



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 08:37 am BST

PDB ID : 6TED
EMDB ID : EMD-10480
Title : Structure of complete, activated transcription complex Pol II-DSIF-PAF-SPT6
uncovers allosteric elongation activation by RTF1
Authors : Vos, S.M.; Farnung, L.; Cramer, P.
Deposited on : 2019-11-11
Resolution : 3.10 Å (reported)
Based on initial models : 4L1U, 6AFO, 6GMH

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

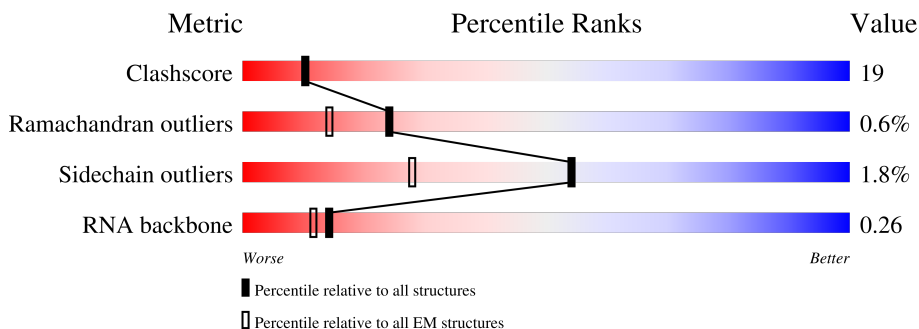
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.




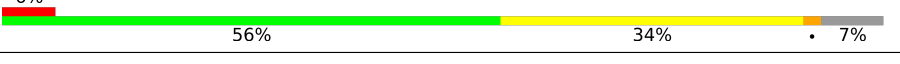



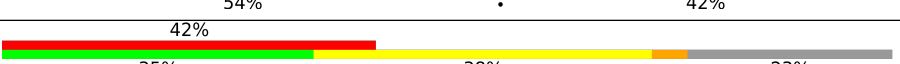
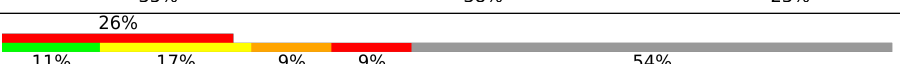


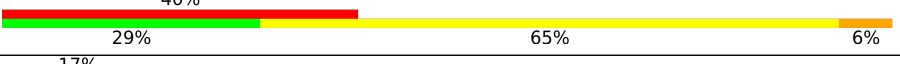
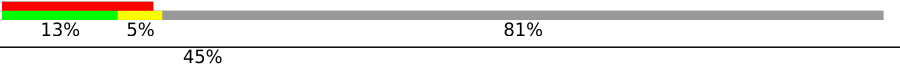
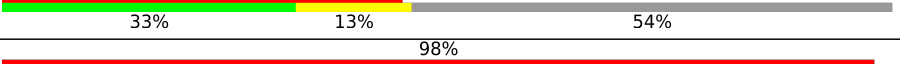

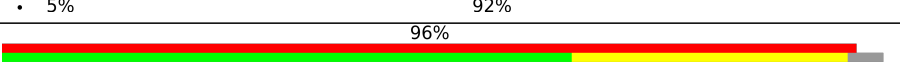
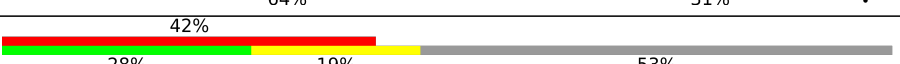


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1984 | |
| 2 | B | 1251 | |
| 3 | C | 275 | |
| 4 | D | 142 | |
| 5 | E | 210 | |
| 6 | F | 127 | |
| 7 | G | 172 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | H | 150 |  |
| 9 | I | 125 |  |
| 10 | J | 67 |  |
| 11 | K | 117 |  |
| 12 | L | 58 |  |
| 13 | M | 1729 |  |
| 14 | N | 48 |  |
| 15 | P | 46 |  |
| 16 | Q | 1179 |  |
| 17 | R | 713 |  |
| 18 | T | 48 |  |
| 19 | U | 666 |  |
| 20 | V | 531 |  |
| 21 | W | 305 |  |
| 22 | X | 531 |  |
| 23 | Y | 121 |  |
| 24 | Z | 1087 |  |

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 57142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|----|---------|-------|
| 1 | A | 1426 | Total | C | N | O | P | S | 0 | 0 |
| | | | 11255 | 7074 | 2014 | 2095 | 2 | 70 | | |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2 | B | 1122 | Total | C | N | O | S | 0 | 0 |
| | | | 8980 | 5684 | 1576 | 1656 | 64 | | |

- Molecule 3 is a protein called RNA polymerase II subunit C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | C | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 2072 | 1300 | 356 | 410 | 6 | | |

- Molecule 4 is a protein called RNA polymerase II subunit D.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | D | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1004 | 630 | 170 | 200 | 4 | | |

- Molecule 5 is a protein called RNA polymerase II subunit E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | E | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1720 | 1089 | 300 | 323 | 8 | | |

- Molecule 6 is a protein called RNA polymerase II subunit F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | F | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 626 | 401 | 106 | 114 | 5 | | |

- Molecule 7 is a protein called RNA polymerase II subunit G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | G | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1333 | 866 | 214 | 245 | 8 | | |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1197 | 759 | 195 | 238 | 5 | | |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9 | I | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 582 | 168 | 181 | 11 | | |

- Molecule 10 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10 | J | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 524 | 339 | 88 | 91 | 6 | | |

- Molecule 11 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 920 | 593 | 152 | 173 | 2 | | |

- Molecule 12 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12 | L | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 390 | 240 | 77 | 67 | 6 | | |

- Molecule 13 is a protein called Transcription elongation factor SPT6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|---------|-------|
| 13 | M | 1002 | Total | C | N | O | S | 0 | 0 |
| | | | 4737 | 2583 | 1071 | 1076 | 7 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | -2 | SER | - | expression tag | UNP Q7KZ85 |
| M | -1 | ASN | - | expression tag | UNP Q7KZ85 |
| M | 0 | ALA | - | expression tag | UNP Q7KZ85 |

- Molecule 14 is a DNA chain called DNA (37-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14 | N | 37 | Total | C | N | O | P | 0 | 0 |
| | | | 773 | 361 | 158 | 217 | 37 | | |

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 15 | P | 21 | Total | C | N | O | P | 0 | 0 |
| | | | 452 | 202 | 87 | 142 | 21 | | |

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 16 | Q | 890 | Total | C | N | O | S | 0 | 0 |
| | | | 7226 | 4579 | 1264 | 1352 | 31 | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Q | 1174 | GLU | - | expression tag | UNP Q6PD62 |
| Q | 1175 | ASN | - | expression tag | UNP Q6PD62 |
| Q | 1176 | LEU | - | expression tag | UNP Q6PD62 |
| Q | 1177 | TYR | - | expression tag | UNP Q6PD62 |
| Q | 1178 | PHE | - | expression tag | UNP Q6PD62 |
| Q | 1179 | GLN | - | expression tag | UNP Q6PD62 |

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | R | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1832 | 1148 | 340 | 337 | 7 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| R | -2 | SER | - | expression tag | UNP Q92541 |
| R | -1 | ASN | - | expression tag | UNP Q92541 |
| R | 0 | ALA | - | expression tag | UNP Q92541 |

- Molecule 18 is a DNA chain called Template DNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18 | T | 48 | Total | C | N | O | P | 0 | 0 |
| | | | 974 | 462 | 168 | 296 | 48 | | |

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | U | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 852 | 534 | 151 | 166 | 1 | | |

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20 | V | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1703 | 1061 | 305 | 333 | 4 | | |

- Molecule 21 is a protein called WD repeat-containing protein 61.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | W | 300 | Total | C | N | O | S | 0 | 0 |
| | | | 2333 | 1483 | 392 | 454 | 4 | | |

- Molecule 22 is a protein called Parafibromin.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 22 | X | 43 | Total | C | N | O | 0 | 0 |
| | | | 353 | 220 | 69 | 64 | | |

- Molecule 23 is a protein called Transcription elongation factor SPT4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | Y | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 911 | 570 | 159 | 173 | 9 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Y | -3 | GLY | - | expression tag | UNP P63272 |
| Y | -2 | PRO | - | expression tag | UNP P63272 |
| Y | -1 | GLY | - | expression tag | UNP P63272 |
| Y | 0 | SER | - | expression tag | UNP P63272 |

- Molecule 24 is a protein called Transcription elongation factor SPT5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|-------|
| 24 | Z | 510 | Total | C | N | O | P | S | 0 | 0 |
| | | | 4023 | 2550 | 709 | 745 | 1 | 18 | | |

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 25 | A | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 25 | B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 25 | C | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 25 | I | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 25 | J | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 25 | L | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 25 | Y | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

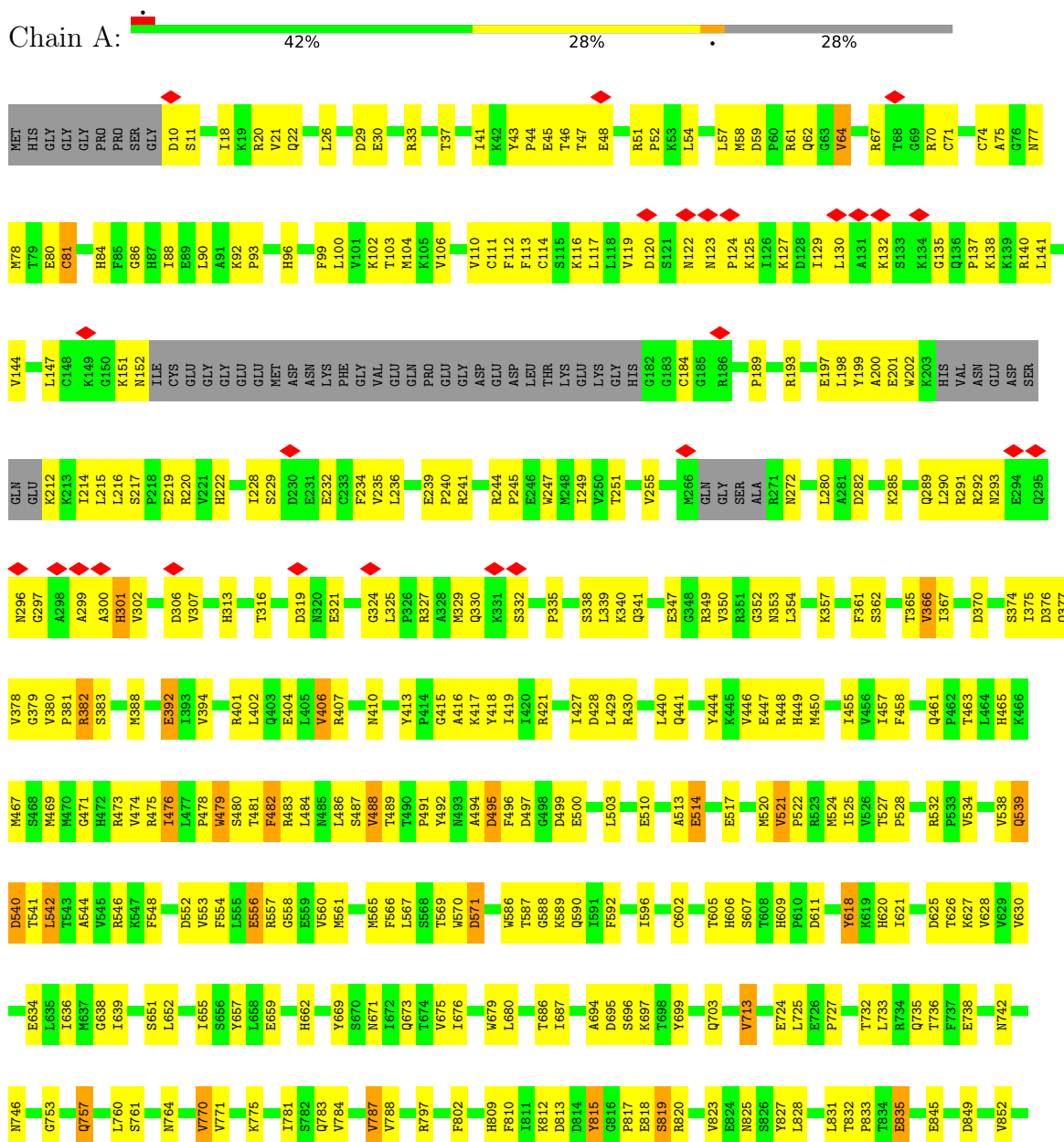
- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 26 | A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit



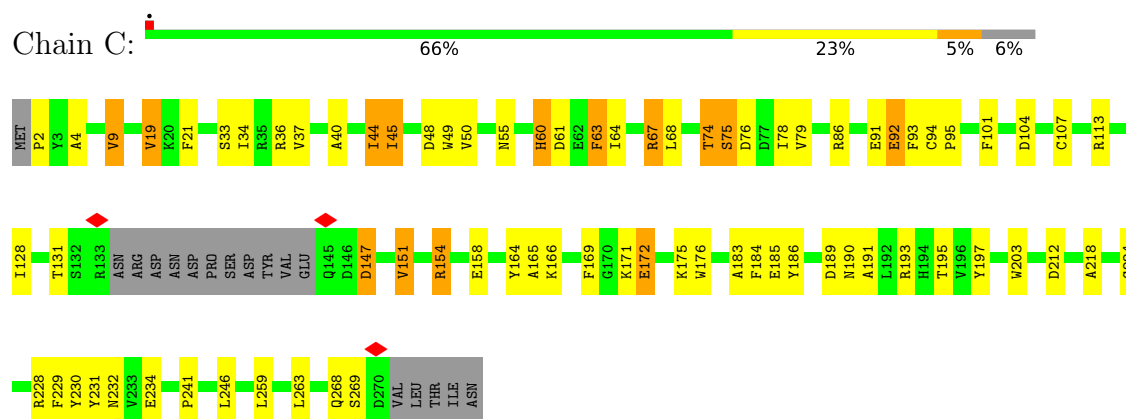


Chain B:

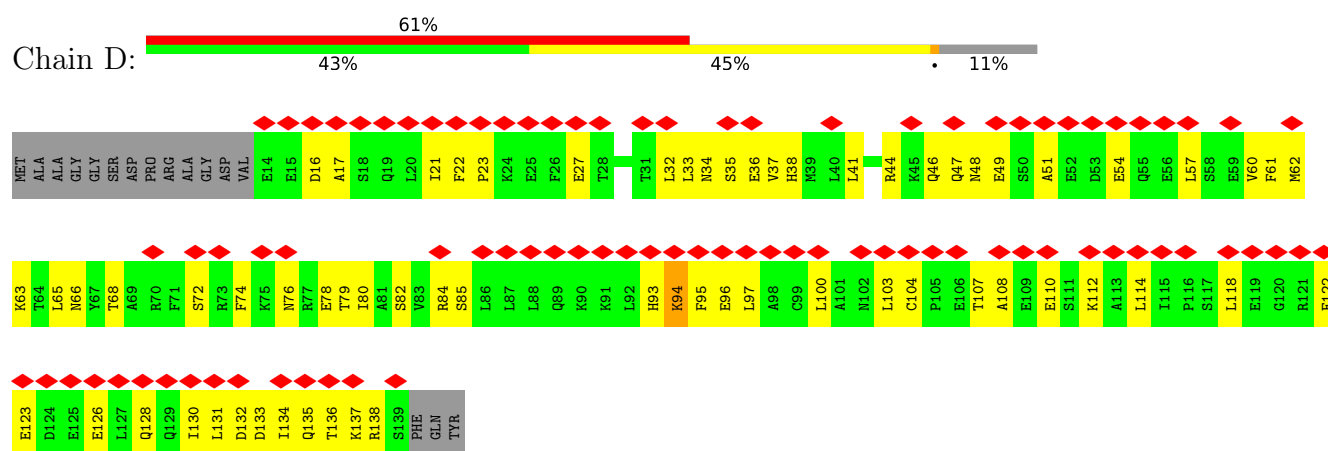


| | | | | | | | | | | | | |
|-----|-----|-----|------|------|------|------|------|------|------|-------|-------|-------|
| MET | VAL | GLN | K146 | ALA | A339 | F544 | L634 | P720 | F810 | S899 | D1004 | M1125 |
| CYS | SER | ALA | T147 | LYS | V342 | L545 | R638 | R721 | Y811 | E900 | A1005 | N1129 |
| THR | VAL | GLN | F148 | SER | E346 | E546 | H639 | M728 | Y814 | T901 | M1006 | T1130 |
| LEU | ASN | HIS | P153 | ALA | K347 | W548 | L643 | Q731 | E815 | V904 | K1010 | R1131 |
| SER | LEU | ALA | I154 | G253 | L348 | E551 | R646 | V735 | Q817 | V907 | I1011 | T1134 |
| GLN | ARG | SER | M155 | Q254 | F349 | R552 | E647 | Y736 | R821 | T910 | L1014 | Y1135 |
| LEU | ARG | GLY | L156 | R255 | H350 | L553 | E648 | T737 | G822 | L911 | L1015 | E1136 |
| ALA | GLY | GLY | R157 | T259 | V351 | Q456 | R649 | T738 | F823 | N912 | L1142 | N1143 |
| LEU | GLY | GLY | S158 | T259 | V351 | Q456 | R650 | W739 | F823 | F918 | Y1018 | K1143 |
| ALA | ALA | GLY | T159 | V267 | S354 | R457 | W651 | H740 | D824 | C919 | G1019 | T1144 |
| THR | PRO | GLY | L163 | M164 | D355 | R458 | R652 | V742 | T833 | R921 | H1021 | Q1145 |
| PHE | GLY | SER | M164 | G165 | F356 | R458 | S652 | R743 | R834 | I921 | L1022 | L1148 |
| ARG | SER | CYS | L166 | L166 | C357 | H460 | D655 | W744 | E835 | R922 | R1023 | V1149 |
| ALA | ALA | ALA | R83 | R83 | C357 | H460 | D655 | W744 | E835 | R923 | R1023 | R1150 |
| ALA | ASN | ASN | Y84 | Y84 | T359 | H461 | S659 | P754 | R847 | R924 | V1027 | M1151 |
| LEU | LEU | THR | L86 | L86 | K360 | Q461 | S660 | Q755 | L848 | S925 | L1028 | P1152 |
| THR | THR | ASP | D170 | D170 | K361 | Q461 | S660 | Q755 | L848 | V926 | Y1029 | Y1153 |
| ALA | ALA | ALA | E176 | E176 | Y367 | S467 | S661 | W750 | D851 | R937 | Y1047 | K1156 |
| ALA | ALA | ASP | C177 | C177 | R472 | S467 | S661 | L751 | R841 | R938 | V1047 | L1157 |
| ALA | ASP | GLY | P178 | P178 | L473 | S467 | S661 | Y752 | H842 | H939 | R1049 | M1171 |
| SER | GLY | GLY | L179 | L179 | R473 | S467 | S661 | Y753 | H842 | G940 | Q1050 | M1172 |
| LEU | LEU | ASP | L93 | L93 | R473 | S467 | S661 | Y753 | H842 | G941 | R1062 | S1173 |
| THR | THR | MET | S94 | S94 | R473 | S467 | S661 | Y753 | H842 | K942 | G1065 | V1174 |
| ALA | ALA | GLN | D180 | D180 | R473 | S467 | S661 | Y753 | H842 | R945 | R1065 | |
| ALA | ALA | TYR | Y184 | Y184 | R473 | S467 | S661 | Y753 | H842 | C946 | M1071 | |
| GLY | GLY | ASP | F185 | F185 | R473 | S467 | S661 | Y753 | H842 | R949 | R1072 | |
| PHE | PHE | ASP | I186 | I186 | R473 | S467 | S661 | Y753 | H842 | R950 | Q1073 | |
| TRP | TRP | ASP | I187 | I187 | R473 | S467 | S661 | Y753 | H842 | D953 | P1074 | |
| GLU | GLU | ASP | E191 | E191 | R473 | S467 | S661 | Y753 | H842 | T957 | E1088 | |
| ARG | ARG | ASP | K192 | K192 | R473 | S467 | S661 | Y753 | H842 | C958 | C1093 | |
| ARG | ARG | ASP | V193 | V193 | R473 | S467 | S661 | Y753 | H842 | E959 | Q1101 | |
| LYS | LYS | ASP | E198 | E198 | R473 | S467 | S661 | Y753 | H842 | N968 | R1104 | |
| LYS | LYS | ASP | K199 | K199 | R473 | S467 | S661 | Y753 | H842 | S974 | E1105 | |
| LEU | LEU | ASP | D211 | D211 | R473 | S467 | S661 | Y753 | H842 | R975 | F1108 | |
| CYS | CYS | ASP | D212 | D212 | R473 | S467 | S661 | Y753 | H842 | C984 | Y1118 | |
| LEU | LEU | ASP | T218 | T218 | R473 | S467 | S661 | Y753 | H842 | K993 | Q1112 | |
| ALA | ALA | ASP | R222 | R222 | R473 | S467 | S661 | Y753 | H842 | G994 | Q1115 | |
| LEU | LEU | ASP | S223 | S223 | R473 | S467 | S661 | Y753 | H842 | E995 | H1116 | |
| ALA | ALA | ASP | S228 | S228 | R473 | S467 | S661 | Y753 | H842 | I996 | V1117 | |
| LEU | LEU | ASP | S229 | S229 | R473 | S467 | S661 | Y753 | H842 | G997 | V1118 | |
| ARG | ARG | ASP | R230 | R230 | R473 | S467 | S661 | Y753 | H842 | P1001 | N1119 | |
| PRO | PRO | ASP | M53 | M53 | R473 | S467 | S661 | Y753 | H842 | F1002 | M1120 | |
| GLY | GLY | ASP | S54 | S54 | R473 | S467 | S661 | Y753 | H842 | N1003 | | |
| ALA | ALA | ASP | Q56 | Q56 | R473 | S467 | S661 | Y753 | H842 | | | |
| CYS | CYS | ASP | R57 | R57 | R473 | S467 | S661 | Y753 | H842 | | | |
| TRP | TRP | ASP | L58 | L58 | R473 | S467 | S661 | Y753 | H842 | | | |
| ARG | ARG | ASP | V59 | V59 | R473 | S467 | S661 | Y753 | H842 | | | |
| TRP | TRP | ASP | D66 | D66 | R473 | S467 | S661 | Y753 | H842 | | | |
| LEU | LEU | ASP | L67 | L67 | R473 | S467 | S661 | Y753 | H842 | | | |
| ALA | ALA | ASP | Q145 | Q145 | R473 | S467 | S661 | Y753 | H842 | | | |

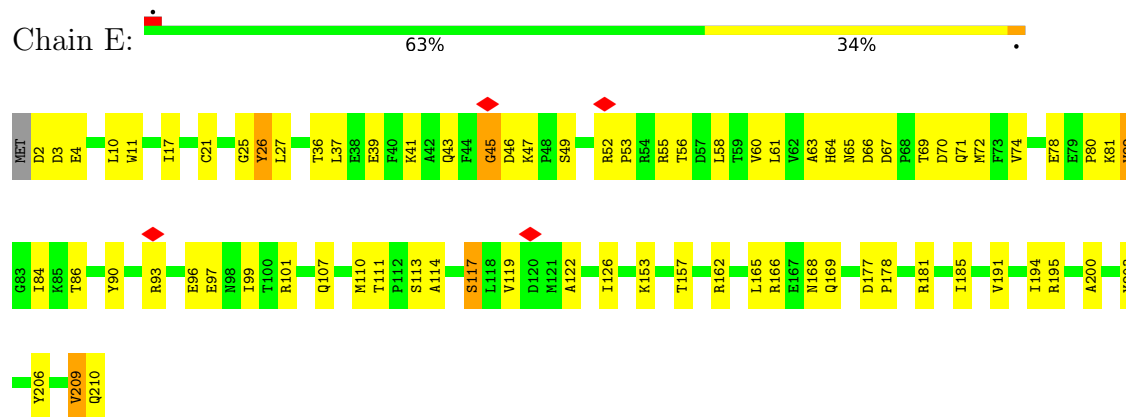
- Molecule 3: RNA polymerase II subunit C



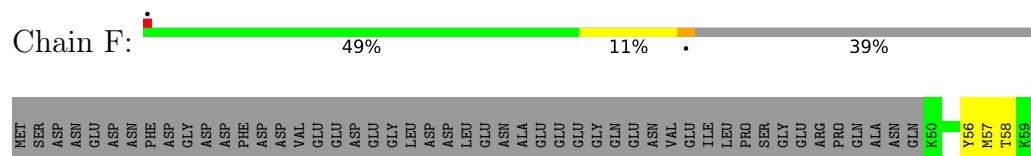
- Molecule 4: RNA polymerase II subunit D

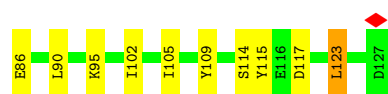


- Molecule 5: RNA polymerase II subunit E

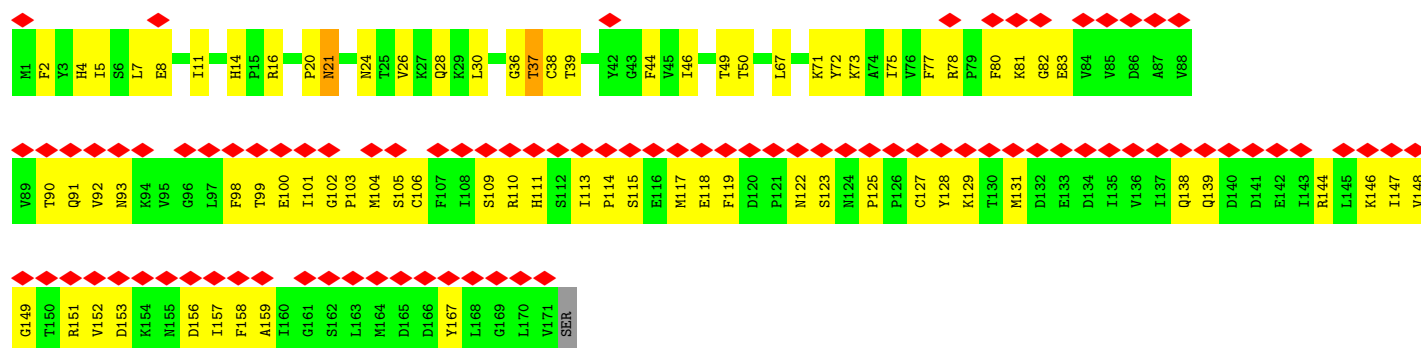


- Molecule 6: RNA polymerase II subunit F

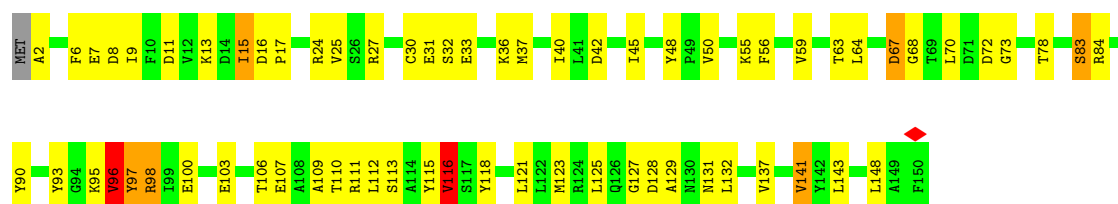




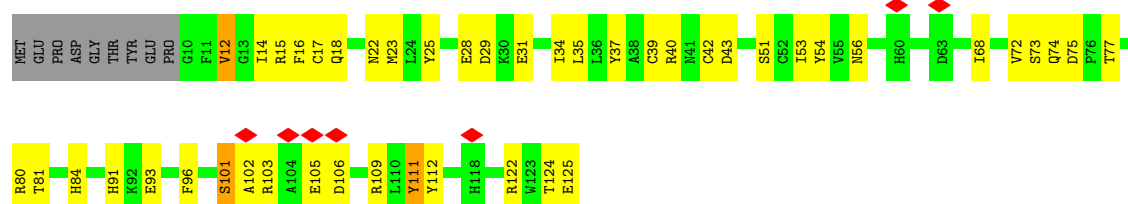
- Molecule 7: RNA polymerase II subunit G



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



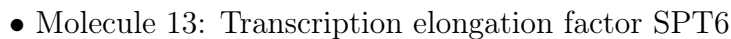
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: Uncharacterized protein



- Molecule 11: Uncharacterized protein



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| ARG | LYS | GLN | ARG | THR | THR | ILE | LYS | ARG | VAL | I1327 | A1328 | H1329 | P1330 | S1331 | F1332 | H1333 | N1334 | I1338 | N1339 | F1340 | K1341 | Q1342 | A1343 | E1344 | K1345 | M1346 | M1347 | E1348 | T1349 | M1350 | D1351 | Q1352 | G1353 | D1354 | V1355 | I1356 | I1357 | R1358 | P1359 | S1360 | S1361 | K1362 | G1363 | E1364 | N1365 | H1366 | L1367 | T1368 | V1369 | T1370 | K1372 | V1373 | S1374 | D1375 | G1376 | I1377 | | | | | |
| K1258 | V1259 | G1260 | M1261 | T1262 | V1263 | H1264 | C1265 | L1266 | I1267 | M1268 | K1269 | I1270 | D1271 | I1272 | E1273 | K1274 | F1275 | S1276 | A1277 | D1278 | L1279 | T1280 | C1281 | R1282 | T1283 | S1284 | D1285 | L1286 | M1287 | ASP | ASN | ASN | GLU | TRP | LYS | LEU | PRO | LYS | THR | TYR | ASP | THR | ASP | ALA | GLU | ALA | ASP | HIS | LYS | GLN | GLU | GLU | ASP | MET | LYS | | | | | | |
| E1078 | R1138 | T1139 | A1140 | Y1141 | I1142 | S1143 | P1144 | N1145 | T1146 | E1147 | E1148 | T1149 | F1150 | M1151 | M1152 | L1153 | T1154 | K1155 | E1156 | T1157 | P1158 | T1160 | F1161 | Y1162 | I1163 | L1164 | K1165 | L1166 | I1167 | I1168 | C1169 | N1170 | V1171 | T1172 | G1173 | I1174 | A1175 | H1176 | ARG | ARG | PRO | GLN | GLY | GLU | SER | ASP | GLN | ILE | ARG | ASN | ASP | GLU | THR | GLY | TRP | GLN | | | | | |
| CYS | PRO | PHE | CYS | GLN | GLN | ASP | ASN | PRO | LEU | SER | GLU | TRP | ASN | HIS | ASP | SER | GLY | SER | CYS | PRO | GLY | ALA | I1226 | G1227 | V1228 | K1229 | T1230 | R1231 | L1232 | D1233 | M1234 | G1235 | V1236 | T1237 | G1238 | F1239 | I1240 | P1241 | T1242 | K1243 | F1244 | L1245 | S1246 | D1247 | K1248 | V1249 | V1250 | K1251 | R1252 | P1253 | E1254 | E1255 | R1256 | V1257 | | | | | | | |
| ARG | LYS | GLN | ARG | THR | THR | ILE | LYS | ARG | VAL | I1327 | A1328 | H1329 | P1330 | S1331 | F1332 | H1333 | N1334 | I1338 | N1339 | F1340 | K1341 | Q1342 | A1343 | E1344 | K1345 | M1346 | M1347 | E1348 | T1349 | M1350 | D1351 | Q1352 | G1353 | D1354 | V1355 | I1356 | I1357 | R1358 | P1359 | S1360 | S1361 | K1362 | G1363 | E1364 | N1365 | H1366 | L1367 | T1368 | V1369 | T1370 | K1372 | V1373 | S1374 | D1375 | G1376 | I1377 | | | | | |
| L658 | A659 | E660 | D661 | E662 | G663 | L664 | L665 | T666 | T667 | D668 | I669 | S670 | D672 | L673 | K674 | G675 | VAL | GLU | GLY | TYR | GLY | ASN | ASP | GLN | T684 | Y685 | F686 | E687 | E688 | I689 | K690 | Q691 | F692 | Y693 | Y694 | R695 | D696 | E697 | F698 | S699 | H700 | Q701 | V702 | Q703 | E704 | W705 | N706 | R707 | Q708 | R709 | T710 | M711 | A712 | I713 | E714 | R715 | A716 | L717 | | | |
| Q718 | Q719 | F720 | L721 | Y722 | Y723 | M725 | A726 | K727 | E728 | L729 | K730 | N731 | K732 | L733 | L734 | A735 | E736 | A737 | E738 | E739 | Y740 | Y741 | I742 | K743 | A744 | C745 | S746 | R747 | K748 | L749 | Y750 | N751 | W752 | L753 | R754 | V755 | A756 | F757 | Y758 | R759 | P760 | D761 | Q762 | Q763 | VAL | GLU | GLU | ASP | ASP | ASP | PHE | MET | ASP | GLU | ASN | Q775 | G776 | K777 | | | |
| G778 | I779 | R780 | V781 | G783 | I784 | A785 | F786 | S787 | S788 | A789 | R790 | D791 | H792 | P793 | V794 | F795 | C796 | A797 | L798 | V799 | N800 | G801 | E802 | G803 | E804 | V805 | T806 | D807 | F808 | L809 | R810 | L811 | P812 | H813 | F814 | T815 | LYS | ARG | THR | ALA | TRP | ARG | GLU | E824 | E825 | R826 | E827 | K828 | K829 | A830 | Q831 | D832 | I833 | E834 | T835 | L836 | K837 | | | | |
| K838 | F839 | L840 | L841 | N842 | K843 | K844 | P845 | H846 | V847 | V848 | T849 | V850 | G852 | E853 | N854 | R855 | D856 | A857 | Q858 | M859 | L860 | I861 | E862 | D863 | V864 | K865 | R866 | T867 | F868 | H869 | E870 | L871 | D872 | Q873 | G874 | Q875 | Q876 | L877 | S878 | S879 | I880 | G881 | V882 | E883 | L884 | V885 | D886 | N887 | E888 | L889 | A890 | I891 | L892 | Y893 | M894 | N895 | S896 | K897 | | | |
| K898 | S899 | E900 | A901 | E902 | F903 | R904 | D905 | Y906 | P907 | F908 | Y909 | R911 | Q912 | A913 | N914 | S915 | L916 | A917 | R918 | M919 | Y920 | Q921 | D922 | P923 | L924 | N925 | E926 | F927 | A928 | Q929 | V930 | C931 | S932 | SER | ASP | E935 | D936 | I937 | L938 | C939 | L940 | K941 | F942 | H943 | P944 | L945 | Q946 | E947 | H948 | V949 | V950 | K951 | E952 | E953 | L954 | L955 | N956 | A957 | | | |
| L958 | Y959 | C960 | E961 | F962 | I963 | N964 | V965 | V966 | N967 | E968 | V969 | G970 | V971 | D972 | V973 | N974 | R975 | A976 | I977 | A978 | H979 | P980 | Y981 | S982 | Q983 | A984 | L985 | I986 | Q987 | Y988 | V989 | C990 | G991 | L992 | G993 | P994 | R995 | K996 | G997 | T998 | H999 | L1000 | L1001 | K1002 | I1003 | L1004 | K1005 | Q1006 | E997 | H998 | V999 | N1008 | T1009 | R1010 | L1011 | E1012 | S1013 | R1014 | T1015 | Q1016 | L1017 |
| V1018 | T1019 | M1020 | C1021 | D1022 | M1023 | G1024 | P1025 | K1026 | V1027 | F1028 | M1029 | N1030 | C1031 | A1032 | G1033 | F1034 | L1035 | K1036 | I1037 | D1038 | ALA | SER | LEU | GLY | ASP | SER | THR | ASP | TYR | ILE | E1051 | V1052 | L1053 | D1054 | G1055 | S1056 | R1057 | V1058 | H1059 | P1060 | E1061 | T1062 | Y1063 | E1064 | V1065 | A1066 | R1067 | K1068 | M1069 | A1070 | V1071 | D1072 | A1073 | L1074 | E1075 | Y1076 | D1077 | | | | |
| E1078 | S1079 | A1080 | E1081 | D1082 | A1083 | N1084 | P1085 | A1086 | G1087 | A1088 | L1089 | E1090 | E1091 | I1092 | L1093 | E1094 | N1095 | P1096 | E1097 | R1098 | K1100 | D1101 | L1102 | D1103 | L1104 | D1105 | A1106 | F1107 | A1108 | E1109 | E1110 | L1111 | E1112 | R1113 | Q1114 | G1115 | Y1116 | D1117 | D1118 | K1119 | H1120 | I1121 | T1122 | TYR | ASP | GLN | ALA | ILE | ARG | ASN | ASP | GLU | THR | GLY | TRP | GLN | | | | | |
| R1138 | T1139 | A1140 | Y1141 | I1142 | S1143 | P1144 | N1145 | T1146 | E1147 | E1148 | T1149 | F1150 | M1151 | M1152 | L1153 | T1154 | K1155 | E1156 | T1157 | P1158 | T1160 | F1161 | Y1162 | I1163 | L1164 | K1165 | L1166 | I1167 | I1168 | C1169 | N1170 | V1171 | T1172 | G1173 | I1174 | A1175 | H1176 | ARG | ARG | PRO | GLN | GLY | GLU | SER | ASP | GLN | ALA | ILE | ARG | ASN | ASP | GLU | THR | GLY | TRP | GLN | | | | | |
| CYS | PRO | PHE | CYS | GLN | GLN | ASP | ASN | PRO | LEU | SER | GLU | TRP | ASN | HIS | ASP | SER | GLY | SER | CYS | PRO | GLY | ALA | I1226 | G1227 | V1228 | K1229 | T1230 | R1231 | L1232 | D1233 | M1234 | G1235 | V1236 | T1237 | G1238 | F1239 | I1240 | P1241 | T1242 | K1243 | F1244 | L1245 | S1246 | D1247 | K1248 | V1249 | V1250 | K1251 | R1252 | P1253 | E1254 | E1255 | R1256 | V1257 | | | | | | | |
| K1258 | V1259 | G1260 | M1261 | T1262 | V1263 | H1264 | C1265 | L1266 | I1267 | M1268 | K1269 | I1270 | D1271 | I1272 | E1273 | K1274 | F1275 | S1276 | A1277 | D1278 | L1279 | T1280 | C1281 | R1282 | T1283 | S1284 | D1285 | L1286 | M1287 | ASP | ASN | ASN | GLU | TRP | LYS | LEU | PRO | LYS | THR | TYR | ASP | THR | ASP | ALA | GLU | ALA | ASP | HIS | LYS | GLN | GLU | GLU | ASP | MET | LYS | | | | | | |



[illegible]

- Molecule 17: RNA polymerase-associated protein RTF1 homolog



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| SER | ASN | ALA | ALA | MET | ARG | GLY | ARG | VAL | CYS | LEU | GLY | ARG | ALA | ALA | ALA | ALA | ALA | ALA | ALA | PRO | LEU | ALA | GLY | GLN | GLY | GLY | SER | PRO | GLY | GLY | GLY | GLY | ARG | ARG | GLY | GLY | THR | THR | MET | VAL | LYS | LYS | ARG | LYS | GLY | ARG | GLY | VAL | VAL | ILE | ASP | SER | THR | THR | GLU | ASP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| SER | GLY | SER | ASP | GLU | ASN | LEU | ASP | GLN | GLU | LEU | LEU | SER | SER | LEU | ALA | LYS | ARG | LYS | ARG | ASP | SER | SER | GLU | GLU | LYS | GLU | GLU | PRO | PRO | VAL | SER | SER | GLN | ALA | ALA | SER | SER | SER | ASP | ASP | ASP | GLU | GLU | THR | THR | THR | PHE | GLY | GLY | ASN | ASN | LYS | LYS | LYS | LYS | LYS | LYS | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| ARG | LYS | ILE | GLU | LYS | LYS | THR | THR | NET | LYS | LYS | GLN | ALA | ASN | LYS | THR | ALA | ASP | LYS | ASP | SER | SER | SER | SER | PRO | ALA | GLU | SER | SER | ALA | VAL | GLY | GLY | GLY | GLU | GLU | ASP | SER | ASP | ASN | SER | SER | SER | SER | ASP | ASP | SER | SER | GLU | GLU | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| PHE | HIS | ASP | TYR | GLY | GLU | ASP | LEU | MET | GLY | ASP | GLU | ASP | ARG | ALA | ARG | LEU | GLU | GLN | MET | THR | GLU | LYS | GLU | LEU | PHE | ASN | ARG | ILE | GLU | LYS | ARG | ARG | PHE | GLU | ILE | LYS | LYS | LYS | ALA | LYS | LYS | LYS | GLU | LYS | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| E358 | L359 | N360 | R361 | V362 | R363 | L364 | S365 | R366 | H367 | K368 | L369 | E370 | R371 | W372 | C373 | H374 | M375 | F376 | F377 | F378 | A379 | K380 | T381 | V382 | T383 | G384 | C385 | F386 | V387 | R388 | I389 | G390 | I391 | G392 | ASN | ASN | HIS | ASN | ASN | SER | K397 | P398 | V399 | Y400 | R401 | V402 | A403 | A404 | I405 | T406 | A407 | V408 | E409 | T411 | A412 | K413 | V414 | Y415 | A416 | L417 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| G418 | G419 | T420 | R421 | T422 | M423 | K424 | G425 | L426 | Q427 | L428 | R429 | H430 | G431 | D432 | D433 | Q434 | R435 | V436 | F437 | R438 | L439 | E440 | F441 | V442 | S443 | M444 | Q445 | E446 | F447 | T448 | E449 | S450 | E451 | F452 | M453 | K454 | M455 | K456 | E457 | A458 | M459 | F460 | S461 | A462 | G463 | Q464 | Q465 | L466 | F467 | T468 | L469 | D470 | E471 | L472 | M473 | K474 | K475 | E476 | L477 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| S478 | I479 | K480 | E481 | A482 | L483 | M484 | Y485 | K486 | F487 | M488 | D489 | K490 | D491 | I492 | E493 | E494 | I495 | V496 | K497 | A498 | K499 | E500 | R501 | F502 | R503 | R504 | A505 | P506 | P507 | N508 | Y509 | A510 | M511 | K512 | K513 | T514 | Q515 | L516 | L517 | L518 | E519 | K520 | A521 | M522 | A523 | E524 | D525 | L526 | G527 | D528 | Q529 | D530 | K531 | A532 | K533 | Q534 | I535 | Q536 | M537 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

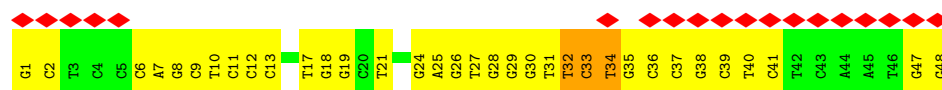
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Q538 | L539 | N540 | E541 | L542 | E543 | E544 | R545 | A546 | E547 | A548 | L549 | D550 | R551 | Q552 | R553 | T554 | K555 | N556 | E557 | S558 | A559 | T560 | S561 | E562 | I563 | N564 | Q565 | R566 | N567 | R568 | E569 | W570 | N571 | T572 | V573 | E574 | S575 | E576 | K577 | A578 | L579 | V580 | A581 | E582 | S583 | H584 | N585 | M586 | K587 | N588 | Q589 | Q590 | N591 | D592 | P593 | F594 | T595 | R596 | E597 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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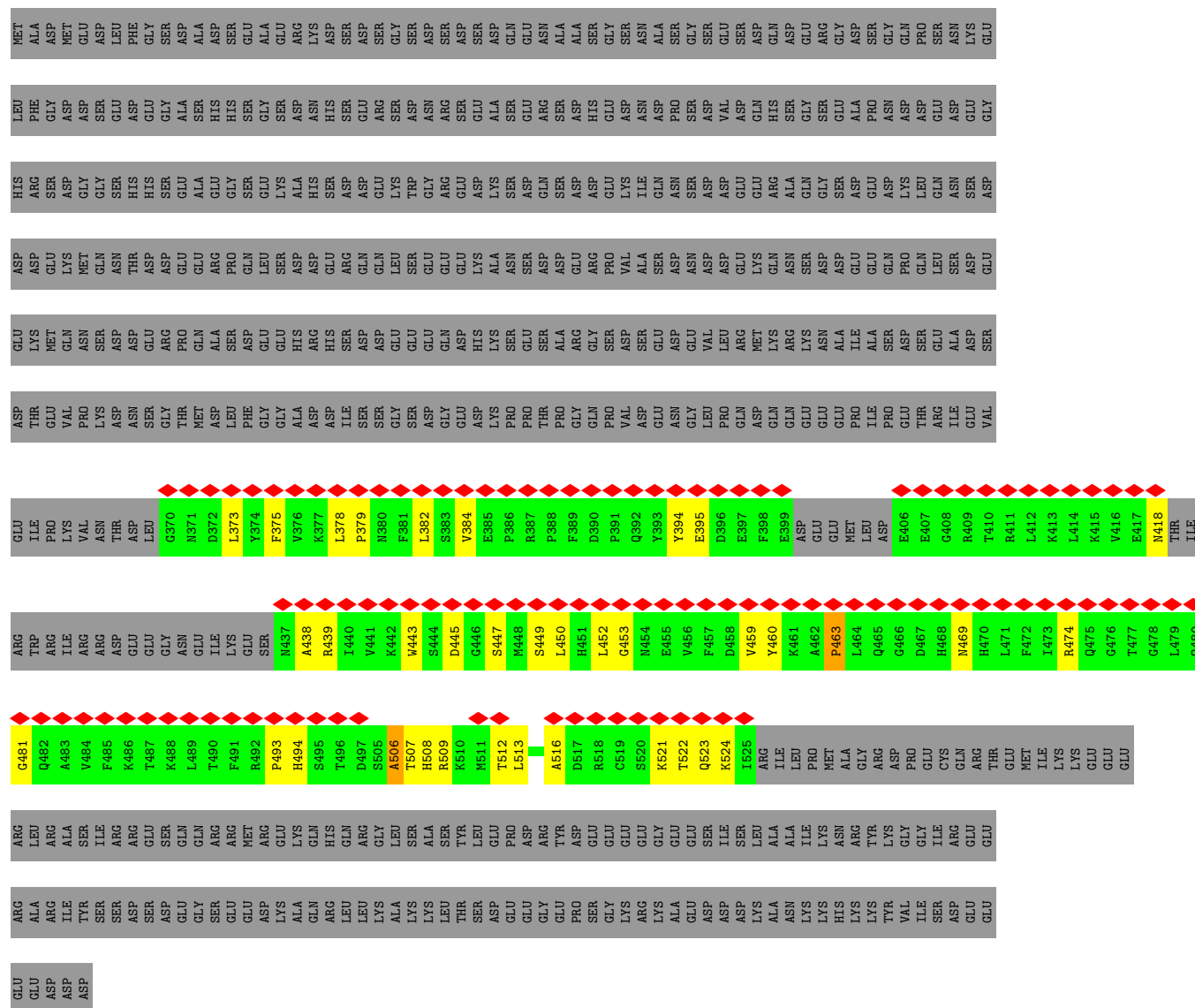
LEU PHE LYS VAL HIS ASP PHE ASP ASP VAL LYS ILE LEU ASP ASP LEU GLN VAL VAL PRO PRO SER SER SER SER LYS LEU LEU ALA ALA ILE THR SER SER LYS ALA ALA PRO PRO PRO ALA ALA LYS ASP ASP GLY GLY ALA PRO PRO ARG ARG SER SER LEU LEU ASN LEU LEU GLU GLU ASP TYR LYS LYS ARG ARG ARG GLY GLY LEU LEU

