# Full wwPDB EM Validation Report

May 19, 2025 – 02:29 pm BST

| | | |
|---|---|---|
| PDB ID | : | 9ESI / pdb_00009esi |
| EMDB ID | : | EMD-19942 |
| Title | : | Structure of a B-state intermediate committed to discard (Bd-II state) |
| Authors | : | Soni, K.; Wild, K.; Sinning, I. |
| Deposited on | : | 2024-03-26 |
| Resolution | : | 3.10 Å(reported) |

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.

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

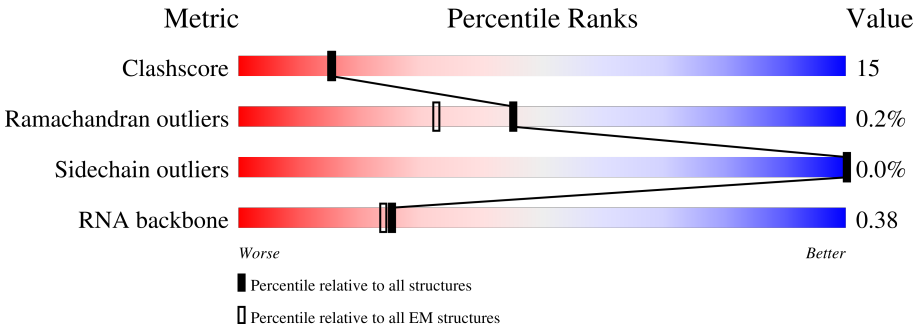
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev118 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.43.1 |

# 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 <=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 | e | 384 | 14% 34% 9% 57% |
| 2 | p | 299 | 12% 13% 7% 80% |
| 3 | 2 | 186 | 7% 5% 5% · 87% |
| 4 | 5 | 120 | 49% 28% 8% 15% |
| 5 | A | 2363 | 12% 62% 22% 16% |
| 6 | B | 984 | · 68% 25% 7% |
| 7 | C | 340 | · 54% 35% 11% |

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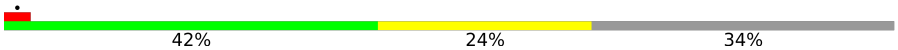
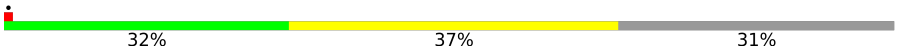
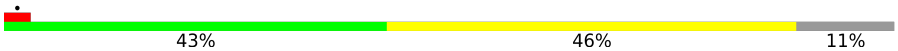
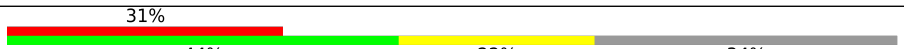
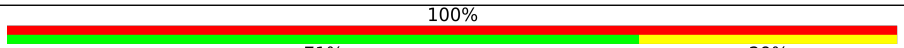
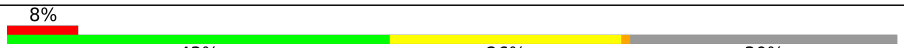
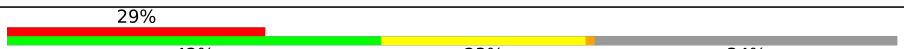
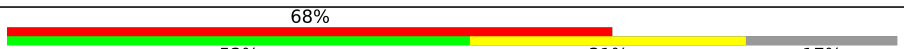
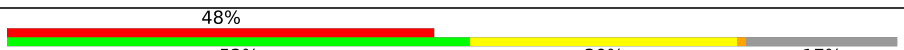
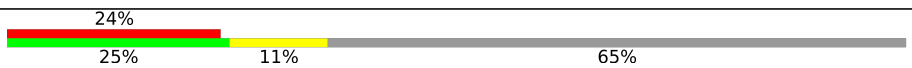
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | D | 97 |   |
| 9 | E | 147 |   |
| 10 | F | 117 |   |
| 11 | G | 115 |   |
| 12 | H | 84 |   |
| 13 | I | 78 |   |
| 14 | J | 77 |   |
| 15 | K | 473 |   |
| 16 | L | 557 |   |
| 17 | M | 354 |   |
| 18 | N | 1284 |   |
| 19 | O | 146 |   |
| 20 | P | 388 |   |
| 21 | Q | 265 |   |
| 22 | R | 674 |   |
| 23 | S | 488 |   |
| 23 | T | 488 |   |
| 23 | U | 488 |   |
| 23 | V | 488 |   |
| 24 | W | 757 |   |
| 25 | X | 790 |   |
| 26 | Y | 229 |   |
| 27 | Z | 187 |   |
| 28 | a | 558 |   |
| 29 | b | 293 |   |

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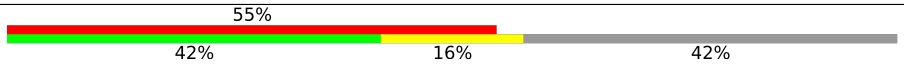
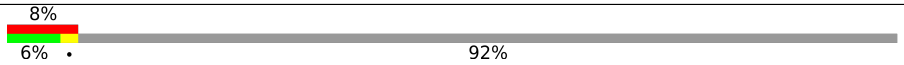
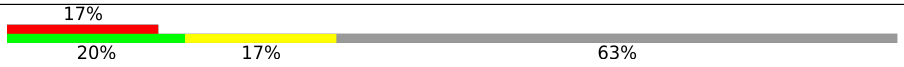
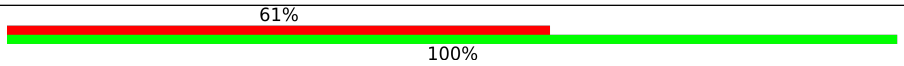
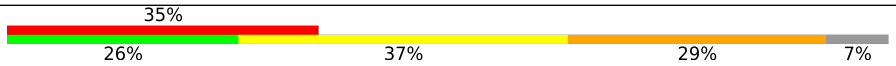
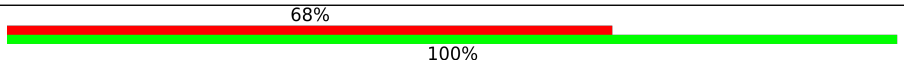
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 30 | c | 887 |   |
| 31 | d | 155 |   |
| 32 | m | 797 |   |
| 33 | n | 361 |   |
| 34 | y | 534 |   |
| 35 | z | 647 |   |
| 36 | r | 346 |   |
| 37 | q | 56 |   |
| 38 | 6 | 99 |   |
| 39 | 1 | 29 |   |
| 40 | f | 22 |   |

# 2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 98220 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 Stress response protein bis1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | e | 166 | 1329 | 838 | 221 | 268 | 2 | 0 | 0 |

- Molecule 2 is a protein called Protein saf4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 2 | p | 60 | 487 | 304 | 89 | 94 | 0 | 0 |

- Molecule 3 is a RNA chain called U2snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | 2 | 24 | 500 | 224 | 79 | 173 | 24 | 0 | 0 |

- Molecule 4 is a RNA chain called U5snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | 5 | 102 | 2149 | 963 | 358 | 726 | 102 | 0 | 0 |

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | A | 1986 | 16424 | 10532 | 2887 | 2938 | 67 | 0 | 0 |

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | B | 918 | 7298 | 4650 | 1251 | 1362 | 35 | 0 | 0 |

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | C | 301 | Total | C | N | O | S | 0 | 0 |
| | | | 2328 | 1460 | 415 | 442 | 11 | | |

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | D | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 760 | 470 | 147 | 136 | 7 | | |

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | E | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 726 | 462 | 129 | 130 | 5 | | |

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | F | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 638 | 407 | 109 | 118 | 4 | | |

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | G | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 819 | 516 | 150 | 149 | 4 | | |

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | H | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 652 | 422 | 113 | 115 | 2 | | |

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | I | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 574 | 373 | 95 | 104 | 2 | | |

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | J | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 366 | 98 | 108 | 1 | | |

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | K | 391 | Total | C | N | O | S | 0 | 0 |
| | | | 3053 | 1925 | 551 | 563 | 14 | | |

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | L | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1954 | 1221 | 364 | 363 | 6 | | |

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | M | 234 | Total | C | N | O | S | 0 | 0 |
| | | | 1818 | 1131 | 329 | 343 | 15 | | |

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | N | 1284 | Total | C | N | O | S | 0 | 0 |
| | | | 10461 | 6715 | 1732 | 1969 | 45 | | |

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | O | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1176 | 733 | 216 | 214 | 13 | | |

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | P | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1354 | 397 | 416 | 11 | | |

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | Q | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 752 | 467 | 146 | 138 | 1 | | |

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | R | 603 | Total | C | N | O | S | 0 | 0 |
| | | | 5108 | 3280 | 892 | 913 | 23 | | |

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | S | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1055 | 664 | 181 | 207 | 3 | | |
| 23 | T | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1069 | 671 | 183 | 212 | 3 | | |
| 23 | U | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 2870 | 1806 | 492 | 563 | 9 | | |
| 23 | V | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1044 | 655 | 180 | 206 | 3 | | |

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | W | 498 | Total | C | N | O | S | 0 | 0 |
| | | | 4126 | 2577 | 750 | 788 | 11 | | |

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | X | 654 | Total | C | N | O | S | 0 | 0 |
| | | | 5467 | 3534 | 918 | 996 | 19 | | |

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 26 | Y | 98 | Total | C | N | O | 0 | 0 |
| | | | 845 | 522 | 157 | 166 | | |

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | Z | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1232 | 766 | 220 | 243 | 3 | | |

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | a | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1035 | 644 | 185 | 205 | 1 | | |

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | b | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 822 | 503 | 148 | 169 | 2 | | |

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | c | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1678 | 1071 | 280 | 315 | 12 | | |

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | d | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1179 | 750 | 202 | 223 | 4 | | |

- Molecule 32 is a protein called G-patch domain-containing protein C1486.03.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | m | 461 | Total | C | N | O | S | 0 | 0 |
| | | | 3813 | 2488 | 616 | 693 | 16 | | |

- Molecule 33 is a protein called Uncharacterized protein C17A2.08c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | n | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 248 | 153 | 44 | 50 | 1 | | |

- Molecule 34 is a protein called Uncharacterized protein C20H4.06c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | y | 200 | Total | C | N | O | S | 0 | 0 |
| | | | 1606 | 1000 | 279 | 323 | 4 | | |

- Molecule 35 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | z | 626 | Total | C | N | O | S | 0 | 0 |
| | | | 4980 | 3193 | 835 | 933 | 19 | | |

- Molecule 36 is a protein called UNK1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 36 | r | 67 | Total | C | N | O | 0 | 0 |
| | | | 335 | 201 | 67 | 67 | | |

- Molecule 37 is a protein called UNK2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 37 | q | 56 | Total | C | N | O | 0 | 0 |
| | | | 295 | 182 | 57 | 56 | | |

- Molecule 38 is a RNA chain called U6snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | 6 | 92 | Total | C | N | O | P | 0 | 0 |
| | | | 1970 | 882 | 365 | 631 | 92 | | |

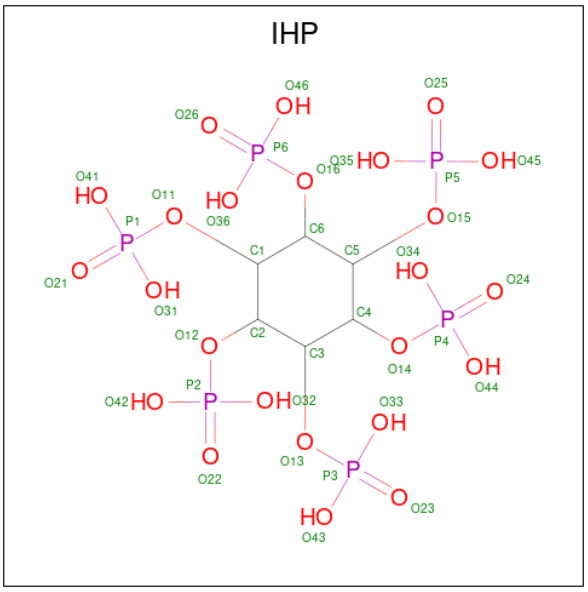
- Molecule 39 is a RNA chain called pre-mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | 1 | 29 | Total | C | N | O | P | 0 | 0 |
| | | | 605 | 272 | 91 | 213 | 29 | | |

- Molecule 40 is a protein called UNK3.

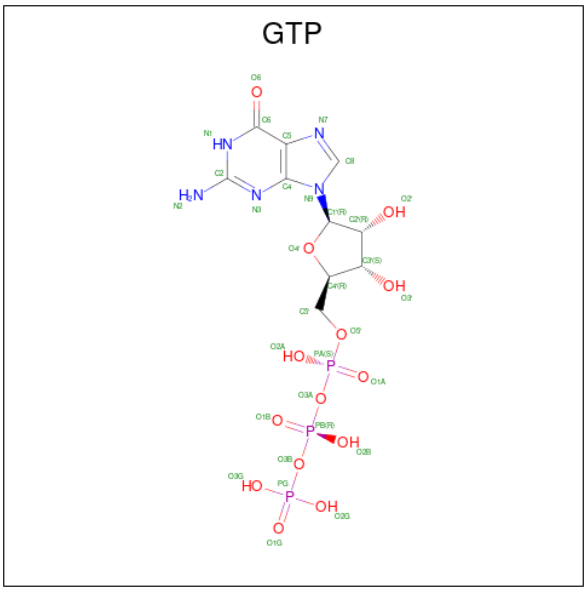
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 40 | f | 22 | Total | C | N | O | 0 | 0 |
| | | | 110 | 66 | 22 | 22 | | |

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | |
| 41 | A | 1 | 36 | 6 | 24 | 6 | 0 |

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | B | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 43 | B | 1 | Total Mg<br>1 1 | 0 |
| 43 | 6 | 3 | Total Mg<br>3 3 | 0 |

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 44 | M | 2 | Total Zn<br>2 2 | 0 |
| 44 | O | 3 | Total Zn<br>3 3 | 0 |
| 44 | P | 1 | Total Zn<br>1 1 | 0 |

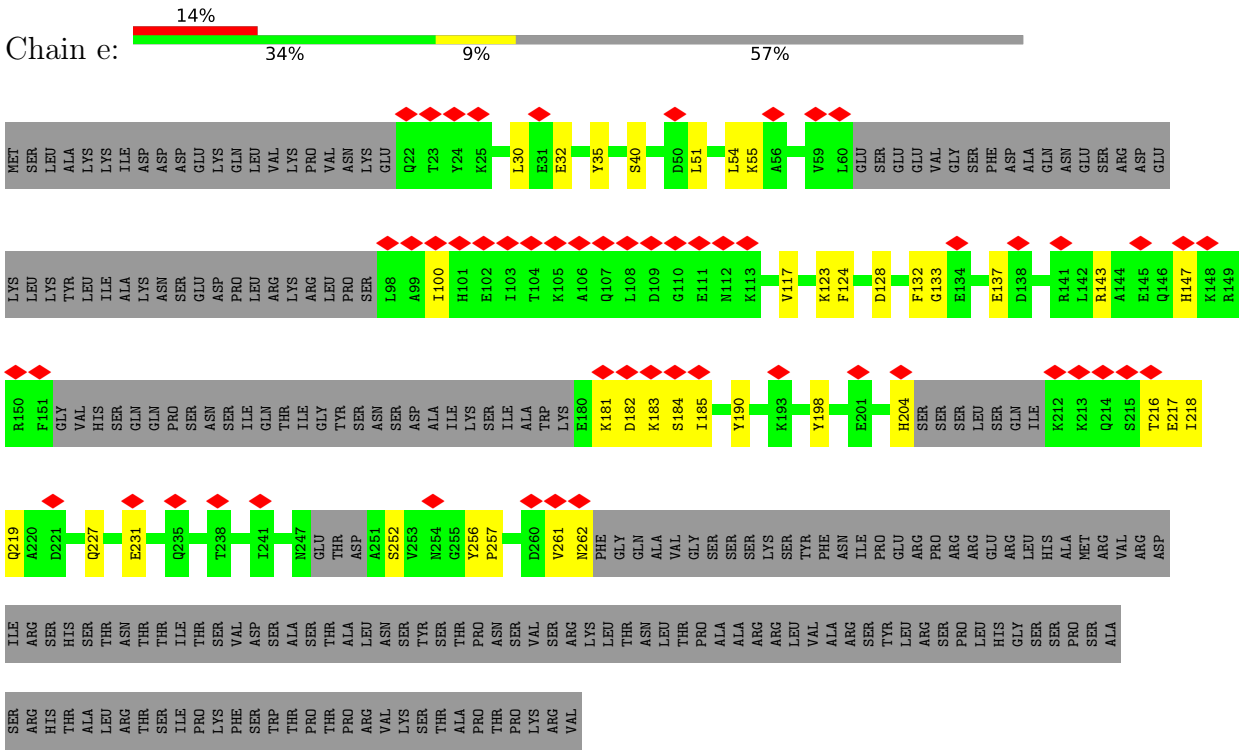
- Molecule 45 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 45 | 6 | 1 | Total K<br>1 1 | 0 |

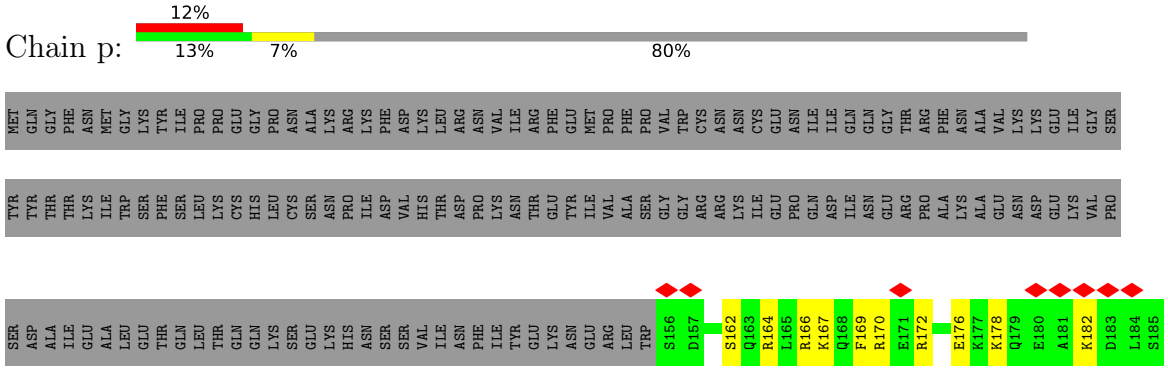
# 3 Residue-property plots (i)

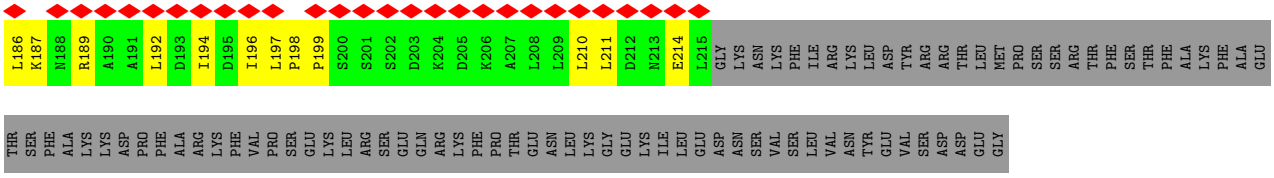
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Stress response protein bis1



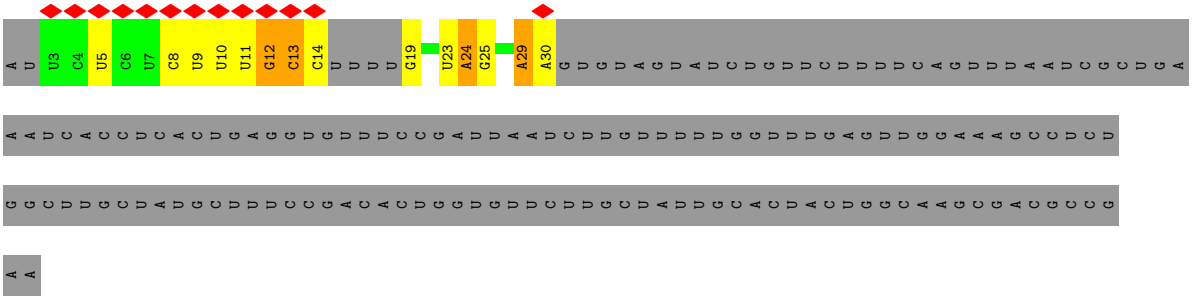

• Molecule 2: Protein saf4





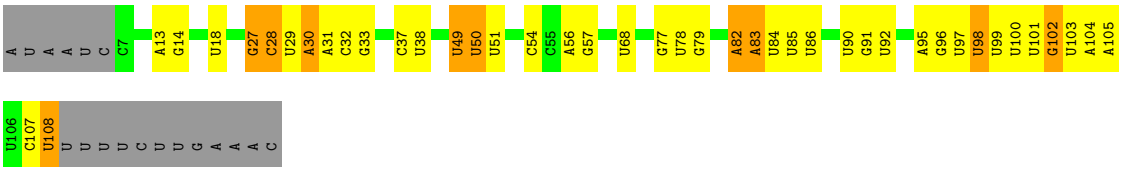

• Molecule 3: U2snRNA

Chain 2:

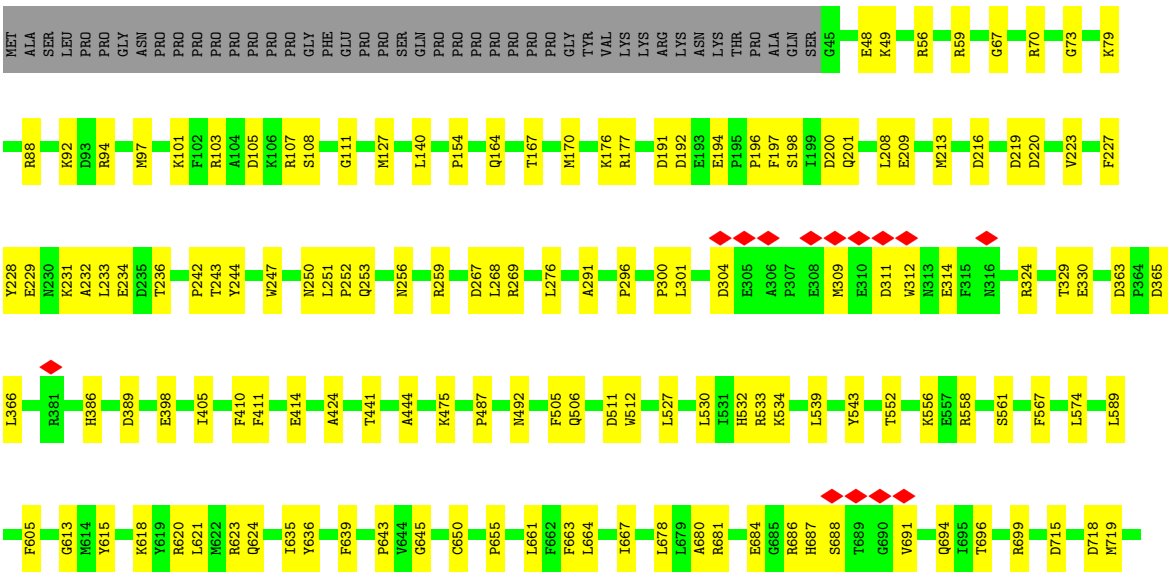

• Molecule 4: U5snRNA

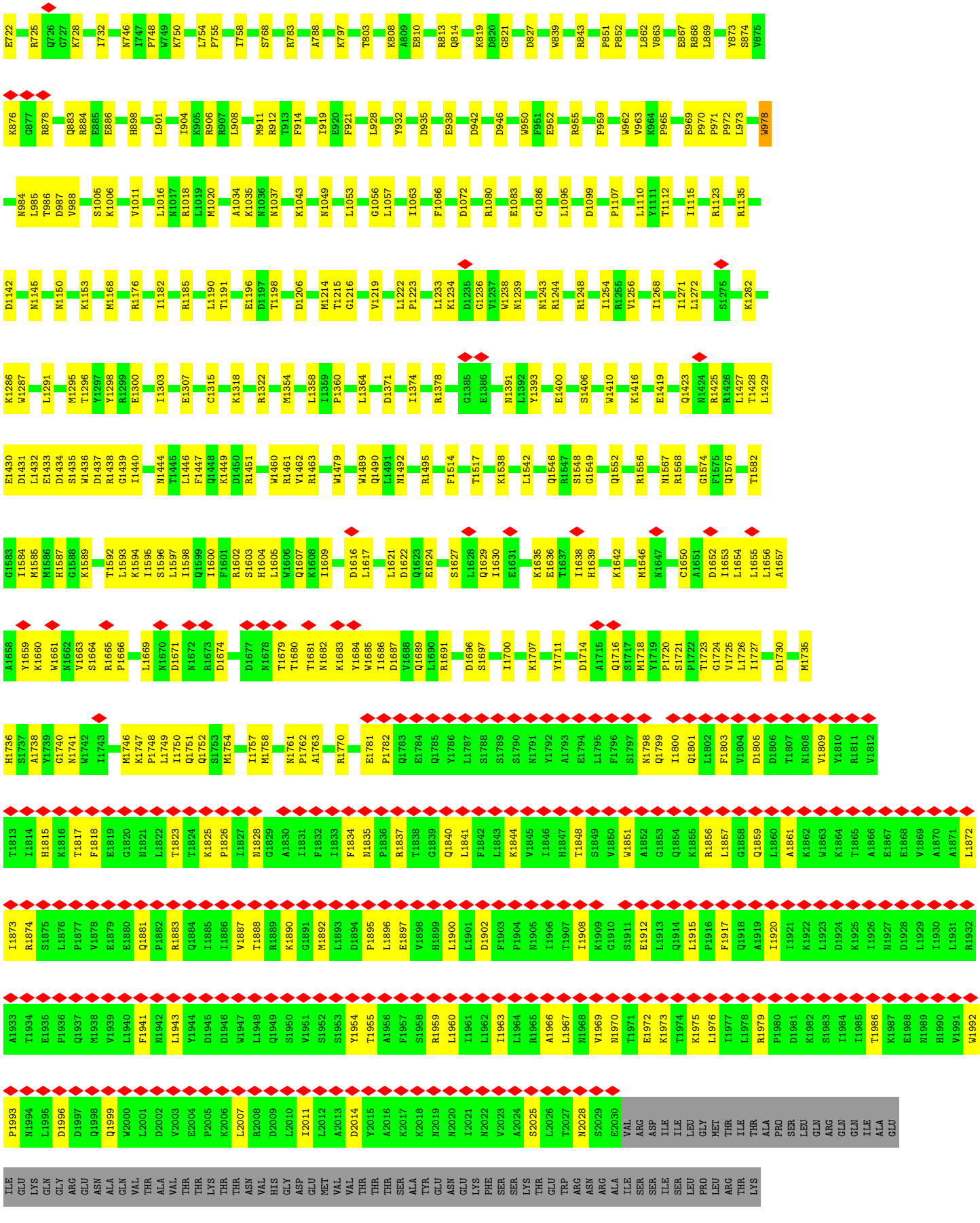
Chain 5:

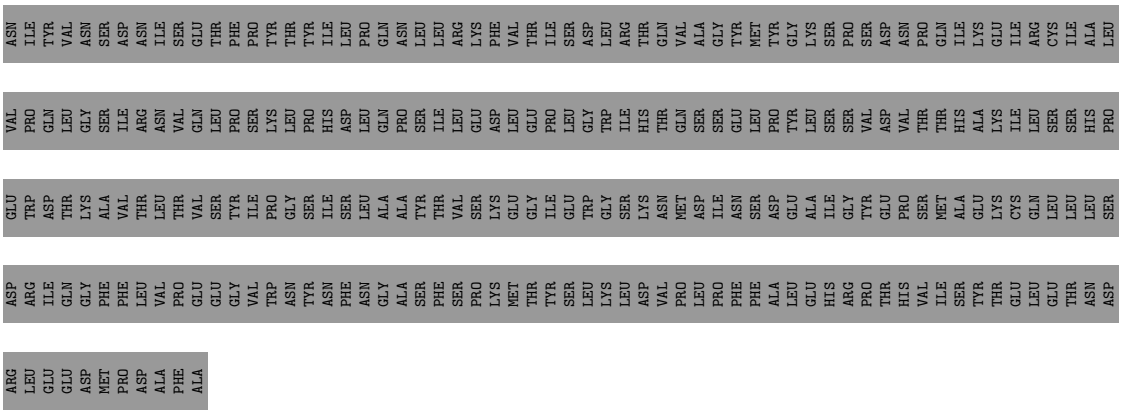




• Molecule 5: Pre-mRNA-splicing factor spp42

Chain A:

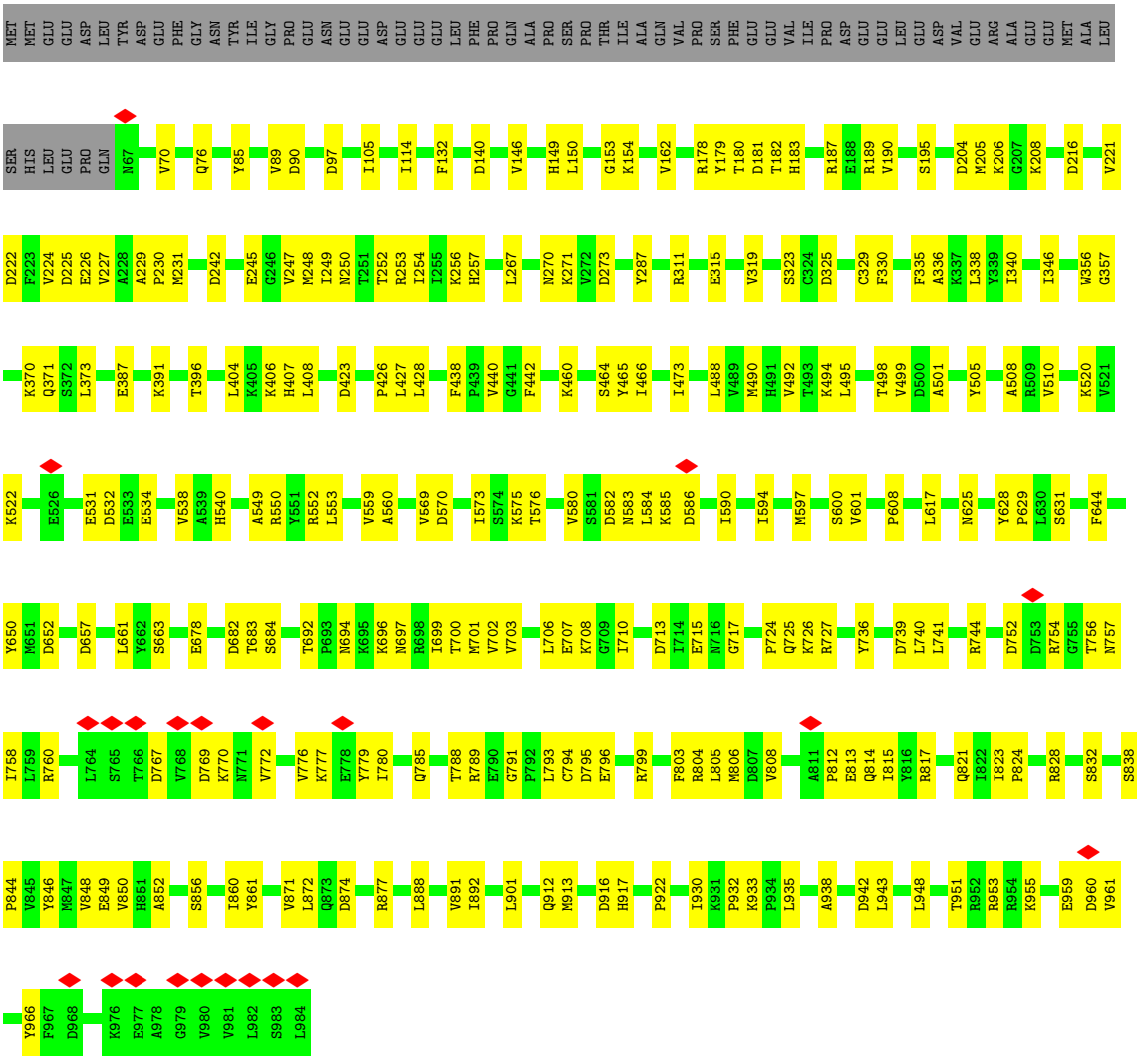




E722 R725 Q726 G727 K728 I732 N746 I747 P748 W749 K750 L754 P755 I758 S768 R783 A788 K797 T803 K808 A809 E810 R813 Q814 K819 D820 G821 D827 W839 R843 P851 P852 L862 V863 E867 R868 L869 Y873 S874 V875
K876 G877 R878 Q883 R884 E885 E886 H898 L901 I904 K905 R906 R907 L908 M911 R912 T913 F914 I919 E920 F921 L928 Y932 D935 E938 D942 D946 W950 F951 E952 R955 F959 W962 V963 K964 P965 E969 P970 P971 P972 L973 W978
N984 L985 T986 D987 V988 S1005 K1006 V1011 L1016 N1017 R1018 L1019 M1020 A1034 K1035 N1036 N1037 K1043 N1049 L1053 G1056 L1057 I1063 F1066 D1072 R1080 E1083 G1086 L1095 D1099 P1107 L1110 Y1111 T1112 I1115 R1123 R1135
D1142 N1145 N1150 K1153 M1168 R1176 I1182 R1185 L1190 T1191 E1196 D1197 T1198 D1206 M1214 T1215 G1216 V1219 L1222 P1223 L1233 K1234 D1235 G1236 V1237 W1238 N1239 N1243 R1244 R1248 I1254 R1255 V1256 I1268 I1271 L1272 S1275 K1282
K1286 W1287 L1291 M1295 T1296 Y1297 Y1298 R1299 E1300 I1303 E1307 C1315 K1318 R1322 M1354 L1358 I1359 P1360 L1364 D1371 I1374 R1378 G1385 E1386 N1391 L1392 Y1393 E1400 S1406 W1410 K1416 E1419 Q1423 N1424 R1425 R1426 L1427 T1428 L1429
E1430 D1431 L1432 E1433 D1434 S1435 W1436 D1437 R1438 G1439 I1440 N1444 T1445 L1446 F1447 Q1448 K1449 D1450 R1451 W1460 R1461 V1462 R1463 W1479 W1489 Q1490 L1491 N1492 R1495 F1514 T1517 K1538 L1542 Q1546 R1547 S1548 G1549 Q1552 R1556 N1567 R1568 G1574 F1575 Q1576 T1582
G1583 I1584 M1585 M1586 H1587 G1588 K1589 T1592 L1593 K1594 I1595 S1596 L1597 I1598 Q1599 I1600 F1601 R1602 S1603 H1604 L1605 W1606 Q1607 K1608 I1609 D1616 L1617 L1621 D1622 Q1623 E1624 S1627 L1628 Q1629 I1630 E1631 K1635 E1636 T1637 I1638 H1639 K1642 M1646 N1647 C1650 A1651 D1652 I1653 L1654 L1655 L1656 A1657
A1658 Y1659 K1660 W1661 N1662 V1663 S1664 R1665 P1666 L1669 N1670 D1671 N1672 R1673 D1674 D1677 N1678 T1679 T1680 T1681 N1682 K1683 Y1684 W1685 I1686 D1687 V1688 Q1689 L1690 R1691 D1696 S1697 I1700 K1707 Y1711 D1714 A1715 Q1716 S1717 M1718 Y1719 P1720 S1721 P1722 T1723 G1724 V1725 L1726 I1727 D1730 M1735
H1736 S1737 A1738 Y1739 G1740 N1741 W1742 I1743 M1746 K1747 P1748 L1749 I1750 Q1751 Q1752 S1753 M1754 I1757 M1758 N1761 P1762 A1763 R1770 E1781 P1782 Q1783 E1784 Q1785 Y1786 L1787 S1788 S1789 S1790 N1791 Y1792 A1793 E1794 L1795 F1796 S1797 N1798 Q1799 I1800 Q1801 L1802 F1803 V1804 D1805 D1806 T1807 N1808 V1809 Y1810 R1811 V1812
T1813 I1814 H1815 K1816 T1817 F1818 E1819 G1820 N1821 L1822 T1823 T1824 K1825 P1826 I1827 N1828 G1829 A1830 I1831 F1832 I1833 F1834 N1835 P1836 R1837 T1838 G1839 Q1840 L1841 F1842 L1843 K1844 V1845 I1846 H1847 T1848 S1849 V1850 W1851 A1852 G1853 Q1854 K1855 R1856 L1857 G1858 Q1859 L1860 A1861 K1862 W1863 K1864 T1865 A1866 E1867 E1868 V1869 A1870 A1871 L1872
I1873 R1874 S1875 L1876 P1877 V1878 E1879 E1880 Q1881 P1882 R1883 Q1884 I1885 I1886 V1887 T1888 R1889 K1890 G1891 M1892 L1893 D1894 P1895 L1896 E1897 V1898 H1899 L1900 L1901 D1902 F1903 P1904 N1905 I1906 T1907 I1908 K1909 G1910 S1911 E1912 L1913 Q1914 L1915 P1916 F1917 Q1918 A1919 I1920 I1921 K1922 L1923 D1924 K1925 I1926 N1927 D1928 L1929 I1930 I1931 R1932
A1933 T1934 E1935 P1936 Q1937 M1938 V1939 L1940 F1941 N1942 L1943 Y1944 D1945 D1946 W1947 L1948 Q1949 S1950 V1951 S1952 S1953 Y1954 T1955 A1956 F1957 S1958 R1959 L1960 I1961 L1962 I1963 L1964 R1965 A1966 L1967 N1968 V1969 N1970 T1971 E1972 K1973 T1974 K1975 L1976 I1977 L1978 R1979 P1980 D1981 K1982 S1983 I1984 I1985 T1986 K1987 E1988 N1989 H1990 V1991 W1992
P1993 N1994 L1995 D1996 D1997 Q1998 Q1999 W2000 L2001 D2002 V2003 E2004 P2005 K2006 L2007 R2008 D2009 L2010 I2011 L2012 A2013 D2014 Y2015 A2016 K2017 K2018 N2019 N2020 I2021 N2022 V2023 A2024 S2025 L2026 T2027 N2028 S2029 E2030 VAL ARG ASP ILE ILE LEU GLY MET THR ILE THR ALA PRO SER LEU GLN ARG GLN GLN ILE ALA GLU
ILE GLU LYS GLN GLY ARG GLU ASN ALA GLN VAL THR ALA VAL THR THR LYS THR THR ASN VAL HIS GLY ASP GLU MET VAL VAL THR THR THR SER ALA TYR GLU ASN GLU LYS PHE SER SER LYS THR GLU TRP ARG ASN ARG ALA ILE SER SER ILE SER LEU PRO LEU ARG THR LYS



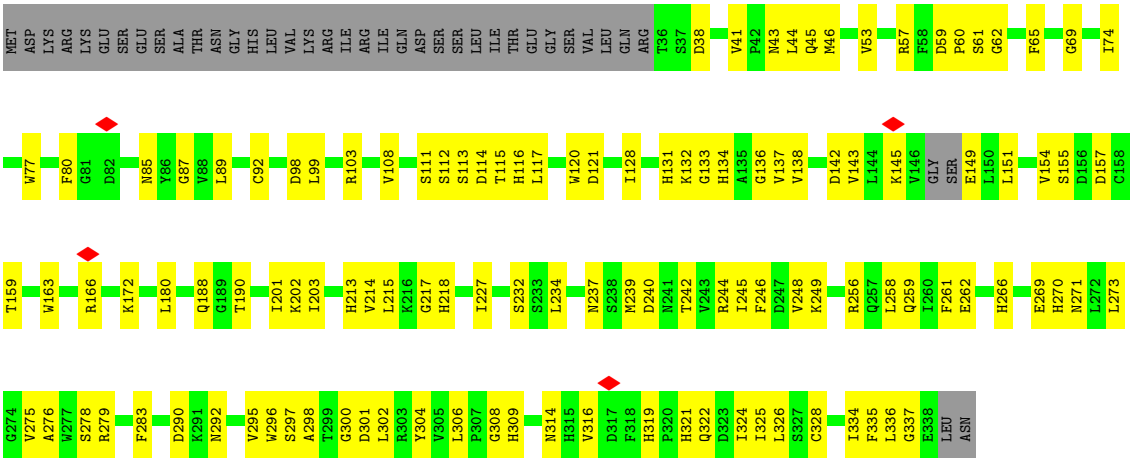

• Molecule 6: Pre-mRNA-splicing factor cwf10

Chain B:


• Molecule 7: Pre-mRNA-splicing factor cwf17

Chain C:

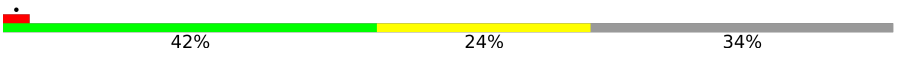


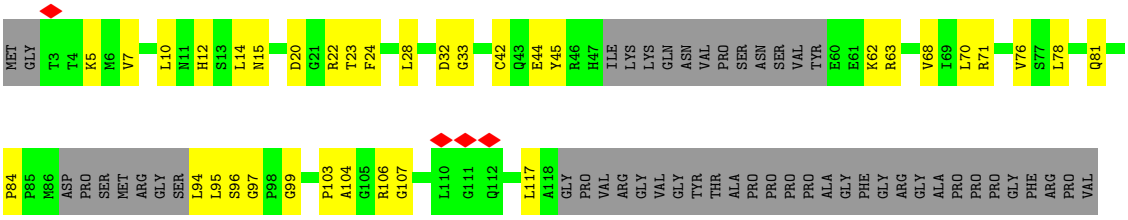
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain D:


• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

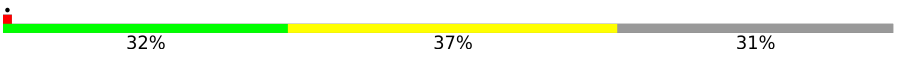
Chain E:

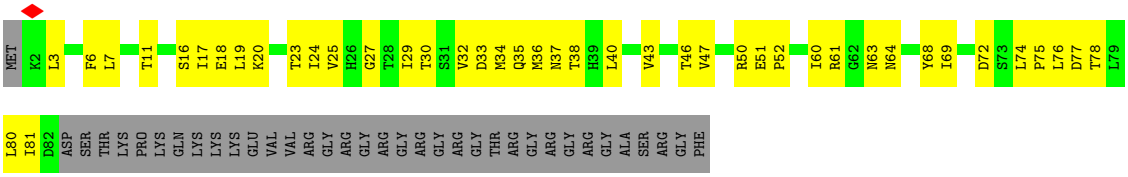


• Molecule 10: Small nuclear ribonucleoprotein Sm D1

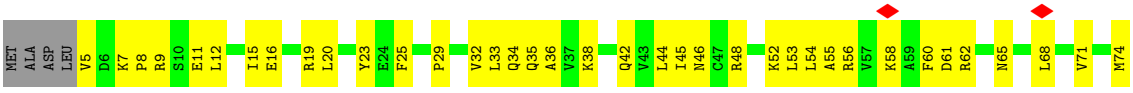
Chain F:



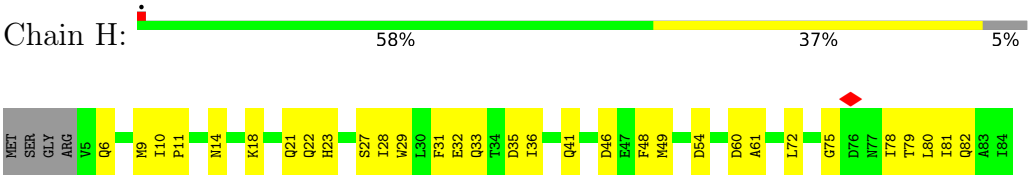



• Molecule 11: Small nuclear ribonucleoprotein Sm D2

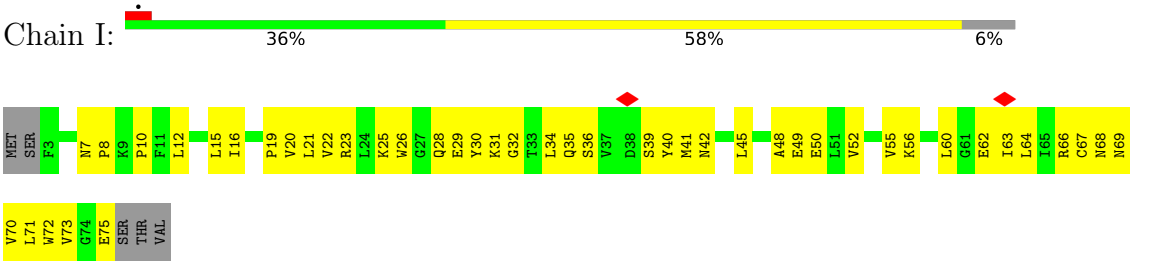
Chain G:

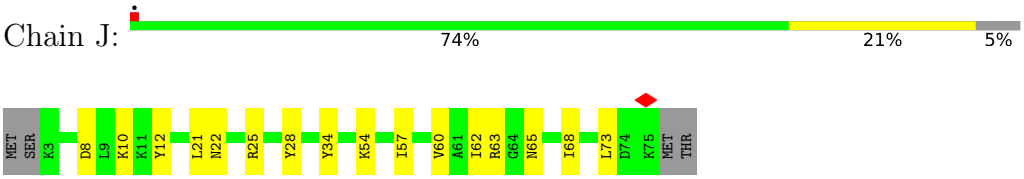

• Molecule 12: Small nuclear ribonucleoprotein E



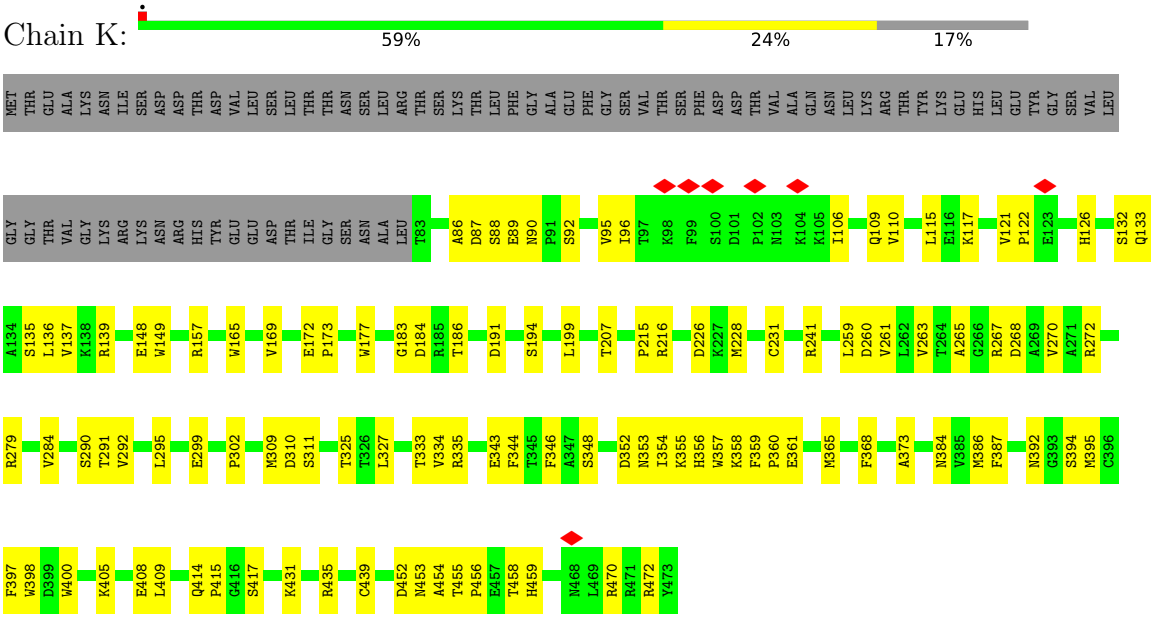

• Molecule 13: Small nuclear ribonucleoprotein F




• Molecule 14: Small nuclear ribonucleoprotein G

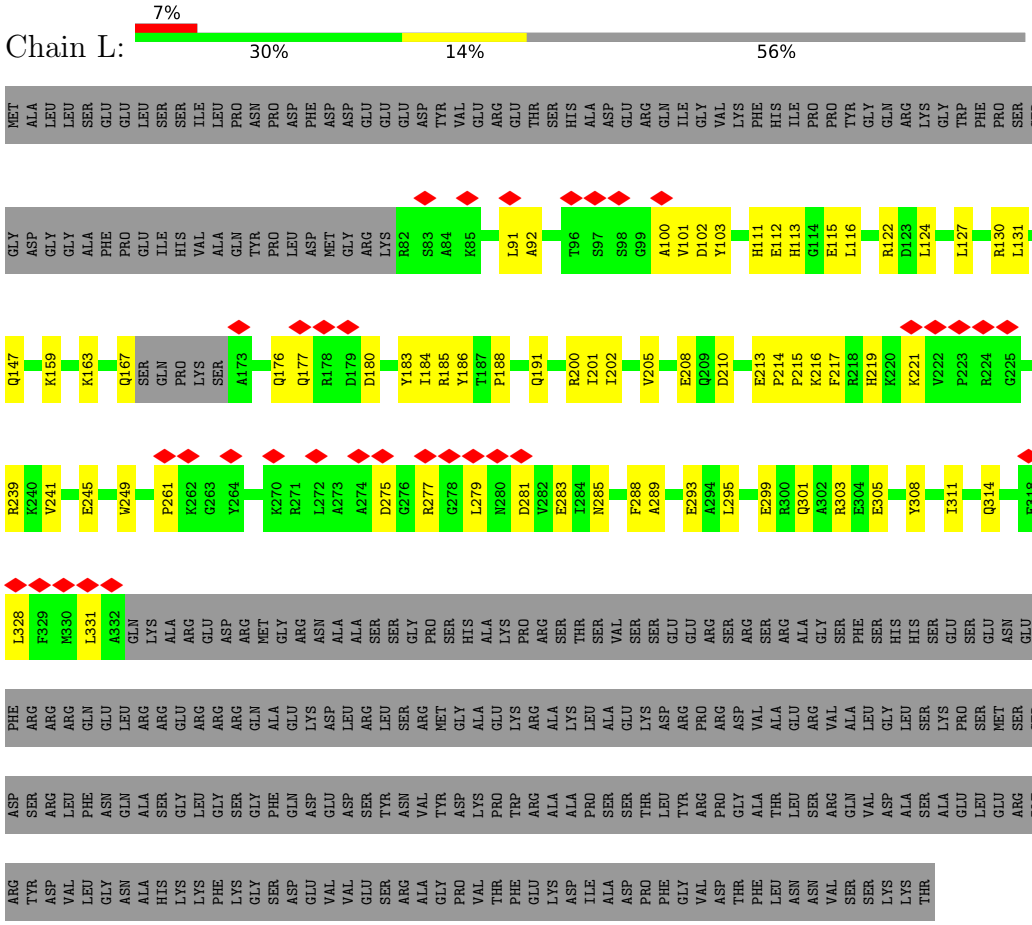



• Molecule 15: Pre-mRNA-splicing factor prp5



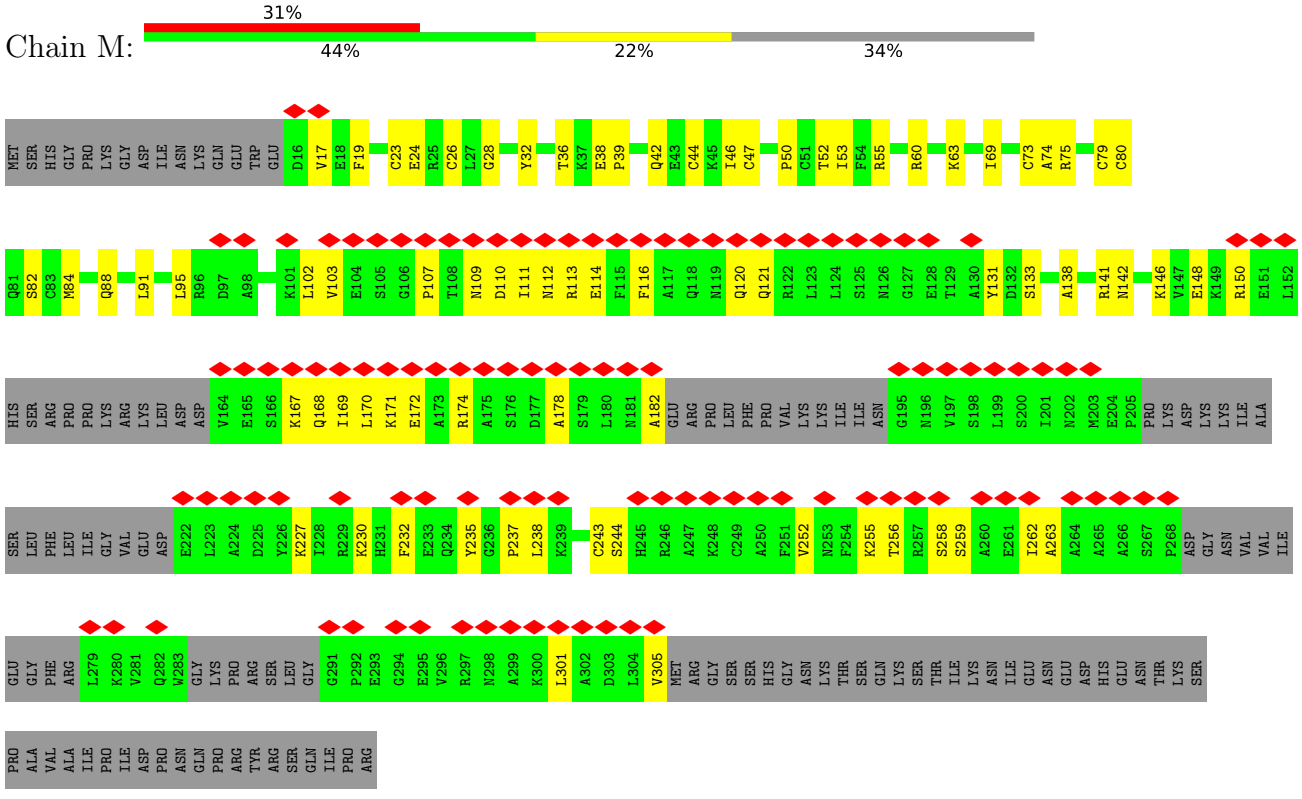

• Molecule 16: Pre-mRNA-processing protein 45

Chain L:



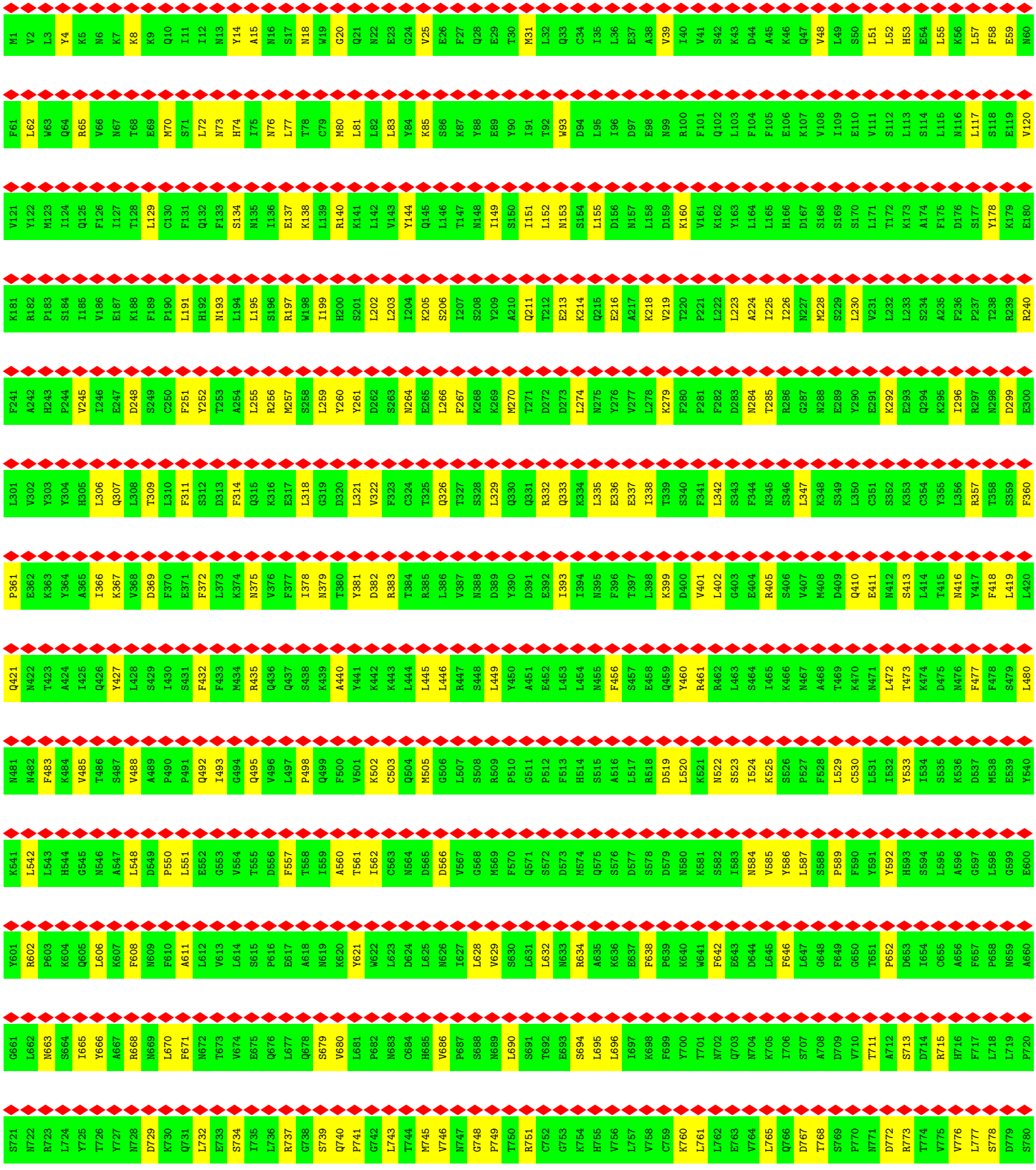

• Molecule 17: Pre-mRNA-splicing factor cwf5

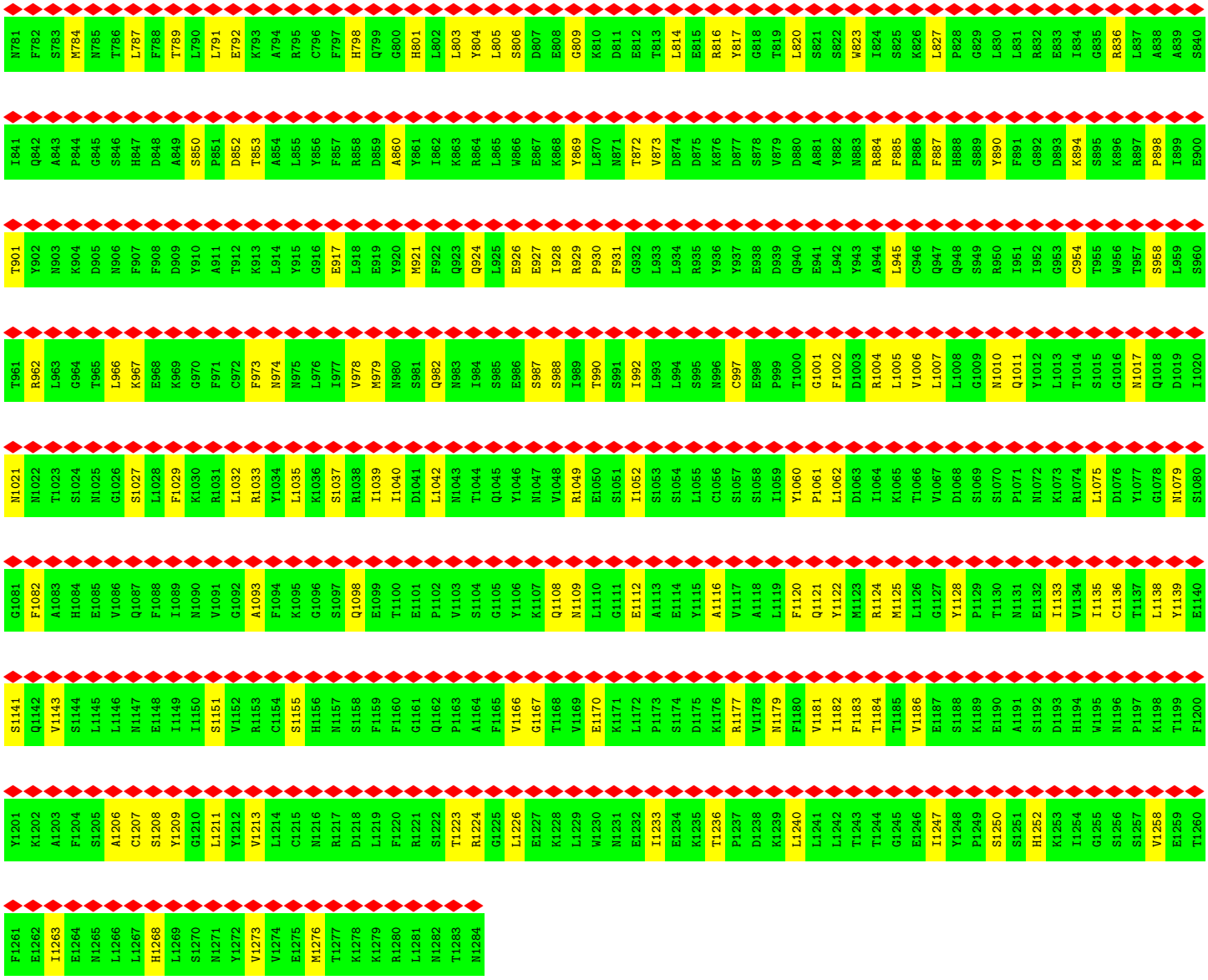
Chain M:



• Molecule 18: Pre-mRNA-splicing factor cwf11

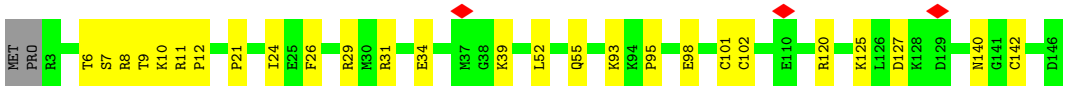
Chain N:



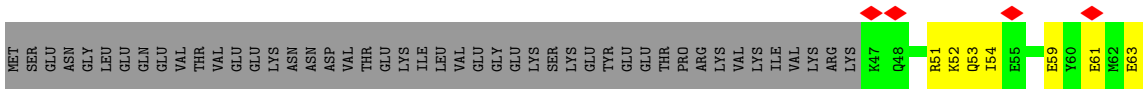

• Molecule 19: Pre-mRNA-splicing factor cwf14

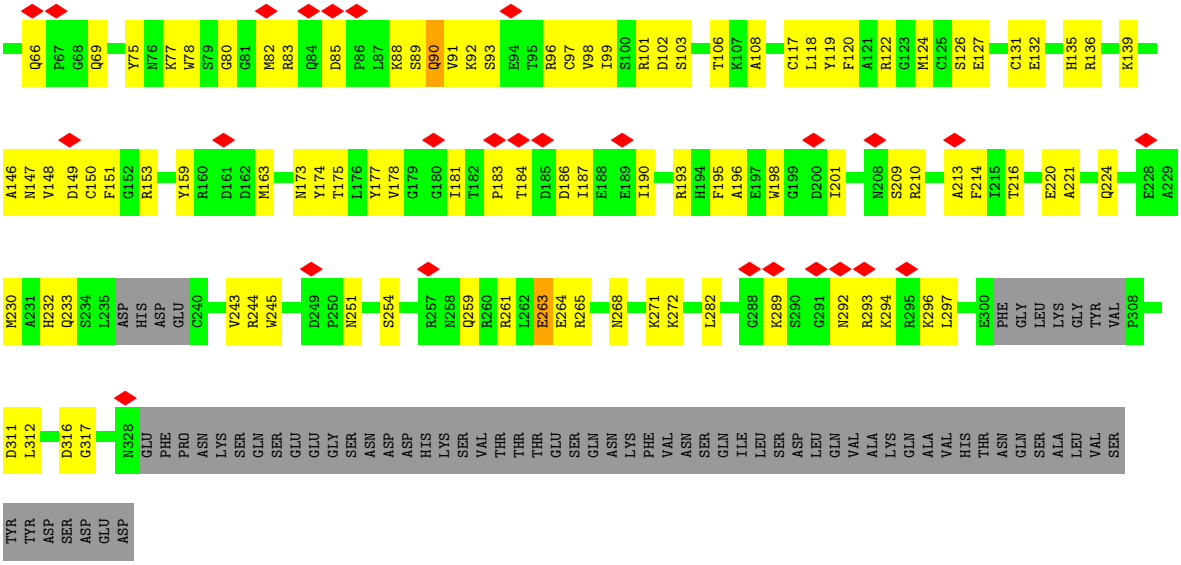
Chain O:


• Molecule 20: Pre-mRNA-splicing factor cwf2

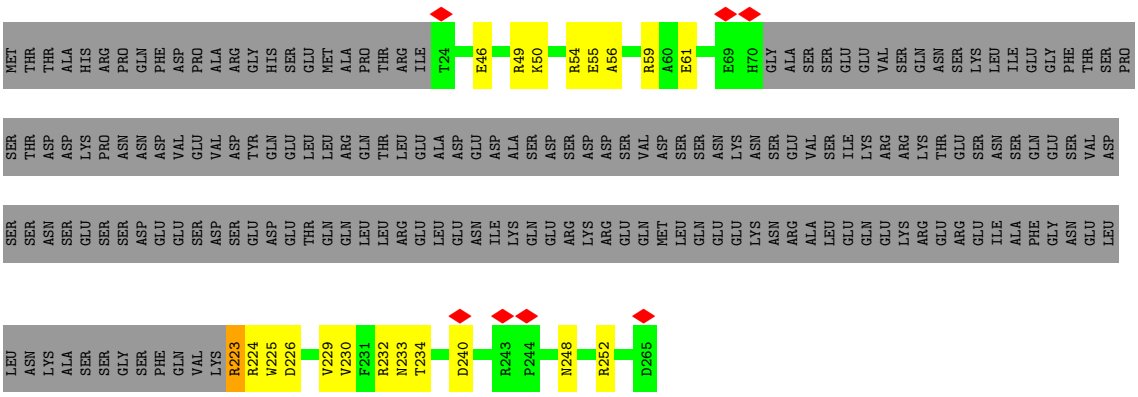
Chain P:



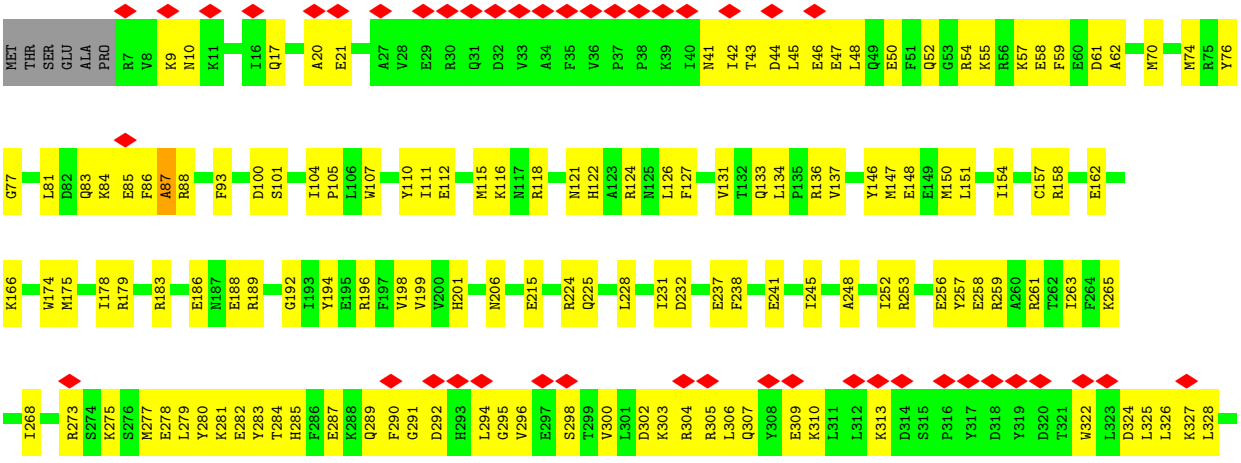
• Molecule 21: Pre-mRNA-splicing factor cwf15

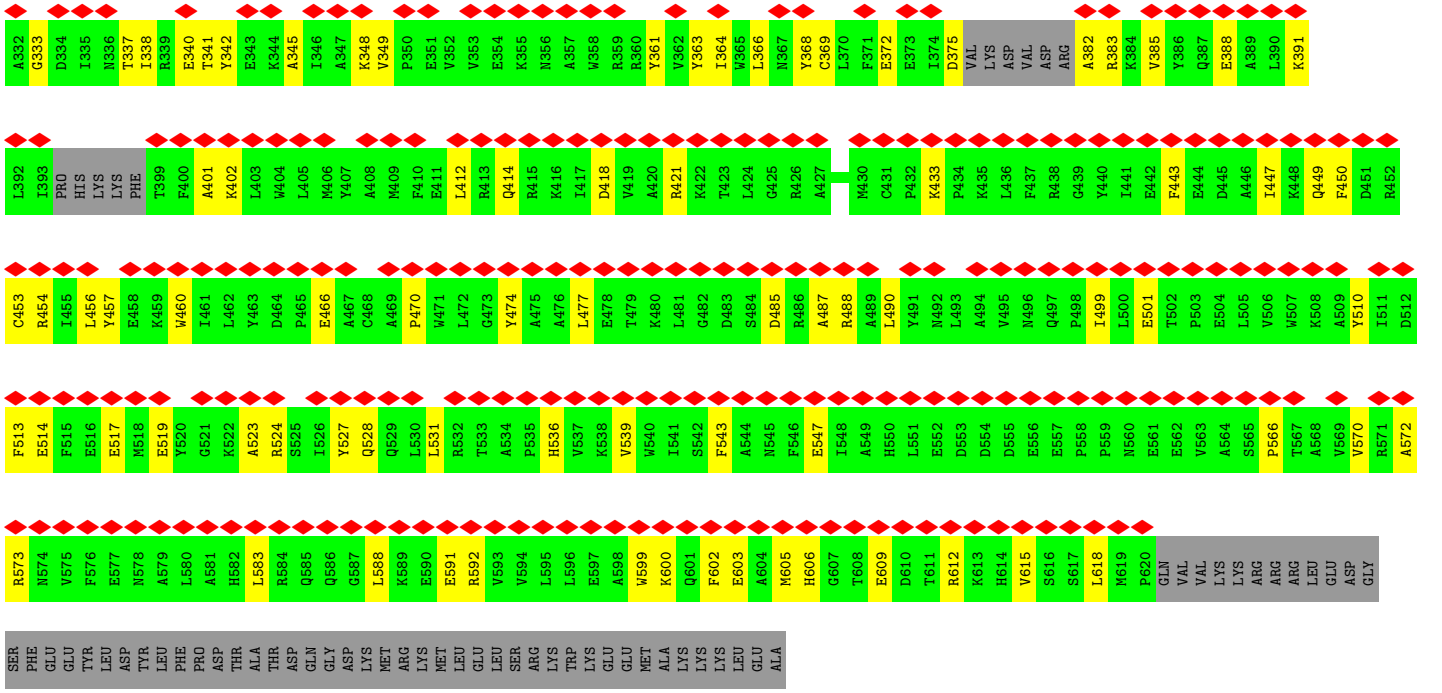
Chain Q:

• Molecule 22: Pre-mRNA-splicing factor cwf4

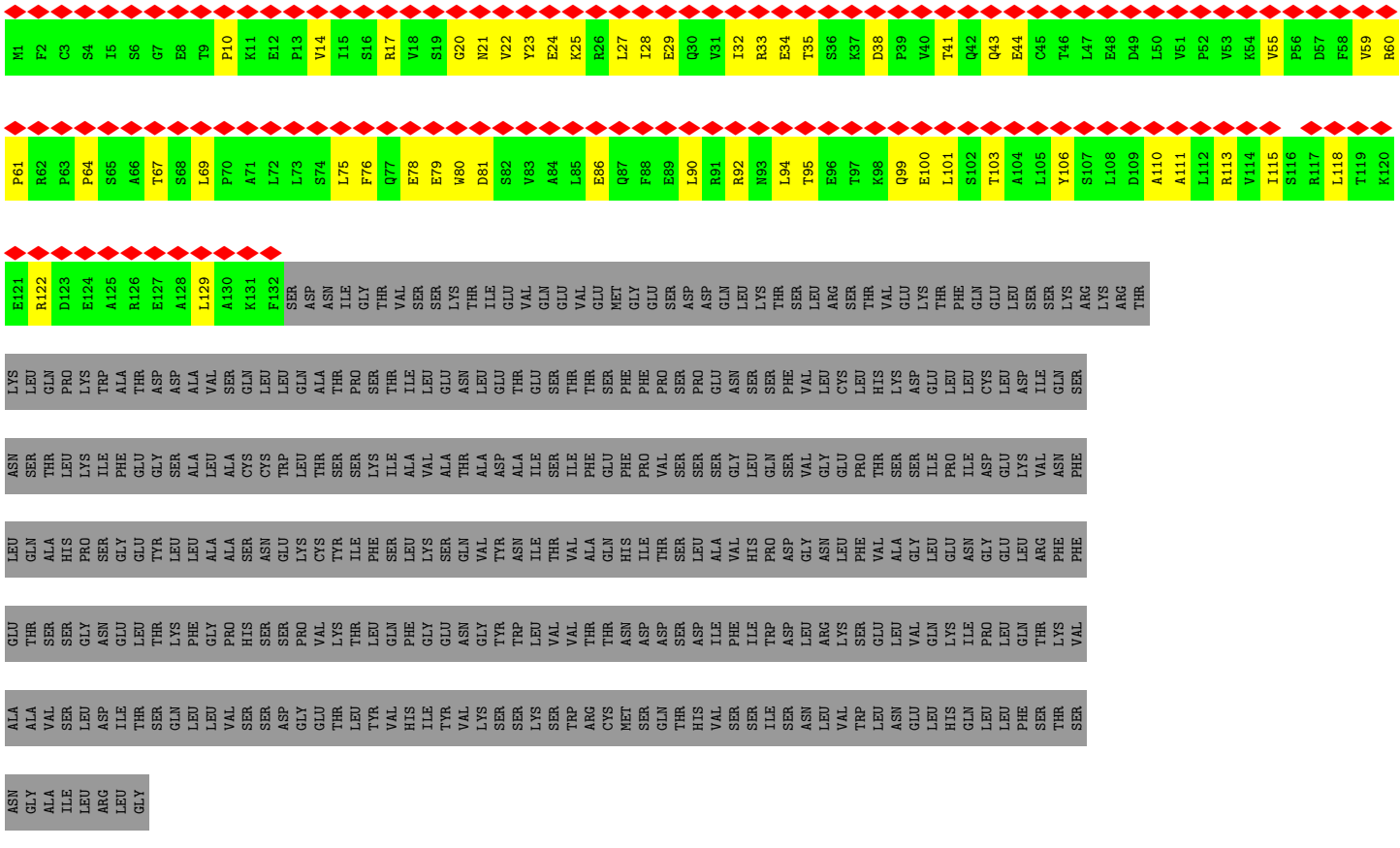
Chain R:



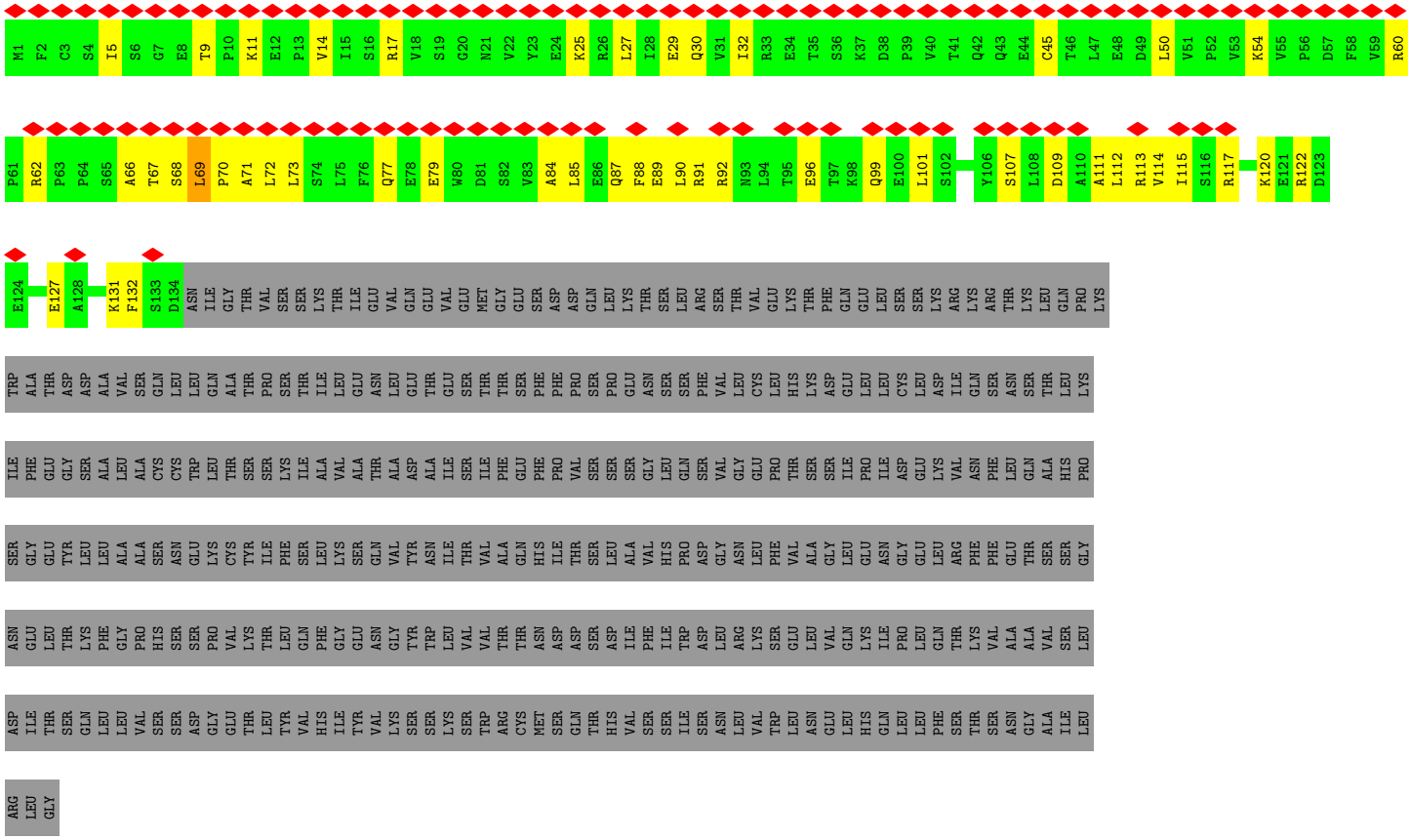

• Molecule 23: Pre-mRNA-processing factor 19

Chain S:

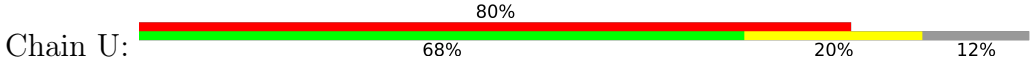
• Molecule 23: Pre-mRNA-processing factor 19

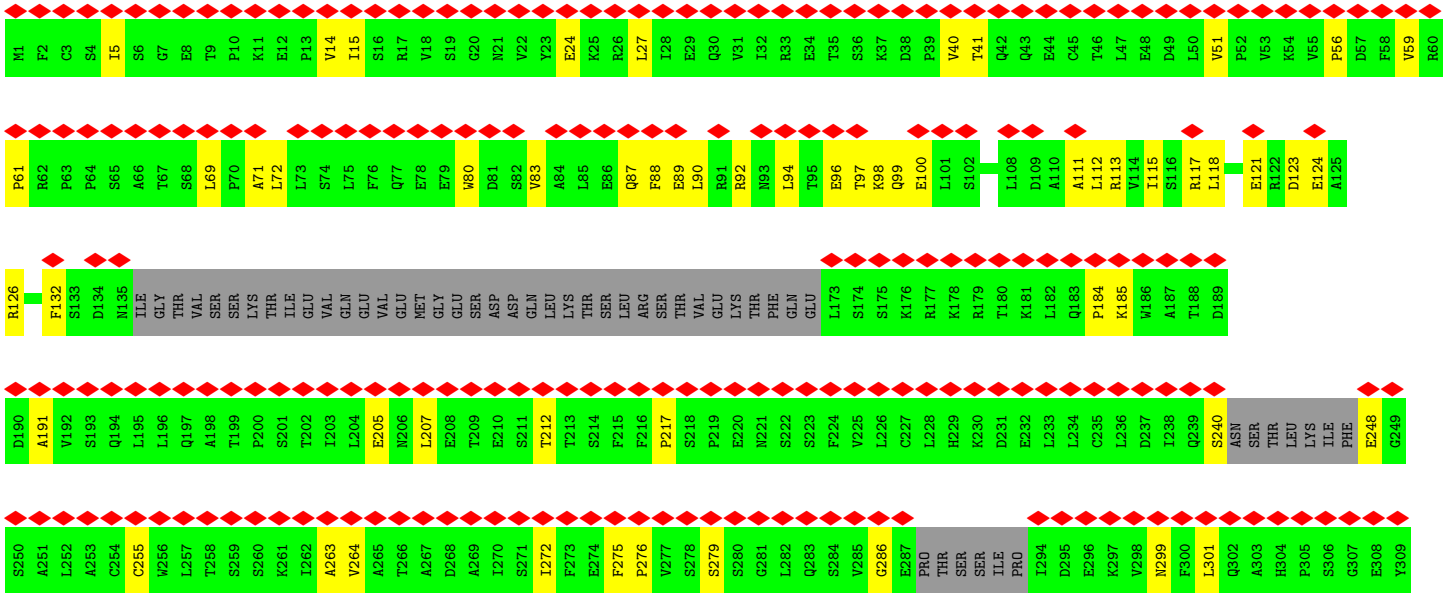
Chain T:

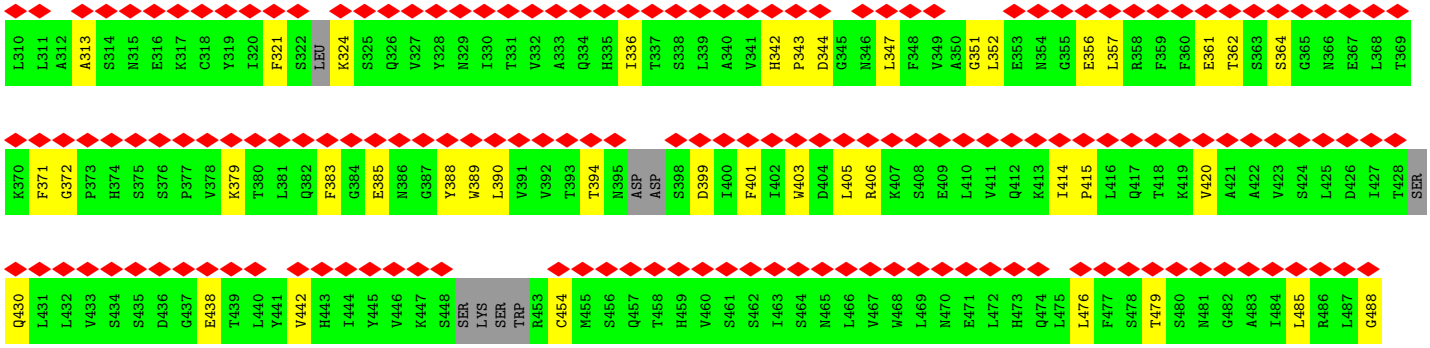




• Molecule 23: Pre-mRNA-processing factor 19

Chain U:

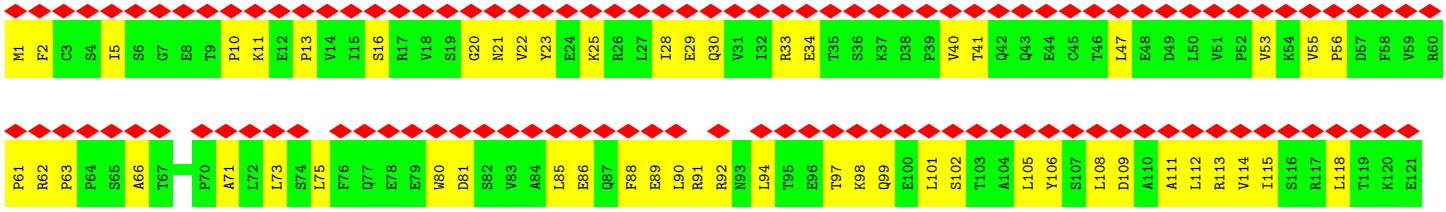




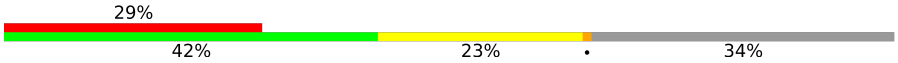

• Molecule 23: Pre-mRNA-processing factor 19

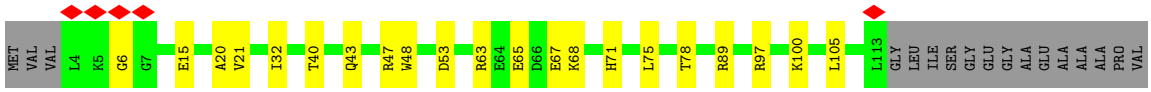
Chain V:

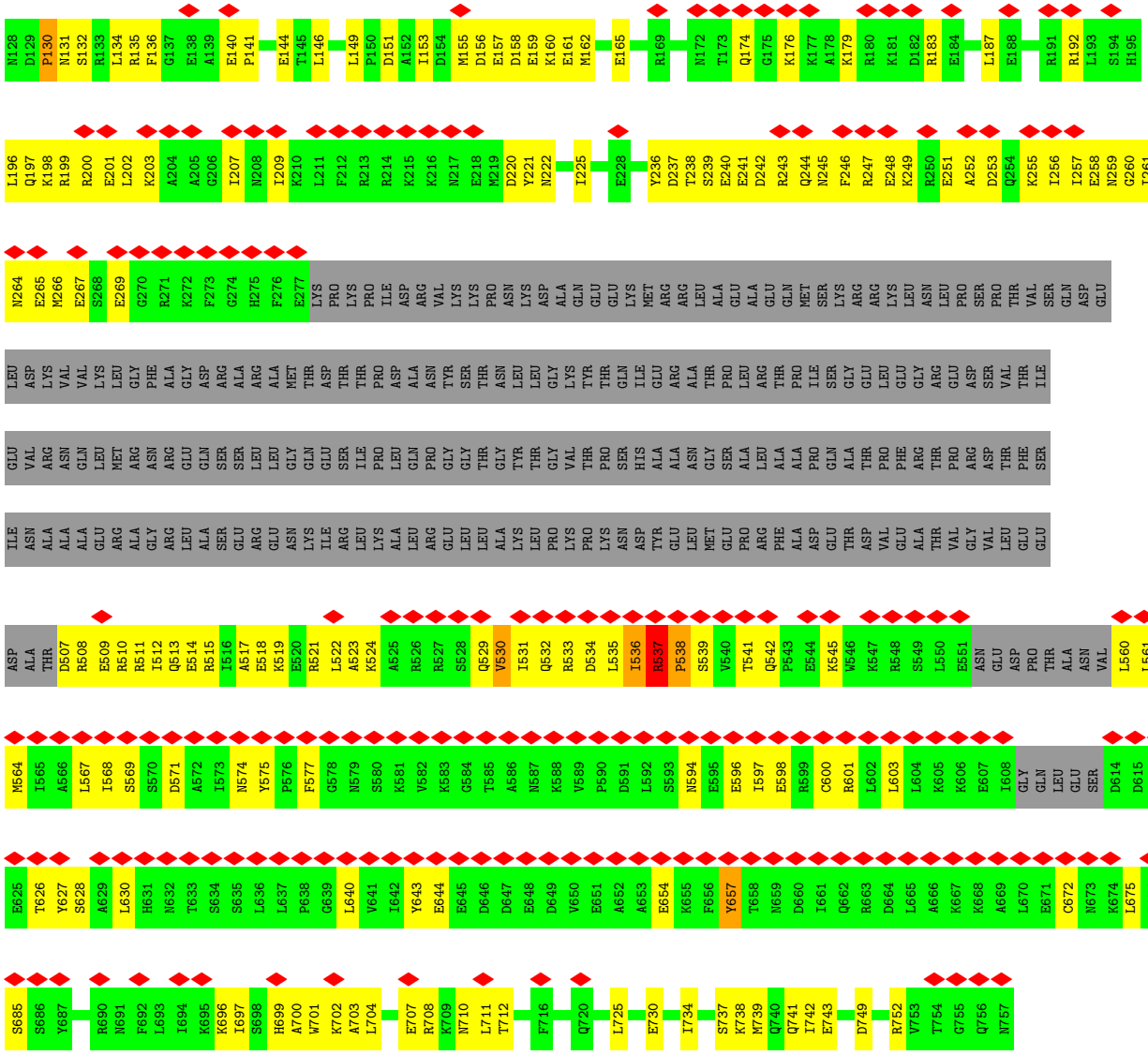




• Molecule 24: Pre-mRNA-splicing factor cdc5

Chain W:

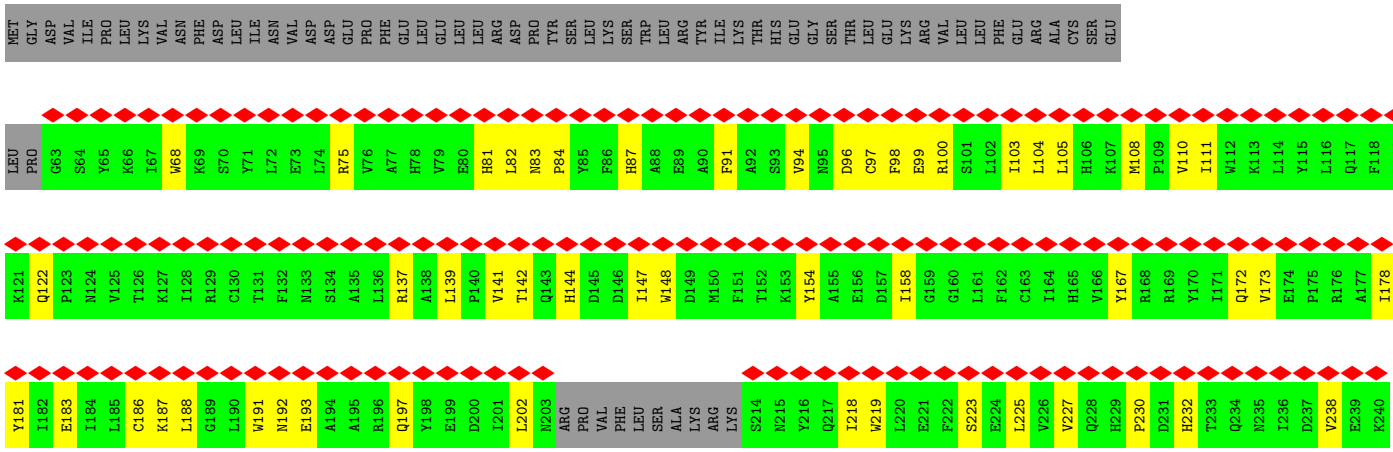


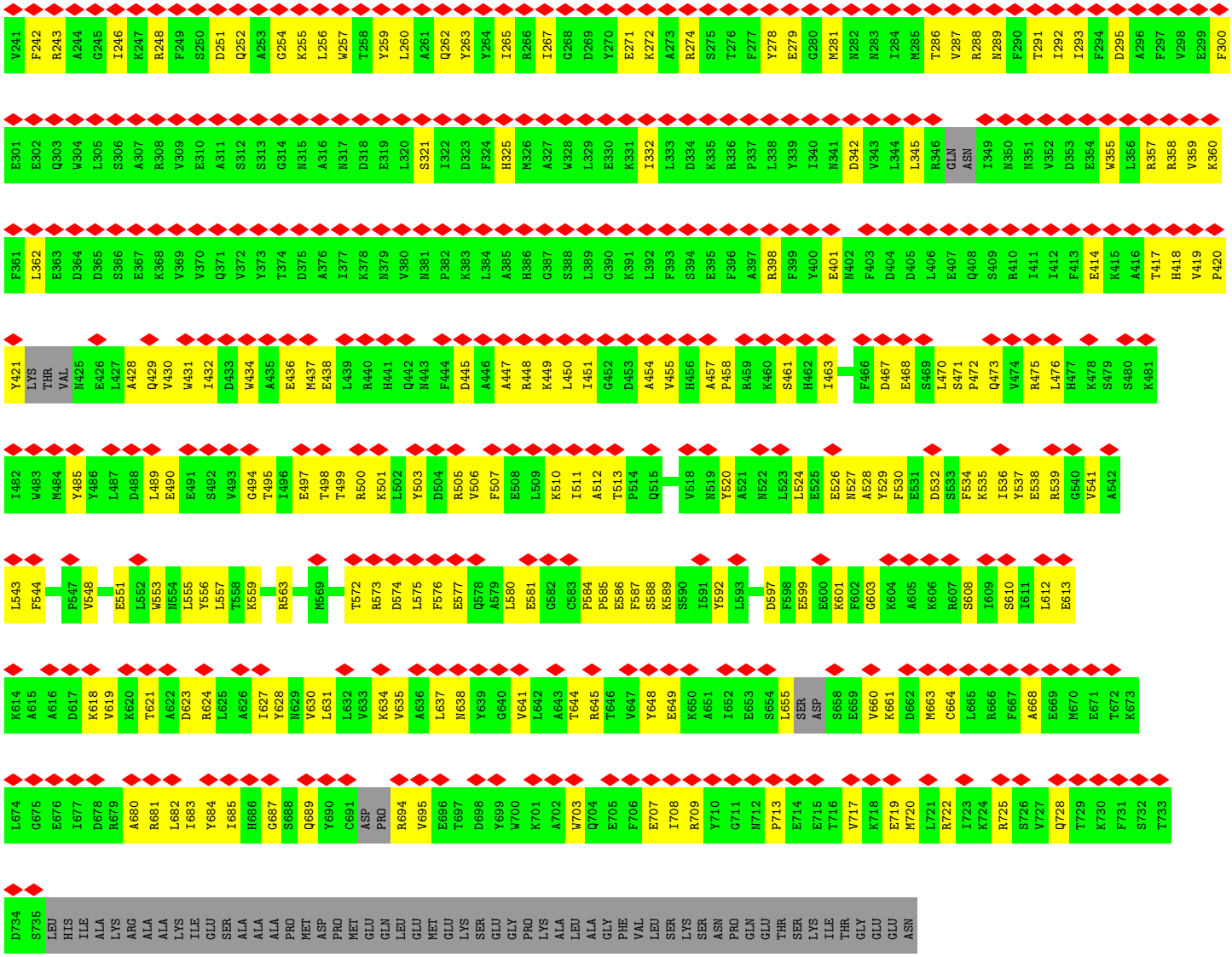





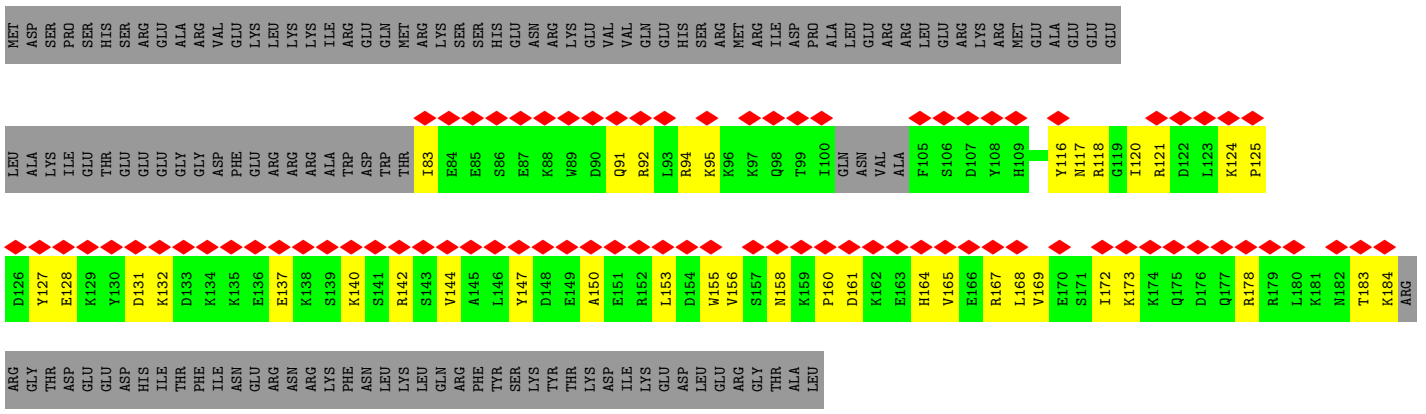
• Molecule 25: Pre-mRNA-splicing factor cwf3

Chain X:

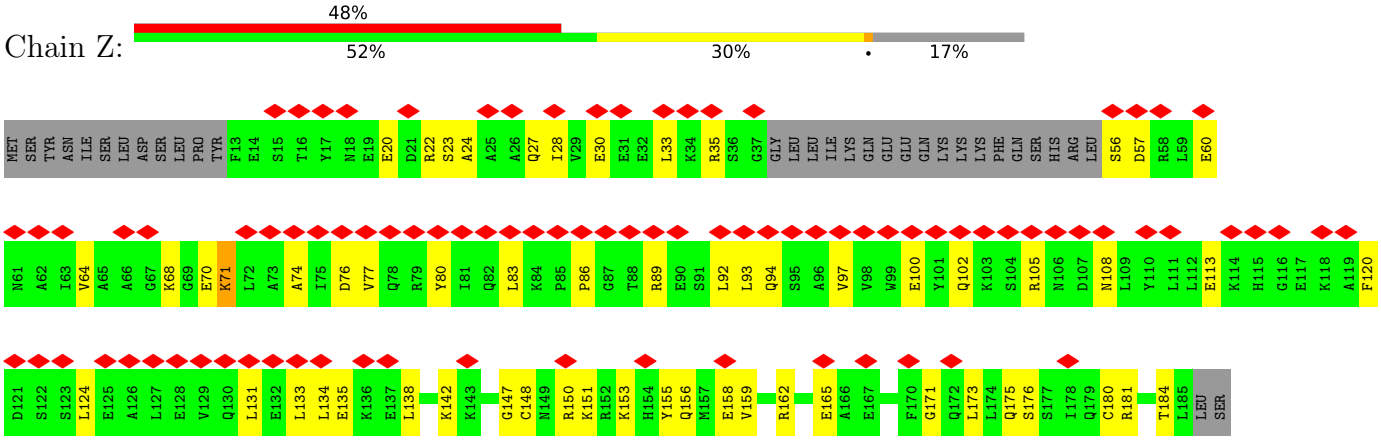



• Molecule 26: Pre-mRNA-splicing factor syf2

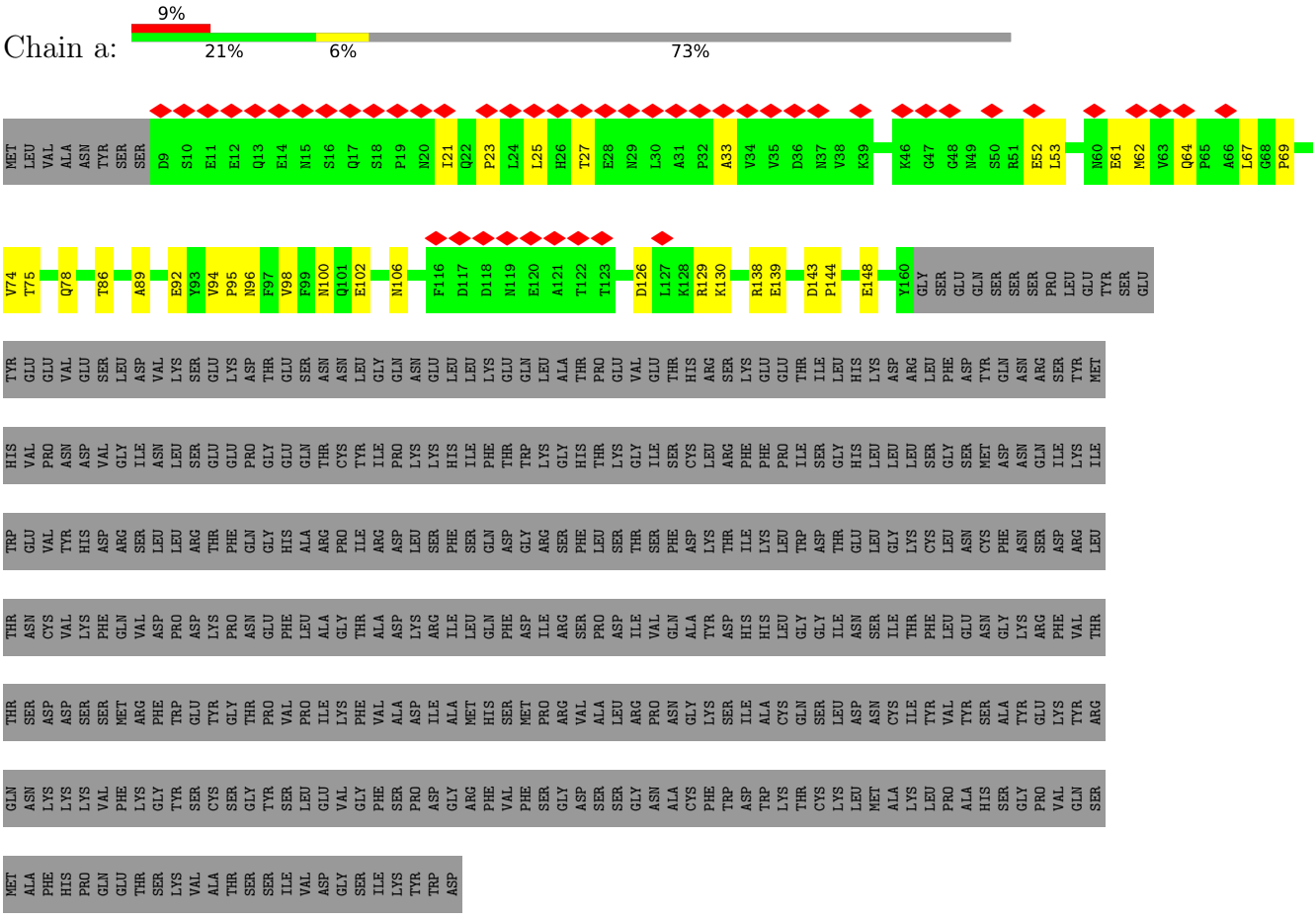

• Molecule 27: Pre-mRNA-splicing factor cwf7

Chain Z:



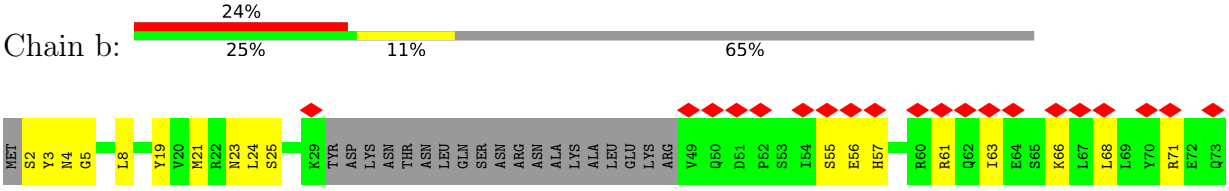

• Molecule 28: Pre-mRNA-processing factor 17

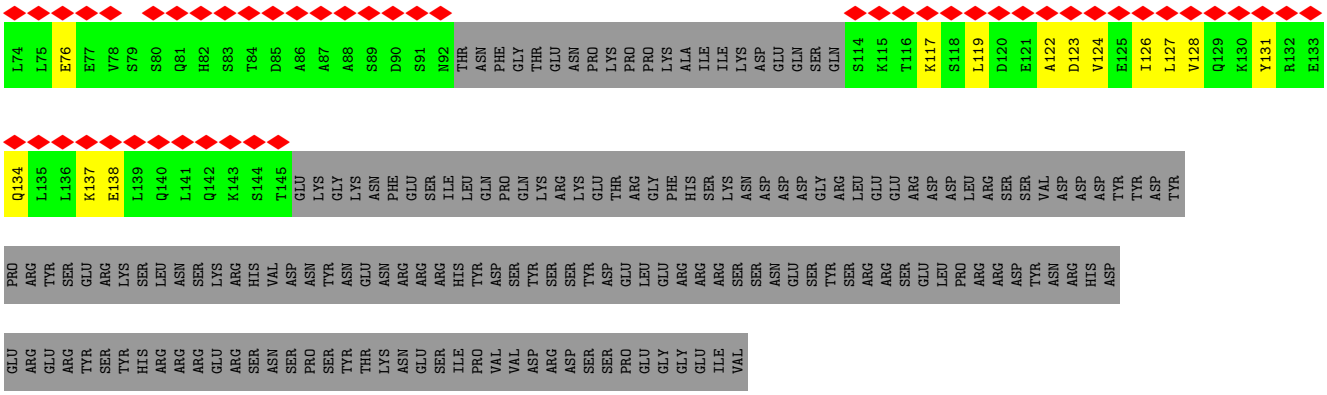
Chain a:




• Molecule 29: Pre-mRNA-splicing factor cwf21

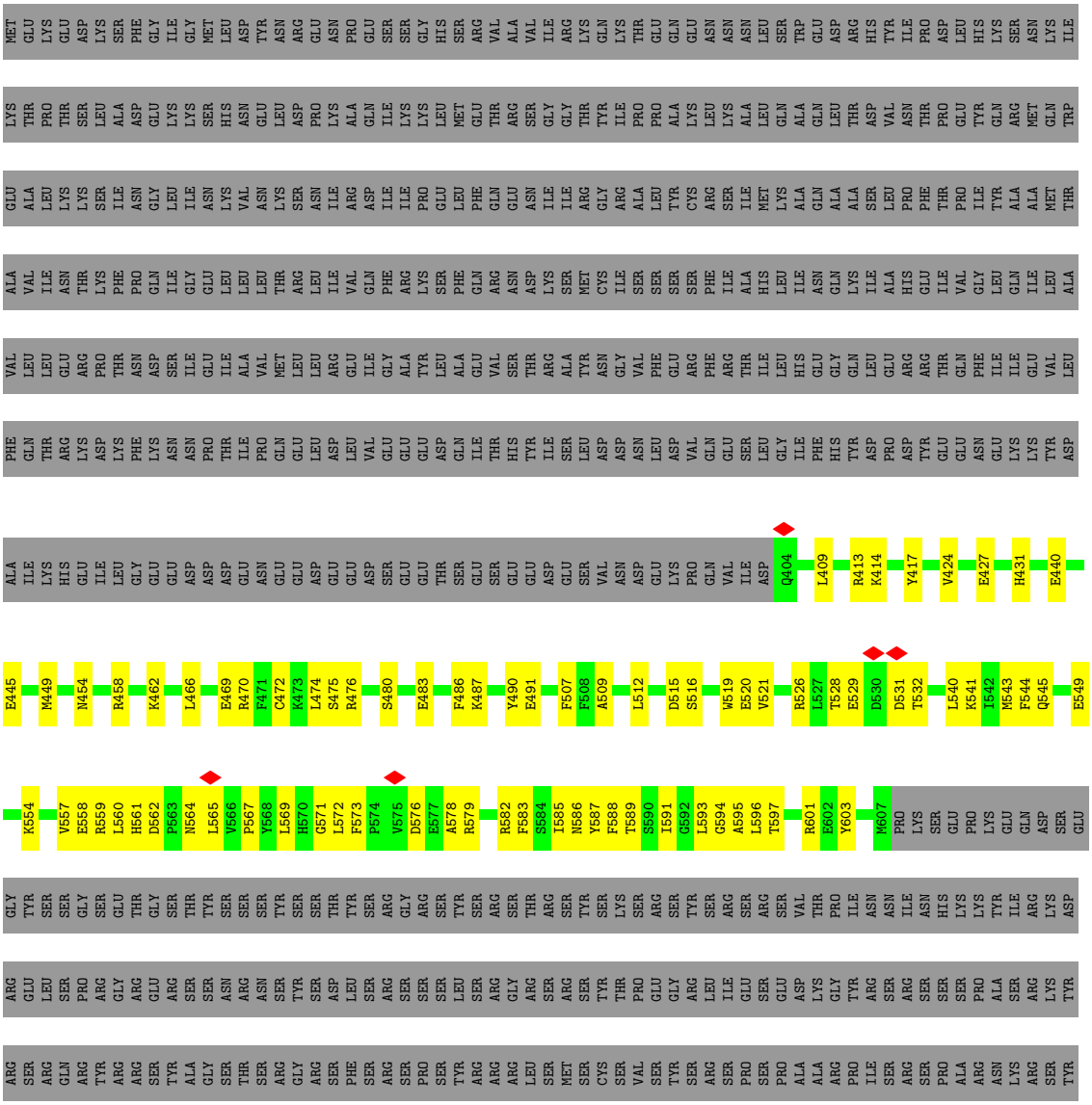
Chain b:

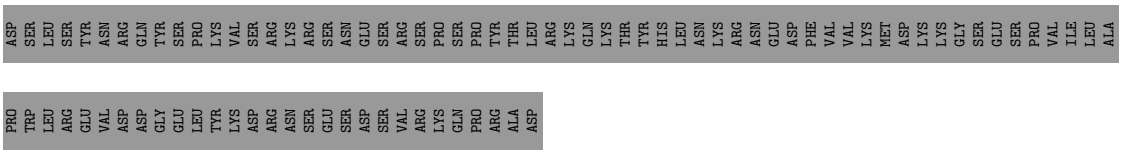




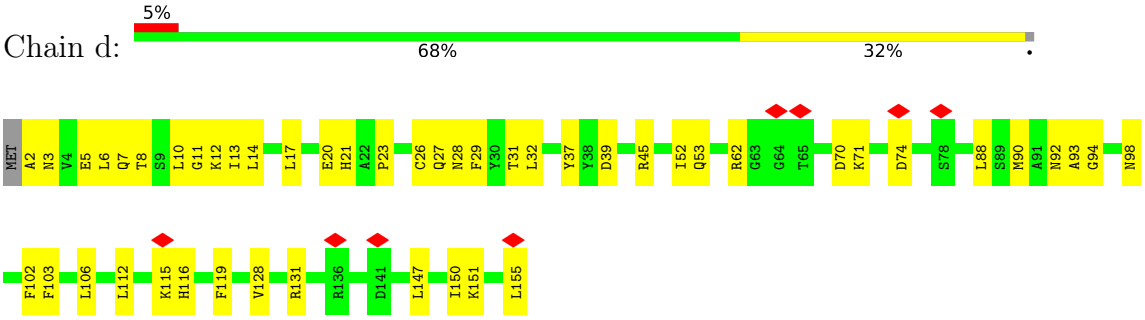

• Molecule 30: Pre-mRNA-splicing factor cwf22

Chain c:

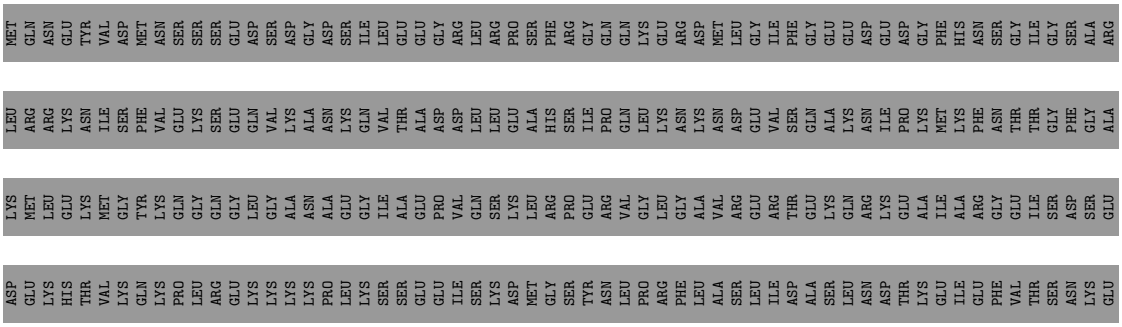





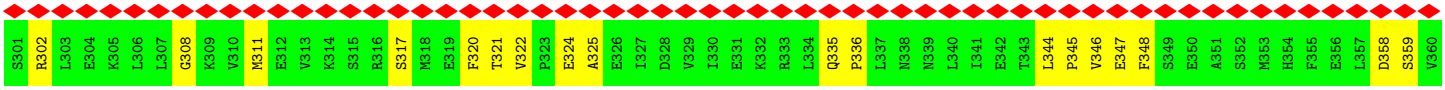

• Molecule 31: Peptidyl-prolyl cis-trans isomerase ppi1

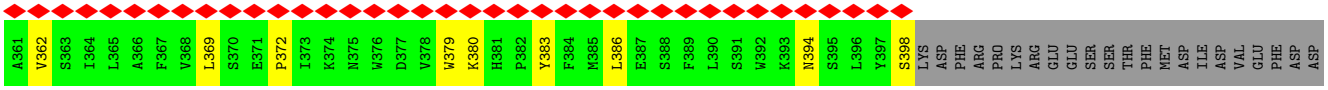


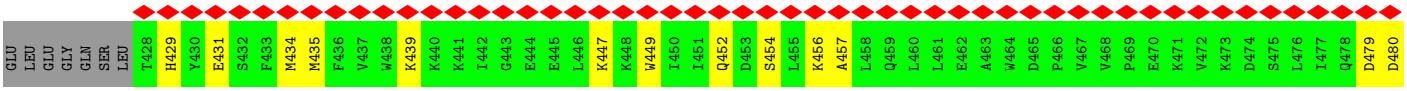

• Molecule 32: G-patch domain-containing protein C1486.03

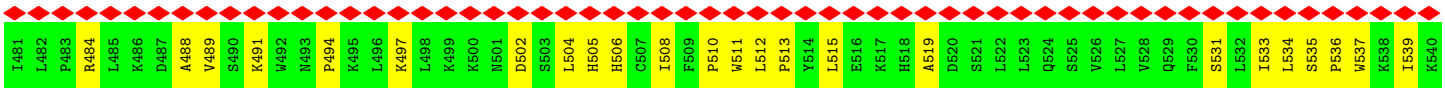



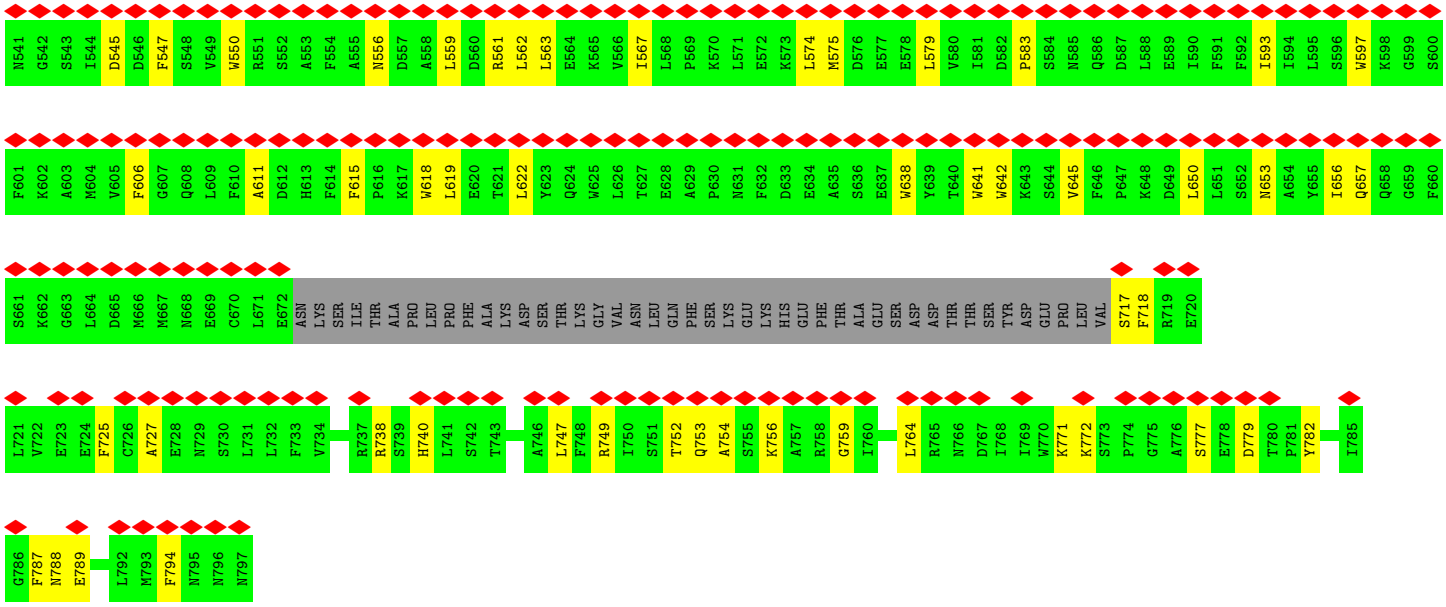




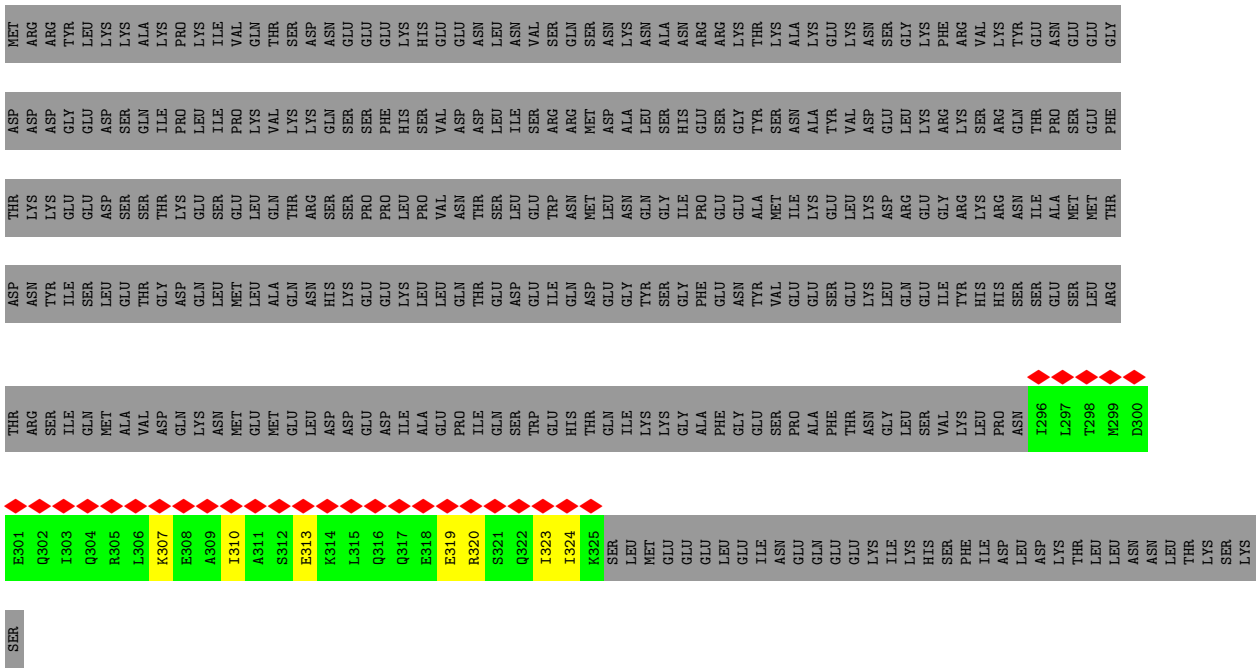



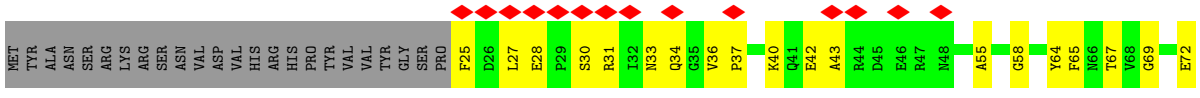



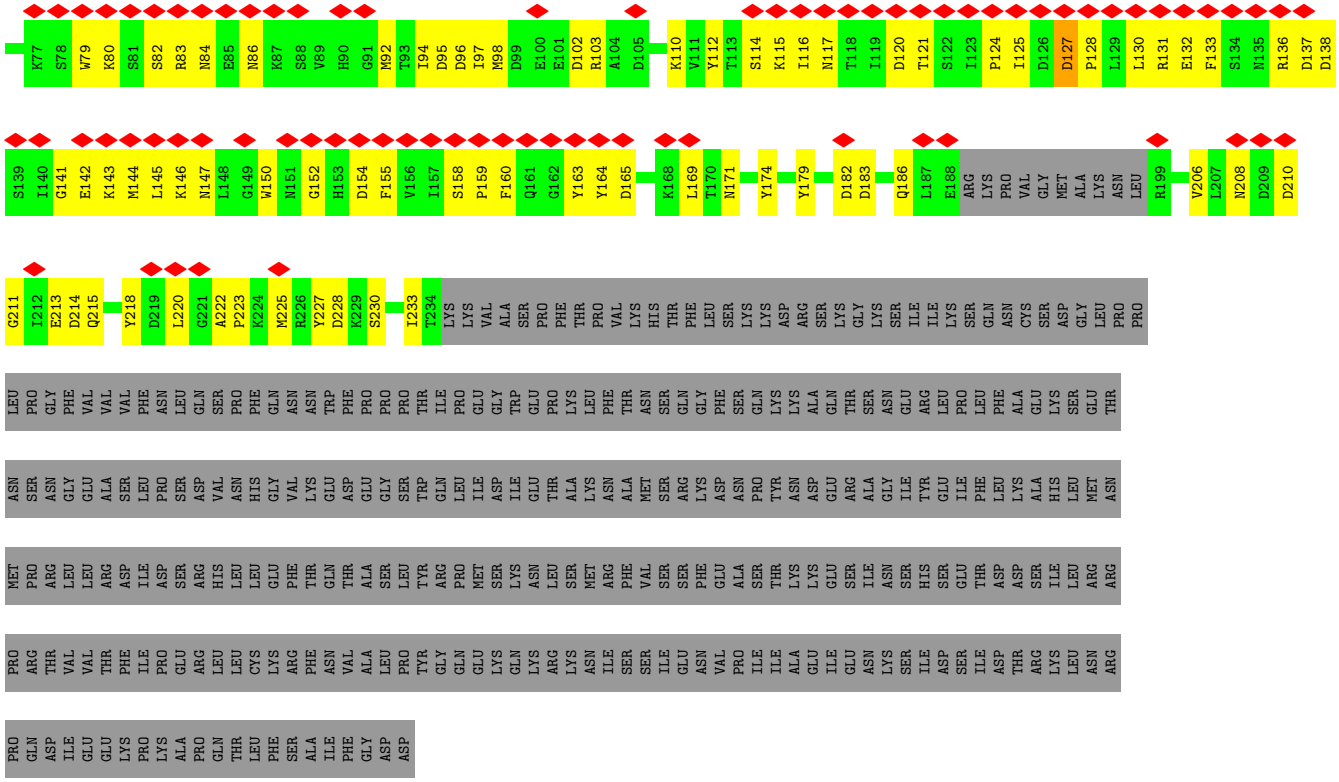



• Molecule 33: Uncharacterized protein C17A2.08c

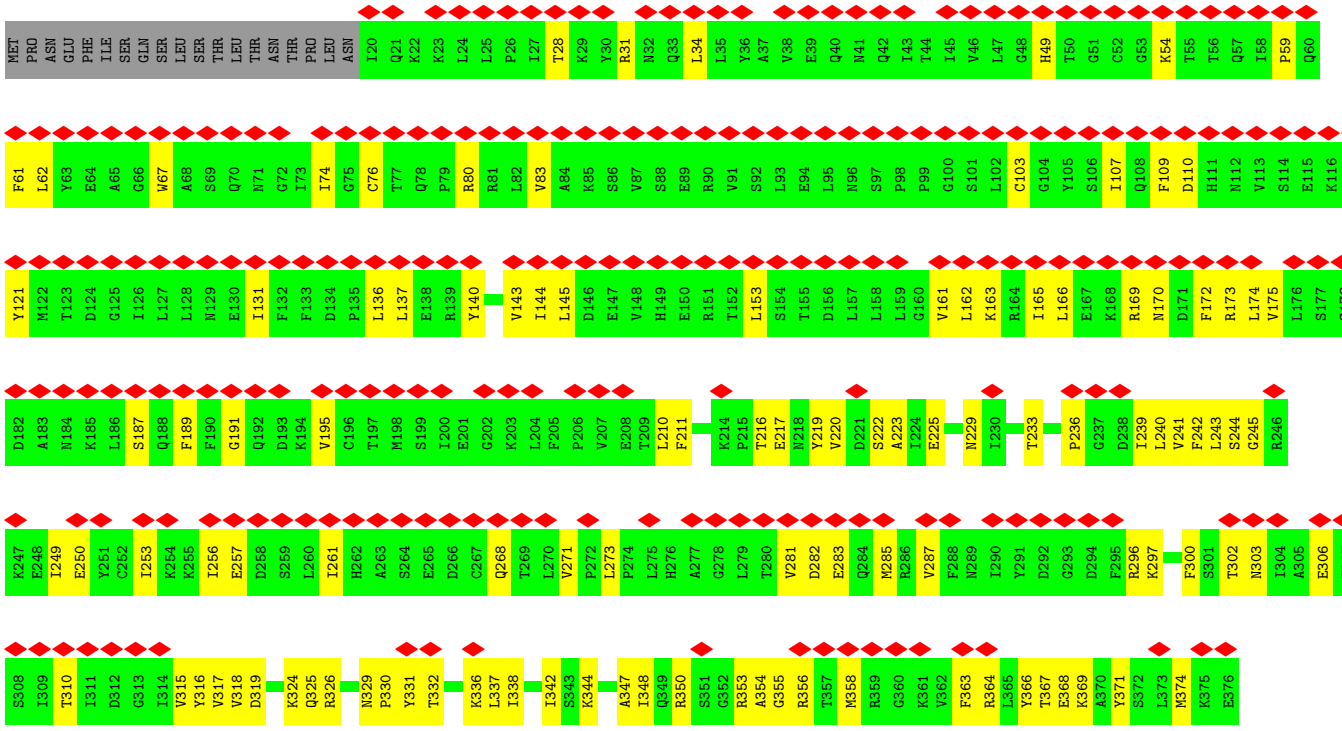

• Molecule 34: Uncharacterized protein C20H4.06c

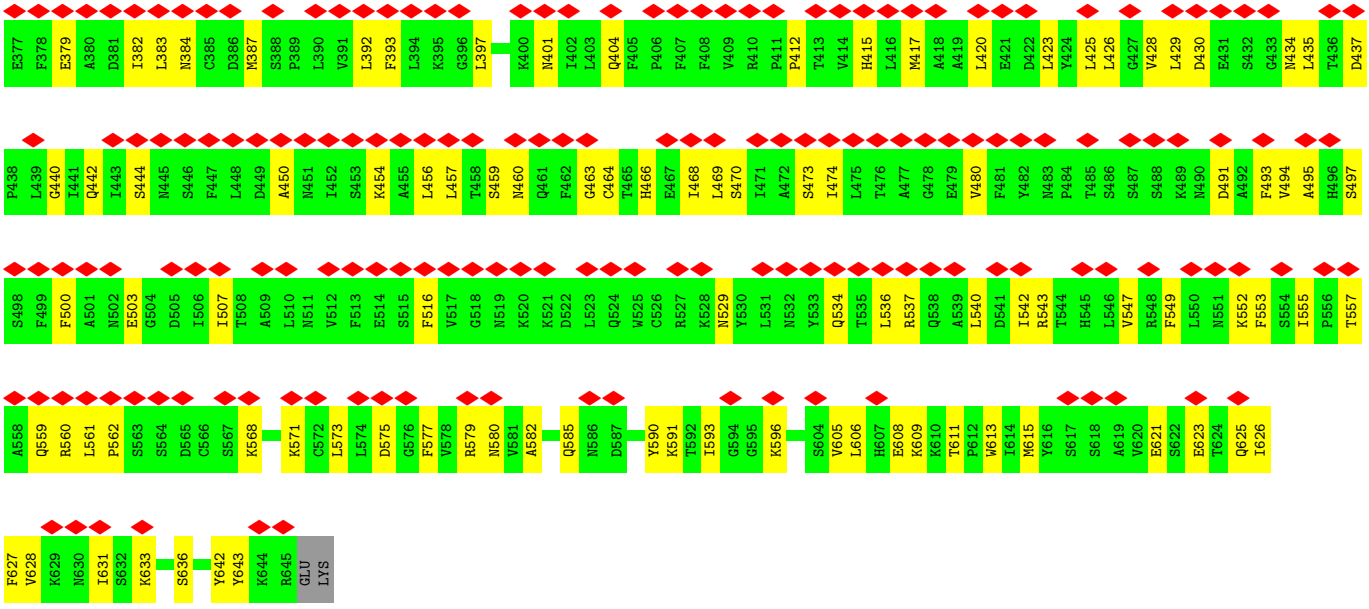





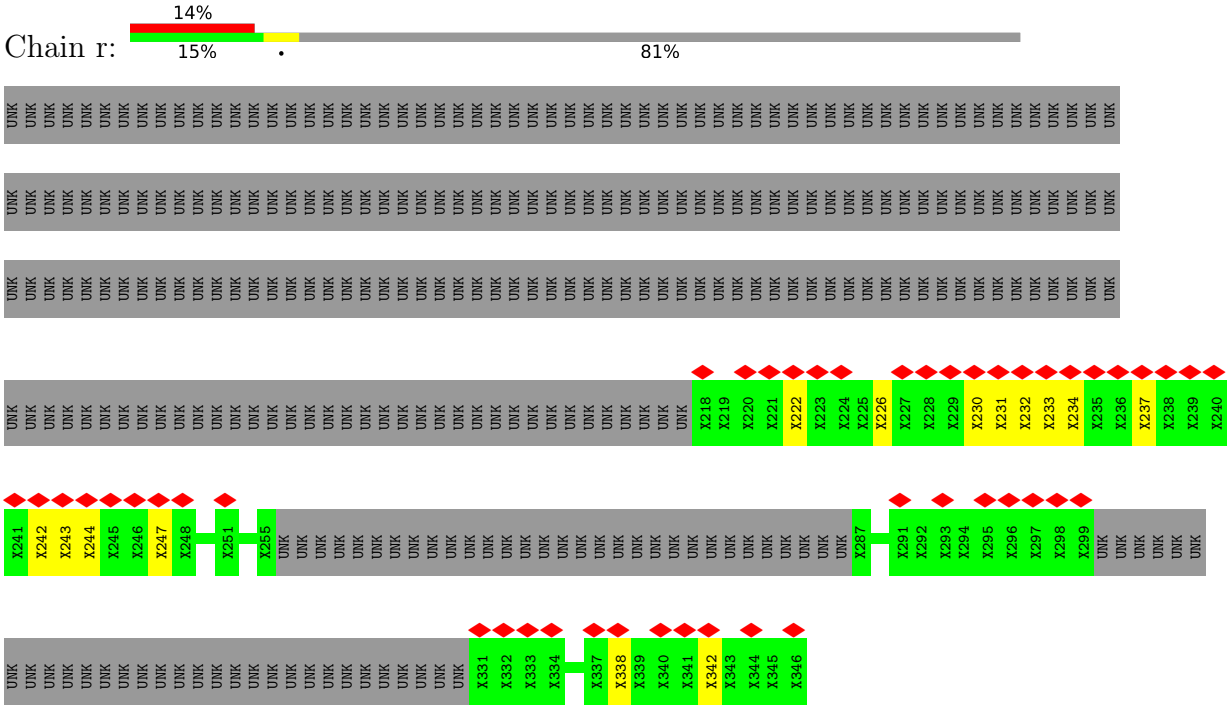

• Molecule 35: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09

Chain z:

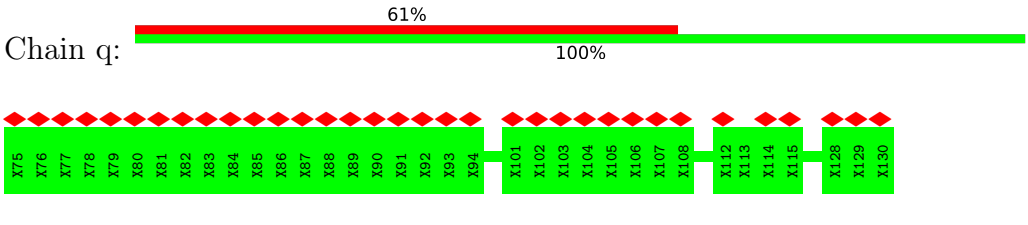






- Molecule 36: UNK1

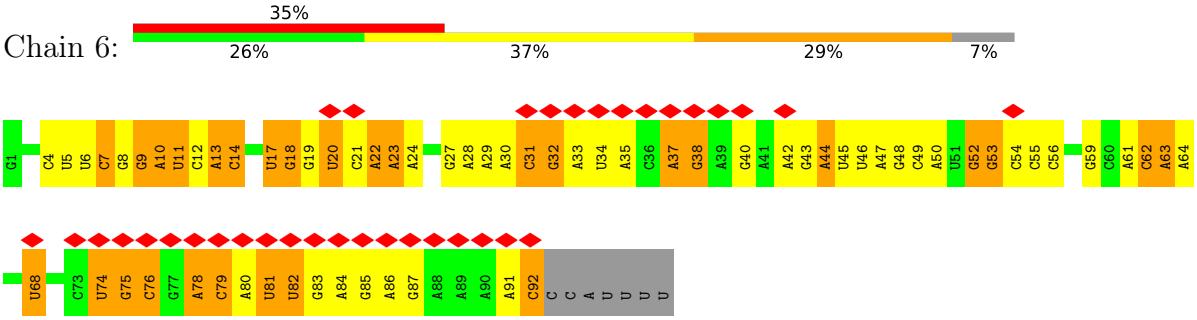



- Molecule 37: UNK2



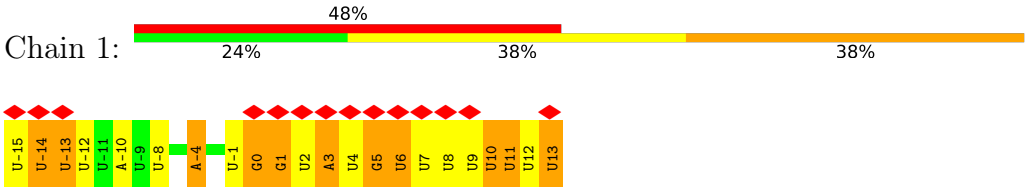

- Molecule 38: U6snRNA

Chain 6:



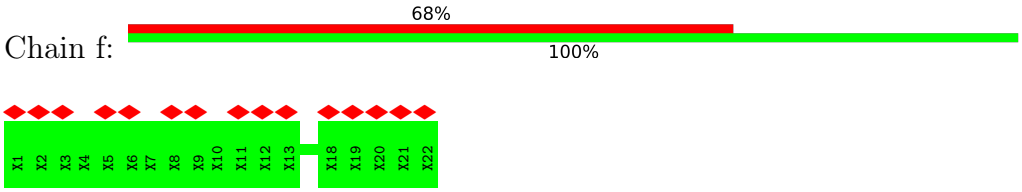

• Molecule 39: pre-mRNA

Chain 1:




• Molecule 40: UNK3

Chain f:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 72631 | 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 ($e^-/Å^2$) | 49.4 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOCONTINUUM (6k x 4k) | Depositor |
| Maximum map value | 37.664 | Depositor |
| Minimum map value | -23.068 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.904 | Depositor |
| Recommended contour level | 3.2 | Depositor |
| Map size (Å) | 460.32, 460.32, 460.32 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.822, 0.822, 0.822 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, GTP, ZN, IHP

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 | e | 0.24 | 0/1354 | 0.43 | 0/1831 |
| 2 | p | 0.18 | 0/491 | 0.43 | 0/654 |
| 3 | 2 | 0.24 | 0/554 | 0.29 | 0/856 |
| 4 | 5 | 0.44 | 0/2397 | 0.33 | 0/3727 |
| 5 | A | 0.45 | 0/16857 | 0.46 | 2/22848 (0.0%) |
| 6 | B | 0.42 | 0/7459 | 0.44 | 0/10117 |
| 7 | C | 0.28 | 0/2376 | 0.41 | 0/3216 |
| 8 | D | 0.40 | 0/772 | 0.40 | 0/1038 |
| 9 | E | 0.30 | 0/737 | 0.46 | 0/993 |
| 10 | F | 0.31 | 0/646 | 0.57 | 0/875 |
| 11 | G | 0.25 | 0/829 | 0.47 | 0/1111 |
| 12 | H | 0.29 | 0/662 | 0.47 | 0/894 |
| 13 | I | 0.28 | 0/585 | 0.60 | 0/794 |
| 14 | J | 0.37 | 0/578 | 0.46 | 0/774 |
| 15 | K | 0.47 | 0/3130 | 0.49 | 0/4251 |
| 16 | L | 0.32 | 0/1991 | 0.46 | 0/2684 |
| 17 | M | 0.25 | 0/1841 | 0.44 | 0/2468 |
| 18 | N | 0.13 | 0/10690 | 0.33 | 0/14463 |
| 19 | O | 0.40 | 0/1199 | 0.48 | 0/1609 |
| 20 | P | 0.33 | 0/2222 | 0.57 | 1/2991 (0.0%) |
| 21 | Q | 0.36 | 0/767 | 0.46 | 0/1028 |
| 22 | R | 0.26 | 0/5235 | 0.45 | 0/7067 |
| 23 | S | 0.20 | 0/1072 | 0.50 | 0/1453 |
| 23 | T | 0.19 | 0/1086 | 0.43 | 0/1472 |
| 23 | U | 0.14 | 0/2897 | 0.37 | 0/3914 |
| 23 | V | 0.19 | 0/1060 | 0.50 | 0/1437 |
| 24 | W | 0.25 | 0/4187 | 0.52 | 3/5613 (0.1%) |
| 25 | X | 0.17 | 0/5599 | 0.44 | 0/7566 |
| 26 | Y | 0.16 | 0/857 | 0.41 | 0/1138 |
| 27 | Z | 0.20 | 0/1244 | 0.47 | 0/1667 |
| 28 | a | 0.28 | 0/1055 | 0.44 | 0/1443 |
| 29 | b | 0.27 | 0/829 | 0.38 | 0/1111 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 30 | c | 0.40 | 0/1711 | 0.49 | 0/2312 |
| 31 | d | 0.24 | 0/1206 | 0.43 | 0/1636 |
| 32 | m | 0.15 | 0/3916 | 0.36 | 0/5300 |
| 33 | n | 0.12 | 0/247 | 0.31 | 0/327 |
| 34 | y | 0.26 | 0/1641 | 0.58 | 0/2211 |
| 35 | z | 0.19 | 0/5079 | 0.41 | 0/6875 |
| 37 | q | 0.23 | 0/32 | 0.19 | 0/43 |
| 38 | 6 | 0.22 | 0/2207 | 0.36 | 0/3438 |
| 39 | 1 | 0.33 | 0/673 | 0.47 | 0/1043 |
| All | All | 0.31 | 0/99970 | 0.44 | 6/136288 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 21 | Q | 0 | 1 |
| 24 | W | 0 | 3 |
| 35 | z | 0 | 1 |
| All | All | 0 | 5 |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | W | 130 | PRO | CA-N-CD | -6.83 | 102.43 | 112.00 |
| 24 | W | 626 | THR | CA-C-N | -6.03 | 112.44 | 120.63 |
| 24 | W | 626 | THR | C-N-CA | -6.03 | 112.44 | 120.63 |
| 5 | A | 1043 | LYS | CB-CA-C | -5.86 | 109.80 | 116.54 |
| 5 | A | 978 | TRP | CB-CG-CD2 | -5.34 | 119.32 | 126.80 |
| 20 | P | 263 | GLU | N-CA-CB | 5.02 | 117.59 | 110.16 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 21 | Q | 223 | ARG | Sidechain |
| 24 | W | 533 | ARG | Sidechain |
| 24 | W | 537 | ARG | Sidechain |
| 24 | W | 657 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | z | 326 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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 | e | 1329 | 0 | 1293 | 41 | 0 |
| 2 | p | 487 | 0 | 515 | 23 | 0 |
| 3 | 2 | 500 | 0 | 257 | 17 | 0 |
| 4 | 5 | 2149 | 0 | 1085 | 36 | 0 |
| 5 | A | 16424 | 0 | 16380 | 403 | 0 |
| 6 | B | 7298 | 0 | 7336 | 175 | 0 |
| 7 | C | 2328 | 0 | 2276 | 95 | 0 |
| 8 | D | 760 | 0 | 776 | 22 | 0 |
| 9 | E | 726 | 0 | 750 | 40 | 0 |
| 10 | F | 638 | 0 | 682 | 42 | 0 |
| 11 | G | 819 | 0 | 845 | 63 | 0 |
| 12 | H | 652 | 0 | 680 | 33 | 0 |
| 13 | I | 574 | 0 | 591 | 49 | 0 |
| 14 | J | 573 | 0 | 602 | 19 | 0 |
| 15 | K | 3053 | 0 | 3011 | 95 | 0 |
| 16 | L | 1954 | 0 | 1991 | 79 | 0 |
| 17 | M | 1818 | 0 | 1822 | 64 | 0 |
| 18 | N | 10461 | 0 | 10412 | 246 | 0 |
| 19 | O | 1176 | 0 | 1167 | 23 | 0 |
| 20 | P | 2178 | 0 | 2101 | 110 | 0 |
| 21 | Q | 752 | 0 | 729 | 25 | 0 |
| 22 | R | 5108 | 0 | 5024 | 200 | 0 |
| 23 | S | 1055 | 0 | 1075 | 58 | 0 |
| 23 | T | 1069 | 0 | 1084 | 48 | 0 |
| 23 | U | 2870 | 0 | 2403 | 79 | 0 |
| 23 | V | 1044 | 0 | 1066 | 71 | 0 |
| 24 | W | 4126 | 0 | 4148 | 185 | 0 |
| 25 | X | 5467 | 0 | 5372 | 211 | 0 |
| 26 | Y | 845 | 0 | 842 | 39 | 0 |
| 27 | Z | 1232 | 0 | 1242 | 58 | 0 |
| 28 | a | 1035 | 0 | 837 | 34 | 0 |
| 29 | b | 822 | 0 | 820 | 29 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 30 | c | 1678 | 0 | 1659 | 62 | 0 |
| 31 | d | 1179 | 0 | 1169 | 38 | 0 |
| 32 | m | 3813 | 0 | 3794 | 90 | 0 |
| 33 | n | 248 | 0 | 262 | 8 | 0 |
| 34 | y | 1606 | 0 | 1502 | 94 | 0 |
| 35 | z | 4980 | 0 | 5047 | 178 | 0 |
| 36 | r | 335 | 0 | 79 | 10 | 0 |
| 37 | q | 295 | 0 | 85 | 0 | 0 |
| 38 | 6 | 1970 | 0 | 994 | 52 | 0 |
| 39 | 1 | 605 | 0 | 302 | 14 | 0 |
| 40 | f | 110 | 0 | 29 | 0 | 0 |
| 41 | A | 36 | 0 | 6 | 0 | 0 |
| 42 | B | 32 | 0 | 12 | 4 | 0 |
| 43 | 6 | 3 | 0 | 0 | 0 | 0 |
| 43 | B | 1 | 0 | 0 | 0 | 0 |
| 44 | M | 2 | 0 | 0 | 0 | 0 |
| 44 | O | 3 | 0 | 0 | 0 | 0 |
| 44 | P | 1 | 0 | 0 | 0 | 0 |
| 45 | 6 | 1 | 0 | 0 | 0 | 0 |
| All | All | 98220 | 0 | 94154 | 2803 | 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 15.

