



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:50 PM GMT

PDB ID : 2B76
Title : E. coli Quinol fumarate reductase FrdA E49Q mutation
Authors : Maklashina, E.; Iverson, T.M.; Sher, Y.; Kotlyar, V.; Mirza, O.; Andrell, J.;
Hudson, J.M.; Armstrong, F.A.; Cecchini, G.
Deposited on : 2005-10-03
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

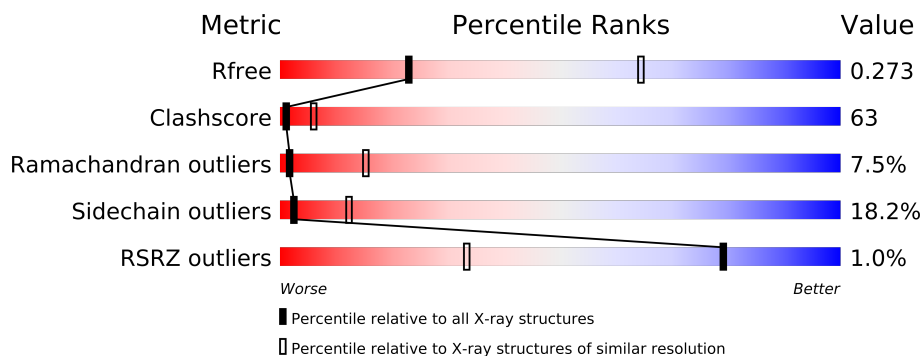
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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} | 66092 | 1341 (3.40-3.20) |
| Clashscore | 79885 | 1696 (3.40-3.20) |
| Ramachandran outliers | 78287 | 1664 (3.40-3.20) |
| Sidechain outliers | 78261 | 1662 (3.40-3.20) |
| RSRZ outliers | 66119 | 1342 (3.40-3.20) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 602 | |
| 1 | M | 602 | |
| 2 | B | 243 | |
| 2 | N | 243 | |
| 3 | C | 130 | |
| 3 | O | 130 | |
| 4 | D | 119 | |
| 4 | P | 119 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 10 | MQ7 | D | 700 | - | X |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 10 | MQ7 | P | 800 | - | X |
| 5 | FLC | A | 702 | - | X |
| 8 | SF4 | B | 246 | - | X |

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16840 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fumarate reductase flavoprotein subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 577 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4448 | 2775 | 803 | 839 | 31 | | | |
| 1 | M | 572 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4414 | 2752 | 798 | 833 | 31 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|-----------|
| A | 49 | GLN | GLU | ENGINEERED | GB P00363 |
| M | 49 | GLN | GLU | ENGINEERED | GB P00363 |

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1888 | 1189 | 323 | 357 | 19 | | | |
| 2 | N | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1888 | 1189 | 323 | 357 | 19 | | | |

- Molecule 3 is a protein called Fumarate reductase subunit C.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | C | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1058 | 720 | 166 | 169 | 3 | | | |
| 3 | O | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1058 | 720 | 166 | 169 | 3 | | | |

- Molecule 4 is a protein called Fumarate reductase subunit D.

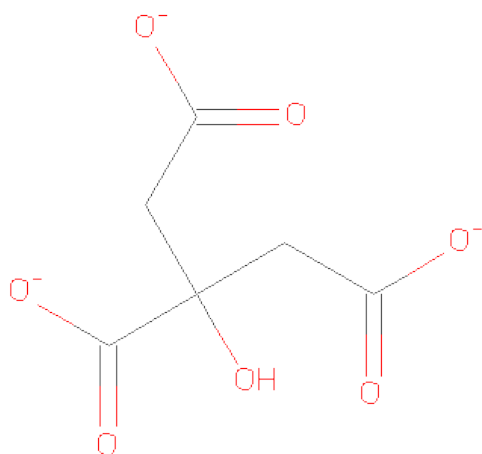
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 626 | 151 | 142 | 7 | | | |

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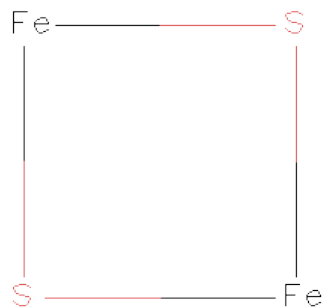
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | P | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 626 | 151 | 142 | 7 | | | |

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



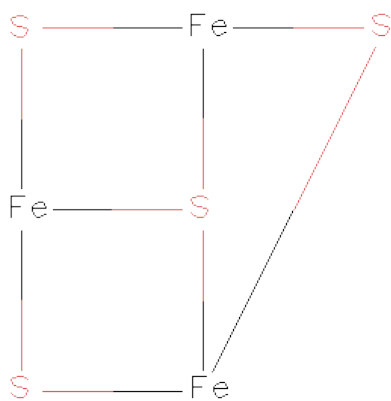
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | A | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 6 | 7 | | |
| 5 | M | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 6 | 7 | | |

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



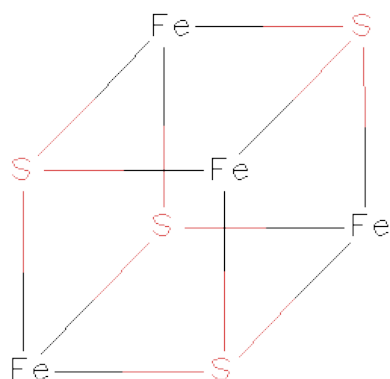
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 6 | N | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



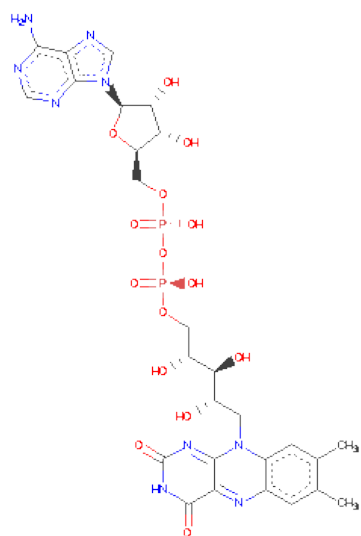
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 7 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 7 | 3 | 4 | | |
| 7 | N | 1 | Total | Fe | S | 0 | 0 |
| | | | 7 | 3 | 4 | | |

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



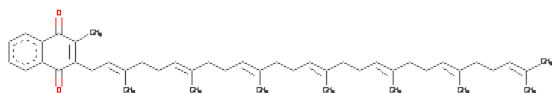
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 8 | N | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 9 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 27 | 9 | 14 | 2 | | |
| 9 | M | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 27 | 9 | 14 | 2 | | |

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).



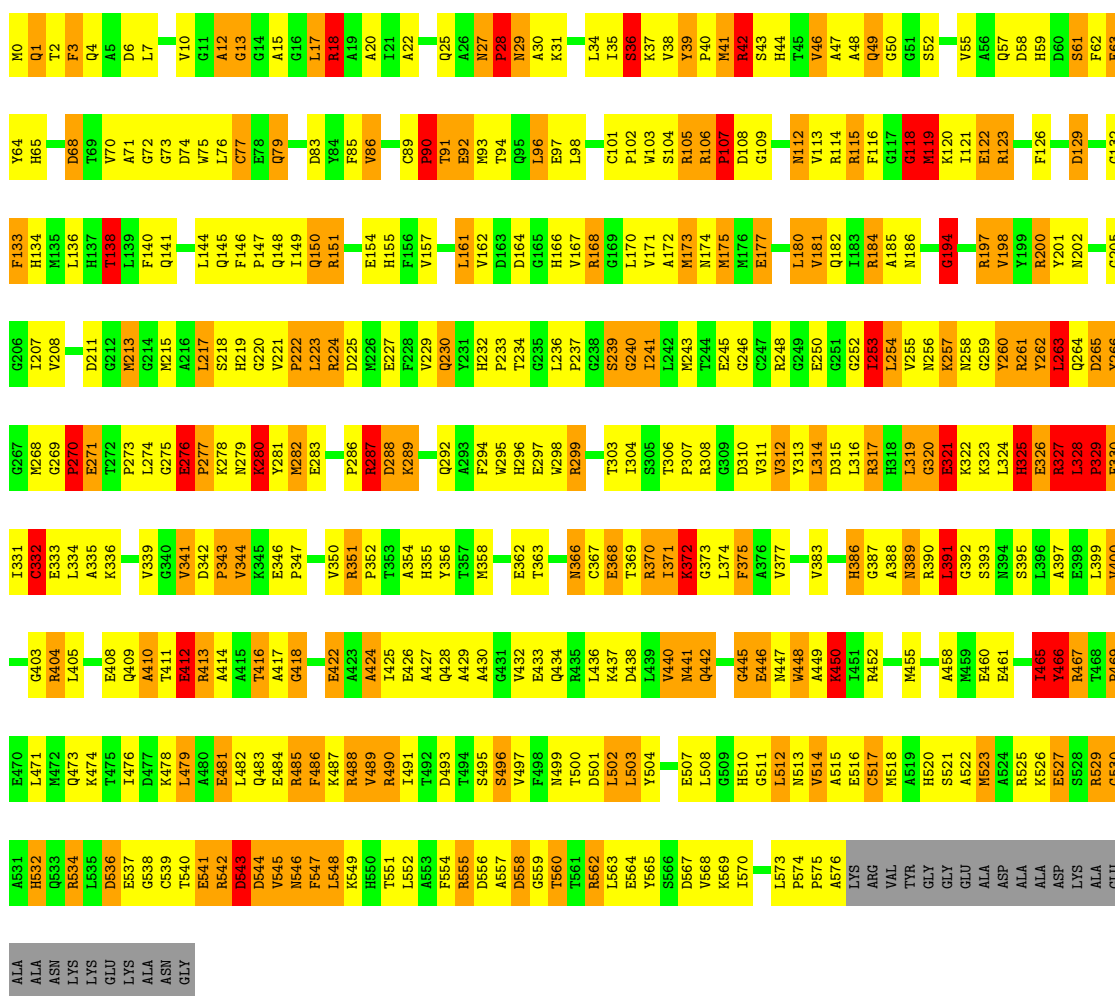
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10 | D | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |
| 10 | P | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |

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: Fumarate reductase flavoprotein subunit

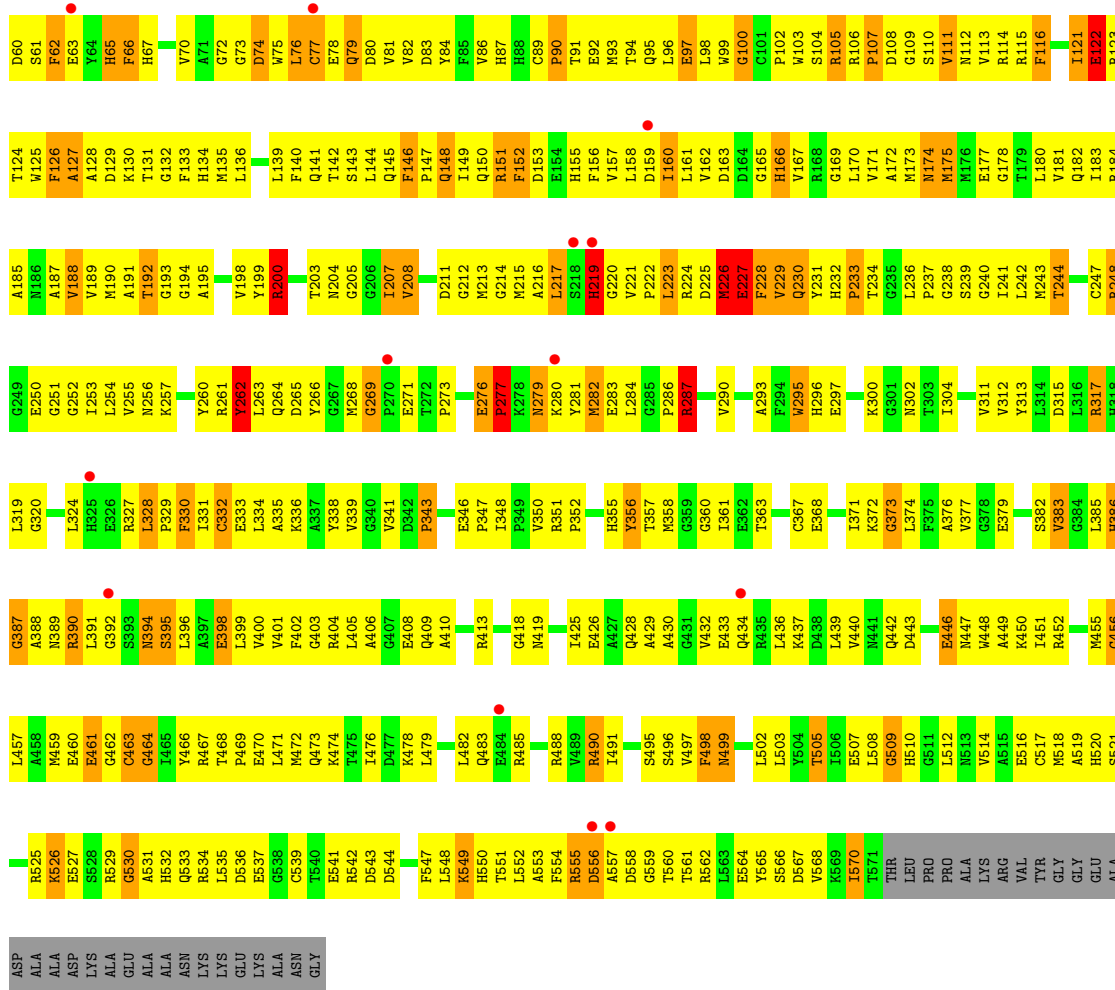
Chain A: 



- Molecule 1: Fumarate reductase flavoprotein subunit

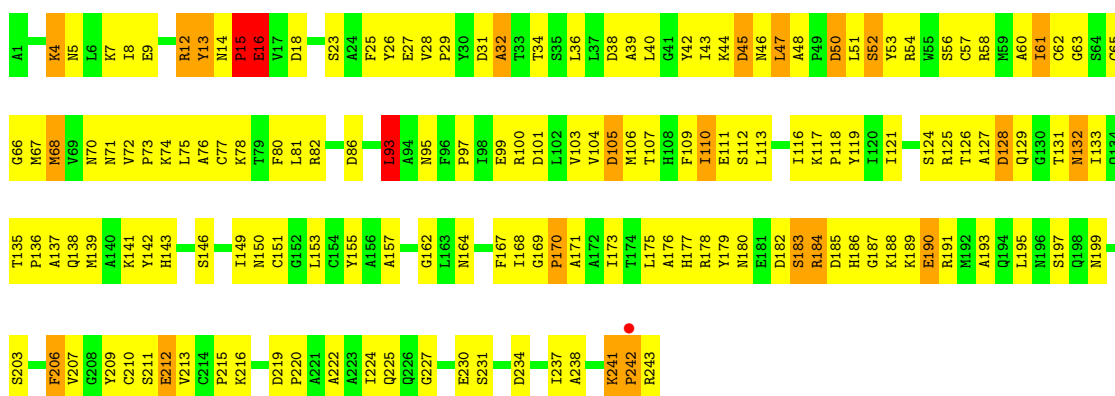
Chain M: 





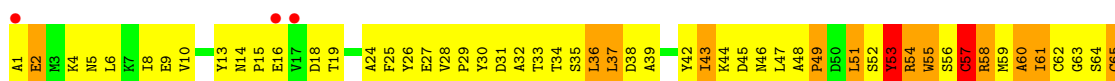
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain B:



• Molecule 2: Fumarate reductase iron-sulfur protein

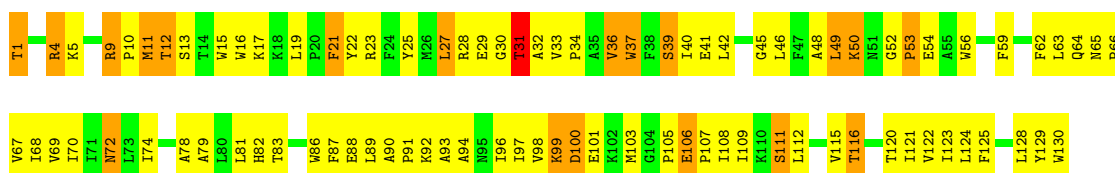
Chain N:





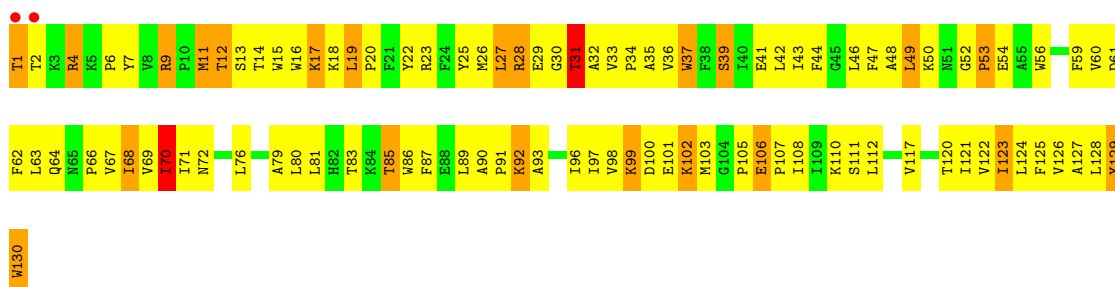
• Molecule 3: Fumarate reductase subunit C

Chain C:



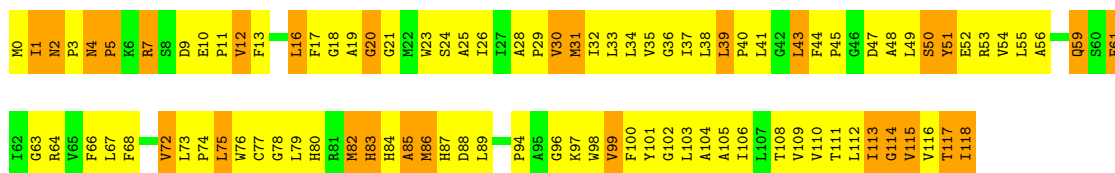
• Molecule 3: Fumarate reductase subunit C

Chain O:



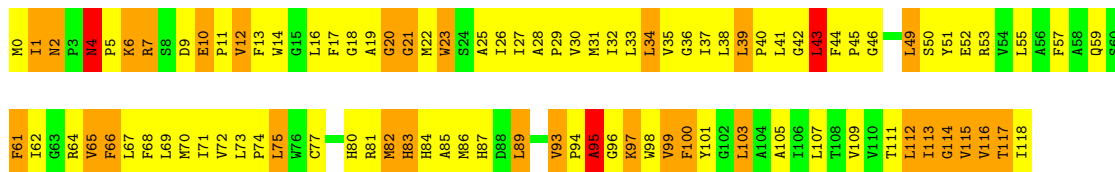
• Molecule 4: Fumarate reductase subunit D

Chain D:



• Molecule 4: Fumarate reductase subunit D

Chain P:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 96.80Å 139.53Å 273.97Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.30 39.53 – 3.30 | Depositor EDS |
| % Data completeness (in resolution range) | 83.5 (20.00-3.30) 83.4 (39.53-3.30) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 5.12 (at 3.32Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.248 , 0.284 0.243 , 0.273 | Depositor DCC |
| R_{free} test set | 923 reflections (1.99%) | DCC |
| Wilson B-factor (Å ²) | 60.4 | Xtriage |
| Anisotropy | 0.046 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 19.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 0 of 56072 reflections | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 16840 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, FES, MQ7, FLC, FAD

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 | 1.71 | 79/4540 (1.7%) | 1.81 | 109/6139 (1.8%) |
| 1 | M | 0.36 | 0/4504 | 0.71 | 0/6087 |
| 2 | B | 1.01 | 2/1931 (0.1%) | 1.15 | 8/2617 (0.3%) |
| 2 | N | 0.41 | 0/1931 | 0.71 | 0/2617 |
| 3 | C | 0.98 | 0/1094 | 1.12 | 6/1496 (0.4%) |
| 3 | O | 0.92 | 1/1094 (0.1%) | 1.11 | 5/1496 (0.3%) |
| 4 | D | 0.77 | 0/956 | 1.03 | 1/1303 (0.1%) |
| 4 | P | 0.70 | 1/956 (0.1%) | 1.06 | 3/1303 (0.2%) |
| All | All | 1.06 | 83/17006 (0.5%) | 1.22 | 132/23058 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 4 |
| 2 | B | 0 | 3 |
| 3 | O | 0 | 1 |
| All | All | 0 | 8 |

All (83) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 450 | LYS | CD-CE | 10.77 | 1.78 | 1.51 |
| 1 | A | 372 | LYS | CB-CG | 9.71 | 1.78 | 1.52 |
| 1 | A | 277 | PRO | CA-C | 9.18 | 1.71 | 1.52 |
| 1 | A | 484 | GLU | CG-CD | 8.83 | 1.65 | 1.51 |
| 1 | A | 240 | GLY | C-O | -8.45 | 1.10 | 1.23 |
| 1 | A | 129 | ASP | CB-CG | 8.43 | 1.69 | 1.51 |
| 1 | A | 576 | ALA | CA-CB | 8.32 | 1.70 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 517 | CYS | CB-SG | -8.04 | 1.68 | 1.82 |
| 1 | A | 352 | PRO | CA-C | 8.02 | 1.68 | 1.52 |
| 1 | A | 269 | GLY | N-CA | -7.89 | 1.34 | 1.46 |
| 1 | A | 270 | PRO | CA-C | 7.79 | 1.68 | 1.52 |
| 1 | A | 63 | GLU | C-O | -7.52 | 1.09 | 1.23 |
| 1 | A | 220 | GLY | C-O | -7.09 | 1.12 | 1.23 |
| 1 | A | 543 | ASP | CA-CB | 6.98 | 1.69 | 1.53 |
| 1 | A | 90 | PRO | CA-CB | -6.80 | 1.40 | 1.53 |
| 1 | A | 333 | GLU | CG-CD | 6.76 | 1.62 | 1.51 |
| 1 | A | 22 | ALA | CA-CB | -6.76 | 1.38 | 1.52 |
| 1 | A | 77 | CYS | CB-SG | -6.73 | 1.70 | 1.82 |
| 1 | A | 85 | PHE | CE2-CZ | -6.66 | 1.24 | 1.37 |
| 3 | O | 1 | THR | C-O | 6.66 | 1.35 | 1.23 |
| 1 | A | 221 | VAL | CA-CB | -6.64 | 1.40 | 1.54 |
| 1 | A | 424 | ALA | CA-CB | 6.58 | 1.66 | 1.52 |
| 1 | A | 287 | ARG | C-O | -6.57 | 1.10 | 1.23 |
| 1 | A | 36 | SER | CA-CB | -6.57 | 1.43 | 1.52 |
| 1 | A | 469 | PRO | CA-C | -6.56 | 1.39 | 1.52 |
| 1 | A | 113 | VAL | CB-CG1 | -6.51 | 1.39 | 1.52 |
| 1 | A | 465 | ILE | CA-CB | -6.51 | 1.39 | 1.54 |
| 1 | A | 276 | GLU | N-CA | -6.35 | 1.33 | 1.46 |
| 1 | A | 64 | TYR | CD2-CE2 | 6.32 | 1.48 | 1.39 |
| 1 | A | 145 | GLN | C-O | -6.31 | 1.11 | 1.23 |
| 1 | A | 172 | ALA | CA-CB | -6.25 | 1.39 | 1.52 |
| 1 | A | 372 | LYS | CG-CD | 6.24 | 1.73 | 1.52 |
| 1 | A | 177 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | A | 229 | VAL | C-O | -6.21 | 1.11 | 1.23 |
| 1 | A | 276 | GLU | CA-CB | 6.19 | 1.67 | 1.53 |
| 1 | A | 372 | LYS | CD-CE | 6.19 | 1.66 | 1.51 |
| 2 | B | 56 | SER | C-O | -6.15 | 1.11 | 1.23 |
| 1 | A | 327 | ARG | CG-CD | 6.07 | 1.67 | 1.51 |
| 1 | A | 330 | PHE | CB-CG | 6.01 | 1.61 | 1.51 |
| 1 | A | 90 | PRO | N-CD | -6.00 | 1.39 | 1.47 |
| 1 | A | 119 | MET | CA-C | 5.96 | 1.68 | 1.52 |
| 1 | A | 386 | HIS | C-O | -5.89 | 1.12 | 1.23 |
| 2 | B | 207 | VAL | CA-CB | -5.89 | 1.42 | 1.54 |
| 1 | A | 574 | PRO | CA-CB | -5.88 | 1.41 | 1.53 |
| 1 | A | 138 | THR | CA-CB | 5.85 | 1.68 | 1.53 |
| 1 | A | 90 | PRO | CA-C | -5.81 | 1.41 | 1.52 |
| 1 | A | 312 | VAL | CA-CB | -5.77 | 1.42 | 1.54 |
| 1 | A | 28 | PRO | CA-C | -5.75 | 1.41 | 1.52 |
| 1 | A | 460 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 522 | ALA | CA-CB | 5.73 | 1.64 | 1.52 |
| 1 | A | 61 | SER | CA-CB | -5.72 | 1.44 | 1.52 |
| 1 | A | 371 | ILE | CA-CB | 5.63 | 1.67 | 1.54 |
| 1 | A | 410 | ALA | C-O | -5.63 | 1.12 | 1.23 |
| 1 | A | 481 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | A | 198 | VAL | CB-CG2 | -5.50 | 1.41 | 1.52 |
| 1 | A | 328 | LEU | N-CA | 5.48 | 1.57 | 1.46 |
| 1 | A | 486 | PHE | CE2-CZ | 5.47 | 1.47 | 1.37 |
| 4 | P | 95 | ALA | CA-CB | -5.43 | 1.41 | 1.52 |
| 1 | A | 157 | VAL | CB-CG1 | -5.38 | 1.41 | 1.52 |
| 1 | A | 514 | VAL | CA-CB | -5.38 | 1.43 | 1.54 |
| 1 | A | 375 | PHE | CE1-CZ | 5.34 | 1.47 | 1.37 |
| 1 | A | 450 | LYS | CE-NZ | 5.33 | 1.62 | 1.49 |
| 1 | A | 549 | LYS | CG-CD | 5.32 | 1.70 | 1.52 |
| 1 | A | 46 | VAL | CB-CG1 | -5.31 | 1.41 | 1.52 |
| 1 | A | 28 | PRO | N-CA | -5.26 | 1.38 | 1.47 |
| 1 | A | 400 | VAL | CA-CB | -5.26 | 1.43 | 1.54 |
| 1 | A | 473 | GLN | CB-CG | -5.23 | 1.38 | 1.52 |
| 1 | A | 253 | ILE | CA-CB | 5.20 | 1.66 | 1.54 |
| 1 | A | 368 | GLU | CA-CB | -5.16 | 1.42 | 1.53 |
| 1 | A | 270 | PRO | N-CD | 5.13 | 1.55 | 1.47 |
| 1 | A | 146 | PHE | CE1-CZ | 5.13 | 1.47 | 1.37 |
| 1 | A | 461 | GLU | CA-CB | 5.12 | 1.65 | 1.53 |
| 1 | A | 547 | PHE | CE2-CZ | -5.12 | 1.27 | 1.37 |
| 1 | A | 173 | MET | SD-CE | 5.10 | 2.06 | 1.77 |
| 1 | A | 35 | ILE | C-O | -5.09 | 1.13 | 1.23 |
| 1 | A | 460 | GLU | CD-OE1 | 5.07 | 1.31 | 1.25 |
| 1 | A | 10 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 1 | A | 474 | LYS | CD-CE | 5.06 | 1.64 | 1.51 |
| 1 | A | 136 | LEU | C-O | -5.05 | 1.13 | 1.23 |
| 1 | A | 391 | LEU | CA-CB | -5.03 | 1.42 | 1.53 |
| 1 | A | 64 | TYR | CZ-OH | 5.03 | 1.46 | 1.37 |
| 1 | A | 3 | PHE | CD2-CE2 | 5.01 | 1.49 | 1.39 |
| 1 | A | 213 | MET | CG-SD | 5.01 | 1.94 | 1.81 |

All (132) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 269 | GLY | C-N-CD | -13.40 | 91.12 | 120.60 |
| 1 | A | 370 | ARG | NE-CZ-NH1 | -13.35 | 113.63 | 120.30 |
| 1 | A | 68 | ASP | CB-CG-OD1 | -10.64 | 108.72 | 118.30 |
| 1 | A | 68 | ASP | CB-CG-OD2 | 10.35 | 127.61 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 501 | ASP | CB-CG-OD2 | 10.22 | 127.50 | 118.30 |
| 1 | A | 164 | ASP | CB-CG-OD2 | 9.37 | 126.73 | 118.30 |
| 1 | A | 161 | LEU | CA-CB-CG | -8.92 | 94.78 | 115.30 |
| 1 | A | 269 | GLY | CA-C-N | -8.85 | 92.31 | 117.10 |
| 1 | A | 501 | ASP | CB-CG-OD1 | -8.76 | 110.42 | 118.30 |
| 1 | A | 200 | ARG | NE-CZ-NH2 | -8.57 | 116.01 | 120.30 |
| 1 | A | 467 | ARG | NE-CZ-NH1 | -8.56 | 116.02 | 120.30 |
| 1 | A | 269 | GLY | O-C-N | 8.51 | 137.26 | 121.10 |
| 2 | B | 13 | TYR | CB-CG-CD1 | -8.50 | 115.90 | 121.00 |
| 1 | A | 325 | HIS | C-N-CA | -8.45 | 100.58 | 121.70 |
| 1 | A | 269 | GLY | N-CA-C | 8.29 | 133.82 | 113.10 |
| 1 | A | 266 | TYR | N-CA-CB | -8.14 | 95.94 | 110.60 |
| 1 | A | 18 | ARG | CG-CD-NE | -8.10 | 94.79 | 111.80 |
| 1 | A | 42 | ARG | NE-CZ-NH1 | 8.08 | 124.34 | 120.30 |
| 1 | A | 151 | ARG | NE-CZ-NH1 | -7.91 | 116.35 | 120.30 |
| 1 | A | 120 | LYS | CA-CB-CG | 7.80 | 130.57 | 113.40 |
| 1 | A | 351 | ARG | NE-CZ-NH1 | 7.67 | 124.14 | 120.30 |
| 1 | A | 563 | LEU | CB-CG-CD1 | -7.63 | 98.04 | 111.00 |
| 1 | A | 164 | ASP | CB-CG-OD1 | -7.47 | 111.57 | 118.30 |
| 1 | A | 391 | LEU | CB-CG-CD1 | -7.47 | 98.31 | 111.00 |
| 1 | A | 391 | LEU | CB-CA-C | -7.42 | 96.11 | 110.20 |
| 1 | A | 277 | PRO | N-CA-C | -7.39 | 92.88 | 112.10 |
| 1 | A | 248 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | A | 42 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | A | 545 | VAL | CB-CA-C | -7.28 | 97.57 | 111.40 |
| 3 | C | 99 | LYS | N-CA-C | -7.20 | 91.55 | 111.00 |
| 1 | A | 225 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | A | 488 | ARG | NE-CZ-NH2 | -7.14 | 116.73 | 120.30 |
| 1 | A | 106 | ARG | NE-CZ-NH2 | -6.77 | 116.92 | 120.30 |
| 1 | A | 321 | GLU | N-CA-C | 6.66 | 128.98 | 111.00 |
| 1 | A | 276 | GLU | CB-CA-C | -6.64 | 97.12 | 110.40 |
| 1 | A | 544 | ASP | N-CA-CB | 6.62 | 122.52 | 110.60 |
| 1 | A | 372 | LYS | CB-CG-CD | 6.61 | 128.79 | 111.60 |
| 1 | A | 460 | GLU | OE1-CD-OE2 | 6.59 | 131.21 | 123.30 |
| 1 | A | 106 | ARG | CB-CA-C | -6.58 | 97.24 | 110.40 |
| 1 | A | 544 | ASP | CB-CG-OD2 | 6.55 | 124.19 | 118.30 |
| 1 | A | 479 | LEU | CB-CG-CD2 | -6.54 | 99.88 | 111.00 |
| 1 | A | 270 | PRO | N-CA-C | -6.53 | 95.12 | 112.10 |
| 1 | A | 466 | TYR | CB-CG-CD2 | -6.51 | 117.09 | 121.00 |
| 1 | A | 270 | PRO | CB-CA-C | 6.51 | 128.27 | 112.00 |
| 1 | A | 194 | GLY | N-CA-C | 6.50 | 129.35 | 113.10 |
| 1 | A | 485 | ARG | NE-CZ-NH1 | -6.46 | 117.07 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | P | 39 | LEU | CA-CB-CG | -6.45 | 100.46 | 115.30 |
| 1 | A | 418 | GLY | N-CA-C | -6.44 | 97.00 | 113.10 |
| 1 | A | 270 | PRO | CA-C-N | 6.34 | 131.15 | 117.20 |
| 1 | A | 136 | LEU | CA-CB-CG | -6.31 | 100.80 | 115.30 |
| 1 | A | 229 | VAL | O-C-N | -6.28 | 112.65 | 122.70 |
| 1 | A | 327 | ARG | NE-CZ-NH1 | 6.26 | 123.43 | 120.30 |
| 1 | A | 543 | ASP | CB-CG-OD2 | 6.23 | 123.91 | 118.30 |
| 1 | A | 517 | CYS | CB-CA-C | 6.22 | 122.84 | 110.40 |
| 1 | A | 118 | GLY | O-C-N | -6.15 | 112.86 | 122.70 |
| 1 | A | 448 | TRP | CB-CA-C | -6.10 | 98.21 | 110.40 |
| 2 | B | 13 | TYR | CB-CA-C | -6.07 | 98.27 | 110.40 |
| 1 | A | 64 | TYR | CB-CG-CD2 | 6.04 | 124.62 | 121.00 |
| 1 | A | 223 | LEU | N-CA-C | -5.97 | 94.87 | 111.00 |
| 1 | A | 549 | LYS | CD-CE-NZ | 5.96 | 125.40 | 111.70 |
| 1 | A | 517 | CYS | N-CA-CB | -5.95 | 99.89 | 110.60 |
| 1 | A | 446 | GLU | C-N-CA | -5.94 | 106.85 | 121.70 |
| 1 | A | 445 | GLY | N-CA-C | 5.89 | 127.83 | 113.10 |
| 1 | A | 556 | ASP | O-C-N | -5.89 | 113.27 | 122.70 |
| 1 | A | 61 | SER | CB-CA-C | -5.88 | 98.92 | 110.10 |
| 3 | C | 100 | ASP | CB-CG-OD2 | 5.88 | 123.59 | 118.30 |
| 1 | A | 556 | ASP | CA-C-N | 5.87 | 130.11 | 117.20 |
| 1 | A | 28 | PRO | C-N-CA | -5.86 | 107.05 | 121.70 |
| 3 | O | 70 | ILE | N-CA-C | -5.86 | 95.18 | 111.00 |
| 3 | C | 27 | LEU | CA-CB-CG | -5.78 | 102.00 | 115.30 |
| 1 | A | 412 | GLU | CG-CD-OE2 | -5.75 | 106.80 | 118.30 |
| 1 | A | 13 | GLY | N-CA-C | -5.75 | 98.73 | 113.10 |
| 1 | A | 263 | LEU | CB-CG-CD1 | -5.74 | 101.24 | 111.00 |
| 1 | A | 366 | ASN | CB-CA-C | -5.74 | 98.92 | 110.40 |
| 2 | B | 13 | TYR | CB-CG-CD2 | 5.73 | 124.44 | 121.00 |
| 1 | A | 105 | ARG | NE-CZ-NH2 | -5.71 | 117.45 | 120.30 |
| 1 | A | 332 | CYS | CA-CB-SG | 5.68 | 124.22 | 114.00 |
| 1 | A | 502 | LEU | CB-CG-CD2 | -5.64 | 101.40 | 111.00 |
| 3 | C | 1 | THR | C-N-CA | -5.64 | 107.60 | 121.70 |
| 2 | B | 93 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 1 | A | 262 | TYR | N-CA-C | 5.61 | 126.14 | 111.00 |
| 1 | A | 254 | LEU | CA-CB-CG | 5.60 | 128.18 | 115.30 |
| 2 | B | 13 | TYR | CA-CB-CG | -5.59 | 102.78 | 113.40 |
| 1 | A | 265 | ASP | CB-CA-C | -5.58 | 99.24 | 110.40 |
| 1 | A | 479 | LEU | CA-CB-CG | -5.56 | 102.52 | 115.30 |
| 1 | A | 248 | ARG | CG-CD-NE | -5.55 | 100.15 | 111.80 |
| 1 | A | 326 | GLU | CA-C-N | -5.54 | 105.00 | 117.20 |
| 1 | A | 312 | VAL | N-CA-C | -5.52 | 96.09 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 83 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 1 | A | 39 | TYR | CB-CG-CD1 | -5.47 | 117.72 | 121.00 |
| 1 | A | 412 | GLU | OE1-CD-OE2 | 5.46 | 129.85 | 123.30 |
| 1 | A | 269 | GLY | CA-C-O | 5.45 | 130.41 | 120.60 |
| 1 | A | 448 | TRP | N-CA-CB | 5.45 | 120.41 | 110.60 |
| 1 | A | 466 | TYR | CB-CG-CD1 | 5.45 | 124.27 | 121.00 |
| 1 | A | 185 | ALA | N-CA-CB | 5.43 | 117.70 | 110.10 |
| 1 | A | 503 | LEU | CB-CG-CD2 | -5.43 | 101.77 | 111.00 |
| 1 | A | 277 | PRO | CA-N-CD | -5.41 | 103.93 | 111.50 |
| 3 | O | 63 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 1 | A | 330 | PHE | CB-CA-C | 5.37 | 121.15 | 110.40 |
| 1 | A | 465 | ILE | CB-CA-C | -5.37 | 100.85 | 111.60 |
| 1 | A | 233 | PRO | N-CD-CG | -5.37 | 95.15 | 103.20 |
| 1 | A | 1 | GLN | N-CA-C | -5.35 | 96.55 | 111.00 |
| 1 | A | 177 | GLU | OE1-CD-OE2 | 5.35 | 129.72 | 123.30 |
| 1 | A | 486 | PHE | N-CA-CB | -5.33 | 101.00 | 110.60 |
| 3 | C | 130 | TRP | N-CA-C | 5.30 | 125.32 | 111.00 |
| 2 | B | 16 | GLU | CA-CB-CG | 5.29 | 125.05 | 113.40 |
| 3 | C | 4 | ARG | NE-CZ-NH2 | 5.29 | 122.94 | 120.30 |
| 1 | A | 123 | ARG | NE-CZ-NH1 | -5.29 | 117.66 | 120.30 |
| 2 | B | 15 | PRO | C-N-CA | -5.29 | 108.49 | 121.70 |
| 1 | A | 68 | ASP | CB-CA-C | -5.27 | 99.86 | 110.40 |
| 1 | A | 488 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 3 | O | 99 | LYS | N-CA-C | -5.24 | 96.84 | 111.00 |
| 1 | A | 311 | VAL | CB-CA-C | -5.22 | 101.48 | 111.40 |
| 1 | A | 538 | GLY | C-N-CA | -5.22 | 108.66 | 121.70 |
| 2 | B | 13 | TYR | C-N-CA | -5.21 | 108.66 | 121.70 |
| 3 | O | 28 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 4 | P | 49 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 4 | P | 4 | ASN | N-CA-C | -5.19 | 97.00 | 111.00 |
| 1 | A | 329 | PRO | N-CA-C | 5.17 | 125.55 | 112.10 |
| 1 | A | 106 | ARG | NE-CZ-NH1 | 5.15 | 122.87 | 120.30 |
| 1 | A | 274 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 1 | A | 548 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 1 | A | 239 | SER | CB-CA-C | -5.11 | 100.38 | 110.10 |
| 4 | D | 39 | LEU | C-N-CD | 5.11 | 139.13 | 128.40 |
| 3 | O | 27 | LEU | CA-CB-CG | -5.10 | 103.57 | 115.30 |
| 1 | A | 12 | ALA | N-CA-C | 5.06 | 124.66 | 111.00 |
| 1 | A | 496 | SER | N-CA-CB | -5.06 | 102.92 | 110.50 |
| 1 | A | 180 | LEU | CB-CA-C | -5.05 | 100.60 | 110.20 |
| 1 | A | 112 | ASN | CB-CA-C | -5.05 | 100.31 | 110.40 |
| 1 | A | 280 | LYS | CD-CE-NZ | 5.04 | 123.28 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 150 | GLN | N-CA-CB | -5.03 | 101.54 | 110.60 |
| 1 | A | 555 | ARG | C-N-CA | -5.02 | 109.14 | 121.70 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 118 | GLY | Mainchain |
| 1 | A | 276 | GLU | Mainchain |
| 1 | A | 341 | VAL | Mainchain |
| 1 | A | 422 | GLU | Mainchain |
| 2 | B | 15 | PRO | Mainchain |
| 2 | B | 16 | GLU | Mainchain |
| 2 | B | 185 | ASP | Mainchain |
| 3 | O | 129 | TYR | Sidechain |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4448 | 0 | 4337 | 456 | 0 |
| 1 | M | 4414 | 0 | 4300 | 754 | 0 |
| 2 | B | 1888 | 0 | 1837 | 172 | 0 |
| 2 | N | 1888 | 0 | 1837 | 315 | 0 |
| 3 | C | 1058 | 0 | 1108 | 122 | 0 |
| 3 | O | 1058 | 0 | 1108 | 133 | 0 |
| 4 | D | 926 | 0 | 971 | 140 | 0 |
| 4 | P | 926 | 0 | 971 | 130 | 0 |
| 5 | A | 13 | 0 | 5 | 14 | 0 |
| 5 | M | 13 | 0 | 5 | 3 | 0 |
| 6 | B | 4 | 0 | 0 | 0 | 0 |
| 6 | N | 4 | 0 | 0 | 0 | 0 |
| 7 | B | 7 | 0 | 0 | 0 | 0 |
| 7 | N | 7 | 0 | 0 | 1 | 0 |
| 8 | B | 8 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | N | 8 | 0 | 0 | 3 | 0 |
| 9 | A | 52 | 0 | 29 | 16 | 0 |
| 9 | M | 52 | 0 | 29 | 13 | 0 |
| 10 | D | 33 | 0 | 37 | 7 | 0 |
| 10 | P | 33 | 0 | 37 | 12 | 0 |
| All | All | 16840 | 0 | 16611 | 2097 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 63.

