:LYS:HG2 | 2.01 | 0.43 |
| 1:C:722:ILE:HG12 | 1:C:763:LEU:HB2 | 1.99 | 0.43 |
| 1:A:408:LEU:C | 1:A:408:LEU:CD2 | 2.86 | 0.43 |
| 1:A:370:LEU:HD11 | 1:A:455:TYR:CD1 | 2.53 | 0.43 |
| 1:A:323:ASN:HD22 | 1:A:323:ASN:C | 2.22 | 0.43 |
| 2:F:102:ALA:O | 2:F:103:ALA:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:39:LEU:HG | 2:E:39:LEU:O | 2.18 | 0.43 |
| 1:A:302:LEU:HD12 | 1:A:602:PHE:HE1 | 1.84 | 0.43 |
| 2:F:26:THR:HA | 2:F:63:ILE:O | 2.17 | 0.43 |
| 1:A:712:PHE:CE2 | 1:A:716:LYS:HE2 | 2.54 | 0.43 |
| 1:C:516:VAL:O | 1:C:516:VAL:CG1 | 2.58 | 0.43 |
| 2:E:44:THR:HG22 | 2:E:47:GLU:CG | 2.45 | 0.43 |
| 1:A:700:TYR:HB3 | 1:A:728:ALA:HB2 | 2.00 | 0.43 |
| 2:D:79:THR:C | 2:D:81:SER:H | 2.22 | 0.43 |
| 1:A:762:LEU:O | 1:A:766:HIS:HB2 | 2.19 | 0.43 |
| 1:B:744:GLU:HG2 | 1:C:397:GLU:CG | 2.48 | 0.43 |
| 1:A:730:ASN:C | 1:A:732:ILE:H | 2.22 | 0.43 |
| 1:A:445:ARG:HH22 | 1:A:456:LYS:HG2 | 1.83 | 0.43 |
| 1:B:323:ASN:ND2 | 1:B:500:SER:CB | 2.82 | 0.43 |
| 1:B:745:TYR:O | 1:B:749:PHE:CD1 | 2.72 | 0.43 |
| 1:B:727:GLN:HG3 | 1:B:786:GLU:CG | 2.48 | 0.43 |
| 1:A:387:ASN:HB3 | 1:A:477:MET:HE1 | 1.99 | 0.43 |
| 1:A:345:THR:HG21 | 1:A:574:VAL:HG22 | 2.00 | 0.43 |
| 1:C:463:THR:CG2 | 1:C:464:VAL:N | 2.82 | 0.43 |
| 2:D:95:ASP:OD1 | 2:D:104:GLU:OE2 | 2.36 | 0.43 |
| 1:B:320:ARG:HH21 | 1:B:320:ARG:CG | 2.31 | 0.43 |
| 1:C:320:ARG:HA | 1:C:598:PRO:O | 2.19 | 0.43 |
| 1:C:329:ARG:HD2 | 1:C:590:ASP:OD2 | 2.18 | 0.43 |
| 1:B:570:THR:O | 1:B:572:GLY:N | 2.51 | 0.43 |
| 1:B:629:ASN:ND2 | 1:B:631:SER:CA | 2.79 | 0.43 |
| 1:A:354:SER:N | 5:A:999:DOT:O2G | 2.42 | 0.43 |
| 1:A:304:ALA:HB3 | 1:A:604:LEU:CD1 | 2.49 | 0.43 |
| 1:B:318:ILE:HD12 | 1:B:319:ALA:H | 1.83 | 0.43 |
| 1:A:385:LEU:HD23 | 1:C:640:LYS:HB3 | 2.00 | 0.43 |
| 1:C:793:PHE:O | 1:C:794:GLN:C | 2.57 | 0.43 |
| 1:C:324:THR:OG1 | 1:C:499:PRO:HB3 | 2.18 | 0.43 |
| 2:E:92:PHE:CZ | 2:E:108:VAL:HG11 | 2.53 | 0.43 |
| 1:A:337:ASN:CB | 1:A:412:GLU:OE2 | 2.64 | 0.43 |
| 1:C:773:PHE:CD2 | 1:C:774:LYS:N | 2.87 | 0.43 |
| 1:A:647:ASP:OD2 | 2:D:90:ARG:NE | 2.52 | 0.43 |
| 1:B:313:ASP:O | 1:B:315:PHE:N | 2.52 | 0.43 |
| 1:C:712:PHE:CE2 | 1:C:716:LYS:HE2 | 2.54 | 0.43 |
| 1:C:321:GLU:HB3 | 1:C:322:LEU:HD12 | 2.00 | 0.43 |
| 1:C:522:SER:HA | 1:C:525:LYS:HG3 | 2.00 | 0.43 |
| 1:C:754:GLU:O | 1:C:758:ASN:ND2 | 2.52 | 0.43 |
| 1:A:663:PHE:CD1 | 1:A:752:LEU:HD11 | 2.54 | 0.43 |
| 1:B:555:GLN:O | 1:B:558:ASP:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:9:ILE:HG22 | 2:F:9:ILE:O | 2.19 | 0.43 |
| 1:B:327:LEU:CD2 | 1:B:595:ILE:HG23 | 2.48 | 0.43 |
| 1:C:332:ASN:O | 1:C:335:ALA:HB3 | 2.19 | 0.43 |
| 2:F:118:ASP:N | 2:F:118:ASP:OD2 | 2.52 | 0.43 |
| 1:A:747:ASN:O | 1:A:748:TYR:C | 2.56 | 0.42 |
| 1:B:381:GLU:O | 1:B:382:LYS:C | 2.55 | 0.42 |
| 1:A:773:PHE:CD2 | 1:A:774:LYS:N | 2.86 | 0.42 |
| 2:E:145:MET:HE2 | 2:E:145:MET:HB2 | 1.72 | 0.42 |
| 1:A:700:TYR:CD1 | 1:A:728:ALA:HA | 2.47 | 0.42 |
| 2:F:145:MET:HG3 | 2:F:145:MET:O | 2.19 | 0.42 |
| 1:A:776:LEU:CD1 | 1:A:776:LEU:N | 2.81 | 0.42 |
| 2:E:118:ASP:N | 2:E:118:ASP:OD2 | 2.52 | 0.42 |
| 1:B:434:LEU:HA | 1:B:445:ARG:HA | 2.01 | 0.42 |
| 2:E:27:ILE:HG13 | 2:E:63:ILE:HB | 2.01 | 0.42 |
| 1:B:726:ILE:O | 1:B:729:TYR:HB2 | 2.19 | 0.42 |
| 1:B:317:LYS:O | 1:B:320:ARG:N | 2.51 | 0.42 |
| 1:B:415:GLU:O | 1:B:417:GLY:N | 2.52 | 0.42 |
| 1:B:774:LYS:O | 1:B:774:LYS:CG | 2.66 | 0.42 |
| 1:C:666:ASN:HD22 | 1:C:666:ASN:N | 2.15 | 0.42 |
| 2:D:89:PHE:HD2 | 2:D:90:ARG:N | 2.17 | 0.42 |
| 2:F:27:ILE:HG13 | 2:F:63:ILE:HB | 2.00 | 0.42 |
| 1:B:648:PRO:C | 1:B:650:THR:H | 2.22 | 0.42 |
| 1:B:315:PHE:O | 1:B:318:ILE:HD12 | 2.19 | 0.42 |
| 1:C:712:PHE:N | 1:C:712:PHE:CD1 | 2.87 | 0.42 |
| 1:A:721:SER:O | 1:A:724:ARG:N | 2.53 | 0.42 |
| 1:A:440:GLN:O | 1:A:458:LYS:HE2 | 2.20 | 0.42 |
| 1:A:340:LYS:O | 1:A:342:GLY:N | 2.52 | 0.42 |
| 2:D:89:PHE:CE1 | 2:D:138:TYR:N | 2.87 | 0.42 |
| 1:B:728:ALA:CA | 1:B:731:GLU:CG | 2.90 | 0.42 |