All (2803) 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) |
|---|---|---|---|
| 20:P:82:MET:HG2 | 38:6:32:G:H21 | 1.06 | 1.18 |
| 35:z:379:GLU:HG3 | 35:z:384:ASN:ND2 | 1.58 | 1.18 |
| 20:P:82:MET:HG2 | 38:6:32:G:N2 | 1.63 | 1.11 |
| 35:z:379:GLU:CG | 35:z:384:ASN:HD21 | 1.68 | 1.06 |
| 20:P:118:LEU:HD11 | 20:P:153:ARG:NH2 | 1.71 | 1.04 |
| 34:y:171:ASN:OD1 | 35:z:338:ILE:HG13 | 1.60 | 1.00 |
| 27:Z:153:LYS:HD3 | 27:Z:156:GLN:HE21 | 1.26 | 1.00 |
| 20:P:85:ASP:HB2 | 20:P:88:LYS:HB2 | 1.41 | 0.99 |
| 25:X:490:GLU:HG3 | 25:X:494:GLY:HA3 | 1.43 | 0.99 |
| 35:z:379:GLU:HG3 | 35:z:384:ASN:HD21 | 0.84 | 0.97 |
| 20:P:82:MET:CG | 38:6:32:G:N2 | 2.28 | 0.97 |
| 23:S:122:ARG:HH21 | 23:V:114:VAL:HG13 | 1.28 | 0.97 |
| 25:X:621:THR:HA | 25:X:624:ARG:HE | 1.30 | 0.96 |
| 35:z:568:LYS:HA | 35:z:571:LYS:HG2 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:285:HIS:O | 22:R:289:GLN:HB2 | 1.66 | 0.95 |
| 24:W:537:ARG:HH11 | 24:W:577:PHE:HB2 | 1.32 | 0.94 |
| 1:e:204:HIS:HB3 | 6:B:76:GLN:HB2 | 1.50 | 0.94 |
| 24:W:207:ILE:HG12 | 24:W:209:ILE:H | 1.34 | 0.93 |
| 30:c:520:GLU:HA | 30:c:567:PRO:HG3 | 1.51 | 0.93 |
| 35:z:371:TYR:HA | 35:z:374:MET:HE3 | 1.53 | 0.91 |
| 1:e:40:SER:OG | 16:L:301:GLN:NE2 | 2.03 | 0.91 |
| 24:W:155:MET:HG2 | 24:W:159:GLU:HG3 | 1.54 | 0.90 |
| 20:P:82:MET:CG | 38:6:32:G:H21 | 1.86 | 0.89 |
| 24:W:536:ILE:HG22 | 24:W:537:ARG:H | 1.36 | 0.88 |
| 23:S:122:ARG:HH22 | 23:V:115:ILE:HD13 | 1.38 | 0.88 |
| 20:P:118:LEU:HD11 | 20:P:153:ARG:HH21 | 1.37 | 0.87 |
| 23:S:110:ALA:HA | 23:S:113:ARG:HE | 1.40 | 0.87 |
| 18:N:206:SER:HB3 | 18:N:225:ILE:HD13 | 1.56 | 0.87 |
| 20:P:150:CYS:SG | 20:P:224:GLN:NE2 | 2.49 | 0.86 |
| 16:L:115:GLU:HG2 | 16:L:116:LEU:HD12 | 1.59 | 0.84 |
| 24:W:192:ARG:HH12 | 24:W:196:LEU:HB2 | 1.42 | 0.84 |
| 17:M:82:SER:O | 20:P:147:ASN:ND2 | 2.09 | 0.84 |
| 16:L:191:GLN:HE21 | 28:a:86:THR:HG23 | 1.42 | 0.84 |
| 5:A:1723:THR:OG1 | 5:A:1741:ASN:OD1 | 1.96 | 0.84 |
| 32:m:653:ASN:O | 32:m:657:GLN:NE2 | 2.10 | 0.84 |
| 17:M:60:ARG:NH1 | 19:O:127:ASP:OD2 | 2.10 | 0.83 |
| 5:A:1665:ARG:HE | 5:A:1666:PRO:HD2 | 1.44 | 0.83 |
| 23:T:69:LEU:HD12 | 23:T:71:ALA:H | 1.42 | 0.83 |
| 14:J:8:ASP:OD1 | 14:J:10:LYS:NZ | 2.11 | 0.82 |
| 23:S:122:ARG:HE | 23:V:114:VAL:HG22 | 1.41 | 0.82 |
| 5:A:1605:LEU:HD22 | 5:A:1770:ARG:HH11 | 1.42 | 0.82 |
| 2:p:197:LEU:O | 25:X:722:ARG:NH1 | 2.11 | 0.81 |
| 10:F:40:LEU:HB3 | 10:F:43:VAL:HG11 | 1.63 | 0.81 |
| 25:X:68:TRP:HE1 | 25:X:104:LEU:HD23 | 1.42 | 0.81 |
| 1:e:183:LYS:HG2 | 1:e:184:SER:H | 1.45 | 0.81 |
| 7:C:203:ILE:HD11 | 7:C:215:LEU:HG | 1.63 | 0.81 |
| 5:A:1757:ILE:HG23 | 5:A:1761:ASN:HD21 | 1.45 | 0.81 |
| 1:e:256:TYR:HE2 | 30:c:595:ALA:HA | 1.46 | 0.80 |
| 12:H:82:GLN:NE2 | 14:J:57:ILE:O | 2.14 | 0.80 |
| 1:e:217:GLU:OE2 | 21:Q:233:ASN:ND2 | 2.15 | 0.80 |
| 30:c:562:ASP:OD1 | 30:c:564:ASN:ND2 | 2.14 | 0.80 |
| 11:G:7:LYS:HB2 | 11:G:20:LEU:HD21 | 1.64 | 0.80 |
| 35:z:387:MET:HE2 | 35:z:415:HIS:HB3 | 1.64 | 0.79 |
| 22:R:118:ARG:HG3 | 26:Y:165:VAL:HG11 | 1.64 | 0.79 |
| 28:a:62:MET:HA | 28:a:64:GLN:HE21 | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:285:HIS:O | 22:R:289:GLN:CB | 2.30 | 0.79 |
| 5:A:1604:HIS:HB3 | 5:A:1607:GLN:HE21 | 1.47 | 0.79 |
| 17:M:102:LEU:HD23 | 17:M:103:VAL:HG23 | 1.62 | 0.79 |
| 2:p:192:LEU:HD11 | 2:p:194:ILE:HG22 | 1.65 | 0.78 |
| 7:C:297:SER:OG | 7:C:301:ASP:OD1 | 2.01 | 0.78 |
| 18:N:665:ILE:HD11 | 18:N:740:GLN:HG2 | 1.64 | 0.78 |
| 24:W:537:ARG:HD2 | 24:W:577:PHE:CG | 2.19 | 0.78 |
| 24:W:242:ASP:HA | 24:W:249:LYS:HZ1 | 1.46 | 0.78 |
| 23:S:92:ARG:HH21 | 23:V:5:ILE:HG12 | 1.47 | 0.78 |
| 24:W:192:ARG:NH1 | 24:W:196:LEU:HB2 | 1.98 | 0.78 |
| 22:R:121:ASN:ND2 | 24:W:237:ASP:O | 2.17 | 0.78 |
| 22:R:265:LYS:NZ | 22:R:283:TYR:OH | 2.16 | 0.78 |
| 24:W:176:LYS:HG3 | 38:6:42:A:H5" | 1.66 | 0.78 |
| 8:D:64:SER:HA | 9:E:71:ARG:HH21 | 1.50 | 0.77 |
| 5:A:1609:ILE:HG12 | 5:A:1763:ALA:HB1 | 1.67 | 0.77 |
| 20:P:96:ARG:NH1 | 20:P:97:CYS:O | 2.16 | 0.77 |
| 17:M:47:CYS:SG | 17:M:121:GLN:NE2 | 2.57 | 0.77 |
| 21:Q:46:GLU:OE1 | 21:Q:49:ARG:NH2 | 2.18 | 0.77 |
| 20:P:259:GLN:NE2 | 20:P:263:GLU:OE2 | 2.16 | 0.77 |
| 23:T:122:ARG:HH22 | 23:U:121:GLU:HB3 | 1.48 | 0.77 |
| 23:U:191:ALA:HB3 | 23:U:485:LEU:HB3 | 1.66 | 0.77 |
| 35:z:412:PRO:HB2 | 35:z:415:HIS:HD2 | 1.49 | 0.77 |
| 18:N:634:ARG:NH2 | 18:N:997:CYS:SG | 2.58 | 0.77 |
| 5:A:1762:PRO:HB3 | 34:y:94:ILE:HD13 | 1.67 | 0.77 |
| 5:A:1602:ARG:HE | 5:A:1770:ARG:NH2 | 1.83 | 0.77 |
| 5:A:1691:ARG:NH2 | 5:A:1697:SER:O | 2.16 | 0.77 |
| 5:A:1736:HIS:ND1 | 5:A:1758:MET:SD | 2.58 | 0.77 |
| 24:W:725:LEU:HD13 | 27:Z:159:VAL:HG21 | 1.67 | 0.77 |
| 24:W:245:ASN:HB2 | 24:W:248:GLU:HB2 | 1.67 | 0.76 |
| 7:C:306:LEU:HD13 | 9:E:106:ARG:HE | 1.50 | 0.76 |
| 17:M:63:LYS:NZ | 38:6:22:A:OP2 | 2.17 | 0.76 |
| 32:m:539:ILE:HD11 | 32:m:574:LEU:HD13 | 1.64 | 0.76 |
| 5:A:1817:THR:HG22 | 5:A:1818:PHE:H | 1.50 | 0.76 |
| 22:R:17:GLN:NE2 | 24:W:151:ASP:OD1 | 2.18 | 0.76 |
| 24:W:246:PHE:HA | 24:W:249:LYS:HG2 | 1.67 | 0.76 |
| 25:X:538:GLU:HA | 25:X:541:VAL:HG12 | 1.67 | 0.76 |
| 5:A:1630:ILE:O | 34:y:83:ARG:NH2 | 2.19 | 0.76 |
| 16:L:208:GLU:O | 38:6:18:G:N1 | 2.19 | 0.76 |
| 5:A:1602:ARG:HE | 5:A:1770:ARG:HH21 | 1.32 | 0.76 |
| 24:W:259:ASN:OD1 | 24:W:262:ARG:NH2 | 2.19 | 0.76 |
| 22:R:292:ASP:OD2 | 22:R:298:SER:OG | 2.02 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:200:ASP:OD1 | 19:O:31:ARG:NH1 | 2.19 | 0.75 |
| 20:P:118:LEU:HD21 | 20:P:153:ARG:HH21 | 1.51 | 0.75 |
| 23:S:90:LEU:HB2 | 23:V:90:LEU:HD11 | 1.68 | 0.75 |
| 24:W:509:GLU:HA | 24:W:512:ILE:HB | 1.68 | 0.75 |
| 17:M:237:PRO:HB2 | 17:M:255:LYS:HD3 | 1.68 | 0.75 |
| 22:R:281:LYS:O | 22:R:285:HIS:ND1 | 2.20 | 0.75 |
| 1:e:132:PHE:HE1 | 24:W:68:LYS:HG3 | 1.51 | 0.75 |
| 15:K:106:ILE:HG12 | 15:K:109:GLN:HG2 | 1.69 | 0.75 |
| 18:N:279:LYS:NZ | 18:N:382:ASP:O | 2.18 | 0.75 |
| 5:A:231:LYS:HB3 | 5:A:244:TYR:CE2 | 2.22 | 0.75 |
| 5:A:1576:GLN:HB3 | 5:A:1585:MET:HE1 | 1.69 | 0.74 |
| 8:D:17:THR:HG22 | 8:D:27:ARG:HD2 | 1.68 | 0.74 |
| 5:A:1282:LYS:HG2 | 34:y:208:ASN:HD21 | 1.51 | 0.74 |
| 5:A:1660:LYS:NZ | 5:A:1661:TRP:O | 2.20 | 0.74 |
| 18:N:778:SER:HB2 | 18:N:979:MET:HE3 | 1.68 | 0.74 |
| 5:A:1616:ASP:OD2 | 5:A:1761:ASN:ND2 | 2.21 | 0.74 |
| 5:A:1972:GLU:HG3 | 5:A:1975:LYS:HE2 | 1.69 | 0.74 |
| 35:z:605:VAL:O | 35:z:609:LYS:NZ | 2.20 | 0.74 |
| 22:R:88:ARG:HB3 | 24:W:225:ILE:HD12 | 1.70 | 0.74 |
| 23:V:99:GLN:NE2 | 36:r:230:UNK:O | 2.21 | 0.74 |
| 18:N:694:SER:HB3 | 18:N:713:SER:HB3 | 1.69 | 0.73 |
| 20:P:147:ASN:OD1 | 20:P:148:VAL:N | 2.21 | 0.73 |
| 10:F:77:ASP:OD1 | 11:G:58:LYS:NZ | 2.20 | 0.73 |
| 18:N:306:LEU:HD23 | 18:N:329:LEU:HD23 | 1.68 | 0.73 |
| 5:A:191:ASP:OD1 | 5:A:192:ASP:N | 2.21 | 0.73 |
| 15:K:290:SER:HB2 | 15:K:309:MET:HB3 | 1.69 | 0.73 |
| 18:N:772:ASP:HB2 | 18:N:974:ASN:HB2 | 1.70 | 0.73 |
| 18:N:988:SER:O | 18:N:992:ILE:HD12 | 1.87 | 0.73 |
| 25:X:262:GLN:HA | 25:X:265:ILE:HD12 | 1.71 | 0.73 |
| 5:A:1888:THR:HG22 | 5:A:1915:LEU:HB2 | 1.71 | 0.73 |
| 6:B:182:THR:O | 6:B:183:HIS:ND1 | 2.20 | 0.73 |
| 10:F:46:THR:HG22 | 10:F:52:PRO:HB3 | 1.69 | 0.73 |
| 22:R:44:ASP:N | 22:R:47:GLU:OE2 | 2.19 | 0.73 |
| 5:A:59:ARG:NH1 | 38:6:11:U:OP1 | 2.22 | 0.73 |
| 18:N:226:ILE:HG23 | 18:N:274:LEU:HD12 | 1.70 | 0.73 |
| 22:R:375:ASP:OD1 | 22:R:382:ALA:N | 2.22 | 0.73 |
| 23:V:106:TYR:HB2 | 24:W:568:ILE:HG13 | 1.71 | 0.73 |
| 30:c:569:LEU:HD22 | 30:c:572:LEU:HD12 | 1.70 | 0.73 |
| 20:P:118:LEU:CD1 | 20:P:153:ARG:HH21 | 2.01 | 0.73 |
| 24:W:531:ILE:HG12 | 24:W:537:ARG:CZ | 2.19 | 0.73 |
| 5:A:1430:GLU:HA | 5:A:1433:GLU:HG2 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:176:LYS:NZ | 5:A:645:GLY:O | 2.23 | 0.72 |
| 18:N:801:HIS:NE2 | 18:N:927:GLU:OE2 | 2.21 | 0.72 |
| 24:W:203:LYS:HA | 24:W:207:ILE:HB | 1.70 | 0.72 |
| 6:B:585:LYS:NZ | 6:B:586:ASP:O | 2.23 | 0.72 |
| 5:A:1635:LYS:HB2 | 5:A:1653:ILE:HG22 | 1.72 | 0.72 |
| 25:X:599:GLU:OE1 | 25:X:608:SER:OG | 2.08 | 0.72 |
| 7:C:203:ILE:HB | 7:C:213:HIS:HD2 | 1.54 | 0.72 |
| 5:A:1236:GLY:HA2 | 5:A:1300:GLU:HG3 | 1.72 | 0.72 |
| 18:N:307:GLN:NE2 | 18:N:322:VAL:O | 2.23 | 0.72 |
| 28:a:106:ASN:HD22 | 28:a:106:ASN:C | 1.94 | 0.72 |
| 16:L:210:ASP:HB3 | 16:L:213:GLU:HG2 | 1.70 | 0.72 |
| 18:N:1179:ASN:HA | 18:N:1208:SER:HB2 | 1.70 | 0.72 |
| 23:T:70:PRO:HA | 23:T:73:LEU:HG | 1.70 | 0.71 |
| 24:W:749:ASP:HA | 24:W:752:ARG:HE | 1.54 | 0.71 |
| 7:C:259:GLN:NE2 | 7:C:298:ALA:O | 2.22 | 0.71 |
| 17:M:110:ASP:OD1 | 17:M:111:ILE:HD12 | 1.90 | 0.71 |
| 22:R:84:LYS:NZ | 22:R:87:ALA:HB3 | 2.04 | 0.71 |
| 35:z:187:SER:HA | 35:z:195:VAL:HG21 | 1.72 | 0.71 |
| 6:B:204:ASP:OD1 | 6:B:205:MET:N | 2.22 | 0.71 |
| 16:L:191:GLN:HE22 | 17:M:23:CYS:HA | 1.56 | 0.71 |
| 23:U:383:PHE:HD1 | 23:U:390:LEU:HD22 | 1.54 | 0.71 |
| 25:X:108:MET:HE3 | 25:X:110:VAL:HB | 1.71 | 0.71 |
| 25:X:271:GLU:OE1 | 25:X:274:ARG:NH1 | 2.24 | 0.71 |
| 34:y:127:ASP:H | 34:y:131:ARG:HH21 | 1.39 | 0.71 |
| 12:H:9:MET:HE3 | 14:J:34:TYR:H | 1.56 | 0.71 |
| 23:S:129:LEU:HD22 | 23:V:125:ALA:HB2 | 1.73 | 0.71 |
| 1:e:51:LEU:HD13 | 16:L:305:GLU:HG2 | 1.73 | 0.71 |
| 15:K:86:ALA:O | 22:R:259:ARG:NH1 | 2.22 | 0.71 |
| 6:B:814:GLN:HA | 6:B:817:ARG:HD3 | 1.71 | 0.71 |
| 25:X:139:LEU:HD13 | 25:X:147:ILE:HG23 | 1.73 | 0.71 |
| 32:m:638:TRP:NE1 | 32:m:642:TRP:HE1 | 1.89 | 0.71 |
| 34:y:136:ARG:NH1 | 34:y:142:GLU:OE2 | 2.24 | 0.71 |
| 38:6:34:U:H2' | 38:6:35:A:H8 | 1.56 | 0.71 |
| 5:A:1020:MET:HG2 | 5:A:1066:PHE:CZ | 2.26 | 0.70 |
| 10:F:32:VAL:HG23 | 10:F:38:THR:HG22 | 1.73 | 0.70 |
| 34:y:42:GLU:HG2 | 34:y:43:ALA:H | 1.56 | 0.70 |
| 6:B:254:ILE:HD13 | 6:B:597:MET:HE1 | 1.70 | 0.70 |
| 18:N:1273:VAL:HA | 18:N:1276:MET:HE2 | 1.73 | 0.70 |
| 5:A:1725:VAL:HA | 5:A:1740:GLY:HA3 | 1.74 | 0.70 |
| 20:P:118:LEU:CD1 | 20:P:153:ARG:NH2 | 2.51 | 0.70 |
| 20:P:122:ARG:HG2 | 20:P:124:MET:HE1 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1684:TYR:HB2 | 5:A:1724:GLY:HA2 | 1.74 | 0.70 |
| 6:B:741:LEU:H | 29:b:66:LYS:HG2 | 1.55 | 0.70 |
| 29:b:23:ASN:ND2 | 30:c:427:GLU:OE2 | 2.23 | 0.70 |
| 12:H:35:ASP:OD1 | 12:H:36:ILE:HD12 | 1.92 | 0.70 |
| 20:P:209:SER:OG | 20:P:210:ARG:NH1 | 2.24 | 0.70 |
| 5:A:220:ASP:HA | 5:A:256:ASN:HD21 | 1.57 | 0.70 |
| 18:N:529:LEU:HD11 | 18:N:611:ALA:HB1 | 1.74 | 0.70 |
| 5:A:680:ALA:O | 5:A:684:GLU:HB2 | 1.92 | 0.70 |
| 16:L:163:LYS:O | 16:L:167:GLN:NE2 | 2.24 | 0.70 |
| 6:B:245:GLU:HB3 | 6:B:248:MET:HE2 | 1.74 | 0.70 |
| 18:N:357:ARG:HH21 | 18:N:361:PRO:HD3 | 1.57 | 0.70 |
| 5:A:1542:LEU:HD23 | 5:A:1546:GLN:HB3 | 1.73 | 0.69 |
| 26:Y:118:ARG:NH2 | 38:6:82:U:OP1 | 2.26 | 0.69 |
| 2:p:186:LEU:HA | 2:p:189:ARG:HE | 1.57 | 0.69 |
| 5:A:1429:LEU:HD12 | 5:A:1430:GLU:H | 1.57 | 0.69 |
| 8:D:2:SER:OG | 9:E:32:ASP:OD2 | 2.09 | 0.69 |
| 22:R:333:GLY:O | 22:R:337:THR:OG1 | 2.09 | 0.69 |
| 3:2:29:A:OP1 | 5:A:884:ARG:NH2 | 2.25 | 0.69 |
| 5:A:1582:THR:HG22 | 5:A:1584:ILE:H | 1.57 | 0.69 |
| 6:B:534:GLU:OE1 | 32:m:772:LYS:NZ | 2.23 | 0.69 |
| 5:A:1185:ARG:HE | 21:Q:229:VAL:HG11 | 1.56 | 0.69 |
| 5:A:1809:VAL:HG11 | 5:A:1861:ALA:HB1 | 1.75 | 0.69 |
| 5:A:1874:ARG:NH2 | 5:A:1902:ASP:OD2 | 2.26 | 0.69 |
| 18:N:926:GLU:HG3 | 25:X:137:ARG:HH21 | 1.57 | 0.69 |
| 22:R:294:LEU:O | 22:R:298:SER:OG | 2.11 | 0.69 |
| 24:W:537:ARG:NH1 | 24:W:577:PHE:HB2 | 2.07 | 0.69 |
| 35:z:162:LEU:HA | 35:z:165:ILE:HG22 | 1.73 | 0.69 |
| 1:e:190:TYR:OH | 5:A:750:LYS:NZ | 2.25 | 0.69 |
| 18:N:225:ILE:HA | 18:N:228:MET:HE2 | 1.75 | 0.69 |
| 5:A:164:GLN:NE2 | 5:A:227:PHE:O | 2.23 | 0.69 |
| 1:e:216:THR:HG22 | 21:Q:234:THR:HA | 1.74 | 0.69 |
| 23:U:336:ILE:HA | 23:U:352:LEU:HA | 1.73 | 0.69 |
| 25:X:584:PRO:HD2 | 25:X:587:PHE:HB2 | 1.75 | 0.69 |
| 25:X:668:ALA:HB2 | 25:X:683:ILE:HD11 | 1.73 | 0.69 |
| 35:z:318:VAL:HG12 | 35:z:363:PHE:HB2 | 1.75 | 0.69 |
| 21:Q:223:ARG:C | 21:Q:225:TRP:H | 2.00 | 0.69 |
| 35:z:319:ASP:OD1 | 35:z:350:ARG:NH1 | 2.25 | 0.69 |
| 2:p:196:ILE:HG23 | 25:X:722:ARG:HD3 | 1.74 | 0.69 |
| 5:A:1296:THR:HG21 | 5:A:1489:TRP:CE3 | 2.28 | 0.69 |
| 16:L:191:GLN:NE2 | 17:M:24:GLU:OE1 | 2.26 | 0.69 |
| 35:z:428:VAL:HG13 | 35:z:429:LEU:HD12 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1629:GLN:HA | 5:A:1657:ALA:HA | 1.75 | 0.68 |
| 7:C:103:ARG:HD3 | 7:C:145:LYS:HA | 1.75 | 0.68 |
| 11:G:42:GLN:HG2 | 11:G:56:ARG:HH12 | 1.58 | 0.68 |
| 17:M:24:GLU:OE1 | 17:M:24:GLU:N | 2.26 | 0.68 |
| 30:c:558:GLU:OE1 | 30:c:558:GLU:N | 2.26 | 0.68 |
| 35:z:131:ILE:HG21 | 35:z:161:VAL:HG11 | 1.75 | 0.68 |
| 23:U:357:LEU:HB2 | 23:U:371:PHE:HB2 | 1.75 | 0.68 |
| 25:X:139:LEU:HD22 | 25:X:147:ILE:HG12 | 1.75 | 0.68 |
| 10:F:51:GLU:N | 10:F:51:GLU:OE1 | 2.26 | 0.68 |
| 18:N:93:TRP:O | 18:N:138:LYS:NZ | 2.27 | 0.68 |
| 20:P:268:ASN:HA | 20:P:271:LYS:HE3 | 1.75 | 0.68 |
| 31:d:7:GLN:OE1 | 31:d:12:LYS:NZ | 2.27 | 0.68 |
| 5:A:1749:LEU:HD12 | 5:A:1752:GLN:HE21 | 1.58 | 0.68 |
| 38:6:47:A:H5” | 38:6:47:A:H8 | 1.58 | 0.68 |
| 15:K:106:ILE:HG21 | 15:K:137:VAL:HA | 1.76 | 0.68 |
| 17:M:88:GLN:NE2 | 17:M:131:TYR:OH | 2.27 | 0.68 |
| 34:y:79:TRP:O | 34:y:80:LYS:HD3 | 1.93 | 0.68 |
| 5:A:681:ARG:NH2 | 38:6:59:G:OP2 | 2.27 | 0.68 |
| 5:A:1589:LYS:HG3 | 39:1:-4:A:H5’ | 1.75 | 0.68 |
| 22:R:289:GLN:HA | 25:X:538:GLU:OE2 | 1.93 | 0.68 |
| 30:c:515:ASP:OD2 | 30:c:559:ARG:NH2 | 2.26 | 0.68 |
| 5:A:1700:ILE:HD12 | 5:A:1730:ASP:HB2 | 1.75 | 0.68 |
| 5:A:1798:ASN:O | 5:A:1801:GLN:HG2 | 1.93 | 0.68 |
| 17:M:148:GLU:HG3 | 20:P:282:LEU:HD21 | 1.75 | 0.68 |
| 22:R:418:ASP:OD1 | 22:R:421:ARG:NH1 | 2.26 | 0.68 |
| 31:d:28:ASN:OD1 | 31:d:29:PHE:N | 2.27 | 0.68 |
| 17:M:91:LEU:HD13 | 17:M:95:LEU:HD22 | 1.74 | 0.68 |
| 19:O:140:ASN:O | 28:a:138:ARG:NH2 | 2.27 | 0.68 |
| 5:A:1892:MET:HE2 | 5:A:1896:LEU:HD21 | 1.76 | 0.68 |
| 9:E:12:HIS:CD2 | 9:E:84:PRO:HG3 | 2.29 | 0.68 |
| 7:C:271:ASN:ND2 | 7:C:314:ASN:OD1 | 2.26 | 0.67 |
| 17:M:243:CYS:SG | 17:M:244:SER:N | 2.66 | 0.67 |
| 27:Z:102:GLN:OE1 | 27:Z:105:ARG:NH1 | 2.27 | 0.67 |
| 5:A:1844:LYS:HE2 | 5:A:1872:LEU:HD21 | 1.76 | 0.67 |
| 7:C:74:ILE:HB | 7:C:89:LEU:HB2 | 1.76 | 0.67 |
| 11:G:61:ASP:OD1 | 11:G:62:ARG:N | 2.27 | 0.67 |
| 13:I:23:ARG:NH1 | 13:I:29:GLU:OE1 | 2.26 | 0.67 |
| 17:M:26:CYS:SG | 17:M:82:SER:OG | 2.52 | 0.67 |
| 20:P:198:TRP:HE1 | 20:P:230:MET:HE3 | 1.59 | 0.67 |
| 22:R:338:ILE:HG23 | 22:R:340:GLU:H | 1.59 | 0.67 |
| 23:V:108:LEU:HB2 | 24:W:600:CYS:SG | 2.35 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:K:417:SER:OG | 21:Q:248:ASN:ND2 | 2.27 | 0.67 |
| 5:A:984:ASN:ND2 | 5:A:1243:ASN:OD1 | 2.27 | 0.67 |
| 18:N:53:HIS:O | 18:N:1224:ARG:NH1 | 2.27 | 0.67 |
| 24:W:202:LEU:HG | 24:W:207:ILE:HA | 1.75 | 0.67 |
| 5:A:1374:ILE:O | 29:b:23:ASN:ND2 | 2.28 | 0.67 |
| 20:P:190:ILE:HG22 | 20:P:193:ARG:HH22 | 1.57 | 0.67 |
| 21:Q:223:ARG:O | 21:Q:225:TRP:N | 2.27 | 0.67 |
| 30:c:472:CYS:SG | 30:c:516:SER:HB3 | 2.35 | 0.67 |
| 7:C:43:ASN:HD21 | 9:E:106:ARG:HH11 | 1.42 | 0.67 |
| 32:m:489:VAL:HG22 | 32:m:504:LEU:HD11 | 1.75 | 0.67 |
| 5:A:1976:LEU:HA | 5:A:1979:ARG:HG2 | 1.77 | 0.67 |
| 20:P:98:VAL:HG12 | 20:P:101:ARG:HH11 | 1.60 | 0.67 |
| 22:R:337:THR:OG1 | 22:R:342:TYR:OH | 2.06 | 0.67 |
| 23:V:112:LEU:HD21 | 24:W:600:CYS:HB2 | 1.76 | 0.67 |
| 5:A:1416:LYS:NZ | 5:A:1431:ASP:O | 2.27 | 0.67 |
| 24:W:130:PRO:O | 24:W:134:LEU:N | 2.27 | 0.67 |
| 30:c:578:ALA:O | 30:c:582:ARG:NH2 | 2.26 | 0.67 |
| 24:W:743:GLU:HG3 | 27:Z:173:LEU:HD11 | 1.75 | 0.66 |
| 25:X:420:PRO:O | 25:X:471:SER:OG | 2.13 | 0.66 |
| 7:C:149:GLU:OE1 | 7:C:166:ARG:NH2 | 2.28 | 0.66 |
| 25:X:97:CYS:SG | 25:X:100:ARG:NH2 | 2.69 | 0.66 |
| 23:T:62:ARG:NH1 | 23:T:66:ALA:O | 2.28 | 0.66 |
| 34:y:117:ASN:HD22 | 35:z:593:ILE:HG13 | 1.60 | 0.66 |
| 5:A:1020:MET:HG2 | 5:A:1066:PHE:HZ | 1.61 | 0.66 |
| 29:b:76:GLU:OE2 | 29:b:117:LYS:NZ | 2.26 | 0.66 |
| 34:y:144:MET:HE3 | 34:y:145:LEU:HD22 | 1.77 | 0.66 |
| 35:z:80:ARG:HB2 | 35:z:83:VAL:HB | 1.78 | 0.66 |
| 11:G:25:PHE:HZ | 11:G:62:ARG:HA | 1.60 | 0.66 |
| 20:P:53:GLN:NE2 | 20:P:102:ASP:OD1 | 2.28 | 0.66 |
| 23:V:98:LYS:HE2 | 24:W:535:LEU:HB2 | 1.76 | 0.66 |
| 30:c:579:ARG:HA | 30:c:582:ARG:HE | 1.60 | 0.66 |
| 10:F:35:GLN:OE1 | 10:F:37:ASN:ND2 | 2.28 | 0.66 |
| 12:H:23:HIS:O | 12:H:41:GLN:NE2 | 2.28 | 0.66 |
| 20:P:118:LEU:HA | 20:P:151:PHE:CE2 | 2.31 | 0.66 |
| 34:y:171:ASN:ND2 | 35:z:623:GLU:OE2 | 2.28 | 0.66 |
| 35:z:239:ILE:HD11 | 35:z:296:ARG:HH11 | 1.61 | 0.66 |
| 35:z:245:GLY:HA3 | 35:z:324:LYS:CE | 2.25 | 0.66 |
| 5:A:56:ARG:NH2 | 38:6:10:A:OP1 | 2.21 | 0.66 |
| 6:B:583:ASN:ND2 | 6:B:583:ASN:O | 2.29 | 0.66 |
| 17:M:178:ALA:HA | 17:M:182:ALA:HB3 | 1.77 | 0.66 |
| 23:S:61:PRO:HG2 | 24:W:697:ILE:HD11 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:U:112:LEU:HD23 | 23:U:113:ARG:HE | 1.61 | 0.66 |
| 23:U:272:ILE:HD13 | 23:U:301:LEU:HD13 | 1.77 | 0.66 |
| 5:A:251:LEU:HD21 | 5:A:424:ALA:HB2 | 1.78 | 0.66 |
| 5:A:962:TRP:NE1 | 5:A:1072:ASP:OD2 | 2.22 | 0.66 |
| 19:O:21:PRO:O | 19:O:24:ILE:HG22 | 1.96 | 0.66 |
| 21:Q:55:GLU:CD | 21:Q:59:ARG:HH21 | 2.04 | 0.66 |
| 23:V:111:ALA:O | 23:V:115:ILE:HG12 | 1.97 | 0.66 |
| 24:W:174:GLN:HB3 | 24:W:179:LYS:HE3 | 1.77 | 0.66 |
| 5:A:103:ARG:NH1 | 38:6:20:U:O3' | 2.28 | 0.65 |
| 5:A:1685:TRP:O | 5:A:1725:VAL:N | 2.27 | 0.65 |
| 6:B:724:PRO:HG2 | 6:B:727:ARG:HG3 | 1.78 | 0.65 |
| 23:S:17:ARG:HD3 | 23:T:17:ARG:HG3 | 1.76 | 0.65 |
| 18:N:73:ASN:HA | 18:N:76:ASN:HD21 | 1.61 | 0.65 |
| 18:N:628:LEU:HD11 | 18:N:987:SER:HB2 | 1.79 | 0.65 |
| 27:Z:64:VAL:O | 27:Z:68:LYS:HG2 | 1.96 | 0.65 |
| 5:A:1629:GLN:HE22 | 5:A:1661:TRP:CD1 | 2.14 | 0.65 |
| 21:Q:223:ARG:HB2 | 21:Q:226:ASP:OD1 | 1.96 | 0.65 |
| 32:m:505:HIS:HA | 32:m:508:ILE:HG22 | 1.79 | 0.65 |
| 5:A:873:TYR:CE1 | 5:A:883:GLN:HG2 | 2.30 | 0.65 |
| 35:z:310:THR:HA | 35:z:356:ARG:HH12 | 1.61 | 0.65 |
| 5:A:1689:GLN:HE22 | 5:A:1726:LEU:HD21 | 1.61 | 0.65 |
| 25:X:191:TRP:HB3 | 25:X:225:LEU:HD13 | 1.76 | 0.65 |
| 5:A:1666:PRO:HD3 | 5:A:1741:ASN:HD21 | 1.62 | 0.65 |
| 6:B:713:ASP:OD2 | 6:B:736:TYR:OH | 2.14 | 0.65 |
| 20:P:264:GLU:O | 20:P:268:ASN:ND2 | 2.29 | 0.65 |
| 5:A:969:GLU:HB2 | 5:A:973:LEU:HB3 | 1.79 | 0.65 |
| 18:N:1060:TYR:CE2 | 18:N:1062:LEU:HB2 | 2.31 | 0.65 |
| 25:X:511:ILE:HG13 | 25:X:512:ALA:H | 1.62 | 0.65 |
| 31:d:20:GLU:HG2 | 31:d:21:HIS:HD2 | 1.62 | 0.65 |
| 5:A:108:SER:OG | 16:L:213:GLU:OE2 | 2.14 | 0.65 |
| 11:G:45:ILE:HG12 | 11:G:109:VAL:HG12 | 1.77 | 0.65 |
| 34:y:210:ASP:OD1 | 34:y:211:GLY:N | 2.29 | 0.65 |
| 5:A:1135:ARG:NH1 | 21:Q:223:ARG:HD2 | 2.13 | 0.64 |
| 15:K:89:GLU:OE2 | 22:R:259:ARG:NE | 2.30 | 0.64 |
| 23:V:80:TRP:HB3 | 27:Z:100:GLU:CD | 2.22 | 0.64 |
| 27:Z:83:LEU:HD23 | 27:Z:94:GLN:HE22 | 1.62 | 0.64 |
| 30:c:528:THR:OG1 | 30:c:531:ASP:OD1 | 2.14 | 0.64 |
| 34:y:125:ILE:HG13 | 34:y:131:ARG:HD3 | 1.78 | 0.64 |
| 20:P:289:LYS:O | 20:P:293:ARG:NH1 | 2.30 | 0.64 |
| 22:R:44:ASP:OD1 | 22:R:45:LEU:N | 2.26 | 0.64 |
| 24:W:530:VAL:HG23 | 24:W:531:ILE:HG13 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:z:423:LEU:HB3 | 35:z:429:LEU:HD13 | 1.78 | 0.64 |
| 5:A:414:GLU:OE2 | 6:B:407:HIS:NE2 | 2.22 | 0.64 |
| 9:E:117:LEU:O | 16:L:185:ARG:NH2 | 2.26 | 0.64 |
| 22:R:47:GLU:HA | 22:R:50:GLU:HG3 | 1.78 | 0.64 |
| 24:W:262:ARG:O | 24:W:266:MET:HG2 | 1.97 | 0.64 |
| 32:m:556:ASN:O | 32:m:561:ARG:NH1 | 2.30 | 0.64 |
| 34:y:160:PHE:O | 34:y:164:TYR:N | 2.30 | 0.64 |
| 17:M:38:GLU:OE2 | 17:M:55:ARG:NH1 | 2.31 | 0.64 |
| 18:N:226:ILE:HG21 | 18:N:270:MET:HG3 | 1.79 | 0.64 |
| 23:U:321:PHE:O | 23:U:324:LYS:N | 2.30 | 0.64 |
| 5:A:1490:GLN:HE21 | 5:A:1492:ASN:HD22 | 1.46 | 0.64 |
| 7:C:62:GLY:O | 7:C:319:HIS:NE2 | 2.29 | 0.64 |
| 9:E:12:HIS:NE2 | 9:E:84:PRO:HG3 | 2.12 | 0.64 |
| 11:G:108:LEU:HD11 | 13:I:30:TYR:HE2 | 1.62 | 0.64 |
| 18:N:401:VAL:HG22 | 18:N:446:LEU:HD11 | 1.78 | 0.64 |
| 20:P:82:MET:SD | 38:6:32:G:N2 | 2.70 | 0.64 |
| 23:V:66:ALA:HB1 | 27:Z:60:GLU:HG2 | 1.79 | 0.64 |
| 24:W:176:LYS:NZ | 38:6:42:A:OP1 | 2.27 | 0.64 |
| 25:X:645:ARG:O | 25:X:649:GLU:HG3 | 1.97 | 0.64 |
| 3:2:19:G:H22 | 38:6:50:A:H2 | 1.45 | 0.64 |
| 5:A:208:LEU:O | 19:O:8:ARG:NH1 | 2.29 | 0.64 |
| 5:A:1803:PHE:HB2 | 5:A:1834:PHE:HB3 | 1.80 | 0.64 |
| 18:N:930:PRO:HD3 | 25:X:137:ARG:NH1 | 2.13 | 0.64 |
| 22:R:284:THR:HG21 | 22:R:306:LEU:HD22 | 1.79 | 0.64 |
| 35:z:547:VAL:HG22 | 35:z:557:THR:HG21 | 1.79 | 0.64 |
| 18:N:314:PHE:HB3 | 18:N:318:LEU:HG | 1.80 | 0.64 |
| 22:R:201:HIS:O | 22:R:206:ASN:ND2 | 2.30 | 0.64 |
| 24:W:536:ILE:O | 24:W:537:ARG:HB2 | 1.97 | 0.64 |
| 24:W:537:ARG:O | 24:W:539:SER:N | 2.30 | 0.64 |
| 6:B:90:ASP:HB3 | 15:K:157:ARG:HG3 | 1.80 | 0.63 |
| 6:B:227:VAL:HG11 | 6:B:254:ILE:HD12 | 1.79 | 0.63 |
| 23:T:77:GLN:NE2 | 27:Z:74:ALA:O | 2.31 | 0.63 |
| 24:W:203:LYS:HB3 | 24:W:207:ILE:HD12 | 1.79 | 0.63 |
| 25:X:321:SER:O | 25:X:325:HIS:ND1 | 2.21 | 0.63 |
| 29:b:24:LEU:HB3 | 30:c:431:HIS:HD1 | 1.63 | 0.63 |
| 35:z:245:GLY:HA3 | 35:z:324:LYS:HD2 | 1.79 | 0.63 |
| 35:z:428:VAL:HG23 | 35:z:440:GLY:HA2 | 1.80 | 0.63 |
| 5:A:952:GLU:OE2 | 5:A:955:ARG:NH2 | 2.22 | 0.63 |
| 27:Z:64:VAL:HG23 | 27:Z:68:LYS:HZ3 | 1.63 | 0.63 |
| 35:z:62:LEU:HB2 | 35:z:67:TRP:CD1 | 2.33 | 0.63 |
| 18:N:715:ARG:NH1 | 18:N:767:ASP:O | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:O:98:GLU:OE1 | 19:O:98:GLU:N | 2.31 | 0.63 |
| 20:P:177:TYR:HD1 | 20:P:214:PHE:HE1 | 1.45 | 0.63 |
| 22:R:48:LEU:HD13 | 24:W:257:ILE:HG23 | 1.79 | 0.63 |
| 23:S:100:GLU:OE1 | 23:V:97:THR:OG1 | 2.15 | 0.63 |
| 25:X:510:LYS:HZ3 | 26:Y:83:ILE:HB | 1.64 | 0.63 |
| 5:A:1656:LEU:HA | 5:A:1683:LYS:HD2 | 1.80 | 0.63 |
| 20:P:251:ASN:ND2 | 39:1:13:U:OP1 | 2.31 | 0.63 |
| 1:e:219:GLN:HE21 | 21:Q:232:ARG:HD3 | 1.62 | 0.63 |
| 5:A:1185:ARG:NE | 21:Q:229:VAL:HG11 | 2.13 | 0.63 |
| 11:G:55:ALA:HB2 | 11:G:71:VAL:HA | 1.80 | 0.63 |
| 15:K:405:LYS:HD3 | 15:K:408:GLU:HG2 | 1.80 | 0.63 |
| 35:z:608:GLU:N | 35:z:608:GLU:OE1 | 2.31 | 0.63 |
| 5:A:1835:ASN:HB2 | 5:A:1840:GLN:H | 1.63 | 0.63 |
| 12:H:80:LEU:HD21 | 14:J:60:VAL:HG13 | 1.81 | 0.63 |
| 20:P:117:CYS:SG | 20:P:135:HIS:HD2 | 2.11 | 0.63 |
| 23:S:24:GLU:OE2 | 23:S:27:LEU:N | 2.31 | 0.63 |
| 23:V:88:PHE:O | 23:V:92:ARG:HG2 | 1.97 | 0.63 |
| 24:W:260:GLY:O | 24:W:264:ASN:ND2 | 2.31 | 0.63 |
| 2:p:172:ARG:NH1 | 24:W:63:ARG:HH11 | 1.97 | 0.63 |
| 6:B:777:LYS:HA | 6:B:780:ILE:HG22 | 1.81 | 0.63 |
| 7:C:217:GLY:O | 7:C:244:ARG:NH1 | 2.32 | 0.63 |
| 10:F:68:TYR:HB2 | 11:G:100:PHE:HB3 | 1.81 | 0.63 |
| 23:U:83:VAL:HG22 | 23:U:87:GLN:HE21 | 1.64 | 0.63 |
| 23:U:420:VAL:HG13 | 23:U:438:GLU:HB2 | 1.81 | 0.63 |
| 7:C:308:GLY:HA3 | 9:E:106:ARG:HG2 | 1.79 | 0.63 |
| 22:R:42:ILE:HG23 | 22:R:47:GLU:HG2 | 1.79 | 0.63 |
| 24:W:247:ARG:O | 24:W:251:GLU:HB2 | 1.99 | 0.63 |
| 24:W:672:CYS:HA | 24:W:675:LEU:HG | 1.81 | 0.63 |
| 32:m:296:LYS:NZ | 33:n:313:GLU:HG3 | 2.13 | 0.63 |
| 11:G:8:PRO:HD2 | 11:G:9:ARG:HH12 | 1.64 | 0.63 |
| 18:N:199:ILE:O | 18:N:203:LEU:HD12 | 1.99 | 0.63 |
| 18:N:369:ASP:H | 18:N:372:PHE:HB3 | 1.63 | 0.63 |
| 23:U:255:CYS:HB3 | 23:U:264:VAL:HG23 | 1.81 | 0.63 |
| 32:m:511:TRP:O | 32:m:515:LEU:N | 2.31 | 0.63 |
| 35:z:245:GLY:HA3 | 35:z:324:LYS:NZ | 2.14 | 0.63 |
| 36:r:222:UNK:O | 36:r:226:UNK:N | 2.31 | 0.63 |
| 25:X:437:MET:SD | 25:X:438:GLU:HG3 | 2.39 | 0.62 |
| 11:G:44:LEU:HD13 | 11:G:54:LEU:HD12 | 1.81 | 0.62 |
| 24:W:509:GLU:O | 24:W:513:GLN:HG3 | 1.99 | 0.62 |
| 25:X:108:MET:HG3 | 25:X:110:VAL:HG12 | 1.80 | 0.62 |
| 5:A:1429:LEU:O | 5:A:1430:GLU:HG3 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:I:26:TRP:HZ3 | 13:I:69:ASN:HD22 | 1.47 | 0.62 |
| 18:N:160:LYS:NZ | 18:N:248:ASP:OD1 | 2.27 | 0.62 |
| 22:R:256:GLU:OE1 | 22:R:259:ARG:NH1 | 2.32 | 0.62 |
| 35:z:210:LEU:HB3 | 35:z:363:PHE:HD1 | 1.62 | 0.62 |
| 23:T:11:LYS:HD3 | 23:T:60:ARG:HH22 | 1.64 | 0.62 |
| 3:2:5:U:O2 | 38:6:87:G:N2 | 2.21 | 0.62 |
| 5:A:196:PRO:HD3 | 5:A:543:TYR:CE2 | 2.35 | 0.62 |
| 5:A:873:TYR:HE1 | 5:A:883:GLN:HG2 | 1.65 | 0.62 |
| 11:G:55:ALA:HB3 | 11:G:68:LEU:HD12 | 1.81 | 0.62 |
| 18:N:1183:PHE:HB3 | 18:N:1213:VAL:HG22 | 1.82 | 0.62 |
| 21:Q:55:GLU:OE1 | 21:Q:59:ARG:NH2 | 2.30 | 0.62 |
| 28:a:126:ASP:O | 28:a:130:LYS:HG3 | 2.00 | 0.62 |
| 38:6:53:G:O2' | 38:6:55:C:OP1 | 2.17 | 0.62 |
| 5:A:986:THR:HG22 | 5:A:1244:ARG:HH22 | 1.65 | 0.62 |
| 25:X:513:THR:H | 25:X:544:PHE:HZ | 1.47 | 0.62 |
| 25:X:581:GLU:OE1 | 25:X:581:GLU:N | 2.33 | 0.62 |
| 6:B:85:TYR:HB3 | 6:B:89:VAL:HG21 | 1.80 | 0.62 |
| 24:W:240:GLU:HB2 | 24:W:244:GLN:HB3 | 1.82 | 0.62 |
| 36:r:242:UNK:O | 36:r:244:UNK:N | 2.33 | 0.62 |
| 6:B:769:ASP:HB2 | 6:B:772:VAL:HB | 1.80 | 0.62 |
| 18:N:836:ARG:NH2 | 18:N:890:TYR:O | 2.30 | 0.62 |
| 18:N:929:ARG:HE | 25:X:137:ARG:NH2 | 1.97 | 0.62 |
| 5:A:935:ASP:HB3 | 5:A:938:GLU:HG3 | 1.82 | 0.62 |
| 5:A:1354:MET:O | 5:A:1354:MET:HG3 | 2.00 | 0.62 |
| 18:N:562:ILE:HA | 18:N:585:VAL:HG22 | 1.81 | 0.62 |
| 35:z:387:MET:SD | 35:z:387:MET:N | 2.67 | 0.62 |
| 1:e:32:GLU:OE2 | 2:p:170:ARG:NH2 | 2.33 | 0.62 |
| 6:B:189:ARG:NH2 | 6:B:652:ASP:OD2 | 2.33 | 0.62 |
| 6:B:938:ALA:HB3 | 6:B:943:LEU:HD23 | 1.81 | 0.62 |
| 20:P:63:GLU:O | 20:P:66:GLN:NE2 | 2.27 | 0.62 |
| 24:W:537:ARG:C | 24:W:539:SER:H | 2.06 | 0.62 |
| 25:X:512:ALA:HB2 | 26:Y:83:ILE:HG13 | 1.82 | 0.62 |
| 23:U:342:HIS:HE1 | 23:U:344:ASP:HB2 | 1.65 | 0.61 |
| 24:W:40:THR:OG1 | 24:W:43:GLN:OE1 | 2.18 | 0.61 |
| 18:N:872:THR:O | 18:N:884:ARG:NH1 | 2.34 | 0.61 |
| 23:S:100:GLU:HA | 23:S:103:THR:HG22 | 1.82 | 0.61 |
| 24:W:207:ILE:HG12 | 24:W:209:ILE:N | 2.11 | 0.61 |
| 27:Z:131:LEU:O | 27:Z:135:GLU:HG2 | 2.01 | 0.61 |
| 32:m:449:TRP:HE1 | 32:m:457:ALA:HB2 | 1.64 | 0.61 |
| 5:A:694:GLN:O | 5:A:699:ARG:NH2 | 2.24 | 0.61 |
| 5:A:1654:LEU:HD12 | 5:A:1720:PRO:HG2 | 1.80 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:C:111:SER:OG | 7:C:138:VAL:HG13 | 2.00 | 0.61 |
| 18:N:480:LEU:HD21 | 18:N:483:PHE:HB2 | 1.83 | 0.61 |
| 30:c:576:ASP:HB3 | 30:c:603:TYR:CZ | 2.35 | 0.61 |
| 6:B:532:ASP:OD2 | 32:m:738:ARG:NH2 | 2.33 | 0.61 |
| 11:G:29:PRO:HG3 | 13:I:36:SER:O | 2.00 | 0.61 |
| 13:I:26:TRP:CZ3 | 13:I:69:ASN:ND2 | 2.69 | 0.61 |
| 32:m:317:SER:HA | 32:m:320:PHE:HB2 | 1.82 | 0.61 |
| 7:C:155:SER:OG | 7:C:157:ASP:OD1 | 2.18 | 0.61 |
| 23:S:60:ARG:CZ | 24:W:701:TRP:HD1 | 2.13 | 0.61 |
| 24:W:174:GLN:O | 24:W:179:LYS:NZ | 2.29 | 0.61 |
| 25:X:87:HIS:HB2 | 25:X:91:PHE:HE1 | 1.66 | 0.61 |
| 32:m:431:GLU:O | 32:m:435:MET:HG2 | 2.00 | 0.61 |
| 34:y:132:GLU:HG2 | 34:y:133:PHE:CD1 | 2.35 | 0.61 |
| 2:p:162:SER:OG | 2:p:166:ARG:NH1 | 2.34 | 0.61 |
| 7:C:85:ASN:HB3 | 9:E:97:GLY:HA3 | 1.82 | 0.61 |
| 24:W:737:SER:O | 24:W:741:GLN:HG2 | 2.01 | 0.61 |
| 25:X:219:TRP:HE1 | 25:X:256:LEU:HD22 | 1.66 | 0.61 |
| 35:z:317:VAL:HG23 | 35:z:354:ALA:HB2 | 1.82 | 0.61 |
| 6:B:628:TYR:OH | 6:B:657:ASP:OD2 | 2.14 | 0.61 |
| 23:V:99:GLN:HE22 | 36:r:231:UNK:HA | 1.66 | 0.61 |
| 24:W:131:ASN:HA | 24:W:134:LEU:HB3 | 1.82 | 0.61 |
| 34:y:30:SER:O | 34:y:33:ASN:ND2 | 2.33 | 0.61 |
| 6:B:146:VAL:HG12 | 6:B:154:LYS:HB2 | 1.82 | 0.61 |
| 25:X:592:TYR:OH | 25:X:618:LYS:HE3 | 2.01 | 0.61 |
| 35:z:241:VAL:HG21 | 35:z:300:PHE:HD1 | 1.65 | 0.61 |
| 5:A:1762:PRO:HB2 | 34:y:97:ILE:HD11 | 1.82 | 0.61 |
| 5:A:1828:ASN:OD1 | 5:A:1848:THR:OG1 | 2.15 | 0.61 |
| 11:G:109:VAL:HG22 | 13:I:64:LEU:HB3 | 1.83 | 0.61 |
| 12:H:78:ILE:H | 12:H:78:ILE:HD12 | 1.65 | 0.61 |
| 25:X:398:ARG:HH22 | 25:X:437:MET:HA | 1.65 | 0.61 |
| 26:Y:137:GLU:OE1 | 26:Y:137:GLU:N | 2.29 | 0.61 |
| 29:b:128:VAL:HA | 29:b:131:TYR:HD2 | 1.66 | 0.61 |
| 30:c:541:LYS:O | 30:c:545:GLN:HG3 | 2.00 | 0.61 |
| 31:d:6:LEU:HB2 | 31:d:13:ILE:HB | 1.82 | 0.61 |
| 6:B:505:TYR:OH | 6:B:552:ARG:NH1 | 2.34 | 0.60 |
| 7:C:115:THR:HG22 | 7:C:136:GLY:O | 2.00 | 0.60 |
| 18:N:492:GLN:O | 25:X:248:ARG:NH2 | 2.34 | 0.60 |
| 25:X:286:THR:HG21 | 25:X:289:ASN:HB2 | 1.83 | 0.60 |
| 19:O:11:ARG:HG2 | 19:O:12:PRO:HD2 | 1.82 | 0.60 |
| 31:d:92:ASN:ND2 | 31:d:115:LYS:O | 2.33 | 0.60 |
| 5:A:978:TRP:CD1 | 5:A:1214:MET:HE1 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:m:545:ASP:OD2 | 32:m:550:TRP:NE1 | 2.33 | 0.60 |
| 11:G:32:VAL:O | 11:G:111:ARG:NH2 | 2.34 | 0.60 |
| 5:A:127:MET:HE1 | 5:A:605:PHE:HZ | 1.66 | 0.60 |
| 22:R:84:LYS:HZ1 | 22:R:87:ALA:HB3 | 1.66 | 0.60 |
| 24:W:141:PRO:HB2 | 24:W:146:LEU:HD21 | 1.84 | 0.60 |
| 24:W:159:GLU:HA | 24:W:162:MET:HG2 | 1.81 | 0.60 |
| 28:a:67:LEU:HA | 31:d:93:ALA:HB2 | 1.82 | 0.60 |
| 3:2:24:A:H5' | 3:2:25:G:H5" | 1.83 | 0.60 |
| 5:A:1307:GLU:N | 5:A:1307:GLU:OE1 | 2.34 | 0.60 |
| 6:B:221:VAL:HG21 | 6:B:912:GLN:HB3 | 1.82 | 0.60 |
| 7:C:295:VAL:HB | 7:C:304:TYR:HB2 | 1.83 | 0.60 |
| 24:W:537:ARG:HH11 | 24:W:577:PHE:CB | 2.11 | 0.60 |
| 25:X:467:ASP:O | 25:X:475:ARG:NH2 | 2.34 | 0.60 |
| 25:X:543:LEU:HD13 | 26:Y:83:ILE:HD11 | 1.82 | 0.60 |
| 28:a:64:GLN:OE1 | 31:d:62:ARG:NH1 | 2.31 | 0.60 |
| 30:c:417:TYR:HB2 | 30:c:449:MET:HE2 | 1.82 | 0.60 |
| 31:d:23:PRO:O | 31:d:27:GLN:HG3 | 2.02 | 0.60 |
| 32:m:439:LYS:NZ | 32:m:479:ASP:OD2 | 2.26 | 0.60 |
| 4:5:68:U:O4 | 5:A:492:ASN:ND2 | 2.33 | 0.60 |
| 5:A:1660:LYS:HZ1 | 5:A:1681:THR:N | 2.00 | 0.60 |
| 8:D:37:MET:HE1 | 9:E:71:ARG:HD2 | 1.82 | 0.60 |
| 18:N:495:GLN:O | 25:X:248:ARG:NH2 | 2.34 | 0.60 |
| 3:2:23:U:OP1 | 5:A:797:LYS:NZ | 2.34 | 0.60 |
| 12:H:75:GLY:O | 14:J:63:ARG:NH1 | 2.34 | 0.60 |
| 20:P:118:LEU:CD2 | 20:P:153:ARG:HH21 | 2.14 | 0.60 |
| 32:m:284:MET:O | 32:m:288:ARG:HG2 | 2.02 | 0.60 |
| 34:y:138:ASP:OD1 | 34:y:141:GLY:HA3 | 2.01 | 0.60 |
| 12:H:31:PHE:O | 14:J:22:ASN:ND2 | 2.31 | 0.60 |
| 22:R:485:ASP:OD1 | 22:R:488:ARG:NH1 | 2.35 | 0.60 |
| 23:S:110:ALA:HA | 23:S:113:ARG:NE | 2.15 | 0.60 |
| 29:b:68:LEU:HG | 29:b:127:LEU:HD22 | 1.84 | 0.60 |
| 30:c:519:TRP:HZ3 | 30:c:560:LEU:HD22 | 1.67 | 0.60 |
| 1:e:143:ARG:NH2 | 16:L:281:ASP:OD1 | 2.35 | 0.59 |
| 5:A:635:ILE:O | 5:A:639:PHE:HB2 | 2.02 | 0.59 |
| 5:A:722:GLU:OE1 | 5:A:722:GLU:N | 2.34 | 0.59 |
| 5:A:1966:ALA:HB1 | 5:A:2007:LEU:HD22 | 1.84 | 0.59 |
| 17:M:170:LEU:HG | 17:M:171:LYS:HE3 | 1.84 | 0.59 |
| 18:N:751:ARG:NH2 | 18:N:1206:ALA:O | 2.35 | 0.59 |
| 20:P:69:GLN:NE2 | 20:P:80:GLY:O | 2.35 | 0.59 |
| 35:z:497:SER:HA | 35:z:500:PHE:CD2 | 2.37 | 0.59 |
| 5:A:1358:LEU:HD22 | 29:b:21:MET:HE1 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1400:GLU:OE1 | 30:c:462:LYS:NZ | 2.35 | 0.59 |
| 16:L:127:LEU:HA | 16:L:130:ARG:HG3 | 1.83 | 0.59 |
| 20:P:214:PHE:HZ | 39:1:10:U:H1' | 1.66 | 0.59 |
| 22:R:112:GLU:OE2 | 22:R:116:LYS:HE2 | 2.02 | 0.59 |
| 23:S:55:VAL:HG11 | 27:Z:133:LEU:HD21 | 1.82 | 0.59 |
| 24:W:531:ILE:HG12 | 24:W:537:ARG:NH2 | 2.17 | 0.59 |
| 25:X:534:PHE:O | 25:X:538:GLU:HG2 | 2.02 | 0.59 |
| 32:m:650:LEU:HB3 | 32:m:656:ILE:HD12 | 1.84 | 0.59 |
| 1:e:133:GLY:O | 1:e:137:GLU:HG3 | 2.02 | 0.59 |
| 6:B:767:ASP:HB3 | 6:B:770:LYS:HE3 | 1.85 | 0.59 |
| 23:S:38:ASP:N | 23:S:43:GLN:O | 2.35 | 0.59 |
| 35:z:319:ASP:HB3 | 35:z:364:ARG:HG2 | 1.83 | 0.59 |
| 22:R:46:GLU:OE2 | 24:W:199:ARG:NH2 | 2.34 | 0.59 |
| 22:R:248:ALA:O | 22:R:252:ILE:HG12 | 2.03 | 0.59 |
| 32:m:449:TRP:O | 32:m:484:ARG:NH2 | 2.35 | 0.59 |
| 35:z:457:LEU:O | 35:z:460:ASN:ND2 | 2.35 | 0.59 |
| 2:p:169:PHE:CZ | 24:W:67:GLU:HB3 | 2.38 | 0.59 |
| 5:A:1514:PHE:O | 5:A:1517:THR:OG1 | 2.20 | 0.59 |
| 15:K:117:LYS:HG3 | 22:R:225:GLN:NE2 | 2.18 | 0.59 |
| 24:W:514:GLU:O | 24:W:518:GLU:N | 2.35 | 0.59 |
| 24:W:514:GLU:HG2 | 24:W:521:ARG:HH22 | 1.68 | 0.59 |
| 31:d:112:LEU:HG | 31:d:116:HIS:HD2 | 1.68 | 0.59 |
| 32:m:718:PHE:HE2 | 32:m:764:LEU:HD22 | 1.67 | 0.59 |
| 5:A:1295:MET:SD | 5:A:1354:MET:HE2 | 2.42 | 0.59 |
| 5:A:1639:HIS:HE1 | 5:A:1718:MET:HE1 | 1.67 | 0.59 |
| 6:B:250:ASN:O | 6:B:254:ILE:HG12 | 2.02 | 0.59 |
| 7:C:245:ILE:HG23 | 7:C:258:LEU:HB2 | 1.85 | 0.59 |
| 17:M:38:GLU:OE1 | 17:M:38:GLU:N | 2.36 | 0.59 |
| 18:N:224:ALA:HA | 18:N:418:PHE:CE1 | 2.38 | 0.59 |
| 22:R:488:ARG:NH2 | 22:R:517:GLU:OE1 | 2.35 | 0.59 |
| 16:L:191:GLN:NE2 | 28:a:86:THR:HG23 | 2.15 | 0.59 |
| 18:N:230:LEU:HD21 | 18:N:274:LEU:HA | 1.85 | 0.59 |
| 23:T:84:ALA:HB1 | 27:Z:68:LYS:HE3 | 1.85 | 0.59 |
| 25:X:503:TYR:HA | 25:X:506:VAL:HG12 | 1.83 | 0.59 |
| 3:2:13:C:O2' | 5:A:725:ARG:NH2 | 2.35 | 0.59 |
| 5:A:1943:LEU:O | 5:A:1992:TRP:NE1 | 2.35 | 0.59 |
| 22:R:412:LEU:HD13 | 22:R:443:PHE:HE1 | 1.67 | 0.59 |
| 24:W:677:ASN:OD1 | 24:W:678:ARG:N | 2.36 | 0.59 |
| 5:A:1873:ILE:O | 5:A:1881:GLN:NE2 | 2.36 | 0.59 |
| 18:N:214:LYS:HE3 | 18:N:259:LEU:HD12 | 1.85 | 0.59 |
| 20:P:93:SER:N | 20:P:232:HIS:O | 2.30 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:P:98:VAL:HG12 | 20:P:101:ARG:NH1 | 2.17 | 0.59 |
| 5:A:94:ARG:NH2 | 5:A:105:ASP:OD2 | 2.35 | 0.59 |
| 5:A:1095:LEU:HD22 | 5:A:1110:LEU:HD22 | 1.83 | 0.59 |
| 20:P:150:CYS:SG | 20:P:221:ALA:HA | 2.43 | 0.59 |
| 20:P:163:MET:HB3 | 20:P:245:TRP:HB2 | 1.83 | 0.59 |
| 23:S:69:LEU:HD22 | 23:U:80:TRP:HD1 | 1.68 | 0.59 |
| 23:S:75:LEU:O | 23:S:78:GLU:HG3 | 2.03 | 0.59 |
| 23:U:385:GLU:OE2 | 23:U:430:GLN:N | 2.36 | 0.59 |
| 14:J:21:LEU:HB2 | 14:J:25:ARG:HB2 | 1.84 | 0.58 |
| 15:K:110:VAL:HG11 | 22:R:199:VAL:HG22 | 1.84 | 0.58 |
| 18:N:333:GLN:O | 18:N:336:GLU:HG2 | 2.03 | 0.58 |
| 18:N:393:ILE:HD11 | 18:N:435:ARG:HH21 | 1.67 | 0.58 |
| 24:W:518:GLU:O | 24:W:522:LEU:N | 2.33 | 0.58 |
| 27:Z:162:ARG:O | 27:Z:165:GLU:HG3 | 2.03 | 0.58 |
| 30:c:565:LEU:HB3 | 30:c:567:PRO:HD2 | 1.84 | 0.58 |
| 5:A:1605:LEU:O | 5:A:1609:ILE:HG13 | 2.03 | 0.58 |
| 18:N:852:ASP:OD1 | 18:N:929:ARG:NH1 | 2.35 | 0.58 |
| 18:N:929:ARG:HE | 25:X:137:ARG:CZ | 2.17 | 0.58 |
| 22:R:70:MET:HE3 | 22:R:100:ASP:HB3 | 1.83 | 0.58 |
| 5:A:746:ASN:OD1 | 5:A:808:LYS:NZ | 2.34 | 0.58 |
| 11:G:104:ASP:HA | 13:I:66:ARG:HH12 | 1.68 | 0.58 |
| 18:N:153:ASN:HB2 | 18:N:178:TYR:HE2 | 1.68 | 0.58 |
| 18:N:1060:TYR:HE2 | 18:N:1062:LEU:HB2 | 1.68 | 0.58 |
| 22:R:111:ILE:HG21 | 22:R:127:PHE:CZ | 2.39 | 0.58 |
| 23:U:71:ALA:HB2 | 23:V:61:PRO:HG2 | 1.86 | 0.58 |
| 30:c:440:GLU:OE1 | 30:c:440:GLU:N | 2.35 | 0.58 |
| 6:B:371:GLN:HE22 | 6:B:373:LEU:HB2 | 1.68 | 0.58 |
| 6:B:473:ILE:H | 6:B:473:ILE:HD12 | 1.69 | 0.58 |
| 18:N:15:ALA:O | 18:N:20:GLY:N | 2.37 | 0.58 |
| 23:U:71:ALA:HB1 | 23:V:63:PRO:HD3 | 1.85 | 0.58 |
| 32:m:749:ARG:HE | 32:m:759:GLY:HA3 | 1.68 | 0.58 |
| 6:B:791:GLY:N | 6:B:796:GLU:O | 2.33 | 0.58 |
| 18:N:746:VAL:HG22 | 18:N:1040:ILE:HD12 | 1.85 | 0.58 |
| 24:W:65:GLU:OE2 | 24:W:89:ARG:NH2 | 2.36 | 0.58 |
| 25:X:457:ALA:H | 25:X:505:ARG:HH22 | 1.52 | 0.58 |
| 34:y:179:TYR:CZ | 35:z:217:GLU:HG3 | 2.39 | 0.58 |
| 2:p:164:ARG:HB3 | 24:W:105:LEU:HD21 | 1.84 | 0.58 |
| 7:C:157:ASP:OD1 | 7:C:159:THR:HG22 | 2.03 | 0.58 |
| 28:a:75:THR:H | 28:a:78:GLN:NE2 | 2.01 | 0.58 |
| 32:m:749:ARG:HH21 | 32:m:759:GLY:HA3 | 1.68 | 0.58 |
| 35:z:466:HIS:CE1 | 35:z:560:ARG:HH22 | 2.22 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:48:GLU:HG2 | 5:A:49:LYS:HD3 | 1.85 | 0.58 |
| 5:A:1272:LEU:O | 5:A:1322:ARG:NH2 | 2.36 | 0.58 |
| 5:A:1800:ILE:HG12 | 5:A:1837:ARG:HG2 | 1.85 | 0.58 |
| 9:E:76:VAL:HA | 10:F:64:ASN:ND2 | 2.18 | 0.58 |
| 13:I:60:LEU:HB3 | 13:I:63:ILE:HD11 | 1.86 | 0.58 |
| 23:U:342:HIS:CE1 | 23:U:344:ASP:HB2 | 2.38 | 0.58 |
| 26:Y:164:HIS:O | 26:Y:168:LEU:HD23 | 2.04 | 0.58 |
| 5:A:911:MET:O | 5:A:912:ARG:NH1 | 2.33 | 0.58 |
| 9:E:14:LEU:HD23 | 9:E:78:LEU:HD12 | 1.85 | 0.58 |
| 18:N:224:ALA:HA | 18:N:418:PHE:HE1 | 1.69 | 0.58 |
| 22:R:127:PHE:O | 22:R:131:VAL:HG22 | 2.03 | 0.58 |
| 22:R:186:GLU:OE2 | 22:R:189:ARG:HD2 | 2.03 | 0.58 |
| 23:T:67:THR:HG22 | 27:Z:108:ASN:HB2 | 1.86 | 0.58 |
| 24:W:700:ALA:HB1 | 27:Z:134:LEU:HD22 | 1.84 | 0.58 |
| 5:A:88:ARG:HG2 | 5:A:92:LYS:NZ | 2.19 | 0.58 |
| 5:A:987:ASP:O | 5:A:1123:ARG:NH2 | 2.37 | 0.58 |
| 23:U:379:LYS:H | 23:U:394:THR:HA | 1.69 | 0.58 |
| 23:V:55:VAL:HG22 | 23:V:56:PRO:HD2 | 1.84 | 0.58 |
| 23:V:101:LEU:O | 23:V:105:LEU:HG | 2.04 | 0.58 |
| 24:W:200:ARG:HA | 24:W:203:LYS:HG2 | 1.85 | 0.58 |
| 31:d:17:LEU:HD23 | 31:d:26:CYS:HB2 | 1.86 | 0.58 |
| 33:n:320:ARG:O | 33:n:324:ILE:HG12 | 2.03 | 0.58 |
| 5:A:191:ASP:HB3 | 5:A:194:GLU:HG2 | 1.84 | 0.58 |
| 5:A:296:PRO:HB3 | 5:A:475:LYS:HB2 | 1.84 | 0.58 |
| 6:B:710:ILE:HD12 | 6:B:710:ILE:H | 1.69 | 0.58 |
| 18:N:751:ARG:NH1 | 18:N:1207:CYS:O | 2.36 | 0.58 |
| 24:W:508:ARG:O | 24:W:512:ILE:N | 2.34 | 0.58 |
| 25:X:414:GLU:O | 25:X:418:HIS:ND1 | 2.28 | 0.58 |
| 35:z:540:LEU:O | 35:z:543:ARG:HG3 | 2.02 | 0.58 |
| 35:z:573:LEU:HD22 | 35:z:577:PHE:HE1 | 1.67 | 0.58 |
| 23:U:347:LEU:HA | 23:U:362:THR:H | 1.69 | 0.57 |
| 35:z:74:ILE:HB | 35:z:119:ILE:HA | 1.86 | 0.57 |
| 5:A:1429:LEU:C | 5:A:1431:ASP:H | 2.12 | 0.57 |
| 18:N:745:MET:HE3 | 18:N:1029:PHE:HD1 | 1.69 | 0.57 |
| 25:X:500:ARG:HA | 25:X:500:ARG:CZ | 2.34 | 0.57 |
| 30:c:588:PHE:CD2 | 30:c:596:LEU:HD11 | 2.39 | 0.57 |
| 5:A:48:GLU:OE1 | 5:A:48:GLU:N | 2.27 | 0.57 |
| 6:B:90:ASP:OD2 | 15:K:157:ARG:NH1 | 2.37 | 0.57 |
| 6:B:178:ARG:HB3 | 6:B:181:ASP:OD2 | 2.04 | 0.57 |
| 6:B:225:ASP:HB3 | 6:B:629:PRO:HB2 | 1.86 | 0.57 |
| 6:B:703:VAL:HG12 | 6:B:803:PHE:HA | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:108:LEU:HD11 | 13:I:30:TYR:CE2 | 2.39 | 0.57 |
| 18:N:560:ALA:HB2 | 18:N:587:LEU:HD12 | 1.85 | 0.57 |
| 22:R:241:GLU:O | 22:R:245:ILE:HG12 | 2.05 | 0.57 |
| 23:S:80:TRP:CZ2 | 23:U:69:LEU:HB3 | 2.39 | 0.57 |
| 27:Z:24:ALA:O | 27:Z:28:ILE:HG12 | 2.04 | 0.57 |
| 1:e:181:LYS:NZ | 1:e:182:ASP:O | 2.36 | 0.57 |
| 6:B:154:LYS:NZ | 42:B:1001:GTP:O2G | 2.37 | 0.57 |
| 18:N:1122:TYR:HD1 | 18:N:1276:MET:HE1 | 1.69 | 0.57 |
| 26:Y:91:GLN:OE1 | 26:Y:94:ARG:NH2 | 2.37 | 0.57 |
| 26:Y:178:ARG:NH1 | 38:6:81:U:OP2 | 2.37 | 0.57 |
| 34:y:144:MET:HE2 | 35:z:417:MET:SD | 2.44 | 0.57 |
| 23:U:89:GLU:O | 23:U:92:ARG:HG2 | 2.03 | 0.57 |
| 35:z:282:ASP:OD1 | 35:z:283:GLU:N | 2.37 | 0.57 |
| 5:A:1410:TRP:HH2 | 5:A:1446:LEU:HD21 | 1.70 | 0.57 |
| 5:A:1969:VAL:HG12 | 5:A:1970:ASN:OD1 | 2.04 | 0.57 |
| 7:C:283:PHE:HD1 | 7:C:297:SER:HA | 1.69 | 0.57 |
| 15:K:133:GLN:OE1 | 22:R:199:VAL:HG13 | 2.04 | 0.57 |
| 25:X:141:VAL:HG12 | 25:X:142:THR:HG23 | 1.86 | 0.57 |
| 32:m:534:LEU:HD13 | 32:m:567:ILE:HD11 | 1.86 | 0.57 |
| 39:1:-1:U:H5' | 39:1:0:G:H5" | 1.86 | 0.57 |
| 6:B:793:LEU:HD11 | 6:B:948:LEU:HD11 | 1.87 | 0.57 |
| 6:B:823:ILE:HG13 | 6:B:824:PRO:HD3 | 1.85 | 0.57 |
| 15:K:267:ARG:HG3 | 15:K:291:THR:HG22 | 1.87 | 0.57 |
| 15:K:344:PHE:HB2 | 16:L:140:LYS:HD3 | 1.86 | 0.57 |
| 22:R:609:GLU:HA | 22:R:612:ARG:HD2 | 1.87 | 0.57 |
| 35:z:344:LYS:O | 35:z:348:ILE:HD12 | 2.04 | 0.57 |
| 1:e:183:LYS:HG2 | 1:e:184:SER:N | 2.17 | 0.57 |
| 5:A:728:LYS:NZ | 16:L:249:TRP:O | 2.37 | 0.57 |
| 5:A:863:VAL:O | 5:A:867:GLU:HG3 | 2.05 | 0.57 |
| 7:C:151:LEU:HB2 | 7:C:163:TRP:HB2 | 1.87 | 0.57 |
| 15:K:226:ASP:OD1 | 15:K:228:MET:HG2 | 2.05 | 0.57 |
| 23:S:14:VAL:HG11 | 23:S:28:ILE:HG21 | 1.85 | 0.57 |
| 31:d:8:THR:HG23 | 31:d:11:GLY:H | 1.70 | 0.57 |
| 4:5:96:G:C5 | 12:H:48:PHE:HE2 | 2.23 | 0.57 |
| 5:A:250:ASN:HB2 | 5:A:253:GLN:HG3 | 1.87 | 0.57 |
| 20:P:214:PHE:HE2 | 39:1:11:U:C6 | 2.22 | 0.57 |
| 22:R:9:LYS:NZ | 35:z:257:GLU:OE2 | 2.38 | 0.57 |
| 22:R:158:ARG:NH1 | 22:R:186:GLU:OE2 | 2.37 | 0.57 |
| 5:A:1447:PHE:O | 34:y:227:TYR:HD1 | 1.88 | 0.57 |
| 16:L:289:ALA:HA | 24:W:75:LEU:HD22 | 1.86 | 0.56 |
| 18:N:59:GLU:OE1 | 18:N:85:LYS:NZ | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:183:ARG:HD3 | 26:Y:125:PRO:HG3 | 1.85 | 0.56 |
| 22:R:302:ASP:HA | 22:R:305:ARG:HG2 | 1.87 | 0.56 |
| 25:X:637:LEU:HD23 | 25:X:638:ASN:H | 1.69 | 0.56 |
| 30:c:487:LYS:NZ | 30:c:491:GLU:OE1 | 2.38 | 0.56 |
| 32:m:788:ASN:OD1 | 32:m:789:GLU:N | 2.38 | 0.56 |
| 18:N:917:GLU:O | 18:N:921:MET:HG2 | 2.05 | 0.56 |
| 18:N:958:SER:O | 18:N:962:ARG:NH1 | 2.37 | 0.56 |
| 21:Q:252:ARG:HH11 | 21:Q:252:ARG:HG3 | 1.69 | 0.56 |
| 1:e:257:PRO:O | 30:c:601:ARG:NH2 | 2.39 | 0.56 |
| 5:A:539:LEU:HD11 | 5:A:561:SER:HB2 | 1.88 | 0.56 |
| 5:A:687:HIS:NE2 | 16:L:219:HIS:HB2 | 2.20 | 0.56 |
| 5:A:1239:ASN:HB3 | 5:A:1248:ARG:HD3 | 1.86 | 0.56 |
| 6:B:872:LEU:HD21 | 6:B:888:LEU:HD13 | 1.87 | 0.56 |
| 23:S:111:ALA:O | 23:S:115:ILE:HG12 | 2.05 | 0.56 |
| 25:X:227:VAL:HG21 | 25:X:259:TYR:HD1 | 1.70 | 0.56 |
| 27:Z:60:GLU:O | 27:Z:64:VAL:HG22 | 2.04 | 0.56 |
| 30:c:486:PHE:CD2 | 30:c:521:VAL:HB | 2.41 | 0.56 |
| 35:z:464:CYS:SG | 35:z:568:LYS:HD2 | 2.45 | 0.56 |
| 5:A:718:ASP:OD2 | 15:K:335:ARG:NH1 | 2.39 | 0.56 |
| 5:A:1654:LEU:HD21 | 5:A:1656:LEU:HG | 1.87 | 0.56 |
| 5:A:1917:PHE:HD1 | 5:A:1920:ILE:HD11 | 1.71 | 0.56 |
| 7:C:283:PHE:CD1 | 7:C:297:SER:HA | 2.41 | 0.56 |
| 15:K:346:PHE:HD1 | 15:K:359:PHE:CE1 | 2.24 | 0.56 |
| 15:K:352:ASP:OD1 | 15:K:353:ASN:N | 2.38 | 0.56 |
| 23:S:20:GLY:O | 23:S:21:ASN:ND2 | 2.38 | 0.56 |
| 24:W:521:ARG:O | 24:W:524:LYS:HG2 | 2.05 | 0.56 |
| 25:X:98:PHE:HD1 | 25:X:111:ILE:HG23 | 1.71 | 0.56 |
| 31:d:32:LEU:HD11 | 31:d:37:TYR:CE1 | 2.40 | 0.56 |
| 5:A:1639:HIS:CE1 | 5:A:1718:MET:HE1 | 2.40 | 0.56 |
| 7:C:77:TRP:HH2 | 9:E:99:GLY:HA3 | 1.71 | 0.56 |
| 18:N:25:VAL:O | 18:N:65:ARG:NH2 | 2.38 | 0.56 |
| 22:R:55:LYS:O | 22:R:58:GLU:HG2 | 2.06 | 0.56 |
| 24:W:257:ILE:O | 24:W:261:ILE:HG12 | 2.05 | 0.56 |
| 5:A:932:TYR:HB2 | 5:A:1056:GLY:HA3 | 1.87 | 0.56 |
| 5:A:1684:TYR:HA | 5:A:1723:THR:O | 2.06 | 0.56 |
| 6:B:162:VAL:HG21 | 6:B:179:TYR:CD2 | 2.41 | 0.56 |
| 22:R:281:LYS:C | 22:R:285:HIS:HD1 | 2.14 | 0.56 |
| 23:S:43:GLN:NE2 | 23:S:44:GLU:OE1 | 2.39 | 0.56 |
| 23:S:80:TRP:CH2 | 23:U:69:LEU:HB3 | 2.41 | 0.56 |
| 35:z:211:PHE:CD2 | 35:z:368:GLU:HG3 | 2.40 | 0.56 |
| 35:z:401:ASN:HB2 | 35:z:404:GLN:OE1 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:678:GLU:HG2 | 6:B:793:LEU:HB3 | 1.88 | 0.56 |
| 15:K:358:LYS:NZ | 15:K:361:GLU:OE2 | 2.39 | 0.56 |
| 18:N:748:GLY:HA3 | 18:N:1042:LEU:HD12 | 1.88 | 0.56 |
| 18:N:1116:ALA:HB1 | 18:N:1182:ILE:HD12 | 1.87 | 0.56 |
| 20:P:136:ARG:HH12 | 20:P:139:LYS:HG2 | 1.70 | 0.56 |
| 23:S:94:LEU:HD13 | 23:V:90:LEU:HD23 | 1.88 | 0.56 |
| 24:W:132:SER:O | 24:W:135:ARG:HG2 | 2.05 | 0.56 |
| 35:z:249:ILE:O | 35:z:253:ILE:HG12 | 2.05 | 0.56 |
| 35:z:621:GLU:HG2 | 35:z:626:ILE:HG13 | 1.87 | 0.56 |
| 2:p:167:LYS:HD3 | 2:p:170:ARG:NH1 | 2.20 | 0.56 |
| 2:p:176:GLU:OE1 | 24:W:63:ARG:NH1 | 2.38 | 0.56 |
| 5:A:1892:MET:O | 5:A:1895:PRO:HD2 | 2.04 | 0.56 |
| 6:B:953:ARG:NE | 6:B:959:GLU:OE2 | 2.23 | 0.56 |
| 7:C:328:CYS:HA | 7:C:334:ILE:HG22 | 1.88 | 0.56 |
| 16:L:122:ARG:NH2 | 16:L:130:ARG:O | 2.39 | 0.56 |
| 16:L:319:LYS:HD3 | 16:L:322:GLN:HE21 | 1.69 | 0.56 |
| 20:P:89:SER:O | 20:P:90:GLN:C | 2.48 | 0.56 |
| 24:W:507:ASP:N | 25:X:529:TYR:O | 2.38 | 0.56 |
| 35:z:163:LYS:NZ | 35:z:189:PHE:O | 2.23 | 0.56 |
| 35:z:393:PHE:O | 35:z:397:LEU:HG | 2.05 | 0.56 |
| 20:P:292:ASN:HD21 | 20:P:293:ARG:HH11 | 1.54 | 0.56 |
| 24:W:149:LEU:HD13 | 35:z:261:ILE:HG21 | 1.86 | 0.56 |
| 25:X:178:ILE:HA | 25:X:181:TYR:CE1 | 2.40 | 0.56 |
| 38:6:74:U:H4' | 38:6:75:G:OP1 | 2.05 | 0.56 |
| 5:A:140:LEU:HD12 | 5:A:506:GLN:O | 2.06 | 0.56 |
| 5:A:1423:GLN:HG3 | 5:A:1425:ARG:HG2 | 1.87 | 0.56 |
| 6:B:336:ALA:O | 6:B:340:ILE:HG12 | 2.05 | 0.56 |
| 6:B:657:ASP:HA | 6:B:661:LEU:HD23 | 1.88 | 0.56 |
| 11:G:25:PHE:CE1 | 11:G:60:PHE:HE1 | 2.23 | 0.56 |
| 15:K:183:GLY:HA2 | 15:K:207:THR:HG23 | 1.88 | 0.56 |
| 18:N:332:ARG:NH1 | 18:N:379:ASN:OD1 | 2.27 | 0.56 |
| 18:N:411:GLU:OE1 | 18:N:1021:ASN:ND2 | 2.39 | 0.56 |
| 35:z:143:VAL:HB | 35:z:172:PHE:HZ | 1.71 | 0.56 |
| 38:6:38:G:O2' | 39:1:3:A:N6 | 2.38 | 0.56 |
| 7:C:98:ASP:OD1 | 7:C:99:LEU:N | 2.39 | 0.55 |
| 10:F:61:ARG:HH21 | 10:F:63:ASN:HD22 | 1.54 | 0.55 |
| 17:M:46:ILE:HG23 | 17:M:113:ARG:HE | 1.71 | 0.55 |
| 18:N:306:LEU:HD13 | 18:N:381:TYR:OH | 2.06 | 0.55 |
| 22:R:20:ALA:N | 24:W:15:GLU:OE2 | 2.38 | 0.55 |
| 23:S:38:ASP:OD2 | 23:S:41:THR:OG1 | 2.23 | 0.55 |
| 27:Z:153:LYS:HD3 | 27:Z:156:GLN:NE2 | 2.09 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1635:LYS:NZ | 5:A:1636:GLU:O | 2.37 | 0.55 |
| 6:B:706:LEU:HD23 | 6:B:710:ILE:HB | 1.88 | 0.55 |
| 7:C:269:GLU:OE1 | 7:C:269:GLU:N | 2.35 | 0.55 |
| 18:N:741:PRO:HA | 18:N:1004:ARG:HG2 | 1.88 | 0.55 |
| 23:T:25:LYS:O | 23:T:29:GLU:HG2 | 2.05 | 0.55 |
| 23:T:27:LEU:O | 23:T:30:GLN:HG2 | 2.06 | 0.55 |
| 25:X:448:ARG:HH12 | 25:X:498:THR:HG21 | 1.71 | 0.55 |
| 25:X:680:ALA:O | 25:X:684:TYR:HD1 | 1.89 | 0.55 |
| 6:B:267:LEU:HB3 | 6:B:319:VAL:HG22 | 1.88 | 0.55 |
| 15:K:344:PHE:CE2 | 15:K:360:PRO:HD3 | 2.42 | 0.55 |
| 18:N:299:ASP:HB3 | 18:N:383:ARG:HH12 | 1.71 | 0.55 |
| 22:R:294:LEU:HD23 | 22:R:298:SER:HB3 | 1.89 | 0.55 |
| 23:S:103:THR:HA | 23:S:106:TYR:CE2 | 2.42 | 0.55 |
| 28:a:106:ASN:C | 28:a:106:ASN:ND2 | 2.65 | 0.55 |
| 5:A:664:LEU:HA | 5:A:667:ILE:HG22 | 1.89 | 0.55 |
| 5:A:1841:LEU:N | 5:A:1941:PHE:O | 2.39 | 0.55 |
| 7:C:218:HIS:CE1 | 7:C:244:ARG:HG3 | 2.41 | 0.55 |
| 10:F:19:LEU:HD21 | 10:F:60:ILE:HD12 | 1.87 | 0.55 |
| 13:I:12:LEU:HD12 | 13:I:41:MET:HE2 | 1.86 | 0.55 |
| 16:L:188:PRO:HB3 | 17:M:24:GLU:OE2 | 2.06 | 0.55 |
| 20:P:196:ALA:HA | 20:P:201:ILE:HD11 | 1.89 | 0.55 |
| 22:R:121:ASN:HA | 22:R:124:ARG:HG2 | 1.88 | 0.55 |
| 22:R:237:GLU:HG2 | 22:R:238:PHE:HD1 | 1.71 | 0.55 |
| 5:A:1660:LYS:HZ1 | 5:A:1680:THR:C | 2.14 | 0.55 |
| 16:L:205:VAL:HG23 | 17:M:36:THR:HG22 | 1.88 | 0.55 |
| 18:N:522:ASN:HA | 18:N:525:LYS:HE3 | 1.87 | 0.55 |
| 22:R:50:GLU:CD | 22:R:54:ARG:HH21 | 2.15 | 0.55 |
| 24:W:739:MET:SD | 24:W:742:ILE:HD11 | 2.46 | 0.55 |
| 32:m:779:ASP:N | 32:m:779:ASP:OD1 | 2.39 | 0.55 |
| 5:A:1801:GLN:HE22 | 5:A:1883:ARG:HB2 | 1.71 | 0.55 |
| 15:K:184:ASP:OD1 | 15:K:186:THR:OG1 | 2.21 | 0.55 |
| 23:T:115:ILE:HG22 | 23:U:115:ILE:HD11 | 1.89 | 0.55 |
| 9:E:23:THR:HB | 9:E:45:TYR:HB2 | 1.89 | 0.55 |
| 10:F:78:THR:O | 10:F:81:ILE:HG22 | 2.06 | 0.55 |
| 23:U:342:HIS:CD2 | 23:U:343:PRO:HD2 | 2.40 | 0.55 |
| 25:X:627:ILE:HA | 25:X:630:VAL:HG22 | 1.89 | 0.55 |
| 25:X:681:ARG:O | 25:X:685:ILE:HD12 | 2.06 | 0.55 |
| 27:Z:150:ARG:HE | 28:a:33:ALA:HA | 1.70 | 0.55 |
| 32:m:296:LYS:HZ3 | 33:n:313:GLU:HG3 | 1.71 | 0.55 |
| 15:K:96:ILE:HG21 | 22:R:228:LEU:HB3 | 1.88 | 0.55 |
| 18:N:52:LEU:HD22 | 18:N:57:LEU:HD13 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:694:ARG:NH2 | 25:X:728:GLN:OE1 | 2.40 | 0.55 |
| 27:Z:138:LEU:O | 27:Z:142:LYS:HG2 | 2.07 | 0.55 |
| 29:b:134:GLN:O | 29:b:138:GLU:HG2 | 2.07 | 0.55 |
| 6:B:149:HIS:CG | 6:B:150:LEU:H | 2.24 | 0.55 |
| 10:F:61:ARG:HH21 | 10:F:63:ASN:ND2 | 2.04 | 0.55 |
| 10:F:72:ASP:OD1 | 11:G:97:SER:OG | 2.24 | 0.55 |
| 16:L:289:ALA:O | 16:L:293:GLU:HG2 | 2.07 | 0.55 |
| 18:N:663:ASN:O | 18:N:740:GLN:NE2 | 2.37 | 0.55 |
| 20:P:127:GLU:HG2 | 20:P:131:CYS:HB2 | 1.88 | 0.55 |
| 27:Z:89:ARG:HA | 27:Z:92:LEU:HD13 | 1.89 | 0.55 |
| 34:y:65:PHE:H | 34:y:67:THR:HG22 | 1.70 | 0.55 |
| 35:z:59:PRO:HA | 35:z:62:LEU:CD2 | 2.36 | 0.55 |
| 5:A:1434:ASP:OD1 | 5:A:1435:SER:N | 2.39 | 0.55 |
| 17:M:232:PHE:HD1 | 17:M:235:TYR:HD2 | 1.54 | 0.55 |
| 18:N:498:PRO:HG2 | 18:N:589:PRO:HB3 | 1.88 | 0.55 |
| 4:5:49:U:H2' | 4:5:50:U:C6 | 2.41 | 0.54 |
| 16:L:91:LEU:HD12 | 16:L:92:ALA:H | 1.72 | 0.54 |
| 29:b:134:GLN:HA | 29:b:137:LYS:HE2 | 1.89 | 0.54 |
| 32:m:611:ALA:HA | 32:m:615:PHE:HD2 | 1.72 | 0.54 |
| 34:y:127:ASP:N | 34:y:131:ARG:HH21 | 2.04 | 0.54 |
| 35:z:107:ILE:HG13 | 35:z:110:ASP:HB3 | 1.88 | 0.54 |
| 7:C:85:ASN:HD22 | 9:E:99:GLY:H | 1.55 | 0.54 |
| 7:C:154:VAL:HB | 7:C:180:LEU:HB2 | 1.88 | 0.54 |
| 11:G:44:LEU:HB3 | 11:G:110:VAL:CG2 | 2.38 | 0.54 |
| 12:H:49:MET:HE2 | 14:J:63:ARG:HD2 | 1.88 | 0.54 |
| 17:M:42:GLN:HB2 | 17:M:53:ILE:HD11 | 1.89 | 0.54 |
| 18:N:850:SER:O | 18:N:853:THR:OG1 | 2.23 | 0.54 |
| 20:P:311:ASP:OD1 | 20:P:312:LEU:N | 2.40 | 0.54 |
| 32:m:515:LEU:HD23 | 32:m:519:ALA:HA | 1.88 | 0.54 |
| 35:z:216:THR:OG1 | 35:z:222:SER:OG | 2.21 | 0.54 |
| 35:z:229:ASN:O | 35:z:233:THR:OG1 | 2.25 | 0.54 |
| 1:e:227:GLN:NE2 | 1:e:231:GLU:OE2 | 2.37 | 0.54 |
| 5:A:1714:ASP:OD2 | 5:A:1716:GLN:NE2 | 2.40 | 0.54 |
| 6:B:206:LYS:HE3 | 8:D:9:HIS:CD2 | 2.41 | 0.54 |
| 12:H:41:GLN:HB2 | 12:H:54:ASP:HB2 | 1.88 | 0.54 |
| 12:H:41:GLN:O | 12:H:54:ASP:N | 2.40 | 0.54 |
| 18:N:252:TYR:OH | 18:N:256:ARG:NH1 | 2.40 | 0.54 |
| 18:N:696:LEU:N | 18:N:711:THR:O | 2.36 | 0.54 |
| 23:T:109:ASP:O | 23:T:113:ARG:HG3 | 2.08 | 0.54 |
| 24:W:132:SER:OG | 24:W:135:ARG:NH1 | 2.40 | 0.54 |
| 24:W:521:ARG:O | 24:W:524:LYS:NZ | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:445:ASP:HB2 | 25:X:449:LYS:NZ | 2.23 | 0.54 |
| 27:Z:64:VAL:HG23 | 27:Z:68:LYS:NZ | 2.22 | 0.54 |
| 35:z:170:ASN:O | 35:z:173:ARG:NH1 | 2.40 | 0.54 |
| 5:A:620:ARG:HD3 | 5:A:623:ARG:NH2 | 2.23 | 0.54 |
| 5:A:810:GLU:OE2 | 5:A:814:GLN:NE2 | 2.32 | 0.54 |
| 11:G:93:ASP:OD1 | 11:G:94:ARG:N | 2.38 | 0.54 |
| 15:K:109:GLN:HA | 15:K:133:GLN:NE2 | 2.23 | 0.54 |
| 23:T:112:LEU:HA | 23:T:115:ILE:HG12 | 1.90 | 0.54 |
| 25:X:635:VAL:HG11 | 25:X:644:THR:HG22 | 1.90 | 0.54 |
| 31:d:3:ASN:HD22 | 31:d:155:LEU:HG | 1.70 | 0.54 |
| 32:m:452:GLN:NE2 | 32:m:502:ASP:OD1 | 2.40 | 0.54 |
| 38:6:52:G:H2' | 38:6:53:G:C8 | 2.42 | 0.54 |
| 5:A:67:GLY:HA3 | 5:A:70:ARG:HD2 | 1.88 | 0.54 |
| 17:M:232:PHE:CE2 | 17:M:252:VAL:HG11 | 2.43 | 0.54 |
| 18:N:1151:SER:HA | 18:N:1155:SER:HB3 | 1.90 | 0.54 |
| 20:P:118:LEU:HA | 20:P:151:PHE:CZ | 2.43 | 0.54 |
| 24:W:536:ILE:HG22 | 24:W:537:ARG:N | 2.16 | 0.54 |
| 25:X:243:ARG:NH1 | 25:X:279:GLU:OE1 | 2.38 | 0.54 |
| 25:X:637:LEU:HD23 | 25:X:638:ASN:N | 2.22 | 0.54 |
| 35:z:423:LEU:HD22 | 35:z:428:VAL:HG11 | 1.89 | 0.54 |
| 4:5:29:U:H4' | 4:5:30:A:H5' | 1.89 | 0.54 |
| 5:A:1268:ILE:HG21 | 5:A:1315:CYS:HB2 | 1.90 | 0.54 |
| 5:A:1663:VAL:HG11 | 5:A:1741:ASN:HB3 | 1.88 | 0.54 |
| 5:A:1799:GLN:HA | 34:y:133:PHE:CD2 | 2.42 | 0.54 |
| 6:B:701:MET:HE2 | 6:B:805:LEU:HD13 | 1.88 | 0.54 |
| 6:B:739:ASP:OD2 | 29:b:66:LYS:HD3 | 2.08 | 0.54 |
| 11:G:42:GLN:HB2 | 11:G:112:ILE:HB | 1.90 | 0.54 |
| 18:N:151:ILE:HG12 | 18:N:245:VAL:HG21 | 1.89 | 0.54 |
| 35:z:392:LEU:HD11 | 35:z:450:ALA:HB2 | 1.89 | 0.54 |
| 2:p:211:LEU:HD21 | 25:X:713:PRO:HB3 | 1.89 | 0.54 |
| 5:A:1653:ILE:HD11 | 5:A:1686:ILE:HB | 1.89 | 0.54 |
| 13:I:52:VAL:O | 13:I:55:VAL:HG22 | 2.08 | 0.54 |
| 18:N:798:HIS:NE2 | 18:N:924:GLN:HG2 | 2.23 | 0.54 |
| 20:P:268:ASN:O | 20:P:272:LYS:NZ | 2.39 | 0.54 |
| 34:y:138:ASP:OD2 | 35:z:417:MET:HE2 | 2.08 | 0.54 |
| 35:z:243:LEU:HD12 | 35:z:249:ILE:HD13 | 1.89 | 0.54 |
| 3:2:30:A:C5 | 34:y:37:PRO:HD2 | 2.42 | 0.54 |
| 5:A:216:ASP:HB3 | 5:A:219:ASP:HB3 | 1.90 | 0.54 |
| 5:A:1063:ILE:HA | 5:A:1066:PHE:CE1 | 2.42 | 0.54 |
| 18:N:777:LEU:O | 18:N:979:MET:N | 2.40 | 0.54 |
| 23:V:105:LEU:O | 23:V:108:LEU:HG | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:485:TYR:O | 25:X:489:LEU:HG | 2.07 | 0.54 |
| 5:A:365:ASP:OD1 | 5:A:366:LEU:N | 2.41 | 0.54 |
| 5:A:862:LEU:HD22 | 5:A:901:LEU:HG | 1.90 | 0.54 |
| 17:M:84:MET:HB2 | 20:P:146:ALA:HB3 | 1.90 | 0.54 |
| 18:N:8:LYS:HE3 | 18:N:51:LEU:HD13 | 1.89 | 0.54 |
| 18:N:73:ASN:HA | 18:N:76:ASN:ND2 | 2.23 | 0.54 |
| 18:N:485:VAL:HG22 | 18:N:503:CYS:SG | 2.48 | 0.54 |
| 23:U:399:ASP:HB2 | 23:U:414:ILE:O | 2.08 | 0.54 |
| 25:X:541:VAL:HG21 | 25:X:553:TRP:CE2 | 2.43 | 0.54 |
| 25:X:577:GLU:HA | 25:X:580:LEU:HG | 1.89 | 0.54 |
| 32:m:358:ASP:N | 32:m:358:ASP:OD1 | 2.41 | 0.54 |
| 34:y:31:ARG:NH2 | 35:z:497:SER:OG | 2.41 | 0.54 |
| 35:z:245:GLY:HA3 | 35:z:324:LYS:CD | 2.37 | 0.54 |
| 5:A:869:LEU:HD23 | 5:A:886:GLU:OE2 | 2.08 | 0.54 |
| 15:K:92:SER:HA | 15:K:95:VAL:HG12 | 1.89 | 0.54 |
| 16:L:237:PRO:HD3 | 22:R:136:ARG:HH12 | 1.73 | 0.54 |
| 22:R:248:ALA:HA | 22:R:263:ILE:HD11 | 1.90 | 0.54 |
| 22:R:261:ARG:O | 22:R:265:LYS:HG2 | 2.08 | 0.54 |
| 22:R:599:TRP:CH2 | 22:R:615:VAL:HG22 | 2.43 | 0.54 |
| 23:V:118:LEU:HD21 | 23:V:122:ARG:NH1 | 2.23 | 0.54 |
| 5:A:363:ASP:N | 5:A:363:ASP:OD1 | 2.41 | 0.53 |
| 5:A:635:ILE:HD11 | 5:A:655:PRO:HG2 | 1.89 | 0.53 |
| 7:C:46:MET:HB3 | 7:C:334:ILE:HG13 | 1.88 | 0.53 |
| 18:N:773:ARG:HB2 | 18:N:973:PHE:HA | 1.90 | 0.53 |
| 20:P:213:ALA:C | 20:P:214:PHE:HD1 | 2.15 | 0.53 |
| 24:W:159:GLU:OE1 | 24:W:159:GLU:N | 2.38 | 0.53 |
| 5:A:1622:ASP:OD2 | 34:y:86:ASN:ND2 | 2.41 | 0.53 |
| 7:C:325:ILE:HG22 | 7:C:337:GLY:HA3 | 1.91 | 0.53 |
| 30:c:512:LEU:HD22 | 30:c:519:TRP:CD1 | 2.43 | 0.53 |
| 9:E:95:LEU:HD12 | 9:E:96:SER:N | 2.23 | 0.53 |
| 10:F:7:LEU:HB3 | 10:F:32:VAL:HG11 | 1.91 | 0.53 |
| 12:H:18:LYS:O | 12:H:22:GLN:HG2 | 2.09 | 0.53 |
| 12:H:82:GLN:HE22 | 14:J:57:ILE:HD12 | 1.74 | 0.53 |
| 18:N:58:PHE:HA | 18:N:62:LEU:HG | 1.90 | 0.53 |
| 23:V:10:PRO:HG2 | 23:V:13:PRO:HG3 | 1.89 | 0.53 |
| 23:V:30:GLN:NE2 | 23:V:34:GLU:OE2 | 2.30 | 0.53 |
| 24:W:594:ASN:O | 24:W:598:GLU:HG3 | 2.08 | 0.53 |
| 31:d:27:GLN:O | 31:d:31:THR:HG22 | 2.09 | 0.53 |
| 35:z:153:LEU:HD12 | 35:z:382:ILE:HG13 | 1.90 | 0.53 |
| 35:z:367:THR:HG22 | 35:z:369:LYS:H | 1.72 | 0.53 |
| 5:A:636:TYR:HE1 | 5:A:650:CYS:HB3 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:102:ARG:HH11 | 11:G:104:ASP:HB2 | 1.74 | 0.53 |
| 16:L:202:ILE:HD12 | 17:M:19:PHE:CZ | 2.43 | 0.53 |
| 18:N:836:ARG:HH22 | 18:N:894:LYS:HB2 | 1.74 | 0.53 |
| 23:S:29:GLU:HG3 | 23:S:33:ARG:HH21 | 1.72 | 0.53 |
| 35:z:225:GLU:OE2 | 35:z:229:ASN:ND2 | 2.41 | 0.53 |
| 35:z:456:LEU:O | 35:z:459:SER:OG | 2.25 | 0.53 |
| 38:6:6:U:O2' | 38:6:7:C:O5' | 2.24 | 0.53 |
| 4:5:77:G:OP1 | 19:O:93:LYS:NZ | 2.39 | 0.53 |
| 15:K:148:GLU:OE1 | 15:K:148:GLU:N | 2.42 | 0.53 |
| 16:L:183:TYR:OH | 28:a:96:ASN:OD1 | 2.13 | 0.53 |
| 18:N:399:LYS:HA | 18:N:402:LEU:HD12 | 1.89 | 0.53 |
| 18:N:666:TYR:HB2 | 18:N:768:THR:HA | 1.90 | 0.53 |
| 22:R:302:ASP:O | 22:R:305:ARG:HG2 | 2.09 | 0.53 |
| 23:U:14:VAL:HG12 | 23:U:51:VAL:HB | 1.89 | 0.53 |
| 24:W:236:TYR:CD1 | 26:Y:156:VAL:HG13 | 2.44 | 0.53 |
| 24:W:623:PHE:CZ | 24:W:627:TYR:CZ | 2.96 | 0.53 |
| 25:X:238:VAL:O | 25:X:242:PHE:HD2 | 1.92 | 0.53 |
| 34:y:114:SER:O | 35:z:643:TYR:OH | 2.22 | 0.53 |
| 5:A:978:TRP:HZ2 | 5:A:1112:THR:HB | 1.73 | 0.53 |
| 6:B:242:ASP:CG | 6:B:271:LYS:HD2 | 2.33 | 0.53 |
| 17:M:238:LEU:O | 17:M:255:LYS:NZ | 2.41 | 0.53 |
| 18:N:737:ARG:HD3 | 18:N:1040:ILE:HD11 | 1.90 | 0.53 |
| 25:X:398:ARG:NH2 | 25:X:437:MET:HA | 2.23 | 0.53 |
| 5:A:715:ASP:O | 5:A:719:MET:HG2 | 2.08 | 0.53 |
| 11:G:45:ILE:HB | 11:G:53:LEU:HB2 | 1.91 | 0.53 |
| 20:P:177:TYR:HD1 | 20:P:214:PHE:CE1 | 2.25 | 0.53 |