All (2097) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:450:LYS:CE | 1:A:450:LYS:CD | 1.78 | 1.57 |
| 1:A:207:ILE:CD1 | 1:A:207:ILE:CG1 | 1.79 | 1.57 |
| 1:A:372:LYS:CG | 1:A:372:LYS:CB | 1.78 | 1.56 |
| 1:A:173:MET:CE | 1:A:173:MET:SD | 2.06 | 1.43 |
| 1:M:44:HIS:NE2 | 9:M:803:FAD:HM82 | 1.13 | 1.42 |
| 1:A:44:HIS:NE2 | 9:A:703:FAD:HM82 | 1.27 | 1.42 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:CB | 1.72 | 1.18 |
| 1:A:253:ILE:CG2 | 1:A:315:ASP:HB3 | 1.74 | 1.16 |
| 1:A:27:ASN:HD22 | 1:A:27:ASN:C | 1.35 | 1.16 |
| 1:A:275:GLY:O | 1:A:277:PRO:HD2 | 1.45 | 1.16 |
| 1:A:261:ARG:NH1 | 1:A:282:MET:HE3 | 1.58 | 1.16 |
| 1:M:48:ALA:HB3 | 1:M:132:GLY:HA3 | 1.18 | 1.12 |
| 5:A:702:FLC:HA1 | 5:A:702:FLC:OG2 | 1.33 | 1.12 |
| 2:N:162:GLY:O | 3:O:11:MET:HG3 | 1.50 | 1.12 |
| 3:C:50:LYS:NZ | 4:D:118:ILE:HD12 | 1.65 | 1.12 |
| 1:M:74:ASP:HB3 | 1:M:388:ALA:HB3 | 1.27 | 1.11 |
| 1:A:543:ASP:OD2 | 1:A:546:ASN:ND2 | 1.85 | 1.10 |
| 1:M:38:VAL:HB | 2:N:54:ARG:HH22 | 1.15 | 1.10 |
| 1:M:391:LEU:HG | 1:M:392:GLY:H | 1.14 | 1.10 |
| 2:N:65:CYS:HB2 | 2:N:76:ALA:HB3 | 1.30 | 1.09 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:HB3 | 1.30 | 1.09 |
| 1:M:227:GLU:HG2 | 1:M:518:MET:HB3 | 1.34 | 1.09 |
| 4:D:55:LEU:HG | 4:D:59:GLN:NE2 | 1.69 | 1.08 |
| 2:B:225:GLN:HG2 | 3:C:93:ALA:HB2 | 1.36 | 1.08 |
| 3:O:87:PHE:HD2 | 3:O:112:LEU:HD13 | 1.08 | 1.07 |
| 1:M:72:GLY:HA3 | 1:M:391:LEU:HD22 | 1.33 | 1.06 |
| 1:M:227:GLU:HG3 | 1:M:463:CYS:SG | 1.95 | 1.06 |
| 1:A:18:ARG:NH1 | 1:A:92:GLU:OE1 | 1.88 | 1.05 |
| 1:M:225:ASP:H | 1:M:550:HIS:HB3 | 1.18 | 1.05 |
| 1:A:263:LEU:O | 1:A:268:MET:HB2 | 1.55 | 1.05 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:287:ARG:HG3 | 1:A:287:ARG:NH1 | 1.56 | 1.04 |
| 1:A:263:LEU:HB3 | 1:A:268:MET:CE | 1.88 | 1.04 |
| 1:A:287:ARG:HH11 | 1:A:287:ARG:CG | 1.70 | 1.04 |
| 4:D:55:LEU:HG | 4:D:59:GLN:HE22 | 1.18 | 1.04 |
| 3:O:2:THR:HG22 | 3:O:4:ARG:H | 1.19 | 1.03 |
| 2:B:180:ASN:ND2 | 2:B:188:LYS:HG3 | 1.72 | 1.03 |
| 1:M:360:GLY:H | 1:M:382:SER:HB2 | 1.24 | 1.02 |
| 1:M:527:GLU:HA | 1:M:539:CYS:SG | 1.97 | 1.02 |
| 1:M:467:ARG:NH2 | 1:M:532:HIS:HA | 1.73 | 1.02 |
| 2:N:98:ILE:HG12 | 3:O:9:ARG:HH21 | 1.23 | 1.02 |
| 1:A:101:CYS:HB2 | 1:A:138:THR:HG21 | 1.40 | 1.02 |
| 1:M:15:ALA:HB2 | 1:M:399:LEU:HD22 | 1.40 | 1.02 |
| 1:A:261:ARG:HH11 | 1:A:282:MET:HE3 | 1.23 | 1.01 |
| 4:P:10:GLU:O | 4:P:10:GLU:HG3 | 1.56 | 1.01 |
| 2:N:69:VAL:HG11 | 2:N:79:THR:HG21 | 1.43 | 1.01 |
| 2:B:110:ILE:HA | 2:B:113:LEU:HD12 | 1.42 | 1.00 |
| 2:B:210:CYS:SG | 2:B:220:PRO:HG2 | 2.02 | 1.00 |
| 1:M:476:ILE:HG12 | 1:M:519:ALA:HB1 | 1.42 | 0.99 |
| 1:A:253:ILE:HG12 | 1:A:261:ARG:HD3 | 1.41 | 0.99 |
| 3:O:87:PHE:CD2 | 3:O:112:LEU:HD13 | 1.97 | 0.99 |
| 1:A:184:ARG:HH11 | 1:A:184:ARG:HG2 | 1.19 | 0.99 |
| 1:M:360:GLY:N | 1:M:382:SER:HB2 | 1.77 | 0.99 |
| 2:B:238:ALA:HA | 2:B:241:LYS:HB3 | 1.43 | 0.98 |
| 3:O:50:LYS:HE2 | 4:P:118:ILE:HG22 | 1.42 | 0.98 |
| 1:A:527:GLU:HG2 | 1:A:547:PHE:CB | 1.94 | 0.97 |
| 1:M:74:ASP:HB3 | 1:M:388:ALA:CB | 1.95 | 0.97 |
| 1:M:548:LEU:HD21 | 1:M:570:ILE:HD11 | 1.46 | 0.97 |
| 1:A:234:THR:HG22 | 1:A:350:VAL:HG21 | 1.46 | 0.97 |
| 1:A:236:LEU:HD21 | 1:A:243:MET:CE | 1.95 | 0.96 |
| 1:A:115:ARG:HG3 | 1:A:115:ARG:HH11 | 1.24 | 0.96 |
| 1:A:253:ILE:CG2 | 1:A:315:ASP:CB | 2.39 | 0.96 |
| 1:M:55:VAL:HB | 1:M:90:PRO:HG3 | 1.48 | 0.96 |
| 1:M:106:ARG:HB3 | 1:M:112:ASN:HB2 | 1.48 | 0.96 |
| 3:O:4:ARG:HE | 3:O:6:PRO:HG3 | 1.31 | 0.95 |
| 1:M:232:HIS:O | 1:M:352:PRO:HA | 1.64 | 0.95 |
| 2:N:149:ILE:HG13 | 2:N:151:CYS:HB3 | 1.45 | 0.95 |
| 1:A:427:ALA:O | 1:A:430:ALA:HB3 | 1.67 | 0.95 |
| 1:M:178:GLY:HA3 | 1:M:496:SER:HB2 | 1.48 | 0.95 |
| 1:A:295:TRP:CZ3 | 1:A:299:ARG:HD2 | 2.00 | 0.95 |
| 1:M:227:GLU:HB2 | 1:M:518:MET:O | 1.67 | 0.94 |
| 1:A:44:HIS:NE2 | 9:A:703:FAD:HM81 | 1.80 | 0.94 |
| 1:A:542:ARG:NE | 1:A:544:ASP:OD2 | 2.00 | 0.94 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:82:VAL:HG22 | 1:M:385:LEU:HA | 1.46 | 0.94 |
| 1:M:53:ALA:H | 1:M:394:ASN:HD22 | 1.16 | 0.94 |
| 1:A:27:ASN:C | 1:A:27:ASN:ND2 | 2.09 | 0.94 |
| 1:M:113:VAL:HB | 1:M:124:THR:O | 1.69 | 0.93 |
| 1:M:223:LEU:HG | 1:M:360:GLY:HA2 | 1.49 | 0.93 |
| 1:A:562:ARG:HG3 | 1:A:562:ARG:HH11 | 1.32 | 0.93 |
| 1:M:448:TRP:O | 1:M:452:ARG:HD3 | 1.67 | 0.93 |
| 2:N:214:CYS:SG | 2:N:218:VAL:HG23 | 2.09 | 0.93 |
| 3:C:50:LYS:HD3 | 4:D:118:ILE:HB | 1.48 | 0.93 |
| 1:M:93:MET:HB3 | 1:M:125:TRP:CZ3 | 2.03 | 0.92 |
| 1:M:474:LYS:HD2 | 1:M:478:LYS:HE2 | 1.52 | 0.92 |
| 1:A:261:ARG:NH1 | 1:A:282:MET:CE | 2.33 | 0.92 |
| 1:M:361:ILE:H | 1:M:382:SER:H | 0.94 | 0.92 |
| 1:A:288:ASP:OD2 | 1:A:288:ASP:N | 1.98 | 0.92 |
| 1:M:217:LEU:HD11 | 1:M:555:ARG:HD2 | 1.50 | 0.92 |
| 2:N:75:LEU:HD21 | 2:N:215:PRO:HB3 | 1.51 | 0.92 |
| 1:M:151:ARG:HH11 | 1:M:151:ARG:HB2 | 1.35 | 0.92 |
| 1:A:44:HIS:CE1 | 9:A:703:FAD:HM82 | 2.04 | 0.92 |
| 1:M:273:PRO:HG2 | 1:M:276:GLU:HB2 | 1.49 | 0.92 |
| 3:O:4:ARG:NE | 3:O:6:PRO:HG3 | 1.86 | 0.91 |
| 1:M:44:HIS:HE1 | 1:M:204:ASN:HA | 1.33 | 0.91 |
| 1:M:44:HIS:NE2 | 9:M:803:FAD:HM81 | 1.84 | 0.91 |
| 4:P:43:LEU:HD23 | 4:P:43:LEU:N | 1.84 | 0.91 |
| 2:B:44:LYS:HA | 2:B:48:ALA:O | 1.71 | 0.90 |
| 1:A:275:GLY:O | 1:A:277:PRO:CD | 2.19 | 0.90 |
| 2:N:30:TYR:HB3 | 2:N:81:LEU:HD13 | 1.54 | 0.90 |
| 1:A:493:ASP:HB3 | 1:A:499:ASN:HD21 | 1.36 | 0.90 |
| 1:M:391:LEU:HG | 1:M:392:GLY:N | 1.86 | 0.90 |
| 2:B:7:LYS:HE2 | 2:B:27:GLU:HG3 | 1.53 | 0.90 |
| 1:M:361:ILE:H | 1:M:382:SER:N | 1.70 | 0.89 |
| 3:C:63:LEU:HB3 | 4:D:40:PRO:HG3 | 1.53 | 0.89 |
| 2:B:14:ASN:N | 2:B:18:ASP:OD2 | 2.06 | 0.89 |
| 2:N:144:GLN:HG3 | 3:O:102:LYS:NZ | 1.88 | 0.89 |
| 1:M:242:LEU:CD2 | 1:M:244:THR:H | 1.85 | 0.89 |
| 3:C:50:LYS:HZ3 | 4:D:118:ILE:HD12 | 1.22 | 0.89 |
| 3:O:53:PRO:HB3 | 4:P:51:TYR:CD2 | 2.08 | 0.88 |
| 2:N:44:LYS:HA | 2:N:48:ALA:O | 1.73 | 0.88 |
| 1:A:13:GLY:O | 1:A:17:LEU:HB2 | 1.72 | 0.88 |
| 3:C:28:ARG:O | 3:C:31:THR:HB | 1.73 | 0.88 |
| 2:N:169:GLY:O | 2:N:173:ILE:HG13 | 1.73 | 0.88 |
| 1:A:416:THR:CG2 | 1:A:416:THR:O | 2.22 | 0.88 |
| 1:M:403:GLY:HA2 | 1:M:406:ALA:HB3 | 1.55 | 0.87 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:287:ARG:HG3 | 1:A:287:ARG:HH11 | 0.77 | 0.87 |
| 3:O:87:PHE:HD2 | 3:O:112:LEU:CD1 | 1.88 | 0.87 |
| 3:O:123:ILE:HD11 | 10:P:800:MQ7:H162 | 1.54 | 0.87 |
| 1:M:433:GLU:HG3 | 1:M:434:GLN:N | 1.89 | 0.87 |
| 1:M:224:ARG:HE | 1:M:550:HIS:CD2 | 1.91 | 0.87 |
| 1:M:38:VAL:HB | 2:N:54:ARG:NH2 | 1.89 | 0.87 |
| 5:A:702:FLC:CA | 5:A:702:FLC:OG2 | 2.22 | 0.86 |
| 1:A:184:ARG:CG | 1:A:184:ARG:HH11 | 1.88 | 0.86 |
| 3:C:111:SER:O | 3:C:115:VAL:HG23 | 1.73 | 0.86 |
| 2:N:196:ASN:N | 2:N:196:ASN:HD22 | 1.74 | 0.86 |
| 1:M:471:LEU:HD12 | 1:M:472:MET:N | 1.90 | 0.86 |
| 1:M:490:ARG:HD3 | 1:M:490:ARG:H | 1.41 | 0.86 |
| 1:M:167:VAL:HG21 | 1:M:374:LEU:HD13 | 1.56 | 0.86 |
| 3:O:123:ILE:CD1 | 10:P:800:MQ7:H162 | 2.06 | 0.86 |
| 1:M:224:ARG:HE | 1:M:550:HIS:HD2 | 1.21 | 0.86 |
| 1:M:279:ASN:HD22 | 1:M:280:LYS:N | 1.74 | 0.85 |
| 1:A:263:LEU:HB3 | 1:A:268:MET:HE3 | 1.58 | 0.85 |
| 2:N:14:ASN:O | 2:N:18:ASP:HB3 | 1.76 | 0.85 |
| 1:A:540:THR:O | 1:A:541:GLU:OE2 | 1.94 | 0.85 |
| 1:M:230:GLN:HE21 | 1:M:287:ARG:NH1 | 1.73 | 0.85 |
| 1:M:53:ALA:CB | 1:M:394:ASN:HD22 | 1.89 | 0.85 |
| 1:A:27:ASN:ND2 | 1:A:27:ASN:O | 2.06 | 0.85 |
| 2:B:12:ARG:NH2 | 2:B:101:ASP:OD1 | 2.10 | 0.85 |
| 1:M:42:ARG:HH22 | 2:N:54:ARG:HB3 | 1.42 | 0.85 |
| 3:O:4:ARG:HE | 3:O:6:PRO:CG | 1.90 | 0.85 |
| 3:C:50:LYS:HA | 3:C:50:LYS:CE | 2.07 | 0.85 |
| 1:M:44:HIS:CE1 | 9:M:803:FAD:HM82 | 2.12 | 0.84 |
| 1:A:261:ARG:HH11 | 1:A:282:MET:CE | 1.88 | 0.84 |
| 2:N:144:GLN:HG3 | 3:O:102:LYS:HZ2 | 1.42 | 0.84 |
| 4:D:0:MET:HG3 | 4:D:1:ILE:H | 1.41 | 0.84 |
| 4:D:99:VAL:HG12 | 4:D:100:PHE:N | 1.91 | 0.84 |
| 2:N:54:ARG:HH11 | 2:N:54:ARG:HG2 | 1.41 | 0.84 |
| 1:M:92:GLU:HA | 1:M:95:GLN:HB3 | 1.60 | 0.83 |
| 2:B:241:LYS:O | 2:B:243:ARG:N | 2.11 | 0.83 |
| 2:N:196:ASN:H | 2:N:196:ASN:HD22 | 1.24 | 0.83 |
| 1:M:44:HIS:CE1 | 1:M:204:ASN:HA | 2.13 | 0.83 |
| 1:A:65:HIS:ND1 | 1:A:86:VAL:HG22 | 1.92 | 0.83 |
| 3:O:60:VAL:HG12 | 3:O:64:GLN:HE21 | 1.41 | 0.83 |
| 1:M:225:ASP:N | 1:M:550:HIS:HB3 | 1.94 | 0.83 |
| 1:A:446:GLU:HG2 | 1:A:488:ARG:O | 1.77 | 0.83 |
| 3:O:87:PHE:CD2 | 3:O:112:LEU:HB3 | 2.13 | 0.83 |
| 3:C:87:PHE:CD1 | 3:C:112:LEU:HB3 | 2.14 | 0.83 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:1:ILE:HG22 | 4:D:1:ILE:O | 1.79 | 0.83 |
| 1:M:49:GLN:HE21 | 1:M:49:GLN:H | 1.22 | 0.82 |
| 1:A:57:GLN:NE2 | 1:A:122:GLU:HG2 | 1.94 | 0.82 |
| 3:C:49:LEU:O | 3:C:49:LEU:HD23 | 1.80 | 0.82 |
| 2:N:145:PHE:HA | 2:N:218:VAL:HG13 | 1.60 | 0.82 |
| 1:A:314:LEU:HD11 | 1:A:316:LEU:HD21 | 1.59 | 0.82 |
| 4:P:26:ILE:HG22 | 4:P:27:ILE:HG13 | 1.61 | 0.82 |
| 2:N:168:ILE:HD11 | 2:N:173:ILE:HG12 | 1.61 | 0.82 |
| 1:M:49:GLN:NE2 | 1:M:49:GLN:H | 1.76 | 0.82 |
| 3:C:45:GLY:HA3 | 10:D:700:MQ7:H8 | 1.61 | 0.82 |
| 1:M:24:ALA:O | 1:M:26:ALA:N | 2.13 | 0.82 |
| 2:B:26:TYR:HD2 | 2:B:47:LEU:HD13 | 1.42 | 0.82 |
| 1:A:200:ARG:HD3 | 1:A:201:TYR:CE1 | 2.15 | 0.82 |
| 1:M:256:ASN:HD21 | 1:M:260:TYR:HB3 | 1.44 | 0.82 |
| 1:M:526:LYS:O | 1:M:526:LYS:HD2 | 1.80 | 0.81 |
| 1:M:551:THR:O | 1:M:552:LEU:HD23 | 1.81 | 0.81 |
| 1:M:52:SER:HB2 | 1:M:396:LEU:CB | 2.10 | 0.81 |
| 2:N:69:VAL:HG21 | 2:N:74:LYS:HB2 | 1.61 | 0.81 |
| 1:A:263:LEU:CB | 1:A:268:MET:HE3 | 2.10 | 0.81 |
| 1:A:548:LEU:HD23 | 1:A:548:LEU:O | 1.81 | 0.81 |
| 1:M:53:ALA:H | 1:M:394:ASN:ND2 | 1.78 | 0.81 |
| 1:A:306:THR:HB | 1:A:307:PRO:CD | 2.10 | 0.81 |
| 1:M:77:CYS:SG | 1:M:387:GLY:HA2 | 2.20 | 0.81 |
| 3:O:17:LYS:HG3 | 3:O:23:ARG:HH21 | 1.47 | 0.81 |
| 3:O:128:LEU:HD13 | 4:P:45:PRO:HD2 | 1.63 | 0.80 |
| 1:A:306:THR:HB | 1:A:307:PRO:HD2 | 1.60 | 0.80 |
| 1:A:253:ILE:O | 1:A:314:LEU:HA | 1.82 | 0.80 |
| 1:A:388:ALA:O | 1:A:389:ASN:HB2 | 1.80 | 0.80 |
| 3:O:90:ALA:N | 3:O:91:PRO:HD2 | 1.97 | 0.80 |
| 1:M:356:TYR:HE2 | 1:M:379:GLU:HG3 | 1.46 | 0.80 |
| 1:M:180:LEU:HD13 | 1:M:433:GLU:HB2 | 1.62 | 0.80 |
| 1:M:116:PHE:HB2 | 1:M:124:THR:HG21 | 1.64 | 0.80 |
| 1:A:90:PRO:HG2 | 1:A:91:THR:N | 1.95 | 0.80 |
| 1:M:65:HIS:HB2 | 1:M:123:ARG:NH1 | 1.96 | 0.80 |
| 1:M:377:VAL:HG22 | 1:M:402:PHE:HE2 | 1.47 | 0.80 |
| 2:B:50:ASP:C | 2:B:50:ASP:OD1 | 2.19 | 0.80 |
| 1:A:155:HIS:CD2 | 1:A:174:ASN:HA | 2.17 | 0.80 |
| 1:M:130:LYS:NZ | 2:N:216:LYS:HD3 | 1.97 | 0.79 |
| 2:B:211:SER:OG | 2:B:220:PRO:HD2 | 1.82 | 0.79 |
| 1:M:439:LEU:HD23 | 1:M:442:GLN:NE2 | 1.98 | 0.79 |
| 1:M:230:GLN:HE21 | 1:M:287:ARG:HH11 | 1.26 | 0.79 |
| 4:P:41:LEU:O | 4:P:43:LEU:HD23 | 1.81 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:361:ILE:HG12 | 1:M:376:ALA:HB3 | 1.64 | 0.79 |
| 1:M:60:ASP:HB2 | 1:M:123:ARG:CZ | 2.12 | 0.79 |
| 2:N:155:TYR:CE2 | 2:N:169:GLY:HA3 | 2.18 | 0.79 |
| 3:C:124:LEU:HD23 | 4:D:34:LEU:HD21 | 1.62 | 0.79 |
| 1:M:133:PHE:HZ | 2:N:149:ILE:HA | 1.46 | 0.79 |
| 2:B:180:ASN:HD22 | 2:B:188:LYS:HG3 | 1.42 | 0.79 |
| 1:M:242:LEU:C | 1:M:242:LEU:HD23 | 2.03 | 0.79 |
| 1:M:38:VAL:CG1 | 2:N:54:ARG:HH12 | 1.96 | 0.79 |
| 2:N:6:LEU:HD13 | 2:N:81:LEU:HD21 | 1.65 | 0.79 |
| 1:M:113:VAL:HG21 | 1:M:123:ARG:HA | 1.65 | 0.78 |
| 1:M:53:ALA:N | 1:M:394:ASN:HD22 | 1.80 | 0.78 |
| 1:M:226:MET:HG2 | 1:M:517:CYS:HB2 | 1.65 | 0.78 |
| 3:C:90:ALA:N | 3:C:91:PRO:HD2 | 1.97 | 0.78 |
| 1:M:479:LEU:HD13 | 1:M:516:GLU:OE1 | 1.83 | 0.78 |
| 2:B:238:ALA:HA | 2:B:241:LYS:CB | 2.13 | 0.78 |
| 1:A:198:VAL:HG23 | 1:A:455:MET:CE | 2.14 | 0.78 |
| 2:N:113:LEU:O | 2:N:116:ILE:HG12 | 1.84 | 0.78 |
| 1:M:361:ILE:N | 1:M:382:SER:H | 1.78 | 0.78 |
| 1:M:467:ARG:HH22 | 1:M:532:HIS:HA | 1.46 | 0.78 |
| 3:C:31:THR:HG21 | 3:C:82:HIS:HB2 | 1.64 | 0.78 |
| 1:A:497:VAL:HG12 | 1:A:497:VAL:O | 1.82 | 0.78 |
| 2:B:211:SER:HA | 2:B:220:PRO:HD2 | 1.64 | 0.77 |
| 1:M:514:VAL:O | 1:M:518:MET:HG3 | 1.83 | 0.77 |
| 1:M:549:LYS:HG3 | 1:M:565:TYR:HB3 | 1.67 | 0.77 |
| 1:M:159:ASP:HB3 | 1:M:432:VAL:HG13 | 1.66 | 0.77 |
| 1:A:493:ASP:HB3 | 1:A:499:ASN:ND2 | 1.99 | 0.77 |
| 1:M:222:PRO:HB3 | 1:M:552:LEU:HD22 | 1.66 | 0.77 |
| 1:A:253:ILE:HG21 | 1:A:315:ASP:HB3 | 1.67 | 0.77 |
| 1:M:52:SER:HB2 | 1:M:396:LEU:HB3 | 1.66 | 0.77 |
| 1:M:229:VAL:HG12 | 1:M:531:ALA:HB1 | 1.66 | 0.77 |
| 3:C:36:VAL:HG22 | 4:D:75:LEU:HD22 | 1.66 | 0.77 |
| 1:M:227:GLU:HG2 | 1:M:518:MET:CB | 2.14 | 0.77 |
| 1:A:416:THR:HG23 | 1:A:416:THR:O | 1.85 | 0.77 |
| 2:N:28:VAL:HG22 | 2:N:43:ILE:HG13 | 1.65 | 0.77 |
| 1:A:262:TYR:CD1 | 1:A:297:GLU:HG3 | 2.19 | 0.77 |
| 1:A:545:VAL:HG12 | 1:A:546:ASN:N | 1.99 | 0.77 |
| 1:M:433:GLU:HG3 | 1:M:434:GLN:H | 1.48 | 0.77 |
| 2:B:97:PRO:C | 2:B:104:VAL:HG23 | 2.05 | 0.77 |
| 3:O:49:LEU:HG | 3:O:49:LEU:O | 1.85 | 0.77 |
| 1:A:491:ILE:HG22 | 1:A:491:ILE:O | 1.85 | 0.77 |
| 1:A:147:PRO:HD2 | 1:A:148:GLN:OE1 | 1.85 | 0.77 |
| 1:M:46:VAL:HG13 | 1:M:136:LEU:HD23 | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:213:MET:O | 1:A:217:LEU:HD12 | 1.85 | 0.77 |
| 2:N:69:VAL:N | 2:N:72:VAL:O | 2.14 | 0.76 |
| 3:C:50:LYS:HE3 | 3:C:50:LYS:HA | 1.67 | 0.76 |
| 1:M:242:LEU:HD21 | 1:M:244:THR:H | 1.51 | 0.76 |
| 4:P:80:HIS:CD2 | 4:P:84:HIS:CD2 | 2.72 | 0.76 |
| 1:M:226:MET:HG3 | 1:M:518:MET:HG2 | 1.68 | 0.76 |
| 1:M:230:GLN:HG2 | 1:M:390:ARG:HH21 | 1.51 | 0.76 |
| 1:M:48:ALA:HB3 | 1:M:132:GLY:CA | 2.09 | 0.76 |
| 1:A:253:ILE:CG1 | 1:A:261:ARG:HD3 | 2.14 | 0.76 |
| 3:O:53:PRO:HD3 | 4:P:51:TYR:CZ | 2.19 | 0.76 |
| 4:D:44:PHE:CE1 | 4:D:49:LEU:HB2 | 2.20 | 0.76 |
| 4:P:43:LEU:H | 4:P:43:LEU:HD23 | 1.46 | 0.76 |
| 4:D:83:HIS:O | 4:D:86:MET:HB2 | 1.86 | 0.76 |
| 1:M:368:GLU:HG2 | 1:M:409:GLN:OE1 | 1.85 | 0.76 |
| 1:M:220:GLY:N | 1:M:371:ILE:HD11 | 2.00 | 0.76 |
| 4:P:67:LEU:O | 4:P:71:ILE:HD12 | 1.86 | 0.76 |
| 3:C:94:ALA:HB1 | 3:C:96:ILE:HD11 | 1.68 | 0.76 |
| 1:A:114:ARG:HD3 | 1:A:126:PHE:CD2 | 2.20 | 0.76 |
| 1:M:42:ARG:NH2 | 2:N:64:SER:OG | 2.18 | 0.76 |
| 1:M:346:GLU:HG3 | 1:M:347:PRO:HD2 | 1.66 | 0.76 |
| 1:A:527:GLU:HG2 | 1:A:547:PHE:HB3 | 1.65 | 0.76 |
| 1:A:46:VAL:HG23 | 1:A:47:ALA:N | 2.00 | 0.76 |
| 2:B:32:ALA:O | 2:B:82:ARG:NH1 | 2.18 | 0.76 |
| 1:M:223:LEU:HA | 1:M:360:GLY:O | 1.86 | 0.76 |
| 1:M:227:GLU:CG | 1:M:518:MET:HB3 | 2.15 | 0.76 |
| 4:D:0:MET:HG3 | 4:D:1:ILE:N | 2.00 | 0.76 |
| 1:A:328:LEU:CD1 | 1:A:331:ILE:HG13 | 2.16 | 0.76 |
| 1:A:44:HIS:CD2 | 9:A:703:FAD:C8M | 2.69 | 0.75 |
| 2:N:81:LEU:O | 2:N:81:LEU:HD23 | 1.86 | 0.75 |
| 4:P:10:GLU:CG | 4:P:10:GLU:O | 2.34 | 0.75 |
| 2:B:43:ILE:HG23 | 2:B:47:LEU:HD12 | 1.68 | 0.75 |
| 2:N:168:ILE:HG23 | 2:N:199:ASN:O | 1.86 | 0.75 |
| 1:A:390:ARG:HH12 | 5:A:702:FLC:CAC | 1.99 | 0.75 |
| 4:D:12:VAL:HG12 | 4:D:13:PHE:N | 2.02 | 0.75 |
| 2:B:155:TYR:HE1 | 2:B:171:ALA:HB3 | 1.52 | 0.75 |
| 2:B:13:TYR:CD2 | 2:B:13:TYR:O | 2.40 | 0.75 |
| 1:M:296:HIS:O | 1:M:300:LYS:HB2 | 1.85 | 0.75 |
| 1:M:226:MET:HG3 | 1:M:518:MET:CA | 2.16 | 0.75 |
| 4:P:117:THR:O | 4:P:118:ILE:HB | 1.85 | 0.75 |
| 2:B:43:ILE:HG23 | 2:B:47:LEU:CD1 | 2.17 | 0.75 |
| 2:N:233:LYS:O | 2:N:237:ILE:HD13 | 1.86 | 0.75 |
| 2:N:97:PRO:HA | 3:O:7:TYR:O | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:467:ARG:CZ | 1:M:532:HIS:HA | 2.15 | 0.75 |
| 1:M:551:THR:HG22 | 1:M:552:LEU:N | 2.00 | 0.75 |
| 1:A:27:ASN:ND2 | 1:A:29:ASN:N | 2.34 | 0.75 |
| 4:D:41:LEU:O | 4:D:43:LEU:HD23 | 1.86 | 0.74 |
| 1:M:256:ASN:HB3 | 1:M:262:TYR:HD2 | 1.51 | 0.74 |
| 2:N:75:LEU:O | 2:N:77:CYS:N | 2.21 | 0.74 |
| 3:O:60:VAL:CG1 | 3:O:64:GLN:HE21 | 1.99 | 0.74 |
| 1:A:73:GLY:O | 1:A:74:ASP:HB2 | 1.87 | 0.74 |
| 2:B:99:GLU:OE2 | 3:C:4:ARG:NH1 | 2.19 | 0.74 |
| 1:M:242:LEU:HD23 | 1:M:244:THR:H | 1.52 | 0.74 |
| 4:D:48:ALA:HA | 4:D:53:ARG:HD3 | 1.68 | 0.74 |
| 3:O:50:LYS:HE2 | 4:P:118:ILE:CG2 | 2.16 | 0.74 |
| 1:A:115:ARG:H | 1:A:115:ARG:HD2 | 1.52 | 0.74 |
| 1:M:9:ILE:HD13 | 1:M:19:ALA:HB3 | 1.68 | 0.74 |
| 1:A:324:LEU:O | 1:A:328:LEU:N | 2.19 | 0.74 |
| 1:M:447:ASN:HB3 | 1:M:450:LYS:HG2 | 1.70 | 0.74 |
| 2:B:97:PRO:O | 2:B:104:VAL:HG23 | 1.87 | 0.73 |
| 1:M:42:ARG:NH2 | 2:N:54:ARG:NE | 2.36 | 0.73 |
| 1:M:356:TYR:CE2 | 1:M:379:GLU:HG3 | 2.22 | 0.73 |
| 1:M:57:GLN:O | 1:M:58:ASP:HB2 | 1.88 | 0.73 |
| 1:M:133:PHE:CZ | 2:N:149:ILE:HG22 | 2.23 | 0.73 |
| 2:N:8:ILE:HG22 | 2:N:9:GLU:N | 2.04 | 0.73 |
| 2:B:182:ASP:OD1 | 2:B:184:ARG:NH1 | 2.20 | 0.73 |
| 1:A:255:VAL:HG12 | 1:A:261:ARG:HG2 | 1.70 | 0.73 |
| 1:M:42:ARG:NH2 | 2:N:54:ARG:CZ | 2.52 | 0.73 |
| 1:A:493:ASP:CB | 1:A:499:ASN:HD21 | 2.00 | 0.73 |
| 2:N:206:PHE:CE1 | 2:N:225:GLN:HG2 | 2.24 | 0.73 |
| 2:N:210:CYS:SG | 2:N:221:ALA:HB2 | 2.27 | 0.73 |
| 1:A:44:HIS:CD2 | 9:A:703:FAD:HM81 | 2.23 | 0.73 |
| 2:N:8:ILE:HG22 | 2:N:9:GLU:H | 1.52 | 0.73 |
| 1:M:187:ALA:HB1 | 1:M:410:ALA:HB1 | 1.70 | 0.73 |
| 1:M:256:ASN:HB3 | 1:M:262:TYR:CD2 | 2.24 | 0.73 |
| 4:D:73:LEU:HB2 | 4:D:74:PRO:HD3 | 1.70 | 0.73 |
| 4:D:55:LEU:CG | 4:D:59:GLN:HE22 | 2.01 | 0.73 |
| 1:M:93:MET:HB3 | 1:M:125:TRP:CH2 | 2.23 | 0.72 |
| 2:N:36:LEU:HB2 | 2:N:76:ALA:O | 1.89 | 0.72 |
| 1:M:113:VAL:CG2 | 1:M:123:ARG:HA | 2.18 | 0.72 |
| 2:B:13:TYR:CG | 2:B:13:TYR:O | 2.38 | 0.72 |
| 2:B:155:TYR:CE2 | 2:B:169:GLY:HA3 | 2.23 | 0.72 |
| 1:M:248:ARG:HH11 | 1:M:248:ARG:HG2 | 1.52 | 0.72 |
| 2:N:155:TYR:CE1 | 2:N:171:ALA:HB3 | 2.24 | 0.72 |
| 1:A:523:MET:O | 1:A:526:LYS:NZ | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:377:VAL:HG13 | 1:M:402:PHE:CD2 | 2.25 | 0.72 |
| 1:A:103:TRP:O | 2:B:139:MET:HE1 | 1.90 | 0.72 |
| 2:B:72:VAL:HG12 | 2:B:73:PRO:HD2 | 1.71 | 0.72 |
| 2:N:215:PRO:HD2 | 8:N:246:SF4:S3 | 2.29 | 0.72 |
| 1:A:40:PRO:HG2 | 1:A:140:PHE:CE1 | 2.25 | 0.72 |
| 4:P:113:ILE:HG22 | 4:P:117:THR:HG21 | 1.71 | 0.72 |
| 3:C:53:PRO:HD3 | 4:D:51:TYR:CZ | 2.25 | 0.72 |
| 1:M:391:LEU:CG | 1:M:392:GLY:H | 1.97 | 0.72 |
| 2:B:60:ALA:N | 2:B:77:CYS:SG | 2.62 | 0.72 |
| 1:M:399:LEU:HD21 | 9:M:803:FAD:H5'2 | 1.71 | 0.71 |
| 1:M:552:LEU:HB2 | 1:M:564:GLU:HB2 | 1.71 | 0.71 |
| 1:A:79:GLN:HG3 | 1:A:570:ILE:HA | 1.72 | 0.71 |
| 1:A:118:GLY:O | 1:A:280:LYS:NZ | 2.14 | 0.71 |
| 4:P:14:TRP:O | 4:P:17:PHE:HB3 | 1.89 | 0.71 |
| 1:M:228:PHE:CE2 | 1:M:388:ALA:HA | 2.24 | 0.71 |
| 2:N:145:PHE:HD1 | 2:N:218:VAL:HG12 | 1.55 | 0.71 |
| 2:B:212:GLU:HG3 | 3:C:21:PHE:HE1 | 1.56 | 0.71 |
| 1:A:527:GLU:HG2 | 1:A:547:PHE:CG | 2.26 | 0.71 |
| 1:M:200:ARG:HD2 | 1:M:457:LEU:HB2 | 1.71 | 0.71 |
| 4:P:6:LYS:O | 4:P:6:LYS:HG3 | 1.91 | 0.71 |
| 1:M:60:ASP:HB3 | 1:M:121:ILE:HG21 | 1.71 | 0.71 |
| 1:M:227:GLU:OE1 | 1:M:227:GLU:HA | 1.91 | 0.71 |
| 1:M:385:LEU:HD12 | 1:M:386:HIS:N | 2.05 | 0.71 |
| 4:P:2:ASN:ND2 | 4:P:4:ASN:O | 2.24 | 0.71 |
| 1:M:187:ALA:O | 1:M:188:VAL:HG23 | 1.91 | 0.71 |
| 2:N:177:HIS:HA | 2:N:180:ASN:HB2 | 1.70 | 0.71 |
| 3:O:70:ILE:HG22 | 3:O:71:ILE:N | 2.04 | 0.71 |
| 1:M:92:GLU:O | 1:M:96:LEU:HG | 1.90 | 0.71 |
| 4:P:80:HIS:CD2 | 4:P:84:HIS:HD2 | 2.08 | 0.71 |
| 1:M:341:VAL:HG13 | 1:M:346:GLU:HB3 | 1.73 | 0.71 |
| 1:A:182:GLN:NE2 | 1:A:184:ARG:HH12 | 1.88 | 0.71 |
| 2:B:143:HIS:O | 2:B:146:SER:OG | 2.07 | 0.71 |
| 1:M:166:HIS:HD2 | 1:M:413:ARG:HH21 | 1.39 | 0.71 |
| 1:M:383:VAL:HG21 | 1:M:398:GLU:HG2 | 1.73 | 0.70 |
| 3:O:83:THR:CG2 | 3:O:87:PHE:CE1 | 2.74 | 0.70 |
| 1:A:236:LEU:HD21 | 1:A:243:MET:HE1 | 1.72 | 0.70 |
| 1:M:377:VAL:HG22 | 1:M:402:PHE:CE2 | 2.26 | 0.70 |
| 2:N:218:VAL:O | 2:N:219:ASP:HB2 | 1.89 | 0.70 |
| 2:B:238:ALA:CA | 2:B:241:LYS:HB3 | 2.20 | 0.70 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:HB2 | 1.68 | 0.70 |
| 4:P:31:MET:HG3 | 4:P:70:MET:SD | 2.31 | 0.70 |
| 1:M:255:VAL:HG23 | 1:M:313:TYR:HB2 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:455:MET:SD | 1:M:508:LEU:HD11 | 2.31 | 0.70 |
| 2:B:67:MET:HE3 | 2:B:76:ALA:HB2 | 1.74 | 0.70 |
| 1:M:229:VAL:HB | 1:M:467:ARG:HH22 | 1.56 | 0.70 |
| 1:M:242:LEU:HD21 | 1:M:244:THR:N | 2.06 | 0.70 |
| 1:M:94:THR:HB | 2:N:130:GLY:O | 1.92 | 0.70 |
| 1:M:53:ALA:CB | 1:M:394:ASN:ND2 | 2.54 | 0.70 |
| 1:A:211:ASP:HB3 | 9:A:703:FAD:H61A | 1.56 | 0.70 |
| 2:B:68:MET:HE3 | 2:B:72:VAL:O | 1.92 | 0.70 |
| 2:N:241:LYS:C | 2:N:243:ARG:H | 1.94 | 0.70 |
| 3:O:97:ILE:HG23 | 3:O:101:GLU:O | 1.92 | 0.70 |
| 1:M:194:GLY:H | 1:M:208:VAL:HG13 | 1.55 | 0.70 |
| 4:D:105:ALA:O | 4:D:109:VAL:HG23 | 1.92 | 0.70 |
| 1:A:177:GLU:HA | 1:A:177:GLU:OE2 | 1.92 | 0.70 |
| 1:M:255:VAL:O | 1:M:312:VAL:HG13 | 1.92 | 0.69 |
| 2:N:240:LEU:HD23 | 2:N:240:LEU:N | 2.06 | 0.69 |
| 1:M:358:MET:SD | 1:M:386:HIS:HB2 | 2.32 | 0.69 |
| 1:M:550:HIS:O | 1:M:565:TYR:HA | 1.92 | 0.69 |
| 2:N:149:ILE:HG23 | 2:N:216:LYS:HG3 | 1.73 | 0.69 |
| 2:N:26:TYR:HE2 | 2:N:48:ALA:HB3 | 1.56 | 0.69 |
| 2:B:9:GLU:OE2 | 2:B:23:SER:HB3 | 1.92 | 0.69 |
| 1:M:106:ARG:HG2 | 1:M:110:SER:O | 1.93 | 0.69 |
| 1:M:130:LYS:HZ1 | 2:N:216:LYS:HD3 | 1.55 | 0.69 |
| 1:M:76:LEU:HD21 | 1:M:525:ARG:HH12 | 1.57 | 0.69 |
| 2:N:6:LEU:HD21 | 2:N:81:LEU:HD11 | 1.75 | 0.69 |
| 2:N:241:LYS:HB3 | 2:N:242:PRO:HD3 | 1.74 | 0.69 |
| 2:N:37:LEU:HD11 | 2:N:58:ARG:HA | 1.74 | 0.69 |
| 1:A:184:ARG:NH1 | 1:A:184:ARG:HG2 | 2.01 | 0.69 |
| 1:M:555:ARG:NE | 1:M:560:THR:H | 1.91 | 0.69 |
| 3:O:125:PHE:CZ | 3:O:130:TRP:CZ3 | 2.81 | 0.69 |
| 1:A:294:PHE:O | 1:A:298:TRP:N | 2.23 | 0.69 |
| 2:N:73:PRO:HG2 | 2:N:213:VAL:HG11 | 1.75 | 0.69 |
| 1:A:62:PHE:HD2 | 1:A:86:VAL:HG13 | 1.56 | 0.69 |
| 1:M:227:GLU:H | 1:M:518:MET:HA | 1.58 | 0.69 |
| 1:M:467:ARG:NH2 | 1:M:532:HIS:CA | 2.53 | 0.69 |
| 1:A:314:LEU:HD11 | 1:A:316:LEU:CD2 | 2.23 | 0.69 |
| 1:A:341:VAL:HG13 | 1:A:346:GLU:HG3 | 1.75 | 0.69 |
| 1:M:177:GLU:OE2 | 3:O:2:THR:HG23 | 1.91 | 0.68 |
| 1:M:554:PHE:HB3 | 1:M:562:ARG:H | 1.58 | 0.68 |
| 3:C:59:PHE:CE1 | 3:C:63:LEU:HD11 | 2.27 | 0.68 |
| 2:N:155:TYR:HE1 | 2:N:171:ALA:HB3 | 1.59 | 0.68 |
| 4:D:34:LEU:HD23 | 4:D:38:LEU:HD12 | 1.75 | 0.68 |
| 4:D:44:PHE:CD1 | 4:D:49:LEU:HB2 | 2.28 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:194:GLY:H | 1:M:208:VAL:CG1 | 2.05 | 0.68 |
| 1:M:53:ALA:HA | 1:M:125:TRP:CD1 | 2.28 | 0.68 |
| 2:N:151:CYS:SG | 2:N:153:LEU:HB2 | 2.34 | 0.68 |
| 1:A:446:GLU:HB2 | 1:A:489:VAL:HB | 1.74 | 0.68 |
| 3:C:87:PHE:CE1 | 3:C:112:LEU:HB3 | 2.28 | 0.68 |
| 1:M:22:ALA:HB2 | 1:M:404:ARG:HA | 1.74 | 0.68 |
| 1:A:27:ASN:ND2 | 1:A:30:ALA:H | 1.91 | 0.68 |
| 4:P:113:ILE:HG22 | 4:P:117:THR:CG2 | 2.24 | 0.68 |
| 1:A:321:GLU:O | 1:A:324:LEU:N | 2.27 | 0.68 |
| 1:A:328:LEU:HD13 | 1:A:331:ILE:HG13 | 1.74 | 0.68 |
| 4:P:73:LEU:HD23 | 4:P:73:LEU:N | 2.08 | 0.68 |
| 1:M:52:SER:O | 1:M:125:TRP:HB2 | 1.94 | 0.68 |
| 2:N:220:PRO:O | 2:N:223:ALA:N | 2.27 | 0.68 |
| 1:A:390:ARG:HD2 | 1:A:395:SER:HB2 | 1.75 | 0.68 |
| 1:M:433:GLU:CG | 1:M:434:GLN:H | 2.07 | 0.68 |
| 4:P:72:VAL:O | 4:P:75:LEU:HB2 | 1.94 | 0.68 |
| 4:D:111:THR:O | 4:D:115:VAL:HG22 | 1.93 | 0.68 |
| 1:M:455:MET:HE2 | 1:M:482:LEU:HD13 | 1.75 | 0.68 |
| 1:M:151:ARG:HH11 | 1:M:151:ARG:CB | 2.06 | 0.68 |
| 4:D:113:ILE:HG22 | 4:D:114:GLY:N | 2.09 | 0.68 |
| 1:M:329:PRO:HA | 1:M:332:CYS:SG | 2.34 | 0.68 |
| 1:M:46:VAL:HA | 1:M:132:GLY:O | 1.93 | 0.67 |
| 1:A:27:ASN:ND2 | 1:A:30:ALA:N | 2.42 | 0.67 |
| 4:P:57:PHE:CZ | 10:P:800:MQ7:H151 | 2.29 | 0.67 |
| 1:A:198:VAL:HG23 | 1:A:455:MET:HE1 | 1.75 | 0.67 |
| 1:M:192:THR:HG21 | 1:M:212:GLY:H | 1.58 | 0.67 |
| 1:M:72:GLY:CA | 1:M:391:LEU:HD22 | 2.18 | 0.67 |
| 1:M:46:VAL:HA | 1:M:133:PHE:HA | 1.75 | 0.67 |
| 1:M:390:ARG:HD3 | 1:M:395:SER:OG | 1.93 | 0.67 |
| 3:O:87:PHE:CE2 | 3:O:112:LEU:HB3 | 2.29 | 0.67 |
| 4:P:68:PHE:O | 4:P:72:VAL:HG22 | 1.94 | 0.67 |
| 1:A:436:LEU:HD23 | 1:A:436:LEU:C | 2.14 | 0.67 |
| 1:A:168:ARG:HG2 | 1:A:425:ILE:CD1 | 2.24 | 0.67 |
| 2:N:36:LEU:HD13 | 2:N:79:THR:HB | 1.76 | 0.67 |
| 1:M:555:ARG:HE | 1:M:560:THR:H | 1.43 | 0.67 |
| 1:M:220:GLY:H | 1:M:371:ILE:HD11 | 1.60 | 0.67 |
| 1:M:226:MET:HG3 | 1:M:518:MET:HA | 1.76 | 0.67 |
| 1:M:76:LEU:HD21 | 1:M:525:ARG:NH1 | 2.10 | 0.67 |
| 1:A:262:TYR:CE1 | 1:A:263:LEU:HD23 | 2.30 | 0.67 |
| 3:O:83:THR:CG2 | 3:O:87:PHE:HE1 | 2.06 | 0.67 |
| 3:C:37:TRP:CZ2 | 3:C:41:GLU:OE2 | 2.47 | 0.67 |
| 2:B:105:ASP:C | 2:B:105:ASP:OD1 | 2.32 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:251:GLY:HA2 | 1:M:277:PRO:HG2 | 1.76 | 0.67 |
| 2:N:235:PHE:C | 2:N:237:ILE:H | 1.98 | 0.67 |
| 2:N:10:VAL:HG13 | 2:N:90:VAL:HB | 1.77 | 0.67 |
| 1:M:225:ASP:O | 1:M:226:MET:O | 2.13 | 0.66 |
| 1:A:254:LEU:HD12 | 1:A:283:GLU:HG3 | 1.77 | 0.66 |
| 2:N:75:LEU:HD21 | 2:N:215:PRO:CB | 2.23 | 0.66 |
| 1:M:242:LEU:CD2 | 1:M:244:THR:N | 2.56 | 0.66 |
| 4:D:50:SER:O | 4:D:51:TYR:C | 2.34 | 0.66 |
| 4:P:13:PHE:HE2 | 4:P:97:LYS:HG2 | 1.59 | 0.66 |
| 1:M:230:GLN:NE2 | 1:M:287:ARG:HH11 | 1.92 | 0.66 |
| 1:M:551:THR:HG22 | 1:M:552:LEU:H | 1.59 | 0.66 |
| 1:M:144:LEU:HD21 | 2:N:114:GLU:O | 1.95 | 0.66 |
| 4:P:105:ALA:O | 4:P:109:VAL:HG23 | 1.94 | 0.66 |
| 1:A:263:LEU:HB3 | 1:A:268:MET:HE2 | 1.76 | 0.66 |
| 1:A:182:GLN:NE2 | 1:A:184:ARG:NH1 | 2.43 | 0.66 |
| 1:M:233:PRO:HG2 | 1:M:234:THR:H | 1.59 | 0.66 |
| 2:B:26:TYR:HD2 | 2:B:47:LEU:CD1 | 2.07 | 0.66 |
| 1:M:346:GLU:HG3 | 1:M:347:PRO:CD | 2.25 | 0.66 |
| 2:N:167:PHE:HA | 2:N:199:ASN:HA | 1.78 | 0.66 |
| 1:M:192:THR:HG21 | 1:M:212:GLY:N | 2.10 | 0.66 |
| 2:N:75:LEU:CD2 | 2:N:215:PRO:HB3 | 2.23 | 0.66 |
| 1:A:181:VAL:HG23 | 1:A:182:GLN:N | 2.11 | 0.66 |
| 1:A:529:ARG:O | 1:A:530:GLY:C | 2.34 | 0.66 |
| 2:N:6:LEU:CD2 | 2:N:81:LEU:HD11 | 2.26 | 0.66 |
| 1:M:46:VAL:HB | 1:M:133:PHE:HD1 | 1.60 | 0.66 |
| 1:M:53:ALA:HB2 | 1:M:124:THR:HG23 | 1.77 | 0.66 |
| 1:A:234:THR:HG22 | 1:A:350:VAL:CG2 | 2.24 | 0.66 |
| 2:B:116:ILE:HD13 | 2:B:176:ALA:HB2 | 1.77 | 0.66 |
| 1:M:78:GLU:H | 1:M:224:ARG:HH22 | 1.44 | 0.66 |
| 2:N:97:PRO:O | 2:N:104:VAL:HA | 1.96 | 0.66 |
| 1:A:166:HIS:HB3 | 1:A:168:ARG:NH2 | 2.11 | 0.66 |
| 2:N:120:ILE:O | 2:N:121:ILE:HG23 | 1.94 | 0.66 |
| 2:N:145:PHE:HE1 | 2:N:219:ASP:HB3 | 1.61 | 0.66 |
| 3:O:130:TRP:CE3 | 3:O:130:TRP:HA | 2.29 | 0.66 |
| 1:A:437:LYS:HA | 1:A:440:VAL:HG23 | 1.77 | 0.66 |
| 3:C:9:ARG:HG2 | 3:C:9:ARG:HH11 | 1.61 | 0.66 |
| 2:N:54:ARG:HG2 | 2:N:54:ARG:NH1 | 2.07 | 0.65 |
| 1:M:195:ALA:O | 1:M:198:VAL:HG22 | 1.96 | 0.65 |
| 3:C:30:GLY:O | 3:C:32:ALA:N | 2.29 | 0.65 |
| 1:M:433:GLU:CG | 1:M:434:GLN:N | 2.59 | 0.65 |
| 3:O:50:LYS:CE | 4:P:118:ILE:HG22 | 2.22 | 0.65 |
| 1:M:78:GLU:N | 1:M:224:ARG:HH22 | 1.94 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:98:ILE:N | 2:N:98:ILE:HD12 | 2.11 | 0.65 |
| 2:N:149:ILE:CG1 | 2:N:151:CYS:HB3 | 2.25 | 0.65 |
| 1:M:217:LEU:HD11 | 1:M:555:ARG:CD | 2.26 | 0.65 |
| 3:C:53:PRO:HD3 | 4:D:51:TYR:OH | 1.97 | 0.65 |
| 1:M:452:ARG:CD | 1:M:508:LEU:HD22 | 2.26 | 0.65 |
| 2:B:14:ASN:OD1 | 2:B:16:GLU:N | 2.17 | 0.65 |
| 4:D:72:VAL:HG12 | 4:D:73:LEU:HD23 | 1.78 | 0.65 |
| 4:D:67:LEU:CD1 | 10:D:700:MQ7:H6 | 2.26 | 0.65 |
| 1:M:103:TRP:CZ3 | 1:M:131:THR:HG23 | 2.32 | 0.65 |
| 1:M:194:GLY:O | 1:M:357:THR:HG21 | 1.97 | 0.65 |
| 1:M:38:VAL:HG12 | 2:N:54:ARG:HH12 | 1.60 | 0.65 |
| 1:M:467:ARG:O | 1:M:534:ARG:HA | 1.97 | 0.65 |
| 1:M:188:VAL:HG12 | 1:M:188:VAL:O | 1.96 | 0.65 |
| 1:M:121:ILE:HD12 | 1:M:123:ARG:NH2 | 2.12 | 0.65 |
| 3:C:48:ALA:C | 3:C:50:LYS:H | 1.99 | 0.65 |
| 1:M:247:CYS:HB3 | 1:M:331:ILE:HD13 | 1.79 | 0.65 |
| 3:C:50:LYS:HZ2 | 4:D:118:ILE:HD12 | 1.57 | 0.64 |
| 2:N:106:MET:O | 2:N:110:ILE:HG12 | 1.96 | 0.64 |
| 1:A:253:ILE:CG2 | 1:A:315:ASP:HB2 | 2.26 | 0.64 |
| 2:B:65:CYS:O | 2:B:67:MET:HE3 | 1.97 | 0.64 |
| 4:D:72:VAL:O | 4:D:75:LEU:HB2 | 1.97 | 0.64 |
| 4:D:87:HIS:O | 4:D:89:LEU:N | 2.30 | 0.64 |
| 1:M:51:GLY:HA3 | 1:M:125:TRP:O | 1.96 | 0.64 |
| 1:A:562:ARG:NH1 | 1:A:562:ARG:HG3 | 2.09 | 0.64 |
| 2:N:155:TYR:HE1 | 2:N:171:ALA:CB | 2.10 | 0.64 |
| 1:A:65:HIS:ND1 | 1:A:86:VAL:CG2 | 2.60 | 0.64 |
| 1:M:226:MET:SD | 1:M:518:MET:HG2 | 2.38 | 0.64 |
| 1:A:455:MET:SD | 1:A:512:LEU:HD23 | 2.37 | 0.64 |
| 1:A:18:ARG:HH22 | 1:A:404:ARG:HD2 | 1.62 | 0.64 |
| 1:M:232:HIS:O | 1:M:352:PRO:CA | 2.44 | 0.64 |
| 2:N:192:MET:O | 2:N:195:LEU:N | 2.29 | 0.64 |
| 4:D:36:GLY:C | 4:D:37:ILE:HD12 | 2.18 | 0.64 |
| 2:N:44:LYS:HB2 | 2:N:49:PRO:HA | 1.80 | 0.64 |
| 1:M:230:GLN:NE2 | 1:M:287:ARG:NH1 | 2.46 | 0.64 |
| 2:B:206:PHE:CD2 | 2:B:206:PHE:O | 2.51 | 0.64 |
| 2:N:73:PRO:O | 2:N:74:LYS:HG3 | 1.98 | 0.64 |
| 2:N:30:TYR:CB | 2:N:81:LEU:HD13 | 2.27 | 0.64 |
| 4:P:30:VAL:O | 4:P:33:LEU:HB3 | 1.98 | 0.64 |
| 1:M:53:ALA:N | 1:M:394:ASN:HB2 | 2.14 | 0.63 |
| 1:A:542:ARG:NH2 | 1:A:544:ASP:OD1 | 2.31 | 0.63 |
| 1:A:38:VAL:CG2 | 1:A:38:VAL:O | 2.44 | 0.63 |
| 1:M:15:ALA:HB2 | 1:M:399:LEU:CD2 | 2.25 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:214:GLY:HA3 | 1:M:510:HIS:HB3 | 1.81 | 0.63 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:CA | 2.29 | 0.63 |
| 1:A:527:GLU:OE2 | 1:A:529:ARG:NH1 | 2.30 | 0.63 |
| 1:A:388:ALA:O | 1:A:389:ASN:CB | 2.41 | 0.63 |
| 2:B:132:ASN:ND2 | 2:B:184:ARG:HD3 | 2.13 | 0.63 |
| 1:M:32:ILE:HG23 | 1:M:149:ILE:HA | 1.79 | 0.63 |
| 3:C:65:ASN:O | 3:C:69:VAL:HG23 | 1.98 | 0.63 |
| 1:M:466:TYR:O | 1:M:467:ARG:HG3 | 1.97 | 0.63 |
| 1:M:527:GLU:HB3 | 1:M:543:ASP:OD2 | 1.98 | 0.63 |
| 2:N:206:PHE:CD1 | 2:N:225:GLN:HG2 | 2.34 | 0.63 |
| 1:A:279:ASN:O | 1:A:280:LYS:HB2 | 1.99 | 0.63 |
| 1:A:41:MET:CE | 2:B:150:ASN:HD22 | 2.11 | 0.63 |
| 1:A:455:MET:O | 1:A:458:ALA:HB3 | 1.98 | 0.63 |
| 1:A:479:LEU:HB3 | 1:A:516:GLU:HG2 | 1.81 | 0.63 |
| 1:M:403:GLY:HA2 | 1:M:406:ALA:CB | 2.27 | 0.63 |
| 1:A:529:ARG:NH2 | 1:A:544:ASP:OD2 | 2.32 | 0.63 |
| 1:A:279:ASN:HD21 | 1:A:280:LYS:HD3 | 1.63 | 0.63 |
| 2:B:4:LYS:HZ2 | 2:B:4:LYS:HB2 | 1.62 | 0.63 |
| 1:A:90:PRO:HG2 | 1:A:91:THR:H | 1.62 | 0.63 |
| 2:N:99:GLU:HB2 | 2:N:103:VAL:HB | 1.80 | 0.63 |
| 1:M:161:LEU:HD21 | 1:M:429:ALA:HA | 1.79 | 0.62 |
| 1:M:9:ILE:HG12 | 1:M:189:VAL:HB | 1.81 | 0.62 |
| 1:M:83:ASP:O | 1:M:87:HIS:ND1 | 2.33 | 0.62 |
| 1:M:182:GLN:NE2 | 1:M:429:ALA:HB1 | 2.15 | 0.62 |
| 2:B:67:MET:CE | 2:B:76:ALA:HB2 | 2.29 | 0.62 |
| 2:N:160:GLN:NE2 | 2:N:160:GLN:HA | 2.13 | 0.62 |
| 1:M:311:VAL:HB | 1:M:350:VAL:O | 1.99 | 0.62 |
| 1:M:105:ARG:HH12 | 1:M:109:GLY:HA2 | 1.64 | 0.62 |
| 1:M:228:PHE:HE2 | 1:M:387:GLY:O | 1.82 | 0.62 |
| 2:N:152:GLY:N | 8:N:246:SF4:S4 | 2.72 | 0.62 |
| 1:A:412:GLU:HG3 | 1:A:413:ARG:N | 2.06 | 0.62 |
| 2:N:4:LYS:C | 2:N:5:ASN:HD22 | 2.02 | 0.62 |
| 1:A:44:HIS:CE1 | 1:A:205:GLY:H | 2.16 | 0.62 |
| 1:M:18:ARG:HD3 | 1:M:18:ARG:O | 1.99 | 0.62 |
| 2:N:37:LEU:HD23 | 2:N:38:ASP:H | 1.64 | 0.62 |
| 2:N:192:MET:O | 2:N:193:ALA:C | 2.38 | 0.62 |
| 2:N:109:PHE:CE1 | 2:N:113:LEU:HD11 | 2.34 | 0.62 |
| 1:M:73:GLY:CA | 1:M:387:GLY:HA3 | 2.30 | 0.62 |
| 1:M:53:ALA:H | 1:M:394:ASN:HB2 | 1.64 | 0.62 |
| 2:N:75:LEU:H | 2:N:75:LEU:HD23 | 1.64 | 0.62 |
| 1:A:27:ASN:HD21 | 1:A:30:ALA:N | 1.98 | 0.62 |
| 2:B:211:SER:CA | 2:B:220:PRO:HD2 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:196:ASN:O | 2:N:197:SER:HB3 | 2.00 | 0.62 |
| 2:B:118:PRO:O | 2:B:179:TYR:CE2 | 2.53 | 0.62 |
| 3:O:48:ALA:C | 3:O:50:LYS:H | 2.03 | 0.62 |
| 1:M:328:LEU:HD12 | 1:M:331:ILE:HD11 | 1.82 | 0.62 |
| 2:B:189:LYS:HE3 | 2:B:190:GLU:OE1 | 2.00 | 0.62 |
| 1:A:467:ARG:O | 1:A:534:ARG:HA | 1.99 | 0.62 |
| 2:B:206:PHE:O | 2:B:206:PHE:HD2 | 1.83 | 0.62 |
| 1:M:5:ALA:O | 1:M:185:ALA:HA | 2.00 | 0.62 |
| 1:A:536:ASP:OD1 | 1:A:536:ASP:N | 2.32 | 0.62 |
| 2:B:157:ALA:HB1 | 2:B:209:TYR:CD2 | 2.34 | 0.62 |
| 1:A:447:ASN:O | 1:A:448:TRP:C | 2.36 | 0.62 |
| 1:A:115:ARG:HG3 | 1:A:115:ARG:NH1 | 2.02 | 0.62 |
| 1:M:182:GLN:HG3 | 1:M:182:GLN:O | 2.00 | 0.62 |
| 3:O:60:VAL:HG12 | 3:O:64:GLN:NE2 | 2.13 | 0.62 |
| 1:A:408:GLU:O | 1:A:411:THR:N | 2.33 | 0.62 |
| 1:M:103:TRP:HZ3 | 1:M:131:THR:HG23 | 1.65 | 0.61 |
| 1:M:43:SER:HB3 | 1:M:136:LEU:HD21 | 1.82 | 0.61 |
| 1:M:229:VAL:HB | 1:M:467:ARG:NH2 | 2.14 | 0.61 |
| 1:M:549:LYS:HB2 | 1:M:566:SER:H | 1.65 | 0.61 |
| 4:D:35:VAL:HG13 | 10:D:700:MQ7:O1 | 2.00 | 0.61 |
| 1:A:335:ALA:O | 1:A:339:VAL:HG23 | 2.00 | 0.61 |
| 1:A:335:ALA:O | 1:A:339:VAL:CG2 | 2.49 | 0.61 |
| 1:M:525:ARG:HA | 1:M:547:PHE:CE2 | 2.35 | 0.61 |
| 1:M:223:LEU:HD22 | 1:M:517:CYS:SG | 2.39 | 0.61 |
| 1:M:46:VAL:HG23 | 1:M:47:ALA:N | 2.16 | 0.61 |
| 1:M:78:GLU:O | 1:M:80:ASP:N | 2.33 | 0.61 |
| 2:N:149:ILE:O | 2:N:151:CYS:N | 2.33 | 0.61 |
| 1:M:434:GLN:O | 1:M:437:LYS:N | 2.30 | 0.61 |
| 1:A:155:HIS:CD2 | 1:A:174:ASN:CA | 2.84 | 0.61 |
| 4:D:12:VAL:CG1 | 4:D:13:PHE:N | 2.63 | 0.61 |
| 3:O:76:LEU:O | 3:O:76:LEU:HD12 | 2.01 | 0.61 |
| 3:O:49:LEU:HD21 | 4:P:55:LEU:HA | 1.81 | 0.61 |
| 1:A:166:HIS:HB3 | 1:A:168:ARG:HH21 | 1.66 | 0.61 |
| 1:A:41:MET:HE2 | 2:B:150:ASN:HD22 | 1.65 | 0.61 |
| 1:A:562:ARG:HH11 | 1:A:562:ARG:CG | 2.09 | 0.61 |
| 1:M:439:LEU:HD23 | 1:M:442:GLN:HE22 | 1.64 | 0.61 |
| 1:A:27:ASN:HD21 | 1:A:29:ASN:N | 1.97 | 0.61 |
| 1:A:236:LEU:HD21 | 1:A:243:MET:SD | 2.39 | 0.61 |
| 1:M:236:LEU:HG | 1:M:237:PRO:HD2 | 1.81 | 0.61 |
| 1:A:287:ARG:NH2 | 5:A:702:FLC:OB1 | 2.33 | 0.61 |
| 4:P:23:TRP:C | 4:P:23:TRP:CD1 | 2.74 | 0.61 |
| 2:N:189:LYS:O | 2:N:191:ARG:N | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:O:39:SER:OG | 4:P:71:ILE:O | 2.18 | 0.61 |
| 2:B:173:ILE:HG23 | 2:B:195:LEU:CD2 | 2.31 | 0.61 |
| 1:M:356:TYR:HB2 | 1:M:390:ARG:NH2 | 2.15 | 0.61 |
| 1:A:390:ARG:NH1 | 5:A:702:FLC:CAC | 2.64 | 0.61 |
| 1:M:455:MET:HG2 | 1:M:456:GLY:N | 2.15 | 0.61 |
| 1:M:430:ALA:O | 1:M:433:GLU:HG2 | 2.01 | 0.61 |
| 1:M:405:LEU:HA | 1:M:408:GLU:HB2 | 1.82 | 0.61 |
| 1:M:226:MET:HG3 | 1:M:518:MET:N | 2.14 | 0.61 |
| 1:M:356:TYR:HD1 | 1:M:390:ARG:CZ | 2.14 | 0.61 |
| 1:A:263:LEU:CB | 1:A:268:MET:CE | 2.68 | 0.61 |
| 1:M:12:ALA:HB2 | 1:M:36:SER:HB2 | 1.83 | 0.60 |
| 1:M:208:VAL:O | 1:M:208:VAL:HG12 | 2.01 | 0.60 |
| 1:M:264:GLN:HB3 | 1:M:282:MET:HE1 | 1.82 | 0.60 |
| 2:B:26:TYR:CD2 | 2:B:47:LEU:CD1 | 2.85 | 0.60 |
| 1:A:441:ASN:O | 1:A:442:GLN:C | 2.37 | 0.60 |
| 1:M:446:GLU:HB3 | 1:M:488:ARG:O | 2.01 | 0.60 |
| 1:M:55:VAL:CB | 1:M:90:PRO:HG3 | 2.29 | 0.60 |
| 2:N:75:LEU:CD2 | 2:N:75:LEU:N | 2.63 | 0.60 |
| 4:P:43:LEU:N | 4:P:43:LEU:CD2 | 2.60 | 0.60 |
| 3:C:33:VAL:HB | 3:C:34:PRO:HD3 | 1.82 | 0.60 |
| 1:A:239:SER:CB | 1:A:241:ILE:HD12 | 2.30 | 0.60 |
| 1:M:72:GLY:HA3 | 1:M:391:LEU:CD2 | 2.20 | 0.60 |
| 1:A:211:ASP:CB | 9:A:703:FAD:H61A | 2.12 | 0.60 |
| 1:A:545:VAL:HG12 | 1:A:546:ASN:CG | 2.20 | 0.60 |
| 3:O:83:THR:HG23 | 3:O:87:PHE:CE1 | 2.35 | 0.60 |
| 3:O:53:PRO:HB3 | 4:P:51:TYR:CE2 | 2.35 | 0.60 |
| 4:D:99:VAL:CG1 | 4:D:100:PHE:N | 2.64 | 0.60 |
| 1:M:236:LEU:HD22 | 1:M:241:ILE:HD12 | 1.84 | 0.60 |
| 1:M:226:MET:CG | 1:M:518:MET:HG2 | 2.31 | 0.60 |
| 1:M:395:SER:O | 1:M:398:GLU:HB3 | 2.00 | 0.60 |
| 2:N:204:CYS:O | 2:N:228:LYS:NZ | 2.34 | 0.60 |
| 5:A:702:FLC:OA2 | 9:A:703:FAD:C2 | 2.50 | 0.60 |
| 1:M:553:ALA:O | 1:M:562:ARG:HG2 | 2.01 | 0.60 |
| 1:M:56:ALA:C | 1:M:57:GLN:HG2 | 2.21 | 0.60 |
| 1:M:55:VAL:HG22 | 1:M:65:HIS:HD2 | 1.65 | 0.60 |
| 1:M:462:GLY:HA2 | 1:M:471:LEU:HD13 | 1.84 | 0.60 |
| 3:O:27:LEU:HD23 | 3:O:81:LEU:CD2 | 2.31 | 0.60 |
| 2:N:120:ILE:HD13 | 2:N:185:ASP:HB2 | 1.81 | 0.60 |
| 1:M:551:THR:CG2 | 1:M:552:LEU:H | 2.14 | 0.60 |
| 1:M:554:PHE:O | 1:M:555:ARG:HG3 | 2.02 | 0.60 |
| 1:A:447:ASN:ND2 | 1:A:449:ALA:HB3 | 2.16 | 0.60 |
| 1:A:1:GLN:NE2 | 1:A:3:PHE:CZ | 2.69 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:243:MET:HE2 | 1:M:348:ILE:HG21 | 1.84 | 0.60 |
| 1:M:228:PHE:CZ | 1:M:388:ALA:HA | 2.36 | 0.60 |
| 1:M:35:ILE:HG22 | 1:M:36:SER:N | 2.16 | 0.60 |
| 1:M:57:GLN:O | 1:M:58:ASP:CB | 2.50 | 0.60 |
| 3:C:36:VAL:HG22 | 4:D:75:LEU:CD2 | 2.32 | 0.60 |
| 1:M:42:ARG:CZ | 2:N:54:ARG:NE | 2.64 | 0.60 |
| 4:P:32:ILE:O | 4:P:33:LEU:C | 2.38 | 0.60 |
| 1:M:315:ASP:OD1 | 1:M:317:ARG:HG2 | 2.02 | 0.60 |
| 1:M:175:MET:HG2 | 1:M:503:LEU:HD11 | 1.83 | 0.60 |
| 1:M:552:LEU:HD12 | 1:M:564:GLU:HB3 | 1.84 | 0.59 |
| 1:A:256:ASN:OD1 | 1:A:260:TYR:N | 2.34 | 0.59 |
| 2:N:239:THR:C | 2:N:240:LEU:HD23 | 2.22 | 0.59 |
| 1:M:89:CYS:HB3 | 1:M:90:PRO:HD3 | 1.83 | 0.59 |
| 3:O:4:ARG:HH21 | 3:O:6:PRO:HG2 | 1.66 | 0.59 |
| 1:M:180:LEU:CD1 | 1:M:433:GLU:HB2 | 2.29 | 0.59 |
| 4:D:79:LEU:HD12 | 4:D:104:ALA:HB2 | 1.83 | 0.59 |
| 2:N:236:LEU:HD12 | 2:N:240:LEU:HD21 | 1.84 | 0.59 |
| 1:M:55:VAL:HG22 | 1:M:65:HIS:CD2 | 2.36 | 0.59 |
| 1:M:551:THR:HA | 1:M:564:GLU:O | 2.02 | 0.59 |
| 2:B:225:GLN:HG2 | 3:C:93:ALA:CB | 2.23 | 0.59 |
| 1:M:82:VAL:O | 1:M:86:VAL:HG22 | 2.01 | 0.59 |
| 4:D:67:LEU:HD13 | 10:D:700:MQ7:H6 | 1.83 | 0.59 |
| 2:N:173:ILE:HG23 | 2:N:195:LEU:CD2 | 2.33 | 0.59 |
| 2:N:193:ALA:HB1 | 4:P:5:PRO:HG3 | 1.84 | 0.59 |
| 2:N:13:TYR:O | 2:N:100:ARG:HG3 | 2.02 | 0.59 |
| 1:M:18:ARG:NH1 | 1:M:22:ALA:HB2 | 2.17 | 0.59 |
| 1:M:44:HIS:CE1 | 9:M:803:FAD:C8M | 2.76 | 0.59 |
| 1:M:161:LEU:HD13 | 1:M:425:ILE:HG22 | 1.84 | 0.59 |
| 1:M:43:SER:HB3 | 1:M:136:LEU:CD2 | 2.33 | 0.59 |
| 1:M:281:TYR:O | 1:M:282:MET:HB3 | 2.02 | 0.59 |
| 1:M:295:TRP:CZ3 | 1:M:466:TYR:HB3 | 2.38 | 0.59 |
| 4:P:41:LEU:O | 4:P:43:LEU:CD2 | 2.50 | 0.59 |
| 1:M:171:VAL:HA | 1:M:181:VAL:O | 2.03 | 0.59 |
| 2:B:173:ILE:HG23 | 2:B:195:LEU:HD22 | 1.84 | 0.59 |
| 1:M:304:ILE:N | 1:M:304:ILE:HD12 | 2.18 | 0.59 |
