



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 07:10 AM BST

PDB ID : 6I1P
Title : Respiratory complex I from Thermus thermophilus with bound NADH
Authors : Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on : 2018-10-29
Resolution : 3.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

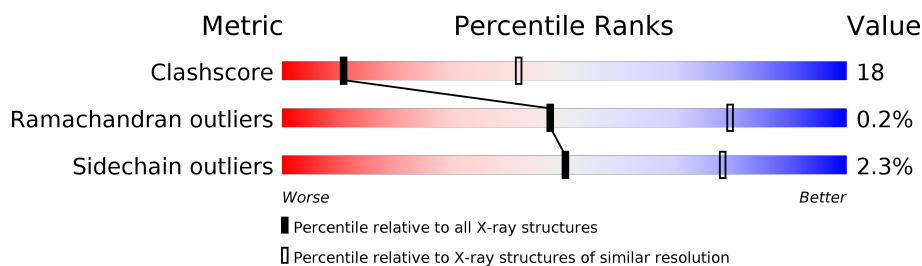
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |



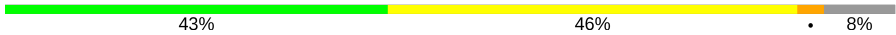
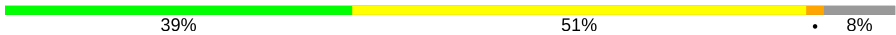




















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1 | 438 | 60% 38% . |
| 1 | B | 438 | 55% 44% . |
| 2 | 2 | 181 | 71% 25% .. |
| 2 | C | 181 | 60% 38% .. |
| 3 | 3 | 783 | 57% 38% .. |
| 3 | D | 783 | 59% 37% . |
| 4 | 4 | 409 | 49% 43% . 6% |
| 4 | E | 409 | 51% 42% . 6% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | 5 | 207 |  |
| 5 | F | 207 |  |
| 6 | 6 | 181 |  |
| 6 | G | 181 |  |
| 7 | 9 | 182 |  |
| 7 | O | 182 |  |
| 8 | 7 | 129 |  |
| 8 | I | 129 |  |
| 9 | W | 131 |  |
| 9 | X | 131 |  |
| 10 | A | 119 |  |
| 10 | P | 119 |  |
| 11 | J | 176 |  |
| 11 | R | 176 |  |
| 12 | K | 95 |  |
| 12 | S | 95 |  |
| 13 | L | 606 |  |
| 13 | T | 606 |  |
| 14 | M | 469 |  |
| 14 | U | 469 |  |
| 15 | N | 427 |  |
| 15 | V | 427 |  |
| 16 | H | 365 |  |
| 16 | Q | 365 |  |

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

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17 | SF4 | 1 | 501 | - | - | X | - |
| 17 | SF4 | 3 | 803 | - | - | X | - |
| 17 | SF4 | 9 | 201 | - | - | X | - |
| 17 | SF4 | 9 | 202 | - | - | X | - |
| 17 | SF4 | G | 201 | - | - | X | - |
| 17 | SF4 | O | 202 | - | - | X | - |
| 20 | FES | C | 201 | - | - | X | - |
| 20 | FES | D | 804 | - | - | X | - |

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 74174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | 1 | 437 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3417 | 2180 | 595 | 624 | 18 | | | |
| 1 | B | 437 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3417 | 2180 | 595 | 624 | 18 | | | |

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | 2 | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1406 | 895 | 238 | 265 | 8 | | | |
| 2 | C | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1406 | 895 | 238 | 265 | 8 | | | |

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3 | 3 | 756 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5895 | 3754 | 1057 | 1053 | 31 | | | |
| 3 | D | 756 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5895 | 3754 | 1057 | 1053 | 31 | | | |

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | 4 | 384 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3067 | 1975 | 522 | 559 | 11 | | | |
| 4 | E | 384 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3067 | 1975 | 522 | 559 | 11 | | | |

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | 5 | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1607 | 1043 | 273 | 288 | 3 | | | |
| 5 | F | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1607 | 1043 | 273 | 288 | 3 | | | |

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 6 | 6 | 166 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1289 | 815 | 235 | 226 | 13 | | | |
| 6 | G | 166 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1289 | 815 | 235 | 226 | 13 | | | |

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7 | 9 | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1388 | 890 | 232 | 255 | 11 | | | |
| 7 | O | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1388 | 890 | 232 | 255 | 11 | | | |

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | 7 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1031 | 664 | 183 | 181 | 3 | | | |
| 8 | I | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1031 | 664 | 183 | 181 | 3 | | | |

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | W | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 623 | 165 | 175 | 4 | | | |
| 9 | X | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 623 | 165 | 175 | 4 | | | |

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | A | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 910 | 624 | 138 | 144 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | P | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 910 | 624 | 138 | 144 | 4 | | | |

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | J | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1183 | 806 | 183 | 191 | 3 | | | |
| 11 | R | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1183 | 806 | 183 | 191 | 3 | | | |

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | K | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 703 | 456 | 118 | 126 | 3 | | | |
| 12 | S | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 703 | 456 | 118 | 126 | 3 | | | |

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 13 | L | 605 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4604 | 3089 | 740 | 756 | 19 | | | |
| 13 | T | 605 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4604 | 3089 | 740 | 756 | 19 | | | |

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 14 | M | 467 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3489 | 2363 | 546 | 572 | 8 | | | |
| 14 | U | 467 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3489 | 2363 | 546 | 572 | 8 | | | |

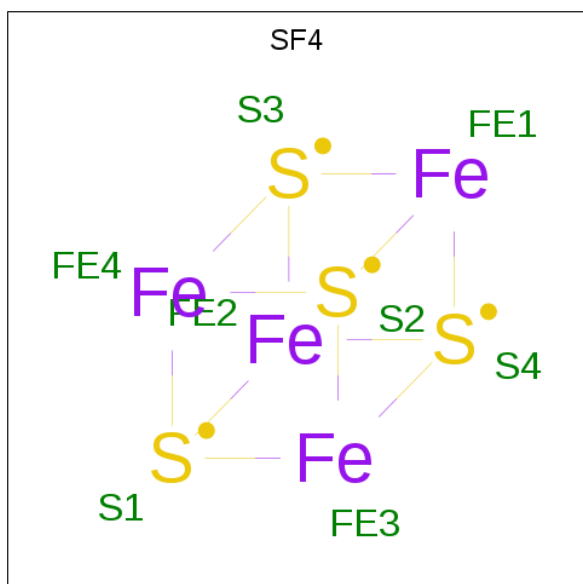
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 15 | N | 427 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3154 | 2125 | 505 | 518 | 6 | | | |
| 15 | V | 427 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3154 | 2125 | 505 | 518 | 6 | | | |

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit 8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 16 | H | 353 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2838 | 1943 | 431 | 457 | 7 | | | |
| 16 | Q | 353 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2838 | 1943 | 431 | 457 | 7 | | | |

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



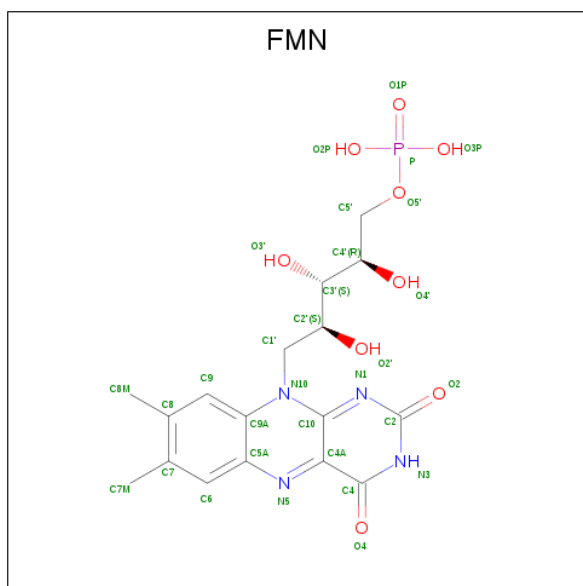
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 17 | 1 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 3 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 3 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 3 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 6 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 9 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | 9 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

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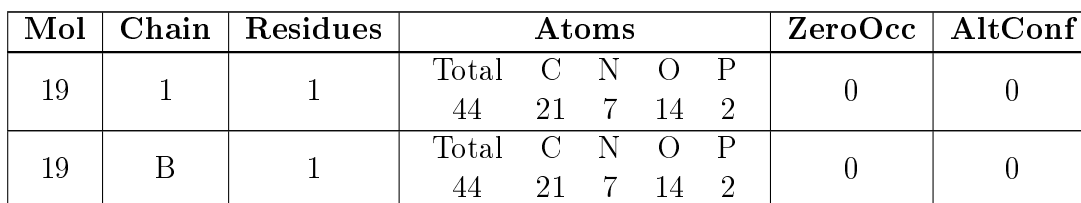
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 17 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | G | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | O | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 17 | O | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 18 | 1 | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 18 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |

- Molecule 19 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by author).



-
- Diagram illustrating the structure of a ferredoxin center (FES), showing two iron atoms (Fe) and two sulfur atoms (S) in a square arrangement. The top-left sulfur is labeled S1, the top-right iron is labeled FE2, the bottom-left iron is labeled FE1, and the bottom-right sulfur is labeled S2. The bonds between S1 and Fe, Fe and S2, and S2 and Fe1 are shown as lines.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 20 | 2 | 1 | Total 4 | Fe 2 | S 2 | 0 | 0 |
| 20 | 3 | 1 | Total 4 | Fe 2 | S 2 | 0 | 0 |



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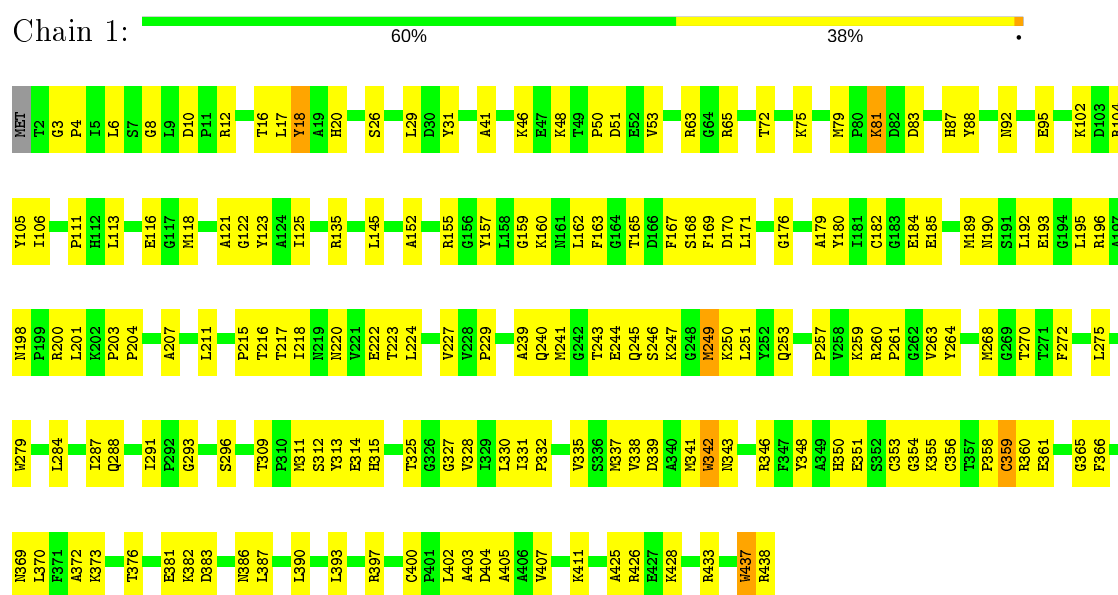
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 20 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |

3 Residue-property plots

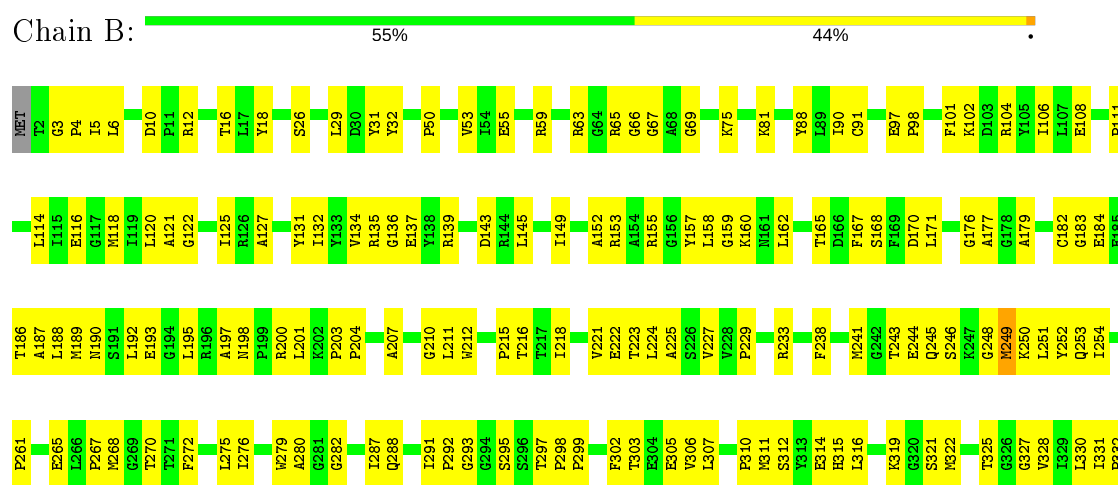
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

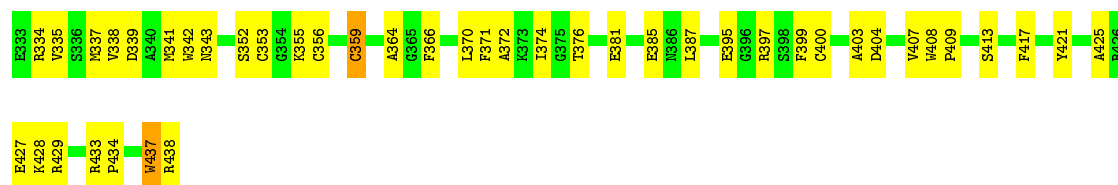
Note EDS failed to run properly.

• Molecule 1: NADH-quinone oxidoreductase subunit 1



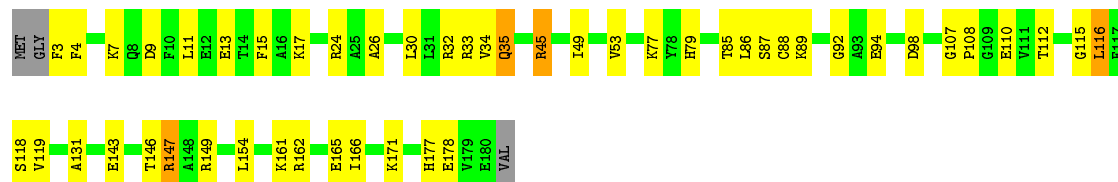
• Molecule 1: NADH-quinone oxidoreductase subunit 1





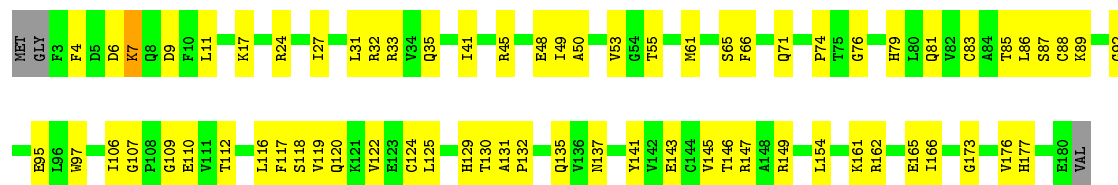
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 71% 25% ..



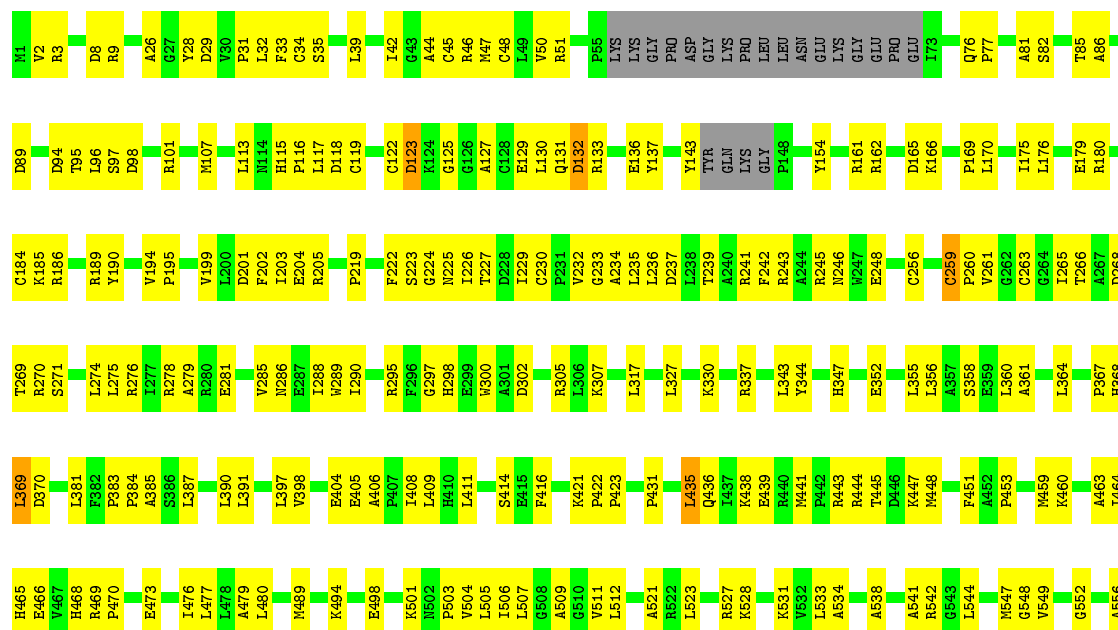
• Molecule 2: NADH-quinone oxidoreductase subunit 2

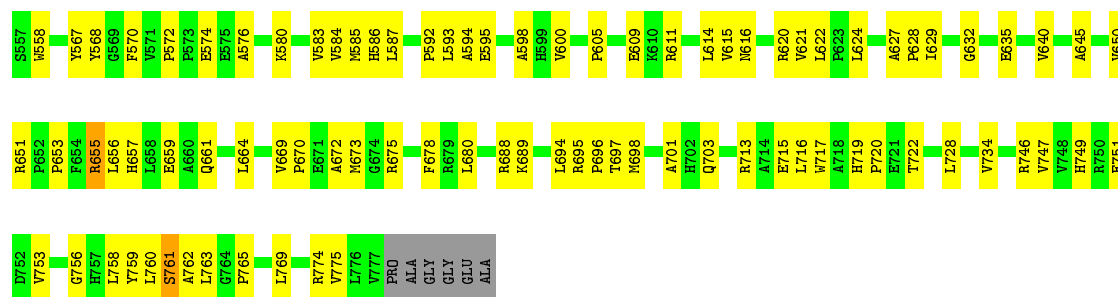
Chain C: 60% 38% ..



• Molecule 3: NADH-quinone oxidoreductase subunit 3

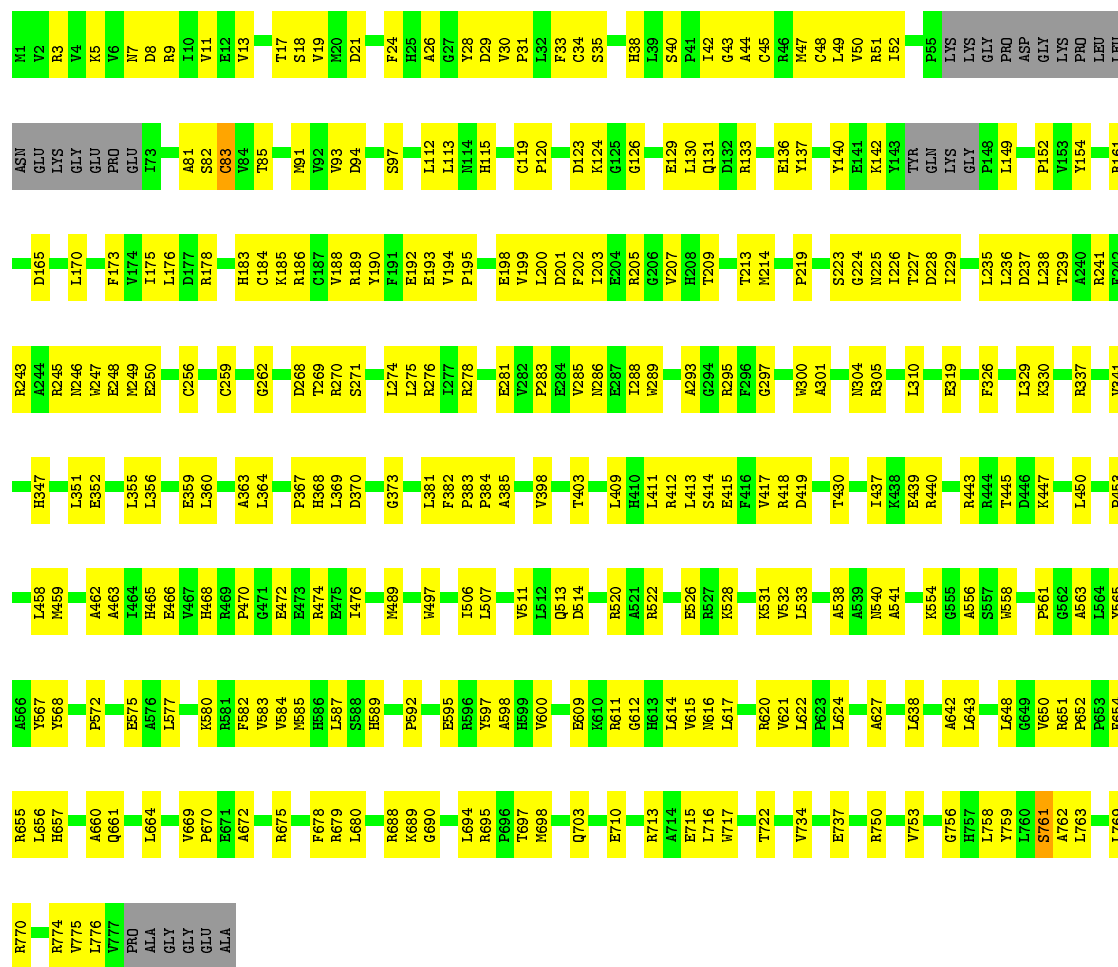
Chain 3: 57% 38% ..





• Molecule 3: NADH-quinone oxidoreductase subunit 3

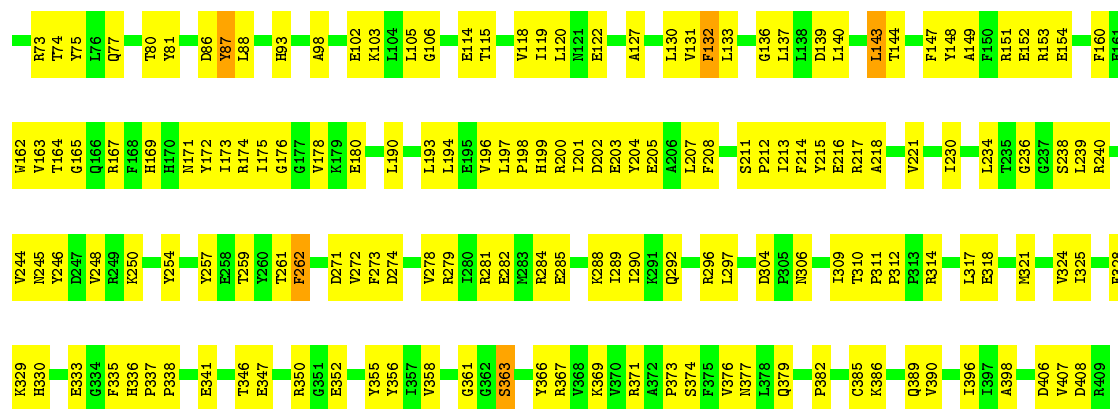
Chain D: 59% 37%



• Molecule 4: NADH-quinone oxidoreductase subunit 4

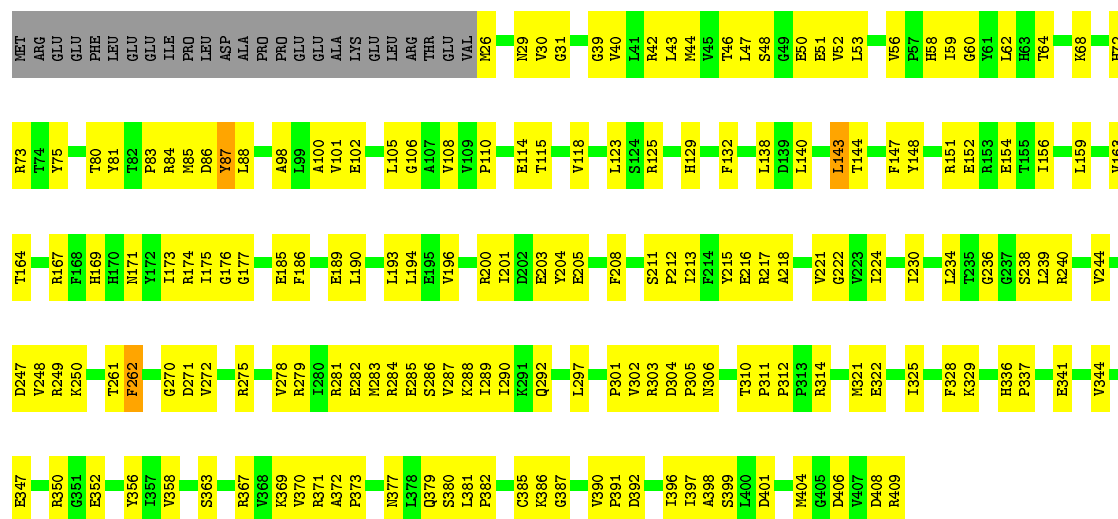
Chain 4: 49% 43% 6%





• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 51% 42% 6%



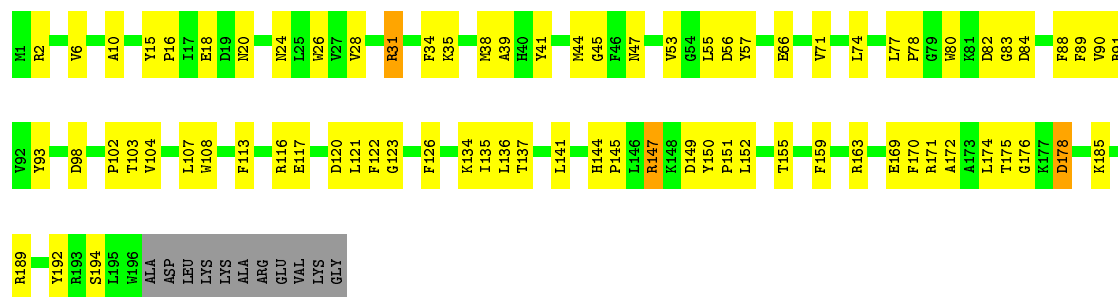
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 55% 39% 5%



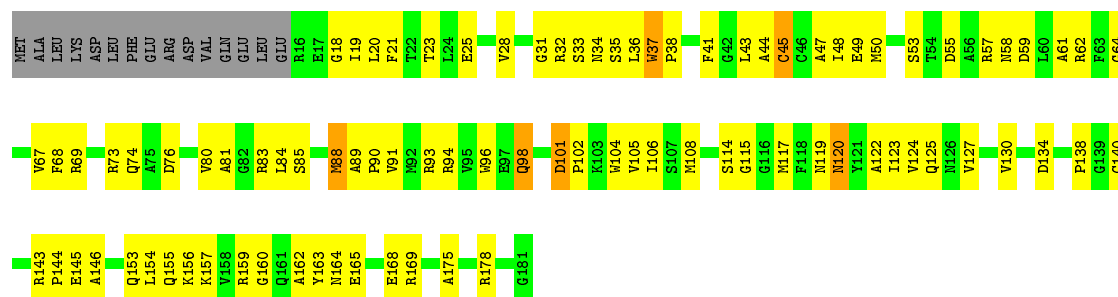
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 57% 36% 5%



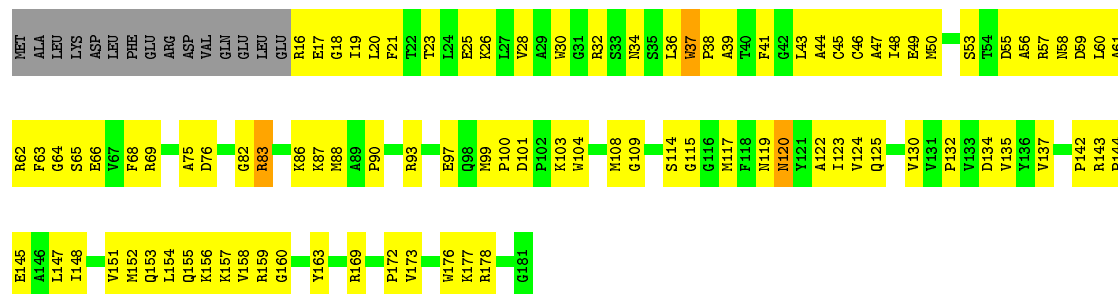
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 43% 46% 8%



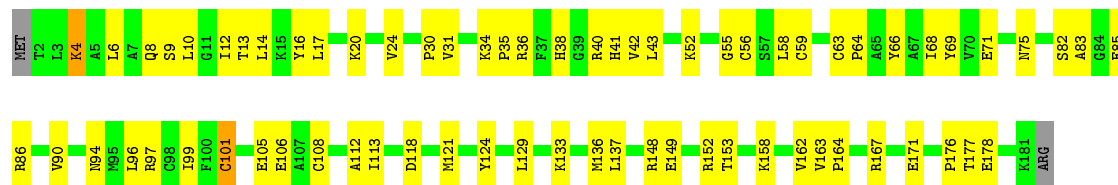
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G: 39% 51% 8%



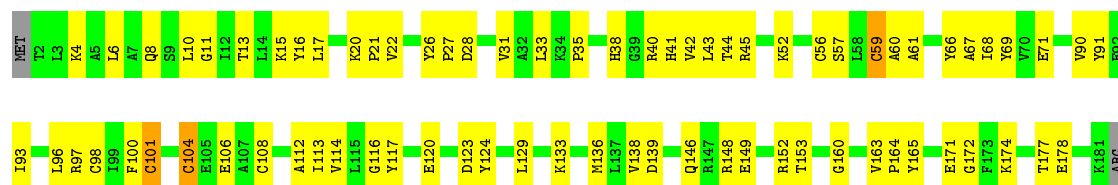
- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9: 61% 37% 2%



- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O: 58% 39% 3%



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 71% 26% ..



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I: 64% 33% ..



- Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain W: 66% 30% ..



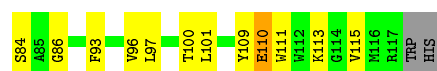
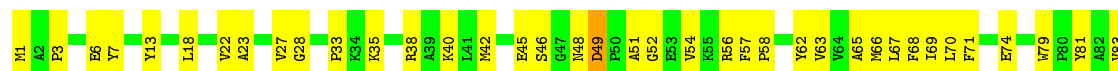
- Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain X: 74% 23% .

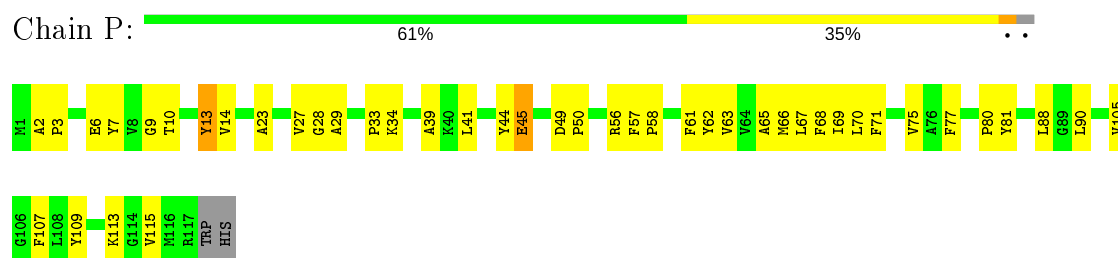


- Molecule 10: NADH-quinone oxidoreductase subunit 7

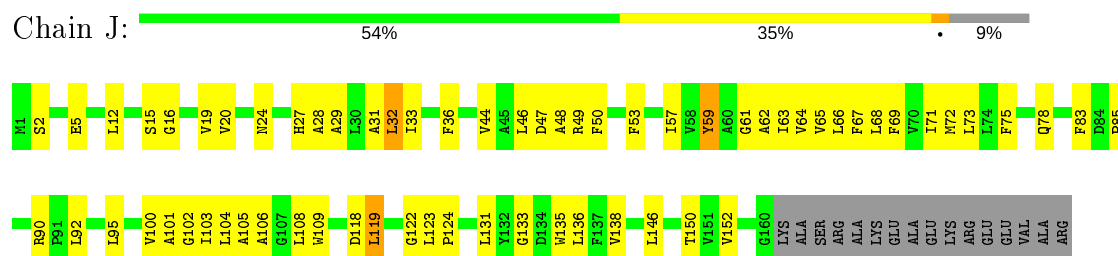
Chain A: 56% 40% ..



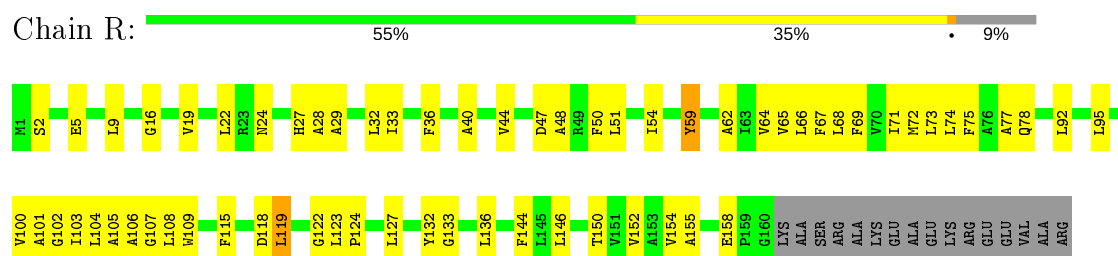
- Molecule 10: NADH-quinone oxidoreductase subunit 7



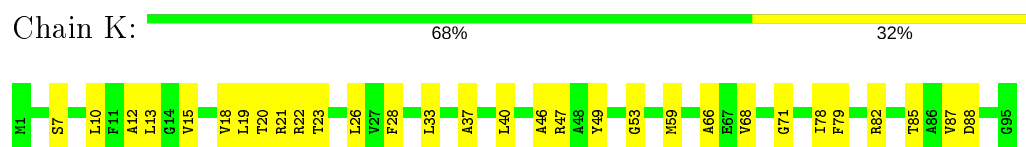
- Molecule 11: NADH-quinone oxidoreductase subunit 10



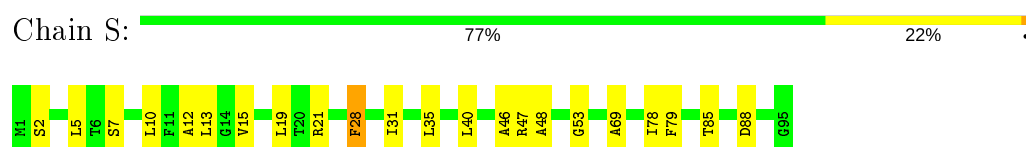
- Molecule 11: NADH-quinone oxidoreductase subunit 10



- Molecule 12: NADH-quinone oxidoreductase subunit 11

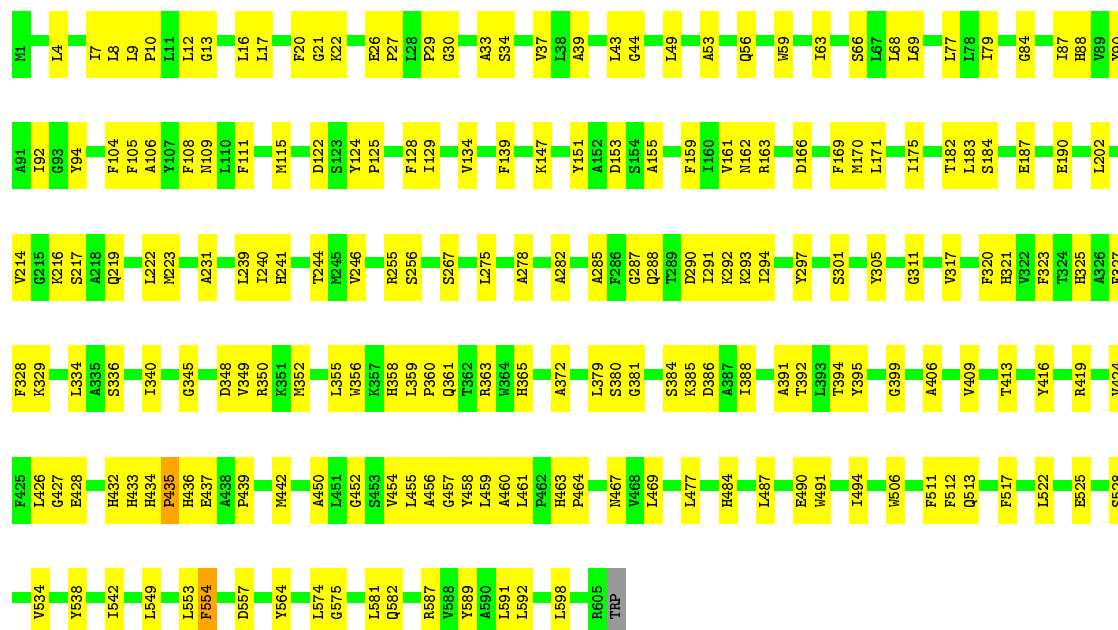


- Molecule 12: NADH-quinone oxidoreductase subunit 11

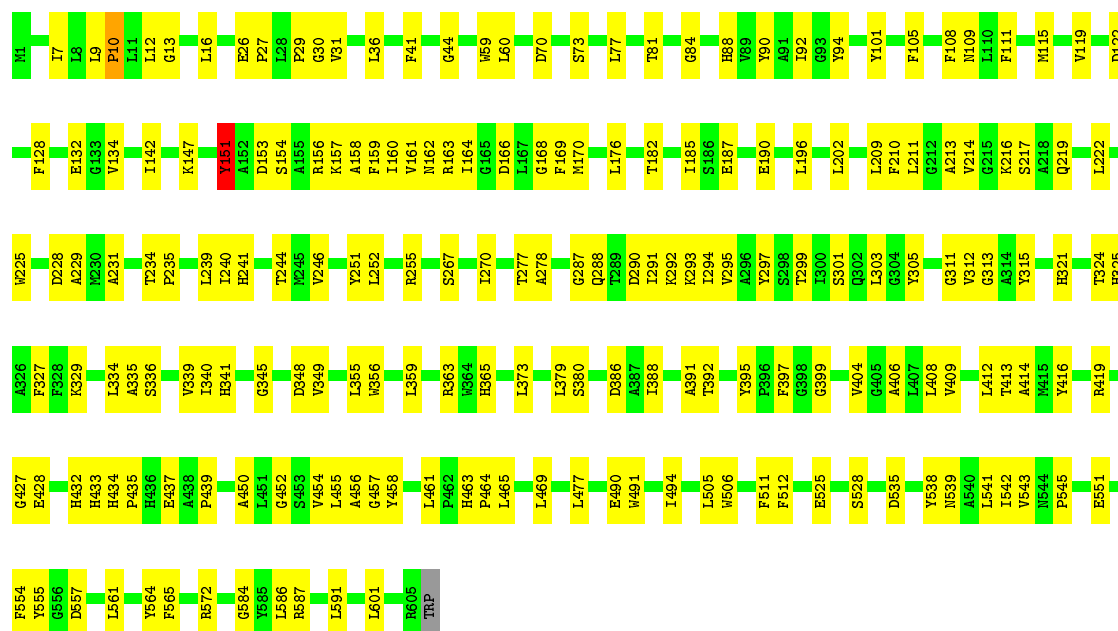


- Molecule 13: NADH-quinone oxidoreductase subunit 12

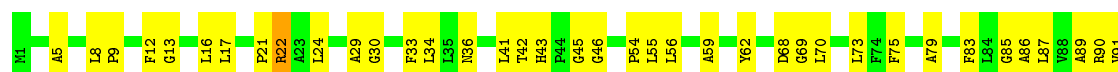


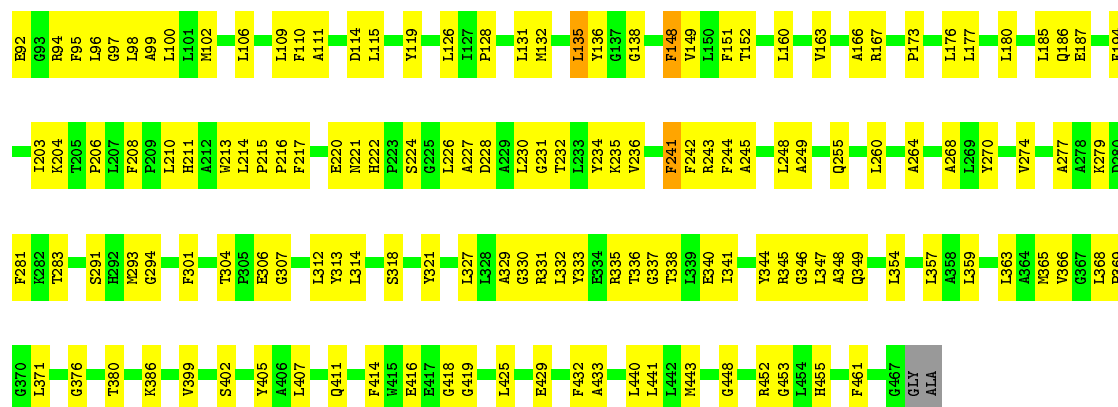


• Molecule 13: NADH-quinone oxidoreductase subunit 12



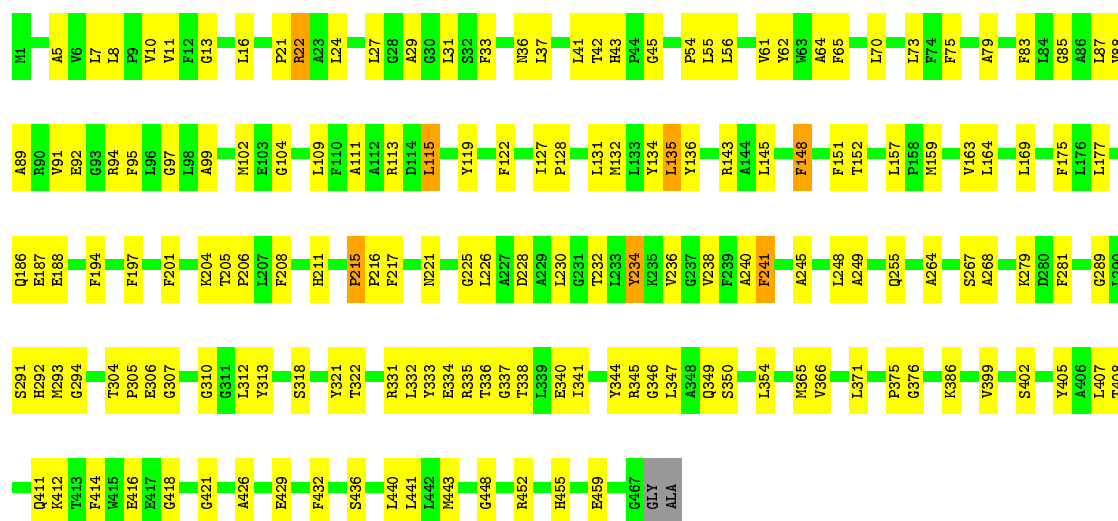
• Molecule 14: NADH-quinone oxidoreductase subunit 13





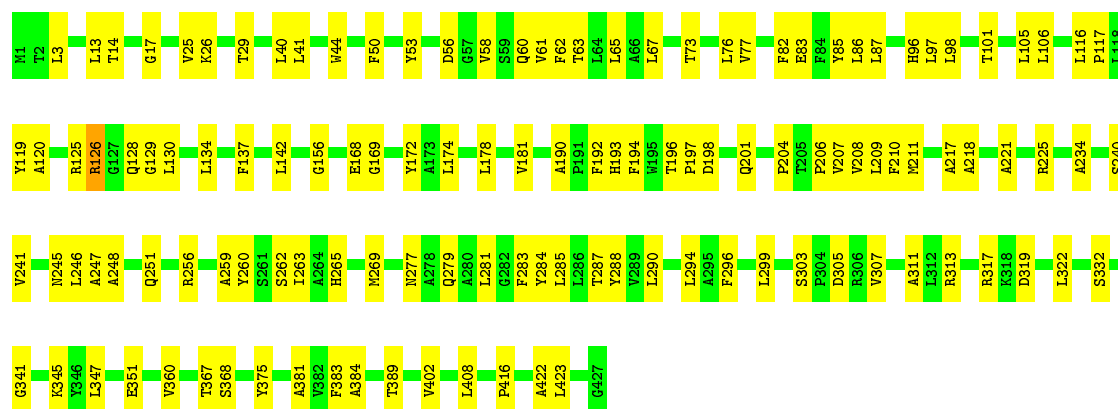
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U: 65% 33%



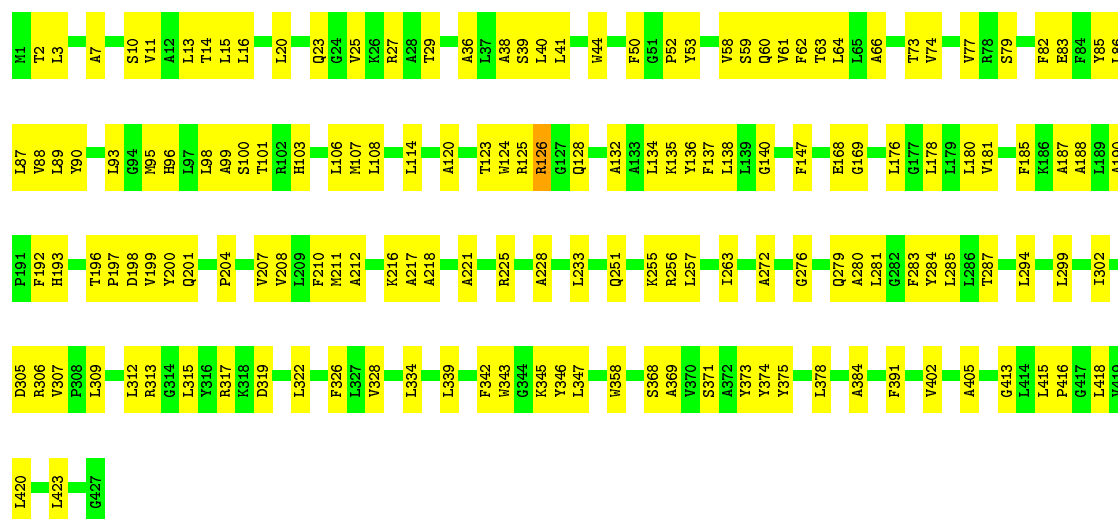
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N: 71% 29%



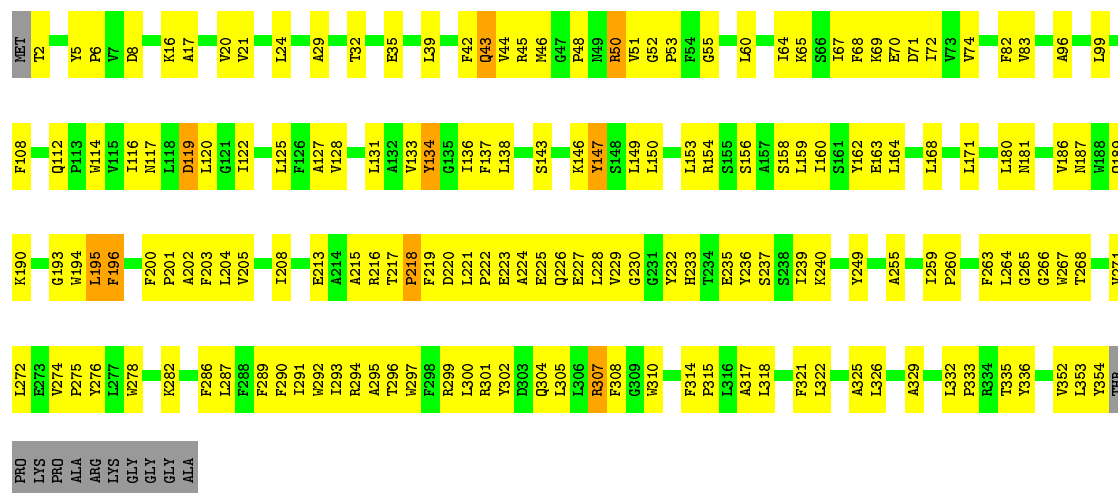
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V:  64% 36%



