# Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 10:41 AM EST

| | | |
|---|---|---|
| PDB ID | : | 5L1D |
| EMDB ID | : | EMD-8303 |
| Title | : | Structure of rabbit RyR2 in complex with FKBP12.6 in a closed state (conformation C1) |
| Authors | : | Dhindwal, S.; Lobo, J.J.; Samso, M. |
| Deposited on | : | 2016-07-29 |
| Resolution | : | 11.00 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:

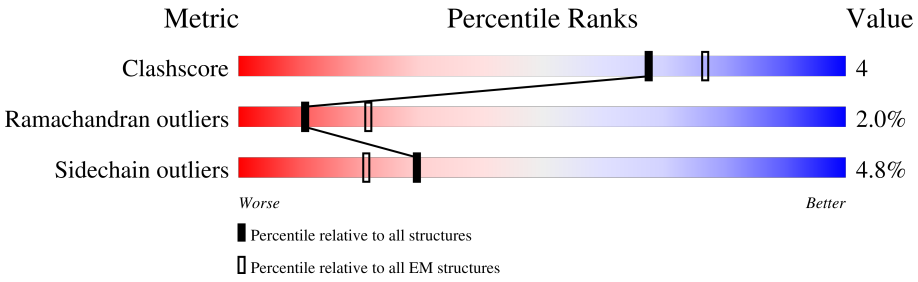
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 11.00 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | A | 4387 | 9% 71% 10% · 19% |
| 1 | C | 4387 | 9% 70% 11% · 19% |
| 1 | E | 4387 | 9% 70% 11% · 19% |
| 1 | G | 4387 | 9% 70% 10% · 19% |
| 2 | B | 158 | 8% 58% 10% 32% |
| 2 | D | 158 | 8% 60% 8% 32% |
| 2 | F | 158 | 8% 56% 12% 32% |
| 2 | H | 158 | 8% 63% · 32% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 112936 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 Ryanodine Receptor.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 3570 | Total<br>27416 | C<br>17427 | N<br>4732 | O<br>5102 | S<br>155 | 0 | 0 |
| 1 | C | 3570 | Total<br>27416 | C<br>17427 | N<br>4732 | O<br>5102 | S<br>155 | 0 | 0 |
| 1 | E | 3570 | Total<br>27416 | C<br>17427 | N<br>4732 | O<br>5102 | S<br>155 | 0 | 0 |
| 1 | G | 3570 | Total<br>27416 | C<br>17427 | N<br>4732 | O<br>5102 | S<br>155 | 0 | 0 |

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | D | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | F | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | H | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |

There are 204 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -50 | MET | - | expression tag | UNP P68106 |
| B | -49 | ASN | - | expression tag | UNP P68106 |
| B | -48 | HIS | - | expression tag | UNP P68106 |
| B | -47 | LYS | - | expression tag | UNP P68106 |
| B | -46 | VAL | - | expression tag | UNP P68106 |
| B | -45 | HIS | - | expression tag | UNP P68106 |
| B | -44 | HIS | - | expression tag | UNP P68106 |
| B | -43 | HIS | - | expression tag | UNP P68106 |
| B | -42 | HIS | - | expression tag | UNP P68106 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -41 | HIS | - | expression tag | UNP P68106 |
| B | -40 | HIS | - | expression tag | UNP P68106 |
| B | -39 | MET | - | expression tag | UNP P68106 |
| B | -38 | ASP | - | expression tag | UNP P68106 |
| B | -37 | GLU | - | expression tag | UNP P68106 |
| B | -36 | LYS | - | expression tag | UNP P68106 |
| B | -35 | THR | - | expression tag | UNP P68106 |
| B | -34 | THR | - | expression tag | UNP P68106 |
| B | -33 | GLY | - | expression tag | UNP P68106 |
| B | -32 | TRP | - | expression tag | UNP P68106 |
| B | -31 | ARG | - | expression tag | UNP P68106 |
| B | -30 | GLY | - | expression tag | UNP P68106 |
| B | -29 | GLY | - | expression tag | UNP P68106 |
| B | -28 | HIS | - | expression tag | UNP P68106 |
| B | -27 | VAL | - | expression tag | UNP P68106 |
| B | -26 | VAL | - | expression tag | UNP P68106 |
| B | -25 | GLU | - | expression tag | UNP P68106 |
| B | -24 | GLY | - | expression tag | UNP P68106 |
| B | -23 | LEU | - | expression tag | UNP P68106 |
| B | -22 | ALA | - | expression tag | UNP P68106 |
| B | -21 | GLY | - | expression tag | UNP P68106 |
| B | -20 | GLU | - | expression tag | UNP P68106 |
| B | -19 | LEU | - | expression tag | UNP P68106 |
| B | -18 | GLU | - | expression tag | UNP P68106 |
| B | -17 | GLN | - | expression tag | UNP P68106 |
| B | -16 | LEU | - | expression tag | UNP P68106 |
| B | -15 | ARG | - | expression tag | UNP P68106 |
| B | -14 | ALA | - | expression tag | UNP P68106 |
| B | -13 | ARG | - | expression tag | UNP P68106 |
| B | -12 | LEU | - | expression tag | UNP P68106 |
| B | -11 | GLU | - | expression tag | UNP P68106 |
| B | -10 | HIS | - | expression tag | UNP P68106 |
| B | -9 | HIS | - | expression tag | UNP P68106 |
| B | -8 | PRO | - | expression tag | UNP P68106 |
| B | -7 | GLN | - | expression tag | UNP P68106 |
| B | -6 | GLY | - | expression tag | UNP P68106 |
| B | -5 | GLN | - | expression tag | UNP P68106 |
| B | -4 | ARG | - | expression tag | UNP P68106 |
| B | -3 | GLU | - | expression tag | UNP P68106 |
| B | -2 | PRO | - | expression tag | UNP P68106 |
| B | -1 | GLU | - | expression tag | UNP P68106 |
| B | 0 | LEU | - | expression tag | UNP P68106 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -50 | MET | - | expression tag | UNP P68106 |
| D | -49 | ASN | - | expression tag | UNP P68106 |
| D | -48 | HIS | - | expression tag | UNP P68106 |
| D | -47 | LYS | - | expression tag | UNP P68106 |
| D | -46 | VAL | - | expression tag | UNP P68106 |
| D | -45 | HIS | - | expression tag | UNP P68106 |
| D | -44 | HIS | - | expression tag | UNP P68106 |
| D | -43 | HIS | - | expression tag | UNP P68106 |
| D | -42 | HIS | - | expression tag | UNP P68106 |
| D | -41 | HIS | - | expression tag | UNP P68106 |
| D | -40 | HIS | - | expression tag | UNP P68106 |
| D | -39 | MET | - | expression tag | UNP P68106 |
| D | -38 | ASP | - | expression tag | UNP P68106 |
| D | -37 | GLU | - | expression tag | UNP P68106 |
| D | -36 | LYS | - | expression tag | UNP P68106 |
| D | -35 | THR | - | expression tag | UNP P68106 |
| D | -34 | THR | - | expression tag | UNP P68106 |
| D | -33 | GLY | - | expression tag | UNP P68106 |
| D | -32 | TRP | - | expression tag | UNP P68106 |
| D | -31 | ARG | - | expression tag | UNP P68106 |
| D | -30 | GLY | - | expression tag | UNP P68106 |
| D | -29 | GLY | - | expression tag | UNP P68106 |
| D | -28 | HIS | - | expression tag | UNP P68106 |
| D | -27 | VAL | - | expression tag | UNP P68106 |
| D | -26 | VAL | - | expression tag | UNP P68106 |
| D | -25 | GLU | - | expression tag | UNP P68106 |
| D | -24 | GLY | - | expression tag | UNP P68106 |
| D | -23 | LEU | - | expression tag | UNP P68106 |
| D | -22 | ALA | - | expression tag | UNP P68106 |
| D | -21 | GLY | - | expression tag | UNP P68106 |
| D | -20 | GLU | - | expression tag | UNP P68106 |
| D | -19 | LEU | - | expression tag | UNP P68106 |
| D | -18 | GLU | - | expression tag | UNP P68106 |
| D | -17 | GLN | - | expression tag | UNP P68106 |
| D | -16 | LEU | - | expression tag | UNP P68106 |
| D | -15 | ARG | - | expression tag | UNP P68106 |
| D | -14 | ALA | - | expression tag | UNP P68106 |
| D | -13 | ARG | - | expression tag | UNP P68106 |
| D | -12 | LEU | - | expression tag | UNP P68106 |
| D | -11 | GLU | - | expression tag | UNP P68106 |
| D | -10 | HIS | - | expression tag | UNP P68106 |
| D | -9 | HIS | - | expression tag | UNP P68106 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -8 | PRO | - | expression tag | UNP P68106 |
| D | -7 | GLN | - | expression tag | UNP P68106 |
| D | -6 | GLY | - | expression tag | UNP P68106 |
| D | -5 | GLN | - | expression tag | UNP P68106 |
| D | -4 | ARG | - | expression tag | UNP P68106 |
| D | -3 | GLU | - | expression tag | UNP P68106 |
| D | -2 | PRO | - | expression tag | UNP P68106 |
| D | -1 | GLU | - | expression tag | UNP P68106 |
| D | 0 | LEU | - | expression tag | UNP P68106 |
| F | -50 | MET | - | expression tag | UNP P68106 |
| F | -49 | ASN | - | expression tag | UNP P68106 |
| F | -48 | HIS | - | expression tag | UNP P68106 |
| F | -47 | LYS | - | expression tag | UNP P68106 |
| F | -46 | VAL | - | expression tag | UNP P68106 |
| F | -45 | HIS | - | expression tag | UNP P68106 |
| F | -44 | HIS | - | expression tag | UNP P68106 |
| F | -43 | HIS | - | expression tag | UNP P68106 |
| F | -42 | HIS | - | expression tag | UNP P68106 |
| F | -41 | HIS | - | expression tag | UNP P68106 |
| F | -40 | HIS | - | expression tag | UNP P68106 |
| F | -39 | MET | - | expression tag | UNP P68106 |
| F | -38 | ASP | - | expression tag | UNP P68106 |
| F | -37 | GLU | - | expression tag | UNP P68106 |
| F | -36 | LYS | - | expression tag | UNP P68106 |
| F | -35 | THR | - | expression tag | UNP P68106 |
| F | -34 | THR | - | expression tag | UNP P68106 |
| F | -33 | GLY | - | expression tag | UNP P68106 |
| F | -32 | TRP | - | expression tag | UNP P68106 |
| F | -31 | ARG | - | expression tag | UNP P68106 |
| F | -30 | GLY | - | expression tag | UNP P68106 |
| F | -29 | GLY | - | expression tag | UNP P68106 |
| F | -28 | HIS | - | expression tag | UNP P68106 |
| F | -27 | VAL | - | expression tag | UNP P68106 |
| F | -26 | VAL | - | expression tag | UNP P68106 |
| F | -25 | GLU | - | expression tag | UNP P68106 |
| F | -24 | GLY | - | expression tag | UNP P68106 |
| F | -23 | LEU | - | expression tag | UNP P68106 |
| F | -22 | ALA | - | expression tag | UNP P68106 |
| F | -21 | GLY | - | expression tag | UNP P68106 |
| F | -20 | GLU | - | expression tag | UNP P68106 |
| F | -19 | LEU | - | expression tag | UNP P68106 |
| F | -18 | GLU | - | expression tag | UNP P68106 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | -17 | GLN | - | expression tag | UNP P68106 |
| F | -16 | LEU | - | expression tag | UNP P68106 |
| F | -15 | ARG | - | expression tag | UNP P68106 |
| F | -14 | ALA | - | expression tag | UNP P68106 |
| F | -13 | ARG | - | expression tag | UNP P68106 |
| F | -12 | LEU | - | expression tag | UNP P68106 |
| F | -11 | GLU | - | expression tag | UNP P68106 |
| F | -10 | HIS | - | expression tag | UNP P68106 |
| F | -9 | HIS | - | expression tag | UNP P68106 |
| F | -8 | PRO | - | expression tag | UNP P68106 |
| F | -7 | GLN | - | expression tag | UNP P68106 |
| F | -6 | GLY | - | expression tag | UNP P68106 |
| F | -5 | GLN | - | expression tag | UNP P68106 |
| F | -4 | ARG | - | expression tag | UNP P68106 |
| F | -3 | GLU | - | expression tag | UNP P68106 |
| F | -2 | PRO | - | expression tag | UNP P68106 |
| F | -1 | GLU | - | expression tag | UNP P68106 |
| F | 0 | LEU | - | expression tag | UNP P68106 |
| H | -50 | MET | - | expression tag | UNP P68106 |
| H | -49 | ASN | - | expression tag | UNP P68106 |
| H | -48 | HIS | - | expression tag | UNP P68106 |
| H | -47 | LYS | - | expression tag | UNP P68106 |
| H | -46 | VAL | - | expression tag | UNP P68106 |
| H | -45 | HIS | - | expression tag | UNP P68106 |
| H | -44 | HIS | - | expression tag | UNP P68106 |
| H | -43 | HIS | - | expression tag | UNP P68106 |
| H | -42 | HIS | - | expression tag | UNP P68106 |
| H | -41 | HIS | - | expression tag | UNP P68106 |
| H | -40 | HIS | - | expression tag | UNP P68106 |
| H | -39 | MET | - | expression tag | UNP P68106 |
| H | -38 | ASP | - | expression tag | UNP P68106 |
| H | -37 | GLU | - | expression tag | UNP P68106 |
| H | -36 | LYS | - | expression tag | UNP P68106 |
| H | -35 | THR | - | expression tag | UNP P68106 |
| H | -34 | THR | - | expression tag | UNP P68106 |
| H | -33 | GLY | - | expression tag | UNP P68106 |
| H | -32 | TRP | - | expression tag | UNP P68106 |
| H | -31 | ARG | - | expression tag | UNP P68106 |
| H | -30 | GLY | - | expression tag | UNP P68106 |
| H | -29 | GLY | - | expression tag | UNP P68106 |
| H | -28 | HIS | - | expression tag | UNP P68106 |
| H | -27 | VAL | - | expression tag | UNP P68106 |

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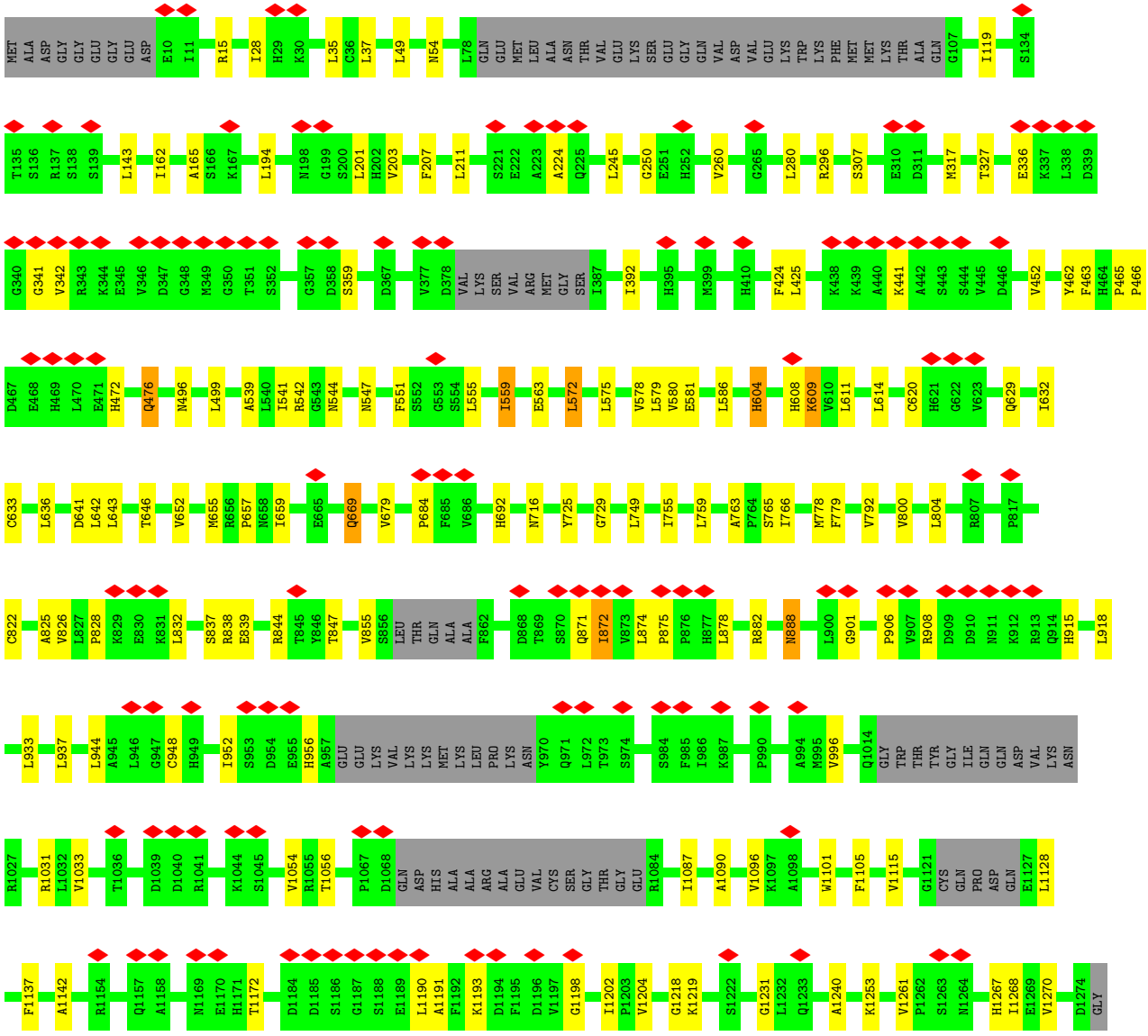
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| H | -26 | VAL | - | expression tag | UNP P68106 |
| H | -25 | GLU | - | expression tag | UNP P68106 |
| H | -24 | GLY | - | expression tag | UNP P68106 |
| H | -23 | LEU | - | expression tag | UNP P68106 |
| H | -22 | ALA | - | expression tag | UNP P68106 |
| H | -21 | GLY | - | expression tag | UNP P68106 |
| H | -20 | GLU | - | expression tag | UNP P68106 |
| H | -19 | LEU | - | expression tag | UNP P68106 |
| H | -18 | GLU | - | expression tag | UNP P68106 |
| H | -17 | GLN | - | expression tag | UNP P68106 |
| H | -16 | LEU | - | expression tag | UNP P68106 |
| H | -15 | ARG | - | expression tag | UNP P68106 |
| H | -14 | ALA | - | expression tag | UNP P68106 |
| H | -13 | ARG | - | expression tag | UNP P68106 |
| H | -12 | LEU | - | expression tag | UNP P68106 |
| H | -11 | GLU | - | expression tag | UNP P68106 |
| H | -10 | HIS | - | expression tag | UNP P68106 |
| H | -9 | HIS | - | expression tag | UNP P68106 |
| H | -8 | PRO | - | expression tag | UNP P68106 |
| H | -7 | GLN | - | expression tag | UNP P68106 |
| H | -6 | GLY | - | expression tag | UNP P68106 |
| H | -5 | GLN | - | expression tag | UNP P68106 |
| H | -4 | ARG | - | expression tag | UNP P68106 |
| H | -3 | GLU | - | expression tag | UNP P68106 |
| H | -2 | PRO | - | expression tag | UNP P68106 |
| H | -1 | GLU | - | expression tag | UNP P68106 |
| H | 0 | LEU | - | expression tag | UNP P68106 |

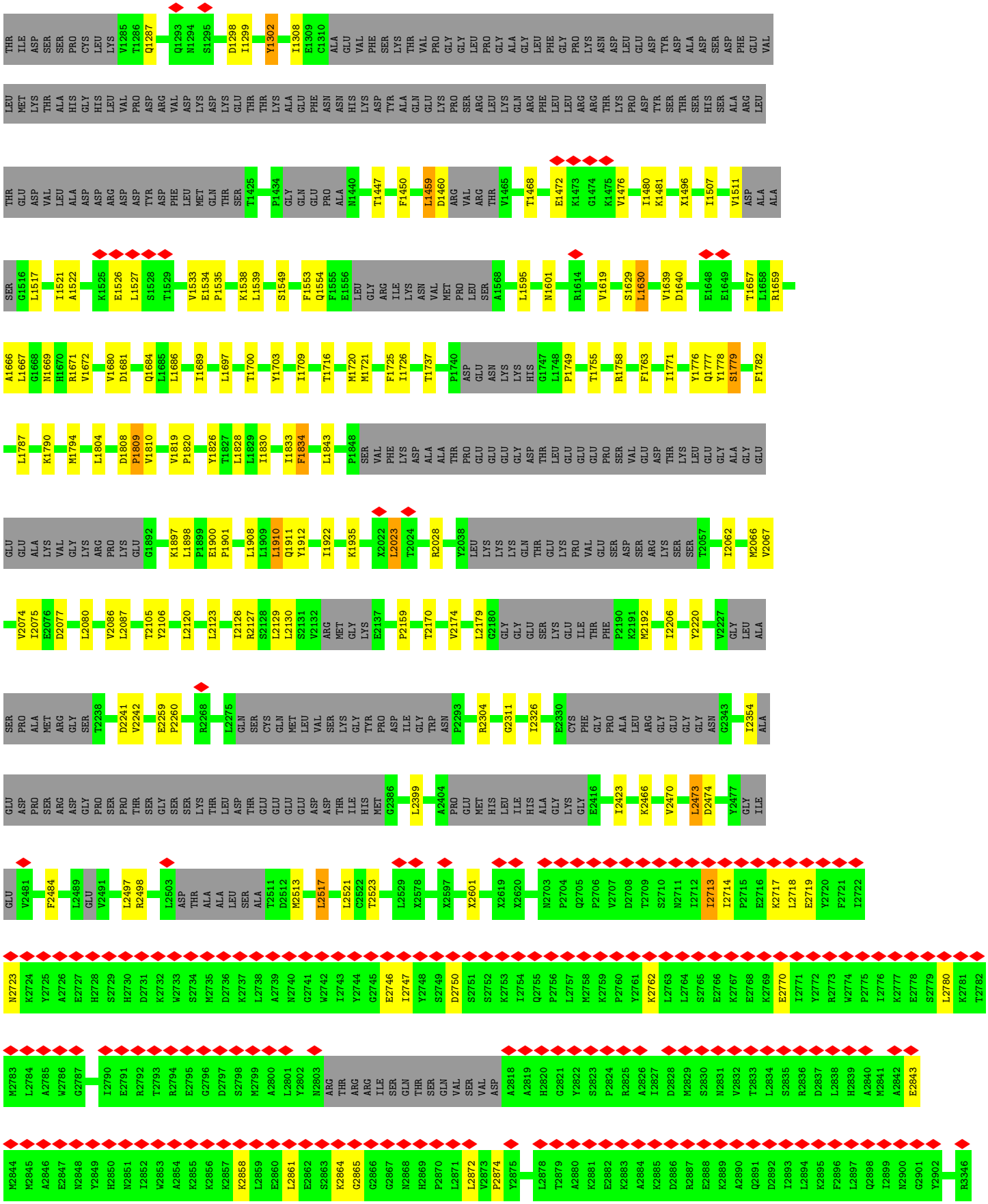
# 3 Residue-property plots (i)

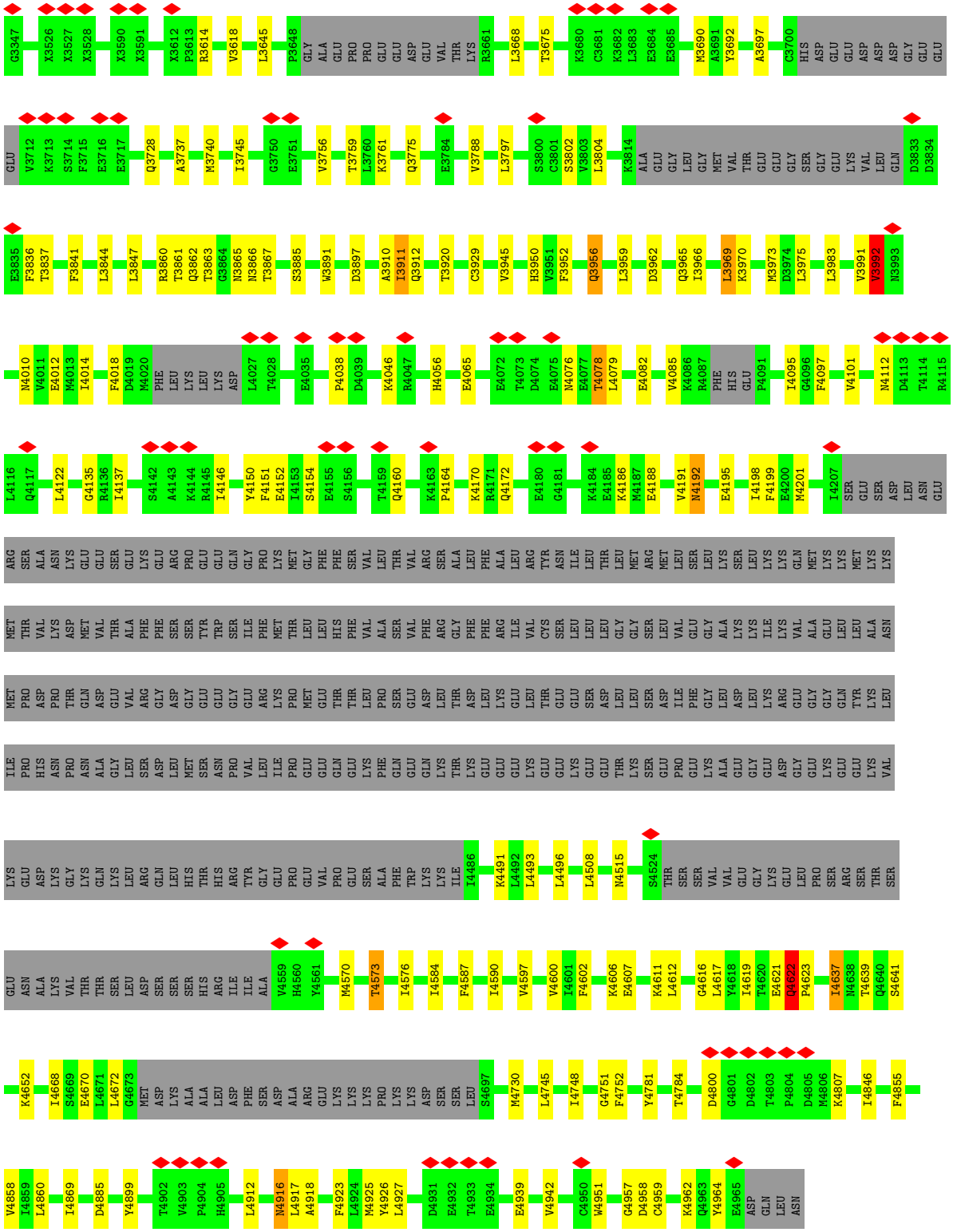
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