| 1:C:549:LEU:CD1 | 1:C:554:LYS:HE2 | 2.49 | 0.42 |
| 1:C:691:LYS:HB2 | 1:C:694:VAL:HG13 | 2.02 | 0.42 |
| 2:F:5:THR:O | 2:F:9:ILE:CG1 | 2.66 | 0.42 |
| 1:A:665:LYS:HE2 | 2:D:11:GLU:OE1 | 2.19 | 0.42 |
| 1:C:295:VAL:CG2 | 1:C:296:LEU:N | 2.81 | 0.42 |
| 2:E:65:PHE:HB2 | 2:E:66:PRO:CD | 2.45 | 0.42 |
| 2:F:65:PHE:HB2 | 2:F:66:PRO:CD | 2.46 | 0.42 |
| 1:B:757:THR:O | 1:B:760:VAL:N | 2.52 | 0.42 |
| 1:A:318:ILE:CG2 | 1:A:322:LEU:HD13 | 2.49 | 0.42 |
| 1:C:307:LEU:HA | 1:C:492:TYR:HE1 | 1.85 | 0.42 |
| 1:C:607:ASN:O | 1:C:608:TRP:C | 2.58 | 0.42 |
| 1:A:403:LEU:CD1 | 1:A:476:VAL:HG21 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:121:VAL:C | 2:D:123:GLU:H | 2.22 | 0.42 |
| 1:B:401:ILE:O | 1:B:401:ILE:HG12 | 2.19 | 0.42 |
| 1:A:376:GLN:HG3 | 1:A:376:GLN:H | 1.68 | 0.42 |
| 1:B:773:PHE:HA | 1:B:775:LEU:HD22 | 2.00 | 0.42 |
| 1:C:415:GLU:C | 1:C:417:GLY:H | 2.23 | 0.42 |
| 1:C:489:THR:OG1 | 1:C:490:ALA:N | 2.53 | 0.42 |
| 1:A:699:GLY:O | 1:A:702:SER:N | 2.53 | 0.42 |
| 1:C:664:ILE:N | 1:C:664:ILE:HD12 | 2.35 | 0.42 |
| 1:C:628:PHE:O | 1:C:628:PHE:CD1 | 2.73 | 0.42 |
| 2:F:92:PHE:CB | 2:F:100:ILE:HD13 | 2.50 | 0.42 |
| 1:B:530:THR:HG22 | 2:E:92:PHE:CE1 | 2.54 | 0.42 |
| 1:A:508:ILE:CG2 | 1:A:532:LEU:HD13 | 2.49 | 0.42 |
| 1:B:614:PHE:CD2 | 1:B:614:PHE:C | 2.93 | 0.42 |
| 1:C:667:LEU:HA | 1:C:670:ILE:CG2 | 2.49 | 0.42 |
| 1:A:523:LEU:O | 1:A:525:LYS:N | 2.52 | 0.42 |
| 1:C:700:TYR:CD1 | 1:C:728:ALA:HA | 2.55 | 0.42 |
| 1:C:502:THR:OG1 | 1:C:503:GLU:N | 2.52 | 0.42 |
| 1:A:463:THR:CG2 | 1:A:464:VAL:N | 2.82 | 0.42 |
| 1:B:715:GLU:O | 1:B:719:LYS:HB2 | 2.19 | 0.42 |
| 1:A:351:HIS:NE2 | 5:A:999:DOT:H3B | 2.34 | 0.42 |
| 1:B:732:ILE:O | 1:B:735:VAL:CG1 | 2.67 | 0.42 |
| 1:B:556:MET:O | 1:B:560:LEU:HD12 | 2.19 | 0.42 |
| 1:A:387:ASN:OD1 | 1:A:477:MET:HE2 | 2.20 | 0.42 |
| 1:B:525:LYS:NZ | 2:E:114:GLU:HG2 | 2.35 | 0.42 |
| 1:C:527:LYS:NZ | 2:F:145:MET:C | 2.74 | 0.42 |
| 1:A:776:LEU:CD1 | 1:A:776:LEU:H | 2.32 | 0.42 |
| 1:C:740:GLN:N | 1:C:740:GLN:CD | 2.72 | 0.42 |
| 2:F:144:MET:SD | 2:F:144:MET:O | 2.77 | 0.42 |
| 2:F:129:ASP:OD1 | 2:F:132:GLY:N | 2.44 | 0.42 |
| 1:A:484:VAL:CG1 | 1:A:485:LEU:N | 2.82 | 0.42 |
| 1:C:659:THR:C | 1:C:701:LEU:HD13 | 2.40 | 0.42 |
| 1:A:593:ILE:HB | 1:A:605:THR:OG1 | 2.20 | 0.42 |
| 1:B:360:VAL:O | 1:B:361:ALA:C | 2.58 | 0.42 |
| 2:F:137:ASN:O | 2:F:138:TYR:C | 2.57 | 0.42 |
| 1:B:751:TYR:CE2 | 1:B:755:ARG:HG3 | 2.55 | 0.42 |
| 1:A:712:PHE:N | 1:A:712:PHE:CD1 | 2.88 | 0.42 |
| 2:D:44:THR:HG22 | 2:D:47:GLU:CG | 2.44 | 0.42 |
| 1:C:387:ASN:OD1 | 1:C:477:MET:HE2 | 2.19 | 0.42 |
| 1:C:478:ALA:CA | 1:C:488:LEU:HD12 | 2.50 | 0.42 |
| 1:C:363:TYR:HB3 | 1:C:476:VAL:HG11 | 2.02 | 0.42 |
| 1:B:629:ASN:ND2 | 1:B:630:ARG:N | 2.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:593:ILE:HB | 1:C:605:THR:OG1 | 2.20 | 0.41 |
| 2:F:89:PHE:HD2 | 2:F:90:ARG:N | 2.18 | 0.41 |
| 1:B:722:ILE:O | 1:B:726:ILE:CG1 | 2.68 | 0.41 |
| 1:A:502:THR:OG1 | 1:A:503:GLU:N | 2.52 | 0.41 |
| 1:B:546:LYS:O | 1:B:547:GLY:O | 2.38 | 0.41 |
| 1:B:453:VAL:HG12 | 1:B:474:ILE:HD12 | 2.02 | 0.41 |
| 1:A:363:TYR:HB3 | 1:A:476:VAL:HG11 | 2.01 | 0.41 |
| 1:B:629:ASN:HB3 | 1:B:632:TYR:CZ | 2.55 | 0.41 |
| 1:C:511:LYS:N | 1:C:514:ASP:OD1 | 2.51 | 0.41 |
| 1:A:749:PHE:C | 1:A:751:TYR:N | 2.72 | 0.41 |
| 1:A:540:ARG:CZ | 1:A:627:TYR:CE1 | 3.03 | 0.41 |
| 1:A:658:PRO:HG3 | 1:A:752:LEU:HD22 | 2.02 | 0.41 |
| 1:A:754:GLU:O | 1:A:758:ASN:ND2 | 2.53 | 0.41 |
| 2:D:130:ILE:O | 2:D:130:ILE:CG2 | 2.68 | 0.41 |
| 2:F:68:PHE:CE1 | 2:F:72:MET:HG2 | 2.55 | 0.41 |
| 1:B:374:HIS:ND1 | 1:B:375:GLY:N | 2.68 | 0.41 |
| 1:B:762:LEU:O | 1:B:766:HIS:HB2 | 2.20 | 0.41 |
| 2:D:99:TYR:HD2 | 2:D:137:ASN:HB3 | 1.79 | 0.41 |
| 1:B:445:ARG:CB | 1:B:471:TRP:CZ3 | 3.02 | 0.41 |
| 1:B:728:ALA:C | 1:B:730:ASN:N | 2.73 | 0.41 |
| 1:A:540:ARG:HB3 | 1:A:549:LEU:O | 2.20 | 0.41 |
| 1:B:461:LYS:HG3 | 1:B:462:ILE:H | 1.85 | 0.41 |
| 2:E:137:ASN:O | 2:E:138:TYR:C | 2.58 | 0.41 |