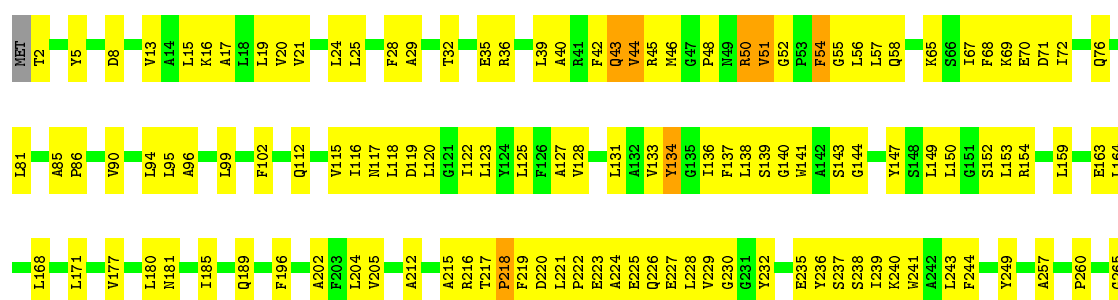
• Molecule 16: NADH-quinone oxidoreductase subunit 8

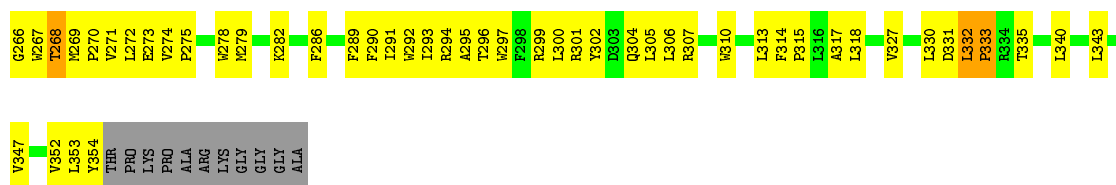
Chain H:  52% 43% • •



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:  49% 45% • •





4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 96.11Å 341.45Å 263.89Å 90.00° 100.52° 90.00° | Depositor |
| Resolution (Å) | 58.71 – 3.21 | Depositor |
| % Data completeness (in resolution range) | 76.1 (58.71-3.21) | Depositor |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.27 (at 3.19Å) | Xtriage |
| Refinement program | PHENIX (1.13rc1_2961: ???) | Depositor |
| R, R_{free} | 0.210 , 0.231 | Depositor |
| Wilson B-factor (Å ²) | 73.9 | Xtriage |
| Anisotropy | 0.034 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$ | Xtriage |
| Estimated twinning fraction | 0.357 for h,-k,-h-l | Xtriage |
| Reported twinning fraction | 0.470 for -H,-K,H+L | Depositor |
| Outliers | 0 of 207039 reflections | Xtriage |
| Total number of atoms | 74174 | wwPDB-VP |
| Average B, all atoms (Å ²) | 74.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, NAI, FES