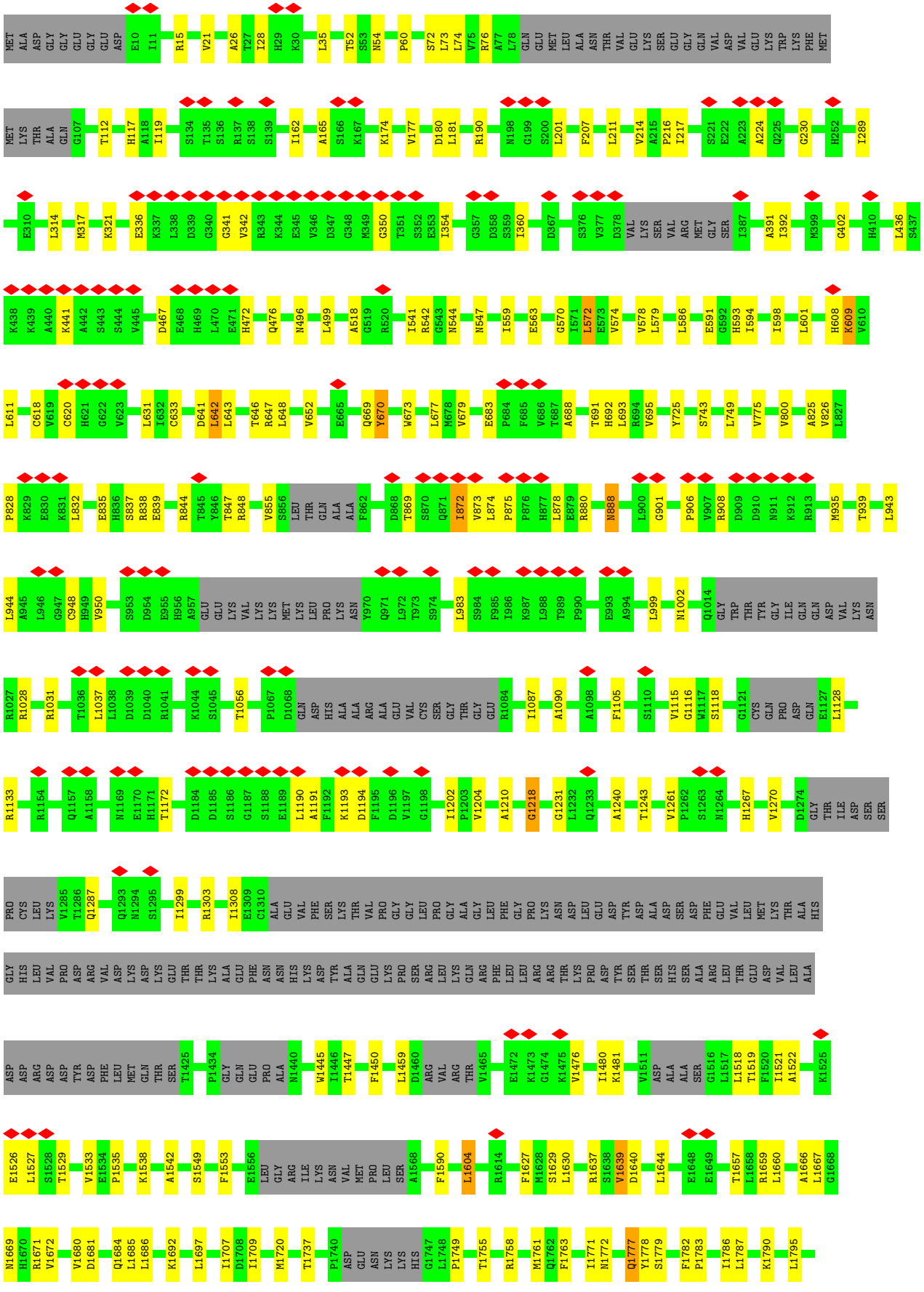



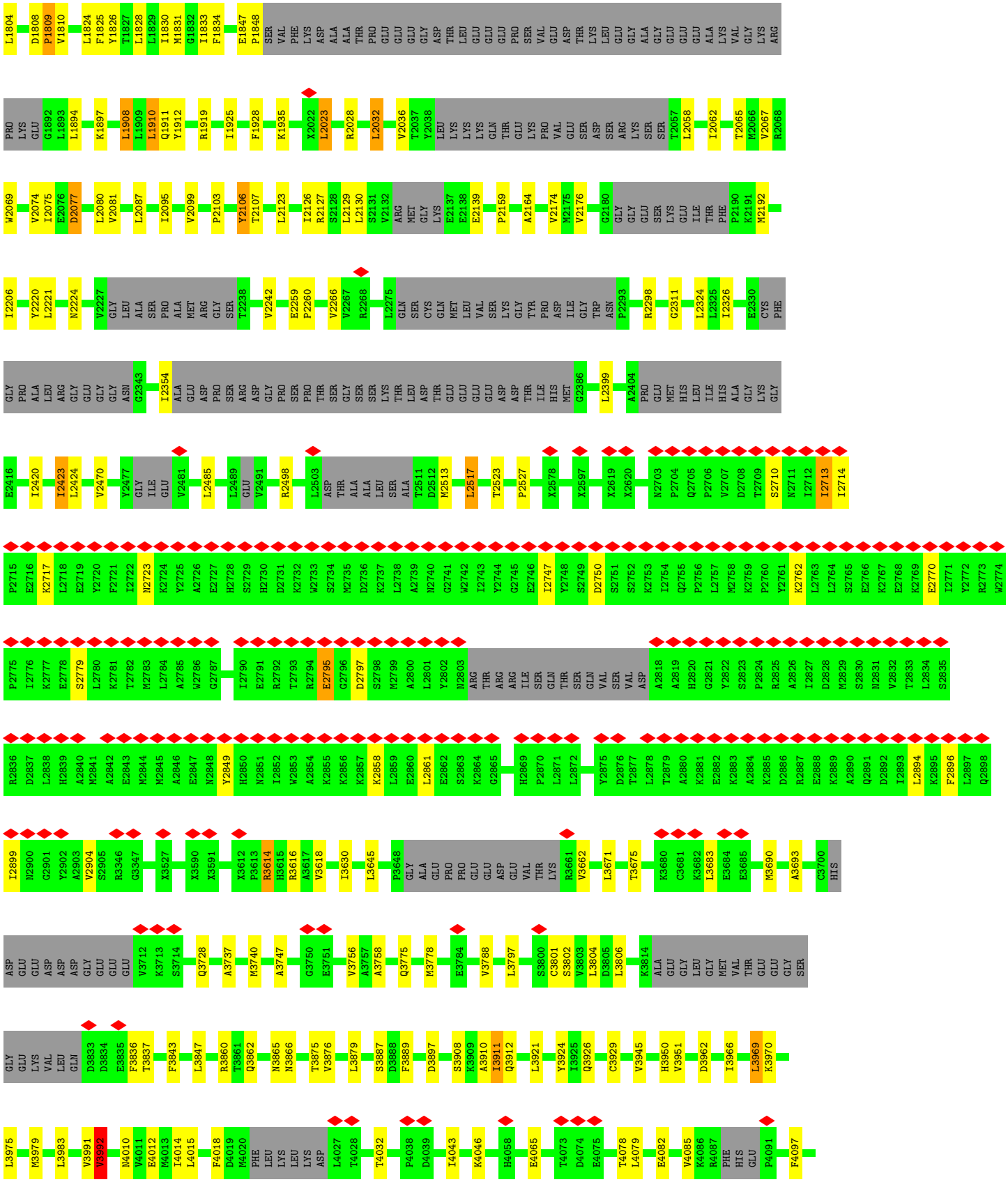


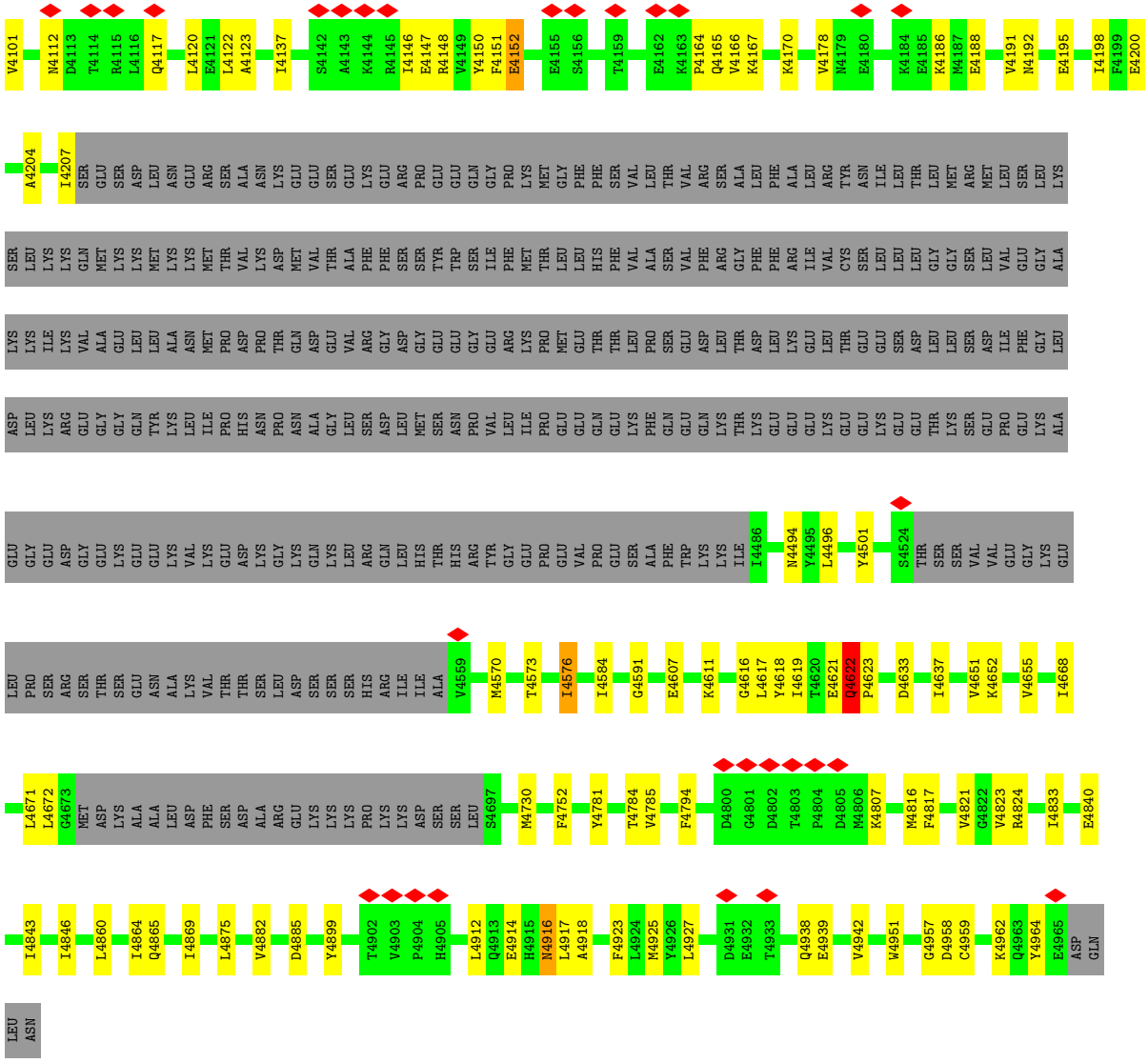


• Molecule 1: Ryanodine Receptor

Chain C:

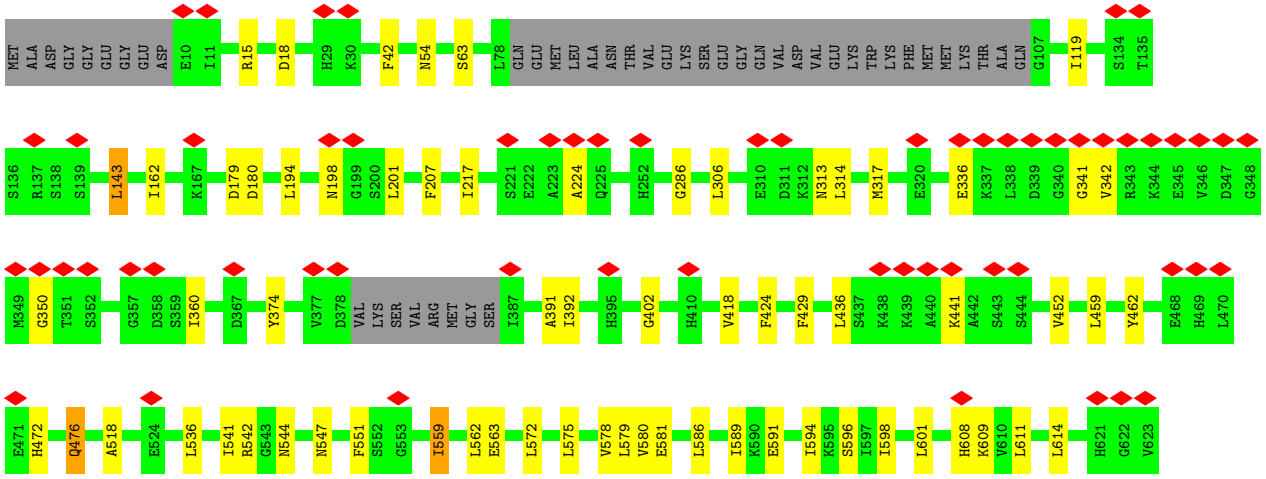

MET ALA ASP GLY GLY GLU GLY GLU ASP E10 I11 R15 V21 A26 T27 I28 H29 K30 L35 T52 S53 N54 P60 S72 L73 L74 V75 R76 A77 L78 GLN GLU MET LEU ALA ASN THR VAL GLU LYS SER GLU GLY GLN VAL ASP VAL GLU LYS TRP LYS PHE MET
MET LYS THR ALA GLN G107 T112 H117 A118 I119 S134 T135 S136 R137 S138 S139 I162 A165 S166 K167 K174 V177 D180 L181 R190 N198 G199 S200 L201 F207 L211 V214 A215 P216 I217 S221 E222 A223 A224 Q225 G230 H252 I289
E310 L314 M317 K321 E336 K337 L338 D339 G340 G341 V342 R343 K344 E345 V346 D347 G348 M349 G350 T351 S352 E353 I354 G357 D358 S359 I360 D367 S376 V377 D378 VAL LYS SER VAL ARG MET GLY SER I387 A391 I392 M399 G402 H410 L436 S437
K438 K439 A440 K441 A442 A442 S443 S444 V445 D467 E468 H469 L470 E471 H472 Q476 N496 L499 A518 G519 R520 I541 R542 G543 N544 N547 I559 E563 G570 I571 L572 E573 V574 V578 L579 L586 E591 G592 H593 I594 I598 L601 H608 K609 V610
L611 C618 V619 C620 H621 G622 V623 L631 I632 C633 D641 L642 L643 T646 R647 L648 V652 E665 Q669 Y670 W673 L677 M678 V679 E683 P684 F685 V686 T687 A688 T691 H692 L693 R694 V695 Y725 S743 L749 V775 V800 A825 V826 L827
P828 K829 E830 K831 L832 E835 H836 S837 R838 E839 R844 T845 Y846 T847 R848 V855 S856 LEU THR GLN ALA ALA F862 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 N888 L900 G901 P906 V907 R908 D909 D910 N911 K912 R913 M935 T939 L943
L944 A945 L946 G947 C948 H949 V950 S953 D954 E955 H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 L983 S984 F985 I986 K987 L988 T989 P990 E993 A994 L999 N1002 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN
R1027 R1028 R1031 T1036 L1037 L1038 D1039 D1040 R1041 K1044 S1045 T1056 P1067 D1068 GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 I1087 A1090 A1098 F1105 S1110 V1115 G1116 W1117 S1118 G1121 CYS GLN PRO ASP GLN E1127 L1128
R1133 R1154 Q1157 A1158 N1169 E1170 H1171 T1172 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 I1202 P1203 V1204 A1210 G1218 G1231 L1232 Q1233 A1240 T1243 V1261 P1262 S1263 N1264 H1267 V1270 D1274 GLY THR ILE ASP SER SER
PRO CYS LEU LYS V1285 T1286 Q1287 Q1293 N1294 S1295 I1299 R1303 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS THR VAL PRO GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS
GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU THR THR LYS ALA GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU VAL LEU THR GLU ASP VAL LEU ALA
ASP ASP ARG ASP ASP TYR ASP PHE LEU MET GLN THR SER T1425 P1434 GLY GLN GLU PRO ALA N1440 W1445 I1446 T1447 F1450 L1459 D1460 ARG VAL ARG THR V1465 E1472 K1473 G1474 K1475 V1476 I1480 K1481 V1511 ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 I1521 A1522 K1525
E1526 L1527 S1528 T1529 V1533 E1534 P1535 K1538 A1542 S1549 F1553 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 F1590 L1604 R1614 F1627 M1628 S1629 L1630 R1637 S1638 V1639 D1640 L1644 E1648 E1649 T1657 L1658 R1659 L1660 A1666 L1667 G1668
N1669 H1670 R1671 V1672 V1680 D1681 Q1684 L1685 L1686 K1692 L1697 I1707 D1708 I1709 M1720 T1737 P1740 ASP GLU ASN LYS LYS HIS G1747 L1748 P1749 T1755 R1758 M1761 Q1762 F1763 I1771 N1772 Q1777 Y1778 S1779 F1782 P1783 I1786 L1787 K1790 L1795

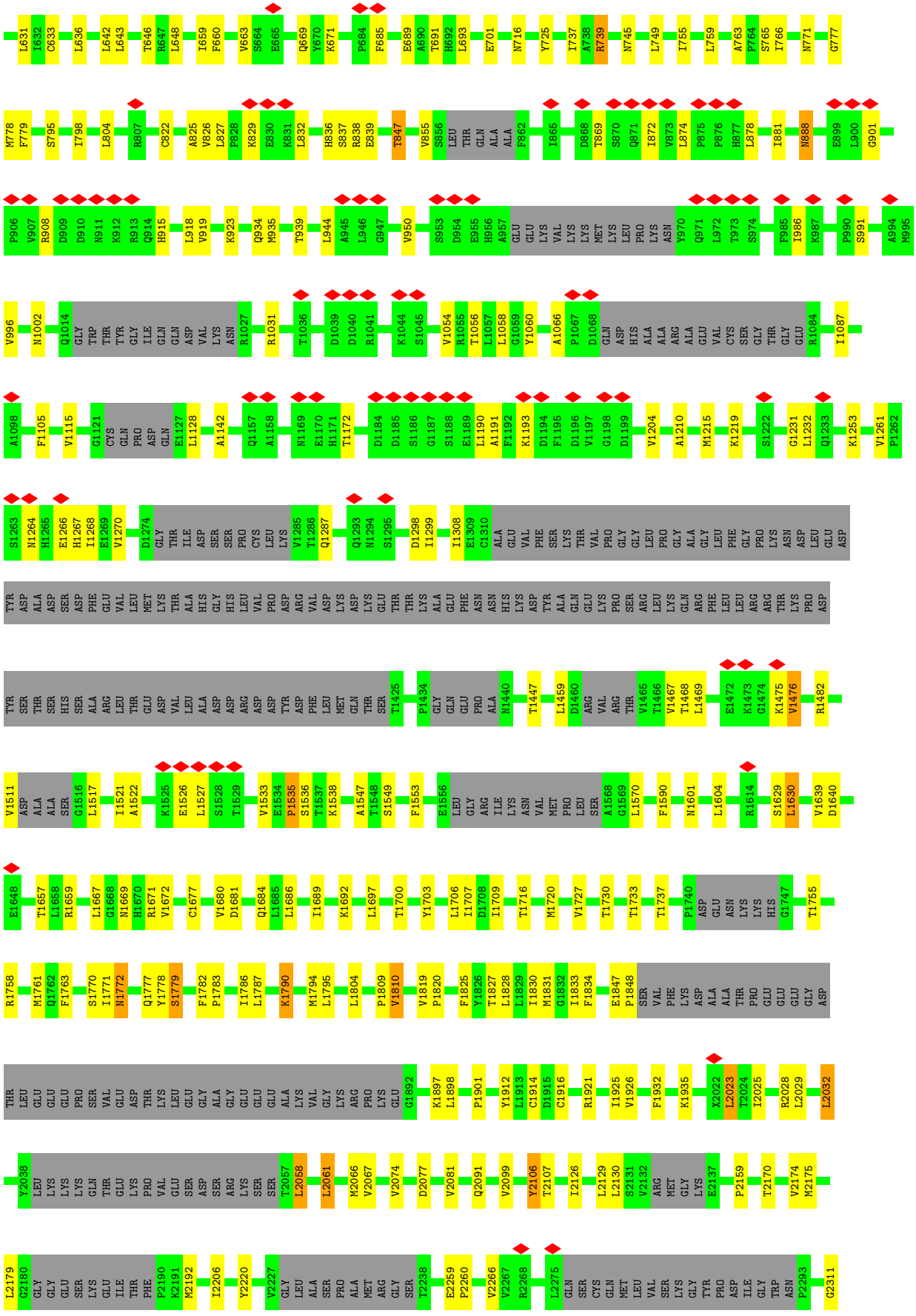


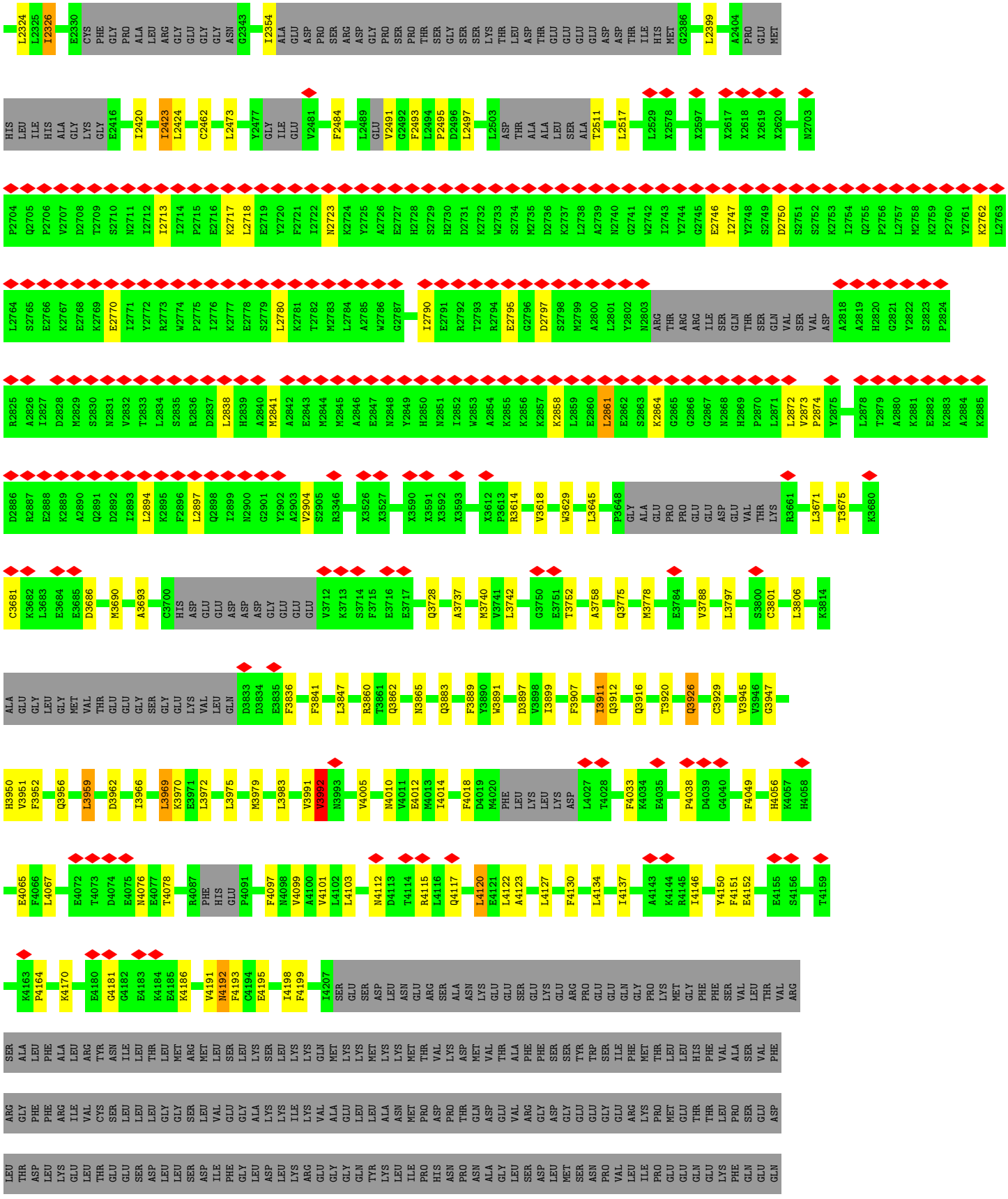


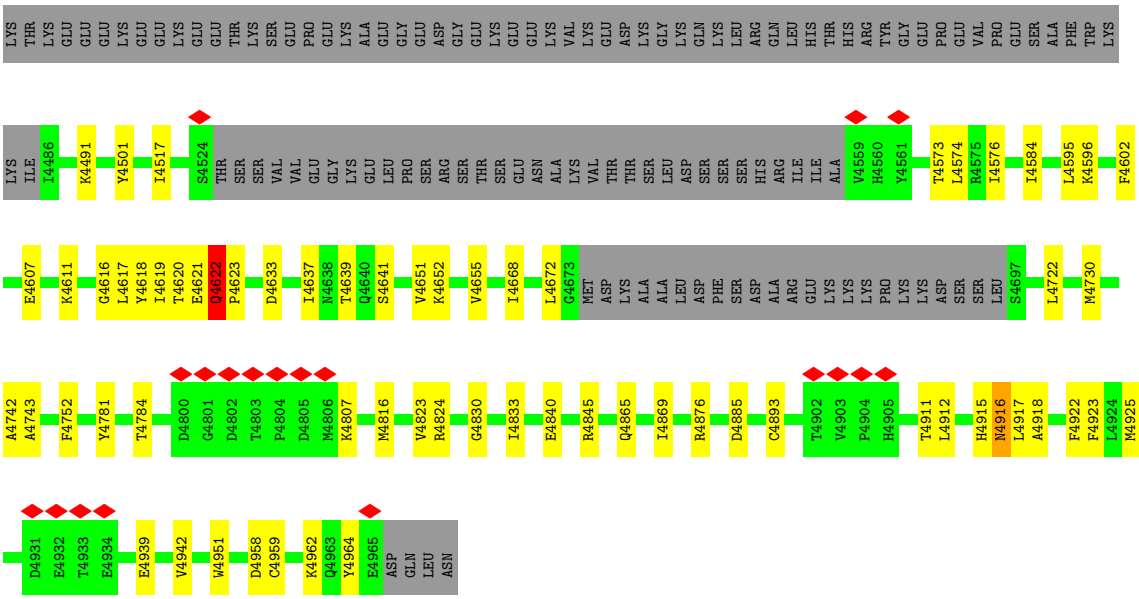
• Molecule 1: Ryanodine Receptor

Chain E:

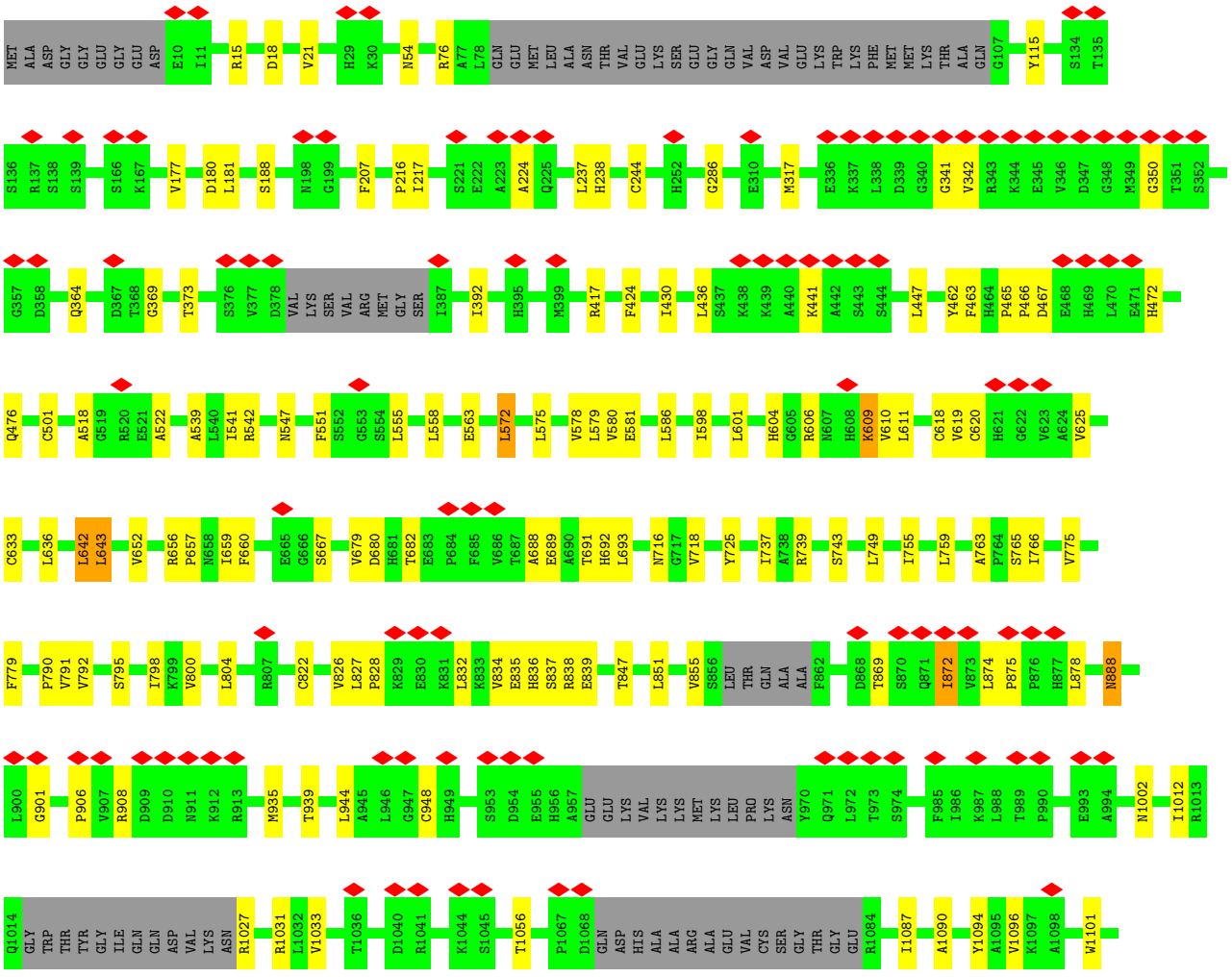


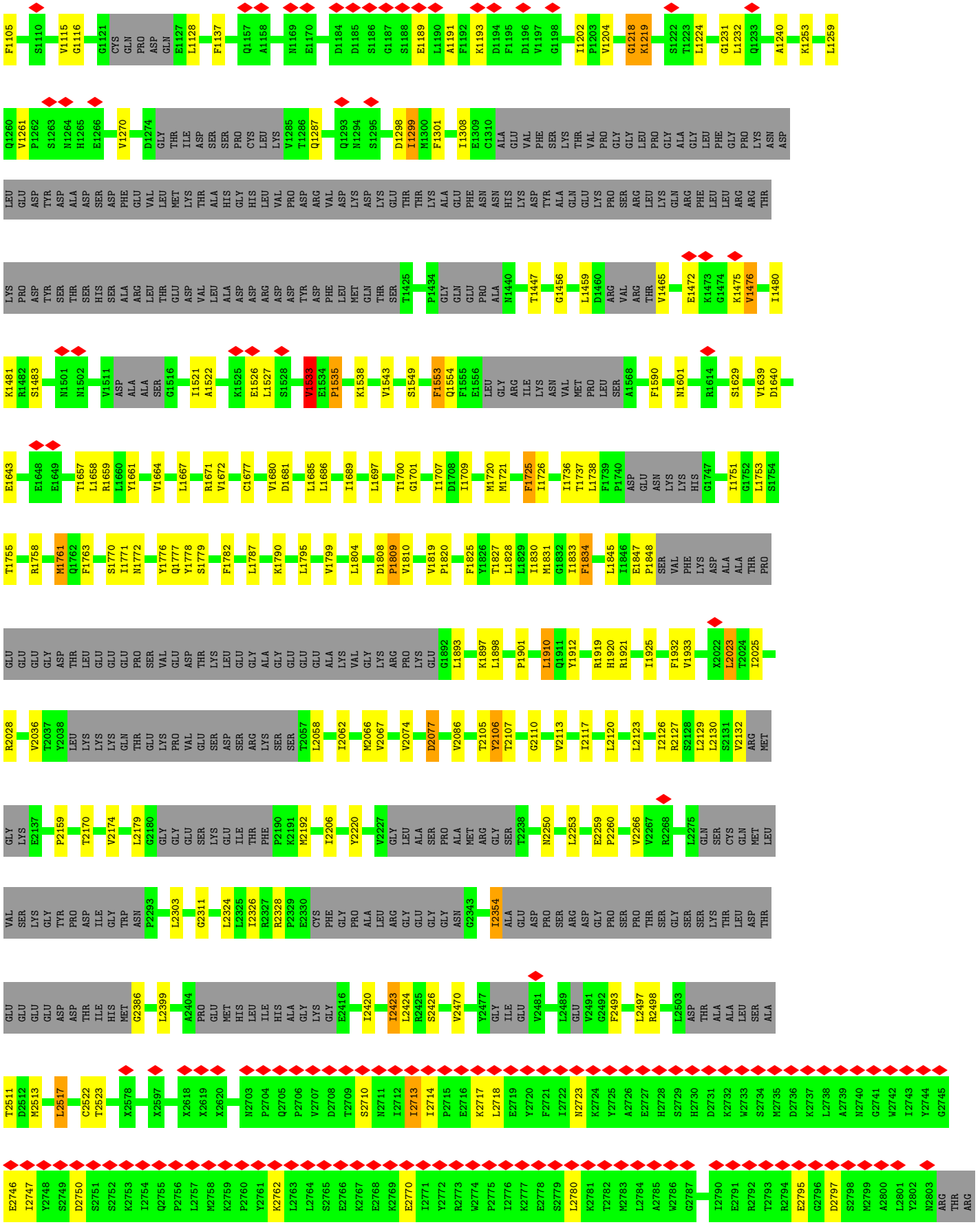


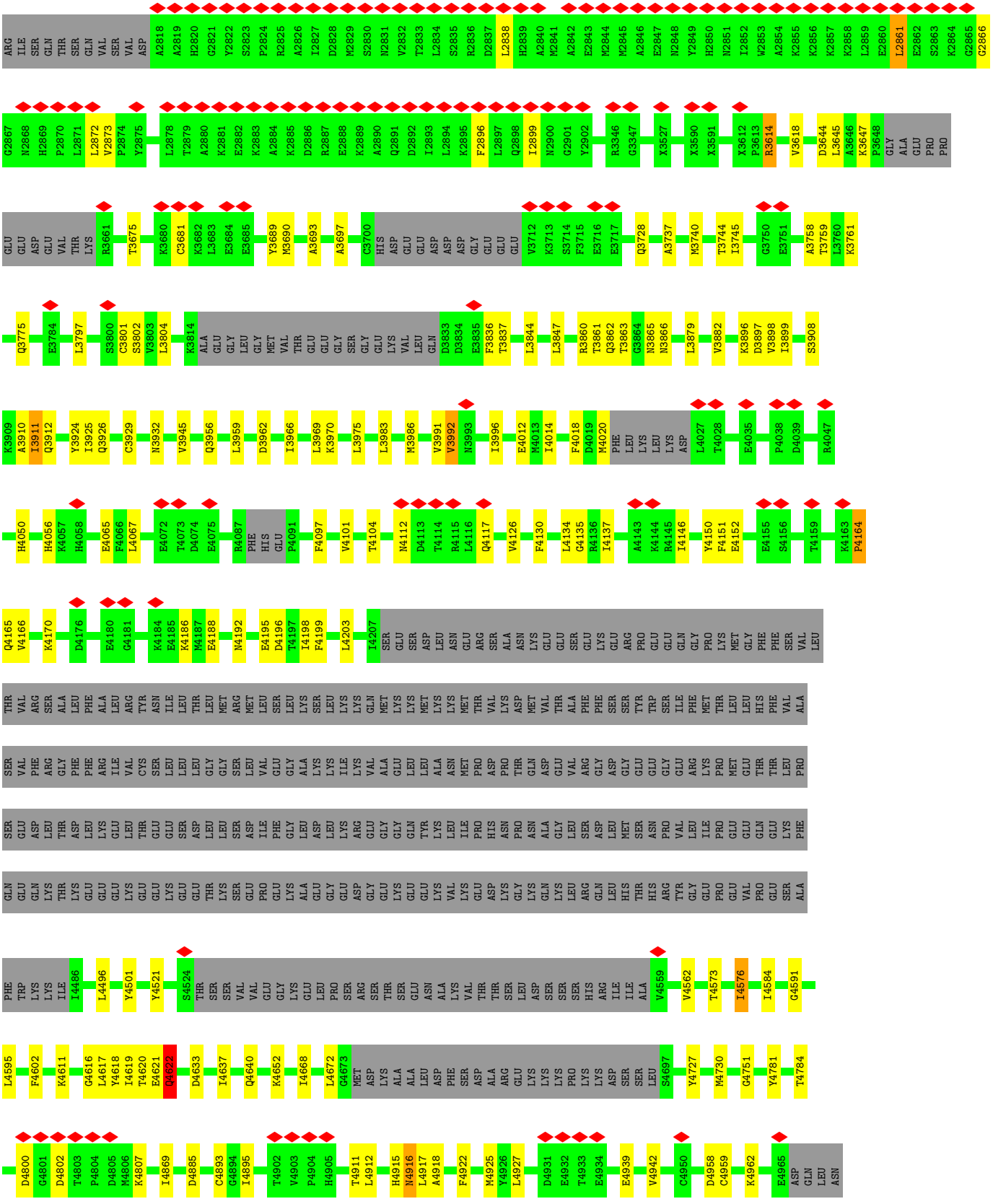


• Molecule 1: Ryanodine Receptor

Chain G:

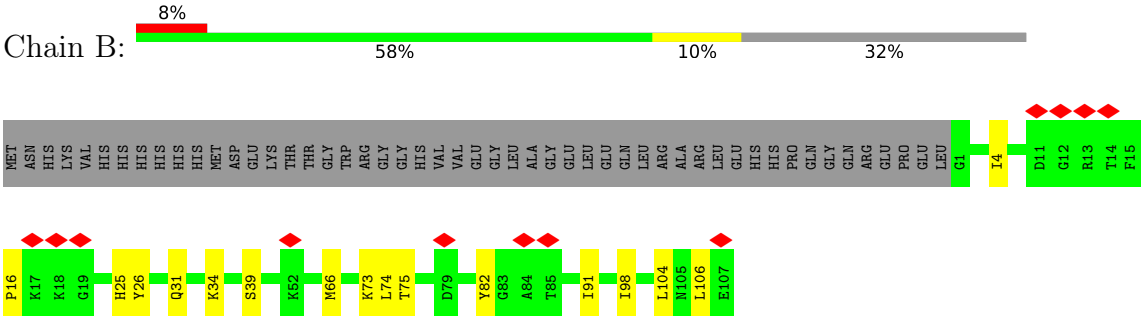




F1105 S1110 V1115 G1116 G1121 CYS GLN PRO ASP GLN E1127 L1128 F1137 Q1157 A1158 N1169 E1170 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 I1202 P1203 V1204 G1218 K1219 S1222 T1223 L1224 G1231 L1232 Q1233 A1240 K1253 L1259
Q1260 V1261 P1262 S1263 N1264 H1265 E1266 V1270 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 Q1293 N1294 S1295 D1298 T1299 M1300 F1301 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS THR VAL PRO GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP
LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU THR THR LYS ALA GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR
LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP PHE LEU MET GLN THR SER T1425 P1434 GLY GLN GLU PRO ALA N1440 T1447 G1456 L1459 D1460 ARG VAL ARG THR V1465 E1472 K1473 G1474 K1475 V1476 I1480
K1481 R1482 S1483 N1501 N1502 V1511 ASP ALA ALA SER G1516 I1521 A1522 K1525 E1526 L1527 S1528 V1533 E1534 P1535 K1538 V1543 S1549 F1553 Q1554 F1555 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 F1590 N1601 R1614 S1629 V1639 D1640
E1643 E1648 E1649 T1657 L1658 R1659 L1660 Y1661 V1664 L1667 R1671 V1672 C1677 V1680 D1681 L1685 L1686 I1689 L1697 T1700 G1701 I1707 D1708 I1709 M1720 M1721 F1725 I1726 I1736 T1737 L1738 F1739 P1740 ASP GLU ASN LYS LYS HIS G1747 I1751 G1752 L1753 S1754
T1755 R1758 M1761 Q1762 F1763 S1770 I1771 N1772 Y1776 Q1777 Y1778 S1779 F1782 L1787 K1790 L1795 V1799 L1804 D1808 P1809 V1810 V1819 P1820 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 G1832 I1833 F1834 L1845 I1846 E1847 P1848 SER VAL PHE LYS ASP ALA ALA THR PRO
GLU GLU GLU GLY ASP THR LEU GLU GLU PRO SER VAL GLU ASP THR LYS LEU GLU GLY ALA GLY GLU GLU GLU ALA ALA LYS VAL GLY LYS ARG PRO LYS GLU G1892 L1893 K1897 L1898 P1901 L1910 Q1911 Y1912 R1919 H1920 R1921 I1925 F1932 V1933 X2022 L2023 T2024 I2025
R2028 V2036 T2037 Y2038 LEU LYS LYS LYS GLN THR GLU LYS PRO VAL GLU SER ASP SER ARG LYS SER SER T2057 L2058 I2062 M2066 V2067 V2074 D2077 V2086 T2105 Y2106 T2107 G2110 V2113 I2117 L2120 L2123 I2126 R2127 S2128 L2129 L2130 S2131 V2132 ARG MET
GLY LYS E2137 P2159 T2170 V2174 L2179 G2180 GLY GLY GLU SER LYS GLU ILE THR PHE P2190 K2191 M2192 I2206 Y2220 V2227 GLY LEU ALA SER PRO ALA MET ARG GLY SER T2238 N2250 L2253 E2259 P2260 V2266 V2267 R2268 L2275 GLN SER CYS GLN MET LEU
VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 L2303 G2311 L2324 L2325 I2326 R2327 R2328 P2329 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS THR LEU ASP THR
GLU GLU GLU GLU ASP ASP THR ILE HIS MET G2386 L2399 A2404 PRO GLU MET HIS LEU ILE HIS ALA GLY LYS GLY E2416 I2420 I2423 L2424 R2425 S2426 V2470 Y2477 GLY ILE GLU V2481 L2489 GLU V2491 G2492 F2493 L2497 R2498 L2503 ASP THR ALA ALA LEU SER ALA
T2511 D2512 M2513 L2517 C2522 T2523 X2578 X2597 X2618 X2619 X2620 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 I2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745
E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 I2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 S2798 M2799 A2800 L2801 Y2802 N2803 ARG THR ARG



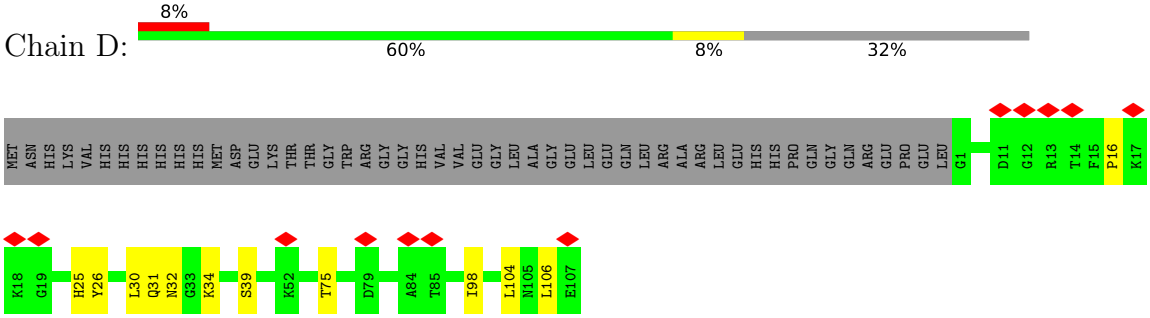
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:



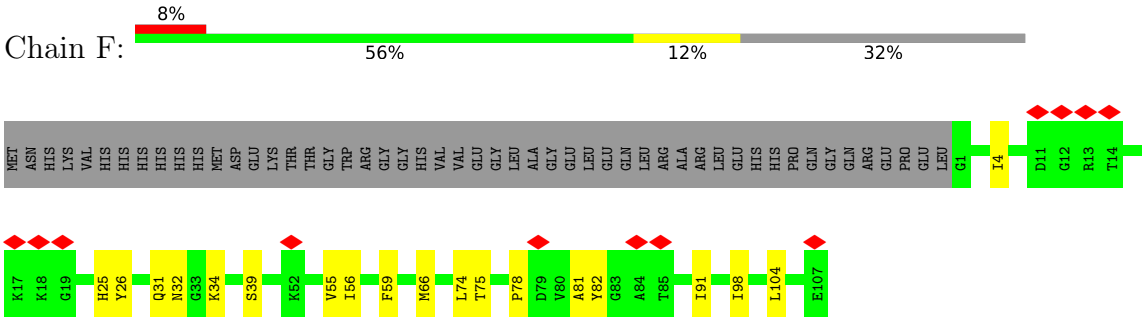

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:



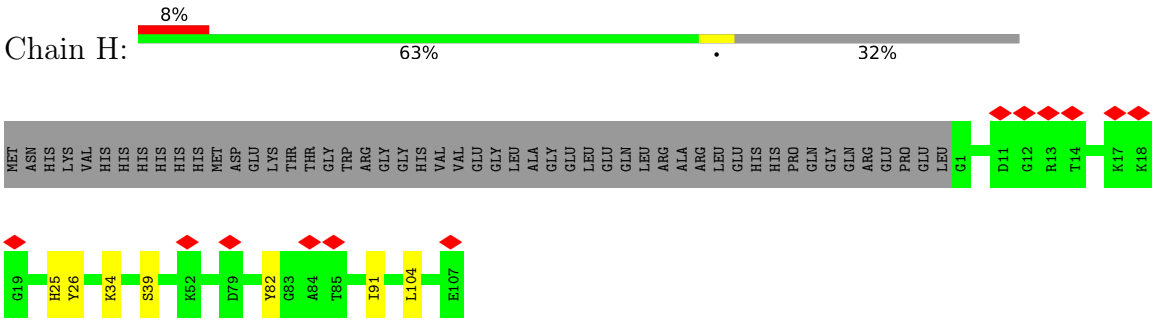

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C4 | Depositor |
| Number of particles used | 13158 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 20 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 6000 | Depositor |
| Magnification | 62000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.090 | Depositor |
| Minimum map value | -0.046 | Depositor |
| Average map value | -0.006 | Depositor |
| Map value standard deviation | 0.010 | Depositor |
| Recommended contour level | 0.035 | Depositor |
| Map size (Å) | 536.0, 536.0, 536.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.34, 1.34, 1.34 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.78 | 0/25831 | 0.64 | 1/34865 (0.0%) |
| 1 | C | 0.78 | 0/25831 | 0.64 | 1/34865 (0.0%) |
| 1 | E | 0.78 | 0/25831 | 0.64 | 1/34865 (0.0%) |
| 1 | G | 0.78 | 0/25831 | 0.64 | 0/34865 |
| 2 | B | 0.85 | 0/834 | 0.64 | 0/1123 |
| 2 | D | 0.85 | 0/834 | 0.63 | 0/1123 |
| 2 | F | 0.84 | 0/834 | 0.64 | 0/1123 |
| 2 | H | 0.86 | 0/834 | 0.65 | 0/1123 |
| All | All | 0.78 | 0/106660 | 0.64 | 3/143952 (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 |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | G | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 1630 | LEU | CA-CB-CG | 6.09 | 129.32 | 115.30 |
| 1 | A | 1630 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |
| 1 | C | 1630 | LEU | CA-CB-CG | 5.38 | 127.68 | 115.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 604 | HIS | Peptide |
| 1 | C | 3614 | ARG | Peptide |
| 1 | G | 3614 | ARG | Peptide |

## 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 | A | 27416 | 0 | 25487 | 197 | 0 |
| 1 | C | 27416 | 0 | 25485 | 217 | 0 |
| 1 | E | 27416 | 0 | 25489 | 211 | 0 |
| 1 | G | 27416 | 0 | 25485 | 206 | 0 |
| 2 | B | 818 | 0 | 824 | 10 | 0 |
| 2 | D | 818 | 0 | 824 | 5 | 0 |
| 2 | F | 818 | 0 | 824 | 9 | 0 |
| 2 | H | 818 | 0 | 824 | 5 | 0 |
| All | All | 112936 | 0 | 105242 | 843 | 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 4.