- Molecule 18: Template DNA

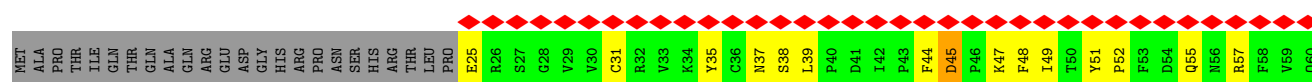
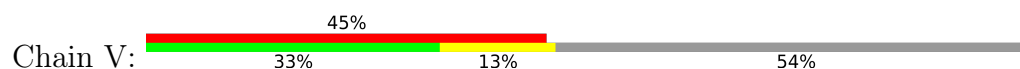




• Molecule 19: RNA polymerase-associated protein LEO1



• Molecule 20: RNA polymerase II-associated factor 1 homolog





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 446195 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 40 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.165 | Depositor |
| Minimum map value | -0.086 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.022 | Depositor |
| Map size (Å) | 377.64, 377.64, 377.64 | wwPDB |
| Map dimensions | 360, 360, 360 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.049, 1.049, 1.049 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.40 | 97/11437 (0.8%) | 0.89 | 18/15433 (0.1%) |
| 2 | B | 1.63 | 126/9158 (1.4%) | 0.97 | 28/12360 (0.2%) |
| 3 | C | 1.77 | 44/2115 (2.1%) | 0.96 | 7/2873 (0.2%) |
| 4 | D | 0.42 | 0/1017 | 0.51 | 0/1368 |
| 5 | E | 1.29 | 10/1751 (0.6%) | 0.81 | 1/2366 (0.0%) |
| 6 | F | 1.69 | 9/636 (1.4%) | 0.89 | 0/859 |
| 7 | G | 0.75 | 0/1364 | 0.62 | 0/1853 |
| 8 | H | 1.78 | 31/1219 (2.5%) | 0.92 | 1/1644 (0.1%) |
| 9 | I | 1.25 | 4/964 (0.4%) | 0.79 | 0/1305 |
| 10 | J | 1.82 | 9/533 (1.7%) | 1.03 | 3/719 (0.4%) |
| 11 | K | 1.68 | 8/939 (0.9%) | 0.92 | 2/1271 (0.2%) |
| 12 | L | 1.57 | 5/395 (1.3%) | 1.00 | 2/525 (0.4%) |
| 13 | M | 0.26 | 0/4763 | 0.48 | 1/6084 (0.0%) |
| 14 | N | 0.98 | 1/870 (0.1%) | 0.87 | 1/1341 (0.1%) |
| 15 | P | 1.34 | 3/506 (0.6%) | 1.82 | 22/787 (2.8%) |
| 16 | Q | 0.36 | 0/7365 | 0.51 | 0/9927 |
| 17 | R | 0.39 | 0/1860 | 0.56 | 2/2509 (0.1%) |
| 18 | T | 1.68 | 11/1087 (1.0%) | 1.13 | 6/1674 (0.4%) |
| 19 | U | 0.34 | 0/864 | 0.58 | 2/1173 (0.2%) |
| 20 | V | 0.32 | 0/1728 | 0.52 | 2/2357 (0.1%) |
| 21 | W | 0.37 | 0/2392 | 0.53 | 0/3257 |
| 22 | X | 0.34 | 0/356 | 0.52 | 0/478 |
| 23 | Y | 0.27 | 0/927 | 0.48 | 0/1250 |
| 24 | Z | 0.45 | 0/4081 | 0.55 | 1/5493 (0.0%) |
| All | All | 1.15 | 358/58327 (0.6%) | 0.79 | 99/78906 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 2 | B | 0 | 3 |
| 17 | R | 0 | 1 |
| All | All | 0 | 6 |

All (358) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | B | 791 | GLU | CA-CB | -15.42 | 1.20 | 1.53 |
| 2 | B | 94 | SER | C-N | -11.45 | 1.07 | 1.34 |
| 8 | H | 116 | VAL | CB-CG1 | -9.52 | 1.32 | 1.52 |
| 2 | B | 690 | CYS | CB-SG | -8.84 | 1.67 | 1.82 |
| 2 | B | 1047 | TYR | CD1-CE1 | -8.57 | 1.26 | 1.39 |
| 2 | B | 753 | TYR | CD2-CE2 | -8.37 | 1.26 | 1.39 |
| 2 | B | 548 | TRP | CB-CG | -8.34 | 1.35 | 1.50 |
| 1 | A | 999 | ARG | C-N | -8.25 | 1.15 | 1.34 |
| 8 | H | 118 | TYR | CD1-CE1 | -8.14 | 1.27 | 1.39 |
| 1 | A | 1050 | CYS | CB-SG | -8.09 | 1.68 | 1.82 |
| 1 | A | 886 | VAL | CB-CG1 | -8.08 | 1.35 | 1.52 |
| 8 | H | 118 | TYR | CD2-CE2 | -8.05 | 1.27 | 1.39 |
| 2 | B | 29 | VAL | CB-CG2 | -8.01 | 1.36 | 1.52 |
| 1 | A | 827 | TYR | CD1-CE1 | -7.83 | 1.27 | 1.39 |
| 3 | C | 19 | VAL | CB-CG2 | -7.76 | 1.36 | 1.52 |
| 2 | B | 664 | TYR | CD1-CE1 | -7.73 | 1.27 | 1.39 |
| 1 | A | 1374 | VAL | CB-CG2 | -7.68 | 1.36 | 1.52 |
| 1 | A | 492 | TYR | CE2-CZ | -7.61 | 1.28 | 1.38 |
| 10 | J | 10 | CYS | CB-SG | -7.54 | 1.69 | 1.82 |
| 1 | A | 492 | TYR | CD2-CE2 | -7.50 | 1.28 | 1.39 |
| 18 | T | 25 | DA | C3'-O3' | -7.48 | 1.34 | 1.44 |
| 2 | B | 664 | TYR | CD2-CE2 | -7.39 | 1.28 | 1.39 |
| 10 | J | 62 | TYR | CD1-CE1 | -7.36 | 1.28 | 1.39 |
| 1 | A | 514 | GLU | CB-CG | -7.34 | 1.38 | 1.52 |
| 8 | H | 118 | TYR | CE1-CZ | -7.25 | 1.29 | 1.38 |
| 2 | B | 1047 | TYR | CD2-CE2 | -7.21 | 1.28 | 1.39 |
| 1 | A | 1396 | ARG | CB-CG | -7.17 | 1.33 | 1.52 |
| 8 | H | 48 | TYR | CD1-CE1 | -7.14 | 1.28 | 1.39 |
| 9 | I | 72 | VAL | CB-CG1 | -7.11 | 1.38 | 1.52 |
| 2 | B | 108 | MET | C-N | -7.10 | 1.17 | 1.34 |
| 2 | B | 1047 | TYR | CE1-CZ | -7.09 | 1.29 | 1.38 |
| 1 | A | 380 | VAL | CB-CG2 | -7.06 | 1.38 | 1.52 |
| 2 | B | 809 | VAL | CB-CG1 | -7.01 | 1.38 | 1.52 |
| 2 | B | 615 | TYR | CD1-CE1 | -7.01 | 1.28 | 1.39 |
| 1 | A | 1379 | GLU | CB-CG | -6.96 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 488 | VAL | CB-CG1 | -6.96 | 1.38 | 1.52 |
| 2 | B | 184 | TYR | CD2-CE2 | -6.95 | 1.28 | 1.39 |
| 18 | T | 28 | DG | C3'-O3' | -6.95 | 1.34 | 1.44 |
| 2 | B | 753 | TYR | CE2-CZ | -6.90 | 1.29 | 1.38 |
| 2 | B | 755 | GLN | C-N | -6.90 | 1.18 | 1.34 |
| 3 | C | 176 | TRP | CE3-CZ3 | -6.89 | 1.26 | 1.38 |
| 1 | A | 560 | VAL | CB-CG2 | -6.86 | 1.38 | 1.52 |
| 10 | J | 45 | CYS | CB-SG | -6.86 | 1.70 | 1.82 |
| 1 | A | 492 | TYR | CD1-CE1 | -6.85 | 1.29 | 1.39 |
| 2 | B | 662 | VAL | CB-CG2 | -6.85 | 1.38 | 1.52 |
| 2 | B | 693 | TYR | CE1-CZ | -6.83 | 1.29 | 1.38 |
| 2 | B | 1029 | TYR | CD2-CE2 | -6.83 | 1.29 | 1.39 |
| 5 | E | 191 | VAL | CB-CG1 | -6.83 | 1.38 | 1.52 |
| 2 | B | 615 | TYR | CD2-CE2 | -6.79 | 1.29 | 1.39 |
| 3 | C | 184 | PHE | CD1-CE1 | -6.79 | 1.25 | 1.39 |
| 2 | B | 1029 | TYR | CE1-CZ | -6.79 | 1.29 | 1.38 |
| 2 | B | 120 | TYR | CD2-CE2 | -6.77 | 1.29 | 1.39 |
| 2 | B | 753 | TYR | CE1-CZ | -6.76 | 1.29 | 1.38 |
| 2 | B | 1047 | TYR | CE2-CZ | -6.75 | 1.29 | 1.38 |
| 2 | B | 509 | VAL | CB-CG1 | -6.74 | 1.38 | 1.52 |
| 3 | C | 186 | TYR | CD1-CE1 | -6.73 | 1.29 | 1.39 |
| 2 | B | 753 | TYR | CD1-CE1 | -6.72 | 1.29 | 1.39 |
| 2 | B | 177 | CYS | CB-SG | -6.70 | 1.70 | 1.82 |
| 2 | B | 504 | THR | CB-CG2 | -6.69 | 1.30 | 1.52 |
| 2 | B | 1105 | GLU | CB-CG | -6.66 | 1.39 | 1.52 |
| 6 | F | 60 | TYR | CD1-CE1 | -6.63 | 1.29 | 1.39 |
| 2 | B | 1029 | TYR | CD1-CE1 | -6.61 | 1.29 | 1.39 |
| 6 | F | 109 | TYR | CD1-CE1 | -6.61 | 1.29 | 1.39 |
| 8 | H | 115 | TYR | CD1-CE1 | -6.61 | 1.29 | 1.39 |
| 3 | C | 184 | PHE | CD2-CE2 | -6.60 | 1.26 | 1.39 |
| 1 | A | 815 | TYR | CD2-CE2 | -6.60 | 1.29 | 1.39 |
| 1 | A | 815 | TYR | CD1-CE1 | -6.59 | 1.29 | 1.39 |
| 8 | H | 97 | TYR | CE1-CZ | -6.58 | 1.29 | 1.38 |
| 18 | T | 33 | DC | N1-C2 | -6.58 | 1.33 | 1.40 |
| 2 | B | 801 | VAL | CB-CG1 | -6.57 | 1.39 | 1.52 |
| 12 | L | 55 | PHE | CB-CG | -6.56 | 1.40 | 1.51 |
| 2 | B | 750 | VAL | CB-CG2 | -6.55 | 1.39 | 1.52 |
| 2 | B | 806 | PHE | CD1-CE1 | -6.54 | 1.26 | 1.39 |
| 3 | C | 229 | PHE | CD1-CE1 | -6.51 | 1.26 | 1.39 |
| 18 | T | 27 | DT | C3'-O3' | -6.51 | 1.35 | 1.44 |
| 2 | B | 811 | TYR | CE1-CZ | -6.48 | 1.30 | 1.38 |
| 3 | C | 172 | GLU | CB-CG | -6.48 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 26 | CYS | CB-SG | -6.47 | 1.71 | 1.82 |
| 8 | H | 115 | TYR | CE1-CZ | -6.46 | 1.30 | 1.38 |
| 3 | C | 186 | TYR | CD2-CE2 | -6.46 | 1.29 | 1.39 |
| 2 | B | 193 | VAL | CB-CG2 | -6.45 | 1.39 | 1.52 |
| 2 | B | 693 | TYR | CD1-CE1 | -6.45 | 1.29 | 1.39 |
| 8 | H | 90 | TYR | CD1-CE1 | -6.44 | 1.29 | 1.39 |
| 1 | A | 787 | VAL | CB-CG2 | -6.43 | 1.39 | 1.52 |
| 3 | C | 169 | PHE | CD1-CE1 | -6.43 | 1.26 | 1.39 |
| 2 | B | 622 | CYS | CB-SG | -6.37 | 1.71 | 1.82 |
| 1 | A | 871 | VAL | CB-CG1 | -6.37 | 1.39 | 1.52 |
| 3 | C | 169 | PHE | CD2-CE2 | -6.35 | 1.26 | 1.39 |
| 1 | A | 835 | GLU | CB-CG | -6.34 | 1.40 | 1.52 |
| 1 | A | 827 | TYR | CD2-CE2 | -6.34 | 1.29 | 1.39 |
| 1 | A | 1140 | THR | CA-CB | -6.33 | 1.36 | 1.53 |
| 1 | A | 521 | VAL | CB-CG2 | -6.33 | 1.39 | 1.52 |
| 2 | B | 922 | ARG | CB-CG | -6.30 | 1.35 | 1.52 |
| 10 | J | 5 | VAL | CB-CG2 | -6.29 | 1.39 | 1.52 |
| 5 | E | 191 | VAL | CB-CG2 | -6.28 | 1.39 | 1.52 |
| 2 | B | 919 | CYS | CB-SG | -6.28 | 1.71 | 1.82 |
| 3 | C | 231 | TYR | CD1-CE1 | -6.27 | 1.29 | 1.39 |
| 10 | J | 62 | TYR | CE1-CZ | -6.26 | 1.30 | 1.38 |
| 6 | F | 109 | TYR | CD2-CE2 | -6.26 | 1.29 | 1.39 |
| 1 | A | 891 | TYR | CD1-CE1 | -6.23 | 1.30 | 1.39 |
| 1 | A | 630 | VAL | CB-CG1 | -6.22 | 1.39 | 1.52 |
| 1 | A | 590 | GLN | CG-CD | -6.22 | 1.36 | 1.51 |
| 2 | B | 33 | TYR | CE1-CZ | -6.21 | 1.30 | 1.38 |
| 11 | K | 56 | VAL | CB-CG1 | -6.21 | 1.39 | 1.52 |
| 18 | T | 33 | DC | N1-C6 | -6.21 | 1.33 | 1.37 |
| 2 | B | 805 | PHE | CD2-CE2 | -6.21 | 1.26 | 1.39 |
| 2 | B | 752 | TYR | CE2-CZ | -6.21 | 1.30 | 1.38 |
| 6 | F | 60 | TYR | CE1-CZ | -6.20 | 1.30 | 1.38 |
| 2 | B | 984 | CYS | CB-SG | -6.20 | 1.71 | 1.82 |
| 2 | B | 809 | VAL | CB-CG2 | -6.19 | 1.39 | 1.52 |
| 8 | H | 90 | TYR | CD2-CE2 | -6.18 | 1.30 | 1.39 |
| 2 | B | 949 | TYR | CD1-CE1 | -6.18 | 1.30 | 1.39 |
| 12 | L | 45 | TYR | CE1-CZ | -6.17 | 1.30 | 1.38 |
| 2 | B | 1029 | TYR | CE2-CZ | -6.17 | 1.30 | 1.38 |
| 18 | T | 26 | DG | C3'-O3' | -6.17 | 1.35 | 1.44 |
| 1 | A | 669 | TYR | CD1-CE1 | -6.14 | 1.30 | 1.39 |
| 8 | H | 115 | TYR | CE2-CZ | -6.11 | 1.30 | 1.38 |
| 8 | H | 98 | ARG | CB-CG | -6.10 | 1.36 | 1.52 |
| 2 | B | 236 | TRP | CB-CG | -6.10 | 1.39 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18 | T | 33 | DC | C1'-N1 | -6.09 | 1.38 | 1.47 |
| 1 | A | 474 | VAL | CB-CG1 | -6.08 | 1.40 | 1.52 |
| 12 | L | 45 | TYR | CD1-CE1 | -6.07 | 1.30 | 1.39 |
| 2 | B | 193 | VAL | CB-CG1 | -6.06 | 1.40 | 1.52 |
| 2 | B | 198 | GLU | CB-CG | -6.06 | 1.40 | 1.52 |
| 2 | B | 924 | ARG | CB-CG | -6.06 | 1.36 | 1.52 |
| 2 | B | 923 | VAL | CB-CG1 | -6.05 | 1.40 | 1.52 |
| 11 | K | 75 | VAL | CB-CG2 | -6.05 | 1.40 | 1.52 |
| 1 | A | 590 | GLN | CB-CG | -6.04 | 1.36 | 1.52 |
| 3 | C | 104 | ASP | CA-CB | -6.02 | 1.40 | 1.53 |
| 1 | A | 873 | VAL | CB-CG2 | -6.01 | 1.40 | 1.52 |
| 2 | B | 707 | CYS | CB-SG | -6.01 | 1.72 | 1.82 |
| 8 | H | 141 | VAL | CB-CG2 | -6.00 | 1.40 | 1.52 |
| 2 | B | 367 | TYR | CD1-CE1 | -6.00 | 1.30 | 1.39 |
| 3 | C | 186 | TYR | CE2-CZ | -5.97 | 1.30 | 1.38 |
| 1 | A | 827 | TYR | CE1-CZ | -5.97 | 1.30 | 1.38 |
| 2 | B | 184 | TYR | CE2-CZ | -5.96 | 1.30 | 1.38 |
| 8 | H | 115 | TYR | CD2-CE2 | -5.94 | 1.30 | 1.39 |
| 18 | T | 24 | DG | C3'-O3' | -5.94 | 1.36 | 1.44 |
| 18 | T | 33 | DC | N3-C4 | -5.93 | 1.29 | 1.33 |
| 3 | C | 151 | VAL | CB-CG1 | -5.90 | 1.40 | 1.52 |
| 1 | A | 366 | VAL | CB-CG1 | -5.89 | 1.40 | 1.52 |
| 2 | B | 92 | TYR | CD2-CE2 | -5.89 | 1.30 | 1.39 |
| 10 | J | 6 | ARG | CB-CG | -5.89 | 1.36 | 1.52 |
| 3 | C | 197 | TYR | CE1-CZ | -5.88 | 1.30 | 1.38 |
| 1 | A | 458 | PHE | CD1-CE1 | -5.87 | 1.27 | 1.39 |
| 3 | C | 186 | TYR | CE1-CZ | -5.87 | 1.30 | 1.38 |
| 2 | B | 184 | TYR | CD1-CE1 | -5.86 | 1.30 | 1.39 |
| 3 | C | 197 | TYR | CE2-CZ | -5.86 | 1.30 | 1.38 |
| 2 | B | 806 | PHE | CD2-CE2 | -5.85 | 1.27 | 1.39 |
| 3 | C | 231 | TYR | CD2-CE2 | -5.85 | 1.30 | 1.39 |
| 1 | A | 377 | GLN | CB-CG | -5.84 | 1.36 | 1.52 |
| 1 | A | 657 | TYR | CD1-CE1 | -5.83 | 1.30 | 1.39 |
| 8 | H | 96 | VAL | CB-CG1 | -5.82 | 1.40 | 1.52 |
| 1 | A | 669 | TYR | CE1-CZ | -5.80 | 1.31 | 1.38 |
| 8 | H | 90 | TYR | CE2-CZ | -5.80 | 1.31 | 1.38 |
| 15 | P | 44 | A | N9-C4 | -5.80 | 1.34 | 1.37 |
| 2 | B | 697 | GLU | CG-CD | -5.80 | 1.43 | 1.51 |
| 2 | B | 1020 | TYR | CD1-CE1 | -5.80 | 1.30 | 1.39 |
| 1 | A | 669 | TYR | CD2-CE2 | -5.79 | 1.30 | 1.39 |
| 1 | A | 771 | VAL | CB-CG2 | -5.77 | 1.40 | 1.52 |
| 2 | B | 794 | VAL | CB-CG2 | -5.76 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 907 | VAL | CB-CG1 | -5.76 | 1.40 | 1.52 |
| 2 | B | 184 | TYR | CE1-CZ | -5.75 | 1.31 | 1.38 |
| 2 | B | 788 | TYR | CE2-CZ | -5.74 | 1.31 | 1.38 |
| 2 | B | 1093 | CYS | CB-SG | -5.74 | 1.72 | 1.81 |
| 2 | B | 811 | TYR | CD1-CE1 | -5.74 | 1.30 | 1.39 |
| 2 | B | 1047 | TYR | CG-CD1 | -5.74 | 1.31 | 1.39 |
| 12 | L | 45 | TYR | CD2-CE2 | -5.72 | 1.30 | 1.39 |
| 1 | A | 482 | PHE | CD2-CE2 | -5.72 | 1.27 | 1.39 |
| 1 | A | 784 | VAL | CB-CG1 | -5.72 | 1.40 | 1.52 |
| 2 | B | 1149 | VAL | CB-CG2 | -5.71 | 1.40 | 1.52 |
| 2 | B | 788 | TYR | CD1-CE1 | -5.71 | 1.30 | 1.39 |
| 3 | C | 197 | TYR | CD1-CE1 | -5.70 | 1.30 | 1.39 |
| 1 | A | 556 | GLU | CB-CG | -5.69 | 1.41 | 1.52 |
| 1 | A | 447 | GLU | CB-CG | -5.68 | 1.41 | 1.52 |
| 8 | H | 48 | TYR | CE1-CZ | -5.68 | 1.31 | 1.38 |
| 5 | E | 209 | VAL | CB-CG2 | -5.67 | 1.41 | 1.52 |
| 2 | B | 120 | TYR | CD1-CE1 | -5.67 | 1.30 | 1.39 |
| 15 | P | 40 | A | N9-C4 | -5.66 | 1.34 | 1.37 |
| 1 | A | 556 | GLU | CG-CD | -5.66 | 1.43 | 1.51 |
| 2 | B | 697 | GLU | CB-CG | -5.66 | 1.41 | 1.52 |
| 1 | A | 406 | VAL | CB-CG1 | -5.65 | 1.41 | 1.52 |
| 1 | A | 1375 | ARG | CG-CD | -5.65 | 1.37 | 1.51 |
| 11 | K | 97 | GLU | CB-CG | -5.64 | 1.41 | 1.52 |
| 1 | A | 901 | VAL | CB-CG2 | -5.64 | 1.41 | 1.52 |
| 3 | C | 169 | PHE | CB-CG | -5.63 | 1.41 | 1.51 |
| 2 | B | 510 | CYS | CB-SG | -5.63 | 1.72 | 1.81 |
| 2 | B | 191 | GLU | CG-CD | -5.63 | 1.43 | 1.51 |
| 2 | B | 785 | TYR | CD2-CE2 | -5.63 | 1.30 | 1.39 |
| 5 | E | 203 | TYR | CD2-CE2 | -5.63 | 1.30 | 1.39 |
| 1 | A | 810 | PHE | CD2-CE2 | -5.62 | 1.28 | 1.39 |
| 2 | B | 788 | TYR | CD2-CE2 | -5.62 | 1.30 | 1.39 |
| 2 | B | 568 | PHE | CD1-CE1 | -5.61 | 1.28 | 1.39 |
| 2 | B | 814 | TYR | CD2-CE2 | -5.61 | 1.30 | 1.39 |
| 1 | A | 815 | TYR | CE2-CZ | -5.60 | 1.31 | 1.38 |
| 11 | K | 63 | VAL | CB-CG1 | -5.60 | 1.41 | 1.52 |
| 2 | B | 1027 | VAL | CB-CG2 | -5.60 | 1.41 | 1.52 |
| 3 | C | 19 | VAL | CB-CG1 | -5.59 | 1.41 | 1.52 |
| 2 | B | 949 | TYR | CD2-CE2 | -5.59 | 1.30 | 1.39 |
| 3 | C | 185 | GLU | CB-CG | -5.59 | 1.41 | 1.52 |
| 2 | B | 176 | GLU | CB-CG | -5.59 | 1.41 | 1.52 |
| 11 | K | 61 | TYR | CD1-CE1 | -5.57 | 1.30 | 1.39 |
| 2 | B | 814 | TYR | CE1-CZ | -5.57 | 1.31 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | H | 115 | TYR | CG-CD2 | -5.57 | 1.31 | 1.39 |
| 5 | E | 26 | TYR | CD2-CE2 | -5.56 | 1.31 | 1.39 |
| 8 | H | 50 | VAL | CB-CG2 | -5.56 | 1.41 | 1.52 |
| 2 | B | 671 | GLU | CB-CG | -5.56 | 1.41 | 1.52 |
| 3 | C | 229 | PHE | CD2-CE2 | -5.56 | 1.28 | 1.39 |
| 2 | B | 367 | TYR | CD2-CE2 | -5.55 | 1.31 | 1.39 |
| 1 | A | 500 | GLU | CB-CG | -5.54 | 1.41 | 1.52 |
| 3 | C | 230 | TYR | CD1-CE1 | -5.54 | 1.31 | 1.39 |
| 3 | C | 45 | ILE | CB-CG2 | -5.54 | 1.35 | 1.52 |
| 2 | B | 1153 | TYR | CE2-CZ | -5.53 | 1.31 | 1.38 |
| 6 | F | 102 | ILE | C-N | -5.53 | 1.23 | 1.34 |
| 1 | A | 479 | TRP | CB-CG | -5.53 | 1.40 | 1.50 |
| 1 | A | 554 | PHE | CD1-CE1 | -5.52 | 1.28 | 1.39 |
| 1 | A | 810 | PHE | CD1-CE1 | -5.52 | 1.28 | 1.39 |
| 1 | A | 446 | VAL | CB-CG2 | -5.50 | 1.41 | 1.52 |
| 9 | I | 111 | TYR | CD1-CE1 | -5.50 | 1.31 | 1.39 |
| 1 | A | 1471 | PHE | CD1-CE1 | -5.50 | 1.28 | 1.39 |
| 3 | C | 37 | VAL | CB-CG1 | -5.49 | 1.41 | 1.52 |
| 1 | A | 378 | VAL | CB-CG1 | -5.48 | 1.41 | 1.52 |
| 2 | B | 466 | VAL | CB-CG2 | -5.48 | 1.41 | 1.52 |
| 2 | B | 791 | GLU | CB-CG | -5.48 | 1.41 | 1.52 |
| 1 | A | 618 | TYR | CD2-CE2 | -5.48 | 1.31 | 1.39 |
| 15 | P | 45 | C | N1-C6 | -5.48 | 1.33 | 1.37 |
| 3 | C | 224 | GLY | C-N | -5.47 | 1.21 | 1.34 |
| 3 | C | 231 | TYR | CE1-CZ | -5.46 | 1.31 | 1.38 |
| 2 | B | 1018 | TYR | CD1-CE1 | -5.46 | 1.31 | 1.39 |
| 2 | B | 1048 | TYR | CB-CG | -5.46 | 1.43 | 1.51 |
| 1 | A | 891 | TYR | CD2-CE2 | -5.46 | 1.31 | 1.39 |
| 8 | H | 93 | TYR | CD1-CE1 | -5.45 | 1.31 | 1.39 |
| 2 | B | 752 | TYR | CD2-CE2 | -5.45 | 1.31 | 1.39 |
| 1 | A | 970 | PHE | CB-CG | -5.44 | 1.42 | 1.51 |
| 1 | A | 548 | PHE | CD2-CE2 | -5.44 | 1.28 | 1.39 |
| 6 | F | 60 | TYR | CD2-CE2 | -5.44 | 1.31 | 1.39 |
| 1 | A | 1085 | GLU | CB-CG | -5.43 | 1.41 | 1.52 |
| 2 | B | 1088 | GLU | CB-CG | -5.43 | 1.41 | 1.52 |
| 6 | F | 60 | TYR | CE2-CZ | -5.43 | 1.31 | 1.38 |
| 1 | A | 64 | VAL | CB-CG1 | -5.42 | 1.41 | 1.52 |
| 3 | C | 231 | TYR | CE2-CZ | -5.40 | 1.31 | 1.38 |
| 11 | K | 61 | TYR | CD2-CE2 | -5.40 | 1.31 | 1.39 |
| 1 | A | 657 | TYR | CD2-CE2 | -5.40 | 1.31 | 1.39 |
| 1 | A | 891 | TYR | CE1-CZ | -5.39 | 1.31 | 1.38 |
| 1 | A | 1087 | VAL | CB-CG1 | -5.39 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 661 | VAL | CB-CG1 | -5.38 | 1.41 | 1.52 |
| 11 | K | 102 | GLU | CB-CG | -5.38 | 1.42 | 1.52 |
| 1 | A | 566 | PHE | CD2-CE2 | -5.38 | 1.28 | 1.39 |
| 8 | H | 118 | TYR | CE2-CZ | -5.38 | 1.31 | 1.38 |
| 1 | A | 978 | VAL | CB-CG1 | -5.37 | 1.41 | 1.52 |
| 1 | A | 553 | VAL | CB-CG2 | -5.36 | 1.41 | 1.52 |
| 3 | C | 158 | GLU | CB-CG | -5.36 | 1.42 | 1.52 |
| 8 | H | 25 | VAL | CB-CG1 | -5.35 | 1.41 | 1.52 |
| 2 | B | 766 | TYR | CD2-CE2 | -5.35 | 1.31 | 1.39 |
| 1 | A | 514 | GLU | CG-CD | -5.35 | 1.44 | 1.51 |
| 8 | H | 90 | TYR | CE1-CZ | -5.34 | 1.31 | 1.38 |
| 8 | H | 137 | VAL | CB-CG2 | -5.34 | 1.41 | 1.52 |
| 5 | E | 206 | TYR | CD1-CE1 | -5.33 | 1.31 | 1.39 |
| 1 | A | 886 | VAL | CB-CG2 | -5.33 | 1.41 | 1.52 |
| 2 | B | 615 | TYR | CE1-CZ | -5.33 | 1.31 | 1.38 |
| 1 | A | 634 | GLU | CB-CG | -5.33 | 1.42 | 1.52 |
| 1 | A | 382 | ARG | CB-CG | -5.31 | 1.38 | 1.52 |
| 2 | B | 766 | TYR | CD1-CE1 | -5.31 | 1.31 | 1.39 |
| 2 | B | 664 | TYR | CB-CG | -5.30 | 1.43 | 1.51 |
| 2 | B | 860 | VAL | CB-CG2 | -5.30 | 1.41 | 1.52 |
| 3 | C | 101 | PHE | CD1-CE1 | -5.30 | 1.28 | 1.39 |
| 2 | B | 568 | PHE | CD2-CE2 | -5.30 | 1.28 | 1.39 |
| 1 | A | 21 | VAL | CB-CG2 | -5.29 | 1.41 | 1.52 |
| 10 | J | 62 | TYR | CD2-CE2 | -5.29 | 1.31 | 1.39 |
| 11 | K | 68 | GLU | CB-CG | -5.29 | 1.42 | 1.52 |
| 2 | B | 752 | TYR | CB-CG | -5.28 | 1.43 | 1.51 |
| 1 | A | 26 | LEU | C-N | -5.28 | 1.22 | 1.34 |
| 1 | A | 787 | VAL | CB-CG1 | -5.27 | 1.41 | 1.52 |
| 3 | C | 197 | TYR | CG-CD1 | -5.27 | 1.32 | 1.39 |
| 9 | I | 111 | TYR | CD2-CE2 | -5.27 | 1.31 | 1.39 |
| 1 | A | 679 | TRP | CE3-CZ3 | -5.26 | 1.29 | 1.38 |
| 6 | F | 56 | TYR | CD1-CE1 | -5.25 | 1.31 | 1.39 |
| 5 | E | 194 | ILE | C-N | -5.25 | 1.22 | 1.34 |
| 2 | B | 176 | GLU | CG-CD | -5.25 | 1.44 | 1.51 |
| 3 | C | 197 | TYR | CD2-CE2 | -5.25 | 1.31 | 1.39 |
| 1 | A | 458 | PHE | CD2-CE2 | -5.25 | 1.28 | 1.39 |
| 2 | B | 1006 | VAL | CB-CG2 | -5.25 | 1.41 | 1.52 |
| 3 | C | 184 | PHE | CB-CG | -5.25 | 1.42 | 1.51 |
| 2 | B | 1153 | TYR | CD2-CE2 | -5.23 | 1.31 | 1.39 |
| 3 | C | 9 | VAL | CB-CG2 | -5.23 | 1.41 | 1.52 |
| 2 | B | 736 | TYR | CD2-CE2 | -5.23 | 1.31 | 1.39 |
| 1 | A | 970 | PHE | CD1-CE1 | -5.23 | 1.28 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 904 | VAL | CB-CG2 | -5.22 | 1.41 | 1.52 |
| 3 | C | 176 | TRP | CB-CG | -5.22 | 1.40 | 1.50 |
| 14 | N | 37 | DG | N9-C4 | -5.22 | 1.33 | 1.38 |
| 2 | B | 743 | ARG | CG-CD | -5.22 | 1.39 | 1.51 |
| 9 | I | 112 | TYR | CD1-CE1 | -5.21 | 1.31 | 1.39 |
| 12 | L | 54 | VAL | CB-CG2 | -5.21 | 1.42 | 1.52 |
| 1 | A | 713 | VAL | CB-CG2 | -5.21 | 1.42 | 1.52 |
| 3 | C | 234 | GLU | CB-CG | -5.21 | 1.42 | 1.52 |
| 2 | B | 735 | VAL | CB-CG2 | -5.21 | 1.42 | 1.52 |
| 18 | T | 27 | DT | N1-C6 | -5.21 | 1.34 | 1.38 |
| 1 | A | 770 | VAL | CB-CG1 | -5.21 | 1.42 | 1.52 |
| 8 | H | 115 | TYR | CG-CD1 | -5.20 | 1.32 | 1.39 |
| 5 | E | 206 | TYR | CD2-CE2 | -5.20 | 1.31 | 1.39 |
| 5 | E | 11 | TRP | CB-CG | -5.20 | 1.40 | 1.50 |
| 6 | F | 65 | VAL | CB-CG1 | -5.19 | 1.42 | 1.52 |
| 3 | C | 50 | VAL | CB-CG2 | -5.18 | 1.42 | 1.52 |
| 2 | B | 1048 | TYR | CD1-CE1 | -5.18 | 1.31 | 1.39 |
| 1 | A | 827 | TYR | CG-CD1 | -5.17 | 1.32 | 1.39 |
| 2 | B | 523 | VAL | CB-CG1 | -5.17 | 1.42 | 1.52 |
| 8 | H | 97 | TYR | CD1-CE1 | -5.17 | 1.31 | 1.39 |
| 18 | T | 32 | DT | N1-C2 | -5.16 | 1.33 | 1.38 |
| 2 | B | 923 | VAL | CB-CG2 | -5.16 | 1.42 | 1.52 |
| 2 | B | 369 | VAL | CB-CG2 | -5.16 | 1.42 | 1.52 |
| 1 | A | 669 | TYR | CG-CD2 | -5.15 | 1.32 | 1.39 |
| 2 | B | 753 | TYR | CG-CD2 | -5.15 | 1.32 | 1.39 |
| 1 | A | 492 | TYR | CG-CD2 | -5.14 | 1.32 | 1.39 |
| 2 | B | 33 | TYR | CD1-CE1 | -5.14 | 1.31 | 1.39 |
| 2 | B | 750 | VAL | CB-CG1 | -5.14 | 1.42 | 1.52 |
| 1 | A | 978 | VAL | CB-CG2 | -5.13 | 1.42 | 1.52 |
| 5 | E | 203 | TYR | CD1-CE1 | -5.13 | 1.31 | 1.39 |
| 3 | C | 101 | PHE | CD2-CE2 | -5.12 | 1.29 | 1.39 |
| 3 | C | 230 | TYR | CD2-CE2 | -5.12 | 1.31 | 1.39 |
| 8 | H | 48 | TYR | CD2-CE2 | -5.12 | 1.31 | 1.39 |
| 2 | B | 918 | PHE | CD2-CE2 | -5.12 | 1.29 | 1.39 |
| 3 | C | 203 | TRP | CB-CG | -5.11 | 1.41 | 1.50 |
| 3 | C | 21 | PHE | CD2-CE2 | -5.11 | 1.29 | 1.39 |
| 10 | J | 18 | TRP | CB-CG | -5.11 | 1.41 | 1.50 |
| 1 | A | 1402 | CYS | CB-SG | -5.10 | 1.73 | 1.81 |
| 2 | B | 666 | ASP | CB-CG | -5.10 | 1.41 | 1.51 |
| 1 | A | 392 | GLU | CB-CG | -5.10 | 1.42 | 1.52 |
| 1 | A | 548 | PHE | CE1-CZ | -5.09 | 1.27 | 1.37 |
| 1 | A | 1392 | TYR | CD2-CE2 | -5.08 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 120 | TYR | CE2-CZ | -5.07 | 1.31 | 1.38 |
| 2 | B | 811 | TYR | CG-CD1 | -5.07 | 1.32 | 1.39 |
| 8 | H | 98 | ARG | CG-CD | -5.07 | 1.39 | 1.51 |
| 2 | B | 782 | ILE | CB-CG2 | -5.07 | 1.37 | 1.52 |
| 10 | J | 53 | VAL | CB-CG2 | -5.07 | 1.42 | 1.52 |
| 1 | A | 570 | TRP | CE3-CZ3 | -5.06 | 1.29 | 1.38 |
| 3 | C | 49 | TRP | CB-CG | -5.06 | 1.41 | 1.50 |
| 1 | A | 554 | PHE | CD2-CE2 | -5.06 | 1.29 | 1.39 |
| 1 | A | 618 | TYR | CD1-CE1 | -5.06 | 1.31 | 1.39 |
| 1 | A | 570 | TRP | CB-CG | -5.05 | 1.41 | 1.50 |
| 1 | A | 521 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 1 | A | 675 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 3 | C | 164 | TYR | CD2-CE2 | -5.04 | 1.31 | 1.39 |
| 2 | B | 926 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 1 | A | 586 | TRP | CD2-CE2 | -5.04 | 1.35 | 1.41 |
| 2 | B | 945 | CYS | CB-SG | -5.03 | 1.73 | 1.81 |
| 8 | H | 116 | VAL | CB-CG2 | -5.03 | 1.42 | 1.52 |
| 2 | B | 736 | TYR | CD1-CE1 | -5.03 | 1.31 | 1.39 |
| 2 | B | 801 | VAL | CB-CG2 | -5.03 | 1.42 | 1.52 |
| 8 | H | 97 | TYR | CE2-CZ | -5.02 | 1.32 | 1.38 |
| 1 | A | 81 | CYS | CB-SG | -5.02 | 1.73 | 1.81 |
| 2 | B | 1018 | TYR | CD2-CE2 | -5.02 | 1.31 | 1.39 |
| 2 | B | 785 | TYR | CD1-CE1 | -5.01 | 1.31 | 1.39 |
| 2 | B | 807 | ARG | CG-CD | -5.01 | 1.39 | 1.51 |
| 8 | H | 115 | TYR | CB-CG | -5.01 | 1.44 | 1.51 |
| 1 | A | 479 | TRP | CE3-CZ3 | -5.01 | 1.29 | 1.38 |
| 2 | B | 466 | VAL | CB-CG1 | -5.01 | 1.42 | 1.52 |
| 1 | A | 458 | PHE | CB-CG | -5.01 | 1.42 | 1.51 |
| 1 | A | 788 | VAL | CB-CG1 | -5.00 | 1.42 | 1.52 |

All (99) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 15 | P | 40 | A | C8-N9-C4 | -13.77 | 100.29 | 105.80 |
| 15 | P | 40 | A | N7-C8-N9 | 12.63 | 120.11 | 113.80 |
| 15 | P | 41 | C | C6-N1-C2 | -11.07 | 115.87 | 120.30 |
| 3 | C | 224 | GLY | C-N-CA | 10.22 | 147.25 | 121.70 |
| 15 | P | 40 | A | C5-N7-C8 | -9.32 | 99.24 | 103.90 |
| 15 | P | 39 | A | C8-N9-C4 | -9.26 | 102.10 | 105.80 |
| 18 | T | 34 | DT | O5'-P-OP1 | -9.09 | 97.52 | 105.70 |
| 1 | A | 457 | ILE | CG1-CB-CG2 | -8.95 | 91.72 | 111.40 |
| 15 | P | 39 | A | N1-C2-N3 | 8.41 | 133.51 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | T | 33 | DC | OP1-P-O3' | 8.23 | 123.31 | 105.20 |
| 2 | B | 473 | LEU | CB-CG-CD2 | -8.05 | 97.32 | 111.00 |
| 2 | B | 411 | LEU | CB-CG-CD2 | -7.96 | 97.46 | 111.00 |
| 15 | P | 40 | A | N9-C4-C5 | 7.60 | 108.84 | 105.80 |
| 2 | B | 583 | LEU | CB-CG-CD1 | -7.48 | 98.28 | 111.00 |
| 14 | N | 40 | DG | O4'-C1'-N9 | 7.36 | 113.15 | 108.00 |
| 15 | P | 39 | A | N9-C4-C5 | 7.34 | 108.74 | 105.80 |
| 2 | B | 567 | ILE | CG1-CB-CG2 | -7.31 | 95.31 | 111.40 |
| 1 | A | 484 | LEU | CB-CG-CD2 | -7.25 | 98.67 | 111.00 |
| 2 | B | 545 | LEU | CB-CG-CD2 | -7.25 | 98.68 | 111.00 |
| 15 | P | 42 | C | C6-N1-C2 | -7.21 | 117.42 | 120.30 |
| 1 | A | 524 | MET | CG-SD-CE | -7.09 | 88.86 | 100.20 |
| 3 | C | 68 | LEU | CB-CG-CD1 | -6.96 | 99.16 | 111.00 |
| 2 | B | 668 | LEU | CB-CG-CD2 | -6.96 | 99.17 | 111.00 |
| 17 | R | 507 | PRO | N-CA-CB | 6.88 | 111.56 | 103.30 |
| 15 | P | 41 | C | N3-C2-O2 | -6.85 | 117.11 | 121.90 |
| 1 | A | 542 | LEU | CB-CG-CD2 | -6.75 | 99.52 | 111.00 |
| 15 | P | 39 | A | C6-N1-C2 | -6.57 | 114.66 | 118.60 |
| 1 | A | 1396 | ARG | CG-CD-NE | -6.55 | 98.03 | 111.80 |
| 15 | P | 37 | G | O4'-C1'-N9 | 6.53 | 113.43 | 108.20 |
| 18 | T | 29 | DG | O4'-C4'-C3' | -6.53 | 101.89 | 104.50 |
| 3 | C | 67 | ARG | NE-CZ-NH1 | -6.49 | 117.06 | 120.30 |
| 1 | A | 1090 | LEU | CB-CG-CD2 | -6.48 | 99.98 | 111.00 |
| 15 | P | 40 | A | N3-C4-N9 | -6.43 | 122.25 | 127.40 |
| 2 | B | 848 | LEU | CB-CG-CD1 | -6.39 | 100.13 | 111.00 |
| 18 | T | 26 | DG | O4'-C4'-C3' | -6.36 | 101.96 | 104.50 |
| 20 | V | 258 | PRO | N-CA-CB | 6.33 | 110.89 | 103.30 |
| 2 | B | 505 | LEU | CA-CB-CG | 6.30 | 129.80 | 115.30 |
| 2 | B | 501 | LEU | CB-CG-CD2 | -6.24 | 100.40 | 111.00 |
| 1 | A | 486 | LEU | CB-CG-CD2 | -6.23 | 100.42 | 111.00 |
| 17 | R | 506 | PRO | N-CA-CB | 6.17 | 110.71 | 103.30 |
| 18 | T | 27 | DT | O4'-C4'-C3' | -6.16 | 102.04 | 104.50 |
| 1 | A | 1463 | LEU | CB-CG-CD1 | -6.11 | 100.61 | 111.00 |
| 1 | A | 1095 | LEU | CB-CG-CD2 | -6.09 | 100.64 | 111.00 |
| 2 | B | 163 | LEU | CB-CG-CD2 | -6.08 | 100.66 | 111.00 |
| 2 | B | 411 | LEU | CA-CB-CG | 6.07 | 129.27 | 115.30 |
| 11 | K | 100 | LEU | CB-CG-CD2 | -6.07 | 100.69 | 111.00 |
| 15 | P | 38 | G | C6-C5-N7 | -5.97 | 126.82 | 130.40 |
| 5 | E | 165 | LEU | CB-CG-CD2 | -5.96 | 100.86 | 111.00 |
| 13 | M | 1330 | PRO | N-CA-CB | 5.95 | 110.44 | 103.30 |
| 1 | A | 26 | LEU | C-N-CA | -5.94 | 106.86 | 121.70 |
| 20 | V | 238 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 15 | P | 41 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 2 | B | 395 | LEU | CB-CG-CD2 | -5.91 | 100.96 | 111.00 |
| 10 | J | 55 | LEU | CB-CG-CD2 | -5.90 | 100.98 | 111.00 |
| 1 | A | 1400 | LEU | CB-CG-CD2 | -5.88 | 101.00 | 111.00 |
| 15 | P | 38 | G | N7-C8-N9 | 5.88 | 116.04 | 113.10 |
| 19 | U | 463 | PRO | N-CA-CB | 5.78 | 110.23 | 103.30 |
| 15 | P | 38 | G | C4-N9-C1' | 5.76 | 133.98 | 126.50 |
| 2 | B | 556 | ILE | C-N-CA | -5.73 | 107.38 | 121.70 |
| 18 | T | 32 | DT | O4'-C1'-N1 | 5.71 | 112.00 | 108.00 |
| 1 | A | 979 | LEU | CB-CG-CD1 | -5.68 | 101.35 | 111.00 |
| 11 | K | 93 | ASP | CB-CG-OD1 | -5.63 | 113.23 | 118.30 |
| 2 | B | 1014 | LEU | CB-CG-CD2 | -5.63 | 101.43 | 111.00 |
| 15 | P | 41 | C | C6-N1-C1' | 5.60 | 127.52 | 120.80 |
| 2 | B | 866 | ILE | CG1-CB-CG2 | -5.58 | 99.12 | 111.40 |
| 1 | A | 1398 | LEU | CB-CG-CD2 | -5.55 | 101.56 | 111.00 |
| 15 | P | 41 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 19 | U | 493 | PRO | N-CA-CB | 5.50 | 109.90 | 103.30 |
| 3 | C | 228 | ARG | NE-CZ-NH1 | -5.49 | 117.56 | 120.30 |
| 2 | B | 1015 | LEU | CB-CG-CD2 | -5.48 | 101.68 | 111.00 |
| 2 | B | 115 | LEU | CB-CG-CD2 | -5.44 | 101.76 | 111.00 |
| 24 | Z | 758 | PRO | N-CA-CB | 5.43 | 109.82 | 103.30 |
| 2 | B | 542 | LEU | CB-CG-CD2 | -5.42 | 101.78 | 111.00 |
| 2 | B | 576 | ILE | CG1-CB-CG2 | -5.39 | 99.54 | 111.40 |
| 2 | B | 21 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 15 | P | 36 | G | P-O3'-C3' | 5.37 | 126.15 | 119.70 |
| 1 | A | 938 | LEU | CB-CG-CD2 | -5.33 | 101.94 | 111.00 |
| 2 | B | 403 | LEU | CB-CG-CD1 | -5.32 | 101.96 | 111.00 |
| 8 | H | 121 | LEU | CB-CG-CD2 | -5.30 | 101.99 | 111.00 |
| 10 | J | 50 | LEU | CB-CG-CD2 | -5.25 | 102.08 | 111.00 |
| 2 | B | 751 | LEU | CB-CG-CD2 | -5.24 | 102.09 | 111.00 |
| 1 | A | 80 | GLU | C-N-CA | -5.23 | 108.63 | 121.70 |
| 2 | B | 371 | ARG | NE-CZ-NH1 | -5.22 | 117.69 | 120.30 |
| 12 | L | 44 | MET | CG-SD-CE | -5.21 | 91.86 | 100.20 |
| 2 | B | 959 | GLU | C-N-CA | -5.18 | 111.42 | 122.30 |
| 2 | B | 395 | LEU | CA-CB-CG | -5.16 | 103.43 | 115.30 |
| 15 | P | 39 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 10 | J | 65 | LEU | CA-CB-CG | 5.14 | 127.13 | 115.30 |
| 3 | C | 67 | ARG | NE-CZ-NH2 | 5.12 | 122.86 | 120.30 |
| 1 | A | 565 | MET | CG-SD-CE | -5.12 | 92.01 | 100.20 |
| 2 | B | 377 | LEU | CB-CG-CD1 | -5.10 | 102.32 | 111.00 |
| 2 | B | 146 | LYS | CA-CB-CG | 5.10 | 124.62 | 113.40 |
| 1 | A | 567 | LEU | CB-CG-CD1 | -5.05 | 102.42 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 15 | P | 38 | G | C8-N9-C4 | -5.04 | 104.38 | 106.40 |
| 1 | A | 484 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 2 | B | 665 | ILE | CG1-CB-CG2 | -5.02 | 100.35 | 111.40 |
| 12 | L | 20 | GLY | N-CA-C | -5.02 | 100.56 | 113.10 |
| 3 | C | 44 | ILE | CG1-CB-CG2 | -5.00 | 100.40 | 111.40 |
| 3 | C | 154 | ARG | CG-CD-NE | -5.00 | 101.30 | 111.80 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 1434 | GLU | Peptide |
| 1 | A | 910 | LYS | Peptide |
| 2 | B | 20 | ASP | Peptide |
| 2 | B | 547 | GLU | Peptide |
| 2 | B | 686 | GLU | Peptide |
| 17 | R | 592 | ASP | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 11255 | 0 | 11374 | 435 | 0 |
| 2 | B | 8980 | 0 | 9017 | 295 | 0 |
| 3 | C | 2072 | 0 | 2019 | 45 | 0 |
| 4 | D | 1004 | 0 | 980 | 55 | 0 |
| 5 | E | 1720 | 0 | 1737 | 73 | 0 |
| 6 | F | 626 | 0 | 657 | 11 | 0 |
| 7 | G | 1333 | 0 | 1321 | 80 | 0 |
| 8 | H | 1197 | 0 | 1156 | 44 | 0 |
| 9 | I | 942 | 0 | 873 | 38 | 0 |
| 10 | J | 524 | 0 | 541 | 19 | 0 |
| 11 | K | 920 | 0 | 942 | 28 | 0 |
| 12 | L | 390 | 0 | 397 | 13 | 0 |
| 13 | M | 4737 | 0 | 2262 | 46 | 0 |
| 14 | N | 773 | 0 | 412 | 38 | 0 |
| 15 | P | 452 | 0 | 229 | 24 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16 | Q | 7226 | 0 | 7169 | 355 | 0 |
| 17 | R | 1832 | 0 | 1687 | 114 | 0 |
| 18 | T | 974 | 0 | 541 | 39 | 0 |
| 19 | U | 852 | 0 | 668 | 31 | 0 |
| 20 | V | 1703 | 0 | 1426 | 85 | 0 |
| 21 | W | 2333 | 0 | 2246 | 155 | 0 |
| 22 | X | 353 | 0 | 371 | 28 | 0 |
| 23 | Y | 911 | 0 | 908 | 27 | 0 |
| 24 | Z | 4023 | 0 | 4035 | 181 | 0 |
| 25 | A | 2 | 0 | 0 | 0 | 0 |
| 25 | B | 1 | 0 | 0 | 0 | 0 |
| 25 | C | 1 | 0 | 0 | 0 | 0 |
| 25 | I | 2 | 0 | 0 | 0 | 0 |
| 25 | J | 1 | 0 | 0 | 0 | 0 |
| 25 | L | 1 | 0 | 0 | 0 | 0 |
| 25 | Y | 1 | 0 | 0 | 0 | 0 |
| 26 | A | 1 | 0 | 0 | 0 | 0 |
| All | All | 57142 | 0 | 52968 | 2040 | 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 19.