| 20:P:316:ASP:OD1 | 20:P:317:GLY:N | 2.33 | 0.53 |
| 22:R:59:PHE:HD2 | 22:R:76:TYR:CD1 | 2.27 | 0.53 |
| 25:X:84:PRO:HG2 | 25:X:122:GLN:HG2 | 1.89 | 0.53 |
| 38:6:37:A:O2' | 38:6:38:G:OP1 | 2.27 | 0.53 |
| 15:K:89:GLU:OE1 | 15:K:89:GLU:N | 2.42 | 0.53 |
| 18:N:240:ARG:HA | 18:N:284:ASN:HB3 | 1.91 | 0.53 |
| 18:N:686:VAL:HG13 | 18:N:690:LEU:HD13 | 1.91 | 0.53 |
| 18:N:809:GLY:HA2 | 18:N:814:LEU:HD12 | 1.90 | 0.53 |
| 20:P:213:ALA:O | 20:P:214:PHE:HD1 | 1.91 | 0.53 |
| 6:B:821:GLN:HG3 | 32:m:727:ALA:HB1 | 1.91 | 0.53 |
| 15:K:344:PHE:HE2 | 15:K:360:PRO:HD3 | 1.73 | 0.53 |
| 18:N:264:ASN:HB3 | 18:N:267:PHE:HB3 | 1.91 | 0.53 |
| 18:N:360:PHE:HB3 | 18:N:366:ILE:HD12 | 1.89 | 0.53 |
| 19:O:26:PHE:HE1 | 19:O:55:GLN:HG2 | 1.74 | 0.53 |
| 23:T:69:LEU:HB2 | 23:T:70:PRO:CD | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:T:90:LEU:HD13 | 23:U:90:LEU:HD22 | 1.89 | 0.53 |
| 23:U:117:ARG:HG3 | 23:U:118:LEU:N | 2.24 | 0.53 |
| 23:V:5:ILE:HD11 | 23:V:23:TYR:HD1 | 1.74 | 0.53 |
| 5:A:1856:ARG:HD2 | 5:A:1856:ARG:O | 2.09 | 0.53 |
| 6:B:249:ILE:HB | 6:B:849:GLU:OE1 | 2.08 | 0.53 |
| 7:C:41:VAL:HG11 | 9:E:103:PRO:HB3 | 1.91 | 0.53 |
| 7:C:46:MET:HE2 | 7:C:77:TRP:CH2 | 2.44 | 0.53 |
| 13:I:26:TRP:HZ3 | 13:I:69:ASN:ND2 | 2.07 | 0.53 |
| 24:W:743:GLU:OE2 | 27:Z:176:SER:OG | 2.25 | 0.53 |
| 5:A:386:HIS:CE1 | 6:B:311:ARG:HG3 | 2.45 | 0.52 |
| 5:A:1080:ARG:NH1 | 5:A:1083:GLU:OE1 | 2.34 | 0.52 |
| 5:A:1576:GLN:HG2 | 5:A:1587:HIS:CE1 | 2.43 | 0.52 |
| 7:C:314:ASN:N | 7:C:328:CYS:O | 2.40 | 0.52 |
| 18:N:749:PRO:HA | 18:N:1010:ASN:HD22 | 1.73 | 0.52 |
| 20:P:181:ILE:HG13 | 20:P:183:PRO:HD3 | 1.91 | 0.52 |
| 22:R:70:MET:O | 22:R:74:MET:HG2 | 2.09 | 0.52 |
| 24:W:47:ARG:HB2 | 24:W:144:GLU:OE1 | 2.09 | 0.52 |
| 29:b:57:HIS:O | 29:b:61:ARG:HG3 | 2.09 | 0.52 |
| 39:1:0:G:H1' | 39:1:1:G:OP2 | 2.09 | 0.52 |
| 6:B:930:ILE:HG22 | 6:B:932:PRO:HD3 | 1.91 | 0.52 |
| 11:G:7:LYS:N | 11:G:8:PRO:HD3 | 2.24 | 0.52 |
| 16:L:275:ASP:HB3 | 16:L:277:ARG:HH11 | 1.74 | 0.52 |
| 16:L:289:ALA:HA | 24:W:75:LEU:CD2 | 2.39 | 0.52 |
| 32:m:434:MET:O | 32:m:439:LYS:N | 2.39 | 0.52 |
| 32:m:447:LYS:NZ | 32:m:480:ASP:OD1 | 2.40 | 0.52 |
| 5:A:921:PHE:HD2 | 5:A:928:LEU:HB3 | 1.73 | 0.52 |
| 6:B:575:LYS:NZ | 6:B:625:ASN:O | 2.41 | 0.52 |
| 18:N:307:GLN:HG3 | 18:N:311:PHE:CZ | 2.44 | 0.52 |
| 18:N:823:TRP:HE1 | 18:N:931:PHE:HE2 | 1.57 | 0.52 |
| 24:W:704:LEU:HD21 | 24:W:708:ARG:HH21 | 1.73 | 0.52 |
| 25:X:470:LEU:O | 25:X:475:ARG:NE | 2.39 | 0.52 |
| 25:X:497:GLU:CD | 25:X:497:GLU:H | 2.17 | 0.52 |
| 30:c:417:TYR:HB2 | 30:c:449:MET:CE | 2.39 | 0.52 |
| 38:6:49:C:OP2 | 38:6:68:U:O2' | 2.23 | 0.52 |
| 5:A:1960:LEU:HA | 5:A:1963:ILE:HD12 | 1.91 | 0.52 |
| 6:B:140:ASP:OD1 | 6:B:208:LYS:NZ | 2.40 | 0.52 |
| 7:C:53:VAL:O | 7:C:314:ASN:ND2 | 2.38 | 0.52 |
| 7:C:113:SER:HA | 7:C:137:VAL:HG13 | 1.91 | 0.52 |
| 10:F:11:THR:HA | 10:F:29:ILE:HD11 | 1.91 | 0.52 |
| 11:G:46:ASN:HB3 | 11:G:52:LYS:NZ | 2.24 | 0.52 |
| 11:G:90:ILE:HG13 | 11:G:92:LYS:HZ3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:N:982:GLN:O | 18:N:1027:SER:OG | 2.25 | 0.52 |
| 18:N:1143:VAL:HG13 | 18:N:1166:VAL:HG12 | 1.91 | 0.52 |
| 24:W:537:ARG:HG3 | 24:W:538:PRO:CD | 2.40 | 0.52 |
| 25:X:597:ASP:O | 25:X:601:LYS:HG2 | 2.09 | 0.52 |
| 38:6:13:A:O2' | 38:6:14:C:OP1 | 2.28 | 0.52 |
| 5:A:312:TRP:CD1 | 5:A:314:GLU:H | 2.27 | 0.52 |
| 5:A:1150:ASN:O | 5:A:1176:ARG:NH2 | 2.43 | 0.52 |
| 5:A:1406:SER:HA | 5:A:1439:GLY:HA2 | 1.90 | 0.52 |
| 18:N:213:GLU:OE1 | 18:N:218:LYS:HD2 | 2.10 | 0.52 |
| 18:N:318:LEU:HB2 | 18:N:322:VAL:HG23 | 1.92 | 0.52 |
| 18:N:449:LEU:HD13 | 18:N:557:PHE:HZ | 1.75 | 0.52 |
| 22:R:215:GLU:OE2 | 22:R:253:ARG:NE | 2.42 | 0.52 |
| 23:S:118:LEU:O | 23:S:122:ARG:HD3 | 2.10 | 0.52 |
| 24:W:262:ARG:HA | 24:W:265:GLU:CD | 2.35 | 0.52 |
| 30:c:579:ARG:HA | 30:c:582:ARG:HH21 | 1.75 | 0.52 |
| 4:5:38:U:P | 5:A:623:ARG:HH21 | 2.33 | 0.52 |
| 4:5:100:U:C2 | 10:F:35:GLN:NE2 | 2.76 | 0.52 |
| 6:B:370:LYS:O | 6:B:370:LYS:NZ | 2.27 | 0.52 |
| 15:K:373:ALA:HB1 | 15:K:392:ASN:HD21 | 1.75 | 0.52 |
| 18:N:137:GLU:HA | 18:N:140:ARG:HG3 | 1.90 | 0.52 |
| 18:N:787:LEU:O | 18:N:791:LEU:HG | 2.09 | 0.52 |
| 22:R:524:ARG:HG2 | 22:R:543:PHE:HE1 | 1.75 | 0.52 |
| 23:T:88:PHE:O | 23:T:92:ARG:HG2 | 2.10 | 0.52 |
| 27:Z:27:GLN:HA | 27:Z:30:GLU:HG3 | 1.91 | 0.52 |
| 31:d:52:ILE:HD11 | 31:d:106:LEU:HD11 | 1.92 | 0.52 |
| 32:m:362:VAL:HG11 | 32:m:429:HIS:CE1 | 2.45 | 0.52 |
| 32:m:718:PHE:CE2 | 32:m:764:LEU:HD22 | 2.44 | 0.52 |
| 5:A:874:SER:OG | 5:A:876:LYS:NZ | 2.28 | 0.52 |
| 6:B:916:ASP:OD2 | 6:B:917:HIS:ND1 | 2.38 | 0.52 |
| 20:P:106:THR:HG23 | 20:P:108:ALA:H | 1.75 | 0.52 |
| 25:X:96:ASP:O | 25:X:99:GLU:HG3 | 2.10 | 0.52 |
| 25:X:490:GLU:OE2 | 25:X:499:THR:OG1 | 2.27 | 0.52 |
| 28:a:69:PRO:HD3 | 31:d:53:GLN:OE1 | 2.10 | 0.52 |
| 5:A:1548:SER:O | 5:A:1552:GLN:HG2 | 2.10 | 0.52 |
| 7:C:121:ASP:HB2 | 7:C:128:ILE:HD11 | 1.91 | 0.52 |
| 15:K:346:PHE:HD1 | 15:K:359:PHE:HE1 | 1.57 | 0.52 |
| 18:N:18:ASN:HA | 18:N:25:VAL:HG21 | 1.92 | 0.52 |
| 18:N:117:LEU:HD11 | 18:N:205:LYS:HB3 | 1.92 | 0.52 |
| 22:R:116:LYS:HZ1 | 26:Y:172:ILE:HG22 | 1.74 | 0.52 |
| 32:m:488:ALA:HA | 32:m:491:LYS:HE3 | 1.92 | 0.52 |
| 32:m:535:SER:OG | 32:m:536:PRO:HD3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1286:LYS:HG3 | 34:y:213:GLU:OE1 | 2.10 | 0.52 |
| 6:B:179:TYR:O | 6:B:180:THR:OG1 | 2.19 | 0.52 |
| 6:B:960:ASP:OD1 | 6:B:961:VAL:N | 2.42 | 0.52 |
| 15:K:231:CYS:HB3 | 15:K:241:ARG:HB2 | 1.92 | 0.52 |
| 16:L:92:ALA:HB1 | 16:L:102:ASP:H | 1.75 | 0.52 |
| 17:M:84:MET:HG2 | 20:P:147:ASN:HB3 | 1.91 | 0.52 |
| 18:N:1177:ARG:NH2 | 18:N:1209:TYR:OH | 2.43 | 0.52 |
| 25:X:263:TYR:CZ | 25:X:267:ILE:HD11 | 2.45 | 0.52 |
| 32:m:300:ILE:HD11 | 33:n:310:ILE:HD12 | 1.92 | 0.52 |
| 32:m:362:VAL:HG11 | 32:m:429:HIS:ND1 | 2.25 | 0.52 |
| 35:z:412:PRO:HB2 | 35:z:415:HIS:CD2 | 2.39 | 0.52 |
| 5:A:1256:VAL:HG22 | 5:A:1298:TYR:CD1 | 2.45 | 0.52 |
| 6:B:105:ILE:HD11 | 15:K:199:LEU:CD2 | 2.40 | 0.52 |
| 13:I:30:TYR:CE1 | 13:I:50:GLU:HG2 | 2.45 | 0.52 |
| 17:M:75:ARG:HG3 | 17:M:75:ARG:HH11 | 1.74 | 0.52 |
| 30:c:409:LEU:O | 30:c:413:ARG:HG3 | 2.10 | 0.52 |
| 38:6:47:A:H5" | 38:6:47:A:C8 | 2.44 | 0.52 |
| 4:5:18:U:OP1 | 5:A:243:THR:OG1 | 2.24 | 0.51 |
| 5:A:389:ASP:N | 5:A:389:ASP:OD1 | 2.43 | 0.51 |
| 5:A:754:LEU:HD12 | 5:A:755:PRO:HD2 | 1.91 | 0.51 |
| 5:A:1238:TRP:NE1 | 5:A:1300:GLU:OE2 | 2.40 | 0.51 |
| 5:A:1410:TRP:CH2 | 5:A:1446:LEU:HD21 | 2.46 | 0.51 |
| 7:C:203:ILE:HB | 7:C:213:HIS:CD2 | 2.40 | 0.51 |
| 9:E:107:GLY:HA2 | 28:a:52:GLU:H | 1.74 | 0.51 |
| 15:K:172:GLU:HG2 | 15:K:177:TRP:CE2 | 2.45 | 0.51 |
| 18:N:256:ARG:HG3 | 18:N:261:TYR:CZ | 2.45 | 0.51 |
| 20:P:117:CYS:HB2 | 20:P:120:PHE:HB3 | 1.91 | 0.51 |
| 23:V:11:LYS:O | 23:V:55:VAL:HG21 | 2.09 | 0.51 |
| 24:W:258:GLU:O | 24:W:262:ARG:HD3 | 2.09 | 0.51 |
| 25:X:445:ASP:HB2 | 25:X:449:LYS:HZ3 | 1.76 | 0.51 |
| 27:Z:171:GLY:O | 27:Z:175:GLN:HG2 | 2.10 | 0.51 |
| 30:c:480:SER:HA | 30:c:483:GLU:OE1 | 2.10 | 0.51 |
| 5:A:750:LYS:HG2 | 16:L:279:LEU:HD22 | 1.90 | 0.51 |
| 8:D:70:ILE:HD13 | 9:E:68:VAL:HG22 | 1.92 | 0.51 |
| 18:N:39:VAL:HG22 | 18:N:48:VAL:HG11 | 1.92 | 0.51 |
| 18:N:739:SER:HA | 18:N:765:LEU:HD21 | 1.92 | 0.51 |
| 20:P:85:ASP:HB2 | 20:P:88:LYS:CB | 2.28 | 0.51 |
| 22:R:84:LYS:HZ3 | 22:R:87:ALA:HB3 | 1.73 | 0.51 |
| 22:R:573:ARG:HG3 | 22:R:602:PHE:HE2 | 1.74 | 0.51 |
| 23:T:96:GLU:HA | 23:T:99:GLN:HG2 | 1.92 | 0.51 |
| 25:X:537:TYR:HB3 | 25:X:556:TYR:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:b:119:LEU:HD13 | 29:b:122:ALA:HB3 | 1.91 | 0.51 |
| 35:z:271:VAL:HG23 | 35:z:297:LYS:HA | 1.92 | 0.51 |
| 5:A:167:THR:HG21 | 5:A:228:TYR:OH | 2.10 | 0.51 |
| 5:A:1642:LYS:HG3 | 5:A:1650:CYS:SG | 2.51 | 0.51 |
| 5:A:1848:THR:HA | 5:A:1851:TRP:HE3 | 1.74 | 0.51 |
| 6:B:114:ILE:HG21 | 6:B:661:LEU:HD11 | 1.91 | 0.51 |
| 6:B:195:SER:HB3 | 6:B:226:GLU:HB3 | 1.93 | 0.51 |
| 6:B:396:THR:HG23 | 6:B:427:LEU:HG | 1.92 | 0.51 |
| 6:B:861:TYR:OH | 6:B:874:ASP:OD2 | 2.20 | 0.51 |
| 7:C:239:MET:HE1 | 7:C:270:HIS:CD2 | 2.45 | 0.51 |
| 16:L:324:LYS:HE2 | 32:m:513:PRO:HA | 1.92 | 0.51 |
| 18:N:460:TYR:CD1 | 18:N:472:LEU:HD21 | 2.45 | 0.51 |
| 5:A:1669:LEU:HD13 | 5:A:1738:ALA:HB3 | 1.93 | 0.51 |
| 8:D:17:THR:HA | 8:D:26:TYR:O | 2.10 | 0.51 |
| 16:L:124:LEU:HD11 | 16:L:234:LEU:HD22 | 1.91 | 0.51 |
| 23:S:122:ARG:NH2 | 23:V:114:VAL:HG13 | 2.10 | 0.51 |
| 25:X:419:VAL:HB | 25:X:421:TYR:CE1 | 2.46 | 0.51 |
| 25:X:429:GLN:HA | 25:X:432:ILE:HG12 | 1.92 | 0.51 |
| 26:Y:127:TYR:HE2 | 26:Y:167:ARG:HH12 | 1.58 | 0.51 |
| 31:d:88:LEU:HD11 | 31:d:102:PHE:CD2 | 2.45 | 0.51 |
| 32:m:593:ILE:O | 32:m:597:TRP:HD1 | 1.94 | 0.51 |
| 35:z:430:ASP:OD1 | 35:z:434:ASN:N | 2.40 | 0.51 |
| 35:z:474:ILE:HD12 | 35:z:480:VAL:HG11 | 1.93 | 0.51 |
| 35:z:606:LEU:HA | 35:z:609:LYS:HG2 | 1.93 | 0.51 |
| 15:K:241:ARG:HG3 | 15:K:279:ARG:HD3 | 1.92 | 0.51 |
| 15:K:346:PHE:HB3 | 15:K:359:PHE:CE1 | 2.45 | 0.51 |
| 21:Q:223:ARG:C | 21:Q:225:TRP:N | 2.65 | 0.51 |
| 22:R:118:ARG:HG3 | 26:Y:165:VAL:CG1 | 2.38 | 0.51 |
| 24:W:574:ASN:OD1 | 24:W:575:TYR:N | 2.43 | 0.51 |
| 25:X:448:ARG:NH2 | 25:X:494:GLY:HA2 | 2.25 | 0.51 |
| 30:c:557:VAL:O | 30:c:561:HIS:HB2 | 2.11 | 0.51 |
| 35:z:144:ILE:HG23 | 35:z:175:VAL:HB | 1.92 | 0.51 |
| 5:A:92:LYS:HE3 | 19:O:34:GLU:HB3 | 1.92 | 0.51 |
| 5:A:1568:ARG:NE | 5:A:1696:ASP:OD2 | 2.31 | 0.51 |
| 5:A:1602:ARG:NE | 5:A:1770:ARG:HH21 | 2.07 | 0.51 |
| 6:B:823:ILE:CG1 | 6:B:824:PRO:HD3 | 2.41 | 0.51 |
| 8:D:17:THR:OG1 | 8:D:70:ILE:HB | 2.11 | 0.51 |
| 14:J:28:TYR:CE2 | 14:J:54:LYS:HE3 | 2.46 | 0.51 |
| 18:N:776:VAL:HG12 | 18:N:979:MET:HE2 | 1.92 | 0.51 |
| 18:N:1017:ASN:ND2 | 18:N:1170:GLU:OE2 | 2.44 | 0.51 |
| 20:P:149:ASP:OD1 | 20:P:224:GLN:NE2 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:T:114:VAL:HG12 | 23:U:115:ILE:HD12 | 1.91 | 0.51 |
| 25:X:289:ASN:O | 25:X:292:ILE:HG22 | 2.11 | 0.51 |
| 34:y:164:TYR:OH | 35:z:329:ASN:OD1 | 2.19 | 0.51 |
| 38:6:84:A:H2' | 38:6:85:G:C8 | 2.45 | 0.51 |
| 5:A:1605:LEU:HD22 | 5:A:1770:ARG:NH1 | 2.20 | 0.51 |
| 18:N:216:GLU:HG2 | 18:N:260:TYR:CD1 | 2.45 | 0.51 |
| 18:N:502:LYS:HE3 | 18:N:584:ASN:HB3 | 1.93 | 0.51 |
| 23:S:122:ARG:NH2 | 23:V:115:ILE:HD13 | 2.17 | 0.51 |
| 25:X:555:LEU:O | 25:X:559:LYS:HG2 | 2.09 | 0.51 |
| 34:y:164:TYR:HE2 | 35:z:330:PRO:HD2 | 1.75 | 0.51 |
| 4:5:101:U:H3 | 11:G:65:ASN:HD21 | 1.57 | 0.51 |
| 5:A:1834:PHE:HA | 5:A:1841:LEU:HD23 | 1.93 | 0.51 |
| 5:A:1897:GLU:HA | 5:A:1900:LEU:HB2 | 1.93 | 0.51 |
| 7:C:319:HIS:HB2 | 7:C:324:ILE:HB | 1.93 | 0.51 |
| 10:F:47:VAL:HB | 10:F:50:ARG:HB2 | 1.93 | 0.51 |
| 18:N:413:SER:OG | 18:N:416:ASN:ND2 | 2.38 | 0.51 |
| 19:O:95:PRO:HA | 19:O:98:GLU:OE2 | 2.10 | 0.51 |
| 24:W:220:ASP:O | 24:W:222:ASN:N | 2.44 | 0.51 |
| 25:X:193:GLU:O | 25:X:197:GLN:HG2 | 2.11 | 0.51 |
| 25:X:278:TYR:HE1 | 25:X:332:ILE:HD13 | 1.75 | 0.51 |
| 30:c:409:LEU:HD11 | 30:c:445:GLU:HG3 | 1.92 | 0.51 |
| 31:d:3:ASN:HD21 | 31:d:14:LEU:HD11 | 1.74 | 0.51 |
| 5:A:965:PRO:HD2 | 5:A:1462:VAL:HG22 | 1.92 | 0.51 |
| 5:A:971:PRO:HB3 | 5:A:1215:THR:HG21 | 1.93 | 0.51 |
| 12:H:60:ASP:OD1 | 12:H:61:ALA:N | 2.35 | 0.51 |
| 15:K:216:ARG:NH2 | 15:K:260:ASP:OD1 | 2.43 | 0.51 |
| 16:L:217:PHE:CZ | 17:M:50:PRO:HG3 | 2.46 | 0.51 |
| 18:N:652:PRO:HB2 | 18:N:1037:SER:HA | 1.92 | 0.51 |
| 25:X:144:HIS:HB2 | 25:X:148:TRP:CD1 | 2.46 | 0.51 |
| 25:X:183:GLU:O | 25:X:187:LYS:HG2 | 2.11 | 0.51 |
| 25:X:719:GLU:O | 25:X:722:ARG:HB3 | 2.11 | 0.51 |
| 2:p:214:GLU:CD | 25:X:708:ILE:HG22 | 2.36 | 0.51 |
| 4:5:49:U:H2' | 4:5:50:U:H6 | 1.76 | 0.51 |
| 5:A:410:PHE:HE2 | 6:B:338:LEU:CD2 | 2.24 | 0.51 |
| 5:A:1762:PRO:HB3 | 34:y:94:ILE:HA | 1.92 | 0.51 |
| 7:C:115:THR:HG22 | 7:C:136:GLY:C | 2.36 | 0.51 |
| 7:C:240:ASP:OD1 | 7:C:242:THR:OG1 | 2.27 | 0.51 |
| 10:F:29:ILE:HA | 10:F:40:LEU:HD23 | 1.93 | 0.51 |
| 11:G:32:VAL:HG23 | 11:G:33:LEU:HD22 | 1.93 | 0.51 |
| 18:N:789:THR:OG1 | 18:N:816:ARG:NH2 | 2.44 | 0.51 |
| 20:P:131:CYS:SG | 20:P:132:GLU:N | 2.84 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:S:122:ARG:HH11 | 23:V:118:LEU:HD22 | 1.76 | 0.51 |
| 25:X:103:ILE:HG22 | 25:X:104:LEU:HD22 | 1.92 | 0.51 |
| 25:X:417:THR:HG22 | 25:X:430:VAL:HG11 | 1.93 | 0.51 |
| 35:z:136:LEU:O | 35:z:169:ARG:HD2 | 2.11 | 0.51 |
| 5:A:1035:LYS:HG3 | 5:A:1057:LEU:HD13 | 1.92 | 0.50 |
| 5:A:1986:THR:HG22 | 5:A:1993:PRO:HA | 1.93 | 0.50 |
| 6:B:180:THR:HG22 | 6:B:549:ALA:HB2 | 1.91 | 0.50 |
| 10:F:76:LEU:O | 10:F:80:LEU:HD23 | 2.10 | 0.50 |
| 15:K:354:ILE:HB | 15:K:368:PHE:HB2 | 1.93 | 0.50 |
| 17:M:171:LYS:NZ | 17:M:174:ARG:HD3 | 2.26 | 0.50 |
| 18:N:483:PHE:HE1 | 18:N:505:MET:HE3 | 1.75 | 0.50 |
| 18:N:1108:GLN:HE21 | 18:N:1141:SER:HB2 | 1.76 | 0.50 |
| 22:R:85:GLU:O | 22:R:86:PHE:HD1 | 1.94 | 0.50 |
| 22:R:174:TRP:O | 22:R:178:ILE:HG12 | 2.11 | 0.50 |
| 22:R:603:GLU:HG3 | 22:R:615:VAL:HG21 | 1.93 | 0.50 |
| 23:S:60:ARG:NH1 | 24:W:701:TRP:HB3 | 2.26 | 0.50 |
| 23:U:59:VAL:HG23 | 23:U:61:PRO:HD3 | 1.91 | 0.50 |
| 28:a:67:LEU:O | 28:a:67:LEU:HD23 | 2.11 | 0.50 |
| 35:z:59:PRO:HG2 | 35:z:121:TYR:OH | 2.11 | 0.50 |
| 4:5:97:U:H1' | 14:J:65:ASN:HB2 | 1.94 | 0.50 |
| 6:B:231:MET:HE1 | 6:B:257:HIS:ND1 | 2.26 | 0.50 |
| 7:C:44:LEU:HD23 | 7:C:336:LEU:HD12 | 1.93 | 0.50 |
| 13:I:50:GLU:OE2 | 13:I:52:VAL:HB | 2.11 | 0.50 |
| 18:N:751:ARG:HH12 | 18:N:1208:SER:HA | 1.77 | 0.50 |
| 23:T:122:ARG:NH2 | 23:U:121:GLU:OE1 | 2.44 | 0.50 |
| 24:W:196:LEU:HD21 | 24:W:200:ARG:HH21 | 1.75 | 0.50 |
| 25:X:631:LEU:O | 25:X:635:VAL:HG23 | 2.10 | 0.50 |
| 32:m:449:TRP:HZ2 | 32:m:456:LYS:HB2 | 1.76 | 0.50 |
| 38:6:55:C:H2' | 38:6:56:C:O4' | 2.11 | 0.50 |
| 5:A:197:PHE:CE2 | 5:A:589:LEU:HD21 | 2.45 | 0.50 |
| 5:A:1018:ARG:HG3 | 16:L:295:LEU:HD13 | 1.93 | 0.50 |
| 5:A:1603:SER:O | 5:A:1605:LEU:N | 2.44 | 0.50 |
| 5:A:1666:PRO:HD3 | 5:A:1741:ASN:ND2 | 2.24 | 0.50 |
| 6:B:404:LEU:O | 6:B:408:LEU:HG | 2.12 | 0.50 |
| 15:K:270:VAL:HG11 | 15:K:284:VAL:HG13 | 1.93 | 0.50 |
| 16:L:186:TYR:HD1 | 28:a:89:ALA:HB2 | 1.77 | 0.50 |
| 22:R:447:ILE:HG22 | 22:R:449:GLN:HG2 | 1.92 | 0.50 |
| 23:T:127:GLU:O | 23:T:131:LYS:HG2 | 2.12 | 0.50 |
| 25:X:154:TYR:O | 25:X:158:ILE:HG22 | 2.12 | 0.50 |
| 31:d:3:ASN:ND2 | 31:d:14:LEU:HD11 | 2.26 | 0.50 |
| 5:A:1495:ARG:HG3 | 34:y:218:TYR:CE1 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:K:455:THR:OG1 | 15:K:458:THR:OG1 | 2.14 | 0.50 |
| 17:M:69:ILE:HG23 | 17:M:84:MET:HE1 | 1.93 | 0.50 |
| 23:S:59:VAL:O | 24:W:701:TRP:NE1 | 2.45 | 0.50 |
| 24:W:238:THR:HG23 | 24:W:241:GLU:HB3 | 1.93 | 0.50 |
| 25:X:398:ARG:NH2 | 25:X:436:GLU:OE1 | 2.37 | 0.50 |
| 31:d:28:ASN:O | 31:d:32:LEU:HB2 | 2.11 | 0.50 |
| 35:z:143:VAL:HB | 35:z:172:PHE:CZ | 2.47 | 0.50 |
| 1:e:182:ASP:HB2 | 16:L:239:ARG:HH21 | 1.77 | 0.50 |
| 5:A:898:HIS:HB2 | 35:z:217:GLU:OE1 | 2.11 | 0.50 |
| 5:A:1099:ASP:N | 5:A:1099:ASP:OD1 | 2.43 | 0.50 |
| 5:A:1371:ASP:OD1 | 5:A:1371:ASP:N | 2.45 | 0.50 |
| 5:A:1490:GLN:NE2 | 5:A:1492:ASN:HD22 | 2.07 | 0.50 |
| 9:E:44:GLU:OE1 | 9:E:63:ARG:NE | 2.38 | 0.50 |
| 10:F:33:ASP:OD1 | 10:F:34:MET:N | 2.44 | 0.50 |
| 22:R:61:ASP:OD1 | 22:R:62:ALA:N | 2.44 | 0.50 |
| 30:c:545:GLN:O | 30:c:549:GLU:OE1 | 2.30 | 0.50 |
| 32:m:619:LEU:HD23 | 32:m:622:LEU:HD12 | 1.93 | 0.50 |
| 38:6:59:G:N2 | 38:6:62:C:OP2 | 2.31 | 0.50 |
| 8:D:27:ARG:HB3 | 8:D:45:SER:OG | 2.12 | 0.50 |
| 9:E:15:ASN:ND2 | 9:E:81:GLN:HE21 | 2.10 | 0.50 |
| 10:F:69:ILE:HD12 | 11:G:96:ILE:HG21 | 1.94 | 0.50 |
| 15:K:346:PHE:HB3 | 15:K:359:PHE:HE1 | 1.76 | 0.50 |
| 22:R:186:GLU:HG3 | 22:R:188:GLU:OE2 | 2.12 | 0.50 |
| 25:X:98:PHE:CD1 | 25:X:111:ILE:HG23 | 2.46 | 0.50 |
| 35:z:145:LEU:HD11 | 35:z:162:LEU:HD22 | 1.94 | 0.50 |
| 35:z:162:LEU:HD23 | 35:z:174:LEU:HD22 | 1.94 | 0.50 |
| 5:A:405:ILE:HG22 | 6:B:346:ILE:HD13 | 1.93 | 0.50 |
| 5:A:1190:LEU:HD12 | 5:A:1191:THR:HG22 | 1.92 | 0.50 |
| 13:I:71:LEU:HD22 | 13:I:72:TRP:CD1 | 2.46 | 0.50 |
| 17:M:79:CYS:SG | 17:M:80:CYS:N | 2.85 | 0.50 |
| 18:N:745:MET:HE1 | 18:N:1007:LEU:HD12 | 1.93 | 0.50 |
| 18:N:898:PRO:HG2 | 18:N:901:THR:HG23 | 1.93 | 0.50 |
| 20:P:175:THR:HB | 20:P:216:THR:HG23 | 1.92 | 0.50 |
| 20:P:178:VAL:HG23 | 20:P:243:VAL:HG22 | 1.93 | 0.50 |
| 23:U:388:TYR:HA | 23:U:405:LEU:HD22 | 1.92 | 0.50 |
| 25:X:707:GLU:OE1 | 25:X:720:MET:HE3 | 2.12 | 0.50 |
| 32:m:725:PHE:CZ | 32:m:787:PHE:HB3 | 2.47 | 0.50 |
| 5:A:810:GLU:OE2 | 5:A:813:ARG:NH2 | 2.42 | 0.50 |
| 9:E:20:ASP:OD2 | 9:E:22:ARG:NH2 | 2.45 | 0.50 |
| 15:K:173:PRO:HG3 | 15:K:215:PRO:HA | 1.92 | 0.50 |
| 17:M:107:PRO:O | 17:M:113:ARG:HD2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:245:ILE:HD11 | 22:R:279:LEU:HA | 1.92 | 0.50 |
| 22:R:460:TRP:CE2 | 22:R:470:PRO:HG3 | 2.46 | 0.50 |
| 24:W:600:CYS:HA | 24:W:603:LEU:HG | 1.93 | 0.50 |
| 35:z:325:GLN:O | 35:z:337:LEU:HD12 | 2.12 | 0.50 |
| 35:z:497:SER:HA | 35:z:500:PHE:CE2 | 2.47 | 0.50 |
| 7:C:232:SER:HB2 | 7:C:249:LYS:HE3 | 1.93 | 0.50 |
| 9:E:106:ARG:O | 28:a:53:LEU:N | 2.44 | 0.50 |
| 11:G:42:GLN:OE1 | 11:G:56:ARG:NH1 | 2.45 | 0.50 |
| 12:H:80:LEU:HD23 | 12:H:81:ILE:N | 2.26 | 0.50 |
| 15:K:346:PHE:CD1 | 15:K:359:PHE:HE1 | 2.29 | 0.50 |
| 22:R:107:TRP:O | 22:R:111:ILE:HG12 | 2.12 | 0.50 |
| 23:V:40:VAL:HG23 | 23:V:41:THR:HG23 | 1.92 | 0.50 |
| 24:W:6:GLY:HA2 | 24:W:43:GLN:HE22 | 1.77 | 0.50 |
| 26:Y:155:TRP:HA | 26:Y:158:ASN:OD1 | 2.11 | 0.50 |
| 5:A:696:THR:OG1 | 38:6:64:A:OP1 | 2.21 | 0.49 |
| 5:A:1233:LEU:O | 30:c:466:LEU:HD11 | 2.12 | 0.49 |
| 7:C:278:SER:OG | 7:C:283:PHE:HB2 | 2.12 | 0.49 |
| 10:F:20:LYS:HB2 | 10:F:64:ASN:HA | 1.94 | 0.49 |
| 13:I:21:LEU:HD11 | 13:I:29:GLU:HB2 | 1.93 | 0.49 |
| 18:N:191:LEU:O | 18:N:195:LEU:HG | 2.12 | 0.49 |
| 18:N:592:TYR:OH | 18:N:602:ARG:NH1 | 2.42 | 0.49 |
| 23:U:476:LEU:H | 23:U:488:GLY:C | 2.20 | 0.49 |
| 25:X:68:TRP:NE1 | 25:X:104:LEU:HD23 | 2.21 | 0.49 |
| 32:m:547:PHE:HA | 32:m:550:TRP:HD1 | 1.77 | 0.49 |
| 34:y:92:MET:HE3 | 34:y:96:ASP:HB2 | 1.94 | 0.49 |
| 5:A:411:PHE:HB2 | 6:B:391:LYS:HD2 | 1.93 | 0.49 |
| 5:A:1815:HIS:HB2 | 5:A:1823:THR:HB | 1.94 | 0.49 |
| 8:D:89:VAL:HG12 | 8:D:91:LEU:HG | 1.92 | 0.49 |
| 18:N:493:ILE:HD12 | 25:X:202:LEU:HD11 | 1.94 | 0.49 |
| 18:N:745:MET:HE3 | 18:N:1029:PHE:CD1 | 2.46 | 0.49 |
| 25:X:703:TRP:O | 25:X:707:GLU:HG3 | 2.11 | 0.49 |
| 28:a:61:GLU:O | 28:a:62:MET:HE2 | 2.12 | 0.49 |
| 6:B:531:GLU:HA | 32:m:756:LYS:HD2 | 1.95 | 0.49 |
| 15:K:356:HIS:CD2 | 15:K:365:MET:HE2 | 2.48 | 0.49 |
| 23:T:5:ILE:HA | 23:U:88:PHE:CD1 | 2.47 | 0.49 |
| 23:V:86:GLU:O | 23:V:89:GLU:HG2 | 2.12 | 0.49 |
| 24:W:198:LYS:O | 24:W:201:GLU:HG3 | 2.12 | 0.49 |
| 24:W:510:ARG:NE | 24:W:510:ARG:O | 2.45 | 0.49 |
| 25:X:265:ILE:HG12 | 25:X:300:PHE:CE1 | 2.47 | 0.49 |
| 38:6:49:C:H2' | 38:6:50:A:O4' | 2.13 | 0.49 |
| 4:5:56:A:O2' | 4:5:57:G:H5" | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:492:VAL:HG22 | 6:B:508:ALA:HB2 | 1.94 | 0.49 |
| 6:B:501:ALA:HB2 | 6:B:661:LEU:HD12 | 1.94 | 0.49 |
| 11:G:111:ARG:HD2 | 13:I:62:GLU:OE2 | 2.12 | 0.49 |
| 15:K:89:GLU:OE1 | 22:R:259:ARG:HG2 | 2.12 | 0.49 |
| 15:K:392:ASN:OD1 | 15:K:394:SER:OG | 2.22 | 0.49 |
| 23:T:67:THR:HG21 | 27:Z:105:ARG:HG3 | 1.93 | 0.49 |
| 23:V:106:TYR:OH | 23:V:113:ARG:NH1 | 2.45 | 0.49 |
| 24:W:266:MET:HA | 24:W:269:GLU:HG2 | 1.93 | 0.49 |
| 24:W:537:ARG:CG | 24:W:538:PRO:HD2 | 2.43 | 0.49 |
| 25:X:585:PRO:HB3 | 25:X:619:VAL:HA | 1.94 | 0.49 |
| 34:y:25:PHE:CE2 | 34:y:27:LEU:HA | 2.48 | 0.49 |
| 35:z:543:ARG:O | 35:z:547:VAL:HG23 | 2.12 | 0.49 |
| 5:A:1282:LYS:NZ | 34:y:214:ASP:OD2 | 2.39 | 0.49 |
| 9:E:5:LYS:HE2 | 10:F:30:THR:HG21 | 1.94 | 0.49 |
| 9:E:32:ASP:OD1 | 9:E:33:GLY:N | 2.45 | 0.49 |
| 23:U:24:GLU:HB3 | 23:U:27:LEU:HD12 | 1.94 | 0.49 |
| 23:U:361:GLU:HB3 | 23:U:364:SER:OG | 2.12 | 0.49 |
| 23:V:102:SER:HA | 23:V:105:LEU:HD12 | 1.95 | 0.49 |
| 32:m:308:GLY:HA2 | 32:m:311:MET:HG2 | 1.94 | 0.49 |
| 35:z:625:GLN:HB2 | 35:z:627:PHE:CE1 | 2.47 | 0.49 |
| 35:z:628:VAL:HG23 | 35:z:631:ILE:HD11 | 1.93 | 0.49 |
| 38:6:34:U:H2' | 38:6:35:A:C8 | 2.43 | 0.49 |
| 5:A:1461:ARG:NH1 | 5:A:1479:TRP:O | 2.45 | 0.49 |
| 6:B:752:ASP:OD2 | 6:B:789:ARG:NH2 | 2.43 | 0.49 |
| 22:R:388:GLU:O | 22:R:391:LYS:HG2 | 2.12 | 0.49 |
| 25:X:251:ASP:OD1 | 25:X:251:ASP:N | 2.45 | 0.49 |
| 34:y:143:LYS:HA | 34:y:146:LYS:HD2 | 1.93 | 0.49 |
| 39:1:0:G:O2' | 39:1:1:G:OP1 | 2.31 | 0.49 |
| 5:A:324:ARG:HG3 | 6:B:892:ILE:HG13 | 1.94 | 0.49 |
| 5:A:839:TRP:CZ2 | 5:A:843:ARG:HD2 | 2.47 | 0.49 |
| 7:C:61:SER:O | 7:C:321:HIS:NE2 | 2.46 | 0.49 |
| 11:G:15:ILE:H | 11:G:15:ILE:HD12 | 1.77 | 0.49 |
| 11:G:74:MET:N | 11:G:74:MET:SD | 2.86 | 0.49 |
| 13:I:15:LEU:HD23 | 13:I:15:LEU:O | 2.12 | 0.49 |
| 14:J:21:LEU:HD21 | 14:J:62:ILE:HD13 | 1.94 | 0.49 |
| 15:K:268:ASP:OD2 | 15:K:272:ARG:NH1 | 2.45 | 0.49 |
| 22:R:302:ASP:OD1 | 22:R:303:LYS:N | 2.46 | 0.49 |
| 22:R:599:TRP:CZ3 | 22:R:615:VAL:HG22 | 2.48 | 0.49 |
| 23:U:69:LEU:HD21 | 23:V:75:LEU:HB2 | 1.94 | 0.49 |
| 25:X:457:ALA:HB3 | 25:X:505:ARG:HH12 | 1.78 | 0.49 |
| 25:X:599:GLU:O | 25:X:603:GLY:N | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:z:268:GLN:OE1 | 35:z:296:ARG:NE | 2.38 | 0.49 |
| 1:e:32:GLU:O | 1:e:35:TYR:N | 2.46 | 0.49 |
| 5:A:1595:ILE:HG12 | 34:y:55:ALA:HB2 | 1.94 | 0.49 |
| 6:B:951:THR:HG22 | 6:B:955:LYS:HD2 | 1.95 | 0.49 |
| 7:C:266:HIS:CD2 | 7:C:273:LEU:HD12 | 2.48 | 0.49 |
| 10:F:27:GLY:HA3 | 10:F:43:VAL:HG12 | 1.95 | 0.49 |
| 17:M:235:TYR:HB3 | 17:M:263:ALA:HB2 | 1.94 | 0.49 |
| 18:N:629:VAL:HA | 18:N:632:LEU:HD23 | 1.94 | 0.49 |
| 22:R:104:ILE:H | 22:R:104:ILE:HD12 | 1.77 | 0.49 |
| 22:R:237:GLU:HG2 | 22:R:238:PHE:CD1 | 2.48 | 0.49 |
| 22:R:287:GLU:HB3 | 22:R:302:ASP:OD2 | 2.12 | 0.49 |
| 22:R:488:ARG:HG2 | 22:R:513:PHE:HE2 | 1.78 | 0.49 |
| 23:U:15:ILE:HD13 | 23:V:53:VAL:HG23 | 1.94 | 0.49 |
| 35:z:131:ILE:HG12 | 35:z:137:LEU:HD11 | 1.94 | 0.49 |
| 35:z:153:LEU:HD13 | 35:z:382:ILE:HA | 1.95 | 0.49 |
| 5:A:1671:ASP:OD1 | 5:A:1671:ASP:N | 2.42 | 0.49 |
| 17:M:150:ARG:HH12 | 20:P:263:GLU:HB2 | 1.77 | 0.49 |
| 18:N:929:ARG:HB3 | 25:X:137:ARG:HH12 | 1.77 | 0.49 |
| 22:R:84:LYS:HA | 24:W:253:ASP:OD1 | 2.13 | 0.49 |
| 22:R:154:ILE:HA | 22:R:157:CYS:SG | 2.52 | 0.49 |
| 22:R:291:GLY:HA3 | 25:X:535:LYS:NZ | 2.28 | 0.49 |
| 23:U:96:GLU:O | 23:U:100:GLU:HG2 | 2.13 | 0.49 |
| 23:U:351:GLY:HA2 | 23:U:357:LEU:HA | 1.95 | 0.49 |
| 24:W:529:GLN:O | 24:W:530:VAL:HG22 | 2.13 | 0.49 |
| 25:X:572:THR:O | 25:X:575:LEU:HG | 2.13 | 0.49 |
| 34:y:223:PRO:HD2 | 34:y:225:MET:HE1 | 1.93 | 0.49 |
| 35:z:242:PHE:HE2 | 35:z:306:GLU:HG3 | 1.78 | 0.49 |
| 35:z:491:ASP:HA | 35:z:494:VAL:HG22 | 1.95 | 0.49 |
| 5:A:1567:ASN:HB2 | 5:A:1593:LEU:HD21 | 1.95 | 0.49 |
| 5:A:1747:LYS:HB3 | 5:A:1748:PRO:HD3 | 1.95 | 0.49 |
| 6:B:570:ASP:N | 6:B:570:ASP:OD1 | 2.44 | 0.49 |
| 6:B:600:SER:HB3 | 6:B:644:PHE:HB3 | 1.95 | 0.49 |
| 13:I:15:LEU:HD21 | 13:I:20:VAL:HG11 | 1.95 | 0.49 |
| 20:P:98:VAL:H | 20:P:101:ARG:HH12 | 1.60 | 0.49 |
| 25:X:192:ASN:ND2 | 25:X:232:HIS:O | 2.33 | 0.49 |
| 35:z:355:GLY:HA2 | 35:z:358:MET:O | 2.13 | 0.49 |
| 5:A:613:GLY:HA2 | 5:A:615:TYR:CE2 | 2.48 | 0.48 |
| 6:B:694:ASN:OD1 | 6:B:696:LYS:HG2 | 2.13 | 0.48 |
| 16:L:241:VAL:O | 16:L:245:GLU:HB2 | 2.13 | 0.48 |
| 18:N:77:LEU:HD12 | 18:N:80:MET:SD | 2.53 | 0.48 |
| 20:P:83:ARG:HD3 | 38:6:31:C:C4 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:300:VAL:HG13 | 22:R:304:ARG:CZ | 2.43 | 0.48 |
| 23:T:32:ILE:HD11 | 23:T:45:CYS:HB3 | 1.95 | 0.48 |
| 23:U:299:ASN:N | 23:U:313:ALA:O | 2.46 | 0.48 |
| 25:X:263:TYR:O | 25:X:267:ILE:HG13 | 2.13 | 0.48 |
| 25:X:621:THR:HA | 25:X:624:ARG:NE | 2.14 | 0.48 |
| 6:B:287:TYR:OH | 6:B:357:GLY:HA2 | 2.13 | 0.48 |
| 6:B:740:LEU:HD23 | 6:B:744:ARG:HG3 | 1.95 | 0.48 |
| 11:G:44:LEU:HD13 | 11:G:54:LEU:CD1 | 2.43 | 0.48 |
| 20:P:82:MET:HG2 | 38:6:32:G:C2 | 2.41 | 0.48 |
| 20:P:93:SER:OG | 20:P:233:GLN:OE1 | 2.31 | 0.48 |
| 24:W:696:LYS:HG3 | 27:Z:131:LEU:HB2 | 1.95 | 0.48 |
| 25:X:230:PRO:HB3 | 25:X:263:TYR:CD1 | 2.48 | 0.48 |
| 4:5:27:G:O2' | 4:5:28:C:OP2 | 2.28 | 0.48 |
| 5:A:1684:TYR:CB | 5:A:1724:GLY:HA2 | 2.42 | 0.48 |
| 5:A:1970:ASN:ND2 | 5:A:2014:ASP:OD2 | 2.46 | 0.48 |
| 6:B:757:ASN:OD1 | 6:B:788:THR:OG1 | 2.32 | 0.48 |
| 13:I:49:GLU:HG3 | 13:I:56:LYS:HD3 | 1.96 | 0.48 |
| 18:N:529:LEU:HD12 | 18:N:530:CYS:H | 1.79 | 0.48 |
| 18:N:1112:GLU:OE2 | 18:N:1184:THR:HB | 2.13 | 0.48 |
| 22:R:21:GLU:CD | 22:R:21:GLU:H | 2.21 | 0.48 |
| 24:W:657:TYR:CE2 | 27:Z:92:LEU:HD23 | 2.48 | 0.48 |
| 34:y:92:MET:HE2 | 34:y:97:ILE:HG23 | 1.95 | 0.48 |
| 5:A:234:GLU:HG3 | 5:A:242:PRO:HA | 1.94 | 0.48 |
| 5:A:1268:ILE:HD13 | 5:A:1271:ILE:HD12 | 1.95 | 0.48 |
| 5:A:1492:ASN:ND2 | 34:y:220:LEU:HG | 2.29 | 0.48 |
| 11:G:90:ILE:HG13 | 11:G:92:LYS:NZ | 2.27 | 0.48 |
| 16:L:111:HIS:NE2 | 16:L:229:PRO:O | 2.43 | 0.48 |
| 18:N:666:TYR:CE1 | 18:N:696:LEU:HD13 | 2.47 | 0.48 |
| 18:N:798:HIS:HD1 | 18:N:801:HIS:H | 1.61 | 0.48 |
| 18:N:805:LEU:HB2 | 18:N:954:CYS:HB3 | 1.96 | 0.48 |
| 18:N:1121:GLN:O | 18:N:1125:MET:HG2 | 2.14 | 0.48 |
| 20:P:261:ARG:HH12 | 20:P:265:ARG:HH21 | 1.61 | 0.48 |
| 22:R:54:ARG:HA | 22:R:57:LYS:HE3 | 1.94 | 0.48 |
| 22:R:147:MET:HE3 | 22:R:148:GLU:OE1 | 2.13 | 0.48 |
| 23:S:129:LEU:CD2 | 23:V:125:ALA:HB2 | 2.43 | 0.48 |
| 27:Z:97:VAL:HA | 27:Z:100:GLU:OE2 | 2.13 | 0.48 |
| 5:A:1584:ILE:HD13 | 5:A:1597:LEU:HD13 | 1.95 | 0.48 |
| 6:B:922:PRO:HG2 | 6:B:943:LEU:HD12 | 1.95 | 0.48 |
| 10:F:18:GLU:HG3 | 10:F:24:ILE:HG13 | 1.94 | 0.48 |
| 15:K:470:ARG:HH12 | 15:K:472:ARG:HD2 | 1.79 | 0.48 |
| 16:L:191:GLN:NE2 | 17:M:23:CYS:HA | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:M:256:THR:HG23 | 17:M:259:SER:H | 1.78 | 0.48 |
| 18:N:202:LEU:HD23 | 18:N:228:MET:HE1 | 1.96 | 0.48 |
| 23:U:191:ALA:O | 23:U:485:LEU:N | 2.46 | 0.48 |
| 25:X:589:LYS:NZ | 25:X:623:ASP:O | 2.45 | 0.48 |
| 28:a:96:ASN:O | 28:a:100:ASN:ND2 | 2.46 | 0.48 |
| 1:e:204:HIS:CB | 6:B:76:GLN:HB2 | 2.33 | 0.48 |
| 4:5:100:U:H4' | 4:5:101:U:H5' | 1.94 | 0.48 |
| 5:A:309:MET:HG3 | 5:A:311:ASP:H | 1.78 | 0.48 |
| 5:A:1182:ILE:HD13 | 5:A:1185:ARG:HH11 | 1.78 | 0.48 |
| 6:B:601:VAL:HB | 6:B:844:PRO:HG3 | 1.95 | 0.48 |
| 6:B:684:SER:HB3 | 6:B:702:VAL:HG23 | 1.96 | 0.48 |
| 13:I:25:LYS:HE2 | 13:I:68:ASN:O | 2.14 | 0.48 |
| 18:N:70:MET:HG3 | 18:N:74:HIS:ND1 | 2.28 | 0.48 |
| 18:N:321:LEU:HD13 | 18:N:338:ILE:HA | 1.96 | 0.48 |
| 21:Q:240:ASP:OD1 | 21:Q:240:ASP:N | 2.44 | 0.48 |
| 22:R:322:TRP:HD1 | 22:R:325:LEU:HB2 | 1.79 | 0.48 |
| 24:W:710:ASN:OD1 | 24:W:711:LEU:N | 2.46 | 0.48 |
| 26:Y:95:LYS:HE2 | 26:Y:121:ARG:HH22 | 1.77 | 0.48 |
| 32:m:575:MET:HE2 | 32:m:579:LEU:HD13 | 1.94 | 0.48 |
| 35:z:561:LEU:HD12 | 35:z:562:PRO:HD2 | 1.95 | 0.48 |
| 35:z:611:THR:HG21 | 35:z:633:LYS:HB2 | 1.96 | 0.48 |
| 3:2:12:G:H2' | 3:2:13:C:H4' | 1.96 | 0.48 |
| 4:5:96:G:N2 | 13:I:41:MET:HG3 | 2.29 | 0.48 |
| 6:B:154:LYS:HG2 | 42:B:1001:GTP:O1B | 2.14 | 0.48 |
| 11:G:8:PRO:HD2 | 11:G:9:ARG:NH1 | 2.27 | 0.48 |
| 18:N:445:LEU:HB2 | 18:N:621:TYR:HB3 | 1.95 | 0.48 |
| 18:N:690:LEU:HD21 | 18:N:695:LEU:HD21 | 1.95 | 0.48 |
| 22:R:111:ILE:HD13 | 22:R:126:LEU:HD23 | 1.96 | 0.48 |
| 31:d:2:ALA:HB1 | 31:d:17:LEU:HB2 | 1.96 | 0.48 |
| 35:z:250:GLU:HA | 35:z:253:ILE:HG12 | 1.94 | 0.48 |
| 5:A:127:MET:HE1 | 5:A:605:PHE:CZ | 2.47 | 0.48 |
| 5:A:1624:GLU:OE2 | 5:A:1627:SER:OG | 2.31 | 0.48 |
| 5:A:1638:ILE:HD12 | 5:A:1642:LYS:HE3 | 1.95 | 0.48 |
| 13:I:34:LEU:H | 13:I:34:LEU:HD23 | 1.78 | 0.48 |
| 15:K:117:LYS:C | 22:R:225:GLN:HE22 | 2.21 | 0.48 |
| 17:M:232:PHE:HE2 | 17:M:252:VAL:HG11 | 1.78 | 0.48 |
| 19:O:10:LYS:HD2 | 19:O:11:ARG:N | 2.28 | 0.48 |
| 22:R:105:PRO:HG3 | 38:6:78:A:C8 | 2.49 | 0.48 |
| 22:R:280:TYR:HB3 | 22:R:306:LEU:CD1 | 2.44 | 0.48 |
| 22:R:453:CYS:HA | 22:R:456:LEU:HD12 | 1.96 | 0.48 |
| 25:X:511:ILE:HG13 | 25:X:512:ALA:N | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:703:TRP:CZ2 | 25:X:720:MET:HB2 | 2.48 | 0.48 |
| 3:2:30:A:H2 | 34:y:40:LYS:HD2 | 1.78 | 0.48 |
| 5:A:329:THR:HG23 | 29:b:4:ASN:H | 1.78 | 0.48 |
| 5:A:942:ASP:OD1 | 5:A:1035:LYS:NZ | 2.47 | 0.48 |
| 5:A:959:PHE:HB3 | 5:A:963:VAL:HG21 | 1.94 | 0.48 |
| 5:A:1817:THR:HG22 | 5:A:1818:PHE:N | 2.23 | 0.48 |
| 6:B:933:LYS:HZ1 | 6:B:935:LEU:HB2 | 1.79 | 0.48 |
| 18:N:58:PHE:CD2 | 18:N:62:LEU:HD11 | 2.49 | 0.48 |
| 18:N:449:LEU:HD13 | 18:N:557:PHE:CZ | 2.49 | 0.48 |
| 20:P:184:THR:O | 20:P:187:ILE:HG23 | 2.13 | 0.48 |
| 25:X:287:VAL:O | 25:X:291:THR:HG23 | 2.14 | 0.48 |
| 25:X:624:ARG:HA | 25:X:627:ILE:HG22 | 1.96 | 0.48 |
| 32:m:278:ARG:NH2 | 33:n:324:ILE:O | 2.47 | 0.48 |
| 35:z:34:LEU:HD21 | 35:z:61:PHE:HD2 | 1.77 | 0.48 |
| 35:z:379:GLU:OE2 | 35:z:384:ASN:OD1 | 2.31 | 0.48 |
| 35:z:393:PHE:CE2 | 35:z:397:LEU:HD11 | 2.49 | 0.48 |
| 5:A:511:ASP:OD1 | 5:A:512:TRP:N | 2.47 | 0.48 |
| 5:A:527:LEU:HD22 | 5:A:567:PHE:CE1 | 2.49 | 0.48 |
| 5:A:1689:GLN:N | 5:A:1689:GLN:OE1 | 2.47 | 0.48 |
| 11:G:5:VAL:HG12 | 11:G:23:TYR:CD2 | 2.48 | 0.48 |
| 15:K:115:LEU:HD23 | 15:K:115:LEU:H | 1.79 | 0.48 |
| 20:P:296:LYS:HG3 | 20:P:297:LEU:N | 2.29 | 0.48 |
| 22:R:224:ARG:O | 22:R:228:LEU:HG | 2.13 | 0.48 |
| 23:U:123:ASP:OD1 | 23:U:124:GLU:N | 2.47 | 0.48 |
| 35:z:456:LEU:HD22 | 35:z:468:ILE:HG22 | 1.95 | 0.48 |
| 3:2:9:U:H2' | 3:2:10:U:H6 | 1.79 | 0.47 |
| 5:A:1011:VAL:HG11 | 5:A:1053:LEU:HD12 | 1.96 | 0.47 |
| 5:A:1153:LYS:HE3 | 5:A:1196:GLU:HA | 1.96 | 0.47 |
| 5:A:1436:TRP:CE2 | 5:A:1444:ASN:ND2 | 2.82 | 0.47 |
| 6:B:776:VAL:HA | 6:B:779:TYR:CE1 | 2.49 | 0.47 |
| 12:H:31:PHE:HA | 12:H:79:THR:OG1 | 2.14 | 0.47 |
| 15:K:384:ASN:HB3 | 15:K:400:TRP:HB3 | 1.95 | 0.47 |
| 18:N:761:LEU:HD21 | 18:N:1006:VAL:HG21 | 1.96 | 0.47 |
| 20:P:174:TYR:CE2 | 20:P:220:GLU:HG2 | 2.49 | 0.47 |
| 22:R:111:ILE:O | 22:R:115:MET:HG2 | 2.14 | 0.47 |
| 24:W:259:ASN:HA | 24:W:262:ARG:HE | 1.79 | 0.47 |
| 25:X:448:ARG:HH21 | 25:X:494:GLY:HA2 | 1.79 | 0.47 |
| 25:X:498:THR:HG22 | 25:X:501:LYS:NZ | 2.28 | 0.47 |
| 3:2:14:C:H2' | 38:6:76:C:C4 | 2.48 | 0.47 |
| 5:A:1215:THR:OG1 | 5:A:1216:GLY:N | 2.45 | 0.47 |
| 7:C:114:ASP:O | 7:C:115:THR:OG1 | 2.24 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:45:TYR:HE1 | 9:E:62:LYS:HE3 | 1.78 | 0.47 |
| 15:K:132:SER:O | 15:K:136:LEU:HD12 | 2.14 | 0.47 |
| 18:N:421:GLN:OE1 | 18:N:440:ALA:HB2 | 2.14 | 0.47 |
| 18:N:519:ASP:O | 18:N:523:SER:N | 2.47 | 0.47 |
| 18:N:926:GLU:HG3 | 25:X:137:ARG:NH2 | 2.27 | 0.47 |
| 22:R:151:LEU:HD12 | 26:Y:160:PRO:HG3 | 1.96 | 0.47 |
| 23:S:115:ILE:HD11 | 23:V:111:ALA:HB2 | 1.95 | 0.47 |
| 34:y:120:ASP:O | 34:y:121:THR:HG23 | 2.15 | 0.47 |
| 35:z:425:LEU:HD12 | 35:z:579:ARG:NH2 | 2.29 | 0.47 |
| 2:p:178:LYS:NZ | 2:p:182:LYS:HB2 | 2.30 | 0.47 |
| 6:B:132:PHE:HZ | 6:B:553:LEU:HB3 | 1.79 | 0.47 |
| 6:B:569:VAL:O | 6:B:569:VAL:HG13 | 2.14 | 0.47 |
| 15:K:191:ASP:OD2 | 15:K:194:SER:OG | 2.26 | 0.47 |
| 15:K:259:LEU:HB2 | 15:K:261:VAL:HG12 | 1.96 | 0.47 |
| 18:N:149:ILE:HG13 | 18:N:152:LEU:HD12 | 1.96 | 0.47 |
| 18:N:945:LEU:HD13 | 18:N:966:LEU:HD21 | 1.97 | 0.47 |
| 22:R:289:GLN:O | 25:X:539:ARG:NH2 | 2.47 | 0.47 |
| 23:S:23:TYR:CG | 23:S:28:ILE:HD13 | 2.50 | 0.47 |
| 25:X:574:ASP:HA | 25:X:577:GLU:CD | 2.39 | 0.47 |
| 32:m:322:VAL:HB | 32:m:325:ALA:HB2 | 1.96 | 0.47 |
| 4:5:102:G:C5 | 10:F:20:LYS:NZ | 2.81 | 0.47 |
| 6:B:356:TRP:CG | 6:B:357:GLY:H | 2.33 | 0.47 |
| 18:N:219:VAL:HG12 | 18:N:223:LEU:HG | 1.94 | 0.47 |
| 18:N:410:GLN:O | 18:N:413:SER:OG | 2.31 | 0.47 |
| 19:O:26:PHE:CE1 | 19:O:55:GLN:HG2 | 2.49 | 0.47 |
| 20:P:261:ARG:O | 20:P:264:GLU:HG3 | 2.14 | 0.47 |
| 32:m:296:LYS:O | 32:m:300:ILE:HG12 | 2.13 | 0.47 |
| 38:6:86:A:H2' | 38:6:87:G:C8 | 2.48 | 0.47 |
| 5:A:1460:TRP:CD1 | 5:A:1460:TRP:H | 2.32 | 0.47 |
| 5:A:1963:ILE:O | 5:A:1967:LEU:HG | 2.15 | 0.47 |
| 7:C:188:GLN:OE1 | 7:C:190:THR:HG22 | 2.15 | 0.47 |
| 7:C:290:ASP:OD2 | 7:C:292:ASN:ND2 | 2.35 | 0.47 |
| 11:G:42:GLN:CG | 11:G:56:ARG:HH12 | 2.27 | 0.47 |
| 18:N:1223:THR:HB | 18:N:1226:LEU:HD12 | 1.97 | 0.47 |
| 22:R:84:LYS:HZ3 | 22:R:88:ARG:H | 1.62 | 0.47 |
| 22:R:158:ARG:O | 22:R:162:GLU:HG2 | 2.15 | 0.47 |
| 23:T:85:LEU:O | 23:T:89:GLU:HG2 | 2.15 | 0.47 |
| 7:C:103:ARG:NE | 7:C:145:LYS:O | 2.47 | 0.47 |
| 7:C:232:SER:O | 7:C:248:VAL:N | 2.44 | 0.47 |
| 11:G:44:LEU:HB3 | 11:G:110:VAL:HG23 | 1.96 | 0.47 |
| 18:N:634:ARG:HD2 | 18:N:967:LYS:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:O:6:THR:O | 19:O:9:THR:OG1 | 2.28 | 0.47 |
| 20:P:209:SER:HG | 20:P:210:ARG:NH1 | 2.12 | 0.47 |
| 23:U:5:ILE:HB | 23:U:27:LEU:HD13 | 1.97 | 0.47 |
| 23:V:88:PHE:O | 23:V:91:ARG:HG2 | 2.14 | 0.47 |
| 25:X:472:PRO:HA | 25:X:475:ARG:HB2 | 1.96 | 0.47 |
| 32:m:435:MET:O | 32:m:439:LYS:HB3 | 2.14 | 0.47 |
| 32:m:494:PRO:HD3 | 32:m:533:ILE:HD13 | 1.95 | 0.47 |
| 34:y:125:ILE:CG1 | 34:y:131:ARG:HD3 | 2.45 | 0.47 |
| 34:y:174:TYR:HE1 | 35:z:220:VAL:HG12 | 1.79 | 0.47 |
| 35:z:241:VAL:HG12 | 35:z:318:VAL:CG2 | 2.45 | 0.47 |
| 5:A:398:GLU:HG3 | 12:H:6:GLN:HE22 | 1.79 | 0.47 |
| 5:A:624:GLN:HG2 | 5:A:663:PHE:HB2 | 1.97 | 0.47 |
| 5:A:1490:GLN:NE2 | 5:A:1492:ASN:HB2 | 2.29 | 0.47 |
| 5:A:1799:GLN:OE1 | 5:A:1954:TYR:OH | 2.22 | 0.47 |
| 6:B:608:PRO:HD3 | 6:B:617:LEU:HD22 | 1.97 | 0.47 |
| 6:B:700:THR:HG23 | 6:B:806:MET:HB2 | 1.96 | 0.47 |
| 6:B:852:ALA:HB1 | 6:B:856:SER:HB2 | 1.96 | 0.47 |
| 11:G:77:GLU:OE2 | 11:G:92:LYS:NZ | 2.47 | 0.47 |
| 15:K:149:TRP:CE2 | 15:K:456:PRO:HA | 2.50 | 0.47 |
| 15:K:327:LEU:HD23 | 15:K:357:TRP:CE2 | 2.50 | 0.47 |
| 15:K:414:GLN:HB2 | 15:K:415:PRO:HD2 | 1.97 | 0.47 |
| 17:M:142:ASN:O | 17:M:146:LYS:HG2 | 2.14 | 0.47 |
| 18:N:240:ARG:HE | 18:N:285:THR:HA | 1.79 | 0.47 |
| 18:N:566:ASP:OD2 | 18:N:584:ASN:N | 2.27 | 0.47 |
| 18:N:745:MET:HB2 | 18:N:1039:ILE:HD12 | 1.96 | 0.47 |
| 18:N:777:LEU:HD23 | 18:N:978:VAL:HG13 | 1.95 | 0.47 |
| 20:P:99:ILE:HG23 | 20:P:103:SER:OG | 2.15 | 0.47 |
| 20:P:187:ILE:HA | 20:P:190:ILE:HG12 | 1.95 | 0.47 |
| 22:R:10:ASN:CG | 24:W:153:ILE:HB | 2.40 | 0.47 |
| 22:R:258:GLU:HA | 22:R:261:ARG:HG2 | 1.97 | 0.47 |
| 22:R:536:HIS:HB3 | 22:R:539:VAL:HG23 | 1.97 | 0.47 |
| 23:T:69:LEU:HB2 | 23:T:70:PRO:HD2 | 1.97 | 0.47 |
| 23:T:87:GLN:O | 23:T:91:ARG:HG2 | 2.15 | 0.47 |
| 24:W:627:TYR:O | 24:W:628:SER:C | 2.56 | 0.47 |
| 25:X:252:GLN:HB2 | 25:X:255:LYS:NZ | 2.29 | 0.47 |
| 25:X:610:SER:HA | 25:X:613:GLU:HG2 | 1.95 | 0.47 |
| 29:b:8:LEU:H | 29:b:8:LEU:HD23 | 1.79 | 0.47 |
| 32:m:753:GLN:HG3 | 32:m:754:ALA:H | 1.79 | 0.47 |
| 34:y:64:TYR:O | 34:y:65:PHE:CD1 | 2.68 | 0.47 |
| 35:z:456:LEU:HD11 | 35:z:469:LEU:HA | 1.96 | 0.47 |
| 5:A:1826:PRO:HG3 | 5:A:1857:LEU:HD11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:D:26:TYR:HD2 | 8:D:44:ILE:HG21 | 1.80 | 0.47 |
| 18:N:1011:GLN:HE21 | 18:N:1033:ARG:HD3 | 1.80 | 0.47 |
| 22:R:338:ILE:O | 22:R:341:THR:HG22 | 2.13 | 0.47 |
| 23:T:68:SER:N | 23:T:72:LEU:HD23 | 2.30 | 0.47 |
| 31:d:45:ARG:HB3 | 31:d:53:GLN:HB3 | 1.97 | 0.47 |
| 32:m:302:ARG:HG2 | 32:m:348:PHE:HD2 | 1.80 | 0.47 |
| 35:z:412:PRO:CB | 35:z:415:HIS:HD2 | 2.23 | 0.47 |
| 1:e:30:LEU:HD21 | 1:e:100:ILE:HG21 | 1.97 | 0.47 |
| 5:A:1594:LYS:O | 5:A:1598:ILE:HG12 | 2.15 | 0.47 |
| 6:B:490:MET:HG2 | 6:B:510:VAL:HA | 1.97 | 0.47 |
| 15:K:87:ASP:HA | 22:R:259:ARG:NH1 | 2.30 | 0.47 |
| 18:N:333:GLN:O | 18:N:337:GLU:OE1 | 2.33 | 0.47 |
| 19:O:101:CYS:SG | 19:O:102:CYS:N | 2.87 | 0.47 |
| 20:P:63:GLU:HG3 | 20:P:78:TRP:CH2 | 2.50 | 0.47 |
| 21:Q:54:ARG:HE | 21:Q:54:ARG:HB2 | 1.60 | 0.47 |
| 23:T:127:GLU:CD | 24:W:738:LYS:HZ1 | 2.21 | 0.47 |
| 23:V:91:ARG:HH12 | 23:V:92:ARG:HH11 | 1.63 | 0.47 |
| 23:V:106:TYR:HD1 | 23:V:109:ASP:HB2 | 1.79 | 0.47 |
| 25:X:541:VAL:HG21 | 25:X:553:TRP:NE1 | 2.30 | 0.47 |
| 26:Y:153:LEU:HD13 | 31:d:131:ARG:NH1 | 2.29 | 0.47 |
| 29:b:25:SER:O | 29:b:25:SER:OG | 2.31 | 0.47 |
| 35:z:162:LEU:O | 35:z:166:LEU:HD23 | 2.14 | 0.47 |
| 35:z:306:GLU:O | 35:z:353:ARG:NH1 | 2.48 | 0.47 |
| 6:B:559:VAL:HG12 | 6:B:560:ALA:N | 2.30 | 0.47 |
| 6:B:760:ARG:HH21 | 6:B:804:ARG:HD3 | 1.79 | 0.47 |
| 10:F:17:ILE:HB | 10:F:25:VAL:CG2 | 2.44 | 0.47 |
| 11:G:104:ASP:HA | 13:I:66:ARG:NH1 | 2.30 | 0.47 |
| 15:K:149:TRP:HH2 | 15:K:454:ALA:HA | 1.80 | 0.47 |
| 15:K:267:ARG:HG3 | 15:K:291:THR:CG2 | 2.44 | 0.47 |
| 20:P:63:GLU:HG3 | 20:P:78:TRP:CZ2 | 2.50 | 0.47 |
| 22:R:84:LYS:NZ | 22:R:88:ARG:H | 2.13 | 0.47 |
| 24:W:519:LYS:O | 24:W:523:ALA:N | 2.47 | 0.47 |
| 25:X:167:TYR:CE2 | 25:X:188:LEU:HD22 | 2.50 | 0.47 |
| 32:m:547:PHE:HA | 32:m:550:TRP:CD1 | 2.49 | 0.47 |
| 32:m:618:TRP:CZ2 | 32:m:622:LEU:HD11 | 2.50 | 0.47 |
| 2:p:187:LYS:HB2 | 2:p:192:LEU:HB3 | 1.97 | 0.46 |
| 5:A:803:THR:HG23 | 5:A:921:PHE:CD1 | 2.50 | 0.46 |
| 5:A:906:ARG:HB3 | 5:A:906:ARG:NH1 | 2.30 | 0.46 |
| 5:A:1996:ASP:N | 5:A:1999:GLN:OE1 | 2.27 | 0.46 |
| 10:F:23:THR:OG1 | 10:F:46:THR:O | 2.23 | 0.46 |
| 15:K:435:ARG:NE | 21:Q:61:GLU:OE2 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:P:292:ASN:ND2 | 20:P:293:ARG:HH11 | 2.13 | 0.46 |
| 23:S:64:PRO:HG3 | 23:T:9:THR:HG21 | 1.96 | 0.46 |
| 23:S:95:THR:O | 23:S:99:GLN:HG3 | 2.14 | 0.46 |
| 23:V:16:SER:HB3 | 23:V:20:GLY:HA2 | 1.97 | 0.46 |
| 23:V:91:ARG:NH1 | 23:V:92:ARG:HH11 | 2.14 | 0.46 |
| 24:W:685:SER:HB3 | 27:Z:120:PHE:CZ | 2.50 | 0.46 |
| 26:Y:116:TYR:O | 26:Y:120:ILE:HG12 | 2.15 | 0.46 |
| 34:y:72:GLU:CD | 34:y:72:GLU:H | 2.24 | 0.46 |
| 35:z:76:CYS:O | 35:z:121:TYR:HA | 2.14 | 0.46 |
| 5:A:111:GLY:HA3 | 16:L:214:PRO:HD3 | 1.97 | 0.46 |
| 5:A:530:LEU:HD21 | 5:A:678:LEU:HD21 | 1.96 | 0.46 |
| 5:A:552:THR:HB | 34:y:65:PHE:HD2 | 1.80 | 0.46 |
| 5:A:1659:TYR:HB2 | 5:A:1661:TRP:CZ2 | 2.51 | 0.46 |
| 13:I:28:GLN:OE1 | 13:I:28:GLN:N | 2.48 | 0.46 |
| 17:M:69:ILE:HD11 | 17:M:74:ALA:HB2 | 1.97 | 0.46 |
| 18:N:551:LEU:H | 18:N:551:LEU:HD23 | 1.80 | 0.46 |
| 18:N:715:ARG:NH1 | 18:N:768:THR:O | 2.46 | 0.46 |
| 23:U:83:VAL:O | 23:U:87:GLN:HG2 | 2.15 | 0.46 |
| 23:V:106:TYR:HB3 | 24:W:564:MET:SD | 2.55 | 0.46 |
| 24:W:158:ASP:OD1 | 24:W:159:GLU:N | 2.48 | 0.46 |
| 25:X:584:PRO:HB2 | 25:X:586:GLU:OE1 | 2.15 | 0.46 |
| 26:Y:183:THR:HG23 | 26:Y:184:LYS:HG2 | 1.97 | 0.46 |
| 32:m:279:ARG:HB3 | 32:m:283:LYS:HE3 | 1.96 | 0.46 |
| 35:z:497:SER:HA | 35:z:500:PHE:HD2 | 1.80 | 0.46 |
| 35:z:582:ALA:HB1 | 35:z:590:TYR:HB3 | 1.97 | 0.46 |
| 1:e:261:VAL:HG13 | 1:e:262:ASN:H | 1.80 | 0.46 |
| 4:5:96:G:H21 | 13:I:41:MET:HG3 | 1.81 | 0.46 |
| 5:A:1427:LEU:HB3 | 34:y:233:ILE:HD11 | 1.97 | 0.46 |
| 18:N:1011:GLN:HG2 | 18:N:1029:PHE:HE2 | 1.80 | 0.46 |
| 20:P:177:TYR:HD2 | 20:P:244:ARG:HB2 | 1.80 | 0.46 |
| 22:R:454:ARG:HG2 | 22:R:474:TYR:HE1 | 1.79 | 0.46 |
| 22:R:487:ALA:HA | 22:R:490:LEU:HD12 | 1.97 | 0.46 |
| 24:W:236:TYR:HD1 | 26:Y:156:VAL:HG13 | 1.81 | 0.46 |
| 25:X:463:ILE:HG23 | 25:X:470:LEU:HD22 | 1.96 | 0.46 |
| 32:m:285:GLU:O | 32:m:289:VAL:HG23 | 2.15 | 0.46 |
| 35:z:330:PRO:HG3 | 35:z:415:HIS:CE1 | 2.51 | 0.46 |
| 4:5:96:G:C5 | 12:H:48:PHE:CE2 | 3.03 | 0.46 |
| 5:A:208:LEU:HG | 5:A:209:GLU:H | 1.80 | 0.46 |
| 5:A:681:ARG:HE | 5:A:686:ARG:HH22 | 1.64 | 0.46 |
| 5:A:718:ASP:OD1 | 15:K:333:THR:HG22 | 2.15 | 0.46 |
| 5:A:1214:MET:HG2 | 5:A:1215:THR:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:183:HIS:O | 6:B:187:ARG:HG2 | 2.16 | 0.46 |
| 6:B:715:GLU:OE2 | 6:B:799:ARG:NH2 | 2.49 | 0.46 |
| 7:C:57:ARG:HG2 | 7:C:57:ARG:HH11 | 1.80 | 0.46 |
| 12:H:33:GLN:HG2 | 12:H:36:ILE:HD13 | 1.98 | 0.46 |
| 13:I:49:GLU:HB2 | 13:I:56:LYS:HZ2 | 1.79 | 0.46 |
| 20:P:159:TYR:OH | 20:P:173:ASN:ND2 | 2.47 | 0.46 |
| 22:R:324:ASP:O | 22:R:327:LYS:HG2 | 2.16 | 0.46 |
| 24:W:514:GLU:HA | 24:W:517:ALA:HB3 | 1.97 | 0.46 |
| 25:X:500:ARG:HA | 25:X:500:ARG:NH1 | 2.30 | 0.46 |
| 28:a:64:GLN:HA | 31:d:62:ARG:NH1 | 2.30 | 0.46 |
| 30:c:427:GLU:OE1 | 30:c:470:ARG:NH1 | 2.48 | 0.46 |
| 32:m:777:SER:OG | 32:m:779:ASP:OD1 | 2.24 | 0.46 |
| 35:z:268:GLN:HE22 | 35:z:296:ARG:HH21 | 1.63 | 0.46 |
| 1:e:218:ILE:HG23 | 21:Q:230:VAL:HG12 | 1.97 | 0.46 |
| 4:5:82:A:HO2' | 4:5:83:A:H8 | 1.57 | 0.46 |
| 13:I:7:ASN:HB2 | 13:I:10:PRO:HD2 | 1.98 | 0.46 |
| 17:M:148:GLU:OE1 | 17:M:148:GLU:HA | 2.16 | 0.46 |
| 19:O:39:LYS:HD2 | 19:O:39:LYS:O | 2.15 | 0.46 |
| 20:P:52:LYS:HD3 | 20:P:54:ILE:O | 2.16 | 0.46 |
| 22:R:273:ARG:NH1 | 22:R:309:GLU:OE1 | 2.48 | 0.46 |
| 23:U:356:GLU:HA | 23:U:372:GLY:HA2 | 1.96 | 0.46 |
| 24:W:242:ASP:OD1 | 24:W:243:ARG:N | 2.46 | 0.46 |
| 25:X:358:ARG:HH12 | 25:X:362:LEU:HB2 | 1.79 | 0.46 |
| 25:X:599:GLU:HG2 | 25:X:603:GLY:HA3 | 1.97 | 0.46 |
| 32:m:278:ARG:HH21 | 33:n:324:ILE:HA | 1.80 | 0.46 |
| 2:p:169:PHE:HD1 | 2:p:172:ARG:HH22 | 1.62 | 0.46 |
| 5:A:267:ASP:N | 5:A:267:ASP:OD1 | 2.46 | 0.46 |
| 5:A:1432:LEU:HD12 | 5:A:1447:PHE:CZ | 2.51 | 0.46 |
| 7:C:112:SER:O | 7:C:138:VAL:HG12 | 2.15 | 0.46 |
| 11:G:12:LEU:HD23 | 11:G:16:GLU:CB | 2.46 | 0.46 |
| 11:G:34:GLN:O | 11:G:38:LYS:HG3 | 2.15 | 0.46 |
| 13:I:30:TYR:HE1 | 13:I:50:GLU:HG2 | 1.79 | 0.46 |
| 17:M:258:SER:O | 17:M:262:ILE:HG23 | 2.16 | 0.46 |
| 18:N:405:ARG:NH1 | 18:N:548:LEU:O | 2.48 | 0.46 |
| 22:R:275:LYS:HA | 22:R:277:MET:HE1 | 1.96 | 0.46 |
| 24:W:196:LEU:HD21 | 24:W:200:ARG:NH2 | 2.30 | 0.46 |
| 25:X:573:ARG:HG3 | 25:X:574:ASP:N | 2.30 | 0.46 |
| 25:X:717:VAL:HA | 25:X:720:MET:HE2 | 1.98 | 0.46 |
| 26:Y:118:ARG:HH11 | 26:Y:121:ARG:HH11 | 1.64 | 0.46 |
| 28:a:23:PRO:O | 28:a:27:THR:N | 2.43 | 0.46 |
| 30:c:593:LEU:O | 30:c:595:ALA:N | 2.41 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:m:358:ASP:HB2 | 32:m:429:HIS:HB3 | 1.98 | 0.46 |
| 32:m:505:HIS:NE2 | 32:m:506:HIS:CE1 | 2.84 | 0.46 |
| 33:n:307:LYS:O | 33:n:310:ILE:HG22 | 2.16 | 0.46 |
| 34:y:179:TYR:OH | 35:z:217:GLU:OE2 | 2.32 | 0.46 |
| 5:A:300:PRO:O | 5:A:301:LEU:HB3 | 2.16 | 0.46 |
| 5:A:1315:CYS:HA | 5:A:1318:LYS:HG2 | 1.97 | 0.46 |
| 5:A:1378:ARG:HD2 | 29:b:8:LEU:HD22 | 1.98 | 0.46 |
| 7:C:57:ARG:HD2 | 7:C:99:LEU:O | 2.16 | 0.46 |
| 22:R:289:GLN:C | 25:X:539:ARG:HH12 | 2.24 | 0.46 |
| 23:S:10:PRO:HG3 | 23:S:22:VAL:HG12 | 1.98 | 0.46 |
| 23:V:71:ALA:O | 23:V:75:LEU:HG | 2.16 | 0.46 |
| 25:X:458:PRO:HG2 | 25:X:461:SER:HB3 | 1.98 | 0.46 |
| 26:Y:165:VAL:O | 26:Y:169:VAL:HG23 | 2.16 | 0.46 |
| 5:A:1669:LEU:HD11 | 5:A:1750:ILE:HD11 | 1.97 | 0.46 |
| 6:B:631:SER:HA | 6:B:644:PHE:O | 2.16 | 0.46 |
| 13:I:22:VAL:HG12 | 13:I:73:VAL:HG22 | 1.98 | 0.46 |
| 17:M:168:GLN:NE2 | 17:M:169:ILE:HG23 | 2.30 | 0.46 |
| 18:N:520:LEU:HD22 | 18:N:524:ILE:HD11 | 1.97 | 0.46 |
| 18:N:974:ASN:ND2 | 18:N:1001:GLY:O | 2.47 | 0.46 |
| 22:R:93:PHE:CD2 | 22:R:110:TYR:HD1 | 2.34 | 0.46 |
| 22:R:363:TYR:O | 22:R:366:LEU:HG | 2.16 | 0.46 |
| 23:U:94:LEU:HG | 23:U:98:LYS:HE3 | 1.98 | 0.46 |
| 23:V:25:LYS:O | 23:V:29:GLU:HG2 | 2.15 | 0.46 |
| 32:m:559:LEU:O | 32:m:563:LEU:HG | 2.16 | 0.46 |
| 34:y:116:ILE:H | 35:z:643:TYR:HH | 1.60 | 0.46 |
| 34:y:124:PRO:HB3 | 34:y:138:ASP:HB2 | 1.98 | 0.46 |
| 35:z:392:LEU:HD22 | 35:z:444:SER:HA | 1.97 | 0.46 |
| 5:A:177:ARG:HD3 | 5:A:643:PRO:HB2 | 1.96 | 0.46 |
| 5:A:1556:ARG:HG2 | 5:A:1592:THR:HG23 | 1.97 | 0.46 |
| 5:A:1657:ALA:O | 5:A:1683:LYS:NZ | 2.49 | 0.46 |
| 5:A:1892:MET:O | 5:A:1896:LEU:HG | 2.16 | 0.46 |
| 6:B:584:LEU:HD23 | 6:B:585:LYS:O | 2.16 | 0.46 |
| 6:B:628:TYR:O | 6:B:631:SER:OG | 2.28 | 0.46 |
| 6:B:812:PRO:O | 6:B:817:ARG:NH2 | 2.49 | 0.46 |
| 6:B:832:SER:OG | 6:B:966:TYR:O | 2.33 | 0.46 |
| 9:E:62:LYS:HA | 9:E:62:LYS:HD2 | 1.75 | 0.46 |
| 11:G:110:VAL:HG12 | 13:I:63:ILE:HD13 | 1.98 | 0.46 |
| 15:K:169:VAL:HB | 15:K:439:CYS:SG | 2.56 | 0.46 |
| 15:K:472:ARG:HD2 | 15:K:472:ARG:HA | 1.77 | 0.46 |
| 16:L:180:ASP:OD1 | 16:L:180:ASP:N | 2.47 | 0.46 |
| 18:N:14:TYR:HB3 | 18:N:31:MET:HE1 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:N:53:HIS:CE1 | 18:N:85:LYS:HG2 | 2.51 | 0.46 |
| 18:N:561:THR:O | 18:N:586:TYR:N | 2.47 | 0.46 |
| 18:N:869:TYR:CE1 | 18:N:873:VAL:HG21 | 2.51 | 0.46 |
| 22:R:41:ASN:OD1 | 24:W:267:GLU:HG3 | 2.16 | 0.46 |
| 22:R:194:TYR:O | 22:R:198:VAL:HG22 | 2.15 | 0.46 |
| 22:R:300:VAL:O | 22:R:304:ARG:HD3 | 2.16 | 0.46 |
| 23:V:106:TYR:HB2 | 24:W:568:ILE:CG1 | 2.45 | 0.46 |
| 26:Y:183:THR:HA | 38:6:79:C:C5 | 2.51 | 0.46 |
| 32:m:335:GLN:N | 32:m:336:PRO:HD2 | 2.31 | 0.46 |
| 34:y:125:ILE:HD11 | 34:y:130:LEU:C | 2.41 | 0.46 |
| 35:z:191:GLY:O | 35:z:195:VAL:HG22 | 2.16 | 0.46 |
| 4:5:107:C:O2' | 4:5:108:U:H5' | 2.16 | 0.46 |
| 5:A:1747:LYS:O | 5:A:1751:GLN:HG3 | 2.16 | 0.46 |
| 6:B:848:VAL:HG12 | 6:B:913:MET:HG2 | 1.98 | 0.46 |
| 14:J:10:LYS:HE2 | 14:J:10:LYS:HB2 | 1.72 | 0.46 |
| 15:K:355:LYS:HB2 | 15:K:357:TRP:CH2 | 2.51 | 0.46 |
| 18:N:1240:LEU:HB3 | 18:N:1263:ILE:HB | 1.98 | 0.46 |
| 24:W:537:ARG:HG3 | 24:W:538:PRO:HD2 | 1.98 | 0.46 |
| 25:X:468:GLU:HA | 25:X:475:ARG:HH22 | 1.81 | 0.46 |
| 25:X:526:GLU:OE2 | 25:X:527:ASN:ND2 | 2.49 | 0.46 |
| 32:m:512:LEU:HB2 | 32:m:513:PRO:HD3 | 1.97 | 0.46 |
| 32:m:534:LEU:HA | 32:m:537:TRP:HB2 | 1.97 | 0.46 |
| 2:p:199:PRO:HD3 | 25:X:722:ARG:HH22 | 1.80 | 0.45 |
| 5:A:1438:ARG:HG2 | 30:c:458:ARG:HH21 | 1.80 | 0.45 |
| 6:B:97:ASP:OD2 | 15:K:199:LEU:HA | 2.16 | 0.45 |
| 9:E:24:PHE:HB3 | 9:E:42:CYS:SG | 2.56 | 0.45 |
| 11:G:38:LYS:HB3 | 11:G:38:LYS:HE3 | 1.83 | 0.45 |
| 16:L:142:SER:OG | 16:L:143:ASP:N | 2.42 | 0.45 |
| 18:N:1124:ARG:NH1 | 18:N:1128:TYR:O | 2.49 | 0.45 |
| 20:P:61:GLU:O | 20:P:61:GLU:HG2 | 2.16 | 0.45 |
| 23:U:99:GLN:OE1 | 24:W:712:THR:OG1 | 2.18 | 0.45 |
| 25:X:703:TRP:HZ2 | 25:X:720:MET:HB2 | 1.81 | 0.45 |
| 30:c:585:ILE:O | 30:c:589:THR:HG23 | 2.16 | 0.45 |
| 5:A:1479:TRP:CD1 | 5:A:1479:TRP:H | 2.33 | 0.45 |
| 6:B:933:LYS:NZ | 6:B:935:LEU:HB2 | 2.31 | 0.45 |
| 18:N:529:LEU:HD12 | 18:N:530:CYS:N | 2.30 | 0.45 |
| 24:W:97:ARG:NH1 | 24:W:100:LYS:HE2 | 2.31 | 0.45 |
| 26:Y:92:ARG:HH22 | 38:6:92:C:H5' | 1.81 | 0.45 |
| 31:d:10:LEU:CD2 | 31:d:147:LEU:HD11 | 2.46 | 0.45 |
| 34:y:165:ASP:O | 34:y:169:LEU:HG | 2.15 | 0.45 |
| 5:A:1746:MET:HE1 | 5:A:1749:LEU:HD23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1825:LYS:HE2 | 5:A:1848:THR:HG21 | 1.99 | 0.45 |
| 6:B:520:LYS:HE2 | 6:B:540:HIS:NE2 | 2.30 | 0.45 |
| 6:B:813:GLU:OE2 | 6:B:815:ILE:HB | 2.16 | 0.45 |
| 19:O:101:CYS:HB3 | 19:O:142:CYS:SG | 2.56 | 0.45 |
| 23:U:389:TRP:O | 23:U:390:LEU:HD23 | 2.17 | 0.45 |
| 25:X:573:ARG:O | 25:X:577:GLU:OE1 | 2.34 | 0.45 |
| 28:a:21:ILE:O | 28:a:25:LEU:N | 2.45 | 0.45 |
| 30:c:509:ALA:HB2 | 30:c:543:MET:HG3 | 1.99 | 0.45 |
| 35:z:383:LEU:O | 35:z:383:LEU:HD23 | 2.16 | 0.45 |
| 1:e:204:HIS:CD2 | 6:B:76:GLN:H | 2.34 | 0.45 |
| 5:A:1664:SER:O | 5:A:1741:ASN:ND2 | 2.50 | 0.45 |
| 5:A:1803:PHE:HB3 | 5:A:1805:ASP:OD1 | 2.17 | 0.45 |
| 6:B:325:ASP:HB2 | 42:B:1001:GTP:C5 | 2.52 | 0.45 |
| 6:B:406:LYS:HB3 | 6:B:406:LYS:HE3 | 1.80 | 0.45 |
| 7:C:57:ARG:HG2 | 7:C:57:ARG:NH1 | 2.31 | 0.45 |
| 8:D:70:ILE:CD1 | 9:E:68:VAL:HG22 | 2.46 | 0.45 |
| 11:G:35:GLN:HG2 | 11:G:111:ARG:HH22 | 1.81 | 0.45 |
| 20:P:119:TYR:HD2 | 38:6:23:A:C6 | 2.34 | 0.45 |
| 24:W:530:VAL:HG23 | 24:W:531:ILE:H | 1.81 | 0.45 |
| 25:X:448:ARG:NH1 | 25:X:498:THR:HG21 | 2.32 | 0.45 |
| 31:d:90:MET:HG2 | 31:d:119:PHE:CE1 | 2.51 | 0.45 |
| 34:y:98:MET:HE3 | 34:y:102:ASP:HB3 | 1.98 | 0.45 |
| 1:e:204:HIS:CE1 | 6:B:70:VAL:HG21 | 2.52 | 0.45 |
| 1:e:256:TYR:CE2 | 30:c:595:ALA:HA | 2.37 | 0.45 |
| 5:A:985:LEU:HB2 | 5:A:988:VAL:HB | 1.98 | 0.45 |
| 5:A:1416:LYS:HA | 5:A:1419:GLU:HG3 | 1.98 | 0.45 |
| 5:A:1955:THR:O | 5:A:1959:ARG:HG2 | 2.16 | 0.45 |
| 6:B:466:ILE:HG12 | 6:B:590:ILE:O | 2.15 | 0.45 |
| 7:C:53:VAL:HG23 | 7:C:328:CYS:SG | 2.57 | 0.45 |
| 7:C:227:ILE:HD11 | 7:C:248:VAL:HG21 | 1.98 | 0.45 |
| 15:K:470:ARG:NH1 | 15:K:472:ARG:HD2 | 2.31 | 0.45 |
| 16:L:124:LEU:CD1 | 16:L:234:LEU:HD22 | 2.46 | 0.45 |
| 16:L:159:LYS:HB2 | 16:L:159:LYS:HE2 | 1.75 | 0.45 |
| 16:L:331:LEU:HD13 | 32:m:513:PRO:HG2 | 1.99 | 0.45 |
| 18:N:638:PHE:HE1 | 18:N:990:THR:HG23 | 1.80 | 0.45 |
| 18:N:670:LEU:HG | 18:N:732:LEU:HD22 | 1.99 | 0.45 |
| 22:R:146:TYR:CE1 | 22:R:150:MET:HE3 | 2.52 | 0.45 |
| 23:S:79:GLU:OE1 | 23:S:80:TRP:HD1 | 1.99 | 0.45 |
| 24:W:135:ARG:HG3 | 24:W:136:PHE:CD2 | 2.51 | 0.45 |
| 24:W:244:GLN:HG2 | 24:W:245:ASN:HD22 | 1.81 | 0.45 |
| 24:W:545:LYS:HG2 | 36:r:233:UNK:HA | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:W:640:LEU:O | 24:W:640:LEU:HD23 | 2.16 | 0.45 |
| 25:X:144:HIS:HB2 | 25:X:148:TRP:NE1 | 2.31 | 0.45 |
| 25:X:434:TRP:HA | 25:X:437:MET:HG3 | 1.98 | 0.45 |
| 26:Y:140:LYS:O | 26:Y:142:ARG:HD3 | 2.17 | 0.45 |
| 28:a:143:ASP:OD1 | 28:a:144:PRO:HD2 | 2.17 | 0.45 |
| 34:y:31:ARG:HA | 35:z:493:PHE:HE2 | 1.81 | 0.45 |
| 35:z:256:ILE:HG13 | 35:z:300:PHE:HZ | 1.80 | 0.45 |
| 35:z:302:THR:OG1 | 35:z:303:ASN:N | 2.48 | 0.45 |
| 4:5:27:G:N3 | 4:5:27:G:H2' | 2.32 | 0.45 |
| 6:B:726:LYS:HD3 | 6:B:726:LYS:N | 2.31 | 0.45 |
| 7:C:239:MET:HA | 7:C:266:HIS:ND1 | 2.31 | 0.45 |
| 10:F:75:PRO:HB2 | 10:F:78:THR:OG1 | 2.16 | 0.45 |
| 13:I:15:LEU:HD21 | 13:I:20:VAL:CG1 | 2.46 | 0.45 |
| 13:I:21:LEU:HD12 | 13:I:30:TYR:O | 2.16 | 0.45 |
| 13:I:26:TRP:CH2 | 13:I:69:ASN:ND2 | 2.84 | 0.45 |
| 16:L:299:GLU:OE1 | 16:L:303:ARG:NH2 | 2.50 | 0.45 |
| 17:M:109:ASN:OD1 | 17:M:112:ASN:HB2 | 2.15 | 0.45 |
| 17:M:111:ILE:O | 17:M:114:GLU:HG3 | 2.17 | 0.45 |
| 18:N:860:ALA:HA | 25:X:103:ILE:HG12 | 1.99 | 0.45 |
| 20:P:51:ARG:HH21 | 20:P:101:ARG:HG3 | 1.82 | 0.45 |
| 20:P:75:TYR:O | 20:P:77:LYS:N | 2.50 | 0.45 |
| 23:S:55:VAL:HG11 | 27:Z:133:LEU:CD2 | 2.47 | 0.45 |
| 23:T:111:ALA:O | 23:T:115:ILE:HG23 | 2.16 | 0.45 |
| 23:U:371:PHE:HE1 | 27:Z:35:ARG:HA | 1.81 | 0.45 |
| 25:X:503:TYR:O | 25:X:507:PHE:HD2 | 1.99 | 0.45 |
| 34:y:164:TYR:OH | 35:z:331:TYR:HD2 | 1.99 | 0.45 |
| 1:e:256:TYR:HB3 | 30:c:601:ARG:HH22 | 1.82 | 0.45 |
| 5:A:247:TRP:HD1 | 5:A:441:THR:HG23 | 1.81 | 0.45 |
| 5:A:819:LYS:HA | 5:A:819:LYS:HD3 | 1.74 | 0.45 |
| 5:A:1617:LEU:O | 5:A:1621:LEU:HD23 | 2.16 | 0.45 |
| 12:H:28:ILE:HG23 | 12:H:78:ILE:HG23 | 1.99 | 0.45 |
| 22:R:257:TYR:CE1 | 22:R:290:PHE:CD2 | 3.04 | 0.45 |
| 25:X:202:LEU:HB2 | 25:X:218:ILE:HG21 | 1.98 | 0.45 |
| 25:X:661:LYS:HA | 25:X:664:CYS:HB2 | 1.99 | 0.45 |
| 35:z:240:LEU:HB3 | 35:z:317:VAL:HG22 | 1.99 | 0.45 |
| 4:5:96:G:C4 | 12:H:48:PHE:CE2 | 3.04 | 0.45 |
| 5:A:906:ARG:HH22 | 24:W:140:GLU:HB2 | 1.82 | 0.45 |
| 5:A:1727:ILE:HG22 | 5:A:1738:ALA:HB2 | 1.99 | 0.45 |
| 6:B:828:ARG:HE | 6:B:828:ARG:HB3 | 1.52 | 0.45 |
| 7:C:142:ASP:OD1 | 7:C:143:VAL:N | 2.50 | 0.45 |
| 8:D:57:ASP:OD1 | 8:D:58:GLN:N | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:36:MET:HE3 | 11:G:102:ARG:HG3 | 1.98 | 0.45 |
| 17:M:39:PRO:HA | 17:M:52:THR:HG22 | 1.98 | 0.45 |
| 17:M:116:PHE:HE1 | 17:M:120:GLN:HE21 | 1.65 | 0.45 |
| 18:N:256:ARG:HG3 | 18:N:261:TYR:CE2 | 2.52 | 0.45 |
| 19:O:120:ARG:HH11 | 19:O:142:CYS:HB3 | 1.81 | 0.45 |
| 25:X:238:VAL:HG13 | 25:X:242:PHE:CD2 | 2.52 | 0.45 |
| 31:d:74:ASP:OD1 | 31:d:74:ASP:N | 2.48 | 0.45 |
| 34:y:64:TYR:O | 34:y:65:PHE:HD1 | 1.99 | 0.45 |
| 35:z:109:PHE:CG | 35:z:542:ILE:HD13 | 2.51 | 0.45 |
| 35:z:241:VAL:HG21 | 35:z:300:PHE:CD1 | 2.49 | 0.45 |
| 35:z:241:VAL:CG2 | 35:z:300:PHE:HD1 | 2.29 | 0.45 |
| 35:z:336:LYS:HB3 | 35:z:621:GLU:OE1 | 2.17 | 0.45 |
| 5:A:229:GLU:HB2 | 5:A:232:ALA:HA | 1.98 | 0.45 |
| 5:A:843:ARG:NH2 | 5:A:1086:GLY:O | 2.40 | 0.45 |
| 5:A:904:ILE:O | 5:A:908:LEU:HD13 | 2.16 | 0.45 |
| 5:A:1686:ILE:HG12 | 5:A:1725:VAL:HB | 1.98 | 0.45 |
| 6:B:179:TYR:CE1 | 6:B:550:ARG:HD2 | 2.52 | 0.45 |
| 6:B:229:ALA:HB3 | 6:B:230:PRO:HD3 | 1.99 | 0.45 |
| 7:C:45:GLN:HB2 | 9:E:104:ALA:HB3 | 1.99 | 0.45 |
| 10:F:16:SER:HB3 | 10:F:69:ILE:HB | 1.99 | 0.45 |
| 12:H:29:TRP:N | 12:H:29:TRP:CD1 | 2.83 | 0.45 |
| 15:K:452:ASP:N | 15:K:452:ASP:OD1 | 2.50 | 0.45 |
| 16:L:311:ILE:O | 16:L:314:GLN:HG3 | 2.17 | 0.45 |
| 18:N:326:GLN:HG3 | 25:X:271:GLU:HG2 | 1.98 | 0.45 |
| 18:N:737:ARG:HH11 | 18:N:1040:ILE:HD11 | 1.82 | 0.45 |
| 22:R:345:ALA:O | 22:R:349:VAL:HG13 | 2.16 | 0.45 |
| 23:S:61:PRO:CG | 24:W:697:ILE:HD11 | 2.44 | 0.45 |
| 23:U:126:ARG:HG2 | 23:U:126:ARG:HH11 | 1.82 | 0.45 |
| 25:X:246:ILE:HA | 25:X:256:LEU:HD12 | 1.99 | 0.45 |
| 25:X:286:THR:HG22 | 25:X:287:VAL:N | 2.31 | 0.45 |
| 26:Y:124:LYS:HG3 | 26:Y:127:TYR:OH | 2.16 | 0.45 |
| 32:m:369:LEU:HA | 32:m:372:PRO:HD2 | 1.99 | 0.45 |
| 35:z:239:ILE:HA | 35:z:316:TYR:O | 2.17 | 0.45 |
| 35:z:580:ASN:O | 35:z:615:MET:HG2 | 2.17 | 0.45 |
| 11:G:103:GLY:O | 13:I:66:ARG:NH1 | 2.50 | 0.45 |
| 19:O:125:LYS:HE3 | 19:O:125:LYS:HB3 | 1.78 | 0.45 |
| 20:P:294:LYS:N | 20:P:294:LYS:HD2 | 2.32 | 0.45 |
| 25:X:588:SER:HB2 | 25:X:592:TYR:CE2 | 2.52 | 0.45 |
| 27:Z:181:ARG:O | 27:Z:184:THR:OG1 | 2.32 | 0.45 |
| 32:m:740:HIS:HB2 | 32:m:747:LEU:HD11 | 1.99 | 0.45 |
| 5:A:783:ARG:HG2 | 5:A:788:ALA:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:95:LEU:HD12 | 9:E:96:SER:H | 1.81 | 0.44 |
| 11:G:46:ASN:OD1 | 11:G:108:LEU:HB2 | 2.16 | 0.44 |
| 18:N:266:LEU:HD11 | 18:N:419:LEU:HD11 | 1.99 | 0.44 |
| 18:N:1032:LEU:HD23 | 18:N:1035:LEU:HD12 | 1.99 | 0.44 |
| 22:R:150:MET:HG3 | 26:Y:168:LEU:HD21 | 1.99 | 0.44 |
| 25:X:288:ARG:O | 25:X:291:THR:OG1 | 2.23 | 0.44 |
| 25:X:401:GLU:OE1 | 25:X:437:MET:HE2 | 2.16 | 0.44 |
| 25:X:534:PHE:HA | 25:X:537:TYR:HD2 | 1.81 | 0.44 |
| 28:a:62:MET:O | 28:a:64:GLN:HG2 | 2.17 | 0.44 |
| 34:y:64:TYR:HB2 | 34:y:69:GLY:O | 2.17 | 0.44 |
| 35:z:428:VAL:HG13 | 35:z:429:LEU:CD1 | 2.45 | 0.44 |
| 1:e:30:LEU:HD11 | 1:e:124:PHE:HD1 | 1.83 | 0.44 |
| 5:A:532:HIS:C | 5:A:534:LYS:H | 2.24 | 0.44 |
| 5:A:533:ARG:HG2 | 5:A:533:ARG:O | 2.17 | 0.44 |
| 6:B:701:MET:SD | 6:B:803:PHE:HB3 | 2.57 | 0.44 |
| 10:F:24:ILE:O | 10:F:46:THR:OG1 | 2.30 | 0.44 |
| 18:N:251:PHE:CE2 | 18:N:255:LEU:HD11 | 2.53 | 0.44 |
| 18:N:488:VAL:HG21 | 18:N:602:ARG:HH12 | 1.82 | 0.44 |
| 18:N:1136:CYS:HA | 18:N:1167:GLY:O | 2.17 | 0.44 |
| 22:R:189:ARG:NH1 | 26:Y:147:TYR:HB3 | 2.32 | 0.44 |
| 22:R:369:CYS:HA | 22:R:372:GLU:HG2 | 2.00 | 0.44 |
| 23:U:217:PRO:HG3 | 23:U:479:THR:HG21 | 1.99 | 0.44 |
| 25:X:355:TRP:O | 25:X:359:VAL:HG23 | 2.17 | 0.44 |
| 25:X:357:ARG:HD3 | 25:X:360:LYS:HD2 | 1.99 | 0.44 |
| 26:Y:117:ASN:O | 26:Y:121:ARG:HG3 | 2.18 | 0.44 |
| 35:z:241:VAL:CG2 | 35:z:300:PHE:HA | 2.47 | 0.44 |
| 6:B:717:GLY:HA2 | 6:B:754:ARG:NH1 | 2.32 | 0.44 |