All (843) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:3945:VAL:HG11 | 1:E:3983:LEU:HD21 | 1.47 | 0.94 |
| 1:A:874:LEU:HD23 | 1:A:878:LEU:HD13 | 1.50 | 0.94 |
| 1:E:1172:THR:HG21 | 1:E:1190:LEU:HD13 | 1.58 | 0.86 |
| 1:G:874:LEU:HD23 | 1:G:878:LEU:HD13 | 1.60 | 0.82 |
| 1:E:1261:VAL:HG11 | 1:E:1270:VAL:HG11 | 1.63 | 0.78 |
| 1:G:3945:VAL:HG11 | 1:G:3983:LEU:HD21 | 1.66 | 0.78 |
| 1:C:1172:THR:HG21 | 1:C:1190:LEU:HD13 | 1.66 | 0.77 |
| 1:G:1933:VAL:HG21 | 1:G:3618:VAL:HG22 | 1.66 | 0.76 |
| 1:A:1172:THR:HG21 | 1:A:1190:LEU:HD13 | 1.68 | 0.75 |
| 1:G:4617:LEU:O | 1:G:4622:GLN:N | 2.19 | 0.75 |
| 1:E:4617:LEU:O | 1:E:4622:GLN:N | 2.20 | 0.74 |
| 1:C:4617:LEU:O | 1:C:4622:GLN:N | 2.19 | 0.74 |
| 1:E:594:ILE:HD12 | 1:E:631:LEU:HD22 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1105:PHE:HB2 | 1:G:1115:VAL:HG21 | 1.72 | 0.71 |
| 1:A:2075:ILE:HG12 | 1:A:2080:LEU:HD23 | 1.74 | 0.69 |
| 1:C:314:LEU:HD12 | 1:C:391:ALA:HB1 | 1.73 | 0.69 |
| 1:G:1543:VAL:HG11 | 1:G:1553:PHE:CZ | 2.27 | 0.69 |
| 1:A:4617:LEU:O | 1:A:4622:GLN:N | 2.20 | 0.69 |
| 1:C:633:CYS:HB3 | 1:C:1672:VAL:HG11 | 1.73 | 0.69 |
| 1:C:874:LEU:HD23 | 1:C:878:LEU:HD13 | 1.75 | 0.68 |
| 1:A:3945:VAL:HG11 | 1:A:3983:LEU:HD21 | 1.74 | 0.68 |
| 1:C:1105:PHE:HB2 | 1:C:1115:VAL:HG21 | 1.76 | 0.67 |
| 2:D:26:TYR:N | 2:D:39:SER:OG | 2.27 | 0.67 |
| 1:E:874:LEU:HD23 | 1:E:878:LEU:HD13 | 1.78 | 0.66 |
| 1:E:1680:VAL:HG11 | 1:E:1709:ILE:HD13 | 1.78 | 0.66 |
| 1:C:26:ALA:HB3 | 1:C:35:LEU:HD13 | 1.77 | 0.65 |
| 1:E:314:LEU:HD12 | 1:E:391:ALA:HB1 | 1.77 | 0.65 |
| 1:G:633:CYS:HB3 | 1:G:1672:VAL:HG11 | 1.79 | 0.65 |
| 2:H:26:TYR:N | 2:H:39:SER:OG | 2.28 | 0.65 |
| 1:A:4192:ASN:HD22 | 1:A:4606:LYS:HE2 | 1.62 | 0.64 |
| 1:G:2266:VAL:HG12 | 1:G:2303:LEU:HD11 | 1.79 | 0.64 |
| 1:A:143:LEU:HD11 | 1:A:207:PHE:CD2 | 2.32 | 0.64 |
| 1:A:1219:LYS:HA | 1:A:1240:ALA:HB3 | 1.80 | 0.64 |
| 1:E:4517:ILE:HG21 | 1:E:4574:LEU:HD23 | 1.80 | 0.64 |
| 2:B:26:TYR:N | 2:B:39:SER:OG | 2.29 | 0.64 |
| 1:A:1261:VAL:HG11 | 1:A:1270:VAL:HG11 | 1.80 | 0.64 |
| 1:A:2123:LEU:HD12 | 1:A:2127:ARG:NH1 | 2.12 | 0.64 |
| 1:A:4097:PHE:CZ | 1:A:4152:GLU:HB2 | 2.32 | 0.64 |
| 1:A:1680:VAL:HG11 | 1:A:1709:ILE:HD13 | 1.80 | 0.63 |
| 1:E:4146:ILE:HD11 | 1:E:4958:ASP:HB3 | 1.80 | 0.63 |
| 1:G:1799:VAL:HG22 | 1:G:1893:LEU:HD22 | 1.80 | 0.63 |
| 1:A:4493:LEU:HD11 | 1:A:4590:ILE:HG21 | 1.81 | 0.63 |
| 1:C:1480:ILE:HG23 | 1:C:1481:LYS:HD2 | 1.81 | 0.63 |
| 1:E:633:CYS:HB3 | 1:E:1672:VAL:HG11 | 1.79 | 0.63 |
| 1:E:591:GLU:HA | 1:E:631:LEU:HD21 | 1.81 | 0.63 |
| 1:A:3862:GLN:HE21 | 1:A:3865:ASN:HD22 | 1.48 | 0.62 |
| 1:C:4652:LYS:HG3 | 1:C:4672:LEU:HD23 | 1.82 | 0.62 |
| 1:G:3862:GLN:HE21 | 1:G:3865:ASN:HD22 | 1.48 | 0.62 |
| 1:A:888:ASN:ND2 | 1:A:1056:THR:HG21 | 2.15 | 0.61 |
| 1:E:2266:VAL:HG21 | 1:E:2324:LEU:HB3 | 1.82 | 0.61 |
| 1:A:37:LEU:HD13 | 1:A:203:VAL:HG11 | 1.81 | 0.61 |
| 1:E:1522:ALA:HB3 | 1:E:1527:LEU:HD11 | 1.81 | 0.61 |
| 1:A:1087:ILE:HD12 | 1:A:1128:LEU:HD23 | 1.82 | 0.61 |
| 1:A:4012:GLU:HG3 | 1:A:4122:LEU:HD21 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1522:ALA:HB3 | 1:G:1527:LEU:HD11 | 1.81 | 0.61 |
| 1:A:1522:ALA:HB3 | 1:A:1527:LEU:HD11 | 1.83 | 0.61 |
| 1:A:4146:ILE:HD11 | 1:A:4958:ASP:HB3 | 1.82 | 0.61 |
| 1:G:1261:VAL:HG11 | 1:G:1270:VAL:HG11 | 1.82 | 0.61 |
| 1:C:693:LEU:HG | 1:C:749:LEU:HD12 | 1.83 | 0.60 |
| 1:E:2130:LEU:HA | 1:E:2174:VAL:HG22 | 1.83 | 0.60 |
| 1:C:2130:LEU:HA | 1:C:2174:VAL:HG22 | 1.82 | 0.60 |
| 1:C:28:ILE:HD11 | 1:C:201:LEU:HD11 | 1.83 | 0.60 |
| 2:H:26:TYR:H | 2:H:39:SER:HG | 1.50 | 0.60 |
| 1:C:4101:VAL:HG13 | 1:C:4150:TYR:HB2 | 1.84 | 0.60 |
| 1:G:1480:ILE:HG23 | 1:G:1481:LYS:HD2 | 1.82 | 0.60 |
| 1:G:766:ILE:HB | 1:G:779:PHE:HB2 | 1.84 | 0.60 |
| 1:A:4916:ASN:O | 1:A:4918:ALA:N | 2.35 | 0.60 |
| 1:E:1727:VAL:HG11 | 1:E:1926:VAL:HG11 | 1.84 | 0.60 |
| 1:E:2067:VAL:HG21 | 1:E:3645:LEU:HD13 | 1.83 | 0.60 |
| 1:G:2130:LEU:HA | 1:G:2174:VAL:HG22 | 1.84 | 0.59 |
| 2:H:26:TYR:N | 2:H:39:SER:HG | 2.00 | 0.59 |
| 1:A:4137:ILE:HG23 | 1:A:4151:PHE:CE2 | 2.37 | 0.59 |
| 1:C:3806:LEU:HD13 | 1:C:3889:PHE:HA | 1.85 | 0.59 |
| 1:E:4101:VAL:HG13 | 1:E:4150:TYR:HB2 | 1.84 | 0.59 |
| 1:G:667:SER:HB2 | 1:G:1012:ILE:HD13 | 1.85 | 0.59 |
| 1:G:1707:ILE:HG23 | 1:G:1827:THR:HG21 | 1.84 | 0.59 |
| 1:E:4097:PHE:CZ | 1:E:4152:GLU:HB2 | 2.37 | 0.59 |
| 1:G:1219:LYS:HA | 1:G:1240:ALA:HB3 | 1.85 | 0.59 |
| 1:A:1480:ILE:HG23 | 1:A:1481:LYS:HD2 | 1.83 | 0.59 |
| 1:A:1090:ALA:HB3 | 1:A:1202:ILE:CG2 | 2.33 | 0.58 |
| 1:C:1090:ALA:HB3 | 1:C:1202:ILE:CG2 | 2.33 | 0.58 |
| 1:G:1700:THR:HG22 | 1:G:1820:PRO:HG3 | 1.85 | 0.58 |
| 1:G:4203:LEU:HD13 | 1:G:4595:LEU:HD12 | 1.85 | 0.58 |
| 1:C:826:VAL:HG21 | 1:C:832:LEU:HD22 | 1.85 | 0.58 |
| 1:A:1922:ILE:HD13 | 1:A:2105:THR:HG21 | 1.84 | 0.58 |
| 1:C:4916:ASN:O | 1:C:4918:ALA:N | 2.36 | 0.58 |
| 1:C:869:THR:HG21 | 1:C:1002:ASN:HD21 | 1.68 | 0.58 |
| 1:E:4014:ILE:HG22 | 1:E:4018:PHE:CE2 | 2.39 | 0.58 |
| 2:F:26:TYR:N | 2:F:39:SER:OG | 2.29 | 0.58 |
| 1:G:4195:GLU:HA | 1:G:4198:ILE:HD12 | 1.85 | 0.58 |
| 1:A:4869:ILE:HG23 | 1:G:4869:ILE:HG21 | 1.85 | 0.58 |
| 1:C:1830:ILE:HG22 | 1:C:1912:TYR:CD1 | 2.39 | 0.58 |
| 1:G:4916:ASN:O | 1:G:4918:ALA:N | 2.37 | 0.58 |
| 1:E:4076:ASN:HB3 | 1:E:4078:THR:HG22 | 1.86 | 0.58 |
| 1:C:3778:MET:CE | 1:C:3847:LEU:HD22 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:3945:VAL:HG11 | 1:C:3983:LEU:HD21 | 1.86 | 0.57 |
| 1:C:4012:GLU:HG3 | 1:C:4122:LEU:HD21 | 1.84 | 0.57 |
| 1:E:4916:ASN:O | 1:E:4918:ALA:N | 2.37 | 0.57 |
| 1:A:4101:VAL:HG13 | 1:A:4150:TYR:HB2 | 1.87 | 0.57 |
| 1:C:4869:ILE:HG21 | 1:E:4869:ILE:HG23 | 1.86 | 0.57 |
| 1:A:2498:ARG:HB3 | 1:A:2517:LEU:HD11 | 1.86 | 0.57 |
| 1:C:611:LEU:HD22 | 1:C:1659:ARG:HD2 | 1.87 | 0.57 |
| 1:C:2159:PRO:HB3 | 1:C:2206:ILE:HD12 | 1.86 | 0.57 |
| 1:E:1087:ILE:HD12 | 1:E:1128:LEU:HD23 | 1.85 | 0.57 |
| 1:C:3879:LEU:HD11 | 1:C:3921:LEU:HD12 | 1.85 | 0.57 |
| 1:G:4014:ILE:HG22 | 1:G:4018:PHE:CE2 | 2.40 | 0.56 |
| 1:C:1519:THR:HG22 | 1:C:1529:THR:HG22 | 1.87 | 0.56 |
| 1:C:1680:VAL:HG11 | 1:C:1709:ILE:HD13 | 1.88 | 0.56 |
| 1:C:4618:TYR:OH | 1:C:4633:ASP:HB2 | 2.05 | 0.56 |
| 1:A:2130:LEU:HA | 1:A:2174:VAL:HG22 | 1.88 | 0.56 |
| 1:E:4618:TYR:OH | 1:E:4633:ASP:HB2 | 2.06 | 0.56 |
| 2:D:25:HIS:CD2 | 2:D:104:LEU:HD11 | 2.41 | 0.56 |
| 1:A:1534:GLU:HG2 | 1:A:1539:LEU:HD11 | 1.87 | 0.56 |
| 1:A:3959:LEU:HD22 | 1:A:3965:GLN:HB3 | 1.87 | 0.56 |
| 1:C:673:TRP:CH2 | 1:C:825:ALA:HB2 | 2.40 | 0.56 |
| 1:G:4652:LYS:HG3 | 1:G:4672:LEU:HD23 | 1.88 | 0.56 |
| 1:G:3911:ILE:HD11 | 1:G:3975:LEU:HB2 | 1.88 | 0.55 |
| 1:A:4137:ILE:HG23 | 1:A:4151:PHE:HE2 | 1.71 | 0.55 |
| 1:E:2159:PRO:HB3 | 1:E:2206:ILE:HD12 | 1.89 | 0.55 |
| 1:A:1105:PHE:HB2 | 1:A:1115:VAL:HG21 | 1.87 | 0.55 |
| 2:B:25:HIS:CD2 | 2:B:104:LEU:HD11 | 2.41 | 0.55 |
| 1:C:4097:PHE:CZ | 1:C:4152:GLU:HB2 | 2.41 | 0.55 |
| 1:G:4146:ILE:HD11 | 1:G:4958:ASP:HB3 | 1.87 | 0.55 |
| 1:A:749:LEU:HD22 | 1:A:755:ILE:HD11 | 1.88 | 0.55 |
| 1:A:1521:ILE:HG22 | 1:A:1526:GLU:HA | 1.88 | 0.55 |
| 1:A:2861:LEU:HD22 | 1:A:2872:LEU:HD11 | 1.88 | 0.55 |
| 1:A:4191:VAL:HG21 | 1:A:4951:TRP:CH2 | 2.42 | 0.55 |
| 1:C:2067:VAL:HG11 | 1:C:3645:LEU:HD22 | 1.88 | 0.55 |
| 1:C:2067:VAL:HG21 | 1:C:3645:LEU:HD13 | 1.89 | 0.55 |
| 1:C:4146:ILE:HD11 | 1:C:4958:ASP:HB3 | 1.88 | 0.55 |
| 1:E:4137:ILE:HG23 | 1:E:4151:PHE:HE2 | 1.72 | 0.55 |
| 1:C:1261:VAL:HG11 | 1:C:1270:VAL:HG11 | 1.87 | 0.55 |
| 1:E:207:PHE:CE2 | 1:G:2326:ILE:HD12 | 2.42 | 0.55 |
| 1:C:4014:ILE:HG22 | 1:C:4018:PHE:CE2 | 2.42 | 0.55 |
| 1:C:1911:GLN:HB2 | 1:C:2087:LEU:HD11 | 1.88 | 0.55 |
| 1:C:3911:ILE:HD11 | 1:C:3975:LEU:HB2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:3614:ARG:O | 1:E:3618:VAL:HG23 | 2.06 | 0.55 |
| 1:G:2861:LEU:HD22 | 1:G:2872:LEU:HD11 | 1.87 | 0.55 |
| 1:C:436:LEU:HD22 | 1:C:518:ALA:HA | 1.89 | 0.55 |
| 1:C:872:ILE:HD13 | 1:C:873:VAL:N | 2.21 | 0.55 |
| 1:E:2497:LEU:HD11 | 1:E:2873:VAL:HG12 | 1.90 | 0.55 |
| 1:G:3924:TYR:HB2 | 1:G:3925:ILE:HD12 | 1.89 | 0.55 |
| 1:C:1522:ALA:HB3 | 1:C:1527:LEU:HD11 | 1.87 | 0.54 |
| 1:C:4191:VAL:HG11 | 1:C:4951:TRP:CH2 | 2.43 | 0.54 |
| 2:F:25:HIS:CD2 | 2:F:104:LEU:HD11 | 2.42 | 0.54 |
| 1:G:3614:ARG:O | 1:G:3618:VAL:HG23 | 2.07 | 0.54 |
| 1:A:1511:VAL:HA | 1:A:1517:LEU:HD13 | 1.89 | 0.54 |
| 1:A:544:ASN:HB2 | 1:A:547:ASN:HD22 | 1.73 | 0.54 |
| 1:A:4199:PHE:CZ | 1:A:4602:PHE:CD1 | 2.96 | 0.54 |
| 2:B:82:TYR:CD2 | 2:B:91:ILE:HG21 | 2.42 | 0.54 |
| 1:G:1736:ILE:HG13 | 1:G:1753:LEU:HD23 | 1.89 | 0.54 |
| 1:A:1268:ILE:HD11 | 1:A:1302:TYR:CE1 | 2.43 | 0.54 |
| 1:C:3614:ARG:O | 1:C:3618:VAL:HG23 | 2.07 | 0.54 |
| 1:A:3614:ARG:O | 1:A:3618:VAL:HG23 | 2.06 | 0.54 |
| 1:A:4014:ILE:HG22 | 1:A:4018:PHE:CE2 | 2.42 | 0.54 |
| 1:A:2067:VAL:HG21 | 1:A:3645:LEU:HD13 | 1.90 | 0.54 |
| 1:C:74:LEU:HD11 | 1:C:117:HIS:CE1 | 2.43 | 0.54 |
| 1:C:3804:LEU:HD13 | 1:C:3910:ALA:HB2 | 1.89 | 0.54 |
| 1:C:360:ILE:HD11 | 1:C:402:GLY:HA3 | 1.89 | 0.54 |
| 1:C:2266:VAL:HG21 | 1:C:2324:LEU:HD13 | 1.89 | 0.54 |
| 1:E:4619:ILE:HD12 | 1:E:4668:ILE:HD12 | 1.90 | 0.54 |
| 1:G:1096:VAL:HG11 | 1:G:1101:TRP:CD1 | 2.43 | 0.54 |
| 1:G:1218:GLY:HA2 | 1:G:1224:LEU:HD11 | 1.90 | 0.54 |
| 1:G:2470:VAL:HG21 | 1:G:2523:THR:CG2 | 2.38 | 0.53 |
| 1:E:1521:ILE:HG22 | 1:E:1526:GLU:HA | 1.90 | 0.53 |
| 1:G:3693:ALA:HB1 | 1:G:3758:ALA:O | 2.08 | 0.53 |
| 1:A:828:PRO:HG3 | 1:A:1033:VAL:HG11 | 1.91 | 0.53 |
| 1:C:3862:GLN:HE21 | 1:C:3865:ASN:HD22 | 1.55 | 0.53 |
| 1:G:601:LEU:HD23 | 1:G:642:LEU:HD21 | 1.89 | 0.53 |
| 1:G:4618:TYR:OH | 1:G:4633:ASP:HB2 | 2.08 | 0.53 |
| 1:A:1460:ASP:HA | 1:A:1496:UNK:H2 | 1.74 | 0.53 |
| 1:A:4570:MET:HA | 1:A:4573:THR:HG22 | 1.91 | 0.53 |
| 1:G:618:CYS:SG | 1:G:619:VAL:HG23 | 2.49 | 0.53 |
| 1:G:749:LEU:HD22 | 1:G:755:ILE:HD11 | 1.90 | 0.53 |
| 1:G:4020:MET:CE | 1:G:4067:LEU:HD21 | 2.39 | 0.53 |
| 1:C:591:GLU:HA | 1:C:631:LEU:HD21 | 1.90 | 0.53 |
| 1:A:4191:VAL:HG21 | 1:A:4951:TRP:CZ3 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:611:LEU:HD22 | 1:A:1659:ARG:HD2 | 1.91 | 0.53 |
| 1:A:4076:ASN:HB3 | 1:A:4078:THR:HG22 | 1.91 | 0.53 |
| 1:E:360:ILE:HD11 | 1:E:402:GLY:HA3 | 1.91 | 0.53 |
| 1:G:828:PRO:HG3 | 1:G:1033:VAL:HG11 | 1.90 | 0.52 |
| 1:G:1680:VAL:HG11 | 1:G:1709:ILE:HD13 | 1.90 | 0.52 |
| 1:E:4195:GLU:HA | 1:E:4198:ILE:HD12 | 1.90 | 0.52 |
| 1:G:4101:VAL:HG13 | 1:G:4150:TYR:HB2 | 1.91 | 0.52 |
| 1:C:688:ALA:HB1 | 1:C:691:THR:CB | 2.39 | 0.52 |
| 1:G:4199:PHE:CZ | 1:G:4602:PHE:CD1 | 2.97 | 0.52 |
| 2:B:26:TYR:N | 2:B:39:SER:HG | 2.07 | 0.52 |
| 1:C:688:ALA:HB1 | 1:C:691:THR:HB | 1.91 | 0.52 |
| 1:E:2790:ILE:HG12 | 1:E:2904:VAL:HG12 | 1.92 | 0.52 |
| 1:G:3911:ILE:O | 1:G:3911:ILE:HD13 | 2.09 | 0.52 |
| 1:A:35:LEU:HD22 | 1:A:49:LEU:HD13 | 1.91 | 0.52 |
| 1:E:4199:PHE:CZ | 1:E:4602:PHE:CD1 | 2.97 | 0.52 |
| 1:E:4617:LEU:HA | 1:E:4621:GLU:HB3 | 1.92 | 0.52 |
| 1:C:1894:LEU:HD12 | 1:C:2069:TRP:CZ2 | 2.44 | 0.52 |
| 1:G:1725:PHE:HB3 | 1:G:2105:THR:HG22 | 1.92 | 0.52 |
| 2:H:25:HIS:CD2 | 2:H:104:LEU:HD11 | 2.44 | 0.52 |
| 1:C:119:ILE:HG21 | 1:C:162:ILE:HD11 | 1.92 | 0.52 |
| 1:E:2718:LEU:HD22 | 1:E:2780:LEU:HD22 | 1.92 | 0.52 |
| 1:G:21:VAL:HG13 | 1:G:217:ILE:HD11 | 1.92 | 0.52 |
| 1:A:872:ILE:HD11 | 1:A:944:LEU:HD13 | 1.92 | 0.52 |
| 1:E:778:MET:O | 1:E:1468:THR:OG1 | 2.28 | 0.52 |
| 1:E:1105:PHE:HB2 | 1:E:1115:VAL:HG21 | 1.91 | 0.52 |
| 1:G:1689:ILE:HD11 | 1:G:1790:LYS:HD3 | 1.91 | 0.52 |
| 1:E:633:CYS:SG | 1:E:1669:ASN:ND2 | 2.83 | 0.52 |
| 1:G:935:MET:O | 1:G:939:THR:HG23 | 2.10 | 0.52 |
| 1:G:2159:PRO:HB3 | 1:G:2206:ILE:HD12 | 1.92 | 0.52 |
| 1:C:572:LEU:HD13 | 1:C:609:LYS:HB2 | 1.90 | 0.51 |
| 1:E:611:LEU:HD22 | 1:E:1659:ARG:CD | 2.40 | 0.51 |
| 1:A:307:SER:HB3 | 1:A:327:THR:HG22 | 1.93 | 0.51 |
| 1:A:2159:PRO:HB3 | 1:A:2206:ILE:HD12 | 1.92 | 0.51 |
| 1:C:3693:ALA:HB1 | 1:C:3758:ALA:O | 2.10 | 0.51 |
| 1:E:804:LEU:HD22 | 1:E:822:CYS:HB3 | 1.92 | 0.51 |
| 1:A:3891:TRP:CZ2 | 1:G:76:ARG:HB2 | 2.45 | 0.51 |
| 1:C:4137:ILE:HG23 | 1:C:4151:PHE:CE2 | 2.45 | 0.51 |
| 1:E:4130:PHE:O | 1:E:4134:LEU:N | 2.43 | 0.51 |
| 1:A:633:CYS:SG | 1:A:1669:ASN:ND2 | 2.83 | 0.51 |
| 1:E:991:SER:HB3 | 1:E:1066:ALA:HB2 | 1.93 | 0.51 |
| 1:G:436:LEU:HD11 | 1:G:447:LEU:HD22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:541:ILE:HD12 | 1:E:578:VAL:HG22 | 1.93 | 0.51 |
| 1:E:659:ILE:HG23 | 1:E:825:ALA:HB1 | 1.92 | 0.51 |
| 1:E:745:ASN:HB2 | 1:E:771:ASN:HD21 | 1.75 | 0.51 |
| 1:G:1726:ILE:HG21 | 1:G:2120:LEU:HD21 | 1.92 | 0.51 |
| 1:C:436:LEU:HD13 | 1:C:518:ALA:HB2 | 1.91 | 0.51 |
| 1:C:4619:ILE:HD12 | 1:C:4668:ILE:HD12 | 1.93 | 0.51 |
| 1:E:888:ASN:ND2 | 1:E:1056:THR:HG21 | 2.25 | 0.51 |
| 1:E:1105:PHE:CB | 1:E:1115:VAL:HG21 | 2.41 | 0.51 |
| 1:A:4958:ASP:O | 1:A:4962:LYS:HB2 | 2.11 | 0.51 |
| 1:E:693:LEU:HD22 | 1:E:798:ILE:HD13 | 1.92 | 0.51 |
| 1:E:4191:VAL:HG21 | 1:E:4951:TRP:CZ3 | 2.46 | 0.51 |
| 1:E:143:LEU:HD21 | 1:E:207:PHE:CE2 | 2.47 | 0.50 |
| 1:E:2170:THR:O | 1:E:2174:VAL:HG23 | 2.11 | 0.50 |
| 1:G:888:ASN:ND2 | 1:G:1056:THR:HG21 | 2.26 | 0.50 |
| 1:A:1830:ILE:HG22 | 1:A:1912:TYR:CD1 | 2.46 | 0.50 |
| 1:E:436:LEU:HD22 | 1:E:518:ALA:HA | 1.94 | 0.50 |
| 1:G:660:PHE:CD2 | 1:G:827:LEU:HD11 | 2.45 | 0.50 |
| 1:G:3689:TYR:OH | 1:G:3744:THR:HG21 | 2.11 | 0.50 |
| 2:F:82:TYR:CD2 | 2:F:91:ILE:HG21 | 2.47 | 0.50 |
| 1:C:677:LEU:HD22 | 1:C:695:VAL:HG21 | 1.93 | 0.50 |
| 1:E:633:CYS:CB | 1:E:1672:VAL:HG11 | 2.40 | 0.50 |
| 1:E:4103:LEU:HD12 | 1:E:4127:LEU:HD11 | 1.94 | 0.50 |
| 1:E:4192:ASN:C | 1:E:4192:ASN:HD22 | 2.14 | 0.50 |
| 1:G:2067:VAL:HG21 | 1:G:3645:LEU:HD13 | 1.93 | 0.50 |
| 1:G:3745:ILE:HG13 | 1:G:3759:THR:HG21 | 1.93 | 0.50 |
| 1:C:2470:VAL:HG21 | 1:C:2523:THR:CG2 | 2.42 | 0.50 |
| 1:E:915:HIS:HB3 | 1:E:918:LEU:HD13 | 1.93 | 0.50 |
| 1:G:688:ALA:HB3 | 1:G:795:SER:OG | 2.12 | 0.50 |
| 1:C:633:CYS:CB | 1:C:1672:VAL:HG11 | 2.41 | 0.50 |
| 1:C:1831:MET:HE1 | 1:C:1833:ILE:HD13 | 1.94 | 0.50 |
| 1:G:872:ILE:HD11 | 1:G:944:LEU:HD13 | 1.92 | 0.50 |
| 1:C:1116:GLY:O | 1:C:1204:VAL:HG12 | 2.11 | 0.50 |
| 1:C:4927:LEU:HD11 | 1:C:4942:VAL:HG13 | 1.94 | 0.50 |
| 1:G:4097:PHE:CZ | 1:G:4152:GLU:HB2 | 2.46 | 0.50 |
| 1:A:759:LEU:HD13 | 1:A:766:ILE:CG1 | 2.41 | 0.49 |
| 1:A:4617:LEU:HD13 | 1:A:4621:GLU:HB3 | 1.94 | 0.49 |
| 1:C:177:VAL:HG13 | 1:C:216:PRO:HD3 | 1.94 | 0.49 |
| 1:A:915:HIS:HB3 | 1:A:918:LEU:HD13 | 1.93 | 0.49 |
| 1:A:1507:ILE:HB | 1:A:1521:ILE:HG13 | 1.94 | 0.49 |
| 1:A:2718:LEU:HD22 | 1:A:2780:LEU:HD22 | 1.94 | 0.49 |
| 1:C:4912:LEU:HA | 1:C:4916:ASN:HB3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:4912:LEU:HA | 1:E:4916:ASN:HB3 | 1.94 | 0.49 |
| 1:G:2423:ILE:HD13 | 1:G:2423:ILE:O | 2.10 | 0.49 |
| 1:E:648:LEU:HD23 | 1:E:1684:GLN:HA | 1.95 | 0.49 |
| 1:E:826:VAL:HG21 | 1:E:832:LEU:HD22 | 1.95 | 0.49 |
| 1:G:177:VAL:HG13 | 1:G:216:PRO:HD3 | 1.94 | 0.49 |
| 1:G:2159:PRO:CB | 1:G:2206:ILE:HD12 | 2.43 | 0.49 |
| 1:G:2497:LEU:CD1 | 1:G:2873:VAL:HG12 | 2.43 | 0.49 |
| 1:A:4912:LEU:HA | 1:A:4916:ASN:HB3 | 1.94 | 0.49 |
| 1:C:181:LEU:HD12 | 1:C:214:VAL:HG21 | 1.94 | 0.49 |
| 1:E:3899:ILE:HD12 | 1:E:3959:LEU:HD23 | 1.93 | 0.49 |
| 1:E:4191:VAL:HG11 | 1:E:4951:TRP:CH2 | 2.46 | 0.49 |
| 1:A:165:ALA:HB1 | 1:A:211:LEU:HD11 | 1.94 | 0.49 |
| 1:A:2473:LEU:HD21 | 1:A:2484:PHE:CE2 | 2.47 | 0.49 |
| 1:C:4046:LYS:HG2 | 1:C:4079:LEU:HD21 | 1.93 | 0.49 |
| 1:E:1782:PHE:CE2 | 1:E:1787:LEU:HD22 | 2.47 | 0.49 |
| 1:G:1689:ILE:HD11 | 1:G:1790:LYS:CD | 2.43 | 0.49 |
| 1:C:3911:ILE:HD13 | 1:C:3911:ILE:O | 2.12 | 0.49 |
| 2:F:78:PRO:HA | 2:F:81:ALA:HB3 | 1.93 | 0.49 |
| 1:G:826:VAL:HG21 | 1:G:832:LEU:HD22 | 1.94 | 0.49 |
| 1:G:4912:LEU:HA | 1:G:4916:ASN:HB3 | 1.94 | 0.49 |
| 1:G:4958:ASP:O | 1:G:4962:LYS:HB2 | 2.11 | 0.49 |
| 1:A:2304:ARG:HB2 | 1:A:2399:LEU:HD21 | 1.94 | 0.49 |
| 1:C:1445:TRP:CD1 | 1:C:1518:LEU:HD22 | 2.47 | 0.49 |
| 1:C:1826:TYR:CZ | 1:C:1908:LEU:HD22 | 2.47 | 0.49 |
| 1:E:4617:LEU:HD13 | 1:E:4621:GLU:HB3 | 1.93 | 0.49 |
| 1:A:2470:VAL:HG11 | 1:A:2523:THR:HG22 | 1.94 | 0.49 |
| 1:C:28:ILE:CG1 | 1:C:201:LEU:HD11 | 2.42 | 0.49 |
| 1:C:1105:PHE:CB | 1:C:1115:VAL:HG21 | 2.42 | 0.49 |
| 1:C:4958:ASP:O | 1:C:4962:LYS:HB2 | 2.13 | 0.49 |
| 1:E:766:ILE:HB | 1:E:779:PHE:HB2 | 1.95 | 0.49 |
| 1:G:660:PHE:CE2 | 1:G:827:LEU:HD11 | 2.48 | 0.49 |
| 1:G:3802:SER:HB2 | 1:G:3837:THR:HG21 | 1.95 | 0.49 |
| 1:A:3861:THR:HG23 | 1:A:3863:THR:HG23 | 1.94 | 0.48 |
| 1:G:659:ILE:N | 1:G:659:ILE:HD12 | 2.28 | 0.48 |
| 1:G:1782:PHE:CE2 | 1:G:1787:LEU:HD22 | 2.47 | 0.48 |
| 1:E:601:LEU:HD23 | 1:E:642:LEU:HD21 | 1.95 | 0.48 |
| 1:E:881:ILE:HD11 | 1:E:1060:TYR:CD2 | 2.47 | 0.48 |
| 1:E:1831:MET:CE | 1:E:1833:ILE:HD13 | 2.43 | 0.48 |
| 1:G:759:LEU:HD13 | 1:G:766:ILE:HG12 | 1.95 | 0.48 |
| 1:E:1087:ILE:HD12 | 1:E:1128:LEU:CD2 | 2.43 | 0.48 |
| 1:E:4099:VAL:O | 1:E:4103:LEU:HG | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1830:ILE:HG22 | 1:G:1912:TYR:CD1 | 2.48 | 0.48 |
| 1:E:2861:LEU:HD22 | 1:E:2872:LEU:HD11 | 1.94 | 0.48 |
| 1:E:3806:LEU:HD13 | 1:E:3889:PHE:HA | 1.96 | 0.48 |
| 1:G:1475:LYS:O | 1:G:1476:VAL:HG22 | 2.12 | 0.48 |
| 1:G:1483:SER:HB2 | 1:G:1533:VAL:HG23 | 1.94 | 0.48 |
| 1:G:4922:PHE:HA | 1:G:4925:MET:HG2 | 1.93 | 0.48 |
| 1:A:2473:LEU:HD21 | 1:A:2484:PHE:HE2 | 1.78 | 0.48 |
| 1:C:579:LEU:HD22 | 1:C:586:LEU:HD23 | 1.95 | 0.48 |
| 1:C:3683:LEU:HD21 | 1:C:3747:ALA:HB1 | 1.95 | 0.48 |
| 1:E:3926:GLN:HA | 1:E:3926:GLN:HE21 | 1.77 | 0.48 |
| 2:F:4:ILE:CD1 | 2:F:74:LEU:HD22 | 2.43 | 0.48 |
| 1:G:579:LEU:HD22 | 1:G:586:LEU:HD23 | 1.94 | 0.48 |
| 1:G:4496:LEU:HD22 | 1:G:4591:GLY:HA3 | 1.95 | 0.48 |
| 1:A:496:ASN:HA | 1:A:499:LEU:HD12 | 1.95 | 0.48 |
| 2:B:4:ILE:CD1 | 2:B:74:LEU:HD22 | 2.44 | 0.48 |
| 1:C:541:ILE:HD12 | 1:C:578:VAL:HG22 | 1.95 | 0.48 |
| 1:E:4192:ASN:HD22 | 1:E:4193:PHE:N | 2.11 | 0.48 |
| 2:F:56:ILE:HD13 | 2:F:82:TYR:CZ | 2.48 | 0.48 |
| 1:G:869:THR:HG21 | 1:G:1002:ASN:HD21 | 1.77 | 0.48 |
| 1:A:1726:ILE:HG21 | 1:A:2120:LEU:HD21 | 1.95 | 0.48 |
| 1:E:986:ILE:HD13 | 1:E:1058:LEU:HB3 | 1.96 | 0.48 |
| 1:C:2123:LEU:HD12 | 1:C:2127:ARG:NE | 2.29 | 0.48 |
| 1:C:3737:ALA:HA | 1:C:3740:MET:HG2 | 1.96 | 0.48 |
| 1:E:4922:PHE:HA | 1:E:4925:MET:HG2 | 1.94 | 0.48 |
| 1:G:759:LEU:HD13 | 1:G:766:ILE:CG1 | 2.44 | 0.48 |
| 1:G:1105:PHE:CB | 1:G:1115:VAL:HG21 | 2.42 | 0.48 |
| 1:C:3775:GLN:NE2 | 1:C:3847:LEU:O | 2.47 | 0.48 |
| 1:C:76:ARG:CB | 1:E:3891:TRP:CZ2 | 2.97 | 0.48 |
| 1:C:4137:ILE:HG23 | 1:C:4151:PHE:HE2 | 1.78 | 0.48 |
| 1:C:4570:MET:HA | 1:C:4573:THR:HG22 | 1.96 | 0.48 |
| 1:E:1686:LEU:HD22 | 1:E:1790:LYS:HE3 | 1.95 | 0.48 |
| 1:G:4521:TYR:CZ | 1:G:4562:VAL:HG22 | 2.49 | 0.48 |
| 1:C:230:GLY:HA3 | 1:C:289:ILE:HD11 | 1.95 | 0.47 |
| 1:C:4617:LEU:HD13 | 1:C:4621:GLU:HB3 | 1.96 | 0.47 |
| 1:E:4652:LYS:HG3 | 1:E:4672:LEU:HD23 | 1.95 | 0.47 |
| 1:G:237:LEU:HD23 | 1:G:244:CYS:SG | 2.53 | 0.47 |
| 1:G:436:LEU:HD13 | 1:G:518:ALA:HB2 | 1.95 | 0.47 |
| 1:C:559:ILE:HG21 | 1:C:593:HIS:HA | 1.96 | 0.47 |
| 1:C:3802:SER:HB2 | 1:C:3837:THR:HG21 | 1.96 | 0.47 |
| 1:E:2497:LEU:CD1 | 1:E:2873:VAL:HG12 | 2.45 | 0.47 |
| 1:E:2861:LEU:HD22 | 1:E:2872:LEU:CD1 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:4869:ILE:HG21 | 1:G:4869:ILE:HG23 | 1.95 | 0.47 |
| 1:E:4923:PHE:HZ | 1:E:4942:VAL:HG11 | 1.79 | 0.47 |
| 1:G:4619:ILE:HD12 | 1:G:4668:ILE:HD12 | 1.96 | 0.47 |
| 1:A:3745:ILE:HG13 | 1:A:3759:THR:HG21 | 1.96 | 0.47 |
| 1:C:652:VAL:HG11 | 1:C:692:HIS:CD2 | 2.49 | 0.47 |
| 1:C:2498:ARG:CB | 1:C:2517:LEU:HD11 | 2.45 | 0.47 |
| 1:E:1707:ILE:HG23 | 1:E:1827:THR:HG21 | 1.97 | 0.47 |
| 1:G:4104:THR:HG21 | 1:G:4134:LEU:HD11 | 1.97 | 0.47 |
| 1:A:4515:ASN:HD22 | 1:A:4745:LEU:HD21 | 1.80 | 0.47 |
| 1:C:935:MET:O | 1:C:939:THR:HG23 | 2.14 | 0.47 |
| 1:C:52:THR:HG22 | 1:C:60:PRO:CB | 2.45 | 0.47 |
| 1:C:1521:ILE:HG22 | 1:C:1526:GLU:HA | 1.96 | 0.47 |
| 1:A:614:LEU:HD13 | 1:A:636:LEU:HD11 | 1.95 | 0.47 |
| 1:A:1686:LEU:HD22 | 1:A:1790:LYS:HE3 | 1.97 | 0.47 |
| 1:A:4619:ILE:HD12 | 1:A:4668:ILE:HD12 | 1.97 | 0.47 |
| 1:C:943:LEU:HD23 | 1:C:999:LEU:HD11 | 1.95 | 0.47 |
| 1:C:1303:ARG:HG2 | 1:C:1542:ALA:HB2 | 1.97 | 0.47 |
| 1:E:4923:PHE:CZ | 1:E:4942:VAL:HG11 | 2.50 | 0.47 |
| 1:G:430:ILE:HD11 | 1:G:501:CYS:SG | 2.55 | 0.47 |
| 1:G:1658:LEU:HD23 | 1:G:1701:GLY:HA3 | 1.96 | 0.47 |
| 1:C:2779:SER:OG | 1:C:2849:TYR:OH | 2.31 | 0.47 |
| 1:C:3778:MET:HE3 | 1:C:3847:LEU:HD13 | 1.96 | 0.47 |
| 1:E:3752:THR:HG23 | 1:E:3836:PHE:CE2 | 2.50 | 0.47 |
| 1:G:826:VAL:HG13 | 1:G:832:LEU:HD13 | 1.97 | 0.47 |
| 1:G:1521:ILE:HG22 | 1:G:1526:GLU:HA | 1.97 | 0.47 |
| 1:G:3911:ILE:HG12 | 1:G:3975:LEU:HD22 | 1.97 | 0.47 |
| 1:A:559:ILE:HG12 | 1:A:575:LEU:HD11 | 1.97 | 0.47 |
| 1:A:3866:ASN:OD1 | 1:A:3867:THR:HG23 | 2.14 | 0.47 |
| 1:A:4652:LYS:HG3 | 1:A:4672:LEU:HD23 | 1.97 | 0.47 |
| 1:C:2259:GLU:N | 1:C:2260:PRO:HD2 | 2.30 | 0.47 |
| 1:C:3911:ILE:HG12 | 1:C:3975:LEU:HD22 | 1.97 | 0.47 |
| 1:E:660:PHE:CD2 | 1:E:827:LEU:HD11 | 2.50 | 0.47 |
| 1:E:749:LEU:HD22 | 1:E:755:ILE:HD11 | 1.97 | 0.47 |
| 1:G:1090:ALA:HB3 | 1:G:1202:ILE:CG2 | 2.45 | 0.47 |
| 1:G:3804:LEU:HD13 | 1:G:3910:ALA:HB2 | 1.97 | 0.47 |
| 1:A:4160:GLN:HG2 | 1:A:4201:MET:HA | 1.97 | 0.47 |
| 1:C:1910:LEU:HG | 1:C:2062:ILE:HD12 | 1.97 | 0.47 |
| 1:E:919:VAL:HG21 | 1:E:923:LYS:HD3 | 1.96 | 0.47 |
| 1:G:436:LEU:HD22 | 1:G:518:ALA:HA | 1.96 | 0.47 |
| 1:C:1087:ILE:HD12 | 1:C:1128:LEU:CD2 | 2.45 | 0.46 |
| 1:C:1118:SER:CB | 1:C:1204:VAL:HG11 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:737:ILE:HG21 | 1:G:1481:LYS:HG2 | 1.98 | 0.46 |
| 1:G:4137:ILE:HG23 | 1:G:4151:PHE:HE2 | 1.78 | 0.46 |
| 1:C:1118:SER:HB3 | 1:C:1204:VAL:HG11 | 1.98 | 0.46 |
| 2:D:16:PRO:HG3 | 2:D:106:LEU:HD21 | 1.97 | 0.46 |
| 1:E:580:VAL:HG23 | 1:E:581:GLU:HG2 | 1.97 | 0.46 |
| 1:E:4607:GLU:O | 1:E:4611:LYS:HG2 | 2.15 | 0.46 |
| 1:C:618:CYS:SG | 1:C:1666:ALA:HA | 2.55 | 0.46 |
| 1:C:1218:GLY:O | 1:C:1240:ALA:HB3 | 2.15 | 0.46 |
| 1:C:2023:LEU:N | 1:C:2023:LEU:HD23 | 2.31 | 0.46 |
| 1:G:2493:PHE:O | 1:G:2497:LEU:HG | 2.15 | 0.46 |
| 1:G:2498:ARG:HB3 | 1:G:2517:LEU:HD11 | 1.98 | 0.46 |
| 1:A:496:ASN:HD22 | 1:A:499:LEU:HD12 | 1.79 | 0.46 |
| 1:A:4611:LYS:O | 1:A:4616:GLY:N | 2.49 | 0.46 |
| 1:C:2075:ILE:HD11 | 1:C:2080:LEU:HD23 | 1.97 | 0.46 |
| 1:C:3756:VAL:HG13 | 1:C:3836:PHE:CE1 | 2.51 | 0.46 |
| 1:E:2491:VAL:O | 1:E:2495:PRO:HD2 | 2.16 | 0.46 |
| 1:E:3737:ALA:HA | 1:E:3740:MET:HG2 | 1.96 | 0.46 |
| 1:G:804:LEU:HD22 | 1:G:822:CYS:HB3 | 1.96 | 0.46 |
| 1:G:3737:ALA:HA | 1:G:3740:MET:HG2 | 1.98 | 0.46 |
| 1:G:3899:ILE:HD12 | 1:G:3959:LEU:HD23 | 1.97 | 0.46 |
| 1:A:572:LEU:HD13 | 1:A:609:LYS:HB2 | 1.98 | 0.46 |
| 1:A:4939:GLU:HA | 1:A:4942:VAL:HG12 | 1.98 | 0.46 |
| 1:C:4611:LYS:O | 1:C:4616:GLY:N | 2.49 | 0.46 |
| 1:E:1475:LYS:O | 1:E:1476:VAL:HG22 | 2.16 | 0.46 |
| 1:E:4927:LEU:HD11 | 1:E:4942:VAL:HG13 | 1.98 | 0.46 |
| 1:A:778:MET:O | 1:A:1468:THR:OG1 | 2.33 | 0.46 |
| 1:A:3737:ALA:HA | 1:A:3740:MET:HG2 | 1.98 | 0.46 |
| 1:C:944:LEU:HD21 | 1:C:950:VAL:HG22 | 1.97 | 0.46 |
| 1:E:579:LEU:HD22 | 1:E:586:LEU:HD23 | 1.98 | 0.46 |
| 1:E:996:VAL:HG12 | 1:E:1054:VAL:HG11 | 1.97 | 0.46 |
| 1:E:3693:ALA:HB1 | 1:E:3758:ALA:O | 2.15 | 0.46 |
| 1:G:4020:MET:HE3 | 1:G:4067:LEU:HD21 | 1.97 | 0.46 |
| 1:G:4617:LEU:HD13 | 1:G:4621:GLU:HB3 | 1.98 | 0.46 |
| 1:A:541:ILE:HG22 | 1:A:547:ASN:HB3 | 1.97 | 0.46 |
| 1:C:601:LEU:HD23 | 1:C:642:LEU:HD21 | 1.96 | 0.46 |
| 1:E:739:ARG:CZ | 1:E:1467:VAL:HG13 | 2.45 | 0.46 |
| 1:E:4501:TYR:OH | 1:E:4595:LEU:HD21 | 2.15 | 0.46 |
| 1:G:633:CYS:CB | 1:G:1672:VAL:HG11 | 2.46 | 0.46 |
| 1:G:1253:LYS:NZ | 1:G:1601:ASN:HD22 | 2.14 | 0.46 |
| 1:C:2485:LEU:HD11 | 1:C:2527:PRO:HB3 | 1.98 | 0.46 |
| 1:G:1738:LEU:HD12 | 1:G:1921:ARG:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:194:LEU:HD11 | 1:A:201:LEU:HD13 | 1.98 | 0.46 |
| 1:C:4198:ILE:HG23 | 1:C:4925:MET:CE | 2.46 | 0.46 |