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 | 1 | 0.34 | 0/3506 | 0.51 | 0/4745 |
| 1 | B | 0.31 | 0/3506 | 0.49 | 0/4745 |
| 2 | 2 | 0.35 | 0/1439 | 0.50 | 0/1953 |
| 2 | C | 0.32 | 0/1439 | 0.50 | 0/1953 |
| 3 | 3 | 0.51 | 2/6035 (0.0%) | 0.73 | 3/8185 (0.0%) |
| 3 | D | 0.40 | 0/6035 | 0.60 | 0/8185 |
| 4 | 4 | 0.44 | 0/3150 | 0.62 | 0/4284 |
| 4 | E | 0.34 | 0/3150 | 0.51 | 0/4284 |
| 5 | 5 | 0.43 | 0/1656 | 0.66 | 1/2246 (0.0%) |
| 5 | F | 0.37 | 0/1656 | 0.57 | 0/2246 |
| 6 | 6 | 0.46 | 0/1319 | 0.64 | 0/1786 |
| 6 | G | 0.46 | 0/1319 | 0.62 | 0/1786 |
| 7 | 9 | 0.53 | 1/1423 (0.1%) | 0.65 | 0/1933 |
| 7 | O | 0.48 | 1/1423 (0.1%) | 0.65 | 1/1933 (0.1%) |
| 8 | 7 | 0.32 | 0/1059 | 0.53 | 0/1429 |
| 8 | I | 0.36 | 0/1059 | 0.57 | 0/1429 |
| 9 | W | 0.43 | 0/985 | 0.62 | 0/1335 |
| 9 | X | 0.37 | 0/985 | 0.57 | 0/1335 |
| 10 | A | 0.33 | 0/940 | 0.52 | 0/1280 |
| 10 | P | 0.35 | 0/940 | 0.51 | 0/1280 |
| 11 | J | 0.31 | 0/1206 | 0.50 | 0/1649 |
| 11 | R | 0.32 | 0/1206 | 0.53 | 0/1649 |
| 12 | K | 0.31 | 0/710 | 0.53 | 0/962 |
| 12 | S | 0.30 | 0/710 | 0.51 | 0/962 |
| 13 | L | 0.29 | 0/4741 | 0.47 | 0/6460 |
| 13 | T | 0.29 | 0/4741 | 0.48 | 1/6460 (0.0%) |
| 14 | M | 0.30 | 0/3591 | 0.48 | 0/4896 |
| 14 | U | 0.32 | 0/3591 | 0.51 | 0/4896 |
| 15 | N | 0.31 | 0/3238 | 0.47 | 0/4434 |
| 15 | V | 0.34 | 0/3238 | 0.52 | 0/4434 |
| 16 | H | 0.34 | 0/2935 | 0.55 | 0/4014 |
| 16 | Q | 0.37 | 0/2935 | 0.56 | 0/4014 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.37 | 4/75866 (0.0%) | 0.56 | 6/103182 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7 | 9 | 0 | 1 |
| 7 | O | 0 | 2 |
| 10 | P | 0 | 1 |
| 16 | H | 0 | 3 |
| 16 | Q | 0 | 3 |
| All | All | 0 | 10 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7 | 9 | 101 | CYS | CB-SG | -6.08 | 1.72 | 1.82 |
| 3 | 3 | 263 | CYS | CB-SG | -5.98 | 1.72 | 1.81 |
| 7 | O | 101 | CYS | CB-SG | -5.30 | 1.73 | 1.81 |
| 3 | 3 | 381 | LEU | C-N | -5.26 | 1.22 | 1.34 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7 | O | 59 | CYS | CA-CB-SG | 7.71 | 127.88 | 114.00 |
| 3 | 3 | 276 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 13 | T | 151 | TYR | N-CA-CB | 5.82 | 121.08 | 110.60 |
| 3 | 3 | 435 | LEU | CB-CG-CD1 | -5.49 | 101.67 | 111.00 |
| 5 | 5 | 189 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 3 | 3 | 276 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 7 | 9 | 20 | LYS | Peptide |
| 16 | H | 217 | THR | Peptide |
| 16 | H | 266 | GLY | Peptide |
| 16 | H | 43 | GLN | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 7 | O | 20 | LYS | Peptide |
| 7 | O | 21 | PRO | Peptide |
| 10 | P | 45 | GLU | Peptide |
| 16 | Q | 217 | THR | Peptide |
| 16 | Q | 266 | GLY | Peptide |
| 16 | Q | 43 | GLN | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1 | 3417 | 0 | 3389 | 116 | 0 |
| 1 | B | 3417 | 0 | 3388 | 152 | 0 |
| 2 | 2 | 1406 | 0 | 1373 | 37 | 0 |
| 2 | C | 1406 | 0 | 1373 | 71 | 0 |
| 3 | 3 | 5895 | 0 | 5929 | 232 | 0 |
| 3 | D | 5895 | 0 | 5930 | 218 | 0 |
| 4 | 4 | 3067 | 0 | 3049 | 167 | 0 |
| 4 | E | 3067 | 0 | 3049 | 162 | 0 |
| 5 | 5 | 1607 | 0 | 1574 | 77 | 0 |
| 5 | F | 1607 | 0 | 1574 | 76 | 0 |
| 6 | 6 | 1289 | 0 | 1298 | 84 | 0 |
| 6 | G | 1289 | 0 | 1298 | 100 | 0 |
| 7 | 9 | 1388 | 0 | 1383 | 72 | 0 |
| 7 | O | 1388 | 0 | 1383 | 69 | 0 |
| 8 | 7 | 1031 | 0 | 1029 | 36 | 0 |
| 8 | I | 1031 | 0 | 1029 | 36 | 0 |
| 9 | W | 967 | 0 | 1010 | 32 | 0 |
| 9 | X | 967 | 0 | 1010 | 23 | 0 |
| 10 | A | 910 | 0 | 939 | 53 | 0 |
| 10 | P | 910 | 0 | 939 | 53 | 0 |
| 11 | J | 1183 | 0 | 1286 | 63 | 0 |
| 11 | R | 1183 | 0 | 1286 | 56 | 0 |
| 12 | K | 703 | 0 | 747 | 29 | 0 |
| 12 | S | 703 | 0 | 747 | 17 | 0 |
| 13 | L | 4604 | 0 | 4734 | 162 | 0 |
| 13 | T | 4604 | 0 | 4734 | 136 | 0 |
| 14 | M | 3489 | 0 | 3606 | 131 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | U | 3489 | 0 | 3606 | 124 | 0 |
| 15 | N | 3154 | 0 | 3343 | 98 | 0 |
| 15 | V | 3154 | 0 | 3343 | 113 | 0 |
| 16 | H | 2838 | 0 | 2903 | 154 | 0 |
| 16 | Q | 2838 | 0 | 2903 | 175 | 0 |
| 17 | 1 | 8 | 0 | 0 | 3 | 0 |
| 17 | 3 | 24 | 0 | 0 | 2 | 0 |
| 17 | 6 | 8 | 0 | 0 | 0 | 0 |
| 17 | 9 | 16 | 0 | 0 | 6 | 0 |
| 17 | B | 8 | 0 | 0 | 1 | 0 |
| 17 | D | 24 | 0 | 0 | 1 | 0 |
| 17 | G | 8 | 0 | 0 | 2 | 0 |
| 17 | O | 16 | 0 | 0 | 3 | 0 |
| 18 | 1 | 31 | 0 | 19 | 8 | 0 |
| 18 | B | 31 | 0 | 19 | 2 | 0 |
| 19 | 1 | 44 | 0 | 27 | 3 | 0 |
| 19 | B | 44 | 0 | 27 | 4 | 0 |
| 20 | 2 | 4 | 0 | 0 | 1 | 0 |
| 20 | 3 | 4 | 0 | 0 | 0 | 0 |
| 20 | C | 4 | 0 | 0 | 2 | 0 |
| 20 | D | 4 | 0 | 0 | 2 | 0 |
| All | All | 74174 | 0 | 75276 | 2718 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2718) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:4:190:LEU:O | 4:4:194:LEU:HD13 | 1.54 | 1.05 |
| 7:9:133:LYS:O | 7:9:137:LEU:HD13 | 1.57 | 1.04 |
| 3:D:286:ASN:ND2 | 3:D:289:TRP:O | 1.96 | 0.98 |
| 4:E:47:LEU:HD13 | 4:E:51:GLU:O | 1.62 | 0.97 |
| 3:3:42:ILE:HD12 | 3:3:42:ILE:O | 1.65 | 0.96 |
| 4:E:47:LEU:CD1 | 4:E:51:GLU:O | 2.16 | 0.94 |
| 3:3:397:LEU:HD21 | 3:3:480:LEU:HD13 | 1.49 | 0.92 |
| 7:9:52:LYS:NZ | 8:7:44:MET:O | 2.03 | 0.92 |
| 16:Q:274:VAL:HG12 | 16:Q:278:TRP:CD1 | 2.03 | 0.91 |
| 6:G:145:GLU:HG2 | 7:O:31:VAL:HG21 | 1.50 | 0.90 |
| 14:M:22:ARG:NH1 | 14:M:92:GLU:OE1 | 2.06 | 0.88 |
| 5:F:38:MET:CE | 5:F:104:VAL:HG11 | 2.03 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:37:PHE:HE1 | 8:I:74:PRO:HA | 1.40 | 0.87 |
| 16:Q:215:ALA:O | 16:Q:294:ARG:NH1 | 2.07 | 0.87 |
| 5:5:175:THR:HG22 | 5:5:178:ASP:HB2 | 1.57 | 0.86 |
| 4:E:169:HIS:NE2 | 6:G:45:CYS:SG | 2.48 | 0.86 |
| 3:3:115:HIS:HB3 | 4:4:321:MET:HE3 | 1.58 | 0.86 |
| 1:B:190:ASN:ND2 | 1:B:198:ASN:O | 2.08 | 0.86 |
| 1:1:437:TRP:HB3 | 2:2:92:GLY:HA3 | 1.57 | 0.85 |
| 4:4:261:THR:H | 4:4:292:GLN:HE22 | 1.23 | 0.85 |
| 6:6:160:GLY:O | 6:6:169:ARG:NH1 | 2.09 | 0.85 |
| 16:Q:333:PRO:HB2 | 16:Q:335:THR:H | 1.41 | 0.85 |
| 2:C:106:ILE:HD11 | 2:C:112:THR:HB | 1.57 | 0.84 |
| 3:D:194:VAL:HG12 | 3:D:411:LEU:HD22 | 1.59 | 0.84 |
| 4:E:314:ARG:NH2 | 7:O:108:CYS:O | 2.11 | 0.83 |
| 5:F:38:MET:HE3 | 5:F:104:VAL:HG11 | 1.60 | 0.83 |
| 10:P:14:VAL:HG22 | 16:Q:95:LEU:HD22 | 1.60 | 0.83 |
| 3:3:286:ASN:ND2 | 3:3:289:TRP:O | 2.12 | 0.83 |
| 16:Q:271:VAL:HG12 | 16:Q:272:LEU:HG | 1.61 | 0.82 |
| 13:L:557:ASP:OD1 | 14:M:211:HIS:NE2 | 2.12 | 0.82 |
| 13:T:94:TYR:HE1 | 13:T:341:HIS:HB2 | 1.44 | 0.82 |
| 16:Q:143:SER:HB2 | 16:Q:235:GLU:HG3 | 1.61 | 0.82 |
| 3:3:31:PRO:HB2 | 3:3:47:MET:HB3 | 1.60 | 0.82 |
| 10:A:70:LEU:HD13 | 11:J:150:THR:HG22 | 1.61 | 0.82 |
| 4:4:152:GLU:OE2 | 4:4:204:TYR:OH | 1.98 | 0.82 |
| 7:9:75:ASN:ND2 | 7:9:82:SER:OG | 2.13 | 0.82 |
| 3:3:584:VAL:HG12 | 3:3:600:VAL:HB | 1.62 | 0.81 |
| 3:3:616:ASN:HD22 | 3:3:622:LEU:HD11 | 1.45 | 0.81 |
| 4:E:261:THR:H | 4:E:292:GLN:HE22 | 1.28 | 0.81 |
| 4:4:373:PRO:O | 4:4:377:ASN:ND2 | 2.14 | 0.81 |
| 1:B:437:TRP:HB3 | 2:C:92:GLY:HA3 | 1.62 | 0.81 |
| 3:D:584:VAL:HG12 | 3:D:600:VAL:HB | 1.61 | 0.81 |
| 3:D:352:GLU:OE2 | 3:D:661:GLN:NE2 | 2.14 | 0.81 |
| 14:M:68:ASP:OD2 | 14:M:243:ARG:NH2 | 2.14 | 0.81 |
| 14:M:268:ALA:HA | 14:M:291:SER:HA | 1.61 | 0.81 |
| 3:3:305:ARG:HH22 | 3:3:605:PRO:HA | 1.46 | 0.80 |
| 10:P:113:LYS:NZ | 15:V:83:GLU:OE2 | 2.11 | 0.80 |
| 15:N:193:HIS:HB2 | 15:N:263:ILE:HD13 | 1.64 | 0.80 |
| 16:H:50:ARG:O | 16:H:52:GLY:N | 2.12 | 0.80 |
| 8:7:23:TYR:HH | 8:7:123:ARG:HH11 | 1.29 | 0.80 |
| 7:O:171:GLU:OE2 | 8:I:43:ARG:NH2 | 2.14 | 0.80 |
| 13:L:458:TYR:HB3 | 13:L:461:LEU:HD11 | 1.64 | 0.80 |
| 15:V:128:GLN:OE1 | 15:V:306:ARG:NH2 | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:115:HIS:HB3 | 4:E:321:MET:HE3 | 1.62 | 0.80 |
| 10:A:35:LYS:O | 10:A:40:LYS:NZ | 2.15 | 0.79 |
| 3:3:609:GLU:HA | 3:3:627:ALA:H | 1.47 | 0.79 |
| 6:G:134:ASP:OD1 | 6:G:157:LYS:NZ | 2.15 | 0.79 |
| 3:3:51:ARG:HB3 | 3:3:94:ASP:HB3 | 1.65 | 0.79 |
| 15:V:309:LEU:HD22 | 15:V:378:LEU:HD11 | 1.62 | 0.79 |
| 2:C:106:ILE:HD13 | 2:C:112:THR:N | 1.98 | 0.79 |
| 3:D:688:ARG:HB3 | 3:D:770:ARG:HB2 | 1.63 | 0.79 |
| 14:U:217:PHE:O | 14:U:221:ASN:ND2 | 2.16 | 0.79 |
| 2:C:24:ARG:HA | 2:C:53:VAL:HG22 | 1.64 | 0.78 |
| 13:T:584:GLY:O | 15:V:135:LYS:NZ | 2.14 | 0.78 |
| 1:1:361:GLU:OE2 | 3:3:162:ARG:NH2 | 2.17 | 0.78 |
| 1:B:425:ALA:O | 1:B:428:LYS:NZ | 2.15 | 0.78 |
| 2:C:106:ILE:HD11 | 2:C:112:THR:CB | 2.14 | 0.78 |
| 3:D:611:ARG:HH21 | 9:X:101:ALA:HB1 | 1.47 | 0.78 |
| 6:G:120:ASN:HD22 | 6:G:122:ALA:H | 1.29 | 0.78 |
| 4:E:306:ASN:ND2 | 5:F:192:TYR:OH | 2.17 | 0.78 |
| 3:3:256:CYS:HB2 | 3:3:265:ILE:HD13 | 1.64 | 0.78 |
| 6:6:120:ASN:HD22 | 6:6:122:ALA:H | 1.30 | 0.77 |
| 3:3:414:SER:OG | 3:3:443:ARG:NH2 | 2.18 | 0.77 |
| 16:H:332:LEU:HB2 | 16:H:333:PRO:HD3 | 1.66 | 0.77 |
| 2:C:109:GLY:O | 8:I:121:ARG:NH2 | 2.17 | 0.77 |
| 3:3:268:ASP:OD2 | 3:3:278:ARG:NH1 | 2.14 | 0.77 |
| 3:D:34:CYS:SG | 3:D:35:SER:N | 2.57 | 0.77 |
| 11:R:69:PHE:O | 11:R:73:LEU:HG | 1.85 | 0.77 |
| 3:3:370:ASP:OD2 | 3:3:558:TRP:HD1 | 1.68 | 0.77 |
| 14:M:115:LEU:HD12 | 14:M:180:LEU:HD13 | 1.64 | 0.77 |
| 15:V:193:HIS:HB2 | 15:V:263:ILE:HD13 | 1.67 | 0.77 |
| 9:X:45:ARG:NH1 | 9:X:61:ASP:OD2 | 2.17 | 0.77 |
| 3:3:290:ILE:HG23 | 17:3:803:SF4:S4 | 2.25 | 0.76 |
| 5:5:185:LYS:HB2 | 5:5:189:ARG:HG3 | 1.65 | 0.76 |
| 6:6:119:ASN:HA | 6:6:125:GLN:HE22 | 1.50 | 0.76 |
| 11:J:68:LEU:HD23 | 11:J:71:ILE:HD11 | 1.67 | 0.76 |
| 1:B:65:ARG:NH1 | 1:B:249:MET:O | 2.19 | 0.76 |
| 7:O:40:ARG:O | 7:O:116:GLY:N | 2.18 | 0.76 |
| 13:T:278:ALA:HA | 13:T:301:SER:HA | 1.65 | 0.76 |
| 14:U:345:ARG:NH1 | 14:U:416:GLU:OE1 | 2.19 | 0.76 |
| 4:4:306:ASN:ND2 | 5:5:192:TYR:OH | 2.18 | 0.76 |
| 13:T:157:LYS:NZ | 13:T:535:ASP:OD2 | 2.19 | 0.76 |
| 6:6:94:ARG:HD2 | 10:A:46:SER:HA | 1.66 | 0.76 |
| 16:Q:50:ARG:O | 16:Q:52:GLY:N | 2.17 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:6:19:ILE:HG23 | 6:6:20:LEU:HG | 1.68 | 0.76 |
| 3:D:717:TRP:HB2 | 3:D:759:TYR:HB2 | 1.66 | 0.76 |
| 4:E:200:ARG:NH1 | 7:O:16:TYR:OH | 2.18 | 0.75 |
| 4:E:216:GLU:OE2 | 16:Q:304:GLN:NE2 | 2.20 | 0.75 |
| 13:L:575:GLY:HA2 | 15:N:246:LEU:HB3 | 1.68 | 0.75 |
| 3:3:635:GLU:OE2 | 9:W:7:ARG:NH1 | 2.20 | 0.75 |
| 1:B:359:CYS:HB2 | 1:B:403:ALA:HB2 | 1.69 | 0.75 |
| 4:E:144:THR:HG22 | 4:E:148:TYR:HE1 | 1.52 | 0.75 |
| 6:G:19:ILE:HG23 | 6:G:20:LEU:HG | 1.66 | 0.75 |
| 3:3:269:THR:HG22 | 3:3:274:LEU:HA | 1.69 | 0.75 |
| 3:3:616:ASN:ND2 | 3:3:622:LEU:HD11 | 2.02 | 0.75 |
| 7:9:96:LEU:HD21 | 7:9:129:LEU:HD13 | 1.69 | 0.75 |
| 14:U:208:PHE:O | 14:U:211:HIS:ND1 | 2.20 | 0.75 |
| 14:U:89:ALA:HB1 | 14:U:91:VAL:HG22 | 1.65 | 0.75 |
| 8:7:63:LEU:HD13 | 8:7:129:ALA:HB3 | 1.69 | 0.74 |
| 3:3:190:TYR:OH | 3:3:222:PHE:O | 2.06 | 0.74 |
| 4:4:352:GLU:OE2 | 5:5:87:ARG:NH1 | 2.20 | 0.74 |
| 11:R:47:ASP:O | 11:R:122:GLY:N | 2.20 | 0.74 |
| 11:R:133:GLY:H | 11:R:136:LEU:HB2 | 1.52 | 0.74 |
| 1:B:29:LEU:HD23 | 1:B:155:ARG:HD2 | 1.68 | 0.74 |
| 16:H:117:ASN:O | 16:H:181:ASN:ND2 | 2.20 | 0.74 |
| 4:E:84:ARG:HG2 | 17:G:201:SF4:S2 | 2.28 | 0.74 |
| 13:L:105:PHE:O | 13:L:109:ASN:ND2 | 2.19 | 0.74 |
| 13:L:162:ASN:OD1 | 13:L:216:LYS:NZ | 2.21 | 0.74 |
| 3:3:203:ILE:HG21 | 8:7:88:ARG:HG2 | 1.70 | 0.74 |
| 3:3:344:TYR:HB3 | 3:3:570:PHE:HE1 | 1.51 | 0.74 |
| 1:B:288:GLN:NE2 | 1:B:335:VAL:O | 2.20 | 0.74 |
| 16:H:16:LYS:NZ | 16:H:114:TRP:O | 2.20 | 0.74 |
| 15:N:294:LEU:HG | 15:N:402:VAL:HG13 | 1.69 | 0.74 |
| 4:4:333:GLU:OE2 | 4:4:336:HIS:NE2 | 2.21 | 0.74 |
| 3:3:113:LEU:O | 3:3:161:ARG:NH1 | 2.21 | 0.74 |
| 14:U:268:ALA:HA | 14:U:291:SER:HA | 1.68 | 0.74 |
| 1:B:305:GLU:OE1 | 1:B:319:LYS:NZ | 2.20 | 0.73 |
| 1:B:4:PRO:HA | 1:B:12:ARG:HH12 | 1.53 | 0.73 |
| 5:F:134:LYS:NZ | 5:F:141:LEU:O | 2.20 | 0.73 |
| 1:B:287:ILE:HA | 1:B:332:PRO:HA | 1.70 | 0.73 |
| 8:I:120:ASP:OD1 | 8:I:123:ARG:NH1 | 2.19 | 0.73 |
| 16:H:216:ARG:HD2 | 16:H:294:ARG:HA | 1.68 | 0.73 |
| 13:L:163:ARG:NH2 | 14:M:366:VAL:O | 2.22 | 0.73 |
| 14:M:89:ALA:HB1 | 14:M:91:VAL:HG22 | 1.68 | 0.73 |
| 7:O:172:GLY:O | 7:O:174:LYS:NZ | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:400:CYS:HG | 17:1:501:SF4:FE3 | 1.01 | 0.73 |
| 16:H:219:PHE:HB3 | 16:H:299:ARG:HG2 | 1.70 | 0.73 |
| 4:4:171:ASN:OD1 | 4:4:174:ARG:NH1 | 2.18 | 0.73 |
| 3:D:247:TRP:CD1 | 5:F:172:ALA:HB2 | 2.24 | 0.73 |
| 3:D:462:ALA:O | 3:D:465:HIS:ND1 | 2.22 | 0.73 |
| 6:G:119:ASN:HA | 6:G:125:GLN:HE22 | 1.54 | 0.73 |
| 15:N:13:LEU:HD22 | 15:N:25:VAL:HG13 | 1.70 | 0.73 |
| 7:O:96:LEU:HD21 | 7:O:129:LEU:HD13 | 1.69 | 0.73 |
| 10:P:3:PRO:HD2 | 16:Q:2:THR:HB | 1.70 | 0.73 |
| 4:4:200:ARG:NH1 | 7:9:16:TYR:OH | 2.21 | 0.73 |
| 16:Q:291:ILE:HA | 16:Q:294:ARG:HG3 | 1.69 | 0.73 |
| 3:D:414:SER:OG | 3:D:443:ARG:NH2 | 2.21 | 0.72 |
| 6:G:34:ASN:O | 16:Q:58:GLN:NE2 | 2.22 | 0.72 |
| 8:7:23:TYR:HH | 8:7:123:ARG:NH1 | 1.86 | 0.72 |
| 3:D:722:THR:HG21 | 3:D:756:GLY:H | 1.53 | 0.72 |
| 14:M:217:PHE:O | 14:M:221:ASN:ND2 | 2.21 | 0.72 |
| 15:V:2:THR:HG1 | 15:V:39:SER:HG | 1.31 | 0.72 |
| 1:1:246:SER:HB3 | 1:1:268:MET:HG2 | 1.69 | 0.72 |
| 4:4:341:GLU:OE1 | 5:5:91:ARG:NH2 | 2.19 | 0.72 |
| 5:5:18:GLU:HB2 | 5:5:26:TRP:HB2 | 1.69 | 0.72 |
| 10:P:109:TYR:OH | 10:P:113:LYS:NZ | 2.21 | 0.72 |
| 13:T:557:ASP:OD1 | 14:U:211:HIS:NE2 | 2.13 | 0.72 |
| 13:T:458:TYR:HB3 | 13:T:461:LEU:HD11 | 1.71 | 0.72 |
| 5:5:168:ALA:HA | 5:5:171:ARG:NH1 | 2.04 | 0.72 |
| 3:D:31:PRO:HB2 | 3:D:47:MET:HB3 | 1.70 | 0.72 |
| 1:1:16:THR:HG21 | 1:1:229:PRO:HB3 | 1.72 | 0.72 |
| 13:L:84:GLY:O | 13:L:88:HIS:ND1 | 2.20 | 0.72 |
| 6:6:114:SER:OG | 7:9:96:LEU:O | 2.06 | 0.72 |
| 4:4:73:ARG:NH2 | 4:4:81:TYR:OH | 2.23 | 0.72 |
| 2:C:106:ILE:CD1 | 2:C:112:THR:N | 2.53 | 0.72 |
| 16:H:271:VAL:HG12 | 16:H:272:LEU:HG | 1.70 | 0.71 |
| 11:R:22:LEU:O | 12:S:21:ARG:NH2 | 2.23 | 0.71 |
| 5:5:38:MET:HE3 | 5:5:104:VAL:HG11 | 1.71 | 0.71 |
| 3:D:412:ARG:NH1 | 3:D:415:GLU:OE1 | 2.23 | 0.71 |
| 16:H:265:GLY:O | 16:H:282:LYS:NZ | 2.17 | 0.71 |
| 16:H:52:GLY:HA3 | 16:H:55:GLY:H | 1.55 | 0.71 |
| 13:T:419:ARG:NH2 | 13:T:525:GLU:OE2 | 2.22 | 0.71 |
| 8:7:120:ASP:OD1 | 8:7:123:ARG:NH1 | 2.23 | 0.71 |
| 3:D:18:SER:OG | 3:D:82:SER:O | 2.07 | 0.71 |
| 3:D:710:GLU:O | 3:D:713:ARG:NH1 | 2.21 | 0.71 |
| 3:3:538:ALA:HB3 | 3:3:541:ALA:HB2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:253:GLN:HG2 | 1:B:327:GLY:HA2 | 1.72 | 0.71 |
| 1:B:433:ARG:HH12 | 2:C:89:LYS:HE2 | 1.55 | 0.71 |
| 13:T:84:GLY:O | 13:T:88:HIS:ND1 | 2.21 | 0.71 |
| 14:U:128:PRO:O | 14:U:132:MET:HG2 | 1.91 | 0.71 |
| 3:3:468:HIS:ND1 | 3:3:469:ARG:O | 2.23 | 0.71 |
| 5:5:3:LEU:HD21 | 5:5:25:LEU:HD22 | 1.71 | 0.71 |
| 6:6:165:GLU:OE2 | 7:9:148:ARG:NH1 | 2.23 | 0.71 |
| 5:F:103:THR:HG22 | 5:F:126:PHE:HB3 | 1.71 | 0.71 |
| 13:L:161:VAL:HG13 | 13:L:222:LEU:HD13 | 1.73 | 0.71 |
| 13:L:278:ALA:HA | 13:L:301:SER:HA | 1.73 | 0.71 |
| 11:J:133:GLY:H | 11:J:136:LEU:HB2 | 1.56 | 0.71 |
| 12:K:7:SER:HB3 | 12:K:40:LEU:HD23 | 1.71 | 0.71 |
| 14:M:345:ARG:NH1 | 14:M:416:GLU:OE1 | 2.24 | 0.71 |
| 3:D:694:LEU:HB3 | 3:D:762:ALA:HB2 | 1.73 | 0.71 |
| 6:G:93:ARG:NH1 | 6:G:130:VAL:O | 2.24 | 0.71 |
| 3:3:115:HIS:CD2 | 3:3:116:PRO:HD2 | 2.26 | 0.70 |
| 4:E:110:PRO:HB3 | 4:E:301:PRO:HG2 | 1.70 | 0.70 |
| 3:D:34:CYS:N | 3:D:45:CYS:SG | 2.61 | 0.70 |
| 2:C:110:GLU:HA | 8:I:121:ARG:HH12 | 1.55 | 0.70 |
| 13:T:105:PHE:O | 13:T:109:ASN:ND2 | 2.23 | 0.70 |
| 2:2:85:THR:HG22 | 2:2:86:LEU:H | 1.56 | 0.70 |
| 4:4:318:GLU:HB2 | 8:7:39:ASP:HA | 1.73 | 0.70 |
| 16:Q:52:GLY:HA3 | 16:Q:55:GLY:H | 1.54 | 0.70 |
| 1:1:287:ILE:HA | 1:1:332:PRO:HA | 1.74 | 0.70 |
| 1:1:342:TRP:HE1 | 1:1:372:ALA:HA | 1.57 | 0.70 |
| 16:H:162:TYR:OH | 16:H:305:LEU:O | 2.07 | 0.70 |
| 4:4:103:LYS:NZ | 5:5:22:LEU:O | 2.25 | 0.70 |
| 2:C:87:SER:HB2 | 20:C:201:FES:S2 | 2.31 | 0.70 |
| 6:G:50:MET:O | 6:G:53:SER:OG | 2.10 | 0.70 |
| 13:L:305:TYR:OH | 13:L:406:ALA:O | 2.08 | 0.70 |
| 1:B:88:TYR:HB2 | 1:B:216:THR:HG22 | 1.72 | 0.70 |
| 3:D:621:VAL:HG23 | 3:D:672:ALA:HA | 1.73 | 0.70 |
| 4:E:372:ALA:HB2 | 4:E:409:ARG:HD3 | 1.74 | 0.70 |
| 14:U:21:PRO:HD2 | 14:U:24:LEU:HG | 1.73 | 0.70 |
| 9:X:60:PRO:HB3 | 9:X:103:LEU:HD13 | 1.74 | 0.70 |
| 16:H:29:ALA:O | 16:H:32:THR:OG1 | 2.08 | 0.70 |
| 7:9:108:CYS:HA | 17:9:202:SF4:S3 | 2.31 | 0.69 |
| 15:N:201:GLN:OE1 | 15:N:256:ARG:NH1 | 2.25 | 0.69 |
| 1:1:79:MET:SD | 1:1:217:THR:OG1 | 2.50 | 0.69 |
| 3:3:435:LEU:O | 3:3:438:LYS:NZ | 2.24 | 0.69 |
| 4:E:154:GLU:OE2 | 4:E:167:ARG:NH2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:370:LEU:HD12 | 1:B:387:LEU:HB2 | 1.73 | 0.69 |
| 3:D:34:CYS:HB3 | 3:D:45:CYS:H | 1.57 | 0.69 |
| 14:M:208:PHE:O | 14:M:211:HIS:ND1 | 2.24 | 0.69 |
| 4:E:392:ASP:OD2 | 16:Q:301:ARG:NH1 | 2.25 | 0.69 |
| 1:1:350:HIS:O | 3:3:205:ARG:NH1 | 2.25 | 0.69 |
| 3:3:576:ALA:O | 3:3:580:LYS:NZ | 2.17 | 0.69 |
| 10:P:69:ILE:HG22 | 11:R:62:ALA:HB1 | 1.75 | 0.69 |
| 1:1:288:GLN:NE2 | 1:1:335:VAL:O | 2.26 | 0.69 |
| 3:3:494:LYS:O | 3:3:498:GLU:HG2 | 1.92 | 0.69 |
| 3:3:507:LEU:HD22 | 3:3:511:VAL:HG11 | 1.75 | 0.69 |
| 8:7:63:LEU:CD1 | 8:7:129:ALA:HB3 | 2.22 | 0.69 |
| 14:U:304:THR:O | 14:U:307:GLY:N | 2.24 | 0.69 |
| 1:B:189:MET:O | 1:B:193:GLU:HB2 | 1.93 | 0.69 |
| 4:E:352:GLU:O | 4:E:371:ARG:NE | 2.19 | 0.69 |
| 13:T:432:HIS:HE1 | 13:T:434:HIS:HB2 | 1.57 | 0.69 |
| 1:1:425:ALA:O | 1:1:428:LYS:NZ | 2.17 | 0.69 |
| 3:3:129:GLU:O | 3:3:133:ARG:HG2 | 1.93 | 0.69 |
| 1:B:16:THR:HG21 | 1:B:229:PRO:HB3 | 1.74 | 0.69 |
| 14:M:166:ALA:HA | 14:M:185:LEU:HD21 | 1.74 | 0.69 |
| 16:Q:168:LEU:HD13 | 16:Q:318:LEU:HB3 | 1.73 | 0.69 |
| 1:B:246:SER:HB3 | 1:B:268:MET:HG2 | 1.73 | 0.68 |
| 16:H:218:PRO:HB3 | 16:H:305:LEU:HD13 | 1.75 | 0.68 |
| 8:I:74:PRO:HG2 | 8:I:77:ALA:HB2 | 1.74 | 0.68 |
| 6:G:63:PHE:HA | 16:Q:50:ARG:HG2 | 1.74 | 0.68 |
| 4:4:167:ARG:HD3 | 6:6:143:ARG:HH12 | 1.59 | 0.68 |
| 7:O:101:CYS:N | 17:O:201:SF4:S4 | 2.66 | 0.68 |
| 10:A:109:TYR:OH | 10:A:113:LYS:NZ | 2.25 | 0.68 |
| 11:J:47:ASP:O | 11:J:122:GLY:N | 2.27 | 0.68 |
| 14:M:86:ALA:HA | 14:M:96:LEU:HD11 | 1.76 | 0.68 |
| 13:T:305:TYR:OH | 13:T:406:ALA:O | 2.10 | 0.68 |
| 3:D:113:LEU:O | 3:D:161:ARG:NH1 | 2.27 | 0.68 |
| 4:4:144:THR:OG1 | 16:H:295:ALA:O | 2.10 | 0.68 |
| 14:M:177:LEU:HD21 | 14:M:243:ARG:HD2 | 1.75 | 0.68 |
| 12:S:7:SER:HB3 | 12:S:40:LEU:HD23 | 1.75 | 0.68 |
| 3:D:48:CYS:HB3 | 20:D:804:FES:S2 | 2.33 | 0.68 |
| 11:R:124:PRO:HA | 11:R:127:LEU:HB2 | 1.74 | 0.68 |
| 3:3:199:VAL:HG11 | 3:3:219:PRO:HD2 | 1.75 | 0.68 |
| 5:F:39:ALA:HA | 5:F:107:LEU:HD21 | 1.74 | 0.68 |
| 4:4:240:ARG:NH1 | 4:4:282:GLU:OE2 | 2.27 | 0.68 |
| 4:E:314:ARG:NH2 | 8:I:44:MET:SD | 2.66 | 0.68 |
| 14:M:371:LEU:HD12 | 14:M:440:LEU:HB3 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:3:611:ARG:HA | 3:3:624:LEU:O | 1.94 | 0.68 |
| 1:B:104:ARG:NH2 | 2:C:143:GLU:OE2 | 2.24 | 0.68 |
| 13:T:288:GLN:NE2 | 13:T:528:SER:O | 2.27 | 0.68 |
| 6:6:69:ARG:NH2 | 16:H:223:GLU:OE2 | 2.27 | 0.68 |
| 14:M:55:LEU:HD11 | 15:N:416:PRO:HD2 | 1.76 | 0.68 |
| 3:3:701:ALA:N | 3:3:763:LEU:O | 2.27 | 0.67 |
| 1:B:195:LEU:HD23 | 2:C:24:ARG:HH12 | 1.56 | 0.67 |
| 16:H:189:GLN:NE2 | 16:H:264:LEU:O | 2.27 | 0.67 |
| 11:J:24:ASN:HB3 | 11:J:27:HIS:HB2 | 1.77 | 0.67 |
| 13:L:432:HIS:HE1 | 13:L:434:HIS:HB2 | 1.58 | 0.67 |
| 13:L:288:GLN:NE2 | 13:L:528:SER:O | 2.27 | 0.67 |
| 3:D:48:CYS:SG | 3:D:83:CYS:N | 2.67 | 0.67 |
| 1:1:4:PRO:HA | 1:1:12:ARG:HH12 | 1.59 | 0.67 |
| 3:3:98:ASP:OD1 | 3:3:101:ARG:NH2 | 2.27 | 0.67 |
| 6:G:37:TRP:HB3 | 6:G:75:ALA:HA | 1.77 | 0.67 |
| 16:H:43:GLN:O | 16:H:45:ARG:N | 2.27 | 0.67 |
| 13:L:182:THR:HB | 13:L:187:GLU:HG3 | 1.76 | 0.67 |
| 3:3:186:ARG:HD3 | 3:3:229:ILE:HG22 | 1.77 | 0.67 |
| 1:1:18:TYR:OH | 1:1:102:LYS:O | 2.11 | 0.67 |
| 3:3:717:TRP:HB2 | 3:3:759:TYR:HB2 | 1.77 | 0.67 |
| 5:5:35:LYS:NZ | 5:5:103:THR:O | 2.28 | 0.67 |
| 1:B:339:ASP:OD1 | 1:B:433:ARG:NH2 | 2.28 | 0.67 |
| 7:O:68:ILE:HG12 | 7:O:93:ILE:HG12 | 1.77 | 0.67 |
| 1:1:433:ARG:HH12 | 2:2:89:LYS:HE2 | 1.58 | 0.67 |
| 10:A:48:ASN:OD1 | 10:A:49:ASP:HB2 | 1.94 | 0.67 |
| 3:3:290:ILE:HB | 3:3:295:ARG:HH21 | 1.58 | 0.67 |
| 7:O:120:GLU:OE1 | 7:O:146:GLN:NE2 | 2.28 | 0.67 |
| 6:6:33:SER:HB2 | 6:6:155:GLN:HG2 | 1.77 | 0.67 |
| 1:B:139:ARG:NH1 | 1:B:143:ASP:OD2 | 2.27 | 0.67 |
| 6:G:125:GLN:OE1 | 7:O:97:ARG:NH1 | 2.26 | 0.67 |
| 13:L:159:PHE:HD2 | 14:M:407:LEU:HD11 | 1.59 | 0.67 |
| 6:6:50:MET:O | 6:6:53:SER:OG | 2.10 | 0.67 |
| 6:6:90:PRO:O | 6:6:93:ARG:HB3 | 1.95 | 0.67 |
| 2:C:106:ILE:HD11 | 2:C:112:THR:CA | 2.24 | 0.67 |
| 3:D:129:GLU:O | 3:D:133:ARG:HG2 | 1.94 | 0.67 |
| 4:E:194:LEU:HD21 | 4:E:290:ILE:HG22 | 1.77 | 0.67 |
| 6:G:17:GLU:HG3 | 10:P:33:PRO:HA | 1.77 | 0.67 |
| 13:T:163:ARG:HE | 14:U:399:VAL:HB | 1.58 | 0.67 |
| 2:2:34:VAL:HG11 | 2:2:45:ARG:HG3 | 1.75 | 0.66 |
| 3:3:367:PRO:O | 3:3:552:GLY:N | 2.29 | 0.66 |
| 3:D:227:THR:HG21 | 3:D:237:ASP:HB2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:381:LEU:HD11 | 4:E:397:ILE:HG12 | 1.77 | 0.66 |
| 4:E:83:PRO:HB2 | 4:E:169:HIS:HA | 1.78 | 0.66 |
| 13:L:582:GLN:NE2 | 15:N:194:PHE:O | 2.29 | 0.66 |
| 13:L:66:SER:HB3 | 13:L:122:ASP:HB3 | 1.77 | 0.66 |
| 14:U:115:LEU:HD13 | 14:U:163:VAL:HG23 | 1.76 | 0.66 |
| 1:B:177:ALA:HA | 2:C:32:ARG:HH21 | 1.61 | 0.66 |
| 1:B:312:SER:OG | 1:B:315:HIS:ND1 | 2.23 | 0.66 |
| 16:H:218:PRO:HA | 16:H:300:LEU:HB2 | 1.77 | 0.66 |
| 4:4:259:THR:O | 4:4:296:ARG:NH2 | 2.28 | 0.66 |
| 13:L:380:SER:HB3 | 13:L:457:GLY:H | 1.60 | 0.66 |
| 16:Q:274:VAL:HG12 | 16:Q:278:TRP:HD1 | 1.56 | 0.66 |
| 16:Q:332:LEU:HB2 | 16:Q:333:PRO:HD3 | 1.76 | 0.66 |
| 16:Q:65:LYS:O | 16:Q:69:LYS:HB2 | 1.96 | 0.66 |
| 3:3:225:ASN:O | 3:3:229:ILE:HG13 | 1.96 | 0.66 |
| 6:G:119:ASN:HA | 6:G:125:GLN:NE2 | 2.11 | 0.66 |
| 13:T:151:TYR:HB3 | 13:T:231:ALA:HB1 | 1.77 | 0.66 |
| 1:1:104:ARG:NH2 | 1:1:105:TYR:OH | 2.29 | 0.66 |
| 3:D:19:VAL:HG21 | 3:D:52:ILE:HD11 | 1.76 | 0.66 |
| 14:M:91:VAL:HG12 | 14:M:222:HIS:CE1 | 2.31 | 0.66 |
| 11:J:85:PRO:HA | 12:K:22:ARG:HH12 | 1.61 | 0.66 |
| 7:9:41:HIS:HB3 | 7:9:113:ILE:HD11 | 1.77 | 0.65 |
| 7:O:43:LEU:HA | 7:O:112:ALA:O | 1.96 | 0.65 |
| 4:4:240:ARG:NH2 | 4:4:347:GLU:OE2 | 2.27 | 0.65 |
| 6:6:93:ARG:NH1 | 6:6:130:VAL:O | 2.30 | 0.65 |
| 7:9:101:CYS:N | 17:9:201:SF4:S4 | 2.68 | 0.65 |
| 6:6:157:LYS:HB2 | 7:9:124:TYR:HE2 | 1.62 | 0.65 |
| 2:C:27:ILE:HG13 | 2:C:53:VAL:HG21 | 1.77 | 0.65 |
| 4:E:81:TYR:OH | 6:G:117:MET:O | 2.13 | 0.65 |
| 6:G:60:LEU:HD21 | 6:G:151:VAL:HG11 | 1.78 | 0.65 |
| 16:H:168:LEU:HD13 | 16:H:318:LEU:HB3 | 1.78 | 0.65 |
| 16:H:71:ASP:OD1 | 16:H:240:LYS:NZ | 2.19 | 0.65 |
| 10:P:65:ALA:HB3 | 11:R:66:LEU:HD13 | 1.79 | 0.65 |
| 13:T:44:GLY:HA3 | 13:T:77:LEU:HD21 | 1.78 | 0.65 |
| 5:5:144:HIS:HB2 | 5:5:147:ARG:HD3 | 1.77 | 0.65 |
| 10:A:63:VAL:HG11 | 10:A:115:VAL:HG21 | 1.77 | 0.65 |
| 4:E:222:GLY:HA3 | 4:E:275:ARG:HH22 | 1.60 | 0.65 |
| 4:E:87:TYR:CG | 6:G:45:CYS:HB3 | 2.32 | 0.65 |
| 15:V:58:VAL:HB | 15:V:225:ARG:HH11 | 1.61 | 0.65 |
| 1:1:88:TYR:HB2 | 1:1:216:THR:HG22 | 1.79 | 0.65 |
| 10:A:3:PRO:HD2 | 16:H:2:THR:HB | 1.78 | 0.65 |
| 11:J:15:SER:OG | 11:J:31:ALA:O | 2.14 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:Q:117:ASN:O | 16:Q:181:ASN:ND2 | 2.28 | 0.65 |
| 9:W:28:GLU:O | 9:W:88:ARG:NH2 | 2.29 | 0.65 |
| 1:B:372:ALA:O | 1:B:376:THR:OG1 | 2.12 | 0.65 |
| 4:E:373:PRO:O | 4:E:377:ASN:ND2 | 2.29 | 0.65 |
| 13:L:487:LEU:HA | 13:L:490:GLU:HG2 | 1.77 | 0.65 |
| 14:U:333:TYR:O | 14:U:337:GLY:N | 2.30 | 0.65 |
| 16:H:333:PRO:HB2 | 16:H:335:THR:H | 1.62 | 0.65 |
| 8:I:20:MET:HG2 | 8:I:115:PHE:CZ | 2.32 | 0.65 |
| 14:M:102:MET:HB3 | 14:M:230:LEU:HD23 | 1.78 | 0.65 |
| 10:P:28:GLY:HA2 | 16:Q:67:ILE:HG22 | 1.77 | 0.65 |
| 4:4:371:ARG:NH2 | 4:4:376:VAL:HG21 | 2.12 | 0.65 |
| 3:3:259:CYS:SG | 3:3:261:VAL:HG22 | 2.36 | 0.64 |
| 4:4:102:GLU:O | 4:4:106:GLY:N | 2.31 | 0.64 |
| 4:4:132:PHE:CE2 | 4:4:279:ARG:HD2 | 2.33 | 0.64 |
| 13:T:162:ASN:OD1 | 13:T:216:LYS:NZ | 2.30 | 0.64 |
| 10:A:69:ILE:HG22 | 11:J:62:ALA:HB1 | 1.79 | 0.64 |
| 15:N:345:LYS:NZ | 15:N:368:SER:OG | 2.30 | 0.64 |
| 7:O:41:HIS:HB3 | 7:O:113:ILE:HD11 | 1.77 | 0.64 |
| 10:P:77:PHE:O | 10:P:80:PRO:HD2 | 1.97 | 0.64 |
| 14:U:33:PHE:HA | 14:U:79:ALA:HB1 | 1.79 | 0.64 |
| 1:B:165:THR:HG23 | 1:B:167:PHE:H | 1.63 | 0.64 |
| 3:D:193:GLU:O | 3:D:443:ARG:NH2 | 2.26 | 0.64 |
| 9:W:59:VAL:HG11 | 9:W:63:PHE:CE2 | 2.32 | 0.64 |
| 3:3:224:GLY:O | 3:3:227:THR:HB | 1.98 | 0.64 |
| 3:3:720:PRO:HG2 | 3:3:751:GLU:HG3 | 1.78 | 0.64 |
| 4:E:52:VAL:O | 4:E:387:GLY:N | 2.24 | 0.64 |
| 11:R:68:LEU:HD23 | 11:R:71:ILE:HD11 | 1.78 | 0.64 |
| 3:3:39:LEU:HB3 | 3:3:189:ARG:HE | 1.63 | 0.64 |
| 14:M:43:HIS:NE2 | 14:M:45:GLY:O | 2.31 | 0.64 |
| 4:4:248:VAL:HB | 4:4:347:GLU:HB2 | 1.80 | 0.64 |
| 14:M:335:ARG:NH2 | 14:M:429:GLU:OE1 | 2.30 | 0.64 |
| 3:3:34:CYS:SG | 3:3:35:SER:N | 2.71 | 0.64 |
| 5:5:126:PHE:H | 5:5:132:LEU:HD11 | 1.63 | 0.64 |
| 5:F:10:ALA:HB1 | 5:F:15:TYR:HB2 | 1.80 | 0.64 |
| 13:L:17:LEU:HB2 | 13:L:106:ALA:HB2 | 1.79 | 0.64 |
| 11:J:135:TRP:HZ3 | 15:N:105:LEU:HD22 | 1.62 | 0.64 |
| 15:V:187:ALA:O | 15:V:216:LYS:NZ | 2.31 | 0.64 |
| 4:4:230:ILE:HG21 | 5:5:47:ASN:HB3 | 1.80 | 0.64 |
| 3:D:149:LEU:HD11 | 4:E:110:PRO:HG3 | 1.79 | 0.64 |
| 4:E:281:ARG:HD3 | 4:E:284:ARG:HH12 | 1.63 | 0.64 |
| 1:1:400:CYS:SG | 17:1:501:SF4:FE3 | 1.88 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:80:VAL:HG11 | 6:6:127:VAL:HG11 | 1.80 | 0.64 |
| 4:4:328:PHE:CE2 | 7:9:58:LEU:HD21 | 2.33 | 0.64 |
| 4:E:80:THR:O | 4:E:84:ARG:NH1 | 2.29 | 0.64 |
| 12:S:88:ASP:OD2 | 13:T:587:ARG:NH1 | 2.31 | 0.64 |
| 14:U:85:GLY:O | 14:U:89:ALA:HB2 | 1.97 | 0.64 |
| 6:G:17:GLU:HA | 10:P:33:PRO:HG3 | 1.79 | 0.64 |
| 3:3:300:TRP:CD1 | 3:3:703:GLN:HA | 2.33 | 0.63 |
| 4:4:31:GLY:HA3 | 10:A:45:GLU:OE2 | 1.98 | 0.63 |
| 13:L:574:LEU:HD22 | 15:N:246:LEU:HD13 | 1.80 | 0.63 |
| 7:O:40:ARG:NH1 | 7:O:41:HIS:O | 2.31 | 0.63 |
| 3:3:567:TYR:HA | 3:3:584:VAL:HG23 | 1.80 | 0.63 |
| 4:4:140:LEU:HD21 | 4:4:217:ARG:HH12 | 1.63 | 0.63 |
| 4:4:311:PRO:HD3 | 4:4:330:HIS:CE1 | 2.34 | 0.63 |
| 5:5:53:VAL:HG13 | 5:5:71:VAL:HB | 1.79 | 0.63 |
| 3:3:592:PRO:HA | 3:3:595:GLU:HG2 | 1.80 | 0.63 |
| 5:5:168:ALA:HA | 5:5:171:ARG:HH11 | 1.62 | 0.63 |
| 10:A:27:VAL:HG12 | 16:H:67:ILE:HG21 | 1.79 | 0.63 |
| 10:P:56:ARG:HD3 | 11:R:74:LEU:HA | 1.79 | 0.63 |
| 13:T:392:THR:HG22 | 13:T:399:GLY:O | 1.98 | 0.63 |
| 4:4:144:THR:HG22 | 4:4:148:TYR:HE1 | 1.62 | 0.63 |
| 5:F:120:ASP:OD2 | 5:F:136:LEU:N | 2.32 | 0.63 |
| 5:F:121:LEU:HA | 5:F:145:PRO:HD2 | 1.80 | 0.63 |
| 6:G:18:GLY:HA2 | 6:G:28:VAL:HG11 | 1.80 | 0.63 |
| 13:T:234:THR:HG23 | 13:T:292:LYS:HE2 | 1.81 | 0.63 |
| 1:B:184:GLU:O | 1:B:188:LEU:N | 2.29 | 0.63 |
| 1:B:275:LEU:HA | 1:B:279:TRP:HD1 | 1.63 | 0.63 |
| 2:C:66:PHE:O | 3:D:205:ARG:NE | 2.30 | 0.63 |
| 5:F:174:LEU:HB3 | 5:F:178:ASP:HB3 | 1.80 | 0.63 |
| 16:Q:120:LEU:HD22 | 16:Q:180:LEU:HD12 | 1.80 | 0.63 |
| 16:Q:332:LEU:HB2 | 16:Q:333:PRO:CD | 2.27 | 0.63 |
| 2:2:110:GLU:OE2 | 8:7:114:ARG:NE | 2.28 | 0.63 |
| 7:9:171:GLU:OE2 | 8:7:43:ARG:NH2 | 2.31 | 0.63 |
| 10:A:81:TYR:HE2 | 16:H:325:ALA:HB1 | 1.64 | 0.63 |
| 4:E:201:ILE:HG21 | 4:E:284:ARG:HG3 | 1.81 | 0.63 |
| 11:J:104:LEU:HA | 15:N:174:LEU:HD21 | 1.80 | 0.63 |
| 3:3:656:LEU:HD11 | 9:W:3:ARG:HD3 | 1.80 | 0.63 |
| 4:4:285:GLU:O | 4:4:289:ILE:HG12 | 1.99 | 0.63 |
| 5:F:35:LYS:NZ | 5:F:103:THR:O | 2.31 | 0.63 |
| 14:M:306:GLU:OE2 | 14:M:386:LYS:NZ | 2.25 | 0.63 |
| 15:N:98:LEU:HD23 | 15:N:218:ALA:HB1 | 1.81 | 0.63 |
| 1:1:354:GLY:O | 1:1:360:ARG:NH1 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:183:HIS:NE2 | 3:D:209:THR:O | 2.31 | 0.63 |
| 16:H:189:GLN:HG2 | 16:H:195:LEU:H | 1.63 | 0.63 |
| 11:J:61:GLY:O | 11:J:65:VAL:HG21 | 1.98 | 0.63 |
| 14:M:115:LEU:HD13 | 14:M:163:VAL:HG23 | 1.80 | 0.63 |
| 3:3:605:PRO:HB2 | 3:3:609:GLU:HG3 | 1.79 | 0.62 |
| 8:7:40:PHE:HA | 8:7:43:ARG:HG2 | 1.80 | 0.62 |
| 1:B:276:ILE:HA | 1:B:280:ALA:HB3 | 1.81 | 0.62 |
| 1:1:196:ARG:NH2 | 3:3:204:GLU:O | 2.30 | 0.62 |
| 15:V:317:ARG:NH1 | 15:V:384:ALA:O | 2.31 | 0.62 |
| 15:V:14:THR:HA | 15:V:86:LEU:HD21 | 1.81 | 0.62 |
| 6:6:58:ASN:ND2 | 6:6:145:GLU:OE2 | 2.33 | 0.62 |
| 2:C:81:GLN:HB3 | 2:C:122:VAL:HG21 | 1.80 | 0.62 |
| 16:H:332:LEU:HB2 | 16:H:333:PRO:CD | 2.29 | 0.62 |
| 13:L:151:TYR:HB3 | 13:L:231:ALA:HB1 | 1.80 | 0.62 |
| 16:Q:43:GLN:O | 16:Q:45:ARG:N | 2.32 | 0.62 |
| 1:1:6:LEU:HD11 | 1:1:240:GLN:HE21 | 1.64 | 0.62 |
| 3:3:384:PRO:HG3 | 3:3:542:ARG:NH1 | 2.14 | 0.62 |
| 2:C:71:GLN:NE2 | 2:C:120:GLN:OE1 | 2.32 | 0.62 |
| 6:G:59:ASP:OD1 | 6:G:62:ARG:NH2 | 2.32 | 0.62 |
| 1:1:365:GLY:O | 1:1:369:ASN:ND2 | 2.33 | 0.62 |
| 4:4:369:LYS:HG3 | 5:5:53:VAL:HG23 | 1.82 | 0.62 |
| 1:B:10:ASP:OD2 | 1:B:12:ARG:NE | 2.26 | 0.62 |
| 15:N:347:LEU:O | 15:N:351:GLU:HG2 | 1.98 | 0.62 |
| 16:Q:72:ILE:HG22 | 16:Q:237:SER:HB3 | 1.80 | 0.62 |
| 15:V:108:LEU:HB2 | 15:V:147:PHE:HE2 | 1.62 | 0.62 |
| 3:3:2:VAL:HG13 | 3:3:89:ASP:HA | 1.81 | 0.62 |
| 7:9:164:PRO:HA | 7:9:178:GLU:HB2 | 1.80 | 0.62 |
| 16:H:147:TYR:CD1 | 16:H:229:VAL:HG22 | 2.35 | 0.62 |
| 16:Q:29:ALA:O | 16:Q:32:THR:OG1 | 2.13 | 0.62 |
| 1:B:293:GLY:HA3 | 1:B:297:THR:HG21 | 1.80 | 0.62 |
| 1:B:201:LEU:HA | 1:B:399:PHE:HZ | 1.65 | 0.62 |
| 16:H:205:VAL:HG21 | 16:H:317:ALA:HB2 | 1.80 | 0.62 |
| 16:H:60:LEU:O | 16:H:64:ILE:HG13 | 2.00 | 0.62 |
| 14:U:70:LEU:O | 14:U:73:LEU:HD23 | 1.99 | 0.62 |
| 1:1:195:LEU:HD23 | 2:2:24:ARG:HH12 | 1.64 | 0.62 |
| 3:D:243:ARG:HB3 | 3:D:275:LEU:HD22 | 1.81 | 0.62 |
| 3:D:737:GLU:HB2 | 3:D:776:LEU:HD11 | 1.81 | 0.62 |
| 3:3:716:LEU:HD21 | 3:3:758:LEU:HD23 | 1.80 | 0.62 |
| 4:4:261:THR:H | 4:4:292:GLN:NE2 | 1.95 | 0.62 |
| 5:5:103:THR:HG22 | 5:5:126:PHE:HB3 | 1.81 | 0.62 |
| 16:H:267:TRP:CG | 16:H:268:THR:N | 2.65 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:T:291:ILE:HD12 | 13:T:336:SER:HB3 | 1.81 | 0.62 |
| 1:1:275:LEU:HA | 1:1:279:TRP:HD1 | 1.63 | 0.61 |
| 1:1:359:CYS:HB2 | 1:1:403:ALA:HB2 | 1.80 | 0.61 |
| 1:B:243:THR:HG22 | 1:B:244:GLU:H | 1.63 | 0.61 |
| 14:M:333:TYR:O | 14:M:337:GLY:N | 2.32 | 0.61 |
| 1:1:46:LYS:HE2 | 1:1:163:PHE:HB3 | 1.82 | 0.61 |
| 8:7:23:TYR:OH | 8:7:123:ARG:NH1 | 2.22 | 0.61 |
| 16:Q:292:TRP:O | 16:Q:296:THR:OG1 | 2.07 | 0.61 |
| 16:Q:302:TYR:HA | 16:Q:305:LEU:HB3 | 1.82 | 0.61 |
| 13:T:278:ALA:HB1 | 13:T:409:VAL:HG11 | 1.82 | 0.61 |
| 15:V:95:MET:HG2 | 15:V:114:LEU:HD22 | 1.82 | 0.61 |
| 3:3:243:ARG:HB3 | 3:3:275:LEU:HD22 | 1.82 | 0.61 |
| 8:7:105:THR:HG23 | 8:7:110:LEU:HB2 | 1.82 | 0.61 |
| 4:E:123:LEU:HG | 4:E:156:ILE:HG23 | 1.83 | 0.61 |
| 5:F:159:PHE:HB2 | 5:F:163:ARG:O | 1.99 | 0.61 |
| 13:L:490:GLU:O | 13:L:494:ILE:HG12 | 2.00 | 0.61 |
| 7:O:28:ASP:OD2 | 16:Q:50:ARG:NH1 | 2.33 | 0.61 |
| 16:Q:216:ARG:HB2 | 16:Q:294:ARG:HD2 | 1.82 | 0.61 |
| 3:3:364:LEU:HB2 | 3:3:650:VAL:HG21 | 1.82 | 0.61 |
| 3:D:51:ARG:HB3 | 3:D:94:ASP:HB3 | 1.82 | 0.61 |
| 5:F:66:GLU:HB2 | 5:F:93:TYR:HB3 | 1.83 | 0.61 |
| 6:G:21:PHE:HD1 | 6:G:23:THR:H | 1.47 | 0.61 |
| 14:M:54:PRO:HA | 14:M:62:TYR:HD1 | 1.65 | 0.61 |
| 16:Q:2:THR:HA | 16:Q:5:TYR:HD2 | 1.65 | 0.61 |
| 14:U:109:LEU:HD21 | 14:U:236:VAL:HG21 | 1.82 | 0.61 |
| 16:Q:127:ALA:O | 16:Q:131:LEU:HG | 2.00 | 0.61 |
| 13:T:490:GLU:O | 13:T:494:ILE:HG12 | 2.01 | 0.61 |
| 5:5:38:MET:HA | 5:5:41:TYR:HD2 | 1.66 | 0.61 |
| 14:M:167:ARG:NH2 | 14:M:173:PRO:O | 2.31 | 0.61 |
| 3:3:722:THR:HG21 | 3:3:756:GLY:H | 1.65 | 0.61 |
| 1:B:254:ILE:HD11 | 1:B:330:LEU:HD11 | 1.82 | 0.61 |
| 15:N:128:GLN:NE2 | 15:N:305:ASP:OD1 | 2.34 | 0.61 |
| 15:V:59:SER:OG | 15:V:100:SER:OG | 2.13 | 0.61 |
| 12:K:88:ASP:OD2 | 13:L:587:ARG:NH1 | 2.33 | 0.61 |
| 14:M:354:LEU:HD13 | 14:M:425:LEU:HG | 1.83 | 0.61 |
| 13:T:432:HIS:CE1 | 13:T:434:HIS:HB2 | 2.36 | 0.61 |
| 6:6:178:ARG:NH1 | 9:W:122:ASP:OD2 | 2.33 | 0.61 |
| 6:6:143:ARG:NE | 6:6:145:GLU:OE1 | 2.33 | 0.61 |
| 1:B:6:LEU:HB2 | 1:B:241:MET:HA | 1.82 | 0.61 |
| 11:J:50:PHE:HB2 | 11:J:124:PRO:HD3 | 1.83 | 0.61 |
| 13:L:325:HIS:NE2 | 13:L:329:LYS:HG3 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:171:ARG:NE | 7:O:66:TYR:OH | 2.34 | 0.61 |
| 16:Q:39:LEU:O | 16:Q:43:GLN:HG2 | 2.00 | 0.61 |
| 14:U:24:LEU:HD22 | 14:U:27:LEU:HD21 | 1.83 | 0.61 |
| 15:V:217:ALA:HA | 15:V:285:LEU:HD23 | 1.82 | 0.61 |
| 16:Q:86:PRO:HG3 | 16:Q:244:PHE:CE2 | 2.35 | 0.60 |
| 1:B:101:PHE:CZ | 1:B:253:GLN:HB2 | 2.35 | 0.60 |
| 1:B:288:GLN:HE21 | 1:B:331:ILE:HG22 | 1.66 | 0.60 |
| 4:4:148:TYR:OH | 16:H:42:PHE:O | 2.17 | 0.60 |
| 9:W:59:VAL:HG11 | 9:W:63:PHE:HE2 | 1.66 | 0.60 |
| 3:3:9:ARG:NH1 | 3:3:26:ALA:O | 2.33 | 0.60 |
| 6:6:117:MET:HE1 | 7:9:99:ILE:HG12 | 1.83 | 0.60 |
| 15:N:14:THR:HA | 15:N:86:LEU:HD21 | 1.81 | 0.60 |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:HZ3 | 1.65 | 0.60 |
| 3:3:352:GLU:OE2 | 3:3:661:GLN:NE2 | 2.35 | 0.60 |
| 4:4:218:ALA:HA | 4:4:221:VAL:HG22 | 1.82 | 0.60 |
| 7:O:108:CYS:HA | 17:O:202:SF4:S3 | 2.41 | 0.60 |
| 10:P:62:TYR:CD2 | 11:R:66:LEU:HD11 | 2.35 | 0.60 |
| 9:W:31:VAL:HG11 | 9:W:81:LEU:HD13 | 1.83 | 0.60 |
| 12:K:49:TYR:OH | 15:N:156:GLY:O | 2.13 | 0.60 |
| 10:P:65:ALA:O | 10:P:69:ILE:HG23 | 2.01 | 0.60 |
| 10:P:70:LEU:HD13 | 11:R:150:THR:HG22 | 1.83 | 0.60 |
| 4:4:250:LYS:HE2 | 4:4:262:PHE:HB3 | 1.84 | 0.60 |
| 12:K:19:LEU:HD22 | 13:L:591:LEU:HD12 | 1.82 | 0.60 |
| 14:M:16:LEU:HD22 | 14:M:97:GLY:H | 1.67 | 0.60 |
| 15:N:126:ARG:HD2 | 15:N:128:GLN:HG2 | 1.82 | 0.60 |
| 16:Q:222:PRO:HD2 | 16:Q:230:GLY:HA2 | 1.82 | 0.60 |
| 3:D:40:SER:O | 3:D:189:ARG:NE | 2.31 | 0.60 |
| 13:L:432:HIS:CE1 | 13:L:434:HIS:HB2 | 2.36 | 0.60 |
| 15:N:317:ARG:NH1 | 15:N:384:ALA:O | 2.35 | 0.60 |
| 15:V:180:LEU:HD21 | 15:V:228:ALA:HB2 | 1.83 | 0.60 |
| 10:A:65:ALA:O | 10:A:69:ILE:HG23 | 2.02 | 0.60 |
| 13:L:68:LEU:HD23 | 13:L:255:ARG:HH22 | 1.66 | 0.60 |
| 13:L:53:ALA:HB3 | 13:L:69:LEU:HB3 | 1.84 | 0.60 |
| 9:W:51:HIS:ND1 | 9:W:56:ASP:OD1 | 2.35 | 0.60 |
| 1:B:253:GLN:NE2 | 1:B:325:THR:O | 2.35 | 0.60 |
| 14:U:201:PHE:HD2 | 14:U:245:ALA:HB2 | 1.66 | 0.60 |
| 6:G:90:PRO:O | 6:G:93:ARG:HB3 | 2.02 | 0.59 |
| 15:N:279:GLN:HG3 | 15:N:423:LEU:HB2 | 1.83 | 0.59 |
| 3:3:223:SER:O | 3:3:226:ILE:HG12 | 2.02 | 0.59 |
| 7:9:9:SER:O | 7:9:12:ILE:HG13 | 2.01 | 0.59 |
| 3:D:19:VAL:HG22 | 3:D:91:MET:HE3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:65:ALA:HB3 | 11:J:66:LEU:HD13 | 1.84 | 0.59 |
| 13:T:287:GLY:HA3 | 13:T:528:SER:HB2 | 1.83 | 0.59 |
| 3:D:198:GLU:OE2 | 3:D:440:ARG:NH1 | 2.36 | 0.59 |
| 4:4:216:GLU:OE2 | 16:H:304:GLN:NE2 | 2.35 | 0.59 |
| 16:H:96:ALA:HB2 | 16:H:128:VAL:HG21 | 1.83 | 0.59 |
| 13:L:287:GLY:HA3 | 13:L:528:SER:HB2 | 1.84 | 0.59 |
| 13:L:581:LEU:HD23 | 15:N:194:PHE:HE1 | 1.67 | 0.59 |
| 3:D:154:TYR:HB3 | 4:E:322:GLU:HB2 | 1.84 | 0.59 |
| 1:1:10:ASP:OD2 | 1:1:12:ARG:NE | 2.29 | 0.59 |
| 3:D:592:PRO:HA | 3:D:595:GLU:HG2 | 1.83 | 0.59 |
| 16:Q:202:ALA:HA | 16:Q:205:VAL:HG22 | 1.84 | 0.59 |
| 1:1:390:LEU:HA | 1:1:393:LEU:HD12 | 1.83 | 0.59 |
| 3:D:538:ALA:HB3 | 3:D:541:ALA:HB2 | 1.85 | 0.59 |
| 6:G:19:ILE:HG12 | 6:G:20:LEU:H | 1.67 | 0.59 |
| 13:L:153:ASP:OD1 | 14:M:411:GLN:NE2 | 2.22 | 0.59 |
| 14:U:448:GLY:O | 14:U:452:ARG:HG2 | 2.02 | 0.59 |
| 15:V:52:PRO:HB3 | 15:V:103:HIS:HB2 | 1.85 | 0.59 |
| 3:3:523:LEU:HD22 | 3:3:527:ARG:HH21 | 1.67 | 0.59 |
| 7:9:99:ILE:HG22 | 17:9:201:SF4:S3 | 2.42 | 0.59 |
| 1:1:243:THR:HG22 | 1:1:244:GLU:H | 1.68 | 0.59 |
| 5:5:55:LEU:HD23 | 5:5:57:TYR:OH | 2.02 | 0.59 |
| 4:4:64:THR:OG1 | 6:6:83:ARG:HD2 | 2.03 | 0.59 |
| 1:B:201:LEU:HG | 1:B:203:PRO:HD2 | 1.85 | 0.59 |
| 3:D:614:LEU:HD11 | 3:D:624:LEU:HG | 1.83 | 0.59 |
| 16:Q:290:PHE:O | 16:Q:294:ARG:HG2 | 2.03 | 0.59 |
| 1:1:92:ASN:ND2 | 18:1:502:FMN:O3' | 2.32 | 0.59 |
| 2:C:106:ILE:HG22 | 2:C:107:GLY:O | 2.03 | 0.59 |
| 4:E:201:ILE:HA | 4:E:204:TYR:HD2 | 1.68 | 0.59 |
| 11:J:146:LEU:HD23 | 12:K:66:ALA:HB2 | 1.85 | 0.59 |
| 5:F:151:PRO:HD3 | 9:X:112:LYS:HE2 | 1.83 | 0.59 |
| 3:3:369:LEU:HD12 | 3:3:369:LEU:O | 2.03 | 0.58 |
| 3:D:94:ASP:OD2 | 3:D:97:SER:OG | 2.18 | 0.58 |
| 4:E:185:GLU:OE2 | 7:O:165:TYR:OH | 2.13 | 0.58 |
| 4:E:26:MET:N | 4:E:47:LEU:O | 2.36 | 0.58 |
| 5:F:175:THR:HG22 | 5:F:178:ASP:HB2 | 1.83 | 0.58 |
| 16:H:302:TYR:HA | 16:H:305:LEU:HB3 | 1.86 | 0.58 |
| 3:3:81:ALA:O | 3:3:85:THR:OG1 | 2.10 | 0.58 |
| 1:B:249:MET:HA | 1:B:267:PRO:HA | 1.85 | 0.58 |
| 16:H:225:GLU:HB3 | 16:H:226:GLN:HG2 | 1.85 | 0.58 |
| 16:H:227:GLU:HG2 | 16:H:228:LEU:H | 1.67 | 0.58 |
| 14:M:109:LEU:HD21 | 14:M:236:VAL:HG21 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:M:22:ARG:HG3 | 14:M:92:GLU:OE1 | 2.02 | 0.58 |
| 16:Q:137:PHE:HA | 16:Q:152:SER:HB2 | 1.83 | 0.58 |
| 4:E:148:TYR:OH | 16:Q:42:PHE:O | 2.13 | 0.58 |
| 1:1:312:SER:OG | 1:1:315:HIS:ND1 | 2.22 | 0.58 |
| 4:4:87:TYR:CB | 6:6:45:CYS:HB3 | 2.34 | 0.58 |
| 8:7:74:PRO:HG2 | 8:7:77:ALA:HB2 | 1.85 | 0.58 |
| 3:D:690:GLY:HA2 | 3:D:770:ARG:HB3 | 1.84 | 0.58 |
| 16:H:274:VAL:HG12 | 16:H:278:TRP:CD1 | 2.37 | 0.58 |
| 14:M:128:PRO:O | 14:M:132:MET:HG2 | 2.03 | 0.58 |
| 16:Q:227:GLU:HG2 | 16:Q:228:LEU:H | 1.67 | 0.58 |
| 13:T:255:ARG:HA | 13:T:477:LEU:HD23 | 1.85 | 0.58 |
| 14:U:232:THR:HG21 | 14:U:322:THR:HB | 1.86 | 0.58 |
| 15:V:132:ALA:HB1 | 15:V:199:VAL:HA | 1.85 | 0.58 |
| 2:2:110:GLU:HA | 8:7:121:ARG:HH12 | 1.68 | 0.58 |
| 5:F:28:VAL:HA | 5:F:91:ARG:O | 2.04 | 0.58 |
| 13:L:278:ALA:HB1 | 13:L:409:VAL:HG11 | 1.83 | 0.58 |
| 16:Q:168:LEU:HD23 | 16:Q:171:LEU:HD12 | 1.86 | 0.58 |
| 13:T:147:LYS:NZ | 14:U:349:GLN:OE1 | 2.33 | 0.58 |
| 3:D:297:GLY:O | 3:D:300:TRP:NE1 | 2.36 | 0.58 |
| 11:J:104:LEU:HD23 | 15:N:174:LEU:HD21 | 1.85 | 0.58 |
| 16:Q:71:ASP:OD1 | 16:Q:240:LYS:NZ | 2.23 | 0.58 |
| 6:G:69:ARG:NH2 | 16:Q:223:GLU:OE2 | 2.32 | 0.58 |
| 16:H:190:LYS:HB2 | 16:H:268:THR:HG21 | 1.86 | 0.58 |
| 11:J:152:VAL:HG13 | 15:N:120:ALA:HB2 | 1.85 | 0.58 |
| 11:J:69:PHE:O | 11:J:73:LEU:HG | 2.04 | 0.58 |
| 13:L:104:PHE:CE2 | 13:L:108:PHE:CE2 | 2.91 | 0.58 |
| 10:A:113:LYS:NZ | 15:N:83:GLU:OE2 | 2.34 | 0.58 |
| 6:G:163:TYR:HD1 | 7:O:152:ARG:HD2 | 1.69 | 0.58 |
| 10:P:63:VAL:HG11 | 10:P:115:VAL:HG21 | 1.84 | 0.58 |
| 16:Q:352:VAL:HG12 | 16:Q:353:LEU:HD12 | 1.85 | 0.58 |
| 10:P:13:TYR:CZ | 16:Q:95:LEU:HA | 2.38 | 0.58 |
| 13:L:355:LEU:HB3 | 13:L:359:LEU:HD12 | 1.85 | 0.58 |
| 1:1:118:MET:HG2 | 1:1:224:LEU:HD13 | 1.84 | 0.58 |
| 1:B:195:LEU:HD23 | 2:C:24:ARG:NH1 | 2.18 | 0.58 |
| 3:D:247:TRP:HE1 | 7:O:61:ALA:HB2 | 1.68 | 0.58 |
| 16:Q:159:LEU:O | 16:Q:163:GLU:HB2 | 2.02 | 0.58 |
| 14:U:201:PHE:CD2 | 14:U:245:ALA:HB2 | 2.39 | 0.58 |
| 4:4:172:TYR:OH | 4:4:180:GLU:O | 2.13 | 0.58 |
| 10:A:62:TYR:CD2 | 11:J:66:LEU:HD11 | 2.39 | 0.58 |
| 3:D:268:ASP:OD2 | 3:D:278:ARG:NH1 | 2.30 | 0.58 |
| 3:D:415:GLU:HG2 | 3:D:418:ARG:HH21 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:150:LEU:HD22 | 16:H:228:LEU:HD12 | 1.85 | 0.58 |
| 9:W:102:LEU:O | 9:W:110:LEU:HD13 | 2.04 | 0.58 |
| 4:4:77:GLN:O | 4:4:80:THR:OG1 | 2.16 | 0.58 |
| 5:5:33:ARG:NH1 | 5:5:36:GLU:OE2 | 2.37 | 0.58 |
| 16:H:147:TYR:HD1 | 16:H:229:VAL:HG22 | 1.69 | 0.58 |
| 13:L:463:HIS:CE1 | 13:L:487:LEU:HD22 | 2.38 | 0.58 |
| 11:J:85:PRO:O | 13:L:587:ARG:NH2 | 2.34 | 0.58 |
| 14:M:206:PRO:HG3 | 14:M:214:LEU:HD22 | 1.85 | 0.58 |
| 16:Q:265:GLY:O | 16:Q:282:LYS:NZ | 2.25 | 0.58 |
| 4:4:62:LEU:HD11 | 6:6:43:LEU:O | 2.04 | 0.57 |
| 3:D:285:VAL:HG13 | 3:D:286:ASN:H | 1.69 | 0.57 |
| 3:D:363:ALA:HB1 | 3:D:650:VAL:HG11 | 1.86 | 0.57 |
| 7:O:69:TYR:HE1 | 7:O:71:GLU:HG3 | 1.68 | 0.57 |
| 13:T:267:SER:HB3 | 13:T:311:GLY:O | 2.04 | 0.57 |
| 13:T:380:SER:HB3 | 13:T:456:ALA:HB3 | 1.86 | 0.57 |
| 9:W:90:TYR:HB3 | 9:W:118:ALA:HB1 | 1.86 | 0.57 |
| 16:H:292:TRP:O | 16:H:296:THR:OG1 | 2.08 | 0.57 |
| 13:L:88:HIS:O | 13:L:92:ILE:HG13 | 2.03 | 0.57 |
| 10:P:2:ALA:HB3 | 16:Q:119:ASP:OD2 | 2.04 | 0.57 |
| 15:V:98:LEU:HD12 | 15:V:107:MET:HG2 | 1.87 | 0.57 |
| 3:3:274:LEU:H | 3:3:302:ASP:HB3 | 1.69 | 0.57 |
| 4:4:30:VAL:HB | 4:4:43:LEU:HB2 | 1.84 | 0.57 |
| 4:E:272:VAL:HG13 | 4:E:399:SER:HB3 | 1.86 | 0.57 |
| 8:I:13:TRP:CE3 | 8:I:72:VAL:HB | 2.38 | 0.57 |
| 14:M:264:ALA:HB1 | 14:M:294:GLY:O | 2.04 | 0.57 |
| 14:M:29:ALA:HB1 | 14:M:83:PHE:HA | 1.87 | 0.57 |
| 7:O:164:PRO:HA | 7:O:178:GLU:HB2 | 1.86 | 0.57 |
| 7:O:59:CYS:SG | 7:O:91:TYR:OH | 2.59 | 0.57 |
| 9:W:87:ARG:HH12 | 10:A:38:ARG:HH12 | 1.52 | 0.57 |
| 1:1:17:LEU:HD22 | 1:1:113:LEU:HD21 | 1.87 | 0.57 |
| 4:4:218:ALA:HB1 | 4:4:272:VAL:HB | 1.87 | 0.57 |
| 8:7:105:THR:OG1 | 8:7:114:ARG:NH2 | 2.35 | 0.57 |
| 3:D:656:LEU:HD11 | 9:X:3:ARG:HD3 | 1.86 | 0.57 |
| 3:D:152:PRO:HD3 | 4:E:305:PRO:HB2 | 1.86 | 0.57 |
| 13:L:291:ILE:HD12 | 13:L:336:SER:HB3 | 1.87 | 0.57 |
| 16:Q:54:PHE:HB3 | 16:Q:56:LEU:HD23 | 1.86 | 0.57 |
| 13:T:433:HIS:ND1 | 13:T:433:HIS:O | 2.38 | 0.57 |
| 4:4:336:HIS:HE1 | 5:5:174:LEU:HD12 | 1.68 | 0.57 |
| 7:9:71:GLU:HB2 | 7:9:90:VAL:HB | 1.86 | 0.57 |
| 2:C:9:ASP:OD1 | 2:C:9:ASP:N | 2.37 | 0.57 |
| 16:Q:150:LEU:HD21 | 16:Q:154:ARG:HH11 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:226:GLN:HB2 | 16:Q:299:ARG:HH22 | 1.70 | 0.57 |
| 8:7:44:MET:HE2 | 8:7:46:ARG:HH22 | 1.69 | 0.57 |
| 10:A:83:VAL:HG23 | 10:A:84:SER:N | 2.20 | 0.57 |
| 3:D:614:LEU:O | 3:D:621:VAL:HA | 2.04 | 0.57 |
| 13:L:433:HIS:O | 13:L:433:HIS:ND1 | 2.37 | 0.57 |
| 16:Q:17:ALA:O | 16:Q:21:VAL:HG23 | 2.05 | 0.57 |
| 3:3:664:LEU:O | 3:3:669:VAL:HG12 | 2.03 | 0.57 |
| 4:4:140:LEU:HD21 | 4:4:217:ARG:NH1 | 2.19 | 0.57 |
| 6:6:102:PRO:HD3 | 10:A:33:PRO:HG2 | 1.87 | 0.57 |
| 6:6:155:GLN:O | 6:6:159:ARG:HG3 | 2.04 | 0.57 |
| 3:D:131:GLN:HG2 | 4:E:325:ILE:HG23 | 1.85 | 0.57 |
| 3:D:678:PHE:CZ | 3:D:680:LEU:HD13 | 2.39 | 0.57 |
| 4:E:224:ILE:HB | 4:E:270:GLY:HA3 | 1.86 | 0.57 |
| 7:O:71:GLU:HB2 | 7:O:90:VAL:HB | 1.85 | 0.57 |
| 16:Q:150:LEU:HD23 | 16:Q:154:ARG:HD2 | 1.87 | 0.57 |
| 15:V:63:THR:HG22 | 15:V:96:HIS:HA | 1.87 | 0.57 |
| 1:1:72:THR:HG21 | 1:1:223:THR:HG21 | 1.85 | 0.57 |
| 7:9:108:CYS:SG | 7:9:112:ALA:N | 2.78 | 0.57 |
| 7:9:162:VAL:HA | 7:9:176:PRO:HG2 | 1.87 | 0.57 |
| 4:E:171:ASN:OD1 | 4:E:174:ARG:NH1 | 2.33 | 0.57 |
| 14:M:232:THR:HA | 14:M:235:LYS:HZ2 | 1.70 | 0.57 |
| 10:P:6:GLU:OE2 | 16:Q:2:THR:OG1 | 2.16 | 0.57 |
| 3:D:185:LYS:O | 3:D:189:ARG:HB2 | 2.05 | 0.57 |
| 6:G:148:ILE:O | 6:G:151:VAL:HG22 | 2.04 | 0.57 |
| 16:H:159:LEU:O | 16:H:163:GLU:HB2 | 2.04 | 0.57 |
| 13:T:187:GLU:HA | 13:T:190:GLU:HG2 | 1.85 | 0.57 |
| 11:J:19:VAL:O | 12:K:21:ARG:NH2 | 2.33 | 0.57 |
| 16:Q:25:LEU:O | 16:Q:28:PHE:CD1 | 2.58 | 0.57 |
| 16:H:39:LEU:O | 16:H:43:GLN:HG2 | 2.04 | 0.56 |
| 14:M:402:SER:HA | 14:M:405:TYR:CE2 | 2.40 | 0.56 |
| 11:R:72:MET:HE3 | 16:Q:149:LEU:HD21 | 1.85 | 0.56 |
| 16:Q:221:LEU:N | 16:Q:222:PRO:HA | 2.19 | 0.56 |
| 14:U:91:VAL:HG23 | 14:U:92:GLU:H | 1.69 | 0.56 |
| 4:E:30:VAL:HB | 4:E:43:LEU:HB2 | 1.86 | 0.56 |
| 11:J:75:PHE:CZ | 11:J:78:GLN:HG2 | 2.40 | 0.56 |
| 13:T:601:LEU:HD21 | 15:V:178:LEU:HD21 | 1.87 | 0.56 |
| 9:X:34:ILE:HA | 9:X:92:ALA:HB3 | 1.86 | 0.56 |
| 1:B:222:GLU:HG3 | 1:B:251:LEU:HD22 | 1.86 | 0.56 |
| 14:M:17:LEU:HD21 | 14:M:98:LEU:HG | 1.87 | 0.56 |
| 7:O:59:CYS:HB2 | 7:O:104:CYS:HB3 | 1.88 | 0.56 |
| 14:U:346:GLY:HA3 | 14:U:418:GLY:HA2 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:285:VAL:HG13 | 3:3:286:ASN:H | 1.71 | 0.56 |
| 6:6:164:ASN:HD21 | 6:6:168:GLU:HB2 | 1.70 | 0.56 |
| 13:L:187:GLU:HA | 13:L:190:GLU:HG2 | 1.87 | 0.56 |
| 1:1:41:ALA:HB2 | 1:1:116:GLU:HG3 | 1.86 | 0.56 |
| 4:4:337:PRO:O | 4:4:361:GLY:HA2 | 2.06 | 0.56 |
| 15:N:245:ASN:ND2 | 15:N:367:THR:HB | 2.21 | 0.56 |
| 15:V:201:GLN:HA | 15:V:255:LYS:HE3 | 1.88 | 0.56 |
| 3:3:269:THR:HG21 | 3:3:629:ILE:HG12 | 1.88 | 0.56 |
| 6:6:19:ILE:HG12 | 6:6:20:LEU:H | 1.70 | 0.56 |
| 3:D:373:GLY:HA3 | 3:D:538:ALA:HB2 | 1.88 | 0.56 |
| 13:L:293:LYS:O | 13:L:297:TYR:HD1 | 1.89 | 0.56 |
| 3:3:31:PRO:HG3 | 3:3:137:TYR:CD2 | 2.40 | 0.56 |
| 10:A:33:PRO:HD2 | 16:H:70:GLU:HB2 | 1.87 | 0.56 |
| 3:D:370:ASP:OD2 | 3:D:558:TRP:HD1 | 1.89 | 0.56 |
| 4:E:174:ARG:N | 4:E:177:GLY:O | 2.34 | 0.56 |
| 16:H:291:ILE:HA | 16:H:294:ARG:HG3 | 1.87 | 0.56 |
| 13:L:87:ILE:HD12 | 13:L:239:LEU:HD13 | 1.88 | 0.56 |
| 4:E:336:HIS:HB2 | 5:F:189:ARG:HA | 1.88 | 0.56 |
| 4:E:341:GLU:OE1 | 4:E:356:TYR:OH | 2.24 | 0.56 |
| 13:T:240:ILE:HG22 | 13:T:241:HIS:HD2 | 1.71 | 0.56 |
| 13:T:60:LEU:HD21 | 14:U:375:PRO:HB3 | 1.87 | 0.56 |
| 1:1:6:LEU:HB2 | 1:1:241:MET:HA | 1.88 | 0.56 |
| 4:4:341:GLU:HG2 | 4:4:358:VAL:HG22 | 1.88 | 0.56 |
| 3:D:19:VAL:HG11 | 3:D:50:VAL:HG21 | 1.88 | 0.56 |
| 16:H:8:ASP:OD2 | 16:H:112:GLN:HB2 | 2.06 | 0.56 |
| 16:Q:205:VAL:HG21 | 16:Q:317:ALA:HB2 | 1.86 | 0.56 |
| 14:U:122:PHE:O | 14:U:234:TYR:OH | 2.21 | 0.56 |
| 18:1:502:FMN:H1'1 | 19:1:503:NAI:H52N | 1.88 | 0.56 |
| 4:4:314:ARG:NH2 | 8:7:44:MET:SD | 2.78 | 0.56 |
| 2:C:146:THR:HG23 | 2:C:149:ARG:H | 1.71 | 0.56 |
| 3:D:616:ASN:HD22 | 3:D:622:LEU:HD11 | 1.70 | 0.56 |
| 16:Q:219:PHE:HB3 | 16:Q:299:ARG:HG2 | 1.87 | 0.56 |
| 15:N:168:GLU:HG2 | 15:N:169:GLY:H | 1.71 | 0.55 |
| 7:O:6:LEU:HD23 | 16:Q:297:TRP:CE2 | 2.41 | 0.55 |
| 14:U:194:PHE:HB2 | 14:U:249:ALA:HB3 | 1.87 | 0.55 |
| 3:3:558:TRP:HB2 | 3:3:570:PHE:CZ | 2.40 | 0.55 |
| 1:B:293:GLY:O | 1:B:327:GLY:N | 2.39 | 0.55 |
| 3:D:43:GLY:HA2 | 20:D:804:FES:S1 | 2.46 | 0.55 |
| 10:P:57:PHE:HB3 | 10:P:58:PRO:HD2 | 1.88 | 0.55 |
| 13:T:115:MET:HG2 | 13:T:244:THR:HG22 | 1.88 | 0.55 |
| 2:2:85:THR:HG22 | 2:2:86:LEU:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:99:PRO:HB2 | 5:5:124:ILE:HA | 1.87 | 0.55 |
| 1:B:184:GLU:HB3 | 1:B:187:ALA:HB3 | 1.89 | 0.55 |
| 3:D:466:GLU:HB2 | 3:D:489:MET:HG3 | 1.87 | 0.55 |
| 4:E:201:ILE:HA | 4:E:204:TYR:CD2 | 2.42 | 0.55 |
| 8:I:104:VAL:HG12 | 8:I:109:PRO:HA | 1.88 | 0.55 |
| 11:J:64:VAL:HA | 11:J:67:PHE:HB2 | 1.86 | 0.55 |
| 14:M:126:LEU:HD11 | 14:M:149:VAL:HG13 | 1.89 | 0.55 |
| 16:Q:16:LYS:HB3 | 16:Q:115:VAL:HG22 | 1.89 | 0.55 |
| 16:Q:35:GLU:OE2 | 16:Q:294:ARG:NE | 2.32 | 0.55 |
| 16:Q:48:PRO:C | 16:Q:50:ARG:H | 2.10 | 0.55 |
| 14:U:54:PRO:HA | 14:U:62:TYR:HD1 | 1.70 | 0.55 |
| 7:9:149:GLU:O | 7:9:153:THR:OG1 | 2.18 | 0.55 |
| 14:U:41:LEU:O | 14:U:42:THR:HG22 | 2.05 | 0.55 |
| 2:2:9:ASP:OD1 | 2:2:9:ASP:N | 2.36 | 0.55 |
| 3:3:343:LEU:HD12 | 3:3:361:ALA:HB2 | 1.89 | 0.55 |
| 3:3:459:MET:HG2 | 3:3:465:HIS:HB2 | 1.89 | 0.55 |
| 3:D:248:GLU:HG2 | 5:F:170:PHE:CE1 | 2.42 | 0.55 |
| 16:H:133:VAL:HG11 | 16:H:160:ILE:HG13 | 1.88 | 0.55 |
| 12:K:7:SER:O | 12:K:37:ALA:HB1 | 2.07 | 0.55 |
| 2:2:87:SER:HB2 | 20:2:201:FES:S2 | 2.47 | 0.55 |
| 5:5:75:VAL:HG13 | 5:5:87:ARG:HB2 | 1.88 | 0.55 |
| 4:E:53:LEU:O | 4:E:386:LYS:HG3 | 2.07 | 0.55 |
| 13:L:139:PHE:HA | 13:L:155:ALA:HB1 | 1.89 | 0.55 |
| 13:T:213:ALA:HB2 | 13:T:252:LEU:HD23 | 1.88 | 0.55 |
| 13:T:325:HIS:CD2 | 13:T:329:LYS:HG3 | 2.41 | 0.55 |
| 1:1:160:LYS:O | 1:1:168:SER:OG | 2.10 | 0.55 |
| 1:1:373:LYS:HD3 | 1:1:383:ASP:OD2 | 2.07 | 0.55 |
| 3:3:131:GLN:HG2 | 4:4:325:ILE:HG23 | 1.87 | 0.55 |
| 3:3:305:ARG:NH2 | 3:3:605:PRO:HA | 2.20 | 0.55 |
| 3:3:297:GLY:O | 3:3:703:GLN:NE2 | 2.38 | 0.55 |
| 4:4:363:SER:HB2 | 5:5:174:LEU:H | 1.72 | 0.55 |
| 4:E:163:VAL:HG13 | 4:E:164:THR:HG23 | 1.88 | 0.55 |
| 15:V:79:SER:O | 15:V:85:TYR:OH | 2.14 | 0.55 |
| 5:5:164:TYR:HB3 | 9:W:37:TRP:HZ3 | 1.71 | 0.55 |
| 3:3:391:LEU:HD12 | 3:3:422:PRO:HG3 | 1.88 | 0.55 |
| 8:7:104:VAL:HG12 | 8:7:109:PRO:HA | 1.88 | 0.55 |
| 8:7:63:LEU:HD22 | 8:7:128:PHE:HB2 | 1.88 | 0.55 |
| 6:6:117:MET:CE | 7:9:99:ILE:HG12 | 2.37 | 0.55 |
| 3:D:293:ALA:HB2 | 3:D:698:MET:HG2 | 1.89 | 0.55 |
| 3:D:34:CYS:HB2 | 3:D:44:ALA:HB3 | 1.89 | 0.55 |
| 4:E:159:LEU:O | 4:E:163:VAL:HG12 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:L:124:TYR:HH | 13:L:256:SER:HG | 1.52 | 0.55 |
| 14:U:332:LEU:HA | 14:U:335:ARG:HG2 | 1.89 | 0.55 |
| 13:T:156:ARG:HG3 | 14:U:407:LEU:HB3 | 1.89 | 0.55 |
| 1:1:8:GLY:HA2 | 1:1:270:THR:HG22 | 1.89 | 0.55 |
| 1:B:18:TYR:N | 1:B:265:GLU:OE1 | 2.33 | 0.55 |
| 1:B:26:SER:HA | 1:B:31:TYR:CG | 2.42 | 0.55 |
| 1:B:291:ILE:HG12 | 1:B:299:PRO:HB3 | 1.88 | 0.55 |
| 3:D:419:ASP:OD1 | 3:D:447:LYS:NZ | 2.23 | 0.55 |
| 5:F:2:ARG:HG3 | 5:F:84:ASP:OD2 | 2.06 | 0.55 |
| 13:L:392:THR:HG22 | 13:L:399:GLY:HA3 | 1.89 | 0.55 |
| 13:L:490:GLU:HG3 | 13:L:491:TRP:N | 2.21 | 0.55 |
| 13:T:325:HIS:NE2 | 13:T:329:LYS:HG3 | 2.22 | 0.55 |
| 4:4:98:ALA:O | 4:4:102:GLU:HG3 | 2.07 | 0.55 |
| 4:4:60:GLY:N | 4:4:408:ASP:OD1 | 2.36 | 0.55 |
| 4:E:87:TYR:CB | 6:G:45:CYS:HB3 | 2.37 | 0.55 |
| 13:L:356:TRP:O | 13:L:363:ARG:HD3 | 2.07 | 0.55 |
| 14:M:332:LEU:O | 14:M:336:THR:OG1 | 2.11 | 0.55 |
| 16:Q:43:GLN:HE21 | 16:Q:45:ARG:NH2 | 2.05 | 0.55 |
| 13:T:312:VAL:HA | 13:T:397:PHE:HD2 | 1.72 | 0.55 |
| 13:T:9:LEU:HB2 | 13:T:10:PRO:HD3 | 1.89 | 0.55 |
| 3:3:166:LYS:NZ | 3:3:179:GLU:OE1 | 2.36 | 0.54 |
| 4:4:88:LEU:HD21 | 6:6:48:ILE:HD13 | 1.88 | 0.54 |
| 3:D:228:ASP:OD2 | 3:D:295:ARG:NH2 | 2.28 | 0.54 |
| 3:D:269:THR:HG22 | 3:D:274:LEU:HA | 1.88 | 0.54 |
| 13:L:223:MET:HE3 | 13:L:534:VAL:HG11 | 1.88 | 0.54 |
| 14:M:357:LEU:HD22 | 14:M:433:ALA:HB2 | 1.89 | 0.54 |
| 1:1:184:GLU:HG2 | 18:1:502:FMN:HM82 | 1.88 | 0.54 |
| 3:3:33:PHE:HB2 | 3:3:45:CYS:SG | 2.46 | 0.54 |
| 6:6:145:GLU:HG2 | 7:9:31:VAL:HG21 | 1.89 | 0.54 |
| 10:A:7:TYR:HD2 | 11:J:44:VAL:HG11 | 1.72 | 0.54 |
| 11:R:64:VAL:HG13 | 16:Q:134:TYR:OH | 2.07 | 0.54 |
| 16:Q:71:ASP:HB2 | 16:Q:238:SER:HB3 | 1.89 | 0.54 |
| 11:R:50:PHE:O | 11:R:54:ILE:HG12 | 2.07 | 0.54 |
| 4:4:144:THR:HG22 | 4:4:148:TYR:CE1 | 2.42 | 0.54 |
| 4:4:341:GLU:OE1 | 4:4:356:TYR:OH | 2.16 | 0.54 |
| 1:B:153:ARG:NH2 | 1:B:171:LEU:O | 2.40 | 0.54 |
| 1:B:177:ALA:HA | 2:C:32:ARG:NH2 | 2.22 | 0.54 |
| 4:E:140:LEU:HD11 | 4:E:217:ARG:HH12 | 1.72 | 0.54 |
| 4:E:200:ARG:NH1 | 4:E:203:GLU:OE1 | 2.40 | 0.54 |
| 4:E:224:ILE:HD11 | 4:E:275:ARG:CZ | 2.37 | 0.54 |
| 8:I:23:TYR:OH | 8:I:123:ARG:NH1 | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:101:ALA:HB2 | 12:K:12:ALA:HB2 | 1.89 | 0.54 |
| 14:U:331:ARG:NH1 | 14:U:334:GLU:OE1 | 2.41 | 0.54 |
| 4:E:64:THR:OG1 | 6:G:83:ARG:HD2 | 2.08 | 0.54 |
| 14:M:21:PRO:HD2 | 14:M:24:LEU:HG | 1.90 | 0.54 |
| 10:P:9:GLY:HA2 | 16:Q:13:VAL:HG11 | 1.88 | 0.54 |
| 15:V:62:PHE:CE2 | 15:V:285:LEU:HD22 | 2.42 | 0.54 |
| 4:4:205:GLU:OE1 | 4:4:284:ARG:NH2 | 2.37 | 0.54 |
| 6:6:162:ALA:HB1 | 7:9:124:TYR:CZ | 2.43 | 0.54 |
| 3:D:413:LEU:O | 3:D:417:VAL:HG23 | 2.07 | 0.54 |
| 3:D:8:ASP:OD1 | 3:D:9:ARG:HG3 | 2.06 | 0.54 |
| 7:9:10:LEU:HA | 16:H:296:THR:HG21 | 1.89 | 0.54 |
| 8:I:13:TRP:CD2 | 8:I:72:VAL:HB | 2.43 | 0.54 |
| 4:E:144:THR:OG1 | 16:Q:295:ALA:O | 2.24 | 0.54 |
| 11:R:119:LEU:HD11 | 12:S:47:ARG:HA | 1.88 | 0.54 |
| 15:V:204:PRO:O | 15:V:208:VAL:HG23 | 2.07 | 0.54 |
| 15:V:62:PHE:HE2 | 15:V:285:LEU:HD22 | 1.72 | 0.54 |
| 12:K:78:ILE:HG12 | 15:N:130:LEU:HD22 | 1.89 | 0.54 |
| 16:Q:122:ILE:HG13 | 16:Q:123:LEU:HD12 | 1.89 | 0.54 |
| 11:R:101:ALA:HB2 | 12:S:12:ALA:HB2 | 1.88 | 0.54 |
| 9:W:6:MET:HG3 | 9:W:9:ALA:HB3 | 1.90 | 0.54 |
| 14:U:7:LEU:O | 14:U:11:VAL:HG12 | 2.08 | 0.54 |
| 1:1:201:LEU:HG | 1:1:203:PRO:HD2 | 1.89 | 0.54 |
| 4:4:162:TRP:CE2 | 7:9:34:LYS:HD2 | 2.43 | 0.54 |
| 3:D:18:SER:HB3 | 3:D:21:ASP:OD2 | 2.07 | 0.54 |
| 16:H:143:SER:HB2 | 16:H:235:GLU:HG3 | 1.89 | 0.54 |
| 13:L:240:ILE:HG22 | 13:L:241:HIS:HD2 | 1.72 | 0.54 |
| 14:M:304:THR:O | 14:M:307:GLY:N | 2.40 | 0.54 |
| 13:L:129:ILE:HG12 | 14:M:369:PRO:HB2 | 1.90 | 0.54 |
| 1:B:203:PRO:HB2 | 1:B:204:PRO:HD3 | 1.90 | 0.54 |
| 3:D:31:PRO:HG3 | 3:D:137:TYR:CD2 | 2.43 | 0.54 |
| 16:H:290:PHE:O | 16:H:294:ARG:HG2 | 2.06 | 0.54 |
| 15:N:56:ASP:OD1 | 15:N:225:ARG:NH1 | 2.41 | 0.54 |
| 7:O:17:LEU:HD12 | 16:Q:42:PHE:CE1 | 2.43 | 0.54 |
| 3:3:713:ARG:HH21 | 3:3:746:ARG:HH21 | 1.56 | 0.54 |
| 3:D:459:MET:HG2 | 3:D:465:HIS:HB2 | 1.89 | 0.54 |
| 4:E:185:GLU:O | 4:E:189:GLU:HG2 | 2.08 | 0.54 |
| 16:Q:267:TRP:CG | 16:Q:268:THR:N | 2.76 | 0.54 |
| 2:2:35:GLN:NE2 | 2:2:35:GLN:C | 2.62 | 0.53 |
| 4:4:26:MET:N | 4:4:47:LEU:O | 2.41 | 0.53 |
| 4:4:278:VAL:O | 4:4:282:GLU:HG3 | 2.08 | 0.53 |
| 5:5:80:TRP:CE3 | 5:5:80:TRP:HA | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:4:32:PRO:HB2 | 6:6:88:MET:HE1 | 1.90 | 0.53 |
| 7:9:6:LEU:HB3 | 16:H:297:TRP:CZ2 | 2.42 | 0.53 |
| 4:4:28:LEU:HD12 | 10:A:51:ALA:HA | 1.90 | 0.53 |
| 5:F:53:VAL:HG13 | 5:F:71:VAL:HB | 1.90 | 0.53 |
| 5:F:31:ARG:NH2 | 5:F:98:ASP:OD2 | 2.41 | 0.53 |
| 11:R:19:VAL:HG23 | 11:R:28:ALA:O | 2.07 | 0.53 |
| 14:U:43:HIS:NE2 | 14:U:45:GLY:O | 2.41 | 0.53 |
| 3:3:728:LEU:HB3 | 3:3:747:VAL:HG11 | 1.90 | 0.53 |
| 4:4:379:GLN:NE2 | 5:5:110:SER:O | 2.35 | 0.53 |
| 10:A:83:VAL:HG23 | 10:A:84:SER:H | 1.74 | 0.53 |
| 16:Q:52:GLY:HA3 | 16:Q:55:GLY:N | 2.23 | 0.53 |
| 14:U:402:SER:HA | 14:U:405:TYR:CE2 | 2.43 | 0.53 |
| 3:3:347:HIS:CD2 | 3:3:765:PRO:HG3 | 2.44 | 0.53 |
| 2:C:88:CYS:HA | 2:C:131:ALA:HB1 | 1.90 | 0.53 |
| 3:D:126:GLY:O | 4:E:329:LYS:NZ | 2.41 | 0.53 |
| 1:1:250:LYS:NZ | 1:1:325:THR:O | 2.41 | 0.53 |
| 3:3:194:VAL:HG12 | 3:3:411:LEU:HD22 | 1.90 | 0.53 |
| 10:P:44:TYR:HB3 | 10:P:50:PRO:HB3 | 1.90 | 0.53 |
| 14:U:313:TYR:OH | 14:U:443:MET:O | 2.22 | 0.53 |
| 3:3:661:GLN:NE2 | 3:3:664:LEU:HD12 | 2.23 | 0.53 |
| 4:E:86:ASP:HB2 | 4:E:406:ASP:OD2 | 2.09 | 0.53 |
| 4:E:68:LYS:HG3 | 5:F:152:LEU:HD13 | 1.90 | 0.53 |
| 11:J:69:PHE:HZ | 16:H:156:SER:HG | 1.56 | 0.53 |
| 11:J:29:ALA:O | 11:J:33:ILE:HG13 | 2.08 | 0.53 |
| 7:O:11:GLY:O | 7:O:15:LYS:HG3 | 2.09 | 0.53 |
| 11:R:102:GLY:O | 11:R:106:ALA:N | 2.38 | 0.53 |
| 15:V:251:GLN:OE1 | 15:V:256:ARG:HD3 | 2.08 | 0.53 |
| 15:V:294:LEU:HG | 15:V:402:VAL:HG13 | 1.89 | 0.53 |
| 1:1:75:LYS:NZ | 1:1:218:ILE:O | 2.32 | 0.53 |
| 2:2:107:GLY:H | 2:2:110:GLU:HG3 | 1.73 | 0.53 |
| 3:3:405:GLU:OE1 | 3:3:509:ALA:N | 2.42 | 0.53 |
| 3:3:544:LEU:HD22 | 3:3:549:VAL:HG21 | 1.90 | 0.53 |
| 3:3:621:VAL:HG23 | 3:3:672:ALA:HA | 1.91 | 0.53 |
| 3:3:85:THR:HG22 | 3:3:86:ALA:O | 2.08 | 0.53 |
| 4:4:68:LYS:HG3 | 5:5:152:LEU:HD13 | 1.91 | 0.53 |
| 6:G:61:ALA:HB1 | 6:G:66:GLU:OE1 | 2.08 | 0.53 |
| 16:H:127:ALA:O | 16:H:131:LEU:HG | 2.08 | 0.53 |
| 10:A:57:PHE:HE2 | 16:H:149:LEU:HD13 | 1.74 | 0.53 |
| 2:C:74:PRO:HD3 | 8:I:125:ALA:HB2 | 1.89 | 0.53 |
| 1:B:160:LYS:O | 1:B:168:SER:OG | 2.18 | 0.53 |
| 8:I:22:GLU:HG2 | 8:I:116:PHE:HZ | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:M:235:LYS:HD3 | 14:M:293:MET:HG3 | 1.90 | 0.53 |
| 13:T:539:ASN:HA | 13:T:543:VAL:HB | 1.89 | 0.53 |
| 14:U:56:LEU:HB2 | 14:U:61:VAL:HB | 1.91 | 0.53 |
| 15:V:2:THR:HG23 | 15:V:36:ALA:HB1 | 1.90 | 0.53 |
| 15:V:345:LYS:NZ | 15:V:368:SER:OG | 2.42 | 0.53 |
| 3:3:42:ILE:O | 3:3:42:ILE:CD1 | 2.48 | 0.53 |
| 3:3:42:ILE:HD13 | 3:3:44:ALA:HB2 | 1.91 | 0.53 |
| 6:6:138:PRO:HG2 | 7:9:121:MET:HG3 | 1.90 | 0.53 |
| 1:B:292:PRO:HG3 | 1:B:316:LEU:HD22 | 1.91 | 0.53 |
| 3:D:326:PHE:CZ | 3:D:330:LYS:HE3 | 2.43 | 0.53 |
| 6:G:99:MET:HB3 | 6:G:103:LYS:HD3 | 1.90 | 0.53 |
| 16:H:186:VAL:HG11 | 16:H:267:TRP:CZ3 | 2.44 | 0.53 |
| 14:M:41:LEU:O | 14:M:42:THR:HG22 | 2.08 | 0.53 |
| 12:S:19:LEU:HD22 | 13:T:591:LEU:HD12 | 1.90 | 0.53 |
| 14:U:346:GLY:O | 14:U:349:GLN:HG2 | 2.07 | 0.53 |
| 3:3:463:ALA:O | 3:3:465:HIS:ND1 | 2.31 | 0.53 |
| 3:D:123:ASP:OD2 | 3:D:241:ARG:HA | 2.08 | 0.53 |
| 3:D:474:ARG:HB3 | 3:D:514:ASP:OD2 | 2.09 | 0.53 |
| 11:J:75:PHE:HZ | 11:J:78:GLN:HG2 | 1.74 | 0.53 |
| 1:1:152:ALA:HB1 | 1:1:157:TYR:HB2 | 1.90 | 0.53 |
| 6:G:66:GLU:HG2 | 16:Q:36:ARG:HD3 | 1.90 | 0.53 |
| 16:H:213:GLU:N | 16:H:213:GLU:OE1 | 2.42 | 0.53 |
| 16:Q:99:LEU:HD12 | 16:Q:116:ILE:HG13 | 1.90 | 0.53 |
| 14:U:215:PRO:HG2 | 14:U:216:PRO:HD3 | 1.91 | 0.53 |
| 14:U:264:ALA:HB1 | 14:U:294:GLY:O | 2.08 | 0.53 |
| 15:V:228:ALA:HB1 | 15:V:233:LEU:CD1 | 2.39 | 0.53 |
| 1:1:203:PRO:HB2 | 1:1:204:PRO:HD3 | 1.90 | 0.52 |
| 3:3:127:ALA:HB3 | 3:3:246:ASN:HD22 | 1.74 | 0.52 |
| 3:3:317:LEU:HD21 | 3:3:595:GLU:HA | 1.92 | 0.52 |
| 4:4:115:THR:HG21 | 4:4:297:LEU:HD13 | 1.91 | 0.52 |
| 7:9:94:ASN:HB3 | 7:9:97:ARG:HB2 | 1.91 | 0.52 |
| 6:G:153:GLN:HG3 | 7:O:124:TYR:CZ | 2.44 | 0.52 |
| 6:G:39:ALA:HB2 | 6:G:75:ALA:HB3 | 1.91 | 0.52 |
| 14:M:215:PRO:HG2 | 14:M:216:PRO:HD3 | 1.90 | 0.52 |
| 3:D:247:TRP:HE1 | 7:O:61:ALA:CB | 2.21 | 0.52 |
| 16:Q:147:TYR:HE1 | 16:Q:229:VAL:H | 1.55 | 0.52 |
| 11:R:64:VAL:HA | 11:R:67:PHE:HB2 | 1.90 | 0.52 |
| 15:V:83:GLU:O | 15:V:87:LEU:HG | 2.09 | 0.52 |
| 3:3:237:ASP:OD1 | 3:3:239:THR:HG22 | 2.10 | 0.52 |
| 3:3:94:ASP:OD2 | 3:3:97:SER:OG | 2.23 | 0.52 |
| 4:4:341:GLU:CD | 5:5:91:ARG:HH22 | 2.11 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:211:SER:HB2 | 4:E:215:TYR:N | 2.24 | 0.52 |
| 16:Q:140:GLY:HA3 | 16:Q:152:SER:HB3 | 1.90 | 0.52 |
| 1:1:111:PRO:HB3 | 1:1:145:LEU:HD23 | 1.91 | 0.52 |
| 2:C:76:GLY:N | 2:C:118:SER:OG | 2.35 | 0.52 |
| 3:D:715:GLU:H | 3:D:761:SER:HB2 | 1.75 | 0.52 |
| 10:A:68:PHE:CD2 | 16:H:164:LEU:HB2 | 2.45 | 0.52 |
| 6:G:153:GLN:HG3 | 7:O:124:TYR:OH | 2.08 | 0.52 |
| 11:R:24:ASN:HB3 | 11:R:27:HIS:HB2 | 1.90 | 0.52 |
| 1:1:159:GLY:H | 1:1:162:LEU:HD21 | 1.72 | 0.52 |
| 3:3:190:TYR:O | 3:3:195:PRO:HD2 | 2.10 | 0.52 |
| 3:3:479:ALA:O | 3:3:494:LYS:HD2 | 2.10 | 0.52 |
| 6:6:73:ARG:HD3 | 6:6:98:GLN:O | 2.09 | 0.52 |
| 3:D:81:ALA:O | 3:D:85:THR:OG1 | 2.23 | 0.52 |
| 5:F:155:THR:N | 6:G:119:ASN:OD1 | 2.30 | 0.52 |
| 8:I:86:LEU:HB3 | 8:I:126:LEU:HD11 | 1.91 | 0.52 |
| 13:L:380:SER:CB | 13:L:457:GLY:H | 2.21 | 0.52 |
| 14:M:13:GLY:HA2 | 14:M:97:GLY:HA2 | 1.91 | 0.52 |
| 7:O:123:ASP:CG | 7:O:148:ARG:HH22 | 2.13 | 0.52 |
| 3:3:32:LEU:HD11 | 3:3:35:SER:HB2 | 1.91 | 0.52 |
| 7:9:40:ARG:NH1 | 7:9:41:HIS:O | 2.43 | 0.52 |
| 3:D:283:PRO:HG3 | 3:D:430:THR:OG1 | 2.10 | 0.52 |
| 4:E:240:ARG:NH1 | 4:E:282:GLU:OE2 | 2.43 | 0.52 |
| 6:G:160:GLY:O | 6:G:169:ARG:NH1 | 2.43 | 0.52 |
| 14:M:448:GLY:O | 14:M:452:ARG:HG2 | 2.10 | 0.52 |
| 15:N:319:ASP:HB3 | 15:N:322:LEU:HB2 | 1.91 | 0.52 |
| 10:P:29:ALA:O | 10:P:34:LYS:NZ | 2.42 | 0.52 |
| 18:1:502:FMN:H9 | 19:1:503:NAI:H52N | 1.91 | 0.52 |
| 3:3:175:ILE:O | 3:3:235:LEU:HA | 2.10 | 0.52 |
| 3:3:34:CYS:HB3 | 3:3:45:CYS:H | 1.75 | 0.52 |
| 3:3:503:PRO:HG3 | 3:3:528:LYS:HD3 | 1.91 | 0.52 |
| 4:4:143:LEU:HD23 | 4:4:143:LEU:H | 1.74 | 0.52 |
| 4:4:47:LEU:HD13 | 4:4:51:GLU:O | 2.10 | 0.52 |
| 1:B:238:PHE:CZ | 1:B:248:GLY:HA3 | 2.45 | 0.52 |
| 2:C:85:THR:HG22 | 2:C:86:LEU:H | 1.74 | 0.52 |
| 4:E:42:ARG:O | 4:E:43:LEU:HD23 | 2.10 | 0.52 |
| 6:G:104:TRP:HE1 | 6:G:173:VAL:HA | 1.74 | 0.52 |
| 15:N:317:ARG:NH1 | 15:N:383:PHE:O | 2.31 | 0.52 |
| 13:T:88:HIS:O | 13:T:92:ILE:HG13 | 2.09 | 0.52 |
| 14:U:134:TYR:HB2 | 14:U:145:LEU:HD13 | 1.92 | 0.52 |
| 4:4:202:ASP:OD1 | 4:4:284:ARG:NE | 2.41 | 0.52 |
| 3:D:199:VAL:HG11 | 3:D:219:PRO:HD2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:222:GLY:HA2 | 4:E:396:ILE:HD11 | 1.92 | 0.52 |
| 6:G:147:LEU:O | 6:G:151:VAL:HG13 | 2.10 | 0.52 |
| 16:H:216:ARG:NH1 | 16:H:294:ARG:O | 2.42 | 0.52 |
| 11:J:12:LEU:HD22 | 12:K:10:LEU:HD11 | 1.91 | 0.52 |
| 14:M:224:SER:HA | 14:M:330:GLY:HA3 | 1.91 | 0.52 |
| 14:U:8:LEU:HD21 | 14:U:31:LEU:HB3 | 1.91 | 0.52 |
| 15:V:280:ALA:HB1 | 15:V:347:LEU:HB3 | 1.91 | 0.52 |
| 9:X:4:VAL:HG22 | 9:X:57:LEU:HD21 | 1.92 | 0.52 |
| 3:3:28:TYR:CE2 | 3:3:96:LEU:HD11 | 2.45 | 0.52 |
| 10:A:7:TYR:CD2 | 11:J:44:VAL:HG11 | 2.44 | 0.52 |
| 6:G:104:TRP:NE1 | 6:G:173:VAL:HA | 2.25 | 0.52 |
| 6:G:114:SER:OG | 7:O:96:LEU:O | 2.28 | 0.52 |
| 7:O:13:THR:HG21 | 16:Q:296:THR:HG23 | 1.92 | 0.52 |
| 1:1:407:VAL:O | 1:1:411:LYS:N | 2.27 | 0.52 |
| 2:2:88:CYS:HA | 2:2:131:ALA:HB1 | 1.91 | 0.52 |
| 4:4:234:LEU:O | 4:4:239:LEU:HB2 | 2.10 | 0.52 |
| 4:4:338:PRO:HG3 | 5:5:193:ARG:HB2 | 1.91 | 0.52 |
| 5:5:67:ARG:HH22 | 5:5:149:ASP:CG | 2.13 | 0.52 |
| 5:5:167:PRO:HB3 | 7:9:66:TYR:CD2 | 2.45 | 0.52 |
| 3:D:33:PHE:HB2 | 3:D:45:CYS:CB | 2.40 | 0.52 |
| 3:D:565:TYR:HA | 3:D:582:PHE:O | 2.10 | 0.52 |
| 3:D:717:TRP:HB3 | 3:D:753:VAL:HG21 | 1.91 | 0.52 |
| 4:E:169:HIS:CE1 | 6:G:45:CYS:SG | 3.03 | 0.52 |
| 5:F:120:ASP:OD1 | 5:F:134:LYS:HG3 | 2.10 | 0.52 |
| 5:F:71:VAL:HG11 | 5:F:89:PHE:HD2 | 1.75 | 0.52 |
| 6:G:21:PHE:O | 6:G:25:GLU:HG2 | 2.10 | 0.52 |
| 16:H:333:PRO:HG2 | 16:H:336:TYR:CD1 | 2.45 | 0.52 |
| 13:L:171:LEU:O | 13:L:175:ILE:HG13 | 2.10 | 0.52 |
| 14:M:91:VAL:HG23 | 14:M:92:GLU:H | 1.74 | 0.52 |
| 13:T:463:HIS:CG | 13:T:464:PRO:HD3 | 2.44 | 0.52 |
| 14:U:22:ARG:NH1 | 14:U:92:GLU:HB3 | 2.25 | 0.52 |
| 14:U:345:ARG:HG2 | 14:U:412:LYS:O | 2.10 | 0.52 |
| 1:1:287:ILE:HG12 | 1:1:330:LEU:HB3 | 1.91 | 0.52 |
| 3:3:451:PHE:HD1 | 3:3:466:GLU:HB3 | 1.75 | 0.52 |
| 3:3:48:CYS:SG | 3:3:82:SER:N | 2.82 | 0.52 |
| 6:G:143:ARG:NE | 6:G:145:GLU:OE1 | 2.43 | 0.52 |
| 14:M:91:VAL:HB | 14:M:95:PHE:HE1 | 1.73 | 0.52 |
| 15:N:44:TRP:CZ3 | 15:N:60:GLN:HB3 | 2.44 | 0.52 |
| 10:P:66:MET:HG3 | 12:S:69:ALA:HB1 | 1.91 | 0.52 |
| 13:T:122:ASP:O | 13:T:185:ILE:N | 2.40 | 0.52 |
| 1:1:95:GLU:O | 1:1:135:ARG:NH1 | 2.30 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:3:657:HIS:O | 3:3:661:GLN:HG2 | 2.10 | 0.51 |
| 5:5:50:ALA:HB3 | 5:5:73:GLU:HB3 | 1.92 | 0.51 |
| 8:7:48:TYR:CZ | 8:7:50:LEU:HB2 | 2.45 | 0.51 |
| 2:C:24:ARG:HE | 2:C:55:THR:CB | 2.22 | 0.51 |
| 3:D:270:ARG:HB3 | 3:D:275:LEU:HD11 | 1.90 | 0.51 |
| 8:I:37:PHE:CE1 | 8:I:74:PRO:HA | 2.31 | 0.51 |
| 15:N:190:ALA:HB3 | 15:N:240:SER:HA | 1.90 | 0.51 |
| 15:N:198:ASP:OD1 | 15:N:256:ARG:NH2 | 2.44 | 0.51 |
| 16:Q:260:PRO:HG3 | 16:Q:286:PHE:CD2 | 2.45 | 0.51 |
| 3:3:614:LEU:O | 3:3:621:VAL:HA | 2.10 | 0.51 |
| 6:6:163:TYR:CD1 | 7:9:152:ARG:HD2 | 2.45 | 0.51 |
| 1:B:135:ARG:HE | 1:B:137:GLU:HB2 | 1.75 | 0.51 |
| 1:B:50:PRO:HA | 1:B:53:VAL:HG12 | 1.91 | 0.51 |
| 4:E:363:SER:N | 5:F:174:LEU:O | 2.43 | 0.51 |
| 14:U:65:PHE:HA | 14:U:111:ALA:O | 2.09 | 0.51 |
| 15:V:53:TYR:HA | 15:V:101:THR:HG22 | 1.92 | 0.51 |
| 1:1:106:ILE:HD11 | 1:1:251:LEU:HD21 | 1.92 | 0.51 |
| 3:3:127:ALA:HB3 | 3:3:246:ASN:ND2 | 2.24 | 0.51 |
| 3:3:416:PHE:HE2 | 3:3:448:MET:HB3 | 1.76 | 0.51 |
| 10:A:23:ALA:O | 10:A:27:VAL:HG23 | 2.10 | 0.51 |
| 1:B:118:MET:HG2 | 1:B:224:LEU:HD13 | 1.92 | 0.51 |
| 13:L:104:PHE:CE2 | 13:L:108:PHE:HE2 | 2.28 | 0.51 |
| 13:T:348:ASP:OD1 | 13:T:349:VAL:N | 2.42 | 0.51 |
| 4:E:222:GLY:HA3 | 4:E:275:ARG:NH2 | 2.26 | 0.51 |
| 13:L:321:HIS:HD2 | 13:L:388:ILE:HD12 | 1.75 | 0.51 |
| 13:L:66:SER:CB | 13:L:122:ASP:HB3 | 2.39 | 0.51 |
| 6:6:84:LEU:HD12 | 6:6:124:VAL:HG21 | 1.91 | 0.51 |
| 1:B:201:LEU:HA | 1:B:399:PHE:CZ | 2.46 | 0.51 |
| 2:C:24:ARG:HA | 2:C:53:VAL:CG2 | 2.40 | 0.51 |
| 4:E:81:TYR:CZ | 6:G:117:MET:HG3 | 2.46 | 0.51 |
| 6:G:97:GLU:HB3 | 10:P:39:ALA:HB3 | 1.91 | 0.51 |
| 16:H:65:LYS:O | 16:H:69:LYS:HB2 | 2.11 | 0.51 |
| 8:I:43:ARG:O | 8:I:43:ARG:HG3 | 2.11 | 0.51 |
| 12:K:79:PHE:CD2 | 12:K:85:THR:HA | 2.46 | 0.51 |
| 15:N:53:TYR:HA | 15:N:101:THR:HG22 | 1.92 | 0.51 |
| 5:F:170:PHE:CE2 | 7:O:61:ALA:HA | 2.45 | 0.51 |
| 1:1:65:ARG:HD2 | 1:1:222:GLU:OE2 | 2.10 | 0.51 |
| 4:4:190:LEU:CD1 | 4:4:194:LEU:HD11 | 2.41 | 0.51 |
| 1:B:364:ALA:HB3 | 3:D:207:VAL:HG13 | 1.92 | 0.51 |
| 3:D:246:ASN:ND2 | 3:D:276:ARG:HH12 | 2.09 | 0.51 |
| 3:D:609:GLU:HA | 3:D:627:ALA:H | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:620:ARG:HA | 3:D:675:ARG:HA | 1.91 | 0.51 |
| 10:A:93:PHE:CE2 | 16:H:326:LEU:HD13 | 2.46 | 0.51 |
| 13:L:12:LEU:O | 13:L:16:LEU:HG | 2.11 | 0.51 |
| 13:L:214:VAL:HG13 | 13:L:219:GLN:HB2 | 1.93 | 0.51 |
| 13:L:454:VAL:HB | 13:L:455:LEU:HD22 | 1.93 | 0.51 |
| 12:K:59:MET:HB2 | 15:N:105:LEU:HD21 | 1.93 | 0.51 |
| 13:T:26:GLU:HB3 | 13:T:27:PRO:HD3 | 1.91 | 0.51 |
| 13:T:340:ILE:O | 13:T:345:GLY:N | 2.28 | 0.51 |
| 14:U:157:LEU:HD12 | 15:V:369:ALA:HB2 | 1.92 | 0.51 |
| 15:V:61:VAL:O | 15:V:64:LEU:HB3 | 2.11 | 0.51 |
| 3:3:385:ALA:HB2 | 3:3:531:LYS:HB2 | 1.92 | 0.51 |
| 3:3:465:HIS:O | 3:3:489:MET:HG3 | 2.11 | 0.51 |
| 1:B:276:ILE:O | 1:B:282:GLY:N | 2.24 | 0.51 |
| 1:B:421:TYR:O | 1:B:425:ALA:N | 2.42 | 0.51 |
| 5:F:71:VAL:HA | 5:F:90:VAL:O | 2.08 | 0.51 |
| 12:K:46:ALA:HB2 | 12:K:53:GLY:HA3 | 1.92 | 0.51 |
| 16:Q:134:TYR:HA | 16:Q:137:PHE:CE2 | 2.45 | 0.51 |
| 1:1:381:GLU:OE1 | 1:1:426:ARG:NH2 | 2.42 | 0.51 |
| 2:2:171:LYS:NZ | 2:2:178:GLU:O | 2.44 | 0.51 |
| 3:3:355:LEU:HB2 | 3:3:547:MET:SD | 2.51 | 0.51 |
| 4:4:310:THR:HG22 | 4:4:311:PRO:O | 2.11 | 0.51 |
| 5:5:34:PHE:CD1 | 5:5:92:VAL:HG11 | 2.46 | 0.51 |
| 8:7:89:ALA:O | 8:7:90:HIS:ND1 | 2.44 | 0.51 |
| 3:D:173:PHE:O | 3:D:238:LEU:N | 2.43 | 0.51 |
| 6:G:152:MET:SD | 7:O:27:PRO:HG3 | 2.50 | 0.51 |
| 11:J:2:SER:HA | 11:J:5:GLU:HB3 | 1.93 | 0.51 |
| 14:M:95:PHE:HB3 | 14:M:136:TYR:CZ | 2.45 | 0.51 |
| 16:Q:332:LEU:H | 16:Q:332:LEU:HD12 | 1.75 | 0.51 |
| 14:U:281:PHE:CE1 | 14:U:341:ILE:HG22 | 2.46 | 0.51 |
| 1:1:165:THR:HG23 | 1:1:167:PHE:H | 1.76 | 0.51 |
| 2:2:3:PHE:HB2 | 2:2:45:ARG:HH11 | 1.76 | 0.51 |
| 3:3:274:LEU:HD21 | 3:3:298:HIS:HB2 | 1.92 | 0.51 |
| 4:4:38:HIS:ND1 | 4:4:139:ASP:OD2 | 2.44 | 0.51 |
| 1:B:190:ASN:OD1 | 1:B:200:ARG:NE | 2.27 | 0.51 |
| 2:C:66:PHE:CE1 | 3:D:205:ARG:HD3 | 2.45 | 0.51 |
| 16:H:136:ILE:HG23 | 16:H:232:TYR:CD2 | 2.45 | 0.51 |
| 7:9:17:LEU:HD12 | 16:H:42:PHE:CE1 | 2.46 | 0.51 |
| 8:I:120:ASP:O | 8:I:124:GLU:HG3 | 2.11 | 0.51 |
| 12:K:21:ARG:CZ | 12:K:26:LEU:HD23 | 2.41 | 0.51 |
| 14:M:203:ILE:HG13 | 14:M:210:LEU:HB3 | 1.92 | 0.51 |
| 15:N:262:SER:OG | 15:N:288:TYR:OH | 2.27 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:205:VAL:HG12 | 16:Q:313:LEU:HD22 | 1.93 | 0.51 |
| 16:Q:291:ILE:HA | 16:Q:294:ARG:CG | 2.40 | 0.51 |
| 15:V:13:LEU:HD22 | 15:V:25:VAL:HG13 | 1.93 | 0.51 |
| 15:V:98:LEU:HD23 | 15:V:218:ALA:HB1 | 1.93 | 0.51 |
| 1:1:192:LEU:HD22 | 1:1:211:LEU:HD21 | 1.93 | 0.51 |
| 1:1:259:LYS:HA | 1:1:284:LEU:HD21 | 1.93 | 0.51 |
| 4:4:190:LEU:HD12 | 4:4:194:LEU:CD1 | 2.41 | 0.51 |
| 5:5:33:ARG:O | 5:5:37:GLU:HB2 | 2.11 | 0.51 |
| 2:C:97:TRP:CH2 | 2:C:119:VAL:HB | 2.45 | 0.51 |
| 5:F:120:ASP:OD2 | 5:F:135:ILE:N | 2.44 | 0.51 |
| 16:H:114:TRP:NE1 | 16:H:117:ASN:HB2 | 2.26 | 0.51 |
| 16:H:201:PRO:O | 16:H:204:LEU:HB2 | 2.10 | 0.51 |
| 13:T:90:TYR:CG | 13:T:334:LEU:HD13 | 2.46 | 0.51 |
| 15:V:29:THR:HG22 | 15:V:89:LEU:HD11 | 1.92 | 0.51 |
| 1:1:193:GLU:OE1 | 1:1:200:ARG:NH2 | 2.40 | 0.50 |
| 7:9:162:VAL:HG12 | 7:9:176:PRO:HB2 | 1.93 | 0.50 |
| 6:G:36:LEU:O | 6:G:38:PRO:HD3 | 2.10 | 0.50 |
| 13:L:340:ILE:HB | 13:L:345:GLY:HA2 | 1.92 | 0.50 |
| 13:L:9:LEU:HB2 | 13:L:10:PRO:HD3 | 1.93 | 0.50 |
| 14:U:208:PHE:N | 14:U:267:SER:OG | 2.44 | 0.50 |
| 15:V:101:THR:HG21 | 15:V:106:LEU:HD23 | 1.92 | 0.50 |
| 3:3:512:LEU:HD21 | 3:3:534:ALA:HB1 | 1.91 | 0.50 |
| 3:3:544:LEU:HB3 | 3:3:549:VAL:HB | 1.92 | 0.50 |
| 5:5:98:ASP:OD1 | 5:5:100:ARG:HD3 | 2.11 | 0.50 |
| 1:B:184:GLU:OE1 | 1:B:186:THR:OG1 | 2.21 | 0.50 |
| 3:D:249:MET:HB3 | 3:D:268:ASP:HB3 | 1.92 | 0.50 |
| 6:G:53:SER:O | 6:G:60:LEU:N | 2.36 | 0.50 |
| 16:H:274:VAL:HG22 | 16:H:275:PRO:HD2 | 1.92 | 0.50 |
| 15:N:283:PHE:O | 15:N:287:THR:HG23 | 2.12 | 0.50 |
| 7:O:44:THR:HA | 7:O:138:VAL:HG13 | 1.92 | 0.50 |
| 16:Q:21:VAL:HG13 | 16:Q:94:LEU:HD22 | 1.92 | 0.50 |
| 13:T:359:LEU:HD21 | 13:T:437:GLU:HB3 | 1.93 | 0.50 |
| 15:V:16:LEU:O | 15:V:20:LEU:N | 2.44 | 0.50 |
| 1:1:121:ALA:O | 1:1:125:ILE:HG12 | 2.11 | 0.50 |
| 1:1:220:ASN:N | 18:1:502:FMN:O3P | 2.30 | 0.50 |
| 3:3:445:THR:HB | 3:3:463:ALA:HB2 | 1.92 | 0.50 |
| 4:4:169:HIS:NE2 | 6:6:45:CYS:SG | 2.84 | 0.50 |
| 7:9:149:GLU:O | 7:9:153:THR:CB | 2.59 | 0.50 |
| 2:C:173:GLY:HA3 | 2:C:176:VAL:O | 2.12 | 0.50 |
| 3:D:351:LEU:HD12 | 3:D:540:ASN:HD21 | 1.76 | 0.50 |
| 11:J:138:VAL:HG22 | 15:N:106:LEU:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:K:18:VAL:HG11 | 15:N:142:LEU:HD13 | 1.93 | 0.50 |
| 15:N:248:ALA:HA | 15:N:251:GLN:HG2 | 1.92 | 0.50 |
| 16:Q:218:PRO:C | 16:Q:220:ASP:H | 2.13 | 0.50 |
| 13:T:463:HIS:CD2 | 13:T:464:PRO:HD3 | 2.46 | 0.50 |
| 13:T:490:GLU:HG3 | 13:T:491:TRP:N | 2.26 | 0.50 |
| 2:2:4:PHE:HB3 | 2:2:11:LEU:HD11 | 1.93 | 0.50 |
| 1:1:260:ARG:HA | 2:2:177:HIS:O | 2.11 | 0.50 |
| 2:C:4:PHE:HB3 | 2:C:11:LEU:HD11 | 1.93 | 0.50 |
| 6:G:86:LYS:HG3 | 6:G:122:ALA:O | 2.12 | 0.50 |
| 11:R:123:LEU:HD22 | 16:Q:120:LEU:HD11 | 1.93 | 0.50 |
| 4:4:73:ARG:NH2 | 6:6:117:MET:O | 2.45 | 0.50 |
| 4:4:87:TYR:CG | 6:6:45:CYS:HB3 | 2.46 | 0.50 |
| 10:A:86:GLY:HA2 | 16:H:329:ALA:HA | 1.93 | 0.50 |
| 3:D:225:ASN:O | 3:D:229:ILE:HG13 | 2.12 | 0.50 |
| 3:D:439:GLU:HG2 | 3:D:440:ARG:HG2 | 1.93 | 0.50 |
| 4:E:212:PRO:HG2 | 4:E:213:ILE:HD12 | 1.93 | 0.50 |
| 16:H:227:GLU:HG2 | 16:H:228:LEU:N | 2.26 | 0.50 |
| 15:N:209:LEU:HB2 | 15:N:296:PHE:HB3 | 1.93 | 0.50 |
| 15:N:422:ALA:O | 15:N:423:LEU:HD23 | 2.12 | 0.50 |
| 7:O:26:TYR:HE1 | 7:O:160:GLY:HA3 | 1.76 | 0.50 |
| 13:T:454:VAL:HB | 13:T:455:LEU:HD22 | 1.94 | 0.50 |
| 13:T:586:LEU:HD13 | 15:V:138:LEU:HD12 | 1.93 | 0.50 |
| 6:G:124:VAL:HG22 | 9:X:120:PRO:HD2 | 1.94 | 0.50 |
| 3:3:165:ASP:HB2 | 8:7:66:PRO:HG2 | 1.93 | 0.50 |
| 3:3:245:ARG:NH1 | 7:9:56:CYS:O | 2.45 | 0.50 |
| 3:3:694:LEU:HB3 | 3:3:762:ALA:HB2 | 1.93 | 0.50 |
| 5:5:38:MET:CE | 5:5:104:VAL:HG11 | 2.39 | 0.50 |
| 4:E:222:GLY:O | 4:E:271:ASP:HA | 2.12 | 0.50 |
| 16:H:159:LEU:HD11 | 16:H:221:LEU:HD21 | 1.92 | 0.50 |
| 13:L:435:PRO:HG2 | 13:L:436:HIS:CD2 | 2.46 | 0.50 |
| 14:M:281:PHE:CE1 | 14:M:341:ILE:HG22 | 2.47 | 0.50 |
| 11:R:19:VAL:HG21 | 11:R:32:LEU:HB2 | 1.93 | 0.50 |
| 11:R:36:PHE:CE2 | 11:R:59:TYR:CD1 | 3.00 | 0.50 |
| 13:T:312:VAL:HA | 13:T:397:PHE:CD2 | 2.47 | 0.50 |
| 1:1:190:ASN:ND2 | 1:1:198:ASN:O | 2.45 | 0.50 |
| 1:1:20:HIS:CG | 1:1:31:TYR:HE1 | 2.30 | 0.50 |
| 1:1:83:ASP:OD1 | 1:1:87:HIS:NE2 | 2.38 | 0.50 |
| 3:D:247:TRP:CG | 5:F:172:ALA:HB2 | 2.46 | 0.50 |
| 5:F:20:ASN:HD21 | 5:F:24:ASN:HB2 | 1.77 | 0.50 |
| 16:H:120:LEU:HD22 | 16:H:180:LEU:HD12 | 1.92 | 0.50 |
| 15:N:29:THR:HG21 | 15:N:85:TYR:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:U:64:ALA:HB1 | 14:U:113:ARG:HB3 | 1.93 | 0.50 |
| 1:1:190:ASN:OD1 | 1:1:200:ARG:NE | 2.38 | 0.50 |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:CZ3 | 2.45 | 0.50 |
| 4:4:34:HIS:HA | 4:4:36:SER:H | 1.76 | 0.50 |
| 7:9:13:THR:HG21 | 16:H:296:THR:HG23 | 1.93 | 0.50 |
| 8:I:86:LEU:HB2 | 8:I:91:ILE:HB | 1.93 | 0.50 |
| 14:M:307:GLY:HA2 | 14:M:380:THR:HA | 1.94 | 0.50 |
| 14:U:305:PRO:HB3 | 14:U:459:GLU:HA | 1.94 | 0.50 |
| 1:1:220:ASN:ND2 | 18:1:502:FMN:O2 | 2.45 | 0.50 |
| 4:4:213:ILE:HD11 | 7:9:6:LEU:HD21 | 1.92 | 0.50 |
| 1:B:16:THR:HG23 | 1:B:233:ARG:HH21 | 1.77 | 0.50 |
| 1:B:91:CYS:HB3 | 1:B:132:ILE:HA | 1.93 | 0.50 |
| 11:J:19:VAL:HG11 | 12:K:33:LEU:HD13 | 1.94 | 0.50 |
| 14:M:46:GLY:HA2 | 14:M:68:ASP:HA | 1.93 | 0.50 |
| 12:S:79:PHE:CD2 | 12:S:85:THR:HA | 2.47 | 0.50 |
| 9:X:52:THR:OG1 | 9:X:55:LYS:O | 2.23 | 0.50 |
| 1:1:179:ALA:HB3 | 1:1:182:CYS:SG | 2.52 | 0.49 |
| 3:3:268:ASP:CG | 3:3:278:ARG:HH11 | 2.13 | 0.49 |
| 3:3:444:ARG:HD3 | 3:3:447:LYS:HD2 | 1.94 | 0.49 |
| 4:4:122:GLU:HB2 | 4:4:290:ILE:HD11 | 1.94 | 0.49 |
| 4:4:93:HIS:ND1 | 4:4:355:TYR:OH | 2.32 | 0.49 |
| 6:6:43:LEU:HD13 | 6:6:83:ARG:O | 2.12 | 0.49 |
| 7:9:43:LEU:HA | 7:9:112:ALA:O | 2.11 | 0.49 |
| 1:B:437:TRP:HD1 | 2:C:95:GLU:OE1 | 1.94 | 0.49 |
| 3:D:133:ARG:NE | 3:D:136:GLU:OE2 | 2.33 | 0.49 |
| 4:E:98:ALA:O | 4:E:102:GLU:HG3 | 2.11 | 0.49 |
| 16:H:2:THR:HA | 16:H:5:TYR:HD2 | 1.77 | 0.49 |
| 8:I:82:ILE:HG23 | 8:I:95:ALA:HB3 | 1.92 | 0.49 |
| 12:S:15:VAL:O | 12:S:19:LEU:HG | 2.11 | 0.49 |
| 15:V:168:GLU:HG2 | 15:V:169:GLY:H | 1.77 | 0.49 |
| 15:V:279:GLN:NE2 | 15:V:420:LEU:O | 2.43 | 0.49 |
| 4:4:201:ILE:HA | 4:4:204:TYR:HD2 | 1.77 | 0.49 |
| 5:5:68:PHE:HB3 | 5:5:124:ILE:HD11 | 1.94 | 0.49 |
| 1:B:341:MET:HB2 | 1:B:371:PHE:CE2 | 2.46 | 0.49 |
| 3:D:11:VAL:HG21 | 3:D:26:ALA:HB2 | 1.93 | 0.49 |
| 6:G:163:TYR:CD1 | 7:O:152:ARG:HD2 | 2.45 | 0.49 |
| 13:L:564:TYR:CG | 14:M:151:PHE:HZ | 2.30 | 0.49 |
| 15:N:194:PHE:O | 15:N:197:PRO:HD2 | 2.11 | 0.49 |
| 16:Q:102:PHE:CD1 | 16:Q:279:MET:HG2 | 2.47 | 0.49 |
| 3:3:133:ARG:HA | 3:3:136:GLU:OE2 | 2.12 | 0.49 |
| 1:B:152:ALA:HB1 | 1:B:157:TYR:HB2 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:146:THR:HG22 | 2:C:149:ARG:HB2 | 1.93 | 0.49 |
| 2:C:161:LYS:HB3 | 2:C:166:ILE:HG12 | 1.93 | 0.49 |
| 2:C:31:LEU:HD22 | 2:C:41:ILE:HD13 | 1.94 | 0.49 |
| 3:D:414:SER:O | 3:D:418:ARG:NE | 2.44 | 0.49 |
| 4:E:285:GLU:O | 4:E:289:ILE:HG12 | 2.11 | 0.49 |
| 5:F:18:GLU:HB2 | 5:F:26:TRP:HB2 | 1.94 | 0.49 |
| 8:I:29:VAL:HG21 | 8:I:67:PHE:CE2 | 2.47 | 0.49 |
| 11:J:19:VAL:HG23 | 11:J:28:ALA:O | 2.12 | 0.49 |
| 10:P:90:LEU:HD12 | 16:Q:330:LEU:HD21 | 1.94 | 0.49 |
| 15:V:319:ASP:HB3 | 15:V:322:LEU:HB2 | 1.94 | 0.49 |
| 15:V:40:LEU:HD22 | 15:V:60:GLN:HG2 | 1.93 | 0.49 |
| 4:4:34:HIS:HA | 4:4:36:SER:N | 2.27 | 0.49 |
| 1:B:338:VAL:HG22 | 1:B:421:TYR:CE2 | 2.47 | 0.49 |
| 13:T:166:ASP:O | 13:T:170:MET:HG3 | 2.12 | 0.49 |
| 13:T:217:SER:HB2 | 13:T:303:LEU:HD22 | 1.94 | 0.49 |
| 13:T:391:ALA:O | 13:T:395:TYR:HB2 | 2.12 | 0.49 |
| 9:W:31:VAL:HG22 | 9:W:50:LEU:HD13 | 1.95 | 0.49 |
| 3:3:416:PHE:O | 3:3:447:LYS:HD3 | 2.12 | 0.49 |
| 7:9:94:ASN:OD1 | 7:9:97:ARG:HG2 | 2.12 | 0.49 |
| 1:B:63:ARG:HB3 | 1:B:69:GLY:HA2 | 1.94 | 0.49 |
| 4:E:85:MET:HE1 | 4:E:370:VAL:HG21 | 1.94 | 0.49 |
| 14:M:363:LEU:HD22 | 14:M:368:LEU:HD13 | 1.92 | 0.49 |
| 7:O:35:PRO:O | 7:O:117:TYR:OH | 2.21 | 0.49 |
| 15:V:126:ARG:HD2 | 15:V:128:GLN:HG2 | 1.95 | 0.49 |
| 3:3:477:LEU:HA | 3:3:480:LEU:HD12 | 1.94 | 0.49 |
| 4:4:118:VAL:HB | 4:4:257:TYR:HE1 | 1.77 | 0.49 |
| 3:D:281:GLU:HB2 | 3:D:288:ILE:HG22 | 1.92 | 0.49 |
| 3:D:398:VAL:HG22 | 3:D:506:ILE:HD12 | 1.95 | 0.49 |
| 3:D:585:MET:SD | 3:D:598:ALA:HB2 | 2.52 | 0.49 |
| 4:E:391:PRO:HG3 | 16:Q:227:GLU:OE2 | 2.13 | 0.49 |
| 16:H:221:LEU:N | 16:H:222:PRO:HA | 2.27 | 0.49 |
| 15:N:217:ALA:HA | 15:N:285:LEU:HD23 | 1.95 | 0.49 |
| 6:G:163:TYR:H | 7:O:152:ARG:NH1 | 2.10 | 0.49 |
| 13:T:196:LEU:HD23 | 13:T:202:LEU:HD23 | 1.94 | 0.49 |
| 15:V:62:PHE:CD2 | 15:V:221:ALA:HB2 | 2.47 | 0.49 |
| 4:4:114:GLU:O | 4:4:118:VAL:HG13 | 2.12 | 0.49 |
| 5:5:103:THR:HG23 | 5:5:127:GLU:O | 2.12 | 0.49 |
| 6:6:31:GLY:O | 6:6:35:SER:HB3 | 2.12 | 0.49 |
| 3:D:716:LEU:HD21 | 3:D:758:LEU:HD23 | 1.94 | 0.49 |
| 4:E:114:GLU:O | 4:E:118:VAL:HG13 | 2.12 | 0.49 |
| 5:F:47:ASN:O | 5:F:108:TRP:NE1 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:N:247:ALA:O | 15:N:251:GLN:NE2 | 2.34 | 0.49 |
| 11:R:75:PHE:CZ | 11:R:78:GLN:HG2 | 2.48 | 0.49 |
| 15:V:315:LEU:O | 15:V:319:ASP:N | 2.37 | 0.49 |
| 1:1:402:LEU:O | 1:1:405:ALA:HB3 | 2.13 | 0.49 |
| 3:3:451:PHE:CD1 | 3:3:466:GLU:HB3 | 2.47 | 0.49 |
| 4:4:254:TYR:CE2 | 4:4:346:THR:HA | 2.47 | 0.49 |
| 4:E:173:ILE:O | 4:E:174:ARG:NH1 | 2.46 | 0.49 |
| 13:L:44:GLY:HA3 | 13:L:77:LEU:HD21 | 1.94 | 0.49 |
| 16:Q:45:ARG:HG2 | 16:Q:46:MET:N | 2.28 | 0.49 |
| 12:S:31:ILE:O | 12:S:35:LEU:HD13 | 2.13 | 0.49 |
| 15:V:14:THR:HG1 | 15:V:90:TYR:HH | 1.58 | 0.49 |
| 3:3:42:ILE:HG21 | 3:3:439:GLU:OE1 | 2.13 | 0.49 |
| 4:4:50:GLU:OE2 | 16:H:154:ARG:NH1 | 2.34 | 0.49 |
| 10:A:68:PHE:HD2 | 16:H:164:LEU:HB2 | 1.77 | 0.49 |
| 6:G:76:ASP:OD1 | 16:Q:65:LYS:NZ | 2.38 | 0.49 |
| 16:H:332:LEU:HD12 | 16:H:332:LEU:H | 1.77 | 0.49 |
| 16:H:6:PRO:HG2 | 16:H:112:GLN:NE2 | 2.28 | 0.49 |
| 13:L:463:HIS:HE1 | 13:L:487:LEU:HD22 | 1.77 | 0.49 |
| 11:R:75:PHE:CE2 | 11:R:78:GLN:HG2 | 2.48 | 0.49 |
| 13:T:461:LEU:HD13 | 13:T:465:LEU:HD13 | 1.95 | 0.49 |
| 10:A:67:LEU:HD21 | 10:A:110:GLU:OE2 | 2.13 | 0.49 |
| 1:B:106:ILE:HD11 | 1:B:251:LEU:HD21 | 1.93 | 0.49 |
| 4:E:50:GLU:OE2 | 16:Q:154:ARG:NH2 | 2.37 | 0.49 |
| 16:Q:302:TYR:O | 16:Q:306:LEU:HG | 2.12 | 0.49 |
| 16:Q:51:VAL:O | 16:Q:57:LEU:HB2 | 2.13 | 0.49 |
| 11:R:75:PHE:HZ | 11:R:78:GLN:HE21 | 1.60 | 0.49 |
| 13:T:551:GLU:O | 13:T:555:TYR:HD1 | 1.95 | 0.49 |
| 1:1:264:TYR:CZ | 1:1:279:TRP:HB3 | 2.48 | 0.48 |
| 1:1:387:LEU:HA | 1:1:390:LEU:HD12 | 1.95 | 0.48 |
| 1:B:131:TYR:OH | 2:C:17:LYS:O | 2.16 | 0.48 |
| 3:D:409:LEU:O | 3:D:413:LEU:N | 2.38 | 0.48 |
| 3:D:42:ILE:HD12 | 3:D:42:ILE:O | 2.12 | 0.48 |
| 5:F:175:THR:H | 5:F:178:ASP:HB2 | 1.77 | 0.48 |
| 5:F:38:MET:HA | 5:F:41:TYR:HB2 | 1.94 | 0.48 |
| 6:G:130:VAL:HG13 | 9:X:120:PRO:O | 2.14 | 0.48 |
| 16:H:8:ASP:OD1 | 16:H:112:GLN:HG2 | 2.13 | 0.48 |
| 13:L:348:ASP:OD1 | 13:L:349:VAL:N | 2.46 | 0.48 |
| 3:D:271:SER:OG | 7:O:69:TYR:OH | 2.25 | 0.48 |
| 10:P:7:TYR:CD1 | 16:Q:118:LEU:HD22 | 2.47 | 0.48 |
| 16:Q:232:TYR:HB2 | 16:Q:244:PHE:CE1 | 2.48 | 0.48 |
| 5:5:137:THR:HB | 5:5:141:LEU:HD22 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:563:ALA:HB3 | 3:D:580:LYS:HE3 | 1.94 | 0.48 |
| 4:E:102:GLU:O | 4:E:106:GLY:N | 2.46 | 0.48 |
| 5:F:137:THR:HB | 5:F:141:LEU:HD22 | 1.96 | 0.48 |
| 6:G:38:PRO:HG2 | 6:G:65:SER:HB3 | 1.95 | 0.48 |
| 14:M:106:LEU:O | 14:M:110:PHE:HD1 | 1.95 | 0.48 |
| 16:Q:81:LEU:HD13 | 16:Q:138:LEU:HD22 | 1.95 | 0.48 |
| 13:T:163:ARG:NH2 | 14:U:366:VAL:O | 2.45 | 0.48 |
| 14:U:127:ILE:HB | 14:U:128:PRO:HD3 | 1.95 | 0.48 |
| 4:4:169:HIS:CE1 | 6:6:45:CYS:SG | 3.06 | 0.48 |
| 3:D:112:LEU:HD23 | 3:D:130:LEU:HD21 | 1.96 | 0.48 |
| 3:D:29:ASP:N | 3:D:29:ASP:OD1 | 2.47 | 0.48 |
| 3:D:450:LEU:HD13 | 3:D:458:LEU:HB2 | 1.95 | 0.48 |
| 6:G:104:TRP:NE1 | 6:G:172:PRO:O | 2.45 | 0.48 |
| 13:L:255:ARG:HA | 13:L:477:LEU:HD23 | 1.93 | 0.48 |
| 13:L:90:TYR:O | 13:L:94:TYR:HB2 | 2.13 | 0.48 |
| 16:Q:35:GLU:OE1 | 16:Q:249:TYR:OH | 2.14 | 0.48 |
| 14:U:371:LEU:HD11 | 14:U:441:LEU:HD12 | 1.94 | 0.48 |
| 6:6:76:ASP:O | 6:6:104:TRP:N | 2.31 | 0.48 |
| 6:6:94:ARG:HH11 | 10:A:46:SER:HB3 | 1.79 | 0.48 |
| 1:B:433:ARG:HH22 | 2:C:89:LYS:NZ | 2.11 | 0.48 |
| 11:J:49:ARG:HD2 | 11:J:123:LEU:HD21 | 1.94 | 0.48 |
| 10:P:105:VAL:HG13 | 15:V:15:LEU:HD21 | 1.95 | 0.48 |
| 13:T:355:LEU:HB3 | 13:T:359:LEU:HD12 | 1.95 | 0.48 |
| 13:T:413:THR:HA | 13:T:416:TYR:CE2 | 2.48 | 0.48 |
| 15:V:315:LEU:HD21 | 15:V:322:LEU:HB3 | 1.95 | 0.48 |
| 1:1:342:TRP:HZ3 | 1:1:346:ARG:HE | 1.60 | 0.48 |
| 2:2:13:GLU:O | 2:2:17:LYS:HG3 | 2.13 | 0.48 |
| 3:3:387:LEU:O | 3:3:390:LEU:HB3 | 2.13 | 0.48 |
| 4:4:199:HIS:NE2 | 4:4:203:GLU:OE2 | 2.43 | 0.48 |
| 7:9:4:LYS:O | 7:9:8:GLN:HG3 | 2.13 | 0.48 |
| 1:B:374:ILE:HD13 | 1:B:421:TYR:HD2 | 1.79 | 0.48 |
| 4:E:275:ARG:O | 4:E:279:ARG:HG3 | 2.13 | 0.48 |
| 11:J:100:VAL:HA | 13:L:598:LEU:HD21 | 1.95 | 0.48 |
| 13:L:159:PHE:CD2 | 14:M:407:LEU:HD11 | 2.45 | 0.48 |
| 7:O:149:GLU:HA | 7:O:152:ARG:HG2 | 1.94 | 0.48 |
| 10:P:105:VAL:HG22 | 15:V:15:LEU:HD11 | 1.95 | 0.48 |
| 16:Q:119:ASP:OD1 | 16:Q:120:LEU:HG | 2.13 | 0.48 |
| 16:Q:67:ILE:HG13 | 16:Q:68:PHE:CD1 | 2.49 | 0.48 |
| 11:R:50:PHE:HB3 | 11:R:122:GLY:O | 2.12 | 0.48 |
| 12:S:10:LEU:HD23 | 12:S:13:LEU:HD12 | 1.96 | 0.48 |
| 13:T:433:HIS:ND1 | 13:T:437:GLU:OE2 | 2.37 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:V:99:ALA:O | 15:V:225:ARG:NH1 | 2.46 | 0.48 |
| 15:V:25:VAL:O | 15:V:29:THR:HG23 | 2.13 | 0.48 |
| 3:3:136:GLU:HG2 | 5:5:189:ARG:HG2 | 1.94 | 0.48 |
| 3:3:697:THR:OG1 | 3:3:762:ALA:O | 2.23 | 0.48 |
| 1:B:134:VAL:O | 1:B:176:GLY:N | 2.39 | 0.48 |
| 3:D:367:PRO:HB2 | 3:D:554:LYS:HB2 | 1.95 | 0.48 |
| 6:G:53:SER:HB3 | 6:G:144:PRO:HB3 | 1.96 | 0.48 |
| 15:N:313:ARG:HA | 15:N:381:ALA:O | 2.14 | 0.48 |
| 7:O:56:CYS:N | 17:O:202:SF4:S1 | 2.86 | 0.48 |
| 13:T:156:ARG:NH1 | 14:U:408:THR:OG1 | 2.46 | 0.48 |
| 1:1:358:PRO:HD3 | 3:3:107:MET:SD | 2.54 | 0.48 |
| 3:3:136:GLU:HG2 | 5:5:186:GLY:O | 2.14 | 0.48 |
| 3:3:117:LEU:H | 4:4:321:MET:CE | 2.26 | 0.48 |
| 5:5:104:VAL:HG12 | 5:5:107:LEU:HD22 | 1.95 | 0.48 |
| 6:6:138:PRO:HG3 | 7:9:129:LEU:HD22 | 1.95 | 0.48 |
| 1:B:241:MET:O | 1:B:248:GLY:N | 2.46 | 0.48 |
| 1:B:55:GLU:OE2 | 1:B:59:ARG:NH2 | 2.44 | 0.48 |
| 3:D:154:TYR:CZ | 4:E:312:PRO:HB3 | 2.48 | 0.48 |
| 4:E:385:CYS:HA | 4:E:396:ILE:HD13 | 1.96 | 0.48 |
| 13:L:327:PHE:CE1 | 13:L:452:GLY:HA3 | 2.48 | 0.48 |
| 13:L:356:TRP:CE3 | 13:L:363:ARG:HD2 | 2.48 | 0.48 |
| 14:M:221:ASN:ND2 | 14:M:228:ASP:OD1 | 2.47 | 0.48 |
| 14:M:241:PHE:HA | 14:M:245:ALA:HB3 | 1.96 | 0.48 |
| 10:P:81:TYR:HB2 | 11:R:132:TYR:CZ | 2.48 | 0.48 |
| 10:P:7:TYR:HD2 | 11:R:44:VAL:HG11 | 1.78 | 0.48 |
| 13:T:182:THR:HB | 13:T:187:GLU:HG3 | 1.96 | 0.48 |
| 13:T:214:VAL:HG22 | 13:T:219:GLN:HB2 | 1.95 | 0.48 |
| 15:V:343:TRP:NE1 | 15:V:413:GLY:O | 2.47 | 0.48 |
| 3:3:501:LYS:HD2 | 3:3:501:LYS:H | 1.78 | 0.48 |
| 6:6:81:ALA:HA | 6:6:108:MET:HB3 | 1.96 | 0.48 |
| 1:B:111:PRO:HB3 | 1:B:145:LEU:HD23 | 1.96 | 0.48 |
| 1:B:136:GLY:HA3 | 2:C:32:ARG:NH2 | 2.29 | 0.48 |
| 3:D:243:ARG:HH11 | 3:D:275:LEU:HD23 | 1.78 | 0.48 |
| 3:D:355:LEU:O | 3:D:359:GLU:HG2 | 2.13 | 0.48 |
| 4:E:171:ASN:CG | 4:E:174:ARG:HH22 | 2.17 | 0.48 |
| 4:E:42:ARG:HB3 | 4:E:58:HIS:HB2 | 1.96 | 0.48 |
| 4:E:154:GLU:OE1 | 6:G:57:ARG:HD3 | 2.14 | 0.48 |
| 6:G:99:MET:HB3 | 6:G:103:LYS:CD | 2.44 | 0.48 |
| 13:L:163:ARG:HD3 | 14:M:399:VAL:O | 2.14 | 0.48 |
| 13:T:241:HIS:HB3 | 13:T:299:THR:HG21 | 1.96 | 0.48 |
| 5:5:49:LEU:HD21 | 5:5:52:ILE:HD11 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:170:ASP:OD1 | 1:B:171:LEU:N | 2.47 | 0.48 |
| 2:C:49:ILE:O | 2:C:53:VAL:HG12 | 2.13 | 0.48 |
| 4:E:341:GLU:OE2 | 5:F:57:TYR:OH | 2.31 | 0.48 |
| 16:H:352:VAL:HG12 | 16:H:353:LEU:HD12 | 1.95 | 0.48 |
| 15:N:181:VAL:HA | 15:N:192:PHE:CE2 | 2.49 | 0.48 |
| 13:L:592:LEU:HB3 | 15:N:194:PHE:CZ | 2.48 | 0.48 |
| 15:N:207:VAL:O | 15:N:211:MET:HG3 | 2.13 | 0.48 |
| 10:P:10:THR:HA | 16:Q:116:ILE:HD13 | 1.96 | 0.48 |
| 15:V:124:TRP:HZ3 | 15:V:305:ASP:HB2 | 1.78 | 0.48 |
| 9:W:28:GLU:C | 9:W:88:ARG:HH21 | 2.17 | 0.48 |
| 4:4:306:ASN:HD21 | 5:5:192:TYR:HH | 1.59 | 0.48 |
| 1:B:65:ARG:HH22 | 1:B:238:PHE:HZ | 1.62 | 0.48 |
| 1:B:395:GLU:HB2 | 1:B:407:VAL:HG21 | 1.95 | 0.48 |
| 3:D:186:ARG:HD3 | 3:D:229:ILE:HG22 | 1.96 | 0.48 |
| 4:E:234:LEU:HD12 | 4:E:380:SER:HB2 | 1.95 | 0.48 |
| 4:E:304:ASP:O | 4:E:310:THR:OG1 | 2.20 | 0.48 |
| 8:I:15:GLU:O | 8:I:18:SER:HB3 | 2.14 | 0.48 |
| 13:L:163:ARG:HE | 14:M:399:VAL:HB | 1.78 | 0.48 |
| 14:M:204:LYS:HE3 | 14:M:234:TYR:O | 2.14 | 0.48 |
| 7:O:60:ALA:HB2 | 7:O:68:ILE:HG22 | 1.96 | 0.48 |
| 13:T:219:GLN:NE2 | 13:T:277:THR:HG21 | 2.29 | 0.48 |
| 13:T:30:GLY:HA3 | 13:T:92:ILE:HG12 | 1.95 | 0.48 |
| 13:T:392:THR:HG22 | 13:T:399:GLY:HA3 | 1.96 | 0.48 |
| 14:U:70:LEU:HD13 | 14:U:312:LEU:HD13 | 1.96 | 0.48 |
| 14:U:338:THR:HG22 | 14:U:340:GLU:H | 1.79 | 0.48 |
| 15:V:66:ALA:HB1 | 15:V:95:MET:HE3 | 1.94 | 0.48 |
| 1:1:176:GLY:O | 2:2:32:ARG:NH2 | 2.44 | 0.47 |
| 3:3:505:LEU:HD21 | 3:3:521:ALA:HB1 | 1.96 | 0.47 |
| 6:6:61:ALA:O | 16:H:48:PRO:HG3 | 2.13 | 0.47 |
| 10:A:57:PHE:CE2 | 16:H:149:LEU:HD13 | 2.49 | 0.47 |
| 13:L:17:LEU:HA | 13:L:21:GLY:HA2 | 1.95 | 0.47 |
| 13:L:26:GLU:HB3 | 13:L:27:PRO:HD3 | 1.95 | 0.47 |
| 13:L:282:ALA:HA | 13:L:416:TYR:HE2 | 1.79 | 0.47 |
| 13:L:4:LEU:HG | 13:L:8:LEU:HG | 1.96 | 0.47 |
| 15:N:269:MET:HB3 | 15:N:281:LEU:HD11 | 1.96 | 0.47 |
| 15:N:25:VAL:HG11 | 15:N:82:PHE:HB2 | 1.96 | 0.47 |
| 14:U:304:THR:HG21 | 14:U:386:LYS:HB2 | 1.95 | 0.47 |
| 14:U:92:GLU:C | 14:U:94:ARG:H | 2.17 | 0.47 |
| 15:V:63:THR:HG21 | 15:V:96:HIS:ND1 | 2.28 | 0.47 |
| 3:3:383:PRO:HG2 | 3:3:531:LYS:HA | 1.96 | 0.47 |
| 4:4:105:LEU:HD21 | 4:4:335:PHE:CE1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:211:LEU:HB2 | 1:B:216:THR:HG21 | 1.96 | 0.47 |
| 3:D:463:ALA:O | 3:D:465:HIS:ND1 | 2.47 | 0.47 |
| 4:E:341:GLU:HG2 | 4:E:358:VAL:HG22 | 1.96 | 0.47 |
| 14:M:126:LEU:HD11 | 14:M:149:VAL:HG22 | 1.96 | 0.47 |
| 14:M:359:LEU:O | 14:M:363:LEU:HG | 2.14 | 0.47 |
| 14:M:36:ASN:OD1 | 14:M:79:ALA:HB2 | 2.14 | 0.47 |
| 13:T:293:LYS:O | 13:T:297:TYR:HD1 | 1.97 | 0.47 |
| 15:V:108:LEU:HB2 | 15:V:147:PHE:CE2 | 2.48 | 0.47 |
| 1:1:343:ASN:O | 1:1:346:ARG:HG2 | 2.14 | 0.47 |
| 3:3:115:HIS:CG | 3:3:116:PRO:HD2 | 2.49 | 0.47 |
| 2:C:81:GLN:HB3 | 2:C:122:VAL:CG2 | 2.45 | 0.47 |
| 3:D:690:GLY:HA3 | 3:D:770:ARG:HH21 | 1.79 | 0.47 |
| 5:F:6:VAL:HG22 | 5:F:41:TYR:HE1 | 1.78 | 0.47 |
| 13:L:340:ILE:O | 13:L:345:GLY:N | 2.28 | 0.47 |
| 15:N:168:GLU:H | 15:N:172:TYR:HB2 | 1.79 | 0.47 |
| 15:N:62:PHE:CD2 | 15:N:221:ALA:HB2 | 2.49 | 0.47 |
| 14:U:221:ASN:ND2 | 14:U:228:ASP:OD1 | 2.48 | 0.47 |
| 3:3:421:LYS:N | 3:3:436:GLN:OE1 | 2.38 | 0.47 |
| 3:3:438:LYS:O | 3:3:441:MET:HG3 | 2.14 | 0.47 |
| 3:3:670:PRO:HG3 | 3:3:675:ARG:O | 2.14 | 0.47 |
| 6:6:28:VAL:O | 6:6:32:ARG:HG3 | 2.14 | 0.47 |
| 4:E:236:GLY:O | 4:E:238:SER:N | 2.48 | 0.47 |
| 16:H:136:ILE:HG23 | 16:H:232:TYR:HD2 | 1.78 | 0.47 |
| 16:H:158:SER:HB2 | 16:H:305:LEU:HD21 | 1.95 | 0.47 |
| 11:J:20:VAL:HG11 | 12:K:13:LEU:O | 2.15 | 0.47 |
| 13:L:582:GLN:HA | 13:L:589:TYR:HE1 | 1.80 | 0.47 |
| 16:Q:133:VAL:HG22 | 16:Q:159:LEU:HD23 | 1.96 | 0.47 |
| 16:Q:50:ARG:C | 16:Q:52:GLY:H | 2.15 | 0.47 |
| 14:U:205:THR:HG23 | 14:U:238:VAL:HG23 | 1.96 | 0.47 |
| 9:W:41:ARG:NH1 | 9:W:91:GLU:OE1 | 2.47 | 0.47 |
| 4:4:371:ARG:HH22 | 4:4:376:VAL:HG21 | 1.76 | 0.47 |
| 3:D:694:LEU:HB3 | 3:D:762:ALA:CB | 2.42 | 0.47 |
| 3:D:7:ASN:ND2 | 3:D:94:ASP:OD1 | 2.45 | 0.47 |
| 16:H:194:TRP:CE2 | 16:H:265:GLY:HA3 | 2.50 | 0.47 |
| 13:L:463:HIS:CG | 13:L:464:PRO:HD3 | 2.49 | 0.47 |
| 14:M:335:ARG:HG3 | 14:M:336:THR:HG23 | 1.96 | 0.47 |
| 14:M:87:LEU:HD11 | 14:M:432:PHE:HB2 | 1.97 | 0.47 |
| 11:R:50:PHE:HB2 | 11:R:124:PRO:HD3 | 1.97 | 0.47 |
| 13:T:161:VAL:HG13 | 13:T:222:LEU:HD22 | 1.97 | 0.47 |
| 15:V:294:LEU:HD12 | 15:V:405:ALA:HB3 | 1.96 | 0.47 |
| 15:V:328:VAL:HG13 | 15:V:339:LEU:HD21 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:211:SER:HB2 | 4:4:215:TYR:N | 2.29 | 0.47 |
| 3:D:297:GLY:HA3 | 3:D:703:GLN:NE2 | 2.29 | 0.47 |
| 3:D:621:VAL:O | 3:D:622:LEU:HD23 | 2.14 | 0.47 |
| 4:E:44:MET:HB2 | 4:E:56:VAL:HB | 1.96 | 0.47 |
| 16:H:146:LYS:HA | 16:H:149:LEU:HB2 | 1.97 | 0.47 |
| 13:L:90:TYR:OH | 13:L:334:LEU:O | 2.29 | 0.47 |
| 7:O:43:LEU:CD1 | 7:O:133:LYS:HG3 | 2.44 | 0.47 |
| 13:T:88:HIS:NE2 | 13:T:108:PHE:HB3 | 2.28 | 0.47 |
| 13:T:176:LEU:HD11 | 13:T:209:LEU:HD11 | 1.96 | 0.47 |
| 14:U:318:SER:HA | 14:U:321:TYR:CZ | 2.50 | 0.47 |
| 1:1:201:LEU:O | 1:1:204:PRO:HD2 | 2.15 | 0.47 |
| 3:3:123:ASP:OD2 | 3:3:241:ARG:HA | 2.15 | 0.47 |
| 5:5:78:PRO:HA | 5:5:83:GLY:HA3 | 1.96 | 0.47 |
| 7:9:105:GLU:OE2 | 7:9:167:ARG:NH2 | 2.47 | 0.47 |
| 3:D:301:ALA:O | 3:D:305:ARG:HD2 | 2.14 | 0.47 |
| 3:D:615:VAL:HG22 | 3:D:621:VAL:HG12 | 1.97 | 0.47 |
| 4:E:248:VAL:HB | 4:E:347:GLU:HB2 | 1.97 | 0.47 |
| 16:H:224:ALA:HA | 16:H:229:VAL:HA | 1.97 | 0.47 |
| 14:M:194:PHE:HB2 | 14:M:249:ALA:HB3 | 1.97 | 0.47 |
| 7:O:40:ARG:HH22 | 7:O:42:VAL:HG12 | 1.79 | 0.47 |
| 14:U:10:VAL:HG23 | 14:U:104:GLY:HA3 | 1.97 | 0.47 |
| 15:V:120:ALA:O | 15:V:123:THR:OG1 | 2.27 | 0.47 |
| 4:E:341:GLU:OE1 | 5:F:91:ARG:NH2 | 2.47 | 0.47 |
| 4:E:84:ARG:O | 6:G:83:ARG:NH2 | 2.47 | 0.47 |
| 13:L:358:HIS:HB3 | 13:L:433:HIS:CE1 | 2.49 | 0.47 |
| 15:N:17:GLY:HA3 | 15:N:82:PHE:CD2 | 2.49 | 0.47 |
| 12:S:2:SER:HA | 12:S:5:LEU:HD12 | 1.96 | 0.47 |
| 15:V:415:LEU:HB3 | 15:V:418:LEU:HD13 | 1.96 | 0.47 |
| 1:1:386:ASN:O | 1:1:390:LEU:HG | 2.15 | 0.47 |
| 3:3:169:PRO:HA | 3:3:175:ILE:HA | 1.96 | 0.47 |
| 4:4:175:ILE:HG13 | 4:4:335:PHE:HZ | 1.80 | 0.47 |
| 5:5:145:PRO:HA | 5:5:150:TYR:CD1 | 2.50 | 0.47 |
| 1:B:211:LEU:HG | 1:B:212:TRP:CE3 | 2.50 | 0.47 |
| 3:D:621:VAL:HG21 | 3:D:670:PRO:O | 2.15 | 0.47 |
| 16:H:219:PHE:HD2 | 16:H:299:ARG:HE | 1.60 | 0.47 |
| 13:L:394:THR:HB | 13:L:484:HIS:O | 2.15 | 0.47 |
| 14:M:331:ARG:HA | 14:M:331:ARG:HD2 | 1.79 | 0.47 |
| 15:N:277:ASN:C | 15:N:279:GLN:H | 2.19 | 0.47 |
| 11:R:2:SER:HA | 11:R:5:GLU:HB3 | 1.96 | 0.47 |
| 10:P:56:ARG:HH11 | 11:R:75:PHE:H | 1.62 | 0.47 |
| 9:X:102:LEU:HG | 9:X:110:LEU:HD13 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:372:ALA:O | 1:1:376:THR:OG1 | 2.21 | 0.47 |
| 13:L:217:SER:HA | 13:L:246:VAL:HG12 | 1.97 | 0.47 |
| 15:N:190:ALA:HA | 15:N:192:PHE:H | 1.80 | 0.47 |
| 16:Q:2:THR:HA | 16:Q:5:TYR:CD2 | 2.47 | 0.47 |
| 15:V:41:LEU:O | 15:V:44:TRP:HB2 | 2.15 | 0.47 |
| 3:3:476:ILE:O | 3:3:480:LEU:HG | 2.15 | 0.47 |
| 4:4:86:ASP:HB3 | 4:4:93:HIS:CD2 | 2.50 | 0.47 |
| 5:5:1:MET:HB3 | 5:5:5:ARG:NH2 | 2.30 | 0.47 |
| 1:B:162:LEU:O | 1:B:165:THR:HG22 | 2.15 | 0.47 |
| 1:B:341:MET:HE1 | 1:B:409:PRO:HB2 | 1.96 | 0.47 |
| 5:F:35:LYS:NZ | 5:F:104:VAL:HA | 2.30 | 0.47 |
| 6:G:25:GLU:HA | 6:G:28:VAL:HG12 | 1.97 | 0.47 |
| 16:H:304:GLN:HE22 | 16:H:307:ARG:HD2 | 1.79 | 0.47 |
| 11:J:19:VAL:HG21 | 11:J:32:LEU:HB2 | 1.95 | 0.47 |
| 13:L:439:PRO:HG2 | 13:L:442:MET:HE3 | 1.96 | 0.47 |
| 7:O:59:CYS:HB2 | 7:O:104:CYS:CB | 2.44 | 0.47 |
| 15:V:272:ALA:HB3 | 15:V:281:LEU:HD13 | 1.97 | 0.47 |
| 15:V:312:LEU:HD13 | 15:V:326:PHE:CZ | 2.50 | 0.47 |
| 13:T:572:ARG:NH2 | 15:V:373:TYR:OH | 2.41 | 0.47 |
| 3:3:125:GLY:HA3 | 3:3:245:ARG:HH21 | 1.78 | 0.46 |
| 3:D:360:LEU:O | 3:D:364:LEU:N | 2.39 | 0.46 |
| 4:E:391:PRO:HB2 | 16:Q:301:ARG:HB2 | 1.97 | 0.46 |
| 5:F:34:PHE:CD2 | 5:F:102:PRO:HG2 | 2.51 | 0.46 |
| 16:H:52:GLY:HA3 | 16:H:55:GLY:N | 2.28 | 0.46 |
| 14:M:151:PHE:CD2 | 14:M:213:TRP:HB3 | 2.49 | 0.46 |
| 15:N:116:LEU:HD23 | 15:N:119:TYR:CE2 | 2.50 | 0.46 |
| 15:N:290:LEU:HD11 | 15:N:408:LEU:HD23 | 1.97 | 0.46 |
| 13:T:132:GLU:OE2 | 13:T:163:ARG:NH1 | 2.47 | 0.46 |
| 14:U:75:PHE:CZ | 14:U:111:ALA:HB2 | 2.50 | 0.46 |
| 15:V:283:PHE:O | 15:V:287:THR:HG23 | 2.14 | 0.46 |
| 1:1:239:ALA:HA | 1:1:247:LYS:HB3 | 1.96 | 0.46 |
| 3:3:230:CYS:SG | 3:3:234:ALA:HB3 | 2.55 | 0.46 |
| 3:3:404:GLU:OE1 | 3:3:698:MET:N | 2.27 | 0.46 |
| 4:4:173:ILE:O | 4:4:174:ARG:NH1 | 2.48 | 0.46 |
| 7:9:158:LYS:O | 7:9:158:LYS:HG3 | 2.15 | 0.46 |
| 1:B:114:LEU:HD13 | 1:B:221:VAL:HG13 | 1.96 | 0.46 |
| 3:D:688:ARG:HA | 3:D:688:ARG:HD3 | 1.56 | 0.46 |
| 4:E:143:LEU:HD23 | 4:E:143:LEU:H | 1.80 | 0.46 |
| 4:E:205:GLU:OE1 | 4:E:284:ARG:NH2 | 2.49 | 0.46 |
| 6:G:163:TYR:O | 7:O:152:ARG:NH1 | 2.49 | 0.46 |
| 16:H:289:PHE:O | 16:H:293:ILE:HG12 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:105:ALA:O | 11:J:109:TRP:HB2 | 2.15 | 0.46 |
| 13:L:63:ILE:HG21 | 13:L:125:PRO:HG2 | 1.98 | 0.46 |
| 14:M:331:ARG:HA | 14:M:331:ARG:HH11 | 1.79 | 0.46 |
| 15:N:241:VAL:O | 15:N:245:ASN:ND2 | 2.48 | 0.46 |
| 11:R:65:VAL:HG23 | 16:Q:134:TYR:CZ | 2.50 | 0.46 |
| 14:U:95:PHE:HB3 | 14:U:136:TYR:CZ | 2.50 | 0.46 |
| 1:1:26:SER:HA | 1:1:31:TYR:CG | 2.50 | 0.46 |
| 1:1:257:PRO:HD2 | 1:1:330:LEU:HB2 | 1.97 | 0.46 |
| 2:2:112:THR:HG23 | 2:2:115:GLY:H | 1.79 | 0.46 |
| 4:4:32:PRO:HG2 | 6:6:91:VAL:HG11 | 1.96 | 0.46 |
| 6:6:32:ARG:HD2 | 6:6:104:TRP:HH2 | 1.81 | 0.46 |
| 1:B:122:GLY:HA2 | 1:B:127:ALA:HB3 | 1.98 | 0.46 |
| 1:B:302:PHE:CZ | 1:B:307:LEU:HD21 | 2.50 | 0.46 |
| 10:A:81:TYR:CE2 | 16:H:325:ALA:HB1 | 2.46 | 0.46 |
| 14:M:186:GLN:HG2 | 14:M:187:GLU:H | 1.81 | 0.46 |
| 14:M:332:LEU:HA | 14:M:335:ARG:HG2 | 1.97 | 0.46 |
| 15:N:299:LEU:HD22 | 15:N:307:VAL:HG11 | 1.98 | 0.46 |
| 10:P:68:PHE:CD2 | 16:Q:164:LEU:HB2 | 2.51 | 0.46 |
| 3:D:611:ARG:NH2 | 9:X:101:ALA:HB1 | 2.24 | 0.46 |
| 3:3:506:ILE:HG12 | 3:3:533:LEU:HB2 | 1.98 | 0.46 |
| 4:4:28:LEU:HD11 | 16:H:147:TYR:CD2 | 2.51 | 0.46 |
| 5:5:164:TYR:HB3 | 9:W:37:TRP:CZ3 | 2.51 | 0.46 |
| 4:4:162:TRP:NE1 | 7:9:34:LYS:HD2 | 2.30 | 0.46 |
| 3:D:203:ILE:HG21 | 8:I:88:ARG:HG2 | 1.96 | 0.46 |
| 4:E:50:GLU:O | 4:E:390:VAL:HG23 | 2.15 | 0.46 |
| 4:4:147:PHE:HE2 | 16:H:45:ARG:HD3 | 1.81 | 0.46 |
| 13:L:458:TYR:HD1 | 13:L:461:LEU:HD21 | 1.80 | 0.46 |
| 13:L:461:LEU:N | 13:L:467:ASN:OD1 | 2.48 | 0.46 |
| 14:M:260:LEU:HB3 | 14:M:301:PHE:CD2 | 2.50 | 0.46 |
| 10:P:67:LEU:HD23 | 16:Q:310:TRP:CZ2 | 2.51 | 0.46 |
| 16:Q:25:LEU:O | 16:Q:28:PHE:HD1 | 1.96 | 0.46 |
| 7:O:10:LEU:HD12 | 16:Q:296:THR:HG21 | 1.97 | 0.46 |
| 15:V:176:LEU:HD23 | 15:V:176:LEU:HA | 1.80 | 0.46 |
| 1:1:291:ILE:O | 1:1:328:VAL:HA | 2.16 | 0.46 |
| 18:1:502:FMN:O4' | 18:1:502:FMN:O2' | 2.33 | 0.46 |
| 2:2:146:THR:HG23 | 2:2:149:ARG:H | 1.81 | 0.46 |
| 3:3:201:ASP:OD1 | 3:3:202:PHE:N | 2.43 | 0.46 |
| 4:4:55:VAL:O | 4:4:382:PRO:HG3 | 2.16 | 0.46 |
| 7:9:133:LYS:HG2 | 7:9:137:LEU:HD11 | 1.97 | 0.46 |
| 1:B:5:ILE:H | 1:B:12:ARG:HH22 | 1.62 | 0.46 |
| 5:F:2:ARG:NH1 | 5:F:45:GLY:O | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:83:PHE:HB3 | 11:J:85:PRO:HG3 | 1.97 | 0.46 |
| 14:M:99:ALA:HB2 | 14:M:226:LEU:HD21 | 1.98 | 0.46 |
| 11:R:154:VAL:O | 11:R:158:GLU:HB2 | 2.15 | 0.46 |
| 2:2:108:PRO:HA | 2:2:119:VAL:HG23 | 1.98 | 0.46 |
| 4:4:193:LEU:HA | 4:4:196:VAL:HG12 | 1.97 | 0.46 |
| 5:5:38:MET:HA | 5:5:41:TYR:CD2 | 2.49 | 0.46 |
| 6:6:101:ASP:OD2 | 10:A:35:LYS:HB2 | 2.15 | 0.46 |
| 10:A:93:PHE:O | 10:A:96:VAL:HG12 | 2.16 | 0.46 |
| 1:B:250:LYS:HB3 | 1:B:252:TYR:CE1 | 2.50 | 0.46 |
| 1:B:291:ILE:O | 1:B:328:VAL:HA | 2.15 | 0.46 |
| 2:C:24:ARG:HE | 2:C:55:THR:HB | 1.80 | 0.46 |
| 4:E:409:ARG:NH2 | 5:F:117:GLU:OE2 | 2.49 | 0.46 |
| 6:G:28:VAL:O | 6:G:32:ARG:HG3 | 2.16 | 0.46 |
| 8:I:58:SER:HB3 | 8:I:69:LEU:HD23 | 1.97 | 0.46 |
| 13:L:13:GLY:O | 13:L:17:LEU:HG | 2.15 | 0.46 |
| 13:L:325:HIS:HA | 13:L:328:PHE:CE2 | 2.50 | 0.46 |
| 15:N:265:HIS:NE2 | 15:N:375:TYR:OH | 2.48 | 0.46 |
| 13:T:153:ASP:OD1 | 14:U:411:GLN:NE2 | 2.37 | 0.46 |
| 3:3:154:TYR:CZ | 4:4:312:PRO:HB3 | 2.50 | 0.46 |
| 2:C:112:THR:HG22 | 2:C:117:PHE:H | 1.80 | 0.46 |
| 3:D:223:SER:O | 3:D:226:ILE:HG12 | 2.16 | 0.46 |
| 3:D:341:VAL:HB | 3:D:364:LEU:HD21 | 1.97 | 0.46 |
| 4:E:140:LEU:HD13 | 4:E:217:ARG:HH22 | 1.80 | 0.46 |
| 4:E:350:ARG:O | 4:E:373:PRO:HB2 | 2.16 | 0.46 |
| 6:G:115:GLY:HA3 | 6:G:125:GLN:CD | 2.36 | 0.46 |
| 16:H:70:GLU:O | 16:H:70:GLU:HG3 | 2.16 | 0.46 |
| 14:M:338:THR:HG22 | 14:M:340:GLU:H | 1.79 | 0.46 |
| 16:Q:150:LEU:O | 16:Q:154:ARG:HG3 | 2.15 | 0.46 |
| 9:W:35:THR:OG1 | 9:W:36:ASP:N | 2.49 | 0.46 |
| 9:X:35:THR:N | 9:X:92:ALA:O | 2.34 | 0.46 |
| 1:1:189:MET:O | 1:1:193:GLU:HB2 | 2.16 | 0.46 |
| 3:3:268:ASP:CG | 3:3:278:ARG:NH1 | 2.68 | 0.46 |
| 3:3:269:THR:OG1 | 3:3:628:PRO:HD2 | 2.16 | 0.46 |
| 4:4:245:ASN:O | 5:5:79:GLY:HA3 | 2.16 | 0.46 |
| 2:C:85:THR:HB | 20:C:201:FES:S2 | 2.56 | 0.46 |
| 3:D:165:ASP:HB3 | 3:D:178:ARG:HD2 | 1.98 | 0.46 |
| 3:D:237:ASP:OD1 | 3:D:239:THR:HG22 | 2.15 | 0.46 |
| 3:D:225:ASN:ND2 | 3:D:289:TRP:HB3 | 2.31 | 0.46 |
| 4:E:85:MET:HE2 | 4:E:370:VAL:HG11 | 1.98 | 0.46 |
| 13:L:26:GLU:O | 13:L:29:PRO:HD2 | 2.16 | 0.46 |
| 13:L:317:VAL:HG12 | 13:L:388:ILE:HG12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:4:LYS:HE2 | 16:Q:352:VAL:O | 2.15 | 0.46 |
| 3:3:397:LEU:HD21 | 3:3:480:LEU:CD1 | 2.34 | 0.46 |
| 3:3:300:TRP:NE1 | 3:3:703:GLN:HG2 | 2.31 | 0.46 |
| 4:4:105:LEU:HD13 | 4:4:309:ILE:HD13 | 1.96 | 0.46 |
| 7:9:30:PRO:HB2 | 7:9:162:VAL:HG22 | 1.96 | 0.46 |
| 18:B:502:FMN:H9 | 19:B:503:NAI:H52N | 1.96 | 0.46 |
| 2:C:61:MET:O | 2:C:65:SER:OG | 2.29 | 0.46 |
| 4:4:144:THR:HA | 16:H:43:GLN:OE1 | 2.16 | 0.46 |
| 15:N:313:ARG:HB2 | 15:N:384:ALA:HB3 | 1.97 | 0.46 |
| 16:Q:43:GLN:HE21 | 16:Q:45:ARG:CZ | 2.28 | 0.46 |
| 11:R:29:ALA:O | 11:R:33:ILE:HG13 | 2.16 | 0.46 |
| 13:T:246:VAL:HB | 13:T:303:LEU:HD21 | 1.98 | 0.46 |
| 13:T:41:PHE:HB2 | 13:T:81:THR:HB | 1.98 | 0.46 |
| 15:V:198:ASP:OD1 | 15:V:256:ARG:NH2 | 2.47 | 0.46 |
| 1:B:352:SER:OG | 1:B:359:CYS:SG | 2.61 | 0.46 |
| 3:D:190:TYR:O | 3:D:195:PRO:HD2 | 2.16 | 0.46 |
| 3:D:654:PHE:CE2 | 3:D:660:ALA:HA | 2.51 | 0.46 |
| 4:E:144:THR:HG22 | 4:E:148:TYR:CE1 | 2.41 | 0.46 |
| 4:E:390:VAL:HB | 4:E:391:PRO:HD3 | 1.98 | 0.46 |
| 4:E:59:ILE:O | 6:G:87:LYS:NZ | 2.46 | 0.46 |
| 4:E:379:GLN:HG2 | 5:F:113:PHE:CD2 | 2.51 | 0.46 |
| 5:F:82:ASP:N | 5:F:82:ASP:OD1 | 2.49 | 0.46 |
| 6:G:82:GLY:HA2 | 17:G:201:SF4:S4 | 2.56 | 0.46 |
| 16:H:138:LEU:HA | 16:H:138:LEU:HD23 | 1.77 | 0.46 |
| 14:U:411:GLN:NE2 | 14:U:416:GLU:OE2 | 2.26 | 0.46 |
| 15:V:257:LEU:HD11 | 15:V:374:TYR:HB2 | 1.98 | 0.46 |
| 9:W:24:LEU:HD21 | 9:W:52:THR:HG21 | 1.96 | 0.46 |
| 3:3:719:HIS:ND1 | 3:3:753:VAL:O | 2.41 | 0.45 |
| 4:4:62:LEU:HD23 | 4:4:62:LEU:HA | 1.72 | 0.45 |
| 1:B:159:GLY:H | 1:B:162:LEU:HD21 | 1.81 | 0.45 |
| 1:B:356:CYS:N | 17:B:501:SF4:S3 | 2.78 | 0.45 |
| 2:C:50:ALA:HA | 2:C:53:VAL:HG12 | 1.98 | 0.45 |
| 3:D:38:HIS:NE2 | 3:D:430:THR:HG21 | 2.31 | 0.45 |
| 3:D:642:ALA:O | 3:D:652:PRO:HG3 | 2.17 | 0.45 |
| 5:F:80:TRP:CE3 | 5:F:80:TRP:HA | 2.51 | 0.45 |
| 16:H:17:ALA:O | 16:H:21:VAL:HG23 | 2.16 | 0.45 |
| 16:H:293:ILE:HG23 | 16:H:297:TRP:CE3 | 2.51 | 0.45 |
| 14:M:119:TYR:OH | 14:M:160:LEU:HB2 | 2.16 | 0.45 |
| 16:Q:20:VAL:O | 16:Q:24:LEU:HD13 | 2.16 | 0.45 |
| 14:U:119:TYR:HE1 | 15:V:342:PHE:CE1 | 2.35 | 0.45 |
| 14:U:75:PHE:HZ | 14:U:111:ALA:HB2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:V:25:VAL:HG11 | 15:V:82:PHE:HB2 | 1.96 | 0.45 |
| 3:3:290:ILE:HB | 3:3:295:ARG:NH2 | 2.30 | 0.45 |
| 4:4:48:SER:H | 4:4:53:LEU:HD23 | 1.80 | 0.45 |
| 4:4:356:TYR:HE1 | 5:5:26:TRP:HZ2 | 1.64 | 0.45 |
| 7:9:112:ALA:HB3 | 17:9:202:SF4:S4 | 2.57 | 0.45 |
| 1:B:303:THR:H | 1:B:306:VAL:HB | 1.80 | 0.45 |
| 2:C:106:ILE:CD1 | 2:C:112:THR:CA | 2.91 | 0.45 |
| 3:D:124:LYS:HG2 | 3:D:236:LEU:HD21 | 1.98 | 0.45 |
| 3:D:40:SER:HB3 | 3:D:437:ILE:HG22 | 1.99 | 0.45 |
| 3:D:651:ARG:NH1 | 3:D:652:PRO:O | 2.50 | 0.45 |
| 4:E:236:GLY:C | 4:E:238:SER:H | 2.20 | 0.45 |
| 5:F:123:GLY:HA2 | 5:F:144:HIS:CE1 | 2.52 | 0.45 |
| 6:G:36:LEU:HD11 | 6:G:155:GLN:HG3 | 1.99 | 0.45 |
| 8:I:27:LYS:HD3 | 8:I:27:LYS:HA | 1.82 | 0.45 |
| 11:J:92:LEU:O | 11:J:95:LEU:HB3 | 2.16 | 0.45 |
| 11:J:119:LEU:HD11 | 12:K:47:ARG:HA | 1.97 | 0.45 |
| 15:N:303:SER:HB3 | 15:N:307:VAL:HG22 | 1.97 | 0.45 |
| 7:O:163:VAL:O | 7:O:177:THR:HA | 2.17 | 0.45 |
| 11:R:105:ALA:O | 11:R:109:TRP:HB2 | 2.16 | 0.45 |
| 13:T:340:ILE:HB | 13:T:345:GLY:HA2 | 1.98 | 0.45 |
| 14:U:54:PRO:HA | 14:U:62:TYR:CD1 | 2.51 | 0.45 |
| 14:U:22:ARG:NH1 | 14:U:92:GLU:HG3 | 2.31 | 0.45 |
| 15:V:207:VAL:O | 15:V:211:MET:HG3 | 2.15 | 0.45 |
| 15:V:38:ALA:HA | 15:V:41:LEU:HD12 | 1.98 | 0.45 |
| 3:3:132:ASP:O | 3:3:136:GLU:HG3 | 2.17 | 0.45 |
| 3:3:76:GLN:HG3 | 3:3:77:PRO:HD2 | 1.98 | 0.45 |
| 3:3:734:VAL:HG13 | 3:3:775:VAL:HG13 | 1.99 | 0.45 |
| 4:4:163:VAL:HG13 | 4:4:164:THR:HG23 | 1.98 | 0.45 |
| 4:4:214:PHE:CE2 | 4:4:273:PHE:HD2 | 2.34 | 0.45 |
| 6:6:59:ASP:OD1 | 6:6:62:ARG:NH2 | 2.49 | 0.45 |
| 7:9:63:CYS:HA | 17:9:201:SF4:S2 | 2.56 | 0.45 |
| 2:C:6:ASP:HB3 | 2:C:7:LYS:HE3 | 1.99 | 0.45 |
| 3:D:120:PRO:O | 3:D:245:ARG:NH1 | 2.49 | 0.45 |
| 3:D:329:LEU:HD12 | 3:D:584:VAL:HG11 | 1.98 | 0.45 |
| 3:D:657:HIS:O | 3:D:661:GLN:HG2 | 2.16 | 0.45 |
| 16:H:300:LEU:O | 16:H:301:ARG:HG2 | 2.17 | 0.45 |
| 12:K:7:SER:HB2 | 12:K:37:ALA:O | 2.17 | 0.45 |
| 13:L:111:PHE:CZ | 13:L:134:VAL:HG13 | 2.51 | 0.45 |
| 11:J:103:ILE:HG13 | 15:N:174:LEU:HD13 | 1.98 | 0.45 |
| 16:Q:136:ILE:HG23 | 16:Q:232:TYR:HD2 | 1.81 | 0.45 |
| 16:Q:76:GLN:O | 16:Q:144:GLY:HA3 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:T:291:ILE:O | 13:T:295:VAL:HG23 | 2.16 | 0.45 |
| 13:T:380:SER:HB3 | 13:T:457:GLY:H | 1.81 | 0.45 |
| 15:V:62:PHE:CG | 15:V:221:ALA:HB2 | 2.51 | 0.45 |
| 7:9:42:VAL:HA | 7:9:136:MET:O | 2.16 | 0.45 |
| 10:A:38:ARG:O | 10:A:42:MET:HG3 | 2.16 | 0.45 |
| 1:B:32:TYR:OH | 1:B:116:GLU:OE1 | 2.21 | 0.45 |
| 1:B:193:GLU:OE1 | 1:B:200:ARG:NH2 | 2.47 | 0.45 |
| 4:E:193:LEU:HA | 4:E:196:VAL:HG12 | 1.98 | 0.45 |
| 4:E:40:VAL:HG21 | 6:G:88:MET:HE1 | 1.98 | 0.45 |
| 11:J:64:VAL:HG13 | 16:H:134:TYR:OH | 2.16 | 0.45 |
| 16:H:215:ALA:O | 16:H:294:ARG:NH1 | 2.39 | 0.45 |
| 16:H:293:ILE:HD12 | 16:H:297:TRP:CZ3 | 2.51 | 0.45 |
| 13:L:356:TRP:CD2 | 13:L:363:ARG:HD2 | 2.51 | 0.45 |
| 13:L:385:LYS:NZ | 13:L:413:THR:OG1 | 2.50 | 0.45 |
| 10:P:23:ALA:O | 10:P:27:VAL:HG23 | 2.17 | 0.45 |
| 10:P:66:MET:O | 10:P:69:ILE:HG12 | 2.15 | 0.45 |
| 11:R:16:GLY:O | 11:R:19:VAL:HG12 | 2.15 | 0.45 |
| 13:T:373:LEU:HD21 | 13:T:416:TYR:HE1 | 1.81 | 0.45 |
| 14:U:238:VAL:O | 14:U:241:PHE:HB2 | 2.17 | 0.45 |
| 9:X:125:ILE:HD11 | 9:X:126:TYR:CZ | 2.51 | 0.45 |
| 3:3:180:ARG:O | 3:3:232:VAL:HG21 | 2.17 | 0.45 |
| 3:3:715:GLU:O | 3:3:760:LEU:HD12 | 2.16 | 0.45 |
| 4:4:197:LEU:N | 4:4:198:PRO:HD2 | 2.31 | 0.45 |
| 4:4:385:CYS:HB3 | 4:4:396:ILE:HG21 | 1.97 | 0.45 |
| 5:5:82:ASP:N | 5:5:82:ASP:OD1 | 2.48 | 0.45 |
| 1:B:121:ALA:O | 1:B:125:ILE:HG12 | 2.17 | 0.45 |
| 3:D:472:GLU:O | 3:D:476:ILE:HD12 | 2.16 | 0.45 |
| 3:D:304:ASN:O | 3:D:589:HIS:NE2 | 2.50 | 0.45 |
| 4:E:283:MET:O | 4:E:287:VAL:HG23 | 2.16 | 0.45 |
| 16:H:147:TYR:CE1 | 16:H:228:LEU:HD13 | 2.51 | 0.45 |
| 8:I:68:LEU:HD11 | 8:I:115:PHE:CE1 | 2.52 | 0.45 |
| 13:L:79:ILE:HD11 | 13:L:323:PHE:HD1 | 1.82 | 0.45 |
| 13:L:33:ALA:O | 13:L:37:VAL:HG23 | 2.17 | 0.45 |
| 13:L:147:LYS:NZ | 14:M:349:GLN:OE1 | 2.47 | 0.45 |
| 7:O:4:LYS:O | 7:O:8:GLN:HG3 | 2.16 | 0.45 |
| 4:E:147:PHE:HE2 | 16:Q:45:ARG:HD3 | 1.81 | 0.45 |
| 13:T:379:LEU:HD22 | 13:T:454:VAL:HA | 1.99 | 0.45 |
| 14:U:332:LEU:O | 14:U:336:THR:OG1 | 2.20 | 0.45 |
| 15:V:272:ALA:O | 15:V:276:GLY:N | 2.45 | 0.45 |
| 3:3:406:ALA:O | 3:3:409:LEU:HB2 | 2.16 | 0.45 |
| 6:6:37:TRP:NE1 | 6:6:67:VAL:HB | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:7:TYR:N | 10:A:7:TYR:CD1 | 2.84 | 0.45 |
| 10:A:7:TYR:N | 10:A:7:TYR:HD1 | 2.15 | 0.45 |
| 1:B:67:GLY:HA3 | 19:B:503:NAI:H1D | 1.99 | 0.45 |
| 3:D:563:ALA:O | 3:D:580:LYS:HG2 | 2.17 | 0.45 |
| 4:E:250:LYS:HE2 | 4:E:262:PHE:HB3 | 1.97 | 0.45 |
| 4:E:369:LYS:HG3 | 5:F:53:VAL:HG23 | 1.98 | 0.45 |
| 5:F:145:PRO:O | 5:F:150:TYR:HB3 | 2.17 | 0.45 |
| 13:L:391:ALA:HA | 13:L:394:THR:OG1 | 2.17 | 0.45 |
| 15:N:126:ARG:O | 15:N:129:GLY:N | 2.48 | 0.45 |
| 15:N:40:LEU:HD12 | 15:N:67:LEU:HD12 | 1.99 | 0.45 |
| 16:Q:138:LEU:HA | 16:Q:138:LEU:HD23 | 1.84 | 0.45 |
| 16:Q:15:LEU:O | 16:Q:19:LEU:HG | 2.17 | 0.45 |
| 16:Q:274:VAL:CG2 | 16:Q:275:PRO:HD2 | 2.47 | 0.45 |
| 16:Q:216:ARG:HD2 | 16:Q:294:ARG:HD2 | 1.98 | 0.45 |
| 10:P:34:LYS:N | 16:Q:70:GLU:OE1 | 2.47 | 0.45 |
| 14:U:16:LEU:HD22 | 14:U:97:GLY:H | 1.82 | 0.45 |
| 14:U:159:MET:HG3 | 14:U:197:PHE:CE1 | 2.52 | 0.45 |
| 14:U:204:LYS:HE3 | 14:U:234:TYR:O | 2.17 | 0.45 |
| 14:U:201:PHE:CZ | 14:U:240:ALA:HB1 | 2.51 | 0.45 |
| 8:7:82:ILE:HG23 | 8:7:95:ALA:HB3 | 1.97 | 0.45 |
| 1:B:275:LEU:O | 1:B:279:TRP:HB2 | 2.16 | 0.45 |
| 1:B:297:THR:HG22 | 1:B:322:MET:HG3 | 1.99 | 0.45 |
| 13:L:34:SER:OG | 13:L:88:HIS:HB3 | 2.16 | 0.45 |
| 13:L:413:THR:HG22 | 13:L:416:TYR:OH | 2.16 | 0.45 |
| 15:N:234:ALA:HB1 | 15:N:360:VAL:HG21 | 1.99 | 0.45 |
| 4:E:314:ARG:NH1 | 7:O:106:GLU:O | 2.49 | 0.45 |
| 14:U:310:GLY:HA2 | 14:U:376:GLY:HA2 | 1.97 | 0.45 |
| 9:X:36:ASP:OD1 | 9:X:36:ASP:N | 2.48 | 0.45 |
| 2:2:154:LEU:HD23 | 2:2:154:LEU:HA | 1.87 | 0.45 |
| 2:C:135:GLN:HB2 | 2:C:141:TYR:HD1 | 1.81 | 0.45 |
| 3:D:119:CYS:N | 17:D:801:SF4:S1 | 2.90 | 0.45 |
| 3:D:224:GLY:HA3 | 3:D:295:ARG:HD2 | 1.98 | 0.45 |
| 4:E:48:SER:H | 4:E:53:LEU:HD23 | 1.82 | 0.45 |
| 16:H:190:LYS:HB2 | 16:H:268:THR:CG2 | 2.46 | 0.45 |
| 13:L:379:LEU:HA | 13:L:379:LEU:HD23 | 1.84 | 0.45 |
| 13:L:426:LEU:HB3 | 13:L:513:GLN:HE22 | 1.82 | 0.45 |
| 11:J:104:LEU:HD21 | 15:N:178:LEU:HD11 | 1.99 | 0.45 |
| 7:O:52:LYS:NZ | 7:O:171:GLU:OE2 | 2.34 | 0.45 |
| 6:G:178:ARG:NE | 9:X:125:ILE:HG22 | 2.31 | 0.45 |
| 5:5:35:LYS:HD3 | 5:5:102:PRO:HB2 | 1.99 | 0.45 |
| 1:B:223:THR:O | 1:B:227:VAL:HG23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:474:ARG:O | 3:D:520:ARG:NH1 | 2.48 | 0.45 |
| 3:D:513:GLN:HG2 | 3:D:769:LEU:HD23 | 1.98 | 0.45 |
| 3:D:654:PHE:CD2 | 3:D:660:ALA:HA | 2.51 | 0.45 |
| 3:D:664:LEU:O | 3:D:669:VAL:HG12 | 2.16 | 0.45 |
| 6:G:108:MET:HA | 6:G:137:VAL:HG13 | 1.99 | 0.45 |
| 16:H:67:ILE:HG13 | 16:H:68:PHE:CD1 | 2.52 | 0.45 |
| 14:M:313:TYR:OH | 14:M:443:MET:O | 2.23 | 0.45 |
| 16:Q:122:ILE:HA | 16:Q:125:LEU:HD12 | 1.98 | 0.45 |
| 16:Q:147:TYR:CD1 | 16:Q:229:VAL:HG22 | 2.52 | 0.45 |
| 1:1:338:VAL:O | 1:1:342:TRP:HB2 | 2.17 | 0.45 |
| 3:3:568:TYR:CD1 | 3:3:572:PRO:HG3 | 2.52 | 0.45 |
| 4:4:73:ARG:CZ | 4:4:81:TYR:OH | 2.65 | 0.45 |
| 7:9:59:CYS:HB3 | 7:9:113:ILE:HG21 | 1.99 | 0.45 |
| 7:9:149:GLU:HA | 7:9:152:ARG:HG2 | 1.98 | 0.45 |
| 1:B:270:THR:O | 1:B:311:MET:HG3 | 2.17 | 0.45 |
| 5:F:74:LEU:HD12 | 5:F:88:PHE:CZ | 2.52 | 0.45 |
| 6:G:56:ALA:HA | 16:Q:45:ARG:HB2 | 1.97 | 0.45 |
| 10:A:28:GLY:HA3 | 16:H:239:ILE:HG21 | 1.99 | 0.45 |
| 13:L:166:ASP:O | 13:L:170:MET:HG3 | 2.17 | 0.45 |
| 16:Q:177:VAL:HG11 | 16:Q:185:ILE:HA | 1.99 | 0.45 |
| 16:Q:40:ALA:HA | 16:Q:45:ARG:HH21 | 1.82 | 0.45 |
| 10:P:80:PRO:HA | 11:R:124:PRO:HB2 | 1.98 | 0.45 |
| 13:T:90:TYR:OH | 13:T:334:LEU:O | 2.14 | 0.45 |
| 14:U:354:LEU:HA | 14:U:354:LEU:HD12 | 1.77 | 0.45 |
| 11:R:152:VAL:HG22 | 15:V:87:LEU:HD22 | 1.99 | 0.45 |
| 9:W:41:ARG:HH12 | 9:W:91:GLU:CD | 2.20 | 0.45 |
| 9:W:74:LEU:HD21 | 9:W:126:TYR:HD1 | 1.81 | 0.45 |
| 9:X:35:THR:OG1 | 9:X:36:ASP:N | 2.49 | 0.45 |
| 3:3:616:ASN:HB2 | 3:3:620:ARG:O | 2.17 | 0.44 |
| 6:6:105:VAL:N | 6:6:134:ASP:OD2 | 2.36 | 0.44 |
| 6:6:21:PHE:HD1 | 6:6:23:THR:H | 1.65 | 0.44 |
| 2:C:130:THR:HB | 2:C:143:GLU:HB3 | 1.99 | 0.44 |
| 3:D:453:PRO:HA | 3:D:468:HIS:O | 2.17 | 0.44 |
| 4:E:62:LEU:HD11 | 6:G:43:LEU:O | 2.17 | 0.44 |
| 5:F:55:LEU:HD23 | 5:F:57:TYR:OH | 2.17 | 0.44 |
| 14:M:70:LEU:HD13 | 14:M:312:LEU:HD13 | 1.99 | 0.44 |
| 16:Q:225:GLU:HB3 | 16:Q:226:GLN:HG2 | 1.99 | 0.44 |
| 16:Q:314:PHE:HB2 | 16:Q:315:PRO:HD3 | 1.98 | 0.44 |
| 11:R:48:ALA:HB1 | 11:R:51:LEU:HB3 | 1.98 | 0.44 |
| 11:R:92:LEU:O | 11:R:95:LEU:HB3 | 2.17 | 0.44 |
| 1:1:288:GLN:NE2 | 1:1:332:PRO:O | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:1:337:MET:O | 1:1:341:MET:HG2 | 2.17 | 0.44 |
| 1:1:370:LEU:HD13 | 1:1:383:ASP:HB3 | 1.99 | 0.44 |
| 3:3:408:ILE:HG23 | 17:3:803:SF4:S1 | 2.57 | 0.44 |
| 3:3:464:ILE:HA | 3:3:489:MET:SD | 2.57 | 0.44 |
| 3:3:76:GLN:CG | 3:3:77:PRO:HD2 | 2.47 | 0.44 |
| 3:3:119:CYS:HB2 | 4:4:324:VAL:HG12 | 1.99 | 0.44 |
| 4:4:374:SER:O | 4:4:407:VAL:HG22 | 2.17 | 0.44 |
| 4:4:81:TYR:CZ | 6:6:117:MET:HG3 | 2.52 | 0.44 |
| 7:9:83:ALA:HB3 | 8:7:41:ILE:HG12 | 1.99 | 0.44 |
| 1:B:225:ALA:O | 1:B:229:PRO:HD2 | 2.16 | 0.44 |
| 3:D:225:ASN:HD21 | 3:D:289:TRP:HB3 | 1.83 | 0.44 |
| 3:D:689:LYS:H | 3:D:689:LYS:HG2 | 1.52 | 0.44 |
| 16:H:224:ALA:HA | 16:H:230:GLY:H | 1.82 | 0.44 |
| 16:H:260:PRO:HG3 | 16:H:286:PHE:CD2 | 2.52 | 0.44 |
| 8:I:96:HIS:O | 8:I:103:LEU:HD12 | 2.17 | 0.44 |
| 7:O:45:ARG:NH2 | 7:O:139:ASP:OD2 | 2.48 | 0.44 |
| 7:O:149:GLU:O | 7:O:153:THR:OG1 | 2.23 | 0.44 |
| 15:V:7:ALA:O | 15:V:11:VAL:HG23 | 2.17 | 0.44 |
| 3:3:307:LYS:HE3 | 3:3:632:GLY:HA2 | 1.99 | 0.44 |
| 3:3:343:LEU:HB2 | 3:3:369:LEU:HB3 | 1.99 | 0.44 |
| 8:7:105:THR:N | 8:7:108:ILE:O | 2.49 | 0.44 |
| 1:B:179:ALA:HB3 | 1:B:182:CYS:SG | 2.57 | 0.44 |
| 1:B:427:GLU:OE1 | 1:B:429:ARG:NH1 | 2.50 | 0.44 |
| 3:D:383:PRO:HD3 | 3:D:679:ARG:HH21 | 1.81 | 0.44 |
| 3:D:497:TRP:O | 3:D:528:LYS:HE3 | 2.17 | 0.44 |
| 3:D:568:TYR:CD1 | 3:D:572:PRO:HG3 | 2.53 | 0.44 |
| 4:E:230:ILE:HG21 | 5:F:47:ASN:HB3 | 1.98 | 0.44 |
| 5:F:34:PHE:HD2 | 5:F:102:PRO:HG2 | 1.83 | 0.44 |
| 5:F:31:ARG:NH2 | 5:F:98:ASP:O | 2.50 | 0.44 |
| 16:H:274:VAL:HG12 | 16:H:278:TRP:HD1 | 1.79 | 0.44 |
| 16:H:50:ARG:C | 16:H:52:GLY:H | 2.11 | 0.44 |
| 11:J:90:ARG:HG2 | 12:K:20:THR:HG23 | 1.99 | 0.44 |
| 13:L:361:GLN:O | 13:L:365:HIS:ND1 | 2.49 | 0.44 |
| 14:M:452:ARG:HA | 14:M:452:ARG:HD3 | 1.74 | 0.44 |
| 14:M:90:ARG:HA | 14:M:90:ARG:HD2 | 1.80 | 0.44 |
| 10:P:71:PHE:O | 10:P:75:VAL:HG23 | 2.16 | 0.44 |
| 9:W:98:GLU:O | 9:W:102:LEU:HB2 | 2.17 | 0.44 |
| 4:4:367:ARG:HH21 | 5:5:146:LEU:CD1 | 2.30 | 0.44 |
| 1:B:201:LEU:O | 1:B:204:PRO:HD2 | 2.18 | 0.44 |
| 1:B:250:LYS:NZ | 1:B:251:LEU:O | 2.50 | 0.44 |
| 1:B:197:ALA:HB3 | 2:C:66:PHE:CE2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:115:THR:HG21 | 4:E:297:LEU:HD13 | 1.99 | 0.44 |
| 16:H:204:LEU:HA | 16:H:204:LEU:HD23 | 1.85 | 0.44 |
| 13:L:20:PHE:O | 13:L:22:LYS:N | 2.48 | 0.44 |
| 14:M:12:PHE:HB3 | 14:M:100:LEU:HD13 | 1.99 | 0.44 |
| 14:M:318:SER:HA | 14:M:321:TYR:CZ | 2.53 | 0.44 |
| 11:R:155:ALA:HB2 | 15:V:83:GLU:HG2 | 2.00 | 0.44 |
| 3:3:270:ARG:HB3 | 3:3:275:LEU:HD11 | 1.99 | 0.44 |
| 3:3:344:TYR:HA | 3:3:370:ASP:O | 2.18 | 0.44 |
| 3:3:635:GLU:OE2 | 9:W:7:ARG:HD2 | 2.17 | 0.44 |
| 4:4:246:TYR:CD1 | 5:5:78:PRO:HD2 | 2.52 | 0.44 |
| 4:4:136:GLY:HA2 | 4:4:398:ALA:HB1 | 1.99 | 0.44 |
| 5:5:105:THR:HA | 5:5:108:TRP:O | 2.18 | 0.44 |
| 5:5:68:PHE:HE1 | 5:5:96:GLU:HA | 1.82 | 0.44 |
| 6:6:34:ASN:O | 6:6:64:GLY:HA3 | 2.18 | 0.44 |
| 6:6:84:LEU:HD11 | 6:6:89:ALA:HA | 2.00 | 0.44 |
| 6:6:96:TRP:HZ2 | 6:6:175:ALA:HB1 | 1.83 | 0.44 |
| 10:A:66:MET:O | 10:A:69:ILE:HG12 | 2.17 | 0.44 |
| 3:D:224:GLY:O | 3:D:227:THR:HB | 2.18 | 0.44 |
| 4:E:261:THR:H | 4:E:292:GLN:NE2 | 2.06 | 0.44 |
| 5:F:149:ASP:O | 9:X:112:LYS:NZ | 2.30 | 0.44 |
| 5:F:16:PRO:HD2 | 5:F:28:VAL:HG13 | 2.00 | 0.44 |
| 6:G:16:ARG:O | 6:G:19:ILE:HG22 | 2.18 | 0.44 |
| 16:H:6:PRO:HG2 | 16:H:112:GLN:HE21 | 1.83 | 0.44 |
| 16:H:72:ILE:HG22 | 16:H:237:SER:HB3 | 2.00 | 0.44 |
| 13:L:183:LEU:HA | 13:L:183:LEU:HD23 | 1.78 | 0.44 |
| 13:L:325:HIS:CD2 | 13:L:329:LYS:HG3 | 2.53 | 0.44 |
| 13:T:158:ALA:HA | 13:T:225:TRP:HB2 | 1.99 | 0.44 |
| 15:V:86:LEU:O | 15:V:89:LEU:HB2 | 2.17 | 0.44 |
| 1:1:382:LYS:O | 1:1:386:ASN:ND2 | 2.51 | 0.44 |
| 2:2:146:THR:HG22 | 2:2:149:ARG:HB2 | 1.99 | 0.44 |
| 3:3:285:VAL:HG21 | 3:3:616:ASN:HD21 | 1.83 | 0.44 |
| 5:5:131:ASP:HB2 | 5:5:133:ARG:HE | 1.82 | 0.44 |
| 3:3:143:TYR:OH | 5:5:195:LEU:O | 2.20 | 0.44 |
| 4:4:61:TYR:O | 6:6:85:SER:HB3 | 2.17 | 0.44 |
| 10:A:57:PHE:HB3 | 10:A:58:PRO:HD2 | 2.00 | 0.44 |
| 1:B:310:PRO:O | 1:B:315:HIS:HB2 | 2.18 | 0.44 |
| 3:D:583:VAL:HG21 | 3:D:597:TYR:O | 2.18 | 0.44 |
| 3:D:694:LEU:CB | 3:D:762:ALA:HB2 | 2.45 | 0.44 |
| 3:D:734:VAL:HG13 | 3:D:775:VAL:HG13 | 1.99 | 0.44 |
| 4:E:186:PHE:CZ | 4:E:190:LEU:HD22 | 2.52 | 0.44 |
| 16:Q:293:ILE:HD12 | 16:Q:297:TRP:CZ3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:35:GLU:CD | 16:Q:294:ARG:HH21 | 2.20 | 0.44 |
| 14:U:279:LYS:HA | 14:U:279:LYS:HD3 | 1.80 | 0.44 |
| 9:X:46:TYR:N | 9:X:63:PHE:O | 2.48 | 0.44 |
| 4:4:193:LEU:HD23 | 4:4:194:LEU:HD12 | 1.99 | 0.44 |
| 4:4:30:VAL:HG13 | 4:4:35:PRO:HD2 | 2.00 | 0.44 |
| 4:4:336:HIS:CE1 | 5:5:174:LEU:HD12 | 2.50 | 0.44 |
| 6:6:21:PHE:O | 6:6:25:GLU:HG2 | 2.18 | 0.44 |
| 6:6:163:TYR:H | 7:9:152:ARG:NH1 | 2.15 | 0.44 |
| 1:B:201:LEU:HD12 | 1:B:399:PHE:CZ | 2.52 | 0.44 |
| 3:D:409:LEU:HA | 3:D:409:LEU:HD23 | 1.61 | 0.44 |
| 4:E:341:GLU:HG2 | 4:E:358:VAL:HG13 | 1.99 | 0.44 |
| 4:E:350:ARG:HG2 | 4:E:401:ASP:O | 2.18 | 0.44 |
| 6:G:58:ASN:ND2 | 6:G:145:GLU:OE2 | 2.51 | 0.44 |
| 6:G:155:GLN:O | 6:G:159:ARG:HG3 | 2.18 | 0.44 |
| 6:G:26:LYS:HA | 6:G:26:LYS:HD3 | 1.82 | 0.44 |
| 11:J:72:MET:HE3 | 16:H:149:LEU:HD21 | 1.99 | 0.44 |
| 11:J:63:ILE:HG23 | 12:K:68:VAL:HG11 | 1.99 | 0.44 |
| 13:L:115:MET:HG2 | 13:L:244:THR:HG22 | 2.00 | 0.44 |
| 13:L:553:LEU:O | 14:M:270:TYR:OH | 2.15 | 0.44 |
| 16:Q:224:ALA:HA | 16:Q:230:GLY:H | 1.83 | 0.44 |
| 14:U:143:ARG:HD3 | 14:U:143:ARG:HA | 1.67 | 0.44 |
| 14:U:169:LEU:HD21 | 15:V:358:TRP:HZ2 | 1.82 | 0.44 |
| 12:S:28:PHE:CZ | 15:V:137:PHE:HZ | 2.36 | 0.44 |
| 15:V:190:ALA:HA | 15:V:192:PHE:H | 1.81 | 0.44 |
| 15:V:10:SER:HB3 | 15:V:90:TYR:HE1 | 1.82 | 0.44 |
| 5:5:163:ARG:O | 9:W:37:TRP:HH2 | 2.01 | 0.44 |
| 2:2:161:LYS:NZ | 2:2:166:ILE:HA | 2.32 | 0.44 |
| 3:3:405:GLU:HG2 | 3:3:696:PRO:HB2 | 2.00 | 0.44 |
| 4:4:205:GLU:OE2 | 4:4:281:ARG:NE | 2.50 | 0.44 |
| 4:4:239:LEU:HG | 4:4:244:VAL:HB | 2.00 | 0.44 |
| 4:4:333:GLU:O | 4:4:363:SER:OG | 2.19 | 0.44 |
| 4:4:369:LYS:HE2 | 5:5:53:VAL:HA | 2.00 | 0.44 |
| 5:5:49:LEU:HD12 | 5:5:73:GLU:O | 2.18 | 0.44 |
| 8:7:27:LYS:HD3 | 8:7:27:LYS:HA | 1.90 | 0.44 |
| 1:B:98:PRO:HB2 | 1:B:295:SER:HB2 | 1.99 | 0.44 |
| 1:B:245:GLN:HB2 | 1:B:314:GLU:CD | 2.38 | 0.44 |
| 2:C:83:CYS:HA | 2:C:122:VAL:O | 2.17 | 0.44 |
| 3:D:352:GLU:OE2 | 3:D:612:GLY:HA2 | 2.16 | 0.44 |
| 4:E:176:GLY:HA3 | 4:E:303:ARG:HB2 | 1.98 | 0.44 |
| 4:E:64:THR:HG23 | 6:G:123:ILE:HG13 | 2.00 | 0.44 |
| 4:E:87:TYR:HB3 | 4:E:169:HIS:HE1 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:292:TRP:HD1 | 16:H:296:THR:OG1 | 2.01 | 0.44 |
| 12:K:87:VAL:HG23 | 15:N:134:LEU:HD21 | 2.00 | 0.44 |
| 13:L:10:PRO:HB2 | 13:L:109:ASN:O | 2.17 | 0.44 |
| 14:U:87:LEU:HD11 | 14:U:432:PHE:HB2 | 2.00 | 0.44 |
| 15:V:188:ALA:HB3 | 15:V:216:LYS:HZ1 | 1.82 | 0.44 |
| 15:V:95:MET:HB3 | 15:V:218:ALA:HB2 | 1.99 | 0.44 |
| 1:1:296:SER:OG | 1:1:348:TYR:OH | 2.25 | 0.44 |
| 1:1:48:LYS:O | 1:1:123:TYR:OH | 2.17 | 0.44 |
| 2:2:26:ALA:O | 2:2:30:LEU:HG | 2.18 | 0.44 |
| 3:3:453:PRO:HA | 3:3:468:HIS:O | 2.17 | 0.44 |
| 3:3:586:HIS:NE2 | 3:3:640:VAL:HG21 | 2.33 | 0.44 |
| 3:3:615:VAL:HG22 | 3:3:621:VAL:HG12 | 2.00 | 0.44 |
| 1:B:186:THR:O | 1:B:200:ARG:HG3 | 2.17 | 0.44 |
| 1:B:438:ARG:OXT | 2:C:146:THR:OG1 | 2.35 | 0.44 |
| 3:D:382:PHE:HB3 | 3:D:532:VAL:HB | 1.99 | 0.44 |
| 4:E:369:LYS:HD3 | 4:E:370:VAL:N | 2.32 | 0.44 |
| 4:E:87:TYR:HD1 | 6:G:48:ILE:HD12 | 1.83 | 0.44 |
| 16:H:122:ILE:HA | 16:H:125:LEU:HD12 | 2.00 | 0.44 |
| 7:9:14:LEU:HB2 | 16:H:292:TRP:CZ2 | 2.52 | 0.44 |
| 16:H:35:GLU:OE1 | 16:H:249:TYR:OH | 2.28 | 0.44 |
| 14:M:314:LEU:HB2 | 14:M:376:GLY:HA3 | 2.00 | 0.44 |
| 15:N:196:THR:HG22 | 15:N:259:ALA:HB1 | 2.00 | 0.44 |
| 16:Q:327:VAL:O | 16:Q:331:ASP:N | 2.51 | 0.44 |
| 14:U:344:TYR:O | 14:U:347:LEU:HD23 | 2.18 | 0.44 |
| 1:1:185:GLU:HB2 | 1:1:218:ILE:HD13 | 1.99 | 0.43 |
| 4:4:50:GLU:C | 4:4:389:GLN:HE21 | 2.19 | 0.43 |
| 1:B:18:TYR:OH | 1:B:102:LYS:O | 2.27 | 0.43 |
| 1:B:310:PRO:HG2 | 1:B:315:HIS:CD2 | 2.52 | 0.43 |
| 4:E:100:ALA:HB2 | 4:E:344:VAL:HG22 | 1.99 | 0.43 |
| 4:E:171:ASN:ND2 | 4:E:174:ARG:HH22 | 2.15 | 0.43 |
| 5:F:74:LEU:HD22 | 5:F:108:TRP:CH2 | 2.52 | 0.43 |
| 6:G:41:PHE:CE2 | 6:G:43:LEU:HD21 | 2.52 | 0.43 |
| 16:H:203:PHE:HB2 | 16:H:263:PHE:CD2 | 2.52 | 0.43 |
| 13:L:104:PHE:HE2 | 13:L:108:PHE:HE2 | 1.66 | 0.43 |
| 13:L:380:SER:HA | 13:L:457:GLY:HA2 | 2.00 | 0.43 |
| 13:L:287:GLY:HA2 | 13:L:525:GLU:CG | 2.48 | 0.43 |
| 16:Q:216:ARG:NH1 | 16:Q:294:ARG:HB3 | 2.33 | 0.43 |
| 16:Q:28:PHE:O | 16:Q:32:THR:HG23 | 2.17 | 0.43 |
| 14:U:350:SER:OG | 14:U:421:GLY:HA2 | 2.18 | 0.43 |
| 15:V:93:LEU:O | 15:V:96:HIS:HB3 | 2.18 | 0.43 |
| 3:3:185:LYS:O | 3:3:189:ARG:HB2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:281:GLU:HB2 | 3:3:288:ILE:HG22 | 2.01 | 0.43 |
| 3:D:526:GLU:HG2 | 3:D:679:ARG:HH22 | 1.83 | 0.43 |
| 8:I:97:TYR:CE1 | 8:I:102:GLY:HA2 | 2.53 | 0.43 |
| 14:M:242:PHE:CE2 | 14:M:461:PHE:HD2 | 2.36 | 0.43 |
| 14:M:346:GLY:HA3 | 14:M:419:GLY:H | 1.82 | 0.43 |
| 15:N:299:LEU:HD23 | 15:N:299:LEU:HA | 1.83 | 0.43 |
| 7:O:6:LEU:O | 7:O:10:LEU:HD13 | 2.18 | 0.43 |
| 6:G:64:GLY:HA2 | 16:Q:58:GLN:NE2 | 2.33 | 0.43 |
| 13:T:12:LEU:O | 13:T:16:LEU:HG | 2.18 | 0.43 |
| 14:U:24:LEU:O | 14:U:27:LEU:HG | 2.17 | 0.43 |
| 9:W:1:MET:HG3 | 9:W:56:ASP:HB2 | 1.99 | 0.43 |
| 3:3:279:ALA:HB2 | 3:3:295:ARG:HH22 | 1.83 | 0.43 |
| 3:3:695:ARG:O | 3:3:762:ALA:HB3 | 2.18 | 0.43 |
| 4:4:329:LYS:HD2 | 4:4:329:LYS:HA | 1.80 | 0.43 |
| 5:5:68:PHE:CE1 | 5:5:96:GLU:HA | 2.53 | 0.43 |
| 6:6:25:GLU:HA | 6:6:28:VAL:HG12 | 1.99 | 0.43 |
| 1:B:157:TYR:O | 1:B:158:LEU:HD23 | 2.18 | 0.43 |
| 3:D:200:LEU:HD12 | 3:D:213:THR:HB | 2.00 | 0.43 |
| 3:D:356:LEU:HD22 | 3:D:638:LEU:HD12 | 2.01 | 0.43 |
| 16:H:45:ARG:HG2 | 16:H:46:MET:N | 2.33 | 0.43 |
| 13:L:538:TYR:O | 13:L:542:ILE:HB | 2.19 | 0.43 |
| 15:N:206:PRO:O | 15:N:209:LEU:HB3 | 2.18 | 0.43 |
| 7:O:52:LYS:HB2 | 7:O:112:ALA:HB2 | 1.99 | 0.43 |
| 16:Q:204:LEU:HA | 16:Q:204:LEU:HD23 | 1.89 | 0.43 |
| 13:T:255:ARG:HD2 | 13:T:255:ARG:HA | 1.83 | 0.43 |
| 14:U:61:VAL:HG22 | 14:U:175:PHE:CD2 | 2.54 | 0.43 |
| 14:U:91:VAL:HB | 14:U:95:PHE:CE1 | 2.53 | 0.43 |
| 3:3:33:PHE:HZ | 3:3:130:LEU:HA | 1.82 | 0.43 |
| 3:3:123:ASP:HB2 | 3:3:236:LEU:HD13 | 2.00 | 0.43 |
| 4:4:288:LYS:HA | 4:4:288:LYS:HD3 | 1.74 | 0.43 |
| 7:9:163:VAL:O | 7:9:177:THR:HA | 2.18 | 0.43 |
| 3:D:9:ARG:NH1 | 3:D:26:ALA:O | 2.51 | 0.43 |
| 14:M:69:GLY:HA3 | 14:M:453:GLY:HA3 | 2.00 | 0.43 |
| 4:E:31:GLY:HA3 | 10:P:45:GLU:OE2 | 2.18 | 0.43 |
| 16:Q:90:VAL:HG21 | 16:Q:243:LEU:HB3 | 2.00 | 0.43 |
| 13:T:477:LEU:HD12 | 13:T:477:LEU:HA | 1.86 | 0.43 |
| 13:T:7:ILE:O | 13:T:10:PRO:HD2 | 2.19 | 0.43 |
| 15:V:124:TRP:CZ3 | 15:V:305:ASP:HB2 | 2.53 | 0.43 |
| 5:5:38:MET:HA | 5:5:41:TYR:HB2 | 2.00 | 0.43 |
| 1:B:374:ILE:HD13 | 1:B:421:TYR:CD2 | 2.54 | 0.43 |
| 1:B:298:PRO:HG3 | 1:B:408:TRP:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:13:VAL:HG21 | 3:D:17:THR:HG21 | 2.01 | 0.43 |
| 3:D:326:PHE:CD2 | 3:D:643:LEU:HD11 | 2.54 | 0.43 |
| 16:H:255:ALA:O | 16:H:259:ILE:HG13 | 2.18 | 0.43 |
| 16:H:287:LEU:O | 16:H:291:ILE:HG13 | 2.19 | 0.43 |
| 11:J:53:PHE:HE2 | 16:H:120:LEU:O | 2.01 | 0.43 |
| 14:M:274:VAL:O | 14:M:277:ALA:N | 2.51 | 0.43 |
| 14:M:279:LYS:HD3 | 14:M:279:LYS:HA | 1.77 | 0.43 |
| 10:P:88:LEU:HD23 | 11:R:132:TYR:HB2 | 2.00 | 0.43 |
| 16:Q:300:LEU:HD23 | 16:Q:305:LEU:HA | 2.00 | 0.43 |
| 13:T:210:PHE:CD1 | 13:T:270:ILE:HG12 | 2.52 | 0.43 |
| 13:T:409:VAL:HA | 13:T:412:LEU:HD12 | 2.00 | 0.43 |
| 15:V:98:LEU:HD12 | 15:V:107:MET:CG | 2.47 | 0.43 |
| 2:2:98:ASP:HB3 | 8:7:107:LYS:HZ2 | 1.84 | 0.43 |
| 4:4:115:THR:O | 4:4:118:VAL:HG22 | 2.19 | 0.43 |
| 4:4:165:GLY:HA3 | 7:9:36:ARG:O | 2.18 | 0.43 |
| 4:4:207:LEU:HD21 | 7:9:12:ILE:HD11 | 2.00 | 0.43 |
| 10:A:110:GLU:HG3 | 10:A:111:TRP:N | 2.31 | 0.43 |
| 1:B:275:LEU:HA | 1:B:279:TRP:CD1 | 2.48 | 0.43 |
| 1:B:364:ALA:HB1 | 3:D:207:VAL:HG22 | 2.00 | 0.43 |
| 4:E:39:GLY:O | 4:E:404:MET:HG3 | 2.18 | 0.43 |
| 16:H:43:GLN:HG2 | 16:H:43:GLN:H | 1.71 | 0.43 |
| 13:L:477:LEU:HA | 13:L:477:LEU:HD12 | 1.85 | 0.43 |
| 14:M:131:LEU:O | 14:M:135:LEU:HD23 | 2.18 | 0.43 |
| 15:N:26:LYS:HD3 | 15:N:85:TYR:OH | 2.19 | 0.43 |
| 10:P:44:TYR:O | 10:P:50:PRO:HG3 | 2.18 | 0.43 |
| 13:T:94:TYR:CE1 | 13:T:341:HIS:HB2 | 2.37 | 0.43 |
| 13:T:287:GLY:HA2 | 13:T:525:GLU:HG3 | 2.00 | 0.43 |
| 14:U:347:LEU:HB2 | 14:U:414:PHE:HA | 2.00 | 0.43 |
| 9:W:102:LEU:HG | 9:W:110:LEU:HD13 | 2.00 | 0.43 |
| 1:1:223:THR:O | 1:1:227:VAL:HG23 | 2.19 | 0.43 |
| 1:1:288:GLN:HE21 | 1:1:331:ILE:HG22 | 1.84 | 0.43 |
| 1:1:293:GLY:O | 1:1:327:GLY:N | 2.52 | 0.43 |
| 3:3:358:SER:HB2 | 3:3:548:GLY:O | 2.19 | 0.43 |
| 5:5:116:ARG:HB3 | 5:5:135:ILE:HG13 | 2.01 | 0.43 |
| 6:6:19:ILE:HG12 | 6:6:20:LEU:N | 2.34 | 0.43 |
| 8:7:43:ARG:HA | 8:7:46:ARG:HH21 | 1.84 | 0.43 |
| 7:9:133:LYS:O | 7:9:137:LEU:CD1 | 2.47 | 0.43 |
| 7:9:94:ASN:OD1 | 7:9:97:ARG:N | 2.52 | 0.43 |
| 7:9:9:SER:OG | 16:H:296:THR:HG22 | 2.18 | 0.43 |
| 1:B:272:PHE:CZ | 1:B:311:MET:HG2 | 2.54 | 0.43 |
| 6:G:154:LEU:O | 6:G:158:VAL:HG13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:43:LEU:HB2 | 6:G:82:GLY:HA3 | 2.00 | 0.43 |
| 16:H:20:VAL:O | 16:H:24:LEU:HD13 | 2.19 | 0.43 |
| 16:H:2:THR:HG23 | 16:H:5:TYR:HB2 | 2.00 | 0.43 |
| 13:L:433:HIS:O | 13:L:433:HIS:CG | 2.71 | 0.43 |
| 7:O:42:VAL:HG22 | 7:O:114:VAL:O | 2.19 | 0.43 |
| 16:Q:181:ASN:O | 16:Q:185:ILE:HG13 | 2.18 | 0.43 |
| 14:U:22:ARG:HH11 | 14:U:92:GLU:HG3 | 1.83 | 0.43 |
| 4:4:26:MET:HG2 | 10:A:54:VAL:HB | 2.00 | 0.43 |
| 4:4:366:TYR:CZ | 5:5:148:LYS:HE3 | 2.54 | 0.43 |
| 1:B:246:SER:OG | 1:B:312:SER:HB2 | 2.19 | 0.43 |
| 1:B:433:ARG:NH1 | 2:C:89:LYS:HE2 | 2.26 | 0.43 |
| 4:E:381:LEU:HB3 | 4:E:382:PRO:HD3 | 2.01 | 0.43 |
| 4:E:62:LEU:HA | 4:E:62:LEU:HD23 | 1.78 | 0.43 |
| 6:G:99:MET:HG2 | 6:G:100:PRO:HD2 | 2.00 | 0.43 |
| 13:L:427:GLY:O | 13:L:428:GLU:HG2 | 2.18 | 0.43 |
| 16:Q:147:TYR:CE1 | 16:Q:228:LEU:HD13 | 2.54 | 0.43 |
| 16:Q:212:ALA:HA | 16:Q:218:PRO:HG3 | 2.00 | 0.43 |
| 16:Q:289:PHE:O | 16:Q:293:ILE:HG12 | 2.19 | 0.43 |
| 14:U:206:PRO:HD2 | 14:U:293:MET:HG3 | 2.01 | 0.43 |
| 14:U:27:LEU:O | 14:U:31:LEU:HD13 | 2.19 | 0.43 |
| 1:1:18:TYR:CZ | 1:1:263:VAL:HG11 | 2.53 | 0.43 |
| 3:3:266:THR:HG21 | 3:3:278:ARG:HH12 | 1.83 | 0.43 |
| 3:3:347:HIS:HB2 | 3:3:538:ALA:CB | 2.49 | 0.43 |
| 3:3:583:VAL:HG23 | 3:3:598:ALA:HA | 2.01 | 0.43 |
| 6:6:164:ASN:ND2 | 6:6:168:GLU:HB2 | 2.33 | 0.43 |
| 6:6:140:CYS:SG | 7:9:99:ILE:HG13 | 2.59 | 0.43 |
| 3:D:149:LEU:HD12 | 4:E:108:VAL:HG23 | 2.01 | 0.43 |
| 3:D:5:LYS:O | 3:D:93:VAL:N | 2.48 | 0.43 |
| 5:F:144:HIS:HB2 | 5:F:147:ARG:HD3 | 2.00 | 0.43 |
| 11:J:36:PHE:CE2 | 11:J:59:TYR:HB3 | 2.54 | 0.43 |
| 15:N:87:LEU:HB3 | 15:N:117:PRO:HB2 | 2.01 | 0.43 |
| 7:O:93:ILE:HD12 | 7:O:136:MET:SD | 2.59 | 0.43 |
| 16:Q:150:LEU:HD21 | 16:Q:154:ARG:NH1 | 2.33 | 0.43 |
| 13:T:214:VAL:HG12 | 13:T:222:LEU:HB2 | 2.01 | 0.43 |
| 14:U:148:PHE:O | 14:U:152:THR:HG23 | 2.19 | 0.43 |
| 14:U:88:VAL:HG22 | 14:U:331:ARG:HE | 1.84 | 0.43 |
| 15:V:181:VAL:HA | 15:V:192:PHE:CE2 | 2.54 | 0.43 |
| 1:1:171:LEU:HA | 1:1:171:LEU:HD23 | 1.79 | 0.43 |
| 1:1:50:PRO:HA | 1:1:53:VAL:HG12 | 2.01 | 0.43 |
| 3:3:398:VAL:HG22 | 3:3:506:ILE:HD12 | 2.01 | 0.43 |
| 3:3:34:CYS:HB2 | 3:3:44:ALA:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:106:ILE:HD11 | 6:6:154:LEU:HD22 | 2.00 | 0.43 |
| 4:4:73:ARG:NH2 | 7:9:64:PRO:O | 2.52 | 0.43 |
| 3:D:585:MET:HB3 | 3:D:587:LEU:CD1 | 2.49 | 0.43 |
| 3:D:5:LYS:HA | 3:D:9:ARG:O | 2.19 | 0.43 |
| 3:D:526:GLU:OE2 | 3:D:679:ARG:NH1 | 2.51 | 0.43 |
| 5:F:78:PRO:HA | 5:F:83:GLY:HA3 | 2.00 | 0.43 |
| 13:L:30:GLY:HA3 | 13:L:92:ILE:HG12 | 2.01 | 0.43 |
| 14:M:75:PHE:CZ | 14:M:111:ALA:HB2 | 2.54 | 0.43 |
| 14:M:217:PHE:CE2 | 14:M:231:GLY:HA3 | 2.54 | 0.43 |
| 16:Q:96:ALA:HB2 | 16:Q:128:VAL:HG21 | 2.01 | 0.43 |
| 16:Q:141:TRP:CE3 | 16:Q:149:LEU:HD11 | 2.54 | 0.43 |
| 16:Q:236:TYR:HB2 | 16:Q:241:TRP:HB2 | 2.01 | 0.43 |
| 2:2:162:ARG:NH2 | 2:2:165:GLU:OE1 | 2.51 | 0.42 |
| 3:3:356:LEU:CD1 | 3:3:653:PRO:HD2 | 2.49 | 0.42 |
| 4:4:130:LEU:HD22 | 4:4:149:ALA:HB1 | 2.01 | 0.42 |
| 4:4:382:PRO:O | 4:4:386:LYS:HB2 | 2.19 | 0.42 |
| 2:C:106:ILE:HG22 | 2:C:107:GLY:N | 2.34 | 0.42 |
| 3:D:310:LEU:HD23 | 3:D:319:GLU:HA | 1.99 | 0.42 |
| 3:D:648:LEU:HD23 | 3:D:648:LEU:HA | 1.83 | 0.42 |
| 4:E:138:LEU:HD13 | 4:E:143:LEU:HA | 2.01 | 0.42 |
| 4:E:247:ASP:OD1 | 4:E:249:ARG:HG3 | 2.19 | 0.42 |
| 4:E:306:ASN:HD21 | 5:F:192:TYR:HH | 1.61 | 0.42 |
| 16:H:208:ILE:HG21 | 16:H:308:PHE:CE1 | 2.54 | 0.42 |
| 8:I:105:THR:N | 8:I:108:ILE:O | 2.45 | 0.42 |
| 8:I:71:ASP:OD2 | 8:I:81:ARG:NH2 | 2.46 | 0.42 |
| 13:L:202:LEU:HA | 13:L:202:LEU:HD12 | 1.82 | 0.42 |
| 13:L:285:ALA:O | 13:L:294:ILE:HG13 | 2.18 | 0.42 |
| 13:L:549:LEU:O | 13:L:553:LEU:HG | 2.19 | 0.42 |
| 14:M:114:ASP:HB3 | 14:M:176:LEU:HD23 | 1.99 | 0.42 |
| 14:M:138:GLY:HA3 | 14:M:220:GLU:HB3 | 2.00 | 0.42 |
| 15:N:260:TYR:HA | 15:N:263:ILE:HD12 | 2.01 | 0.42 |
| 16:Q:39:LEU:CD2 | 16:Q:295:ALA:HB2 | 2.48 | 0.42 |
| 13:T:561:LEU:HG | 13:T:565:PHE:CE2 | 2.54 | 0.42 |
| 14:U:157:LEU:HD23 | 14:U:157:LEU:HA | 1.87 | 0.42 |
| 1:1:404:ASP:OD1 | 1:1:404:ASP:N | 2.50 | 0.42 |
| 18:1:502:FMN:C9 | 19:1:503:NAI:H52N | 2.49 | 0.42 |
| 3:3:50:VAL:HG12 | 3:3:95:THR:HG22 | 2.01 | 0.42 |
| 3:3:368:HIS:HB2 | 3:3:556:ALA:O | 2.19 | 0.42 |
| 3:3:585:MET:HB3 | 3:3:587:LEU:HD13 | 2.00 | 0.42 |
| 4:4:350:ARG:O | 4:4:373:PRO:HB2 | 2.18 | 0.42 |
| 4:4:86:ASP:HB3 | 4:4:93:HIS:HD2 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:5:41:TYR:HD1 | 5:5:46:PHE:HE2 | 1.67 | 0.42 |
| 1:B:104:ARG:O | 1:B:108:GLU:HG3 | 2.19 | 0.42 |
| 4:E:240:ARG:HG3 | 4:E:278:VAL:HG11 | 2.00 | 0.42 |
| 4:E:72:HIS:ND1 | 5:F:152:LEU:HD22 | 2.34 | 0.42 |
| 5:F:176:GLY:O | 5:F:185:LYS:NZ | 2.43 | 0.42 |
| 6:G:115:GLY:HA3 | 6:G:125:GLN:OE1 | 2.18 | 0.42 |
| 13:L:162:ASN:ND2 | 13:L:166:ASP:OD2 | 2.51 | 0.42 |
| 14:M:371:LEU:HA | 14:M:371:LEU:HD13 | 1.87 | 0.42 |
| 13:T:321:HIS:HD2 | 13:T:388:ILE:HD12 | 1.84 | 0.42 |
| 13:T:419:ARG:HB2 | 13:T:512:PHE:CE2 | 2.53 | 0.42 |
| 9:W:102:LEU:HG | 9:W:110:LEU:CD1 | 2.49 | 0.42 |
| 9:W:72:GLU:O | 9:W:76:GLU:HG3 | 2.19 | 0.42 |
| 1:1:241:MET:SD | 1:1:249:MET:HB3 | 2.59 | 0.42 |
| 3:3:688:ARG:HA | 3:3:688:ARG:HD3 | 1.65 | 0.42 |
| 4:4:115:THR:O | 4:4:119:ILE:HG13 | 2.19 | 0.42 |
| 4:4:131:VAL:HG23 | 4:4:153:ARG:HD2 | 2.01 | 0.42 |
| 4:4:304:ASP:O | 4:4:310:THR:OG1 | 2.11 | 0.42 |
| 3:D:188:VAL:HG11 | 3:D:201:ASP:HA | 2.02 | 0.42 |
| 2:C:66:PHE:CZ | 3:D:205:ARG:HD3 | 2.54 | 0.42 |
| 4:E:310:THR:HG22 | 4:E:311:PRO:O | 2.18 | 0.42 |
| 5:F:41:TYR:HA | 5:F:44:MET:HE3 | 2.01 | 0.42 |
| 6:G:19:ILE:HG12 | 6:G:20:LEU:N | 2.33 | 0.42 |
| 6:G:56:ALA:O | 7:O:22:VAL:HG12 | 2.19 | 0.42 |
| 8:I:23:TYR:OH | 8:I:120:ASP:HA | 2.18 | 0.42 |
| 13:L:33:ALA:HB2 | 13:L:109:ASN:HD21 | 1.84 | 0.42 |
| 13:L:39:ALA:O | 13:L:43:LEU:HG | 2.19 | 0.42 |
| 14:U:131:LEU:O | 14:U:135:LEU:HD23 | 2.19 | 0.42 |
| 15:V:114:LEU:C | 15:V:114:LEU:HD12 | 2.39 | 0.42 |
| 15:V:3:LEU:HD13 | 15:V:96:HIS:CD2 | 2.54 | 0.42 |
| 1:1:253:GLN:HG2 | 1:1:327:GLY:HA2 | 2.01 | 0.42 |
| 1:1:291:ILE:HD11 | 1:1:331:ILE:HD11 | 2.01 | 0.42 |
| 3:3:46:ARG:HH22 | 3:3:81:ALA:HB2 | 1.84 | 0.42 |
| 3:3:722:THR:HG21 | 3:3:756:GLY:N | 2.34 | 0.42 |
| 4:4:261:THR:N | 4:4:292:GLN:HE22 | 2.03 | 0.42 |
| 6:6:143:ARG:HG3 | 6:6:144:PRO:HD2 | 2.00 | 0.42 |
| 6:6:83:ARG:HB2 | 6:6:123:ILE:HD12 | 2.01 | 0.42 |
| 10:A:97:LEU:O | 10:A:101:LEU:HG | 2.19 | 0.42 |
| 1:B:145:LEU:HA | 1:B:145:LEU:HD23 | 1.89 | 0.42 |
| 1:B:189:MET:HE1 | 1:B:210:GLY:HA2 | 2.02 | 0.42 |
| 2:C:132:PRO:HG2 | 2:C:145:VAL:HB | 2.00 | 0.42 |
| 3:D:256:CYS:O | 3:D:262:GLY:HA2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:341:VAL:HA | 3:D:565:TYR:O | 2.19 | 0.42 |
| 3:D:513:GLN:NE2 | 3:D:769:LEU:HD21 | 2.35 | 0.42 |
| 11:J:146:LEU:O | 11:J:150:THR:HG23 | 2.19 | 0.42 |
| 12:K:15:VAL:O | 12:K:19:LEU:HG | 2.19 | 0.42 |
| 13:L:239:LEU:HD12 | 13:L:239:LEU:HA | 1.86 | 0.42 |
| 13:L:348:ASP:OD1 | 13:L:350:ARG:HG2 | 2.19 | 0.42 |
| 13:L:380:SER:CB | 13:L:456:ALA:HB3 | 2.49 | 0.42 |
| 13:L:459:LEU:HD23 | 13:L:459:LEU:HA | 1.90 | 0.42 |
| 15:N:97:LEU:HD23 | 15:N:97:LEU:HA | 1.94 | 0.42 |
| 11:R:72:MET:HG2 | 16:Q:141:TRP:CE3 | 2.54 | 0.42 |
| 16:Q:185:ILE:HG22 | 16:Q:189:GLN:OE1 | 2.19 | 0.42 |
| 16:Q:267:TRP:CD1 | 16:Q:275:PRO:HA | 2.53 | 0.42 |
| 6:G:62:ARG:HB3 | 16:Q:50:ARG:HB2 | 2.00 | 0.42 |
| 12:S:78:ILE:CD1 | 15:V:134:LEU:HB2 | 2.48 | 0.42 |
| 14:U:318:SER:HA | 14:U:321:TYR:CE1 | 2.54 | 0.42 |
| 3:3:271:SER:HG | 7:9:69:TYR:HH | 1.55 | 0.42 |
| 3:3:46:ARG:NH2 | 3:3:81:ALA:HB2 | 2.34 | 0.42 |
| 4:4:127:ALA:O | 4:4:153:ARG:NH1 | 2.52 | 0.42 |
| 6:6:43:LEU:HD11 | 6:6:84:LEU:HD23 | 2.01 | 0.42 |
| 1:B:292:PRO:HA | 1:B:328:VAL:HG13 | 2.01 | 0.42 |
| 3:D:445:THR:HB | 3:D:463:ALA:HB2 | 2.02 | 0.42 |
| 3:D:385:ALA:O | 3:D:533:LEU:HD21 | 2.19 | 0.42 |
| 4:E:29:ASN:HD22 | 10:P:49:ASP:HB3 | 1.84 | 0.42 |
| 6:G:151:VAL:O | 6:G:155:GLN:HB2 | 2.19 | 0.42 |
| 14:M:33:PHE:HA | 14:M:79:ALA:HB1 | 2.00 | 0.42 |
| 15:N:61:VAL:O | 15:N:65:LEU:HG | 2.20 | 0.42 |
| 10:P:41:LEU:HD23 | 16:Q:72:ILE:HD11 | 2.02 | 0.42 |
| 14:U:13:GLY:HA2 | 14:U:97:GLY:HA2 | 2.01 | 0.42 |
| 14:U:304:THR:O | 14:U:306:GLU:N | 2.52 | 0.42 |
| 14:U:436:SER:O | 14:U:440:LEU:HD13 | 2.19 | 0.42 |
| 14:U:55:LEU:HD11 | 15:V:416:PRO:HD2 | 2.00 | 0.42 |
| 15:V:77:VAL:HG12 | 15:V:85:TYR:HE1 | 1.83 | 0.42 |
| 1:1:245:GLN:HB2 | 1:1:314:GLU:CD | 2.40 | 0.42 |
| 2:2:110:GLU:OE1 | 8:7:114:ARG:HG3 | 2.20 | 0.42 |
| 2:2:15:PHE:HE1 | 2:2:53:VAL:HG23 | 1.84 | 0.42 |
| 3:3:470:PRO:HD3 | 3:3:759:TYR:OH | 2.19 | 0.42 |
| 1:B:90:ILE:HB | 1:B:218:ILE:HG12 | 2.01 | 0.42 |
| 2:C:162:ARG:NH2 | 2:C:165:GLU:OE2 | 2.53 | 0.42 |
| 3:D:572:PRO:HD2 | 3:D:577:LEU:HD21 | 2.01 | 0.42 |
| 3:D:697:THR:OG1 | 3:D:763:LEU:HA | 2.19 | 0.42 |
| 16:H:131:LEU:HA | 16:H:134:TYR:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:218:PRO:C | 16:H:220:ASP:H | 2.22 | 0.42 |
| 16:H:99:LEU:HD12 | 16:H:116:ILE:HG13 | 2.02 | 0.42 |
| 13:L:128:PHE:CZ | 13:L:166:ASP:HB3 | 2.55 | 0.42 |
| 15:N:332:SER:O | 15:N:341:GLY:HA3 | 2.20 | 0.42 |
| 10:P:61:PHE:HE1 | 16:Q:302:TYR:OH | 2.03 | 0.42 |
| 11:R:146:LEU:O | 11:R:150:THR:HG23 | 2.20 | 0.42 |
| 11:R:40:ALA:O | 11:R:44:VAL:HG23 | 2.20 | 0.42 |
| 13:T:365:HIS:HD2 | 13:T:450:ALA:HB2 | 1.85 | 0.42 |
| 13:T:287:GLY:HA2 | 13:T:525:GLU:CG | 2.50 | 0.42 |
| 14:U:452:ARG:HD3 | 14:U:452:ARG:HA | 1.83 | 0.42 |
| 15:V:368:SER:O | 15:V:371:SER:OG | 2.25 | 0.42 |
| 9:W:113:ARG:O | 9:W:117:ILE:HG12 | 2.20 | 0.42 |
| 1:1:211:LEU:HA | 1:1:211:LEU:HD12 | 1.75 | 0.42 |
| 3:3:574:GLU:HG3 | 3:3:593:LEU:HD11 | 2.00 | 0.42 |
| 3:3:672:ALA:O | 3:3:673:MET:HB2 | 2.19 | 0.42 |
| 4:4:236:GLY:O | 4:4:238:SER:N | 2.51 | 0.42 |
| 1:B:193:GLU:OE1 | 1:B:211:LEU:HD12 | 2.20 | 0.42 |
| 1:B:381:GLU:O | 1:B:385:GLU:HG3 | 2.20 | 0.42 |
| 1:B:334:ARG:HG2 | 1:B:434:PRO:HG3 | 2.02 | 0.42 |
| 3:D:381:LEU:HD12 | 3:D:522:ARG:HD3 | 2.02 | 0.42 |
| 4:E:46:THR:O | 4:E:53:LEU:HB2 | 2.19 | 0.42 |
| 4:E:73:ARG:NH2 | 6:G:117:MET:O | 2.52 | 0.42 |
| 6:G:30:TRP:O | 6:G:34:ASN:ND2 | 2.48 | 0.42 |
| 11:J:53:PHE:O | 11:J:57:ILE:HG13 | 2.19 | 0.42 |
| 13:L:214:VAL:HG22 | 13:L:219:GLN:HB2 | 2.01 | 0.42 |
| 13:L:90:TYR:CG | 13:L:334:LEU:HD13 | 2.54 | 0.42 |
| 14:M:329:ALA:O | 14:M:332:LEU:HG | 2.19 | 0.42 |
| 13:L:582:GLN:CD | 15:N:194:PHE:HA | 2.40 | 0.42 |
| 15:N:204:PRO:O | 15:N:208:VAL:HG23 | 2.20 | 0.42 |
| 15:N:290:LEU:HD13 | 15:N:408:LEU:HB3 | 2.02 | 0.42 |
| 13:T:290:ASP:OD1 | 13:T:291:ILE:N | 2.53 | 0.42 |
| 1:1:3:GLY:HA2 | 1:1:4:PRO:HD3 | 1.87 | 0.42 |
| 3:3:248:GLU:HG2 | 5:5:170:PHE:CE1 | 2.54 | 0.42 |
| 6:6:163:TYR:OH | 6:6:169:ARG:NH2 | 2.53 | 0.42 |
| 10:A:71:PHE:O | 10:A:74:GLU:HB3 | 2.20 | 0.42 |
| 1:B:176:GLY:O | 2:C:32:ARG:NH2 | 2.51 | 0.42 |
| 2:C:4:PHE:HB2 | 2:C:48:GLU:OE2 | 2.20 | 0.42 |
| 3:D:507:LEU:HD22 | 3:D:511:VAL:HG11 | 2.01 | 0.42 |
| 3:D:716:LEU:HD21 | 3:D:758:LEU:HB3 | 2.00 | 0.42 |
| 4:E:60:GLY:N | 4:E:408:ASP:OD1 | 2.48 | 0.42 |
| 16:H:108:PHE:O | 16:H:108:PHE:CG | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:82:PHE:HA | 16:H:236:TYR:OH | 2.20 | 0.42 |
| 16:H:48:PRO:C | 16:H:50:ARG:H | 2.23 | 0.42 |
| 11:J:102:GLY:O | 11:J:106:ALA:N | 2.50 | 0.42 |
| 11:J:104:LEU:O | 11:J:108:LEU:HD12 | 2.20 | 0.42 |
| 13:L:7:ILE:O | 13:L:10:PRO:HD2 | 2.20 | 0.42 |
| 14:M:203:ILE:HA | 14:M:210:LEU:HB3 | 2.01 | 0.42 |
| 14:M:244:PHE:O | 14:M:248:LEU:HB2 | 2.20 | 0.42 |
| 11:J:135:TRP:CZ3 | 15:N:105:LEU:HD22 | 2.49 | 0.42 |
| 15:N:190:ALA:HA | 15:N:192:PHE:N | 2.35 | 0.42 |
| 11:R:144:PHE:CE1 | 15:V:93:LEU:HD22 | 2.55 | 0.42 |
| 12:S:46:ALA:HB2 | 12:S:53:GLY:HA3 | 2.01 | 0.42 |
| 13:T:291:ILE:O | 13:T:294:ILE:HG22 | 2.19 | 0.42 |
| 13:T:27:PRO:O | 13:T:31:VAL:HG23 | 2.19 | 0.42 |
| 14:U:37:LEU:O | 14:U:41:LEU:HG | 2.20 | 0.42 |
| 9:X:51:HIS:HA | 9:X:56:ASP:OD1 | 2.20 | 0.42 |
| 3:3:585:MET:SD | 3:3:594:ALA:HB2 | 2.60 | 0.42 |
| 4:4:202:ASP:HA | 4:4:284:ARG:HH21 | 1.84 | 0.42 |
| 4:4:236:GLY:C | 4:4:238:SER:H | 2.23 | 0.42 |
| 10:A:18:LEU:O | 10:A:22:VAL:HG23 | 2.19 | 0.42 |
| 3:D:459:MET:HG2 | 3:D:465:HIS:CB | 2.49 | 0.42 |
| 3:D:470:PRO:HD3 | 3:D:759:TYR:OH | 2.20 | 0.42 |
| 4:E:101:VAL:O | 4:E:105:LEU:HG | 2.20 | 0.42 |
| 4:E:239:LEU:HG | 4:E:244:VAL:HB | 2.01 | 0.42 |
| 6:G:109:GLY:HA2 | 6:G:142:PRO:HD3 | 2.01 | 0.42 |
| 6:G:135:VAL:HG21 | 6:G:154:LEU:HB2 | 2.02 | 0.42 |
| 13:L:290:ASP:OD1 | 13:L:291:ILE:N | 2.53 | 0.42 |
| 13:L:574:LEU:HD22 | 15:N:246:LEU:CD1 | 2.49 | 0.42 |
| 13:L:554:PHE:CZ | 14:M:283:THR:HG21 | 2.54 | 0.42 |
| 14:M:327:LEU:O | 14:M:331:ARG:HG2 | 2.20 | 0.42 |
| 14:M:30:GLY:O | 14:M:34:LEU:HG | 2.20 | 0.42 |
| 14:M:348:ALA:HB2 | 14:M:414:PHE:HB3 | 2.02 | 0.42 |
| 15:N:217:ALA:HA | 15:N:285:LEU:CD2 | 2.49 | 0.42 |
| 15:N:259:ALA:O | 15:N:263:ILE:HG13 | 2.20 | 0.42 |
| 7:O:33:LEU:HB2 | 7:O:163:VAL:HG12 | 2.00 | 0.42 |
| 16:Q:147:TYR:CE1 | 16:Q:229:VAL:HG22 | 2.54 | 0.42 |
| 16:Q:237:SER:OG | 16:Q:238:SER:N | 2.52 | 0.42 |
| 16:Q:293:ILE:HG23 | 16:Q:297:TRP:CE3 | 2.55 | 0.42 |
| 16:Q:343:LEU:O | 16:Q:347:VAL:HG23 | 2.20 | 0.42 |
| 14:U:186:GLN:HG2 | 14:U:187:GLU:H | 1.85 | 0.42 |
| 15:V:73:THR:HG21 | 15:V:210:PHE:HB2 | 2.02 | 0.42 |
| 1:1:343:ASN:HA | 1:1:346:ARG:HG2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:268:ASP:OD1 | 3:3:278:ARG:NH1 | 2.53 | 0.42 |
| 8:7:20:MET:HG2 | 8:7:115:PHE:CZ | 2.55 | 0.42 |
| 1:B:75:LYS:NZ | 1:B:218:ILE:O | 2.48 | 0.42 |
| 16:H:189:GLN:O | 16:H:193:GLY:HA2 | 2.20 | 0.42 |
| 16:H:310:TRP:HA | 16:H:314:PHE:CD2 | 2.55 | 0.42 |
| 13:L:435:PRO:HG2 | 13:L:436:HIS:HD2 | 1.84 | 0.42 |
| 15:N:190:ALA:N | 15:N:240:SER:OG | 2.53 | 0.42 |
| 13:T:159:PHE:HD2 | 14:U:407:LEU:HD11 | 1.85 | 0.42 |
| 13:T:313:GLY:HA2 | 13:T:315:TYR:CZ | 2.54 | 0.42 |
| 1:1:339:ASP:OD1 | 1:1:433:ARG:NH2 | 2.53 | 0.41 |
| 3:3:384:PRO:O | 3:3:531:LYS:HD3 | 2.19 | 0.41 |
| 3:3:409:LEU:HD23 | 3:3:409:LEU:HA | 1.63 | 0.41 |
| 4:4:167:ARG:HD3 | 6:6:143:ARG:NH1 | 2.28 | 0.41 |
| 4:4:172:TYR:CE2 | 4:4:178:VAL:HB | 2.55 | 0.41 |
| 4:4:176:GLY:HA3 | 4:4:304:ASP:H | 1.83 | 0.41 |
| 4:4:59:ILE:HB | 4:4:408:ASP:OD1 | 2.20 | 0.41 |
| 4:4:50:GLU:O | 4:4:390:VAL:HG23 | 2.20 | 0.41 |
| 8:7:120:ASP:O | 8:7:124:GLU:HG3 | 2.20 | 0.41 |
| 1:B:404:ASP:HA | 1:B:407:VAL:HG22 | 2.02 | 0.41 |
| 3:D:248:GLU:OE2 | 7:O:57:SER:OG | 2.36 | 0.41 |
| 4:E:84:ARG:CZ | 4:E:169:HIS:HB3 | 2.50 | 0.41 |
| 13:L:433:HIS:ND1 | 13:L:437:GLU:OE2 | 2.44 | 0.41 |
| 14:M:131:LEU:HA | 14:M:131:LEU:HD23 | 1.85 | 0.41 |
| 14:M:371:LEU:HD11 | 14:M:441:LEU:HD12 | 2.02 | 0.41 |
| 15:N:3:LEU:HD13 | 15:N:96:HIS:HD2 | 1.84 | 0.41 |
| 15:N:63:THR:HG22 | 15:N:96:HIS:HA | 2.02 | 0.41 |
| 7:O:43:LEU:HD12 | 7:O:133:LYS:HG3 | 2.01 | 0.41 |
| 14:U:163:VAL:HG22 | 14:U:175:PHE:CE1 | 2.55 | 0.41 |
| 14:U:292:HIS:NE2 | 14:U:365:MET:HG3 | 2.35 | 0.41 |
| 14:U:426:ALA:HB3 | 14:U:429:GLU:HG3 | 2.02 | 0.41 |
| 15:V:196:THR:HB | 15:V:197:PRO:HD3 | 2.01 | 0.41 |
| 9:W:38:GLN:HG3 | 9:W:93:VAL:HG21 | 2.02 | 0.41 |
| 3:3:29:ASP:OD1 | 3:3:29:ASP:N | 2.54 | 0.41 |
| 3:3:387:LEU:HA | 3:3:387:LEU:HD23 | 1.74 | 0.41 |
| 3:3:460:LYS:HA | 3:3:460:LYS:HD3 | 1.94 | 0.41 |
| 3:3:504:VAL:HG12 | 3:3:506:ILE:HG13 | 2.02 | 0.41 |
| 3:3:533:LEU:HA | 3:3:533:LEU:HD23 | 1.75 | 0.41 |
| 3:3:689:LYS:HG2 | 3:3:689:LYS:H | 1.34 | 0.41 |
| 8:7:23:TYR:OH | 8:7:123:ARG:HD3 | 2.20 | 0.41 |
| 4:4:314:ARG:NH1 | 7:9:106:GLU:O | 2.53 | 0.41 |
| 3:D:149:LEU:HG | 4:E:305:PRO:HD2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:561:PRO:HB3 | 3:D:575:GLU:O | 2.20 | 0.41 |
| 4:E:59:ILE:HB | 4:E:408:ASP:OD1 | 2.19 | 0.41 |
| 4:E:88:LEU:HD21 | 6:G:48:ILE:HD13 | 2.02 | 0.41 |
| 5:F:31:ARG:HH22 | 5:F:98:ASP:CG | 2.23 | 0.41 |
| 11:J:16:GLY:O | 11:J:19:VAL:HG12 | 2.20 | 0.41 |
| 14:M:17:LEU:HD11 | 14:M:98:LEU:HD23 | 2.01 | 0.41 |
| 14:M:321:TYR:CE1 | 14:M:365:MET:HA | 2.55 | 0.41 |
| 14:M:346:GLY:HA3 | 14:M:418:GLY:HA2 | 2.02 | 0.41 |
| 14:M:8:LEU:HB3 | 14:M:9:PRO:HD3 | 2.02 | 0.41 |
| 15:N:101:THR:HG21 | 15:N:106:LEU:HD23 | 2.01 | 0.41 |
| 10:P:7:TYR:N | 10:P:7:TYR:HD1 | 2.18 | 0.41 |
| 16:Q:269:MET:HG3 | 16:Q:270:PRO:HD2 | 2.01 | 0.41 |
| 16:Q:48:PRO:C | 16:Q:50:ARG:N | 2.73 | 0.41 |
| 11:R:100:VAL:O | 11:R:104:LEU:HG | 2.20 | 0.41 |
| 13:T:437:GLU:O | 13:T:439:PRO:HD3 | 2.19 | 0.41 |
| 13:T:469:LEU:HD12 | 13:T:469:LEU:HA | 1.82 | 0.41 |
| 14:U:426:ALA:N | 14:U:429:GLU:OE1 | 2.39 | 0.41 |
| 1:1:207:ALA:O | 1:1:215:PRO:HB3 | 2.21 | 0.41 |
| 3:3:327:LEU:HA | 3:3:327:LEU:HD23 | 1.83 | 0.41 |
| 3:3:715:GLU:H | 3:3:761:SER:HB2 | 1.85 | 0.41 |
| 8:7:63:LEU:HD11 | 8:7:129:ALA:HB3 | 2.00 | 0.41 |
| 6:6:57:ARG:O | 7:9:24:VAL:HG22 | 2.20 | 0.41 |
| 1:B:298:PRO:HD2 | 1:B:321:SER:HA | 2.02 | 0.41 |
| 1:B:4:PRO:HA | 1:B:12:ARG:NH1 | 2.29 | 0.41 |
| 2:C:79:HIS:N | 2:C:137:ASN:OD1 | 2.52 | 0.41 |
| 3:D:175:ILE:HG22 | 3:D:236:LEU:HB2 | 2.02 | 0.41 |
| 3:D:347:HIS:HB2 | 3:D:538:ALA:HB1 | 2.02 | 0.41 |
| 4:E:272:VAL:N | 4:E:275:ARG:HH21 | 2.18 | 0.41 |
| 5:F:116:ARG:CZ | 5:F:135:ILE:HD11 | 2.49 | 0.41 |
| 6:G:36:LEU:CD1 | 6:G:155:GLN:HG3 | 2.50 | 0.41 |
| 16:H:153:LEU:HA | 16:H:153:LEU:HD23 | 1.75 | 0.41 |
| 16:H:187:ASN:O | 16:H:190:LYS:HB3 | 2.19 | 0.41 |
| 8:I:8:GLU:HG2 | 8:I:97:TYR:CZ | 2.55 | 0.41 |
| 13:L:128:PHE:CE1 | 13:L:166:ASP:HB3 | 2.55 | 0.41 |
| 13:L:352:MET:SD | 13:L:424:VAL:HG13 | 2.60 | 0.41 |
| 13:L:372:ALA:O | 13:L:381:GLY:HA3 | 2.21 | 0.41 |
| 14:M:306:GLU:H | 14:M:306:GLU:HG3 | 1.63 | 0.41 |
| 15:N:73:THR:O | 15:N:77:VAL:HG23 | 2.20 | 0.41 |
| 10:P:10:THR:OG1 | 16:Q:118:LEU:HD21 | 2.21 | 0.41 |
| 16:Q:134:TYR:HA | 16:Q:137:PHE:HE2 | 1.84 | 0.41 |
| 16:Q:224:ALA:HA | 16:Q:229:VAL:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:S:7:SER:CB | 12:S:40:LEU:HD23 | 2.47 | 0.41 |
| 15:V:136:TYR:HB2 | 15:V:199:VAL:HG21 | 2.02 | 0.41 |
| 9:X:113:ARG:O | 9:X:117:ILE:HG12 | 2.20 | 0.41 |
| 2:2:45:ARG:O | 2:2:49:ILE:HG13 | 2.20 | 0.41 |
| 3:3:118:ASP:O | 3:3:122:CYS:N | 2.53 | 0.41 |
| 4:4:74:THR:HG22 | 4:4:75:TYR:N | 2.35 | 0.41 |
| 7:9:34:LYS:HB3 | 7:9:35:PRO:HD2 | 2.02 | 0.41 |
| 1:B:97:GLU:HB2 | 19:B:503:NAI:H42N | 2.02 | 0.41 |
| 2:C:129:HIS:CD2 | 2:C:130:THR:HG23 | 2.55 | 0.41 |
| 8:I:105:THR:HG1 | 8:I:108:ILE:HB | 1.86 | 0.41 |
| 12:K:23:THR:HG22 | 12:K:85:THR:OG1 | 2.21 | 0.41 |
| 13:L:450:ALA:O | 13:L:454:VAL:HG23 | 2.21 | 0.41 |
| 13:T:327:PHE:CE1 | 13:T:452:GLY:HA3 | 2.55 | 0.41 |
| 13:T:564:TYR:CZ | 14:U:151:PHE:HZ | 2.38 | 0.41 |
| 14:U:289:GLY:O | 14:U:293:MET:HG2 | 2.19 | 0.41 |
| 15:V:302:ILE:HG12 | 15:V:391:PHE:HD1 | 1.84 | 0.41 |
| 1:1:29:LEU:HD23 | 1:1:155:ARG:HD2 | 2.02 | 0.41 |
| 3:3:242:PHE:HE2 | 7:9:85:GLU:O | 2.04 | 0.41 |
| 3:3:661:GLN:HE22 | 3:3:664:LEU:HD12 | 1.85 | 0.41 |
| 4:4:154:GLU:OE1 | 6:6:57:ARG:HD3 | 2.21 | 0.41 |
| 4:4:374:SER:HB2 | 4:4:406:ASP:HB3 | 2.02 | 0.41 |
| 3:3:127:ALA:HB2 | 5:5:181:LEU:HB3 | 2.03 | 0.41 |
| 6:6:115:GLY:HA3 | 6:6:125:GLN:OE1 | 2.21 | 0.41 |
| 6:6:143:ARG:O | 6:6:146:ALA:N | 2.54 | 0.41 |
| 2:C:154:LEU:HD23 | 2:C:154:LEU:HA | 1.86 | 0.41 |
| 1:B:343:ASN:OD1 | 2:C:86:LEU:N | 2.54 | 0.41 |
| 3:D:8:ASP:OD2 | 3:D:28:TYR:OH | 2.39 | 0.41 |
| 4:E:125:ARG:HD2 | 4:E:286:SER:OG | 2.21 | 0.41 |
| 5:F:6:VAL:HG22 | 5:F:41:TYR:CE1 | 2.56 | 0.41 |
| 16:H:134:TYR:HA | 16:H:137:PHE:CE2 | 2.55 | 0.41 |
| 12:K:71:GLY:HA3 | 15:N:137:PHE:CZ | 2.55 | 0.41 |
| 13:L:419:ARG:HB2 | 13:L:512:PHE:CE2 | 2.56 | 0.41 |
| 13:L:553:LEU:HB3 | 14:M:270:TYR:CE2 | 2.55 | 0.41 |
| 14:M:70:LEU:O | 14:M:73:LEU:HD23 | 2.20 | 0.41 |
| 16:Q:267:TRP:O | 16:Q:269:MET:N | 2.53 | 0.41 |
| 13:T:356:TRP:O | 13:T:363:ARG:HD3 | 2.20 | 0.41 |
| 15:V:140:GLY:HA2 | 15:V:185:PHE:CZ | 2.56 | 0.41 |
| 15:V:334:LEU:HD13 | 15:V:375:TYR:HD2 | 1.85 | 0.41 |
| 1:1:261:PRO:HD2 | 2:2:177:HIS:O | 2.20 | 0.41 |
| 3:3:678:PHE:CZ | 3:3:680:LEU:HD13 | 2.56 | 0.41 |
| 6:6:41:PHE:HE2 | 6:6:88:MET:HE2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:74:PRO:HG2 | 8:7:77:ALA:CB | 2.51 | 0.41 |
| 1:B:261:PRO:HD2 | 2:C:177:HIS:O | 2.21 | 0.41 |
| 3:D:140:TYR:CE2 | 3:D:142:LYS:HA | 2.56 | 0.41 |
| 6:G:44:ALA:O | 6:G:47:ALA:N | 2.41 | 0.41 |
| 16:H:333:PRO:HG2 | 16:H:336:TYR:CG | 2.55 | 0.41 |
| 16:H:70:GLU:O | 16:H:237:SER:OG | 2.31 | 0.41 |
| 11:J:46:LEU:HA | 11:J:46:LEU:HD23 | 1.81 | 0.41 |
| 13:L:267:SER:HB3 | 13:L:311:GLY:O | 2.21 | 0.41 |
| 13:L:469:LEU:HD12 | 13:L:469:LEU:HA | 1.79 | 0.41 |
| 13:L:517:PHE:O | 13:L:522:LEU:HG | 2.20 | 0.41 |
| 15:N:58:VAL:O | 15:N:62:PHE:HD1 | 2.03 | 0.41 |
| 11:R:103:ILE:O | 11:R:107:GLY:N | 2.45 | 0.41 |
| 13:T:13:GLY:HA3 | 13:T:36:LEU:HD13 | 2.02 | 0.41 |
| 13:T:335:ALA:O | 13:T:339:VAL:HG23 | 2.20 | 0.41 |
| 13:T:414:ALA:HB1 | 13:T:505:LEU:HD23 | 2.02 | 0.41 |
| 14:U:177:LEU:HD11 | 14:U:248:LEU:HD11 | 2.03 | 0.41 |
| 15:V:73:THR:O | 15:V:77:VAL:HG23 | 2.20 | 0.41 |
| 15:V:74:VAL:HG23 | 15:V:88:VAL:HG11 | 2.02 | 0.41 |
| 1:1:51:ASP:OD1 | 1:1:81:LYS:HD3 | 2.20 | 0.41 |
| 2:2:77:LYS:H | 2:2:116:LEU:HA | 1.86 | 0.41 |
| 3:3:423:PRO:HB2 | 3:3:431:PRO:HG3 | 2.03 | 0.41 |
| 4:4:271:ASP:OD1 | 4:4:274:ASP:HB2 | 2.20 | 0.41 |
| 1:B:183:GLY:HA3 | 18:B:502:FMN:O4 | 2.21 | 0.41 |
| 16:H:202:ALA:O | 16:H:205:VAL:HG22 | 2.21 | 0.41 |
| 14:M:215:PRO:CG | 14:M:216:PRO:HD3 | 2.50 | 0.41 |
| 14:M:221:ASN:HB3 | 14:M:227:ALA:HB3 | 2.03 | 0.41 |
| 14:M:344:TYR:O | 14:M:347:LEU:HD23 | 2.20 | 0.41 |
| 15:N:62:PHE:CE2 | 15:N:285:LEU:HD22 | 2.56 | 0.41 |
| 16:Q:8:ASP:OD2 | 16:Q:112:GLN:HB2 | 2.21 | 0.41 |
| 13:T:119:VAL:HA | 13:T:251:TYR:CZ | 2.55 | 0.41 |
| 14:U:187:GLU:HG2 | 14:U:188:GLU:HG3 | 2.02 | 0.41 |
| 14:U:102:MET:HB3 | 14:U:230:LEU:HD23 | 2.03 | 0.41 |
| 1:1:41:ALA:N | 1:1:116:GLU:OE2 | 2.48 | 0.41 |
| 3:3:360:LEU:HD11 | 3:3:645:ALA:HB2 | 2.03 | 0.41 |
| 4:4:212:PRO:HG2 | 4:4:213:ILE:HD12 | 2.02 | 0.41 |
| 5:5:80:TRP:HE3 | 5:5:80:TRP:HA | 1.85 | 0.41 |
| 5:5:2:ARG:HG3 | 5:5:84:ASP:OD2 | 2.21 | 0.41 |
| 1:B:193:GLU:CD | 1:B:200:ARG:HH22 | 2.24 | 0.41 |
| 1:B:3:GLY:HA2 | 1:B:4:PRO:HD3 | 1.89 | 0.41 |
| 3:D:533:LEU:HD23 | 3:D:533:LEU:HA | 1.77 | 0.41 |
| 4:E:177:GLY:HA3 | 4:E:302:VAL:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:L:321:HIS:HA | 13:L:384:SER:HB2 | 2.02 | 0.41 |
| 13:L:391:ALA:O | 13:L:395:TYR:HB2 | 2.19 | 0.41 |
| 13:L:598:LEU:HA | 13:L:598:LEU:HD23 | 1.84 | 0.41 |
| 15:N:41:LEU:O | 15:N:44:TRP:HB2 | 2.20 | 0.41 |
| 16:Q:268:THR:HA | 16:Q:273:GLU:OE1 | 2.21 | 0.41 |
| 7:O:22:VAL:HB | 16:Q:44:VAL:CG1 | 2.51 | 0.41 |
| 16:Q:85:ALA:CB | 16:Q:139:SER:HB2 | 2.50 | 0.41 |
| 11:R:72:MET:CE | 16:Q:153:LEU:HD21 | 2.51 | 0.41 |
| 13:T:154:SER:HB2 | 13:T:228:ASP:HB3 | 2.03 | 0.41 |
| 13:T:168:GLY:HA3 | 13:T:211:LEU:HD22 | 2.02 | 0.41 |
| 13:T:538:TYR:O | 13:T:542:ILE:HB | 2.20 | 0.41 |
| 14:U:164:LEU:HD21 | 15:V:346:TYR:HE1 | 1.85 | 0.41 |
| 2:2:147:ARG:HB2 | 2:2:147:ARG:HE | 1.58 | 0.41 |
| 3:3:688:ARG:CZ | 3:3:769:LEU:HD22 | 2.51 | 0.41 |
| 6:6:163:TYR:H | 7:9:152:ARG:HH12 | 1.67 | 0.41 |
| 1:B:145:LEU:O | 1:B:149:ILE:HG13 | 2.20 | 0.41 |
| 1:B:66:GLY:O | 19:B:503:NAI:H2N | 2.21 | 0.41 |
| 3:D:201:ASP:OD1 | 3:D:202:PHE:N | 2.49 | 0.41 |
| 3:D:49:LEU:HD23 | 3:D:81:ALA:HA | 2.02 | 0.41 |
| 4:E:132:PHE:HE1 | 4:E:398:ALA:O | 2.03 | 0.41 |
| 4:E:288:LYS:HD3 | 4:E:288:LYS:HA | 1.69 | 0.41 |
| 16:H:119:ASP:OD1 | 16:H:120:LEU:HG | 2.20 | 0.41 |
| 14:M:85:GLY:O | 14:M:89:ALA:HB2 | 2.20 | 0.41 |
| 15:N:73:THR:HG21 | 15:N:210:PHE:HB2 | 2.03 | 0.41 |
| 7:O:98:CYS:SG | 7:O:100:PHE:CD1 | 3.14 | 0.41 |
| 11:R:5:GLU:O | 11:R:9:LEU:HG | 2.21 | 0.41 |
| 13:T:450:ALA:O | 13:T:454:VAL:HG23 | 2.21 | 0.41 |
| 13:T:541:LEU:C | 13:T:545:PRO:HG2 | 2.41 | 0.41 |
| 13:T:41:PHE:HD1 | 13:T:81:THR:OG1 | 2.04 | 0.41 |
| 14:U:371:LEU:HD12 | 14:U:440:LEU:HB3 | 2.03 | 0.41 |
| 15:V:23:GLN:O | 15:V:27:ARG:HG3 | 2.21 | 0.41 |
| 15:V:299:LEU:HD22 | 15:V:307:VAL:HG11 | 2.03 | 0.41 |
| 1:1:63:ARG:HD3 | 1:1:313:TYR:CD2 | 2.56 | 0.41 |
| 1:1:354:GLY:HA2 | 1:1:360:ARG:HB2 | 2.02 | 0.41 |
| 2:2:89:LYS:HE3 | 2:2:94:GLU:HG2 | 2.02 | 0.41 |
| 3:3:655:ARG:HH22 | 3:3:659:GLU:HG3 | 1.85 | 0.41 |
| 3:3:664:LEU:HB3 | 3:3:669:VAL:HG11 | 2.03 | 0.41 |
| 5:5:35:LYS:HA | 5:5:35:LYS:HD2 | 1.88 | 0.41 |
| 6:6:18:GLY:HA3 | 6:6:32:ARG:HH21 | 1.85 | 0.41 |
| 1:B:404:ASP:N | 1:B:404:ASP:OD1 | 2.54 | 0.41 |
| 3:D:567:TYR:HA | 3:D:584:VAL:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:87:TYR:HB3 | 6:G:45:CYS:HB3 | 2.01 | 0.41 |
| 6:G:132:PRO:HG3 | 6:G:178:ARG:CZ | 2.51 | 0.41 |
| 4:E:154:GLU:OE1 | 6:G:57:ARG:NH1 | 2.54 | 0.41 |
| 10:A:56:ARG:HB3 | 11:J:73:LEU:O | 2.21 | 0.41 |
| 13:L:49:LEU:HD23 | 13:L:49:LEU:HA | 1.96 | 0.41 |
| 13:L:68:LEU:HD23 | 13:L:255:ARG:NH2 | 2.33 | 0.41 |
| 16:Q:274:VAL:CG1 | 16:Q:278:TRP:CD1 | 2.91 | 0.41 |
| 11:R:115:PHE:CD1 | 12:S:48:ALA:HB2 | 2.56 | 0.41 |
| 13:T:29:PRO:HB2 | 13:T:101:TYR:HD2 | 1.85 | 0.41 |
| 13:T:324:THR:HG22 | 13:T:380:SER:HB2 | 2.03 | 0.41 |
| 14:U:99:ALA:HB2 | 14:U:226:LEU:HD21 | 2.03 | 0.41 |
| 14:U:331:ARG:HD2 | 14:U:331:ARG:HA | 1.82 | 0.41 |
| 15:V:3:LEU:HD13 | 15:V:96:HIS:HD2 | 1.85 | 0.41 |
| 15:V:98:LEU:HD22 | 15:V:114:LEU:HD21 | 2.01 | 0.41 |
| 9:X:49:LEU:HD13 | 9:X:58:LEU:HD13 | 2.03 | 0.41 |
| 1:1:272:PHE:CE1 | 1:1:309:THR:HB | 2.56 | 0.41 |
| 3:3:34:CYS:O | 3:3:189:ARG:NH2 | 2.52 | 0.41 |
| 3:3:728:LEU:O | 3:3:749:HIS:NE2 | 2.37 | 0.41 |
| 3:3:8:ASP:OD1 | 3:3:9:ARG:HG3 | 2.21 | 0.41 |
| 4:4:133:LEU:O | 4:4:137:LEU:HD13 | 2.21 | 0.41 |
| 6:6:44:ALA:O | 6:6:47:ALA:N | 2.40 | 0.41 |
| 8:7:60:SER:HA | 8:7:66:PRO:HA | 2.02 | 0.41 |
| 1:B:207:ALA:O | 1:B:215:PRO:HB3 | 2.21 | 0.41 |
| 1:B:98:PRO:HA | 2:C:124:CYS:SG | 2.61 | 0.41 |
| 2:C:61:MET:CE | 3:D:214:MET:HG3 | 2.51 | 0.41 |
| 3:D:176:LEU:HD13 | 3:D:235:LEU:CD2 | 2.51 | 0.41 |
| 3:D:384:PRO:O | 3:D:531:LYS:HD3 | 2.21 | 0.41 |
| 3:D:403:THR:H | 3:D:458:LEU:HD11 | 1.86 | 0.41 |
| 4:4:35:PRO:HB3 | 16:H:229:VAL:HG12 | 2.02 | 0.41 |
| 16:H:171:LEU:HB3 | 16:H:321:PHE:CD1 | 2.56 | 0.41 |
| 11:J:61:GLY:O | 11:J:65:VAL:CG2 | 2.66 | 0.41 |
| 13:L:291:ILE:HG13 | 13:L:292:LYS:N | 2.36 | 0.41 |
| 13:L:360:PRO:HA | 13:L:363:ARG:NH1 | 2.35 | 0.41 |
| 13:L:386:ASP:OD2 | 13:L:494:ILE:HA | 2.21 | 0.41 |
| 14:M:214:LEU:HD11 | 14:M:235:LYS:HZ1 | 1.86 | 0.41 |
| 14:M:5:ALA:HB1 | 14:M:36:ASN:HD21 | 1.85 | 0.41 |
| 15:N:76:LEU:HD12 | 15:N:206:PRO:HB3 | 2.03 | 0.41 |
| 10:P:28:GLY:HA3 | 16:Q:239:ILE:HB | 2.02 | 0.41 |
| 10:P:71:PHE:CZ | 10:P:107:PHE:HB2 | 2.56 | 0.41 |
| 11:R:72:MET:HE2 | 16:Q:153:LEU:HD21 | 2.03 | 0.41 |
| 10:P:107:PHE:HE1 | 16:Q:310:TRP:CD1 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:P:56:ARG:NH1 | 11:R:75:PHE:H | 2.19 | 0.41 |
| 13:T:111:PHE:CZ | 13:T:134:VAL:HG13 | 2.56 | 0.41 |
| 4:4:42:ARG:O | 4:4:43:LEU:HD23 | 2.21 | 0.40 |
| 1:B:65:ARG:NH2 | 1:B:238:PHE:HZ | 2.19 | 0.40 |
| 3:D:170:LEU:HD11 | 3:D:176:LEU:HD22 | 2.03 | 0.40 |
| 3:D:368:HIS:CB | 3:D:556:ALA:HB3 | 2.52 | 0.40 |
| 3:D:717:TRP:CE3 | 3:D:750:ARG:HD3 | 2.57 | 0.40 |
| 10:A:100:THR:HG21 | 16:H:322:LEU:HD11 | 2.02 | 0.40 |
| 16:H:74:VAL:HG23 | 16:H:82:PHE:CZ | 2.56 | 0.40 |
| 11:J:83:PHE:O | 12:K:22:ARG:HD3 | 2.21 | 0.40 |
| 13:L:90:TYR:CD1 | 13:L:334:LEU:HD22 | 2.56 | 0.40 |
| 13:L:463:HIS:CD2 | 13:L:464:PRO:HD3 | 2.56 | 0.40 |
| 14:M:148:PHE:O | 14:M:152:THR:HG23 | 2.20 | 0.40 |
| 14:M:304:THR:O | 14:M:306:GLU:N | 2.54 | 0.40 |
| 14:M:54:PRO:HA | 14:M:62:TYR:CD1 | 2.51 | 0.40 |
| 13:T:160:ILE:O | 13:T:164:ILE:HG13 | 2.20 | 0.40 |
| 13:T:202:LEU:HD12 | 13:T:202:LEU:HA | 1.87 | 0.40 |
| 13:T:427:GLY:O | 13:T:428:GLU:HG2 | 2.20 | 0.40 |
| 14:U:225:GLY:HA2 | 14:U:228:ASP:OD2 | 2.20 | 0.40 |
| 14:U:306:GLU:H | 14:U:306:GLU:HG3 | 1.68 | 0.40 |
| 14:U:29:ALA:HB1 | 14:U:83:PHE:HA | 2.02 | 0.40 |
| 1:1:180:TYR:HB3 | 1:1:351:GLU:HB3 | 2.03 | 0.40 |
| 1:1:356:CYS:N | 17:1:501:SF4:S3 | 2.86 | 0.40 |
| 2:2:79:HIS:ND1 | 2:2:118:SER:HB2 | 2.36 | 0.40 |
| 4:4:120:LEU:HD22 | 4:4:160:PHE:HE1 | 1.85 | 0.40 |
| 5:5:116:ARG:NH2 | 5:5:135:ILE:HG12 | 2.36 | 0.40 |
| 6:6:36:LEU:O | 6:6:38:PRO:HD3 | 2.21 | 0.40 |
| 6:6:94:ARG:HD2 | 10:A:46:SER:CA | 2.45 | 0.40 |
| 10:A:49:ASP:OD1 | 10:A:52:GLY:HA3 | 2.21 | 0.40 |
| 1:B:116:GLU:O | 1:B:120:LEU:HG | 2.21 | 0.40 |
| 3:D:695:ARG:HH11 | 3:D:695:ARG:HD3 | 1.72 | 0.40 |
| 4:E:84:ARG:HA | 4:E:169:HIS:CE1 | 2.57 | 0.40 |
| 5:F:56:ASP:HB2 | 5:F:122:PHE:HE2 | 1.86 | 0.40 |
| 4:E:106:GLY:O | 5:F:194:SER:HB3 | 2.21 | 0.40 |
| 6:G:178:ARG:CZ | 9:X:125:ILE:HG22 | 2.51 | 0.40 |
| 16:H:196:PHE:O | 16:H:200:PHE:N | 2.55 | 0.40 |
| 10:A:67:LEU:HD23 | 16:H:310:TRP:CZ2 | 2.56 | 0.40 |
| 16:H:83:VAL:HA | 16:H:240:LYS:HD3 | 2.03 | 0.40 |
| 8:I:88:ARG:HH21 | 8:I:126:LEU:HB3 | 1.86 | 0.40 |
| 14:M:224:SER:O | 14:M:330:GLY:HA3 | 2.21 | 0.40 |
| 14:M:56:LEU:HB3 | 14:M:59:ALA:HB3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:N:311:ALA:HA | 15:N:389:THR:OG1 | 2.21 | 0.40 |
| 7:O:40:ARG:NH2 | 7:O:42:VAL:HG12 | 2.36 | 0.40 |
| 13:T:128:PHE:CZ | 13:T:166:ASP:HB3 | 2.56 | 0.40 |
| 13:T:142:ILE:HD13 | 13:T:229:ALA:HA | 2.02 | 0.40 |
| 13:T:404:VAL:O | 13:T:408:LEU:HG | 2.21 | 0.40 |
| 14:U:5:ALA:HB1 | 14:U:36:ASN:ND2 | 2.37 | 0.40 |
| 14:U:64:ALA:CB | 14:U:113:ARG:HB3 | 2.51 | 0.40 |
| 3:3:233:GLY:O | 3:3:236:LEU:HG | 2.22 | 0.40 |
| 3:3:327:LEU:HD23 | 3:3:330:LYS:HD2 | 2.03 | 0.40 |
| 4:4:162:TRP:CD1 | 7:9:34:LYS:HD2 | 2.56 | 0.40 |
| 6:6:37:TRP:HB2 | 6:6:76:ASP:OD1 | 2.22 | 0.40 |
| 6:6:69:ARG:HD3 | 6:6:74:GLN:OE1 | 2.20 | 0.40 |
| 7:9:55:GLY:O | 7:9:86:ARG:NE | 2.46 | 0.40 |
| 10:A:6:GLU:OE2 | 16:H:2:THR:OG1 | 2.31 | 0.40 |
| 1:B:192:LEU:HD22 | 1:B:211:LEU:HD21 | 2.04 | 0.40 |
| 2:C:7:LYS:HE2 | 2:C:7:LYS:HB3 | 1.96 | 0.40 |
| 3:D:250:GLU:HG3 | 5:F:169:GLU:OE1 | 2.22 | 0.40 |
| 3:D:33:PHE:CE2 | 3:D:47:MET:HE3 | 2.57 | 0.40 |
| 5:F:147:ARG:HG2 | 5:F:147:ARG:H | 1.68 | 0.40 |
| 4:E:367:ARG:HH12 | 5:F:53:VAL:HG23 | 1.87 | 0.40 |
| 16:H:222:PRO:HD2 | 16:H:230:GLY:HA2 | 2.04 | 0.40 |
| 16:H:260:PRO:HG3 | 16:H:286:PHE:CE2 | 2.55 | 0.40 |
| 8:I:21:ARG:O | 8:I:24:ALA:HB3 | 2.21 | 0.40 |
| 11:J:48:ALA:HA | 11:J:122:GLY:HA3 | 2.03 | 0.40 |
| 11:J:36:PHE:CD2 | 11:J:59:TYR:HB3 | 2.57 | 0.40 |
| 12:K:13:LEU:HD23 | 12:K:13:LEU:HA | 1.77 | 0.40 |
| 14:M:92:GLU:C | 14:M:94:ARG:H | 2.24 | 0.40 |
| 7:O:67:ALA:O | 7:O:93:ILE:HA | 2.22 | 0.40 |
| 10:P:7:TYR:N | 10:P:7:TYR:CD1 | 2.88 | 0.40 |
| 16:Q:50:ARG:HA | 16:Q:50:ARG:HD3 | 1.93 | 0.40 |
| 13:T:234:THR:N | 13:T:235:PRO:HD2 | 2.37 | 0.40 |
| 13:T:239:LEU:HA | 13:T:239:LEU:HD12 | 1.87 | 0.40 |
| 15:V:200:TYR:CE2 | 15:V:212:ALA:HB2 | 2.56 | 0.40 |
| 1:1:122:GLY:HA3 | 1:1:169:PHE:HE1 | 1.86 | 0.40 |
| 1:1:270:THR:O | 1:1:311:MET:HG3 | 2.21 | 0.40 |
| 2:2:143:GLU:O | 2:2:149:ARG:NH1 | 2.55 | 0.40 |
| 3:3:170:LEU:HG | 3:3:176:LEU:HB2 | 2.03 | 0.40 |
| 6:6:93:ARG:HD3 | 6:6:130:VAL:O | 2.21 | 0.40 |
| 1:B:413:SER:O | 1:B:417:PHE:HB2 | 2.21 | 0.40 |
| 2:C:79:HIS:H | 2:C:137:ASN:HD21 | 1.69 | 0.40 |
| 3:D:192:GLU:HG3 | 3:D:440:ARG:HH11 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:24:PHE:CE2 | 3:D:30:VAL:HG12 | 2.56 | 0.40 |
| 4:E:218:ALA:HA | 4:E:221:VAL:HG22 | 2.03 | 0.40 |
| 4:E:75:TYR:CZ | 4:E:337:PRO:HG2 | 2.56 | 0.40 |
| 5:F:122:PHE:O | 5:F:144:HIS:ND1 | 2.55 | 0.40 |
| 4:E:73:ARG:NH1 | 5:F:171:ARG:HH21 | 2.19 | 0.40 |
| 6:G:46:CYS:SG | 6:G:109:GLY:HA3 | 2.61 | 0.40 |
| 8:I:101:LYS:H | 8:I:101:LYS:HG2 | 1.66 | 0.40 |
| 12:K:23:THR:OG1 | 12:K:26:LEU:HD13 | 2.21 | 0.40 |
| 13:L:184:SER:HB3 | 13:L:187:GLU:HG2 | 2.04 | 0.40 |
| 13:L:582:GLN:HA | 13:L:589:TYR:CE1 | 2.57 | 0.40 |
| 10:P:57:PHE:HE2 | 16:Q:149:LEU:HD13 | 1.85 | 0.40 |
| 16:Q:257:ALA:O | 16:Q:260:PRO:HD2 | 2.20 | 0.40 |
| 11:R:104:LEU:O | 11:R:108:LEU:HD12 | 2.21 | 0.40 |
| 13:T:291:ILE:HG13 | 13:T:292:LYS:N | 2.36 | 0.40 |
| 14:U:281:PHE:CE2 | 14:U:332:LEU:HD21 | 2.56 | 0.40 |
| 9:W:10:PRO:HG3 | 9:W:62:ALA:O | 2.21 | 0.40 |
| 1:1:170:ASP:OD1 | 1:1:171:LEU:N | 2.55 | 0.40 |
| 3:3:42:ILE:HD12 | 3:3:42:ILE:C | 2.37 | 0.40 |
| 3:3:473:GLU:O | 3:3:476:ILE:N | 2.55 | 0.40 |
| 4:4:317:LEU:HD12 | 4:4:317:LEU:HA | 1.86 | 0.40 |
| 5:5:3:LEU:HB2 | 5:5:86:SER:HB2 | 2.02 | 0.40 |
| 7:9:68:ILE:HD11 | 17:9:201:SF4:S1 | 2.61 | 0.40 |
| 10:A:1:MET:HG3 | 11:J:123:LEU:HD11 | 2.03 | 0.40 |
| 2:C:125:LEU:HB3 | 2:C:141:TYR:CZ | 2.55 | 0.40 |
| 3:D:7:ASN:ND2 | 3:D:94:ASP:HA | 2.36 | 0.40 |
| 4:E:102:GLU:HG2 | 4:E:175:ILE:O | 2.21 | 0.40 |
| 3:D:120:PRO:HA | 4:E:328:PHE:HE2 | 1.86 | 0.40 |
| 5:F:77:LEU:HA | 5:F:78:PRO:HD3 | 1.98 | 0.40 |
| 16:H:275:PRO:HB2 | 16:H:276:TYR:HD1 | 1.87 | 0.40 |
| 16:H:314:PHE:HB2 | 16:H:315:PRO:HD3 | 2.02 | 0.40 |
| 11:J:131:LEU:HA | 11:J:135:TRP:HB2 | 2.04 | 0.40 |
| 13:L:320:PHE:CE2 | 13:L:460:ALA:HB3 | 2.56 | 0.40 |
| 14:M:232:THR:HA | 14:M:235:LYS:NZ | 2.34 | 0.40 |
| 14:M:206:PRO:HD2 | 14:M:293:MET:HG3 | 2.04 | 0.40 |
| 16:Q:340:LEU:HD23 | 16:Q:340:LEU:HA | 1.83 | 0.40 |
| 11:R:75:PHE:O | 11:R:77:ALA:N | 2.54 | 0.40 |
| 13:T:386:ASP:OD2 | 13:T:494:ILE:HG23 | 2.22 | 0.40 |
| 13:T:70:ASP:H | 13:T:73:SER:HB2 | 1.85 | 0.40 |
| 14:U:215:PRO:CG | 14:U:216:PRO:HD3 | 2.52 | 0.40 |
| 15:V:279:GLN:HG3 | 15:V:423:LEU:HB2 | 2.04 | 0.40 |
| 9:W:43:GLN:O | 9:W:66:ALA:HB2 | 2.22 | 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 | 1 | 435/438 (99%) | 403 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | B | 435/438 (99%) | 404 (93%) | 31 (7%) | 0 | 100 | 100 |
| 2 | 2 | 176/181 (97%) | 168 (96%) | 8 (4%) | 0 | 100 | 100 |
| 2 | C | 176/181 (97%) | 168 (96%) | 8 (4%) | 0 | 100 | 100 |
| 3 | 3 | 750/783 (96%) | 696 (93%) | 54 (7%) | 0 | 100 | 100 |
| 3 | D | 750/783 (96%) | 703 (94%) | 47 (6%) | 0 | 100 | 100 |
| 4 | 4 | 382/409 (93%) | 359 (94%) | 23 (6%) | 0 | 100 | 100 |
| 4 | E | 382/409 (93%) | 360 (94%) | 22 (6%) | 0 | 100 | 100 |
| 5 | 5 | 194/207 (94%) | 185 (95%) | 9 (5%) | 0 | 100 | 100 |
| 5 | F | 194/207 (94%) | 187 (96%) | 7 (4%) | 0 | 100 | 100 |
| 6 | 6 | 164/181 (91%) | 147 (90%) | 16 (10%) | 1 (1%) | 25 | 64 |
| 6 | G | 164/181 (91%) | 145 (88%) | 19 (12%) | 0 | 100 | 100 |
| 7 | 9 | 178/182 (98%) | 172 (97%) | 6 (3%) | 0 | 100 | 100 |
| 7 | O | 178/182 (98%) | 171 (96%) | 7 (4%) | 0 | 100 | 100 |
| 8 | 7 | 125/129 (97%) | 116 (93%) | 9 (7%) | 0 | 100 | 100 |
| 8 | I | 125/129 (97%) | 115 (92%) | 10 (8%) | 0 | 100 | 100 |
| 9 | W | 125/131 (95%) | 121 (97%) | 4 (3%) | 0 | 100 | 100 |
| 9 | X | 125/131 (95%) | 121 (97%) | 4 (3%) | 0 | 100 | 100 |
| 10 | A | 115/119 (97%) | 106 (92%) | 9 (8%) | 0 | 100 | 100 |
| 10 | P | 115/119 (97%) | 106 (92%) | 9 (8%) | 0 | 100 | 100 |
| 11 | J | 158/176 (90%) | 147 (93%) | 11 (7%) | 0 | 100 | 100 |
| 11 | R | 158/176 (90%) | 146 (92%) | 12 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12 | K | 93/95 (98%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 12 | S | 93/95 (98%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 13 | L | 603/606 (100%) | 569 (94%) | 33 (6%) | 1 (0%) | 47 | 79 |
| 13 | T | 603/606 (100%) | 569 (94%) | 33 (6%) | 1 (0%) | 47 | 79 |
| 14 | M | 465/469 (99%) | 437 (94%) | 28 (6%) | 0 | 100 | 100 |
| 14 | U | 465/469 (99%) | 437 (94%) | 28 (6%) | 0 | 100 | 100 |
| 15 | N | 425/427 (100%) | 400 (94%) | 25 (6%) | 0 | 100 | 100 |
| 15 | V | 425/427 (100%) | 404 (95%) | 21 (5%) | 0 | 100 | 100 |
| 16 | H | 351/365 (96%) | 303 (86%) | 42 (12%) | 6 (2%) | 9 | 42 |
| 16 | Q | 351/365 (96%) | 302 (86%) | 42 (12%) | 7 (2%) | 7 | 38 |
| All | All | 9478/9796 (97%) | 8845 (93%) | 617 (6%) | 16 (0%) | 47 | 79 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | H | 51 | VAL |
| 16 | Q | 51 | VAL |
| 16 | H | 50 | ARG |
| 16 | H | 218 | PRO |
| 16 | H | 44 | VAL |
| 13 | T | 435 | PRO |
| 16 | Q | 50 | ARG |
| 16 | Q | 268 | THR |
| 13 | L | 435 | PRO |
| 6 | 6 | 45 | CYS |
| 16 | H | 195 | LEU |
| 16 | Q | 218 | PRO |
| 16 | Q | 44 | VAL |
| 16 | Q | 332 | LEU |
| 16 | Q | 333 | PRO |
| 16 | H | 53 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 1 | 355/356 (100%) | 344 (97%) | 11 (3%) | 40 | 72 |
| 1 | B | 355/356 (100%) | 344 (97%) | 11 (3%) | 40 | 72 |
| 2 | 2 | 150/152 (99%) | 144 (96%) | 6 (4%) | 31 | 66 |
| 2 | C | 150/152 (99%) | 144 (96%) | 6 (4%) | 31 | 66 |
| 3 | 3 | 609/628 (97%) | 597 (98%) | 12 (2%) | 55 | 80 |
| 3 | D | 609/628 (97%) | 599 (98%) | 10 (2%) | 62 | 84 |
| 4 | 4 | 332/355 (94%) | 325 (98%) | 7 (2%) | 53 | 79 |
| 4 | E | 332/355 (94%) | 325 (98%) | 7 (2%) | 53 | 79 |
| 5 | 5 | 167/175 (95%) | 166 (99%) | 1 (1%) | 86 | 94 |
| 5 | F | 167/175 (95%) | 164 (98%) | 3 (2%) | 59 | 82 |
| 6 | 6 | 135/149 (91%) | 125 (93%) | 10 (7%) | 13 | 46 |
| 6 | G | 135/149 (91%) | 125 (93%) | 10 (7%) | 13 | 46 |
| 7 | 9 | 148/150 (99%) | 145 (98%) | 3 (2%) | 55 | 80 |
| 7 | O | 148/150 (99%) | 146 (99%) | 2 (1%) | 67 | 86 |
| 8 | 7 | 104/106 (98%) | 103 (99%) | 1 (1%) | 76 | 90 |
| 8 | I | 104/106 (98%) | 102 (98%) | 2 (2%) | 57 | 81 |
| 9 | W | 99/101 (98%) | 98 (99%) | 1 (1%) | 76 | 90 |
| 9 | X | 99/101 (98%) | 97 (98%) | 2 (2%) | 55 | 80 |
| 10 | A | 90/92 (98%) | 86 (96%) | 4 (4%) | 28 | 64 |
| 10 | P | 90/92 (98%) | 89 (99%) | 1 (1%) | 73 | 88 |
| 11 | J | 118/130 (91%) | 114 (97%) | 4 (3%) | 37 | 70 |
| 11 | R | 118/130 (91%) | 115 (98%) | 3 (2%) | 47 | 77 |
| 12 | K | 71/71 (100%) | 69 (97%) | 2 (3%) | 43 | 74 |
| 12 | S | 71/71 (100%) | 70 (99%) | 1 (1%) | 67 | 86 |
| 13 | L | 453/454 (100%) | 446 (98%) | 7 (2%) | 65 | 85 |
| 13 | T | 453/454 (100%) | 446 (98%) | 7 (2%) | 65 | 85 |
| 14 | M | 332/332 (100%) | 326 (98%) | 6 (2%) | 59 | 82 |
| 14 | U | 332/332 (100%) | 323 (97%) | 9 (3%) | 44 | 75 |
| 15 | N | 302/302 (100%) | 298 (99%) | 4 (1%) | 69 | 87 |
| 15 | V | 302/302 (100%) | 297 (98%) | 5 (2%) | 60 | 83 |
| 16 | H | 293/300 (98%) | 286 (98%) | 7 (2%) | 49 | 77 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 16 | Q | 293/300 (98%) | 288 (98%) | 5 (2%) | 60 | 83 |
| All | All | 7516/7706 (98%) | 7346 (98%) | 170 (2%) | 50 | 78 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 18 | TYR |
| 1 | 1 | 81 | LYS |
| 1 | 1 | 249 | MET |
| 1 | 1 | 342 | TRP |
| 1 | 1 | 353 | CYS |
| 1 | 1 | 355 | LYS |
| 1 | 1 | 359 | CYS |
| 1 | 1 | 366 | PHE |
| 1 | 1 | 397 | ARG |
| 1 | 1 | 437 | TRP |
| 1 | 1 | 438 | ARG |
| 2 | 2 | 7 | LYS |
| 2 | 2 | 33 | ARG |
| 2 | 2 | 35 | GLN |
| 2 | 2 | 45 | ARG |
| 2 | 2 | 116 | LEU |
| 2 | 2 | 147 | ARG |
| 3 | 3 | 3 | ARG |
| 3 | 3 | 123 | ASP |
| 3 | 3 | 132 | ASP |
| 3 | 3 | 184 | CYS |
| 3 | 3 | 259 | CYS |
| 3 | 3 | 260 | PRO |
| 3 | 3 | 337 | ARG |
| 3 | 3 | 369 | LEU |
| 3 | 3 | 651 | ARG |
| 3 | 3 | 655 | ARG |
| 3 | 3 | 761 | SER |
| 3 | 3 | 774 | ARG |
| 4 | 4 | 87 | TYR |
| 4 | 4 | 132 | PHE |
| 4 | 4 | 143 | LEU |
| 4 | 4 | 151 | ARG |
| 4 | 4 | 208 | PHE |
| 4 | 4 | 262 | PHE |
| 4 | 4 | 363 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 5 | 147 | ARG |
| 6 | 6 | 37 | TRP |
| 6 | 6 | 49 | GLU |
| 6 | 6 | 55 | ASP |
| 6 | 6 | 68 | PHE |
| 6 | 6 | 88 | MET |
| 6 | 6 | 98 | GLN |
| 6 | 6 | 101 | ASP |
| 6 | 6 | 120 | ASN |
| 6 | 6 | 153 | GLN |
| 6 | 6 | 156 | LYS |
| 7 | 9 | 4 | LYS |
| 7 | 9 | 38 | HIS |
| 7 | 9 | 118 | ASP |
| 8 | 7 | 43 | ARG |
| 9 | W | 37 | TRP |
| 10 | A | 13 | TYR |
| 10 | A | 49 | ASP |
| 10 | A | 79 | TRP |
| 10 | A | 110 | GLU |
| 11 | J | 32 | LEU |
| 11 | J | 59 | TYR |
| 11 | J | 118 | ASP |
| 11 | J | 119 | LEU |
| 12 | K | 28 | PHE |
| 12 | K | 82 | ARG |
| 13 | L | 56 | GLN |
| 13 | L | 59 | TRP |
| 13 | L | 169 | PHE |
| 13 | L | 275 | LEU |
| 13 | L | 506 | TRP |
| 13 | L | 511 | PHE |
| 13 | L | 554 | PHE |
| 14 | M | 22 | ARG |
| 14 | M | 135 | LEU |
| 14 | M | 148 | PHE |
| 14 | M | 241 | PHE |
| 14 | M | 255 | GLN |
| 14 | M | 455 | HIS |
| 15 | N | 50 | PHE |
| 15 | N | 125 | ARG |
| 15 | N | 126 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | N | 284 | TYR |
| 16 | H | 119 | ASP |
| 16 | H | 134 | TYR |
| 16 | H | 147 | TYR |
| 16 | H | 196 | PHE |
| 16 | H | 233 | HIS |
| 16 | H | 307 | ARG |
| 16 | H | 354 | TYR |
| 1 | B | 81 | LYS |
| 1 | B | 249 | MET |
| 1 | B | 337 | MET |
| 1 | B | 342 | TRP |
| 1 | B | 353 | CYS |
| 1 | B | 355 | LYS |
| 1 | B | 359 | CYS |
| 1 | B | 366 | PHE |
| 1 | B | 397 | ARG |
| 1 | B | 400 | CYS |
| 1 | B | 437 | TRP |
| 2 | C | 7 | LYS |
| 2 | C | 33 | ARG |
| 2 | C | 35 | GLN |
| 2 | C | 45 | ARG |
| 2 | C | 116 | LEU |
| 2 | C | 147 | ARG |
| 3 | D | 3 | ARG |
| 3 | D | 83 | CYS |
| 3 | D | 184 | CYS |
| 3 | D | 259 | CYS |
| 3 | D | 337 | ARG |
| 3 | D | 369 | LEU |
| 3 | D | 617 | LEU |
| 3 | D | 655 | ARG |
| 3 | D | 761 | SER |
| 3 | D | 774 | ARG |
| 4 | E | 87 | TYR |
| 4 | E | 129 | HIS |
| 4 | E | 143 | LEU |
| 4 | E | 151 | ARG |
| 4 | E | 152 | GLU |
| 4 | E | 208 | PHE |
| 4 | E | 262 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 31 | ARG |
| 5 | F | 147 | ARG |
| 5 | F | 178 | ASP |
| 6 | G | 37 | TRP |
| 6 | G | 49 | GLU |
| 6 | G | 55 | ASP |
| 6 | G | 68 | PHE |
| 6 | G | 83 | ARG |
| 6 | G | 101 | ASP |
| 6 | G | 120 | ASN |
| 6 | G | 156 | LYS |
| 6 | G | 176 | TRP |
| 6 | G | 177 | LYS |
| 7 | O | 38 | HIS |
| 7 | O | 104 | CYS |
| 8 | I | 43 | ARG |
| 8 | I | 120 | ASP |
| 9 | X | 37 | TRP |
| 9 | X | 43 | GLN |
| 10 | P | 13 | TYR |
| 11 | R | 59 | TYR |
| 11 | R | 118 | ASP |
| 11 | R | 119 | LEU |
| 12 | S | 28 | PHE |
| 13 | T | 10 | PRO |
| 13 | T | 59 | TRP |
| 13 | T | 151 | TYR |
| 13 | T | 169 | PHE |
| 13 | T | 506 | TRP |
| 13 | T | 511 | PHE |
| 13 | T | 554 | PHE |
| 14 | U | 22 | ARG |
| 14 | U | 115 | LEU |
| 14 | U | 135 | LEU |
| 14 | U | 148 | PHE |
| 14 | U | 215 | PRO |
| 14 | U | 234 | TYR |
| 14 | U | 241 | PHE |
| 14 | U | 255 | GLN |
| 14 | U | 455 | HIS |
| 15 | V | 50 | PHE |
| 15 | V | 125 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | V | 126 | ARG |
| 15 | V | 284 | TYR |
| 15 | V | 313 | ARG |
| 16 | Q | 54 | PHE |
| 16 | Q | 134 | TYR |
| 16 | Q | 196 | PHE |
| 16 | Q | 307 | ARG |
| 16 | Q | 354 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 92 | ASN |
| 1 | 1 | 220 | ASN |
| 1 | 1 | 240 | GLN |
| 1 | 1 | 288 | GLN |
| 2 | 2 | 35 | GLN |
| 2 | 2 | 71 | GLN |
| 2 | 2 | 120 | GLN |
| 3 | 3 | 104 | GLN |
| 3 | 3 | 616 | ASN |
| 3 | 3 | 709 | GLN |
| 4 | 4 | 292 | GLN |
| 4 | 4 | 330 | HIS |
| 5 | 5 | 112 | ASN |
| 5 | 5 | 129 | HIS |
| 6 | 6 | 120 | ASN |
| 6 | 6 | 125 | GLN |
| 6 | 6 | 153 | GLN |
| 9 | W | 43 | GLN |
| 10 | A | 60 | HIS |
| 12 | K | 81 | HIS |
| 13 | L | 241 | HIS |
| 13 | L | 302 | GLN |
| 13 | L | 432 | HIS |
| 13 | L | 447 | HIS |
| 13 | L | 513 | GLN |
| 14 | M | 221 | ASN |
| 15 | N | 128 | GLN |
| 15 | N | 245 | ASN |
| 16 | H | 112 | GLN |
| 16 | H | 117 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | H | 304 | GLN |
| 1 | B | 240 | GLN |
| 1 | B | 288 | GLN |
| 3 | D | 104 | GLN |
| 3 | D | 246 | ASN |
| 3 | D | 436 | GLN |
| 3 | D | 709 | GLN |
| 4 | E | 29 | ASN |
| 4 | E | 292 | GLN |
| 4 | E | 308 | GLN |
| 6 | G | 120 | ASN |
| 6 | G | 153 | GLN |
| 9 | X | 43 | GLN |
| 10 | P | 60 | HIS |
| 11 | R | 78 | GLN |
| 12 | S | 81 | HIS |
| 13 | T | 241 | HIS |
| 13 | T | 288 | GLN |
| 13 | T | 325 | HIS |
| 13 | T | 432 | HIS |
| 13 | T | 447 | HIS |
| 14 | U | 36 | ASN |
| 14 | U | 218 | HIS |
| 14 | U | 221 | ASN |
| 14 | U | 255 | GLN |
| 15 | V | 277 | ASN |
| 16 | Q | 43 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