| 1:B:410:ILE:HD13 | 1:B:419:ILE:HD11 | 2.01 | 0.41 |
| 2:F:39:LEU:HG | 2:F:39:LEU:O | 2.20 | 0.41 |
| 1:A:662:GLU:O | 1:A:666:ASN:HB2 | 2.20 | 0.41 |
| 1:A:517:VAL:HG13 | 2:D:114:GLU:OE2 | 2.20 | 0.41 |
| 1:B:707:SER:C | 1:B:709:ASN:H | 2.24 | 0.41 |
| 1:C:713:SER:O | 1:C:716:LYS:HB3 | 2.19 | 0.41 |
| 1:B:350:VAL:CG2 | 1:B:398:ILE:HG13 | 2.51 | 0.41 |
| 1:A:505:LYS:O | 1:A:507:GLN:N | 2.54 | 0.41 |
| 1:C:340:LYS:O | 1:C:342:GLY:N | 2.54 | 0.41 |
| 1:A:670:ILE:HD12 | 1:A:745:TYR:CD1 | 2.54 | 0.41 |
| 1:B:403:LEU:HB2 | 1:B:476:VAL:HG23 | 2.01 | 0.41 |
| 1:C:522:SER:C | 1:C:524:GLU:H | 2.24 | 0.41 |
| 1:B:656:THR:O | 1:B:705:TYR:CE1 | 2.69 | 0.41 |
| 2:E:121:VAL:C | 2:E:123:GLU:H | 2.24 | 0.41 |
| 2:F:85:ILE:O | 2:F:88:ALA:HB3 | 2.20 | 0.41 |
| 1:A:661:ALA:O | 1:A:662:GLU:C | 2.58 | 0.41 |
| 1:C:581:GLN:O | 1:C:629:ASN:HA | 2.20 | 0.41 |
| 1:A:583:ASN:ND2 | 5:A:999:DOT:C1B | 2.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:784:GLU:HB2 | 1:B:788:ASP:HB2 | 2.03 | 0.41 |
| 1:C:540:ARG:HD3 | 1:C:582:ASP:CG | 2.41 | 0.41 |
| 2:D:92:PHE:O | 2:D:94:LYS:N | 2.44 | 0.41 |
| 1:B:597:ASN:CG | 1:B:601:GLU:HB2 | 2.41 | 0.41 |
| 1:B:410:ILE:HD12 | 1:B:435:LEU:HD21 | 2.02 | 0.41 |
| 1:C:415:GLU:C | 1:C:417:GLY:N | 2.74 | 0.41 |
| 1:B:775:LEU:N | 1:B:775:LEU:HD13 | 2.35 | 0.41 |
| 1:C:540:ARG:CZ | 1:C:627:TYR:CE1 | 3.03 | 0.41 |
| 1:C:691:LYS:HB2 | 1:C:694:VAL:CG1 | 2.51 | 0.41 |
| 1:C:747:ASN:O | 1:C:748:TYR:C | 2.56 | 0.41 |
| 1:A:388:LYS:HD3 | 1:C:642:TYR:HB2 | 2.02 | 0.41 |
| 1:B:629:ASN:HD22 | 1:B:630:ARG:N | 2.19 | 0.41 |
| 2:D:40:GLY:O | 2:D:41:GLN:HG2 | 2.21 | 0.41 |
| 2:F:44:THR:HG22 | 2:F:47:GLU:CG | 2.45 | 0.41 |
| 1:C:463:THR:HB | 1:C:467:GLU:N | 2.33 | 0.41 |
| 2:D:76:MET:HE2 | 2:D:79:THR:HG23 | 2.02 | 0.41 |
| 2:D:79:THR:O | 2:D:81:SER:N | 2.53 | 0.41 |
| 2:D:121:VAL:O | 2:D:123:GLU:N | 2.54 | 0.41 |
| 1:B:630:ARG:HE | 2:E:87:GLU:CD | 2.24 | 0.41 |
| 1:C:456:LYS:HD3 | 1:C:471:TRP:CE2 | 2.56 | 0.41 |
| 1:C:628:PHE:HD1 | 1:C:629:ASN:O | 2.03 | 0.41 |
| 1:A:302:LEU:C | 1:A:302:LEU:CD2 | 2.88 | 0.41 |
| 1:B:457:THR:HG21 | 1:B:468:LYS:HA | 2.01 | 0.41 |
| 1:B:745:TYR:HD2 | 1:B:749:PHE:CZ | 2.39 | 0.41 |
| 1:B:785:ASN:O | 1:B:787:THR:N | 2.54 | 0.41 |
| 1:A:712:PHE:HD2 | 1:A:716:LYS:HE2 | 1.83 | 0.41 |
| 1:C:540:ARG:NH1 | 1:C:630:ARG:HH21 | 2.18 | 0.41 |
| 2:D:92:PHE:CB | 2:D:100:ILE:HD13 | 2.51 | 0.41 |
| 1:C:569:TYR:CE2 | 1:C:574:VAL:HG23 | 2.56 | 0.41 |
| 1:A:768:LYS:HD2 | 1:A:797:ILE:O | 2.21 | 0.41 |
| 1:B:616:GLU:CG | 1:B:617:LYS:H | 2.33 | 0.41 |
| 1:C:421:LYS:HA | 1:C:435:LEU:HD23 | 2.02 | 0.41 |
| 1:A:530:THR:CB | 2:D:145:MET:HE1 | 2.51 | 0.41 |
| 1:A:323:ASN:ND2 | 1:A:323:ASN:C | 2.74 | 0.41 |
| 2:D:120:GLU:O | 2:D:123:GLU:HB2 | 2.21 | 0.41 |
| 1:C:407:HIS:CD2 | 1:C:407:HIS:H | 2.35 | 0.41 |
| 1:C:657:ILE:CG2 | 1:C:658:PRO:HD2 | 2.51 | 0.41 |
| 1:C:604:LEU:C | 1:C:604:LEU:HD23 | 2.42 | 0.41 |
| 1:A:295:VAL:CG2 | 1:A:296:LEU:N | 2.84 | 0.41 |
| 1:B:746:LYS:HG2 | 1:B:750:GLN:HB2 | 2.03 | 0.41 |
| 1:C:621:GLY:HA2 | 2:F:94:LYS:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:540:ARG:HH12 | 1:C:630:ARG:HH21 | 1.69 | 0.41 |
| 2:D:108:VAL:O | 2:D:112:LEU:HG | 2.21 | 0.41 |
| 1:B:703:ASP:OD1 | 1:B:703:ASP:O | 2.38 | 0.41 |
| 1:C:597:ASN:C | 1:C:599:GLU:H | 2.24 | 0.41 |
| 1:B:574:VAL:O | 1:B:574:VAL:HG13 | 2.21 | 0.41 |
| 1:C:777:TYR:CD1 | 1:C:780:LEU:HD21 | 2.56 | 0.41 |
| 2:F:121:VAL:O | 2:F:123:GLU:N | 2.54 | 0.41 |
| 1:B:626:TYR:HD2 | 1:B:626:TYR:C | 2.21 | 0.40 |
| 1:C:629:ASN:CB | 1:C:632:TYR:CE2 | 3.03 | 0.40 |
| 1:A:593:ILE:HG13 | 1:A:611:THR:HG21 | 2.03 | 0.40 |
| 1:B:338:LEU:HD11 | 1:B:409:ARG:CZ | 2.51 | 0.40 |
| 1:B:508:ILE:CG2 | 1:B:532:LEU:HD22 | 2.50 | 0.40 |
| 2:D:85:ILE:O | 2:D:88:ALA:HB3 | 2.20 | 0.40 |
| 1:C:324:THR:HG21 | 1:C:556:MET:HE3 | 1.98 | 0.40 |
| 2:E:108:VAL:O | 2:E:112:LEU:HG | 2.21 | 0.40 |
| 1:C:504:ILE:O | 1:C:505:LYS:C | 2.58 | 0.40 |