| 1:E:3797:LEU:HD21 | 1:E:3836:PHE:HE2 | 1.80 | 0.46 |
| 2:F:75:THR:HG23 | 2:F:98:ILE:CD1 | 2.46 | 0.46 |
| 1:G:2170:THR:O | 1:G:2174:VAL:HG23 | 2.15 | 0.46 |
| 1:C:230:GLY:CA | 1:C:289:ILE:HD11 | 2.46 | 0.46 |
| 1:C:743:SER:OG | 1:C:775:VAL:HG22 | 2.16 | 0.46 |
| 1:C:4794:PHE:HB2 | 1:C:4833:ILE:HD11 | 1.98 | 0.46 |
| 1:A:1105:PHE:CB | 1:A:1115:VAL:HG21 | 2.46 | 0.45 |
| 1:A:2170:THR:O | 1:A:2174:VAL:HG23 | 2.16 | 0.45 |
| 1:A:2521:LEU:HD11 | 1:A:2601:UNK:CB | 2.46 | 0.45 |
| 2:B:75:THR:HG23 | 2:B:98:ILE:CD1 | 2.46 | 0.45 |
| 1:E:611:LEU:HD22 | 1:E:1659:ARG:CG | 2.45 | 0.45 |
| 1:E:4958:ASP:O | 1:E:4962:LYS:HB2 | 2.16 | 0.45 |
| 1:G:541:ILE:HG22 | 1:G:547:ASN:HB3 | 1.97 | 0.45 |
| 1:G:3966:ILE:O | 1:G:3969:LEU:N | 2.49 | 0.45 |
| 1:A:2086:VAL:HG13 | 1:A:2087:LEU:HD12 | 1.98 | 0.45 |
| 1:C:670:TYR:O | 1:C:673:TRP:NE1 | 2.49 | 0.45 |
| 1:C:1782:PHE:CE2 | 1:C:1787:LEU:HD22 | 2.51 | 0.45 |
| 1:C:3992:VAL:HG13 | 1:C:4964:TYR:CE2 | 2.51 | 0.45 |
| 1:E:476:GLN:HE21 | 1:E:476:GLN:HA | 1.81 | 0.45 |
| 1:E:559:ILE:HD12 | 1:E:596:SER:HB2 | 1.98 | 0.45 |
| 1:E:3966:ILE:O | 1:E:3969:LEU:N | 2.48 | 0.45 |
| 1:G:3844:LEU:HD13 | 1:G:3847:LEU:HD12 | 1.97 | 0.45 |
| 1:A:875:PRO:HD2 | 1:A:878:LEU:HD12 | 1.98 | 0.45 |
| 2:B:73:LYS:HZ1 | 2:B:98:ILE:HD12 | 1.80 | 0.45 |
| 1:C:4617:LEU:HA | 1:C:4621:GLU:HB3 | 1.98 | 0.45 |
| 1:G:4165:GLN:HG3 | 1:G:4501:TYR:CZ | 2.52 | 0.45 |
| 1:C:112:THR:HG21 | 1:C:174:LYS:HD3 | 1.99 | 0.45 |
| 1:C:2423:ILE:HD13 | 1:C:2423:ILE:O | 2.16 | 0.45 |
| 1:G:1094:TYR:OH | 1:G:1808:ASP:OD1 | 2.33 | 0.45 |
| 1:E:1253:LYS:NZ | 1:E:1601:ASN:HD22 | 2.14 | 0.45 |
| 1:E:1831:MET:HE1 | 1:E:1833:ILE:HD13 | 1.97 | 0.45 |
| 1:E:3952:PHE:HZ | 1:E:3975:LEU:HD23 | 1.82 | 0.45 |
| 1:E:4152:GLU:HB3 | 1:E:4926:TYR:CD1 | 2.50 | 0.45 |
| 1:G:611:LEU:HD22 | 1:G:1659:ARG:HD2 | 1.98 | 0.45 |
| 1:A:996:VAL:HG12 | 1:A:1054:VAL:HG11 | 1.99 | 0.45 |
| 1:E:2023:LEU:N | 1:E:2023:LEU:HD23 | 2.30 | 0.45 |
| 1:G:1299:ILE:HG23 | 1:G:1301:PHE:CE1 | 2.52 | 0.45 |
| 1:G:4130:PHE:O | 1:G:4134:LEU:N | 2.50 | 0.45 |
| 1:C:72:SER:C | 1:C:73:LEU:HD22 | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2513:MET:O | 1:C:2517:LEU:HD13 | 2.17 | 0.45 |
| 1:G:689:GLU:O | 1:G:691:THR:HG22 | 2.16 | 0.45 |
| 1:G:2896:PHE:HA | 1:G:2899:ILE:HG12 | 1.98 | 0.45 |
| 1:E:459:LEU:HB3 | 1:E:536:LEU:HD13 | 1.99 | 0.45 |
| 1:E:1692:LYS:HG2 | 1:E:1810:VAL:HG13 | 1.97 | 0.45 |
| 1:E:1914:CYS:HB2 | 1:E:2091:GLN:HE22 | 1.82 | 0.45 |
| 1:E:2259:GLU:N | 1:E:2260:PRO:HD2 | 2.32 | 0.45 |
| 1:G:598:ILE:HG23 | 1:G:642:LEU:HD22 | 1.99 | 0.45 |
| 1:G:2259:GLU:N | 1:G:2260:PRO:HD2 | 2.31 | 0.45 |
| 1:A:1782:PHE:CE2 | 1:A:1787:LEU:HD22 | 2.52 | 0.45 |
| 1:C:2095:ILE:HD11 | 1:C:3630:ILE:HG22 | 1.99 | 0.45 |
| 1:C:2176:VAL:HG22 | 1:C:2224:ASN:HD21 | 1.81 | 0.45 |
| 1:A:804:LEU:HD22 | 1:A:822:CYS:HB3 | 1.98 | 0.45 |
| 1:C:4496:LEU:HD22 | 1:C:4591:GLY:HA3 | 1.99 | 0.45 |
| 1:E:739:ARG:NE | 1:E:1467:VAL:HG13 | 2.32 | 0.45 |
| 1:E:935:MET:O | 1:E:939:THR:HG23 | 2.17 | 0.45 |
| 1:E:4137:ILE:HG23 | 1:E:4151:PHE:CE2 | 2.50 | 0.45 |
| 1:E:4939:GLU:HA | 1:E:4942:VAL:HG12 | 1.99 | 0.45 |
| 1:G:217:ILE:HG22 | 1:G:286:GLY:HA3 | 2.00 | 0.45 |
| 1:G:4611:LYS:O | 1:G:4616:GLY:N | 2.50 | 0.45 |
| 1:A:633:CYS:CB | 1:A:1672:VAL:HG11 | 2.47 | 0.44 |
| 1:A:759:LEU:HD13 | 1:A:766:ILE:HG12 | 1.98 | 0.44 |
| 1:A:826:VAL:HG21 | 1:A:832:LEU:HD22 | 1.99 | 0.44 |
| 1:A:2473:LEU:HD13 | 1:A:2473:LEU:O | 2.17 | 0.44 |
| 1:A:3911:ILE:HD11 | 1:A:3975:LEU:HD22 | 1.98 | 0.44 |
| 1:A:4195:GLU:HA | 1:A:4198:ILE:HD12 | 2.00 | 0.44 |
| 1:C:2106:TYR:CG | 1:C:2107:THR:N | 2.85 | 0.44 |
| 1:E:2067:VAL:HG11 | 1:E:3645:LEU:HD22 | 1.99 | 0.44 |
| 1:G:2266:VAL:HG21 | 1:G:2324:LEU:HB3 | 1.99 | 0.44 |
| 1:A:4607:GLU:O | 1:A:4611:LYS:HG2 | 2.17 | 0.44 |
| 1:C:1639:VAL:HG21 | 1:C:1644:LEU:HD23 | 1.99 | 0.44 |
| 1:E:1629:SER:HA | 1:E:1640:ASP:HA | 1.99 | 0.44 |
| 1:G:743:SER:OG | 1:G:775:VAL:HG22 | 2.17 | 0.44 |
| 1:A:3956:GLN:HE21 | 1:A:4014:ILE:HG23 | 1.83 | 0.44 |
| 1:C:76:ARG:HB3 | 1:E:3891:TRP:CZ2 | 2.51 | 0.44 |
| 1:C:598:ILE:HG23 | 1:C:642:LEU:HD22 | 1.98 | 0.44 |
| 1:E:944:LEU:HD21 | 1:E:950:VAL:HG22 | 1.99 | 0.44 |
| 1:E:2473:LEU:HD21 | 1:E:2484:PHE:CE2 | 2.51 | 0.44 |
| 1:G:2718:LEU:HD22 | 1:G:2780:LEU:HD22 | 1.99 | 0.44 |
| 1:G:4164:PRO:HG2 | 1:G:4166:VAL:HG22 | 2.00 | 0.44 |
| 1:G:679:VAL:HA | 1:G:800:VAL:HG12 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2023:LEU:N | 1:A:2023:LEU:HD23 | 2.32 | 0.44 |
| 1:A:4617:LEU:HA | 1:A:4621:GLU:HB3 | 1.98 | 0.44 |
| 1:E:1689:ILE:HD11 | 1:E:1790:LYS:CD | 2.47 | 0.44 |
| 1:E:2838:LEU:HD23 | 1:E:2841:MET:SD | 2.57 | 0.44 |
| 1:A:4612:LEU:HD11 | 1:A:4637:ILE:HG12 | 2.00 | 0.44 |
| 1:E:2130:LEU:CA | 1:E:2174:VAL:HG22 | 2.46 | 0.44 |
| 1:A:1253:LYS:NZ | 1:A:1601:ASN:HD22 | 2.15 | 0.44 |
| 1:A:2259:GLU:N | 1:A:2260:PRO:HD2 | 2.31 | 0.44 |
| 1:A:3992:VAL:HG13 | 1:A:4964:TYR:CE2 | 2.53 | 0.44 |
| 1:C:28:ILE:CD1 | 1:C:201:LEU:HD11 | 2.46 | 0.44 |
| 1:C:4191:VAL:HG21 | 1:C:4951:TRP:CZ3 | 2.52 | 0.44 |
| 1:C:4817:PHE:O | 1:C:4821:VAL:HG22 | 2.18 | 0.44 |
| 1:C:4823:VAL:HG23 | 1:C:4824:ARG:HG3 | 1.99 | 0.44 |
| 1:E:826:VAL:CG2 | 1:E:832:LEU:HD13 | 2.48 | 0.44 |
| 1:G:1116:GLY:O | 1:G:1204:VAL:HG12 | 2.18 | 0.44 |
| 1:G:3966:ILE:HD12 | 1:G:3969:LEU:HD23 | 1.99 | 0.44 |
| 1:G:3986:MET:SD | 1:G:3996:ILE:HD11 | 2.57 | 0.44 |
| 1:A:1703:TYR:HB2 | 1:A:1820:PRO:HB3 | 1.99 | 0.44 |
| 1:A:4617:LEU:HA | 1:A:4621:GLU:CB | 2.48 | 0.44 |
| 1:C:4164:PRO:HG2 | 1:C:4166:VAL:HG22 | 1.99 | 0.44 |
| 1:E:3778:MET:HE1 | 1:E:3847:LEU:HD22 | 2.00 | 0.44 |
| 1:E:4611:LYS:O | 1:E:4616:GLY:N | 2.51 | 0.44 |
| 1:G:3697:ALA:HB2 | 1:G:3761:LYS:HB3 | 2.00 | 0.44 |
| 1:A:280:LEU:HD13 | 1:A:296:ARG:NH1 | 2.33 | 0.44 |
| 1:A:3775:GLN:NE2 | 1:A:3847:LEU:O | 2.51 | 0.44 |
| 1:C:1090:ALA:HB3 | 1:C:1202:ILE:HG22 | 2.00 | 0.44 |
| 1:C:4846:ILE:CD1 | 1:E:4816:MET:HG3 | 2.47 | 0.44 |
| 1:E:759:LEU:HD13 | 1:E:766:ILE:CG1 | 2.48 | 0.44 |
| 1:G:737:ILE:HD13 | 1:G:1535:PRO:HG3 | 2.00 | 0.44 |
| 1:G:3879:LEU:HA | 1:G:3882:VAL:HG22 | 2.00 | 0.44 |
| 1:A:655:MET:SD | 1:A:1619:VAL:HG21 | 2.58 | 0.43 |
| 1:C:633:CYS:SG | 1:C:1669:ASN:ND2 | 2.91 | 0.43 |
| 1:C:4191:VAL:HG21 | 1:C:4951:TRP:CH2 | 2.53 | 0.43 |
| 1:C:4607:GLU:O | 1:C:4611:LYS:HG2 | 2.18 | 0.43 |
| 1:G:580:VAL:HG23 | 1:G:581:GLU:HG2 | 2.00 | 0.43 |
| 1:A:952:ILE:HD12 | 1:A:956:HIS:CE1 | 2.53 | 0.43 |
| 1:A:1090:ALA:HB3 | 1:A:1202:ILE:HG22 | 1.99 | 0.43 |
| 1:A:2075:ILE:CG1 | 1:A:2080:LEU:HD23 | 2.46 | 0.43 |
| 1:A:3802:SER:HB2 | 1:A:3837:THR:HG21 | 2.00 | 0.43 |
| 1:A:3804:LEU:HB3 | 1:A:3885:SER:HB3 | 2.00 | 0.43 |
| 1:C:1808:ASP:HB3 | 1:C:1809:PRO:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:429:PHE:CD1 | 1:E:452:VAL:HG21 | 2.53 | 0.43 |
| 1:E:3916:GLN:O | 1:E:3920:THR:HG23 | 2.19 | 0.43 |
| 1:G:3797:LEU:HD21 | 1:G:3836:PHE:CE2 | 2.53 | 0.43 |
| 1:A:463:PHE:HB3 | 1:A:539:ALA:HB1 | 2.00 | 0.43 |
| 1:A:611:LEU:HD22 | 1:A:1659:ARG:CD | 2.48 | 0.43 |
| 1:A:4496:LEU:HD12 | 1:A:4587:PHE:CZ | 2.53 | 0.43 |
| 1:C:73:LEU:C | 1:C:74:LEU:HD12 | 2.39 | 0.43 |
| 1:E:739:ARG:HG3 | 1:E:1469:LEU:HD21 | 2.01 | 0.43 |
| 1:E:1830:ILE:HG22 | 1:E:1912:TYR:CD1 | 2.53 | 0.43 |
| 1:E:1847:GLU:HB2 | 1:E:1848:PRO:HD3 | 2.00 | 0.43 |
| 1:A:580:VAL:HG23 | 1:A:581:GLU:HG2 | 2.00 | 0.43 |
| 1:A:2497:LEU:HD13 | 1:A:2874:PRO:HD2 | 1.99 | 0.43 |
| 1:A:4152:GLU:HB3 | 1:A:4926:TYR:CE1 | 2.53 | 0.43 |
| 1:A:4508:LEU:HD21 | 1:A:4748:ILE:HD13 | 2.00 | 0.43 |
| 1:A:4858:VAL:CG1 | 1:C:4864:ILE:HG21 | 2.49 | 0.43 |
| 1:C:2498:ARG:HB3 | 1:C:2517:LEU:HD11 | 1.99 | 0.43 |
| 1:C:4668:ILE:HD13 | 1:C:4671:LEU:HD12 | 2.00 | 0.43 |
| 1:C:4899:TYR:CE2 | 1:C:4962:LYS:HG2 | 2.53 | 0.43 |
| 1:E:1268:ILE:HG23 | 1:E:1268:ILE:O | 2.18 | 0.43 |
| 1:E:4005:VAL:HG21 | 1:E:4115:ARG:HD3 | 2.00 | 0.43 |
| 1:G:364:GLN:HE21 | 1:G:369:GLY:HA2 | 1.83 | 0.43 |
| 1:G:656:ARG:NH2 | 1:G:835:GLU:OE2 | 2.51 | 0.43 |
| 1:G:4939:GLU:HA | 1:G:4942:VAL:HG12 | 2.00 | 0.43 |
| 1:C:4651:VAL:O | 1:C:4655:VAL:HG23 | 2.18 | 0.43 |
| 1:E:663:VAL:HG13 | 1:E:671:LYS:HD3 | 2.00 | 0.43 |
| 1:E:847:THR:HG21 | 1:E:1215:MET:O | 2.18 | 0.43 |
| 1:E:1783:PRO:HB2 | 1:E:1786:ILE:HG22 | 2.01 | 0.43 |
| 1:E:1925:ILE:HD13 | 1:E:2032:LEU:HD21 | 2.00 | 0.43 |
| 1:G:2110:GLY:O | 1:G:2113:VAL:HG13 | 2.18 | 0.43 |
| 1:G:2497:LEU:HD12 | 1:G:2873:VAL:HG12 | 2.01 | 0.43 |
| 1:A:4082:GLU:HA | 1:A:4085:VAL:HG22 | 2.00 | 0.43 |
| 1:C:983:LEU:HD21 | 1:C:1056:THR:HG23 | 2.01 | 0.43 |
| 1:C:1783:PRO:HB2 | 1:C:1786:ILE:HG22 | 2.01 | 0.43 |
| 1:C:1894:LEU:HD11 | 1:C:2065:THR:HG21 | 2.01 | 0.43 |
| 1:C:3843:PHE:O | 1:C:3847:LEU:HG | 2.19 | 0.43 |
| 1:E:869:THR:HG21 | 1:E:1002:ASN:HD21 | 1.84 | 0.43 |
| 1:G:21:VAL:CG1 | 1:G:217:ILE:HD11 | 2.48 | 0.43 |
| 1:G:1808:ASP:HB3 | 1:G:1809:PRO:HA | 2.00 | 0.43 |
| 1:G:2713:ILE:HD13 | 1:G:2714:ILE:N | 2.34 | 0.43 |
| 1:G:4781:TYR:HA | 1:G:4784:THR:HG22 | 2.00 | 0.43 |
| 1:C:2779:SER:HG | 1:C:2849:TYR:HH | 1.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1511:VAL:HA | 1:E:1517:LEU:HD13 | 2.01 | 0.43 |
| 1:E:2497:LEU:HD13 | 1:E:2874:PRO:HD3 | 2.00 | 0.43 |
| 1:G:2023:LEU:N | 1:G:2023:LEU:HD23 | 2.34 | 0.43 |
| 1:A:1808:ASP:HB3 | 1:A:1809:PRO:HA | 2.00 | 0.43 |
| 1:A:1826:TYR:CZ | 1:A:1908:LEU:HD22 | 2.54 | 0.43 |
| 1:A:4597:VAL:HA | 1:A:4600:VAL:HG22 | 2.00 | 0.43 |
| 1:C:544:ASN:HB2 | 1:C:547:ASN:HD22 | 1.84 | 0.43 |
| 1:E:2058:LEU:HA | 1:E:2061:LEU:HD23 | 2.01 | 0.43 |
| 1:E:2266:VAL:HG21 | 1:E:2324:LEU:HD13 | 2.00 | 0.43 |
| 1:G:693:LEU:HD13 | 1:G:798:ILE:HD13 | 2.00 | 0.43 |
| 1:A:3697:ALA:HB2 | 1:A:3761:LYS:HB3 | 2.01 | 0.43 |
| 1:A:3973:MET:O | 1:A:4095:ILE:HD11 | 2.19 | 0.43 |
| 1:E:2130:LEU:CB | 1:E:2174:VAL:HG22 | 2.49 | 0.43 |
| 1:E:4103:LEU:HD12 | 1:E:4127:LEU:CD1 | 2.49 | 0.43 |
| 1:G:611:LEU:HD22 | 1:G:1659:ARG:CG | 2.49 | 0.43 |
| 1:G:643:LEU:HD22 | 1:G:1661:TYR:CZ | 2.53 | 0.43 |
| 1:G:2513:MET:O | 1:G:2517:LEU:HD13 | 2.18 | 0.43 |
| 1:A:633:CYS:HB3 | 1:A:1672:VAL:HG11 | 2.01 | 0.42 |
| 1:C:2266:VAL:HG21 | 1:C:2324:LEU:HB3 | 2.01 | 0.42 |
| 1:C:4781:TYR:HA | 1:C:4784:THR:HG22 | 2.01 | 0.42 |
| 1:E:763:ALA:HB3 | 1:E:765:SER:N | 2.34 | 0.42 |
| 1:G:763:ALA:HB3 | 1:G:765:SER:N | 2.33 | 0.42 |
| 1:G:1686:LEU:HD22 | 1:G:1790:LYS:HD2 | 2.01 | 0.42 |
| 1:G:1799:VAL:HG11 | 1:G:1845:LEU:HD11 | 2.01 | 0.42 |
| 1:A:2326:ILE:HG23 | 1:G:207:PHE:CD1 | 2.54 | 0.42 |
| 1:A:4046:LYS:HG2 | 1:A:4079:LEU:HD21 | 2.00 | 0.42 |
| 1:A:4493:LEU:HD21 | 1:A:4590:ILE:CG2 | 2.48 | 0.42 |
| 1:A:4846:ILE:CD1 | 1:C:4816:MET:HG3 | 2.48 | 0.42 |
| 1:C:207:PHE:CG | 1:E:2326:ILE:HG23 | 2.54 | 0.42 |
| 1:C:1928:PHE:CG | 1:C:2032:LEU:HD22 | 2.53 | 0.42 |
| 1:C:2896:PHE:HA | 1:C:2899:ILE:HG12 | 2.01 | 0.42 |
| 1:E:611:LEU:HD22 | 1:E:1659:ARG:HG3 | 2.01 | 0.42 |
| 1:E:614:LEU:HD13 | 1:E:636:LEU:HD11 | 2.00 | 0.42 |
| 1:E:3911:ILE:CD1 | 1:E:3975:LEU:HD22 | 2.49 | 0.42 |
| 1:G:636:LEU:HD13 | 1:G:1664:VAL:HG21 | 2.01 | 0.42 |
| 1:G:1087:ILE:HD12 | 1:G:1128:LEU:HD23 | 2.01 | 0.42 |
| 1:G:2470:VAL:HG21 | 1:G:2523:THR:HG23 | 2.01 | 0.42 |
| 1:A:646:THR:HG23 | 1:A:1684:GLN:NE2 | 2.34 | 0.42 |
| 1:A:763:ALA:HB3 | 1:A:765:SER:N | 2.34 | 0.42 |
| 1:A:1749:PRO:HB2 | 1:A:1843:LEU:HD21 | 2.01 | 0.42 |
| 1:A:4899:TYR:CE2 | 1:A:4962:LYS:HG2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:16:PRO:HG3 | 2:B:106:LEU:HD21 | 2.01 | 0.42 |
| 1:C:289:ILE:HG22 | 1:C:354:ILE:HD12 | 2.01 | 0.42 |
| 1:C:591:GLU:CA | 1:C:631:LEU:HD21 | 2.49 | 0.42 |
| 1:C:875:PRO:HD2 | 1:C:878:LEU:HD12 | 2.01 | 0.42 |
| 1:C:4939:GLU:HA | 1:C:4942:VAL:HG12 | 2.01 | 0.42 |
| 1:E:4617:LEU:HA | 1:E:4621:GLU:CB | 2.49 | 0.42 |
| 1:G:652:VAL:HG11 | 1:G:692:HIS:CD2 | 2.54 | 0.42 |
| 1:G:3797:LEU:HD21 | 1:G:3836:PHE:HE2 | 1.84 | 0.42 |
| 1:G:3924:TYR:HB3 | 1:G:3932:ASN:HD21 | 1.85 | 0.42 |
| 1:C:1680:VAL:HG21 | 1:C:1685:LEU:HD13 | 2.01 | 0.42 |
| 1:C:4195:GLU:HA | 1:C:4198:ILE:HD12 | 2.00 | 0.42 |
| 1:E:1932:PHE:CE2 | 1:E:2025:ILE:HG13 | 2.54 | 0.42 |
| 1:G:606:ARG:HG2 | 1:G:610:VAL:HG21 | 2.00 | 0.42 |
| 1:A:629:GLN:HA | 1:A:632:ILE:HD12 | 2.00 | 0.42 |
| 1:A:1459:LEU:HD13 | 1:A:1459:LEU:N | 2.35 | 0.42 |
| 1:A:1828:LEU:HD23 | 1:A:1834:PHE:CZ | 2.54 | 0.42 |
| 1:A:3911:ILE:CD1 | 1:A:3975:LEU:HD22 | 2.49 | 0.42 |
| 1:C:2420:ILE:O | 1:C:2424:LEU:HD13 | 2.20 | 0.42 |
| 1:C:4082:GLU:HA | 1:C:4085:VAL:HG22 | 2.01 | 0.42 |
| 1:E:611:LEU:HD22 | 1:E:1659:ARG:HD2 | 2.00 | 0.42 |
| 1:E:3950:HIS:N | 1:E:4010:ASN:HD21 | 2.18 | 0.42 |
| 1:E:4097:PHE:O | 1:E:4101:VAL:HG23 | 2.19 | 0.42 |
| 1:E:4781:TYR:HA | 1:E:4784:THR:HG22 | 2.00 | 0.42 |
| 2:F:66:MET:SD | 2:F:74:LEU:HD21 | 2.59 | 0.42 |
| 1:G:682:THR:HG22 | 1:G:798:ILE:HG12 | 2.01 | 0.42 |
| 1:G:3644:ASP:HA | 1:G:3647:LYS:HD2 | 2.02 | 0.42 |
| 1:G:3775:GLN:NE2 | 1:G:3847:LEU:O | 2.53 | 0.42 |
| 1:G:3861:THR:HG23 | 1:G:3863:THR:HG23 | 2.00 | 0.42 |
| 1:A:245:LEU:HD11 | 1:A:260:VAL:CG1 | 2.49 | 0.42 |
| 1:A:652:VAL:HG11 | 1:A:692:HIS:CD2 | 2.55 | 0.42 |
| 1:A:996:VAL:CG1 | 1:A:1054:VAL:HG11 | 2.49 | 0.42 |
| 1:A:3668:LEU:HD21 | 1:A:3692:TYR:CD1 | 2.54 | 0.42 |
| 1:A:4923:PHE:CZ | 1:A:4942:VAL:HG11 | 2.55 | 0.42 |
| 1:C:4043:ILE:HD12 | 1:C:4078:THR:HG21 | 2.01 | 0.42 |
| 1:C:4204:ALA:HA | 1:C:4207:ILE:HG22 | 2.01 | 0.42 |
| 1:E:194:LEU:HD11 | 1:E:201:LEU:HD13 | 2.00 | 0.42 |
| 1:E:3775:GLN:NE2 | 1:E:3847:LEU:O | 2.52 | 0.42 |
| 1:G:1932:PHE:CD2 | 1:G:2025:ILE:HD11 | 2.54 | 0.42 |
| 1:G:3740:MET:O | 1:G:3744:THR:HG22 | 2.19 | 0.42 |
| 1:A:659:ILE:HG23 | 1:A:825:ALA:HB1 | 2.02 | 0.42 |
| 1:A:792:VAL:HG13 | 1:A:792:VAL:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4191:VAL:HG11 | 1:A:4951:TRP:CH2 | 2.55 | 0.42 |
| 1:E:544:ASN:HB2 | 1:E:547:ASN:HD22 | 1.84 | 0.42 |
| 1:E:689:GLU:O | 1:E:691:THR:HG22 | 2.19 | 0.42 |
| 1:E:4639:THR:HG22 | 1:E:4641:SER:H | 1.84 | 0.42 |
| 1:G:625:VAL:HG13 | 1:G:2132:VAL:HG23 | 2.01 | 0.42 |
| 1:G:875:PRO:HD2 | 1:G:878:LEU:HD12 | 2.00 | 0.42 |
| 1:A:629:GLN:CD | 1:A:1666:ALA:HB1 | 2.40 | 0.42 |
| 1:A:2719:GLU:OE1 | 1:A:2719:GLU:O | 2.38 | 0.42 |
| 1:A:3950:HIS:N | 1:A:4010:ASN:HD21 | 2.17 | 0.42 |
| 1:E:559:ILE:HG12 | 1:E:575:LEU:HD11 | 2.02 | 0.42 |
| 1:E:2106:TYR:CG | 1:E:2107:THR:N | 2.88 | 0.42 |
| 1:E:2493:PHE:O | 1:E:2497:LEU:HG | 2.19 | 0.42 |
| 1:E:3883:GLN:HE22 | 1:E:3947:GLY:HA3 | 1.84 | 0.42 |
| 1:E:3956:GLN:NE2 | 1:E:4014:ILE:HG23 | 2.35 | 0.42 |
| 1:E:3992:VAL:HG13 | 1:E:4964:TYR:CE2 | 2.55 | 0.42 |
| 1:G:115:TYR:HE1 | 1:G:181:LEU:HD22 | 1.85 | 0.42 |
| 1:G:555:LEU:HD13 | 1:G:578:VAL:HG11 | 2.02 | 0.42 |
| 1:G:1910:LEU:HD12 | 1:G:2062:ILE:HD12 | 2.01 | 0.42 |
| 1:G:2250:ASN:HB2 | 1:G:2253:LEU:HB2 | 2.01 | 0.42 |
| 1:G:2420:ILE:O | 1:G:2424:LEU:HD13 | 2.19 | 0.42 |
| 1:A:874:LEU:HD22 | 1:A:882:ARG:NH2 | 2.34 | 0.42 |
| 1:A:1819:VAL:HG21 | 1:A:1901:PRO:HB2 | 2.02 | 0.42 |
| 1:A:1911:GLN:HB2 | 1:A:2087:LEU:HD11 | 2.01 | 0.42 |
| 1:A:3862:GLN:HE21 | 1:A:3865:ASN:ND2 | 2.15 | 0.42 |
| 1:C:1847:GLU:HB2 | 1:C:1848:PRO:HD3 | 2.02 | 0.42 |
| 1:C:4576:ILE:HD13 | 1:C:4576:ILE:O | 2.20 | 0.42 |
| 1:E:119:ILE:HD13 | 1:E:162:ILE:HD11 | 2.02 | 0.42 |
| 1:G:718:VAL:HG22 | 1:G:791:VAL:HG13 | 2.00 | 0.42 |
| 1:G:2123:LEU:HD12 | 1:G:2127:ARG:NH1 | 2.35 | 0.42 |
| 1:A:2513:MET:O | 1:A:2517:LEU:HD13 | 2.20 | 0.42 |
| 1:A:3756:VAL:HG13 | 1:A:3836:PHE:CE1 | 2.54 | 0.42 |
| 1:E:2420:ILE:O | 1:E:2424:LEU:HD13 | 2.20 | 0.42 |
| 1:G:1819:VAL:HG21 | 1:G:1901:PRO:HB2 | 2.01 | 0.42 |
| 1:G:2106:TYR:CG | 1:G:2107:THR:N | 2.88 | 0.42 |
| 1:A:766:ILE:HB | 1:A:779:PHE:HB2 | 2.02 | 0.41 |
| 1:C:646:THR:HG23 | 1:C:1684:GLN:NE2 | 2.35 | 0.41 |
| 1:C:4147:GLU:OE1 | 1:C:4938:GLN:NE2 | 2.53 | 0.41 |
| 1:E:1795:LEU:HD11 | 1:E:1825:PHE:HB2 | 2.01 | 0.41 |
| 1:E:3907:PHE:HE2 | 1:E:3972:LEU:HD21 | 1.85 | 0.41 |
| 1:A:207:PHE:CE2 | 1:C:2326:ILE:HD12 | 2.54 | 0.41 |
| 1:A:659:ILE:HD12 | 1:A:659:ILE:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:3742:LEU:HD11 | 1:E:3778:MET:HG2 | 2.02 | 0.41 |
| 1:E:3911:ILE:HD11 | 1:E:3975:LEU:HD22 | 2.02 | 0.41 |
| 1:A:119:ILE:HG21 | 1:A:162:ILE:HD11 | 2.00 | 0.41 |
| 1:A:1096:VAL:HG13 | 1:A:1101:TRP:CD1 | 2.55 | 0.41 |
| 1:A:3952:PHE:HZ | 1:A:3975:LEU:HD23 | 1.84 | 0.41 |
| 1:C:1629:SER:HA | 1:C:1640:ASP:HA | 2.02 | 0.41 |
| 1:C:1707:ILE:HD11 | 1:C:1824:LEU:HA | 2.02 | 0.41 |
| 1:C:1828:LEU:HD23 | 1:C:1834:PHE:HZ | 1.84 | 0.41 |
| 1:E:4833:ILE:HD13 | 1:E:4845:ARG:NH1 | 2.35 | 0.41 |
| 1:G:1761:MET:HB2 | 1:G:1776:TYR:CD2 | 2.55 | 0.41 |
| 1:G:2354:ILE:HG23 | 1:G:2386:GLY:HA3 | 2.02 | 0.41 |
| 1:G:4097:PHE:O | 1:G:4101:VAL:HG23 | 2.20 | 0.41 |
| 1:A:28:ILE:CG1 | 1:A:201:LEU:HD11 | 2.50 | 0.41 |
| 1:A:49:LEU:HD11 | 1:A:194:LEU:HD21 | 2.03 | 0.41 |
| 1:A:657:PRO:CB | 1:A:804:LEU:HD11 | 2.50 | 0.41 |
| 1:A:3966:ILE:O | 1:A:3969:LEU:N | 2.54 | 0.41 |
| 1:C:679:VAL:HA | 1:C:800:VAL:HG12 | 2.02 | 0.41 |
| 1:C:1604:LEU:HD21 | 1:C:1627:PHE:HE1 | 1.86 | 0.41 |
| 1:E:1703:TYR:HB2 | 1:E:1820:PRO:HB3 | 2.02 | 0.41 |
| 1:E:1819:VAL:HG21 | 1:E:1901:PRO:HB2 | 2.02 | 0.41 |
| 1:E:3862:GLN:HG2 | 1:E:3865:ASN:HD22 | 1.85 | 0.41 |
| 1:G:1847:GLU:HB2 | 1:G:1848:PRO:HD3 | 2.03 | 0.41 |
| 1:A:476:GLN:HA | 1:A:476:GLN:HE21 | 1.84 | 0.41 |
| 1:A:4639:THR:HG22 | 1:A:4641:SER:H | 1.85 | 0.41 |
| 1:C:594:ILE:HD12 | 1:C:631:LEU:HD22 | 2.02 | 0.41 |
| 1:E:306:LEU:HD11 | 1:E:314:LEU:HD22 | 2.03 | 0.41 |
| 1:E:4049:PHE:HE2 | 1:E:4067:LEU:HD13 | 1.85 | 0.41 |
| 1:G:1685:LEU:HD22 | 1:G:1709:ILE:HD11 | 2.01 | 0.41 |
| 1:G:3862:GLN:HE21 | 1:G:3865:ASN:ND2 | 2.14 | 0.41 |
| 1:A:425:LEU:HD13 | 1:A:452:VAL:HG22 | 2.03 | 0.41 |
| 1:A:579:LEU:HD22 | 1:A:586:LEU:HD23 | 2.02 | 0.41 |
| 1:A:1629:SER:HA | 1:A:1640:ASP:HA | 2.03 | 0.41 |
| 1:A:4869:ILE:HG21 | 1:C:4869:ILE:HG23 | 2.01 | 0.41 |
| 2:B:66:MET:SD | 2:B:74:LEU:HD21 | 2.60 | 0.41 |
| 1:C:648:LEU:HD23 | 1:C:1684:GLN:HA | 2.02 | 0.41 |
| 1:C:3693:ALA:HB3 | 1:C:3758:ALA:HB1 | 2.02 | 0.41 |
| 1:E:4012:GLU:HG3 | 1:E:4122:LEU:HD21 | 2.03 | 0.41 |
| 1:E:4823:VAL:HG23 | 1:E:4824:ARG:HG3 | 2.02 | 0.41 |
| 1:G:4135:GLY:HA3 | 1:G:4151:PHE:CZ | 2.55 | 0.41 |
| 1:A:4097:PHE:O | 1:A:4101:VAL:HG23 | 2.21 | 0.41 |
| 1:A:4135:GLY:HA3 | 1:A:4151:PHE:CZ | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:21:VAL:CG1 | 1:C:217:ILE:HD11 | 2.51 | 0.41 |
| 1:C:165:ALA:HB3 | 1:C:211:LEU:HD21 | 2.02 | 0.41 |
| 1:C:2081:VAL:HG23 | 1:C:3671:LEU:HD12 | 2.03 | 0.41 |
| 1:E:42:PHE:CG | 1:E:418:VAL:HG22 | 2.56 | 0.41 |
| 1:E:996:VAL:CG1 | 1:E:1054:VAL:HG11 | 2.51 | 0.41 |
| 1:G:1795:LEU:HD11 | 1:G:1825:PHE:CD1 | 2.55 | 0.41 |
| 1:G:2861:LEU:HD22 | 1:G:2872:LEU:CD1 | 2.51 | 0.41 |
| 1:G:3908:SER:HA | 1:G:3911:ILE:HG22 | 2.01 | 0.41 |
| 1:A:4781:TYR:HA | 1:A:4784:THR:HG22 | 2.02 | 0.41 |
| 1:C:572:LEU:HD13 | 1:C:609:LYS:CB | 2.51 | 0.41 |
| 1:E:1730:THR:O | 1:E:1733:THR:OG1 | 2.37 | 0.41 |
| 1:E:1772:ASN:N | 1:E:1772:ASN:HD22 | 2.19 | 0.41 |
| 1:A:555:LEU:HD13 | 1:A:578:VAL:HG11 | 2.03 | 0.41 |
| 1:A:679:VAL:HA | 1:A:800:VAL:HG12 | 2.02 | 0.41 |
| 1:A:933:LEU:O | 1:A:937:LEU:HB2 | 2.21 | 0.41 |
| 1:A:3841:PHE:HB3 | 1:A:3920:THR:HG21 | 2.02 | 0.41 |
| 1:C:888:ASN:ND2 | 1:C:1056:THR:HG21 | 2.35 | 0.41 |
| 1:C:1749:PRO:HB3 | 1:C:2058:LEU:HD23 | 2.02 | 0.41 |
| 1:C:1795:LEU:HD11 | 1:C:1825:PHE:CG | 2.55 | 0.41 |
| 1:C:3950:HIS:N | 1:C:4010:ASN:HD21 | 2.19 | 0.41 |
| 1:E:598:ILE:HG23 | 1:E:642:LEU:HD22 | 2.02 | 0.41 |
| 1:E:3778:MET:CE | 1:E:3847:LEU:HD22 | 2.51 | 0.41 |
| 1:E:4893:CYS:HG | 1:E:4915:HIS:HE2 | 1.68 | 0.41 |
| 2:F:55:VAL:HG21 | 2:F:59:PHE:HD1 | 1.86 | 0.41 |
| 1:G:657:PRO:HG2 | 1:G:790:PRO:HG2 | 2.02 | 0.41 |
| 1:G:792:VAL:O | 1:G:792:VAL:HG13 | 2.21 | 0.41 |
| 1:G:1751:ILE:HD13 | 1:G:1920:HIS:CE1 | 2.56 | 0.41 |
| 1:G:3956:GLN:HE21 | 1:G:4014:ILE:HG23 | 1.84 | 0.41 |
| 1:G:4893:CYS:HG | 1:G:4915:HIS:HE2 | 1.68 | 0.41 |
| 1:G:4911:THR:O | 1:G:4916:ASN:N | 2.50 | 0.41 |
| 1:A:1910:LEU:HG | 1:A:2062:ILE:HD12 | 2.02 | 0.41 |
| 1:C:207:PHE:CZ | 1:E:2423:ILE:HD12 | 2.56 | 0.41 |
| 1:C:570:GLY:O | 1:C:574:VAL:HG23 | 2.21 | 0.41 |
| 1:C:828:PRO:HG2 | 1:C:1037:LEU:HB3 | 2.03 | 0.41 |
| 1:C:4015:LEU:HD13 | 1:C:4123:ALA:HA | 2.03 | 0.41 |
| 1:E:2029:LEU:HD21 | 1:E:3629:TRP:CE3 | 2.56 | 0.41 |
| 1:E:4120:LEU:HA | 1:E:4123:ALA:HB3 | 2.03 | 0.41 |
| 1:E:4611:LYS:HB3 | 1:E:4617:LEU:HD23 | 2.03 | 0.41 |
| 1:E:4911:THR:O | 1:E:4916:ASN:N | 2.51 | 0.41 |
| 1:G:1831:MET:HE1 | 1:G:1833:ILE:HD13 | 2.02 | 0.41 |
| 1:G:3896:LYS:O | 1:G:3898:VAL:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3992:VAL:HG13 | 1:A:4964:TYR:CZ | 2.56 | 0.40 |
| 1:C:496:ASN:HA | 1:C:499:LEU:HD12 | 2.02 | 0.40 |
| 1:C:1828:LEU:HD23 | 1:C:1834:PHE:CZ | 2.56 | 0.40 |
| 1:C:2103:PRO:O | 1:C:2164:ALA:HB1 | 2.20 | 0.40 |
| 1:C:3875:THR:HG21 | 1:C:3924:TYR:HE2 | 1.86 | 0.40 |
| 1:C:4148:ARG:NH2 | 1:C:4914:GLU:OE2 | 2.54 | 0.40 |
| 1:C:4785:VAL:HG21 | 1:E:4742:ALA:CB | 2.50 | 0.40 |
| 1:C:4923:PHE:HZ | 1:C:4942:VAL:HG11 | 1.86 | 0.40 |
| 1:E:646:THR:HG23 | 1:E:1684:GLN:NE2 | 2.36 | 0.40 |
| 1:E:881:ILE:HD11 | 1:E:1060:TYR:CE2 | 2.56 | 0.40 |
| 1:E:2894:LEU:CD1 | 1:E:2897:LEU:HD12 | 2.52 | 0.40 |
| 1:G:463:PHE:HB3 | 1:G:539:ALA:HB1 | 2.03 | 0.40 |
| 1:G:465:PRO:HA | 1:G:466:PRO:HD3 | 1.96 | 0.40 |
| 1:G:1686:LEU:HD22 | 1:G:1790:LYS:HE3 | 2.02 | 0.40 |
| 1:A:207:PHE:CD2 | 1:C:2326:ILE:HD12 | 2.56 | 0.40 |
| 1:C:1686:LEU:HD22 | 1:C:1790:LYS:HE3 | 2.04 | 0.40 |
| 1:C:2159:PRO:CB | 1:C:2206:ILE:HD12 | 2.49 | 0.40 |
| 1:C:2221:LEU:HD21 | 1:C:2242:VAL:HB | 2.03 | 0.40 |
| 1:C:3966:ILE:O | 1:C:3969:LEU:N | 2.54 | 0.40 |
| 2:D:75:THR:HG23 | 2:D:98:ILE:CD1 | 2.51 | 0.40 |
| 1:E:3841:PHE:HB3 | 1:E:3920:THR:HG21 | 2.04 | 0.40 |
| 1:G:447:LEU:HD21 | 1:G:522:ALA:HB2 | 2.03 | 0.40 |
| 1:G:572:LEU:HD13 | 1:G:609:LYS:CB | 2.51 | 0.40 |
| 1:G:1629:SER:HA | 1:G:1640:ASP:HA | 2.03 | 0.40 |
| 1:G:1828:LEU:HD23 | 1:G:1834:PHE:HZ | 1.86 | 0.40 |
| 1:C:572:LEU:HD22 | 1:C:609:LYS:HB3 | 2.04 | 0.40 |
| 1:E:1828:LEU:HD23 | 1:E:1834:PHE:HZ | 1.87 | 0.40 |
| 1:A:465:PRO:HA | 1:A:466:PRO:HD3 | 1.97 | 0.40 |
| 1:A:1268:ILE:O | 1:A:1268:ILE:HG23 | 2.21 | 0.40 |
| 1:A:3804:LEU:HD13 | 1:A:3910:ALA:HB2 | 2.03 | 0.40 |
| 1:C:611:LEU:HB2 | 1:C:1659:ARG:HG3 | 2.02 | 0.40 |
| 1:C:1686:LEU:HD22 | 1:C:1790:LYS:HD2 | 2.02 | 0.40 |
| 1:C:2713:ILE:HD13 | 1:C:2714:ILE:N | 2.36 | 0.40 |
| 1:C:2894:LEU:HD11 | 1:C:2904:VAL:HG21 | 2.04 | 0.40 |
| 1:C:3908:SER:HA | 1:C:3911:ILE:HG22 | 2.02 | 0.40 |
| 1:C:4097:PHE:O | 1:C:4101:VAL:HG23 | 2.22 | 0.40 |
| 1:C:4165:GLN:HG3 | 1:C:4501:TYR:CZ | 2.57 | 0.40 |
| 1:C:4794:PHE:CB | 1:C:4833:ILE:HD11 | 2.52 | 0.40 |
| 1:E:763:ALA:HB3 | 1:E:765:SER:H | 1.86 | 0.40 |
| 2:H:82:TYR:CD2 | 2:H:91:ILE:HG21 | 2.56 | 0.40 |
| 1:A:1782:PHE:CZ | 1:A:1787:LEU:HD22 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2241:ASP:OD1 | 1:A:2242:VAL:N | 2.55 | 0.40 |
| 1:A:2713:ILE:HD13 | 1:A:2714:ILE:N | 2.36 | 0.40 |
| 2:B:4:ILE:HD12 | 2:B:74:LEU:HD22 | 2.03 | 0.40 |
| 1:C:4843:ILE:O | 1:C:4846:ILE:HG22 | 2.22 | 0.40 |
| 2:D:30:LEU:O | 2:D:32:ASN:N | 2.55 | 0.40 |
| 1:E:217:ILE:HG22 | 1:E:286:GLY:HA3 | 2.03 | 0.40 |
| 1:E:737:ILE:HD13 | 1:E:1535:PRO:HG3 | 2.04 | 0.40 |
| 1:E:1706:LEU:O | 1:E:1706:LEU:HD13 | 2.22 | 0.40 |
| 1:E:4651:VAL:O | 1:E:4655:VAL:HG23 | 2.22 | 0.40 |
| 1:G:4573:THR:HA | 1:G:4576:ILE:HG22 | 2.03 | 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 | A | 3065/4387 (70%) | 2784 (91%) | 217 (7%) | 64 (2%) | 7 36 |
| 1 | C | 3065/4387 (70%) | 2773 (90%) | 236 (8%) | 56 (2%) | 8 40 |
| 1 | E | 3065/4387 (70%) | 2765 (90%) | 238 (8%) | 62 (2%) | 7 38 |
| 1 | G | 3065/4387 (70%) | 2789 (91%) | 211 (7%) | 65 (2%) | 7 36 |
| 2 | B | 105/158 (66%) | 97 (92%) | 7 (7%) | 1 (1%) | 15 55 |
| 2 | D | 105/158 (66%) | 96 (91%) | 8 (8%) | 1 (1%) | 15 55 |
| 2 | F | 105/158 (66%) | 97 (92%) | 6 (6%) | 2 (2%) | 8 38 |
| 2 | H | 105/158 (66%) | 97 (92%) | 8 (8%) | 0 | 100 100 |
| All | All | 12680/18180 (70%) | 11498 (91%) | 931 (7%) | 251 (2%) | 11 38 |