| 1:A:282:MET:HE3 | 1:A:283:GLU:OE1 | 2.03 | 0.59 |
| 1:A:493:ASP:CB | 1:A:499:ASN:ND2 | 2.63 | 0.59 |
| 1:A:324:LEU:O | 1:A:326:GLU:N | 2.36 | 0.59 |
| 1:A:279:ASN:ND2 | 1:A:280:LYS:HD3 | 2.17 | 0.59 |
| 1:M:39:TYR:HB3 | 1:M:40:PRO:HD2 | 1.84 | 0.59 |
| 1:M:451:ILE:O | 1:M:455:MET:HB3 | 2.03 | 0.59 |
| 2:N:241:LYS:C | 2:N:243:ARG:N | 2.56 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:O:30:GLY:O | 3:O:32:ALA:N | 2.35 | 0.59 |
| 3:O:105:PRO:HD2 | 3:O:106:GLU:HG3 | 1.84 | 0.59 |
| 3:C:128:LEU:HD22 | 4:D:45:PRO:HD2 | 1.85 | 0.58 |
| 1:M:356:TYR:HD1 | 1:M:390:ARG:NE | 2.01 | 0.58 |
| 1:M:42:ARG:NH2 | 2:N:54:ARG:HB3 | 2.15 | 0.58 |
| 1:A:2:THR:CG2 | 1:A:3:PHE:N | 2.65 | 0.58 |
| 4:P:113:ILE:O | 4:P:114:GLY:C | 2.42 | 0.58 |
| 4:P:35:VAL:HG22 | 10:P:800:MQ7:O1 | 2.03 | 0.58 |
| 2:N:108:HIS:O | 2:N:112:SER:N | 2.30 | 0.58 |
| 1:A:68:ASP:OD2 | 1:A:119:MET:HB3 | 2.03 | 0.58 |
| 1:M:539:CYS:SG | 1:M:541:GLU:O | 2.60 | 0.58 |
| 2:N:6:LEU:HD21 | 2:N:8:ILE:HD11 | 1.85 | 0.58 |
| 2:N:196:ASN:N | 2:N:196:ASN:ND2 | 2.47 | 0.58 |
| 1:A:329:PRO:HD2 | 1:A:330:PHE:H | 1.68 | 0.58 |
| 2:N:36:LEU:HB3 | 2:N:76:ALA:HB1 | 1.85 | 0.58 |
| 1:A:91:THR:HG22 | 1:A:92:GLU:N | 2.17 | 0.58 |
| 2:N:98:ILE:HD11 | 3:O:9:ARG:HE | 1.69 | 0.58 |
| 4:D:23:TRP:C | 4:D:25:ALA:H | 2.06 | 0.58 |
| 1:M:263:LEU:CD1 | 1:M:283:GLU:H | 2.16 | 0.58 |
| 1:M:226:MET:HG3 | 1:M:518:MET:CG | 2.32 | 0.58 |
| 3:C:50:LYS:HD3 | 4:D:118:ILE:CB | 2.26 | 0.58 |
| 2:N:8:ILE:CG2 | 2:N:9:GLU:H | 2.16 | 0.58 |
| 2:B:72:VAL:CG1 | 2:B:73:PRO:HD2 | 2.33 | 0.58 |
| 1:M:15:ALA:HB1 | 1:M:377:VAL:HG12 | 1.86 | 0.58 |
| 1:M:214:GLY:HA3 | 1:M:510:HIS:CG | 2.39 | 0.58 |
| 2:N:68:MET:CE | 2:N:73:PRO:HB3 | 2.33 | 0.58 |
| 2:N:9:GLU:HG3 | 2:N:24:ALA:O | 2.03 | 0.58 |
| 1:M:485:ARG:O | 1:M:485:ARG:HG2 | 2.03 | 0.58 |
| 1:M:53:ALA:HB2 | 1:M:394:ASN:ND2 | 2.18 | 0.58 |
| 2:N:193:ALA:HB1 | 4:P:5:PRO:CG | 2.34 | 0.58 |
| 2:B:75:LEU:CD2 | 2:B:153:LEU:HD11 | 2.33 | 0.58 |
| 1:M:115:ARG:HD3 | 1:M:122:GLU:HA | 1.86 | 0.58 |
| 1:M:54:ALA:N | 1:M:125:TRP:CD1 | 2.71 | 0.58 |
| 1:M:225:ASP:OD2 | 1:M:550:HIS:CE1 | 2.57 | 0.58 |
| 1:A:18:ARG:NH2 | 1:A:404:ARG:HD2 | 2.18 | 0.58 |
| 2:N:196:ASN:HA | 2:N:201:VAL:CG1 | 2.34 | 0.58 |
| 1:M:263:LEU:HD12 | 1:M:283:GLU:N | 2.19 | 0.58 |
| 1:M:84:TYR:CE2 | 1:M:405:LEU:HD11 | 2.39 | 0.58 |
| 2:B:180:ASN:ND2 | 2:B:188:LYS:CG | 2.60 | 0.58 |
| 1:M:147:PRO:C | 1:M:149:ILE:H | 2.07 | 0.58 |
| 4:D:82:MET:HA | 4:D:85:ALA:HB3 | 1.86 | 0.58 |
| 2:B:121:ILE:HB | 2:B:187:GLY:HA3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:306:THR:CB | 1:A:307:PRO:CD | 2.73 | 0.58 |
| 1:M:554:PHE:HD2 | 1:M:560:THR:HB | 1.69 | 0.58 |
| 4:P:72:VAL:O | 4:P:75:LEU:N | 2.36 | 0.58 |
| 1:M:78:GLU:H | 1:M:224:ARG:NH2 | 2.02 | 0.57 |
| 1:M:9:ILE:HB | 1:M:34:LEU:HD12 | 1.84 | 0.57 |
| 2:N:37:LEU:HD22 | 2:N:77:CYS:HA | 1.85 | 0.57 |
| 4:P:117:THR:O | 4:P:118:ILE:CB | 2.51 | 0.57 |
| 3:O:32:ALA:O | 3:O:35:ALA:HB3 | 2.04 | 0.57 |
| 1:M:551:THR:CG2 | 1:M:552:LEU:N | 2.65 | 0.57 |
| 2:N:167:PHE:HA | 2:N:199:ASN:CA | 2.34 | 0.57 |
| 3:O:17:LYS:HG3 | 3:O:23:ARG:NH2 | 2.17 | 0.57 |
| 4:P:75:LEU:HD11 | 4:P:107:LEU:HD13 | 1.86 | 0.57 |
| 1:M:332:CYS:O | 1:M:336:LYS:HG3 | 2.04 | 0.57 |
| 2:B:135:THR:O | 2:B:137:ALA:N | 2.37 | 0.57 |
| 1:A:42:ARG:HD3 | 2:B:62:CYS:O | 2.03 | 0.57 |
| 1:M:92:GLU:CD | 1:M:400:VAL:HG12 | 2.25 | 0.57 |
| 1:A:262:TYR:CE1 | 1:A:263:LEU:CD2 | 2.87 | 0.57 |
| 1:M:207:ILE:HG23 | 1:M:208:VAL:HG23 | 1.86 | 0.57 |
| 1:M:78:GLU:HB3 | 1:M:81:VAL:HG23 | 1.87 | 0.57 |
| 1:M:95:GLN:O | 1:M:98:LEU:HB3 | 2.04 | 0.57 |
| 2:N:149:ILE:O | 2:N:150:ASN:C | 2.42 | 0.57 |
| 2:B:211:SER:HA | 2:B:220:PRO:CD | 2.35 | 0.57 |
| 4:D:2:ASN:OD1 | 4:D:4:ASN:O | 2.23 | 0.57 |
| 1:A:273:PRO:HG2 | 1:A:276:GLU:HB2 | 1.85 | 0.57 |
| 1:A:417:ALA:C | 1:A:418:GLY:O | 2.40 | 0.57 |
| 1:M:77:CYS:O | 1:M:568:VAL:HG13 | 2.04 | 0.57 |
| 1:A:256:ASN:HD21 | 1:A:260:TYR:HB3 | 1.69 | 0.57 |
| 5:A:702:FLC:OA1 | 9:A:703:FAD:C10 | 2.52 | 0.57 |
| 2:B:109:PHE:CD1 | 2:B:113:LEU:HD11 | 2.39 | 0.57 |
| 2:N:196:ASN:ND2 | 2:N:196:ASN:H | 2.00 | 0.57 |
| 4:D:9:ASP:C | 4:D:11:PRO:HD2 | 2.24 | 0.57 |
| 3:O:130:TRP:HE3 | 3:O:130:TRP:HA | 1.70 | 0.57 |
| 4:P:112:LEU:O | 4:P:116:VAL:HG22 | 2.05 | 0.57 |
| 1:A:224:ARG:HB2 | 1:A:552:LEU:HD23 | 1.87 | 0.57 |
| 1:M:103:TRP:O | 1:M:105:ARG:HD2 | 2.05 | 0.57 |
| 2:N:133:ILE:HG23 | 2:N:133:ILE:O | 2.04 | 0.57 |
| 3:C:9:ARG:HD3 | 3:C:9:ARG:H | 1.70 | 0.57 |
| 1:A:465:ILE:HG22 | 1:A:465:ILE:O | 2.02 | 0.57 |
| 2:N:51:LEU:HA | 2:N:101:ASP:OD2 | 2.04 | 0.57 |
| 1:M:194:GLY:N | 1:M:208:VAL:CG1 | 2.67 | 0.57 |
| 1:A:253:ILE:HG12 | 1:A:261:ARG:CD | 2.24 | 0.57 |
| 4:D:55:LEU:O | 4:D:59:GLN:HB2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:12:ALA:HB2 | 1:A:34:LEU:HD21 | 1.87 | 0.57 |
| 1:M:33:ALA:HA | 1:M:150:GLN:O | 2.05 | 0.57 |
| 1:M:103:TRP:HE3 | 1:M:126:PHE:O | 1.88 | 0.57 |
| 2:N:149:ILE:HG13 | 2:N:149:ILE:O | 2.05 | 0.57 |
| 2:N:68:MET:HE3 | 2:N:93:LEU:HD12 | 1.87 | 0.57 |
| 1:M:256:ASN:HD22 | 1:M:262:TYR:HB3 | 1.69 | 0.57 |
| 3:C:21:PHE:O | 3:C:21:PHE:HD2 | 1.88 | 0.57 |
| 1:M:537:GLU:CD | 1:M:537:GLU:H | 2.06 | 0.57 |
| 2:B:31:ASP:C | 2:B:31:ASP:OD2 | 2.43 | 0.57 |
| 2:N:125:ARG:NH2 | 2:N:131:THR:O | 2.38 | 0.57 |
| 1:M:372:LYS:O | 1:M:413:ARG:NE | 2.38 | 0.57 |
| 1:A:70:VAL:HG11 | 1:A:573:LEU:HD23 | 1.87 | 0.57 |
| 1:M:194:GLY:HA3 | 1:M:379:GLU:HG2 | 1.87 | 0.56 |
| 1:M:568:VAL:HG12 | 1:M:570:ILE:HG13 | 1.86 | 0.56 |
| 1:M:129:ASP:HB2 | 1:M:328:LEU:HB3 | 1.87 | 0.56 |
| 1:A:424:ALA:O | 1:A:427:ALA:HB3 | 2.05 | 0.56 |
| 1:M:276:GLU:N | 1:M:277:PRO:CD | 2.66 | 0.56 |
| 1:A:40:PRO:CG | 1:A:140:PHE:CE1 | 2.87 | 0.56 |
| 4:D:23:TRP:O | 4:D:25:ALA:N | 2.37 | 0.56 |
| 1:A:523:MET:HG3 | 1:A:523:MET:O | 2.04 | 0.56 |
| 1:M:40:PRO:HG3 | 1:M:140:PHE:CE1 | 2.40 | 0.56 |
| 3:C:45:GLY:CA | 3:C:59:PHE:CE2 | 2.87 | 0.56 |
| 2:N:112:SER:O | 2:N:116:ILE:HG23 | 2.05 | 0.56 |
| 1:M:102:PRO:HD2 | 1:M:134:HIS:HB3 | 1.86 | 0.56 |
| 1:A:230:GLN:NE2 | 1:A:287:ARG:HE | 2.03 | 0.56 |
| 1:M:452:ARG:HG3 | 1:M:508:LEU:HD22 | 1.86 | 0.56 |
| 1:M:151:ARG:HH12 | 1:M:153:ASP:CG | 2.07 | 0.56 |
| 1:A:324:LEU:C | 1:A:326:GLU:N | 2.56 | 0.56 |
| 3:C:17:LYS:HG2 | 3:C:23:ARG:HH22 | 1.70 | 0.56 |
| 1:M:483:GLN:HG3 | 1:M:512:LEU:HD13 | 1.88 | 0.56 |
| 4:P:42:GLY:O | 4:P:44:PHE:N | 2.35 | 0.56 |
| 1:M:114:ARG:O | 1:M:115:ARG:HG2 | 2.04 | 0.56 |
| 1:M:32:ILE:HG22 | 1:M:148:GLN:O | 2.05 | 0.56 |
| 1:A:282:MET:CE | 1:A:283:GLU:OE1 | 2.54 | 0.56 |
| 4:D:78:GLY:O | 4:D:82:MET:HG2 | 2.05 | 0.56 |
| 1:A:2:THR:HG22 | 1:A:3:PHE:N | 2.20 | 0.56 |
| 3:C:45:GLY:HA2 | 3:C:59:PHE:CE2 | 2.40 | 0.56 |
| 1:M:162:VAL:HG12 | 1:M:163:ASP:N | 2.20 | 0.56 |
| 3:C:83:THR:HG23 | 3:C:87:PHE:CE2 | 2.40 | 0.56 |
| 3:O:28:ARG:O | 3:O:31:THR:HB | 2.06 | 0.56 |
| 4:D:87:HIS:C | 4:D:89:LEU:H | 2.07 | 0.56 |
| 3:C:17:LYS:HG3 | 3:C:23:ARG:HH12 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:180:ASN:HD21 | 2:B:188:LYS:HG3 | 1.68 | 0.56 |
| 1:M:295:TRP:CH2 | 1:M:535:LEU:HD11 | 2.41 | 0.56 |
| 3:C:123:ILE:HG23 | 10:D:700:MQ7:H161 | 1.88 | 0.56 |
| 1:A:416:THR:HG22 | 1:A:416:THR:O | 2.01 | 0.56 |
| 2:B:68:MET:HE3 | 2:B:72:VAL:C | 2.25 | 0.56 |
| 4:D:87:HIS:C | 4:D:89:LEU:N | 2.59 | 0.56 |
| 3:O:15:TRP:CD2 | 3:O:16:TRP:N | 2.74 | 0.56 |
| 1:M:53:ALA:HB2 | 1:M:394:ASN:HD22 | 1.71 | 0.56 |
| 2:N:166:GLU:HB2 | 2:N:199:ASN:OD1 | 2.06 | 0.56 |
| 2:N:175:LEU:O | 2:N:178:ARG:HB3 | 2.05 | 0.56 |
| 4:P:7:ARG:HH11 | 4:P:7:ARG:HB2 | 1.71 | 0.56 |
| 2:N:162:GLY:O | 3:O:11:MET:CG | 2.41 | 0.56 |
| 1:M:222:PRO:CB | 1:M:552:LEU:HD22 | 2.35 | 0.55 |
| 1:M:93:MET:CB | 1:M:125:TRP:CH2 | 2.89 | 0.55 |
| 4:P:28:ALA:N | 4:P:29:PRO:HD2 | 2.21 | 0.55 |
| 3:C:36:VAL:HG12 | 3:C:37:TRP:N | 2.21 | 0.55 |
| 1:M:76:LEU:HB2 | 1:M:529:ARG:HD3 | 1.88 | 0.55 |
| 3:C:45:GLY:N | 3:C:59:PHE:CE2 | 2.74 | 0.55 |
| 1:A:46:VAL:CG2 | 1:A:47:ALA:N | 2.69 | 0.55 |
| 4:P:19:ALA:O | 4:P:20:GLY:O | 2.24 | 0.55 |
| 1:M:252:GLY:O | 1:M:283:GLU:HG2 | 2.06 | 0.55 |
| 1:M:144:LEU:HD13 | 2:N:114:GLU:HG3 | 1.88 | 0.55 |
| 2:N:221:ALA:O | 2:N:225:GLN:NE2 | 2.39 | 0.55 |
| 1:M:555:ARG:CG | 1:M:560:THR:H | 2.19 | 0.55 |
| 2:B:68:MET:CE | 2:B:72:VAL:C | 2.74 | 0.55 |
| 1:M:263:LEU:HD12 | 1:M:283:GLU:CA | 2.36 | 0.55 |
| 1:A:37:LYS:HG3 | 1:A:38:VAL:HG13 | 1.86 | 0.55 |
| 1:M:499:ASN:O | 1:M:503:LEU:HG | 2.07 | 0.55 |
| 2:B:63:GLY:CA | 2:B:149:ILE:HD12 | 2.36 | 0.55 |
| 1:M:115:ARG:HA | 1:M:124:THR:OG1 | 2.07 | 0.55 |
| 1:M:53:ALA:HB2 | 1:M:124:THR:CG2 | 2.37 | 0.55 |
| 1:M:268:MET:HB3 | 1:M:282:MET:HB3 | 1.88 | 0.55 |
| 1:M:57:GLN:C | 1:M:60:ASP:OD1 | 2.45 | 0.55 |
| 1:A:168:ARG:HG2 | 1:A:425:ILE:HD11 | 1.88 | 0.55 |
| 1:A:37:LYS:HG3 | 1:A:38:VAL:CG1 | 2.36 | 0.55 |
| 1:A:286:PRO:O | 1:A:289:LYS:HB2 | 2.06 | 0.55 |
| 1:A:106:ARG:O | 1:A:108:ASP:N | 2.40 | 0.55 |
| 2:B:167:PHE:HA | 2:B:199:ASN:HB3 | 1.87 | 0.55 |
| 1:M:264:GLN:HB3 | 1:M:282:MET:CE | 2.36 | 0.55 |
| 1:A:446:GLU:HB2 | 1:A:489:VAL:HA | 1.88 | 0.55 |
| 3:C:98:VAL:O | 3:C:99:LYS:HB2 | 2.07 | 0.55 |
| 1:M:527:GLU:OE1 | 1:M:543:ASP:HB2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:254:LEU:HA | 1:A:313:TYR:O | 2.07 | 0.55 |
| 1:M:276:GLU:O | 1:M:277:PRO:C | 2.44 | 0.55 |
| 1:M:35:ILE:HA | 1:M:152:PHE:O | 2.06 | 0.55 |
| 1:M:228:PHE:CE1 | 1:M:532:HIS:HB2 | 2.42 | 0.55 |
| 3:C:49:LEU:HD11 | 4:D:54:VAL:HG12 | 1.89 | 0.55 |
| 1:A:298:TRP:HA | 1:A:303:THR:HG23 | 1.89 | 0.55 |
| 4:P:112:LEU:HG | 4:P:112:LEU:O | 2.07 | 0.55 |
| 1:M:279:ASN:HD22 | 1:M:280:LYS:H | 1.55 | 0.55 |
| 1:M:386:HIS:O | 1:M:387:GLY:O | 2.25 | 0.55 |
| 1:A:93:MET:HE1 | 1:A:397:ALA:HA | 1.88 | 0.55 |
| 1:A:236:LEU:HD21 | 1:A:243:MET:HE2 | 1.87 | 0.55 |
| 2:N:210:CYS:SG | 2:N:221:ALA:N | 2.80 | 0.55 |
| 2:N:54:ARG:C | 2:N:55:TRP:CD1 | 2.81 | 0.55 |
| 2:N:121:ILE:N | 2:N:185:ASP:OD1 | 2.39 | 0.55 |
| 4:P:101:TYR:CD1 | 4:P:101:TYR:N | 2.75 | 0.55 |
| 1:M:52:SER:C | 1:M:125:TRP:HB2 | 2.27 | 0.55 |
| 2:N:6:LEU:CD1 | 2:N:81:LEU:HD21 | 2.33 | 0.55 |
| 2:B:75:LEU:C | 2:B:77:CYS:N | 2.52 | 0.55 |
| 1:A:411:THR:O | 1:A:414:ALA:HB3 | 2.07 | 0.55 |
| 1:M:114:ARG:NH1 | 1:M:114:ARG:HB2 | 2.21 | 0.54 |
| 2:N:98:ILE:HG12 | 3:O:9:ARG:NH2 | 2.07 | 0.54 |
| 1:A:429:ALA:O | 1:A:430:ALA:C | 2.45 | 0.54 |
| 1:M:455:MET:CE | 1:M:508:LEU:HD21 | 2.37 | 0.54 |
| 2:N:116:ILE:HG21 | 2:N:172:ALA:HB1 | 1.88 | 0.54 |
| 4:D:73:LEU:N | 4:D:73:LEU:HD23 | 2.22 | 0.54 |
| 1:M:447:ASN:HB3 | 1:M:450:LYS:CG | 2.38 | 0.54 |
| 2:B:75:LEU:C | 2:B:77:CYS:H | 2.06 | 0.54 |
| 1:M:225:ASP:O | 1:M:225:ASP:CG | 2.44 | 0.54 |
| 1:M:467:ARG:HH22 | 1:M:532:HIS:CA | 2.18 | 0.54 |
| 1:M:78:GLU:N | 1:M:224:ARG:NH2 | 2.55 | 0.54 |
| 3:O:50:LYS:HG2 | 4:P:118:ILE:HG23 | 1.89 | 0.54 |
| 1:A:446:GLU:OE1 | 1:A:485:ARG:HD3 | 2.06 | 0.54 |
| 4:D:113:ILE:O | 4:D:114:GLY:C | 2.45 | 0.54 |
| 3:C:65:ASN:OD1 | 3:C:66:PRO:HD2 | 2.06 | 0.54 |
| 1:M:426:GLU:HA | 1:M:429:ALA:HB3 | 1.90 | 0.54 |
| 1:A:324:LEU:HB2 | 1:A:325:HIS:ND1 | 2.22 | 0.54 |
| 2:B:135:THR:C | 2:B:137:ALA:N | 2.58 | 0.54 |
| 4:D:7:ARG:O | 4:D:7:ARG:HG2 | 2.06 | 0.54 |
| 1:M:75:TRP:HB2 | 1:M:529:ARG:NH2 | 2.23 | 0.54 |
| 1:M:96:LEU:HB2 | 1:M:103:TRP:HE1 | 1.72 | 0.54 |
| 1:A:38:VAL:HG23 | 1:A:39:TYR:O | 2.08 | 0.54 |
| 3:O:83:THR:HG22 | 3:O:87:PHE:CE1 | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:128:ASP:OD1 | 2:B:128:ASP:N | 2.40 | 0.54 |
| 1:M:60:ASP:HB3 | 1:M:121:ILE:CG2 | 2.36 | 0.54 |
| 1:M:9:ILE:HB | 1:M:34:LEU:CD1 | 2.37 | 0.54 |
| 1:M:82:VAL:CG2 | 1:M:385:LEU:HA | 2.30 | 0.54 |
| 1:A:89:CYS:N | 1:A:90:PRO:HD2 | 2.22 | 0.54 |
| 2:N:192:MET:O | 2:N:196:ASN:ND2 | 2.41 | 0.54 |
| 2:N:154:CYS:C | 2:N:156:ALA:H | 2.10 | 0.54 |
| 1:M:166:HIS:HB2 | 1:M:373:GLY:HA3 | 1.90 | 0.54 |
| 1:A:541:GLU:HA | 1:A:541:GLU:OE2 | 2.08 | 0.54 |
| 1:M:516:GLU:HA | 1:M:516:GLU:OE1 | 2.08 | 0.54 |
| 2:N:109:PHE:O | 2:N:113:LEU:HG | 2.08 | 0.54 |
| 2:N:175:LEU:O | 2:N:176:ALA:C | 2.44 | 0.54 |
| 1:M:99:TRP:CE3 | 1:M:142:THR:HG21 | 2.42 | 0.54 |
| 1:M:361:ILE:CG1 | 1:M:376:ALA:HB3 | 2.36 | 0.54 |
| 1:M:13:GLY:N | 9:M:803:FAD:H4B | 2.23 | 0.54 |
| 2:N:28:VAL:HG12 | 2:N:29:PRO:HD2 | 1.90 | 0.54 |
| 2:B:241:LYS:O | 2:B:242:PRO:C | 2.46 | 0.54 |
| 4:P:64:ARG:NH2 | 4:P:118:ILE:HA | 2.22 | 0.54 |
| 2:N:120:ILE:CD1 | 2:N:185:ASP:HB2 | 2.38 | 0.54 |
| 2:N:69:VAL:HG11 | 2:N:79:THR:CG2 | 2.29 | 0.54 |
| 2:N:75:LEU:CD2 | 2:N:75:LEU:H | 2.19 | 0.54 |
| 1:A:448:TRP:CG | 1:A:449:ALA:N | 2.75 | 0.54 |
| 1:A:71:ALA:HA | 1:A:75:TRP:CZ3 | 2.42 | 0.54 |
| 1:M:28:PRO:O | 1:M:30:ALA:N | 2.41 | 0.54 |
| 2:B:216:LYS:HA | 2:B:216:LYS:HE2 | 1.88 | 0.54 |
| 1:M:525:ARG:HA | 1:M:547:PHE:CD2 | 2.42 | 0.54 |
| 1:M:130:LYS:HZ3 | 2:N:216:LYS:HD3 | 1.72 | 0.54 |
| 3:O:50:LYS:C | 3:O:52:GLY:H | 2.11 | 0.54 |
| 4:D:37:ILE:N | 4:D:37:ILE:HD12 | 2.22 | 0.54 |
| 4:D:20:GLY:HA3 | 4:D:77:CYS:HB2 | 1.90 | 0.54 |
| 2:N:125:ARG:HA | 2:N:129:GLN:OE1 | 2.08 | 0.54 |
| 1:A:109:GLY:O | 2:B:133:ILE:HG23 | 2.08 | 0.54 |
| 1:M:103:TRP:CE3 | 1:M:126:PHE:O | 2.61 | 0.53 |
| 1:M:467:ARG:HB2 | 1:M:533:GLN:O | 2.08 | 0.53 |
| 1:M:549:LYS:CB | 1:M:566:SER:O | 2.56 | 0.53 |
| 2:N:206:PHE:O | 2:N:206:PHE:CD2 | 2.62 | 0.53 |
| 1:A:263:LEU:HB2 | 1:A:268:MET:HE3 | 1.87 | 0.53 |
| 2:B:26:TYR:CD2 | 2:B:47:LEU:HD13 | 2.33 | 0.53 |
| 3:O:12:THR:OG1 | 3:O:13:SER:N | 2.40 | 0.53 |
| 1:M:363:THR:HA | 1:M:368:GLU:O | 2.08 | 0.53 |
| 1:M:204:ASN:O | 2:N:58:ARG:CZ | 2.56 | 0.53 |
| 1:M:474:LYS:O | 1:M:478:LYS:HG2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:166:GLU:O | 2:N:199:ASN:HB3 | 2.08 | 0.53 |
| 3:O:28:ARG:HG3 | 3:O:85:THR:HG21 | 1.90 | 0.53 |
| 1:A:106:ARG:O | 1:A:107:PRO:C | 2.45 | 0.53 |
| 1:M:53:ALA:CA | 1:M:394:ASN:HD22 | 2.21 | 0.53 |
| 1:M:216:ALA:O | 1:M:217:LEU:C | 2.47 | 0.53 |
| 1:A:319:LEU:HD12 | 1:A:323:LYS:CE | 2.37 | 0.53 |
| 2:B:126:THR:H | 2:B:129:GLN:HG3 | 1.73 | 0.53 |
| 1:M:49:GLN:N | 1:M:49:GLN:HE21 | 2.00 | 0.53 |
| 1:M:228:PHE:HE1 | 1:M:532:HIS:HB2 | 1.73 | 0.53 |
| 1:A:115:ARG:CG | 1:A:115:ARG:HH11 | 2.09 | 0.53 |
| 1:M:162:VAL:HG12 | 1:M:163:ASP:H | 1.74 | 0.53 |
| 2:B:212:GLU:HG3 | 3:C:21:PHE:CE1 | 2.41 | 0.53 |
| 2:N:154:CYS:O | 2:N:156:ALA:N | 2.39 | 0.53 |
| 1:A:366:ASN:HB3 | 1:A:409:GLN:HG3 | 1.89 | 0.53 |
| 1:M:320:GLY:O | 1:M:324:LEU:HB2 | 2.09 | 0.53 |
| 2:N:73:PRO:HB2 | 2:N:153:LEU:CD2 | 2.39 | 0.53 |
| 2:N:8:ILE:CG2 | 2:N:9:GLU:N | 2.71 | 0.53 |
| 3:C:36:VAL:CG2 | 4:D:75:LEU:HD22 | 2.38 | 0.53 |
| 1:M:46:VAL:O | 1:M:48:ALA:N | 2.40 | 0.53 |
| 2:N:70:ASN:C | 2:N:72:VAL:H | 2.11 | 0.53 |
| 4:P:59:GLN:O | 4:P:64:ARG:NH1 | 2.41 | 0.53 |
| 2:N:44:LYS:C | 2:N:46:ASN:H | 2.10 | 0.53 |
| 1:M:157:VAL:HA | 1:M:172:ALA:HA | 1.91 | 0.53 |
| 1:M:194:GLY:N | 1:M:208:VAL:HG12 | 2.24 | 0.53 |
| 1:M:552:LEU:HD12 | 1:M:564:GLU:CB | 2.38 | 0.53 |
| 2:N:144:GLN:HG3 | 3:O:102:LYS:HZ1 | 1.68 | 0.53 |
| 2:N:192:MET:HE3 | 2:N:195:LEU:HB2 | 1.89 | 0.53 |
| 1:M:256:ASN:ND2 | 1:M:260:TYR:HB3 | 2.19 | 0.53 |
| 4:D:103:LEU:HA | 4:D:106:ILE:HD12 | 1.89 | 0.53 |
| 4:P:13:PHE:CE2 | 4:P:97:LYS:HG2 | 2.43 | 0.53 |
| 1:M:363:THR:OG1 | 1:M:367:CYS:HA | 2.09 | 0.53 |
| 2:N:219:ASP:CG | 2:N:222:ALA:HB3 | 2.29 | 0.53 |
| 1:A:57:GLN:HE21 | 1:A:122:GLU:HG2 | 1.72 | 0.53 |
| 1:M:281:TYR:O | 1:M:282:MET:CB | 2.57 | 0.53 |
| 1:M:554:PHE:O | 1:M:560:THR:O | 2.26 | 0.53 |
| 2:N:168:ILE:CD1 | 2:N:173:ILE:HG12 | 2.36 | 0.53 |
| 1:M:8:ALA:HB1 | 1:M:170:LEU:CD1 | 2.39 | 0.53 |
| 4:P:80:HIS:HD2 | 4:P:84:HIS:HD2 | 1.54 | 0.53 |
| 4:P:20:GLY:HA3 | 4:P:77:CYS:HB2 | 1.91 | 0.53 |
| 4:D:110:VAL:O | 4:D:113:ILE:HB | 2.09 | 0.53 |
| 1:A:500:THR:OG1 | 2:B:52:SER:HB3 | 2.09 | 0.53 |
| 2:B:53:TYR:HA | 2:B:103:VAL:HG22 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:74:ASP:O | 1:M:74:ASP:OD1 | 2.26 | 0.52 |
| 2:N:157:ALA:HB2 | 2:N:213:VAL:HG21 | 1.91 | 0.52 |
| 2:N:51:LEU:HD12 | 2:N:51:LEU:C | 2.28 | 0.52 |
| 3:O:126:VAL:CG1 | 10:P:800:MQ7:H141 | 2.38 | 0.52 |
| 1:A:496:SER:OG | 2:B:16:GLU:OE1 | 2.19 | 0.52 |
| 2:N:155:TYR:CZ | 2:N:169:GLY:HA3 | 2.45 | 0.52 |
| 1:M:263:LEU:CD1 | 1:M:283:GLU:HA | 2.39 | 0.52 |
| 2:N:236:LEU:O | 2:N:240:LEU:HD21 | 2.09 | 0.52 |
| 3:O:120:THR:HG23 | 4:P:30:VAL:HB | 1.91 | 0.52 |
| 2:N:94:ALA:O | 2:N:95:ASN:HB2 | 2.09 | 0.52 |
| 1:M:78:GLU:C | 1:M:80:ASP:H | 2.11 | 0.52 |
| 2:N:101:ASP:O | 2:N:102:LEU:HD23 | 2.09 | 0.52 |
| 2:B:110:ILE:CA | 2:B:113:LEU:HD12 | 2.27 | 0.52 |
| 1:M:110:SER:O | 1:M:111:VAL:C | 2.47 | 0.52 |
| 1:M:549:LYS:HB3 | 1:M:566:SER:O | 2.10 | 0.52 |
| 1:M:78:GLU:HB2 | 1:M:224:ARG:HH22 | 1.74 | 0.52 |
| 2:N:134:GLN:O | 2:N:135:THR:O | 2.27 | 0.52 |
| 1:A:390:ARG:NH2 | 5:A:702:FLC:OA1 | 2.42 | 0.52 |
| 2:B:219:ASP:OD2 | 2:B:222:ALA:HB2 | 2.09 | 0.52 |
| 2:N:173:ILE:HG23 | 2:N:195:LEU:HD22 | 1.90 | 0.52 |
| 2:B:15:PRO:HB3 | 3:C:5:LYS:H | 1.75 | 0.52 |
| 1:A:48:ALA:HB3 | 1:A:132:GLY:HA3 | 1.92 | 0.52 |
| 1:M:242:LEU:HD21 | 1:M:244:THR:HA | 1.92 | 0.52 |
| 1:M:363:THR:HB | 1:M:367:CYS:C | 2.30 | 0.52 |
| 1:M:96:LEU:HD12 | 1:M:103:TRP:HZ2 | 1.74 | 0.52 |
| 1:M:174:ASN:ND2 | 1:M:177:GLU:CG | 2.73 | 0.52 |
| 4:D:48:ALA:CA | 4:D:53:ARG:HD3 | 2.38 | 0.52 |
| 1:A:377:VAL:HG21 | 1:A:403:GLY:HA2 | 1.92 | 0.52 |
| 1:A:253:ILE:O | 1:A:314:LEU:CA | 2.55 | 0.52 |
| 1:M:242:LEU:HD21 | 1:M:244:THR:CA | 2.40 | 0.52 |
| 1:M:219:HIS:HB3 | 1:M:371:ILE:HD11 | 1.92 | 0.52 |
| 1:A:446:GLU:CG | 1:A:488:ARG:O | 2.53 | 0.52 |
| 4:D:103:LEU:HD23 | 4:D:103:LEU:O | 2.10 | 0.52 |
| 4:D:112:LEU:HA | 4:D:115:VAL:CG2 | 2.40 | 0.52 |
| 1:M:329:PRO:O | 1:M:333:GLU:HG3 | 2.09 | 0.52 |
| 1:M:79:GLN:CD | 1:M:570:ILE:HG23 | 2.30 | 0.52 |
| 4:P:35:VAL:HG22 | 10:P:800:MQ7:C1 | 2.40 | 0.52 |
| 4:P:50:SER:O | 4:P:51:TYR:C | 2.48 | 0.52 |
| 2:N:108:HIS:HA | 2:N:111:GLU:HB2 | 1.91 | 0.52 |
| 3:C:22:TYR:O | 3:C:25:TYR:HB3 | 2.10 | 0.52 |
| 1:M:211:ASP:CG | 1:M:507:GLU:HA | 2.30 | 0.52 |
| 1:A:253:ILE:HG21 | 1:A:315:ASP:CB | 2.29 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:M:555:ARG:HG2 | 1:M:558:ASP:O | 2.09 | 0.52 |
| 1:A:102:PRO:O | 1:A:103:TRP:C | 2.48 | 0.52 |
| 2:B:95:ASN:HD21 | 2:B:162:GLY:HA3 | 1.74 | 0.52 |
| 4:D:30:VAL:O | 4:D:33:LEU:HB3 | 2.09 | 0.52 |
| 1:A:96:LEU:HD11 | 1:A:400:VAL:HG21 | 1.91 | 0.52 |
| 4:D:41:LEU:O | 4:D:43:LEU:CD2 | 2.57 | 0.52 |
| 3:C:15:TRP:CD2 | 3:C:16:TRP:N | 2.78 | 0.52 |
| 1:M:106:ARG:HD2 | 1:M:110:SER:OG | 2.10 | 0.51 |
| 1:M:41:MET:CE | 1:M:42:ARG:HG3 | 2.39 | 0.51 |
| 1:M:229:VAL:CG2 | 1:M:467:ARG:CZ | 2.87 | 0.51 |
| 1:M:388:ALA:HB1 | 1:M:529:ARG:HB3 | 1.92 | 0.51 |
| 1:M:60:ASP:OD2 | 1:M:123:ARG:HD3 | 2.10 | 0.51 |
| 1:M:242:LEU:O | 1:M:242:LEU:HD23 | 2.10 | 0.51 |
| 1:M:158:LEU:HB3 | 1:M:436:LEU:CD1 | 2.41 | 0.51 |
| 1:M:106:ARG:HG3 | 1:M:108:ASP:OD1 | 2.09 | 0.51 |
| 1:M:211:ASP:HB3 | 9:M:803:FAD:H61A | 1.75 | 0.51 |
| 1:M:73:GLY:HA2 | 1:M:387:GLY:HA3 | 1.90 | 0.51 |
| 2:N:73:PRO:HB2 | 2:N:153:LEU:HD22 | 1.93 | 0.51 |
| 2:B:209:TYR:O | 2:B:213:VAL:HG13 | 2.10 | 0.51 |
| 1:M:92:GLU:OE2 | 1:M:401:VAL:HA | 2.10 | 0.51 |
| 2:B:162:GLY:O | 3:C:11:MET:SD | 2.68 | 0.51 |
| 1:M:495:SER:HB3 | 2:N:16:GLU:OE2 | 2.11 | 0.51 |
| 1:M:97:GLU:OE1 | 2:N:132:ASN:HB2 | 2.10 | 0.51 |
| 1:M:42:ARG:HH22 | 2:N:54:ARG:CB | 2.20 | 0.51 |
| 2:N:149:ILE:CG2 | 2:N:216:LYS:HG3 | 2.41 | 0.51 |
| 1:A:184:ARG:NH1 | 1:A:184:ARG:CG | 2.57 | 0.51 |
| 4:D:72:VAL:HG12 | 4:D:73:LEU:N | 2.24 | 0.51 |
| 4:P:66:PHE:CD2 | 4:P:66:PHE:C | 2.84 | 0.51 |
| 2:B:65:CYS:O | 2:B:67:MET:CE | 2.59 | 0.51 |
| 1:A:410:ALA:O | 1:A:411:THR:C | 2.47 | 0.51 |
| 3:C:97:ILE:HG23 | 3:C:101:GLU:O | 2.10 | 0.51 |
| 1:A:292:GLN:HG2 | 1:A:466:TYR:CZ | 2.45 | 0.51 |
| 1:M:467:ARG:NH2 | 1:M:533:GLN:H | 2.07 | 0.51 |
| 1:M:58:ASP:C | 1:M:60:ASP:H | 2.13 | 0.51 |
| 1:A:493:ASP:CG | 1:A:499:ASN:ND2 | 2.64 | 0.51 |
| 1:M:84:TYR:HE2 | 1:M:405:LEU:HD11 | 1.76 | 0.51 |
| 2:N:31:ASP:CG | 2:N:32:ALA:H | 2.13 | 0.51 |
| 2:B:70:ASN:O | 2:B:71:ASN:HB2 | 2.09 | 0.51 |
| 1:M:295:TRP:C | 1:M:295:TRP:CD1 | 2.83 | 0.51 |
| 2:N:214:CYS:HA | 8:N:246:SF4:S3 | 2.50 | 0.51 |
| 1:A:256:ASN:OD1 | 1:A:259:GLY:N | 2.42 | 0.51 |
| 1:A:12:ALA:HB1 | 1:A:40:PRO:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:468:THR:O | 1:M:472:MET:HG3 | 2.11 | 0.51 |
| 1:A:198:VAL:CG2 | 1:A:455:MET:CE | 2.88 | 0.51 |
| 4:D:68:PHE:CE1 | 4:D:72:VAL:HG21 | 2.45 | 0.51 |
| 1:A:328:LEU:HD11 | 1:A:331:ILE:HG13 | 1.93 | 0.51 |
| 1:A:245:GLU:O | 1:A:246:GLY:C | 2.47 | 0.51 |
| 1:M:382:SER:HG | 1:M:386:HIS:CE1 | 2.25 | 0.51 |
| 3:C:50:LYS:C | 3:C:52:GLY:H | 2.14 | 0.51 |
| 3:O:87:PHE:CD2 | 3:O:112:LEU:CD1 | 2.75 | 0.51 |
| 3:C:121:ILE:O | 3:C:123:ILE:N | 2.44 | 0.51 |
| 3:C:123:ILE:HG13 | 10:D:700:MQ7:H192 | 1.92 | 0.51 |
| 1:M:434:GLN:HA | 1:M:437:LYS:HB2 | 1.93 | 0.51 |
| 3:O:90:ALA:N | 3:O:91:PRO:CD | 2.73 | 0.51 |
| 1:M:191:ALA:HB2 | 1:M:377:VAL:O | 2.10 | 0.51 |
| 1:A:114:ARG:HD3 | 1:A:126:PHE:CE2 | 2.44 | 0.51 |
| 1:M:3:PHE:HB3 | 1:M:183:ILE:HG23 | 1.93 | 0.51 |
| 1:M:106:ARG:HB3 | 1:M:112:ASN:CB | 2.29 | 0.51 |
| 1:M:194:GLY:HA3 | 1:M:379:GLU:CG | 2.41 | 0.51 |
| 1:M:42:ARG:NE | 2:N:54:ARG:NH2 | 2.59 | 0.51 |
| 1:M:467:ARG:NH2 | 1:M:533:GLN:N | 2.59 | 0.51 |
| 1:M:328:LEU:HD23 | 1:M:328:LEU:H | 1.75 | 0.51 |
| 3:C:87:PHE:HD1 | 3:C:112:LEU:HD13 | 1.75 | 0.51 |
| 2:N:204:CYS:CB | 2:N:224:ILE:HG21 | 2.41 | 0.51 |
| 4:P:83:HIS:O | 4:P:86:MET:HB2 | 2.11 | 0.51 |
| 1:M:266:TYR:CE2 | 1:M:296:HIS:HB3 | 2.45 | 0.51 |
| 1:M:53:ALA:HB3 | 1:M:394:ASN:ND2 | 2.26 | 0.51 |
| 1:M:223:LEU:CD2 | 1:M:517:CYS:SG | 2.99 | 0.51 |
| 2:N:37:LEU:CD2 | 2:N:77:CYS:HA | 2.41 | 0.51 |
| 1:A:399:LEU:HD23 | 1:A:399:LEU:N | 2.25 | 0.51 |
| 1:M:221:VAL:HG23 | 1:M:371:ILE:HG13 | 1.92 | 0.51 |
| 1:A:65:HIS:CG | 1:A:86:VAL:CG2 | 2.94 | 0.51 |
| 4:P:103:LEU:HD21 | 4:P:107:LEU:HD11 | 1.93 | 0.51 |
| 3:C:88:GLU:HA | 3:C:109:ILE:HD13 | 1.93 | 0.51 |
| 3:C:12:THR:HG22 | 3:C:13:SER:H | 1.75 | 0.51 |
| 1:M:66:PHE:O | 1:M:70:VAL:HG23 | 2.10 | 0.51 |
| 1:M:104:SER:OG | 1:M:128:ALA:N | 2.43 | 0.50 |
| 1:M:214:GLY:HA3 | 1:M:510:HIS:CB | 2.41 | 0.50 |
| 1:M:461:GLU:HA | 1:M:466:TYR:OH | 2.11 | 0.50 |
| 4:D:28:ALA:O | 4:D:32:ILE:HG13 | 2.11 | 0.50 |
| 2:N:108:HIS:O | 2:N:109:PHE:C | 2.49 | 0.50 |
| 3:O:22:TYR:O | 3:O:25:TYR:HB3 | 2.11 | 0.50 |
| 1:A:557:ALA:C | 1:A:559:GLY:H | 2.15 | 0.50 |
| 3:O:37:TRP:CZ2 | 3:O:41:GLU:OE1 | 2.64 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:O:59:PHE:O | 3:O:62:PHE:HB3 | 2.10 | 0.50 |
| 2:N:28:VAL:HG11 | 2:N:39:ALA:O | 2.11 | 0.50 |
| 1:A:268:MET:O | 1:A:282:MET:HG2 | 2.11 | 0.50 |
| 1:M:167:VAL:CG2 | 1:M:374:LEU:HD13 | 2.36 | 0.50 |
| 1:A:280:LYS:C | 1:A:281:TYR:HD1 | 2.15 | 0.50 |
| 1:A:239:SER:OG | 1:A:240:GLY:N | 2.42 | 0.50 |
| 1:M:105:ARG:NH1 | 1:M:109:GLY:HA2 | 2.25 | 0.50 |
| 1:M:548:LEU:HG | 1:M:568:VAL:HB | 1.93 | 0.50 |
| 2:N:163:LEU:HG | 3:O:11:MET:HE3 | 1.94 | 0.50 |
| 1:M:213:MET:SD | 1:M:216:ALA:HB3 | 2.51 | 0.50 |
| 4:P:30:VAL:O | 4:P:33:LEU:N | 2.44 | 0.50 |
| 2:N:241:LYS:O | 2:N:243:ARG:N | 2.44 | 0.50 |
| 1:A:224:ARG:HB2 | 1:A:552:LEU:CD2 | 2.41 | 0.50 |
| 3:C:17:LYS:CG | 3:C:23:ARG:HH12 | 2.24 | 0.50 |
| 2:N:207:VAL:HG22 | 3:O:25:TYR:CZ | 2.46 | 0.50 |
| 1:M:266:TYR:HE2 | 1:M:296:HIS:HB3 | 1.77 | 0.50 |
| 2:N:134:GLN:OE1 | 2:N:184:ARG:HG3 | 2.12 | 0.50 |
| 1:A:215:MET:O | 1:A:219:HIS:HD2 | 1.93 | 0.50 |
| 1:A:255:VAL:HB | 1:A:259:GLY:HA2 | 1.92 | 0.50 |
| 1:A:527:GLU:HG2 | 1:A:547:PHE:HB2 | 1.90 | 0.50 |
| 1:A:250:GLU:HG3 | 1:A:328:LEU:HD23 | 1.93 | 0.50 |
| 2:N:31:ASP:CG | 2:N:32:ALA:N | 2.64 | 0.50 |
| 1:A:270:PRO:O | 1:A:271:GLU:C | 2.50 | 0.50 |
| 4:P:94:PRO:O | 4:P:95:ALA:C | 2.50 | 0.50 |
| 1:M:39:TYR:H | 1:M:39:TYR:HD1 | 1.58 | 0.50 |
| 1:M:79:GLN:NE2 | 1:M:570:ILE:HG23 | 2.26 | 0.50 |
| 2:N:196:ASN:HB3 | 2:N:231:SER:OG | 2.12 | 0.50 |
| 2:N:120:ILE:C | 2:N:121:ILE:HG13 | 2.32 | 0.50 |
| 1:A:413:ARG:CZ | 1:A:413:ARG:HB2 | 2.41 | 0.50 |
| 1:M:358:MET:SD | 1:M:386:HIS:CB | 3.00 | 0.50 |
| 1:M:92:GLU:CA | 1:M:95:GLN:HB3 | 2.38 | 0.50 |
| 2:N:135:THR:O | 2:N:137:ALA:N | 2.41 | 0.50 |
| 4:P:39:LEU:HD13 | 4:P:49:LEU:CD1 | 2.42 | 0.50 |
| 1:A:525:ARG:O | 1:A:527:GLU:N | 2.42 | 0.50 |
| 4:P:80:HIS:NE2 | 4:P:84:HIS:NE2 | 2.60 | 0.50 |
| 3:O:70:ILE:CG2 | 3:O:71:ILE:N | 2.74 | 0.50 |
| 3:O:106:GLU:HB2 | 3:O:107:PRO:HD3 | 1.94 | 0.50 |
| 2:N:219:ASP:H | 2:N:220:PRO:CD | 2.25 | 0.50 |
| 1:M:166:HIS:HD2 | 1:M:413:ARG:NH2 | 2.09 | 0.50 |
| 1:M:115:ARG:CD | 1:M:122:GLU:HA | 2.42 | 0.50 |
| 1:M:74:ASP:CB | 1:M:388:ALA:HB3 | 2.19 | 0.50 |
| 1:M:396:LEU:O | 1:M:399:LEU:HB2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:52:SER:C | 2:N:53:TYR:HD1 | 2.15 | 0.50 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:H | 1.77 | 0.50 |
| 1:M:151:ARG:NH1 | 1:M:153:ASP:OD1 | 2.39 | 0.50 |
| 4:D:23:TRP:C | 4:D:25:ALA:N | 2.64 | 0.50 |
| 2:B:176:ALA:O | 2:B:177:HIS:C | 2.48 | 0.50 |
| 2:B:57:CYS:HB3 | 2:B:62:CYS:HB3 | 1.94 | 0.50 |
| 1:A:59:HIS:CD2 | 1:A:121:ILE:HD12 | 2.47 | 0.50 |
| 1:A:266:TYR:CE2 | 1:A:296:HIS:HB3 | 2.46 | 0.50 |
| 1:M:527:GLU:CA | 1:M:539:CYS:SG | 2.87 | 0.49 |
| 1:A:232:HIS:HD2 | 1:A:234:THR:H | 1.60 | 0.49 |
| 1:A:0:MET:HG3 | 1:A:182:GLN:HG2 | 1.94 | 0.49 |
| 1:A:237:PRO:HB2 | 1:A:308:ARG:HB3 | 1.94 | 0.49 |
| 4:D:67:LEU:HD11 | 10:D:700:MQ7:H6 | 1.92 | 0.49 |
| 1:A:567:ASP:OD1 | 1:A:568:VAL:N | 2.45 | 0.49 |
| 1:M:203:THR:HA | 1:M:240:GLY:O | 2.12 | 0.49 |
| 1:A:252:GLY:HA2 | 1:A:316:LEU:HD23 | 1.93 | 0.49 |
| 1:A:155:HIS:NE2 | 1:A:174:ASN:HB2 | 2.27 | 0.49 |
| 3:C:36:VAL:CG1 | 3:C:37:TRP:N | 2.75 | 0.49 |
| 1:A:328:LEU:HD13 | 1:A:331:ILE:CG1 | 2.41 | 0.49 |
| 1:A:166:HIS:ND1 | 1:A:167:VAL:N | 2.60 | 0.49 |
| 1:A:239:SER:HB2 | 1:A:241:ILE:HD12 | 1.94 | 0.49 |
| 1:A:141:GLN:NE2 | 2:B:175:LEU:HD21 | 2.27 | 0.49 |
| 1:M:112:ASN:O | 1:M:126:PHE:HE2 | 1.94 | 0.49 |
| 1:M:127:ALA:HB3 | 1:M:131:THR:OG1 | 2.13 | 0.49 |
| 1:M:227:GLU:HB2 | 1:M:518:MET:C | 2.30 | 0.49 |
| 1:M:72:GLY:C | 1:M:74:ASP:H | 2.14 | 0.49 |
| 1:M:162:VAL:HG13 | 1:M:219:HIS:CE1 | 2.48 | 0.49 |
| 2:B:184:ARG:HH11 | 2:B:184:ARG:HG3 | 1.77 | 0.49 |
| 3:O:15:TRP:CE3 | 3:O:16:TRP:N | 2.80 | 0.49 |
| 2:B:142:TYR:CD1 | 2:B:142:TYR:C | 2.86 | 0.49 |
| 1:M:21:ILE:CD1 | 1:M:139:LEU:HD22 | 2.41 | 0.49 |
| 1:M:356:TYR:CD1 | 1:M:390:ARG:CZ | 2.95 | 0.49 |
| 1:A:390:ARG:NH1 | 5:A:702:FLC:OA2 | 2.44 | 0.49 |
| 1:A:133:PHE:CD2 | 1:A:133:PHE:C | 2.86 | 0.49 |
| 2:N:201:VAL:HG13 | 2:N:202:TRP:CD1 | 2.48 | 0.49 |
| 2:N:235:PHE:C | 2:N:237:ILE:N | 2.62 | 0.49 |
| 2:B:50:ASP:OD1 | 2:B:51:LEU:N | 2.44 | 0.49 |
| 2:B:75:LEU:HD21 | 2:B:153:LEU:HD11 | 1.94 | 0.49 |
| 4:P:19:ALA:O | 4:P:20:GLY:C | 2.50 | 0.49 |
| 1:M:257:LYS:HB2 | 1:M:302:ASN:C | 2.32 | 0.49 |
| 1:A:317:ARG:HB2 | 1:A:344:VAL:O | 2.12 | 0.49 |
| 1:M:491:ILE:HD13 | 1:M:502:LEU:HD13 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:45:THR:HB | 1:M:136:LEU:HD22 | 1.95 | 0.49 |
| 1:A:307:PRO:HD2 | 1:A:308:ARG:HG3 | 1.93 | 0.49 |
| 1:M:448:TRP:O | 1:M:452:ARG:NH1 | 2.42 | 0.49 |
| 1:A:489:VAL:HG22 | 1:A:489:VAL:O | 2.12 | 0.49 |
| 4:P:23:TRP:C | 4:P:25:ALA:H | 2.15 | 0.49 |
| 4:D:12:VAL:HG12 | 4:D:13:PHE:H | 1.78 | 0.49 |
| 3:O:125:PHE:HZ | 3:O:130:TRP:CZ3 | 2.29 | 0.49 |
| 4:P:37:ILE:HG22 | 4:P:38:LEU:N | 2.26 | 0.49 |
| 1:M:52:SER:HB2 | 1:M:396:LEU:HB2 | 1.91 | 0.49 |
| 1:M:53:ALA:H | 1:M:394:ASN:CB | 2.25 | 0.49 |
| 1:M:244:THR:O | 1:M:247:CYS:SG | 2.52 | 0.49 |
| 1:M:554:PHE:O | 1:M:555:ARG:CB | 2.61 | 0.49 |
| 3:C:121:ILE:O | 3:C:122:VAL:C | 2.47 | 0.49 |
| 1:M:468:THR:OG1 | 1:M:471:LEU:HG | 2.13 | 0.49 |
| 1:M:165:GLY:O | 1:M:166:HIS:HB3 | 2.11 | 0.49 |
| 1:M:263:LEU:HD13 | 1:M:283:GLU:H | 1.76 | 0.49 |
| 1:M:39:TYR:CD1 | 1:M:39:TYR:N | 2.80 | 0.49 |
| 1:M:461:GLU:H | 1:M:461:GLU:CD | 2.16 | 0.49 |
| 1:M:426:GLU:O | 1:M:430:ALA:N | 2.45 | 0.49 |
| 1:A:446:GLU:HB2 | 1:A:489:VAL:CB | 2.41 | 0.49 |
| 1:A:437:LYS:HG3 | 1:A:441:ASN:HD21 | 1.77 | 0.49 |
| 1:M:32:ILE:HG12 | 1:M:33:ALA:N | 2.27 | 0.49 |
| 3:O:33:VAL:HB | 3:O:34:PRO:CD | 2.43 | 0.49 |
| 2:N:209:TYR:HD1 | 2:N:212:GLU:HB3 | 1.76 | 0.49 |
| 1:M:226:MET:HG2 | 1:M:517:CYS:CB | 2.40 | 0.49 |
| 2:N:37:LEU:N | 2:N:37:LEU:HD23 | 2.27 | 0.49 |
| 1:M:328:LEU:HB2 | 1:M:331:ILE:CD1 | 2.43 | 0.49 |
| 4:P:62:ILE:HD13 | 10:P:800:MQ7:H212 | 1.94 | 0.49 |
| 2:N:192:MET:O | 2:N:195:LEU:HB2 | 2.13 | 0.49 |
| 4:P:30:VAL:HG13 | 4:P:31:MET:N | 2.28 | 0.49 |
| 4:D:72:VAL:HG22 | 4:D:108:THR:HG23 | 1.94 | 0.49 |
| 4:D:13:PHE:CE1 | 4:D:101:TYR:CD1 | 3.00 | 0.49 |
| 2:B:153:LEU:HD12 | 2:B:215:PRO:HD3 | 1.95 | 0.49 |
| 2:B:95:ASN:ND2 | 2:B:162:GLY:HA3 | 2.27 | 0.49 |
| 3:O:53:PRO:HB3 | 4:P:51:TYR:CG | 2.47 | 0.49 |
| 4:D:98:TRP:O | 4:D:99:VAL:C | 2.51 | 0.49 |
| 4:D:51:TYR:O | 4:D:52:GLU:C | 2.49 | 0.49 |
| 1:A:436:LEU:HD23 | 1:A:437:LYS:N | 2.27 | 0.49 |
| 2:B:57:CYS:O | 2:B:58:ARG:HB2 | 2.12 | 0.49 |
| 2:B:36:LEU:O | 2:B:40:LEU:HG | 2.12 | 0.49 |
| 1:M:53:ALA:HA | 1:M:125:TRP:HB2 | 1.94 | 0.49 |
| 1:A:350:VAL:CG2 | 1:A:350:VAL:O | 2.61 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:443:ASP:HA | 1:M:490:ARG:HA | 1.95 | 0.49 |
| 2:N:116:ILE:O | 2:N:191:ARG:HG3 | 2.13 | 0.49 |
| 1:A:103:TRP:O | 2:B:139:MET:CE | 2.60 | 0.49 |
| 1:M:469:PRO:HD3 | 1:M:536:ASP:OD2 | 2.13 | 0.49 |
| 2:N:80:PHE:HB2 | 2:N:82:ARG:HG2 | 1.95 | 0.49 |
| 1:M:106:ARG:HB2 | 1:M:112:ASN:HD22 | 1.78 | 0.48 |
| 1:M:361:ILE:HG22 | 1:M:363:THR:HG23 | 1.96 | 0.48 |
| 1:M:35:ILE:CG2 | 1:M:36:SER:N | 2.75 | 0.48 |
| 1:A:134:HIS:O | 1:A:138:THR:HB | 2.13 | 0.48 |
| 1:M:355:HIS:NE2 | 5:M:802:FLC:OB1 | 2.46 | 0.48 |
| 2:B:111:GLU:OE1 | 4:D:0:MET:HB2 | 2.13 | 0.48 |
| 2:B:54:ARG:NE | 2:B:103:VAL:CG1 | 2.76 | 0.48 |
| 1:A:363:THR:OG1 | 1:A:383:VAL:HA | 2.13 | 0.48 |
| 1:M:377:VAL:HG13 | 1:M:402:PHE:HD2 | 1.75 | 0.48 |
| 1:M:60:ASP:HB2 | 1:M:123:ARG:NH1 | 2.28 | 0.48 |
| 1:A:261:ARG:O | 1:A:264:GLN:NE2 | 2.31 | 0.48 |
| 3:C:48:ALA:C | 3:C:50:LYS:N | 2.66 | 0.48 |
| 4:P:64:ARG:HH22 | 4:P:118:ILE:HA | 1.78 | 0.48 |
| 2:B:26:TYR:CB | 2:B:43:ILE:HD13 | 2.43 | 0.48 |
| 4:P:23:TRP:HE1 | 4:P:70:MET:CE | 2.26 | 0.48 |
| 2:B:182:ASP:OD2 | 2:B:182:ASP:C | 2.51 | 0.48 |
| 1:M:158:LEU:HD13 | 1:M:436:LEU:HD12 | 1.94 | 0.48 |
| 2:N:31:ASP:H | 2:N:34:THR:HG21 | 1.78 | 0.48 |
| 1:M:338:TYR:O | 2:N:33:THR:HG22 | 2.13 | 0.48 |
| 1:M:65:HIS:HB2 | 1:M:123:ARG:CZ | 2.42 | 0.48 |
| 1:M:34:LEU:O | 1:M:152:PHE:N | 2.44 | 0.48 |
| 1:M:8:ALA:HB1 | 1:M:170:LEU:HD12 | 1.95 | 0.48 |
| 4:D:0:MET:CG | 4:D:1:ILE:H | 2.21 | 0.48 |
| 4:D:4:ASN:C | 4:D:4:ASN:ND2 | 2.67 | 0.48 |
| 1:M:159:ASP:OD2 | 1:M:432:VAL:HG22 | 2.14 | 0.48 |
| 3:C:37:TRP:CE2 | 3:C:41:GLU:OE2 | 2.67 | 0.48 |
| 1:A:490:ARG:HG2 | 1:A:491:ILE:N | 2.28 | 0.48 |
| 1:A:294:PHE:CZ | 1:A:351:ARG:HG3 | 2.49 | 0.48 |
| 1:A:366:ASN:O | 1:A:367:CYS:CB | 2.60 | 0.48 |
| 1:M:517:CYS:O | 1:M:521:SER:HB2 | 2.12 | 0.48 |
| 1:A:232:HIS:CD2 | 1:A:234:THR:H | 2.32 | 0.48 |
| 1:M:476:ILE:HG12 | 1:M:519:ALA:CB | 2.29 | 0.48 |
| 1:M:455:MET:HB2 | 1:M:482:LEU:HD21 | 1.95 | 0.48 |
| 4:P:0:MET:O | 4:P:1:ILE:HG12 | 2.12 | 0.48 |
| 2:N:235:PHE:O | 2:N:237:ILE:N | 2.45 | 0.48 |
| 3:O:27:LEU:HD23 | 3:O:81:LEU:HD21 | 1.95 | 0.48 |
| 3:O:15:TRP:CE3 | 3:O:16:TRP:HA | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:529:ARG:O | 1:M:530:GLY:C | 2.52 | 0.48 |
| 1:M:42:ARG:CZ | 2:N:54:ARG:CZ | 2.92 | 0.48 |
| 2:N:53:TYR:O | 2:N:54:ARG:HG3 | 2.13 | 0.48 |
| 1:M:174:ASN:HD22 | 1:M:177:GLU:HB2 | 1.79 | 0.48 |
| 1:M:371:ILE:HD12 | 1:M:374:LEU:HD23 | 1.96 | 0.48 |
| 3:O:62:PHE:CE1 | 3:O:68:ILE:HG12 | 2.48 | 0.48 |
| 1:M:104:SER:H | 1:M:127:ALA:HA | 1.78 | 0.48 |
| 1:M:227:GLU:HG3 | 1:M:463:CYS:HG | 1.74 | 0.48 |
| 1:M:452:ARG:CG | 1:M:508:LEU:HD22 | 2.42 | 0.48 |
| 3:C:63:LEU:CB | 4:D:40:PRO:HG3 | 2.36 | 0.48 |
| 1:M:490:ARG:CD | 1:M:490:ARG:H | 2.21 | 0.48 |
| 2:B:13:TYR:OH | 3:C:5:LYS:HE3 | 2.14 | 0.48 |
| 1:M:192:THR:CG2 | 1:M:212:GLY:H | 2.25 | 0.48 |
| 1:A:448:TRP:CZ2 | 1:A:504:TYR:HD1 | 2.32 | 0.48 |
| 2:B:121:ILE:O | 2:B:186:HIS:N | 2.47 | 0.48 |
| 3:O:56:TRP:O | 3:O:59:PHE:HB3 | 2.13 | 0.48 |
| 1:M:225:ASP:O | 1:M:225:ASP:OD1 | 2.32 | 0.48 |
| 1:M:78:GLU:C | 1:M:80:ASP:N | 2.66 | 0.48 |
| 1:A:540:THR:C | 1:A:541:GLU:OE2 | 2.49 | 0.48 |
| 4:D:20:GLY:HA2 | 4:D:73:LEU:HB3 | 1.94 | 0.48 |
| 1:M:263:LEU:HD12 | 1:M:283:GLU:HA | 1.94 | 0.48 |
| 3:O:79:ALA:O | 3:O:80:LEU:C | 2.50 | 0.48 |
| 1:M:46:VAL:C | 1:M:48:ALA:H | 2.16 | 0.48 |
| 4:P:32:ILE:O | 4:P:36:GLY:N | 2.45 | 0.48 |
| 3:C:124:LEU:O | 3:C:128:LEU:HB2 | 2.14 | 0.48 |
| 4:D:66:PHE:C | 4:D:66:PHE:CD2 | 2.87 | 0.48 |
| 1:M:92:GLU:OE1 | 1:M:400:VAL:HG12 | 2.13 | 0.48 |
| 1:M:440:VAL:HA | 1:M:491:ILE:HD12 | 1.96 | 0.48 |
| 2:N:216:LYS:HA | 2:N:216:LYS:NZ | 2.29 | 0.47 |
| 1:A:253:ILE:HG22 | 1:A:315:ASP:N | 2.29 | 0.47 |
| 1:M:555:ARG:CD | 1:M:559:GLY:HA2 | 2.44 | 0.47 |
| 1:A:17:LEU:HD11 | 1:A:140:PHE:HA | 1.95 | 0.47 |
| 2:N:104:VAL:HG23 | 2:N:106:MET:SD | 2.53 | 0.47 |
| 3:C:98:VAL:HG23 | 3:C:99:LYS:HE3 | 1.96 | 0.47 |
| 1:A:109:GLY:C | 2:B:133:ILE:HG23 | 2.34 | 0.47 |
| 3:O:67:VAL:C | 3:O:69:VAL:N | 2.66 | 0.47 |
| 1:A:427:ALA:HA | 1:A:430:ALA:HB2 | 1.97 | 0.47 |
| 3:C:27:LEU:O | 3:C:28:ARG:C | 2.49 | 0.47 |
| 4:D:10:GLU:N | 4:D:11:PRO:HD2 | 2.29 | 0.47 |
| 2:N:31:ASP:H | 2:N:34:THR:CG2 | 2.27 | 0.47 |
| 1:M:228:PHE:CE2 | 1:M:387:GLY:O | 2.65 | 0.47 |
| 2:N:157:ALA:CB | 2:N:213:VAL:HG21 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:4:LYS:C | 2:N:5:ASN:ND2 | 2.67 | 0.47 |
| 2:N:64:SER:O | 2:N:66:GLY:N | 2.47 | 0.47 |
| 4:D:32:ILE:O | 4:D:36:GLY:N | 2.42 | 0.47 |
| 1:A:43:SER:O | 1:A:46:VAL:HG13 | 2.14 | 0.47 |
| 1:M:255:VAL:CG2 | 1:M:313:TYR:HB2 | 2.42 | 0.47 |
| 2:N:10:VAL:HG22 | 2:N:90:VAL:CG2 | 2.44 | 0.47 |
| 1:M:157:VAL:HG12 | 1:M:215:MET:SD | 2.54 | 0.47 |
| 2:N:145:PHE:CE1 | 2:N:219:ASP:HB3 | 2.45 | 0.47 |
| 1:M:448:TRP:CG | 1:M:449:ALA:N | 2.82 | 0.47 |
| 2:N:201:VAL:O | 2:N:201:VAL:HG22 | 2.14 | 0.47 |
| 1:A:479:LEU:HA | 1:A:479:LEU:HD23 | 1.37 | 0.47 |
| 1:M:483:GLN:CG | 1:M:512:LEU:HD13 | 2.45 | 0.47 |
| 1:A:558:ASP:OD2 | 1:A:560:THR:OG1 | 2.32 | 0.47 |
| 1:M:268:MET:HG2 | 1:M:282:MET:HA | 1.97 | 0.47 |
| 1:M:46:VAL:CG2 | 1:M:47:ALA:N | 2.78 | 0.47 |
| 1:M:53:ALA:HB3 | 1:M:392:GLY:O | 2.14 | 0.47 |
| 2:N:174:THR:HG21 | 2:N:218:VAL:HG11 | 1.96 | 0.47 |
| 1:A:287:ARG:NH1 | 1:A:287:ARG:CG | 2.42 | 0.47 |
| 1:M:555:ARG:HG3 | 1:M:560:THR:H | 1.78 | 0.47 |
| 3:C:27:LEU:C | 3:C:29:GLU:N | 2.65 | 0.47 |
| 2:N:107:THR:O | 2:N:111:GLU:HG3 | 2.14 | 0.47 |
| 1:A:551:THR:O | 1:A:552:LEU:HD23 | 2.15 | 0.47 |
| 4:D:30:VAL:CG1 | 4:D:31:MET:N | 2.78 | 0.47 |
| 1:M:470:GLU:CD | 1:M:470:GLU:O | 2.53 | 0.47 |
| 1:M:131:THR:O | 1:M:135:MET:HB2 | 2.15 | 0.47 |
| 1:A:261:ARG:HD2 | 1:A:282:MET:HE1 | 1.95 | 0.47 |
| 5:A:702:FLC:OA1 | 9:A:703:FAD:N1 | 2.47 | 0.47 |
| 1:A:182:GLN:O | 1:A:182:GLN:HG3 | 2.14 | 0.47 |
| 4:P:39:LEU:HG | 4:P:40:PRO:N | 2.29 | 0.47 |
| 2:B:73:PRO:O | 2:B:74:LYS:HG3 | 2.15 | 0.47 |
| 1:M:224:ARG:HG3 | 1:M:550:HIS:HB2 | 1.97 | 0.47 |
| 2:N:70:ASN:O | 2:N:72:VAL:N | 2.47 | 0.47 |
| 1:A:277:PRO:HG2 | 1:A:277:PRO:O | 2.15 | 0.47 |
| 3:C:50:LYS:NZ | 4:D:118:ILE:CD1 | 2.57 | 0.47 |
| 2:B:180:ASN:OD1 | 2:B:191:ARG:HD2 | 2.14 | 0.47 |
| 1:A:2:THR:OG1 | 1:A:182:GLN:NE2 | 2.47 | 0.47 |
| 2:B:242:PRO:O | 2:B:243:ARG:C | 2.51 | 0.47 |
| 1:M:452:ARG:HD2 | 1:M:452:ARG:N | 2.29 | 0.47 |
| 2:N:30:TYR:CG | 2:N:81:LEU:HD22 | 2.50 | 0.47 |
| 3:O:102:LYS:HG3 | 3:O:102:LYS:O | 2.13 | 0.47 |
| 2:N:44:LYS:C | 2:N:46:ASN:N | 2.68 | 0.47 |
| 3:C:82:HIS:HE2 | 4:D:25:ALA:HB2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:511:GLY:O | 1:A:512:LEU:C | 2.50 | 0.47 |
| 1:M:22:ALA:CB | 1:M:404:ARG:HA | 2.45 | 0.47 |
| 1:A:109:GLY:HA3 | 2:B:133:ILE:CG2 | 2.45 | 0.47 |
| 1:A:154:GLU:OE2 | 2:B:54:ARG:NH2 | 2.48 | 0.47 |
| 4:P:34:LEU:HA | 4:P:38:LEU:HB2 | 1.96 | 0.47 |
| 1:M:526:LYS:CD | 1:M:526:LYS:O | 2.58 | 0.47 |
| 1:M:388:ALA:HB1 | 1:M:529:ARG:CB | 2.45 | 0.47 |
| 2:N:4:LYS:O | 2:N:5:ASN:ND2 | 2.41 | 0.47 |
| 1:A:91:THR:O | 1:A:94:THR:HB | 2.15 | 0.47 |
| 2:B:75:LEU:HB3 | 2:B:77:CYS:HB3 | 1.97 | 0.47 |
| 1:A:298:TRP:HA | 1:A:303:THR:CG2 | 2.45 | 0.47 |
| 4:P:13:PHE:HE2 | 4:P:97:LYS:CG | 2.27 | 0.47 |
| 2:N:175:LEU:O | 2:N:178:ARG:N | 2.48 | 0.47 |
| 1:M:518:MET:O | 1:M:521:SER:HB3 | 2.15 | 0.47 |
| 4:D:64:ARG:HH21 | 4:D:118:ILE:HA | 1.80 | 0.47 |
| 1:M:244:THR:HG23 | 1:M:244:THR:O | 2.14 | 0.47 |
| 3:O:123:ILE:HD12 | 10:P:800:MQ7:H162 | 1.93 | 0.47 |
| 2:B:119:TYR:O | 2:B:121:ILE:HG13 | 2.15 | 0.47 |
| 1:A:386:HIS:O | 1:A:387:GLY:C | 2.49 | 0.47 |
| 1:M:230:GLN:HG2 | 1:M:390:ARG:NH2 | 2.25 | 0.47 |
| 1:M:279:ASN:HD22 | 1:M:279:ASN:C | 2.15 | 0.47 |
| 1:A:230:GLN:CD | 1:A:287:ARG:HE | 2.17 | 0.47 |
| 4:D:61:PHE:HA | 4:D:64:ARG:HB2 | 1.97 | 0.47 |
| 4:D:105:ALA:O | 4:D:106:ILE:C | 2.53 | 0.47 |
| 1:M:194:GLY:HA3 | 1:M:379:GLU:CD | 2.35 | 0.46 |
| 1:M:228:PHE:HE1 | 1:M:532:HIS:CB | 2.28 | 0.46 |
| 3:C:88:GLU:HA | 3:C:109:ILE:CD1 | 2.45 | 0.46 |