| 10:F:68:TYR:HD2 | 11:G:100:PHE:CD1 | 2.35 | 0.44 |
| 23:U:272:ILE:O | 23:U:286:GLY:N | 2.50 | 0.44 |
| 30:c:540:LEU:HD12 | 30:c:544:PHE:HE2 | 1.83 | 0.44 |
| 34:y:158:SER:HB3 | 35:z:412:PRO:HG3 | 1.99 | 0.44 |
| 34:y:171:ASN:HD22 | 35:z:623:GLU:CD | 2.23 | 0.44 |
| 38:6:33:A:H2' | 38:6:34:U:C6 | 2.52 | 0.44 |
| 4:5:102:G:C4 | 10:F:20:LYS:NZ | 2.85 | 0.44 |
| 5:A:79:LYS:NZ | 5:A:505:PHE:O | 2.30 | 0.44 |
| 5:A:1153:LYS:HD3 | 5:A:1153:LYS:N | 2.31 | 0.44 |
| 5:A:1629:GLN:NE2 | 5:A:1657:ALA:HB2 | 2.32 | 0.44 |
| 5:A:1887:VAL:HG11 | 5:A:1892:MET:CG | 2.48 | 0.44 |
| 6:B:387:GLU:O | 6:B:391:LYS:HG3 | 2.17 | 0.44 |
| 6:B:576:THR:HG21 | 6:B:594:ILE:HG12 | 1.99 | 0.44 |
| 6:B:699:ILE:HG13 | 6:B:808:VAL:HG22 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:14:LEU:HD13 | 9:E:28:LEU:HB2 | 1.98 | 0.44 |
| 22:R:83:GLN:HA | 24:W:256:ILE:HG21 | 1.99 | 0.44 |
| 23:S:103:THR:HA | 23:S:106:TYR:CZ | 2.53 | 0.44 |
| 28:a:92:GLU:HG2 | 28:a:94:VAL:HG23 | 1.99 | 0.44 |
| 29:b:3:TYR:HB3 | 39:1:-10:A:C2 | 2.52 | 0.44 |
| 32:m:383:TYR:HA | 32:m:386:LEU:HD12 | 1.99 | 0.44 |
| 38:6:44:A:H2' | 38:6:45:U:C6 | 2.52 | 0.44 |
| 4:5:77:G:H2' | 4:5:78:U:O4' | 2.18 | 0.44 |
| 16:L:235:HIS:O | 22:R:136:ARG:HG3 | 2.17 | 0.44 |
| 18:N:206:SER:CB | 18:N:225:ILE:HD13 | 2.39 | 0.44 |
| 18:N:473:THR:HG22 | 18:N:477:PHE:O | 2.17 | 0.44 |
| 18:N:1181:VAL:HG12 | 18:N:1207:CYS:HB2 | 1.98 | 0.44 |
| 22:R:327:LYS:HG3 | 22:R:328:LEU:HD22 | 1.99 | 0.44 |
| 23:S:76:PHE:HE1 | 23:T:72:LEU:HB3 | 1.83 | 0.44 |
| 24:W:640:LEU:HA | 24:W:643:TYR:HB2 | 1.99 | 0.44 |
| 25:X:263:TYR:CE1 | 25:X:267:ILE:HD11 | 2.52 | 0.44 |
| 25:X:265:ILE:HG12 | 25:X:300:PHE:HE1 | 1.83 | 0.44 |
| 25:X:281:MET:HE3 | 25:X:293:ILE:HG21 | 2.00 | 0.44 |
| 29:b:123:ASP:HA | 29:b:126:ILE:HG22 | 1.98 | 0.44 |
| 30:c:470:ARG:O | 30:c:474:LEU:HG | 2.18 | 0.44 |
| 31:d:94:GLY:O | 31:d:115:LYS:HD3 | 2.16 | 0.44 |
| 35:z:315:VAL:O | 35:z:354:ALA:HB1 | 2.17 | 0.44 |
| 4:5:50:U:H2' | 4:5:51:U:C6 | 2.52 | 0.44 |
| 5:A:574:LEU:HD12 | 5:A:574:LEU:HA | 1.87 | 0.44 |
| 7:C:108:VAL:N | 7:C:120:TRP:O | 2.40 | 0.44 |
| 11:G:71:VAL:HG22 | 11:G:96:ILE:O | 2.18 | 0.44 |
| 19:O:6:THR:HG21 | 19:O:8:ARG:NH1 | 2.33 | 0.44 |
| 22:R:175:MET:O | 22:R:179:ARG:HG3 | 2.17 | 0.44 |
| 22:R:188:GLU:H | 22:R:188:GLU:CD | 2.24 | 0.44 |
| 22:R:189:ARG:HH12 | 26:Y:147:TYR:HB3 | 1.81 | 0.44 |
| 23:T:92:ARG:NH2 | 23:T:96:GLU:OE2 | 2.50 | 0.44 |
| 24:W:640:LEU:HD23 | 24:W:644:GLU:HG3 | 2.00 | 0.44 |
| 34:y:95:ASP:OD1 | 34:y:103:ARG:HD3 | 2.18 | 0.44 |
| 35:z:144:ILE:HG12 | 35:z:175:VAL:HB | 2.00 | 0.44 |
| 35:z:503:GLU:HB2 | 35:z:507:ILE:HD12 | 1.98 | 0.44 |
| 1:e:147:HIS:CE1 | 16:L:279:LEU:HA | 2.53 | 0.44 |
| 5:A:688:SER:O | 5:A:691:VAL:HG22 | 2.18 | 0.44 |
| 5:A:978:TRP:NE1 | 5:A:1214:MET:HE1 | 2.33 | 0.44 |
| 5:A:1674:ASP:OD1 | 5:A:1674:ASP:N | 2.43 | 0.44 |
| 10:F:6:PHE:CE1 | 10:F:80:LEU:HD22 | 2.53 | 0.44 |
| 16:L:185:ARG:HA | 16:L:201:ILE:HG22 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:N:461:ARG:HH22 | 18:N:550:PRO:HB3 | 1.82 | 0.44 |
| 22:R:48:LEU:O | 22:R:52:GLN:HG3 | 2.17 | 0.44 |
| 22:R:303:LYS:HZ1 | 25:X:574:ASP:CG | 2.21 | 0.44 |
| 22:R:528:GLN:HA | 22:R:531:LEU:HB2 | 2.00 | 0.44 |
| 24:W:183:ARG:O | 24:W:187:LEU:HD23 | 2.18 | 0.44 |
| 25:X:573:ARG:O | 25:X:576:PHE:HB2 | 2.17 | 0.44 |
| 25:X:628:TYR:HE2 | 25:X:655:LEU:HD22 | 1.83 | 0.44 |
| 31:d:13:ILE:HD11 | 31:d:128:VAL:HB | 1.99 | 0.44 |
| 35:z:613:TRP:CD1 | 35:z:636:SER:HG | 2.35 | 0.44 |
| 5:A:556:LYS:HA | 5:A:556:LYS:HD3 | 1.71 | 0.44 |
| 5:A:1685:TRP:HE3 | 5:A:1721:SER:HB2 | 1.83 | 0.44 |
| 6:B:273:ASP:OD1 | 6:B:323:SER:OG | 2.25 | 0.44 |
| 6:B:756:THR:HG23 | 6:B:799:ARG:HA | 1.98 | 0.44 |
| 6:B:848:VAL:HG12 | 6:B:913:MET:CG | 2.47 | 0.44 |
| 15:K:348:SER:HG | 15:K:357:TRP:HZ3 | 1.63 | 0.44 |
| 18:N:1060:TYR:CD1 | 18:N:1061:PRO:HD2 | 2.53 | 0.44 |
| 18:N:1247:ILE:O | 18:N:1250:SER:OG | 2.28 | 0.44 |
| 22:R:231:ILE:HG13 | 22:R:232:ASP:N | 2.33 | 0.44 |
| 22:R:514:GLU:HB2 | 22:R:523:ALA:HB2 | 1.99 | 0.44 |
| 23:S:14:VAL:HG13 | 23:S:23:TYR:HB2 | 1.99 | 0.44 |
| 23:T:101:LEU:HD11 | 23:U:100:GLU:HB2 | 2.00 | 0.44 |
| 23:T:107:SER:HA | 27:Z:33:LEU:HD21 | 1.99 | 0.44 |
| 31:d:39:ASP:OD1 | 31:d:151:LYS:HA | 2.18 | 0.44 |
| 31:d:71:LYS:HA | 31:d:98:ASN:O | 2.17 | 0.44 |
| 32:m:752:THR:HB | 32:m:794:PHE:CD2 | 2.52 | 0.44 |
| 34:y:144:MET:SD | 35:z:420:LEU:HD13 | 2.58 | 0.44 |
| 6:B:812:PRO:HD2 | 6:B:817:ARG:HH22 | 1.82 | 0.44 |
| 15:K:86:ALA:C | 22:R:259:ARG:HH22 | 2.26 | 0.44 |
| 18:N:668:ARG:O | 18:N:760:LYS:NZ | 2.46 | 0.44 |
| 23:T:132:PHE:CZ | 23:U:132:PHE:HB3 | 2.53 | 0.44 |
| 27:Z:76:ASP:OD1 | 27:Z:77:VAL:N | 2.48 | 0.44 |
| 28:a:95:PRO:HG2 | 28:a:98:VAL:HG12 | 1.99 | 0.44 |
| 31:d:5:GLU:OE2 | 31:d:14:LEU:HD13 | 2.18 | 0.44 |
| 31:d:88:LEU:HD12 | 31:d:103:PHE:O | 2.18 | 0.44 |
| 34:y:144:MET:O | 34:y:147:ASN:HB3 | 2.17 | 0.44 |
| 35:z:245:GLY:CA | 35:z:324:LYS:HD2 | 2.44 | 0.44 |
| 38:6:5:U:H1' | 38:6:9:G:N2 | 2.33 | 0.44 |
| 4:5:96:G:N2 | 13:I:39:SER:O | 2.46 | 0.43 |
| 5:A:1576:GLN:HG2 | 5:A:1587:HIS:ND1 | 2.32 | 0.43 |
| 5:A:1969:VAL:HG11 | 5:A:2011:ILE:HA | 1.99 | 0.43 |
| 6:B:252:THR:O | 6:B:256:LYS:HG2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:C:59:ASP:OD1 | 7:C:60:PRO:HD2 | 2.17 | 0.43 |
| 7:C:87:GLY:HA3 | 9:E:94:LEU:HD11 | 1.99 | 0.43 |
| 7:C:92:CYS:SG | 7:C:112:SER:OG | 2.58 | 0.43 |
| 8:D:6:LYS:HD2 | 8:D:90:PRO:HG2 | 2.00 | 0.43 |
| 11:G:29:PRO:HG2 | 13:I:42:ASN:O | 2.17 | 0.43 |
| 15:K:398:TRP:CZ3 | 15:K:405:LYS:HB2 | 2.53 | 0.43 |
| 17:M:32:TYR:CE2 | 28:a:102:GLU:OE1 | 2.71 | 0.43 |
| 18:N:642:PHE:O | 18:N:646:PHE:HB2 | 2.17 | 0.43 |
| 18:N:827:LEU:HB2 | 18:N:928:ILE:HG21 | 1.98 | 0.43 |
| 18:N:1233:ILE:O | 18:N:1236:THR:OG1 | 2.34 | 0.43 |
| 20:P:118:LEU:CD1 | 20:P:151:PHE:HE2 | 2.31 | 0.43 |
| 22:R:289:GLN:O | 25:X:539:ARG:NH1 | 2.50 | 0.43 |
| 22:R:401:ALA:CB | 22:R:433:LYS:HD2 | 2.48 | 0.43 |
| 22:R:547:GLU:HB2 | 22:R:572:ALA:HB2 | 1.99 | 0.43 |
| 22:R:570:VAL:HA | 22:R:573:ARG:HD2 | 2.00 | 0.43 |
| 23:S:17:ARG:NH1 | 23:T:17:ARG:HA | 2.33 | 0.43 |
| 23:T:127:GLU:OE1 | 24:W:738:LYS:NZ | 2.40 | 0.43 |
| 24:W:511:ARG:O | 24:W:515:ARG:HG2 | 2.18 | 0.43 |
| 27:Z:180:CYS:O | 27:Z:184:THR:HG23 | 2.19 | 0.43 |
| 32:m:346:VAL:HG23 | 32:m:347:GLU:OE1 | 2.18 | 0.43 |
| 35:z:49:HIS:O | 35:z:54:LYS:NZ | 2.51 | 0.43 |
| 35:z:219:TYR:O | 35:z:223:ALA:N | 2.46 | 0.43 |
| 35:z:575:ASP:HA | 35:z:642:TYR:CZ | 2.53 | 0.43 |
| 5:A:101:LYS:HB2 | 5:A:101:LYS:HE3 | 1.81 | 0.43 |
| 5:A:873:TYR:HE1 | 5:A:883:GLN:HE21 | 1.65 | 0.43 |
| 5:A:1107:PRO:HG2 | 21:Q:225:TRP:CE3 | 2.53 | 0.43 |
| 5:A:1451:ARG:NH1 | 34:y:228:ASP:OD2 | 2.40 | 0.43 |
| 5:A:1754:MET:HE2 | 5:A:1757:ILE:HD12 | 1.99 | 0.43 |
| 7:C:276:ALA:HB2 | 7:C:316:VAL:O | 2.18 | 0.43 |
| 9:E:68:VAL:HG12 | 9:E:70:LEU:HD22 | 1.99 | 0.43 |
| 16:L:221:LYS:HE3 | 38:6:54:C:H4' | 2.00 | 0.43 |
| 18:N:51:LEU:O | 18:N:55:LEU:HD13 | 2.18 | 0.43 |
| 18:N:1263:ILE:HA | 18:N:1268:HIS:ND1 | 2.33 | 0.43 |
| 22:R:43:THR:N | 22:R:47:GLU:OE2 | 2.51 | 0.43 |
| 22:R:342:TYR:HB3 | 22:R:368:TYR:CE1 | 2.53 | 0.43 |
| 23:V:112:LEU:HD13 | 24:W:596:GLU:HB3 | 2.00 | 0.43 |
| 24:W:730:GLU:O | 24:W:734:ILE:HG12 | 2.18 | 0.43 |
| 25:X:252:GLN:HB2 | 25:X:255:LYS:HZ2 | 1.83 | 0.43 |
| 25:X:398:ARG:HA | 25:X:398:ARG:HD3 | 1.70 | 0.43 |
| 25:X:528:ALA:HA | 25:X:530:PHE:CZ | 2.53 | 0.43 |
| 25:X:532:ASP:HA | 25:X:535:LYS:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:660:VAL:HA | 25:X:663:MET:HE3 | 2.00 | 0.43 |
| 28:a:74:VAL:HA | 28:a:78:GLN:HE21 | 1.83 | 0.43 |
| 30:c:520:GLU:CA | 30:c:567:PRO:HG3 | 2.37 | 0.43 |
| 30:c:587:TYR:O | 30:c:591:ILE:HG12 | 2.18 | 0.43 |
| 35:z:347:ALA:HB1 | 35:z:364:ARG:HH11 | 1.82 | 0.43 |
| 35:z:549:PHE:O | 35:z:552:LYS:HB3 | 2.18 | 0.43 |
| 1:e:54:LEU:CD2 | 16:L:308:TYR:HB3 | 2.49 | 0.43 |
| 4:5:32:C:C5 | 5:A:487:PRO:HB2 | 2.54 | 0.43 |
| 4:5:104:A:O2' | 11:G:48:ARG:HB3 | 2.17 | 0.43 |
| 5:A:107:ARG:NH1 | 16:L:213:GLU:OE1 | 2.51 | 0.43 |
| 5:A:1080:ARG:HD2 | 5:A:1080:ARG:HA | 1.80 | 0.43 |
| 5:A:1360:PRO:HB2 | 5:A:1374:ILE:HD12 | 2.01 | 0.43 |
| 6:B:498:THR:HG22 | 6:B:499:VAL:H | 1.84 | 0.43 |
| 16:L:202:ILE:HD12 | 17:M:19:PHE:HZ | 1.83 | 0.43 |
| 16:L:217:PHE:CE1 | 17:M:50:PRO:HG3 | 2.53 | 0.43 |
| 16:L:325:GLU:O | 16:L:328:LEU:HG | 2.17 | 0.43 |
| 18:N:292:LYS:O | 18:N:296:ILE:HG12 | 2.19 | 0.43 |
| 22:R:412:LEU:HD13 | 22:R:443:PHE:CE1 | 2.50 | 0.43 |
| 23:S:34:GLU:OE2 | 23:S:35:THR:HG22 | 2.17 | 0.43 |
| 24:W:678:ARG:CZ | 27:Z:113:GLU:HG3 | 2.48 | 0.43 |
| 30:c:526:ARG:HA | 30:c:571:GLY:HA3 | 1.99 | 0.43 |
| 30:c:529:GLU:HA | 30:c:532:THR:HG22 | 2.00 | 0.43 |
| 5:A:558:ARG:HG2 | 5:A:558:ARG:HH11 | 1.84 | 0.43 |
| 7:C:202:LYS:HG2 | 7:C:214:VAL:HG12 | 2.01 | 0.43 |
| 7:C:306:LEU:HD13 | 9:E:106:ARG:NE | 2.27 | 0.43 |
| 12:H:11:PRO:HG2 | 12:H:14:ASN:OD1 | 2.19 | 0.43 |
| 17:M:17:VAL:O | 17:M:17:VAL:HG12 | 2.18 | 0.43 |
| 22:R:85:GLU:O | 22:R:86:PHE:CD1 | 2.71 | 0.43 |
| 22:R:101:SER:OG | 22:R:133:GLN:OE1 | 2.32 | 0.43 |
| 22:R:268:ILE:HD13 | 22:R:268:ILE:HA | 1.87 | 0.43 |
| 22:R:460:TRP:CD2 | 22:R:470:PRO:HG3 | 2.53 | 0.43 |
| 23:T:54:LYS:HA | 23:T:54:LYS:HD2 | 1.80 | 0.43 |
| 23:T:68:SER:H | 23:T:72:LEU:HD23 | 1.83 | 0.43 |
| 23:V:33:ARG:HH12 | 23:V:47:LEU:HD21 | 1.84 | 0.43 |
| 23:V:66:ALA:CB | 27:Z:60:GLU:HG2 | 2.48 | 0.43 |
| 24:W:627:TYR:O | 24:W:630:LEU:N | 2.51 | 0.43 |
| 25:X:192:ASN:OD1 | 25:X:232:HIS:NE2 | 2.52 | 0.43 |
| 32:m:454:SER:HB3 | 32:m:510:PRO:HG2 | 2.00 | 0.43 |
| 5:A:1168:MET:HG3 | 5:A:1206:ASP:HB3 | 2.00 | 0.43 |
| 6:B:329:CYS:SG | 6:B:442:PHE:HB2 | 2.58 | 0.43 |
| 6:B:494:LYS:C | 6:B:495:LEU:HD12 | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:663:SER:O | 6:B:663:SER:OG | 2.34 | 0.43 |
| 6:B:767:ASP:HB3 | 6:B:770:LYS:CE | 2.48 | 0.43 |
| 6:B:861:TYR:CE1 | 6:B:871:VAL:HG21 | 2.53 | 0.43 |
| 7:C:326:LEU:HD12 | 7:C:326:LEU:HA | 1.79 | 0.43 |
| 15:K:299:GLU:OE1 | 15:K:299:GLU:N | 2.51 | 0.43 |
| 16:L:163:LYS:HE3 | 16:L:163:LYS:HB3 | 1.87 | 0.43 |
| 17:M:172:GLU:OE1 | 17:M:172:GLU:N | 2.50 | 0.43 |
| 18:N:1002:PHE:HZ | 18:N:1005:LEU:HD13 | 1.83 | 0.43 |
| 23:S:100:GLU:OE2 | 23:S:101:LEU:HD12 | 2.19 | 0.43 |
| 23:T:122:ARG:NH1 | 23:U:121:GLU:OE1 | 2.51 | 0.43 |
| 23:U:112:LEU:HD22 | 27:Z:22:ARG:HH11 | 1.84 | 0.43 |
| 23:U:442:VAL:O | 23:U:454:CYS:HB3 | 2.18 | 0.43 |
| 25:X:695:VAL:O | 25:X:695:VAL:HG12 | 2.17 | 0.43 |
| 30:c:526:ARG:HB2 | 30:c:531:ASP:OD2 | 2.18 | 0.43 |
| 32:m:531:SER:HB2 | 32:m:562:LEU:HD11 | 1.98 | 0.43 |
| 35:z:103:CYS:HA | 35:z:119:ILE:O | 2.18 | 0.43 |
| 35:z:236:PRO:HA | 35:z:296:ARG:NH2 | 2.34 | 0.43 |
| 35:z:516:PHE:CD1 | 35:z:536:LEU:HD13 | 2.54 | 0.43 |
| 36:r:338:UNK:O | 36:r:342:UNK:N | 2.52 | 0.43 |
| 5:A:1449:LYS:HD3 | 5:A:1449:LYS:HA | 1.86 | 0.43 |
| 6:B:149:HIS:CG | 6:B:150:LEU:N | 2.87 | 0.43 |
| 7:C:249:LYS:H | 7:C:256:ARG:NH2 | 2.17 | 0.43 |
| 8:D:50:ASP:OD1 | 8:D:51:GLY:N | 2.52 | 0.43 |
| 14:J:73:LEU:O | 14:J:73:LEU:HD12 | 2.19 | 0.43 |
| 18:N:803:LEU:HD22 | 18:N:945:LEU:HD21 | 2.00 | 0.43 |
| 18:N:885:PHE:CZ | 18:N:887:PHE:HB2 | 2.54 | 0.43 |
| 18:N:1139:TYR:HE2 | 18:N:1186:VAL:HB | 1.84 | 0.43 |
| 22:R:10:ASN:OD1 | 24:W:153:ILE:HB | 2.18 | 0.43 |
| 22:R:524:ARG:HA | 22:R:527:TYR:HD2 | 1.83 | 0.43 |
| 23:S:86:GLU:O | 23:S:90:LEU:HG | 2.18 | 0.43 |
| 24:W:155:MET:CG | 24:W:159:GLU:HG3 | 2.34 | 0.43 |
| 24:W:261:ILE:O | 24:W:265:GLU:OE1 | 2.37 | 0.43 |
| 25:X:75:ARG:HB3 | 25:X:94:VAL:HG22 | 2.00 | 0.43 |
| 25:X:557:LEU:HD22 | 25:X:576:PHE:HE1 | 1.83 | 0.43 |
| 25:X:608:SER:O | 25:X:612:LEU:HD23 | 2.19 | 0.43 |
| 30:c:554:LYS:O | 30:c:557:VAL:HG22 | 2.18 | 0.43 |
| 35:z:59:PRO:HA | 35:z:62:LEU:HD23 | 1.99 | 0.43 |
| 5:A:821:GLY:HA2 | 16:L:288:PHE:CE2 | 2.54 | 0.43 |
| 5:A:1757:ILE:HG23 | 5:A:1761:ASN:ND2 | 2.23 | 0.43 |
| 7:C:261:PHE:HE1 | 7:C:300:GLY:HA2 | 1.84 | 0.43 |
| 9:E:7:VAL:O | 9:E:10:LEU:HD13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:H:32:GLU:OE1 | 14:J:22:ASN:ND2 | 2.52 | 0.43 |
| 16:L:176:GLN:OE1 | 16:L:177:GLN:N | 2.52 | 0.43 |
| 17:M:44:CYS:HB3 | 17:M:47:CYS:HB2 | 2.01 | 0.43 |
| 18:N:4:TYR:CZ | 18:N:8:LYS:HD2 | 2.54 | 0.43 |
| 18:N:76:ASN:O | 18:N:80:MET:HG2 | 2.18 | 0.43 |
| 18:N:533:TYR:HB2 | 18:N:608:PHE:HA | 2.00 | 0.43 |
| 19:O:29:ARG:HB2 | 19:O:52:LEU:HD21 | 2.01 | 0.43 |
| 22:R:310:LYS:O | 22:R:313:LYS:HG2 | 2.18 | 0.43 |
| 23:U:185:LYS:HB3 | 23:U:488:GLY:O | 2.19 | 0.43 |
| 23:U:276:PRO:HG2 | 23:U:279:SER:HB2 | 2.00 | 0.43 |
| 23:V:21:ASN:HB3 | 23:V:23:TYR:CE2 | 2.54 | 0.43 |
| 23:V:81:ASP:OD2 | 27:Z:93:LEU:HD11 | 2.18 | 0.43 |
| 24:W:507:ASP:OD2 | 25:X:563:ARG:NH2 | 2.52 | 0.43 |
| 25:X:708:ILE:HG13 | 25:X:709:ARG:N | 2.34 | 0.43 |
| 30:c:409:LEU:HD21 | 30:c:413:ARG:HH21 | 1.83 | 0.43 |
| 32:m:505:HIS:ND1 | 32:m:545:ASP:OD2 | 2.50 | 0.43 |
| 35:z:28:THR:HG23 | 35:z:31:ARG:HH21 | 1.83 | 0.43 |
| 35:z:244:SER:O | 35:z:324:LYS:HG3 | 2.18 | 0.43 |
| 35:z:473:SER:OG | 35:z:543:ARG:HB3 | 2.19 | 0.43 |
| 35:z:503:GLU:HA | 35:z:633:LYS:HE3 | 2.00 | 0.43 |
| 35:z:609:LYS:HD3 | 35:z:609:LYS:N | 2.33 | 0.43 |
| 39:1:-14:U:H3' | 39:1:-13:U:H5" | 2.01 | 0.43 |
| 1:e:261:VAL:HG13 | 1:e:262:ASN:N | 2.33 | 0.43 |
| 4:5:32:C:C4 | 5:A:487:PRO:HB2 | 2.54 | 0.43 |
| 5:A:1034:ALA:HB2 | 24:W:78:THR:HB | 2.01 | 0.43 |
| 5:A:1657:ALA:HB3 | 5:A:1682:ASN:OD1 | 2.19 | 0.43 |
| 6:B:396:THR:HG21 | 6:B:428:LEU:HD23 | 2.00 | 0.43 |
| 7:C:131:HIS:HB3 | 7:C:163:TRP:CE3 | 2.54 | 0.43 |
| 7:C:261:PHE:HB3 | 7:C:296:TRP:CZ2 | 2.54 | 0.43 |
| 9:E:76:VAL:HA | 10:F:64:ASN:HD21 | 1.82 | 0.43 |
| 16:L:186:TYR:N | 16:L:200:ARG:O | 2.40 | 0.43 |
| 18:N:279:LYS:HZ3 | 18:N:383:ARG:HA | 1.83 | 0.43 |
| 22:R:166:LYS:HE2 | 22:R:166:LYS:HB3 | 1.92 | 0.43 |
| 22:R:600:LYS:HA | 22:R:615:VAL:HG11 | 2.00 | 0.43 |
| 23:U:56:PRO:HB3 | 23:V:2:PHE:HD2 | 1.82 | 0.43 |
| 24:W:251:GLU:OE1 | 24:W:255:LYS:HE3 | 2.19 | 0.43 |
| 25:X:431:TRP:HZ3 | 25:X:450:LEU:HD22 | 1.84 | 0.43 |
| 25:X:634:LYS:HA | 25:X:634:LYS:HD2 | 1.77 | 0.43 |
| 30:c:519:TRP:CZ3 | 30:c:560:LEU:HD22 | 2.50 | 0.43 |
| 32:m:394:ASN:O | 32:m:398:SER:OG | 2.28 | 0.43 |
| 32:m:772:LYS:HB3 | 32:m:782:TYR:CZ | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:z:387:MET:CE | 35:z:415:HIS:HB3 | 2.43 | 0.43 |
| 35:z:495:ALA:HB1 | 35:z:529:ASN:HA | 2.01 | 0.43 |
| 5:A:250:ASN:HB3 | 5:A:252:PRO:HD2 | 2.01 | 0.43 |
| 5:A:661:LEU:HD23 | 5:A:661:LEU:HA | 1.83 | 0.43 |
| 6:B:195:SER:HA | 6:B:216:ASP:O | 2.18 | 0.43 |
| 7:C:234:LEU:N | 7:C:246:PHE:O | 2.35 | 0.43 |
| 18:N:120:VAL:O | 18:N:120:VAL:HG12 | 2.18 | 0.43 |
| 22:R:54:ARG:O | 22:R:57:LYS:HG2 | 2.18 | 0.43 |
| 22:R:450:PHE:HA | 22:R:453:CYS:HB2 | 2.01 | 0.43 |
| 23:S:122:ARG:NH1 | 23:V:118:LEU:HD22 | 2.33 | 0.43 |
| 24:W:530:VAL:O | 24:W:534:ASP:N | 2.52 | 0.43 |
| 33:n:319:GLU:O | 33:n:323:ILE:HG12 | 2.18 | 0.43 |
| 35:z:585:GLN:CD | 35:z:591:LYS:HG2 | 2.44 | 0.43 |
| 5:A:821:GLY:HA3 | 16:L:285:ASN:HD22 | 1.83 | 0.43 |
| 5:A:1659:TYR:HB2 | 5:A:1661:TRP:CH2 | 2.54 | 0.43 |
| 5:A:1663:VAL:O | 5:A:1679:THR:OG1 | 2.22 | 0.43 |
| 5:A:1900:LEU:HG | 5:A:1908:ILE:HD11 | 2.00 | 0.43 |
| 6:B:356:TRP:CE3 | 6:B:356:TRP:HA | 2.54 | 0.43 |
| 8:D:60:TYR:HB2 | 14:J:12:TYR:HE2 | 1.84 | 0.43 |
| 8:D:64:SER:HA | 9:E:71:ARG:NH2 | 2.26 | 0.43 |
| 15:K:135:SER:O | 15:K:139:ARG:HG3 | 2.18 | 0.43 |
| 17:M:138:ALA:O | 17:M:141:ARG:HG2 | 2.19 | 0.43 |
| 20:P:52:LYS:HE3 | 20:P:52:LYS:HB3 | 1.83 | 0.43 |
| 24:W:247:ARG:O | 24:W:251:GLU:CB | 2.65 | 0.43 |
| 25:X:513:THR:HG23 | 25:X:513:THR:O | 2.18 | 0.43 |
| 25:X:520:TYR:CD2 | 25:X:536:ILE:HG12 | 2.54 | 0.43 |
| 29:b:19:TYR:HA | 39:1:-10:A:O2' | 2.18 | 0.43 |
| 35:z:342:ILE:HD13 | 35:z:350:ARG:NH1 | 2.34 | 0.43 |
| 1:e:185:ILE:HG23 | 15:K:373:ALA:HA | 2.01 | 0.42 |
| 5:A:1303:ILE:HD12 | 30:c:424:VAL:HG13 | 2.01 | 0.42 |
| 5:A:1364:LEU:HD23 | 29:b:5:GLY:O | 2.19 | 0.42 |
| 5:A:1890:LYS:NZ | 5:A:1912:GLU:HG2 | 2.34 | 0.42 |
| 6:B:850:VAL:HG13 | 6:B:901:LEU:HD21 | 2.01 | 0.42 |
| 7:C:279:ARG:HH21 | 7:C:322:GLN:C | 2.26 | 0.42 |
| 10:F:74:LEU:HD12 | 10:F:74:LEU:O | 2.19 | 0.42 |
| 13:I:67:CYS:O | 13:I:70:VAL:HG22 | 2.19 | 0.42 |
| 15:K:122:PRO:HA | 15:K:126:HIS:HB2 | 2.01 | 0.42 |
| 15:K:302:PRO:HD2 | 15:K:359:PHE:HB3 | 2.00 | 0.42 |
| 17:M:73:CYS:C | 17:M:75:ARG:H | 2.27 | 0.42 |
| 18:N:257:MET:HE2 | 18:N:375:ASN:CB | 2.49 | 0.42 |
| 18:N:743:LEU:HD21 | 18:N:1032:LEU:HD13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:Q:56:ALA:O | 21:Q:59:ARG:HG2 | 2.19 | 0.42 |
| 22:R:85:GLU:C | 22:R:86:PHE:CD1 | 2.97 | 0.42 |
| 22:R:573:ARG:HG3 | 22:R:602:PHE:CE2 | 2.54 | 0.42 |
| 23:S:67:THR:HA | 23:T:79:GLU:OE1 | 2.19 | 0.42 |
| 24:W:537:ARG:HD2 | 24:W:577:PHE:CD1 | 2.52 | 0.42 |
| 24:W:699:HIS:HA | 24:W:702:LYS:HE2 | 2.01 | 0.42 |
| 24:W:703:ALA:O | 24:W:707:GLU:HG2 | 2.19 | 0.42 |
| 25:X:223:SER:O | 25:X:227:VAL:HG23 | 2.19 | 0.42 |
| 25:X:682:LEU:HD23 | 25:X:682:LEU:HA | 1.68 | 0.42 |
| 27:Z:148:CYS:O | 27:Z:151:LYS:HG2 | 2.17 | 0.42 |
| 34:y:182:ASP:OD1 | 34:y:183:ASP:N | 2.52 | 0.42 |
| 34:y:222:ALA:HA | 34:y:225:MET:SD | 2.59 | 0.42 |
| 1:e:128:ASP:OD2 | 2:p:166:ARG:HD2 | 2.18 | 0.42 |
| 2:p:167:LYS:HD3 | 2:p:170:ARG:HH12 | 1.84 | 0.42 |
| 4:5:82:A:O2' | 4:5:83:A:H8 | 2.01 | 0.42 |
| 5:A:223:VAL:O | 5:A:227:PHE:HB2 | 2.18 | 0.42 |
| 5:A:942:ASP:CG | 5:A:1035:LYS:HZ3 | 2.27 | 0.42 |
| 5:A:1437:ASP:OD1 | 5:A:1437:ASP:N | 2.46 | 0.42 |
| 6:B:438:PHE:O | 6:B:440:VAL:N | 2.52 | 0.42 |
| 6:B:794:CYS:SG | 6:B:795:ASP:N | 2.92 | 0.42 |
| 15:K:310:ASP:O | 15:K:311:SER:OG | 2.23 | 0.42 |
| 15:K:346:PHE:CD1 | 15:K:359:PHE:CE1 | 3.04 | 0.42 |
| 17:M:227:LYS:HD3 | 17:M:230:LYS:NZ | 2.34 | 0.42 |
| 18:N:306:LEU:O | 18:N:309:THR:OG1 | 2.28 | 0.42 |
| 18:N:671:PHE:HE1 | 18:N:680:VAL:HG21 | 1.84 | 0.42 |
| 18:N:1049:ARG:HG2 | 18:N:1075:LEU:HD22 | 2.02 | 0.42 |
| 20:P:184:THR:OG1 | 20:P:186:ASP:OD1 | 2.30 | 0.42 |
| 23:V:1:MET:HE1 | 23:V:13:PRO:HG2 | 1.99 | 0.42 |
| 25:X:292:ILE:HA | 25:X:295:ASP:OD2 | 2.19 | 0.42 |
| 26:Y:142:ARG:HD3 | 26:Y:142:ARG:H | 1.84 | 0.42 |
| 28:a:139:GLU:OE1 | 28:a:139:GLU:N | 2.41 | 0.42 |
| 34:y:31:ARG:HE | 35:z:494:VAL:HG12 | 1.83 | 0.42 |
| 5:A:768:SER:HB2 | 15:K:165:TRP:CZ2 | 2.54 | 0.42 |
| 5:A:919:ILE:HD13 | 5:A:932:TYR:CE2 | 2.54 | 0.42 |
| 5:A:1538:LYS:HE2 | 34:y:206:VAL:O | 2.18 | 0.42 |
| 5:A:1707:LYS:HE2 | 5:A:1711:TYR:CZ | 2.54 | 0.42 |
| 6:B:520:LYS:HD2 | 6:B:538:VAL:HG13 | 2.01 | 0.42 |
| 15:K:263:VAL:HG12 | 15:K:295:LEU:HD21 | 2.01 | 0.42 |
| 18:N:734:SER:HB2 | 18:N:746:VAL:HG21 | 2.01 | 0.42 |
| 18:N:1135:ILE:HG13 | 18:N:1182:ILE:HD11 | 2.00 | 0.42 |
| 20:P:259:GLN:O | 20:P:263:GLU:OE1 | 2.36 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:583:LEU:HD13 | 22:R:592:ARG:HA | 2.01 | 0.42 |
| 23:U:405:LEU:HD23 | 23:U:405:LEU:H | 1.84 | 0.42 |
| 32:m:717:SER:OG | 32:m:718:PHE:N | 2.52 | 0.42 |
| 34:y:124:PRO:HA | 34:y:137:ASP:HB3 | 2.01 | 0.42 |
| 34:y:128:PRO:HD3 | 34:y:155:PHE:CE1 | 2.54 | 0.42 |
| 35:z:434:ASN:OD1 | 35:z:435:LEU:N | 2.51 | 0.42 |
| 35:z:534:GLN:O | 35:z:537:ARG:HG2 | 2.18 | 0.42 |
| 2:p:176:GLU:CD | 24:W:63:ARG:HH12 | 2.26 | 0.42 |
| 5:A:868:ARG:HH11 | 5:A:1463:ARG:HD2 | 1.84 | 0.42 |
| 5:A:1635:LYS:HE2 | 5:A:1652:ASP:OD1 | 2.19 | 0.42 |
| 5:A:1856:ARG:HD3 | 5:A:1859:GLN:HB3 | 2.01 | 0.42 |
| 6:B:247:VAL:O | 6:B:877:ARG:NH2 | 2.50 | 0.42 |
| 7:C:237:ASN:HB2 | 7:C:275:VAL:HG13 | 2.01 | 0.42 |
| 11:G:36:ALA:HB2 | 11:G:111:ARG:HH21 | 1.83 | 0.42 |
| 11:G:110:VAL:HG12 | 13:I:63:ILE:CD1 | 2.50 | 0.42 |
| 20:P:251:ASN:HB2 | 20:P:254:SER:HB3 | 2.01 | 0.42 |
| 22:R:77:GLY:O | 22:R:81:LEU:HB2 | 2.19 | 0.42 |
| 22:R:361:TYR:HA | 22:R:364:ILE:HG22 | 2.01 | 0.42 |
| 22:R:466:GLU:HG2 | 22:R:499:ILE:HG22 | 2.00 | 0.42 |
| 23:U:240:SER:O | 23:U:248:GLU:N | 2.53 | 0.42 |
| 23:V:16:SER:H | 23:V:20:GLY:HA2 | 1.84 | 0.42 |
| 23:V:73:LEU:HD11 | 27:Z:80:TYR:HE2 | 1.84 | 0.42 |
| 24:W:537:ARG:CG | 24:W:538:PRO:CD | 2.97 | 0.42 |
| 27:Z:155:TYR:O | 27:Z:158:GLU:HG3 | 2.19 | 0.42 |
| 29:b:124:VAL:HA | 29:b:127:LEU:HD12 | 2.01 | 0.42 |
| 30:c:586:ASN:OD1 | 30:c:587:TYR:N | 2.53 | 0.42 |
| 32:m:497:LYS:NZ | 32:m:545:ASP:OD1 | 2.48 | 0.42 |
| 35:z:379:GLU:HB2 | 35:z:383:LEU:HD22 | 2.01 | 0.42 |
| 3:2:30:A:C6 | 34:y:37:PRO:HD2 | 2.54 | 0.42 |
| 4:5:84:U:H2' | 4:5:85:U:C6 | 2.53 | 0.42 |
| 5:A:154:PRO:O | 5:A:444:ALA:N | 2.51 | 0.42 |
| 5:A:291:ALA:N | 29:b:2:SER:O | 2.40 | 0.42 |
| 7:C:132:LYS:HG2 | 7:C:133:GLY:N | 2.35 | 0.42 |
| 7:C:279:ARG:NE | 7:C:321:HIS:O | 2.53 | 0.42 |
| 12:H:28:ILE:HG12 | 12:H:81:ILE:HD13 | 2.01 | 0.42 |
| 18:N:869:TYR:O | 18:N:873:VAL:HB | 2.19 | 0.42 |
| 20:P:292:ASN:OD1 | 20:P:293:ARG:NH1 | 2.52 | 0.42 |
| 22:R:466:GLU:HB3 | 22:R:501:GLU:HG3 | 2.00 | 0.42 |
| 24:W:237:ASP:OD2 | 24:W:239:SER:HB3 | 2.19 | 0.42 |
| 24:W:542:GLN:NE2 | 24:W:569:SER:O | 2.49 | 0.42 |
| 25:X:548:VAL:HA | 25:X:551:GLU:OE2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:X:584:PRO:CD | 25:X:587:PHE:HB2 | 2.48 | 0.42 |
| 38:6:17:U:O2' | 38:6:18:G:OP2 | 2.34 | 0.42 |
| 2:p:169:PHE:CE2 | 24:W:67:GLU:HB3 | 2.53 | 0.42 |
| 5:A:107:ARG:NH2 | 16:L:215:PRO:O | 2.52 | 0.42 |
| 5:A:1219:VAL:HG22 | 5:A:1254:ILE:HD13 | 2.02 | 0.42 |
| 6:B:330:PHE:CG | 6:B:335:PHE:HE1 | 2.38 | 0.42 |
| 6:B:942:ASP:OD1 | 6:B:942:ASP:N | 2.49 | 0.42 |
| 7:C:134:HIS:ND1 | 7:C:155:SER:OG | 2.53 | 0.42 |
| 14:J:22:ASN:O | 14:J:25:ARG:HD3 | 2.19 | 0.42 |
| 16:L:216:LYS:HE3 | 16:L:216:LYS:HB3 | 1.81 | 0.42 |
| 16:L:237:PRO:HD3 | 22:R:136:ARG:NH1 | 2.33 | 0.42 |
| 18:N:803:LEU:HG | 18:N:820:LEU:HD11 | 2.00 | 0.42 |
| 20:P:120:PHE:HB2 | 20:P:135:HIS:CD2 | 2.55 | 0.42 |
| 23:U:72:LEU:HD12 | 23:V:63:PRO:HG2 | 2.00 | 0.42 |
| 24:W:197:GLN:OE1 | 24:W:200:ARG:NE | 2.50 | 0.42 |
| 25:X:254:GLY:CA | 25:X:293:ILE:HD11 | 2.50 | 0.42 |
| 25:X:455:VAL:HA | 25:X:476:LEU:HD21 | 2.01 | 0.42 |
| 30:c:541:LYS:HG3 | 30:c:591:ILE:HD12 | 2.00 | 0.42 |
| 32:m:606:PHE:CE2 | 32:m:650:LEU:HD11 | 2.55 | 0.42 |
| 34:y:159:PRO:O | 34:y:163:TYR:HD1 | 2.03 | 0.42 |
| 34:y:160:PHE:HB2 | 35:z:383:LEU:CD2 | 2.49 | 0.42 |
| 35:z:442:GLN:HG2 | 35:z:553:PHE:CE1 | 2.55 | 0.42 |
| 3:2:14:C:H2' | 38:6:76:C:C5 | 2.54 | 0.42 |
| 5:A:1287:TRP:CZ2 | 5:A:1291:LEU:HD22 | 2.54 | 0.42 |
| 6:B:739:ASP:CG | 29:b:66:LYS:HD3 | 2.45 | 0.42 |
| 6:B:846:TYR:CE1 | 6:B:891:VAL:HG22 | 2.54 | 0.42 |
| 12:H:46:ASP:OD1 | 12:H:46:ASP:N | 2.52 | 0.42 |
| 15:K:387:PHE:HE1 | 15:K:395:MET:HE3 | 1.83 | 0.42 |
| 16:L:111:HIS:C | 16:L:113:HIS:H | 2.27 | 0.42 |
| 18:N:256:ARG:HA | 18:N:261:TYR:CD1 | 2.55 | 0.42 |
| 20:P:91:VAL:O | 20:P:92:LYS:C | 2.62 | 0.42 |
| 20:P:178:VAL:HG21 | 20:P:195:PHE:HZ | 1.85 | 0.42 |
| 22:R:310:LYS:HA | 22:R:313:LYS:HE3 | 2.01 | 0.42 |
| 22:R:510:TYR:O | 22:R:513:PHE:HB3 | 2.20 | 0.42 |
| 23:S:69:LEU:HD22 | 23:U:80:TRP:CD1 | 2.53 | 0.42 |
| 23:U:207:LEU:HD22 | 23:U:212:THR:O | 2.19 | 0.42 |
| 25:X:186:CYS:HA | 25:X:191:TRP:CZ3 | 2.55 | 0.42 |
| 25:X:357:ARG:HA | 25:X:360:LYS:HG2 | 2.01 | 0.42 |
| 25:X:648:TYR:HE1 | 25:X:663:MET:HB2 | 1.85 | 0.42 |
| 30:c:475:SER:OG | 30:c:476:ARG:N | 2.53 | 0.42 |
| 34:y:142:GLU:O | 34:y:146:LYS:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:398:GLU:HG3 | 12:H:6:GLN:NE2 | 2.35 | 0.42 |
| 5:A:1153:LYS:NZ | 5:A:1198:THR:O | 2.53 | 0.42 |
| 5:A:2025:SER:HB3 | 5:A:2028:ASN:ND2 | 2.35 | 0.42 |
| 6:B:752:ASP:N | 6:B:785:GLN:OE1 | 2.30 | 0.42 |
| 11:G:5:VAL:HG21 | 11:G:19:ARG:NH1 | 2.34 | 0.42 |
| 18:N:211:GLN:NE2 | 18:N:367:LYS:HB2 | 2.35 | 0.42 |
| 20:P:124:MET:HE3 | 20:P:124:MET:HB3 | 1.85 | 0.42 |
| 22:R:42:ILE:HG21 | 22:R:48:LEU:HB2 | 2.01 | 0.42 |
| 23:T:67:THR:HB | 27:Z:105:ARG:HA | 2.01 | 0.42 |
| 24:W:696:LYS:HE3 | 27:Z:131:LEU:HA | 2.00 | 0.42 |
| 25:X:105:LEU:HD12 | 25:X:108:MET:HB3 | 2.01 | 0.42 |
| 25:X:272:LYS:HA | 25:X:272:LYS:HD2 | 1.85 | 0.42 |
| 25:X:428:ALA:O | 25:X:432:ILE:HG23 | 2.20 | 0.42 |
| 27:Z:56:SER:OG | 27:Z:57:ASP:N | 2.48 | 0.42 |
| 34:y:183:ASP:HA | 34:y:186:GLN:HE22 | 1.85 | 0.42 |
| 35:z:463:GLY:HA2 | 35:z:559:GLN:OE1 | 2.19 | 0.42 |
| 1:e:55:LYS:HA | 16:L:308:TYR:CD2 | 2.55 | 0.42 |
| 4:5:85:U:H2' | 4:5:86:U:C6 | 2.55 | 0.42 |
| 5:A:732:ILE:HD13 | 5:A:758:ILE:HD12 | 2.02 | 0.42 |
| 5:A:1016:LEU:O | 5:A:1020:MET:HG3 | 2.19 | 0.42 |
| 6:B:325:ASP:HB2 | 42:B:1001:GTP:C6 | 2.55 | 0.42 |
| 13:I:25:LYS:HA | 13:I:71:LEU:HD12 | 2.01 | 0.42 |
| 16:L:100:ALA:HB1 | 26:Y:150:ALA:O | 2.18 | 0.42 |
| 18:N:1052:ILE:HG13 | 18:N:1211:LEU:HD22 | 2.02 | 0.42 |
| 18:N:1093:ALA:HB2 | 18:N:1098:GLN:NE2 | 2.34 | 0.42 |
| 18:N:1098:GLN:O | 18:N:1109:ASN:ND2 | 2.52 | 0.42 |
| 22:R:349:VAL:HB | 22:R:361:TYR:HE1 | 1.85 | 0.42 |
| 22:R:450:PHE:CE1 | 22:R:477:LEU:HD11 | 2.54 | 0.42 |
| 23:V:61:PRO:O | 23:V:62:ARG:HG2 | 2.20 | 0.42 |
| 23:V:94:LEU:HA | 23:V:97:THR:HG22 | 2.02 | 0.42 |
| 24:W:567:LEU:O | 24:W:571:ASP:N | 2.49 | 0.42 |
| 25:X:238:VAL:HG13 | 25:X:242:PHE:CE2 | 2.55 | 0.42 |
| 25:X:420:PRO:HA | 25:X:473:GLN:HG3 | 2.02 | 0.42 |
| 25:X:447:ALA:O | 25:X:451:ILE:HG12 | 2.20 | 0.42 |
| 25:X:520:TYR:CE1 | 25:X:524:LEU:HB2 | 2.55 | 0.42 |
| 30:c:454:ASN:ND2 | 30:c:507:PHE:HB2 | 2.34 | 0.42 |
| 32:m:322:VAL:HG12 | 32:m:324:GLU:H | 1.83 | 0.42 |
| 32:m:771:LYS:HE2 | 32:m:771:LYS:HB3 | 1.71 | 0.42 |
| 36:r:232:UNK:C | 36:r:234:UNK:H | 2.32 | 0.42 |
| 38:6:85:G:H2' | 38:6:86:A:C8 | 2.55 | 0.42 |
| 1:e:123:LYS:HB2 | 1:e:123:LYS:HE2 | 1.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:2:30:A:H62 | 34:y:37:PRO:HB2 | 1.85 | 0.42 |
| 5:A:1005:SER:O | 5:A:1006:LYS:HD3 | 2.20 | 0.42 |
| 5:A:1429:LEU:C | 5:A:1431:ASP:N | 2.77 | 0.42 |
| 5:A:1440:ILE:HD13 | 5:A:1440:ILE:HA | 1.73 | 0.42 |
| 7:C:262:GLU:O | 7:C:296:TRP:HZ2 | 2.03 | 0.42 |
| 11:G:9:ARG:NE | 11:G:9:ARG:HA | 2.35 | 0.42 |
| 12:H:10:ILE:O | 12:H:10:ILE:HG13 | 2.20 | 0.42 |
| 16:L:184:ILE:O | 16:L:201:ILE:HA | 2.19 | 0.42 |
| 17:M:110:ASP:OD1 | 17:M:111:ILE:N | 2.53 | 0.42 |
| 18:N:679:SER:OG | 18:N:729:ASP:OD2 | 2.28 | 0.42 |
| 20:P:97:CYS:SG | 20:P:98:VAL:N | 2.93 | 0.42 |
| 22:R:292:ASP:OD1 | 22:R:295:GLY:HA2 | 2.20 | 0.42 |
| 22:R:605:MET:HE2 | 22:R:606:HIS:CE1 | 2.55 | 0.42 |
| 23:S:25:LYS:HA | 23:S:25:LYS:HD2 | 1.92 | 0.42 |
| 23:U:99:GLN:NE2 | 23:U:99:GLN:HA | 2.34 | 0.42 |
| 23:U:405:LEU:HG | 23:U:406:ARG:HD2 | 2.01 | 0.42 |
| 24:W:155:MET:HG2 | 24:W:155:MET:O | 2.19 | 0.42 |
| 24:W:537:ARG:HD2 | 24:W:577:PHE:CD2 | 2.55 | 0.42 |
| 24:W:675:LEU:HD11 | 27:Z:105:ARG:HH21 | 1.84 | 0.42 |
| 25:X:260:LEU:HD12 | 25:X:263:TYR:HD2 | 1.84 | 0.42 |
| 27:Z:24:ALA:O | 27:Z:27:GLN:HG3 | 2.20 | 0.42 |
| 32:m:641:TRP:O | 32:m:645:VAL:HG23 | 2.19 | 0.42 |
| 1:e:117:VAL:HB | 5:A:827:ASP:OD1 | 2.19 | 0.41 |
| 5:A:170:MET:SD | 5:A:213:MET:HE1 | 2.60 | 0.41 |
| 5:A:1660:LYS:NZ | 5:A:1681:THR:O | 2.53 | 0.41 |
| 5:A:1687:ASP:OD1 | 5:A:1726:LEU:HA | 2.20 | 0.41 |
| 6:B:702:VAL:HG13 | 6:B:804:ARG:HE | 1.84 | 0.41 |
| 7:C:172:LYS:HB2 | 7:C:172:LYS:HE2 | 1.91 | 0.41 |
| 8:D:19:GLU:HB3 | 8:D:25:THR:HG22 | 2.02 | 0.41 |
| 11:G:42:GLN:O | 11:G:112:ILE:N | 2.32 | 0.41 |
| 15:K:431:LYS:HA | 15:K:431:LYS:HD3 | 1.79 | 0.41 |
| 16:L:281:ASP:OD2 | 16:L:283:GLU:OE1 | 2.37 | 0.41 |
| 17:M:301:LEU:O | 17:M:305:VAL:N | 2.53 | 0.41 |
| 18:N:671:PHE:CE1 | 18:N:732:LEU:HD13 | 2.55 | 0.41 |
| 18:N:792:GLU:OE1 | 18:N:817:TYR:HB2 | 2.20 | 0.41 |
| 22:R:147:MET:O | 22:R:151:LEU:HD23 | 2.20 | 0.41 |
| 24:W:240:GLU:O | 24:W:242:ASP:N | 2.53 | 0.41 |
| 32:m:583:PRO:HG3 | 32:m:638:TRP:CZ2 | 2.55 | 0.41 |
| 34:y:110:LYS:HG3 | 34:y:112:TYR:HE1 | 1.85 | 0.41 |
| 35:z:553:PHE:HB2 | 35:z:555:ILE:HG12 | 2.01 | 0.41 |
| 5:A:197:PHE:CZ | 5:A:589:LEU:HD21 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:970:PRO:HB2 | 5:A:972:PRO:HD2 | 2.02 | 0.41 |
| 5:A:1549:GLY:HA3 | 34:y:58:GLY:O | 2.21 | 0.41 |
| 5:A:1973:LYS:NZ | 5:A:1976:LEU:HD22 | 2.34 | 0.41 |
| 6:B:311:ARG:NH2 | 6:B:315:GLU:OE2 | 2.53 | 0.41 |
| 7:C:65:PHE:CD2 | 7:C:326:LEU:HD21 | 2.55 | 0.41 |
| 8:D:65:HIS:CE1 | 14:J:68:ILE:HD13 | 2.55 | 0.41 |
| 11:G:11:GLU:N | 11:G:12:LEU:HD12 | 2.35 | 0.41 |
| 12:H:21:GLN:OE1 | 12:H:21:GLN:HA | 2.20 | 0.41 |
| 12:H:72:LEU:HD11 | 13:I:8:PRO:HB3 | 2.02 | 0.41 |
| 15:K:387:PHE:CE1 | 15:K:395:MET:HE3 | 2.55 | 0.41 |
| 18:N:606:LEU:HD12 | 18:N:606:LEU:HA | 1.94 | 0.41 |
| 18:N:823:TRP:CZ2 | 18:N:928:ILE:HG13 | 2.56 | 0.41 |
| 18:N:1252:HIS:CG | 18:N:1258:VAL:HG21 | 2.55 | 0.41 |
| 24:W:48:TRP:CE2 | 24:W:53:ASP:HB3 | 2.55 | 0.41 |
| 25:X:624:ARG:O | 25:X:627:ILE:HG22 | 2.20 | 0.41 |
| 34:y:36:VAL:O | 34:y:36:VAL:HG23 | 2.20 | 0.41 |
| 34:y:154:ASP:OD1 | 34:y:154:ASP:N | 2.50 | 0.41 |
| 35:z:364:ARG:HD2 | 35:z:366:TYR:OH | 2.20 | 0.41 |
| 5:A:1222:LEU:HD12 | 5:A:1223:PRO:HD2 | 2.02 | 0.41 |
| 5:A:1538:LYS:HD2 | 34:y:206:VAL:HG22 | 2.02 | 0.41 |
| 6:B:371:GLN:NE2 | 6:B:373:LEU:H | 2.18 | 0.41 |
| 6:B:860:ILE:HG12 | 6:B:901:LEU:HD11 | 2.01 | 0.41 |
| 10:F:17:ILE:HD11 | 10:F:68:TYR:HE1 | 1.85 | 0.41 |
| 10:F:36:MET:HG3 | 10:F:36:MET:O | 2.20 | 0.41 |
| 13:I:16:ILE:HG13 | 13:I:35:GLN:HA | 2.02 | 0.41 |
| 13:I:31:LYS:O | 13:I:48:ALA:HA | 2.20 | 0.41 |
| 13:I:45:LEU:HB2 | 13:I:63:ILE:HB | 2.02 | 0.41 |
| 15:K:87:ASP:HA | 22:R:259:ARG:HH12 | 1.85 | 0.41 |
| 15:K:343:GLU:OE1 | 15:K:400:TRP:NE1 | 2.53 | 0.41 |
| 16:L:319:LYS:HA | 16:L:322:GLN:NE2 | 2.35 | 0.41 |
| 18:N:140:ARG:HB2 | 18:N:144:TYR:CE2 | 2.55 | 0.41 |
| 18:N:480:LEU:CD1 | 18:N:505:MET:HB2 | 2.51 | 0.41 |
| 20:P:127:GLU:CG | 20:P:131:CYS:HB2 | 2.49 | 0.41 |
| 22:R:322:TRP:O | 22:R:326:LEU:HD23 | 2.20 | 0.41 |
| 22:R:402:LYS:HE2 | 22:R:402:LYS:HB2 | 1.90 | 0.41 |
| 22:R:566:PRO:O | 22:R:570:VAL:HG23 | 2.19 | 0.41 |
| 23:V:2:PHE:O | 23:V:22:VAL:HG21 | 2.20 | 0.41 |
| 23:V:23:TYR:HB2 | 23:V:28:ILE:HD11 | 2.03 | 0.41 |
| 24:W:510:ARG:CZ | 24:W:513:GLN:HE22 | 2.32 | 0.41 |
| 25:X:454:ALA:O | 25:X:476:LEU:HD21 | 2.21 | 0.41 |
| 29:b:55:SER:OG | 29:b:56:GLU:OE1 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:y:31:ARG:HA | 35:z:493:PHE:CE2 | 2.55 | 0.41 |
| 3:2:30:A:N3 | 3:2:30:A:H2' | 2.34 | 0.41 |
| 5:A:330:GLU:OE1 | 5:A:330:GLU:N | 2.51 | 0.41 |
| 5:A:1391:ASN:ND2 | 5:A:1393:TYR:HB3 | 2.35 | 0.41 |
| 6:B:222:ASP:HB3 | 6:B:650:TYR:HB2 | 2.02 | 0.41 |
| 7:C:237:ASN:HB2 | 7:C:275:VAL:CG1 | 2.50 | 0.41 |
| 15:K:88:SER:C | 15:K:90:ASN:H | 2.28 | 0.41 |
| 15:K:344:PHE:CE2 | 15:K:359:PHE:HB2 | 2.56 | 0.41 |
| 17:M:88:GLN:OE1 | 17:M:133:SER:HB2 | 2.20 | 0.41 |
| 20:P:52:LYS:HD3 | 20:P:54:ILE:C | 2.45 | 0.41 |
| 22:R:122:HIS:O | 22:R:126:LEU:HD13 | 2.20 | 0.41 |
| 22:R:192:GLY:O | 22:R:196:ARG:HG3 | 2.19 | 0.41 |
| 22:R:277:MET:O | 22:R:281:LYS:HG2 | 2.20 | 0.41 |
| 23:V:81:ASP:O | 23:V:85:LEU:HG | 2.20 | 0.41 |
| 25:X:398:ARG:HH21 | 25:X:436:GLU:CD | 2.27 | 0.41 |
| 25:X:495:THR:O | 25:X:499:THR:OG1 | 2.23 | 0.41 |
| 26:Y:131:ASP:OD1 | 26:Y:132:LYS:N | 2.54 | 0.41 |
| 28:a:61:GLU:OE1 | 28:a:61:GLU:N | 2.47 | 0.41 |
| 28:a:126:ASP:OD1 | 28:a:129:ARG:NH1 | 2.54 | 0.41 |
| 30:c:573:PHE:CZ | 30:c:596:LEU:HD13 | 2.55 | 0.41 |
| 30:c:594:GLY:O | 30:c:597:THR:HG22 | 2.18 | 0.41 |
| 34:y:150:TRP:CE2 | 34:y:152:GLY:HA3 | 2.55 | 0.41 |
| 35:z:426:LEU:HG | 35:z:454:LYS:HD2 | 2.01 | 0.41 |
| 5:A:220:ASP:OD1 | 5:A:259:ARG:NH2 | 2.42 | 0.41 |
| 5:A:946:ASP:OD1 | 5:A:950:TRP:HD1 | 2.03 | 0.41 |
| 5:A:1234:LYS:HA | 5:A:1234:LYS:HD2 | 1.87 | 0.41 |
| 5:A:1781:GLU:O | 5:A:1782:PRO:C | 2.63 | 0.41 |
| 6:B:725:GLN:NE2 | 6:B:744:ARG:O | 2.53 | 0.41 |
| 7:C:296:TRP:CD1 | 7:C:302:LEU:HA | 2.55 | 0.41 |
| 18:N:58:PHE:HB3 | 18:N:85:LYS:NZ | 2.36 | 0.41 |
| 22:R:59:PHE:CD2 | 22:R:76:TYR:HA | 2.55 | 0.41 |
| 22:R:307:GLN:HA | 22:R:310:LYS:HG2 | 2.03 | 0.41 |
| 23:T:91:ARG:HH11 | 23:U:90:LEU:HD12 | 1.85 | 0.41 |
| 23:V:106:TYR:HA | 23:V:109:ASP:HB2 | 2.02 | 0.41 |
| 24:W:529:GLN:HA | 24:W:532:GLN:HB2 | 2.02 | 0.41 |
| 27:Z:20:GLU:OE2 | 27:Z:23:SER:OG | 2.38 | 0.41 |
| 27:Z:70:GLU:O | 27:Z:71:LYS:HB2 | 2.19 | 0.41 |
| 27:Z:147:GLY:HA2 | 27:Z:150:ARG:NH1 | 2.36 | 0.41 |
| 32:m:379:TRP:CD1 | 32:m:380:LYS:HG3 | 2.55 | 0.41 |
| 34:y:82:SER:C | 34:y:84:ASN:H | 2.27 | 0.41 |
| 2:p:198:PRO:O | 25:X:725:ARG:NH2 | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:2:19:G:H5' | 16:L:261:PRO:HG2 | 2.03 | 0.41 |
| 5:A:268:LEU:O | 5:A:269:ARG:HG2 | 2.20 | 0.41 |
| 5:A:1282:LYS:CG | 34:y:208:ASN:HD21 | 2.26 | 0.41 |
| 6:B:707:GLU:HG2 | 6:B:708:LYS:H | 1.85 | 0.41 |
| 7:C:43:ASN:HD21 | 9:E:106:ARG:HD2 | 1.85 | 0.41 |
| 7:C:201:ILE:HB | 7:C:215:LEU:HB2 | 2.03 | 0.41 |
| 17:M:69:ILE:CG2 | 17:M:84:MET:HE1 | 2.50 | 0.41 |
| 18:N:72:LEU:O | 18:N:76:ASN:ND2 | 2.53 | 0.41 |
| 18:N:193:ASN:HB3 | 18:N:197:ARG:HH12 | 1.85 | 0.41 |
| 20:P:82:MET:O | 20:P:83:ARG:C | 2.63 | 0.41 |
| 20:P:108:ALA:HB2 | 20:P:132:GLU:C | 2.44 | 0.41 |
| 22:R:134:LEU:HB3 | 22:R:137:VAL:HG12 | 2.03 | 0.41 |
| 23:U:80:TRP:HA | 23:U:83:VAL:HG12 | 2.01 | 0.41 |
| 24:W:132:SER:HA | 24:W:135:ARG:CZ | 2.51 | 0.41 |
| 28:a:98:VAL:O | 28:a:102:GLU:HG3 | 2.20 | 0.41 |
| 29:b:131:TYR:O | 29:b:134:GLN:HG3 | 2.21 | 0.41 |
| 34:y:31:ARG:O | 34:y:34:GLN:HG2 | 2.20 | 0.41 |
| 35:z:464:CYS:SG | 35:z:561:LEU:HD13 | 2.61 | 0.41 |
| 35:z:585:GLN:CG | 35:z:591:LYS:HG2 | 2.51 | 0.41 |
| 5:A:276:LEU:HD23 | 5:A:276:LEU:HA | 1.88 | 0.41 |
| 5:A:532:HIS:O | 5:A:533:ARG:HB3 | 2.20 | 0.41 |
| 5:A:1142:ASP:OD2 | 5:A:1145:ASN:HA | 2.19 | 0.41 |
| 7:C:116:HIS:C | 7:C:117:LEU:HD12 | 2.46 | 0.41 |
| 12:H:27:SER:HB3 | 12:H:82:GLN:HB3 | 2.03 | 0.41 |
| 15:K:121:VAL:HG13 | 15:K:121:VAL:O | 2.20 | 0.41 |
| 16:L:101:VAL:HG13 | 16:L:103:TYR:CE1 | 2.56 | 0.41 |
| 17:M:167:LYS:O | 17:M:170:LEU:HB3 | 2.20 | 0.41 |
| 20:P:59:GLU:HG2 | 20:P:61:GLU:OE2 | 2.20 | 0.41 |
| 20:P:214:PHE:CE2 | 39:1:11:U:C6 | 3.05 | 0.41 |
| 22:R:383:ARG:HH22 | 22:R:414:GLN:HG3 | 1.86 | 0.41 |
| 26:Y:95:LYS:HE2 | 26:Y:121:ARG:NH2 | 2.35 | 0.41 |
| 31:d:29:PHE:HD2 | 31:d:119:PHE:HE2 | 1.67 | 0.41 |
| 35:z:281:VAL:O | 35:z:285:MET:HG2 | 2.21 | 0.41 |
| 5:A:198:SER:OG | 5:A:201:GLN:HG2 | 2.21 | 0.41 |
| 5:A:876:LYS:HG3 | 5:A:878:ARG:H | 1.86 | 0.41 |
| 5:A:911:MET:HE2 | 5:A:914:PHE:CD2 | 2.56 | 0.41 |
| 5:A:1428:THR:HA | 34:y:230:SER:HA | 2.03 | 0.41 |
| 6:B:460:LYS:HA | 6:B:460:LYS:HD2 | 1.79 | 0.41 |
| 7:C:306:LEU:HD12 | 7:C:306:LEU:O | 2.21 | 0.41 |
| 8:D:91:LEU:HB3 | 8:D:92:PRO:HD2 | 2.01 | 0.41 |
| 13:I:19:PRO:HA | 13:I:32:GLY:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:143:ASP:O | 16:L:147:GLN:HG2 | 2.20 | 0.41 |
| 18:N:427:TYR:HD1 | 18:N:432:PHE:CD2 | 2.38 | 0.41 |
| 18:N:456:PHE:HB2 | 18:N:477:PHE:CE1 | 2.56 | 0.41 |
| 20:P:127:GLU:OE1 | 20:P:127:GLU:N | 2.53 | 0.41 |
| 20:P:261:ARG:HH12 | 20:P:265:ARG:NH2 | 2.18 | 0.41 |
| 22:R:88:ARG:HB3 | 24:W:225:ILE:CD1 | 2.45 | 0.41 |
| 22:R:296:VAL:O | 22:R:300:VAL:HG23 | 2.20 | 0.41 |
| 23:T:117:ARG:HA | 23:T:120:LYS:NZ | 2.36 | 0.41 |
| 23:U:205:GLU:HA | 23:U:217:PRO:HA | 2.03 | 0.41 |
| 23:U:342:HIS:CE1 | 23:U:344:ASP:H | 2.38 | 0.41 |
| 24:W:71:HIS:NE2 | 24:W:75:LEU:HD11 | 2.36 | 0.41 |
| 24:W:159:GLU:CD | 24:W:160:LYS:H | 2.29 | 0.41 |
| 24:W:530:VAL:HG23 | 24:W:531:ILE:N | 2.35 | 0.41 |
| 24:W:536:ILE:CG2 | 24:W:537:ARG:H | 2.17 | 0.41 |
| 25:X:230:PRO:HB3 | 25:X:263:TYR:HD1 | 1.86 | 0.41 |
| 29:b:71:ARG:HH12 | 29:b:126:ILE:HG13 | 1.86 | 0.41 |
| 2:p:210:LEU:O | 2:p:214:GLU:HG3 | 2.21 | 0.41 |
| 4:5:95:A:C6 | 13:I:40:TYR:HD2 | 2.38 | 0.41 |
| 5:A:97:MET:HE3 | 5:A:97:MET:HB3 | 1.93 | 0.41 |
| 5:A:615:TYR:OH | 5:A:1574:GLY:HA2 | 2.21 | 0.41 |
| 5:A:851:PRO:HA | 5:A:852:PRO:HD3 | 1.97 | 0.41 |
| 5:A:1037:ASN:ND2 | 5:A:1049:ASN:O | 2.47 | 0.41 |
| 5:A:1185:ARG:HE | 21:Q:229:VAL:CG1 | 2.31 | 0.41 |
| 5:A:1272:LEU:HA | 5:A:1272:LEU:HD23 | 1.74 | 0.41 |
| 5:A:1635:LYS:HE2 | 5:A:1652:ASP:HA | 2.01 | 0.41 |
| 5:A:1646:MET:N | 5:A:1646:MET:SD | 2.94 | 0.41 |
| 5:A:1654:LEU:C | 5:A:1655:LEU:HD22 | 2.46 | 0.41 |
| 5:A:1973:LYS:HA | 5:A:1973:LYS:HD2 | 1.92 | 0.41 |
| 6:B:153:GLY:HA3 | 6:B:270:ASN:HD22 | 1.86 | 0.41 |
| 6:B:682:ASP:OD1 | 6:B:683:THR:N | 2.54 | 0.41 |
| 7:C:143:VAL:HG12 | 7:C:151:LEU:HD22 | 2.02 | 0.41 |
| 7:C:309:HIS:CE1 | 7:C:335:PHE:CD2 | 3.09 | 0.41 |
| 10:F:40:LEU:HB3 | 10:F:43:VAL:CG1 | 2.41 | 0.41 |
| 11:G:35:GLN:HG2 | 11:G:111:ARG:NH2 | 2.35 | 0.41 |
| 11:G:52:LYS:HB2 | 11:G:74:MET:SD | 2.61 | 0.41 |
| 12:H:80:LEU:CD2 | 14:J:60:VAL:HG13 | 2.49 | 0.41 |
| 13:I:42:ASN:HB3 | 13:I:67:CYS:HB3 | 2.02 | 0.41 |
| 15:K:386:MET:HE2 | 15:K:386:MET:HB3 | 1.95 | 0.41 |
| 16:L:139:GLU:OE1 | 16:L:139:GLU:HA | 2.21 | 0.41 |
| 18:N:81:LEU:HA | 18:N:81:LEU:HD23 | 1.82 | 0.41 |
| 18:N:155:LEU:HD22 | 18:N:160:LYS:HD3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:N:342:LEU:HB3 | 18:N:347:LEU:HG | 2.02 | 0.41 |
| 20:P:119:TYR:CD2 | 38:6:23:A:C6 | 3.09 | 0.41 |
| 20:P:136:ARG:NH1 | 20:P:139:LYS:HG2 | 2.34 | 0.41 |
| 20:P:183:PRO:HD2 | 20:P:187:ILE:HG22 | 2.03 | 0.41 |
| 22:R:116:LYS:NZ | 26:Y:172:ILE:HG22 | 2.35 | 0.41 |
| 22:R:189:ARG:HE | 22:R:189:ARG:HB3 | 1.62 | 0.41 |
| 22:R:278:GLU:O | 22:R:282:GLU:OE1 | 2.39 | 0.41 |
| 22:R:322:TRP:CZ2 | 22:R:348:LYS:HE3 | 2.55 | 0.41 |
| 22:R:453:CYS:HB3 | 22:R:457:TYR:CZ | 2.56 | 0.41 |
| 22:R:588:LEU:HB3 | 22:R:591:GLU:HB2 | 2.02 | 0.41 |
| 23:S:78:GLU:HA | 23:S:81:ASP:OD2 | 2.21 | 0.41 |
| 23:T:73:LEU:HD22 | 23:V:73:LEU:HD13 | 2.03 | 0.41 |
| 23:U:94:LEU:O | 23:U:97:THR:HG22 | 2.21 | 0.41 |
| 23:U:263:ALA:O | 23:U:275:PHE:N | 2.54 | 0.41 |
| 23:V:23:TYR:CD2 | 23:V:28:ILE:HD11 | 2.56 | 0.41 |
| 23:V:91:ARG:NE | 36:r:237:UNK:O | 2.54 | 0.41 |
| 25:X:81:HIS:CE1 | 25:X:82:LEU:HD22 | 2.55 | 0.41 |
| 25:X:219:TRP:HE1 | 25:X:256:LEU:CD2 | 2.33 | 0.41 |
| 25:X:292:ILE:HA | 25:X:292:ILE:HD12 | 1.94 | 0.41 |
| 30:c:414:LYS:HE2 | 30:c:414:LYS:HB2 | 1.85 | 0.41 |
| 30:c:490:TYR:HE1 | 30:c:540:LEU:HD21 | 1.86 | 0.41 |
| 30:c:576:ASP:HB3 | 30:c:603:TYR:CE1 | 2.56 | 0.41 |
| 31:d:32:LEU:HD11 | 31:d:37:TYR:HE1 | 1.83 | 0.41 |
| 35:z:306:GLU:HA | 35:z:353:ARG:CZ | 2.51 | 0.41 |
| 35:z:310:THR:HA | 35:z:356:ARG:NH1 | 2.30 | 0.41 |
| 39:1:-15:U:H2' | 39:1:-14:U:H5" | 2.03 | 0.41 |
| 1:e:198:TYR:CE1 | 5:A:748:PRO:HB3 | 2.55 | 0.41 |
| 1:e:204:HIS:HD2 | 6:B:76:GLN:H | 1.67 | 0.41 |
| 5:A:70:ARG:NH1 | 5:A:73:GLY:O | 2.53 | 0.41 |
| 5:A:366:LEU:HD23 | 5:A:366:LEU:HA | 1.88 | 0.41 |
| 5:A:1654:LEU:O | 5:A:1655:LEU:HD22 | 2.21 | 0.41 |
| 6:B:190:VAL:O | 6:B:190:VAL:HG12 | 2.20 | 0.41 |
| 15:K:149:TRP:HZ2 | 15:K:459:HIS:HB2 | 1.86 | 0.41 |
| 15:K:265:ALA:HB1 | 15:K:292:VAL:HB | 2.03 | 0.41 |
| 16:L:183:TYR:HB2 | 28:a:92:GLU:O | 2.21 | 0.41 |
| 18:N:134:SER:O | 18:N:140:ARG:HB3 | 2.21 | 0.41 |
| 18:N:480:LEU:HD23 | 18:N:608:PHE:O | 2.20 | 0.41 |
| 18:N:745:MET:HB3 | 18:N:1029:PHE:HE1 | 1.85 | 0.41 |
| 18:N:784:MET:HE3 | 18:N:784:MET:HB2 | 1.78 | 0.41 |
| 23:U:111:ALA:O | 23:U:115:ILE:HG12 | 2.20 | 0.41 |
| 24:W:20:ALA:HB1 | 24:W:32:ILE:HG12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:W:248:GLU:HA | 24:W:251:GLU:HB3 | 2.03 | 0.41 |
| 24:W:541:THR:O | 24:W:545:LYS:HD3 | 2.21 | 0.41 |
| 24:W:560:LEU:HG | 24:W:561:LEU:HG | 2.02 | 0.41 |
| 24:W:654:GLU:HG2 | 27:Z:86:PRO:HB3 | 2.03 | 0.41 |
| 24:W:675:LEU:HD21 | 27:Z:105:ARG:NH2 | 2.34 | 0.41 |
| 26:Y:161:ASP:OD1 | 26:Y:164:HIS:ND1 | 2.35 | 0.41 |
| 27:Z:94:GLN:HA | 27:Z:97:VAL:HG22 | 2.03 | 0.41 |
| 27:Z:120:PHE:CZ | 27:Z:124:LEU:HD11 | 2.56 | 0.41 |
| 31:d:70:ASP:OD1 | 31:d:70:ASP:N | 2.54 | 0.41 |
| 32:m:359:SER:HA | 32:m:362:VAL:HG12 | 2.03 | 0.41 |
| 34:y:160:PHE:CD2 | 35:z:415:HIS:NE2 | 2.90 | 0.41 |
| 35:z:140:TYR:O | 35:z:169:ARG:NH1 | 2.43 | 0.41 |
| 4:5:98:U:N3 | 8:D:38:ASN:OD1 | 2.53 | 0.40 |
| 5:A:304:ASP:OD1 | 5:A:304:ASP:N | 2.55 | 0.40 |
| 5:A:1600:ILE:O | 5:A:1770:ARG:HD3 | 2.21 | 0.40 |
| 6:B:488:LEU:O | 6:B:580:VAL:HA | 2.21 | 0.40 |
| 6:B:838:SER:O | 6:B:838:SER:OG | 2.32 | 0.40 |
| 7:C:53:VAL:HA | 7:C:69:GLY:HA3 | 2.03 | 0.40 |
| 15:K:397:PHE:HE1 | 15:K:409:LEU:HD12 | 1.86 | 0.40 |
| 15:K:453:ASN:O | 15:K:455:THR:HG23 | 2.20 | 0.40 |
| 18:N:1017:ASN:HD22 | 18:N:1170:GLU:CD | 2.29 | 0.40 |
| 18:N:1079:ASN:HB3 | 18:N:1082:PHE:HB2 | 2.02 | 0.40 |
| 18:N:1138:LEU:HG | 18:N:1183:PHE:CZ | 2.55 | 0.40 |
| 19:O:29:ARG:NH1 | 28:a:148:GLU:OE2 | 2.52 | 0.40 |
| 20:P:59:GLU:CD | 20:P:59:GLU:H | 2.29 | 0.40 |
| 20:P:77:LYS:HE3 | 20:P:77:LYS:HB3 | 1.75 | 0.40 |
| 22:R:372:GLU:OE2 | 22:R:385:VAL:HB | 2.21 | 0.40 |
| 22:R:457:TYR:CD2 | 22:R:474:TYR:HD1 | 2.39 | 0.40 |
| 23:U:352:LEU:N | 23:U:356:GLU:O | 2.49 | 0.40 |
| 23:V:86:GLU:O | 23:V:90:LEU:HG | 2.21 | 0.40 |
| 23:V:99:GLN:HE22 | 36:r:230:UNK:C | 2.33 | 0.40 |
| 24:W:21:VAL:HG11 | 24:W:48:TRP:CH2 | 2.56 | 0.40 |
| 24:W:161:GLU:O | 24:W:165:GLU:HG3 | 2.21 | 0.40 |
| 25:X:574:ASP:HA | 25:X:577:GLU:OE2 | 2.22 | 0.40 |
| 30:c:540:LEU:HD12 | 30:c:544:PHE:CE2 | 2.57 | 0.40 |
| 36:r:243:UNK:O | 36:r:247:UNK:N | 2.54 | 0.40 |
| 1:e:252:SER:HA | 1:e:257:PRO:HA | 2.03 | 0.40 |
| 5:A:233:LEU:HB3 | 5:A:236:THR:OG1 | 2.20 | 0.40 |
| 5:A:618:LYS:O | 5:A:621:LEU:HD13 | 2.22 | 0.40 |
| 6:B:522:LYS:HD2 | 6:B:582:ASP:HA | 2.03 | 0.40 |
| 7:C:188:GLN:HE22 | 7:C:190:THR:HG22 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:K:334:VAL:O | 15:K:334:VAL:HG13 | 2.22 | 0.40 |
| 18:N:257:MET:HE2 | 18:N:375:ASN:HB2 | 2.02 | 0.40 |
| 20:P:52:LYS:HG2 | 20:P:126:SER:HA | 2.03 | 0.40 |
| 22:R:517:GLU:C | 22:R:519:GLU:H | 2.30 | 0.40 |
| 22:R:599:TRP:HH2 | 22:R:618:LEU:HD12 | 1.86 | 0.40 |
| 23:T:14:VAL:HB | 23:T:50:LEU:HB2 | 2.02 | 0.40 |
| 23:T:14:VAL:HG11 | 23:T:50:LEU:HD13 | 2.03 | 0.40 |
| 23:U:40:VAL:HG12 | 23:U:41:THR:HG23 | 2.03 | 0.40 |
| 24:W:237:ASP:CG | 24:W:239:SER:HB3 | 2.46 | 0.40 |
| 25:X:172:GLN:NE2 | 25:X:173:VAL:HG13 | 2.37 | 0.40 |
| 25:X:414:GLU:HG2 | 25:X:418:HIS:CE1 | 2.56 | 0.40 |
| 29:b:63:ILE:HD12 | 29:b:63:ILE:HA | 1.92 | 0.40 |
| 31:d:150:ILE:HG13 | 31:d:151:LYS:N | 2.36 | 0.40 |
| 32:m:575:MET:HG3 | 32:m:579:LEU:HB3 | 2.03 | 0.40 |
| 34:y:145:LEU:HD12 | 34:y:150:TRP:HB2 | 2.02 | 0.40 |
| 34:y:215:GLN:N | 34:y:215:GLN:OE1 | 2.54 | 0.40 |
| 35:z:273:LEU:HD13 | 35:z:287:VAL:HA | 2.02 | 0.40 |
| 35:z:332:THR:HG22 | 35:z:596:LYS:NZ | 2.36 | 0.40 |
| 39:1:5:G:H2' | 39:1:6:U:C6 | 2.56 | 0.40 |
| 5:A:1495:ARG:HG3 | 34:y:218:TYR:CD1 | 2.56 | 0.40 |
| 5:A:1596:SER:O | 5:A:1600:ILE:HG12 | 2.21 | 0.40 |
| 5:A:1735:MET:H | 5:A:1735:MET:HG2 | 1.78 | 0.40 |
| 6:B:464:SER:OG | 6:B:465:TYR:N | 2.54 | 0.40 |
| 6:B:657:ASP:O | 6:B:661:LEU:HB2 | 2.22 | 0.40 |
| 8:D:40:GLN:HG2 | 8:D:60:TYR:CD2 | 2.56 | 0.40 |
| 19:O:6:THR:HG22 | 19:O:7:SER:N | 2.35 | 0.40 |
| 23:S:75:LEU:HA | 23:S:78:GLU:HG3 | 2.03 | 0.40 |
| 23:S:90:LEU:CD1 | 23:V:86:GLU:HG2 | 2.51 | 0.40 |
| 25:X:687:GLY:C | 25:X:689:GLN:H | 2.29 | 0.40 |
| 26:Y:173:LYS:HB3 | 26:Y:173:LYS:HE2 | 1.78 | 0.40 |
| 29:b:23:ASN:C | 29:b:25:SER:H | 2.29 | 0.40 |
| 32:m:515:LEU:HG | 32:m:519:ALA:N | 2.36 | 0.40 |
| 3:2:8:C:H2' | 3:2:9:U:C6 | 2.56 | 0.40 |
| 5:A:1135:ARG:NH1 | 21:Q:226:ASP:OD2 | 2.54 | 0.40 |
| 5:A:1892:MET:HE3 | 5:A:1892:MET:HB2 | 1.89 | 0.40 |
| 6:B:423:ASP:HB2 | 6:B:426:PRO:CG | 2.50 | 0.40 |
| 6:B:706:LEU:HD21 | 6:B:758:ILE:CD1 | 2.51 | 0.40 |
| 10:F:3:LEU:O | 10:F:3:LEU:HD23 | 2.21 | 0.40 |
| 15:K:325:THR:OG1 | 16:L:116:LEU:HD23 | 2.20 | 0.40 |
| 18:N:1120:PHE:HD1 | 18:N:1133:ILE:HG21 | 1.85 | 0.40 |
| 21:Q:50:LYS:HA | 21:Q:50:LYS:HD3 | 1.91 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:R:74:MET:HG2 | 22:R:74:MET:H | 1.77 | 0.40 |
| 22:R:133:GLN:HB3 | 22:R:134:LEU:HD12 | 2.03 | 0.40 |
| 22:R:310:LYS:HE3 | 22:R:310:LYS:HB3 | 1.77 | 0.40 |
| 22:R:599:TRP:CH2 | 22:R:618:LEU:HD12 | 2.57 | 0.40 |
| 23:U:94:LEU:HA | 23:U:97:THR:HG22 | 2.04 | 0.40 |
| 24:W:156:ASP:CG | 24:W:157:GLU:H | 2.29 | 0.40 |
| 24:W:252:ALA:HA | 24:W:255:LYS:HG2 | 2.02 | 0.40 |
| 24:W:597:ILE:O | 24:W:601:ARG:HG2 | 2.22 | 0.40 |
| 27:Z:153:LYS:HD3 | 27:Z:153:LYS:HA | 1.90 | 0.40 |
| 30:c:583:PHE:HA | 30:c:586:ASN:ND2 | 2.36 | 0.40 |
| 32:m:344:LEU:HB3 | 32:m:345:PRO:HD3 | 2.04 | 0.40 |
| 32:m:505:HIS:HB3 | 32:m:550:TRP:CE2 | 2.57 | 0.40 |
| 35:z:470:SER:O | 35:z:474:ILE:HG12 | 2.22 | 0.40 |
| 1:e:219:GLN:NE2 | 21:Q:232:ARG:HD3 | 2.31 | 0.40 |
| 1:e:256:TYR:HA | 1:e:257:PRO:HD3 | 1.93 | 0.40 |
| 4:5:51:U:O2' | 38:6:63:A:H8 | 2.04 | 0.40 |
| 4:5:96:G:C6 | 13:I:40:TYR:CE1 | 3.10 | 0.40 |
| 6:B:224:VAL:HG11 | 6:B:253:ARG:NH2 | 2.36 | 0.40 |
| 6:B:569:VAL:HG22 | 6:B:573:ILE:HD11 | 2.03 | 0.40 |
| 6:B:692:THR:OG1 | 6:B:697:ASN:HB2 | 2.21 | 0.40 |
| 7:C:38:ASP:HB2 | 7:C:80:PHE:CE1 | 2.57 | 0.40 |
| 7:C:85:ASN:ND2 | 9:E:99:GLY:H | 2.19 | 0.40 |
| 10:F:7:LEU:HD21 | 11:G:100:PHE:CE2 | 2.56 | 0.40 |
| 13:I:20:VAL:HG12 | 13:I:75:GLU:C | 2.46 | 0.40 |
| 15:K:133:GLN:O | 15:K:137:VAL:HG12 | 2.21 | 0.40 |
| 16:L:91:LEU:HD23 | 31:d:131:ARG:NH2 | 2.37 | 0.40 |
| 16:L:200:ARG:NH2 | 17:M:28:GLY:O | 2.43 | 0.40 |
| 18:N:83:LEU:HD23 | 18:N:129:LEU:HD13 | 2.03 | 0.40 |
| 18:N:335:LEU:HB3 | 18:N:378:ILE:HG12 | 2.03 | 0.40 |
| 18:N:542:LEU:HD23 | 18:N:542:LEU:HA | 1.93 | 0.40 |
| 18:N:804:TYR:CZ | 18:N:806:SER:HB3 | 2.57 | 0.40 |
| 23:S:28:ILE:O | 23:S:32:ILE:HG12 | 2.21 | 0.40 |
| 23:U:401:PHE:HB2 | 23:U:403:TRP:HZ3 | 1.86 | 0.40 |
| 24:W:512:ILE:HD13 | 24:W:512:ILE:HA | 2.00 | 0.40 |
| 25:X:246:ILE:HD13 | 25:X:257:TRP:CZ2 | 2.57 | 0.40 |
| 25:X:342:ASP:OD1 | 25:X:345:LEU:HD12 | 2.22 | 0.40 |
| 25:X:641:VAL:O | 25:X:644:THR:HG23 | 2.21 | 0.40 |
| 26:Y:128:GLU:HB3 | 26:Y:132:LYS:NZ | 2.37 | 0.40 |
| 27:Z:57:ASP:N | 27:Z:57:ASP:OD1 | 2.54 | 0.40 |
| 30:c:469:GLU:HA | 30:c:472:CYS:SG | 2.61 | 0.40 |
| 34:y:127:ASP:O | 34:y:131:ARG:HG2 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:6:13:A:HO2' | 38:6:14:C:P | 2.44 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | e | 156/384 (41%) | 146 (94%) | 10 (6%) | 0 | 100 | 100 |
| 2 | p | 58/299 (19%) | 55 (95%) | 3 (5%) | 0 | 100 | 100 |
| 5 | A | 1984/2363 (84%) | 1893 (95%) | 90 (4%) | 1 (0%) | 48 | 79 |
| 6 | B | 916/984 (93%) | 867 (95%) | 49 (5%) | 0 | 100 | 100 |
| 7 | C | 297/340 (87%) | 278 (94%) | 19 (6%) | 0 | 100 | 100 |
| 8 | D | 94/97 (97%) | 93 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | E | 91/147 (62%) | 88 (97%) | 3 (3%) | 0 | 100 | 100 |
| 10 | F | 79/117 (68%) | 73 (92%) | 6 (8%) | 0 | 100 | 100 |
| 11 | G | 98/115 (85%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 12 | H | 78/84 (93%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 13 | I | 71/78 (91%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |
| 14 | J | 71/77 (92%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |
| 15 | K | 389/473 (82%) | 359 (92%) | 30 (8%) | 0 | 100 | 100 |
| 16 | L | 242/557 (43%) | 226 (93%) | 14 (6%) | 2 (1%) | 16 | 48 |
| 17 | M | 222/354 (63%) | 215 (97%) | 7 (3%) | 0 | 100 | 100 |
| 18 | N | 1282/1284 (100%) | 1261 (98%) | 21 (2%) | 0 | 100 | 100 |
| 19 | O | 142/146 (97%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 20 | P | 265/388 (68%) | 247 (93%) | 17 (6%) | 1 (0%) | 30 | 63 |
| 21 | Q | 86/265 (32%) | 82 (95%) | 3 (4%) | 1 (1%) | 11 | 38 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 22 | R | 597/674 (89%) | 585 (98%) | 11 (2%) | 1 (0%) | 44 74 |
| 23 | S | 130/488 (27%) | 121 (93%) | 9 (7%) | 0 | 100 100 |
| 23 | T | 132/488 (27%) | 127 (96%) | 4 (3%) | 1 (1%) | 16 48 |
| 23 | U | 414/488 (85%) | 399 (96%) | 15 (4%) | 0 | 100 100 |
| 23 | V | 129/488 (26%) | 118 (92%) | 11 (8%) | 0 | 100 100 |
| 24 | W | 488/757 (64%) | 450 (92%) | 33 (7%) | 5 (1%) | 13 42 |
| 25 | X | 642/790 (81%) | 608 (95%) | 33 (5%) | 1 (0%) | 44 74 |
| 26 | Y | 94/229 (41%) | 89 (95%) | 4 (4%) | 1 (1%) | 12 39 |
| 27 | Z | 151/187 (81%) | 145 (96%) | 5 (3%) | 1 (1%) | 19 51 |
| 28 | a | 150/558 (27%) | 138 (92%) | 12 (8%) | 0 | 100 100 |
| 29 | b | 98/293 (33%) | 92 (94%) | 6 (6%) | 0 | 100 100 |
| 30 | c | 202/887 (23%) | 194 (96%) | 8 (4%) | 0 | 100 100 |
| 31 | d | 152/155 (98%) | 138 (91%) | 14 (9%) | 0 | 100 100 |
| 32 | m | 455/797 (57%) | 447 (98%) | 7 (2%) | 1 (0%) | 44 74 |
| 33 | n | 28/361 (8%) | 27 (96%) | 1 (4%) | 0 | 100 100 |
| 34 | y | 196/534 (37%) | 168 (86%) | 25 (13%) | 3 (2%) | 8 33 |
| 35 | z | 624/647 (96%) | 611 (98%) | 12 (2%) | 1 (0%) | 44 74 |
| 37 | q | 3/56 (5%) | 3 (100%) | 0 | 0 | 100 100 |
| All | All | 11306/17429 (65%) | 10784 (95%) | 502 (4%) | 20 (0%) | 45 74 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | Y | 144 | VAL |
| 34 | y | 115 | LYS |
| 23 | T | 69 | LEU |
| 24 | W | 536 | ILE |
| 5 | A | 1115 | ILE |
| 16 | L | 131 | LEU |
| 21 | Q | 224 | ARG |
| 20 | P | 90 | GLN |
| 22 | R | 87 | ALA |
| 24 | W | 538 | PRO |
| 27 | Z | 71 | LYS |
| 32 | m | 321 | THR |
| 35 | z | 437 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | W | 221 | TYR |
| 16 | L | 112 | GLU |
| 25 | X | 83 | ASN |
| 24 | W | 537 | ARG |
| 24 | W | 530 | VAL |
| 34 | y | 127 | ASP |
| 34 | y | 28 | GLU |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | e | 149/346 (43%) | 149 (100%) | 0 | 100 | 100 |
| 2 | p | 56/274 (20%) | 56 (100%) | 0 | 100 | 100 |
| 5 | A | 1798/2138 (84%) | 1798 (100%) | 0 | 100 | 100 |
| 6 | B | 821/881 (93%) | 821 (100%) | 0 | 100 | 100 |
| 7 | C | 257/292 (88%) | 257 (100%) | 0 | 100 | 100 |
| 8 | D | 85/86 (99%) | 85 (100%) | 0 | 100 | 100 |
| 9 | E | 80/118 (68%) | 80 (100%) | 0 | 100 | 100 |
| 10 | F | 76/102 (74%) | 76 (100%) | 0 | 100 | 100 |
| 11 | G | 91/101 (90%) | 91 (100%) | 0 | 100 | 100 |
| 12 | H | 73/76 (96%) | 73 (100%) | 0 | 100 | 100 |
| 13 | I | 64/69 (93%) | 64 (100%) | 0 | 100 | 100 |
| 14 | J | 63/67 (94%) | 63 (100%) | 0 | 100 | 100 |
| 15 | K | 333/405 (82%) | 333 (100%) | 0 | 100 | 100 |
| 16 | L | 211/477 (44%) | 211 (100%) | 0 | 100 | 100 |
| 17 | M | 198/306 (65%) | 198 (100%) | 0 | 100 | 100 |
| 18 | N | 1188/1188 (100%) | 1188 (100%) | 0 | 100 | 100 |
| 19 | O | 130/132 (98%) | 130 (100%) | 0 | 100 | 100 |
| 20 | P | 231/340 (68%) | 231 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 21 | Q | 79/240 (33%) | 79 (100%) | 0 | 100 | 100 |
| 22 | R | 532/597 (89%) | 532 (100%) | 0 | 100 | 100 |
| 23 | S | 121/443 (27%) | 121 (100%) | 0 | 100 | 100 |
| 23 | T | 123/443 (28%) | 123 (100%) | 0 | 100 | 100 |
| 23 | U | 222/443 (50%) | 220 (99%) | 2 (1%) | 75 | 88 |
| 23 | V | 120/443 (27%) | 120 (100%) | 0 | 100 | 100 |
| 24 | W | 443/656 (68%) | 443 (100%) | 0 | 100 | 100 |
| 25 | X | 586/707 (83%) | 586 (100%) | 0 | 100 | 100 |
| 26 | Y | 94/214 (44%) | 94 (100%) | 0 | 100 | 100 |
| 27 | Z | 132/163 (81%) | 132 (100%) | 0 | 100 | 100 |
| 28 | a | 79/496 (16%) | 79 (100%) | 0 | 100 | 100 |
| 29 | b | 95/275 (34%) | 95 (100%) | 0 | 100 | 100 |
| 30 | c | 188/816 (23%) | 188 (100%) | 0 | 100 | 100 |
| 31 | d | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 32 | m | 425/719 (59%) | 425 (100%) | 0 | 100 | 100 |
| 33 | n | 28/335 (8%) | 28 (100%) | 0 | 100 | 100 |
| 34 | y | 173/478 (36%) | 173 (100%) | 0 | 100 | 100 |
| 35 | z | 564/585 (96%) | 564 (100%) | 0 | 100 | 100 |
| 37 | q | 2/2 (100%) | 2 (100%) | 0 | 100 | 100 |
| All | All | 10038/15582 (64%) | 10036 (100%) | 2 (0%) | 100 | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | U | 184 | PRO |
| 23 | U | 415 | PRO |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | e | 147 | HIS |
| 1 | e | 204 | HIS |
| 1 | e | 219 | GLN |
| 5 | A | 253 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 256 | ASN |
| 5 | A | 402 | ASN |
| 5 | A | 522 | GLN |
| 5 | A | 640 | ASN |
| 5 | A | 1027 | ASN |
| 5 | A | 1065 | GLN |
| 5 | A | 1134 | GLN |
| 5 | A | 1387 | HIS |
| 5 | A | 1391 | ASN |
| 5 | A | 1444 | ASN |
| 5 | A | 1452 | HIS |
| 5 | A | 1490 | GLN |
| 5 | A | 1511 | HIS |
| 5 | A | 1544 | ASN |
| 5 | A | 1576 | GLN |
| 5 | A | 1587 | HIS |
| 5 | A | 1607 | GLN |
| 5 | A | 1639 | HIS |
| 5 | A | 1752 | GLN |
| 6 | B | 213 | GLN |
| 6 | B | 343 | HIS |
| 6 | B | 497 | ASN |
| 6 | B | 503 | ASN |
| 6 | B | 596 | HIS |
| 6 | B | 733 | GLN |
| 6 | B | 821 | GLN |
| 7 | C | 40 | ASN |
| 7 | C | 139 | ASN |
| 7 | C | 191 | GLN |
| 7 | C | 213 | HIS |
| 7 | C | 322 | GLN |
| 9 | E | 11 | ASN |
| 9 | E | 81 | GLN |
| 10 | F | 37 | ASN |
| 10 | F | 64 | ASN |
| 11 | G | 40 | HIS |
| 12 | H | 33 | GLN |
| 12 | H | 82 | GLN |
| 15 | K | 459 | HIS |
| 16 | L | 113 | HIS |
| 16 | L | 191 | GLN |
| 16 | L | 301 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | L | 322 | GLN |
| 17 | M | 81 | GLN |
| 17 | M | 88 | GLN |
| 17 | M | 134 | GLN |
| 18 | N | 580 | ASN |
| 18 | N | 584 | ASN |
| 18 | N | 659 | ASN |
| 18 | N | 731 | GLN |
| 18 | N | 747 | ASN |
| 18 | N | 1045 | GLN |
| 18 | N | 1047 | ASN |
| 18 | N | 1108 | GLN |
| 19 | O | 35 | ASN |
| 20 | P | 111 | ASN |
| 20 | P | 156 | HIS |
| 20 | P | 224 | GLN |
| 20 | P | 268 | ASN |
| 20 | P | 287 | ASN |
| 20 | P | 323 | ASN |
| 21 | Q | 68 | GLN |
| 22 | R | 22 | GLN |
| 22 | R | 187 | ASN |
| 22 | R | 225 | GLN |
| 22 | R | 289 | GLN |
| 22 | R | 307 | GLN |
| 22 | R | 367 | ASN |
| 22 | R | 529 | GLN |
| 22 | R | 545 | ASN |
| 23 | S | 21 | ASN |
| 23 | S | 99 | GLN |
| 23 | U | 342 | HIS |
| 23 | V | 99 | GLN |
| 24 | W | 28 | GLN |
| 24 | W | 172 | ASN |
| 24 | W | 195 | HIS |
| 24 | W | 222 | ASN |
| 24 | W | 699 | HIS |
| 25 | X | 81 | HIS |
| 25 | X | 117 | GLN |
| 25 | X | 441 | HIS |
| 26 | Y | 98 | GLN |
| 27 | Z | 94 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | Z | 154 | HIS |
| 27 | Z | 156 | GLN |
| 30 | c | 442 | GLN |
| 30 | c | 561 | HIS |
| 31 | d | 3 | ASN |
| 31 | d | 82 | HIS |
| 31 | d | 101 | GLN |
| 31 | d | 116 | HIS |
| 32 | m | 766 | ASN |
| 34 | y | 117 | ASN |
| 34 | y | 208 | ASN |
| 35 | z | 108 | GLN |
| 35 | z | 111 | HIS |
| 35 | z | 289 | ASN |
| 35 | z | 384 | ASN |
| 35 | z | 415 | HIS |
| 35 | z | 451 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 3 | 2 | 22/186 (11%) | 5 (22%) | 0 |
| 38 | 6 | 91/99 (91%) | 44 (48%) | 7 (7%) |
| 39 | 1 | 28/29 (96%) | 19 (67%) | 2 (7%) |
| 4 | 5 | 101/120 (84%) | 22 (21%) | 2 (1%) |
| All | All | 242/434 (55%) | 90 (37%) | 11 (4%) |