All (251) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 472 | HIS |
| 1 | A | 1476 | VAL |
| 1 | A | 1549 | SER |
| 1 | A | 1779 | SER |
| 1 | A | 3897 | ASP |
| 1 | A | 3992 | VAL |
| 1 | A | 4916 | ASN |
| 1 | A | 4917 | LEU |
| 1 | C | 472 | HIS |
| 1 | C | 1476 | VAL |
| 1 | C | 1549 | SER |
| 1 | C | 1779 | SER |
| 1 | C | 3897 | ASP |
| 1 | C | 4916 | ASN |
| 2 | D | 31 | GLN |
| 1 | E | 837 | SER |
| 1 | E | 855 | VAL |
| 1 | E | 1549 | SER |
| 1 | E | 1590 | PHE |
| 1 | E | 1779 | SER |
| 1 | E | 3897 | ASP |
| 1 | E | 3992 | VAL |
| 1 | E | 4916 | ASN |
| 1 | E | 4917 | LEU |
| 1 | E | 4959 | CYS |
| 1 | G | 472 | HIS |
| 1 | G | 837 | SER |
| 1 | G | 855 | VAL |
| 1 | G | 1549 | SER |
| 1 | G | 1639 | VAL |
| 1 | G | 1779 | SER |
| 1 | G | 3897 | ASP |
| 1 | G | 4916 | ASN |
| 1 | G | 4917 | LEU |
| 1 | G | 4959 | CYS |
| 1 | A | 250 | GLY |
| 1 | A | 838 | ARG |
| 1 | A | 855 | VAL |
| 1 | A | 901 | GLY |
| 1 | A | 1191 | ALA |
| 1 | A | 1535 | PRO |
| 1 | A | 1639 | VAL |
| 1 | A | 1737 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4751 | GLY |
| 1 | A | 4959 | CYS |
| 1 | C | 855 | VAL |
| 1 | C | 901 | GLY |
| 1 | C | 906 | PRO |
| 1 | C | 1267 | HIS |
| 1 | C | 1535 | PRO |
| 1 | C | 1639 | VAL |
| 1 | C | 1681 | ASP |
| 1 | C | 1737 | THR |
| 1 | C | 1755 | THR |
| 1 | C | 2795 | GLU |
| 1 | C | 2797 | ASP |
| 1 | C | 3992 | VAL |
| 1 | C | 4917 | LEU |
| 1 | C | 4959 | CYS |
| 1 | E | 350 | GLY |
| 1 | E | 836 | HIS |
| 1 | E | 838 | ARG |
| 1 | E | 1191 | ALA |
| 1 | E | 1476 | VAL |
| 1 | E | 1667 | LEU |
| 1 | E | 1681 | ASP |
| 1 | E | 1737 | THR |
| 1 | E | 1755 | THR |
| 1 | E | 4038 | PRO |
| 1 | G | 188 | SER |
| 1 | G | 350 | GLY |
| 1 | G | 716 | ASN |
| 1 | G | 838 | ARG |
| 1 | G | 901 | GLY |
| 1 | G | 1191 | ALA |
| 1 | G | 1218 | GLY |
| 1 | G | 1456 | GLY |
| 1 | G | 1476 | VAL |
| 1 | G | 1535 | PRO |
| 1 | G | 1681 | ASP |
| 1 | G | 1755 | THR |
| 1 | G | 3992 | VAL |
| 1 | A | 359 | SER |
| 1 | A | 716 | ASN |
| 1 | A | 1667 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1681 | ASP |
| 1 | A | 1755 | THR |
| 1 | A | 2106 | TYR |
| 1 | A | 2864 | LYS |
| 1 | A | 4038 | PRO |
| 1 | A | 4112 | ASN |
| 1 | C | 224 | ALA |
| 1 | C | 838 | ARG |
| 1 | C | 1191 | ALA |
| 1 | C | 1590 | PHE |
| 1 | C | 1667 | LEU |
| 1 | C | 2106 | TYR |
| 1 | C | 4112 | ASN |
| 1 | C | 4957 | GLY |
| 1 | E | 716 | ASN |
| 1 | E | 901 | GLY |
| 1 | E | 1639 | VAL |
| 1 | E | 4112 | ASN |
| 2 | F | 31 | GLN |
| 1 | G | 224 | ALA |
| 1 | G | 906 | PRO |
| 1 | G | 1219 | LYS |
| 1 | G | 1231 | GLY |
| 1 | G | 1590 | PHE |
| 1 | G | 1667 | LEU |
| 1 | G | 2106 | TYR |
| 1 | G | 2797 | ASP |
| 1 | G | 4112 | ASN |
| 1 | A | 224 | ALA |
| 1 | A | 641 | ASP |
| 1 | A | 642 | LEU |
| 1 | A | 669 | GLN |
| 1 | A | 837 | SER |
| 1 | A | 1218 | GLY |
| 1 | A | 1472 | GLU |
| 1 | A | 1725 | PHE |
| 1 | A | 1758 | ARG |
| 1 | A | 1834 | PHE |
| 1 | A | 2074 | VAL |
| 1 | A | 2077 | ASP |
| 1 | A | 4056 | HIS |
| 1 | C | 350 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 620 | CYS |
| 1 | C | 847 | THR |
| 1 | C | 1231 | GLY |
| 1 | C | 1604 | LEU |
| 1 | C | 1758 | ARG |
| 1 | C | 2077 | ASP |
| 1 | C | 2710 | SER |
| 1 | E | 63 | SER |
| 1 | E | 224 | ALA |
| 1 | E | 472 | HIS |
| 1 | E | 1210 | ALA |
| 1 | E | 1535 | PRO |
| 1 | E | 1536 | SER |
| 1 | E | 1758 | ARG |
| 1 | E | 1770 | SER |
| 1 | E | 2074 | VAL |
| 1 | E | 2077 | ASP |
| 1 | E | 2106 | TYR |
| 1 | E | 2797 | ASP |
| 1 | E | 3686 | ASP |
| 2 | F | 32 | ASN |
| 1 | G | 467 | ASP |
| 1 | G | 642 | LEU |
| 1 | G | 836 | HIS |
| 1 | G | 847 | THR |
| 1 | G | 1725 | PHE |
| 1 | G | 1737 | THR |
| 1 | G | 2074 | VAL |
| 1 | G | 2077 | ASP |
| 1 | G | 2710 | SER |
| 1 | G | 3681 | CYS |
| 1 | G | 4056 | HIS |
| 1 | G | 4802 | ASP |
| 1 | A | 620 | CYS |
| 1 | A | 839 | GLU |
| 1 | A | 847 | THR |
| 1 | A | 871 | GLN |
| 1 | A | 1142 | ALA |
| 1 | A | 1267 | HIS |
| 1 | A | 2311 | GLY |
| 1 | A | 4164 | PRO |
| 1 | A | 4622 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 641 | ASP |
| 1 | C | 642 | LEU |
| 1 | C | 837 | SER |
| 1 | C | 839 | GLU |
| 1 | C | 1210 | ALA |
| 1 | C | 1299 | ILE |
| 1 | C | 2074 | VAL |
| 1 | C | 3991 | VAL |
| 1 | C | 4622 | GLN |
| 1 | E | 685 | PHE |
| 1 | E | 829 | LYS |
| 1 | E | 839 | GLU |
| 1 | E | 1142 | ALA |
| 1 | E | 1231 | GLY |
| 1 | E | 1547 | ALA |
| 1 | E | 1604 | LEU |
| 1 | E | 3788 | VAL |
| 1 | E | 4056 | HIS |
| 1 | E | 4164 | PRO |
| 1 | E | 4181 | GLY |
| 1 | E | 4743 | ALA |
| 1 | G | 341 | GLY |
| 1 | G | 620 | CYS |
| 1 | G | 839 | GLU |
| 1 | G | 1299 | ILE |
| 1 | G | 1472 | GLU |
| 1 | G | 1758 | ARG |
| 1 | G | 1770 | SER |
| 1 | G | 1777 | GLN |
| 1 | G | 1834 | PHE |
| 1 | G | 4622 | GLN |
| 1 | G | 4751 | GLY |
| 1 | G | 4800 | ASP |
| 1 | A | 1299 | ILE |
| 1 | A | 4800 | ASP |
| 2 | B | 31 | GLN |
| 1 | C | 341 | GLY |
| 1 | C | 467 | ASP |
| 1 | C | 670 | TYR |
| 1 | C | 1194 | ASP |
| 1 | C | 1777 | GLN |
| 1 | C | 1810 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 2311 | GLY |
| 1 | E | 777 | GLY |
| 1 | E | 847 | THR |
| 1 | E | 1267 | HIS |
| 1 | E | 1299 | ILE |
| 1 | E | 2311 | GLY |
| 1 | E | 3681 | CYS |
| 1 | E | 4622 | GLN |
| 1 | G | 1810 | VAL |
| 1 | A | 341 | GLY |
| 1 | A | 1231 | GLY |
| 1 | A | 1810 | VAL |
| 1 | E | 341 | GLY |
| 1 | E | 3991 | VAL |
| 1 | G | 2866 | GLY |
| 1 | A | 906 | PRO |
| 1 | A | 3991 | VAL |
| 1 | A | 4623 | PRO |
| 1 | E | 1810 | VAL |
| 1 | G | 3991 | VAL |
| 1 | A | 729 | GLY |
| 1 | A | 1198 | GLY |
| 1 | A | 4957 | GLY |
| 1 | C | 1218 | GLY |
| 1 | C | 4623 | PRO |
| 1 | E | 4623 | PRO |
| 1 | G | 4164 | PRO |
| 1 | A | 684 | PRO |
| 1 | C | 3788 | VAL |
| 1 | E | 4830 | GLY |
| 1 | G | 834 | VAL |
| 1 | G | 1533 | VAL |
| 1 | G | 4895 | ILE |
| 1 | A | 2865 | GLY |
| 1 | A | 3788 | VAL |
| 1 | G | 2311 | GLY |
| 1 | G | 1809 | PRO |
| 1 | C | 1809 | PRO |
| 1 | A | 1809 | PRO |
| 1 | E | 1809 | PRO |