| 1:C:654:ILE:HG13 | 1:C:654:ILE:H | 1.59 | 0.40 |
| 2:E:115:LYS:HA | 2:E:115:LYS:HD2 | 1.96 | 0.40 |
| 1:B:501:LEU:O | 1:B:501:LEU:HD23 | 2.20 | 0.40 |
| 1:A:326:ILE:HG22 | 1:A:328:PHE:CE1 | 2.57 | 0.40 |
| 1:C:773:PHE:O | 1:C:774:LYS:C | 2.60 | 0.40 |
| 1:C:509:PRO:C | 1:C:511:LYS:H | 2.25 | 0.40 |
| 1:A:556:MET:HB2 | 1:A:556:MET:HE2 | 1.98 | 0.40 |
| 1:B:322:LEU:O | 1:B:323:ASN:C | 2.59 | 0.40 |
| 1:B:509:PRO:HG2 | 1:B:512:GLU:CB | 2.40 | 0.40 |
| 1:B:394:HIS:O | 1:B:395:GLU:C | 2.59 | 0.40 |
| 1:A:777:TYR:CD1 | 1:A:780:LEU:HD21 | 2.55 | 0.40 |
| 1:C:494:LEU:HB3 | 1:C:579:THR:HG22 | 2.04 | 0.40 |
| 1:C:785:ASN:OD1 | 1:C:786:GLU:HG2 | 2.22 | 0.40 |
| 1:C:587:PRO:HB2 | 1:C:643:ILE:CD1 | 2.49 | 0.40 |
| 1:C:510:GLN:HE21 | 1:C:510:GLN:HA | 1.86 | 0.40 |
| 1:B:717:LYS:HD2 | 2:E:132:GLY:H | 1.78 | 0.40 |
| 1:B:297:LYS:HA | 1:B:602:PHE:O | 2.21 | 0.40 |
| 1:A:549:LEU:CD1 | 1:A:554:LYS:HE2 | 2.51 | 0.40 |
| 2:E:41:GLN:HA | 2:E:41:GLN:HE21 | 1.86 | 0.40 |
| 1:C:526:GLN:HB3 | 2:F:144:MET:CE | 2.52 | 0.40 |
| 2:D:145:MET:HB2 | 2:D:145:MET:HE2 | 1.83 | 0.40 |
| 1:C:779:GLN:O | 1:C:779:GLN:HG3 | 2.22 | 0.40 |
| 1:B:310:GLU:CB | 1:B:567:THR:HG21 | 2.51 | 0.40 |
| 1:C:317:LYS:HB2 | 1:C:317:LYS:HE2 | 1.96 | 0.40 |
| 2:E:89:PHE:CD1 | 2:E:138:TYR:HA | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:730:ASN:C | 1:C:732:ILE:H | 2.24 | 0.40 |
| 1:A:597:ASN:C | 1:A:599:GLU:H | 2.24 | 0.40 |
| 1:B:329:ARG:HB3 | 1:B:329:ARG:HE | 1.61 | 0.40 |
| 1:A:785:ASN:OD1 | 1:A:786:GLU:HG2 | 2.22 | 0.40 |
| 2:D:102:ALA:O | 2:D:103:ALA:C | 2.59 | 0.40 |
| 1:C:671:ARG:C | 1:C:672:ARG:HE | 2.25 | 0.40 |
| 1:A:432:TYR:CE1 | 1:A:471:TRP:CZ3 | 3.07 | 0.40 |
| 1:B:777:TYR:CD1 | 1:B:780:LEU:CD1 | 2.92 | 0.40 |
| 1:A:517:VAL:CA | 1:A:525:LYS:NZ | 2.85 | 0.40 |
| 1:B:717:LYS:CD | 2:E:132:GLY:H | 2.32 | 0.40 |
| 2:E:83:GLU:O | 2:E:84:GLU:C | 2.60 | 0.40 |
| 1:B:325:TYR:HB2 | 1:B:498:ALA:HB3 | 2.03 | 0.40 |
| 1:C:443:GLU:HB2 | 1:C:458:LYS:HG2 | 2.02 | 0.40 |
| 1:C:440:GLN:O | 1:C:458:LYS:HE2 | 2.21 | 0.40 |
| 2:E:121:VAL:C | 2:E:123:GLU:N | 2.72 | 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 | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 479/510 (94%) | 386 (81%) | 71 (15%) | 22 (5%) | 3 | 31 |
| 1 | B | 457/510 (90%) | 335 (73%) | 89 (20%) | 33 (7%) | 1 | 19 |
| 1 | C | 499/510 (98%) | 384 (77%) | 93 (19%) | 22 (4%) | 3 | 32 |
| 2 | D | 141/149 (95%) | 105 (74%) | 28 (20%) | 8 (6%) | 2 | 25 |
| 2 | E | 141/149 (95%) | 108 (77%) | 24 (17%) | 9 (6%) | 2 | 23 |
| 2 | F | 141/149 (95%) | 108 (77%) | 23 (16%) | 10 (7%) | 1 | 19 |
| All | All | 1858/1977 (94%) | 1426 (77%) | 328 (18%) | 104 (6%) | 2 | 26 |

All (104) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 368 | GLN |
| 1 | A | 521 | ASN |
| 1 | B | 566 | TYR |
| 1 | B | 571 | GLY |
| 1 | B | 757 | THR |
| 1 | C | 368 | GLN |
| 1 | C | 519 | THR |
| 1 | C | 521 | ASN |
| 2 | D | 82 | GLU |
| 2 | E | 82 | GLU |
| 2 | F | 82 | GLU |
| 1 | A | 378 | LEU |
| 1 | A | 629 | ASN |
| 1 | A | 653 | LYS |
| 1 | B | 299 | GLU |
| 1 | B | 460 | GLY |
| 1 | B | 525 | LYS |
| 1 | B | 547 | GLY |
| 1 | B | 575 | VAL |
| 1 | B | 722 | ILE |
| 1 | B | 734 | ASN |
| 1 | B | 735 | VAL |
| 1 | B | 736 | LEU |
| 1 | B | 739 | LYS |
| 1 | B | 774 | LYS |
| 1 | B | 786 | GLU |
| 1 | B | 796 | ILE |
| 1 | C | 378 | LEU |
| 1 | C | 569 | TYR |
| 2 | D | 93 | ASP |
| 2 | D | 141 | PHE |
| 2 | E | 141 | PHE |
| 2 | F | 93 | ASP |
| 2 | F | 141 | PHE |
| 1 | A | 294 | ASP |
| 1 | A | 317 | LYS |
| 1 | A | 347 | GLY |
| 1 | A | 377 | GLN |
| 1 | A | 510 | GLN |
| 1 | B | 309 | PRO |
| 1 | B | 317 | LYS |
| 1 | B | 354 | SER |
| 1 | B | 463 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 563 | ALA |
| 1 | B | 591 | ASN |
| 1 | B | 702 | SER |
| 1 | B | 706 | ASN |
| 1 | B | 793 | PHE |
| 1 | C | 317 | LYS |
| 1 | C | 332 | ASN |
| 1 | C | 623 | ASP |
| 2 | D | 73 | ALA |