All (2040) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:37:MET:HE2 | 8:H:127:GLY:HA3 | 1.42 | 0.99 |
| 2:B:953:ASP:OD1 | 3:C:36:ARG:NH2 | 1.96 | 0.98 |
| 1:A:609:HIS:HD1 | 1:A:626:THR:HG1 | 1.04 | 0.94 |
| 16:Q:505:ARG:HH21 | 20:V:44:PHE:HB2 | 1.32 | 0.93 |
| 1:A:904:GLN:NE2 | 1:A:981:CYS:O | 2.01 | 0.91 |
| 2:B:105:PRO:HG2 | 19:U:512:THR:HA | 1.51 | 0.91 |
| 16:Q:830:ARG:HA | 16:Q:833:LYS:HE2 | 1.54 | 0.90 |
| 21:W:278:TRP:HB2 | 21:W:293:GLY:HA2 | 1.51 | 0.90 |
| 1:A:1227:THR:H | 1:A:1230:GLN:HE21 | 1.19 | 0.90 |
| 14:N:30:DC:H42 | 18:T:19:DG:H1 | 1.18 | 0.89 |
| 23:Y:7:PRO:HG3 | 23:Y:23:LYS:HA | 1.53 | 0.89 |
| 2:B:332:LYS:NZ | 2:B:333:GLU:OE1 | 2.07 | 0.88 |
| 21:W:40:LEU:HD12 | 21:W:66:GLY:HA3 | 1.53 | 0.88 |
| 16:Q:727:LEU:HB3 | 16:Q:732:LYS:HB3 | 1.57 | 0.87 |
| 17:R:388:ARG:NH1 | 17:R:446:GLU:O | 2.08 | 0.87 |
| 16:Q:768:VAL:HG21 | 16:Q:778:GLU:HG3 | 1.55 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:103:ARG:NH2 | 9:I:105:GLU:OE2 | 2.08 | 0.86 |
| 17:R:387:VAL:HG13 | 17:R:405:ILE:HD11 | 1.58 | 0.86 |
| 24:Z:478:VAL:HB | 24:Z:518:LEU:HD11 | 1.58 | 0.85 |
| 2:B:387:HIS:NE2 | 2:B:671:GLU:OE2 | 2.10 | 0.85 |
| 1:A:922:PHE:H | 1:A:1052:ARG:HD2 | 1.40 | 0.85 |
| 18:T:41:DC:H4' | 24:Z:283:ARG:HE | 1.41 | 0.85 |
| 3:C:193:ARG:NH2 | 3:C:218:ALA:O | 2.09 | 0.85 |
| 21:W:35:VAL:HB | 21:W:47:TRP:HB2 | 1.59 | 0.85 |
| 8:H:98:ARG:NH2 | 8:H:100:GLU:OE1 | 2.09 | 0.85 |
| 2:B:85:LEU:HB2 | 2:B:131:THR:HB | 1.59 | 0.85 |
| 23:Y:75:GLN:O | 23:Y:111:ARG:NH1 | 2.09 | 0.85 |
| 16:Q:682:ASP:O | 16:Q:686:ASN:ND2 | 2.09 | 0.84 |
| 1:A:197:GLU:HB2 | 1:A:215:LEU:HD11 | 1.60 | 0.84 |
| 17:R:570:TRP:HB3 | 20:V:133:LYS:HE2 | 1.61 | 0.83 |
| 1:A:404:GLU:OE2 | 1:A:407:ARG:NH1 | 2.12 | 0.82 |
| 9:I:54:TYR:OH | 9:I:56:ASN:ND2 | 2.12 | 0.82 |
| 2:B:613:ARG:NH1 | 2:B:615:TYR:OH | 2.12 | 0.82 |
| 4:D:107:THR:HG23 | 4:D:110:GLU:H | 1.43 | 0.82 |
| 14:N:37:DG:N1 | 18:T:12:DC:N3 | 2.27 | 0.82 |
| 1:A:392:GLU:OE2 | 1:A:401:ARG:NH2 | 2.11 | 0.81 |
| 5:E:166:ARG:HH22 | 5:E:168:ASN:HD22 | 1.26 | 0.81 |
| 16:Q:387:ALA:N | 16:Q:390:ASP:OD2 | 2.13 | 0.81 |
| 21:W:14:ALA:N | 21:W:296:GLN:O | 2.13 | 0.81 |
| 21:W:172:ILE:HB | 21:W:186:LEU:HB2 | 1.61 | 0.81 |
| 2:B:179:LEU:HD22 | 2:B:768:ARG:HD3 | 1.62 | 0.81 |
| 16:Q:643:ASP:OD2 | 22:X:239:GLN:NE2 | 2.11 | 0.81 |
| 4:D:76:ASN:HD22 | 4:D:79:THR:HG23 | 1.45 | 0.81 |
| 10:J:25:LEU:HB3 | 17:R:563:ILE:HD11 | 1.61 | 0.81 |
| 21:W:237:ASN:HD22 | 21:W:279:GLY:HA2 | 1.45 | 0.81 |
| 23:Y:3:LEU:O | 23:Y:8:LYS:NZ | 2.12 | 0.81 |
| 21:W:95:ASN:O | 21:W:97:LYS:NZ | 2.12 | 0.81 |
| 16:Q:276:ALA:HB1 | 16:Q:288:VAL:HG23 | 1.61 | 0.81 |
| 16:Q:737:LYS:HZ2 | 16:Q:764:LEU:HD13 | 1.46 | 0.80 |
| 1:A:1182:GLN:O | 1:A:1192:TRP:NE1 | 2.14 | 0.80 |
| 21:W:35:VAL:N | 21:W:47:TRP:O | 2.12 | 0.80 |
| 2:B:756:LYS:NZ | 20:V:134:THR:OG1 | 2.15 | 0.80 |
| 1:A:1525:TPO:O3P | 13:M:1358:ARG:NH2 | 2.15 | 0.80 |
| 15:P:39:A:H3' | 15:P:40:A:H8 | 1.47 | 0.80 |
| 16:Q:268:ASN:HD22 | 16:Q:271:VAL:H | 1.29 | 0.79 |
| 1:A:1536:GLY:O | 13:M:1483:ARG:NH2 | 2.16 | 0.79 |
| 7:G:111:HIS:HB3 | 24:Z:494:ARG:HB2 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:237:ASN:HB3 | 21:W:280:VAL:HG22 | 1.65 | 0.79 |
| 16:Q:41:LEU:HD23 | 16:Q:81:ASP:HB3 | 1.65 | 0.79 |
| 16:Q:534:TYR:HH | 16:Q:553:TRP:HD1 | 1.31 | 0.79 |
| 1:A:1180:ASN:O | 1:A:1183:SER:OG | 2.00 | 0.79 |
| 20:V:47:LYS:HB3 | 22:X:228:GLU:HB2 | 1.63 | 0.79 |
| 1:A:539:GLN:O | 1:A:541:THR:N | 2.16 | 0.78 |
| 2:B:297:MET:HG2 | 2:B:377:LEU:HD11 | 1.65 | 0.78 |
| 3:C:154:ARG:NH1 | 10:J:63:ALA:HB2 | 1.98 | 0.78 |
| 1:A:349:ARG:HE | 2:B:1157:LEU:HD22 | 1.46 | 0.78 |
| 15:P:38:G:H2' | 15:P:39:A:H8 | 1.49 | 0.78 |
| 15:P:40:A:H2' | 15:P:41:C:C6 | 2.19 | 0.78 |
| 1:A:1189:ASP:HA | 1:A:1192:TRP:HE3 | 1.49 | 0.78 |
| 14:N:14:DC:N4 | 18:T:35:DG:O6 | 2.16 | 0.78 |
| 16:Q:268:ASN:HD21 | 16:Q:270:MET:HB3 | 1.49 | 0.78 |
| 1:A:413:TYR:O | 1:A:415:GLY:N | 2.17 | 0.78 |
| 16:Q:568:TRP:HE1 | 16:Q:591:ILE:HD12 | 1.49 | 0.78 |
| 24:Z:216:VAL:HB | 24:Z:226:TYR:HB2 | 1.65 | 0.77 |
| 9:I:101:SER:OG | 9:I:102:ALA:O | 2.03 | 0.77 |
| 12:L:16:ILE:HD11 | 12:L:25:GLU:HB3 | 1.66 | 0.77 |
| 19:U:394:TYR:O | 20:V:172:ARG:NH2 | 2.17 | 0.77 |
| 24:Z:728:THR:O | 24:Z:747:ARG:NH1 | 2.18 | 0.77 |
| 16:Q:624:LYS:HG3 | 16:Q:627:ARG:HH21 | 1.47 | 0.76 |
| 1:A:272:ASN:ND2 | 18:T:34:DT:O2 | 2.19 | 0.76 |
| 1:A:1189:ASP:HA | 1:A:1192:TRP:CE3 | 2.20 | 0.76 |
| 2:B:622:CYS:HB3 | 2:B:666:ASP:HB3 | 1.68 | 0.76 |
| 1:A:571:ASP:OD1 | 1:A:571:ASP:N | 2.13 | 0.76 |
| 2:B:629:GLU:HG2 | 2:B:634:LEU:HD21 | 1.66 | 0.76 |
| 11:K:77:THR:OG1 | 11:K:81:TYR:O | 2.04 | 0.76 |
| 17:R:562:TYR:O | 17:R:566:ARG:NE | 2.18 | 0.76 |
| 20:V:47:LYS:HE3 | 22:X:230:VAL:HG22 | 1.67 | 0.76 |
| 16:Q:353:TYR:OH | 20:V:57:ARG:O | 2.04 | 0.76 |
| 1:A:659:GLU:OE1 | 1:A:985:ARG:NH1 | 2.19 | 0.75 |
| 1:A:1434:GLU:O | 1:A:1436:VAL:N | 2.19 | 0.75 |
| 16:Q:314:ARG:HH12 | 16:Q:349:GLN:HE22 | 1.33 | 0.75 |
| 2:B:834:ARG:NH2 | 2:B:841:ARG:O | 2.20 | 0.75 |
| 1:A:819:SER:O | 1:A:819:SER:OG | 2.05 | 0.74 |
| 2:B:1142:ASN:HD21 | 2:B:1145:GLN:HB2 | 1.52 | 0.74 |
| 1:A:713:VAL:HG21 | 1:A:817:PRO:HD3 | 1.67 | 0.74 |
| 8:H:7:GLU:HG2 | 8:H:59:VAL:HG22 | 1.68 | 0.74 |
| 14:N:37:DG:O6 | 18:T:12:DC:N4 | 2.20 | 0.74 |
| 1:A:296:ASN:OD1 | 1:A:297:GLY:N | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:299:ALA:HB3 | 1:A:302:VAL:HG12 | 1.69 | 0.74 |
| 1:A:1467:GLY:O | 1:A:1469:GLY:N | 2.20 | 0.74 |
| 2:B:677:MET:H | 2:B:682:LEU:HD22 | 1.52 | 0.74 |
| 20:V:193:HIS:HB2 | 20:V:199:VAL:HG12 | 1.70 | 0.74 |
| 1:A:239:GLU:OE2 | 1:A:241:ARG:NH1 | 2.21 | 0.74 |
| 1:A:863:ARG:NH2 | 1:A:1129:ASN:OD1 | 2.21 | 0.74 |
| 24:Z:438:GLY:HA3 | 24:Z:452:PRO:HB2 | 1.68 | 0.74 |
| 2:B:388:TYR:H | 2:B:504:THR:HG21 | 1.51 | 0.73 |
| 24:Z:492:ILE:HG22 | 24:Z:502:LEU:HB3 | 1.70 | 0.73 |
| 24:Z:554:GLU:OE2 | 24:Z:559:GLN:NE2 | 2.21 | 0.73 |
| 15:P:39:A:C3' | 15:P:40:A:H8 | 2.01 | 0.73 |
| 21:W:214:ILE:N | 21:W:228:LEU:O | 2.21 | 0.73 |
| 24:Z:353:ALA:HB3 | 24:Z:360:ILE:HB | 1.69 | 0.73 |
| 16:Q:424:GLN:HB2 | 22:X:231:TRP:CE3 | 2.24 | 0.73 |
| 24:Z:188:GLU:O | 24:Z:192:THR:OG1 | 2.05 | 0.73 |
| 24:Z:295:TYR:N | 24:Z:304:SER:OG | 2.17 | 0.73 |
| 1:A:1184:THR:O | 1:A:1186:VAL:N | 2.22 | 0.73 |
| 21:W:169:ASP:N | 21:W:169:ASP:OD1 | 2.22 | 0.73 |
| 2:B:898:THR:O | 2:B:899:SER:OG | 2.05 | 0.72 |
| 8:H:32:SER:HB3 | 8:H:37:MET:H | 1.52 | 0.72 |
| 2:B:84:TYR:HB3 | 2:B:132:VAL:HG23 | 1.70 | 0.72 |
| 2:B:309:PHE:O | 9:I:40:ARG:NH2 | 2.22 | 0.72 |
| 2:B:650:ASN:N | 19:U:460:TYR:OH | 2.17 | 0.72 |
| 4:D:131:LEU:HA | 4:D:134:ILE:HD12 | 1.71 | 0.72 |
| 5:E:81:LYS:NZ | 14:N:39:DA:OP1 | 2.19 | 0.72 |
| 1:A:539:GLN:O | 1:A:542:LEU:N | 2.21 | 0.72 |
| 21:W:272:ASP:O | 21:W:274:GLN:NE2 | 2.22 | 0.72 |
| 8:H:103:GLU:HG3 | 8:H:109:ALA:HB2 | 1.71 | 0.72 |
| 19:U:438:ALA:O | 19:U:439:ARG:NH1 | 2.20 | 0.72 |
| 20:V:110:GLU:HG3 | 20:V:111:GLU:H | 1.53 | 0.72 |
| 1:A:289:GLN:O | 1:A:293:ASN:HB2 | 1.89 | 0.72 |
| 12:L:19:CYS:SG | 12:L:20:GLY:N | 2.62 | 0.72 |
| 21:W:251:SER:OG | 21:W:253:ASP:OD1 | 2.05 | 0.72 |
| 2:B:348:LEU:O | 2:B:361:LYS:NZ | 2.22 | 0.72 |
| 7:G:11:ILE:HD11 | 7:G:26:VAL:HG13 | 1.70 | 0.72 |
| 23:Y:93:LEU:HD22 | 23:Y:97:ILE:HD11 | 1.70 | 0.72 |
| 2:B:595:ASP:OD1 | 2:B:596:ILE:N | 2.20 | 0.71 |
| 16:Q:163:ILE:HB | 16:Q:194:PRO:HG3 | 1.72 | 0.71 |
| 21:W:81:SER:HB3 | 21:W:91:TRP:HE1 | 1.55 | 0.71 |
| 16:Q:302:GLU:HG3 | 16:Q:305:GLN:HE21 | 1.55 | 0.71 |
| 8:H:128:ASP:OD1 | 8:H:131:ASN:ND2 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:401:LEU:HD22 | 16:Q:418:LEU:HG | 1.72 | 0.71 |
| 17:R:405:ILE:HG23 | 17:R:426:LEU:HD11 | 1.72 | 0.71 |
| 5:E:80:PRO:HA | 5:E:107:GLN:HB3 | 1.72 | 0.71 |
| 10:J:64:PRO:O | 12:L:23:HIS:NE2 | 2.23 | 0.71 |
| 18:T:8:DG:H1' | 18:T:9:DC:H5' | 1.73 | 0.71 |
| 21:W:256:VAL:HB | 21:W:270:PHE:HB2 | 1.72 | 0.71 |
| 24:Z:504:SER:OG | 24:Z:507:THR:O | 2.08 | 0.71 |
| 16:Q:384:LEU:HD13 | 16:Q:397:ALA:HB2 | 1.73 | 0.71 |
| 19:U:507:THR:O | 19:U:509:ARG:N | 2.24 | 0.71 |
| 24:Z:470:LYS:HB2 | 24:Z:516:ARG:HA | 1.72 | 0.71 |
| 5:E:36:THR:N | 5:E:39:GLU:OE2 | 2.16 | 0.70 |
| 9:I:109:ARG:HD3 | 9:I:124:THR:HG21 | 1.72 | 0.70 |
| 16:Q:799:VAL:O | 16:Q:802:LYS:NZ | 2.23 | 0.70 |
| 17:R:405:ILE:HG12 | 17:R:426:LEU:HD21 | 1.72 | 0.70 |
| 7:G:151:ARG:O | 7:G:158:PHE:N | 2.22 | 0.70 |
| 10:J:44:CYS:O | 10:J:47:ARG:NH1 | 2.25 | 0.70 |
| 1:A:77:ASN:OD1 | 1:A:78:MET:N | 2.25 | 0.70 |
| 16:Q:729:LYS:HE2 | 16:Q:732:LYS:HD2 | 1.72 | 0.70 |
| 1:A:244:ARG:HE | 1:A:245:PRO:HD2 | 1.57 | 0.70 |
| 3:C:74:THR:OG1 | 3:C:74:THR:O | 2.09 | 0.70 |
| 1:A:1372:GLU:OE2 | 5:E:195:ARG:NH1 | 2.25 | 0.70 |
| 7:G:110:ARG:HH21 | 7:G:118:GLU:HA | 1.56 | 0.70 |
| 9:I:42:CYS:SG | 9:I:43:ASP:N | 2.65 | 0.70 |
| 24:Z:563:MET:HA | 24:Z:637:VAL:HG11 | 1.73 | 0.70 |
| 24:Z:759:GLY:O | 24:Z:761:MET:N | 2.24 | 0.70 |
| 2:B:85:LEU:N | 2:B:131:THR:O | 2.25 | 0.70 |
| 1:A:100:LEU:HD23 | 1:A:193:ARG:HE | 1.57 | 0.69 |
| 19:U:450:LEU:HD21 | 19:U:452:LEU:HD23 | 1.73 | 0.69 |
| 4:D:37:VAL:HG21 | 7:G:2:PHE:CD2 | 2.27 | 0.69 |
| 1:A:357:LYS:NZ | 2:B:1112:ASP:OD1 | 2.26 | 0.69 |
| 1:A:686:THR:OG1 | 1:A:687:ILE:N | 2.25 | 0.69 |
| 16:Q:624:LYS:HG3 | 16:Q:627:ARG:NH2 | 2.07 | 0.69 |
| 5:E:97:GLU:HB2 | 5:E:99:ILE:HG12 | 1.74 | 0.69 |
| 13:M:1379:GLN:HG2 | 13:M:1469:PRO:HB2 | 1.73 | 0.69 |
| 17:R:428:LEU:HB2 | 17:R:437:PHE:CD2 | 2.27 | 0.69 |
| 21:W:231:HIS:HD1 | 21:W:235:VAL:HG22 | 1.57 | 0.69 |
| 24:Z:502:LEU:HG | 24:Z:511:LEU:HB3 | 1.75 | 0.69 |
| 2:B:1040:GLN:NE2 | 3:C:195:THR:OG1 | 2.25 | 0.69 |
| 7:G:91:GLN:HG2 | 7:G:93:ASN:HD21 | 1.58 | 0.69 |
| 24:Z:525:ALA:HB1 | 24:Z:552:ARG:HH22 | 1.58 | 0.69 |
| 1:A:917:GLU:OE2 | 1:A:921:ARG:NH1 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:M:1462:ILE:HD11 | 13:M:1472:PHE:HB3 | 1.74 | 0.69 |
| 21:W:113:ALA:HB3 | 21:W:122:ALA:HB3 | 1.74 | 0.69 |
| 1:A:999:ARG:NH2 | 8:H:103:GLU:OE2 | 2.24 | 0.69 |
| 4:D:34:ASN:O | 4:D:68:THR:OG1 | 2.09 | 0.69 |
| 17:R:564:ASN:HD21 | 20:V:136:TYR:C | 1.96 | 0.69 |
| 1:A:1212:LEU:HD21 | 1:A:1289:GLU:HB3 | 1.75 | 0.69 |
| 16:Q:752:VAL:HG22 | 16:Q:803:MET:HE2 | 1.75 | 0.69 |
| 24:Z:450:ILE:HG23 | 24:Z:452:PRO:HD3 | 1.74 | 0.69 |
| 5:E:2:ASP:OD2 | 5:E:4:GLU:N | 2.25 | 0.69 |
| 7:G:152:VAL:HG22 | 7:G:157:ILE:HG22 | 1.74 | 0.69 |
| 17:R:410:GLU:OE1 | 17:R:423:ASN:ND2 | 2.25 | 0.69 |
| 8:H:36:LYS:HG3 | 16:Q:709:ARG:HH22 | 1.57 | 0.68 |
| 17:R:366:ARG:NH1 | 24:Z:775:TPO:OG1 | 2.26 | 0.68 |
| 4:D:23:PRO:HG2 | 7:G:78:ARG:HH12 | 1.58 | 0.68 |
| 13:M:1488:THR:HB | 13:M:1495:ARG:HB3 | 1.75 | 0.68 |
| 17:R:570:TRP:HD1 | 20:V:133:LYS:HD2 | 1.57 | 0.68 |
| 20:V:192:GLN:HB2 | 20:V:197:PRO:HB3 | 1.74 | 0.68 |
| 13:M:1512:LYS:O | 13:M:1516:GLN:NE2 | 2.24 | 0.68 |
| 16:Q:886:LYS:O | 16:Q:890:MET:HG2 | 1.94 | 0.68 |
| 15:P:39:A:H3' | 15:P:40:A:C8 | 2.29 | 0.68 |
| 1:A:487:SER:OG | 1:A:673:GLN:NE2 | 2.26 | 0.68 |
| 24:Z:433:LEU:HB3 | 24:Z:436:LEU:HD12 | 1.75 | 0.68 |
| 24:Z:478:VAL:HG21 | 24:Z:502:LEU:HD22 | 1.74 | 0.68 |
| 21:W:289:ILE:HB | 21:W:301:TYR:HB2 | 1.74 | 0.68 |
| 16:Q:86:LEU:HD11 | 16:Q:116:LEU:HB3 | 1.76 | 0.68 |
| 7:G:123:SER:OG | 7:G:125:PRO:O | 2.11 | 0.68 |
| 16:Q:590:ARG:HA | 16:Q:593:LYS:HG3 | 1.76 | 0.67 |
| 2:B:633:LEU:HD11 | 2:B:679:PRO:HB2 | 1.76 | 0.67 |
| 2:B:649:ASN:HB2 | 19:U:460:TYR:OH | 1.93 | 0.67 |
| 6:F:86:GLU:OE2 | 6:F:95:LYS:NZ | 2.17 | 0.67 |
| 1:A:1212:LEU:HD12 | 1:A:1285:LEU:HD13 | 1.77 | 0.67 |
| 16:Q:394:ARG:HB3 | 16:Q:398:LYS:HE3 | 1.76 | 0.67 |
| 24:Z:419:ASN:OD1 | 24:Z:516:ARG:NH1 | 2.27 | 0.67 |
| 1:A:140:ARG:HH22 | 1:A:234:PHE:HD1 | 1.41 | 0.67 |
| 1:A:611:ASP:N | 1:A:611:ASP:OD1 | 2.25 | 0.67 |
| 1:A:1024:ASN:O | 5:E:162:ARG:NH2 | 2.28 | 0.67 |
| 5:E:82:VAL:HG22 | 5:E:86:THR:OG1 | 1.93 | 0.67 |
| 21:W:13:GLN:NE2 | 21:W:15:HIS:O | 2.27 | 0.67 |
| 17:R:406:THR:OG1 | 17:R:427:GLN:O | 2.11 | 0.67 |
| 1:A:112:PHE:O | 1:A:113:PHE:HB2 | 1.93 | 0.67 |
| 1:A:116:LYS:NZ | 1:A:184:CYS:SG | 2.66 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:22:TRP:CE2 | 2:B:679:PRO:HG3 | 2.30 | 0.67 |
| 2:B:565:THR:HG21 | 2:B:580:PRO:HB3 | 1.77 | 0.67 |
| 2:B:1136:GLU:HB2 | 2:B:1143:LYS:HG2 | 1.77 | 0.67 |
| 16:Q:484:GLU:HB3 | 16:Q:487:HIS:HB2 | 1.76 | 0.66 |
| 24:Z:295:TYR:H | 24:Z:304:SER:HG | 1.42 | 0.66 |
| 2:B:1157:LEU:O | 2:B:1161:GLU:HG3 | 1.95 | 0.66 |
| 4:D:128:GLN:NE2 | 4:D:132:ASP:OD1 | 2.27 | 0.66 |
| 24:Z:184:CYS:SG | 24:Z:185:LYS:N | 2.68 | 0.66 |
| 7:G:21:ASN:OD1 | 7:G:21:ASN:N | 2.23 | 0.66 |
| 7:G:109:SER:HB3 | 24:Z:493:VAL:HG21 | 1.77 | 0.66 |
| 19:U:474:ARG:H | 20:V:218:GLN:HA | 1.60 | 0.66 |
| 21:W:236:LEU:N | 21:W:250:SER:O | 2.27 | 0.66 |
| 21:W:292:VAL:HG12 | 21:W:298:ILE:HG12 | 1.76 | 0.66 |
| 1:A:200:ALA:HB3 | 1:A:214:ILE:HG12 | 1.78 | 0.66 |
| 14:N:37:DG:N2 | 18:T:12:DC:O2 | 2.26 | 0.66 |
| 1:A:413:TYR:O | 1:A:449:HIS:HD2 | 1.77 | 0.66 |
| 1:A:1118:THR:O | 1:A:1123:ARG:HB2 | 1.96 | 0.66 |
| 2:B:1003:ASN:O | 2:B:1005:ALA:N | 2.27 | 0.66 |
| 16:Q:534:TYR:OH | 16:Q:556:GLU:OE1 | 2.12 | 0.66 |
| 3:C:212:ASP:OD1 | 3:C:212:ASP:N | 2.28 | 0.66 |
| 13:M:1373:VAL:HG21 | 13:M:1379:GLN:HG3 | 1.76 | 0.66 |
| 21:W:66:GLY:O | 21:W:83:SER:OG | 2.11 | 0.66 |
| 1:A:539:GLN:NE2 | 2:B:790:GLN:O | 2.28 | 0.66 |
| 14:N:34:DC:H2'' | 14:N:35:DA:C8 | 2.30 | 0.66 |
| 16:Q:268:ASN:ND2 | 16:Q:271:VAL:H | 1.93 | 0.66 |
| 16:Q:420:GLN:O | 22:X:229:ARG:NH1 | 2.28 | 0.66 |
| 24:Z:613:GLU:O | 24:Z:625:HIS:N | 2.28 | 0.66 |
| 14:N:10:DG:H2'' | 14:N:11:DC:C5 | 2.30 | 0.66 |
| 21:W:46:VAL:HB | 21:W:58:TRP:HB2 | 1.77 | 0.66 |
| 2:B:354:SER:OG | 2:B:355:ASP:N | 2.26 | 0.65 |
| 3:C:154:ARG:HH11 | 10:J:63:ALA:HB2 | 1.61 | 0.65 |
| 21:W:130:VAL:HB | 21:W:144:LEU:HD12 | 1.78 | 0.65 |
| 6:F:105:ILE:HD12 | 6:F:117:ASP:HB3 | 1.78 | 0.65 |
| 11:K:13:PHE:HB2 | 11:K:16:GLU:HG3 | 1.77 | 0.65 |
| 16:Q:494:ALA:HB1 | 22:X:224:ILE:HG12 | 1.78 | 0.65 |
| 17:R:494:GLU:HA | 17:R:497:LYS:HD2 | 1.79 | 0.65 |
| 23:Y:4:GLU:O | 23:Y:27:GLN:NE2 | 2.29 | 0.65 |
| 5:E:27:LEU:O | 16:Q:877:GLN:NE2 | 2.29 | 0.65 |
| 5:E:41:LYS:NZ | 5:E:46:ASP:OD1 | 2.19 | 0.65 |
| 5:E:93:ARG:HA | 5:E:96:GLU:OE1 | 1.97 | 0.65 |
| 14:N:30:DC:N3 | 18:T:19:DG:N2 | 2.37 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:342:LEU:HD11 | 20:V:67:GLU:HG2 | 1.78 | 0.65 |
| 16:Q:86:LEU:HG | 16:Q:120:ALA:HB2 | 1.76 | 0.65 |
| 2:B:1071:ASN:O | 2:B:1073:GLN:N | 2.29 | 0.65 |
| 14:N:30:DC:N4 | 18:T:19:DG:H1 | 1.93 | 0.65 |
| 16:Q:211:LEU:HD12 | 16:Q:213:LYS:HZ1 | 1.62 | 0.65 |
| 1:A:1184:THR:C | 1:A:1186:VAL:H | 2.00 | 0.65 |
| 8:H:72:ASP:OD1 | 8:H:73:GLY:N | 2.29 | 0.65 |
| 21:W:218:ASP:N | 21:W:223:ASN:O | 2.29 | 0.65 |
| 23:Y:14:ARG:HH21 | 23:Y:54:SER:HA | 1.61 | 0.65 |
| 24:Z:539:LEU:HD22 | 24:Z:616:HIS:HB3 | 1.79 | 0.65 |
| 21:W:195:SER:OG | 21:W:236:LEU:O | 2.15 | 0.65 |
| 1:A:419:ILE:HG23 | 1:A:427:ILE:HB | 1.79 | 0.65 |
| 16:Q:856:LEU:HD23 | 16:Q:857:LEU:HD22 | 1.78 | 0.65 |
| 24:Z:558:PHE:N | 24:Z:570:VAL:O | 2.30 | 0.65 |
| 2:B:223:SER:OG | 2:B:350:HIS:ND1 | 2.26 | 0.64 |
| 16:Q:605:LEU:O | 16:Q:609:ASN:ND2 | 2.30 | 0.64 |
| 5:E:71:GLN:HB2 | 5:E:99:ILE:HG22 | 1.78 | 0.64 |
| 16:Q:568:TRP:CZ3 | 16:Q:592:LEU:HB2 | 2.32 | 0.64 |
| 20:V:45:ASP:N | 20:V:45:ASP:OD1 | 2.30 | 0.64 |
| 24:Z:470:LYS:NZ | 24:Z:518:LEU:O | 2.31 | 0.64 |
| 4:D:76:ASN:HD21 | 4:D:78:GLU:HB2 | 1.61 | 0.64 |
| 5:E:113:SER:OG | 14:N:40:DG:OP1 | 2.15 | 0.64 |
| 1:A:609:HIS:ND1 | 1:A:626:THR:OG1 | 2.13 | 0.64 |
| 21:W:214:ILE:HB | 21:W:228:LEU:HB3 | 1.78 | 0.64 |
| 24:Z:282:LYS:O | 24:Z:287:LYS:NZ | 2.28 | 0.64 |
| 17:R:569:GLU:O | 17:R:573:VAL:HG23 | 1.97 | 0.64 |
| 20:V:48:PHE:HB2 | 22:X:229:ARG:HB2 | 1.78 | 0.64 |
| 1:A:329:MET:HA | 1:A:335:PRO:HA | 1.80 | 0.64 |
| 1:A:1140:THR:OG1 | 1:A:1140:THR:O | 2.12 | 0.64 |
| 2:B:100:GLU:OE1 | 2:B:100:GLU:N | 2.24 | 0.64 |
| 7:G:153:ASP:N | 7:G:156:ASP:O | 2.23 | 0.64 |
| 21:W:26:THR:HG23 | 21:W:284:GLY:HA2 | 1.80 | 0.64 |
| 16:Q:710:LYS:HB2 | 16:Q:712:TYR:CD1 | 2.32 | 0.64 |
| 2:B:497:LYS:HG3 | 2:B:498:PRO:HD3 | 1.80 | 0.64 |
| 14:N:31:DC:H2" | 14:N:32:DA:C8 | 2.32 | 0.64 |
| 2:B:577:HIS:NE2 | 2:B:583:LEU:HD11 | 2.13 | 0.64 |
| 24:Z:519:GLN:NE2 | 24:Z:521:CYS:SG | 2.71 | 0.64 |
| 1:A:376:ASP:CG | 1:A:473:ARG:HH21 | 2.01 | 0.63 |
| 17:R:355:LEU:HG | 17:R:357:GLU:H | 1.62 | 0.63 |
| 2:B:787:GLY:O | 2:B:790:GLN:HG3 | 1.98 | 0.63 |
| 21:W:92:ASP:HB3 | 21:W:95:ASN:OD1 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:59:VAL:HG23 | 2:B:408:PHE:CZ | 2.33 | 0.63 |
| 2:B:184:TYR:CE2 | 2:B:191:GLU:HG2 | 2.33 | 0.63 |
| 3:C:2:PRO:HB3 | 11:K:54:PRO:HD2 | 1.79 | 0.63 |
| 14:N:38:DG:H2'' | 14:N:39:DA:C8 | 2.34 | 0.63 |
| 1:A:1540:THR:HG23 | 13:M:1479:ARG:HE | 1.62 | 0.63 |
| 2:B:93:LEU:O | 19:U:507:THR:HA | 1.99 | 0.63 |
| 8:H:2:ALA:C | 8:H:84:ARG:HH22 | 2.02 | 0.63 |
| 16:Q:123:ILE:HG13 | 16:Q:124:ILE:HG12 | 1.80 | 0.63 |
| 16:Q:398:LYS:O | 16:Q:402:LYS:HD3 | 1.99 | 0.63 |
| 2:B:310:VAL:HG23 | 2:B:311:ILE:HD12 | 1.81 | 0.63 |
| 18:T:38:DG:H2'' | 18:T:39:DC:C5 | 2.33 | 0.63 |
| 21:W:48:LYS:N | 21:W:55:ASP:O | 2.27 | 0.63 |
| 5:E:166:ARG:NH2 | 5:E:168:ASN:HD22 | 1.95 | 0.63 |
| 7:G:36:GLY:O | 24:Z:628:LYS:NZ | 2.23 | 0.63 |
| 8:H:8:ASP:OD1 | 8:H:32:SER:OG | 2.05 | 0.63 |
| 17:R:355:LEU:HD12 | 17:R:356:PRO:HD2 | 1.81 | 0.63 |
| 17:R:404:GLU:OE1 | 17:R:455:TRP:NE1 | 2.32 | 0.63 |
| 24:Z:733:ARG:NH1 | 24:Z:744:SER:OG | 2.31 | 0.63 |
| 8:H:30:CYS:HG | 8:H:56:PHE:HZ | 1.47 | 0.63 |
| 16:Q:286:SER:O | 16:Q:290:HIS:ND1 | 2.32 | 0.63 |
| 16:Q:611:TRP:HE1 | 16:Q:628:HIS:HA | 1.63 | 0.63 |
| 2:B:67:LEU:H | 2:B:83:ARG:HB2 | 1.64 | 0.63 |
| 16:Q:239:ALA:HB2 | 16:Q:257:LEU:HB3 | 1.81 | 0.63 |
| 1:A:694:ALA:HB3 | 1:A:699:TYR:CE1 | 2.34 | 0.62 |
| 16:Q:576:LEU:HD21 | 16:Q:585:GLN:HE22 | 1.64 | 0.62 |
| 16:Q:128:GLN:HE22 | 20:V:86:LEU:HD13 | 1.64 | 0.62 |
| 16:Q:835:ASP:OD1 | 16:Q:839:ARG:NE | 2.32 | 0.62 |
| 21:W:206:VAL:HG11 | 21:W:238:VAL:HG21 | 1.81 | 0.62 |
| 5:E:64:HIS:N | 5:E:70:ASP:O | 2.31 | 0.62 |
| 1:A:481:THR:O | 1:A:483:ARG:NH1 | 2.32 | 0.62 |
| 4:D:114:LEU:HD21 | 7:G:167:TYR:HB2 | 1.80 | 0.62 |
| 4:D:135:GLN:OE1 | 4:D:138:ARG:NH1 | 2.32 | 0.62 |
| 1:A:381:PRO:HB3 | 1:A:480:SER:HA | 1.81 | 0.62 |
| 1:A:922:PHE:H | 1:A:1052:ARG:HH11 | 1.48 | 0.62 |
| 8:H:110:THR:O | 8:H:129:ALA:N | 2.32 | 0.62 |
| 11:K:5:PRO:HG2 | 11:K:8:GLU:HG3 | 1.81 | 0.62 |
| 1:A:556:GLU:OE1 | 1:A:556:GLU:N | 2.33 | 0.62 |
| 2:B:100:GLU:HA | 2:B:105:PRO:HG3 | 1.82 | 0.62 |
| 5:E:55:ARG:HB2 | 5:E:78:GLU:HG3 | 1.82 | 0.62 |
| 5:E:56:THR:OG1 | 5:E:78:GLU:OE2 | 2.11 | 0.62 |
| 9:I:35:LEU:HD21 | 9:I:53:ILE:HD11 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:67:LEU:HG | 2:B:84:TYR:OH | 2.00 | 0.62 |
| 1:A:1016:LEU:HD22 | 1:A:1069:LEU:HD22 | 1.82 | 0.62 |
| 16:Q:394:ARG:HD2 | 16:Q:421:ILE:HG23 | 1.82 | 0.62 |
| 16:Q:849:LYS:O | 16:Q:852:LEU:HG | 2.00 | 0.62 |
| 24:Z:506:LEU:HD11 | 24:Z:552:ARG:HH21 | 1.63 | 0.62 |
| 8:H:83:SER:OG | 8:H:84:ARG:N | 2.33 | 0.62 |
| 9:I:12:VAL:HG21 | 9:I:53:ILE:O | 2.00 | 0.62 |
| 21:W:206:VAL:HG22 | 21:W:216:ILE:HG12 | 1.81 | 0.62 |
| 8:H:32:SER:OG | 8:H:33:GLU:N | 2.33 | 0.61 |
| 12:L:56:ASP:O | 12:L:58:ARG:N | 2.33 | 0.61 |
| 17:R:564:ASN:OD1 | 20:V:136:TYR:N | 2.29 | 0.61 |
| 1:A:797:ARG:NH2 | 1:A:815:TYR:O | 2.32 | 0.61 |
| 1:A:876:ASP:HB3 | 1:A:878:THR:HG22 | 1.82 | 0.61 |
| 5:E:39:GLU:OE1 | 5:E:39:GLU:N | 2.24 | 0.61 |
| 8:H:2:ALA:O | 8:H:84:ARG:NH2 | 2.30 | 0.61 |
| 16:Q:86:LEU:HD12 | 16:Q:89:LEU:HB2 | 1.80 | 0.61 |
| 1:A:30:GLU:HA | 1:A:33:ARG:HE | 1.63 | 0.61 |
| 1:A:200:ALA:HB2 | 1:A:216:LEU:HD21 | 1.81 | 0.61 |
| 1:A:1468:THR:H | 6:F:60:TYR:HB3 | 1.66 | 0.61 |
| 2:B:19:PRO:O | 2:B:21:LEU:N | 2.32 | 0.61 |
| 16:Q:249:ASP:O | 16:Q:253:ASN:ND2 | 2.33 | 0.61 |
| 17:R:364:LEU:HB2 | 17:R:387:VAL:HG12 | 1.81 | 0.61 |
| 24:Z:366:TYR:O | 24:Z:373:PHE:N | 2.28 | 0.61 |
| 2:B:765:GLU:OE1 | 2:B:770:ARG:NE | 2.34 | 0.61 |
| 16:Q:715:GLN:HB2 | 16:Q:746:VAL:HG11 | 1.83 | 0.61 |
| 20:V:110:GLU:HG3 | 20:V:111:GLU:N | 2.14 | 0.61 |
| 1:A:88:ILE:O | 1:A:90:LEU:N | 2.33 | 0.61 |
| 16:Q:38:HIS:HE1 | 16:Q:73:LEU:HD13 | 1.66 | 0.61 |
| 16:Q:68:ARG:HE | 16:Q:89:LEU:HD12 | 1.65 | 0.61 |
| 24:Z:390:LEU:HD12 | 24:Z:393:LEU:HD12 | 1.82 | 0.61 |
| 1:A:1303:GLN:O | 1:A:1340:GLY:HA3 | 2.01 | 0.61 |
| 3:C:190:ASN:ND2 | 3:C:195:THR:O | 2.20 | 0.61 |
| 16:Q:862:GLU:HA | 16:Q:865:LEU:HG | 1.82 | 0.61 |
| 2:B:228:SER:O | 2:B:405:ARG:NH1 | 2.34 | 0.61 |
| 3:C:91:GLU:OE1 | 24:Z:713:SER:HB2 | 2.01 | 0.61 |
| 5:E:45:GLY:HA3 | 5:E:53:PRO:HD3 | 1.82 | 0.61 |
| 16:Q:729:LYS:HB2 | 16:Q:732:LYS:HD2 | 1.82 | 0.61 |
| 1:A:47:THR:HA | 1:A:52:PRO:HA | 1.81 | 0.61 |
| 1:A:1244:ASN:HB2 | 1:A:1262:MET:HE1 | 1.81 | 0.61 |
| 1:A:1481:LYS:O | 13:M:1384:ARG:NH1 | 2.34 | 0.61 |
| 2:B:144:HIS:CD2 | 2:B:431:LEU:HD21 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:158:GLN:HG3 | 16:Q:159:SER:H | 1.66 | 0.61 |
| 1:A:1301:ILE:HG22 | 1:A:1345:ARG:HH21 | 1.65 | 0.60 |
| 16:Q:379:LYS:HZ1 | 20:V:61:TYR:HE2 | 1.47 | 0.60 |
| 21:W:26:THR:HA | 21:W:284:GLY:HA2 | 1.83 | 0.60 |
| 1:A:222:HIS:HB2 | 1:A:249:ILE:HD11 | 1.82 | 0.60 |
| 16:Q:646:ASN:HA | 22:X:239:GLN:HA | 1.82 | 0.60 |
| 20:V:196:LYS:O | 20:V:198:ARG:HG3 | 2.01 | 0.60 |
| 21:W:53:ARG:NH1 | 21:W:54:LEU:O | 2.34 | 0.60 |
| 23:Y:66:PRO:HB2 | 23:Y:78:SER:HA | 1.82 | 0.60 |
| 24:Z:554:GLU:OE1 | 24:Z:557:THR:OG1 | 2.18 | 0.60 |
| 7:G:151:ARG:HB3 | 7:G:158:PHE:O | 2.01 | 0.60 |
| 4:D:48:ASN:HD22 | 4:D:57:LEU:HG | 1.66 | 0.60 |
| 16:Q:65:GLU:OE1 | 16:Q:93:TYR:OH | 2.15 | 0.60 |
| 1:A:123:ASN:O | 1:A:127:LYS:HG2 | 2.02 | 0.60 |
| 16:Q:80:LYS:O | 16:Q:83:MET:HG3 | 2.01 | 0.60 |
| 16:Q:222:SER:O | 16:Q:226:GLU:HG2 | 2.01 | 0.60 |
| 21:W:27:ASN:O | 21:W:32:SER:OG | 2.19 | 0.60 |
| 6:F:114:SER:OG | 6:F:115:TYR:N | 2.33 | 0.60 |
| 16:Q:163:ILE:HG21 | 16:Q:189:ALA:HA | 1.83 | 0.60 |
| 16:Q:313:ALA:HB2 | 16:Q:328:TYR:HB2 | 1.83 | 0.60 |
| 23:Y:19:CYS:SG | 23:Y:21:LEU:HB2 | 2.42 | 0.60 |
| 3:C:55:ASN:ND2 | 3:C:60:HIS:O | 2.34 | 0.60 |
| 16:Q:48:ALA:HB2 | 16:Q:63:LEU:HD11 | 1.84 | 0.60 |
| 16:Q:65:GLU:HA | 16:Q:89:LEU:HD11 | 1.82 | 0.60 |
| 21:W:176:ASP:HB2 | 21:W:183:LEU:HD11 | 1.83 | 0.60 |
| 1:A:760:LEU:HD22 | 1:A:764:ASN:ND2 | 2.16 | 0.60 |
| 20:V:233:VAL:O | 20:V:238:PRO:N | 2.35 | 0.60 |
| 2:B:784:SER:O | 2:B:784:SER:OG | 2.14 | 0.60 |
| 10:J:36:ASP:OD1 | 10:J:36:ASP:N | 2.28 | 0.60 |
| 21:W:125:THR:OG1 | 21:W:131:ASN:ND2 | 2.34 | 0.60 |
| 1:A:217:SER:OG | 1:A:220:ARG:N | 2.35 | 0.60 |
| 5:E:45:GLY:CA | 5:E:53:PRO:HD3 | 2.32 | 0.60 |
| 16:Q:581:TRP:O | 16:Q:585:GLN:HB2 | 2.02 | 0.60 |
| 16:Q:620:ARG:HG3 | 16:Q:625:GLU:HB2 | 1.84 | 0.60 |
| 24:Z:629:LEU:HB2 | 24:Z:634:GLY:HA2 | 1.83 | 0.60 |
| 1:A:894:ASP:OD2 | 1:A:1396:ARG:NH2 | 2.35 | 0.59 |
| 1:A:1222:THR:O | 1:A:1225:LYS:N | 2.34 | 0.59 |
| 3:C:189:ASP:O | 3:C:191:ALA:N | 2.34 | 0.59 |
| 1:A:1210:TRP:CZ2 | 1:A:1281:ASP:HB3 | 2.37 | 0.59 |
| 4:D:60:VAL:HA | 4:D:63:LYS:HG2 | 1.82 | 0.59 |
| 7:G:109:SER:HB2 | 24:Z:503:PHE:CZ | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:690:CYS:O | 2:B:691:SER:OG | 2.21 | 0.59 |
| 2:B:743:ARG:NH1 | 2:B:745:ASP:OD1 | 2.35 | 0.59 |
| 16:Q:351:TYR:HB2 | 16:Q:360:ALA:HB2 | 1.83 | 0.59 |
| 16:Q:708:LEU:HD21 | 16:Q:719:VAL:HG21 | 1.83 | 0.59 |
| 1:A:1128:ILE:HG23 | 1:A:1414:ILE:HB | 1.84 | 0.59 |
| 11:K:49:GLN:NE2 | 11:K:93:ASP:OD2 | 2.34 | 0.59 |
| 1:A:64:VAL:HG11 | 1:A:78:MET:HA | 1.84 | 0.59 |
| 24:Z:365:ARG:HD3 | 24:Z:374:LYS:HD2 | 1.84 | 0.59 |
| 24:Z:499:PHE:HD1 | 24:Z:512:LYS:HB3 | 1.67 | 0.59 |
| 16:Q:776:LEU:O | 16:Q:779:VAL:HG22 | 2.03 | 0.59 |
| 1:A:379:GLY:HA2 | 1:A:475:ARG:O | 2.02 | 0.59 |
| 1:A:1231:ILE:O | 1:A:1235:ILE:HB | 2.03 | 0.59 |
| 2:B:650:ASN:N | 2:B:650:ASN:OD1 | 2.36 | 0.59 |
| 3:C:60:HIS:HB2 | 3:C:63:PHE:HB2 | 1.83 | 0.59 |
| 16:Q:371:TYR:HE2 | 16:Q:373:ASN:HD21 | 1.51 | 0.59 |
| 16:Q:505:ARG:NH2 | 20:V:44:PHE:HB2 | 2.12 | 0.59 |
| 16:Q:419:ALA:HB2 | 16:Q:433:ALA:HB3 | 1.83 | 0.59 |
| 1:A:620:HIS:O | 8:H:97:TYR:OH | 2.15 | 0.59 |
| 1:A:1004:LEU:HD13 | 1:A:1062:GLY:HA2 | 1.85 | 0.59 |
| 16:Q:201:ARG:HH12 | 16:Q:227:LEU:HD13 | 1.68 | 0.59 |
| 1:A:1005:HIS:HD2 | 1:A:1007:ILE:H | 1.49 | 0.59 |
| 2:B:177:CYS:SG | 2:B:180:ASP:N | 2.74 | 0.59 |
| 4:D:103:LEU:O | 7:G:144:ARG:NH2 | 2.36 | 0.59 |
| 16:Q:24:LEU:HD11 | 16:Q:56:LYS:HZ3 | 1.68 | 0.59 |
| 16:Q:624:LYS:HA | 16:Q:627:ARG:HH21 | 1.67 | 0.59 |
| 15:P:39:A:C2 | 15:P:40:A:C5 | 2.91 | 0.58 |
| 21:W:8:LEU:N | 21:W:300:ILE:O | 2.30 | 0.58 |
| 1:A:476:ILE:O | 1:A:476:ILE:HG13 | 2.00 | 0.58 |
| 2:B:912:ASN:OD1 | 2:B:912:ASN:N | 2.26 | 0.58 |
| 9:I:17:CYS:N | 9:I:22:ASN:O | 2.27 | 0.58 |
| 14:N:11:DC:H2" | 14:N:12:DG:C8 | 2.38 | 0.58 |
| 16:Q:884:LYS:O | 16:Q:887:ASN:N | 2.34 | 0.58 |
| 16:Q:774:SER:H | 16:Q:830:ARG:NH1 | 1.99 | 0.58 |
| 17:R:574:GLU:HA | 17:R:577:LYS:HG2 | 1.84 | 0.58 |
| 2:B:565:THR:HA | 2:B:610:ARG:HB3 | 1.86 | 0.58 |
| 5:E:93:ARG:HB2 | 16:Q:891:PHE:CE1 | 2.38 | 0.58 |
| 8:H:63:THR:HG21 | 8:H:68:GLY:HA2 | 1.85 | 0.58 |
| 8:H:78:THR:O | 8:H:78:THR:OG1 | 2.21 | 0.58 |
| 17:R:353:VAL:HG12 | 17:R:469:LEU:HD13 | 1.86 | 0.58 |
| 19:U:445:ASP:OD2 | 19:U:447:SER:OG | 2.19 | 0.58 |
| 1:A:202:TRP:CE3 | 1:A:212:LYS:HB2 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1052:ARG:NE | 1:A:1056:GLU:OE2 | 2.36 | 0.58 |
| 15:P:37:G:HO2' | 15:P:38:G:H8 | 1.52 | 0.58 |
| 20:V:88:ASN:OD1 | 20:V:89:PRO:HD3 | 2.04 | 0.58 |
| 24:Z:562:ASN:HD21 | 24:Z:566:LYS:HG3 | 1.67 | 0.58 |
| 1:A:367:ILE:HA | 1:A:482:PHE:O | 2.04 | 0.58 |
| 1:A:394:VAL:HG23 | 1:A:444:TYR:O | 2.04 | 0.58 |
| 2:B:743:ARG:HB3 | 2:B:743:ARG:HH11 | 1.69 | 0.58 |
| 5:E:66:ASP:OD1 | 5:E:67:ASP:N | 2.36 | 0.58 |
| 17:R:363:ARG:NH2 | 17:R:365:SER:OG | 2.36 | 0.58 |
| 1:A:11:SER:O | 2:B:1135:TYR:OH | 2.14 | 0.58 |
| 1:A:370:ASP:OD2 | 11:K:65:HIS:NE2 | 2.36 | 0.58 |
| 2:B:577:HIS:CD2 | 2:B:583:LEU:HD11 | 2.38 | 0.58 |
| 2:B:646:ARG:C | 2:B:648:TYR:H | 2.07 | 0.58 |
| 1:A:552:ASP:OD1 | 8:H:24:ARG:NH1 | 2.37 | 0.58 |
| 2:B:83:ARG:O | 2:B:83:ARG:NH2 | 2.37 | 0.58 |
| 1:A:1190:GLN:O | 1:A:1193:VAL:HG12 | 2.04 | 0.58 |
| 1:A:1244:ASN:HB2 | 1:A:1262:MET:CE | 2.34 | 0.58 |
| 4:D:46:GLN:HA | 4:D:49:GLU:CD | 2.24 | 0.58 |
| 13:M:1356:ILE:HG22 | 13:M:1370:THR:HB | 1.85 | 0.58 |
| 15:P:37:G:O2' | 15:P:38:G:H8 | 1.86 | 0.58 |
| 15:P:38:G:H2' | 15:P:39:A:C8 | 2.35 | 0.58 |
| 16:Q:95:GLN:NE2 | 20:V:84:ILE:O | 2.37 | 0.58 |
| 17:R:493:GLU:OE1 | 17:R:493:GLU:N | 2.22 | 0.58 |
| 2:B:715:ASP:OD1 | 2:B:715:ASP:N | 2.19 | 0.58 |
| 24:Z:416:ARG:HE | 24:Z:466:GLN:HE21 | 1.52 | 0.57 |
| 2:B:1115:GLN:HG2 | 2:B:1150:ARG:HG2 | 1.86 | 0.57 |
| 16:Q:156:LEU:HD11 | 16:Q:169:LYS:HE2 | 1.87 | 0.57 |
| 16:Q:504:ALA:HB2 | 16:Q:519:LEU:HB3 | 1.86 | 0.57 |
| 17:R:407:GLY:H | 17:R:427:GLN:HB3 | 1.69 | 0.57 |
| 24:Z:424:ASP:HB2 | 24:Z:440:ILE:HD12 | 1.84 | 0.57 |
| 1:A:1177:TYR:OH | 1:A:1282:ASP:HA | 2.04 | 0.57 |
| 2:B:721:ARG:NH1 | 2:B:940:GLY:O | 2.36 | 0.57 |
| 5:E:90:TYR:HA | 16:Q:891:PHE:HZ | 1.69 | 0.57 |
| 1:A:392:GLU:HG2 | 1:A:402:LEU:HD11 | 1.86 | 0.57 |
| 1:A:699:TYR:O | 1:A:703:GLN:HG2 | 2.05 | 0.57 |
| 2:B:235:ILE:HG13 | 2:B:348:LEU:HD13 | 1.85 | 0.57 |
| 7:G:37:THR:HA | 24:Z:628:LYS:NZ | 2.20 | 0.57 |
| 11:K:63:VAL:HG22 | 11:K:71:ILE:HG22 | 1.86 | 0.57 |
| 7:G:122:ASN:OD1 | 7:G:123:SER:N | 2.38 | 0.57 |
| 16:Q:384:LEU:HG | 16:Q:386:ALA:H | 1.69 | 0.57 |
| 24:Z:280:ARG:HH21 | 24:Z:288:ASP:HB3 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:823:VAL:HG22 | 1:A:835:GLU:HB2 | 1.86 | 0.57 |
| 21:W:27:ASN:HB2 | 21:W:31:ASN:HD21 | 1.70 | 0.57 |
| 24:Z:192:THR:HG23 | 24:Z:245:LEU:HD21 | 1.85 | 0.57 |
| 1:A:96:HIS:HD2 | 1:A:99:PHE:CD2 | 2.23 | 0.57 |
| 1:A:546:ARG:HG2 | 1:A:546:ARG:O | 2.04 | 0.57 |
| 1:A:1146:GLN:NE2 | 1:A:1150:ASP:OD2 | 2.36 | 0.57 |
| 1:A:1484:MET:HB2 | 13:M:1362:LYS:HE3 | 1.87 | 0.57 |
| 11:K:39:ASP:OD1 | 11:K:39:ASP:N | 2.35 | 0.57 |
| 16:Q:474:PHE:HB2 | 16:Q:503:LEU:HD13 | 1.85 | 0.57 |
| 1:A:628:VAL:HA | 1:A:638:GLY:HA3 | 1.87 | 0.57 |
| 1:A:962:ASP:CG | 1:A:1046:ARG:HH21 | 2.08 | 0.57 |
| 16:Q:208:PHE:HD1 | 16:Q:213:LYS:HD2 | 1.70 | 0.57 |
| 21:W:48:LYS:HB2 | 21:W:57:GLN:HB2 | 1.85 | 0.57 |
| 1:A:282:ASP:HB3 | 1:A:313:HIS:CE1 | 2.39 | 0.57 |
| 1:A:1146:GLN:OE1 | 1:A:1153:ARG:HD3 | 2.05 | 0.57 |
| 20:V:55:GLN:OE1 | 20:V:57:ARG:NE | 2.35 | 0.57 |
| 24:Z:450:ILE:HG21 | 24:Z:468:LEU:HD11 | 1.86 | 0.57 |
| 1:A:92:LYS:HD2 | 1:A:307:VAL:HG11 | 1.87 | 0.56 |
| 1:A:117:LEU:HG | 1:A:232:GLU:OE2 | 2.05 | 0.56 |
| 21:W:152:LEU:HD12 | 21:W:168:ILE:HA | 1.85 | 0.56 |
| 1:A:1005:HIS:CD2 | 1:A:1007:ILE:H | 2.23 | 0.56 |
| 3:C:4:ALA:HB2 | 11:K:93:ASP:HB2 | 1.86 | 0.56 |
| 16:Q:188:LYS:HB3 | 16:Q:191:ARG:HH11 | 1.70 | 0.56 |
| 16:Q:678:ALA:O | 16:Q:684:TRP:NE1 | 2.38 | 0.56 |
| 17:R:560:ILE:HA | 17:R:563:ILE:HG22 | 1.87 | 0.56 |
| 24:Z:501:ILE:HD11 | 24:Z:510:GLU:HB3 | 1.87 | 0.56 |
| 1:A:140:ARG:NH2 | 1:A:234:PHE:HD1 | 2.03 | 0.56 |
| 1:A:299:ALA:O | 1:A:301:HIS:N | 2.39 | 0.56 |
| 1:A:538:VAL:O | 1:A:538:VAL:HG12 | 2.06 | 0.56 |
| 1:A:809:HIS:HE1 | 2:B:506:TRP:CZ2 | 2.23 | 0.56 |
| 2:B:177:CYS:HB2 | 2:B:738:THR:OG1 | 2.06 | 0.56 |
| 2:B:995:GLU:OE1 | 20:V:131:MET:HB3 | 2.05 | 0.56 |
| 5:E:55:ARG:O | 5:E:56:THR:OG1 | 2.23 | 0.56 |
| 13:M:1505:ASN:O | 13:M:1509:ARG:HG2 | 2.05 | 0.56 |
| 2:B:285:LEU:HD23 | 9:I:16:PHE:HZ | 1.70 | 0.56 |
| 7:G:110:ARG:HH12 | 7:G:115:SER:HA | 1.69 | 0.56 |
| 14:N:12:DG:H2" | 14:N:13:DG:H8 | 1.70 | 0.56 |
| 21:W:68:VAL:HG13 | 21:W:83:SER:HA | 1.87 | 0.56 |
| 9:I:25:TYR:O | 9:I:37:TYR:HA | 2.04 | 0.56 |
| 18:T:33:DC:H2" | 18:T:34:DT:OP1 | 2.04 | 0.56 |
| 20:V:61:TYR:N | 20:V:62:LYS:HA | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:U:384:VAL:HA | 19:U:418:ASN:HB3 | 1.86 | 0.56 |
| 1:A:353:ASN:OD1 | 2:B:1071:ASN:ND2 | 2.39 | 0.56 |
| 2:B:897:ARG:HB2 | 2:B:900:GLU:HG3 | 1.88 | 0.56 |
| 16:Q:802:LYS:HE2 | 16:Q:807:LEU:HB2 | 1.87 | 0.56 |
| 23:Y:14:ARG:NH1 | 23:Y:55:SER:OG | 2.39 | 0.56 |
| 1:A:886:VAL:HG12 | 5:E:169:GLN:O | 2.06 | 0.56 |
| 1:A:1370:GLY:O | 1:A:1374:VAL:HG23 | 2.06 | 0.56 |
| 15:P:39:A:C3' | 15:P:40:A:C8 | 2.87 | 0.56 |
| 16:Q:777:LYS:HE3 | 16:Q:781:ASN:HD21 | 1.71 | 0.56 |
| 19:U:395:GLU:HA | 20:V:172:ARG:HH21 | 1.71 | 0.56 |
| 24:Z:478:VAL:HG11 | 24:Z:492:ILE:HG23 | 1.87 | 0.56 |
| 1:A:1211:LEU:HD12 | 1:A:1213:ARG:N | 2.21 | 0.56 |
| 1:A:1234:LYS:HE2 | 1:A:1298:LEU:HA | 1.87 | 0.56 |
| 2:B:639:HIS:O | 2:B:643:LEU:HB2 | 2.06 | 0.56 |
| 4:D:104:CYS:HB3 | 4:D:135:GLN:HE22 | 1.70 | 0.56 |
| 17:R:415:TYR:CZ | 17:R:438:ARG:HB3 | 2.41 | 0.56 |
| 24:Z:420:PHE:HB3 | 24:Z:440:ILE:HD13 | 1.88 | 0.56 |
| 2:B:218:THR:HG23 | 2:B:238:SER:HB3 | 1.88 | 0.56 |
| 2:B:1129:ASN:HB3 | 2:B:1134:THR:HG22 | 1.87 | 0.56 |
| 18:T:12:DC:H2'' | 18:T:13:DC:H5' | 1.88 | 0.56 |
| 20:V:127:VAL:HG23 | 20:V:128:VAL:H | 1.71 | 0.56 |
| 21:W:163:LEU:O | 21:W:175:PHE:N | 2.34 | 0.56 |
| 1:A:469:MET:HG3 | 2:B:1093:CYS:SG | 2.46 | 0.55 |
| 3:C:60:HIS:HB2 | 3:C:63:PHE:H | 1.71 | 0.55 |
| 14:N:39:DA:H2'' | 14:N:40:DG:O4' | 2.07 | 0.55 |
| 20:V:95:ASP:OD1 | 20:V:95:ASP:N | 2.39 | 0.55 |
| 1:A:1302:GLU:OE1 | 1:A:1302:GLU:N | 2.38 | 0.55 |
| 2:B:866:ILE:HG22 | 2:B:867:ILE:HG13 | 1.87 | 0.55 |
| 21:W:81:SER:HB3 | 21:W:91:TRP:NE1 | 2.20 | 0.55 |
| 21:W:112:LEU:HD22 | 21:W:121:LEU:HD21 | 1.87 | 0.55 |
| 24:Z:472:PHE:HB3 | 24:Z:476:ASP:OD2 | 2.06 | 0.55 |
| 2:B:588:ARG:O | 2:B:592:ARG:HD3 | 2.07 | 0.55 |
| 17:R:492:ILE:O | 17:R:496:VAL:HG13 | 2.07 | 0.55 |
| 21:W:9:PHE:HB3 | 21:W:300:ILE:CG1 | 2.35 | 0.55 |
| 24:Z:364:ASN:O | 24:Z:374:LYS:NZ | 2.39 | 0.55 |
| 1:A:760:LEU:HD13 | 1:A:764:ASN:HD22 | 1.71 | 0.55 |
| 2:B:789:ASN:HB3 | 2:B:795:ILE:HG13 | 1.88 | 0.55 |
| 16:Q:302:GLU:HG3 | 16:Q:305:GLN:NE2 | 2.20 | 0.55 |
| 17:R:592:ASP:O | 17:R:594:PHE:N | 2.37 | 0.55 |
| 1:A:365:THR:HG22 | 1:A:366:VAL:H | 1.70 | 0.55 |
| 7:G:118:GLU:O | 7:G:128:TYR:HA | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:W:108:ASP:HA | 21:W:126:HIS:CE1 | 2.41 | 0.55 |
| 2:B:279:VAL:HG23 | 2:B:312:GLN:O | 2.06 | 0.55 |
| 4:D:74:PHE:HE2 | 4:D:80:ILE:HG12 | 1.72 | 0.55 |
| 16:Q:451:PRO:HD3 | 16:Q:480:ARG:HG3 | 1.88 | 0.55 |
| 16:Q:772:GLU:HA | 16:Q:773:LYS:HB2 | 1.88 | 0.55 |
| 24:Z:542:LEU:HD22 | 24:Z:570:VAL:HG11 | 1.87 | 0.55 |
| 1:A:528:PRO:HB3 | 1:A:899:GLU:HG3 | 1.87 | 0.55 |
| 17:R:363:ARG:NE | 17:R:446:GLU:HA | 2.21 | 0.55 |
| 18:T:31:DT:H2'' | 18:T:32:DT:H5' | 1.89 | 0.55 |
| 22:X:250:PHE:CE1 | 22:X:253:LEU:HD22 | 2.42 | 0.55 |
| 1:A:1208:SER:O | 1:A:1260:ARG:HD3 | 2.07 | 0.55 |
| 2:B:756:LYS:NZ | 20:V:134:THR:HG1 | 2.02 | 0.55 |
| 7:G:46:ILE:HB | 7:G:75:ILE:HG13 | 1.89 | 0.55 |
| 16:Q:772:GLU:HB3 | 16:Q:774:SER:CB | 2.37 | 0.55 |
| 24:Z:416:ARG:NE | 24:Z:466:GLN:HE21 | 2.04 | 0.55 |
| 1:A:874:LYS:HG3 | 1:A:880:ARG:HG3 | 1.89 | 0.55 |
| 2:B:649:ASN:ND2 | 19:U:460:TYR:OH | 2.40 | 0.55 |
| 13:M:1369:VAL:HG11 | 13:M:1416:VAL:HG21 | 1.88 | 0.55 |
| 17:R:569:GLU:O | 17:R:572:ILE:HG22 | 2.07 | 0.55 |
| 1:A:229:SER:OG | 1:A:232:GLU:HB2 | 2.07 | 0.55 |
| 14:N:43:DG:H2'' | 14:N:44:DG:C8 | 2.42 | 0.55 |
| 16:Q:94:VAL:HG23 | 16:Q:140:LEU:HD11 | 1.89 | 0.55 |
| 16:Q:313:ALA:HB2 | 16:Q:328:TYR:CB | 2.37 | 0.55 |
| 16:Q:761:LEU:HD22 | 16:Q:785:GLU:HB3 | 1.89 | 0.55 |
| 17:R:449:GLU:O | 17:R:453:MET:HG2 | 2.07 | 0.55 |
| 7:G:7:LEU:N | 7:G:72:TYR:O | 2.40 | 0.54 |
| 9:I:17:CYS:HB3 | 9:I:22:ASN:H | 1.72 | 0.54 |
| 13:M:1476:TYR:OH | 13:M:1483:ARG:NH1 | 2.40 | 0.54 |
| 16:Q:568:TRP:CD2 | 16:Q:592:LEU:HD13 | 2.42 | 0.54 |
| 17:R:360:ASN:HA | 17:R:363:ARG:HB2 | 1.89 | 0.54 |
| 21:W:31:ASN:HB2 | 21:W:72:ILE:HG21 | 1.90 | 0.54 |
| 21:W:41:ASP:OD1 | 21:W:41:ASP:N | 2.40 | 0.54 |
| 1:A:350:VAL:HA | 1:A:354:LEU:HB2 | 1.89 | 0.54 |
| 8:H:27:ARG:HD3 | 8:H:42:ASP:OD2 | 2.06 | 0.54 |
| 2:B:714:PRO:HD2 | 2:B:1001:PRO:HG3 | 1.88 | 0.54 |
| 2:B:859:ARG:HH12 | 2:B:901:THR:HG22 | 1.72 | 0.54 |
| 10:J:57:GLU:OE1 | 17:R:557:ILE:HG12 | 2.06 | 0.54 |
| 17:R:471:GLU:HG2 | 17:R:474:LYS:HE3 | 1.88 | 0.54 |
| 1:A:62:GLN:HE22 | 1:A:255:VAL:HG13 | 1.71 | 0.54 |
| 1:A:117:LEU:C | 1:A:119:VAL:H | 2.11 | 0.54 |
| 2:B:342:VAL:HG23 | 2:B:346:GLU:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:309:CYS:HB3 | 16:Q:328:TYR:HD1 | 1.73 | 0.54 |
| 16:Q:546:ASN:HD22 | 16:Q:577:ALA:HB2 | 1.73 | 0.54 |
| 24:Z:610:ARG:HD2 | 24:Z:629:LEU:HD21 | 1.89 | 0.54 |
| 1:A:340:LYS:HG3 | 1:A:1436:VAL:HG11 | 1.90 | 0.54 |
| 1:A:522:PRO:O | 1:A:662:HIS:HB2 | 2.07 | 0.54 |
| 2:B:309:PHE:HD2 | 9:I:40:ARG:NE | 2.04 | 0.54 |
| 5:E:166:ARG:HH22 | 5:E:168:ASN:ND2 | 1.99 | 0.54 |
| 16:Q:316:PHE:HB2 | 16:Q:325:ALA:HB2 | 1.90 | 0.54 |
| 16:Q:525:ARG:HG3 | 16:Q:526:GLU:HG3 | 1.88 | 0.54 |
| 16:Q:776:LEU:HD22 | 16:Q:831:ALA:HA | 1.88 | 0.54 |
| 21:W:76:LEU:HD12 | 21:W:77:PRO:HD2 | 1.89 | 0.54 |
| 24:Z:235:VAL:O | 24:Z:239:ILE:HG12 | 2.07 | 0.54 |
| 1:A:48:GLU:OE1 | 1:A:51:ARG:HB2 | 2.08 | 0.54 |
| 1:A:606:HIS:HB3 | 1:A:626:THR:HB | 1.89 | 0.54 |
| 5:E:111:THR:HG23 | 5:E:114:ALA:H | 1.73 | 0.54 |
| 15:P:39:A:C2 | 18:T:33:DC:O2 | 2.61 | 0.54 |
| 17:R:385:CYS:O | 17:R:405:ILE:HD12 | 2.08 | 0.54 |
| 21:W:236:LEU:HD13 | 21:W:278:TRP:CE3 | 2.42 | 0.54 |
| 1:A:1130:ILE:HD11 | 1:A:1405:MET:CE | 2.38 | 0.54 |
| 1:A:1141:VAL:HB | 1:A:1336:LEU:HB2 | 1.90 | 0.54 |
| 1:A:1248:ASN:ND2 | 1:A:1254:LYS:O | 2.40 | 0.54 |
| 16:Q:46:ALA:O | 16:Q:50:GLU:HG2 | 2.08 | 0.54 |
| 19:U:450:LEU:CD2 | 19:U:452:LEU:HD23 | 2.37 | 0.54 |
| 21:W:19:ILE:HG12 | 21:W:39:SER:OG | 2.06 | 0.54 |
| 1:A:255:VAL:HG23 | 1:A:280:LEU:HD13 | 1.89 | 0.54 |
| 16:Q:274:HIS:HA | 16:Q:277:ASN:ND2 | 2.23 | 0.54 |
| 16:Q:505:ARG:HE | 20:V:44:PHE:HB3 | 1.73 | 0.54 |
| 2:B:169:ARG:NH2 | 20:V:139:THR:OG1 | 2.40 | 0.54 |
| 2:B:933:ASP:OD2 | 2:B:1050:ARG:NH2 | 2.38 | 0.54 |
| 4:D:133:ASP:O | 4:D:136:THR:OG1 | 2.22 | 0.54 |
| 9:I:39:CYS:SG | 9:I:40:ARG:N | 2.81 | 0.54 |
| 16:Q:364:PHE:HB3 | 16:Q:380:ILE:HD11 | 1.90 | 0.54 |
| 21:W:29:LYS:O | 21:W:77:PRO:HB3 | 2.08 | 0.54 |
| 2:B:159:THR:HA | 2:B:164:ASN:ND2 | 2.22 | 0.54 |
| 17:R:452:PHE:CZ | 17:R:456:LYS:HE2 | 2.43 | 0.54 |
| 19:U:379:PRO:HD2 | 19:U:382:LEU:HD12 | 1.89 | 0.54 |
| 21:W:233:SER:HG | 21:W:251:SER:HB2 | 1.71 | 0.54 |
| 13:M:1463:CYS:O | 13:M:1473:LEU:N | 2.30 | 0.53 |
| 16:Q:147:GLN:O | 16:Q:151:GLN:HG2 | 2.08 | 0.53 |
| 16:Q:392:GLU:HG2 | 16:Q:393:LYS:HG2 | 1.90 | 0.53 |
| 16:Q:553:TRP:HD1 | 16:Q:556:GLU:OE1 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:760:LEU:HD11 | 1:A:781:ILE:HG21 | 1.90 | 0.53 |
| 2:B:22:TRP:CH2 | 2:B:679:PRO:HD3 | 2.43 | 0.53 |
| 2:B:141:GLN:O | 2:B:143:GLN:N | 2.42 | 0.53 |
| 2:B:959:GLU:OE1 | 2:B:959:GLU:N | 2.41 | 0.53 |
| 17:R:356:PRO:HB3 | 17:R:452:PHE:HB2 | 1.90 | 0.53 |
| 17:R:560:ILE:O | 17:R:563:ILE:HG22 | 2.08 | 0.53 |
| 1:A:606:HIS:CG | 1:A:607:SER:H | 2.26 | 0.53 |
| 1:A:727:PRO:HA | 1:A:736:THR:HG21 | 1.89 | 0.53 |
| 3:C:36:ARG:NH1 | 11:K:41:THR:OG1 | 2.40 | 0.53 |
| 7:G:100:GLU:OE1 | 7:G:105:SER:HB3 | 2.08 | 0.53 |
| 7:G:117:MET:HB3 | 7:G:128:TYR:HB3 | 1.89 | 0.53 |
| 9:I:29:ASP:HB3 | 9:I:34:ILE:HG13 | 1.89 | 0.53 |
| 16:Q:772:GLU:HB3 | 16:Q:774:SER:HB3 | 1.89 | 0.53 |
| 21:W:228:LEU:HD13 | 21:W:264:ARG:HB3 | 1.90 | 0.53 |
| 21:W:256:VAL:O | 21:W:269:THR:HA | 2.07 | 0.53 |
| 1:A:64:VAL:HG12 | 1:A:81:CYS:SG | 2.48 | 0.53 |
| 2:B:388:TYR:CE2 | 2:B:505:LEU:HD21 | 2.43 | 0.53 |
| 16:Q:190:LEU:O | 16:Q:193:ASN:ND2 | 2.41 | 0.53 |
| 16:Q:454:LEU:HA | 16:Q:457:VAL:HG12 | 1.91 | 0.53 |
| 16:Q:867:GLU:O | 16:Q:871:GLN:HG3 | 2.08 | 0.53 |
| 20:V:45:ASP:HB3 | 22:X:232:ARG:HE | 1.73 | 0.53 |
| 21:W:33:GLU:O | 21:W:49:TRP:N | 2.41 | 0.53 |
| 23:Y:40:LEU:HD22 | 23:Y:42:MET:HB3 | 1.89 | 0.53 |
| 24:Z:244:ASN:HB3 | 24:Z:245:LEU:HD22 | 1.90 | 0.53 |
| 1:A:141:LEU:HA | 1:A:144:VAL:HG22 | 1.89 | 0.53 |
| 5:E:45:GLY:HA3 | 5:E:52:ARG:HB2 | 1.91 | 0.53 |
| 8:H:9:ILE:HD12 | 8:H:148:LEU:HD11 | 1.90 | 0.53 |
| 12:L:35:ARG:HH21 | 12:L:40:GLY:CA | 2.20 | 0.53 |
| 13:M:1440:ARG:O | 13:M:1444:GLU:HG2 | 2.08 | 0.53 |
| 16:Q:631:ARG:O | 16:Q:635:ILE:HG12 | 2.09 | 0.53 |
| 1:A:589:LYS:NZ | 1:A:625:ASP:OD2 | 2.36 | 0.53 |
| 1:A:802:PHE:HD2 | 2:B:671:GLU:HG2 | 1.74 | 0.53 |
| 1:A:1227:THR:N | 1:A:1230:GLN:HE21 | 1.98 | 0.53 |