All (90) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 2 | 11 | U |
| 3 | 2 | 12 | G |
| 3 | 2 | 13 | C |
| 3 | 2 | 24 | A |
| 3 | 2 | 29 | A |
| 4 | 5 | 13 | A |
| 4 | 5 | 14 | G |
| 4 | 5 | 27 | G |
| 4 | 5 | 28 | C |
| 4 | 5 | 30 | A |
| 4 | 5 | 31 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 5 | 33 | G |
| 4 | 5 | 37 | C |
| 4 | 5 | 50 | U |
| 4 | 5 | 54 | C |
| 4 | 5 | 79 | G |
| 4 | 5 | 82 | A |
| 4 | 5 | 83 | A |
| 4 | 5 | 90 | U |
| 4 | 5 | 91 | G |
| 4 | 5 | 92 | U |
| 4 | 5 | 98 | U |
| 4 | 5 | 99 | U |
| 4 | 5 | 102 | G |
| 4 | 5 | 103 | U |
| 4 | 5 | 105 | A |
| 4 | 5 | 108 | U |
| 38 | 6 | 4 | C |
| 38 | 6 | 7 | C |
| 38 | 6 | 8 | G |
| 38 | 6 | 9 | G |
| 38 | 6 | 10 | A |
| 38 | 6 | 11 | U |
| 38 | 6 | 12 | C |
| 38 | 6 | 14 | C |
| 38 | 6 | 18 | G |
| 38 | 6 | 19 | G |
| 38 | 6 | 20 | U |
| 38 | 6 | 21 | C |
| 38 | 6 | 22 | A |
| 38 | 6 | 23 | A |
| 38 | 6 | 24 | A |
| 38 | 6 | 27 | G |
| 38 | 6 | 28 | A |
| 38 | 6 | 29 | A |
| 38 | 6 | 30 | A |
| 38 | 6 | 31 | C |
| 38 | 6 | 32 | G |
| 38 | 6 | 38 | G |
| 38 | 6 | 40 | G |
| 38 | 6 | 43 | G |
| 38 | 6 | 44 | A |
| 38 | 6 | 46 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | 6 | 48 | G |
| 38 | 6 | 52 | G |
| 38 | 6 | 53 | G |
| 38 | 6 | 61 | A |
| 38 | 6 | 62 | C |
| 38 | 6 | 63 | A |
| 38 | 6 | 68 | U |
| 38 | 6 | 74 | U |
| 38 | 6 | 75 | G |
| 38 | 6 | 76 | C |
| 38 | 6 | 78 | A |
| 38 | 6 | 79 | C |
| 38 | 6 | 80 | A |
| 38 | 6 | 81 | U |
| 38 | 6 | 82 | U |
| 38 | 6 | 83 | G |
| 38 | 6 | 91 | A |
| 38 | 6 | 92 | C |
| 39 | 1 | -14 | U |
| 39 | 1 | -13 | U |
| 39 | 1 | -12 | U |
| 39 | 1 | -8 | U |
| 39 | 1 | -4 | A |
| 39 | 1 | 0 | G |
| 39 | 1 | 1 | G |
| 39 | 1 | 2 | U |
| 39 | 1 | 3 | A |
| 39 | 1 | 4 | U |
| 39 | 1 | 5 | G |
| 39 | 1 | 6 | U |
| 39 | 1 | 7 | U |
| 39 | 1 | 8 | U |
| 39 | 1 | 9 | U |
| 39 | 1 | 10 | U |
| 39 | 1 | 11 | U |
| 39 | 1 | 12 | U |
| 39 | 1 | 13 | U |