22 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 |
| 20 | FES | 3 | 804 | 3 | 0,4,4 | 0.00 | - | - | | |
| 17 | SF4 | 3 | 802 | 3 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | 3 | 801 | 3 | 0,12,12 | 0.00 | - | - | | |
| 18 | FMN | 1 | 502 | - | 31,33,33 | 1.39 | 4 (12%) | 40,50,50 | 1.65 | 7 (17%) |
| 19 | NAI | B | 503 | - | 42,48,48 | 0.57 | 0 | 47,73,73 | 0.66 | 1 (2%) |
| 17 | SF4 | B | 501 | 1 | 0,12,12 | 0.00 | - | - | | |
| 18 | FMN | B | 502 | - | 31,33,33 | 1.44 | 4 (12%) | 40,50,50 | 1.50 | 5 (12%) |
| 17 | SF4 | 9 | 202 | 7 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | D | 801 | 3 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | 9 | 201 | 7 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | 1 | 501 | 1 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | 3 | 803 | 3 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | O | 202 | 7 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | G | 201 | 6 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | D | 803 | 3 | 0,12,12 | 0.00 | - | - | | |
| 19 | NAI | 1 | 503 | - | 42,48,48 | 0.53 | 0 | 47,73,73 | 0.66 | 1 (2%) |
| 17 | SF4 | O | 201 | 7 | 0,12,12 | 0.00 | - | - | | |
| 17 | SF4 | 6 | 201 | 6 | 0,12,12 | 0.00 | - | - | | |
| 20 | FES | C | 201 | 2 | 0,4,4 | 0.00 | - | - | | |
| 17 | SF4 | D | 802 | 3 | 0,12,12 | 0.00 | - | - | | |
| 20 | FES | 2 | 201 | 2 | 0,4,4 | 0.00 | - | - | | |
| 20 | FES | D | 804 | 3 | 0,4,4 | 0.00 | - | - | | |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 20 | FES | 3 | 804 | 3 | - | - | 0/1/1/1 |
| 17 | SF4 | 3 | 802 | 3 | - | - | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 17 | SF4 | 3 | 801 | 3 | - | - | 0/6/5/5 |
| 18 | FMN | 1 | 502 | - | - | 8/18/18/18 | 0/3/3/3 |
| 19 | NAI | B | 503 | - | - | 9/25/72/72 | 0/5/5/5 |
| 17 | SF4 | B | 501 | 1 | - | - | 0/6/5/5 |
| 18 | FMN | B | 502 | - | - | 8/18/18/18 | 0/3/3/3 |
| 17 | SF4 | 9 | 202 | 7 | - | - | 0/6/5/5 |
| 17 | SF4 | D | 801 | 3 | - | - | 0/6/5/5 |
| 17 | SF4 | 9 | 201 | 7 | - | - | 0/6/5/5 |
| 17 | SF4 | 1 | 501 | 1 | - | - | 0/6/5/5 |
| 17 | SF4 | 3 | 803 | 3 | - | - | 0/6/5/5 |
| 17 | SF4 | O | 202 | 7 | - | - | 0/6/5/5 |
| 17 | SF4 | G | 201 | 6 | - | - | 0/6/5/5 |
| 17 | SF4 | D | 803 | 3 | - | - | 0/6/5/5 |
| 19 | NAI | 1 | 503 | - | - | 11/25/72/72 | 0/5/5/5 |
| 17 | SF4 | O | 201 | 7 | - | - | 0/6/5/5 |
| 17 | SF4 | 6 | 201 | 6 | - | - | 0/6/5/5 |
| 20 | FES | C | 201 | 2 | - | - | 0/1/1/1 |
| 17 | SF4 | D | 802 | 3 | - | - | 0/6/5/5 |
| 20 | FES | 2 | 201 | 2 | - | - | 0/1/1/1 |
| 20 | FES | D | 804 | 3 | - | - | 0/1/1/1 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 18 | B | 502 | FMN | C10-N1 | 4.25 | 1.38 | 1.33 |
| 18 | 1 | 502 | FMN | C10-N1 | 3.63 | 1.37 | 1.33 |
| 18 | B | 502 | FMN | C4A-N5 | 3.42 | 1.38 | 1.33 |
| 18 | 1 | 502 | FMN | C4A-N5 | 3.21 | 1.37 | 1.33 |
| 18 | 1 | 502 | FMN | C4-N3 | 3.17 | 1.38 | 1.33 |
| 18 | B | 502 | FMN | C4-N3 | 3.12 | 1.38 | 1.33 |
| 18 | B | 502 | FMN | C1'-N10 | 2.61 | 1.50 | 1.48 |
| 18 | 1 | 502 | FMN | C1'-N10 | 2.56 | 1.50 | 1.48 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 18 | 1 | 502 | FMN | C4-N3-C2 | 6.14 | 120.32 | 115.14 |
| 18 | B | 502 | FMN | C4-N3-C2 | 5.78 | 120.02 | 115.14 |
| 18 | 1 | 502 | FMN | C5A-C9A-N10 | 3.61 | 120.33 | 117.72 |
| 18 | B | 502 | FMN | C4A-N5-C5A | 3.39 | 120.16 | 116.77 |
| 18 | B | 502 | FMN | C5A-C9A-N10 | 3.35 | 120.14 | 117.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18 | 1 | 502 | FMN | C4A-C4-N3 | -3.10 | 119.19 | 123.43 |
| 18 | 1 | 502 | FMN | C4A-N5-C5A | 2.91 | 119.68 | 116.77 |
| 18 | B | 502 | FMN | C1'-N10-C10 | 2.59 | 120.73 | 118.41 |
| 18 | 1 | 502 | FMN | C1'-N10-C10 | 2.51 | 120.66 | 118.41 |
| 18 | 1 | 502 | FMN | P-O5'-C5' | 2.34 | 124.75 | 118.30 |
| 18 | B | 502 | FMN | C4A-C4-N3 | -2.31 | 120.27 | 123.43 |
| 19 | 1 | 503 | NAI | C5A-C6A-N6A | 2.30 | 123.85 | 120.35 |
| 19 | B | 503 | NAI | C5A-C6A-N6A | 2.29 | 123.84 | 120.35 |
| 18 | 1 | 502 | FMN | C1'-N10-C9A | 2.11 | 119.96 | 118.29 |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | 1 | 502 | FMN | N10-C1'-C2'-O2' |
| 18 | 1 | 502 | FMN | C1'-C2'-C3'-O3' |
| 18 | 1 | 502 | FMN | C1'-C2'-C3'-C4' |
| 18 | 1 | 502 | FMN | O2'-C2'-C3'-O3' |
| 18 | 1 | 502 | FMN | O2'-C2'-C3'-C4' |
| 18 | 1 | 502 | FMN | O4'-C4'-C5'-O5' |
| 19 | B | 503 | NAI | C5D-O5D-PN-O2N |
| 19 | B | 503 | NAI | C3D-C4D-C5D-O5D |
| 18 | B | 502 | FMN | N10-C1'-C2'-O2' |
| 18 | B | 502 | FMN | C1'-C2'-C3'-O3' |
| 18 | B | 502 | FMN | C1'-C2'-C3'-C4' |
| 18 | B | 502 | FMN | O2'-C2'-C3'-O3' |
| 18 | B | 502 | FMN | O2'-C2'-C3'-C4' |
| 18 | B | 502 | FMN | O4'-C4'-C5'-O5' |
| 19 | 1 | 503 | NAI | C5D-O5D-PN-O3 |
| 19 | 1 | 503 | NAI | C5D-O5D-PN-O2N |
| 19 | 1 | 503 | NAI | C3D-C4D-C5D-O5D |
| 19 | 1 | 503 | NAI | O4D-C4D-C5D-O5D |
| 19 | B | 503 | NAI | O4D-C4D-C5D-O5D |
| 19 | B | 503 | NAI | C2D-C1D-N1N-C2N |
| 19 | 1 | 503 | NAI | C2D-C1D-N1N-C2N |
| 19 | B | 503 | NAI | C2D-C1D-N1N-C6N |
| 19 | 1 | 503 | NAI | C2D-C1D-N1N-C6N |
| 19 | B | 503 | NAI | O4D-C1D-N1N-C2N |
| 19 | B | 503 | NAI | O4D-C1D-N1N-C6N |
| 19 | B | 503 | NAI | C5D-O5D-PN-O3 |
| 19 | 1 | 503 | NAI | O4D-C1D-N1N-C2N |
| 18 | 1 | 502 | FMN | N10-C1'-C2'-C3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | B | 502 | FMN | N10-C1'-C2'-C3' |
| 19 | 1 | 503 | NAI | O4D-C1D-N1N-C6N |
| 19 | 1 | 503 | NAI | PA-O3-PN-O1N |
| 19 | B | 503 | NAI | PA-O3-PN-O1N |
| 19 | 1 | 503 | NAI | PA-O3-PN-O2N |
| 18 | 1 | 502 | FMN | C3'-C4'-C5'-O5' |
| 18 | B | 502 | FMN | C3'-C4'-C5'-O5' |
| 19 | 1 | 503 | NAI | C5B-O5B-PA-O1A |