| 7:G:117:MET:N | 7:G:117:MET:SD | 2.80 | 0.53 |
| 22:X:233:THR:O | 22:X:236:THR:OG1 | 2.22 | 0.53 |
| 24:Z:279:VAL:HA | 24:Z:386:VAL:HG21 | 1.90 | 0.53 |
| 1:A:241:ARG:HB2 | 1:A:241:ARG:CZ | 2.39 | 0.53 |
| 2:B:393:LEU:HD22 | 2:B:485:LEU:HD22 | 1.89 | 0.53 |
| 2:B:957:THR:HG22 | 2:B:1028:LEU:HD22 | 1.90 | 0.53 |
| 5:E:119:VAL:HA | 5:E:122:ALA:HB2 | 1.90 | 0.53 |
| 2:B:395:LEU:HD11 | 2:B:532:ILE:HD12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:Q:623:GLU:O | 16:Q:627:ARG:NE | 2.42 | 0.53 |
| 16:Q:776:LEU:O | 16:Q:780:LEU:HD12 | 2.08 | 0.53 |
| 1:A:845:GLU:OE2 | 2:B:500:GLN:NE2 | 2.42 | 0.53 |
| 2:B:741:HIS:CD2 | 2:B:742:VAL:HG23 | 2.43 | 0.53 |
| 2:B:789:ASN:O | 2:B:968:ASN:HB2 | 2.09 | 0.53 |
| 2:B:833:THR:C | 2:B:835:GLU:H | 2.11 | 0.53 |
| 7:G:109:SER:HB3 | 24:Z:493:VAL:HG11 | 1.91 | 0.53 |
| 13:M:1352:GLN:HE22 | 13:M:1373:VAL:C | 2.11 | 0.53 |
| 16:Q:769:LEU:HD13 | 16:Q:824:ALA:HB2 | 1.91 | 0.53 |
| 16:Q:777:LYS:HA | 16:Q:780:LEU:HD13 | 1.91 | 0.53 |
| 21:W:9:PHE:H | 21:W:300:ILE:HB | 1.73 | 0.53 |
| 24:Z:479:LYS:NZ | 24:Z:521:CYS:O | 2.28 | 0.53 |
| 4:D:130:ILE:HA | 4:D:133:ASP:OD2 | 2.09 | 0.53 |
| 9:I:68:ILE:HB | 9:I:122:ARG:HD3 | 1.91 | 0.53 |
| 11:K:93:ASP:OD1 | 11:K:93:ASP:N | 2.41 | 0.53 |
| 16:Q:26:GLU:HG3 | 16:Q:28:ASP:H | 1.74 | 0.53 |
| 21:W:108:ASP:HA | 21:W:126:HIS:ND1 | 2.23 | 0.53 |
| 21:W:248:VAL:HG12 | 21:W:258:VAL:HG22 | 1.90 | 0.53 |
| 1:A:1180:ASN:ND2 | 1:A:1182:GLN:HE21 | 2.07 | 0.52 |
| 7:G:8:GLU:HA | 7:G:71:LYS:HA | 1.91 | 0.52 |
| 7:G:37:THR:OG1 | 7:G:38:CYS:N | 2.42 | 0.52 |
| 10:J:65:LEU:HD12 | 10:J:66:GLU:OE1 | 2.09 | 0.52 |
| 16:Q:244:ASN:ND2 | 20:V:69:GLN:HA | 2.24 | 0.52 |
| 3:C:19:VAL:HG23 | 3:C:241:PRO:HB2 | 1.91 | 0.52 |
| 4:D:61:PHE:CE2 | 4:D:65:LEU:HD21 | 2.44 | 0.52 |
| 10:J:40:LEU:HD11 | 10:J:49:LEU:HD12 | 1.91 | 0.52 |
| 17:R:355:LEU:HD11 | 17:R:357:GLU:HG2 | 1.90 | 0.52 |
| 17:R:403:ALA:HB1 | 17:R:428:LEU:HB3 | 1.91 | 0.52 |
| 18:T:17:DT:H2" | 18:T:18:DG:C8 | 2.44 | 0.52 |
| 18:T:35:DG:C2 | 18:T:36:DC:C2 | 2.97 | 0.52 |
| 16:Q:384:LEU:HD21 | 16:Q:386:ALA:HB3 | 1.91 | 0.52 |
| 16:Q:763:ARG:HG2 | 20:V:25:GLU:HG3 | 1.91 | 0.52 |
| 2:B:414:GLU:HG3 | 2:B:439:ILE:HD11 | 1.90 | 0.52 |
| 2:B:609:GLU:O | 2:B:609:GLU:HG2 | 2.09 | 0.52 |
| 13:M:1447:LEU:HB3 | 13:M:1477:GLN:HG3 | 1.91 | 0.52 |
| 17:R:577:LYS:O | 17:R:580:VAL:HG22 | 2.09 | 0.52 |
| 24:Z:422:PRO:HG3 | 24:Z:443:VAL:HG21 | 1.91 | 0.52 |
| 1:A:129:ILE:HD13 | 1:A:132:LYS:NZ | 2.24 | 0.52 |
| 16:Q:420:GLN:HA | 22:X:229:ARG:HH22 | 1.75 | 0.52 |
| 21:W:172:ILE:N | 21:W:186:LEU:O | 2.42 | 0.52 |
| 21:W:289:ILE:N | 21:W:301:TYR:O | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:193:ALA:O | 24:Z:197:MET:HG3 | 2.10 | 0.52 |
| 2:B:1136:GLU:HA | 2:B:1143:LYS:HA | 1.90 | 0.52 |
| 4:D:51:ALA:O | 4:D:54:GLU:HB2 | 2.10 | 0.52 |
| 4:D:82:SER:O | 4:D:85:SER:OG | 2.25 | 0.52 |
| 5:E:209:VAL:O | 5:E:210:GLN:HB2 | 2.10 | 0.52 |
| 7:G:93:ASN:O | 7:G:128:TYR:OH | 2.27 | 0.52 |
| 16:Q:239:ALA:HA | 16:Q:257:LEU:HD13 | 1.92 | 0.52 |
| 16:Q:774:SER:O | 16:Q:830:ARG:NH2 | 2.41 | 0.52 |
| 18:T:9:DC:C6 | 18:T:10:DT:H72 | 2.45 | 0.52 |
| 2:B:1010:LYS:HE3 | 20:V:130:TRP:CZ3 | 2.43 | 0.52 |
| 4:D:63:LYS:HA | 4:D:66:ASN:HD21 | 1.75 | 0.52 |
| 4:D:63:LYS:HE2 | 7:G:102:GLY:O | 2.10 | 0.52 |
| 16:Q:380:ILE:HD12 | 16:Q:400:HIS:HE1 | 1.75 | 0.52 |
| 17:R:473:ASN:HA | 17:R:476:GLU:CD | 2.30 | 0.52 |
| 21:W:39:SER:HB2 | 21:W:41:ASP:OD1 | 2.10 | 0.52 |
| 21:W:217:TYR:HA | 21:W:224:LEU:HA | 1.91 | 0.52 |
| 1:A:525:ILE:O | 1:A:534:VAL:HG22 | 2.09 | 0.52 |
| 1:A:1229:GLU:O | 1:A:1233:GLU:HG3 | 2.10 | 0.52 |
| 3:C:183:ALA:HB3 | 3:C:232:ASN:HB3 | 1.92 | 0.52 |
| 7:G:7:LEU:O | 7:G:72:TYR:N | 2.27 | 0.52 |
| 16:Q:511:CYS:O | 21:W:229:SER:OG | 2.24 | 0.52 |
| 16:Q:790:HIS:HA | 16:Q:793:PHE:CD2 | 2.45 | 0.52 |
| 17:R:452:PHE:HB3 | 17:R:453:MET:HE2 | 1.92 | 0.52 |
| 21:W:176:ASP:HB2 | 21:W:183:LEU:HD21 | 1.92 | 0.52 |
| 24:Z:588:ASP:HA | 24:Z:640:THR:O | 2.10 | 0.52 |
| 1:A:1546:PHE:HD2 | 13:M:1516:GLN:HG3 | 1.75 | 0.51 |
| 2:B:388:TYR:OH | 2:B:524:LYS:HE3 | 2.10 | 0.51 |
| 2:B:651:TYR:HB2 | 19:U:460:TYR:CZ | 2.44 | 0.51 |
| 5:E:36:THR:HG1 | 5:E:39:GLU:CD | 2.13 | 0.51 |
| 5:E:67:ASP:OD2 | 5:E:69:THR:OG1 | 2.22 | 0.51 |
| 16:Q:768:VAL:HG13 | 16:Q:769:LEU:HG | 1.91 | 0.51 |
| 1:A:922:PHE:N | 1:A:1052:ARG:HH11 | 2.09 | 0.51 |
| 4:D:63:LYS:HD3 | 7:G:103:PRO:HA | 1.92 | 0.51 |
| 17:R:581:ALA:O | 17:R:585:ASN:ND2 | 2.43 | 0.51 |
| 24:Z:568:VAL:HG13 | 24:Z:570:VAL:HG13 | 1.91 | 0.51 |
| 2:B:1062:ARG:CZ | 2:B:1074:PRO:HB3 | 2.39 | 0.51 |
| 7:G:118:GLU:HG2 | 7:G:129:LYS:O | 2.11 | 0.51 |
| 24:Z:206:THR:OG1 | 24:Z:207:ASP:N | 2.43 | 0.51 |
| 24:Z:232:GLN:HE21 | 24:Z:252:GLN:HB2 | 1.75 | 0.51 |
| 24:Z:454:HIS:HE2 | 24:Z:463:PHE:HE2 | 1.58 | 0.51 |
| 1:A:43:TYR:HB3 | 1:A:45:GLU:OE1 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:695:ASP:O | 1:A:697:LYS:N | 2.39 | 0.51 |
| 10:J:21:TYR:HB2 | 10:J:38:LEU:HD11 | 1.92 | 0.51 |
| 13:M:1443:LEU:HD13 | 13:M:1473:LEU:HD22 | 1.92 | 0.51 |
| 9:I:81:THR:HG23 | 9:I:96:PHE:CE1 | 2.45 | 0.51 |
| 13:M:1473:LEU:HD11 | 13:M:1484:ILE:HD12 | 1.92 | 0.51 |
| 14:N:34:DC:H2" | 14:N:35:DA:H8 | 1.76 | 0.51 |
| 24:Z:470:LYS:HD2 | 24:Z:472:PHE:CZ | 2.46 | 0.51 |
| 24:Z:745:VAL:HG11 | 24:Z:750:LEU:HD21 | 1.92 | 0.51 |
| 2:B:851:ASP:HB2 | 12:L:15:MET:HG2 | 1.91 | 0.51 |
| 2:B:997:GLY:HA2 | 20:V:131:MET:HG2 | 1.91 | 0.51 |
| 4:D:123:GLU:OE1 | 4:D:123:GLU:N | 2.44 | 0.51 |
| 16:Q:513:PHE:HB2 | 21:W:213:TYR:HE1 | 1.75 | 0.51 |
| 22:X:248:ASN:OD1 | 22:X:249:ILE:HG13 | 2.10 | 0.51 |
| 24:Z:478:VAL:HG22 | 24:Z:490:GLY:O | 2.11 | 0.51 |
| 1:A:927:GLU:HG3 | 1:A:943:LEU:HD11 | 1.92 | 0.51 |
| 2:B:993:LYS:HG2 | 2:B:1018:TYR:OH | 2.11 | 0.51 |
| 2:B:1007:ASN:N | 2:B:1007:ASN:OD1 | 2.42 | 0.51 |
| 16:Q:744:ARG:HG2 | 16:Q:748:PRO:HA | 1.93 | 0.51 |
| 17:R:417:LEU:N | 17:R:420:THR:O | 2.40 | 0.51 |
| 20:V:193:HIS:H | 20:V:197:PRO:HA | 1.73 | 0.51 |
| 21:W:17:ASP:HB2 | 21:W:41:ASP:HB3 | 1.93 | 0.51 |
| 21:W:22:VAL:HG23 | 21:W:37:THR:HG22 | 1.92 | 0.51 |
| 1:A:428:ASP:OD1 | 1:A:430:ARG:NH1 | 2.44 | 0.51 |
| 2:B:177:CYS:SG | 2:B:737:ILE:HD11 | 2.50 | 0.51 |
| 5:E:84:ILE:HG12 | 5:E:114:ALA:HA | 1.92 | 0.51 |
| 16:Q:530:TYR:HD2 | 16:Q:533:CYS:HB2 | 1.76 | 0.51 |
| 16:Q:682:ASP:OD1 | 16:Q:683:VAL:N | 2.43 | 0.51 |
| 18:T:36:DC:C2 | 18:T:37:DC:C5 | 2.99 | 0.51 |
| 23:Y:45:ASN:HD21 | 23:Y:48:MET:HB2 | 1.75 | 0.51 |
| 24:Z:478:VAL:O | 24:Z:489:THR:HG23 | 2.11 | 0.51 |
| 1:A:120:ASP:O | 1:A:122:ASN:ND2 | 2.44 | 0.51 |
| 1:A:419:ILE:HD12 | 1:A:440:LEU:HD23 | 1.92 | 0.51 |
| 1:A:1474:LEU:HB2 | 6:F:105:ILE:HG12 | 1.93 | 0.51 |
| 2:B:624:PRO:HA | 2:B:663:GLU:O | 2.09 | 0.51 |
| 7:G:46:ILE:HD11 | 7:G:77:PHE:CB | 2.40 | 0.51 |
| 16:Q:244:ASN:HD22 | 20:V:69:GLN:HA | 1.76 | 0.51 |
| 17:R:493:GLU:O | 17:R:496:VAL:HG22 | 2.11 | 0.51 |
| 21:W:110:TRP:H | 21:W:123:THR:HG23 | 1.76 | 0.51 |
| 24:Z:312:ASP:O | 24:Z:315:ARG:HG2 | 2.11 | 0.51 |
| 1:A:44:PRO:HG2 | 1:A:285:LYS:HD3 | 1.93 | 0.51 |
| 1:A:725:LEU:HD23 | 1:A:733:LEU:HD11 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1370:GLY:HA2 | 5:E:178:PRO:HD2 | 1.93 | 0.51 |
| 1:A:1423:ASP:OD2 | 1:A:1423:ASP:N | 2.38 | 0.51 |
| 16:Q:815:ARG:O | 16:Q:818:SER:OG | 2.25 | 0.51 |
| 17:R:454:LYS:NZ | 17:R:458:ALA:HB2 | 2.26 | 0.51 |
| 21:W:44:VAL:HB | 21:W:60:LEU:HB2 | 1.93 | 0.51 |
| 21:W:231:HIS:ND1 | 21:W:251:SER:HB3 | 2.26 | 0.51 |
| 22:X:252:ILE:HG13 | 22:X:253:LEU:N | 2.26 | 0.51 |
| 23:Y:40:LEU:HD21 | 23:Y:52:CYS:SG | 2.51 | 0.51 |
| 1:A:410:ASN:HD22 | 1:A:430:ARG:HD2 | 1.76 | 0.50 |
| 1:A:1288:ILE:HA | 1:A:1291:ASN:ND2 | 2.27 | 0.50 |
| 1:A:1314:THR:OG1 | 1:A:1316:ASN:OD1 | 2.29 | 0.50 |
| 2:B:56:GLN:HG2 | 2:B:91:ILE:HG22 | 1.92 | 0.50 |
| 5:E:21:CYS:O | 5:E:26:TYR:HB2 | 2.11 | 0.50 |
| 7:G:91:GLN:HA | 7:G:139:GLN:NE2 | 2.26 | 0.50 |
| 16:Q:93:TYR:HB3 | 16:Q:113:ALA:HB2 | 1.93 | 0.50 |
| 17:R:564:ASN:ND2 | 20:V:136:TYR:C | 2.64 | 0.50 |
| 19:U:373:LEU:HD23 | 19:U:375:PHE:H | 1.76 | 0.50 |
| 21:W:159:ASP:OD2 | 21:W:161:LYS:HE3 | 2.11 | 0.50 |
| 21:W:295:ASP:OD2 | 21:W:297:GLU:HB2 | 2.11 | 0.50 |
| 24:Z:436:LEU:HB3 | 24:Z:454:HIS:CE1 | 2.45 | 0.50 |
| 2:B:848:LEU:HD23 | 2:B:865:VAL:HG13 | 1.93 | 0.50 |
| 16:Q:106:LYS:O | 16:Q:110:ILE:HG12 | 2.12 | 0.50 |
| 16:Q:880:GLN:HB2 | 16:Q:884:LYS:HZ3 | 1.75 | 0.50 |
| 21:W:116:PRO:HD3 | 21:W:156:TYR:HB3 | 1.92 | 0.50 |
| 24:Z:215:VAL:HG12 | 24:Z:227:VAL:HG23 | 1.94 | 0.50 |
| 1:A:202:TRP:HE3 | 1:A:212:LYS:HB2 | 1.76 | 0.50 |
| 1:A:471:GLY:O | 1:A:521:VAL:HG23 | 2.12 | 0.50 |
| 1:A:1177:TYR:CE1 | 1:A:1210:TRP:HB3 | 2.46 | 0.50 |
| 1:A:1302:GLU:C | 1:A:1304:ILE:H | 2.15 | 0.50 |
| 4:D:37:VAL:HG21 | 7:G:2:PHE:HD2 | 1.75 | 0.50 |
| 13:M:1398:LEU:HD23 | 13:M:1400:ILE:HG23 | 1.93 | 0.50 |
| 13:M:1494:PHE:HE2 | 13:M:1504:VAL:HG12 | 1.75 | 0.50 |
| 23:Y:63:MET:SD | 23:Y:72:SER:HB2 | 2.51 | 0.50 |
| 1:A:140:ARG:O | 1:A:144:VAL:HG13 | 2.11 | 0.50 |
| 1:A:383:SER:HB3 | 11:K:2:ASN:HD21 | 1.76 | 0.50 |
| 1:A:1180:ASN:CG | 1:A:1182:GLN:HE21 | 2.14 | 0.50 |
| 2:B:130:LYS:HB3 | 2:B:142:THR:HG23 | 1.94 | 0.50 |
| 4:D:61:PHE:O | 4:D:65:LEU:HG | 2.11 | 0.50 |
| 16:Q:38:HIS:CE1 | 16:Q:73:LEU:HD22 | 2.47 | 0.50 |
| 16:Q:164:PRO:HA | 16:Q:167:LEU:HB2 | 1.93 | 0.50 |
| 16:Q:310:TYR:CE2 | 16:Q:342:LEU:HD13 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:635:ILE:O | 16:Q:639:VAL:HG22 | 2.11 | 0.50 |
| 17:R:441:PHE:HA | 24:Z:776:PRO:O | 2.11 | 0.50 |
| 4:D:33:LEU:HB2 | 4:D:36:GLU:HB2 | 1.93 | 0.50 |
| 14:N:39:DA:C6 | 14:N:40:DG:C6 | 3.00 | 0.50 |
| 15:P:39:A:H2' | 15:P:40:A:C8 | 2.47 | 0.50 |
| 16:Q:163:ILE:HB | 16:Q:164:PRO:HD3 | 1.94 | 0.50 |
| 16:Q:841:LEU:HD23 | 16:Q:844:LYS:HD3 | 1.93 | 0.50 |
| 17:R:404:GLU:O | 17:R:428:LEU:HA | 2.11 | 0.50 |
| 24:Z:440:ILE:HA | 24:Z:450:ILE:HD11 | 1.94 | 0.50 |
| 1:A:123:ASN:HD22 | 1:A:125:LYS:HD3 | 1.75 | 0.50 |
| 1:A:738:GLU:OE2 | 1:A:797:ARG:NH1 | 2.45 | 0.50 |
| 2:B:169:ARG:NH2 | 20:V:139:THR:O | 2.43 | 0.50 |
| 2:B:1142:ASN:ND2 | 2:B:1145:GLN:O | 2.45 | 0.50 |
| 2:B:1142:ASN:O | 2:B:1144:THR:HG22 | 2.10 | 0.50 |
| 3:C:9:VAL:HG11 | 11:K:105:PHE:HD1 | 1.75 | 0.50 |
| 5:E:47:LYS:O | 5:E:53:PRO:HD2 | 2.11 | 0.50 |
| 5:E:64:HIS:HB2 | 5:E:70:ASP:OD1 | 2.12 | 0.50 |
| 15:P:38:G:N3 | 15:P:39:A:C8 | 2.80 | 0.50 |
| 18:T:37:DC:H2'' | 18:T:38:DG:C8 | 2.46 | 0.50 |
| 1:A:324:GLY:O | 1:A:325:LEU:HD22 | 2.12 | 0.50 |
| 1:A:1147:SER:OG | 1:A:1351:ASP:OD1 | 2.29 | 0.50 |
| 16:Q:166:LEU:HA | 16:Q:169:LYS:NZ | 2.26 | 0.50 |
| 16:Q:837:GLU:O | 16:Q:840:GLU:HG3 | 2.11 | 0.50 |
| 17:R:414:VAL:HG22 | 17:R:423:ASN:HB3 | 1.94 | 0.50 |
| 1:A:651:SER:O | 1:A:655:ILE:HG12 | 2.11 | 0.50 |
| 13:M:1347:MET:HB2 | 13:M:1372:LYS:HE3 | 1.94 | 0.50 |
| 16:Q:288:VAL:HG13 | 16:Q:289:GLN:HG3 | 1.93 | 0.50 |
| 24:Z:444:ASP:HB3 | 24:Z:448:ILE:HA | 1.93 | 0.50 |
| 1:A:894:ASP:HB3 | 5:E:200:ALA:HB2 | 1.93 | 0.49 |
| 2:B:1022:LEU:HD23 | 2:B:1022:LEU:H | 1.76 | 0.49 |
| 7:G:46:ILE:HD11 | 7:G:77:PHE:HB3 | 1.94 | 0.49 |
| 14:N:39:DA:H2' | 14:N:40:DG:C8 | 2.47 | 0.49 |
| 16:Q:163:ILE:O | 16:Q:166:LEU:HG | 2.12 | 0.49 |
| 21:W:258:VAL:O | 21:W:267:VAL:HG22 | 2.11 | 0.49 |
| 1:A:833:PRO:HB2 | 2:B:677:MET:SD | 2.52 | 0.49 |
| 2:B:649:ASN:OD1 | 2:B:649:ASN:N | 2.46 | 0.49 |
| 2:B:728:MET:SD | 2:B:942:LYS:HB3 | 2.52 | 0.49 |
| 3:C:86:ARG:NH1 | 24:Z:716:PRO:O | 2.45 | 0.49 |
| 4:D:133:ASP:O | 4:D:137:LYS:HG2 | 2.12 | 0.49 |
| 5:E:177:ASP:O | 5:E:181:ARG:HG3 | 2.11 | 0.49 |
| 16:Q:524:LEU:HD11 | 16:Q:537:LEU:HD12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:Q:735:GLU:OE1 | 16:Q:738:GLN:HB2 | 2.13 | 0.49 |
| 17:R:403:ALA:HB3 | 17:R:428:LEU:HD13 | 1.93 | 0.49 |
| 21:W:65:LEU:HG | 21:W:85:ASP:HB3 | 1.94 | 0.49 |
| 22:X:233:THR:HG22 | 22:X:236:THR:HG23 | 1.94 | 0.49 |
| 24:Z:529:ASP:HB3 | 24:Z:553:LEU:HD23 | 1.94 | 0.49 |
| 1:A:290:LEU:HD13 | 1:A:306:ASP:CG | 2.33 | 0.49 |
| 1:A:1374:VAL:HG11 | 1:A:1411:LEU:HD21 | 1.93 | 0.49 |
| 2:B:218:THR:HG22 | 2:B:236:TRP:HD1 | 1.77 | 0.49 |
| 10:J:22:LEU:HD22 | 17:R:563:ILE:HG21 | 1.94 | 0.49 |
| 16:Q:743:ALA:O | 16:Q:746:VAL:HG22 | 2.12 | 0.49 |
| 16:Q:829:ALA:HA | 16:Q:832:ARG:HD2 | 1.94 | 0.49 |
| 1:A:742:ASN:O | 1:A:746:ASN:ND2 | 2.45 | 0.49 |
| 2:B:237:VAL:HG11 | 2:B:369:VAL:HG22 | 1.94 | 0.49 |
| 20:V:126:LYS:HE3 | 20:V:126:LYS:HA | 1.94 | 0.49 |
| 24:Z:470:LYS:HB3 | 24:Z:472:PHE:HE2 | 1.78 | 0.49 |
| 24:Z:588:ASP:HB3 | 24:Z:594:ILE:HG13 | 1.95 | 0.49 |
| 24:Z:735:GLU:HG3 | 24:Z:735:GLU:O | 2.13 | 0.49 |
| 1:A:316:THR:HA | 1:A:319:ASP:O | 2.11 | 0.49 |
| 1:A:428:ASP:OD1 | 1:A:430:ARG:HG3 | 2.11 | 0.49 |
| 1:A:441:GLN:HG2 | 1:A:444:TYR:CE2 | 2.47 | 0.49 |
| 1:A:1295:ASP:OD2 | 1:A:1295:ASP:N | 2.46 | 0.49 |
| 4:D:44:ARG:HA | 4:D:47:GLN:OE1 | 2.12 | 0.49 |
| 16:Q:183:LEU:O | 16:Q:187:LYS:HG2 | 2.13 | 0.49 |
| 17:R:363:ARG:HE | 17:R:446:GLU:HG2 | 1.78 | 0.49 |
| 17:R:410:GLU:HA | 17:R:424:LYS:HA | 1.93 | 0.49 |
| 17:R:416:GLN:HE21 | 17:R:421:ARG:CZ | 2.26 | 0.49 |
| 17:R:471:GLU:O | 17:R:474:LYS:HG3 | 2.13 | 0.49 |
| 2:B:537:GLN:HG3 | 2:B:538:PRO:HD2 | 1.93 | 0.49 |
| 2:B:626:LEU:HD13 | 2:B:698:ILE:HG12 | 1.94 | 0.49 |
| 14:N:35:DA:H2'' | 14:N:36:DG:H8 | 1.75 | 0.49 |
| 16:Q:68:ARG:NE | 16:Q:89:LEU:HD12 | 2.27 | 0.49 |
| 19:U:443:TRP:HE1 | 19:U:449:SER:HG | 1.58 | 0.49 |
| 21:W:228:LEU:HD11 | 21:W:259:TRP:CZ3 | 2.48 | 0.49 |
| 1:A:587:THR:HG22 | 1:A:588:GLY:N | 2.27 | 0.49 |
| 7:G:151:ARG:HG3 | 24:Z:477:HIS:NE2 | 2.26 | 0.49 |
| 13:M:1374:SER:HB2 | 13:M:1377:ILE:HD13 | 1.93 | 0.49 |
| 13:M:1485:GLU:OE1 | 13:M:1497:ARG:NE | 2.34 | 0.49 |
| 16:Q:750:ASP:HB3 | 16:Q:753:LEU:HG | 1.93 | 0.49 |
| 21:W:108:ASP:HB3 | 21:W:125:THR:HG23 | 1.95 | 0.49 |
| 1:A:1128:ILE:CG2 | 1:A:1414:ILE:HB | 2.43 | 0.49 |
| 2:B:130:LYS:NZ | 2:B:429:PHE:O | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:60:VAL:HG11 | 7:G:44:PHE:CZ | 2.48 | 0.49 |
| 7:G:110:ARG:HD2 | 7:G:113:ILE:HB | 1.95 | 0.49 |
| 12:L:16:ILE:HG13 | 12:L:26:ASN:O | 2.13 | 0.49 |
| 17:R:416:GLN:HG2 | 17:R:421:ARG:HB3 | 1.95 | 0.49 |
| 19:U:453:GLY:HA2 | 20:V:185:ASP:OD2 | 2.12 | 0.49 |
| 22:X:242:GLY:O | 22:X:243:LYS:HE2 | 2.13 | 0.49 |
| 24:Z:257:ILE:O | 24:Z:260:MET:HG2 | 2.13 | 0.49 |
| 1:A:54:LEU:O | 1:A:61:ARG:NH2 | 2.45 | 0.49 |
| 1:A:496:PHE:HB2 | 2:B:791:GLU:O | 2.12 | 0.49 |
| 1:A:963:ARG:O | 1:A:967:ARG:HG3 | 2.13 | 0.49 |
| 1:A:1000:LEU:O | 1:A:1059:ARG:NH1 | 2.45 | 0.49 |
| 2:B:22:TRP:CZ2 | 2:B:679:PRO:HG3 | 2.48 | 0.49 |
| 2:B:824:ASP:O | 2:B:872:THR:HG23 | 2.13 | 0.49 |
| 13:M:783:GLY:N | 13:M:797:ALA:O | 2.46 | 0.49 |
| 17:R:358:GLU:HA | 17:R:361:ARG:NE | 2.27 | 0.49 |
| 17:R:389:ILE:O | 17:R:400:TYR:HD1 | 1.95 | 0.49 |
| 24:Z:199:LYS:HG2 | 24:Z:210:LEU:HD21 | 1.93 | 0.49 |
| 24:Z:426:VAL:HG21 | 24:Z:468:LEU:HD13 | 1.95 | 0.49 |
| 1:A:926:ASN:O | 1:A:930:LEU:HG | 2.13 | 0.49 |
| 1:A:1007:ILE:HD12 | 1:A:1007:ILE:HA | 1.63 | 0.49 |
| 2:B:792:ASP:CG | 2:B:975:ARG:HH22 | 2.16 | 0.49 |
| 14:N:37:DG:N2 | 18:T:12:DC:C2 | 2.77 | 0.49 |
| 16:Q:128:GLN:HA | 16:Q:158:GLN:NE2 | 2.26 | 0.49 |
| 16:Q:129:ASN:OD1 | 16:Q:132:LEU:HD13 | 2.12 | 0.49 |
| 17:R:416:GLN:HA | 17:R:421:ARG:HA | 1.94 | 0.49 |
| 1:A:1311:LEU:HD22 | 1:A:1332:GLN:HG2 | 1.95 | 0.48 |
| 2:B:431:LEU:HD23 | 2:B:431:LEU:H | 1.77 | 0.48 |
| 2:B:679:PRO:HG2 | 2:B:680:ASP:H | 1.78 | 0.48 |
| 2:B:816:GLU:OE2 | 2:B:869:LYS:HE3 | 2.13 | 0.48 |
| 2:B:1120:ASN:HD22 | 2:B:1145:GLN:HB3 | 1.77 | 0.48 |
| 4:D:108:ALA:N | 4:D:128:GLN:OE1 | 2.46 | 0.48 |
| 16:Q:764:LEU:HD22 | 16:Q:785:GLU:OE1 | 2.12 | 0.48 |
| 17:R:563:ILE:O | 17:R:566:ARG:HG2 | 2.13 | 0.48 |
| 21:W:35:VAL:O | 21:W:47:TRP:N | 2.44 | 0.48 |
| 21:W:231:HIS:ND1 | 21:W:235:VAL:HG22 | 2.26 | 0.48 |
| 1:A:84:HIS:H | 1:A:84:HIS:CD2 | 2.31 | 0.48 |
| 1:A:1073:GLU:HG3 | 1:A:1074:SER:N | 2.28 | 0.48 |
| 1:A:1087:VAL:HG23 | 1:A:1400:LEU:HD21 | 1.95 | 0.48 |
| 2:B:92:TYR:HD1 | 19:U:506:ALA:HB3 | 1.79 | 0.48 |
| 2:B:420:GLN:C | 2:B:422:PHE:H | 2.17 | 0.48 |
| 2:B:910:THR:OG1 | 2:B:911:LEU:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:90:THR:HG23 | 7:G:99:THR:HA | 1.95 | 0.48 |
| 8:H:11:ASP:OD1 | 8:H:11:ASP:N | 2.46 | 0.48 |
| 8:H:36:LYS:CE | 16:Q:709:ARG:HH12 | 2.26 | 0.48 |
| 9:I:96:PHE:HA | 9:I:111:TYR:O | 2.13 | 0.48 |
| 16:Q:663:PHE:HB3 | 16:Q:690:ILE:HG23 | 1.95 | 0.48 |
| 21:W:204:LEU:HD22 | 21:W:216:ILE:HG22 | 1.95 | 0.48 |
| 23:Y:33:CYS:SG | 23:Y:36:CYS:N | 2.85 | 0.48 |
| 1:A:1359:SER:O | 1:A:1359:SER:OG | 2.16 | 0.48 |
| 1:A:1400:LEU:O | 1:A:1404:THR:HG23 | 2.14 | 0.48 |
| 8:H:13:LYS:HG3 | 8:H:31:GLU:HG2 | 1.95 | 0.48 |
| 14:N:4:DT:OP2 | 14:N:4:DT:H71 | 2.13 | 0.48 |
| 16:Q:188:LYS:HB3 | 16:Q:191:ARG:NH1 | 2.29 | 0.48 |
| 16:Q:236:VAL:O | 16:Q:240:VAL:HG23 | 2.13 | 0.48 |
| 16:Q:454:LEU:HB3 | 16:Q:477:SER:OG | 2.13 | 0.48 |
| 16:Q:855:LYS:O | 16:Q:858:LYS:HG3 | 2.13 | 0.48 |
| 23:Y:56:SER:HA | 24:Z:271:ALA:HA | 1.96 | 0.48 |
| 24:Z:436:LEU:HD13 | 24:Z:454:HIS:CD2 | 2.49 | 0.48 |
| 24:Z:746:ASP:OD1 | 24:Z:747:ARG:N | 2.46 | 0.48 |
| 2:B:299:GLU:HA | 2:B:302:LYS:HD3 | 1.95 | 0.48 |
| 3:C:74:THR:HG23 | 3:C:128:ILE:O | 2.14 | 0.48 |
| 5:E:114:ALA:O | 5:E:117:SER:OG | 2.23 | 0.48 |
| 16:Q:80:LYS:O | 16:Q:84:THR:HG23 | 2.13 | 0.48 |
| 16:Q:268:ASN:HB3 | 16:Q:271:VAL:HG12 | 1.95 | 0.48 |
| 16:Q:854:GLN:HB2 | 16:Q:855:LYS:NZ | 2.28 | 0.48 |
| 19:U:522:THR:O | 19:U:524:LYS:N | 2.46 | 0.48 |
| 20:V:97:ASN:ND2 | 20:V:98:VAL:O | 2.46 | 0.48 |
| 21:W:89:ARG:HA | 21:W:101:SER:HA | 1.94 | 0.48 |
| 1:A:111:CYS:SG | 1:A:114:CYS:HB2 | 2.54 | 0.48 |
| 1:A:330:GLN:C | 1:A:332:SER:H | 2.17 | 0.48 |
| 1:A:733:LEU:HB2 | 9:I:106:ASP:HB2 | 1.96 | 0.48 |
| 17:R:576:GLU:O | 17:R:580:VAL:HG13 | 2.14 | 0.48 |
| 24:Z:548:GLY:CA | 24:Z:562:ASN:HA | 2.44 | 0.48 |
| 24:Z:615:ARG:HB2 | 24:Z:616:HIS:CD2 | 2.49 | 0.48 |
| 4:D:76:ASN:O | 4:D:79:THR:OG1 | 2.31 | 0.48 |
| 7:G:49:THR:OG1 | 7:G:50:THR:N | 2.47 | 0.48 |
| 15:P:40:A:C2 | 18:T:32:DT:N3 | 2.81 | 0.48 |
| 16:Q:211:LEU:HB2 | 16:Q:213:LYS:NZ | 2.29 | 0.48 |
| 24:Z:342:ALA:HB1 | 24:Z:346:ARG:NH2 | 2.28 | 0.48 |
| 1:A:86:GLY:C | 1:A:255:VAL:HG12 | 2.34 | 0.48 |
| 1:A:606:HIS:CG | 1:A:607:SER:N | 2.82 | 0.48 |
| 1:A:922:PHE:N | 1:A:1052:ARG:HD2 | 2.19 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1173:THR:HG23 | 1:A:1214:VAL:HG22 | 1.94 | 0.48 |
| 1:A:1218:ARG:HH22 | 1:A:1253:GLU:HA | 1.77 | 0.48 |
| 16:Q:211:LEU:HB2 | 16:Q:213:LYS:HE3 | 1.94 | 0.48 |
| 16:Q:346:GLY:HA2 | 16:Q:349:GLN:HE21 | 1.79 | 0.48 |
| 16:Q:423:GLU:OE1 | 22:X:231:TRP:NE1 | 2.43 | 0.48 |
| 16:Q:568:TRP:CE2 | 16:Q:592:LEU:HD13 | 2.49 | 0.48 |
| 17:R:366:ARG:HH22 | 24:Z:773:SER:H | 1.62 | 0.48 |
| 18:T:7:DA:H2" | 18:T:8:DG:C8 | 2.48 | 0.48 |
| 21:W:76:LEU:HG | 21:W:78:ILE:HG23 | 1.95 | 0.48 |
| 21:W:130:VAL:HG22 | 21:W:151:ILE:HG13 | 1.95 | 0.48 |
| 24:Z:206:THR:HG23 | 24:Z:208:THR:H | 1.79 | 0.48 |
| 2:B:425:ARG:HH21 | 2:B:427:LYS:HD3 | 1.78 | 0.48 |
| 16:Q:542:ARG:NH2 | 16:Q:574:LEU:HA | 2.28 | 0.48 |
| 17:R:359:LEU:HD22 | 17:R:452:PHE:CE1 | 2.48 | 0.48 |
| 17:R:370:GLU:HA | 17:R:373:CYS:SG | 2.54 | 0.48 |
| 21:W:46:VAL:HG11 | 21:W:58:TRP:HD1 | 1.78 | 0.48 |
| 21:W:89:ARG:HG2 | 21:W:101:SER:OG | 2.13 | 0.48 |
| 21:W:110:TRP:CD2 | 21:W:150:PHE:HZ | 2.32 | 0.48 |
| 24:Z:310:ARG:CZ | 24:Z:337:GLN:HB2 | 2.44 | 0.48 |
| 24:Z:366:TYR:HB2 | 24:Z:374:LYS:HA | 1.95 | 0.48 |
| 1:A:104:MET:CE | 1:A:193:ARG:HD2 | 2.44 | 0.48 |
| 1:A:488:VAL:O | 1:A:491:PRO:HD2 | 2.14 | 0.48 |
| 1:A:1129:ASN:O | 1:A:1131:SER:N | 2.47 | 0.48 |
| 1:A:1263:ASN:N | 1:A:1263:ASN:OD1 | 2.47 | 0.48 |
| 2:B:355:ASP:OD2 | 2:B:356:PHE:N | 2.46 | 0.48 |
| 2:B:551:GLU:HB3 | 2:B:556:ILE:HD13 | 1.96 | 0.48 |
| 14:N:12:DG:C4 | 14:N:13:DG:C8 | 3.02 | 0.48 |
| 16:Q:153:HIS:HA | 16:Q:169:LYS:HE3 | 1.96 | 0.48 |
| 16:Q:568:TRP:CZ2 | 16:Q:591:ILE:HB | 2.48 | 0.48 |
| 16:Q:645:LYS:HD2 | 22:X:242:GLY:O | 2.14 | 0.48 |
| 16:Q:835:ASP:O | 16:Q:839:ARG:HG3 | 2.14 | 0.48 |
| 1:A:489:THR:HG23 | 1:A:494:ALA:HB3 | 1.96 | 0.48 |
| 1:A:557:ARG:O | 1:A:561:MET:HG3 | 2.14 | 0.48 |
| 1:A:1162:GLU:HG2 | 1:A:1163:HIS:N | 2.29 | 0.48 |
| 2:B:281:ASP:HB3 | 9:I:22:ASN:HA | 1.95 | 0.48 |
| 2:B:1021:HIS:CE1 | 2:B:1023:ARG:HB2 | 2.49 | 0.48 |
| 7:G:38:CYS:SG | 7:G:39:THR:N | 2.87 | 0.48 |
| 7:G:82:GLY:N | 7:G:147:ILE:O | 2.34 | 0.48 |
| 7:G:101:ILE:N | 7:G:104:MET:O | 2.43 | 0.48 |
| 8:H:15:ILE:O | 8:H:16:ASP:C | 2.51 | 0.48 |
| 8:H:106:THR:OG1 | 8:H:107:GLU:N | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:232:VAL:O | 16:Q:236:VAL:HG22 | 2.13 | 0.48 |
| 16:Q:390:ASP:HB2 | 16:Q:392:GLU:OE1 | 2.14 | 0.48 |
| 16:Q:578:LYS:HB2 | 16:Q:580:GLU:HG3 | 1.94 | 0.48 |
| 16:Q:682:ASP:OD1 | 16:Q:683:VAL:HG13 | 2.14 | 0.48 |
| 16:Q:844:LYS:O | 16:Q:848:GLU:HG3 | 2.14 | 0.48 |
| 17:R:359:LEU:HD11 | 17:R:386:PHE:CE2 | 2.49 | 0.48 |
| 19:U:443:TRP:HA | 20:V:201:PRO:HA | 1.95 | 0.48 |
| 21:W:237:ASN:ND2 | 21:W:279:GLY:HA2 | 2.21 | 0.48 |
| 21:W:248:VAL:HG13 | 21:W:282:TYR:OH | 2.14 | 0.48 |
| 21:W:254:LYS:HB3 | 21:W:273:HIS:O | 2.14 | 0.48 |
| 24:Z:426:VAL:HG13 | 24:Z:440:ILE:HD11 | 1.95 | 0.48 |
| 1:A:495:ASP:HB3 | 1:A:499:ASP:OD2 | 2.14 | 0.47 |
| 1:A:896:LEU:HD13 | 1:A:980:PRO:HG3 | 1.95 | 0.47 |
| 1:A:1245:CYS:O | 1:A:1246:ILE:HD13 | 2.13 | 0.47 |
| 1:A:1416:ARG:O | 1:A:1420:ASN:HB2 | 2.14 | 0.47 |
| 3:C:92:GLU:HG2 | 24:Z:711:ARG:CZ | 2.43 | 0.47 |
| 16:Q:39:THR:OG1 | 16:Q:43:ILE:HD13 | 2.14 | 0.47 |
| 16:Q:576:LEU:CD2 | 16:Q:585:GLN:HE22 | 2.27 | 0.47 |
| 16:Q:850:GLU:O | 16:Q:854:GLN:NE2 | 2.44 | 0.47 |
| 17:R:363:ARG:HA | 17:R:386:PHE:O | 2.14 | 0.47 |
| 17:R:485:TYR:OH | 17:R:489:ASP:OD2 | 2.32 | 0.47 |
| 1:A:141:LEU:HB2 | 1:A:236:LEU:O | 2.14 | 0.47 |
| 2:B:108:MET:HE2 | 2:B:113:ALA:HB2 | 1.96 | 0.47 |
| 2:B:166:LEU:HG | 2:B:170:ASP:HB2 | 1.96 | 0.47 |
| 2:B:320:PHE:O | 2:B:323:SER:OG | 2.31 | 0.47 |
| 2:B:719:SER:OG | 2:B:720:PRO:HD3 | 2.13 | 0.47 |
| 2:B:768:ARG:HG3 | 2:B:771:GLU:OE2 | 2.15 | 0.47 |
| 7:G:109:SER:HB2 | 24:Z:503:PHE:CE2 | 2.48 | 0.47 |
| 16:Q:128:GLN:NE2 | 20:V:86:LEU:HD13 | 2.26 | 0.47 |
| 16:Q:336:ALA:HB1 | 16:Q:339:SER:OG | 2.14 | 0.47 |
| 16:Q:358:GLU:O | 16:Q:361:SER:OG | 2.32 | 0.47 |
| 16:Q:689:HIS:HA | 16:Q:692:VAL:HG12 | 1.96 | 0.47 |
| 16:Q:753:LEU:O | 16:Q:757:VAL:HG13 | 2.14 | 0.47 |
| 1:A:46:THR:HB | 1:A:58:MET:HB2 | 1.96 | 0.47 |
| 1:A:376:ASP:HB3 | 1:A:522:PRO:HD3 | 1.95 | 0.47 |
| 1:A:1177:TYR:HD2 | 9:I:28:GLU:OE1 | 1.97 | 0.47 |
| 2:B:44:LEU:HD23 | 2:B:155:MET:CE | 2.44 | 0.47 |
| 5:E:2:ASP:OD2 | 5:E:3:ASP:N | 2.47 | 0.47 |
| 10:J:64:PRO:HG2 | 10:J:65:LEU:H | 1.78 | 0.47 |
| 21:W:191:MET:HB2 | 21:W:209:SER:HB3 | 1.96 | 0.47 |
| 1:A:10:ASP:O | 2:B:1130:THR:HG21 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:406:VAL:HG13 | 1:A:429:LEU:HD11 | 1.97 | 0.47 |
| 1:A:514:GLU:OE1 | 2:B:1101:GLN:HB2 | 2.14 | 0.47 |
| 1:A:527:THR:HG22 | 1:A:532:ARG:O | 2.14 | 0.47 |
| 1:A:760:LEU:HD22 | 1:A:764:ASN:HD22 | 1.79 | 0.47 |
| 1:A:1060:LEU:HA | 1:A:1060:LEU:HD23 | 1.60 | 0.47 |
| 1:A:1083:PRO:HD2 | 6:F:58:THR:HG21 | 1.96 | 0.47 |
| 3:C:2:PRO:HB3 | 11:K:54:PRO:CD | 2.44 | 0.47 |
| 5:E:78:GLU:OE1 | 5:E:78:GLU:N | 2.48 | 0.47 |
| 8:H:45:ILE:HA | 8:H:45:ILE:HD12 | 1.68 | 0.47 |
| 16:Q:143:ASP:N | 16:Q:143:ASP:OD1 | 2.44 | 0.47 |
| 21:W:112:LEU:HB3 | 21:W:121:LEU:HD11 | 1.96 | 0.47 |
| 24:Z:626:CYS:HB3 | 24:Z:629:LEU:HD12 | 1.95 | 0.47 |
| 2:B:313:GLU:HG2 | 2:B:316:VAL:HG12 | 1.95 | 0.47 |
| 2:B:680:ASP:O | 2:B:684:GLU:HG2 | 2.14 | 0.47 |
| 4:D:93:HIS:HB3 | 4:D:96:GLU:OE1 | 2.14 | 0.47 |
| 7:G:4:HIS:CG | 7:G:73:LYS:HE3 | 2.50 | 0.47 |
| 16:Q:172:ILE:HG22 | 16:Q:176:LYS:HZ1 | 1.79 | 0.47 |
| 16:Q:786:LEU:HD21 | 16:Q:820:LEU:HB3 | 1.96 | 0.47 |
| 17:R:363:ARG:HG3 | 17:R:447:PHE:CZ | 2.49 | 0.47 |
| 17:R:587:LYS:O | 17:R:588:ASN:ND2 | 2.48 | 0.47 |
| 1:A:199:TYR:CE2 | 1:A:215:LEU:HD13 | 2.49 | 0.47 |
| 7:G:119:PHE:HA | 7:G:128:TYR:CD1 | 2.49 | 0.47 |
| 15:P:39:A:H2' | 15:P:39:A:N3 | 2.29 | 0.47 |
| 16:Q:68:ARG:HE | 16:Q:86:LEU:HD13 | 1.80 | 0.47 |
| 1:A:70:ARG:HD2 | 2:B:1131:ARG:HH12 | 1.79 | 0.47 |
| 1:A:416:ALA:HA | 1:A:448:ARG:HA | 1.97 | 0.47 |
| 1:A:513:ALA:O | 1:A:517:GLU:HG2 | 2.14 | 0.47 |
| 1:A:1027:ASP:HB3 | 1:A:1030:SER:HB3 | 1.96 | 0.47 |
| 1:A:1177:TYR:CD2 | 9:I:28:GLU:OE1 | 2.68 | 0.47 |
| 2:B:170:ASP:N | 2:B:170:ASP:OD1 | 2.43 | 0.47 |
| 2:B:1007:ASN:O | 2:B:1011:ILE:HG13 | 2.14 | 0.47 |
| 14:N:12:DG:C6 | 14:N:13:DG:C6 | 3.02 | 0.47 |
| 16:Q:76:ARG:HH11 | 16:Q:76:ARG:HG3 | 1.80 | 0.47 |
| 16:Q:366:LYS:HG3 | 16:Q:369:LYS:HZ3 | 1.79 | 0.47 |
| 16:Q:721:LEU:HD11 | 20:V:31:CYS:HA | 1.97 | 0.47 |
| 16:Q:737:LYS:HE3 | 16:Q:760:VAL:HG22 | 1.96 | 0.47 |
| 21:W:11:GLN:HB3 | 21:W:298:ILE:HB | 1.97 | 0.47 |
| 24:Z:479:LYS:HD3 | 24:Z:521:CYS:HB2 | 1.96 | 0.47 |
| 1:A:724:GLU:OE1 | 1:A:724:GLU:N | 2.47 | 0.47 |
| 1:A:951:GLU:HG2 | 1:A:1007:ILE:HD11 | 1.97 | 0.47 |
| 1:A:1236:ASN:O | 1:A:1240:GLY:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1415:THR:O | 1:A:1419:VAL:HG22 | 2.14 | 0.47 |
| 2:B:255:ARG:CD | 2:B:307:GLU:HG3 | 2.44 | 0.47 |
| 2:B:347:MET:HG3 | 2:B:347:MET:O | 2.15 | 0.47 |
| 4:D:62:MET:O | 4:D:66:ASN:ND2 | 2.47 | 0.47 |
| 16:Q:167:LEU:HD21 | 16:Q:189:ALA:HB2 | 1.96 | 0.47 |
| 16:Q:373:ASN:HB2 | 16:Q:376:GLU:HG2 | 1.96 | 0.47 |
| 16:Q:750:ASP:OD1 | 16:Q:752:VAL:N | 2.48 | 0.47 |
| 19:U:394:TYR:C | 20:V:172:ARG:HH21 | 2.18 | 0.47 |
| 1:A:621:ILE:HG23 | 1:A:621:ILE:O | 2.14 | 0.47 |
| 1:A:831:LEU:HB3 | 1:A:835:GLU:HG3 | 1.97 | 0.47 |
| 2:B:84:TYR:HA | 2:B:132:VAL:HA | 1.97 | 0.47 |
| 4:D:79:THR:O | 4:D:82:SER:OG | 2.33 | 0.47 |
| 7:G:147:ILE:HG23 | 7:G:159:ALA:HB1 | 1.96 | 0.47 |
| 15:P:38:G:C2' | 15:P:39:A:H8 | 2.24 | 0.47 |
| 16:Q:347:LEU:HB2 | 16:Q:363:CYS:SG | 2.54 | 0.47 |
| 16:Q:411:ASP:HB3 | 16:Q:415:TRP:CZ3 | 2.50 | 0.47 |
| 16:Q:624:LYS:HA | 16:Q:627:ARG:HE | 1.79 | 0.47 |
| 16:Q:712:TYR:O | 16:Q:713:LYS:HG3 | 2.15 | 0.47 |
| 16:Q:833:LYS:O | 16:Q:836:GLU:HG3 | 2.15 | 0.47 |
| 17:R:573:VAL:O | 17:R:576:GLU:HG3 | 2.15 | 0.47 |
| 21:W:5:TYR:CE1 | 21:W:303:CYS:HB3 | 2.50 | 0.47 |
| 24:Z:433:LEU:HD13 | 24:Z:461:LEU:HD13 | 1.96 | 0.47 |
| 1:A:1016:LEU:HD23 | 1:A:1045:LEU:HD21 | 1.97 | 0.47 |
| 2:B:690:CYS:SG | 2:B:693:TYR:CZ | 3.08 | 0.47 |
| 2:B:1136:GLU:CB | 2:B:1143:LYS:HG2 | 2.44 | 0.47 |
| 7:G:113:ILE:HG22 | 7:G:114:PRO:O | 2.15 | 0.47 |
| 8:H:112:LEU:HB2 | 8:H:132:LEU:HD12 | 1.97 | 0.47 |
| 9:I:84:HIS:CD2 | 9:I:125:GLU:OE1 | 2.68 | 0.47 |
| 16:Q:7:GLU:OE2 | 16:Q:18:GLU:HB3 | 2.14 | 0.47 |
| 16:Q:716:ASN:HB3 | 16:Q:719:VAL:HG22 | 1.96 | 0.47 |
| 20:V:96:PRO:HA | 20:V:97:ASN:HA | 1.57 | 0.47 |
| 24:Z:521:CYS:HB3 | 24:Z:523:GLU:OE1 | 2.15 | 0.47 |
| 1:A:71:CYS:HB3 | 1:A:74:CYS:O | 2.15 | 0.46 |
| 1:A:239:GLU:HG3 | 1:A:240:PRO:HD2 | 1.96 | 0.46 |
| 1:A:1184:THR:C | 1:A:1186:VAL:N | 2.64 | 0.46 |
| 2:B:451:GLY:HA2 | 2:B:467:SER:HB3 | 1.97 | 0.46 |
| 5:E:3:ASP:OD1 | 5:E:47:LYS:HD2 | 2.15 | 0.46 |
| 5:E:82:VAL:HG12 | 5:E:110:MET:CB | 2.45 | 0.46 |
| 8:H:112:LEU:HA | 8:H:112:LEU:HD23 | 1.59 | 0.46 |
| 12:L:16:ILE:HD12 | 12:L:27:GLU:OE2 | 2.16 | 0.46 |
| 13:M:848:VAL:O | 13:M:883:GLU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:N:42:DT:H2'' | 14:N:43:DG:C8 | 2.51 | 0.46 |
| 21:W:215:LYS:HG2 | 21:W:227:THR:HG22 | 1.97 | 0.46 |
| 23:Y:22:VAL:HB | 23:Y:84:VAL:HG12 | 1.97 | 0.46 |
| 24:Z:547:VAL:HG12 | 24:Z:563:MET:SD | 2.54 | 0.46 |
| 1:A:866:LYS:HG3 | 1:A:1432:PHE:CD1 | 2.49 | 0.46 |
| 1:A:1162:GLU:O | 1:A:1300:GLY:HA3 | 2.15 | 0.46 |
| 2:B:425:ARG:NH2 | 2:B:427:LYS:HD3 | 2.30 | 0.46 |
| 4:D:48:ASN:HB3 | 4:D:57:LEU:HD11 | 1.97 | 0.46 |
| 7:G:5:ILE:O | 7:G:73:LYS:HD2 | 2.15 | 0.46 |
| 13:M:1362:LYS:HD3 | 13:M:1363:GLY:N | 2.31 | 0.46 |
| 16:Q:211:LEU:HB2 | 16:Q:213:LYS:HZ2 | 1.80 | 0.46 |
| 16:Q:380:ILE:HB | 16:Q:400:HIS:CE1 | 2.50 | 0.46 |
| 24:Z:571:ARG:H | 24:Z:574:ALA:HB3 | 1.80 | 0.46 |
| 1:A:1474:LEU:HD12 | 6:F:105:ILE:HD11 | 1.97 | 0.46 |
| 2:B:285:LEU:HD12 | 2:B:285:LEU:HA | 1.61 | 0.46 |
| 11:K:7:PHE:CD2 | 11:K:11:LEU:HD12 | 2.50 | 0.46 |
| 13:M:1447:LEU:HA | 13:M:1450:THR:HG22 | 1.97 | 0.46 |
| 15:P:43:C:H2' | 15:P:44:A:O4' | 2.16 | 0.46 |
| 16:Q:30:VAL:HA | 16:Q:33:ILE:HG12 | 1.96 | 0.46 |
| 16:Q:830:ARG:HH21 | 16:Q:834:GLN:HG3 | 1.79 | 0.46 |
| 17:R:562:TYR:HB3 | 17:R:566:ARG:HH21 | 1.80 | 0.46 |
| 24:Z:340:PHE:HD2 | 24:Z:370:GLY:HA2 | 1.81 | 0.46 |
| 1:A:93:PRO:HG2 | 1:A:219:GLU:OE2 | 2.15 | 0.46 |
| 1:A:228:ILE:HG23 | 1:A:232:GLU:HG2 | 1.96 | 0.46 |
| 1:A:1148:ALA:HB1 | 1:A:1333:GLU:HB3 | 1.97 | 0.46 |
| 2:B:285:LEU:HD23 | 9:I:16:PHE:CZ | 2.51 | 0.46 |
| 2:B:329:GLY:HA3 | 2:B:334:LYS:HB3 | 1.97 | 0.46 |
| 3:C:78:ILE:H | 3:C:78:ILE:HG12 | 1.48 | 0.46 |
| 5:E:63:ALA:HB3 | 16:Q:880:GLN:HE22 | 1.80 | 0.46 |
| 5:E:153:LYS:O | 5:E:157:THR:HG23 | 2.14 | 0.46 |
| 7:G:82:GLY:HA2 | 7:G:146:LYS:HE3 | 1.96 | 0.46 |
| 9:I:29:ASP:CB | 9:I:34:ILE:HG13 | 2.45 | 0.46 |
| 16:Q:637:LYS:O | 16:Q:641:ARG:HD3 | 2.15 | 0.46 |
| 21:W:151:ILE:HG23 | 21:W:165:SER:OG | 2.15 | 0.46 |
| 1:A:1176:TYR:HD1 | 9:I:51:SER:O | 1.99 | 0.46 |
| 1:A:1177:TYR:CE2 | 1:A:1210:TRP:HE3 | 2.34 | 0.46 |
| 1:A:1416:ARG:HD2 | 1:A:1434:GLU:OE2 | 2.15 | 0.46 |
| 2:B:566:LYS:HA | 2:B:576:ILE:HD12 | 1.97 | 0.46 |
| 2:B:646:ARG:O | 2:B:647:GLU:HG2 | 2.16 | 0.46 |
| 16:Q:386:ALA:HB1 | 16:Q:394:ARG:HG3 | 1.97 | 0.46 |
| 16:Q:452:GLU:OE1 | 16:Q:490:HIS:NE2 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:527:HIS:CE1 | 22:X:220:VAL:HB | 2.51 | 0.46 |
| 16:Q:834:GLN:O | 16:Q:838:GLU:HG2 | 2.15 | 0.46 |
| 1:A:609:HIS:HA | 1:A:626:THR:HG21 | 1.98 | 0.46 |
| 1:A:1150:ASP:OD1 | 1:A:1150:ASP:N | 2.48 | 0.46 |
| 1:A:1305:SER:OG | 1:A:1306:LYS:N | 2.48 | 0.46 |
| 2:B:26:CYS:O | 2:B:30:ILE:HG12 | 2.15 | 0.46 |
| 8:H:67:ASP:OD1 | 8:H:67:ASP:N | 2.46 | 0.46 |
| 9:I:17:CYS:SG | 9:I:18:GLN:N | 2.89 | 0.46 |
| 9:I:75:ASP:OD1 | 9:I:77:THR:HG22 | 2.16 | 0.46 |
| 10:J:26:GLN:HA | 17:R:566:ARG:HD2 | 1.98 | 0.46 |
| 16:Q:41:LEU:HD13 | 16:Q:75:TYR:HE2 | 1.81 | 0.46 |
| 16:Q:460:LEU:O | 16:Q:464:LEU:HG | 2.14 | 0.46 |
| 16:Q:855:LYS:HD3 | 16:Q:855:LYS:HA | 1.59 | 0.46 |
| 17:R:574:GLU:HA | 17:R:577:LYS:NZ | 2.31 | 0.46 |
| 19:U:443:TRP:NE1 | 19:U:449:SER:OG | 2.47 | 0.46 |
| 21:W:152:LEU:N | 21:W:166:GLY:O | 2.34 | 0.46 |
| 21:W:252:SER:HA | 21:W:276:GLN:HB3 | 1.98 | 0.46 |
| 24:Z:182:VAL:O | 24:Z:224:TYR:HB2 | 2.14 | 0.46 |
| 1:A:123:ASN:HB3 | 1:A:125:LYS:HG2 | 1.98 | 0.46 |
| 1:A:1547:SEP:HA | 1:A:1548:PRO:HD3 | 1.78 | 0.46 |
| 2:B:133:ILE:HD12 | 2:B:139:GLN:HB3 | 1.98 | 0.46 |
| 2:B:548:TRP:CZ2 | 2:B:586:THR:HG21 | 2.51 | 0.46 |
| 7:G:111:HIS:ND1 | 24:Z:494:ARG:HB3 | 2.31 | 0.46 |
| 8:H:30:CYS:SG | 8:H:56:PHE:HZ | 2.39 | 0.46 |
| 11:K:99:SER:O | 11:K:103:GLU:HG3 | 2.16 | 0.46 |
| 16:Q:566:ASP:OD1 | 22:X:234:ARG:HD3 | 2.16 | 0.46 |
| 18:T:30:DG:H2' | 18:T:31:DT:C6 | 2.50 | 0.46 |
| 19:U:469:ASN:HA | 20:V:222:ARG:HA | 1.98 | 0.46 |
| 21:W:46:VAL:CB | 21:W:58:TRP:HB2 | 2.45 | 0.46 |
| 21:W:182:LEU:HD21 | 21:W:185:THR:OG1 | 2.16 | 0.46 |
| 21:W:233:SER:HB3 | 21:W:253:ASP:HB3 | 1.98 | 0.46 |
| 24:Z:571:ARG:HB2 | 24:Z:574:ALA:HB2 | 1.98 | 0.46 |
| 1:A:732:THR:HG23 | 1:A:735:GLN:OE1 | 2.14 | 0.46 |
| 1:A:1054:MET:SD | 1:A:1060:LEU:HD12 | 2.56 | 0.46 |
| 1:A:1176:TYR:C | 1:A:1177:TYR:HD1 | 2.19 | 0.46 |
| 16:Q:386:ALA:HB2 | 16:Q:393:LYS:CB | 2.46 | 0.46 |
| 16:Q:563:ASP:O | 16:Q:565:PRO:HD3 | 2.15 | 0.46 |
| 16:Q:803:MET:HE1 | 16:Q:807:LEU:HD11 | 1.98 | 0.46 |
| 24:Z:182:VAL:HG23 | 24:Z:225:ILE:HG13 | 1.98 | 0.46 |
| 24:Z:239:ILE:O | 24:Z:242:VAL:HG22 | 2.15 | 0.46 |
| 24:Z:539:LEU:O | 24:Z:578:LYS:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:112:PHE:CZ | 1:A:220:ARG:NH1 | 2.84 | 0.46 |
| 5:E:126:ILE:H | 5:E:126:ILE:HD12 | 1.81 | 0.46 |
| 6:F:57:MET:HB2 | 6:F:123:LEU:HD13 | 1.98 | 0.46 |
| 8:H:143:LEU:HD12 | 8:H:143:LEU:HA | 1.62 | 0.46 |
| 10:J:25:LEU:HD23 | 17:R:567:ASN:HD21 | 1.81 | 0.46 |
| 16:Q:265:ASP:OD1 | 16:Q:268:ASN:HB2 | 2.16 | 0.46 |
| 16:Q:289:GLN:O | 16:Q:293:LEU:HD23 | 2.16 | 0.46 |
| 16:Q:872:LYS:O | 16:Q:875:LEU:HG | 2.16 | 0.46 |
| 18:T:37:DC:H6 | 18:T:37:DC:H5' | 1.81 | 0.46 |
| 18:T:41:DC:H4' | 24:Z:283:ARG:NE | 2.21 | 0.46 |
| 20:V:88:ASN:O | 20:V:90:ASP:N | 2.49 | 0.46 |
| 21:W:86:ALA:HB1 | 21:W:105:GLY:HA2 | 1.97 | 0.46 |
| 24:Z:705:LEU:HD21 | 24:Z:747:ARG:HD2 | 1.96 | 0.46 |
| 1:A:37:THR:O | 1:A:37:THR:OG1 | 2.30 | 0.46 |
| 1:A:117:LEU:HD21 | 1:A:232:GLU:HG3 | 1.98 | 0.46 |
| 1:A:347:GLU:HA | 1:A:352:GLY:HA3 | 1.98 | 0.46 |
| 1:A:753:GLY:O | 1:A:757:GLN:HG2 | 2.16 | 0.46 |
| 1:A:1379:GLU:O | 1:A:1379:GLU:HG2 | 2.16 | 0.46 |
| 3:C:60:HIS:HB3 | 3:C:61:ASP:H | 1.33 | 0.46 |
| 16:Q:208:PHE:CD1 | 16:Q:213:LYS:HD2 | 2.51 | 0.46 |
| 16:Q:450:PRO:HB2 | 16:Q:452:GLU:HG2 | 1.98 | 0.46 |
| 19:U:378:LEU:HD23 | 19:U:382:LEU:O | 2.16 | 0.46 |
| 24:Z:280:ARG:HG3 | 24:Z:386:VAL:HG13 | 1.98 | 0.46 |
| 24:Z:294:ASP:HB2 | 24:Z:306:LYS:HE2 | 1.98 | 0.46 |
| 24:Z:480:VAL:HG13 | 24:Z:487:GLY:H | 1.81 | 0.46 |
| 1:A:465:HIS:HB3 | 1:A:1097:GLU:HG3 | 1.97 | 0.45 |
| 1:A:966:LEU:HA | 1:A:966:LEU:HD23 | 1.74 | 0.45 |
| 1:A:971:PRO:O | 1:A:972:THR:OG1 | 2.26 | 0.45 |
| 1:A:1117:VAL:HA | 1:A:1136:THR:HG21 | 1.97 | 0.45 |
| 2:B:236:TRP:HB2 | 2:B:259:THR:HB | 1.98 | 0.45 |
| 2:B:684:GLU:OE2 | 2:B:684:GLU:HA | 2.16 | 0.45 |
| 12:L:52:LEU:HA | 12:L:52:LEU:HD12 | 1.69 | 0.45 |
| 16:Q:620:ARG:NH1 | 16:Q:659:HIS:O | 2.47 | 0.45 |
| 17:R:429:ARG:NE | 17:R:431:GLY:O | 2.42 | 0.45 |
| 21:W:13:GLN:H | 21:W:297:GLU:HG2 | 1.80 | 0.45 |
| 22:X:253:LEU:O | 22:X:256:VAL:HG12 | 2.16 | 0.45 |
| 1:A:18:ILE:HD12 | 2:B:1171:MET:HB3 | 1.99 | 0.45 |
| 1:A:124:PRO:HA | 1:A:127:LYS:CG | 2.45 | 0.45 |
| 1:A:1254:LYS:HD3 | 1:A:1254:LYS:HA | 1.77 | 0.45 |
| 1:A:1298:LEU:HA | 1:A:1298:LEU:HD23 | 1.77 | 0.45 |
| 2:B:121:SER:HA | 2:B:153:PRO:HA | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:255:ARG:HD3 | 2:B:307:GLU:HG3 | 1.98 | 0.45 |
| 2:B:621:ILE:HD13 | 2:B:621:ILE:HG21 | 1.66 | 0.45 |
| 2:B:1006:VAL:HG22 | 20:V:130:TRP:CB | 2.45 | 0.45 |
| 4:D:38:HIS:HB2 | 4:D:68:THR:OG1 | 2.16 | 0.45 |
| 11:K:71:ILE:HG21 | 11:K:71:ILE:HD13 | 1.61 | 0.45 |
| 16:Q:64:LEU:HA | 16:Q:64:LEU:HD23 | 1.82 | 0.45 |
| 17:R:565:GLN:HA | 17:R:568:ARG:CZ | 2.47 | 0.45 |
| 20:V:38:SER:OG | 20:V:39:LEU:N | 2.49 | 0.45 |
| 21:W:7:ILE:HA | 21:W:301:TYR:HA | 1.98 | 0.45 |
| 21:W:233:SER:OG | 21:W:252:SER:N | 2.44 | 0.45 |
| 23:Y:35:ASN:ND2 | 23:Y:85:TYR:OH | 2.49 | 0.45 |
| 24:Z:470:LYS:HB3 | 24:Z:472:PHE:CE2 | 2.51 | 0.45 |
| 1:A:189:PRO:HB2 | 1:A:201:GLU:H | 1.81 | 0.45 |
| 1:A:989:ASN:O | 1:A:993:ILE:HG13 | 2.16 | 0.45 |
| 1:A:1371:ILE:HD11 | 1:A:1406:THR:HB | 1.99 | 0.45 |
| 2:B:317:ALA:O | 2:B:321:ILE:HD12 | 2.15 | 0.45 |
| 2:B:681:ASP:OD2 | 2:B:681:ASP:N | 2.50 | 0.45 |
| 11:K:51:LEU:HA | 11:K:51:LEU:HD23 | 1.62 | 0.45 |
| 14:N:12:DG:C4 | 14:N:13:DG:N7 | 2.84 | 0.45 |
| 1:A:1044:HIS:O | 1:A:1048:THR:HG23 | 2.17 | 0.45 |
| 2:B:757:PRO:HB2 | 2:B:760:THR:HG22 | 1.99 | 0.45 |
| 3:C:92:GLU:HG2 | 24:Z:711:ARG:NH1 | 2.32 | 0.45 |
| 8:H:70:LEU:HD12 | 8:H:70:LEU:HA | 1.76 | 0.45 |
| 9:I:73:SER:O | 9:I:80:ARG:NH2 | 2.50 | 0.45 |
| 9:I:74:GLN:H | 9:I:74:GLN:HG2 | 1.51 | 0.45 |
| 9:I:91:HIS:CD2 | 9:I:93:GLU:H | 2.35 | 0.45 |
| 16:Q:474:PHE:CB | 16:Q:503:LEU:HD13 | 2.46 | 0.45 |
| 16:Q:591:ILE:HG22 | 16:Q:592:LEU:HD12 | 1.97 | 0.45 |
| 23:Y:116:LYS:HD3 | 23:Y:116:LYS:HA | 1.74 | 0.45 |
| 24:Z:469:ARG:NH2 | 24:Z:497:GLU:O | 2.49 | 0.45 |
| 1:A:775:LYS:HD2 | 2:B:974:SER:HB3 | 1.97 | 0.45 |
| 2:B:332:LYS:HB3 | 2:B:332:LYS:HE3 | 1.57 | 0.45 |
| 2:B:388:TYR:HB2 | 2:B:504:THR:HG23 | 1.99 | 0.45 |
| 2:B:395:LEU:HA | 2:B:395:LEU:HD23 | 1.67 | 0.45 |
| 3:C:44:ILE:HD13 | 3:C:44:ILE:HG21 | 1.48 | 0.45 |
| 7:G:151:ARG:NE | 7:G:153:ASP:OD1 | 2.50 | 0.45 |
| 21:W:235:VAL:HA | 21:W:251:SER:HA | 1.98 | 0.45 |
| 23:Y:66:PRO:HD3 | 23:Y:82:PRO:HG3 | 1.98 | 0.45 |
| 2:B:834:ARG:HH22 | 2:B:842:HIS:HA | 1.80 | 0.45 |
| 14:N:12:DG:N1 | 18:T:38:DG:N2 | 2.64 | 0.45 |
| 16:Q:246:LYS:HD2 | 16:Q:246:LYS:HA | 1.73 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:620:ARG:HH22 | 16:Q:660:LYS:HA | 1.81 | 0.45 |
| 17:R:388:ARG:HD3 | 17:R:445:GLN:HB2 | 1.99 | 0.45 |
| 17:R:570:TRP:CD1 | 20:V:133:LYS:HD2 | 2.43 | 0.45 |
| 20:V:103:ALA:O | 20:V:107:LEU:HG | 2.17 | 0.45 |
| 21:W:29:LYS:HE2 | 21:W:75:THR:HA | 1.99 | 0.45 |
| 22:X:222:ARG:HA | 22:X:225:VAL:HG22 | 1.97 | 0.45 |
| 23:Y:65:SER:O | 23:Y:65:SER:OG | 2.33 | 0.45 |
| 1:A:111:CYS:HG | 1:A:114:CYS:HB2 | 1.81 | 0.45 |
| 1:A:825:ASN:ND2 | 1:A:835:GLU:OE1 | 2.47 | 0.45 |
| 1:A:1369:LEU:HD23 | 1:A:1369:LEU:HA | 1.73 | 0.45 |
| 2:B:1134:THR:HG23 | 2:B:1134:THR:O | 2.17 | 0.45 |
| 4:D:74:PHE:CE2 | 4:D:80:ILE:HG12 | 2.52 | 0.45 |
| 16:Q:763:ARG:HE | 20:V:25:GLU:N | 2.14 | 0.45 |
| 17:R:566:ARG:HA | 17:R:569:GLU:OE1 | 2.16 | 0.45 |
| 21:W:56:LEU:HD21 | 21:W:59:SER:OG | 2.16 | 0.45 |
| 24:Z:546:THR:HG22 | 24:Z:547:VAL:N | 2.32 | 0.45 |
| 1:A:291:ARG:HG3 | 1:A:292:ARG:N | 2.32 | 0.45 |
| 1:A:1226:LEU:HA | 1:A:1230:GLN:NE2 | 2.31 | 0.45 |
| 2:B:357:CYS:SG | 2:B:360:LYS:NZ | 2.85 | 0.45 |
| 2:B:651:TYR:N | 19:U:460:TYR:OH | 2.49 | 0.45 |
| 2:B:714:PRO:CD | 2:B:1001:PRO:HG3 | 2.47 | 0.45 |
| 2:B:1104:ARG:O | 2:B:1108:PHE:HB3 | 2.16 | 0.45 |
| 3:C:45:ILE:HG22 | 3:C:165:ALA:HB1 | 1.98 | 0.45 |
| 4:D:32:LEU:HD23 | 4:D:32:LEU:HA | 1.83 | 0.45 |
| 12:L:22:CYS:SG | 12:L:39:CYS:SG | 3.06 | 0.45 |
| 13:M:1463:CYS:SG | 13:M:1464:ALA:N | 2.90 | 0.45 |
| 16:Q:123:ILE:HG23 | 16:Q:124:ILE:H | 1.82 | 0.45 |
| 16:Q:134:ARG:HA | 16:Q:134:ARG:HD2 | 1.76 | 0.45 |
| 16:Q:170:ALA:HB2 | 16:Q:185:TYR:HB2 | 1.99 | 0.45 |
| 17:R:402:VAL:HG23 | 17:R:451:GLU:HG2 | 1.98 | 0.45 |
| 20:V:190:ILE:O | 20:V:190:ILE:HG13 | 2.17 | 0.45 |
| 21:W:64:GLN:OE1 | 21:W:89:ARG:NH2 | 2.48 | 0.45 |
| 24:Z:243:GLY:O | 24:Z:246:ARG:HG2 | 2.17 | 0.45 |
| 2:B:319:ASN:HD21 | 2:B:332:LYS:HG2 | 1.82 | 0.45 |
| 8:H:64:LEU:HD23 | 8:H:64:LEU:HA | 1.79 | 0.45 |
| 16:Q:386:ALA:HB2 | 16:Q:393:LYS:HB3 | 1.99 | 0.45 |
| 17:R:356:PRO:HB3 | 17:R:452:PHE:CB | 2.47 | 0.45 |
| 1:A:557:ARG:HG3 | 1:A:558:GLY:N | 2.27 | 0.45 |
| 2:B:479:LEU:O | 2:B:483:ARG:HG3 | 2.17 | 0.45 |
| 5:E:185:ILE:HD12 | 5:E:209:VAL:HG21 | 1.98 | 0.45 |