| 4:P:65:VAL:O | 4:P:69:LEU:HG | 2.16 | 0.46 |
| 2:N:56:SER:O | 2:N:57:CYS:HB3 | 2.15 | 0.46 |
| 3:O:43:ILE:O | 3:O:44:PHE:C | 2.53 | 0.46 |
| 1:M:279:ASN:O | 1:M:280:LYS:HG2 | 2.15 | 0.46 |
| 1:M:49:GLN:O | 1:M:50:GLY:C | 2.54 | 0.46 |
| 2:N:35:SER:HB3 | 2:N:77:CYS:HA | 1.97 | 0.46 |
| 1:A:324:LEU:C | 1:A:326:GLU:H | 2.18 | 0.46 |
| 1:M:263:LEU:CD1 | 1:M:283:GLU:N | 2.77 | 0.46 |
| 1:M:236:LEU:CB | 1:M:241:ILE:H | 2.28 | 0.46 |
| 1:M:418:GLY:O | 1:M:419:ASN:CG | 2.53 | 0.46 |
| 1:M:193:GLY:HA3 | 1:M:208:VAL:HA | 1.96 | 0.46 |
| 1:M:521:SER:O | 1:M:525:ARG:HG3 | 2.16 | 0.46 |
| 2:N:220:PRO:HG2 | 2:N:221:ALA:H | 1.80 | 0.46 |
| 1:A:2:THR:O | 1:A:3:PHE:CD1 | 2.68 | 0.46 |
| 1:A:427:ALA:C | 1:A:430:ALA:HB3 | 2.35 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:1:ILE:CG2 | 4:D:1:ILE:O | 2.56 | 0.46 |
| 4:D:100:PHE:C | 4:D:102:GLY:N | 2.68 | 0.46 |
| 1:M:297:GLU:OE1 | 1:M:297:GLU:HA | 2.14 | 0.46 |
| 3:O:14:THR:O | 3:O:17:LYS:HB3 | 2.16 | 0.46 |
| 3:O:49:LEU:HD11 | 4:P:55:LEU:HB2 | 1.98 | 0.46 |
| 4:D:10:GLU:C | 4:D:12:VAL:H | 2.18 | 0.46 |
| 1:A:197:ARG:HB2 | 1:A:208:VAL:O | 2.16 | 0.46 |
| 1:M:103:TRP:CE3 | 1:M:127:ALA:HB2 | 2.51 | 0.46 |
| 4:P:10:GLU:N | 4:P:11:PRO:HD3 | 2.31 | 0.46 |
| 1:A:181:VAL:CG2 | 1:A:182:GLN:N | 2.78 | 0.46 |
| 2:N:108:HIS:CE1 | 2:N:112:SER:OG | 2.68 | 0.46 |
| 1:M:147:PRO:C | 1:M:149:ILE:N | 2.69 | 0.46 |
| 1:A:504:TYR:HA | 1:A:507:GLU:OE1 | 2.16 | 0.46 |
| 1:M:237:PRO:O | 1:M:239:SER:N | 2.37 | 0.46 |
| 2:N:209:TYR:CD1 | 2:N:212:GLU:HB3 | 2.50 | 0.46 |
| 1:M:56:ALA:O | 1:M:57:GLN:HG2 | 2.16 | 0.46 |
| 1:M:80:ASP:O | 1:M:83:ASP:HB3 | 2.16 | 0.46 |
| 3:O:48:ALA:C | 3:O:50:LYS:N | 2.68 | 0.46 |
| 1:M:187:ALA:CB | 1:M:410:ALA:HB1 | 2.43 | 0.46 |
| 2:N:189:LYS:C | 2:N:191:ARG:H | 2.15 | 0.46 |
| 4:D:53:ARG:O | 4:D:56:ALA:HB3 | 2.15 | 0.46 |
| 1:M:503:LEU:C | 1:M:505:THR:H | 2.18 | 0.46 |
| 4:P:98:TRP:O | 4:P:99:VAL:C | 2.52 | 0.46 |
| 1:M:130:LYS:HB2 | 1:M:134:HIS:CE1 | 2.51 | 0.46 |
| 1:M:383:VAL:HG13 | 1:M:402:PHE:CD1 | 2.50 | 0.46 |
| 1:M:42:ARG:NE | 2:N:54:ARG:HH21 | 2.14 | 0.46 |
| 1:A:255:VAL:CG1 | 1:A:261:ARG:HG2 | 2.43 | 0.46 |
| 3:C:27:LEU:O | 3:C:29:GLU:N | 2.48 | 0.46 |
| 2:B:97:PRO:O | 2:B:104:VAL:CG2 | 2.62 | 0.46 |
| 4:D:84:HIS:O | 4:D:86:MET:N | 2.48 | 0.46 |
| 1:A:328:LEU:CD1 | 1:A:331:ILE:CG1 | 2.91 | 0.46 |
| 4:P:103:LEU:CD2 | 4:P:107:LEU:HD11 | 2.46 | 0.46 |
| 1:A:391:LEU:O | 1:A:392:GLY:C | 2.51 | 0.46 |
| 2:B:127:ALA:C | 2:B:129:GLN:N | 2.68 | 0.46 |
| 1:M:10:VAL:CG1 | 1:M:157:VAL:HG21 | 2.46 | 0.46 |
| 1:M:360:GLY:C | 1:M:361:ILE:HD12 | 2.36 | 0.46 |
| 1:M:52:SER:HB2 | 1:M:396:LEU:CD2 | 2.45 | 0.46 |
| 2:B:43:ILE:HG22 | 2:B:48:ALA:HB3 | 1.97 | 0.46 |
| 4:P:29:PRO:HG2 | 4:P:30:VAL:H | 1.81 | 0.46 |
| 1:A:168:ARG:HD3 | 1:A:168:ARG:HA | 1.67 | 0.46 |
| 3:C:17:LYS:HG2 | 3:C:23:ARG:NH2 | 2.30 | 0.46 |
| 1:M:61:SER:O | 1:M:62:PHE:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:N:54:ARG:C | 2:N:55:TRP:HD1 | 2.18 | 0.46 |
| 3:C:49:LEU:HD21 | 4:D:55:LEU:HD12 | 1.98 | 0.46 |
| 1:A:541:GLU:CA | 1:A:541:GLU:OE2 | 2.63 | 0.46 |
| 4:D:75:LEU:O | 4:D:76:TRP:C | 2.54 | 0.46 |
| 1:A:280:LYS:O | 1:A:281:TYR:CD1 | 2.68 | 0.46 |
| 4:P:18:GLY:O | 4:P:19:ALA:C | 2.53 | 0.46 |
| 4:P:72:VAL:O | 4:P:75:LEU:CB | 2.64 | 0.46 |
| 1:M:143:SER:O | 1:M:149:ILE:HD12 | 2.15 | 0.46 |
| 1:A:342:ASP:O | 1:A:344:VAL:N | 2.49 | 0.46 |
| 1:A:49:GLN:CG | 1:A:129:ASP:O | 2.63 | 0.46 |
| 1:A:161:LEU:HD23 | 1:A:161:LEU:HA | 1.70 | 0.46 |
| 1:M:363:THR:HB | 1:M:368:GLU:N | 2.31 | 0.46 |
| 1:M:229:VAL:CB | 1:M:467:ARG:NH2 | 2.78 | 0.46 |
| 1:M:399:LEU:HD11 | 9:M:803:FAD:C4' | 2.45 | 0.46 |
| 2:N:37:LEU:HD23 | 2:N:38:ASP:N | 2.29 | 0.46 |
| 1:A:133:PHE:CD2 | 1:A:134:HIS:N | 2.84 | 0.46 |
| 1:M:449:ALA:O | 1:M:452:ARG:HB2 | 2.15 | 0.46 |
| 1:M:151:ARG:NH1 | 1:M:151:ARG:HB2 | 2.16 | 0.46 |
| 4:P:49:LEU:HD22 | 10:P:800:MQ7:H2M3 | 1.98 | 0.46 |
| 3:O:27:LEU:O | 3:O:28:ARG:C | 2.52 | 0.46 |
| 2:B:121:ILE:O | 2:B:186:HIS:HB2 | 2.15 | 0.46 |
| 1:M:142:THR:O | 1:M:145:GLN:HB3 | 2.16 | 0.46 |
| 1:M:42:ARG:CZ | 2:N:54:ARG:HE | 2.28 | 0.46 |
| 1:M:203:THR:OG1 | 9:M:803:FAD:HM83 | 2.16 | 0.46 |
| 1:M:133:PHE:CZ | 2:N:149:ILE:HA | 2.38 | 0.46 |
| 2:N:37:LEU:CD2 | 2:N:37:LEU:N | 2.79 | 0.46 |
| 4:D:84:HIS:C | 4:D:86:MET:N | 2.69 | 0.46 |
| 1:A:425:ILE:O | 1:A:426:GLU:C | 2.53 | 0.46 |
| 1:A:38:VAL:O | 1:A:38:VAL:HG22 | 2.14 | 0.46 |
| 1:M:106:ARG:HB2 | 1:M:107:PRO:HD2 | 1.98 | 0.45 |
| 1:M:11:GLY:HA3 | 1:M:191:ALA:O | 2.16 | 0.45 |
| 1:M:570:ILE:H | 1:M:570:ILE:HD12 | 1.81 | 0.45 |
| 1:M:11:GLY:HA2 | 9:M:803:FAD:H1B | 1.98 | 0.45 |
| 1:A:399:LEU:HD13 | 9:A:703:FAD:O1P | 2.15 | 0.45 |
| 1:M:555:ARG:NE | 1:M:560:THR:N | 2.61 | 0.45 |
| 1:M:555:ARG:HE | 1:M:560:THR:N | 2.10 | 0.45 |
| 1:M:490:ARG:O | 1:M:490:ARG:HG2 | 2.16 | 0.45 |
| 2:B:50:ASP:O | 2:B:100:ARG:NH2 | 2.49 | 0.45 |
| 3:C:21:PHE:CD2 | 3:C:21:PHE:O | 2.67 | 0.45 |
| 2:B:9:GLU:OE2 | 2:B:23:SER:CB | 2.62 | 0.45 |
| 1:M:330:PHE:HA | 1:M:333:GLU:HB2 | 1.97 | 0.45 |
| 3:C:86:TRP:CH2 | 4:D:21:GLY:HA3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:13:GLY:C | 1:M:15:ALA:N | 2.67 | 0.45 |
| 1:M:269:GLY:O | 1:M:282:MET:HE3 | 2.15 | 0.45 |
| 2:N:75:LEU:HD22 | 2:N:75:LEU:N | 2.30 | 0.45 |
| 4:D:55:LEU:CG | 4:D:59:GLN:NE2 | 2.61 | 0.45 |
| 1:M:476:ILE:HG21 | 1:M:520:HIS:CE1 | 2.51 | 0.45 |
| 1:M:170:LEU:O | 1:M:182:GLN:HA | 2.16 | 0.45 |
| 4:P:30:VAL:CG1 | 4:P:31:MET:N | 2.78 | 0.45 |
| 1:M:428:GLN:O | 1:M:432:VAL:HG23 | 2.16 | 0.45 |
| 3:O:49:LEU:CG | 3:O:49:LEU:O | 2.59 | 0.45 |
| 3:O:125:PHE:HZ | 3:O:130:TRP:HZ3 | 1.63 | 0.45 |
| 1:A:332:CYS:HA | 1:A:343:PRO:HG2 | 1.97 | 0.45 |
| 1:A:515:ALA:O | 1:A:516:GLU:C | 2.55 | 0.45 |
| 3:C:15:TRP:CE3 | 3:C:16:TRP:HA | 2.51 | 0.45 |
| 1:M:113:VAL:CB | 1:M:124:THR:O | 2.53 | 0.45 |
| 1:M:53:ALA:HA | 1:M:125:TRP:HD1 | 1.78 | 0.45 |
| 2:N:206:PHE:O | 2:N:206:PHE:HD2 | 1.98 | 0.45 |
| 2:N:73:PRO:CG | 2:N:213:VAL:HG11 | 2.43 | 0.45 |
| 1:M:174:ASN:HD22 | 1:M:177:GLU:CG | 2.30 | 0.45 |
| 1:A:237:PRO:CB | 1:A:308:ARG:HB3 | 2.46 | 0.45 |
| 4:D:28:ALA:N | 4:D:29:PRO:CD | 2.80 | 0.45 |
| 1:A:326:GLU:HB3 | 1:A:327:ARG:HG3 | 1.99 | 0.45 |
| 4:P:94:PRO:O | 4:P:96:GLY:N | 2.49 | 0.45 |
| 1:M:60:ASP:O | 1:M:123:ARG:NH1 | 2.49 | 0.45 |
| 1:M:38:VAL:HG12 | 2:N:54:ARG:NH1 | 2.29 | 0.45 |
| 1:M:42:ARG:CZ | 2:N:64:SER:CB | 2.94 | 0.45 |
| 2:N:162:GLY:O | 3:O:11:MET:CE | 2.64 | 0.45 |
| 1:A:97:GLU:OE2 | 1:A:98:LEU:HD23 | 2.17 | 0.45 |
| 1:A:520:HIS:O | 1:A:521:SER:C | 2.53 | 0.45 |
| 2:B:43:ILE:HG23 | 2:B:47:LEU:HD11 | 1.93 | 0.45 |
| 3:C:30:GLY:C | 3:C:32:ALA:H | 2.19 | 0.45 |
| 2:N:188:LYS:O | 2:N:192:MET:HB2 | 2.15 | 0.45 |
| 2:N:231:SER:O | 2:N:234:ASP:HB3 | 2.17 | 0.45 |
| 1:M:371:ILE:O | 1:M:372:LYS:HB2 | 2.16 | 0.45 |
| 3:C:112:LEU:HA | 3:C:112:LEU:HD23 | 1.68 | 0.45 |
| 4:D:34:LEU:HA | 4:D:38:LEU:HB2 | 1.98 | 0.45 |
| 2:B:95:ASN:ND2 | 2:B:162:GLY:CA | 2.79 | 0.45 |
| 3:C:120:THR:CG2 | 4:D:30:VAL:HG23 | 2.45 | 0.45 |
| 1:M:158:LEU:HB3 | 1:M:436:LEU:HD12 | 1.99 | 0.45 |
| 1:M:44:HIS:CE1 | 1:M:204:ASN:ND2 | 2.85 | 0.45 |
| 1:M:356:TYR:HD2 | 1:M:357:THR:H | 1.60 | 0.45 |
| 1:M:55:VAL:HB | 1:M:90:PRO:CG | 2.32 | 0.45 |
| 2:B:211:SER:CB | 2:B:220:PRO:HD2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:M:554:PHE:HD1 | 1:M:562:ARG:CZ | 2.29 | 0.45 |
| 2:N:195:LEU:O | 2:N:197:SER:N | 2.50 | 0.45 |
| 4:D:84:HIS:C | 4:D:86:MET:H | 2.18 | 0.45 |
| 1:M:346:GLU:HG3 | 1:M:347:PRO:N | 2.30 | 0.45 |
| 1:M:192:THR:HG21 | 1:M:212:GLY:CA | 2.46 | 0.45 |
| 1:A:167:VAL:HG11 | 1:A:373:GLY:C | 2.37 | 0.45 |
| 2:B:135:THR:O | 2:B:138:GLN:N | 2.49 | 0.45 |
| 1:A:289:LYS:HD3 | 1:A:289:LYS:HA | 1.62 | 0.45 |
| 1:M:115:ARG:HH21 | 1:M:279:ASN:HB2 | 1.82 | 0.45 |
| 1:M:124:THR:HG22 | 1:M:125:TRP:H | 1.80 | 0.45 |
| 5:A:702:FLC:CAC | 9:A:703:FAD:C2 | 2.95 | 0.45 |
| 4:D:1:ILE:O | 4:D:2:ASN:C | 2.54 | 0.45 |
| 1:A:515:ALA:C | 1:A:517:CYS:N | 2.66 | 0.45 |
| 1:A:273:PRO:HB2 | 1:A:276:GLU:H | 1.80 | 0.45 |
| 1:A:405:LEU:O | 1:A:409:GLN:HG2 | 2.16 | 0.45 |
| 1:M:334:LEU:HD23 | 1:M:338:TYR:CE1 | 2.52 | 0.45 |
| 1:M:106:ARG:CB | 1:M:112:ASN:HD22 | 2.30 | 0.45 |
| 1:M:223:LEU:HD12 | 1:M:360:GLY:O | 2.17 | 0.45 |
| 1:M:41:MET:HE3 | 1:M:42:ARG:HG3 | 1.98 | 0.45 |
| 2:N:196:ASN:HA | 2:N:201:VAL:HG11 | 1.97 | 0.45 |
| 1:M:260:TYR:CE2 | 1:M:262:TYR:HA | 2.51 | 0.45 |
| 3:O:127:ALA:O | 3:O:128:LEU:HD23 | 2.17 | 0.45 |
| 3:O:30:GLY:C | 3:O:32:ALA:N | 2.70 | 0.45 |
| 1:A:514:VAL:H | 1:A:514:VAL:HG23 | 1.46 | 0.45 |
| 1:A:151:ARG:HH11 | 1:A:151:ARG:HD2 | 1.50 | 0.45 |
| 1:M:264:GLN:C | 1:M:266:TYR:H | 2.19 | 0.45 |
| 1:M:382:SER:O | 1:M:383:VAL:C | 2.55 | 0.45 |
| 1:A:94:THR:O | 1:A:97:GLU:N | 2.48 | 0.45 |
| 3:O:126:VAL:HG11 | 10:P:800:MQ7:H141 | 1.99 | 0.45 |
| 2:N:196:ASN:HB3 | 2:N:231:SER:CB | 2.47 | 0.45 |
| 1:A:433:GLU:O | 1:A:434:GLN:C | 2.54 | 0.45 |
| 1:M:542:ARG:NH2 | 1:M:544:ASP:OD1 | 2.49 | 0.45 |
| 3:C:49:LEU:HB2 | 3:C:56:TRP:CE3 | 2.51 | 0.45 |
| 3:O:50:LYS:NZ | 4:P:117:THR:OG1 | 2.48 | 0.45 |
| 1:M:560:THR:HG22 | 1:M:561:THR:N | 2.31 | 0.45 |
| 4:D:18:GLY:O | 4:D:19:ALA:C | 2.55 | 0.45 |
| 4:D:13:PHE:CE1 | 4:D:101:TYR:CG | 3.05 | 0.45 |
| 2:N:241:LYS:CB | 2:N:242:PRO:HD3 | 2.45 | 0.45 |
| 3:O:33:VAL:O | 3:O:36:VAL:HG22 | 2.16 | 0.45 |
| 1:M:509:GLY:O | 1:M:512:LEU:HD12 | 2.17 | 0.45 |
| 2:N:36:LEU:N | 2:N:76:ALA:O | 2.42 | 0.45 |
| 1:A:50:GLY:N | 9:A:703:FAD:O4 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:242:LEU:HD12 | 5:M:802:FLC:OB1 | 2.17 | 0.45 |
| 1:A:12:ALA:CB | 1:A:34:LEU:HD21 | 2.46 | 0.45 |
| 2:B:9:GLU:OE2 | 2:B:25:PHE:CZ | 2.70 | 0.45 |
| 1:A:36:SER:OG | 1:A:37:LYS:N | 2.47 | 0.45 |
| 1:A:154:GLU:O | 1:A:175:MET:HB2 | 2.17 | 0.45 |
| 3:C:62:PHE:CZ | 3:C:68:ILE:CD1 | 3.00 | 0.45 |
| 1:M:60:ASP:HB2 | 1:M:123:ARG:NH2 | 2.31 | 0.44 |
| 1:M:91:THR:O | 1:M:95:GLN:N | 2.50 | 0.44 |
| 2:B:211:SER:OG | 2:B:219:ASP:HA | 2.17 | 0.44 |
| 1:M:232:HIS:ND1 | 1:M:233:PRO:HD2 | 2.32 | 0.44 |
| 3:C:30:GLY:C | 3:C:32:ALA:N | 2.70 | 0.44 |
| 2:B:155:TYR:CZ | 2:B:169:GLY:HA3 | 2.52 | 0.44 |
| 1:M:248:ARG:HG2 | 1:M:248:ARG:NH1 | 2.28 | 0.44 |
| 4:P:75:LEU:HA | 4:P:75:LEU:HD23 | 1.80 | 0.44 |
| 1:M:146:PHE:O | 1:M:149:ILE:HG13 | 2.18 | 0.44 |
| 2:B:175:LEU:HA | 2:B:175:LEU:HD12 | 1.79 | 0.44 |
| 1:M:74:ASP:O | 1:M:529:ARG:NH2 | 2.51 | 0.44 |
| 4:D:73:LEU:HB2 | 4:D:74:PRO:CD | 2.42 | 0.44 |
| 1:A:319:LEU:O | 1:A:320:GLY:O | 2.35 | 0.44 |
| 4:D:113:ILE:O | 4:D:116:VAL:N | 2.50 | 0.44 |
| 1:A:437:LYS:HE3 | 1:A:441:ASN:OD1 | 2.18 | 0.44 |
| 1:M:32:ILE:CG2 | 1:M:149:ILE:HA | 2.47 | 0.44 |
| 2:N:178:ARG:NH1 | 2:N:179:TYR:CE1 | 2.85 | 0.44 |
| 2:N:31:ASP:N | 2:N:34:THR:HG21 | 2.32 | 0.44 |
| 3:O:62:PHE:CE1 | 3:O:68:ILE:CG1 | 2.99 | 0.44 |
| 3:O:80:LEU:HD23 | 3:O:80:LEU:HA | 1.87 | 0.44 |
| 1:A:49:GLN:HG2 | 1:A:129:ASP:O | 2.17 | 0.44 |
| 2:B:8:ILE:HD12 | 2:B:28:VAL:HG21 | 1.99 | 0.44 |
| 1:M:78:GLU:CB | 1:M:224:ARG:HH22 | 2.30 | 0.44 |
| 1:M:227:GLU:CG | 1:M:463:CYS:SG | 2.88 | 0.44 |
| 1:M:243:MET:CE | 1:M:348:ILE:HG21 | 2.46 | 0.44 |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:HA | 1.83 | 0.44 |
| 1:A:504:TYR:N | 1:A:504:TYR:CD2 | 2.81 | 0.44 |
| 4:D:7:ARG:O | 4:D:7:ARG:CG | 2.65 | 0.44 |
| 1:A:532:HIS:O | 1:A:532:HIS:CD2 | 2.70 | 0.44 |
| 1:M:105:ARG:NH1 | 2:N:134:GLN:HB2 | 2.32 | 0.44 |
| 2:N:98:ILE:CD1 | 3:O:9:ARG:HE | 2.30 | 0.44 |
| 4:P:61:PHE:O | 4:P:64:ARG:N | 2.44 | 0.44 |
| 1:A:115:ARG:CG | 1:A:115:ARG:NH1 | 2.74 | 0.44 |
| 2:N:173:ILE:HG23 | 2:N:195:LEU:HD21 | 1.99 | 0.44 |
| 1:M:160:ILE:HD12 | 1:M:170:LEU:HD23 | 1.99 | 0.44 |
| 1:M:1:GLN:O | 1:M:182:GLN:HG2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:97:PRO:C | 2:B:104:VAL:CG2 | 2.82 | 0.44 |
| 1:M:248:ARG:HH11 | 1:M:248:ARG:CG | 2.24 | 0.44 |
| 1:A:168:ARG:HD2 | 1:A:186:ASN:OD1 | 2.18 | 0.44 |
| 1:A:37:LYS:CG | 1:A:38:VAL:HG13 | 2.47 | 0.44 |
| 1:M:156:PHE:O | 1:M:173:MET:N | 2.50 | 0.44 |
| 3:O:19:LEU:HA | 3:O:20:PRO:HD3 | 1.79 | 0.44 |
| 2:N:153:LEU:HD12 | 2:N:215:PRO:HD3 | 2.00 | 0.44 |
| 3:C:50:LYS:CA | 3:C:50:LYS:CE | 2.86 | 0.44 |
| 1:A:307:PRO:CD | 1:A:308:ARG:H | 2.26 | 0.44 |
| 2:B:151:CYS:SG | 2:B:153:LEU:HG | 2.58 | 0.44 |
| 1:M:104:SER:OG | 1:M:127:ALA:HA | 2.17 | 0.44 |
| 1:M:467:ARG:CZ | 1:M:533:GLN:H | 2.31 | 0.44 |
| 3:C:48:ALA:O | 3:C:50:LYS:N | 2.50 | 0.44 |
| 1:A:92:GLU:HG3 | 1:A:400:VAL:HG12 | 1.99 | 0.44 |
| 1:A:89:CYS:O | 1:A:93:MET:HG2 | 2.16 | 0.44 |
| 4:P:40:PRO:HG2 | 4:P:41:LEU:H | 1.83 | 0.44 |
| 1:A:17:LEU:HD23 | 1:A:17:LEU:HA | 1.81 | 0.44 |
| 4:P:27:ILE:CG2 | 4:P:27:ILE:O | 2.65 | 0.44 |
| 3:C:90:ALA:N | 3:C:91:PRO:CD | 2.72 | 0.44 |
| 2:B:15:PRO:HB3 | 3:C:5:LYS:N | 2.31 | 0.44 |
| 1:M:253:ILE:HA | 1:M:283:GLU:CD | 2.38 | 0.44 |
| 4:P:82:MET:O | 4:P:86:MET:HG2 | 2.18 | 0.44 |
| 3:C:72:ASN:HD22 | 3:C:72:ASN:HA | 1.59 | 0.44 |
| 1:A:450:LYS:HD3 | 1:A:450:LYS:HA | 1.67 | 0.44 |
| 1:M:191:ALA:CB | 1:M:377:VAL:O | 2.65 | 0.44 |
| 1:M:89:CYS:N | 1:M:90:PRO:CD | 2.81 | 0.44 |
| 1:A:232:HIS:HE1 | 5:A:702:FLC:HG2 | 1.83 | 0.44 |
| 1:A:356:TYR:HE1 | 9:A:703:FAD:O3' | 1.99 | 0.44 |
| 3:C:50:LYS:C | 3:C:52:GLY:N | 2.69 | 0.44 |
| 3:C:121:ILE:C | 3:C:123:ILE:N | 2.70 | 0.44 |
| 3:O:125:PHE:HD1 | 3:O:129:TYR:HB2 | 1.83 | 0.44 |
| 1:M:236:LEU:HD23 | 1:M:239:SER:OG | 2.17 | 0.44 |
| 3:O:86:TRP:CH2 | 4:P:21:GLY:HA3 | 2.53 | 0.44 |
| 2:N:36:LEU:O | 2:N:39:ALA:N | 2.51 | 0.44 |
| 2:N:51:LEU:HD12 | 2:N:51:LEU:O | 2.18 | 0.44 |
| 2:B:112:SER:O | 2:B:113:LEU:C | 2.54 | 0.44 |
| 1:M:162:VAL:O | 1:M:163:ASP:HB2 | 2.17 | 0.44 |
| 1:M:261:ARG:NH2 | 1:M:283:GLU:OE1 | 2.51 | 0.44 |
| 1:A:335:ALA:O | 1:A:339:VAL:HG22 | 2.18 | 0.44 |
| 2:B:105:ASP:O | 2:B:105:ASP:OD1 | 2.36 | 0.44 |
| 2:N:120:ILE:HA | 2:N:185:ASP:OD1 | 2.18 | 0.44 |
| 3:C:9:ARG:NH1 | 3:C:9:ARG:HG2 | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:250:GLU:OE2 | 1:M:327:ARG:HG3 | 2.17 | 0.44 |
| 4:P:111:THR:O | 4:P:115:VAL:HG23 | 2.17 | 0.44 |
| 1:A:202:ASN:HB3 | 1:A:354:ALA:HB3 | 1.99 | 0.44 |
| 1:M:81:VAL:HG11 | 1:M:383:VAL:O | 2.18 | 0.44 |
| 1:M:229:VAL:HG21 | 1:M:464:GLY:O | 2.18 | 0.44 |
| 1:M:466:TYR:CD2 | 1:M:466:TYR:N | 2.84 | 0.44 |
| 2:N:150:ASN:OD1 | 2:N:150:ASN:N | 2.51 | 0.44 |
| 1:A:390:ARG:CD | 1:A:395:SER:HB2 | 2.46 | 0.44 |
| 1:M:160:ILE:HD11 | 1:M:188:VAL:HG11 | 1.99 | 0.44 |
| 1:A:495:SER:OG | 2:B:100:ARG:NH1 | 2.49 | 0.44 |
| 4:D:2:ASN:HA | 4:D:3:PRO:HD3 | 1.75 | 0.44 |
| 4:P:27:ILE:C | 4:P:29:PRO:HD2 | 2.37 | 0.44 |
| 3:O:32:ALA:HB2 | 4:P:81:ARG:HD2 | 1.99 | 0.44 |
| 1:A:391:LEU:HD12 | 1:A:391:LEU:HA | 1.47 | 0.44 |
| 3:C:46:LEU:HD12 | 3:C:46:LEU:HA | 1.75 | 0.44 |
| 3:C:105:PRO:HD2 | 3:C:106:GLU:H | 1.83 | 0.44 |
| 1:M:356:TYR:HE1 | 1:M:395:SER:OG | 2.01 | 0.43 |
| 1:M:162:VAL:HG22 | 1:M:219:HIS:NE2 | 2.33 | 0.43 |
| 1:A:446:GLU:HB2 | 1:A:489:VAL:CA | 2.48 | 0.43 |
| 3:C:89:LEU:C | 3:C:91:PRO:HD2 | 2.37 | 0.43 |
| 3:O:32:ALA:O | 3:O:33:VAL:C | 2.57 | 0.43 |
| 1:M:199:TYR:HE1 | 1:M:459:MET:O | 2.01 | 0.43 |
| 1:M:92:GLU:O | 1:M:96:LEU:N | 2.45 | 0.43 |
| 1:A:92:GLU:HG3 | 1:A:400:VAL:CG1 | 2.49 | 0.43 |
| 1:M:242:LEU:HD23 | 1:M:243:MET:N | 2.33 | 0.43 |
| 1:A:427:ALA:HA | 1:A:430:ALA:CB | 2.48 | 0.43 |
| 4:D:0:MET:CG | 4:D:1:ILE:N | 2.77 | 0.43 |
| 3:O:106:GLU:HB2 | 3:O:107:PRO:CD | 2.48 | 0.43 |
| 3:O:105:PRO:CG | 3:O:106:GLU:H | 2.31 | 0.43 |
| 1:M:295:TRP:CD1 | 1:M:296:HIS:N | 2.86 | 0.43 |
| 1:A:97:GLU:OE1 | 1:A:105:ARG:NH2 | 2.52 | 0.43 |
| 3:O:2:THR:HG22 | 3:O:4:ARG:N | 2.04 | 0.43 |
| 1:M:232:HIS:NE2 | 1:M:242:LEU:HD12 | 2.34 | 0.43 |
| 1:A:562:ARG:NH1 | 1:A:562:ARG:CG | 2.73 | 0.43 |
| 3:C:36:VAL:O | 3:C:39:SER:N | 2.52 | 0.43 |
| 1:M:346:GLU:CG | 1:M:347:PRO:HD2 | 2.44 | 0.43 |
| 2:B:29:PRO:HG3 | 2:B:42:TYR:CE1 | 2.53 | 0.43 |
| 1:M:13:GLY:C | 1:M:15:ALA:H | 2.20 | 0.43 |
| 1:M:268:MET:O | 1:M:269:GLY:C | 2.56 | 0.43 |
| 1:M:467:ARG:NH2 | 1:M:531:ALA:O | 2.52 | 0.43 |
| 1:M:65:HIS:O | 1:M:67:HIS:N | 2.51 | 0.43 |
| 1:A:253:ILE:HG23 | 1:A:255:VAL:HG13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:27:ASN:HA | 1:A:28:PRO:HD3 | 1.42 | 0.43 |
| 3:O:50:LYS:C | 3:O:52:GLY:N | 2.71 | 0.43 |
| 3:O:50:LYS:CE | 4:P:117:THR:OG1 | 2.66 | 0.43 |
| 1:M:554:PHE:O | 1:M:555:ARG:CG | 2.66 | 0.43 |
| 3:O:91:PRO:O | 3:O:93:ALA:N | 2.49 | 0.43 |
| 1:M:171:VAL:HB | 1:M:432:VAL:HG11 | 2.00 | 0.43 |
| 1:A:500:THR:HB | 1:A:504:TYR:CE2 | 2.52 | 0.43 |
| 1:M:145:GLN:HA | 2:N:119:TYR:CZ | 2.53 | 0.43 |
| 1:M:4:GLN:OE1 | 1:M:31:LYS:HD3 | 2.19 | 0.43 |
| 1:M:112:ASN:O | 1:M:126:PHE:CE2 | 2.71 | 0.43 |
| 1:M:43:SER:OG | 1:M:44:HIS:N | 2.52 | 0.43 |
| 1:M:527:GLU:OE2 | 1:M:529:ARG:HG3 | 2.18 | 0.43 |
| 1:M:77:CYS:O | 1:M:568:VAL:CG1 | 2.65 | 0.43 |
| 2:N:100:ARG:O | 2:N:102:LEU:N | 2.52 | 0.43 |
| 1:M:243:MET:HE3 | 1:M:331:ILE:HG23 | 2.00 | 0.43 |
| 1:M:452:ARG:NE | 1:M:508:LEU:HD22 | 2.32 | 0.43 |
| 2:N:48:ALA:HA | 2:N:49:PRO:HD3 | 1.78 | 0.43 |
| 1:A:279:ASN:O | 1:A:280:LYS:CB | 2.65 | 0.43 |
| 2:N:160:GLN:HE21 | 2:N:160:GLN:HA | 1.84 | 0.43 |
| 2:B:126:THR:O | 2:B:129:GLN:HB2 | 2.18 | 0.43 |
| 1:M:106:ARG:HD2 | 1:M:108:ASP:OD1 | 2.18 | 0.43 |
| 2:N:43:ILE:HG21 | 2:N:51:LEU:HD21 | 2.01 | 0.43 |
| 1:A:510:HIS:O | 1:A:513:ASN:N | 2.51 | 0.43 |
| 1:A:306:THR:CB | 1:A:307:PRO:HD2 | 2.38 | 0.43 |
| 1:A:15:ALA:C | 1:A:17:LEU:N | 2.71 | 0.43 |
| 3:O:26:MET:O | 3:O:29:GLU:HB2 | 2.18 | 0.43 |
| 3:O:32:ALA:HA | 3:O:35:ALA:HB3 | 2.00 | 0.43 |
| 3:O:56:TRP:C | 3:O:56:TRP:CD1 | 2.91 | 0.43 |
| 1:M:106:ARG:HB2 | 1:M:107:PRO:CD | 2.48 | 0.43 |
| 1:M:52:SER:HB2 | 1:M:396:LEU:HD23 | 2.01 | 0.43 |
| 1:A:255:VAL:CG2 | 1:A:259:GLY:HA2 | 2.48 | 0.43 |
| 1:A:227:GLU:OE1 | 1:A:525:ARG:NE | 2.49 | 0.43 |
| 4:P:35:VAL:O | 4:P:40:PRO:HD3 | 2.19 | 0.43 |
| 3:C:31:THR:CG2 | 3:C:82:HIS:HB2 | 2.42 | 0.43 |
| 4:P:4:ASN:HA | 4:P:5:PRO:HD3 | 1.77 | 0.43 |
| 1:M:253:ILE:HG22 | 1:M:255:VAL:HG13 | 2.00 | 0.43 |
| 2:B:4:LYS:H | 2:B:4:LYS:HZ1 | 1.67 | 0.43 |
| 1:A:119:MET:HE2 | 1:A:391:LEU:HD23 | 2.00 | 0.43 |
| 4:D:96:GLY:O | 4:D:97:LYS:C | 2.55 | 0.43 |
| 1:A:362:GLU:OE1 | 1:A:370:ARG:NE | 2.52 | 0.43 |
| 2:N:54:ARG:CG | 2:N:54:ARG:HH11 | 2.19 | 0.43 |
| 1:M:242:LEU:C | 1:M:242:LEU:CD2 | 2.75 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:26:TYR:CG | 2:B:43:ILE:HD13 | 2.54 | 0.43 |
| 3:O:89:LEU:C | 3:O:91:PRO:HD2 | 2.38 | 0.43 |
| 4:D:103:LEU:C | 4:D:103:LEU:HD23 | 2.39 | 0.43 |
| 2:N:117:LYS:C | 2:N:119:TYR:H | 2.22 | 0.43 |
| 2:B:39:ALA:O | 2:B:40:LEU:C | 2.56 | 0.43 |
| 1:A:194:GLY:O | 1:A:208:VAL:HG12 | 2.19 | 0.43 |
| 1:A:162:VAL:O | 1:A:428:GLN:NE2 | 2.52 | 0.43 |
| 1:M:113:VAL:HG23 | 1:M:123:ARG:HA | 1.97 | 0.43 |
| 1:M:126:PHE:CD2 | 1:M:126:PHE:N | 2.87 | 0.43 |
| 1:M:60:ASP:OD1 | 1:M:60:ASP:N | 2.52 | 0.43 |
| 1:M:243:MET:HE1 | 1:M:348:ILE:HD13 | 2.00 | 0.43 |
| 3:O:126:VAL:HG12 | 10:P:800:MQ7:H141 | 1.99 | 0.43 |
| 2:N:167:PHE:HD1 | 2:N:199:ASN:C | 2.22 | 0.43 |
| 2:N:232:SER:C | 2:N:234:ASP:N | 2.72 | 0.43 |
| 3:C:124:LEU:CD2 | 4:D:34:LEU:HD21 | 2.41 | 0.43 |
| 1:A:503:LEU:O | 1:A:504:TYR:C | 2.53 | 0.43 |
| 1:A:504:TYR:HD2 | 1:A:504:TYR:N | 2.17 | 0.43 |
| 2:B:231:SER:O | 2:B:234:ASP:HB3 | 2.19 | 0.43 |
| 1:A:483:GLN:OE1 | 1:A:483:GLN:CA | 2.67 | 0.43 |
| 1:M:225:ASP:HB2 | 1:M:550:HIS:CG | 2.54 | 0.43 |
| 2:N:28:VAL:HG12 | 2:N:29:PRO:CD | 2.48 | 0.43 |
| 4:D:37:ILE:N | 4:D:37:ILE:CD1 | 2.82 | 0.43 |
| 1:M:162:VAL:HG13 | 1:M:219:HIS:HE1 | 1.84 | 0.43 |
| 1:A:330:PHE:CZ | 2:B:61:ILE:CG1 | 3.02 | 0.43 |
| 1:A:280:LYS:O | 1:A:281:TYR:HD1 | 2.01 | 0.43 |
| 2:N:239:THR:HG22 | 2:N:239:THR:O | 2.17 | 0.43 |
| 2:N:158:CYS:HB2 | 7:N:245:F3S:S4 | 2.58 | 0.43 |
| 1:M:446:GLU:CB | 1:M:488:ARG:O | 2.67 | 0.43 |
| 4:P:81:ARG:HG3 | 4:P:81:ARG:HH11 | 1.83 | 0.43 |
| 3:C:15:TRP:CE3 | 3:C:16:TRP:N | 2.87 | 0.43 |
| 1:M:473:GLN:OE1 | 1:M:473:GLN:HA | 2.19 | 0.43 |
| 1:M:189:VAL:CG1 | 1:M:377:VAL:HG23 | 2.49 | 0.42 |
| 2:N:29:PRO:HD2 | 2:N:42:TYR:HB3 | 2.01 | 0.42 |
| 1:A:211:ASP:HB3 | 9:A:703:FAD:N6A | 2.30 | 0.42 |
| 1:A:211:ASP:O | 1:A:215:MET:HG3 | 2.19 | 0.42 |
| 1:A:230:GLN:CD | 1:A:287:ARG:HH21 | 2.22 | 0.42 |
| 1:M:129:ASP:O | 1:M:129:ASP:OD1 | 2.37 | 0.42 |
| 1:M:452:ARG:CD | 1:M:452:ARG:N | 2.82 | 0.42 |
| 1:A:37:LYS:C | 1:A:38:VAL:CG1 | 2.86 | 0.42 |
| 2:B:164:ASN:C | 2:B:164:ASN:OD1 | 2.57 | 0.42 |
| 3:C:116:THR:HA | 4:D:26:ILE:HG23 | 2.01 | 0.42 |
| 1:A:27:ASN:ND2 | 1:A:29:ASN:H | 2.17 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:474:LYS:HD3 | 1:M:474:LYS:HA | 1.86 | 0.42 |
| 2:N:6:LEU:HD22 | 2:N:81:LEU:HD21 | 2.00 | 0.42 |
| 4:P:28:ALA:N | 4:P:29:PRO:CD | 2.82 | 0.42 |
| 3:O:91:PRO:HA | 3:O:108:ILE:HD12 | 2.01 | 0.42 |
| 1:A:551:THR:HG23 | 1:A:565:TYR:CE2 | 2.53 | 0.42 |
| 2:N:117:LYS:HD2 | 2:N:190:GLU:O | 2.18 | 0.42 |
| 2:B:193:ALA:O | 4:D:5:PRO:HG2 | 2.19 | 0.42 |
| 1:M:124:THR:HG22 | 1:M:125:TRP:N | 2.34 | 0.42 |
| 1:M:276:GLU:N | 1:M:277:PRO:HD3 | 2.35 | 0.42 |
| 1:A:62:PHE:CD2 | 1:A:86:VAL:HG13 | 2.45 | 0.42 |
| 3:O:91:PRO:C | 3:O:93:ALA:H | 2.22 | 0.42 |
| 3:C:128:LEU:HD23 | 3:C:128:LEU:HA | 1.77 | 0.42 |
| 1:A:319:LEU:HD12 | 1:A:323:LYS:HE2 | 2.02 | 0.42 |
| 4:P:72:VAL:HG23 | 4:P:73:LEU:H | 1.83 | 0.42 |
| 1:A:371:ILE:HG21 | 1:A:371:ILE:HD13 | 1.60 | 0.42 |
| 1:M:243:MET:O | 1:M:244:THR:O | 2.38 | 0.42 |
| 2:N:188:LYS:HG2 | 2:N:188:LYS:H | 1.37 | 0.42 |
| 2:B:12:ARG:NH2 | 2:B:50:ASP:OD1 | 2.43 | 0.42 |
| 4:D:4:ASN:HD22 | 4:D:4:ASN:C | 2.22 | 0.42 |
| 2:N:105:ASP:C | 2:N:107:THR:H | 2.22 | 0.42 |
| 4:D:19:ALA:O | 4:D:20:GLY:C | 2.58 | 0.42 |
| 4:D:31:MET:HB3 | 4:D:31:MET:HE3 | 1.81 | 0.42 |
| 3:C:108:ILE:O | 3:C:109:ILE:C | 2.56 | 0.42 |
| 1:M:17:LEU:HD21 | 1:M:139:LEU:HB2 | 2.00 | 0.42 |
| 2:B:170:PRO:HA | 2:B:224:ILE:HD11 | 2.00 | 0.42 |
| 2:B:34:THR:HG22 | 2:B:81:LEU:HG | 2.01 | 0.42 |
| 1:M:53:ALA:HA | 1:M:125:TRP:CB | 2.49 | 0.42 |
| 1:M:266:TYR:CE2 | 1:M:296:HIS:CB | 3.02 | 0.42 |
| 1:M:228:PHE:HE2 | 1:M:388:ALA:HA | 1.80 | 0.42 |
| 1:M:224:ARG:HA | 1:M:551:THR:O | 2.19 | 0.42 |
| 2:N:133:ILE:O | 2:N:133:ILE:CG2 | 2.66 | 0.42 |
| 1:A:122:GLU:OE2 | 1:A:122:GLU:N | 2.35 | 0.42 |
| 1:M:455:MET:HB2 | 1:M:482:LEU:CD2 | 2.49 | 0.42 |
| 2:N:193:ALA:HB1 | 4:P:5:PRO:HG2 | 2.02 | 0.42 |
| 3:O:27:LEU:O | 3:O:29:GLU:N | 2.52 | 0.42 |
| 2:B:68:MET:HE1 | 2:B:73:PRO:N | 2.35 | 0.42 |
| 3:O:30:GLY:C | 3:O:32:ALA:H | 2.22 | 0.42 |
| 1:A:392:GLY:O | 1:A:393:SER:CB | 2.64 | 0.42 |
| 1:A:478:LYS:O | 1:A:481:GLU:HB3 | 2.19 | 0.42 |
| 1:A:334:LEU:HD23 | 1:A:334:LEU:HA | 1.93 | 0.42 |
| 1:M:45:THR:O | 1:M:132:GLY:O | 2.37 | 0.42 |
| 1:M:211:ASP:OD2 | 1:M:510:HIS:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:132:ASN:HD22 | 2:B:184:ARG:HD3 | 1.84 | 0.42 |
| 2:N:177:HIS:CA | 2:N:180:ASN:HB2 | 2.46 | 0.42 |
| 1:A:437:LYS:HA | 1:A:440:VAL:CG2 | 2.46 | 0.42 |
| 2:B:135:THR:C | 2:B:137:ALA:H | 2.22 | 0.42 |
| 2:B:135:THR:O | 2:B:136:PRO:C | 2.57 | 0.42 |
| 4:P:95:ALA:O | 4:P:99:VAL:HG23 | 2.20 | 0.42 |
| 3:C:106:GLU:CG | 3:C:107:PRO:HD3 | 2.50 | 0.42 |
| 4:P:85:ALA:O | 4:P:89:LEU:HD12 | 2.20 | 0.42 |
| 1:M:35:ILE:HG23 | 1:M:155:HIS:HB2 | 2.02 | 0.42 |
| 1:M:389:ASN:O | 1:M:391:LEU:N | 2.53 | 0.42 |
| 1:M:377:VAL:HG21 | 1:M:406:ALA:HB1 | 2.01 | 0.42 |
| 1:M:40:PRO:O | 1:M:41:MET:C | 2.57 | 0.42 |
| 1:M:555:ARG:NE | 1:M:559:GLY:HA2 | 2.34 | 0.42 |
| 1:A:34:LEU:HA | 1:A:34:LEU:HD12 | 1.81 | 0.42 |
| 4:P:80:HIS:HD2 | 4:P:84:HIS:CD2 | 2.32 | 0.42 |
| 4:D:13:PHE:HB3 | 4:D:80:HIS:ND1 | 2.35 | 0.42 |
| 1:M:329:PRO:O | 1:M:333:GLU:N | 2.47 | 0.42 |
| 4:P:81:ARG:NH1 | 4:P:81:ARG:HG3 | 2.35 | 0.42 |
| 2:N:59:MET:SD | 2:N:59:MET:O | 2.77 | 0.42 |
| 2:N:37:LEU:HD12 | 2:N:55:TRP:CB | 2.50 | 0.42 |
| 1:A:48:ALA:HA | 9:A:703:FAD:C5X | 2.50 | 0.42 |
| 4:D:117:THR:O | 4:D:118:ILE:HG12 | 2.19 | 0.42 |
| 1:A:543:ASP:OD1 | 1:A:546:ASN:N | 2.41 | 0.42 |
| 1:A:236:LEU:HA | 1:A:237:PRO:HD3 | 1.89 | 0.42 |
| 1:M:233:PRO:CG | 1:M:234:THR:H | 2.31 | 0.42 |
| 1:A:61:SER:OG | 1:A:62:PHE:N | 2.49 | 0.42 |
| 3:O:28:ARG:O | 3:O:31:THR:CG2 | 2.68 | 0.42 |
| 3:C:21:PHE:CD2 | 3:C:21:PHE:C | 2.93 | 0.42 |
| 4:P:13:PHE:HE2 | 4:P:97:LYS:HD3 | 1.85 | 0.42 |
| 3:O:67:VAL:O | 3:O:69:VAL:N | 2.53 | 0.42 |
| 2:N:57:CYS:SG | 2:N:61:ILE:HG22 | 2.60 | 0.42 |
| 1:A:222:PRO:HB3 | 1:A:554:PHE:CE2 | 2.55 | 0.42 |
| 1:A:27:ASN:HD22 | 1:A:28:PRO:N | 2.01 | 0.42 |
| 1:A:89:CYS:N | 1:A:90:PRO:CD | 2.83 | 0.42 |
| 2:B:109:PHE:CZ | 2:B:113:LEU:HD21 | 2.55 | 0.42 |
| 1:A:1:GLN:O | 1:A:181:VAL:HA | 2.20 | 0.42 |
| 4:D:37:ILE:O | 4:D:40:PRO:HD2 | 2.20 | 0.42 |
| 3:C:27:LEU:O | 3:C:30:GLY:N | 2.53 | 0.42 |
| 1:M:372:LYS:O | 1:M:413:ARG:HG2 | 2.20 | 0.42 |
| 2:B:12:ARG:NH2 | 2:B:51:LEU:HA | 2.35 | 0.42 |
| 4:P:28:ALA:O | 4:P:32:ILE:HG13 | 2.20 | 0.42 |
| 3:O:27:LEU:C | 3:O:29:GLU:N | 2.71 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:80:PHE:CD1 | 2:B:82:ARG:NH2 | 2.88 | 0.42 |
| 1:A:330:PHE:O | 1:A:331:ILE:C | 2.58 | 0.42 |
| 1:A:369:THR:HG23 | 1:A:374:LEU:O | 2.20 | 0.42 |
| 1:M:73:GLY:C | 1:M:388:ALA:H | 2.24 | 0.42 |
| 1:M:11:GLY:HA2 | 9:M:803:FAD:C1B | 2.50 | 0.42 |
| 1:A:261:ARG:NH1 | 1:A:283:GLU:OE1 | 2.51 | 0.42 |
| 1:M:129:ASP:HB2 | 1:M:328:LEU:CB | 2.50 | 0.42 |
| 1:M:182:GLN:HE22 | 1:M:429:ALA:HB1 | 1.84 | 0.42 |
| 4:D:98:TRP:O | 4:D:102:GLY:N | 2.52 | 0.42 |
| 4:D:83:HIS:HB3 | 4:D:84:HIS:H | 1.59 | 0.42 |
| 1:A:554:PHE:HE1 | 1:A:564:GLU:HB2 | 1.85 | 0.42 |
| 1:M:335:ALA:O | 1:M:339:VAL:HB | 2.20 | 0.42 |
| 1:M:526:LYS:HE3 | 1:M:547:PHE:CE1 | 2.55 | 0.41 |
| 1:M:92:GLU:HA | 1:M:95:GLN:CB | 2.40 | 0.41 |
| 2:N:60:ALA:N | 2:N:77:CYS:SG | 2.87 | 0.41 |
| 3:C:49:LEU:CD2 | 4:D:55:LEU:HD12 | 2.50 | 0.41 |
| 1:M:555:ARG:HD3 | 1:M:559:GLY:HA2 | 2.00 | 0.41 |
| 2:N:44:LYS:O | 2:N:46:ASN:N | 2.53 | 0.41 |
| 1:A:320:GLY:O | 1:A:321:GLU:C | 2.58 | 0.41 |
| 1:A:469:PRO:HA | 1:A:523:MET:HE3 | 2.02 | 0.41 |
| 2:B:66:GLY:HA2 | 2:B:74:LYS:O | 2.20 | 0.41 |
| 4:P:73:LEU:HB2 | 4:P:74:PRO:HD3 | 2.02 | 0.41 |
| 1:A:413:ARG:HA | 1:A:413:ARG:NH1 | 2.35 | 0.41 |
| 1:A:448:TRP:CH2 | 1:A:504:TYR:HB3 | 2.55 | 0.41 |
| 2:N:224:ILE:H | 2:N:224:ILE:HG13 | 1.74 | 0.41 |
| 1:M:99:TRP:CZ3 | 1:M:142:THR:HG21 | 2.55 | 0.41 |
| 3:C:106:GLU:HG3 | 3:C:106:GLU:H | 1.65 | 0.41 |
| 2:B:227:GLY:O | 2:B:230:GLU:N | 2.51 | 0.41 |
| 3:C:78:ALA:O | 3:C:79:ALA:C | 2.58 | 0.41 |
| 1:A:173:MET:CE | 1:A:173:MET:CG | 2.95 | 0.41 |
| 1:M:265:ASP:C | 1:M:266:TYR:CD1 | 2.94 | 0.41 |
| 1:M:135:MET:SD | 1:M:396:LEU:HG | 2.60 | 0.41 |
| 1:A:211:ASP:HA | 1:A:510:HIS:CD2 | 2.54 | 0.41 |
| 4:D:61:PHE:C | 4:D:63:GLY:H | 2.22 | 0.41 |
| 1:M:219:HIS:HB3 | 1:M:371:ILE:CD1 | 2.51 | 0.41 |
| 1:A:486:PHE:HA | 1:A:489:VAL:HG12 | 2.01 | 0.41 |
| 4:D:73:LEU:O | 4:D:74:PRO:C | 2.55 | 0.41 |
| 4:D:76:TRP:O | 4:D:77:CYS:C | 2.58 | 0.41 |
| 1:A:70:VAL:CG1 | 1:A:573:LEU:HD23 | 2.49 | 0.41 |
| 3:O:68:ILE:CG2 | 3:O:68:ILE:O | 2.65 | 0.41 |
| 1:A:144:LEU:HA | 1:A:144:LEU:HD23 | 1.82 | 0.41 |
| 1:A:532:HIS:C | 1:A:532:HIS:CD2 | 2.94 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:C:125:PHE:CD1 | 3:C:129:TYR:CD2 | 3.08 | 0.41 |
| 1:A:368:GLU:HG3 | 1:A:375:PHE:CE2 | 2.55 | 0.41 |
| 1:M:74:ASP:O | 1:M:529:ARG:NE | 2.54 | 0.41 |
| 2:N:214:CYS:SG | 2:N:218:VAL:CG2 | 2.96 | 0.41 |
| 2:N:5:ASN:ND2 | 2:N:29:PRO:HA | 2.35 | 0.41 |
| 1:M:355:HIS:CD2 | 5:M:802:FLC:OHB | 2.73 | 0.41 |
| 4:D:1:ILE:O | 4:D:2:ASN:O | 2.38 | 0.41 |
| 3:C:40:ILE:O | 3:C:41:GLU:C | 2.58 | 0.41 |
| 4:P:66:PHE:HD2 | 4:P:67:LEU:N | 2.18 | 0.41 |
| 1:A:71:ALA:O | 1:A:72:GLY:C | 2.58 | 0.41 |
| 2:N:175:LEU:HD12 | 2:N:178:ARG:HB3 | 2.02 | 0.41 |
| 4:P:100:PHE:N | 4:P:100:PHE:CD1 | 2.87 | 0.41 |
| 1:A:482:LEU:HD23 | 1:A:482:LEU:HA | 1.57 | 0.41 |
| 1:M:108:ASP:O | 2:N:133:ILE:HG13 | 2.20 | 0.41 |
| 3:O:53:PRO:HD3 | 4:P:51:TYR:OH | 2.20 | 0.41 |
| 4:D:101:TYR:HA | 4:D:104:ALA:HB3 | 2.02 | 0.41 |
| 1:M:139:LEU:C | 1:M:141:GLN:H | 2.23 | 0.41 |
| 1:M:334:LEU:HD23 | 1:M:338:TYR:HE1 | 1.84 | 0.41 |
| 1:M:250:GLU:O | 1:M:319:LEU:HD11 | 2.20 | 0.41 |
| 2:B:168:ILE:HG21 | 2:B:168:ILE:HD13 | 1.84 | 0.41 |
| 1:A:471:LEU:HA | 1:A:471:LEU:HD23 | 1.64 | 0.41 |
| 1:M:127:ALA:N | 1:M:131:THR:OG1 | 2.54 | 0.41 |
| 1:M:204:ASN:OD1 | 1:M:208:VAL:HB | 2.21 | 0.41 |
| 1:M:228:PHE:HD1 | 1:M:228:PHE:HA | 1.56 | 0.41 |
| 1:M:396:LEU:HD13 | 9:M:803:FAD:C2 | 2.51 | 0.41 |
| 1:M:42:ARG:HG2 | 2:N:62:CYS:O | 2.20 | 0.41 |
| 2:N:53:TYR:CD1 | 2:N:53:TYR:N | 2.87 | 0.41 |
| 4:D:59:GLN:HB2 | 4:D:59:GLN:HE21 | 1.63 | 0.41 |
| 1:A:55:VAL:HG21 | 1:A:62:PHE:CE2 | 2.55 | 0.41 |
| 1:M:262:TYR:CB | 1:M:297:GLU:OE2 | 2.68 | 0.41 |
| 3:O:28:ARG:NH2 | 3:O:89:LEU:HD11 | 2.35 | 0.41 |
| 1:A:20:ALA:HB1 | 1:A:149:ILE:HD13 | 2.02 | 0.41 |
| 1:M:144:LEU:HD22 | 2:N:114:GLU:HG3 | 2.02 | 0.41 |
| 1:M:156:PHE:CG | 1:M:503:LEU:HD22 | 2.55 | 0.41 |
| 1:M:334:LEU:O | 1:M:338:TYR:N | 2.46 | 0.41 |
| 1:A:194:GLY:C | 1:A:208:VAL:HG12 | 2.41 | 0.41 |
| 1:M:199:TYR:CE1 | 1:M:459:MET:HB3 | 2.56 | 0.41 |
| 1:M:556:ASP:HB3 | 1:M:557:ALA:H | 1.65 | 0.41 |
| 2:N:68:MET:HE1 | 2:N:73:PRO:HB3 | 2.00 | 0.41 |
| 2:B:110:ILE:HG12 | 2:B:110:ILE:H | 1.54 | 0.41 |
| 3:O:91:PRO:HB3 | 3:O:108:ILE:HD12 | 2.01 | 0.41 |
| 4:P:17:PHE:O | 4:P:18:GLY:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:D:94:PRO:HA | 2:N:243:ARG:O | 2.20 | 0.41 |
| 1:A:335:ALA:HB1 | 1:A:341:VAL:O | 2.20 | 0.41 |
| 2:N:158:CYS:SG | 2:N:160:GLN:HB2 | 2.61 | 0.41 |
| 3:O:67:VAL:O | 3:O:68:ILE:C | 2.57 | 0.41 |
| 4:P:9:ASP:O | 4:P:12:VAL:HG23 | 2.21 | 0.41 |
| 1:M:49:GLN:HE22 | 9:M:803:FAD:H6 | 1.85 | 0.41 |
| 1:M:42:ARG:HG2 | 2:N:63:GLY:O | 2.20 | 0.41 |
| 1:A:232:HIS:CE1 | 5:A:702:FLC:HG2 | 2.55 | 0.41 |
| 1:A:97:GLU:CD | 2:B:131:THR:HB | 2.41 | 0.41 |
| 2:B:241:LYS:O | 2:B:243:ARG:HG3 | 2.20 | 0.41 |
| 1:A:527:GLU:CG | 1:A:547:PHE:HB3 | 2.43 | 0.41 |
| 4:P:41:LEU:HD23 | 4:P:41:LEU:HA | 1.72 | 0.41 |
| 3:O:60:VAL:O | 3:O:60:VAL:HG12 | 2.21 | 0.41 |
| 4:D:16:LEU:O | 4:D:18:GLY:N | 2.54 | 0.41 |
| 1:A:526:LYS:HZ2 | 1:A:534:ARG:HH12 | 1.69 | 0.41 |
| 1:A:177:GLU:CA | 1:A:177:GLU:OE2 | 2.60 | 0.41 |
| 2:N:34:THR:HG23 | 2:N:34:THR:O | 2.20 | 0.41 |
| 4:P:95:ALA:O | 4:P:96:GLY:C | 2.58 | 0.41 |
| 1:M:526:LYS:HA | 1:M:534:ARG:CD | 2.51 | 0.41 |
| 2:N:137:ALA:N | 2:N:139:MET:SD | 2.94 | 0.41 |
| 2:N:36:LEU:CB | 2:N:76:ALA:O | 2.65 | 0.41 |
| 1:A:262:TYR:OH | 1:A:312:VAL:HG11 | 2.21 | 0.41 |
| 1:A:355:HIS:NE2 | 5:A:702:FLC:OHB | 2.54 | 0.41 |
| 3:C:50:LYS:HD3 | 4:D:118:ILE:CG1 | 2.50 | 0.41 |
| 1:A:227:GLU:HB3 | 1:A:521:SER:CB | 2.51 | 0.41 |
| 10:P:800:MQ7:H17 | 10:P:800:MQ7:H141 | 2.02 | 0.41 |
| 1:M:471:LEU:HD12 | 1:M:472:MET:H | 1.76 | 0.41 |
| 1:A:55:VAL:HG21 | 1:A:62:PHE:CD2 | 2.56 | 0.41 |
| 3:O:128:LEU:HB3 | 4:P:45:PRO:HG2 | 2.02 | 0.41 |
| 1:A:445:GLY:H | 1:A:490:ARG:HB3 | 1.86 | 0.41 |
| 1:A:502:LEU:O | 1:A:503:LEU:C | 2.56 | 0.41 |
| 1:A:141:GLN:O | 1:A:144:LEU:HB2 | 2.21 | 0.41 |
| 2:B:40:LEU:HA | 2:B:40:LEU:HD23 | 1.74 | 0.41 |
| 2:N:37:LEU:HD22 | 2:N:77:CYS:CA | 2.49 | 0.41 |
| 2:N:68:MET:HE2 | 2:N:73:PRO:HB3 | 2.00 | 0.41 |
| 1:M:103:TRP:HZ3 | 1:M:131:THR:CG2 | 2.31 | 0.41 |
| 1:M:205:GLY:HA2 | 2:N:58:ARG:HD2 | 2.02 | 0.41 |
| 1:M:226:MET:O | 1:M:227:GLU:C | 2.59 | 0.41 |
| 1:M:228:PHE:CE2 | 1:M:388:ALA:CA | 3.01 | 0.41 |
| 2:N:36:LEU:CB | 2:N:76:ALA:HB1 | 2.49 | 0.41 |
| 1:A:513:ASN:OD1 | 1:A:555:ARG:CZ | 2.69 | 0.41 |
| 1:A:253:ILE:HD13 | 1:A:253:ILE:HG21 | 1.67 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:52:SER:HB3 | 1:A:93:MET:CE | 2.51 | 0.41 |
| 2:B:109:PHE:CE1 | 2:B:113:LEU:HD11 | 2.55 | 0.41 |
| 1:A:115:ARG:NH1 | 1:A:122:GLU:OE1 | 2.53 | 0.41 |
| 1:M:452:ARG:HD2 | 1:M:508:LEU:HD22 | 2.02 | 0.41 |
| 1:M:273:PRO:HG3 | 1:M:276:GLU:OE1 | 2.21 | 0.41 |
| 4:D:16:LEU:HA | 4:D:16:LEU:HD23 | 1.69 | 0.41 |
| 1:A:73:GLY:O | 1:A:74:ASP:CB | 2.54 | 0.41 |
| 3:C:21:PHE:HD2 | 3:C:21:PHE:C | 2.23 | 0.41 |
| 4:P:13:PHE:CE2 | 4:P:97:LYS:HD3 | 2.56 | 0.41 |
| 2:N:160:GLN:HG3 | 2:N:203:SER:O | 2.21 | 0.41 |
| 1:M:5:ALA:O | 1:M:185:ALA:CA | 2.68 | 0.41 |
| 2:N:123:ASN:OD1 | 2:N:124:SER:N | 2.48 | 0.41 |
| 2:N:124:SER:O | 2:N:125:ARG:C | 2.59 | 0.41 |
| 2:N:179:TYR:HA | 2:N:182:ASP:HB2 | 2.03 | 0.41 |
| 4:P:95:ALA:O | 4:P:98:TRP:N | 2.49 | 0.41 |
| 3:C:78:ALA:O | 3:C:81:LEU:N | 2.54 | 0.41 |
| 3:O:121:ILE:O | 3:O:124:LEU:N | 2.54 | 0.41 |
| 2:N:142:TYR:O | 2:N:143:HIS:C | 2.59 | 0.41 |
| 1:M:190:MET:H | 1:M:376:ALA:HA | 1.86 | 0.41 |
| 1:M:89:CYS:N | 1:M:90:PRO:HD2 | 2.36 | 0.41 |
| 1:M:456:GLY:O | 1:M:457:LEU:C | 2.58 | 0.41 |
| 2:B:68:MET:HB3 | 2:B:68:MET:HE2 | 1.93 | 0.41 |
| 1:A:79:GLN:HG3 | 1:A:569:LYS:O | 2.21 | 0.41 |
| 2:N:240:LEU:N | 2:N:240:LEU:CD2 | 2.78 | 0.41 |
| 1:A:452:ARG:NH2 | 2:B:45:ASP:OD2 | 2.50 | 0.41 |
| 2:N:37:LEU:HD13 | 2:N:77:CYS:HB3 | 2.03 | 0.40 |
| 1:A:312:VAL:HG22 | 1:A:350:VAL:O | 2.21 | 0.40 |
| 4:D:117:THR:C | 4:D:118:ILE:HG12 | 2.41 | 0.40 |
| 1:M:198:VAL:O | 1:M:456:GLY:HA2 | 2.20 | 0.40 |
| 4:P:39:LEU:HA | 4:P:39:LEU:HD12 | 1.79 | 0.40 |
| 1:M:161:LEU:HB2 | 1:M:169:GLY:O | 2.21 | 0.40 |
| 1:M:1:GLN:O | 1:M:182:GLN:CG | 2.69 | 0.40 |
| 1:M:433:GLU:HG3 | 1:M:434:GLN:HG3 | 2.03 | 0.40 |
| 4:P:22:MET:O | 4:P:26:ILE:HD13 | 2.21 | 0.40 |
| 1:M:516:GLU:CA | 1:M:516:GLU:OE1 | 2.68 | 0.40 |
| 1:M:263:LEU:HD21 | 1:M:290:VAL:HG13 | 2.03 | 0.40 |
| 3:C:9:ARG:HA | 3:C:10:PRO:HD3 | 1.82 | 0.40 |
| 1:M:497:VAL:O | 1:M:498:PHE:C | 2.59 | 0.40 |
| 1:M:10:VAL:HG11 | 1:M:157:VAL:HG21 | 2.03 | 0.40 |
| 1:A:171:VAL:HG11 | 1:A:432:VAL:HG11 | 2.03 | 0.40 |
| 1:M:225:ASP:CA | 1:M:550:HIS:HB3 | 2.51 | 0.40 |
| 1:M:100:GLY:HA2 | 2:N:184:ARG:HH21 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:N:37:LEU:HD12 | 2:N:55:TRP:HB2 | 2.03 | 0.40 |
| 3:C:50:LYS:HZ3 | 4:D:118:ILE:CD1 | 2.11 | 0.40 |
| 1:M:554:PHE:CD2 | 1:M:560:THR:HB | 2.51 | 0.40 |
| 2:N:235:PHE:O | 2:N:238:ALA:N | 2.55 | 0.40 |
| 4:P:23:TRP:HE1 | 4:P:70:MET:HE3 | 1.85 | 0.40 |
| 2:N:109:PHE:CE1 | 2:N:113:LEU:CD1 | 3.04 | 0.40 |
| 1:A:341:VAL:O | 1:A:343:PRO:HD3 | 2.21 | 0.40 |
| 4:D:112:LEU:O | 4:D:116:VAL:HG22 | 2.21 | 0.40 |
| 3:C:9:ARG:CG | 3:C:9:ARG:HH11 | 2.32 | 0.40 |
| 1:M:32:ILE:CG1 | 1:M:33:ALA:N | 2.83 | 0.40 |
| 1:A:41:MET:HE3 | 2:B:150:ASN:HD22 | 1.85 | 0.40 |
| 4:P:93:VAL:HA | 4:P:94:PRO:HD2 | 1.74 | 0.40 |
| 2:B:81:LEU:HA | 2:B:81:LEU:HD23 | 1.57 | 0.40 |
| 1:M:226:MET:HB3 | 1:M:517:CYS:O | 2.22 | 0.40 |
| 2:N:73:PRO:O | 2:N:74:LYS:CG | 2.68 | 0.40 |
| 1:A:262:TYR:CD1 | 1:A:263:LEU:HD23 | 2.57 | 0.40 |
| 2:B:219:ASP:OD2 | 3:C:92:LYS:HE2 | 2.22 | 0.40 |
| 1:A:182:GLN:HE22 | 1:A:184:ARG:NH1 | 2.16 | 0.40 |
| 4:P:40:PRO:HG2 | 4:P:41:LEU:N | 2.36 | 0.40 |
| 1:A:147:PRO:O | 1:A:149:ILE:N | 2.54 | 0.40 |
| 1:A:319:LEU:CD1 | 1:A:323:LYS:HE3 | 2.52 | 0.40 |
| 1:M:144:LEU:HD22 | 2:N:114:GLU:HA | 2.03 | 0.40 |
| 1:M:146:PHE:HA | 1:M:147:PRO:HD2 | 1.82 | 0.40 |
| 3:O:66:PRO:HG2 | 3:O:67:VAL:H | 1.85 | 0.40 |
| 1:A:257:LYS:HA | 1:A:304:ILE:HD11 | 2.03 | 0.40 |
| 3:O:46:LEU:HA | 3:O:46:LEU:HD12 | 1.75 | 0.40 |
| 1:M:214:GLY:HA3 | 1:M:510:HIS:ND1 | 2.36 | 0.40 |
| 1:M:89:CYS:HA | 1:M:401:VAL:CG2 | 2.51 | 0.40 |
| 1:M:41:MET:HE2 | 1:M:42:ARG:HG3 | 2.03 | 0.40 |
| 1:M:211:ASP:OD1 | 1:M:507:GLU:HA | 2.22 | 0.40 |
| 1:M:229:VAL:O | 1:M:531:ALA:HB1 | 2.20 | 0.40 |
| 2:N:73:PRO:C | 2:N:74:LYS:HG3 | 2.40 | 0.40 |
| 1:M:151:ARG:NH1 | 1:M:153:ASP:OD2 | 2.55 | 0.40 |
| 3:C:53:PRO:CA | 4:D:51:TYR:CE1 | 3.04 | 0.40 |
| 1:M:263:LEU:CD1 | 1:M:283:GLU:CA | 2.99 | 0.40 |
| 3:C:65:ASN:OD1 | 3:C:66:PRO:CD | 2.68 | 0.40 |
| 3:O:105:PRO:HG2 | 3:O:106:GLU:H | 1.86 | 0.40 |
| 4:P:111:THR:O | 4:P:115:VAL:CG2 | 2.69 | 0.40 |
| 1:M:184:ARG:HH11 | 1:M:184:ARG:HG2 | 1.87 | 0.40 |
| 1:M:114:ARG:HB2 | 1:M:114:ARG:HH11 | 1.85 | 0.40 |
| 1:M:229:VAL:HG13 | 1:M:230:GLN:N | 2.37 | 0.40 |
| 2:N:232:SER:O | 2:N:235:PHE:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 3:O:127:ALA:C | 3:O:128:LEU:HD23 | 2.42 | 0.40 |
| 2:N:108:HIS:NE2 | 2:N:112:SER:OG | 2.54 | 0.40 |
| 2:B:68:MET:HG2 | 2:B:93:LEU:HA | 2.03 | 0.40 |
| 3:C:53:PRO:N | 4:D:51:TYR:CE1 | 2.89 | 0.40 |
| 1:M:175:MET:O | 1:M:498:PHE:HA | 2.20 | 0.40 |
| 1:A:70:VAL:O | 1:A:71:ALA:C | 2.58 | 0.40 |
| 2:B:54:ARG:CD | 2:B:103:VAL:HG13 | 2.51 | 0.40 |
| 2:N:80:PHE:CB | 2:N:82:ARG:HG2 | 2.51 | 0.40 |
| 2:N:1:ALA:O | 2:N:2:GLU:C | 2.60 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 575/602 (96%) | 492 (86%) | 69 (12%) | 14 (2%) | 9 | 53 |
| 1 | M | 570/602 (95%) | 402 (70%) | 103 (18%) | 65 (11%) | 1 | 5 |
| 2 | B | 241/243 (99%) | 207 (86%) | 30 (12%) | 4 (2%) | 14 | 62 |
| 2 | N | 241/243 (99%) | 126 (52%) | 79 (33%) | 36 (15%) | 0 | 2 |
| 3 | C | 128/130 (98%) | 99 (77%) | 25 (20%) | 4 (3%) | 7 | 45 |
| 3 | O | 128/130 (98%) | 103 (80%) | 18 (14%) | 7 (6%) | 3 | 25 |
| 4 | D | 117/119 (98%) | 68 (58%) | 35 (30%) | 14 (12%) | 1 | 4 |
| 4 | P | 117/119 (98%) | 76 (65%) | 26 (22%) | 15 (13%) | 0 | 3 |
| All | All | 2117/2188 (97%) | 1573 (74%) | 385 (18%) | 159 (8%) | 2 | 15 |