### 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 | A | 2774/3480 (80%) | 2648 (96%) | 126 (4%) | 27 | 52 |
| 1 | C | 2774/3480 (80%) | 2639 (95%) | 135 (5%) | 25 | 50 |
| 1 | E | 2774/3480 (80%) | 2624 (95%) | 150 (5%) | 22 | 47 |
| 1 | G | 2774/3480 (80%) | 2642 (95%) | 132 (5%) | 25 | 51 |
| 2 | B | 88/131 (67%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 2 | D | 88/131 (67%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 2 | F | 88/131 (67%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 2 | H | 88/131 (67%) | 87 (99%) | 1 (1%) | 73 | 84 |
| All | All | 11448/14444 (79%) | 10901 (95%) | 547 (5%) | 29 | 51 |

All (547) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 15 | ARG |
| 1 | A | 54 | ASN |
| 1 | A | 317 | MET |
| 1 | A | 336 | GLU |
| 1 | A | 342 | VAL |
| 1 | A | 392 | ILE |
| 1 | A | 424 | PHE |
| 1 | A | 441 | LYS |
| 1 | A | 462 | TYR |
| 1 | A | 476 | GLN |
| 1 | A | 542 | ARG |
| 1 | A | 551 | PHE |
| 1 | A | 559 | ILE |
| 1 | A | 563 | GLU |
| 1 | A | 572 | LEU |
| 1 | A | 604 | HIS |
| 1 | A | 608 | HIS |
| 1 | A | 609 | LYS |
| 1 | A | 643 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 669 | GLN |
| 1 | A | 725 | TYR |
| 1 | A | 844 | ARG |
| 1 | A | 872 | ILE |
| 1 | A | 888 | ASN |
| 1 | A | 908 | ARG |
| 1 | A | 948 | CYS |
| 1 | A | 1031 | ARG |
| 1 | A | 1137 | PHE |
| 1 | A | 1193 | LYS |
| 1 | A | 1204 | VAL |
| 1 | A | 1287 | GLN |
| 1 | A | 1298 | ASP |
| 1 | A | 1302 | TYR |
| 1 | A | 1308 | ILE |
| 1 | A | 1447 | THR |
| 1 | A | 1450 | PHE |
| 1 | A | 1459 | LEU |
| 1 | A | 1533 | VAL |
| 1 | A | 1538 | LYS |
| 1 | A | 1553 | PHE |
| 1 | A | 1554 | GLN |
| 1 | A | 1595 | LEU |
| 1 | A | 1630 | LEU |
| 1 | A | 1657 | THR |
| 1 | A | 1671 | ARG |
| 1 | A | 1689 | ILE |
| 1 | A | 1697 | LEU |
| 1 | A | 1700 | THR |
| 1 | A | 1716 | THR |
| 1 | A | 1720 | MET |
| 1 | A | 1721 | MET |
| 1 | A | 1763 | PHE |
| 1 | A | 1771 | ILE |
| 1 | A | 1776 | TYR |
| 1 | A | 1777 | GLN |
| 1 | A | 1778 | TYR |
| 1 | A | 1779 | SER |
| 1 | A | 1794 | MET |
| 1 | A | 1804 | LEU |
| 1 | A | 1833 | ILE |
| 1 | A | 1897 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1898 | LEU |
| 1 | A | 1900 | GLU |
| 1 | A | 1910 | LEU |
| 1 | A | 1935 | LYS |
| 1 | A | 2023 | LEU |
| 1 | A | 2028 | ARG |
| 1 | A | 2066 | MET |
| 1 | A | 2126 | ILE |
| 1 | A | 2129 | LEU |
| 1 | A | 2179 | LEU |
| 1 | A | 2192 | MET |
| 1 | A | 2220 | TYR |
| 1 | A | 2354 | ILE |
| 1 | A | 2423 | ILE |
| 1 | A | 2466 | LYS |
| 1 | A | 2473 | LEU |
| 1 | A | 2474 | ASP |
| 1 | A | 2517 | LEU |
| 1 | A | 2713 | ILE |
| 1 | A | 2717 | LYS |
| 1 | A | 2723 | ASN |
| 1 | A | 2746 | GLU |
| 1 | A | 2747 | ILE |
| 1 | A | 2750 | ASP |
| 1 | A | 2762 | LYS |
| 1 | A | 2770 | GLU |
| 1 | A | 2843 | GLU |
| 1 | A | 2858 | LYS |
| 1 | A | 3675 | THR |
| 1 | A | 3690 | MET |
| 1 | A | 3728 | GLN |
| 1 | A | 3797 | LEU |
| 1 | A | 3844 | LEU |
| 1 | A | 3860 | ARG |
| 1 | A | 3911 | ILE |
| 1 | A | 3912 | GLN |
| 1 | A | 3929 | CYS |
| 1 | A | 3956 | GLN |
| 1 | A | 3962 | ASP |
| 1 | A | 3969 | LEU |
| 1 | A | 3970 | LYS |
| 1 | A | 3992 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4065 | GLU |
| 1 | A | 4078 | THR |
| 1 | A | 4154 | SER |
| 1 | A | 4170 | LYS |
| 1 | A | 4172 | GLN |
| 1 | A | 4186 | LYS |
| 1 | A | 4188 | GLU |
| 1 | A | 4192 | ASN |
| 1 | A | 4491 | LYS |
| 1 | A | 4573 | THR |
| 1 | A | 4576 | ILE |
| 1 | A | 4584 | ILE |
| 1 | A | 4622 | GLN |
| 1 | A | 4637 | ILE |
| 1 | A | 4670 | GLU |
| 1 | A | 4730 | MET |
| 1 | A | 4752 | PHE |
| 1 | A | 4807 | LYS |
| 1 | A | 4855 | PHE |
| 1 | A | 4860 | LEU |
| 1 | A | 4885 | ASP |
| 1 | A | 4925 | MET |
| 1 | A | 4927 | LEU |
| 2 | B | 34 | LYS |
| 1 | C | 15 | ARG |
| 1 | C | 54 | ASN |
| 1 | C | 180 | ASP |
| 1 | C | 190 | ARG |
| 1 | C | 317 | MET |
| 1 | C | 321 | LYS |
| 1 | C | 336 | GLU |
| 1 | C | 342 | VAL |
| 1 | C | 392 | ILE |
| 1 | C | 441 | LYS |
| 1 | C | 476 | GLN |
| 1 | C | 542 | ARG |
| 1 | C | 563 | GLU |
| 1 | C | 572 | LEU |
| 1 | C | 608 | HIS |
| 1 | C | 609 | LYS |
| 1 | C | 643 | LEU |
| 1 | C | 647 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 669 | GLN |
| 1 | C | 683 | GLU |
| 1 | C | 725 | TYR |
| 1 | C | 835 | GLU |
| 1 | C | 844 | ARG |
| 1 | C | 848 | ARG |
| 1 | C | 872 | ILE |
| 1 | C | 880 | ARG |
| 1 | C | 888 | ASN |
| 1 | C | 908 | ARG |
| 1 | C | 948 | CYS |
| 1 | C | 1028 | ARG |
| 1 | C | 1031 | ARG |
| 1 | C | 1133 | ARG |
| 1 | C | 1193 | LYS |
| 1 | C | 1243 | THR |
| 1 | C | 1287 | GLN |
| 1 | C | 1308 | ILE |
| 1 | C | 1447 | THR |
| 1 | C | 1450 | PHE |
| 1 | C | 1459 | LEU |
| 1 | C | 1533 | VAL |
| 1 | C | 1538 | LYS |
| 1 | C | 1553 | PHE |
| 1 | C | 1637 | ARG |
| 1 | C | 1657 | THR |
| 1 | C | 1660 | LEU |
| 1 | C | 1671 | ARG |
| 1 | C | 1692 | LYS |
| 1 | C | 1697 | LEU |
| 1 | C | 1720 | MET |
| 1 | C | 1761 | MET |
| 1 | C | 1763 | PHE |
| 1 | C | 1771 | ILE |
| 1 | C | 1772 | ASN |
| 1 | C | 1777 | GLN |
| 1 | C | 1778 | TYR |
| 1 | C | 1804 | LEU |
| 1 | C | 1897 | LYS |
| 1 | C | 1908 | LEU |
| 1 | C | 1910 | LEU |
| 1 | C | 1919 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 1925 | ILE |
| 1 | C | 1935 | LYS |
| 1 | C | 2023 | LEU |
| 1 | C | 2028 | ARG |
| 1 | C | 2032 | LEU |
| 1 | C | 2036 | VAL |
| 1 | C | 2077 | ASP |
| 1 | C | 2099 | VAL |
| 1 | C | 2126 | ILE |
| 1 | C | 2129 | LEU |
| 1 | C | 2139 | GLU |
| 1 | C | 2192 | MET |
| 1 | C | 2220 | TYR |
| 1 | C | 2298 | ARG |
| 1 | C | 2354 | ILE |
| 1 | C | 2399 | LEU |
| 1 | C | 2423 | ILE |
| 1 | C | 2517 | LEU |
| 1 | C | 2713 | ILE |
| 1 | C | 2717 | LYS |
| 1 | C | 2723 | ASN |
| 1 | C | 2747 | ILE |
| 1 | C | 2750 | ASP |
| 1 | C | 2762 | LYS |
| 1 | C | 2770 | GLU |
| 1 | C | 2795 | GLU |
| 1 | C | 2858 | LYS |
| 1 | C | 2861 | LEU |
| 1 | C | 3616 | ARG |
| 1 | C | 3662 | VAL |
| 1 | C | 3675 | THR |
| 1 | C | 3690 | MET |
| 1 | C | 3728 | GLN |
| 1 | C | 3797 | LEU |
| 1 | C | 3801 | CYS |
| 1 | C | 3860 | ARG |
| 1 | C | 3866 | ASN |
| 1 | C | 3876 | VAL |
| 1 | C | 3887 | SER |
| 1 | C | 3911 | ILE |
| 1 | C | 3912 | GLN |
| 1 | C | 3926 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 3929 | CYS |
| 1 | C | 3951 | VAL |
| 1 | C | 3962 | ASP |
| 1 | C | 3969 | LEU |
| 1 | C | 3970 | LYS |
| 1 | C | 3979 | MET |
| 1 | C | 3992 | VAL |
| 1 | C | 4032 | THR |
| 1 | C | 4065 | GLU |
| 1 | C | 4117 | GLN |
| 1 | C | 4120 | LEU |
| 1 | C | 4152 | GLU |
| 1 | C | 4167 | LYS |
| 1 | C | 4170 | LYS |
| 1 | C | 4178 | VAL |
| 1 | C | 4186 | LYS |
| 1 | C | 4188 | GLU |
| 1 | C | 4192 | ASN |
| 1 | C | 4200 | GLU |
| 1 | C | 4494 | ASN |
| 1 | C | 4576 | ILE |
| 1 | C | 4584 | ILE |
| 1 | C | 4622 | GLN |
| 1 | C | 4637 | ILE |
| 1 | C | 4730 | MET |
| 1 | C | 4752 | PHE |
| 1 | C | 4807 | LYS |
| 1 | C | 4840 | GLU |
| 1 | C | 4860 | LEU |
| 1 | C | 4865 | GLN |
| 1 | C | 4875 | LEU |
| 1 | C | 4882 | VAL |
| 1 | C | 4885 | ASP |
| 2 | D | 34 | LYS |
| 1 | E | 15 | ARG |
| 1 | E | 18 | ASP |
| 1 | E | 54 | ASN |
| 1 | E | 143 | LEU |
| 1 | E | 179 | ASP |
| 1 | E | 180 | ASP |
| 1 | E | 198 | ASN |
| 1 | E | 313 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 317 | MET |
| 1 | E | 336 | GLU |
| 1 | E | 342 | VAL |
| 1 | E | 374 | TYR |
| 1 | E | 392 | ILE |
| 1 | E | 424 | PHE |
| 1 | E | 441 | LYS |
| 1 | E | 462 | TYR |
| 1 | E | 476 | GLN |
| 1 | E | 542 | ARG |
| 1 | E | 551 | PHE |
| 1 | E | 559 | ILE |
| 1 | E | 562 | LEU |
| 1 | E | 563 | GLU |
| 1 | E | 572 | LEU |
| 1 | E | 589 | ILE |
| 1 | E | 608 | HIS |
| 1 | E | 609 | LYS |
| 1 | E | 643 | LEU |
| 1 | E | 669 | GLN |
| 1 | E | 701 | GLU |
| 1 | E | 725 | TYR |
| 1 | E | 739 | ARG |
| 1 | E | 795 | SER |
| 1 | E | 872 | ILE |
| 1 | E | 888 | ASN |
| 1 | E | 908 | ARG |
| 1 | E | 934 | GLN |
| 1 | E | 1031 | ARG |
| 1 | E | 1193 | LYS |
| 1 | E | 1204 | VAL |
| 1 | E | 1219 | LYS |
| 1 | E | 1232 | LEU |
| 1 | E | 1264 | ASN |
| 1 | E | 1266 | GLU |
| 1 | E | 1287 | GLN |
| 1 | E | 1298 | ASP |
| 1 | E | 1308 | ILE |
| 1 | E | 1447 | THR |
| 1 | E | 1459 | LEU |
| 1 | E | 1482 | ARG |
| 1 | E | 1533 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 1538 | LYS |
| 1 | E | 1553 | PHE |
| 1 | E | 1570 | LEU |
| 1 | E | 1630 | LEU |
| 1 | E | 1657 | THR |
| 1 | E | 1671 | ARG |
| 1 | E | 1677 | CYS |
| 1 | E | 1697 | LEU |
| 1 | E | 1700 | THR |
| 1 | E | 1716 | THR |
| 1 | E | 1720 | MET |
| 1 | E | 1761 | MET |
| 1 | E | 1763 | PHE |
| 1 | E | 1771 | ILE |
| 1 | E | 1772 | ASN |
| 1 | E | 1777 | GLN |
| 1 | E | 1778 | TYR |
| 1 | E | 1779 | SER |
| 1 | E | 1790 | LYS |
| 1 | E | 1794 | MET |
| 1 | E | 1804 | LEU |
| 1 | E | 1897 | LYS |
| 1 | E | 1898 | LEU |
| 1 | E | 1916 | CYS |
| 1 | E | 1921 | ARG |
| 1 | E | 1935 | LYS |
| 1 | E | 2023 | LEU |
| 1 | E | 2028 | ARG |
| 1 | E | 2032 | LEU |
| 1 | E | 2058 | LEU |
| 1 | E | 2061 | LEU |
| 1 | E | 2066 | MET |
| 1 | E | 2081 | VAL |
| 1 | E | 2099 | VAL |
| 1 | E | 2126 | ILE |
| 1 | E | 2129 | LEU |
| 1 | E | 2175 | MET |
| 1 | E | 2179 | LEU |
| 1 | E | 2192 | MET |
| 1 | E | 2220 | TYR |
| 1 | E | 2326 | ILE |
| 1 | E | 2354 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 2399 | LEU |
| 1 | E | 2423 | ILE |
| 1 | E | 2462 | CYS |
| 1 | E | 2511 | THR |
| 1 | E | 2517 | LEU |
| 1 | E | 2713 | ILE |
| 1 | E | 2717 | LYS |
| 1 | E | 2723 | ASN |
| 1 | E | 2746 | GLU |
| 1 | E | 2747 | ILE |
| 1 | E | 2750 | ASP |
| 1 | E | 2762 | LYS |
| 1 | E | 2770 | GLU |
| 1 | E | 2795 | GLU |
| 1 | E | 2858 | LYS |
| 1 | E | 2861 | LEU |
| 1 | E | 2864 | LYS |
| 1 | E | 3671 | LEU |
| 1 | E | 3675 | THR |
| 1 | E | 3690 | MET |
| 1 | E | 3728 | GLN |
| 1 | E | 3801 | CYS |
| 1 | E | 3860 | ARG |
| 1 | E | 3911 | ILE |
| 1 | E | 3912 | GLN |
| 1 | E | 3926 | GLN |
| 1 | E | 3929 | CYS |
| 1 | E | 3951 | VAL |
| 1 | E | 3959 | LEU |
| 1 | E | 3962 | ASP |
| 1 | E | 3969 | LEU |
| 1 | E | 3970 | LYS |
| 1 | E | 3979 | MET |
| 1 | E | 3992 | VAL |
| 1 | E | 4033 | PHE |
| 1 | E | 4065 | GLU |
| 1 | E | 4117 | GLN |
| 1 | E | 4120 | LEU |
| 1 | E | 4170 | LYS |
| 1 | E | 4186 | LYS |
| 1 | E | 4192 | ASN |
| 1 | E | 4491 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 4573 | THR |
| 1 | E | 4576 | ILE |
| 1 | E | 4584 | ILE |
| 1 | E | 4596 | LYS |
| 1 | E | 4620 | THR |
| 1 | E | 4622 | GLN |
| 1 | E | 4637 | ILE |
| 1 | E | 4722 | LEU |
| 1 | E | 4730 | MET |
| 1 | E | 4752 | PHE |
| 1 | E | 4807 | LYS |
| 1 | E | 4840 | GLU |
| 1 | E | 4865 | GLN |
| 1 | E | 4876 | ARG |
| 1 | E | 4885 | ASP |
| 1 | E | 4927 | LEU |
| 2 | F | 34 | LYS |
| 1 | G | 15 | ARG |
| 1 | G | 18 | ASP |
| 1 | G | 54 | ASN |
| 1 | G | 180 | ASP |
| 1 | G | 238 | HIS |
| 1 | G | 317 | MET |
| 1 | G | 342 | VAL |
| 1 | G | 373 | THR |
| 1 | G | 392 | ILE |
| 1 | G | 417 | ARG |
| 1 | G | 424 | PHE |
| 1 | G | 441 | LYS |
| 1 | G | 462 | TYR |
| 1 | G | 476 | GLN |
| 1 | G | 542 | ARG |
| 1 | G | 551 | PHE |
| 1 | G | 558 | LEU |
| 1 | G | 563 | GLU |
| 1 | G | 572 | LEU |
| 1 | G | 575 | LEU |
| 1 | G | 604 | HIS |
| 1 | G | 609 | LYS |
| 1 | G | 643 | LEU |
| 1 | G | 680 | ASP |
| 1 | G | 725 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 739 | ARG |
| 1 | G | 851 | LEU |
| 1 | G | 872 | ILE |
| 1 | G | 888 | ASN |
| 1 | G | 908 | ARG |
| 1 | G | 948 | CYS |
| 1 | G | 1027 | ARG |
| 1 | G | 1031 | ARG |
| 1 | G | 1137 | PHE |
| 1 | G | 1189 | GLU |
| 1 | G | 1193 | LYS |
| 1 | G | 1232 | LEU |
| 1 | G | 1259 | LEU |
| 1 | G | 1287 | GLN |
| 1 | G | 1298 | ASP |
| 1 | G | 1308 | ILE |
| 1 | G | 1447 | THR |
| 1 | G | 1459 | LEU |
| 1 | G | 1465 | VAL |
| 1 | G | 1533 | VAL |
| 1 | G | 1538 | LYS |
| 1 | G | 1553 | PHE |
| 1 | G | 1554 | GLN |
| 1 | G | 1643 | GLU |
| 1 | G | 1657 | THR |
| 1 | G | 1671 | ARG |
| 1 | G | 1677 | CYS |
| 1 | G | 1697 | LEU |
| 1 | G | 1720 | MET |
| 1 | G | 1721 | MET |
| 1 | G | 1761 | MET |
| 1 | G | 1763 | PHE |
| 1 | G | 1771 | ILE |
| 1 | G | 1772 | ASN |
| 1 | G | 1778 | TYR |
| 1 | G | 1804 | LEU |
| 1 | G | 1897 | LYS |
| 1 | G | 1898 | LEU |
| 1 | G | 1910 | LEU |
| 1 | G | 1919 | ARG |
| 1 | G | 1925 | ILE |
| 1 | G | 2023 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 2028 | ARG |
| 1 | G | 2036 | VAL |
| 1 | G | 2058 | LEU |
| 1 | G | 2066 | MET |
| 1 | G | 2077 | ASP |
| 1 | G | 2086 | VAL |
| 1 | G | 2117 | ILE |
| 1 | G | 2126 | ILE |
| 1 | G | 2129 | LEU |
| 1 | G | 2179 | LEU |
| 1 | G | 2192 | MET |
| 1 | G | 2220 | TYR |
| 1 | G | 2328 | ARG |
| 1 | G | 2354 | ILE |
| 1 | G | 2399 | LEU |
| 1 | G | 2423 | ILE |
| 1 | G | 2426 | SER |
| 1 | G | 2511 | THR |
| 1 | G | 2517 | LEU |
| 1 | G | 2522 | CYS |
| 1 | G | 2713 | ILE |
| 1 | G | 2717 | LYS |
| 1 | G | 2723 | ASN |
| 1 | G | 2746 | GLU |
| 1 | G | 2747 | ILE |
| 1 | G | 2750 | ASP |
| 1 | G | 2762 | LYS |
| 1 | G | 2770 | GLU |
| 1 | G | 2795 | GLU |
| 1 | G | 2838 | LEU |
| 1 | G | 2861 | LEU |
| 1 | G | 3675 | THR |
| 1 | G | 3690 | MET |
| 1 | G | 3728 | GLN |
| 1 | G | 3801 | CYS |
| 1 | G | 3860 | ARG |
| 1 | G | 3866 | ASN |
| 1 | G | 3911 | ILE |
| 1 | G | 3912 | GLN |
| 1 | G | 3926 | GLN |
| 1 | G | 3929 | CYS |
| 1 | G | 3962 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 3970 | LYS |
| 1 | G | 3992 | VAL |
| 1 | G | 4012 | GLU |
| 1 | G | 4050 | HIS |
| 1 | G | 4065 | GLU |
| 1 | G | 4117 | GLN |
| 1 | G | 4126 | VAL |
| 1 | G | 4170 | LYS |
| 1 | G | 4186 | LYS |
| 1 | G | 4188 | GLU |
| 1 | G | 4192 | ASN |
| 1 | G | 4196 | ASP |
| 1 | G | 4576 | ILE |
| 1 | G | 4584 | ILE |
| 1 | G | 4620 | THR |
| 1 | G | 4622 | GLN |
| 1 | G | 4637 | ILE |
| 1 | G | 4640 | GLN |
| 1 | G | 4727 | TYR |
| 1 | G | 4730 | MET |
| 1 | G | 4807 | LYS |
| 1 | G | 4885 | ASP |
| 1 | G | 4927 | LEU |
| 2 | H | 34 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 375 | GLN |
| 1 | A | 476 | GLN |
| 1 | A | 486 | GLN |
| 1 | A | 487 | ASN |
| 1 | A | 496 | ASN |
| 1 | A | 547 | ASN |
| 1 | A | 669 | GLN |
| 1 | A | 692 | HIS |
| 1 | A | 746 | GLN |
| 1 | A | 888 | ASN |
| 1 | A | 956 | HIS |
| 1 | A | 1002 | ASN |
| 1 | A | 1046 | ASN |
| 1 | A | 1063 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1601 | ASN |
| 1 | A | 1684 | GLN |
| 1 | A | 1772 | ASN |
| 1 | A | 1773 | ASN |
| 1 | A | 1905 | GLN |
| 1 | A | 2152 | ASN |
| 1 | A | 2209 | GLN |
| 1 | A | 2891 | GLN |
| 1 | A | 3775 | GLN |
| 1 | A | 3865 | ASN |
| 1 | A | 3956 | GLN |
| 1 | A | 4010 | ASN |
| 1 | A | 4192 | ASN |
| 1 | A | 4515 | ASN |
| 1 | A | 4644 | ASN |
| 1 | A | 4738 | ASN |
| 1 | A | 4765 | ASN |
| 1 | A | 4818 | HIS |
| 1 | A | 4879 | GLN |
| 1 | A | 4919 | ASN |
| 2 | B | 25 | HIS |
| 2 | B | 65 | GLN |
| 1 | C | 54 | ASN |
| 1 | C | 364 | GLN |
| 1 | C | 476 | GLN |
| 1 | C | 487 | ASN |
| 1 | C | 496 | ASN |
| 1 | C | 547 | ASN |
| 1 | C | 669 | GLN |
| 1 | C | 692 | HIS |
| 1 | C | 771 | ASN |
| 1 | C | 888 | ASN |
| 1 | C | 956 | HIS |
| 1 | C | 1002 | ASN |
| 1 | C | 1772 | ASN |
| 1 | C | 1773 | ASN |
| 1 | C | 1905 | GLN |
| 1 | C | 2152 | ASN |
| 1 | C | 2224 | ASN |
| 1 | C | 2891 | GLN |
| 1 | C | 3775 | GLN |
| 1 | C | 3862 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 3932 | ASN |
| 1 | C | 3956 | GLN |
| 1 | C | 3976 | GLN |
| 1 | C | 4010 | ASN |
| 1 | C | 4192 | ASN |
| 1 | C | 4644 | ASN |
| 1 | C | 4818 | HIS |
| 1 | C | 4879 | GLN |
| 1 | C | 4919 | ASN |
| 2 | D | 25 | HIS |
| 1 | E | 476 | GLN |
| 1 | E | 547 | ASN |
| 1 | E | 607 | ASN |
| 1 | E | 746 | GLN |
| 1 | E | 771 | ASN |
| 1 | E | 888 | ASN |
| 1 | E | 1002 | ASN |
| 1 | E | 1147 | GLN |
| 1 | E | 1601 | ASN |
| 1 | E | 1772 | ASN |
| 1 | E | 1773 | ASN |
| 1 | E | 1905 | GLN |
| 1 | E | 2091 | GLN |
| 1 | E | 2482 | GLN |
| 1 | E | 2848 | ASN |
| 1 | E | 3775 | GLN |
| 1 | E | 3865 | ASN |
| 1 | E | 3912 | GLN |
| 1 | E | 3926 | GLN |
| 1 | E | 3932 | ASN |
| 1 | E | 4192 | ASN |
| 1 | E | 4631 | GLN |
| 1 | E | 4644 | ASN |
| 1 | E | 4818 | HIS |
| 1 | E | 4919 | ASN |
| 2 | F | 25 | HIS |
| 1 | G | 33 | GLN |
| 1 | G | 54 | ASN |
| 1 | G | 476 | GLN |
| 1 | G | 487 | ASN |
| 1 | G | 544 | ASN |
| 1 | G | 547 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 692 | HIS |
| 1 | G | 746 | GLN |
| 1 | G | 771 | ASN |
| 1 | G | 773 | GLN |
| 1 | G | 888 | ASN |
| 1 | G | 956 | HIS |
| 1 | G | 1002 | ASN |
| 1 | G | 1147 | GLN |
| 1 | G | 1601 | ASN |
| 1 | G | 1631 | HIS |
| 1 | G | 1691 | ASN |
| 1 | G | 1772 | ASN |
| 1 | G | 1773 | ASN |
| 1 | G | 2071 | GLN |
| 1 | G | 2091 | GLN |
| 1 | G | 2152 | ASN |
| 1 | G | 2848 | ASN |
| 1 | G | 2891 | GLN |
| 1 | G | 3775 | GLN |
| 1 | G | 3799 | GLN |
| 1 | G | 3865 | ASN |
| 1 | G | 3912 | GLN |
| 1 | G | 3916 | GLN |
| 1 | G | 3926 | GLN |
| 1 | G | 3932 | ASN |
| 1 | G | 3965 | GLN |
| 1 | G | 4010 | ASN |
| 1 | G | 4192 | ASN |
| 1 | G | 4768 | GLN |
| 1 | G | 4879 | GLN |
| 1 | G | 4919 | ASN |
| 2 | H | 25 | HIS |
| 2 | H | 65 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | C | 27 |
| 1 | G | 27 |
| 1 | E | 27 |
| 1 | A | 27 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 3612:UNK | C | 3613:PRO | N | 76.52 |
| 1 | G | 3612:UNK | C | 3613:PRO | N | 75.29 |
| 1 | E | 3612:UNK | C | 3613:PRO | N | 74.52 |
| 1 | A | 3612:UNK | C | 3613:PRO | N | 74.10 |
| 1 | E | 2701:UNK | C | 2702:PHE | N | 43.29 |
| 1 | C | 2701:UNK | C | 2702:PHE | N | 43.25 |
| 1 | G | 2701:UNK | C | 2702:PHE | N | 42.68 |
| 1 | A | 2701:UNK | C | 2702:PHE | N | 41.57 |
| 1 | E | 3589:UNK | C | 3590:UNK | N | 41.47 |
| 1 | A | 3589:UNK | C | 3590:UNK | N | 40.67 |
| 1 | G | 3589:UNK | C | 3590:UNK | N | 38.79 |
| 1 | C | 3589:UNK | C | 3590:UNK | N | 37.92 |
| 1 | G | 3436:UNK | C | 3437:UNK | N | 22.01 |
| 1 | A | 3347:GLY | C | 3348:UNK | N | 21.94 |
| 1 | E | 3347:GLY | C | 3348:UNK | N | 21.63 |
| 1 | C | 2529:LEU | C | 2578:UNK | N | 21.47 |
| 1 | E | 3436:UNK | C | 3437:UNK | N | 21.40 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 3347:GLY | C | 3348:UNK | N | 21.29 |
| 1 | E | 2529:LEU | C | 2578:UNK | N | 20.68 |
| 1 | G | 3347:GLY | C | 3348:UNK | N | 20.37 |
| 1 | C | 3436:UNK | C | 3437:UNK | N | 20.35 |
| 1 | A | 2529:LEU | C | 2578:UNK | N | 20.28 |
| 1 | A | 3436:UNK | C | 3437:UNK | N | 20.21 |
| 1 | A | 2659:UNK | C | 2660:UNK | N | 19.56 |
| 1 | G | 2529:LEU | C | 2578:UNK | N | 19.18 |
| 1 | G | 2659:UNK | C | 2660:UNK | N | 18.25 |
| 1 | E | 1943:ARG | C | 2008:UNK | N | 18.00 |
| 1 | G | 1943:ARG | C | 2008:UNK | N | 17.56 |
| 1 | C | 3414:UNK | C | 3415:UNK | N | 17.36 |
| 1 | G | 3496:UNK | C | 3497:UNK | N | 17.23 |
| 1 | E | 3371:UNK | C | 3372:UNK | N | 17.18 |
| 1 | A | 1943:ARG | C | 2008:UNK | N | 17.12 |
| 1 | E | 2659:UNK | C | 2660:UNK | N | 16.94 |
| 1 | G | 3478:UNK | C | 3479:UNK | N | 16.94 |
| 1 | G | 1500:UNK | C | 1501:ASN | N | 16.90 |
| 1 | E | 3478:UNK | C | 3479:UNK | N | 16.86 |
| 1 | C | 3478:UNK | C | 3479:UNK | N | 16.82 |
| 1 | A | 3414:UNK | C | 3415:UNK | N | 16.74 |
| 1 | C | 1500:UNK | C | 1501:ASN | N | 16.69 |
| 1 | E | 2597:UNK | C | 2598:UNK | N | 16.38 |
| 1 | C | 2659:UNK | C | 2660:UNK | N | 16.36 |
| 1 | C | 1943:ARG | C | 2008:UNK | N | 16.33 |
| 1 | E | 3414:UNK | C | 3415:UNK | N | 16.18 |
| 1 | C | 3496:UNK | C | 3497:UNK | N | 16.05 |
| 1 | E | 1500:UNK | C | 1501:ASN | N | 16.00 |
| 1 | A | 3510:UNK | C | 3511:UNK | N | 15.98 |
| 1 | A | 1500:UNK | C | 1501:ASN | N | 15.96 |
| 1 | C | 2597:UNK | C | 2598:UNK | N | 15.85 |
| 1 | G | 3414:UNK | C | 3415:UNK | N | 15.79 |
| 1 | C | 2679:UNK | C | 2680:UNK | N | 15.57 |
| 1 | A | 3478:UNK | C | 3479:UNK | N | 15.52 |
| 1 | G | 3510:UNK | C | 3511:UNK | N | 15.50 |
| 1 | E | 2636:UNK | C | 2637:UNK | N | 15.08 |
| 1 | G | 3371:UNK | C | 3372:UNK | N | 15.08 |
| 1 | G | 2022:UNK | C | 2023:LEU | N | 14.88 |
| 1 | A | 3496:UNK | C | 3497:UNK | N | 14.87 |
| 1 | E | 3510:UNK | C | 3511:UNK | N | 14.76 |
| 1 | A | 2022:UNK | C | 2023:LEU | N | 14.71 |
| 1 | A | 2597:UNK | C | 2598:UNK | N | 14.71 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 2022:UNK | C | 2023:LEU | N | 14.64 |
| 1 | G | 3548:UNK | C | 3549:UNK | N | 14.53 |
| 1 | E | 2022:UNK | C | 2023:LEU | N | 14.45 |
| 1 | G | 3571:UNK | C | 3572:UNK | N | 14.26 |
| 1 | C | 3510:UNK | C | 3511:UNK | N | 13.96 |
| 1 | G | 2679:UNK | C | 2680:UNK | N | 13.82 |
| 1 | C | 2636:UNK | C | 2637:UNK | N | 13.74 |
| 1 | C | 3571:UNK | C | 3572:UNK | N | 13.65 |
| 1 | G | 2636:UNK | C | 2637:UNK | N | 13.56 |
| 1 | C | 3371:UNK | C | 3372:UNK | N | 13.49 |
| 1 | A | 2679:UNK | C | 2680:UNK | N | 13.34 |
| 1 | A | 3548:UNK | C | 3549:UNK | N | 13.33 |
| 1 | E | 3496:UNK | C | 3497:UNK | N | 12.80 |
| 1 | C | 3528:UNK | C | 3529:UNK | N | 12.75 |
| 1 | A | 2636:UNK | C | 2637:UNK | N | 12.73 |
| 1 | G | 2597:UNK | C | 2598:UNK | N | 12.44 |
| 1 | E | 3528:UNK | C | 3529:UNK | N | 12.40 |
| 1 | G | 3391:UNK | C | 3392:UNK | N | 12.33 |
| 1 | E | 3571:UNK | C | 3572:UNK | N | 12.27 |
| 1 | C | 3548:UNK | C | 3549:UNK | N | 12.03 |
| 1 | E | 3457:UNK | C | 3458:UNK | N | 11.91 |
| 1 | E | 3391:UNK | C | 3392:UNK | N | 11.75 |
| 1 | E | 2679:UNK | C | 2680:UNK | N | 11.67 |
| 1 | C | 3457:UNK | C | 3458:UNK | N | 11.62 |
| 1 | A | 3528:UNK | C | 3529:UNK | N | 11.43 |
| 1 | A | 2460:UNK | C | 2461:PHE | N | 10.92 |
| 1 | A | 3571:UNK | C | 3572:UNK | N | 10.38 |
| 1 | A | 3371:UNK | C | 3372:UNK | N | 10.05 |
| 1 | E | 2460:UNK | C | 2461:PHE | N | 9.63 |
| 1 | G | 2460:UNK | C | 2461:PHE | N | 9.03 |
| 1 | C | 2460:UNK | C | 2461:PHE | N | 9.00 |
| 1 | G | 3528:UNK | C | 3529:UNK | N | 8.96 |
| 1 | A | 3457:UNK | C | 3458:UNK | N | 8.73 |
| 1 | A | 3391:UNK | C | 3392:UNK | N | 8.48 |
| 1 | E | 2616:UNK | C | 2617:UNK | N | 8.34 |
| 1 | G | 3457:UNK | C | 3458:UNK | N | 8.29 |
| 1 | E | 3548:UNK | C | 3549:UNK | N | 6.74 |
| 1 | C | 2616:UNK | C | 2617:UNK | N | 6.50 |
| 1 | G | 2616:UNK | C | 2617:UNK | N | 6.26 |
| 1 | C | 1484:ASN | C | 1496:UNK | N | 5.85 |
| 1 | A | 1484:ASN | C | 1496:UNK | N | 5.47 |
| 1 | C | 2427:LEU | C | 2447:UNK | N | 5.34 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | E | 2427:LEU | C | 2447:UNK | N | 5.15 |
| 1 | G | 1484:ASN | C | 1496:UNK | N | 4.71 |
| 1 | A | 2616:UNK | C | 2617:UNK | N | 4.70 |
| 1 | C | 3391:UNK | C | 3392:UNK | N | 4.48 |
| 1 | A | 2427:LEU | C | 2447:UNK | N | 4.21 |
| 1 | E | 1484:ASN | C | 1496:UNK | N | 4.12 |
| 1 | G | 2427:LEU | C | 2447:UNK | N | 3.84 |