| 16:Q:95:GLN:HG3 | 20:V:85:ASP:OD1 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:131:LEU:HD12 | 16:Q:155:VAL:HG22 | 1.98 | 0.45 |
| 16:Q:133:GLY:HA2 | 16:Q:136:CYS:SG | 2.57 | 0.45 |
| 16:Q:200:VAL:HA | 20:V:82:VAL:HG22 | 1.97 | 0.45 |
| 16:Q:380:ILE:HG21 | 16:Q:396:ILE:HD12 | 1.98 | 0.45 |
| 16:Q:568:TRP:CE3 | 16:Q:592:LEU:HB2 | 2.51 | 0.45 |
| 16:Q:736:CYS:O | 16:Q:739:THR:HG22 | 2.17 | 0.45 |
| 23:Y:8:LYS:HE2 | 23:Y:27:GLN:NE2 | 2.32 | 0.45 |
| 24:Z:272:ASN:ND2 | 24:Z:384:GLU:HB2 | 2.32 | 0.45 |
| 24:Z:729:GLU:O | 24:Z:747:ARG:NH2 | 2.50 | 0.45 |
| 1:A:74:CYS:SG | 1:A:81:CYS:HB2 | 2.56 | 0.44 |
| 1:A:902:GLU:O | 1:A:978:VAL:HA | 2.17 | 0.44 |
| 1:A:1040:LEU:HA | 1:A:1040:LEU:HD12 | 1.75 | 0.44 |
| 1:A:1118:THR:HG21 | 1:A:1135:LYS:HB2 | 1.99 | 0.44 |
| 1:A:1184:THR:O | 1:A:1184:THR:OG1 | 2.28 | 0.44 |
| 2:B:655:ASP:O | 2:B:659:SER:HB3 | 2.17 | 0.44 |
| 7:G:4:HIS:CD2 | 7:G:73:LYS:HE3 | 2.52 | 0.44 |
| 8:H:111:ARG:HA | 8:H:128:ASP:HA | 1.99 | 0.44 |
| 15:P:37:G:H2' | 15:P:38:G:C8 | 2.52 | 0.44 |
| 20:V:75:LEU:HD12 | 20:V:75:LEU:HA | 1.82 | 0.44 |
| 21:W:37:THR:HA | 21:W:70:VAL:HG21 | 1.99 | 0.44 |
| 1:A:57:LEU:HA | 1:A:57:LEU:HD23 | 1.73 | 0.44 |
| 1:A:465:HIS:NE2 | 1:A:467:MET:HB2 | 2.31 | 0.44 |
| 2:B:67:LEU:HD13 | 2:B:420:GLN:OE1 | 2.17 | 0.44 |
| 4:D:93:HIS:CE1 | 4:D:94:LYS:HG3 | 2.52 | 0.44 |
| 14:N:44:DG:H2'' | 14:N:45:DG:C8 | 2.51 | 0.44 |
| 16:Q:716:ASN:OD1 | 16:Q:717:THR:N | 2.50 | 0.44 |
| 17:R:428:LEU:HB2 | 17:R:437:PHE:CE2 | 2.52 | 0.44 |
| 23:Y:19:CYS:SG | 23:Y:35:ASN:ND2 | 2.84 | 0.44 |
| 24:Z:280:ARG:HB2 | 24:Z:382:ILE:HG23 | 2.00 | 0.44 |
| 1:A:299:ALA:C | 1:A:301:HIS:H | 2.20 | 0.44 |
| 2:B:139:GLN:OE1 | 2:B:139:GLN:N | 2.49 | 0.44 |
| 2:B:718:GLN:HG2 | 2:B:720:PRO:HD2 | 1.99 | 0.44 |
| 3:C:48:ASP:OD1 | 3:C:175:LYS:NZ | 2.51 | 0.44 |
| 16:Q:667:ARG:HD3 | 16:Q:691:TYR:HE1 | 1.83 | 0.44 |
| 17:R:353:VAL:HG23 | 17:R:456:LYS:NZ | 2.32 | 0.44 |
| 18:T:11:DC:H2'' | 18:T:12:DC:C6 | 2.51 | 0.44 |
| 21:W:203:GLN:OE1 | 21:W:204:LEU:HG | 2.17 | 0.44 |
| 21:W:295:ASP:O | 21:W:297:GLU:HG3 | 2.17 | 0.44 |
| 23:Y:76:ARG:HH11 | 23:Y:109:LYS:HD3 | 1.83 | 0.44 |
| 24:Z:639:LYS:HB2 | 24:Z:642:HIS:HB2 | 1.99 | 0.44 |
| 2:B:92:TYR:N | 2:B:92:TYR:CD2 | 2.84 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:528:LEU:HD23 | 2:B:528:LEU:HA | 1.78 | 0.44 |
| 3:C:107:CYS:HB3 | 3:C:154:ARG:O | 2.17 | 0.44 |
| 14:N:42:DT:C2 | 14:N:43:DG:C6 | 3.06 | 0.44 |
| 16:Q:415:TRP:HA | 16:Q:418:LEU:HD12 | 2.00 | 0.44 |
| 16:Q:868:LYS:HD3 | 16:Q:868:LYS:HA | 1.79 | 0.44 |
| 17:R:353:VAL:HG11 | 17:R:472:ILE:HD12 | 1.99 | 0.44 |
| 24:Z:258:LYS:HB3 | 24:Z:258:LYS:HE2 | 1.73 | 0.44 |
| 24:Z:614:ILE:HA | 24:Z:624:LEU:HA | 1.98 | 0.44 |
| 1:A:59:ASP:OD2 | 1:A:61:ARG:HB2 | 2.18 | 0.44 |
| 1:A:1124:LEU:HA | 1:A:1124:LEU:HD12 | 1.67 | 0.44 |
| 1:A:1168:LYS:HA | 1:A:1168:LYS:HD2 | 1.89 | 0.44 |
| 2:B:652:SER:N | 2:B:655:ASP:OD1 | 2.38 | 0.44 |
| 2:B:737:ILE:HD12 | 2:B:737:ILE:HA | 1.79 | 0.44 |
| 5:E:97:GLU:OE1 | 5:E:97:GLU:N | 2.50 | 0.44 |
| 5:E:99:ILE:O | 5:E:99:ILE:HG13 | 2.18 | 0.44 |
| 7:G:30:LEU:HD12 | 7:G:30:LEU:HA | 1.72 | 0.44 |
| 16:Q:841:LEU:HA | 16:Q:844:LYS:HG2 | 1.99 | 0.44 |
| 20:V:193:HIS:HB3 | 20:V:196:LYS:O | 2.18 | 0.44 |
| 24:Z:479:LYS:O | 24:Z:519:GLN:HG2 | 2.17 | 0.44 |
| 24:Z:489:THR:HB | 24:Z:505:ASP:OD2 | 2.17 | 0.44 |
| 1:A:602:CYS:SG | 1:A:652:LEU:HD13 | 2.57 | 0.44 |
| 1:A:982:ASN:HD22 | 1:A:985:ARG:HB2 | 1.83 | 0.44 |
| 2:B:897:ARG:CB | 2:B:900:GLU:HG3 | 2.48 | 0.44 |
| 8:H:40:ILE:O | 8:H:123:MET:HA | 2.17 | 0.44 |
| 15:P:40:A:H2' | 15:P:41:C:H6 | 1.77 | 0.44 |
| 17:R:366:ARG:HH12 | 24:Z:775:TPO:HA | 1.83 | 0.44 |
| 1:A:249:ILE:HG13 | 1:A:249:ILE:O | 2.16 | 0.44 |
| 1:A:354:LEU:HD23 | 1:A:354:LEU:HA | 1.70 | 0.44 |
| 5:E:37:LEU:HD21 | 5:E:41:LYS:HZ3 | 1.82 | 0.44 |
| 14:N:31:DC:H2'' | 14:N:32:DA:H8 | 1.80 | 0.44 |
| 16:Q:847:GLN:O | 16:Q:851:LEU:HG | 2.17 | 0.44 |
| 20:V:127:VAL:HG23 | 20:V:128:VAL:N | 2.32 | 0.44 |
| 21:W:65:LEU:HD12 | 21:W:84:LEU:C | 2.38 | 0.44 |
| 24:Z:242:VAL:HG23 | 24:Z:245:LEU:HB2 | 2.00 | 0.44 |
| 1:A:198:LEU:O | 1:A:215:LEU:HD12 | 2.18 | 0.44 |
| 2:B:650:ASN:C | 19:U:460:TYR:CE2 | 2.91 | 0.44 |
| 13:M:540:GLY:HA2 | 13:M:560:GLU:H | 1.83 | 0.44 |
| 16:Q:128:GLN:HA | 16:Q:158:GLN:HE22 | 1.82 | 0.44 |
| 16:Q:750:ASP:OD1 | 16:Q:753:LEU:N | 2.40 | 0.44 |
| 16:Q:870:GLU:HA | 16:Q:873:LYS:NZ | 2.32 | 0.44 |
| 17:R:455:TRP:O | 17:R:459:MET:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:W:171:ILE:HG23 | 21:W:187:GLU:HG2 | 1.99 | 0.44 |
| 21:W:253:ASP:OD1 | 21:W:253:ASP:N | 2.51 | 0.44 |
| 24:Z:499:PHE:HB3 | 24:Z:512:LYS:HD2 | 2.00 | 0.44 |
| 1:A:365:THR:HG22 | 1:A:366:VAL:N | 2.31 | 0.44 |
| 1:A:676:ILE:HD12 | 1:A:676:ILE:HG23 | 1.76 | 0.44 |
| 1:A:1467:GLY:C | 1:A:1469:GLY:H | 2.21 | 0.44 |
| 2:B:1151:MET:HE2 | 2:B:1151:MET:HB2 | 1.71 | 0.44 |
| 6:F:105:ILE:HG21 | 6:F:105:ILE:HD13 | 1.63 | 0.44 |
| 11:K:37:LYS:HA | 11:K:37:LYS:HD3 | 1.80 | 0.44 |
| 14:N:37:DG:C2 | 18:T:12:DC:N3 | 2.86 | 0.44 |
| 15:P:39:A:N1 | 15:P:40:A:C6 | 2.86 | 0.44 |
| 16:Q:527:HIS:CD2 | 16:Q:530:TYR:HB2 | 2.53 | 0.44 |
| 16:Q:677:THR:HG22 | 16:Q:679:ASP:H | 1.83 | 0.44 |
| 20:V:182:THR:HA | 20:V:185:ASP:OD2 | 2.17 | 0.44 |
| 21:W:17:ASP:OD2 | 21:W:40:LEU:HB3 | 2.17 | 0.44 |
| 1:A:488:VAL:O | 1:A:488:VAL:HG12 | 2.18 | 0.43 |
| 1:A:812:LYS:HE2 | 9:I:77:THR:HG23 | 1.99 | 0.43 |
| 1:A:1484:MET:N | 1:A:1484:MET:SD | 2.91 | 0.43 |
| 2:B:332:LYS:HZ1 | 2:B:333:GLU:HB2 | 1.83 | 0.43 |
| 2:B:556:ILE:HD12 | 2:B:556:ILE:HA | 1.59 | 0.43 |
| 4:D:60:VAL:HG11 | 7:G:44:PHE:HZ | 1.83 | 0.43 |
| 5:E:58:LEU:HD23 | 5:E:58:LEU:H | 1.81 | 0.43 |
| 5:E:61:LEU:HA | 5:E:61:LEU:HD12 | 1.77 | 0.43 |
| 7:G:151:ARG:HH11 | 24:Z:477:HIS:CD2 | 2.36 | 0.43 |
| 8:H:11:ASP:HB3 | 8:H:55:LYS:HG2 | 2.00 | 0.43 |
| 16:Q:513:PHE:HB2 | 21:W:213:TYR:CE1 | 2.53 | 0.43 |
| 16:Q:530:TYR:CE2 | 16:Q:532:ASP:HB2 | 2.53 | 0.43 |
| 21:W:191:MET:HG3 | 21:W:211:ASP:HB3 | 1.99 | 0.43 |
| 1:A:539:GLN:O | 1:A:540:ASP:C | 2.56 | 0.43 |
| 2:B:705:GLY:O | 2:B:709:SER:HB3 | 2.18 | 0.43 |
| 4:D:93:HIS:HE1 | 4:D:94:LYS:HE3 | 1.83 | 0.43 |
| 7:G:131:MET:SD | 7:G:131:MET:N | 2.92 | 0.43 |
| 10:J:60:LEU:HD23 | 10:J:60:LEU:HA | 1.79 | 0.43 |
| 13:M:1398:LEU:HD11 | 13:M:1415:TYR:CD1 | 2.53 | 0.43 |
| 13:M:1435:CYS:SG | 13:M:1442:LYS:HG2 | 2.58 | 0.43 |
| 16:Q:120:ALA:HB1 | 16:Q:130:HIS:HE1 | 1.83 | 0.43 |
| 16:Q:538:GLY:HA2 | 16:Q:553:TRP:HE3 | 1.83 | 0.43 |
| 18:T:47:DG:H2'' | 18:T:48:DG:H5' | 1.99 | 0.43 |
| 20:V:106:LYS:HA | 20:V:106:LYS:HD2 | 1.87 | 0.43 |
| 21:W:281:LYS:HD2 | 21:W:281:LYS:HA | 1.80 | 0.43 |
| 24:Z:389:THR:O | 24:Z:393:LEU:HG | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:593:ASN:HB3 | 24:Z:595:HIS:CE1 | 2.54 | 0.43 |
| 1:A:75:ALA:O | 2:B:1131:ARG:NH1 | 2.52 | 0.43 |
| 1:A:1403:ASP:O | 1:A:1407:CYS:HB2 | 2.18 | 0.43 |
| 2:B:1173:SER:O | 2:B:1173:SER:OG | 2.36 | 0.43 |
| 4:D:137:LYS:HA | 4:D:137:LYS:HD3 | 1.83 | 0.43 |
| 9:I:53:ILE:HA | 9:I:53:ILE:HD13 | 1.70 | 0.43 |
| 13:M:1476:TYR:CE2 | 13:M:1483:ARG:HD3 | 2.54 | 0.43 |
| 16:Q:218:ARG:HD3 | 16:Q:238:LEU:HD11 | 2.00 | 0.43 |
| 16:Q:710:LYS:HB2 | 16:Q:712:TYR:CE1 | 2.52 | 0.43 |
| 24:Z:188:GLU:OE1 | 24:Z:188:GLU:N | 2.51 | 0.43 |
| 24:Z:420:PHE:HE1 | 24:Z:470:LYS:HG2 | 1.83 | 0.43 |
| 24:Z:464:PRO:HD2 | 24:Z:467:GLU:HB3 | 1.99 | 0.43 |
| 1:A:106:VAL:O | 1:A:110:VAL:HG22 | 2.19 | 0.43 |
| 1:A:818:GLU:OE2 | 17:R:599:CYS:HA | 2.18 | 0.43 |
| 1:A:996:ILE:HD13 | 1:A:996:ILE:HA | 1.62 | 0.43 |
| 2:B:83:ARG:HH22 | 2:B:133:ILE:CG2 | 2.31 | 0.43 |
| 2:B:399:LEU:HA | 2:B:399:LEU:HD23 | 1.80 | 0.43 |
| 2:B:576:ILE:HD12 | 2:B:576:ILE:HA | 1.79 | 0.43 |
| 5:E:55:ARG:HA | 5:E:58:LEU:CD2 | 2.48 | 0.43 |
| 16:Q:68:ARG:NH1 | 16:Q:82:GLN:HE22 | 2.16 | 0.43 |
| 16:Q:503:LEU:HG | 16:Q:507:TYR:CE2 | 2.53 | 0.43 |
| 1:A:413:TYR:OH | 1:A:450:MET:O | 2.32 | 0.43 |
| 2:B:472:ARG:HA | 2:B:472:ARG:HD2 | 1.92 | 0.43 |
| 2:B:497:LYS:HG3 | 2:B:498:PRO:CD | 2.46 | 0.43 |
| 2:B:553:LEU:HA | 2:B:553:LEU:HD12 | 1.73 | 0.43 |
| 5:E:3:ASP:OD1 | 5:E:49:SER:OG | 2.20 | 0.43 |
| 5:E:27:LEU:HD12 | 5:E:27:LEU:HA | 1.77 | 0.43 |
| 5:E:72:MET:HB2 | 5:E:72:MET:HE3 | 1.77 | 0.43 |
| 7:G:104:MET:HG3 | 7:G:157:ILE:O | 2.19 | 0.43 |
| 16:Q:268:ASN:HD22 | 16:Q:271:VAL:HG12 | 1.84 | 0.43 |
| 16:Q:456:ASN:OD1 | 20:V:48:PHE:HA | 2.18 | 0.43 |
| 16:Q:772:GLU:HB3 | 16:Q:774:SER:OG | 2.18 | 0.43 |
| 16:Q:877:GLN:OE1 | 16:Q:881:TYR:CE1 | 2.72 | 0.43 |
| 17:R:359:LEU:HD22 | 17:R:452:PHE:HE1 | 1.84 | 0.43 |
| 17:R:456:LYS:NZ | 17:R:466:LEU:HD13 | 2.33 | 0.43 |
| 21:W:40:LEU:HA | 21:W:66:GLY:HA3 | 2.01 | 0.43 |
| 21:W:152:LEU:HD12 | 21:W:167:ALA:O | 2.19 | 0.43 |
| 21:W:252:SER:HB3 | 21:W:276:GLN:OE1 | 2.18 | 0.43 |
| 24:Z:291:ALA:HB2 | 24:Z:307:MET:HG2 | 2.00 | 0.43 |
| 24:Z:502:LEU:HD21 | 24:Z:511:LEU:HD22 | 2.00 | 0.43 |
| 24:Z:557:THR:O | 24:Z:558:PHE:CD1 | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:520:VAL:HG13 | 2:B:520:VAL:O | 2.19 | 0.43 |
| 7:G:91:GLN:HB3 | 7:G:98:PHE:HD2 | 1.83 | 0.43 |
| 13:M:1037:ILE:H | 13:M:1055:GLY:HA2 | 1.84 | 0.43 |
| 13:M:1341:LYS:HA | 13:M:1341:LYS:HD2 | 1.85 | 0.43 |
| 14:N:10:DG:H2" | 14:N:11:DC:C6 | 2.54 | 0.43 |
| 16:Q:69:ILE:H | 16:Q:69:ILE:HD12 | 1.84 | 0.43 |
| 16:Q:239:ALA:O | 16:Q:243:LEU:HG | 2.17 | 0.43 |
| 16:Q:464:LEU:HB2 | 16:Q:466:ASN:HD22 | 1.84 | 0.43 |
| 16:Q:527:HIS:HD2 | 16:Q:530:TYR:HB2 | 1.83 | 0.43 |
| 16:Q:691:TYR:HB3 | 16:Q:699:SER:OG | 2.19 | 0.43 |
| 23:Y:29:GLU:HG3 | 23:Y:45:ASN:O | 2.19 | 0.43 |
| 24:Z:200:PHE:HA | 24:Z:210:LEU:HD13 | 2.00 | 0.43 |
| 24:Z:540:VAL:HB | 24:Z:575:VAL:CG2 | 2.49 | 0.43 |
| 1:A:417:LYS:HE2 | 1:A:418:TYR:CE2 | 2.53 | 0.43 |
| 1:A:479:TRP:CD1 | 1:A:479:TRP:N | 2.87 | 0.43 |
| 2:B:472:ARG:HH11 | 2:B:472:ARG:HD3 | 1.65 | 0.43 |
| 2:B:679:PRO:HG2 | 2:B:680:ASP:N | 2.33 | 0.43 |
| 2:B:907:VAL:HG22 | 2:B:921:ILE:HG12 | 2.00 | 0.43 |
| 3:C:94:CYS:SG | 3:C:95:PRO:HD2 | 2.59 | 0.43 |
| 16:Q:762:GLN:O | 16:Q:766:THR:HG22 | 2.18 | 0.43 |
| 1:A:37:THR:HG21 | 1:A:41:ILE:HD11 | 2.01 | 0.43 |
| 1:A:1178:ASP:OD1 | 1:A:1185:VAL:HG13 | 2.18 | 0.43 |
| 2:B:254:GLN:O | 2:B:303:PRO:HB2 | 2.19 | 0.43 |
| 2:B:577:HIS:CE1 | 2:B:583:LEU:HD11 | 2.53 | 0.43 |
| 2:B:625:LEU:HA | 2:B:625:LEU:HD23 | 1.87 | 0.43 |
| 2:B:866:ILE:HG23 | 2:B:866:ILE:HD12 | 1.57 | 0.43 |
| 2:B:1142:ASN:ND2 | 2:B:1145:GLN:HB2 | 2.27 | 0.43 |
| 7:G:151:ARG:HA | 24:Z:477:HIS:CE1 | 2.54 | 0.43 |
| 8:H:15:ILE:HG23 | 8:H:16:ASP:N | 2.33 | 0.43 |
| 11:K:12:LEU:HD23 | 11:K:12:LEU:HA | 1.86 | 0.43 |
| 16:Q:380:ILE:HD12 | 16:Q:400:HIS:CE1 | 2.53 | 0.43 |
| 17:R:454:LYS:HA | 17:R:454:LYS:HD2 | 1.77 | 0.43 |
| 2:B:100:GLU:HA | 2:B:105:PRO:HB3 | 1.99 | 0.43 |
| 2:B:313:GLU:HG3 | 2:B:315:ASN:H | 1.82 | 0.43 |
| 4:D:33:LEU:HD21 | 4:D:97:LEU:HD23 | 2.00 | 0.43 |
| 7:G:81:LYS:HG3 | 7:G:148:VAL:C | 2.39 | 0.43 |
| 16:Q:471:LYS:O | 16:Q:475:LEU:HD23 | 2.18 | 0.43 |
| 16:Q:484:GLU:HB2 | 16:Q:492:TYR:HB3 | 2.00 | 0.43 |
| 21:W:25:GLY:N | 21:W:72:ILE:HD12 | 2.34 | 0.43 |
| 21:W:84:LEU:HD21 | 21:W:110:TRP:CZ3 | 2.53 | 0.43 |
| 21:W:231:HIS:CG | 21:W:251:SER:HB3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:189:PRO:HA | 1:A:201:GLU:O | 2.19 | 0.43 |
| 1:A:592:PHE:CD2 | 1:A:592:PHE:O | 2.71 | 0.43 |
| 1:A:770:VAL:HG21 | 1:A:781:ILE:HD11 | 2.01 | 0.43 |
| 1:A:783:GLN:HA | 1:A:787:VAL:O | 2.19 | 0.43 |
| 1:A:1006:PRO:O | 1:A:1010:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1551:ALA:O | 13:M:1509:ARG:HD2 | 2.19 | 0.43 |
| 4:D:17:ALA:HB1 | 4:D:95:PHE:CZ | 2.54 | 0.43 |
| 7:G:80:PHE:HB2 | 7:G:83:GLU:CD | 2.40 | 0.43 |
| 16:Q:645:LYS:HE3 | 22:X:243:LYS:NZ | 2.33 | 0.43 |
| 16:Q:651:ASN:HB3 | 20:V:37:ASN:HD21 | 1.82 | 0.43 |
| 16:Q:651:ASN:ND2 | 16:Q:682:ASP:OD2 | 2.52 | 0.43 |
| 16:Q:653:ILE:O | 16:Q:656:VAL:HG22 | 2.19 | 0.43 |
| 17:R:378:PHE:CZ | 17:R:382:VAL:HG11 | 2.54 | 0.43 |
| 18:T:35:DG:N2 | 18:T:36:DC:O2 | 2.51 | 0.43 |
| 19:U:459:VAL:HG23 | 19:U:494:HIS:C | 2.39 | 0.43 |
| 24:Z:196:LEU:HD12 | 24:Z:196:LEU:HA | 1.79 | 0.43 |
| 24:Z:478:VAL:O | 24:Z:489:THR:HA | 2.19 | 0.43 |
| 1:A:1132:LYS:H | 1:A:1132:LYS:HG2 | 1.65 | 0.42 |
| 1:A:1463:LEU:HA | 1:A:1463:LEU:HD12 | 1.59 | 0.42 |
| 2:B:501:LEU:HD12 | 2:B:505:LEU:HD12 | 2.01 | 0.42 |
| 2:B:1038:THR:HA | 3:C:195:THR:HA | 1.99 | 0.42 |
| 15:P:35:A:H5' | 15:P:36:G:OP2 | 2.18 | 0.42 |
| 16:Q:689:HIS:HB2 | 20:V:35:TYR:HE1 | 1.84 | 0.42 |
| 16:Q:725:ARG:NE | 20:V:31:CYS:SG | 2.92 | 0.42 |
| 16:Q:729:LYS:HB2 | 16:Q:732:LYS:CD | 2.46 | 0.42 |
| 16:Q:750:ASP:OD1 | 16:Q:753:LEU:HG | 2.18 | 0.42 |
| 21:W:9:PHE:CE2 | 21:W:54:LEU:HB3 | 2.54 | 0.42 |
| 24:Z:261:THR:O | 24:Z:264:LEU:HG | 2.18 | 0.42 |
| 24:Z:492:ILE:HA | 24:Z:502:LEU:HA | 1.99 | 0.42 |
| 24:Z:602:VAL:HG21 | 24:Z:636:PHE:HE2 | 1.83 | 0.42 |
| 24:Z:705:LEU:HD12 | 24:Z:724:VAL:HG11 | 2.01 | 0.42 |
| 1:A:130:LEU:HD11 | 1:A:235:VAL:HG13 | 2.01 | 0.42 |
| 1:A:510:GLU:OE1 | 2:B:1101:GLN:NE2 | 2.52 | 0.42 |
| 1:A:639:ILE:HG21 | 1:A:639:ILE:HD13 | 1.81 | 0.42 |
| 1:A:1179:PRO:HA | 1:A:1209:PRO:CB | 2.49 | 0.42 |
| 1:A:1323:THR:HG22 | 1:A:1329:LYS:HD2 | 2.01 | 0.42 |
| 2:B:568:PHE:CE1 | 2:B:573:TRP:HB2 | 2.54 | 0.42 |
| 3:C:67:ARG:NH1 | 10:J:2:ILE:HG23 | 2.33 | 0.42 |
| 3:C:75:SER:HB3 | 3:C:79:VAL:HB | 2.01 | 0.42 |
| 4:D:22:PHE:HB2 | 4:D:27:GLU:OE1 | 2.18 | 0.42 |
| 16:Q:508:GLU:OE2 | 16:Q:540:MET:HG3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:W:163:LEU:HB2 | 21:W:177:ILE:HG23 | 2.00 | 0.42 |
| 24:Z:439:LYS:O | 24:Z:452:PRO:HA | 2.19 | 0.42 |
| 1:A:20:ARG:NH1 | 1:A:22:GLN:OE1 | 2.52 | 0.42 |
| 1:A:1177:TYR:CE2 | 1:A:1210:TRP:CE3 | 3.06 | 0.42 |
| 2:B:186:ILE:HG21 | 2:B:186:ILE:HD13 | 1.74 | 0.42 |
| 3:C:268:GLN:HG3 | 3:C:269:SER:N | 2.34 | 0.42 |
| 4:D:16:ASP:H | 4:D:21:ILE:CG2 | 2.32 | 0.42 |
| 4:D:122:PHE:HD1 | 4:D:126:GLU:CD | 2.23 | 0.42 |
| 16:Q:182:ALA:O | 16:Q:186:TYR:CD2 | 2.72 | 0.42 |
| 16:Q:365:GLU:HG2 | 16:Q:369:LYS:NZ | 2.34 | 0.42 |
| 16:Q:745:HIS:HB2 | 21:W:20:TRP:CH2 | 2.53 | 0.42 |
| 20:V:196:LYS:O | 20:V:198:ARG:N | 2.49 | 0.42 |
| 21:W:135:VAL:HG23 | 21:W:136:GLU:HG2 | 2.01 | 0.42 |
| 21:W:170:GLY:HA2 | 21:W:193:ILE:HG13 | 2.01 | 0.42 |
| 24:Z:525:ALA:O | 24:Z:552:ARG:NH1 | 2.49 | 0.42 |
| 1:A:104:MET:HE1 | 1:A:193:ARG:HD2 | 2.01 | 0.42 |
| 1:A:338:SER:OG | 1:A:341:GLN:HG2 | 2.20 | 0.42 |
| 1:A:421:ARG:HA | 1:A:444:TYR:CD1 | 2.55 | 0.42 |
| 1:A:421:ARG:HE | 1:A:427:ILE:HD11 | 1.85 | 0.42 |
| 1:A:461:GLN:O | 1:A:463:THR:N | 2.52 | 0.42 |
| 1:A:1137:PRO:O | 1:A:1341:VAL:HG23 | 2.20 | 0.42 |
| 7:G:127:CYS:SG | 7:G:138:GLN:HB3 | 2.60 | 0.42 |
| 14:N:35:DA:H2'' | 14:N:36:DG:C8 | 2.53 | 0.42 |
| 16:Q:611:TRP:HZ2 | 16:Q:631:ARG:HH11 | 1.65 | 0.42 |
| 16:Q:880:GLN:HE21 | 16:Q:884:LYS:CE | 2.32 | 0.42 |
| 17:R:578:ALA:HA | 20:V:127:VAL:HB | 2.01 | 0.42 |
| 1:A:427:ILE:N | 1:A:427:ILE:HD12 | 2.35 | 0.42 |
| 1:A:569:THR:HG23 | 1:A:671:ASN:HD21 | 1.85 | 0.42 |
| 1:A:820:ARG:HH11 | 1:A:820:ARG:HD3 | 1.66 | 0.42 |
| 1:A:1343:LEU:HD12 | 1:A:1343:LEU:HA | 1.76 | 0.42 |
| 2:B:319:ASN:ND2 | 2:B:332:LYS:HG2 | 2.34 | 0.42 |
| 2:B:544:PHE:CE2 | 2:B:548:TRP:NE1 | 2.81 | 0.42 |
| 2:B:544:PHE:CZ | 2:B:548:TRP:NE1 | 2.87 | 0.42 |
| 2:B:574:VAL:O | 2:B:574:VAL:HG22 | 2.20 | 0.42 |
| 2:B:841:ARG:HD3 | 2:B:841:ARG:HA | 1.77 | 0.42 |
| 13:M:1408:LEU:HD23 | 13:M:1408:LEU:H | 1.84 | 0.42 |
| 13:M:1490:THR:OG1 | 13:M:1493:GLY:N | 2.53 | 0.42 |
| 14:N:37:DG:C6 | 18:T:12:DC:N4 | 2.79 | 0.42 |
| 15:P:37:G:C2' | 15:P:38:G:H8 | 2.33 | 0.42 |
| 16:Q:62:LYS:HA | 16:Q:62:LYS:HD3 | 1.74 | 0.42 |
| 16:Q:240:VAL:HG11 | 20:V:72:HIS:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:598:GLN:HA | 16:Q:599:SER:HA | 1.76 | 0.42 |
| 16:Q:719:VAL:HG23 | 16:Q:720:VAL:N | 2.35 | 0.42 |
| 17:R:581:ALA:CB | 20:V:127:VAL:HG21 | 2.48 | 0.42 |
| 21:W:11:GLN:HE21 | 21:W:54:LEU:HD23 | 1.85 | 0.42 |
| 21:W:288:LYS:HA | 21:W:288:LYS:HD3 | 1.77 | 0.42 |
| 1:A:503:LEU:O | 1:A:503:LEU:HD23 | 2.19 | 0.42 |
| 1:A:909:LEU:O | 1:A:910:LYS:HG2 | 2.20 | 0.42 |
| 1:A:932:ARG:HD3 | 8:H:106:THR:O | 2.19 | 0.42 |
| 1:A:1166:LEU:HA | 1:A:1166:LEU:HD23 | 1.84 | 0.42 |
| 1:A:1401:LEU:O | 1:A:1405:MET:HG3 | 2.19 | 0.42 |
| 2:B:412:LEU:HD23 | 2:B:412:LEU:HA | 1.71 | 0.42 |
| 2:B:428:ASP:OD1 | 2:B:429:PHE:N | 2.52 | 0.42 |
| 2:B:638:ARG:HH21 | 2:B:639:HIS:CE1 | 2.38 | 0.42 |
| 2:B:1125:MET:HE3 | 2:B:1156:LYS:HG2 | 2.02 | 0.42 |
| 3:C:263:LEU:HD13 | 11:K:19:ILE:HD13 | 2.00 | 0.42 |
| 5:E:96:GLU:OE1 | 5:E:96:GLU:N | 2.52 | 0.42 |
| 7:G:106:CYS:SG | 7:G:159:ALA:HB3 | 2.59 | 0.42 |
| 11:K:101:LEU:HA | 11:K:101:LEU:HD12 | 1.85 | 0.42 |
| 14:N:12:DG:C6 | 18:T:38:DG:N2 | 2.87 | 0.42 |
| 14:N:14:DC:OP2 | 24:Z:186:ILE:HD12 | 2.19 | 0.42 |
| 16:Q:384:LEU:HD11 | 16:Q:393:LYS:O | 2.20 | 0.42 |
| 16:Q:542:ARG:HD2 | 16:Q:554:PHE:HE2 | 1.83 | 0.42 |
| 16:Q:553:TRP:HA | 16:Q:556:GLU:OE1 | 2.19 | 0.42 |
| 17:R:397:LYS:O | 24:Z:777:MET:HE3 | 2.19 | 0.42 |
| 17:R:429:ARG:HB2 | 17:R:434:GLN:HB3 | 2.02 | 0.42 |
| 17:R:492:ILE:H | 17:R:492:ILE:HD12 | 1.83 | 0.42 |
| 22:X:250:PHE:HA | 22:X:253:LEU:HB3 | 2.02 | 0.42 |
| 23:Y:18:LEU:HD23 | 23:Y:18:LEU:HA | 1.86 | 0.42 |
| 24:Z:178:ASN:OD1 | 24:Z:179:LEU:N | 2.47 | 0.42 |
| 1:A:1038:THR:O | 1:A:1042:ASN:ND2 | 2.52 | 0.42 |
| 2:B:235:ILE:HD12 | 2:B:235:ILE:HG23 | 1.64 | 0.42 |
| 2:B:479:LEU:HD23 | 2:B:479:LEU:HA | 1.79 | 0.42 |
| 2:B:557:SER:O | 2:B:559:ALA:N | 2.53 | 0.42 |
| 2:B:666:ASP:N | 2:B:666:ASP:OD1 | 2.48 | 0.42 |
| 2:B:1062:ARG:CZ | 2:B:1065:GLY:H | 2.32 | 0.42 |
| 5:E:27:LEU:HD13 | 5:E:65:ASN:ND2 | 2.35 | 0.42 |
| 13:M:1421:SER:OG | 13:M:1424:ARG:NH2 | 2.53 | 0.42 |
| 21:W:228:LEU:HD11 | 21:W:259:TRP:CE3 | 2.54 | 0.42 |
| 24:Z:450:ILE:O | 24:Z:462:GLU:HA | 2.20 | 0.42 |
| 1:A:361:PHE:HA | 1:A:388:MET:HE2 | 2.02 | 0.42 |
| 1:A:362:SER:O | 1:A:388:MET:HE1 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:933:THR:OG1 | 1:A:934:LEU:HG | 2.19 | 0.42 |
| 1:A:965:VAL:O | 1:A:968:VAL:HG22 | 2.19 | 0.42 |
| 2:B:355:ASP:N | 2:B:355:ASP:OD2 | 2.52 | 0.42 |
| 3:C:131:THR:HG22 | 3:C:147:ASP:OD1 | 2.20 | 0.42 |
| 3:C:172:GLU:HG2 | 11:K:10:PHE:CE1 | 2.54 | 0.42 |
| 4:D:100:LEU:HD11 | 4:D:118:LEU:HD21 | 2.01 | 0.42 |
| 5:E:61:LEU:HD23 | 16:Q:884:LYS:HG2 | 2.02 | 0.42 |
| 16:Q:188:LYS:HA | 16:Q:191:ARG:HG2 | 2.01 | 0.42 |
| 16:Q:310:TYR:OH | 20:V:67:GLU:OE2 | 2.36 | 0.42 |
| 16:Q:773:LYS:HE2 | 16:Q:827:HIS:HE1 | 1.84 | 0.42 |
| 20:V:49:ILE:HG22 | 22:X:227:ARG:HG3 | 2.01 | 0.42 |
| 21:W:83:SER:HB3 | 21:W:85:ASP:OD1 | 2.20 | 0.42 |
| 22:X:221:THR:O | 22:X:225:VAL:HG22 | 2.19 | 0.42 |
| 1:A:374:SER:OG | 1:A:375:ILE:N | 2.53 | 0.42 |
| 1:A:621:ILE:HG21 | 1:A:621:ILE:HD13 | 1.78 | 0.42 |
| 1:A:1417:HIS:HA | 1:A:1421:ARG:NH1 | 2.35 | 0.42 |
| 2:B:44:LEU:HD23 | 2:B:155:MET:HE2 | 2.01 | 0.42 |
| 2:B:839:GLY:O | 2:B:891:ASP:HB2 | 2.20 | 0.42 |
| 7:G:119:PHE:HA | 7:G:128:TYR:CE1 | 2.54 | 0.42 |
| 8:H:132:LEU:HA | 8:H:132:LEU:HD23 | 1.81 | 0.42 |
| 16:Q:132:LEU:HD11 | 20:V:85:ASP:HA | 2.01 | 0.42 |
| 16:Q:211:LEU:HB2 | 16:Q:213:LYS:CE | 2.49 | 0.42 |
| 16:Q:639:VAL:HA | 16:Q:642:ASN:OD1 | 2.20 | 0.42 |
| 16:Q:652:GLY:O | 16:Q:656:VAL:HG13 | 2.20 | 0.42 |
| 17:R:414:VAL:HA | 17:R:423:ASN:HB3 | 2.02 | 0.42 |
| 17:R:429:ARG:NH2 | 17:R:431:GLY:O | 2.51 | 0.42 |
| 17:R:452:PHE:HD2 | 17:R:453:MET:CE | 2.33 | 0.42 |
| 20:V:47:LYS:HA | 20:V:47:LYS:HD3 | 1.75 | 0.42 |
| 21:W:108:ASP:OD1 | 21:W:126:HIS:ND1 | 2.53 | 0.42 |
| 21:W:214:ILE:HD12 | 21:W:228:LEU:HD23 | 2.02 | 0.42 |
| 21:W:231:HIS:CE1 | 21:W:249:SER:HG | 2.38 | 0.42 |
| 24:Z:490:GLY:HA3 | 24:Z:503:PHE:O | 2.20 | 0.42 |
| 24:Z:526:SER:OG | 24:Z:527:GLY:N | 2.53 | 0.42 |
| 1:A:339:LEU:HD23 | 1:A:339:LEU:HA | 1.77 | 0.42 |
| 1:A:680:LEU:HD12 | 1:A:680:LEU:HA | 1.85 | 0.42 |
| 1:A:828:LEU:HD12 | 1:A:828:LEU:HA | 1.85 | 0.42 |
| 2:B:53:MET:HB3 | 2:B:57:ARG:HH21 | 1.84 | 0.42 |
| 2:B:583:LEU:O | 2:B:587:LEU:HD23 | 2.20 | 0.42 |
| 2:B:847:LYS:HE3 | 2:B:864:ASP:OD2 | 2.20 | 0.42 |
| 3:C:113:ARG:HD2 | 3:C:113:ARG:HA | 1.90 | 0.42 |
| 5:E:64:HIS:ND1 | 5:E:65:ASN:N | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:16:ASN:N | 10:J:16:ASN:OD1 | 2.24 | 0.42 |
| 12:L:35:ARG:HH21 | 12:L:40:GLY:HA3 | 1.83 | 0.42 |
| 15:P:27:A:O2' | 15:P:28:A:O5' | 2.36 | 0.42 |
| 16:Q:152:PHE:HD1 | 16:Q:172:ILE:HD11 | 1.83 | 0.42 |
| 17:R:452:PHE:O | 17:R:456:LYS:HG2 | 2.20 | 0.42 |
| 20:V:121:SER:O | 20:V:121:SER:OG | 2.37 | 0.42 |
| 21:W:155:ALA:O | 21:W:163:LEU:HG | 2.20 | 0.42 |
| 24:Z:176:ASP:OD2 | 24:Z:176:ASP:N | 2.53 | 0.42 |
| 1:A:465:HIS:CD2 | 1:A:467:MET:HB2 | 2.54 | 0.41 |
| 1:A:636:ILE:HG23 | 1:A:636:ILE:HD12 | 1.66 | 0.41 |
| 1:A:832:THR:HG23 | 1:A:833:PRO:HD2 | 2.02 | 0.41 |
| 1:A:1316:ASN:OD1 | 1:A:1317:LYS:N | 2.52 | 0.41 |
| 2:B:309:PHE:CD2 | 9:I:40:ARG:NE | 2.88 | 0.41 |
| 2:B:835:GLU:OE1 | 2:B:835:GLU:N | 2.53 | 0.41 |
| 2:B:1116:VAL:HG11 | 2:B:1125:MET:HE3 | 2.02 | 0.41 |
| 5:E:10:LEU:HD23 | 5:E:10:LEU:HA | 1.79 | 0.41 |
| 7:G:111:HIS:CD2 | 24:Z:501:ILE:HD13 | 2.54 | 0.41 |
| 9:I:31:GLU:OE1 | 9:I:31:GLU:N | 2.53 | 0.41 |
| 16:Q:707:CYS:SG | 16:Q:708:LEU:N | 2.93 | 0.41 |
| 16:Q:744:ARG:HG3 | 16:Q:753:LEU:HD12 | 2.02 | 0.41 |
| 17:R:563:ILE:HD12 | 17:R:566:ARG:HD2 | 2.02 | 0.41 |
| 18:T:6:DC:H1' | 18:T:7:DA:C8 | 2.55 | 0.41 |
| 20:V:51:TYR:CD1 | 20:V:52:PRO:HD2 | 2.55 | 0.41 |
| 23:Y:14:ARG:NH1 | 24:Z:300:GLN:OE1 | 2.53 | 0.41 |
| 1:A:321:GLU:HG2 | 1:A:327:ARG:NH2 | 2.35 | 0.41 |
| 1:A:912:SER:O | 1:A:914:LYS:N | 2.54 | 0.41 |
| 1:A:1216:LEU:HA | 1:A:1216:LEU:HD23 | 1.86 | 0.41 |
| 2:B:86:LEU:HD12 | 2:B:86:LEU:HA | 1.84 | 0.41 |
| 2:B:544:PHE:O | 2:B:547:GLU:N | 2.48 | 0.41 |
| 2:B:679:PRO:CG | 2:B:680:ASP:N | 2.84 | 0.41 |
| 2:B:993:LYS:HD3 | 20:V:131:MET:SD | 2.60 | 0.41 |
| 5:E:37:LEU:O | 5:E:41:LYS:HG3 | 2.20 | 0.41 |
| 5:E:166:ARG:NH1 | 5:E:168:ASN:HB3 | 2.35 | 0.41 |
| 7:G:24:ASN:O | 7:G:28:GLN:HG2 | 2.20 | 0.41 |
| 9:I:109:ARG:HD3 | 9:I:124:THR:CG2 | 2.46 | 0.41 |
| 16:Q:858:LYS:HA | 16:Q:861:GLU:HG3 | 2.03 | 0.41 |
| 24:Z:199:LYS:HG3 | 24:Z:203:TYR:HD2 | 1.84 | 0.41 |
| 1:A:993:ILE:HD13 | 1:A:993:ILE:HG21 | 1.81 | 0.41 |
| 1:A:1217:ASP:OD2 | 1:A:1218:ARG:N | 2.53 | 0.41 |
| 2:B:199:LYS:HB3 | 2:B:199:LYS:HE2 | 1.87 | 0.41 |
| 2:B:566:LYS:HG2 | 2:B:576:ILE:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:597:ILE:HG22 | 2:B:601:VAL:HB | 2.01 | 0.41 |
| 2:B:739:ASN:N | 2:B:739:ASN:OD1 | 2.53 | 0.41 |
| 4:D:112:LYS:HE3 | 4:D:112:LYS:HB2 | 1.74 | 0.41 |
| 13:M:758:TYR:N | 13:M:920:ILE:O | 2.49 | 0.41 |
| 16:Q:215:GLU:HG2 | 16:Q:216:LYS:NZ | 2.35 | 0.41 |
| 16:Q:431:LEU:HD23 | 16:Q:431:LEU:HA | 1.83 | 0.41 |
| 16:Q:791:ARG:HH12 | 21:W:87:HIS:CD2 | 2.38 | 0.41 |
| 17:R:397:LYS:HA | 17:R:397:LYS:HD2 | 1.85 | 0.41 |
| 17:R:402:VAL:HB | 17:R:455:TRP:HB2 | 2.02 | 0.41 |
| 17:R:485:TYR:HD1 | 17:R:487:PHE:CE1 | 2.38 | 0.41 |
| 21:W:25:GLY:HA3 | 21:W:31:ASN:C | 2.40 | 0.41 |
| 1:A:140:ARG:NH2 | 1:A:234:PHE:O | 2.50 | 0.41 |
| 1:A:561:MET:SD | 11:K:58:PHE:HA | 2.59 | 0.41 |
| 1:A:1165:THR:HG22 | 1:A:1297:THR:H | 1.85 | 0.41 |
| 1:A:1255:LEU:HD12 | 1:A:1255:LEU:N | 2.34 | 0.41 |
| 2:B:105:PRO:HG2 | 19:U:512:THR:CA | 2.37 | 0.41 |
| 3:C:64:ILE:HG23 | 3:C:64:ILE:HD12 | 1.70 | 0.41 |
| 3:C:166:LYS:HE2 | 3:C:166:LYS:HB3 | 1.74 | 0.41 |
| 4:D:41:LEU:HB3 | 4:D:65:LEU:CD2 | 2.50 | 0.41 |
| 4:D:84:ARG:HG3 | 4:D:97:LEU:HD11 | 2.02 | 0.41 |
| 6:F:90:LEU:HA | 6:F:90:LEU:HD23 | 1.82 | 0.41 |
| 10:J:49:LEU:HD23 | 10:J:49:LEU:HA | 1.82 | 0.41 |
| 16:Q:345:PHE:O | 16:Q:349:GLN:HG2 | 2.20 | 0.41 |
| 16:Q:537:LEU:HB3 | 16:Q:553:TRP:CZ3 | 2.55 | 0.41 |
| 16:Q:572:GLY:O | 16:Q:576:LEU:HG | 2.20 | 0.41 |
| 16:Q:851:LEU:O | 16:Q:855:LYS:HG2 | 2.21 | 0.41 |
| 21:W:8:LEU:HD13 | 21:W:288:LYS:HE3 | 2.01 | 0.41 |
| 22:X:246:SER:HA | 22:X:249:ILE:HD12 | 2.02 | 0.41 |
| 24:Z:439:LYS:H | 24:Z:453:LYS:H | 1.66 | 0.41 |
| 24:Z:548:GLY:HA3 | 24:Z:562:ASN:HA | 2.01 | 0.41 |
| 24:Z:593:ASN:HB3 | 24:Z:595:HIS:HE1 | 1.84 | 0.41 |
| 1:A:544:ALA:HB2 | 1:A:680:LEU:HD22 | 2.03 | 0.41 |
| 1:A:618:TYR:HB3 | 1:A:621:ILE:O | 2.21 | 0.41 |
| 1:A:1321:ILE:O | 1:A:1328:PHE:O | 2.38 | 0.41 |
| 2:B:305:LEU:HD12 | 2:B:305:LEU:HA | 1.74 | 0.41 |
| 3:C:259:LEU:HA | 3:C:259:LEU:HD12 | 1.81 | 0.41 |
| 5:E:39:GLU:O | 5:E:43:GLN:HB2 | 2.20 | 0.41 |
| 10:J:30:THR:HG22 | 10:J:33:ASP:HB2 | 2.02 | 0.41 |
| 11:K:109:ILE:HD13 | 11:K:109:ILE:HA | 1.88 | 0.41 |
| 16:Q:202:LEU:HD21 | 16:Q:233:GLY:HA3 | 2.02 | 0.41 |
| 16:Q:424:GLN:HB2 | 22:X:231:TRP:CZ3 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:T:37:DC:C4 | 18:T:38:DG:C6 | 3.08 | 0.41 |
| 21:W:84:LEU:HD23 | 21:W:84:LEU:HA | 1.77 | 0.41 |
| 1:A:725:LEU:HD21 | 1:A:736:THR:HG23 | 2.02 | 0.41 |
| 2:B:186:ILE:O | 2:B:187:ILE:HD13 | 2.20 | 0.41 |
| 2:B:322:GLY:CA | 2:B:339:ALA:HB2 | 2.50 | 0.41 |
| 2:B:422:PHE:HB3 | 2:B:429:PHE:CB | 2.50 | 0.41 |
| 2:B:509:VAL:HG11 | 2:B:524:LYS:HD2 | 2.01 | 0.41 |
| 2:B:937:SER:OG | 2:B:938:ARG:N | 2.53 | 0.41 |
| 4:D:110:GLU:O | 4:D:114:LEU:HD23 | 2.21 | 0.41 |
| 5:E:36:THR:OG1 | 5:E:39:GLU:OE1 | 2.29 | 0.41 |
| 13:M:623:LYS:O | 13:M:627:ASP:N | 2.51 | 0.41 |
| 16:Q:285:TYR:HA | 16:Q:288:VAL:HG12 | 2.01 | 0.41 |
| 16:Q:720:VAL:HG21 | 16:Q:743:ALA:HB2 | 2.01 | 0.41 |
| 16:Q:733:LEU:HA | 16:Q:733:LEU:HD23 | 1.72 | 0.41 |
| 17:R:507:PRO:HA | 17:R:508:ASN:HA | 1.49 | 0.41 |
| 21:W:46:VAL:CG2 | 21:W:58:TRP:HB2 | 2.51 | 0.41 |
| 24:Z:601:LYS:HG3 | 24:Z:611:GLU:OE2 | 2.20 | 0.41 |
| 24:Z:736:LEU:HA | 24:Z:736:LEU:HD23 | 1.79 | 0.41 |
| 1:A:46:THR:OG1 | 1:A:47:THR:N | 2.53 | 0.41 |
| 1:A:626:THR:O | 1:A:627:LYS:HB3 | 2.21 | 0.41 |
| 1:A:849:ASP:HA | 1:A:852:VAL:HG22 | 2.03 | 0.41 |
| 1:A:875:TYR:OH | 6:F:61:GLU:OE2 | 2.28 | 0.41 |
| 2:B:273:PHE:CG | 2:B:284:ILE:HG23 | 2.56 | 0.41 |
| 2:B:312:GLN:OE1 | 9:I:40:ARG:NH2 | 2.54 | 0.41 |
| 5:E:111:THR:O | 5:E:114:ALA:N | 2.52 | 0.41 |
| 7:G:7:LEU:HB2 | 7:G:72:TYR:CE2 | 2.55 | 0.41 |
| 13:M:1354:ASP:O | 13:M:1372:LYS:HG2 | 2.20 | 0.41 |
| 13:M:1474:LEU:HD21 | 13:M:1511:PHE:CE1 | 2.55 | 0.41 |
| 17:R:440:GLU:HG3 | 17:R:441:PHE:CE1 | 2.55 | 0.41 |
| 21:W:27:ASN:ND2 | 21:W:74:HIS:O | 2.53 | 0.41 |
| 24:Z:192:THR:OG1 | 24:Z:244:ASN:ND2 | 2.54 | 0.41 |
| 1:A:151:LYS:O | 1:A:152:ASN:ND2 | 2.53 | 0.41 |
| 1:A:954:ARG:HH11 | 1:A:954:ARG:HD2 | 1.74 | 0.41 |
| 1:A:1290:SER:O | 1:A:1294:THR:HG23 | 2.21 | 0.41 |
| 2:B:817:GLN:HB3 | 2:B:918:PHE:HD1 | 1.84 | 0.41 |
| 3:C:34:ILE:HG21 | 3:C:34:ILE:HD13 | 1.80 | 0.41 |
| 5:E:17:ILE:HD13 | 5:E:17:ILE:HA | 1.87 | 0.41 |
| 5:E:60:VAL:HG23 | 5:E:74:VAL:HB | 2.03 | 0.41 |
| 5:E:185:ILE:HG21 | 5:E:185:ILE:HD13 | 1.67 | 0.41 |
| 7:G:81:LYS:HE2 | 7:G:149:GLY:HA2 | 2.03 | 0.41 |
| 8:H:96:VAL:HA | 8:H:116:VAL:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:235:LEU:HD23 | 16:Q:261:ALA:HB2 | 2.02 | 0.41 |
| 16:Q:468:GLY:O | 16:Q:472:LYS:HG2 | 2.20 | 0.41 |
| 16:Q:790:HIS:NE2 | 16:Q:817:CYS:SG | 2.94 | 0.41 |
| 1:A:18:ILE:H | 1:A:1462:GLN:HE22 | 1.69 | 0.41 |
| 1:A:120:ASP:O | 1:A:122:ASN:N | 2.54 | 0.41 |
| 1:A:290:LEU:HD12 | 1:A:290:LEU:HA | 1.78 | 0.41 |
| 1:A:419:ILE:HD13 | 1:A:419:ILE:HG21 | 1.70 | 0.41 |
| 1:A:421:ARG:NE | 1:A:427:ILE:HD11 | 2.36 | 0.41 |
| 1:A:461:GLN:O | 1:A:461:GLN:NE2 | 2.53 | 0.41 |
| 1:A:497:ASP:HB3 | 2:B:792:ASP:HB3 | 2.01 | 0.41 |
| 1:A:596:ILE:HG21 | 1:A:596:ILE:HD13 | 1.76 | 0.41 |
| 1:A:738:GLU:OE1 | 1:A:797:ARG:HD3 | 2.21 | 0.41 |
| 1:A:1121:VAL:N | 1:A:1122:PRO:CD | 2.84 | 0.41 |
| 1:A:1164:THR:O | 1:A:1298:LEU:N | 2.53 | 0.41 |
| 2:B:19:PRO:C | 2:B:21:LEU:N | 2.74 | 0.41 |
| 2:B:222:ARG:HH11 | 2:B:222:ARG:HD3 | 1.72 | 0.41 |
| 2:B:889:LYS:HB2 | 2:B:889:LYS:HE2 | 1.46 | 0.41 |
| 2:B:1010:LYS:HE3 | 20:V:130:TRP:CH2 | 2.56 | 0.41 |
| 3:C:246:LEU:HA | 3:C:246:LEU:HD23 | 1.87 | 0.41 |
| 7:G:14:HIS:O | 7:G:16:ARG:N | 2.54 | 0.41 |
| 7:G:50:THR:HG22 | 7:G:73:LYS:HB3 | 2.03 | 0.41 |
| 7:G:92:VAL:H | 7:G:139:GLN:HE21 | 1.68 | 0.41 |
| 11:K:93:ASP:OD1 | 11:K:94:LEU:N | 2.53 | 0.41 |
| 15:P:40:A:C2 | 15:P:41:C:C4 | 3.08 | 0.41 |
| 16:Q:258:LEU:HD23 | 16:Q:258:LEU:HA | 1.90 | 0.41 |
| 16:Q:858:LYS:O | 16:Q:861:GLU:HG3 | 2.21 | 0.41 |
| 17:R:388:ARG:HG2 | 17:R:443:SER:HB2 | 2.03 | 0.41 |
| 17:R:390:GLY:HA2 | 17:R:400:TYR:CD1 | 2.55 | 0.41 |
| 17:R:582:GLU:HA | 17:R:585:ASN:HD21 | 1.85 | 0.41 |
| 21:W:196:LEU:HD13 | 21:W:205:LEU:HD11 | 2.01 | 0.41 |
| 21:W:222:ALA:O | 21:W:223:ASN:ND2 | 2.54 | 0.41 |
| 24:Z:389:THR:HG23 | 24:Z:391:SER:H | 1.85 | 0.41 |
| 24:Z:491:LEU:HD23 | 24:Z:491:LEU:HA | 1.83 | 0.41 |
| 24:Z:562:ASN:ND2 | 24:Z:566:LYS:HG3 | 2.33 | 0.41 |
| 1:A:33:ARG:H | 1:A:33:ARG:HG2 | 1.69 | 0.41 |
| 1:A:102:LYS:HE2 | 1:A:138:LYS:NZ | 2.36 | 0.41 |
| 1:A:117:LEU:O | 1:A:119:VAL:N | 2.53 | 0.41 |
| 1:A:455:ILE:HD12 | 1:A:520:MET:HE1 | 2.03 | 0.41 |
| 1:A:939:VAL:O | 1:A:943:LEU:HD12 | 2.21 | 0.41 |
| 1:A:1090:LEU:HD23 | 1:A:1090:LEU:HA | 1.79 | 0.41 |
| 2:B:650:ASN:C | 19:U:460:TYR:HE2 | 2.25 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:123:SER:HB2 | 7:G:125:PRO:HD2 | 2.03 | 0.41 |
| 8:H:6:PHE:CZ | 8:H:37:MET:SD | 3.14 | 0.41 |
| 11:K:103:GLU:O | 11:K:107:VAL:HG13 | 2.20 | 0.41 |
| 12:L:18:ILE:HD11 | 12:L:47:LYS:HG3 | 2.02 | 0.41 |
| 16:Q:218:ARG:HH11 | 16:Q:238:LEU:CD2 | 2.33 | 0.41 |
| 16:Q:467:LEU:HD12 | 16:Q:506:LEU:HG | 2.02 | 0.41 |
| 16:Q:790:HIS:CD2 | 16:Q:817:CYS:SG | 3.14 | 0.41 |
| 18:T:37:DC:H5' | 18:T:37:DC:C6 | 2.56 | 0.41 |
| 18:T:39:DC:H2'' | 18:T:40:DT:H72 | 2.02 | 0.41 |
| 21:W:5:TYR:CD1 | 21:W:303:CYS:HB3 | 2.56 | 0.41 |
| 21:W:250:SER:OG | 21:W:277:VAL:HG23 | 2.21 | 0.41 |
| 1:A:217:SER:O | 1:A:220:ARG:N | 2.53 | 0.40 |
| 1:A:812:LYS:O | 1:A:813:ASP:HB2 | 2.21 | 0.40 |
| 1:A:1177:TYR:HH | 1:A:1282:ASP:HA | 1.86 | 0.40 |
| 1:A:1212:LEU:CD1 | 1:A:1285:LEU:HD13 | 2.48 | 0.40 |
| 1:A:1376:LYS:O | 1:A:1380:ARG:HG3 | 2.21 | 0.40 |
| 1:A:1481:LYS:HA | 7:G:20:PRO:HA | 2.03 | 0.40 |
| 2:B:123:PRO:HB2 | 2:B:148:PHE:HE1 | 1.86 | 0.40 |
| 3:C:40:ALA:HB1 | 3:C:171:LYS:HB2 | 2.02 | 0.40 |
| 16:Q:18:GLU:N | 16:Q:18:GLU:OE1 | 2.53 | 0.40 |
| 16:Q:274:HIS:HA | 16:Q:277:ASN:HD21 | 1.84 | 0.40 |
| 16:Q:296:PHE:CE1 | 16:Q:305:GLN:HB2 | 2.56 | 0.40 |
| 16:Q:398:LYS:HE2 | 16:Q:421:ILE:HG21 | 2.03 | 0.40 |
| 24:Z:525:ALA:CB | 24:Z:552:ARG:HH22 | 2.31 | 0.40 |
| 1:A:99:PHE:O | 1:A:103:THR:HG23 | 2.21 | 0.40 |
| 1:A:247:TRP:N | 1:A:247:TRP:CD1 | 2.87 | 0.40 |
| 1:A:539:GLN:C | 1:A:541:THR:N | 2.74 | 0.40 |
| 1:A:991:GLN:HA | 1:A:996:ILE:HG12 | 2.04 | 0.40 |
| 1:A:1222:THR:C | 1:A:1225:LYS:H | 2.23 | 0.40 |
| 1:A:1288:ILE:HA | 1:A:1291:ASN:HD21 | 1.86 | 0.40 |
| 2:B:583:LEU:N | 2:B:583:LEU:HD12 | 2.36 | 0.40 |
| 4:D:35:SER:OG | 4:D:72:SER:HA | 2.21 | 0.40 |
| 7:G:110:ARG:HG2 | 7:G:119:PHE:CZ | 2.56 | 0.40 |
| 7:G:152:VAL:HA | 7:G:157:ILE:HA | 2.03 | 0.40 |
| 16:Q:238:LEU:HD12 | 16:Q:238:LEU:HA | 1.96 | 0.40 |
| 16:Q:393:LYS:HB3 | 16:Q:393:LYS:HE3 | 1.70 | 0.40 |
| 18:T:21:DT:H6 | 18:T:21:DT:H2' | 1.67 | 0.40 |
| 21:W:251:SER:HG | 21:W:255:SER:HG | 1.68 | 0.40 |
| 24:Z:551:VAL:HG21 | 24:Z:632:ASN:OD1 | 2.20 | 0.40 |
| 24:Z:571:ARG:HB2 | 24:Z:574:ALA:CB | 2.51 | 0.40 |
| 1:A:92:LYS:CD | 1:A:307:VAL:HG11 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:350:VAL:HG21 | 1:A:1435:THR:HG23 | 2.03 | 0.40 |
| 1:A:413:TYR:O | 1:A:449:HIS:CD2 | 2.67 | 0.40 |
| 1:A:713:VAL:CG2 | 1:A:817:PRO:HD3 | 2.45 | 0.40 |
| 1:A:1150:ASP:OD2 | 1:A:1153:ARG:HG3 | 2.21 | 0.40 |
| 1:A:1182:GLN:O | 1:A:1192:TRP:CE2 | 2.73 | 0.40 |
| 1:A:1261:ILE:C | 1:A:1262:MET:HE3 | 2.41 | 0.40 |
| 2:B:157:ARG:NH2 | 2:B:177:CYS:O | 2.54 | 0.40 |
| 2:B:665:ILE:HA | 2:B:665:ILE:HD12 | 1.78 | 0.40 |
| 2:B:833:THR:HG22 | 2:B:835:GLU:OE1 | 2.22 | 0.40 |
| 5:E:101:ARG:HA | 5:E:126:ILE:O | 2.20 | 0.40 |
| 7:G:110:ARG:NH2 | 7:G:117:MET:O | 2.55 | 0.40 |
| 8:H:125:LEU:HD12 | 8:H:125:LEU:HA | 1.79 | 0.40 |
| 11:K:80:ASP:N | 11:K:80:ASP:OD1 | 2.32 | 0.40 |
| 12:L:13:GLN:HA | 12:L:14:PRO:HD3 | 1.88 | 0.40 |
| 14:N:42:DT:H6 | 14:N:42:DT:H2' | 1.71 | 0.40 |
| 16:Q:3:ARG:HB3 | 16:Q:4:GLY:H | 1.67 | 0.40 |
| 16:Q:153:HIS:CE1 | 16:Q:156:LEU:HD12 | 2.56 | 0.40 |
| 16:Q:333:THR:HG21 | 16:Q:347:LEU:HD12 | 2.02 | 0.40 |
| 16:Q:415:TRP:CZ3 | 16:Q:440:ILE:HG12 | 2.57 | 0.40 |
| 17:R:392:GLY:HA2 | 17:R:397:LYS:O | 2.20 | 0.40 |
| 17:R:587:LYS:HE2 | 17:R:587:LYS:HB2 | 1.93 | 0.40 |
| 20:V:282:ALA:C | 20:V:284:GLU:H | 2.25 | 0.40 |
| 21:W:243:ASP:OD2 | 21:W:243:ASP:N | 2.54 | 0.40 |
| 21:W:254:LYS:HG2 | 21:W:275:ASP:C | 2.42 | 0.40 |
| 23:Y:93:LEU:HD23 | 23:Y:93:LEU:HA | 1.87 | 0.40 |
| 24:Z:260:MET:N | 24:Z:260:MET:SD | 2.94 | 0.40 |
| 1:A:54:LEU:HD12 | 1:A:54:LEU:HA | 1.85 | 0.40 |
| 1:A:135:GLY:O | 1:A:137:PRO:HD3 | 2.21 | 0.40 |
| 1:A:538:VAL:O | 1:A:539:GLN:HG2 | 2.22 | 0.40 |
| 1:A:1182:GLN:C | 1:A:1192:TRP:HE1 | 2.18 | 0.40 |
| 2:B:84:TYR:CB | 2:B:132:VAL:HA | 2.52 | 0.40 |
| 2:B:95:LYS:HA | 2:B:95:LYS:HD2 | 1.92 | 0.40 |
| 2:B:332:LYS:HD2 | 2:B:332:LYS:C | 2.41 | 0.40 |
| 2:B:388:TYR:H | 2:B:504:THR:CG2 | 2.27 | 0.40 |
| 2:B:620:ARG:HH11 | 2:B:620:ARG:HD2 | 1.69 | 0.40 |
| 2:B:791:GLU:O | 2:B:792:ASP:HB2 | 2.21 | 0.40 |
| 5:E:25:GLY:O | 5:E:65:ASN:HB2 | 2.22 | 0.40 |
| 13:M:1429:HIS:CE1 | 13:M:1460:TYR:HH | 2.37 | 0.40 |
| 16:Q:24:LEU:HD11 | 16:Q:56:LYS:NZ | 2.36 | 0.40 |
| 16:Q:95:GLN:OE1 | 20:V:83:THR:OG1 | 2.38 | 0.40 |
| 16:Q:689:HIS:HB2 | 20:V:35:TYR:CE1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:W:14:ALA:CB | 21:W:298:ILE:HG13 | 2.52 | 0.40 |
| 24:Z:200:PHE:HB2 | 24:Z:210:LEU:HD22 | 2.02 | 0.40 |
| 24:Z:420:PHE:CE1 | 24:Z:470:LYS:HG2 | 2.56 | 0.40 |
| 1:A:29:ASP:O | 1:A:33:ARG:HG2 | 2.21 | 0.40 |
| 1:A:955:GLU:OE1 | 1:A:1010:VAL:HG22 | 2.22 | 0.40 |
| 1:A:1163:HIS:CD2 | 1:A:1297:THR:HG23 | 2.57 | 0.40 |
| 2:B:50:PHE:HA | 2:B:54:SER:HB3 | 2.02 | 0.40 |
| 2:B:242:ARG:NH2 | 2:B:252:ILE:HD12 | 2.37 | 0.40 |
| 9:I:14:ILE:HG23 | 9:I:23:MET:HG3 | 2.03 | 0.40 |
| 16:Q:386:ALA:HB1 | 16:Q:394:ARG:CG | 2.51 | 0.40 |
| 16:Q:636:TYR:CE2 | 16:Q:652:GLY:HA3 | 2.56 | 0.40 |
| 18:T:1:DG:H2" | 18:T:2:DC:C6 | 2.56 | 0.40 |
| 21:W:172:ILE:O | 21:W:186:LEU:N | 2.54 | 0.40 |
| 21:W:273:HIS:CE1 | 21:W:291:SER:HG | 2.39 | 0.40 |
| 24:Z:501:ILE:HA | 24:Z:511:LEU:O | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 1408/1984 (71%) | 1281 (91%) | 117 (8%) | 10 (1%) | 19 | 51 |
| 2 | B | 1112/1251 (89%) | 998 (90%) | 105 (9%) | 9 (1%) | 16 | 48 |
| 3 | C | 254/275 (92%) | 232 (91%) | 19 (8%) | 3 (1%) | 11 | 38 |
| 4 | D | 124/142 (87%) | 118 (95%) | 6 (5%) | 0 | 100 | 100 |
| 5 | E | 207/210 (99%) | 199 (96%) | 7 (3%) | 1 (0%) | 25 | 58 |
| 6 | F | 76/127 (60%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |
| 7 | G | 169/172 (98%) | 157 (93%) | 12 (7%) | 0 | 100 | 100 |
| 8 | H | 147/150 (98%) | 130 (88%) | 16 (11%) | 1 (1%) | 19 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 9 | I | 114/125 (91%) | 104 (91%) | 10 (9%) | 0 | 100 | 100 |
| 10 | J | 64/67 (96%) | 60 (94%) | 2 (3%) | 2 (3%) | 3 | 19 |
| 11 | K | 113/117 (97%) | 107 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | L | 45/58 (78%) | 39 (87%) | 6 (13%) | 0 | 100 | 100 |
| 13 | M | 976/1729 (56%) | 903 (92%) | 72 (7%) | 1 (0%) | 48 | 79 |
| 16 | Q | 888/1179 (75%) | 836 (94%) | 52 (6%) | 0 | 100 | 100 |
| 17 | R | 240/713 (34%) | 225 (94%) | 14 (6%) | 1 (0%) | 30 | 63 |
| 19 | U | 117/666 (18%) | 88 (75%) | 21 (18%) | 8 (7%) | 1 | 6 |
| 20 | V | 234/531 (44%) | 199 (85%) | 31 (13%) | 4 (2%) | 7 | 30 |
| 21 | W | 298/305 (98%) | 268 (90%) | 30 (10%) | 0 | 100 | 100 |
| 22 | X | 41/531 (8%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 23 | Y | 114/121 (94%) | 109 (96%) | 5 (4%) | 0 | 100 | 100 |
| 24 | Z | 497/1087 (46%) | 460 (93%) | 36 (7%) | 1 (0%) | 44 | 74 |
| All | All | 7238/11540 (63%) | 6624 (92%) | 573 (8%) | 41 (1%) | 24 | 53 |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 540 | ASP |
| 1 | A | 1185 | VAL |
| 1 | A | 1468 | THR |
| 2 | B | 19 | PRO |
| 3 | C | 93 | PHE |
| 13 | M | 1330 | PRO |
| 17 | R | 507 | PRO |
| 19 | U | 506 | ALA |
| 19 | U | 508 | HIS |
| 20 | V | 238 | PRO |
| 24 | Z | 760 | GLY |
| 1 | A | 1435 | THR |
| 19 | U | 481 | GLY |
| 19 | U | 521 | LYS |
| 2 | B | 20 | ASP |
| 2 | B | 142 | THR |
| 2 | B | 1004 | ASP |
| 10 | J | 28 | GLU |
| 19 | U | 463 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 19 | U | 513 | LEU |
| 19 | U | 516 | ALA |
| 19 | U | 523 | GLN |
| 20 | V | 228 | GLU |
| 20 | V | 249 | ASP |
| 20 | V | 291 | ASN |
| 1 | A | 300 | ALA |
| 1 | A | 696 | SER |
| 2 | B | 950 | ARG |
| 1 | A | 495 | ASP |
| 1 | A | 1130 | ILE |
| 2 | B | 679 | PRO |
| 2 | B | 834 | ARG |
| 3 | C | 60 | HIS |
| 3 | C | 92 | GLU |
| 2 | B | 650 | ASN |
| 2 | B | 1001 | PRO |
| 1 | A | 478 | PRO |
| 5 | E | 45 | GLY |
| 8 | H | 17 | PRO |
| 10 | J | 64 | PRO |
| 1 | A | 980 | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 1245/1761 (71%) | 1226 (98%) | 19 (2%) | 60 | 80 |
| 2 | B | 986/1084 (91%) | 949 (96%) | 37 (4%) | 28 | 59 |
| 3 | C | 235/252 (93%) | 228 (97%) | 7 (3%) | 36 | 64 |
| 4 | D | 109/126 (86%) | 108 (99%) | 1 (1%) | 75 | 88 |
| 5 | E | 191/192 (100%) | 189 (99%) | 2 (1%) | 73 | 86 |
| 6 | F | 68/111 (61%) | 67 (98%) | 1 (2%) | 60 | 80 |
| 7 | G | 146/153 (95%) | 143 (98%) | 3 (2%) | 48 | 72 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 8 | H | 130/131 (99%) | 122 (94%) | 8 (6%) | 15 | 43 |
| 9 | I | 104/112 (93%) | 101 (97%) | 3 (3%) | 37 | 65 |
| 10 | J | 55/56 (98%) | 54 (98%) | 1 (2%) | 54 | 76 |
| 11 | K | 104/106 (98%) | 103 (99%) | 1 (1%) | 73 | 86 |
| 12 | L | 43/55 (78%) | 40 (93%) | 3 (7%) | 12 | 39 |
| 13 | M | 154/1524 (10%) | 154 (100%) | 0 | 100 | 100 |
| 16 | Q | 761/1011 (75%) | 755 (99%) | 6 (1%) | 79 | 89 |
| 17 | R | 168/625 (27%) | 166 (99%) | 2 (1%) | 67 | 83 |
| 19 | U | 63/590 (11%) | 63 (100%) | 0 | 100 | 100 |
| 20 | V | 144/462 (31%) | 141 (98%) | 3 (2%) | 48 | 72 |
| 21 | W | 255/260 (98%) | 254 (100%) | 1 (0%) | 89 | 94 |
| 22 | X | 40/467 (9%) | 40 (100%) | 0 | 100 | 100 |
| 23 | Y | 102/105 (97%) | 102 (100%) | 0 | 100 | 100 |
| 24 | Z | 434/939 (46%) | 432 (100%) | 2 (0%) | 86 | 92 |
| All | All | 5537/10122 (55%) | 5437 (98%) | 100 (2%) | 54 | 76 |