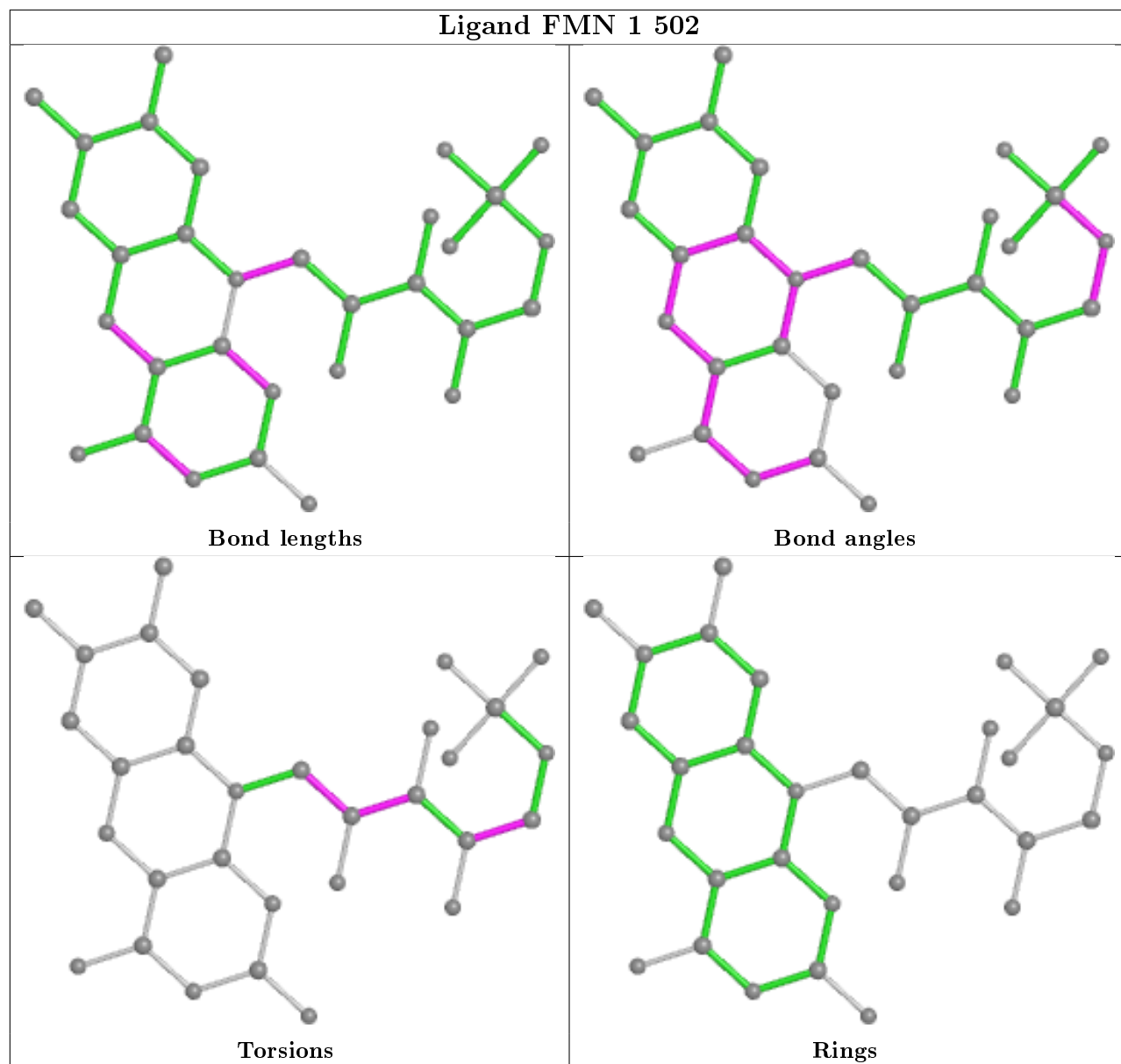
There are no ring outliers.