All (159) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 194 | GLY |
| 1 | A | 270 | PRO |
| 1 | A | 321 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 242 | PRO |
| 3 | C | 31 | THR |
| 4 | D | 61 | PHE |
| 1 | M | 25 | GLN |
| 1 | M | 29 | ASN |
| 1 | M | 47 | ALA |
| 1 | M | 58 | ASP |
| 1 | M | 62 | PHE |
| 1 | M | 111 | VAL |
| 1 | M | 219 | HIS |
| 1 | M | 226 | MET |
| 1 | M | 227 | GLU |
| 1 | M | 244 | THR |
| 1 | M | 282 | MET |
| 1 | M | 284 | LEU |
| 1 | M | 394 | ASN |
| 1 | M | 464 | GLY |
| 1 | M | 530 | GLY |
| 2 | N | 19 | THR |
| 2 | N | 65 | CYS |
| 2 | N | 76 | ALA |
| 2 | N | 121 | ILE |
| 2 | N | 135 | THR |
| 2 | N | 150 | ASN |
| 2 | N | 189 | LYS |
| 2 | N | 190 | GLU |
| 2 | N | 219 | ASP |
| 3 | O | 18 | LYS |
| 3 | O | 31 | THR |
| 3 | O | 92 | LYS |
| 4 | P | 10 | GLU |
| 4 | P | 34 | LEU |
| 4 | P | 61 | PHE |
| 4 | P | 99 | VAL |
| 1 | A | 287 | ARG |
| 1 | A | 343 | PRO |
| 1 | A | 389 | ASN |
| 2 | B | 32 | ALA |
| 4 | D | 2 | ASN |
| 4 | D | 17 | PHE |
| 4 | D | 88 | ASP |
| 1 | M | 40 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 49 | GLN |
| 1 | M | 50 | GLY |
| 1 | M | 74 | ASP |
| 1 | M | 79 | GLN |
| 1 | M | 122 | GLU |
| 1 | M | 127 | ALA |
| 1 | M | 166 | HIS |
| 1 | M | 175 | MET |
| 1 | M | 188 | VAL |
| 1 | M | 217 | LEU |
| 1 | M | 230 | GLN |
| 1 | M | 238 | GLY |
| 1 | M | 277 | PRO |
| 1 | M | 287 | ARG |
| 1 | M | 293 | ALA |
| 1 | M | 387 | GLY |
| 1 | M | 390 | ARG |
| 1 | M | 395 | SER |
| 1 | M | 498 | PHE |
| 1 | M | 555 | ARG |
| 2 | N | 2 | GLU |
| 2 | N | 57 | CYS |
| 2 | N | 61 | ILE |
| 2 | N | 141 | LYS |
| 2 | N | 155 | TYR |
| 2 | N | 186 | HIS |
| 2 | N | 187 | GLY |
| 2 | N | 197 | SER |
| 2 | N | 201 | VAL |
| 2 | N | 218 | VAL |
| 2 | N | 236 | LEU |
| 4 | P | 20 | GLY |
| 4 | P | 43 | LEU |
| 4 | P | 46 | GLY |
| 4 | P | 114 | GLY |
| 1 | A | 282 | MET |
| 4 | D | 20 | GLY |
| 4 | D | 24 | SER |
| 4 | D | 51 | TYR |
| 4 | D | 99 | VAL |
| 1 | M | 63 | GLU |
| 1 | M | 66 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 107 | PRO |
| 1 | M | 174 | ASN |
| 1 | M | 269 | GLY |
| 1 | M | 446 | GLU |
| 2 | N | 15 | PRO |
| 2 | N | 53 | TYR |
| 2 | N | 60 | ALA |
| 2 | N | 101 | ASP |
| 2 | N | 115 | ALA |
| 2 | N | 128 | ASP |
| 2 | N | 137 | ALA |
| 2 | N | 196 | ASN |
| 4 | P | 95 | ALA |
| 1 | A | 271 | GLU |
| 1 | A | 329 | PRO |
| 1 | A | 347 | PRO |
| 3 | C | 49 | LEU |
| 4 | D | 16 | LEU |
| 1 | M | 26 | ALA |
| 1 | M | 59 | HIS |
| 1 | M | 77 | CYS |
| 1 | M | 200 | ARG |
| 1 | M | 262 | TYR |
| 1 | M | 317 | ARG |
| 1 | M | 343 | PRO |
| 1 | M | 460 | GLU |
| 2 | N | 47 | LEU |
| 4 | P | 1 | ILE |
| 1 | A | 320 | GLY |
| 1 | A | 530 | GLY |
| 1 | A | 575 | PRO |
| 2 | B | 170 | PRO |
| 2 | B | 183 | SER |
| 4 | D | 5 | PRO |
| 4 | D | 85 | ALA |
| 1 | M | 43 | SER |
| 1 | M | 65 | HIS |
| 1 | M | 148 | GLN |
| 1 | M | 233 | PRO |
| 1 | M | 286 | PRO |
| 1 | M | 456 | GLY |
| 1 | M | 461 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | N | 45 | ASP |
| 4 | P | 100 | PHE |
| 4 | P | 113 | ILE |
| 3 | C | 53 | PRO |
| 4 | D | 113 | ILE |
| 1 | M | 271 | GLU |
| 1 | M | 276 | GLU |
| 1 | M | 373 | GLY |
| 2 | N | 195 | LEU |
| 2 | N | 220 | PRO |
| 3 | O | 49 | LEU |
| 4 | P | 83 | HIS |
| 1 | M | 208 | VAL |
| 3 | O | 53 | PRO |
| 4 | P | 2 | ASN |
| 1 | A | 107 | PRO |
| 3 | C | 67 | VAL |
| 4 | D | 114 | GLY |
| 1 | M | 509 | GLY |
| 4 | P | 21 | GLY |
| 4 | D | 72 | VAL |
| 2 | N | 136 | PRO |
| 2 | N | 162 | GLY |
| 3 | O | 122 | VAL |
| 1 | M | 383 | VAL |
| 2 | N | 49 | PRO |
| 1 | M | 100 | GLY |
| 1 | M | 121 | ILE |
| 2 | N | 149 | ILE |
| 3 | O | 106 | GLU |