All (100) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 67 | ARG |
| 1 | A | 147 | LEU |
| 1 | A | 251 | THR |
| 1 | A | 301 | HIS |
| 1 | A | 382 | ARG |
| 1 | A | 476 | ILE |
| 1 | A | 539 | GLN |
| 1 | A | 571 | ASP |
| 1 | A | 605 | THR |
| 1 | A | 757 | GLN |
| 1 | A | 761 | SER |
| 1 | A | 819 | SER |
| 1 | A | 884 | ASN |
| 1 | A | 931 | ARG |
| 1 | A | 937 | ASP |
| 1 | A | 1030 | SER |
| 1 | A | 1074 | SER |
| 1 | A | 1210 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1286 | ARG |
| 2 | B | 20 | ASP |
| 2 | B | 83 | ARG |
| 2 | B | 90 | GLN |
| 2 | B | 92 | TYR |
| 2 | B | 115 | LEU |
| 2 | B | 147 | THR |
| 2 | B | 170 | ASP |
| 2 | B | 180 | ASP |
| 2 | B | 218 | THR |
| 2 | B | 236 | TRP |
| 2 | B | 267 | VAL |
| 2 | B | 331 | THR |
| 2 | B | 332 | LYS |
| 2 | B | 348 | LEU |
| 2 | B | 351 | VAL |
| 2 | B | 354 | SER |
| 2 | B | 359 | THR |
| 2 | B | 386 | ASP |
| 2 | B | 411 | LEU |
| 2 | B | 429 | PHE |
| 2 | B | 453 | TRP |
| 2 | B | 592 | ARG |
| 2 | B | 597 | ILE |
| 2 | B | 610 | ARG |
| 2 | B | 626 | LEU |
| 2 | B | 649 | ASN |
| 2 | B | 650 | ASN |
| 2 | B | 659 | SER |
| 2 | B | 715 | ASP |
| 2 | B | 731 | GLN |
| 2 | B | 738 | THR |
| 2 | B | 743 | ARG |
| 2 | B | 784 | SER |
| 2 | B | 931 | ILE |
| 2 | B | 1118 | VAL |
| 2 | B | 1148 | LEU |
| 2 | B | 1174 | VAL |
| 3 | C | 33 | SER |
| 3 | C | 63 | PHE |
| 3 | C | 74 | THR |
| 3 | C | 75 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 76 | ASP |
| 3 | C | 147 | ASP |
| 3 | C | 151 | VAL |
| 4 | D | 94 | LYS |
| 5 | E | 82 | VAL |
| 5 | E | 117 | SER |
| 6 | F | 123 | LEU |
| 7 | G | 21 | ASN |
| 7 | G | 37 | THR |
| 7 | G | 67 | LEU |
| 8 | H | 15 | ILE |
| 8 | H | 67 | ASP |
| 8 | H | 83 | SER |
| 8 | H | 95 | LYS |
| 8 | H | 96 | VAL |
| 8 | H | 113 | SER |
| 8 | H | 116 | VAL |
| 8 | H | 141 | VAL |
| 9 | I | 12 | VAL |
| 9 | I | 15 | ARG |
| 9 | I | 101 | SER |
| 10 | J | 47 | ARG |
| 11 | K | 99 | SER |
| 12 | L | 34 | ILE |
| 12 | L | 39 | CYS |
| 12 | L | 44 | MET |
| 16 | Q | 180 | ARG |
| 16 | Q | 191 | ARG |
| 16 | Q | 697 | TYR |
| 16 | Q | 707 | CYS |
| 16 | Q | 820 | LEU |
| 16 | Q | 858 | LYS |
| 17 | R | 422 | THR |
| 17 | R | 474 | LYS |
| 20 | V | 45 | ASP |
| 20 | V | 132 | ARG |
| 20 | V | 181 | LYS |
| 21 | W | 169 | ASP |
| 24 | Z | 176 | ASP |
| 24 | Z | 720 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 62 | GLN |
| 1 | A | 96 | HIS |
| 1 | A | 122 | ASN |
| 1 | A | 123 | ASN |
| 1 | A | 152 | ASN |
| 1 | A | 288 | ASN |
| 1 | A | 313 | HIS |
| 1 | A | 449 | HIS |
| 1 | A | 704 | ASN |
| 1 | A | 742 | ASN |
| 1 | A | 780 | ASN |
| 1 | A | 809 | HIS |
| 1 | A | 935 | GLN |
| 1 | A | 982 | ASN |
| 1 | A | 1005 | HIS |
| 1 | A | 1182 | GLN |
| 1 | A | 1230 | GLN |
| 2 | B | 52 | GLN |
| 2 | B | 175 | ASN |
| 2 | B | 319 | ASN |
| 2 | B | 471 | ASN |
| 2 | B | 631 | GLN |
| 2 | B | 649 | ASN |
| 2 | B | 1003 | ASN |
| 2 | B | 1040 | GLN |
| 2 | B | 1120 | ASN |
| 2 | B | 1142 | ASN |
| 3 | C | 60 | HIS |
| 3 | C | 114 | HIS |
| 3 | C | 262 | GLN |
| 4 | D | 34 | ASN |
| 4 | D | 48 | ASN |
| 4 | D | 66 | ASN |
| 4 | D | 76 | ASN |
| 4 | D | 129 | GLN |
| 5 | E | 107 | GLN |
| 5 | E | 168 | ASN |
| 7 | G | 93 | ASN |
| 7 | G | 139 | GLN |
| 8 | H | 131 | ASN |
| 9 | I | 84 | HIS |
| 9 | I | 91 | HIS |
| 11 | K | 49 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 13 | M | 1352 | GLN |
| 16 | Q | 38 | HIS |
| 16 | Q | 40 | GLN |
| 16 | Q | 82 | GLN |
| 16 | Q | 105 | ASN |
| 16 | Q | 128 | GLN |
| 16 | Q | 161 | ASN |
| 16 | Q | 244 | ASN |
| 16 | Q | 268 | ASN |
| 16 | Q | 289 | GLN |
| 16 | Q | 294 | HIS |
| 16 | Q | 298 | ASN |
| 16 | Q | 305 | GLN |
| 16 | Q | 349 | GLN |
| 16 | Q | 359 | ASN |
| 16 | Q | 373 | ASN |
| 16 | Q | 407 | GLN |
| 16 | Q | 466 | ASN |
| 16 | Q | 502 | ASN |
| 16 | Q | 527 | HIS |
| 16 | Q | 561 | ASN |
| 16 | Q | 573 | ASN |
| 16 | Q | 585 | GLN |
| 16 | Q | 616 | HIS |
| 16 | Q | 706 | ASN |
| 16 | Q | 714 | HIS |
| 16 | Q | 877 | GLN |
| 16 | Q | 880 | GLN |
| 16 | Q | 887 | ASN |
| 17 | R | 416 | GLN |
| 17 | R | 432 | ASN |
| 17 | R | 484 | ASN |
| 17 | R | 585 | ASN |
| 17 | R | 588 | ASN |
| 20 | V | 37 | ASN |
| 20 | V | 69 | GLN |
| 20 | V | 72 | HIS |
| 20 | V | 97 | ASN |
| 20 | V | 122 | GLN |
| 20 | V | 193 | HIS |
| 21 | W | 11 | GLN |
| 21 | W | 15 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | W | 27 | ASN |
| 21 | W | 98 | GLN |
| 21 | W | 131 | ASN |
| 21 | W | 173 | ASN |
| 21 | W | 223 | ASN |
| 21 | W | 268 | HIS |
| 21 | W | 273 | HIS |
| 23 | Y | 27 | GLN |
| 24 | Z | 232 | GLN |
| 24 | Z | 251 | ASN |
| 24 | Z | 466 | GLN |
| 24 | Z | 519 | GLN |
| 24 | Z | 595 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 15 | P | 20/46 (43%) | 7 (35%) | 3 (15%) |