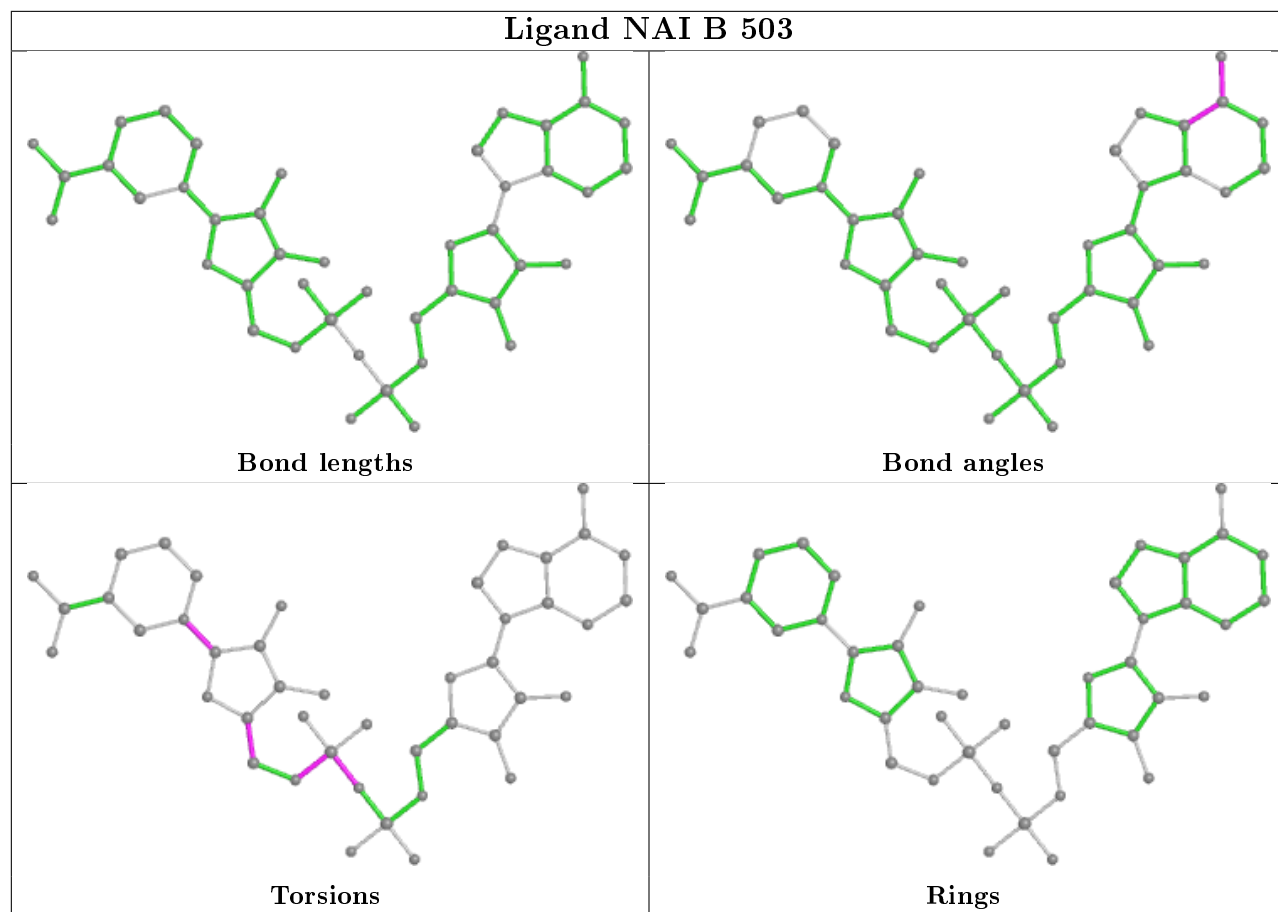
16 monomers are involved in 36 short contacts:

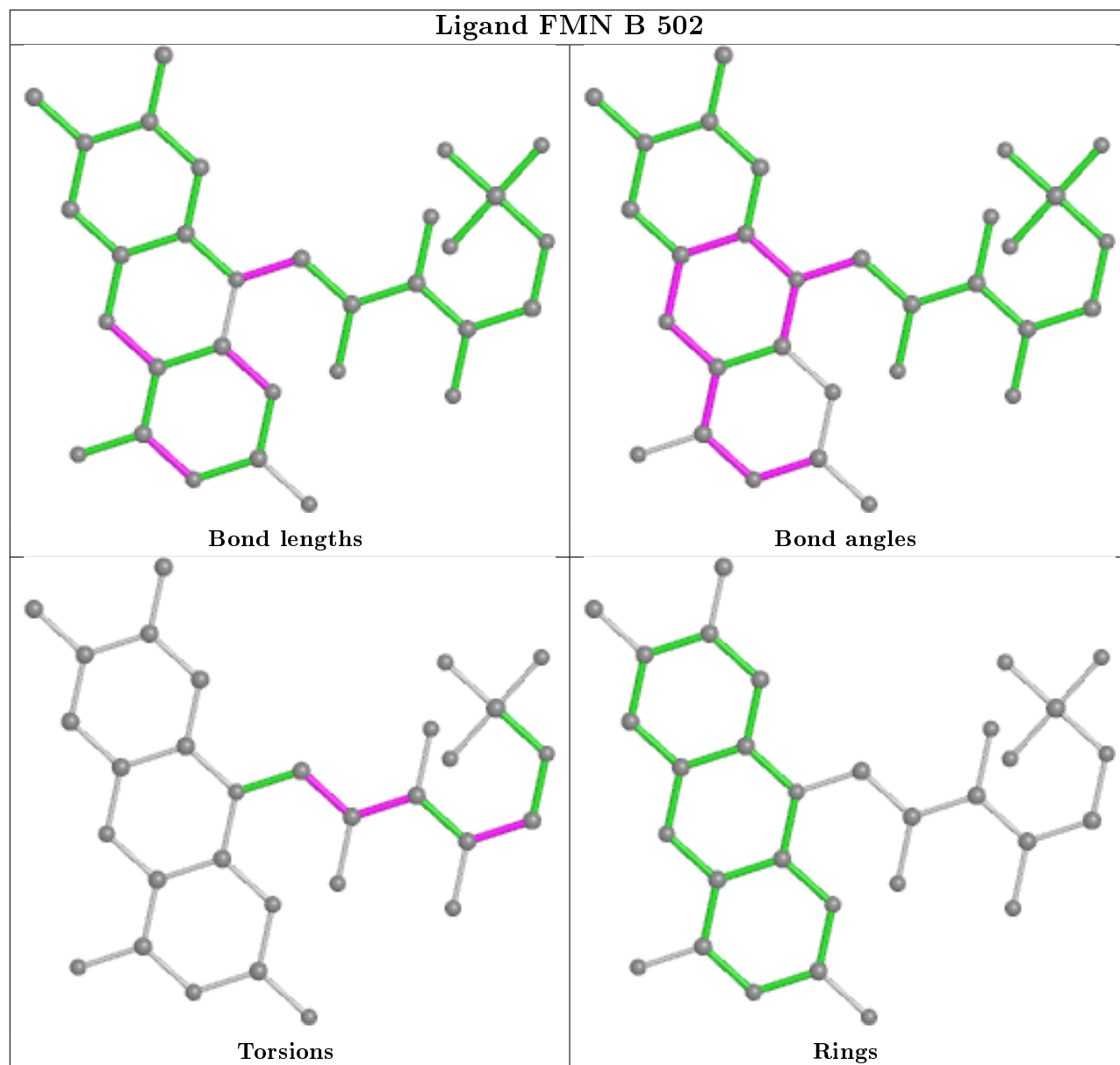
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18 | 1 | 502 | FMN | 8 | 0 |
| 19 | B | 503 | NAI | 4 | 0 |
| 17 | B | 501 | SF4 | 1 | 0 |
| 18 | B | 502 | FMN | 2 | 0 |
| 17 | 9 | 202 | SF4 | 2 | 0 |
| 17 | D | 801 | SF4 | 1 | 0 |
| 17 | 9 | 201 | SF4 | 4 | 0 |
| 17 | 1 | 501 | SF4 | 3 | 0 |
| 17 | 3 | 803 | SF4 | 2 | 0 |
| 17 | O | 202 | SF4 | 2 | 0 |
| 17 | G | 201 | SF4 | 2 | 0 |
| 19 | 1 | 503 | NAI | 3 | 0 |
| 17 | O | 201 | SF4 | 1 | 0 |
| 20 | C | 201 | FES | 2 | 0 |
| 20 | 2 | 201 | FES | 1 | 0 |
| 20 | D | 804 | FES | 2 | 0 |