| 2 | D | 76 | MET |
| 2 | D | 80 | ASP |
| 2 | E | 73 | ALA |
| 2 | E | 76 | MET |
| 2 | F | 73 | ALA |
| 2 | F | 76 | MET |
| 2 | F | 80 | ASP |
| 1 | A | 330 | PRO |
| 1 | A | 332 | ASN |
| 1 | A | 511 | LYS |
| 1 | A | 520 | PRO |
| 1 | A | 708 | ALA |
| 1 | B | 332 | ASN |
| 1 | B | 361 | ALA |
| 1 | B | 629 | ASN |
| 1 | B | 794 | GLN |
| 1 | C | 347 | GLY |
| 1 | C | 407 | HIS |
| 1 | C | 523 | LEU |
| 1 | C | 708 | ALA |
| 2 | D | 118 | ASP |
| 2 | E | 80 | ASP |
| 2 | E | 118 | ASP |
| 2 | F | 94 | LYS |
| 2 | F | 118 | ASP |
| 1 | A | 503 | GLU |
| 1 | A | 569 | TYR |
| 1 | A | 608 | TRP |
| 1 | B | 694 | VAL |
| 1 | B | 792 | VAL |
| 1 | C | 330 | PRO |
| 1 | C | 377 | GLN |
| 1 | C | 658 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 54 | GLU |
| 2 | E | 49 | GLN |
| 2 | E | 54 | GLU |
| 2 | E | 94 | LYS |
| 2 | F | 54 | GLU |
| 1 | A | 598 | PRO |
| 1 | A | 784 | GLU |
| 1 | B | 295 | VAL |
| 1 | B | 373 | LYS |
| 1 | C | 578 | GLY |
| 1 | C | 608 | TRP |
| 2 | F | 49 | GLN |
| 1 | A | 358 | GLY |
| 1 | C | 537 | GLY |
| 1 | C | 598 | PRO |
| 1 | C | 694 | VAL |
| 1 | A | 534 | ILE |
| 1 | C | 520 | PRO |
| 1 | C | 657 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 433/455 (95%) | 394 (91%) | 39 (9%) | 12 | 49 |
| 1 | B | 414/455 (91%) | 351 (85%) | 63 (15%) | 3 | 24 |
| 1 | C | 448/455 (98%) | 405 (90%) | 43 (10%) | 10 | 45 |
| 2 | D | 121/127 (95%) | 113 (93%) | 8 (7%) | 21 | 63 |
| 2 | E | 121/127 (95%) | 112 (93%) | 9 (7%) | 17 | 57 |
| 2 | F | 121/127 (95%) | 111 (92%) | 10 (8%) | 14 | 52 |
| All | All | 1658/1746 (95%) | 1486 (90%) | 172 (10%) | 9 | 42 |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 322 | LEU |
| 1 | A | 323 | ASN |
| 1 | A | 329 | ARG |
| 1 | A | 376 | GLN |
| 1 | A | 384 | ASN |
| 1 | A | 407 | HIS |
| 1 | A | 423 | LYS |
| 1 | A | 438 | ASN |
| 1 | A | 445 | ARG |
| 1 | A | 455 | TYR |
| 1 | A | 469 | PHE |
| 1 | A | 471 | TRP |
| 1 | A | 485 | LEU |
| 1 | A | 540 | ARG |
| 1 | A | 549 | LEU |
| 1 | A | 557 | LEU |
| 1 | A | 559 | ARG |
| 1 | A | 567 | THR |
| 1 | A | 570 | THR |
| 1 | A | 574 | VAL |
| 1 | A | 620 | THR |
| 1 | A | 622 | LYS |
| 1 | A | 629 | ASN |
| 1 | A | 639 | ASN |
| 1 | A | 646 | THR |
| 1 | A | 656 | THR |
| 1 | A | 659 | THR |
| 1 | A | 666 | ASN |
| 1 | A | 670 | ILE |
| 1 | A | 701 | LEU |
| 1 | A | 709 | ASN |
| 1 | A | 737 | LYS |
| 1 | A | 739 | LYS |
| 1 | A | 759 | GLN |
| 1 | A | 775 | LEU |
| 1 | A | 780 | LEU |
| 1 | A | 781 | ASN |
| 1 | A | 782 | PHE |
| 1 | A | 784 | GLU |
| 1 | B | 305 | SER |
| 1 | B | 320 | ARG |
| 1 | B | 327 | LEU |
| 1 | B | 332 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 333 | LYS |
| 1 | B | 336 | THR |
| 1 | B | 355 | SER |
| 1 | B | 370 | LEU |
| 1 | B | 372 | LYS |
| 1 | B | 382 | LYS |
| 1 | B | 388 | LYS |
| 1 | B | 398 | ILE |
| 1 | B | 401 | ILE |
| 1 | B | 403 | LEU |
| 1 | B | 406 | ASP |
| 1 | B | 425 | GLU |
| 1 | B | 433 | TYR |
| 1 | B | 440 | GLN |
| 1 | B | 447 | SER |
| 1 | B | 455 | TYR |
| 1 | B | 458 | LYS |
| 1 | B | 462 | ILE |
| 1 | B | 463 | THR |
| 1 | B | 477 | MET |
| 1 | B | 480 | ASN |
| 1 | B | 485 | LEU |
| 1 | B | 493 | ASP |
| 1 | B | 501 | LEU |
| 1 | B | 503 | GLU |
| 1 | B | 524 | GLU |
| 1 | B | 531 | ASN |
| 1 | B | 535 | LYS |
| 1 | B | 539 | GLU |
| 1 | B | 540 | ARG |
| 1 | B | 541 | LYS |
| 1 | B | 544 | SER |
| 1 | B | 545 | THR |
| 1 | B | 549 | LEU |
| 1 | B | 552 | TRP |
| 1 | B | 562 | GLU |
| 1 | B | 576 | ASN |
| 1 | B | 577 | HIS |
| 1 | B | 590 | ASP |
| 1 | B | 595 | ILE |
| 1 | B | 611 | THR |
| 1 | B | 626 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 629 | ASN |
| 1 | B | 631 | SER |
| 1 | B | 639 | ASN |
| 1 | B | 646 | THR |
| 1 | B | 711 | ILE |
| 1 | B | 712 | PHE |
| 1 | B | 723 | PHE |
| 1 | B | 724 | ARG |
| 1 | B | 729 | TYR |
| 1 | B | 730 | ASN |
| 1 | B | 731 | GLU |
| 1 | B | 741 | ILE |