All (7) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | P | 28 | A |
| 15 | P | 29 | C |
| 15 | P | 30 | C |
| 15 | P | 31 | G |
| 15 | P | 36 | G |
| 15 | P | 37 | G |
| 15 | P | 39 | A |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | P | 28 | A |
| 15 | P | 36 | G |
| 15 | P | 38 | G |

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

3 non-standard protein/DNA/RNA residues 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$ |
| 24 | TPO | Z | 775 | 24 | 8,10,11 | 1.54 | 1 (12%) | 10,14,16 | 1.99 | 1 (10%) |
| 1 | SEP | A | 1547 | 1 | 8,9,10 | 1.49 | 1 (12%) | 8,12,14 | 1.39 | 2 (25%) |
| 1 | TPO | A | 1525 | 1 | 8,10,11 | 1.60 | 1 (12%) | 10,14,16 | 1.83 | 1 (10%) |

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 |
|-----|------|-------|------|------|---------|-----------|-------|
| 24 | TPO | Z | 775 | 24 | - | 1/9/11/13 | - |
| 1 | SEP | A | 1547 | 1 | - | 0/5/8/10 | - |
| 1 | TPO | A | 1525 | 1 | - | 4/9/11/13 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1 | A | 1525 | TPO | P-O1P | 3.41 | 1.61 | 1.50 |
| 24 | Z | 775 | TPO | P-O1P | 3.34 | 1.61 | 1.50 |
| 1 | A | 1547 | SEP | P-O1P | 3.25 | 1.61 | 1.50 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 24 | Z | 775 | TPO | P-OG1-CB | -5.85 | 105.53 | 123.21 |
| 1 | A | 1525 | TPO | P-OG1-CB | -4.96 | 108.22 | 123.21 |
| 1 | A | 1547 | SEP | P-OG-CB | -2.69 | 110.89 | 118.30 |
| 1 | A | 1547 | SEP | OG-CB-CA | 2.01 | 110.10 | 108.14 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 1 | A | 1525 | TPO | N-CA-CB-CG2 |
| 1 | A | 1525 | TPO | N-CA-CB-OG1 |
| 1 | A | 1525 | TPO | C-CA-CB-CG2 |
| 24 | Z | 775 | TPO | C-CA-CB-CG2 |
| 1 | A | 1525 | TPO | O-C-CA-CB |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24 | Z | 775 | TPO | 2 | 0 |
| 1 | A | 1547 | SEP | 1 | 0 |
| 1 | A | 1525 | TPO | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2 | B | 3 |
| 19 | U | 1 |
| 20 | V | 1 |
| 13 | M | 1 |
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | U | 497:ASP | C | 505:SER | N | 25.86 |
| 1 | V | 299:GLU | C | 310:ASN | N | 12.74 |
| 1 | M | 1334:ASN | C | 1338:ILE | N | 5.29 |
| 1 | B | 755:GLN | C | 756:LYS | N | 1.18 |
| 1 | B | 108:MET | C | 109:MET | N | 1.17 |
| 1 | A | 999:ARG | C | 1000:LEU | N | 1.15 |
| 1 | B | 94:SER | C | 95:LYS | N | 1.07 |

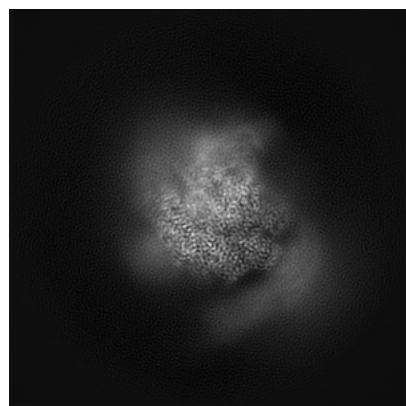
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10480. These allow visual inspection of the internal detail of the map and identification of artifacts.