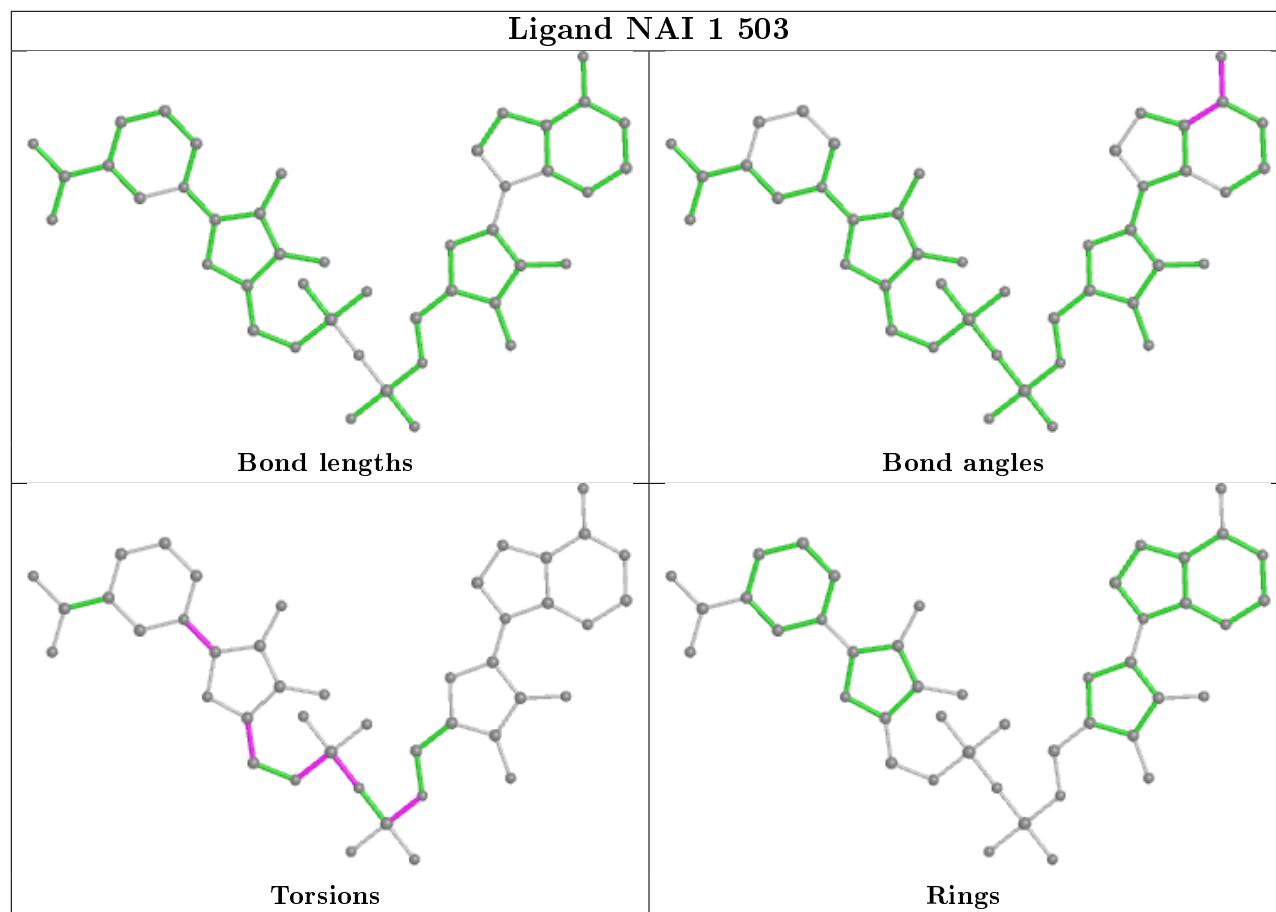
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FMN 1 502









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.