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 | 460/475 (97%) | 349 (76%) | 111 (24%) | 1 4 |
| 1 | M | 456/475 (96%) | 406 (89%) | 50 (11%) | 9 38 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2 | B | 205/205 (100%) | 171 (83%) | 34 (17%) | 3 | 16 |
| 2 | N | 205/205 (100%) | 175 (85%) | 30 (15%) | 5 | 23 |
| 3 | C | 111/111 (100%) | 89 (80%) | 22 (20%) | 2 | 9 |
| 3 | O | 111/111 (100%) | 81 (73%) | 30 (27%) | 1 | 2 |
| 4 | D | 97/97 (100%) | 79 (81%) | 18 (19%) | 2 | 11 |
| 4 | P | 97/97 (100%) | 75 (77%) | 22 (23%) | 1 | 5 |
| All | All | 1742/1776 (98%) | 1425 (82%) | 317 (18%) | 2 | 12 |

All (317) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | GLN |
| 1 | A | 6 | ASP |
| 1 | A | 7 | LEU |
| 1 | A | 17 | LEU |
| 1 | A | 18 | ARG |
| 1 | A | 25 | GLN |
| 1 | A | 27 | ASN |
| 1 | A | 28 | PRO |
| 1 | A | 29 | ASN |
| 1 | A | 31 | LYS |
| 1 | A | 36 | SER |
| 1 | A | 41 | MET |
| 1 | A | 42 | ARG |
| 1 | A | 49 | GLN |
| 1 | A | 58 | ASP |
| 1 | A | 63 | GLU |
| 1 | A | 76 | LEU |
| 1 | A | 77 | CYS |
| 1 | A | 79 | GLN |
| 1 | A | 86 | VAL |
| 1 | A | 90 | PRO |
| 1 | A | 91 | THR |
| 1 | A | 92 | GLU |
| 1 | A | 96 | LEU |
| 1 | A | 104 | SER |
| 1 | A | 107 | PRO |
| 1 | A | 112 | ASN |
| 1 | A | 115 | ARG |
| 1 | A | 116 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 119 | MET |
| 1 | A | 122 | GLU |
| 1 | A | 123 | ARG |
| 1 | A | 133 | PHE |
| 1 | A | 138 | THR |
| 1 | A | 150 | GLN |
| 1 | A | 168 | ARG |
| 1 | A | 170 | LEU |
| 1 | A | 175 | MET |
| 1 | A | 180 | LEU |
| 1 | A | 181 | VAL |
| 1 | A | 184 | ARG |
| 1 | A | 197 | ARG |
| 1 | A | 217 | LEU |
| 1 | A | 218 | SER |
| 1 | A | 222 | PRO |
| 1 | A | 223 | LEU |
| 1 | A | 224 | ARG |
| 1 | A | 230 | GLN |
| 1 | A | 241 | ILE |
| 1 | A | 253 | ILE |
| 1 | A | 257 | LYS |
| 1 | A | 258 | ASN |
| 1 | A | 260 | TYR |
| 1 | A | 261 | ARG |
| 1 | A | 263 | LEU |
| 1 | A | 265 | ASP |
| 1 | A | 278 | LYS |
| 1 | A | 280 | LYS |
| 1 | A | 287 | ARG |
| 1 | A | 288 | ASP |
| 1 | A | 289 | LYS |
| 1 | A | 299 | ARG |
| 1 | A | 310 | ASP |
| 1 | A | 314 | LEU |
| 1 | A | 317 | ARG |
| 1 | A | 319 | LEU |
| 1 | A | 321 | GLU |
| 1 | A | 322 | LYS |
| 1 | A | 325 | HIS |
| 1 | A | 327 | ARG |
| 1 | A | 328 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 332 | CYS |
| 1 | A | 336 | LYS |
| 1 | A | 344 | VAL |
| 1 | A | 358 | MET |
| 1 | A | 372 | LYS |
| 1 | A | 391 | LEU |
| 1 | A | 404 | ARG |
| 1 | A | 412 | GLU |
| 1 | A | 413 | ARG |
| 1 | A | 416 | THR |
| 1 | A | 422 | GLU |
| 1 | A | 438 | ASP |
| 1 | A | 440 | VAL |
| 1 | A | 441 | ASN |
| 1 | A | 442 | GLN |
| 1 | A | 450 | LYS |
| 1 | A | 465 | ILE |
| 1 | A | 466 | TYR |
| 1 | A | 476 | ILE |
| 1 | A | 487 | LYS |
| 1 | A | 489 | VAL |
| 1 | A | 490 | ARG |
| 1 | A | 508 | LEU |
| 1 | A | 512 | LEU |
| 1 | A | 518 | MET |
| 1 | A | 523 | MET |
| 1 | A | 527 | GLU |
| 1 | A | 529 | ARG |
| 1 | A | 532 | HIS |
| 1 | A | 534 | ARG |
| 1 | A | 536 | ASP |
| 1 | A | 537 | GLU |
| 1 | A | 539 | CYS |
| 1 | A | 541 | GLU |
| 1 | A | 542 | ARG |
| 1 | A | 543 | ASP |
| 1 | A | 546 | ASN |
| 1 | A | 558 | ASP |
| 1 | A | 560 | THR |
| 1 | A | 562 | ARG |
| 2 | B | 4 | LYS |
| 2 | B | 5 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 12 | ARG |
| 2 | B | 38 | ASP |
| 2 | B | 45 | ASP |
| 2 | B | 46 | ASN |
| 2 | B | 47 | LEU |
| 2 | B | 50 | ASP |
| 2 | B | 52 | SER |
| 2 | B | 61 | ILE |
| 2 | B | 68 | MET |
| 2 | B | 78 | LYS |
| 2 | B | 86 | ASP |
| 2 | B | 93 | LEU |
| 2 | B | 105 | ASP |
| 2 | B | 106 | MET |
| 2 | B | 107 | THR |
| 2 | B | 110 | ILE |
| 2 | B | 117 | LYS |
| 2 | B | 124 | SER |
| 2 | B | 125 | ARG |
| 2 | B | 128 | ASP |
| 2 | B | 132 | ASN |
| 2 | B | 141 | LYS |
| 2 | B | 178 | ARG |
| 2 | B | 183 | SER |
| 2 | B | 184 | ARG |
| 2 | B | 190 | GLU |
| 2 | B | 197 | SER |
| 2 | B | 203 | SER |
| 2 | B | 206 | PHE |
| 2 | B | 212 | GLU |
| 2 | B | 237 | ILE |
| 2 | B | 241 | LYS |
| 3 | C | 1 | THR |
| 3 | C | 9 | ARG |
| 3 | C | 11 | MET |
| 3 | C | 12 | THR |
| 3 | C | 19 | LEU |
| 3 | C | 21 | PHE |
| 3 | C | 31 | THR |
| 3 | C | 36 | VAL |
| 3 | C | 37 | TRP |
| 3 | C | 39 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 42 | LEU |
| 3 | C | 50 | LYS |
| 3 | C | 54 | GLU |
| 3 | C | 64 | GLN |
| 3 | C | 70 | ILE |
| 3 | C | 72 | ASN |
| 3 | C | 74 | ILE |
| 3 | C | 100 | ASP |
| 3 | C | 103 | MET |
| 3 | C | 106 | GLU |
| 3 | C | 111 | SER |
| 3 | C | 116 | THR |
| 4 | D | 1 | ILE |
| 4 | D | 4 | ASN |
| 4 | D | 7 | ARG |
| 4 | D | 12 | VAL |
| 4 | D | 30 | VAL |
| 4 | D | 31 | MET |
| 4 | D | 39 | LEU |
| 4 | D | 43 | LEU |
| 4 | D | 47 | ASP |
| 4 | D | 50 | SER |
| 4 | D | 59 | GLN |
| 4 | D | 75 | LEU |
| 4 | D | 82 | MET |
| 4 | D | 83 | HIS |
| 4 | D | 86 | MET |
| 4 | D | 115 | VAL |
| 4 | D | 117 | THR |
| 4 | D | 118 | ILE |
| 1 | M | 6 | ASP |
| 1 | M | 18 | ARG |
| 1 | M | 49 | GLN |
| 1 | M | 52 | SER |
| 1 | M | 57 | GLN |
| 1 | M | 76 | LEU |
| 1 | M | 90 | PRO |
| 1 | M | 97 | GLU |
| 1 | M | 105 | ARG |
| 1 | M | 116 | PHE |
| 1 | M | 122 | GLU |
| 1 | M | 126 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 146 | PHE |
| 1 | M | 151 | ARG |
| 1 | M | 152 | PHE |
| 1 | M | 160 | ILE |
| 1 | M | 192 | THR |
| 1 | M | 200 | ARG |
| 1 | M | 207 | ILE |
| 1 | M | 219 | HIS |
| 1 | M | 223 | LEU |
| 1 | M | 226 | MET |
| 1 | M | 227 | GLU |
| 1 | M | 228 | PHE |
| 1 | M | 229 | VAL |
| 1 | M | 231 | TYR |
| 1 | M | 248 | ARG |
| 1 | M | 254 | LEU |
| 1 | M | 262 | TYR |
| 1 | M | 277 | PRO |
| 1 | M | 279 | ASN |
| 1 | M | 287 | ARG |
| 1 | M | 295 | TRP |
| 1 | M | 328 | LEU |
| 1 | M | 330 | PHE |
| 1 | M | 332 | CYS |
| 1 | M | 343 | PRO |
| 1 | M | 351 | ARG |
| 1 | M | 356 | TYR |
| 1 | M | 386 | HIS |
| 1 | M | 398 | GLU |
| 1 | M | 463 | CYS |
| 1 | M | 490 | ARG |
| 1 | M | 499 | ASN |
| 1 | M | 505 | THR |
| 1 | M | 526 | LYS |
| 1 | M | 549 | LYS |
| 1 | M | 556 | ASP |
| 1 | M | 567 | ASP |
| 1 | M | 570 | ILE |
| 2 | N | 25 | PHE |
| 2 | N | 27 | GLU |
| 2 | N | 36 | LEU |
| 2 | N | 37 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | N | 43 | ILE |
| 2 | N | 51 | LEU |
| 2 | N | 53 | TYR |
| 2 | N | 54 | ARG |
| 2 | N | 55 | TRP |
| 2 | N | 57 | CYS |
| 2 | N | 58 | ARG |
| 2 | N | 69 | VAL |
| 2 | N | 75 | LEU |
| 2 | N | 133 | ILE |
| 2 | N | 139 | MET |
| 2 | N | 144 | GLN |
| 2 | N | 150 | ASN |
| 2 | N | 153 | LEU |
| 2 | N | 158 | CYS |
| 2 | N | 178 | ARG |
| 2 | N | 183 | SER |
| 2 | N | 186 | HIS |
| 2 | N | 188 | LYS |
| 2 | N | 192 | MET |
| 2 | N | 196 | ASN |
| 2 | N | 206 | PHE |
| 2 | N | 213 | VAL |
| 2 | N | 216 | LYS |
| 2 | N | 235 | PHE |
| 2 | N | 240 | LEU |
| 3 | O | 1 | THR |
| 3 | O | 4 | ARG |
| 3 | O | 9 | ARG |
| 3 | O | 11 | MET |
| 3 | O | 12 | THR |
| 3 | O | 17 | LYS |
| 3 | O | 19 | LEU |
| 3 | O | 31 | THR |
| 3 | O | 37 | TRP |
| 3 | O | 39 | SER |
| 3 | O | 42 | LEU |
| 3 | O | 47 | PHE |
| 3 | O | 54 | GLU |
| 3 | O | 61 | ASP |
| 3 | O | 68 | ILE |
| 3 | O | 70 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | O | 72 | ASN |
| 3 | O | 85 | THR |
| 3 | O | 92 | LYS |
| 3 | O | 96 | ILE |
| 3 | O | 98 | VAL |
| 3 | O | 99 | LYS |
| 3 | O | 100 | ASP |
| 3 | O | 102 | LYS |
| 3 | O | 103 | MET |
| 3 | O | 110 | LYS |
| 3 | O | 111 | SER |
| 3 | O | 117 | VAL |
| 3 | O | 123 | ILE |
| 3 | O | 130 | TRP |
| 4 | P | 4 | ASN |
| 4 | P | 6 | LYS |
| 4 | P | 7 | ARG |
| 4 | P | 12 | VAL |
| 4 | P | 16 | LEU |
| 4 | P | 23 | TRP |
| 4 | P | 43 | LEU |
| 4 | P | 52 | GLU |
| 4 | P | 53 | ARG |
| 4 | P | 65 | VAL |
| 4 | P | 66 | PHE |
| 4 | P | 75 | LEU |
| 4 | P | 82 | MET |
| 4 | P | 87 | HIS |
| 4 | P | 89 | LEU |
| 4 | P | 93 | VAL |
| 4 | P | 97 | LYS |
| 4 | P | 103 | LEU |
| 4 | P | 112 | LEU |
| 4 | P | 115 | VAL |
| 4 | P | 116 | VAL |
| 4 | P | 117 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1 | GLN |
| 1 | A | 27 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | GLN |
| 1 | A | 95 | GLN |
| 1 | A | 182 | GLN |
| 1 | A | 204 | ASN |
| 1 | A | 219 | HIS |
| 1 | A | 232 | HIS |
| 1 | A | 279 | ASN |
| 1 | A | 318 | HIS |
| 1 | A | 366 | ASN |
| 1 | A | 409 | GLN |
| 1 | A | 421 | ASN |
| 1 | A | 434 | GLN |
| 1 | A | 499 | ASN |
| 1 | A | 510 | HIS |
| 1 | A | 532 | HIS |
| 2 | B | 95 | ASN |
| 2 | B | 123 | ASN |
| 2 | B | 144 | GLN |
| 2 | B | 150 | ASN |
| 2 | B | 160 | GLN |
| 2 | B | 180 | ASN |
| 2 | B | 194 | GLN |
| 2 | B | 199 | ASN |
| 3 | C | 72 | ASN |
| 4 | D | 4 | ASN |
| 4 | D | 59 | GLN |
| 1 | M | 44 | HIS |
| 1 | M | 49 | GLN |
| 1 | M | 65 | HIS |
| 1 | M | 79 | GLN |
| 1 | M | 112 | ASN |
| 1 | M | 137 | HIS |
| 1 | M | 166 | HIS |
| 1 | M | 174 | ASN |
| 1 | M | 182 | GLN |
| 1 | M | 230 | GLN |
| 1 | M | 279 | ASN |
| 1 | M | 302 | ASN |
| 1 | M | 355 | HIS |
| 1 | M | 394 | ASN |
| 1 | M | 442 | GLN |
| 1 | M | 520 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 532 | HIS |
| 1 | M | 533 | GLN |
| 1 | M | 550 | HIS |
| 2 | N | 5 | ASN |
| 2 | N | 138 | GLN |
| 2 | N | 144 | GLN |
| 2 | N | 160 | GLN |
| 2 | N | 196 | ASN |
| 2 | N | 226 | GLN |
| 3 | O | 64 | GLN |
| 3 | O | 65 | ASN |
| 3 | O | 72 | ASN |
| 3 | O | 82 | HIS |
| 3 | O | 95 | ASN |
| 4 | P | 4 | ASN |
| 4 | P | 59 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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 | FLC | A | 702 | - | 5,12,12 | 14.14 | 4 (80%) | 7,17,17 | 6.06 | 2 (28%) |
| 9 | FAD | A | 703 | 1 | 56,57,58 | 4.06 | 32 (57%) | 79,87,89 | 2.18 | 16 (20%) |
| 6 | FES | B | 244 | 2 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 7 | F3S | B | 245 | 2 | 3,9,9 | 13.24 | 3 (100%) | 0,15,15 | 0.00 | - |
| 8 | SF4 | B | 246 | 2 | 12,12,12 | 16.77 | 12 (100%) | 0,24,24 | 0.00 | - |
| 10 | MQ7 | D | 700 | - | 34,34,49 | 3.69 | 16 (47%) | 43,45,63 | 2.32 | 14 (32%) |
| 5 | FLC | M | 802 | - | 5,12,12 | 7.24 | 4 (80%) | 7,17,17 | 4.10 | 2 (28%) |
| 9 | FAD | M | 803 | 1 | 56,57,58 | 3.89 | 27 (48%) | 79,87,89 | 2.17 | 14 (17%) |
| 6 | FES | N | 244 | 2 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 7 | F3S | N | 245 | 2 | 3,9,9 | 7.26 | 3 (100%) | 0,15,15 | 0.00 | - |
| 8 | SF4 | N | 246 | 2 | 12,12,12 | 8.16 | 12 (100%) | 0,24,24 | 0.00 | - |
| 10 | MQ7 | P | 800 | - | 34,34,49 | 3.74 | 16 (47%) | 43,45,63 | 2.54 | 16 (37%) |