| 1 | B | 744 | GLU |
| 1 | B | 775 | LEU |
| 1 | B | 785 | ASN |
| 1 | B | 790 | PHE |
| 1 | B | 794 | GLN |
| 1 | C | 292 | ARG |
| 1 | C | 323 | ASN |
| 1 | C | 329 | ARG |
| 1 | C | 345 | THR |
| 1 | C | 376 | GLN |
| 1 | C | 384 | ASN |
| 1 | C | 401 | ILE |
| 1 | C | 406 | ASP |
| 1 | C | 407 | HIS |
| 1 | C | 423 | LYS |
| 1 | C | 438 | ASN |
| 1 | C | 455 | TYR |
| 1 | C | 469 | PHE |
| 1 | C | 485 | LEU |
| 1 | C | 509 | PRO |
| 1 | C | 510 | GLN |
| 1 | C | 511 | LYS |
| 1 | C | 523 | LEU |
| 1 | C | 526 | GLN |
| 1 | C | 540 | ARG |
| 1 | C | 549 | LEU |
| 1 | C | 557 | LEU |
| 1 | C | 559 | ARG |
| 1 | C | 567 | THR |
| 1 | C | 570 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 574 | VAL |
| 1 | C | 620 | THR |
| 1 | C | 622 | LYS |
| 1 | C | 629 | ASN |
| 1 | C | 639 | ASN |
| 1 | C | 646 | THR |
| 1 | C | 650 | THR |
| 1 | C | 656 | THR |
| 1 | C | 657 | ILE |
| 1 | C | 658 | PRO |
| 1 | C | 709 | ASN |
| 1 | C | 737 | LYS |
| 1 | C | 739 | LYS |
| 1 | C | 759 | GLN |
| 1 | C | 775 | LEU |
| 1 | C | 780 | LEU |
| 1 | C | 781 | ASN |
| 1 | C | 782 | PHE |
| 2 | D | 14 | GLU |
| 2 | D | 18 | LEU |
| 2 | D | 22 | ASP |
| 2 | D | 64 | ASP |
| 2 | D | 65 | PHE |
| 2 | D | 89 | PHE |
| 2 | D | 135 | GLN |
| 2 | D | 136 | VAL |
| 2 | E | 14 | GLU |
| 2 | E | 18 | LEU |
| 2 | E | 22 | ASP |
| 2 | E | 64 | ASP |
| 2 | E | 65 | PHE |
| 2 | E | 74 | ARG |
| 2 | E | 89 | PHE |
| 2 | E | 135 | GLN |
| 2 | E | 136 | VAL |
| 2 | F | 14 | GLU |
| 2 | F | 18 | LEU |
| 2 | F | 22 | ASP |
| 2 | F | 41 | GLN |
| 2 | F | 64 | ASP |
| 2 | F | 65 | PHE |
| 2 | F | 74 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 89 | PHE |
| 2 | F | 135 | GLN |
| 2 | F | 136 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 323 | ASN |
| 1 | A | 349 | ASN |
| 1 | A | 376 | GLN |
| 1 | A | 407 | HIS |
| 1 | A | 438 | ASN |
| 1 | A | 451 | ASN |
| 1 | A | 507 | GLN |
| 1 | A | 510 | GLN |
| 1 | A | 521 | ASN |
| 1 | A | 555 | GLN |
| 1 | A | 581 | GLN |
| 1 | A | 583 | ASN |
| 1 | A | 607 | ASN |
| 1 | A | 629 | ASN |
| 1 | A | 633 | ASN |
| 1 | A | 639 | ASN |
| 1 | A | 666 | ASN |
| 1 | A | 714 | GLN |
| 1 | A | 727 | GLN |
| 1 | A | 730 | ASN |
| 1 | A | 747 | ASN |
| 1 | A | 758 | ASN |
| 1 | A | 759 | GLN |
| 1 | A | 781 | ASN |
| 1 | B | 323 | ASN |
| 1 | B | 332 | ASN |
| 1 | B | 368 | GLN |
| 1 | B | 384 | ASN |
| 1 | B | 407 | HIS |
| 1 | B | 439 | ASN |
| 1 | B | 507 | GLN |
| 1 | B | 518 | ASN |
| 1 | B | 526 | GLN |
| 1 | B | 551 | ASN |
| 1 | B | 553 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 555 | GLN |
| 1 | B | 581 | GLN |
| 1 | B | 629 | ASN |
| 1 | B | 639 | ASN |
| 1 | B | 655 | ASN |
| 1 | B | 706 | ASN |
| 1 | B | 709 | ASN |
| 1 | B | 730 | ASN |
| 1 | B | 734 | ASN |
| 1 | B | 750 | GLN |
| 1 | B | 785 | ASN |
| 1 | C | 323 | ASN |
| 1 | C | 349 | ASN |
| 1 | C | 376 | GLN |
| 1 | C | 377 | GLN |
| 1 | C | 438 | ASN |
| 1 | C | 507 | GLN |
| 1 | C | 510 | GLN |
| 1 | C | 518 | ASN |
| 1 | C | 555 | GLN |
| 1 | C | 581 | GLN |
| 1 | C | 583 | ASN |
| 1 | C | 607 | ASN |
| 1 | C | 629 | ASN |
| 1 | C | 633 | ASN |
| 1 | C | 639 | ASN |
| 1 | C | 655 | ASN |
| 1 | C | 714 | GLN |
| 1 | C | 727 | GLN |
| 1 | C | 730 | ASN |
| 1 | C | 747 | ASN |
| 1 | C | 758 | ASN |
| 1 | C | 759 | GLN |
| 1 | C | 781 | ASN |
| 2 | D | 41 | GLN |
| 2 | D | 42 | ASN |
| 2 | E | 41 | GLN |
| 2 | F | 41 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 5 | DOT | A | 999 | 4 | 34,42,42 | 4.87 | 19 (55%) | 46,64,64 | 7.51 | 23 (50%) |
| 5 | DOT | C | 1999 | 4 | 34,42,42 | 4.85 | 19 (55%) | 46,64,64 | 7.49 | 24 (52%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 5 | DOT | A | 999 | 4 | - | 0/26/42/42 | 0/4/4/4 |
| 5 | DOT | C | 1999 | 4 | - | 0/26/42/42 | 0/4/4/4 |

All (38) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | A | 999 | DOT | C2B-C3B | -4.56 | 1.42 | 1.52 |