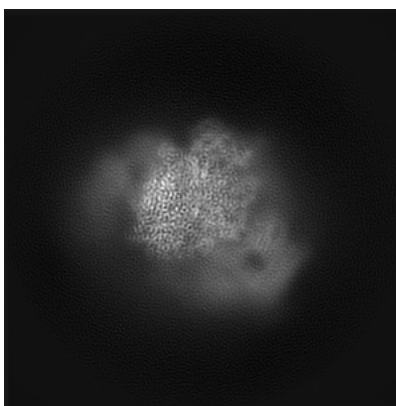
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

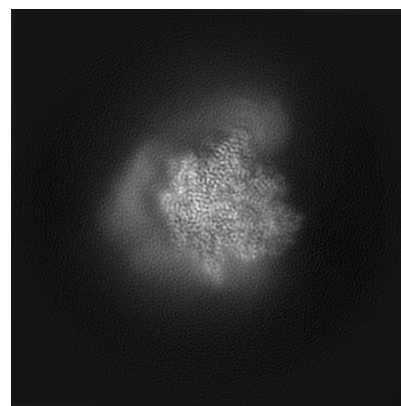
6.1.1 Primary map



X

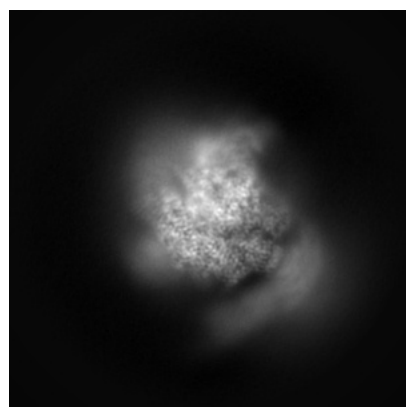


Y

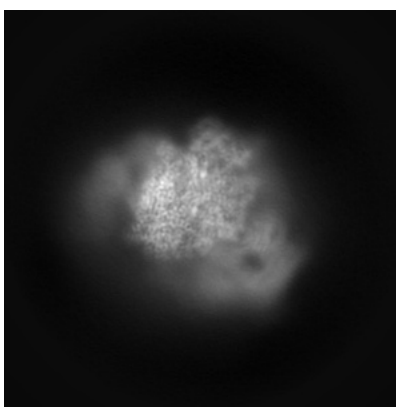


Z

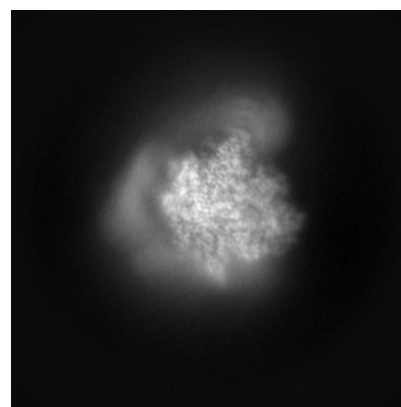
6.1.2 Raw map



X



Y

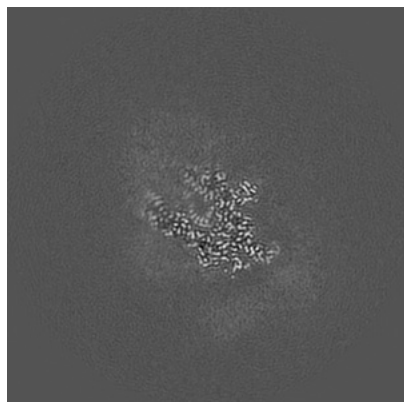


Z

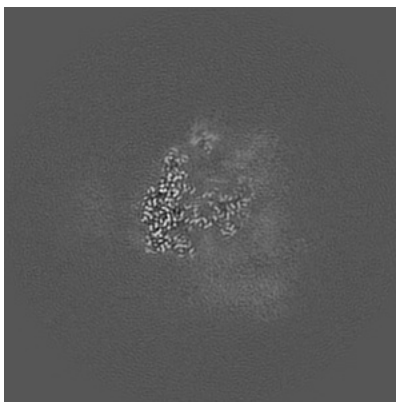
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

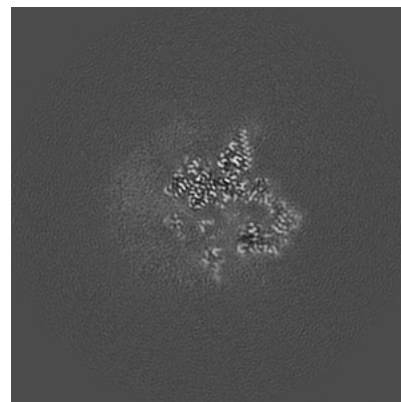
6.2.1 Primary map



X Index: 180

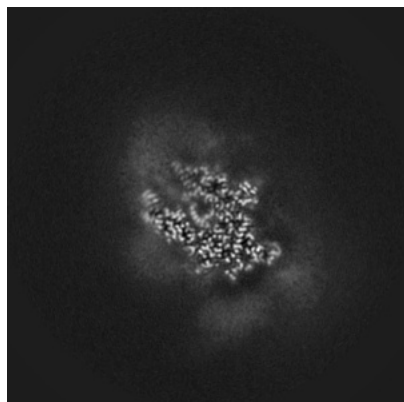


Y Index: 180

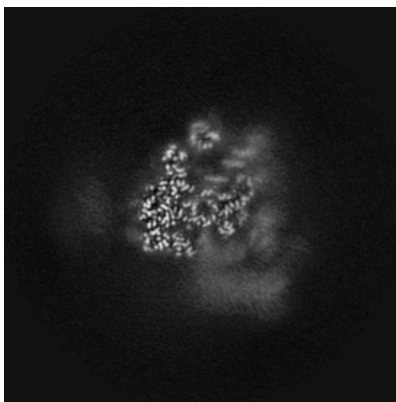


Z Index: 180

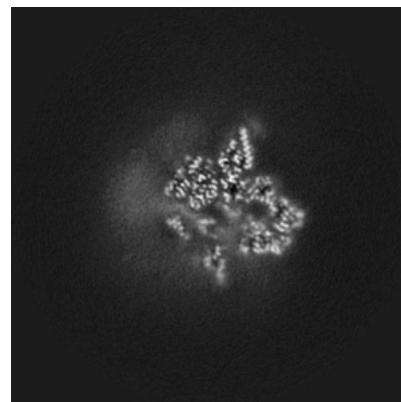
6.2.2 Raw map



X Index: 180



Y Index: 180

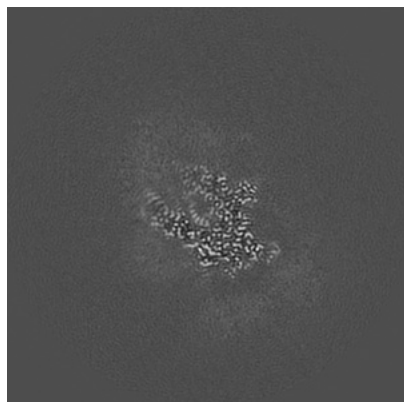


Z Index: 180

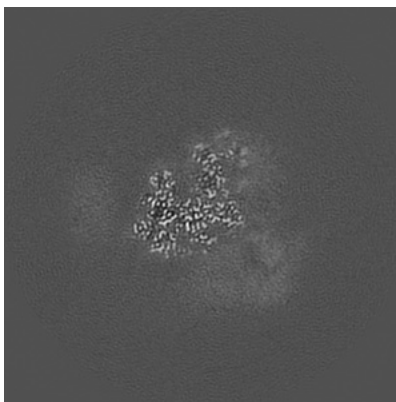
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

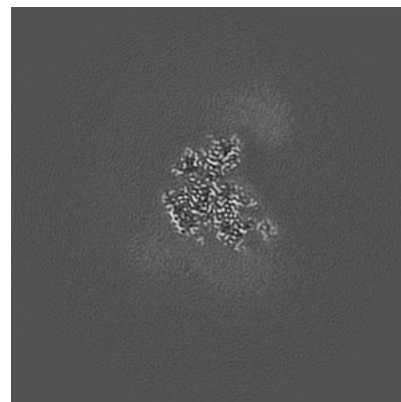
6.3.1 Primary map



X Index: 179

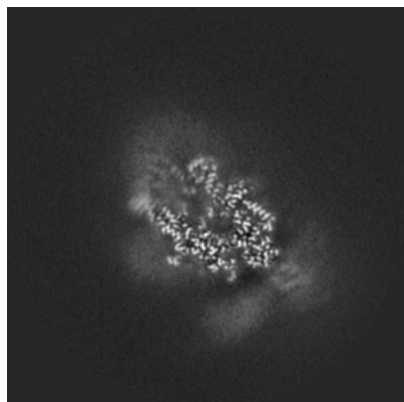


Y Index: 193

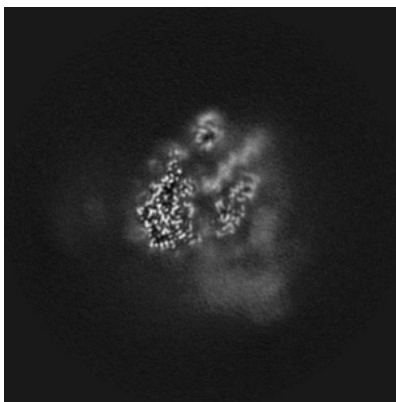


Z Index: 143

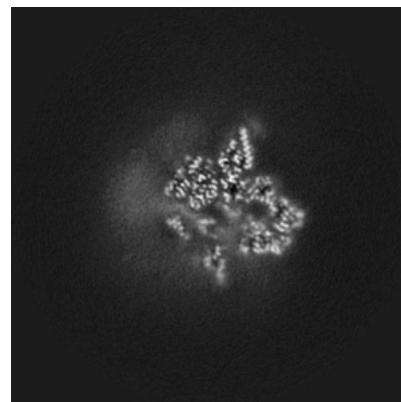
6.3.2 Raw map



X Index: 189



Y Index: 174

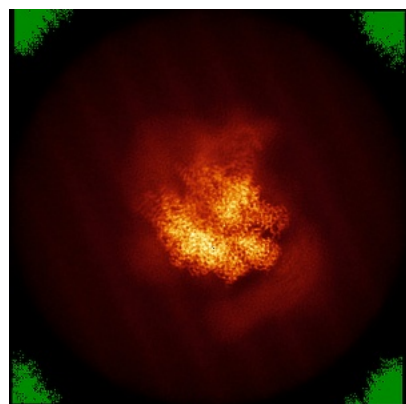


Z Index: 180

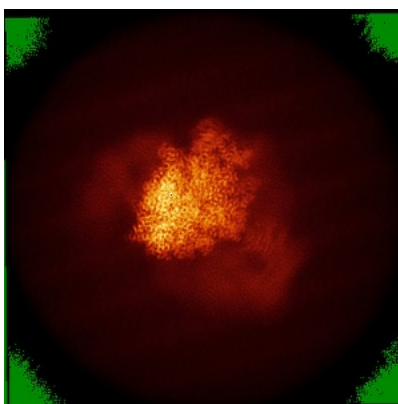
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

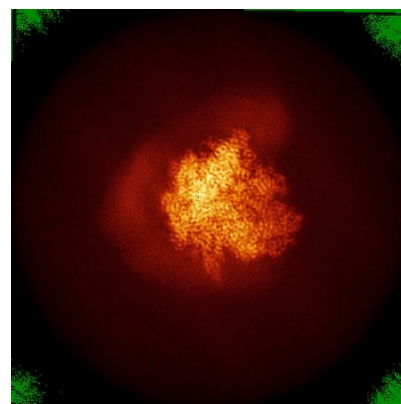
6.4.1 Primary map



X

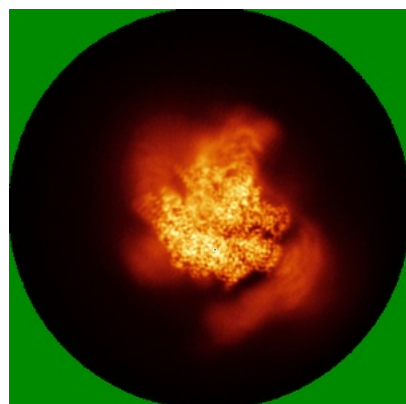


Y

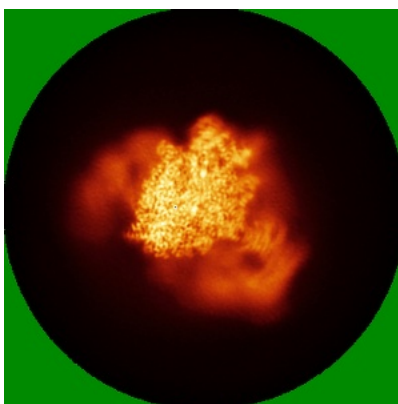


Z

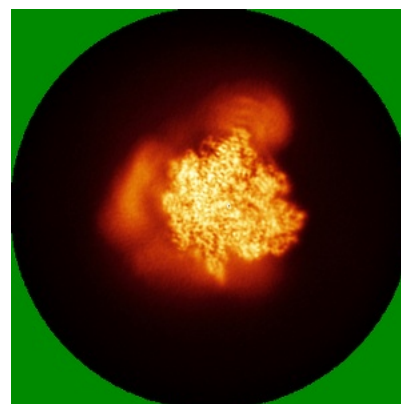
6.4.2 Raw map



X



Y

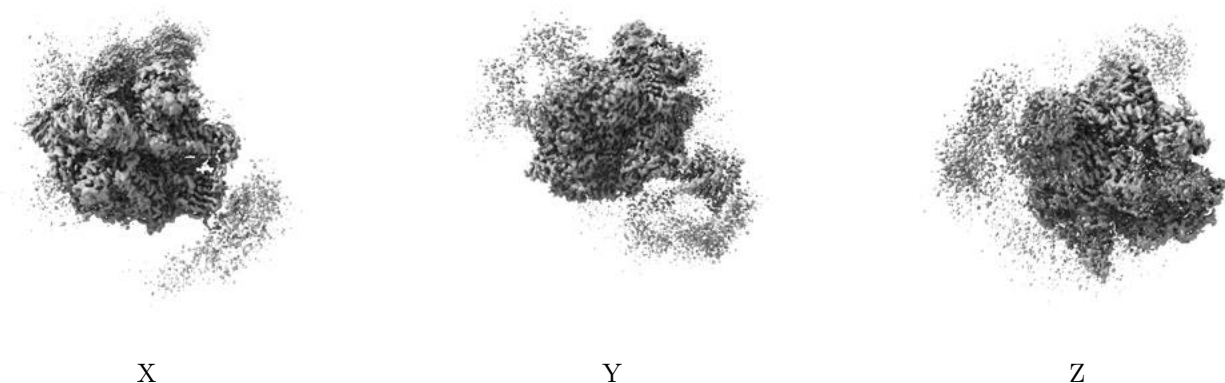


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

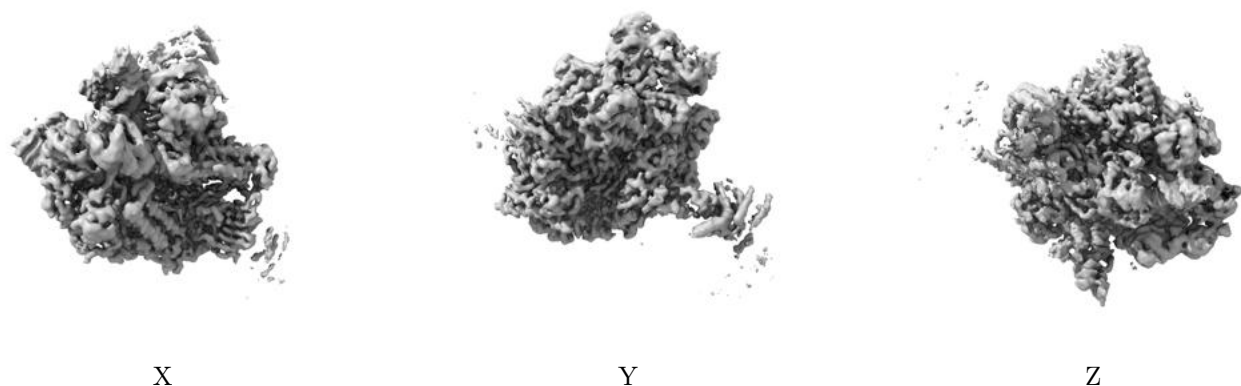
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

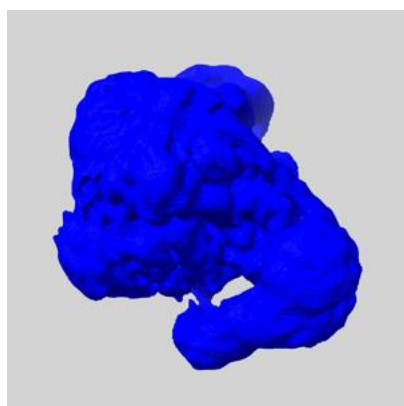
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

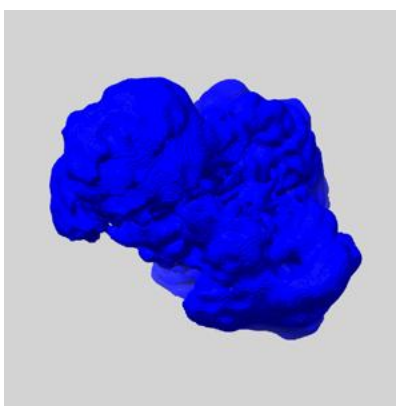
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

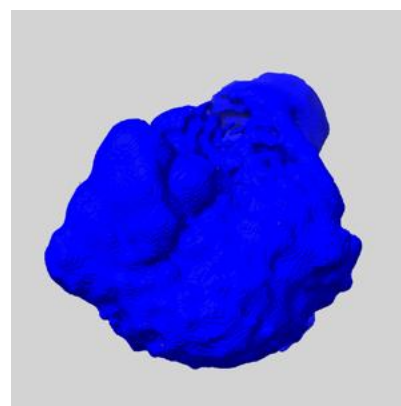
6.6.1 emd_10480_msk_1.map [i](#)



X

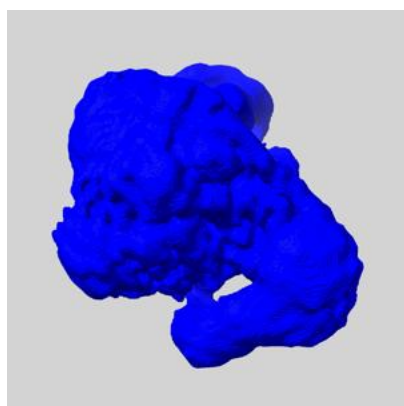


Y

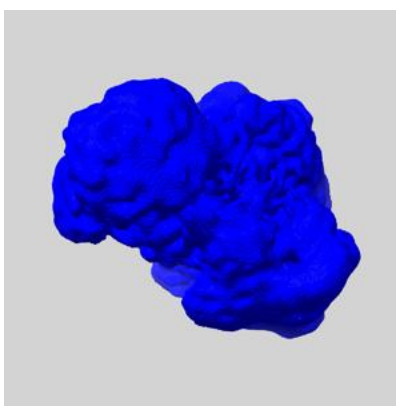


Z

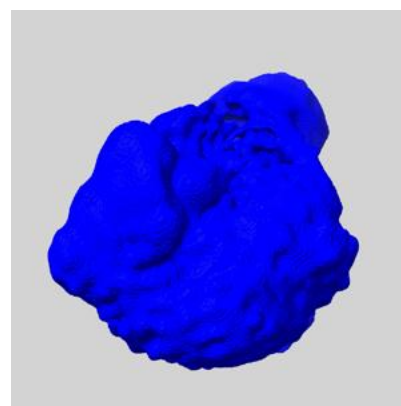
6.6.2 emd_10480_msk_2.map [i](#)



X



Y

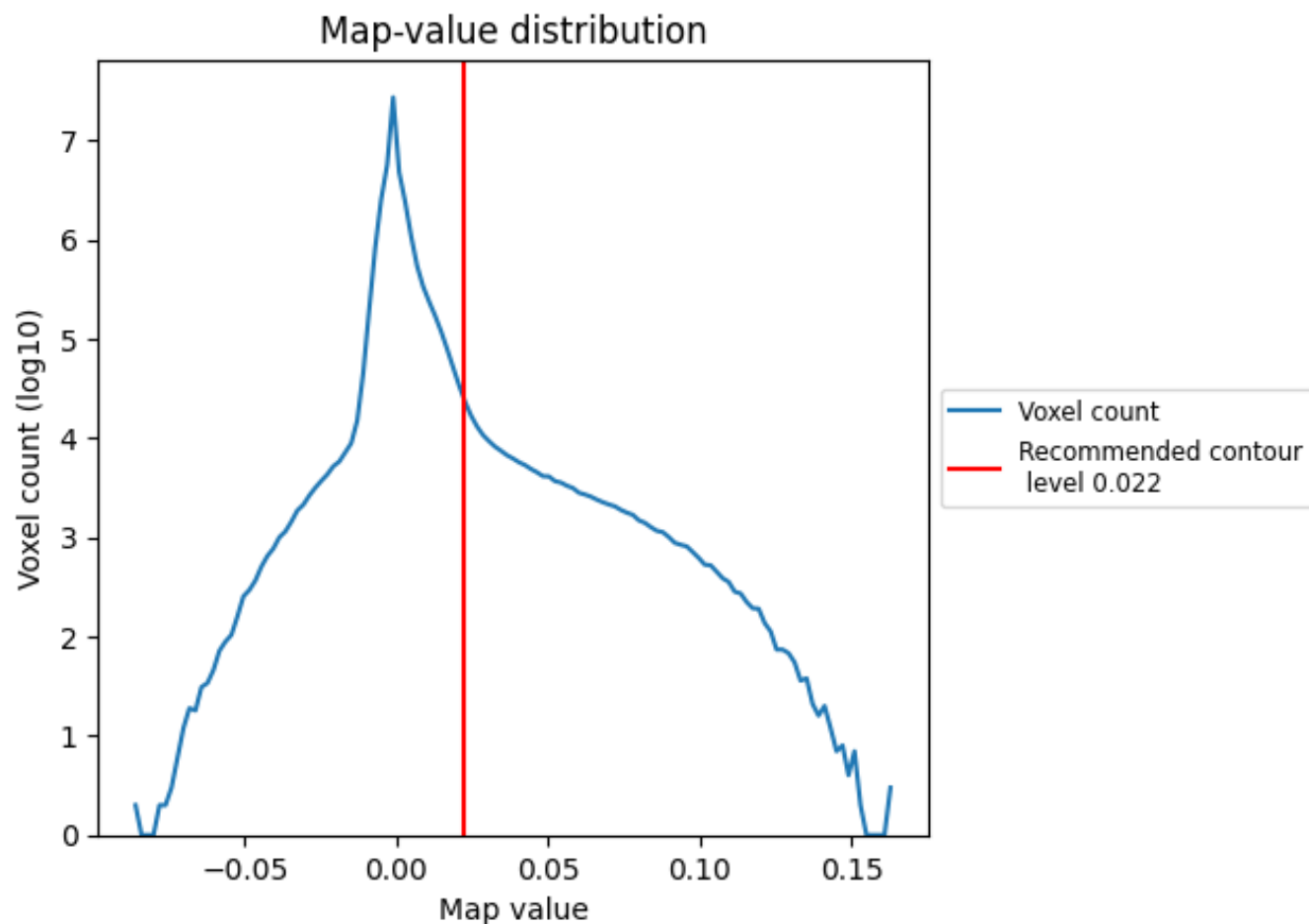


Z

7 Map analysis [i](#)

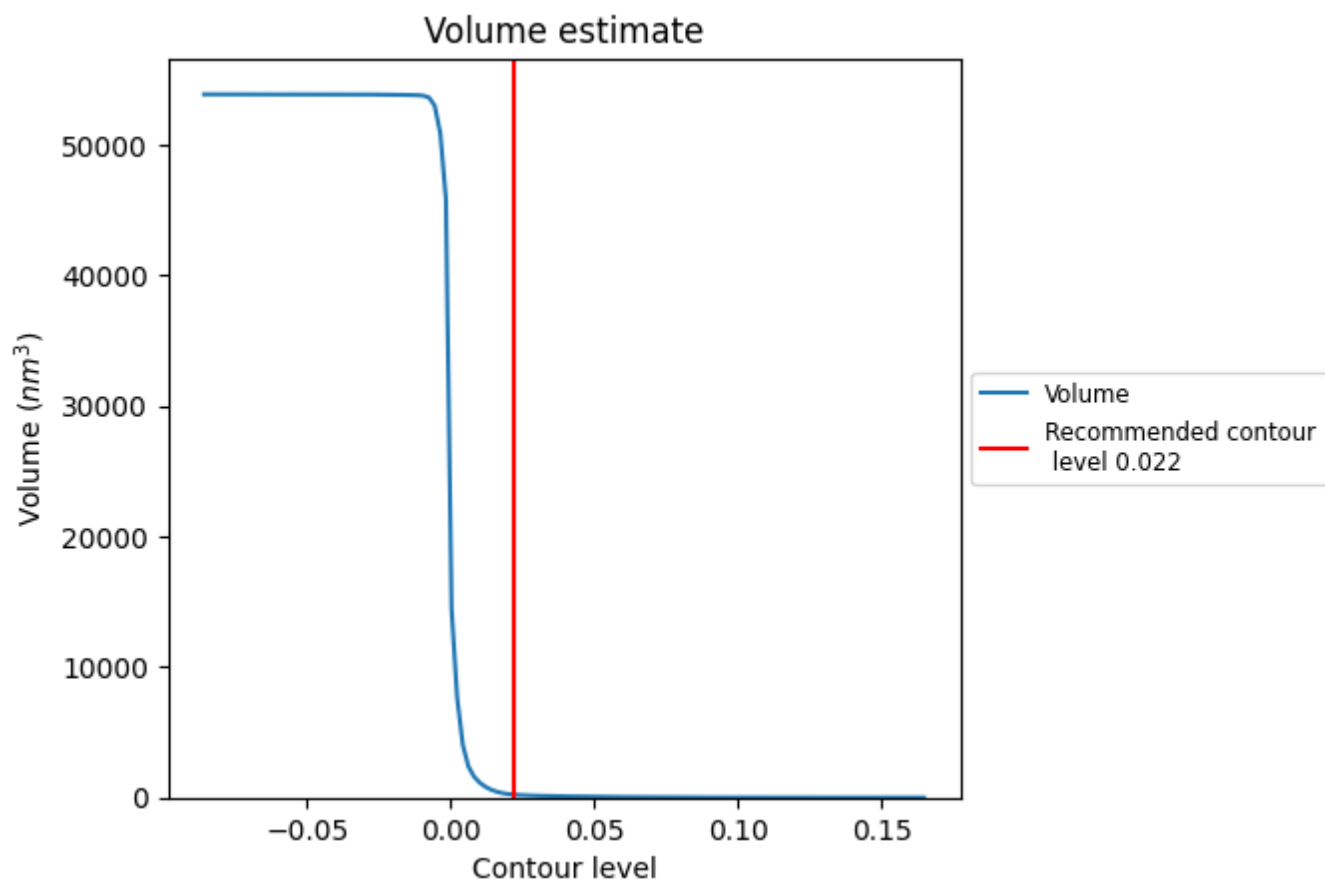
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

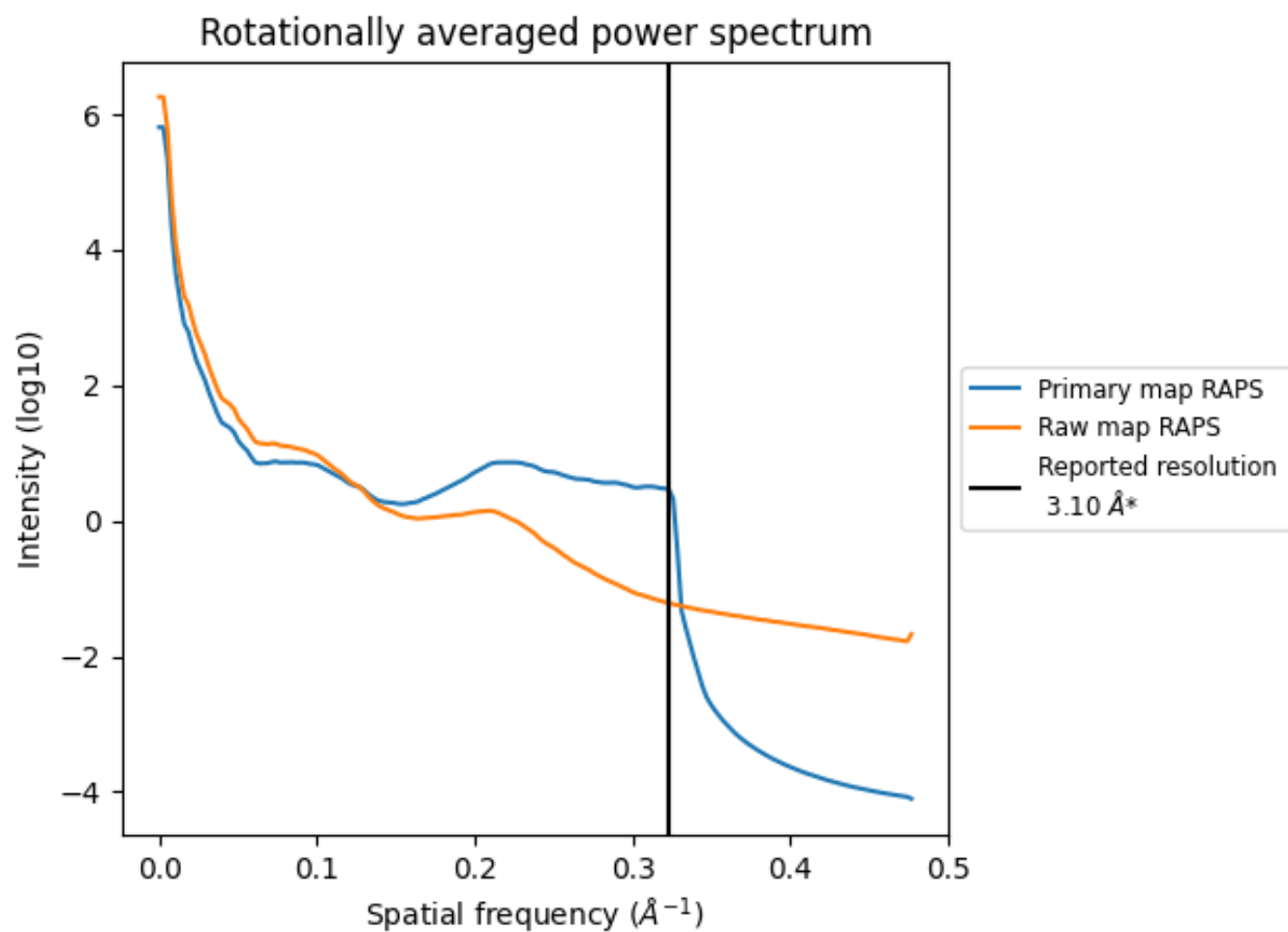
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

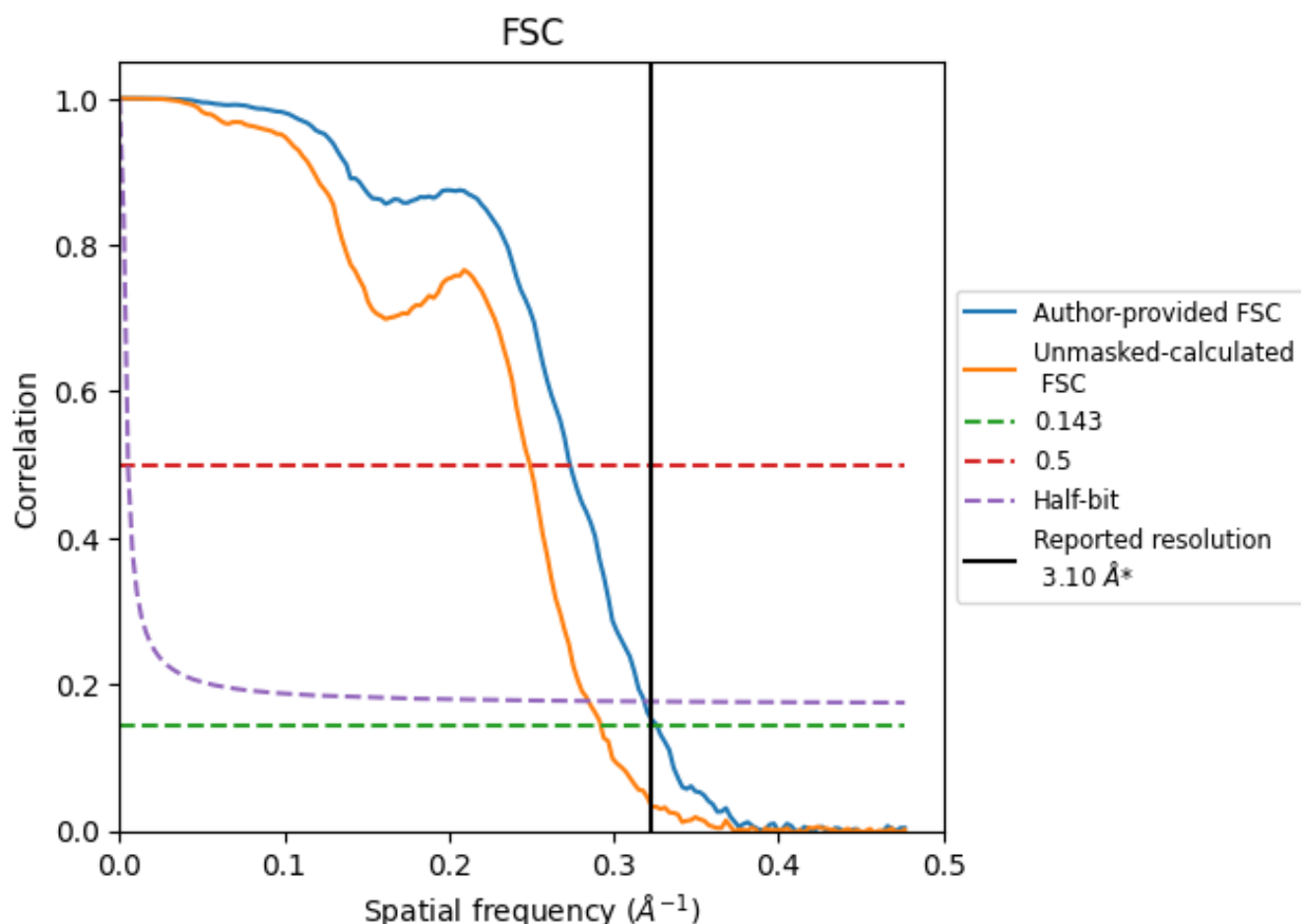


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

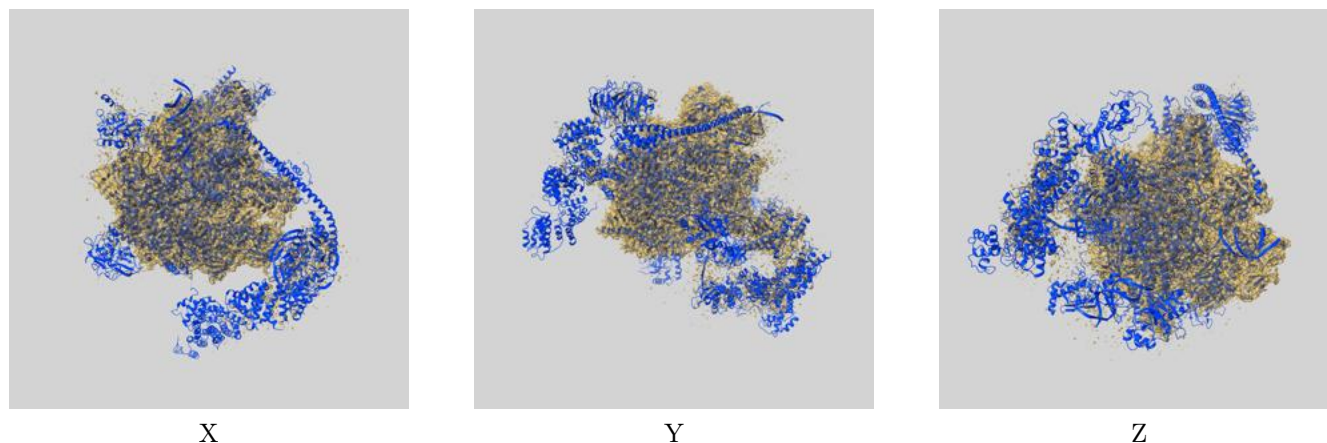
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.10 | - | - |
| Author-provided FSC curve | 3.07 | 3.66 | 3.14 |
| Unmasked-calculated* | 3.42 | 4.01 | 3.51 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

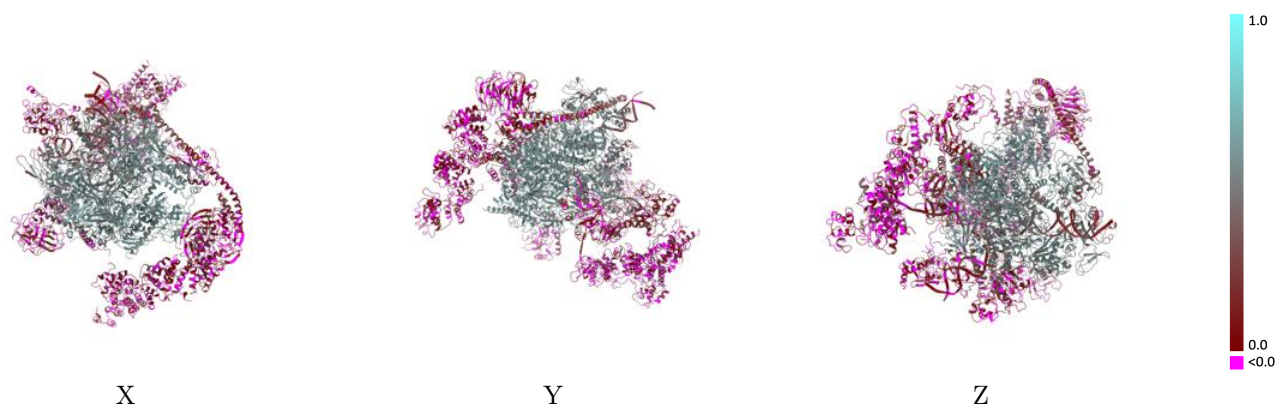
This section contains information regarding the fit between EMDB map EMD-10480 and PDB model 6TED. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



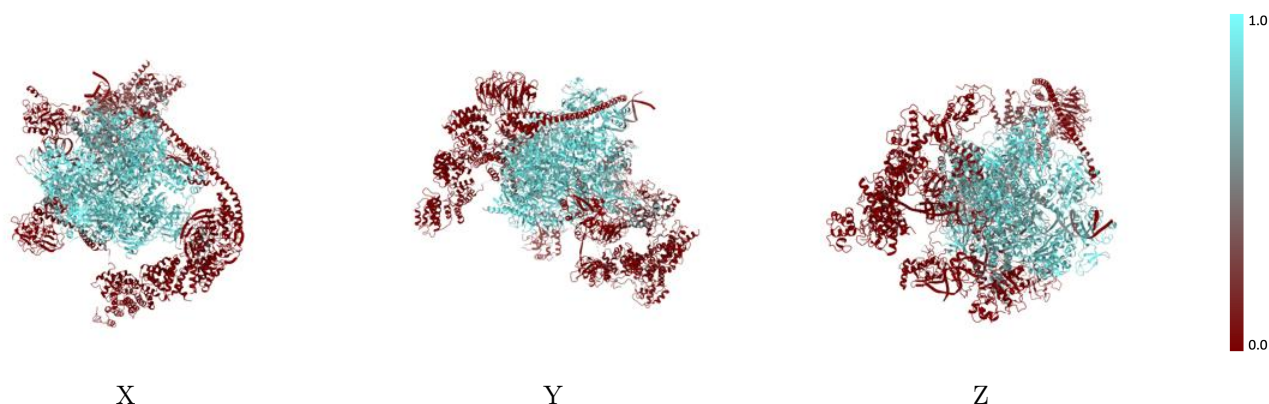
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



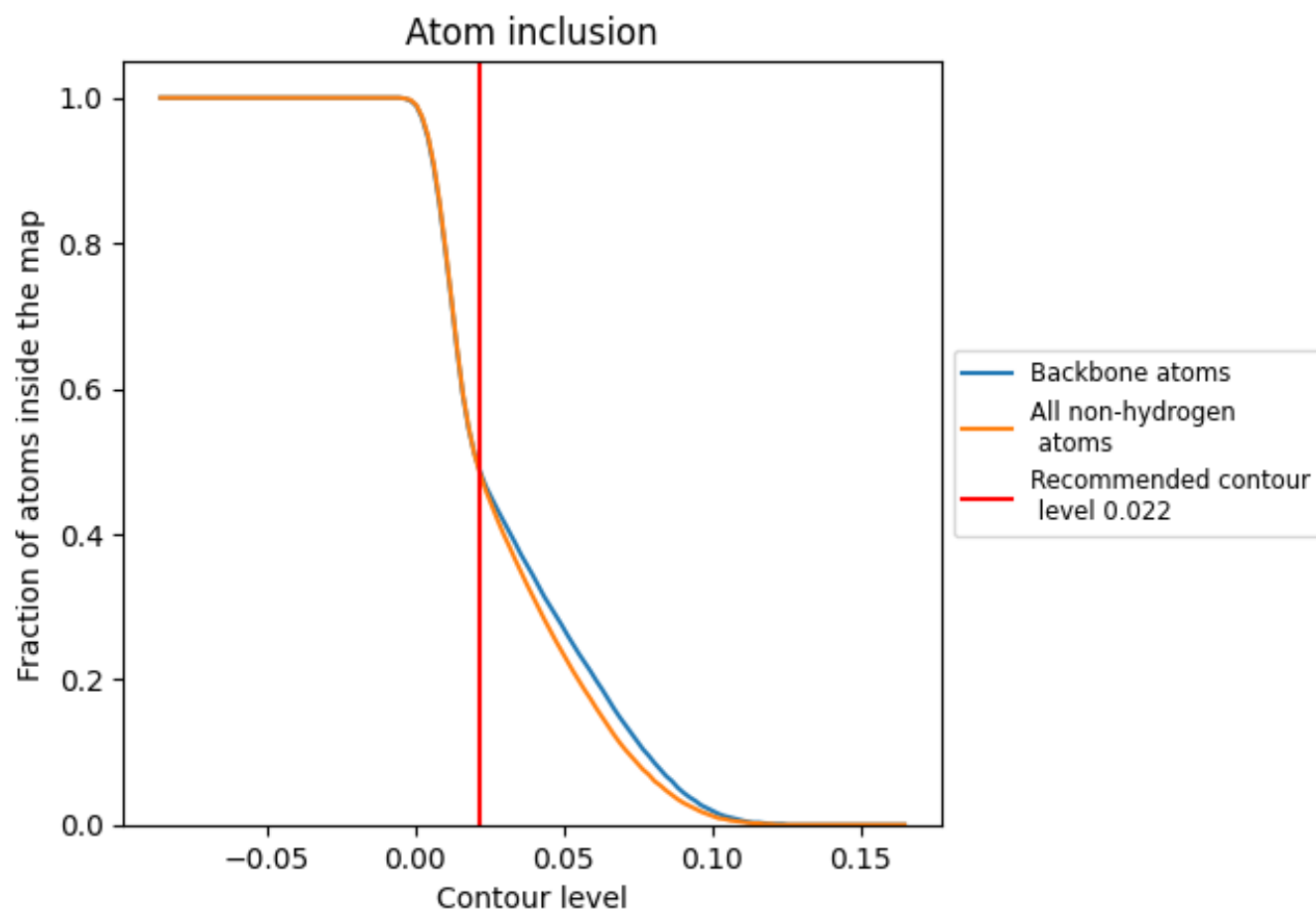
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.4810 |  0.3380 |
| A |  0.8490 |  0.5370 |
| B |  0.8820 |  0.5560 |
| C |  0.9110 |  0.5800 |
| D |  0.2730 |  0.1850 |
| E |  0.8540 |  0.5210 |
| F |  0.8960 |  0.5740 |
| G |  0.4390 |  0.3110 |
| H |  0.8510 |  0.5590 |
| I |  0.8470 |  0.5110 |
| J |  0.9180 |  0.5730 |
| K |  0.9210 |  0.5890 |
| L |  0.8480 |  0.5090 |
| M |  0.0150 |  0.0750 |
| N |  0.3470 |  0.2200 |
| P |  0.4250 |  0.2780 |
| Q |  0.0280 |  0.1020 |
| R |  0.0120 |  0.0880 |
| T |  0.5190 |  0.3100 |
| U |  0.0550 |  0.1140 |
| V |  0.0260 |  0.1270 |
| W |  0.0110 |  0.0430 |
| X |  0.0240 |  0.1060 |
| Y |  0.0060 |  0.0770 |
| Z |  0.0990 |  0.1660 |