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 | FLC | A | 702 | - | - | 0/6/16/16 | 0/0/0/0 |
| 9 | FAD | A | 703 | 1 | - | 0/34/46/50 | 0/1/6/6 |
| 6 | FES | B | 244 | 2 | - | 0/0/4/4 | 0/0/1/1 |
| 7 | F3S | B | 245 | 2 | - | 0/0/24/24 | 0/0/3/3 |
| 8 | SF4 | B | 246 | 2 | - | 0/0/48/48 | 0/0/5/5 |
| 10 | MQ7 | D | 700 | - | - | 0/23/43/61 | 0/0/2/2 |
| 5 | FLC | M | 802 | - | - | 0/6/16/16 | 0/0/0/0 |
| 9 | FAD | M | 803 | 1 | - | 0/34/46/50 | 0/1/6/6 |
| 6 | FES | N | 244 | 2 | - | 0/0/4/4 | 0/0/1/1 |
| 7 | F3S | N | 245 | 2 | - | 0/0/24/24 | 0/0/3/3 |
| 8 | SF4 | N | 246 | 2 | - | 0/0/48/48 | 0/0/5/5 |
| 10 | MQ7 | P | 800 | - | - | 0/23/43/61 | 0/0/2/2 |

All (129) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 5 | A | 702 | FLC | CG-CGC | -30.94 | 1.30 | 1.49 |
| 8 | B | 246 | SF4 | S3-FE2 | -22.27 | 2.18 | 2.33 |
| 8 | B | 246 | SF4 | S4-FE1 | -21.09 | 2.19 | 2.33 |
| 8 | B | 246 | SF4 | S1-FE4 | -19.21 | 2.20 | 2.33 |
| 8 | B | 246 | SF4 | S3-FE4 | -17.80 | 2.21 | 2.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 8 | B | 246 | SF4 | S1-FE2 | -17.32 | 2.21 | 2.33 |
| 8 | B | 246 | SF4 | S2-FE3 | -17.26 | 2.21 | 2.33 |
| 8 | B | 246 | SF4 | S4-FE3 | -16.81 | 2.21 | 2.33 |
| 9 | A | 703 | FAD | C2B-C3B | -15.99 | 1.42 | 1.52 |
| 8 | B | 246 | SF4 | S2-FE1 | -15.65 | 2.22 | 2.33 |
| 8 | B | 246 | SF4 | S1-FE3 | -15.58 | 2.22 | 2.33 |
| 7 | B | 245 | F3S | S3-FE1 | -15.54 | 2.22 | 2.33 |
| 5 | M | 802 | FLC | CA-CAC | 13.70 | 1.58 | 1.49 |
| 8 | B | 246 | SF4 | S4-FE2 | -13.43 | 2.24 | 2.33 |
| 8 | B | 246 | SF4 | S3-FE1 | -12.84 | 2.24 | 2.33 |
| 8 | N | 246 | SF4 | S3-FE1 | -12.82 | 2.24 | 2.33 |
| 8 | N | 246 | SF4 | S1-FE3 | -12.68 | 2.24 | 2.33 |
| 9 | M | 803 | FAD | PA-O3P | 12.02 | 1.81 | 1.59 |
| 7 | B | 245 | F3S | S3-FE3 | -12.00 | 2.25 | 2.33 |
| 7 | B | 245 | F3S | S3-FE4 | -11.86 | 2.25 | 2.33 |
| 9 | M | 803 | FAD | C2B-C3B | -10.81 | 1.45 | 1.52 |
| 10 | P | 800 | MQ7 | C12-C13 | 10.50 | 1.54 | 1.32 |
| 10 | D | 700 | MQ7 | C12-C13 | 10.41 | 1.54 | 1.32 |
| 8 | N | 246 | SF4 | S2-FE3 | -9.66 | 2.26 | 2.33 |
| 9 | A | 703 | FAD | PA-O3P | 9.29 | 1.76 | 1.59 |
| 8 | N | 246 | SF4 | S3-FE2 | -9.28 | 2.27 | 2.33 |
| 8 | N | 246 | SF4 | S4-FE1 | -9.15 | 2.27 | 2.33 |
| 10 | P | 800 | MQ7 | C17-C18 | 8.73 | 1.50 | 1.32 |
| 9 | M | 803 | FAD | C9A-N10 | 8.48 | 1.51 | 1.38 |
| 10 | D | 700 | MQ7 | C17-C18 | 8.34 | 1.49 | 1.32 |
| 9 | A | 703 | FAD | C9A-N10 | 8.16 | 1.50 | 1.38 |
| 9 | M | 803 | FAD | C1'-N10 | 8.06 | 1.57 | 1.48 |
| 7 | N | 245 | F3S | S3-FE1 | -7.88 | 2.27 | 2.33 |
| 8 | N | 246 | SF4 | S2-FE4 | -7.63 | 2.28 | 2.33 |
| 10 | P | 800 | MQ7 | C22-C23 | 7.61 | 1.48 | 1.32 |
| 10 | D | 700 | MQ7 | C22-C23 | 7.54 | 1.48 | 1.32 |
| 7 | N | 245 | F3S | S3-FE3 | -7.51 | 2.28 | 2.33 |
| 10 | P | 800 | MQ7 | C27-C28 | 7.50 | 1.49 | 1.34 |
| 8 | N | 246 | SF4 | S1-FE4 | -7.29 | 2.28 | 2.33 |
| 10 | D | 700 | MQ7 | C27-C28 | 7.18 | 1.48 | 1.34 |
| 8 | N | 246 | SF4 | S4-FE2 | -6.84 | 2.28 | 2.33 |
| 9 | A | 703 | FAD | C4A-N3A | 6.41 | 1.45 | 1.35 |
| 9 | M | 803 | FAD | C4A-N3A | 6.40 | 1.45 | 1.35 |
| 7 | N | 245 | F3S | S3-FE4 | -6.29 | 2.29 | 2.33 |
| 9 | M | 803 | FAD | C10-N10 | 6.18 | 1.52 | 1.38 |
| 8 | B | 246 | SF4 | S2-FE4 | -6.02 | 2.29 | 2.33 |
| 9 | A | 703 | FAD | C4X-N5 | 5.77 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9 | M | 803 | FAD | C2A-N3A | 5.74 | 1.43 | 1.32 |
| 9 | M | 803 | FAD | C10-N1 | 5.64 | 1.45 | 1.35 |
| 9 | A | 703 | FAD | C1'-N10 | 5.47 | 1.54 | 1.48 |
| 5 | M | 802 | FLC | CG-CB | 5.35 | 1.63 | 1.54 |
| 5 | M | 802 | FLC | CA-CB | 5.30 | 1.63 | 1.54 |
| 9 | M | 803 | FAD | C4X-N5 | 5.24 | 1.47 | 1.36 |
| 9 | A | 703 | FAD | P-O3P | -5.11 | 1.50 | 1.59 |
| 9 | A | 703 | FAD | C10-N10 | 5.07 | 1.49 | 1.38 |
| 9 | A | 703 | FAD | C10-N1 | 5.03 | 1.44 | 1.35 |
| 8 | N | 246 | SF4 | S3-FE4 | -4.87 | 2.30 | 2.33 |
| 9 | A | 703 | FAD | C5X-N5 | 4.85 | 1.42 | 1.35 |
| 10 | D | 700 | MQ7 | C9-C10 | 4.78 | 1.48 | 1.39 |
| 9 | M | 803 | FAD | C9A-C5X | 4.77 | 1.52 | 1.42 |
| 10 | P | 800 | MQ7 | C9-C10 | 4.59 | 1.47 | 1.39 |
| 9 | A | 703 | FAD | C4B-C3B | 4.55 | 1.58 | 1.53 |
| 9 | A | 703 | FAD | C8-C7 | 4.54 | 1.54 | 1.40 |
| 9 | M | 803 | FAD | C4-C4X | 4.46 | 1.48 | 1.41 |
| 9 | M | 803 | FAD | C4-N3 | 4.45 | 1.44 | 1.37 |
| 9 | A | 703 | FAD | C2A-N3A | 4.45 | 1.41 | 1.32 |
| 9 | M | 803 | FAD | C6-C7 | 4.39 | 1.49 | 1.37 |
| 9 | M | 803 | FAD | C4X-C10 | 4.38 | 1.48 | 1.40 |
| 10 | P | 800 | MQ7 | C2-C1 | 4.30 | 1.57 | 1.48 |
| 9 | A | 703 | FAD | C9-C9A | 4.27 | 1.49 | 1.40 |
| 9 | A | 703 | FAD | C4-N3 | 4.25 | 1.44 | 1.37 |
| 10 | D | 700 | MQ7 | C11-C12 | -4.24 | 1.43 | 1.50 |
| 9 | A | 703 | FAD | C4-C4X | 4.22 | 1.48 | 1.41 |
| 10 | D | 700 | MQ7 | C7-C6 | 4.11 | 1.48 | 1.39 |
| 10 | P | 800 | MQ7 | C7-C6 | 4.09 | 1.48 | 1.39 |
| 9 | M | 803 | FAD | C8-C7 | 4.08 | 1.52 | 1.40 |
| 9 | A | 703 | FAD | C6-C7 | 4.08 | 1.49 | 1.37 |
| 10 | D | 700 | MQ7 | C2-C1 | 4.06 | 1.56 | 1.48 |
| 5 | M | 802 | FLC | CG-CGC | 4.00 | 1.52 | 1.49 |
| 10 | D | 700 | MQ7 | C5-C4 | 4.00 | 1.56 | 1.48 |
| 9 | M | 803 | FAD | C8A-N9A | 3.99 | 1.42 | 1.36 |
| 10 | P | 800 | MQ7 | C8-C7 | 3.97 | 1.49 | 1.37 |
| 9 | A | 703 | FAD | C1'-C2' | -3.93 | 1.47 | 1.51 |
| 9 | M | 803 | FAD | C9-C9A | 3.92 | 1.48 | 1.40 |
| 10 | D | 700 | MQ7 | C8-C7 | 3.92 | 1.49 | 1.37 |
| 9 | A | 703 | FAD | C9A-C5X | 3.91 | 1.50 | 1.42 |
| 9 | M | 803 | FAD | C6-C5X | 3.91 | 1.46 | 1.41 |
| 5 | A | 702 | FLC | CA-CAC | 3.87 | 1.52 | 1.49 |
| 9 | A | 703 | FAD | C5A-C4A | -3.85 | 1.31 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9 | M | 803 | FAD | C9-C8 | 3.78 | 1.48 | 1.37 |
| 5 | A | 702 | FLC | CA-CB | 3.77 | 1.60 | 1.54 |
| 9 | A | 703 | FAD | C8A-N9A | 3.77 | 1.42 | 1.36 |
| 9 | A | 703 | FAD | C7M-C7 | -3.76 | 1.43 | 1.51 |
| 10 | P | 800 | MQ7 | C11-C12 | -3.54 | 1.45 | 1.50 |
| 9 | A | 703 | FAD | C6-C5X | 3.53 | 1.46 | 1.41 |
| 9 | A | 703 | FAD | C9-C8 | 3.48 | 1.47 | 1.37 |
| 10 | P | 800 | MQ7 | C5-C4 | 3.42 | 1.55 | 1.48 |
| 8 | N | 246 | SF4 | S2-FE1 | -3.41 | 2.31 | 2.33 |
| 10 | P | 800 | MQ7 | C3-C4 | 3.39 | 1.56 | 1.47 |
| 9 | M | 803 | FAD | C7M-C7 | -3.38 | 1.43 | 1.51 |
| 9 | M | 803 | FAD | C5X-N5 | 3.38 | 1.40 | 1.35 |
| 9 | M | 803 | FAD | C5A-C4A | -3.37 | 1.32 | 1.40 |
| 5 | A | 702 | FLC | CG-CB | 3.30 | 1.60 | 1.54 |
| 9 | A | 703 | FAD | C4'-C3' | -3.26 | 1.46 | 1.53 |
| 9 | M | 803 | FAD | P-O3P | -3.24 | 1.54 | 1.59 |
| 8 | N | 246 | SF4 | S1-FE2 | -3.23 | 2.31 | 2.33 |
| 9 | A | 703 | FAD | C4X-C10 | 3.22 | 1.46 | 1.40 |
| 10 | D | 700 | MQ7 | C3-C4 | 2.90 | 1.54 | 1.47 |
| 10 | P | 800 | MQ7 | C6-C5 | 2.80 | 1.44 | 1.39 |
| 10 | P | 800 | MQ7 | C8-C9 | 2.78 | 1.45 | 1.39 |
| 9 | A | 703 | FAD | O4-C4 | -2.78 | 1.19 | 1.24 |
| 10 | D | 700 | MQ7 | C8-C9 | 2.78 | 1.45 | 1.39 |
| 9 | M | 803 | FAD | C5'-C4' | 2.77 | 1.56 | 1.51 |
| 10 | D | 700 | MQ7 | C6-C5 | 2.75 | 1.44 | 1.39 |
| 9 | M | 803 | FAD | C4B-C3B | 2.70 | 1.56 | 1.53 |
| 10 | D | 700 | MQ7 | C30-C28 | 2.68 | 1.55 | 1.40 |
| 10 | P | 800 | MQ7 | C30-C28 | 2.63 | 1.54 | 1.40 |
| 9 | A | 703 | FAD | C2'-C3' | -2.51 | 1.48 | 1.53 |
| 8 | N | 246 | SF4 | S4-FE3 | -2.45 | 2.31 | 2.33 |
| 10 | P | 800 | MQ7 | C15-C13 | 2.44 | 1.57 | 1.51 |
| 10 | D | 700 | MQ7 | O4-C4 | 2.43 | 1.28 | 1.23 |
| 9 | A | 703 | FAD | C2-N3 | 2.39 | 1.42 | 1.37 |
| 9 | M | 803 | FAD | C2-N3 | 2.26 | 1.41 | 1.37 |
| 9 | A | 703 | FAD | P-O5' | -2.22 | 1.49 | 1.59 |
| 9 | M | 803 | FAD | C8A-N7A | -2.16 | 1.30 | 1.34 |
| 9 | A | 703 | FAD | C4A-N9A | 2.14 | 1.40 | 1.37 |
| 10 | P | 800 | MQ7 | C19-C18 | 2.14 | 1.56 | 1.50 |
| 10 | D | 700 | MQ7 | C19-C18 | 2.11 | 1.56 | 1.50 |
| 9 | A | 703 | FAD | C8A-N7A | -2.09 | 1.30 | 1.34 |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | A | 702 | FLC | CB-CA-CAC | 15.70 | 138.46 | 115.01 |
| 10 | P | 800 | MQ7 | C16-C15-C13 | 9.17 | 143.11 | 112.74 |
| 5 | M | 802 | FLC | CB-CA-CAC | 8.94 | 128.37 | 115.01 |
| 9 | M | 803 | FAD | C8A-N9A-C4A | -8.92 | 100.09 | 106.90 |
| 9 | A | 703 | FAD | C8A-N9A-C4A | -8.70 | 100.26 | 106.90 |
| 9 | A | 703 | FAD | C2-N1-C10 | 7.94 | 122.98 | 114.98 |
| 9 | M | 803 | FAD | C2-N1-C10 | 7.65 | 122.69 | 114.98 |
| 10 | D | 700 | MQ7 | C16-C15-C13 | 6.85 | 135.43 | 112.74 |
| 9 | M | 803 | FAD | C4X-C10-N10 | -6.34 | 117.34 | 120.51 |
| 9 | A | 703 | FAD | C4X-C10-N10 | -6.13 | 117.45 | 120.51 |
| 9 | M | 803 | FAD | N3A-C2A-N1A | -6.02 | 123.67 | 128.71 |
| 10 | D | 700 | MQ7 | C12-C11-C3 | 6.00 | 130.77 | 111.61 |
| 9 | A | 703 | FAD | N3A-C2A-N1A | -5.97 | 123.72 | 128.71 |
| 5 | M | 802 | FLC | CB-CG-CGC | 5.73 | 123.56 | 115.01 |
| 9 | M | 803 | FAD | C4X-N5-C5X | 5.69 | 123.09 | 116.69 |
| 9 | A | 703 | FAD | C4X-N5-C5X | 5.63 | 123.02 | 116.69 |
| 10 | D | 700 | MQ7 | C11-C3-C4 | -5.40 | 113.03 | 118.67 |
| 10 | P | 800 | MQ7 | C12-C11-C3 | 4.91 | 127.28 | 111.61 |
| 10 | P | 800 | MQ7 | C11-C3-C4 | -4.76 | 113.70 | 118.67 |
| 10 | P | 800 | MQ7 | C14-C13-C15 | 4.39 | 122.07 | 115.39 |
| 10 | P | 800 | MQ7 | C21-C20-C18 | -3.72 | 100.40 | 112.74 |
| 10 | P | 800 | MQ7 | C11-C12-C13 | 3.67 | 132.96 | 126.76 |
| 9 | M | 803 | FAD | C4X-C10-N1 | -3.46 | 119.27 | 122.73 |
| 10 | D | 700 | MQ7 | C21-C20-C18 | -3.43 | 101.39 | 112.74 |
| 9 | M | 803 | FAD | N3A-C4A-N9A | -3.29 | 119.49 | 125.43 |
| 10 | P | 800 | MQ7 | O1-C1-C10 | -3.18 | 116.04 | 121.58 |
| 9 | A | 703 | FAD | N3A-C4A-N9A | -3.15 | 119.74 | 125.43 |
| 10 | D | 700 | MQ7 | O1-C1-C10 | -2.95 | 116.44 | 121.58 |
| 10 | D | 700 | MQ7 | C29-C28-C27 | -2.93 | 116.60 | 123.62 |
| 9 | A | 703 | FAD | C5A-C4A-N9A | 2.85 | 111.27 | 107.16 |
| 9 | M | 803 | FAD | N1-C10-N10 | 2.82 | 123.39 | 115.97 |
| 9 | M | 803 | FAD | C5A-C4A-N9A | 2.80 | 111.21 | 107.16 |
| 10 | D | 700 | MQ7 | C25-C23-C22 | -2.79 | 115.72 | 121.08 |
| 10 | D | 700 | MQ7 | C26-C25-C23 | 2.78 | 121.93 | 112.74 |
| 9 | A | 703 | FAD | O4'-C4'-C5' | -2.77 | 104.43 | 110.12 |
| 9 | A | 703 | FAD | C4X-C10-N1 | -2.77 | 119.97 | 122.73 |
| 10 | P | 800 | MQ7 | C26-C25-C23 | 2.76 | 121.88 | 112.74 |
| 10 | P | 800 | MQ7 | C29-C28-C27 | -2.75 | 117.03 | 123.62 |
| 9 | M | 803 | FAD | O4'-C4'-C5' | -2.73 | 104.52 | 110.12 |
| 10 | P | 800 | MQ7 | C25-C23-C22 | -2.71 | 115.86 | 121.08 |
| 5 | A | 702 | FLC | CG-CB-CA | -2.67 | 103.23 | 109.61 |
| 10 | D | 700 | MQ7 | C19-C18-C20 | 2.63 | 119.39 | 115.39 |
| 10 | D | 700 | MQ7 | C14-C13-C15 | 2.61 | 119.36 | 115.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | P | 800 | MQ7 | C5-C10-C1 | -2.59 | 117.77 | 120.70 |
| 9 | A | 703 | FAD | O3'-C3'-C2' | -2.55 | 102.30 | 108.74 |
| 9 | A | 703 | FAD | N1-C10-N10 | 2.52 | 122.58 | 115.97 |
| 10 | P | 800 | MQ7 | C24-C23-C25 | 2.51 | 119.21 | 115.39 |
| 10 | D | 700 | MQ7 | C5-C10-C1 | -2.49 | 117.89 | 120.70 |
| 9 | M | 803 | FAD | C8A-N9A-C1B | 2.48 | 131.26 | 126.38 |
| 10 | D | 700 | MQ7 | C20-C18-C17 | -2.44 | 116.40 | 121.08 |
| 9 | A | 703 | FAD | C4-N3-C2 | -2.42 | 120.43 | 125.39 |
| 10 | D | 700 | MQ7 | C24-C23-C25 | 2.41 | 119.06 | 115.39 |
| 9 | A | 703 | FAD | C8A-N9A-C1B | 2.32 | 130.95 | 126.38 |
| 9 | M | 803 | FAD | O3P-P-O5' | 2.29 | 113.64 | 103.41 |
| 9 | M | 803 | FAD | C4-N3-C2 | -2.25 | 120.76 | 125.39 |
| 10 | D | 700 | MQ7 | C2M-C2-C1 | -2.21 | 112.47 | 116.33 |
| 10 | P | 800 | MQ7 | C2M-C2-C1 | -2.15 | 112.57 | 116.33 |
| 10 | P | 800 | MQ7 | C20-C18-C17 | -2.14 | 116.96 | 121.08 |
| 9 | A | 703 | FAD | P-O3P-PA | -2.08 | 125.58 | 131.68 |
| 10 | P | 800 | MQ7 | C10-C1-C2 | 2.06 | 121.52 | 118.84 |
| 9 | M | 803 | FAD | O3P-PA-O5B | -2.05 | 94.23 | 103.41 |
| 9 | A | 703 | FAD | C4X-C4-N3 | 2.02 | 121.29 | 115.39 |
| 9 | A | 703 | FAD | C2'-C1'-N10 | 2.02 | 115.12 | 112.45 |
| 10 | P | 800 | MQ7 | C19-C18-C20 | 2.01 | 118.45 | 115.39 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 577/602 (95%) | -0.40 | 0 100 100 | 9, 14, 62, 85 | 0 |
| 1 | M | 572/602 (95%) | 0.41 | 13 (2%) 57 15 | 30, 92, 127, 142 | 0 |
| 2 | B | 243/243 (100%) | -0.43 | 1 (0%) 90 57 | 9, 15, 36, 85 | 0 |
| 2 | N | 243/243 (100%) | -0.01 | 3 (1%) 75 29 | 9, 62, 119, 147 | 0 |
| 3 | C | 130/130 (100%) | -0.36 | 0 100 100 | 10, 32, 59, 76 | 0 |
| 3 | O | 130/130 (100%) | -0.17 | 2 (1%) 70 24 | 24, 55, 106, 123 | 0 |
| 4 | D | 119/119 (100%) | -0.42 | 0 100 100 | 18, 36, 61, 70 | 0 |
| 4 | P | 119/119 (100%) | -0.31 | 0 100 100 | 27, 49, 80, 118 | 0 |
| All | All | 2133/2188 (97%) | -0.12 | 19 (0%) 79 37 | 9, 45, 114, 147 | 0 |