| 5 | C | 1999 | DOT | C2B-C3B | -4.51 | 1.42 | 1.52 |
| 5 | C | 1999 | DOT | PB-O1B | -2.41 | 1.42 | 1.51 |
| 5 | A | 999 | DOT | PB-O1B | -2.39 | 1.42 | 1.51 |
| 5 | C | 1999 | DOT | O1'-C' | 2.10 | 1.28 | 1.22 |
| 5 | A | 999 | DOT | O1'-C' | 2.11 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | A | 999 | DOT | C5B-C4B | 2.42 | 1.59 | 1.51 |
| 5 | C | 1999 | DOT | C5B-C4B | 2.43 | 1.59 | 1.51 |
| 5 | A | 999 | DOT | C1'-C' | 2.65 | 1.56 | 1.50 |
| 5 | C | 1999 | DOT | C1'-C' | 2.65 | 1.56 | 1.50 |
| 5 | A | 999 | DOT | C3B-C4B | 2.70 | 1.63 | 1.52 |
| 5 | C | 1999 | DOT | C3B-C4B | 2.72 | 1.63 | 1.52 |
| 5 | C | 1999 | DOT | O3'-C' | 3.01 | 1.41 | 1.34 |
| 5 | A | 999 | DOT | O3'-C' | 3.02 | 1.41 | 1.34 |
| 5 | C | 1999 | DOT | PA-O1A | 3.06 | 1.62 | 1.51 |
| 5 | A | 999 | DOT | PA-O1A | 3.07 | 1.62 | 1.51 |
| 5 | C | 1999 | DOT | C4'-C3' | 3.16 | 1.45 | 1.38 |
| 5 | A | 999 | DOT | C4'-C3' | 3.22 | 1.45 | 1.38 |
| 5 | C | 1999 | DOT | C2-N3 | 3.57 | 1.38 | 1.32 |
| 5 | A | 999 | DOT | C2-N3 | 3.57 | 1.38 | 1.32 |
| 5 | A | 999 | DOT | O3'-C3B | 3.89 | 1.53 | 1.46 |
| 5 | C | 1999 | DOT | O3'-C3B | 3.95 | 1.53 | 1.46 |
| 5 | C | 1999 | DOT | C5-C4 | 4.10 | 1.49 | 1.40 |
| 5 | A | 999 | DOT | C5-C4 | 4.16 | 1.49 | 1.40 |
| 5 | C | 1999 | DOT | C5'-C6' | 4.24 | 1.47 | 1.38 |
| 5 | A | 999 | DOT | C5'-C6' | 4.25 | 1.47 | 1.38 |
| 5 | A | 999 | DOT | C5'-C4' | 4.50 | 1.49 | 1.38 |
| 5 | C | 1999 | DOT | C5'-C4' | 4.50 | 1.49 | 1.38 |
| 5 | C | 1999 | DOT | C2-N1 | 4.89 | 1.43 | 1.33 |
| 5 | A | 999 | DOT | C2-N1 | 4.91 | 1.43 | 1.33 |
| 5 | C | 1999 | DOT | C6'-C1' | 6.12 | 1.50 | 1.39 |
| 5 | A | 999 | DOT | C6'-C1' | 6.13 | 1.50 | 1.39 |
| 5 | A | 999 | DOT | C8-N7 | 6.15 | 1.46 | 1.34 |
| 5 | C | 1999 | DOT | C8-N7 | 6.20 | 1.46 | 1.34 |
| 5 | C | 1999 | DOT | C3'-C2' | 13.71 | 1.74 | 1.40 |
| 5 | A | 999 | DOT | C3'-C2' | 13.72 | 1.74 | 1.40 |
| 5 | C | 1999 | DOT | C1'-C2' | 18.29 | 1.70 | 1.41 |
| 5 | A | 999 | DOT | C1'-C2' | 18.39 | 1.70 | 1.41 |

All (47) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | A | 999 | DOT | C1'-C2'-N2' | -25.44 | 90.26 | 122.74 |
| 5 | C | 1999 | DOT | C1'-C2'-N2' | -25.41 | 90.30 | 122.74 |
| 5 | A | 999 | DOT | C3'-C2'-C1' | -23.65 | 94.08 | 118.06 |
| 5 | C | 1999 | DOT | C3'-C2'-C1' | -23.60 | 94.13 | 118.06 |
| 5 | C | 1999 | DOT | C2'-C1'-C' | -11.80 | 104.95 | 120.92 |
| 5 | A | 999 | DOT | C2'-C1'-C' | -11.80 | 104.95 | 120.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | C | 1999 | DOT | O3'-C'-O1' | -10.10 | 106.63 | 123.53 |
| 5 | A | 999 | DOT | O3'-C'-O1' | -10.07 | 106.67 | 123.53 |
| 5 | C | 1999 | DOT | N6-C6-N1 | -7.03 | 104.11 | 119.20 |
| 5 | A | 999 | DOT | N6-C6-N1 | -6.98 | 104.23 | 119.20 |
| 5 | C | 1999 | DOT | C6'-C1'-C' | -4.37 | 109.69 | 118.68 |
| 5 | A | 999 | DOT | C6'-C1'-C' | -4.36 | 109.72 | 118.68 |
| 5 | A | 999 | DOT | O5'-PA-O1A | -3.45 | 96.21 | 109.62 |
| 5 | C | 1999 | DOT | O5'-PA-O1A | -3.45 | 96.23 | 109.62 |
| 5 | C | 1999 | DOT | O3G-PG-O3B | -2.78 | 92.50 | 105.09 |
| 5 | A | 999 | DOT | C4'-C5'-C6' | -2.22 | 116.94 | 120.19 |
| 5 | C | 1999 | DOT | C4'-C5'-C6' | -2.21 | 116.95 | 120.19 |
| 5 | A | 999 | DOT | C1B-N9-C4 | -2.08 | 123.64 | 127.16 |
| 5 | C | 1999 | DOT | C1B-N9-C4 | -2.06 | 123.67 | 127.16 |
| 5 | C | 1999 | DOT | N3-C2-N1 | 2.25 | 130.62 | 128.89 |
| 5 | C | 1999 | DOT | C5B-C4B-C3B | 2.33 | 120.10 | 114.46 |
| 5 | A | 999 | DOT | C5B-C4B-C3B | 2.35 | 120.14 | 114.46 |
| 5 | A | 999 | DOT | N3-C2-N1 | 2.39 | 130.72 | 128.89 |
| 5 | C | 1999 | DOT | C2B-C1B-N9 | 2.41 | 120.01 | 114.16 |
| 5 | A | 999 | DOT | O2A-PA-O1A | 2.75 | 127.44 | 112.53 |
| 5 | C | 1999 | DOT | O2A-PA-O1A | 2.75 | 127.44 | 112.53 |
| 5 | C | 1999 | DOT | O3A-PA-O5' | 3.22 | 111.48 | 102.94 |
| 5 | A | 999 | DOT | O3A-PA-O5' | 3.23 | 111.51 | 102.94 |
| 5 | A | 999 | DOT | C4-C5-N7 | 3.54 | 112.73 | 109.48 |