All (11) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 5 | 27 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 5 | 49 | U |
| 38 | 6 | 13 | A |
| 38 | 6 | 17 | U |
| 38 | 6 | 29 | A |
| 38 | 6 | 30 | A |
| 38 | 6 | 37 | A |
| 38 | 6 | 52 | G |
| 38 | 6 | 74 | U |
| 39 | 1 | 0 | G |
| 39 | 1 | 1 | G |

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 42 | GTP | B | 1001 | 43 | 26,34,34 | 1.45 | 3 (11%) | 32,54,54 | 1.75 | 8 (25%) |
| 41 | IHP | A | 2401 | - | 36,36,36 | 1.54 | 13 (36%) | 54,60,60 | 1.48 | 10 (18%) |

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 |
|---|---|---|---|---|---|---|---|
| 42 | GTP | B | 1001 | 43 | - | 0/18/38/38 | 0/3/3/3 |
| 41 | IHP | A | 2401 | - | - | 4/30/54/54 | 0/1/1/1 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | B | 1001 | GTP | C5-C6 | -4.74 | 1.37 | 1.47 |
| 42 | B | 1001 | GTP | C2'-C1' | -2.47 | 1.50 | 1.53 |
| 41 | A | 2401 | IHP | P1-O31 | -2.46 | 1.45 | 1.54 |
| 41 | A | 2401 | IHP | P3-O33 | -2.36 | 1.45 | 1.54 |
| 41 | A | 2401 | IHP | P6-O46 | -2.35 | 1.45 | 1.54 |
| 41 | A | 2401 | IHP | P5-O45 | -2.33 | 1.45 | 1.54 |
| 41 | A | 2401 | IHP | P3-O43 | -2.32 | 1.45 | 1.54 |
| 41 | A | 2401 | IHP | P4-O34 | -2.29 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P1-O11 | 2.29 | 1.63 | 1.59 |
| 42 | B | 1001 | GTP | C5-C4 | -2.26 | 1.37 | 1.43 |
| 41 | A | 2401 | IHP | P6-O36 | -2.24 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P1-O41 | -2.22 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P5-O35 | -2.21 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P4-O44 | -2.21 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P2-O42 | -2.20 | 1.46 | 1.54 |
| 41 | A | 2401 | IHP | P2-O32 | -2.13 | 1.46 | 1.54 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | B | 1001 | GTP | PB-O3B-PG | -5.21 | 114.95 | 132.83 |
| 42 | B | 1001 | GTP | C5-C6-N1 | 3.71 | 120.51 | 113.95 |
| 42 | B | 1001 | GTP | C2-N1-C6 | -3.26 | 119.09 | 125.10 |
| 41 | A | 2401 | IHP | C5-C6-C1 | 3.18 | 117.38 | 110.41 |
| 42 | B | 1001 | GTP | PA-O3A-PB | -3.16 | 121.99 | 132.83 |
| 42 | B | 1001 | GTP | C8-N7-C5 | 3.10 | 108.90 | 102.99 |
| 41 | A | 2401 | IHP | O11-P1-O21 | -2.87 | 98.32 | 109.39 |
| 41 | A | 2401 | IHP | C6-C1-C2 | 2.82 | 116.58 | 110.41 |
| 41 | A | 2401 | IHP | C6-C5-C4 | 2.62 | 116.14 | 110.41 |
| 41 | A | 2401 | IHP | O41-P1-O31 | 2.61 | 117.60 | 107.64 |
| 42 | B | 1001 | GTP | O6-C6-C5 | -2.37 | 119.74 | 124.37 |
| 42 | B | 1001 | GTP | O4'-C1'-C2' | -2.23 | 103.67 | 106.93 |
| 41 | A | 2401 | IHP | C3-C2-C1 | 2.22 | 115.27 | 110.41 |
| 41 | A | 2401 | IHP | O12-P2-O22 | -2.14 | 101.13 | 109.39 |
| 42 | B | 1001 | GTP | O3G-PG-O3B | 2.06 | 111.55 | 104.64 |
| 41 | A | 2401 | IHP | O44-P4-O34 | 2.03 | 115.40 | 107.64 |
| 41 | A | 2401 | IHP | O42-P2-O32 | 2.02 | 115.37 | 107.64 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | A | 2401 | IHP | O41-P1-O21 | 2.02 | 118.59 | 110.68 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | A | 2401 | IHP | C6-O16-P6-O26 |
| 41 | A | 2401 | IHP | C1-O11-P1-O41 |
| 41 | A | 2401 | IHP | C6-O16-P6-O36 |
| 41 | A | 2401 | IHP | C5-O15-P5-O35 |

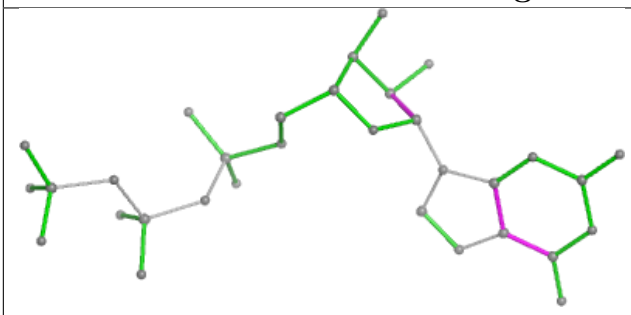
There are no ring outliers.

1 monomer is involved in 4 short contacts:

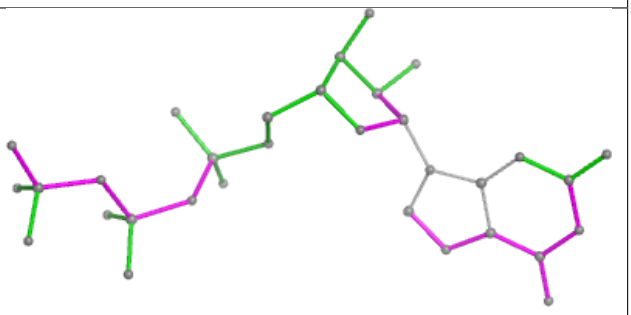
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 42 | B | 1001 | GTP | 4 | 0 |

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

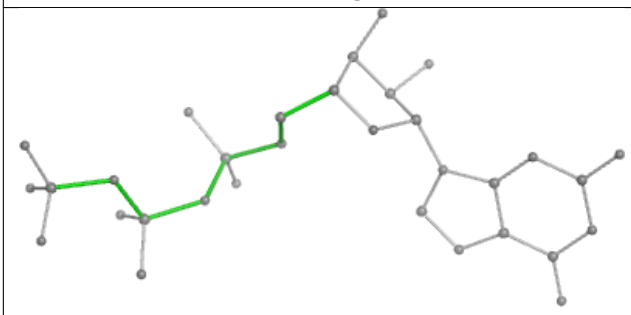
**Ligand GTP B 1001**



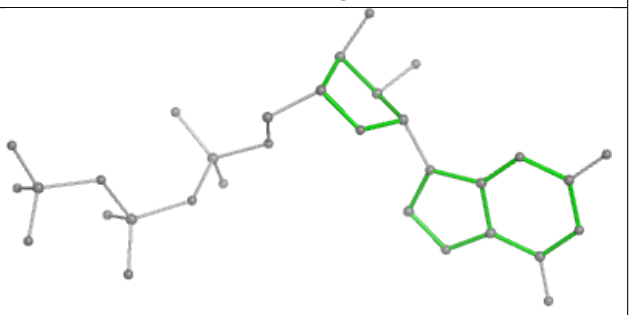
**Bond lengths**



**Bond angles**

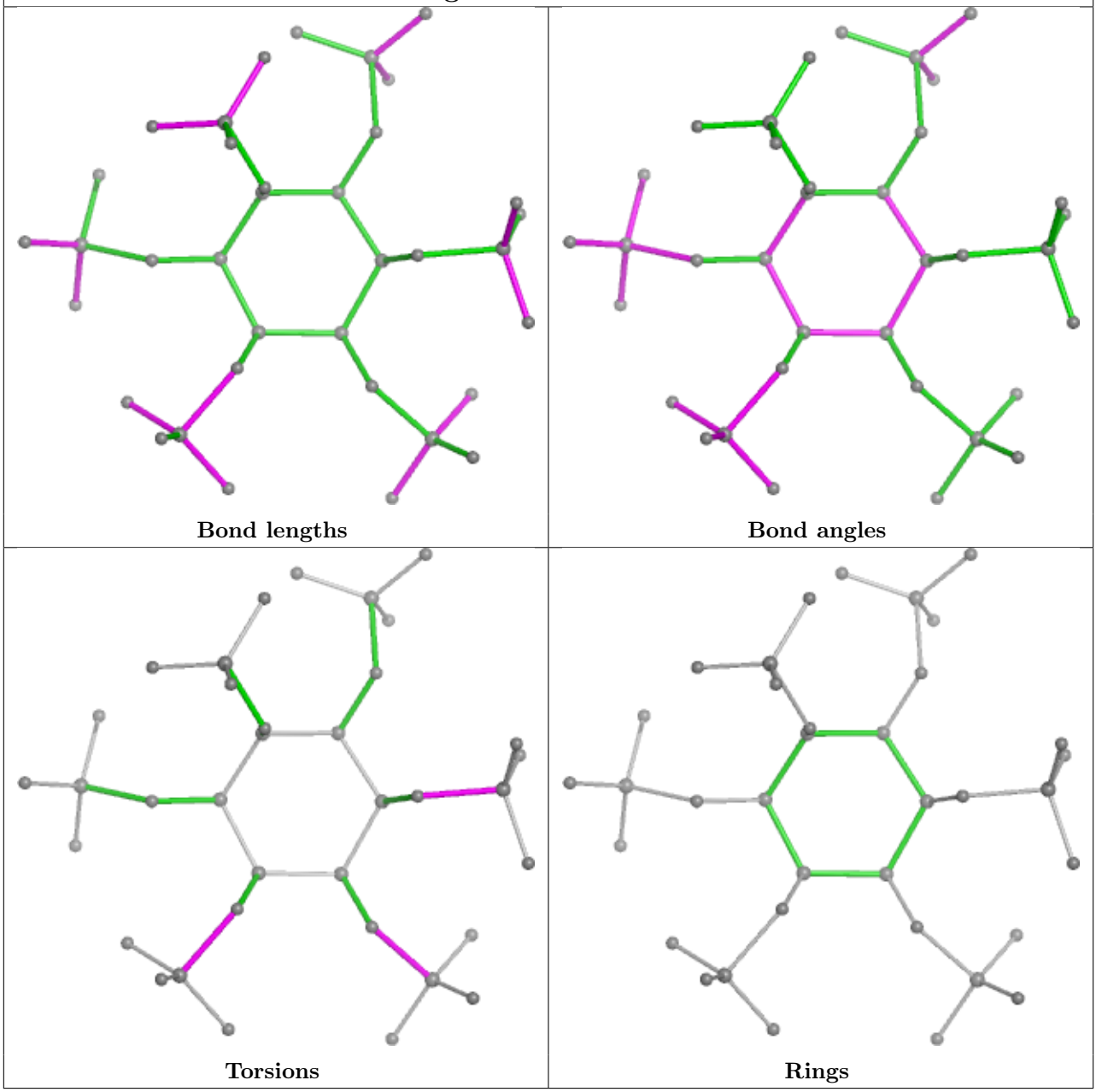


**Torsions**



**Rings**

**Ligand IHP A 2401**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

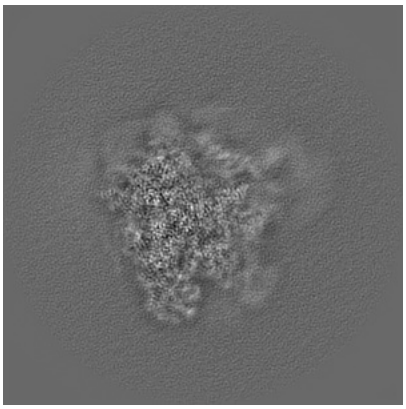
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19942. These allow visual inspection of the internal detail of the map and identification of artifacts.

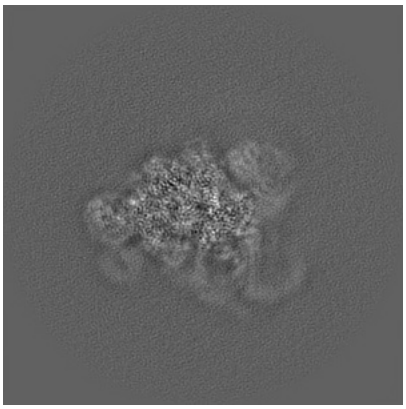
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

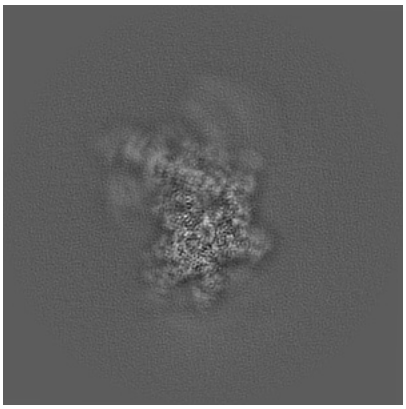
### 6.1.1 Primary map



X

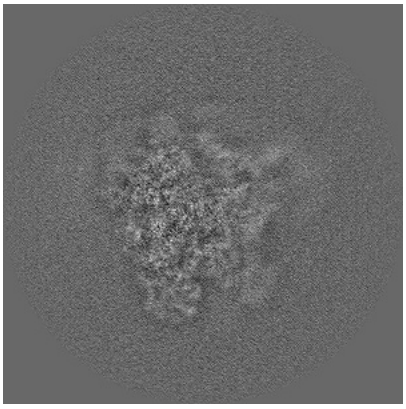


Y

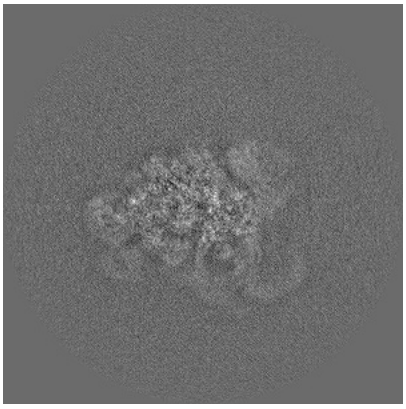


Z

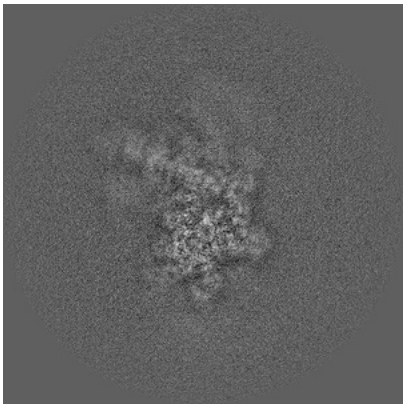
### 6.1.2 Raw map



X



Y

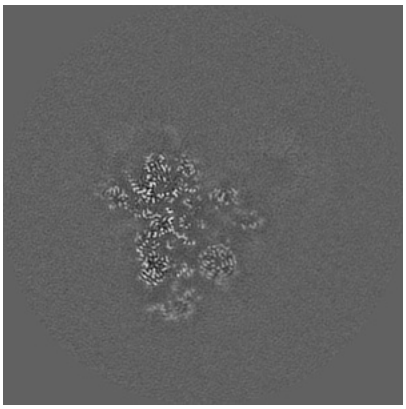


Z

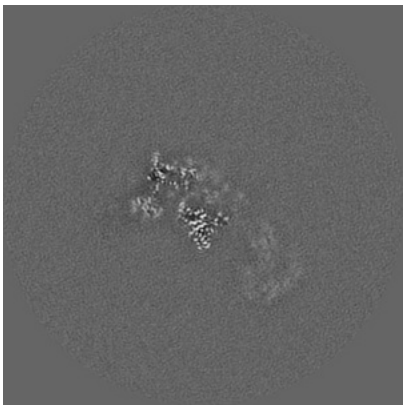
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

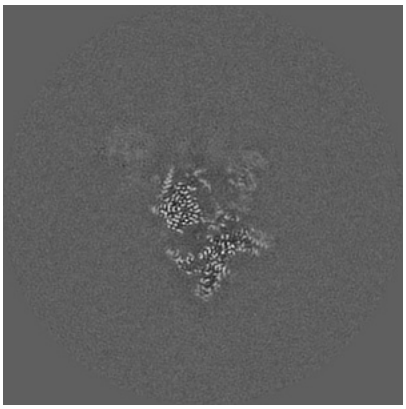
### 6.2.1 Primary map



X Index: 280

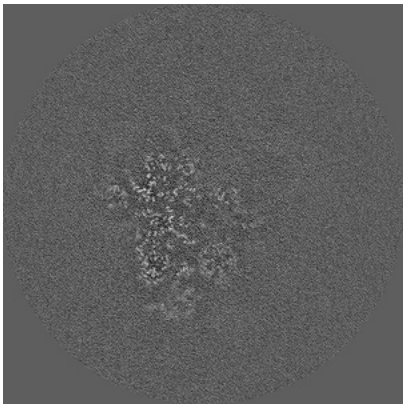


Y Index: 280

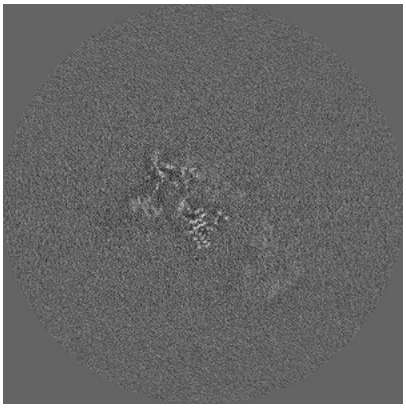


Z Index: 280

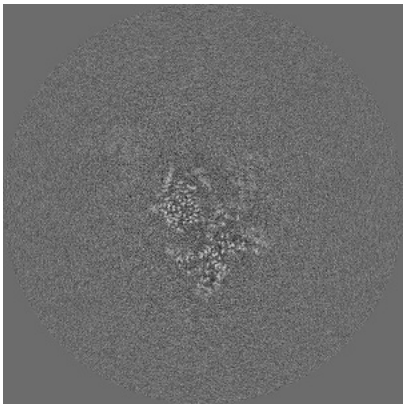
### 6.2.2 Raw map



X Index: 280



Y Index: 280

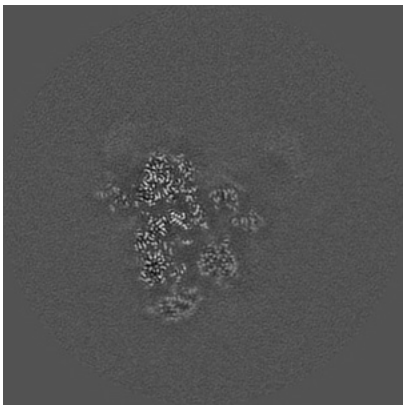


Z Index: 280

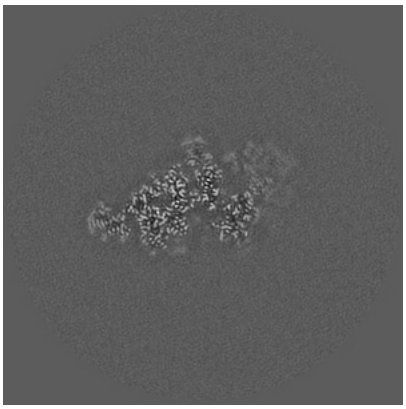
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

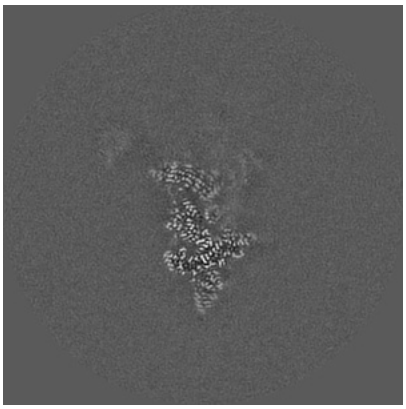
### 6.3.1 Primary map



X Index: 276

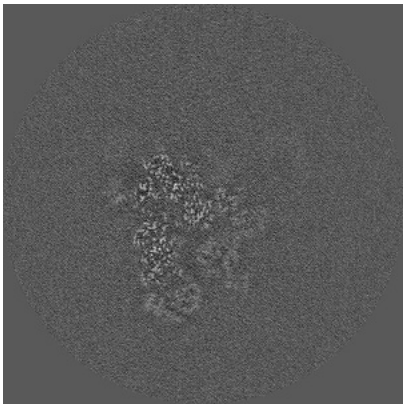


Y Index: 219

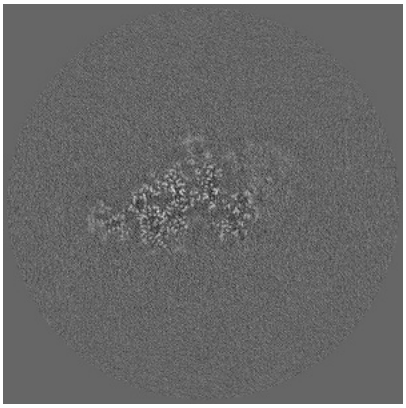


Z Index: 295

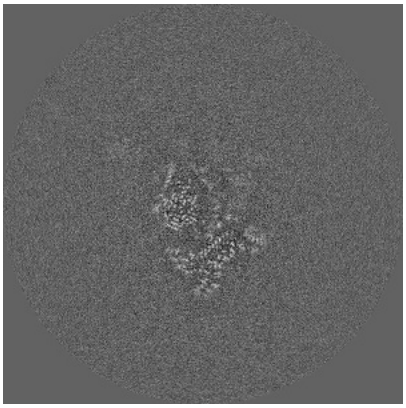
### 6.3.2 Raw map



X Index: 269



Y Index: 219

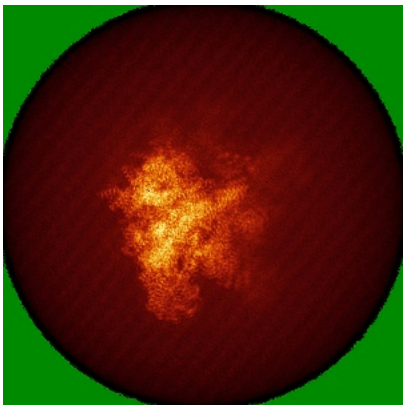


Z Index: 282

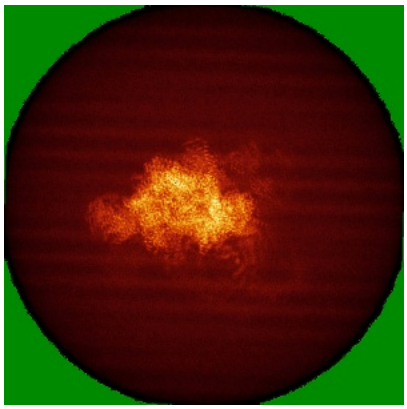
The images above show the largest variance slices of the map in three orthogonal directions.

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

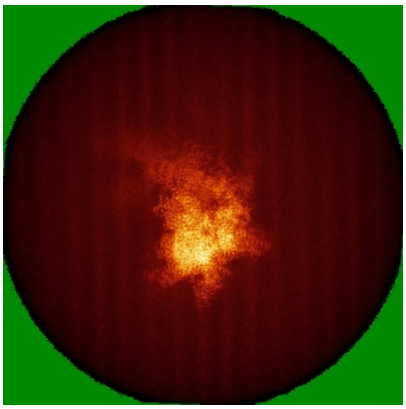
### 6.4.1 Primary map



X

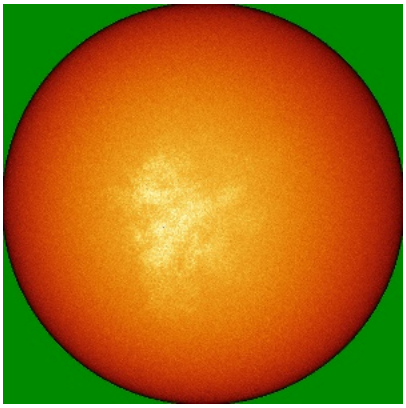


Y

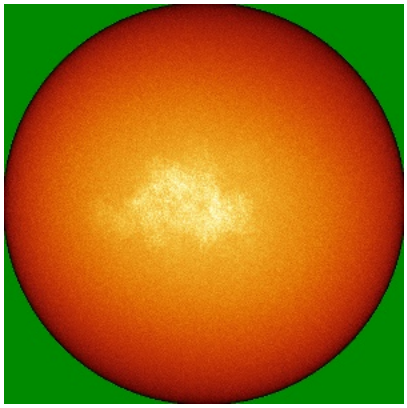


Z

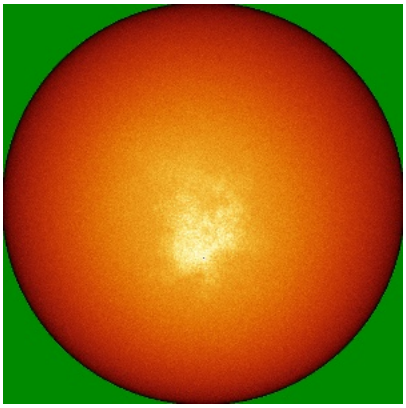
### 6.4.2 Raw map



X



Y

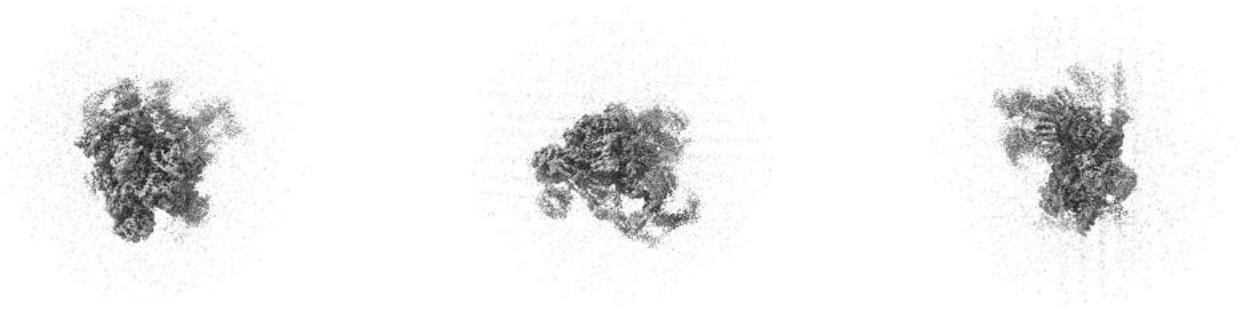


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. 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

X Y Z

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.

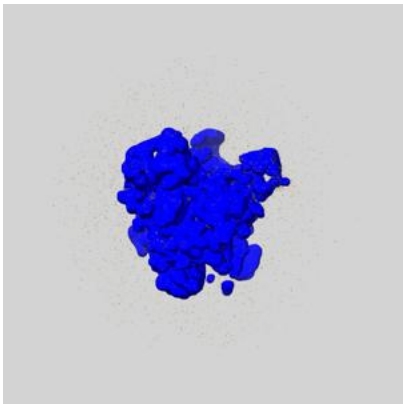
## 6.6 Mask visualisation

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

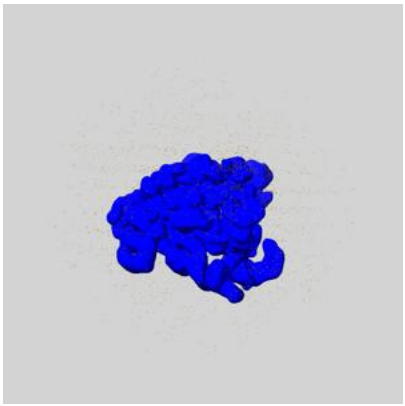
A mask typically either:

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

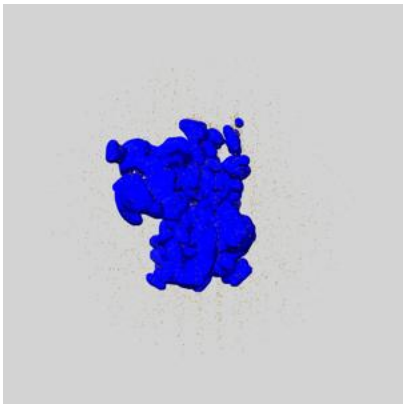
### 6.6.1 emd_19942_msk_1.map



X



Y

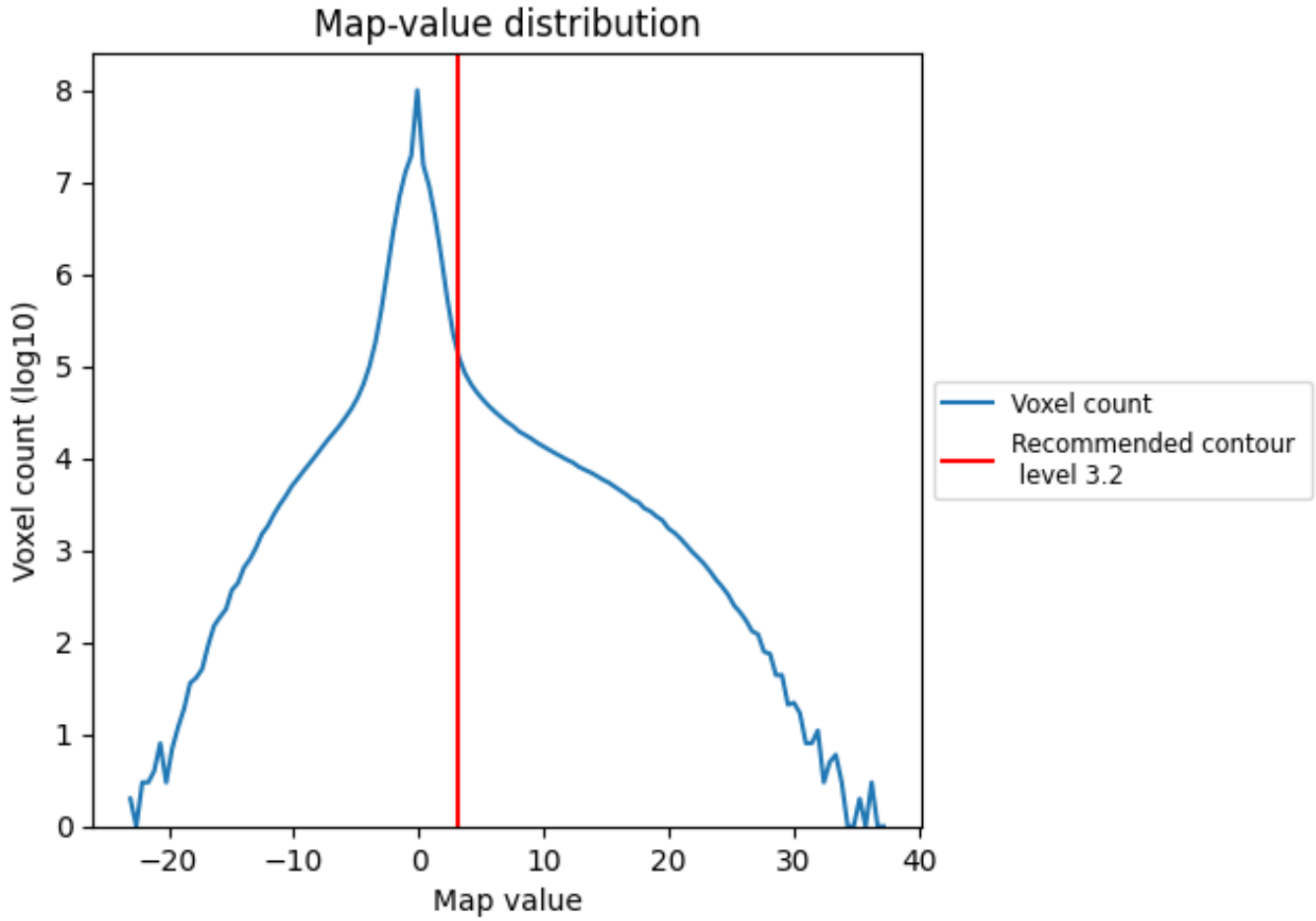


Z

# 7 Map analysis

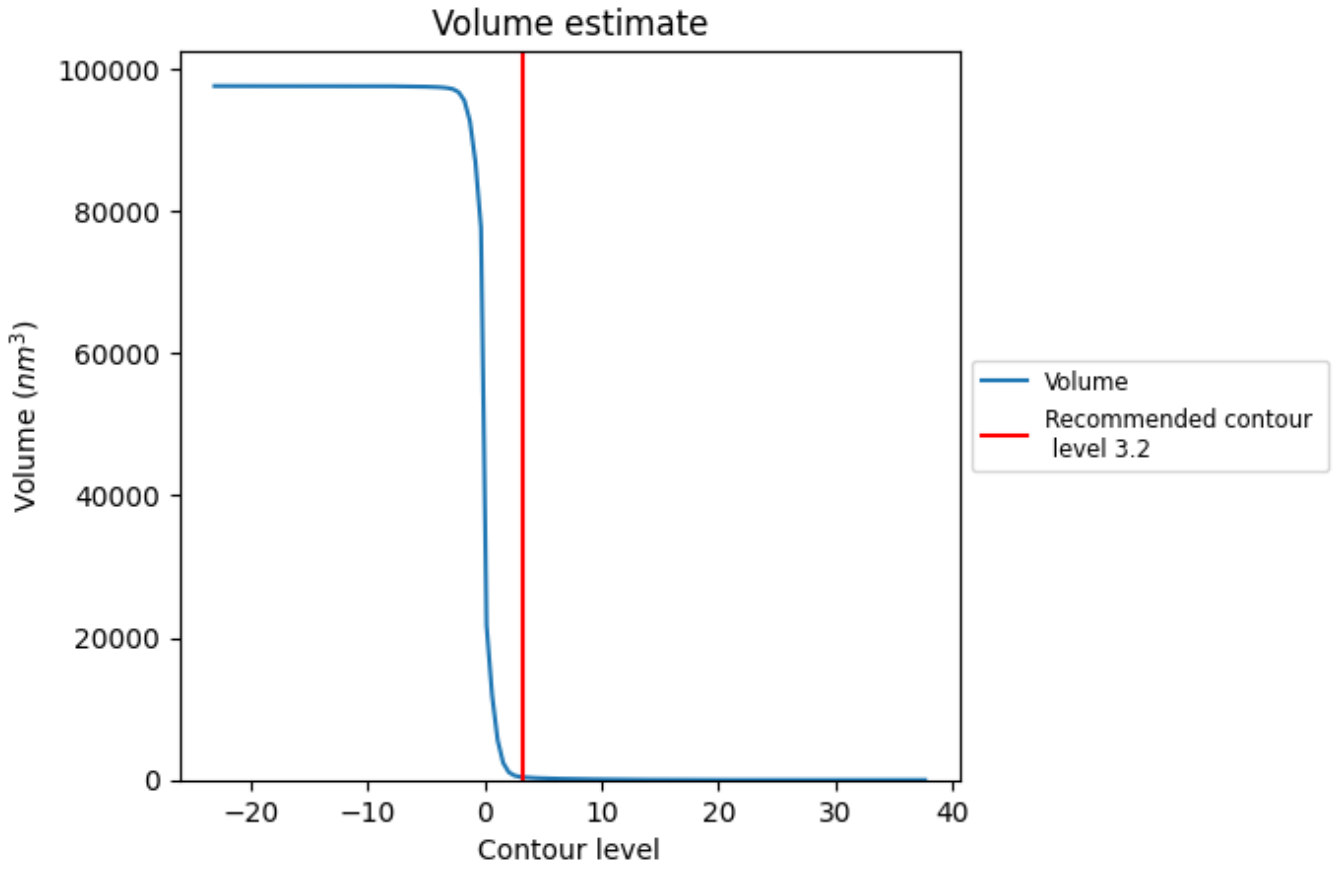
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

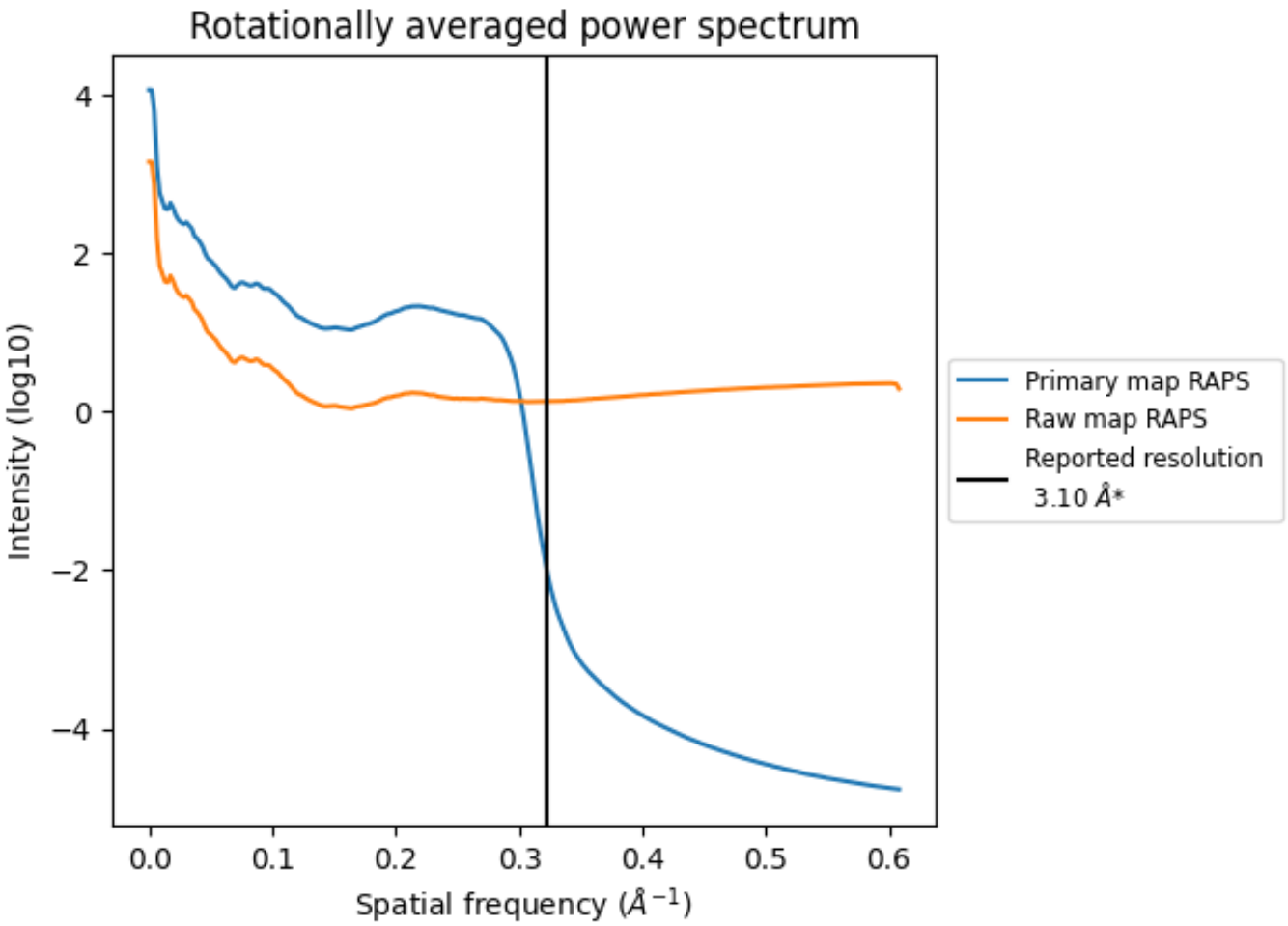
## 7.2 Volume estimate




The volume at the recommended contour level is 415 $nm^3$; this corresponds to an approximate mass of 375 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 (i)

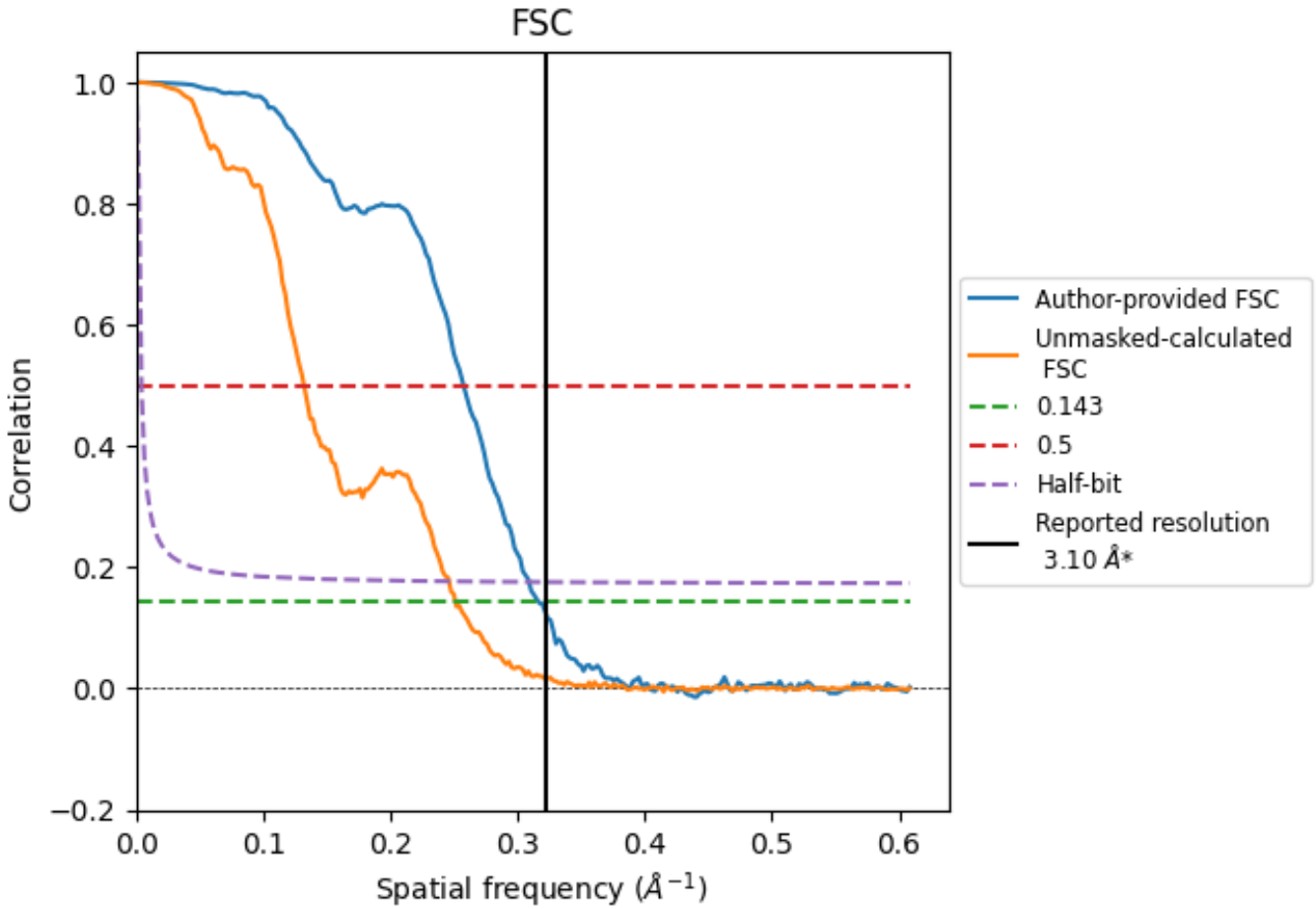



*Reported resolution corresponds to spatial frequency of 0.323 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.323 Å$^{-1}$

## 8.2 Resolution estimates (i)

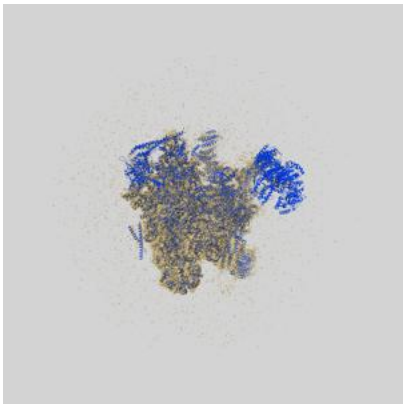
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.10 | - | - |
| Author-provided FSC curve | 3.16 | 3.88 | 3.24 |
| Unmasked-calculated* | 3.98 | 7.58 | 4.06 |

*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 3.98 differs from the reported value 3.1 by more than 10 %

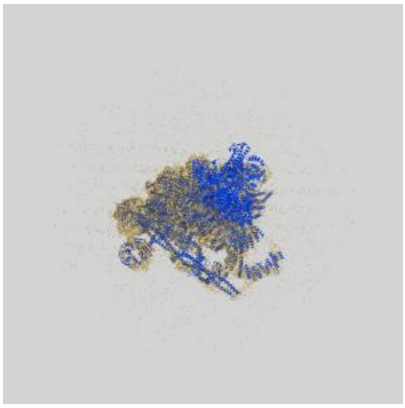
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

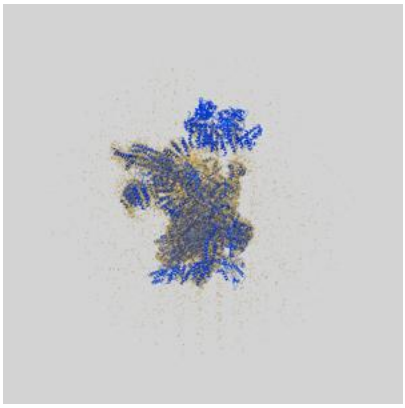
## 9.1 Map-model overlay



X



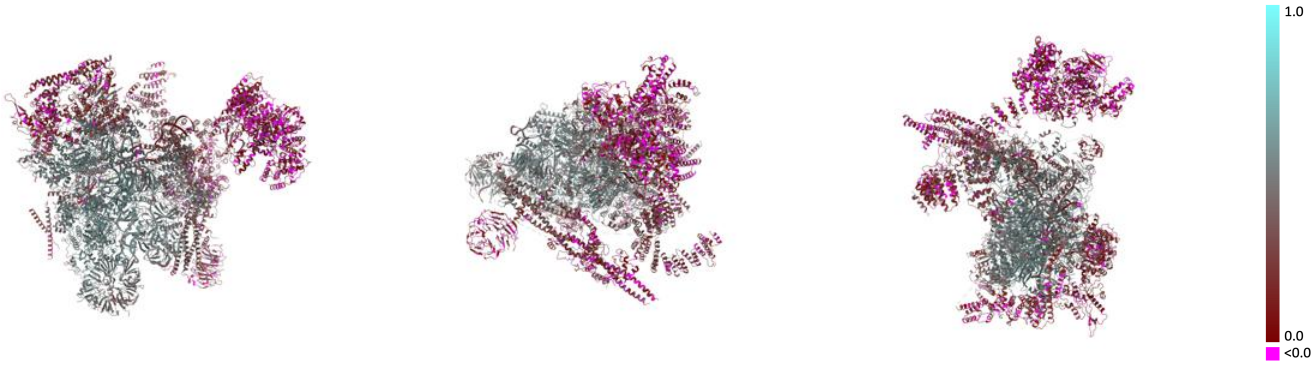
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2 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.

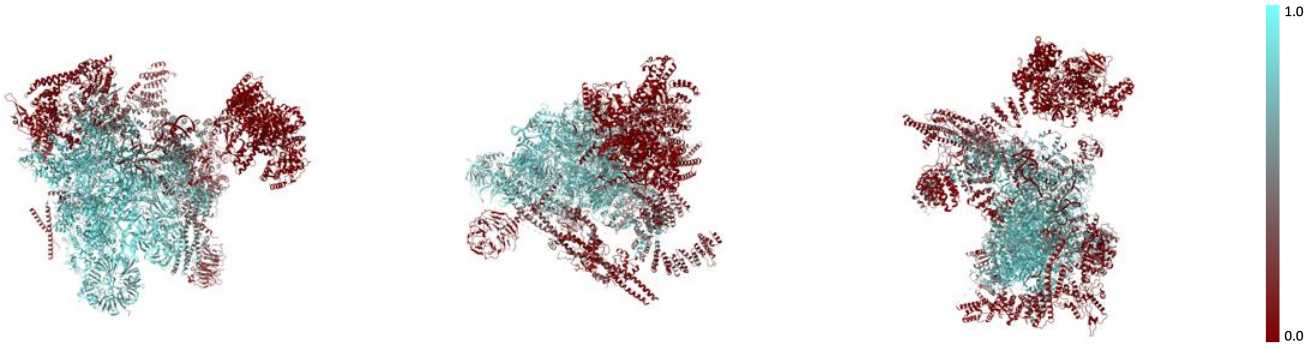
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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.

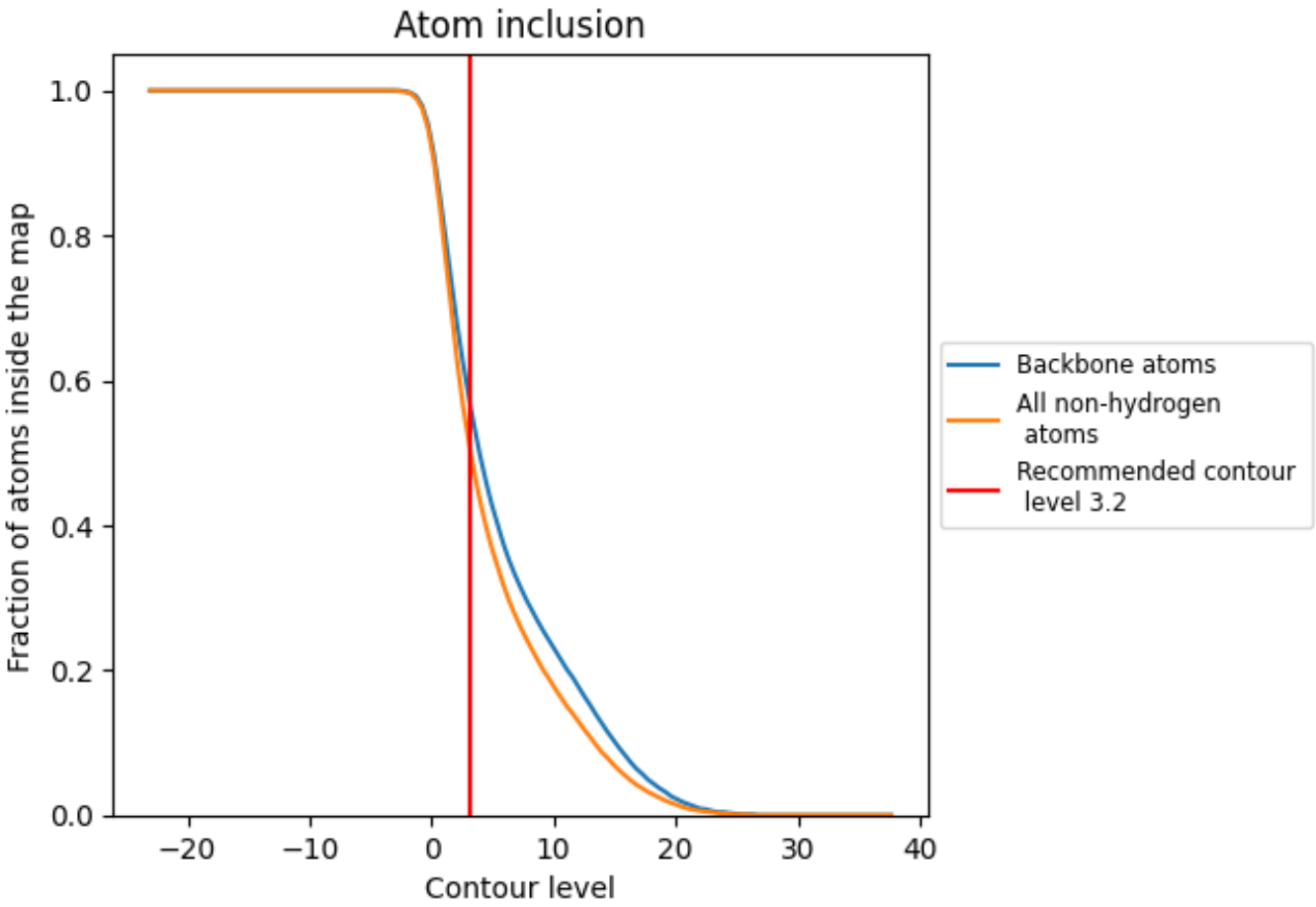
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (3.2).

## 9.4 Atom inclusion (i)




At the recommended contour level, 56% of all backbone atoms, 50% 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 (3.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4990 | 0.3640 |
| 1 | 0.5170 | 0.4200 |
| 2 | 0.4320 | 0.3200 |
| 5 | 0.9380 | 0.5360 |
| 6 | 0.5180 | 0.4060 |
| A | 0.7590 | 0.4960 |
| B | 0.8490 | 0.5310 |
| C | 0.7990 | 0.5030 |
| D | 0.8680 | 0.5490 |
| E | 0.7970 | 0.5080 |
| F | 0.7330 | 0.4680 |
| G | 0.7130 | 0.4240 |
| H | 0.7930 | 0.5050 |
| I | 0.7390 | 0.4490 |
| J | 0.8260 | 0.5340 |
| K | 0.8780 | 0.5480 |
| L | 0.7030 | 0.4700 |
| M | 0.4680 | 0.3830 |
| N | 0.0050 | 0.1040 |
| O | 0.8500 | 0.5400 |
| P | 0.6750 | 0.4450 |
| Q | 0.7790 | 0.5310 |
| R | 0.4450 | 0.3280 |
| S | 0.0530 | 0.1340 |
| T | 0.2000 | 0.2100 |
| U | 0.1300 | 0.1600 |
| V | 0.0770 | 0.1340 |
| W | 0.4690 | 0.3200 |
| X | 0.1770 | 0.1980 |
| Y | 0.1780 | 0.3150 |
| Z | 0.3780 | 0.2660 |
| a | 0.6470 | 0.4370 |
| b | 0.3050 | 0.3220 |
| c | 0.8220 | 0.5050 |
| d | 0.7110 | 0.4720 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| e | 0.4730 | 0.4550 |
| f | 0.3910 | 0.3230 |
| m | 0.0830 | 0.1860 |
| n | 0.0210 | 0.1600 |
| p | 0.3440 | 0.3510 |
| q | 0.3880 | 0.4780 |
| r | 0.3490 | 0.2780 |
| y | 0.4500 | 0.3500 |
| z | 0.2880 | 0.2760 |