All (19) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | N | 17 | VAL | 4.0 |
| 1 | M | 484 | GLU | 3.6 |
| 1 | M | 392 | GLY | 3.1 |
| 1 | M | 557 | ALA | 3.0 |
| 1 | M | 219 | HIS | 2.9 |
| 3 | O | 1 | THR | 2.6 |
| 2 | N | 1 | ALA | 2.4 |
| 1 | M | 159 | ASP | 2.4 |
| 1 | M | 63 | GLU | 2.4 |
| 1 | M | 434 | GLN | 2.4 |
| 1 | M | 325 | HIS | 2.4 |
| 1 | M | 270 | PRO | 2.1 |
| 3 | O | 2 | THR | 2.1 |
| 2 | N | 16 | GLU | 2.1 |
| 1 | M | 218 | SER | 2.1 |
| 1 | M | 280 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | M | 556 | ASP | 2.1 |
| 1 | M | 77 | CYS | 2.0 |
| 2 | B | 242 | PRO | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|----------------------------|-------|
| 10 | MQ7 | P | 800 | 33/48 | 0.97 | 17.74 | 83,106,120,123 | 0 |
| 10 | MQ7 | D | 700 | 33/48 | 0.74 | 12.18 | 59,100,117,127 | 0 |
| 5 | FLC | A | 702 | 13/13 | 0.31 | 4.26 | 31,37,38,39 | 0 |
| 8 | SF4 | B | 246 | 8/8 | 0.18 | 2.25 | 9,21,27,27 | 0 |
| 5 | FLC | M | 802 | 13/13 | 0.43 | 1.09 | 60,74,92,97 | 0 |
| 9 | FAD | M | 803 | 52/53 | 0.43 | 0.95 | 23,87,158,164 | 0 |
| 9 | FAD | A | 703 | 52/53 | 0.19 | -0.09 | 0,1,17,36 | 0 |
| 6 | FES | B | 244 | 4/4 | 0.17 | -0.12 | 0,4,5,8 | 0 |
| 7 | F3S | B | 245 | 7/7 | 0.13 | -0.64 | 7,11,15,24 | 0 |
| 8 | SF4 | N | 246 | 8/8 | 0.14 | -0.81 | 20,29,49,53 | 0 |
| 6 | FES | N | 244 | 4/4 | 0.12 | -2.05 | 21,24,44,53 | 0 |
| 7 | F3S | N | 245 | 7/7 | 0.07 | -2.70 | 14,16,29,49 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.