| 5 | A | 999 | DOT | C3B-C2B-C1B | 3.61 | 110.49 | 103.07 |
| 5 | C | 1999 | DOT | C4-C5-N7 | 3.62 | 112.81 | 109.48 |
| 5 | C | 1999 | DOT | C3B-C2B-C1B | 3.62 | 110.52 | 103.07 |
| 5 | C | 1999 | DOT | O3'-C3B-C2B | 3.94 | 118.43 | 109.07 |
| 5 | A | 999 | DOT | O3'-C3B-C2B | 3.95 | 118.44 | 109.07 |
| 5 | A | 999 | DOT | C2B-C1B-N9 | 4.18 | 124.32 | 114.16 |
| 5 | C | 1999 | DOT | O3'-C3B-C4B | 4.19 | 118.80 | 109.67 |
| 5 | A | 999 | DOT | O3'-C3B-C4B | 4.20 | 118.83 | 109.67 |
| 5 | C | 1999 | DOT | C3B-O3'-C' | 4.28 | 124.88 | 117.43 |
| 5 | A | 999 | DOT | C3B-O3'-C' | 4.29 | 124.89 | 117.43 |
| 5 | A | 999 | DOT | O3'-C'-C1' | 7.46 | 124.10 | 111.77 |
| 5 | C | 1999 | DOT | O3'-C'-C1' | 7.47 | 124.12 | 111.77 |
| 5 | C | 1999 | DOT | C4'-C3'-C2' | 8.61 | 134.50 | 121.01 |
| 5 | A | 999 | DOT | C4'-C3'-C2' | 8.63 | 134.54 | 121.01 |
| 5 | A | 999 | DOT | C6'-C1'-C2' | 10.76 | 131.61 | 119.01 |
| 5 | C | 1999 | DOT | C6'-C1'-C2' | 10.76 | 131.62 | 119.01 |
| 5 | C | 1999 | DOT | C3'-C2'-N2' | 25.79 | 171.90 | 120.15 |
| 5 | A | 999 | DOT | C3'-C2'-N2' | 25.80 | 171.91 | 120.15 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5 | A | 999 | DOT | 8 | 0 |
| 5 | C | 1999 | DOT | 5 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1 | A | 485/510 (95%) | -0.41 | 1 (0%) 95 92 | 14, 58, 137, 162 | 16 (3%) |
| 1 | B | 457/510 (89%) | -0.26 | 13 (2%) 56 42 | 13, 58, 158, 165 | 12 (2%) |
| 1 | C | 491/510 (96%) | -0.35 | 3 (0%) 90 83 | 13, 61, 137, 162 | 19 (3%) |
| 2 | D | 143/149 (95%) | 0.15 | 5 (3%) 48 34 | 49, 143, 180, 183 | 0 |
| 2 | E | 143/149 (95%) | 0.19 | 10 (6%) 19 13 | 48, 144, 180, 182 | 0 |
| 2 | F | 143/149 (95%) | 0.19 | 9 (6%) 23 15 | 49, 143, 180, 183 | 0 |
| All | All | 1862/1977 (94%) | -0.22 | 41 (2%) 65 50 | 13, 66, 166, 183 | 47 (2%) |

All (41) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 697 | ILE | 5.3 |
| 2 | F | 62 | THR | 4.1 |
| 2 | E | 79 | THR | 3.5 |
| 2 | E | 19 | PHE | 3.4 |
| 2 | E | 21 | LYS | 3.3 |
| 2 | F | 46 | ALA | 3.2 |
| 1 | B | 778 | LYS | 3.2 |
| 2 | E | 62 | THR | 3.2 |
| 1 | C | 744 | GLU | 3.1 |
| 1 | B | 702 | SER | 3.0 |
| 2 | E | 61 | GLY | 2.9 |
| 2 | D | 58 | ASP | 2.8 |
| 1 | C | 708 | ALA | 2.7 |
| 1 | B | 741 | ILE | 2.7 |
| 2 | E | 60 | ASN | 2.6 |
| 1 | B | 740 | GLN | 2.6 |
| 2 | F | 61 | GLY | 2.6 |
| 2 | E | 55 | VAL | 2.6 |
| 2 | F | 53 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 741 | ILE | 2.5 |
| 1 | B | 658 | PRO | 2.5 |
| 1 | B | 776 | LEU | 2.5 |
| 2 | F | 50 | ASP | 2.5 |
| 2 | F | 19 | PHE | 2.5 |
| 2 | F | 28 | THR | 2.5 |
| 2 | E | 23 | GLY | 2.4 |
| 2 | D | 43 | PRO | 2.3 |
| 2 | E | 59 | GLY | 2.3 |
| 1 | B | 774 | LYS | 2.2 |
| 1 | B | 783 | THR | 2.2 |
| 2 | D | 49 | GLN | 2.2 |
| 2 | F | 44 | THR | 2.2 |
| 1 | B | 779 | GLN | 2.1 |
| 2 | E | 42 | ASN | 2.1 |
| 1 | B | 773 | PHE | 2.1 |
| 2 | D | 53 | ASN | 2.1 |
| 1 | B | 737 | LYS | 2.1 |
| 2 | D | 30 | LYS | 2.0 |
| 1 | A | 296 | LEU | 2.0 |
| 2 | F | 29 | THR | 2.0 |
| 1 | B | 521 | ASN | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 5 | DOT | A | 999 | 39/39 | 0.87 | 0.29 | 1.51 | 52,80,92,92 | 0 |
| 5 | DOT | C | 1999 | 39/39 | 0.88 | 0.26 | 0.70 | 45,80,83,84 | 0 |
| 3 | CA | F | 805 | 1/1 | 0.86 | 0.12 | -1.59 | 82,82,82,82 | 0 |
| 3 | CA | F | 804 | 1/1 | 0.88 | 0.14 | -1.62 | 70,70,70,70 | 0 |
| 3 | CA | E | 803 | 1/1 | 0.99 | 0.06 | -1.71 | 70,70,70,70 | 0 |
| 3 | CA | D | 801 | 1/1 | 0.98 | 0.04 | -1.90 | 51,51,51,51 | 0 |
| 3 | CA | D | 800 | 1/1 | 0.94 | 0.11 | -2.36 | 65,65,65,65 | 0 |
| 3 | CA | E | 802 | 1/1 | 0.86 | 0.04 | -2.93 | 75,75,75,75 | 0 |
| 4 | YB | B | 902 | 1/1 | 0.98 | 0.09 | - | 142,142,142,142 | 0 |
| 4 | YB | C | 903 | 1/1 | 0.96 | 0.04 | - | 124,124,124,124 | 0 |
| 4 | YB | A | 901 | 1/1 | 0.87 | 0.08 | - | 135,135,135,135 | 0 |

6.5 Other polymers

There are no such residues in this entry.