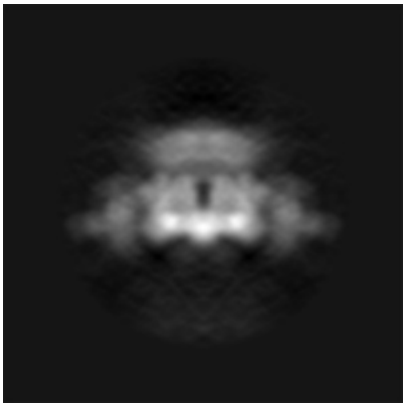
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8303. These allow visual inspection of the internal detail of the map and identification of artifacts.

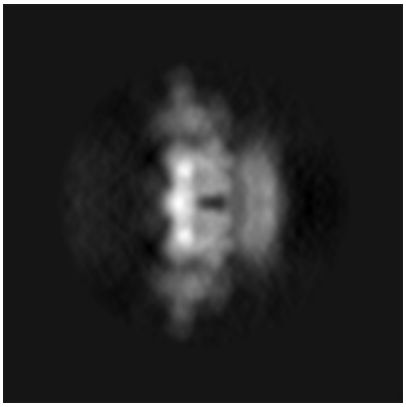
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

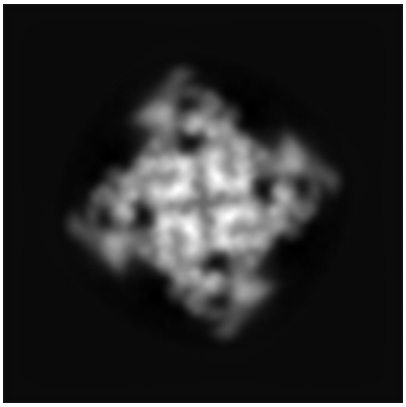
### 6.1.1 Primary map



X



Y

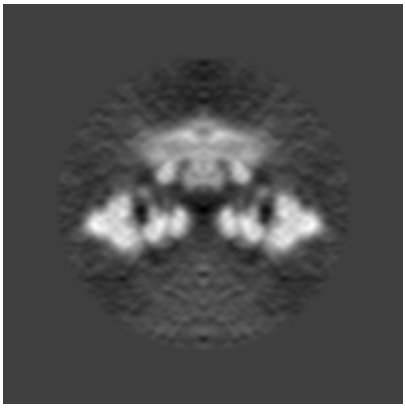


Z

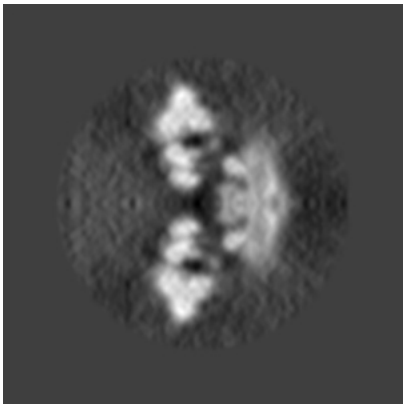
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

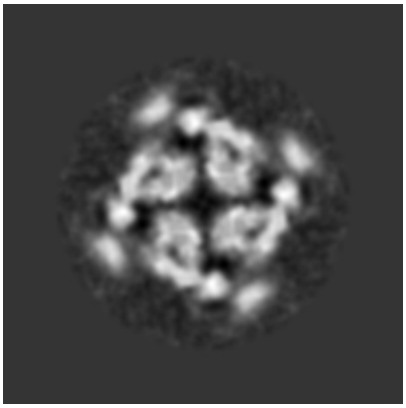
### 6.2.1 Primary map



X Index: 200



Y Index: 200

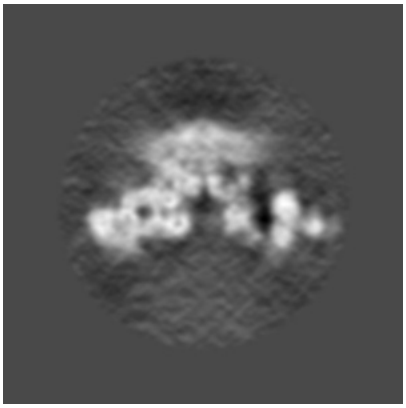


Z Index: 200

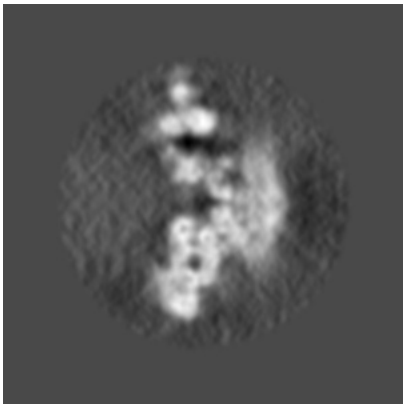
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

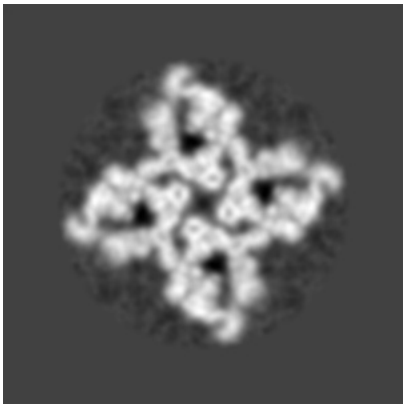
### 6.3.1 Primary map



X Index: 190



Y Index: 210

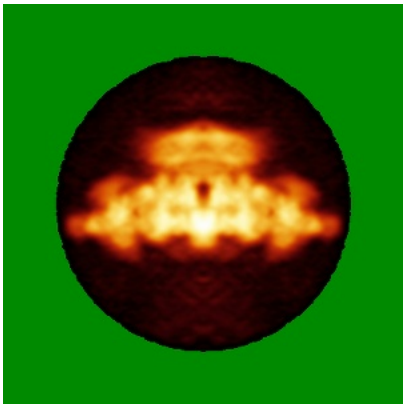


Z Index: 181

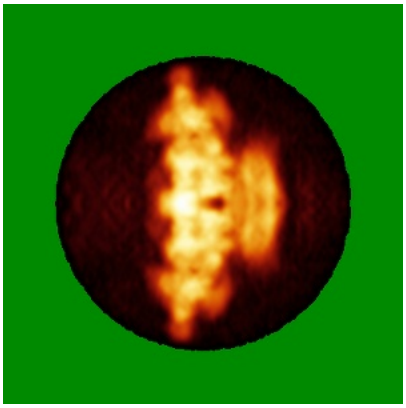
The images above show the largest variance slices of the map in three orthogonal directions.

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

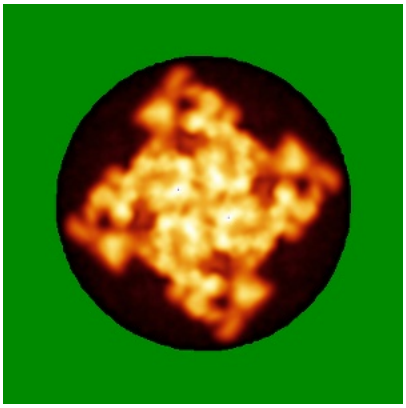
### 6.4.1 Primary map



X



Y



Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

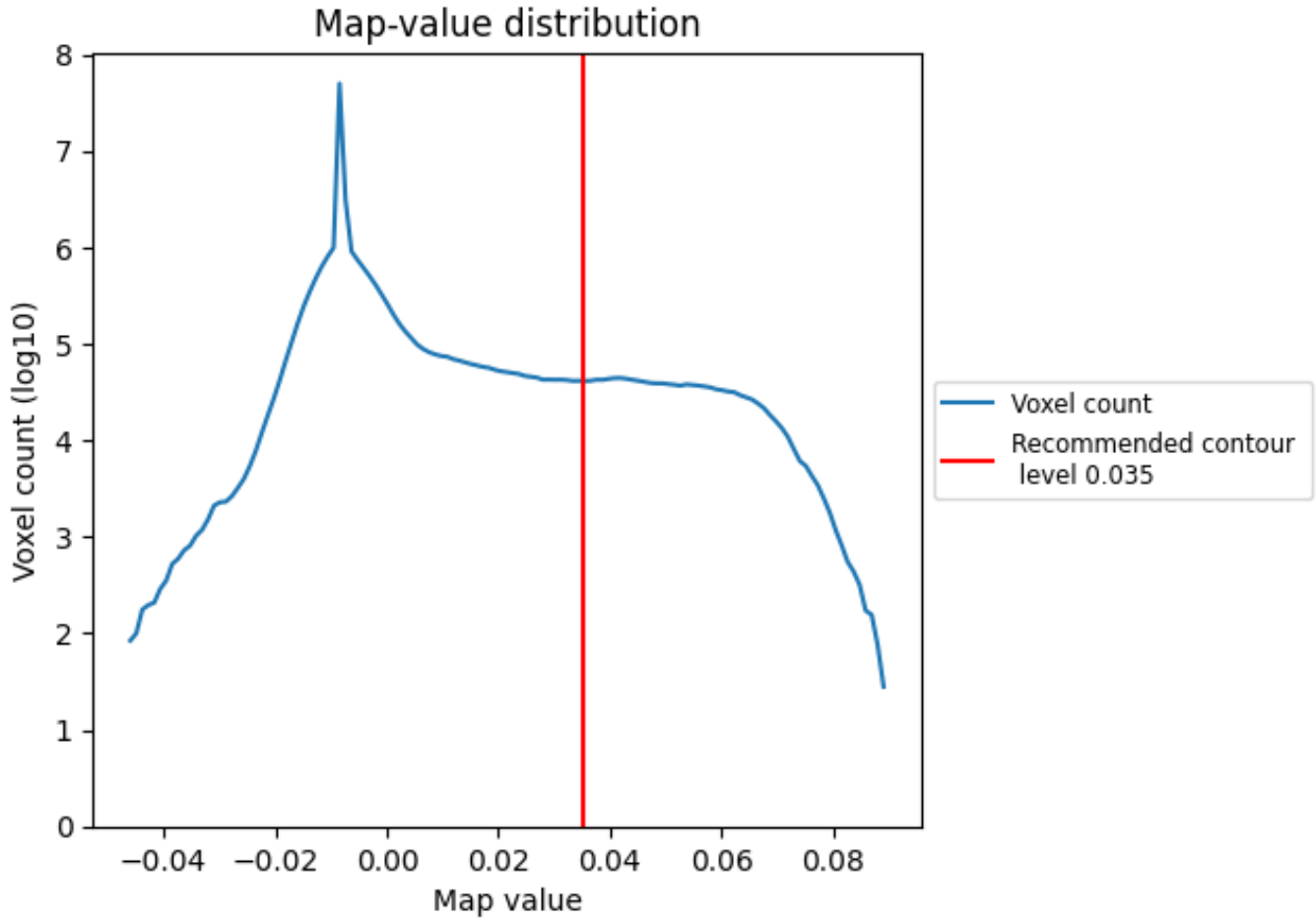
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

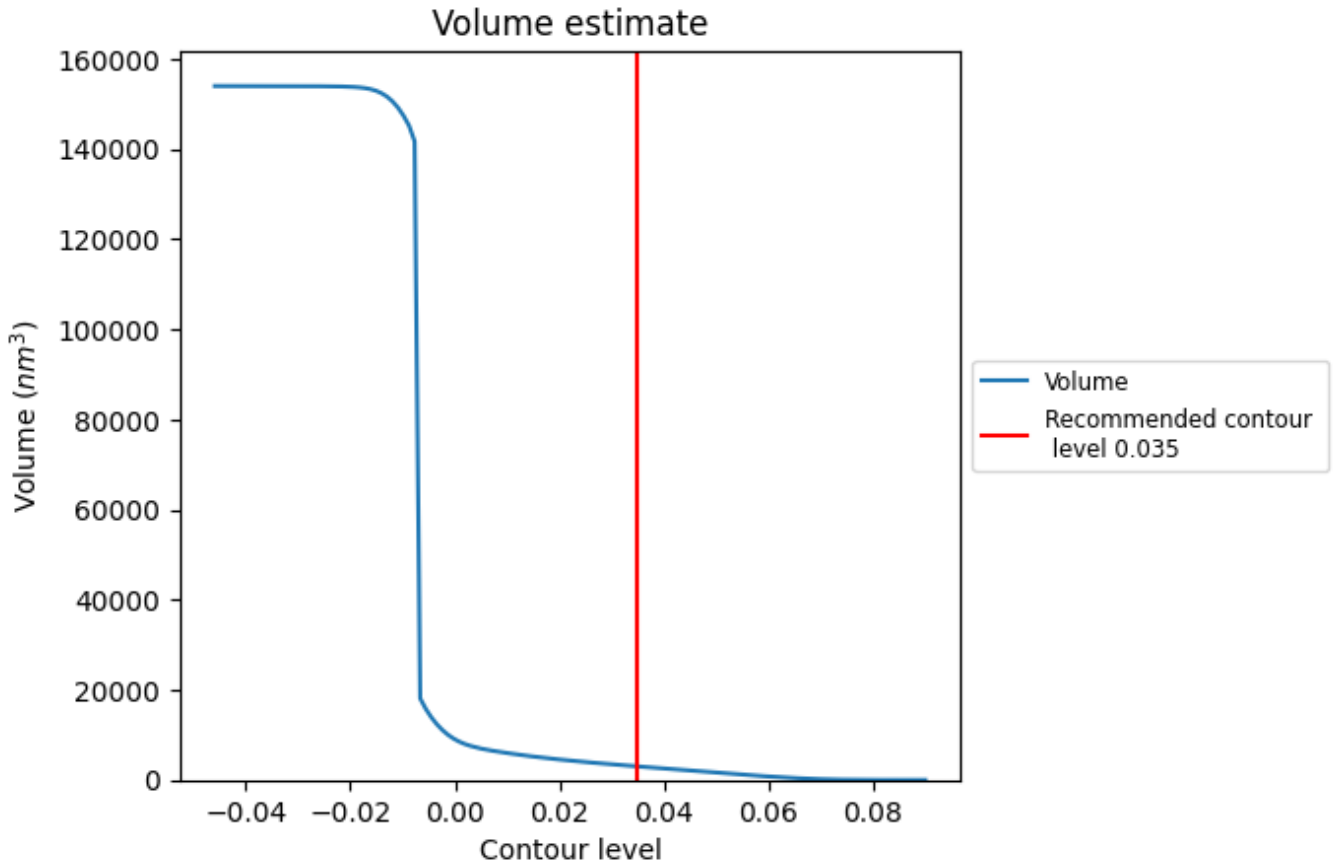
This section contains the results of statistical analysis of the map.

## 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.

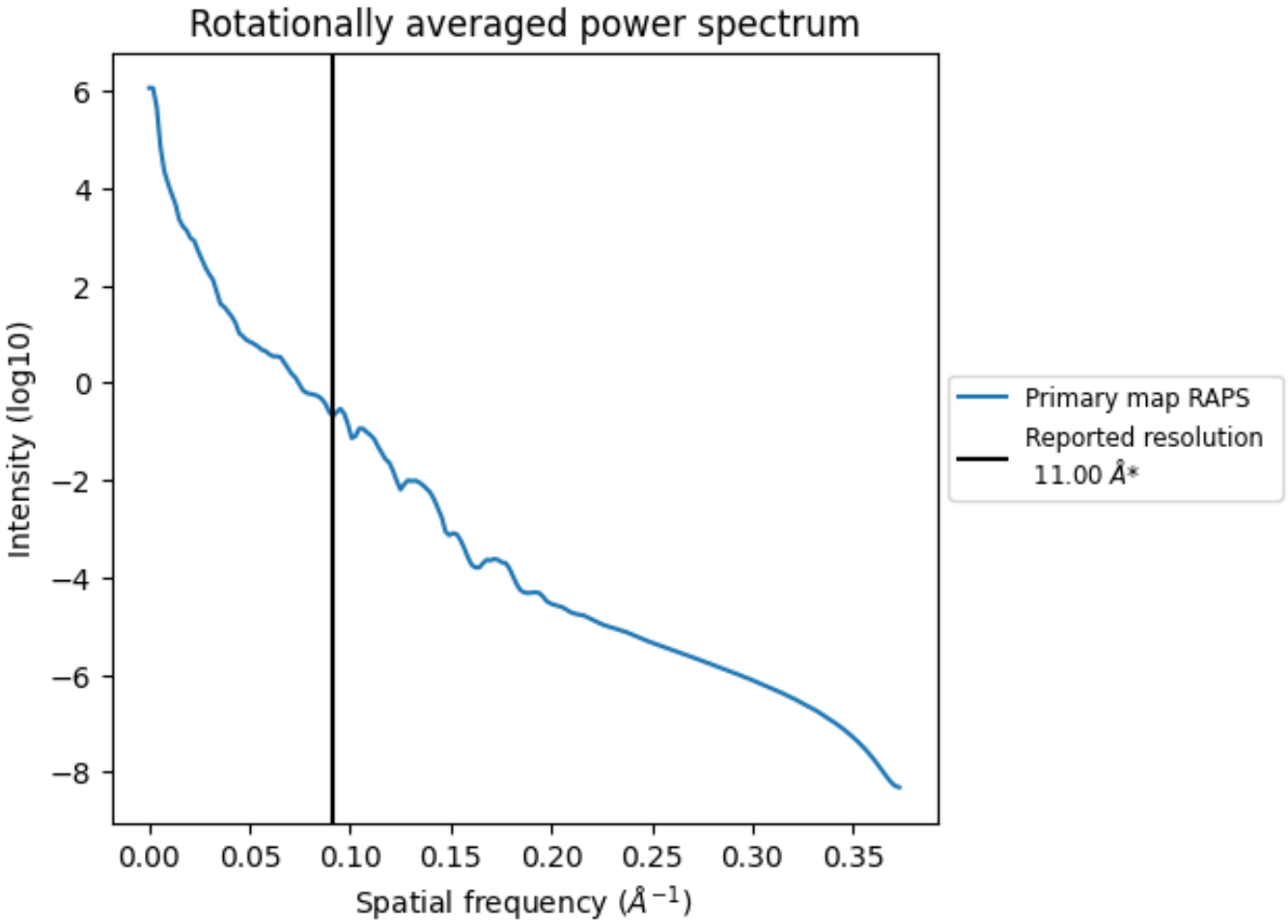
## 7.2 Volume estimate




The volume at the recommended contour level is 3008 $nm^3$; this corresponds to an approximate mass of 2718 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 0.091 $Å^{-1}$

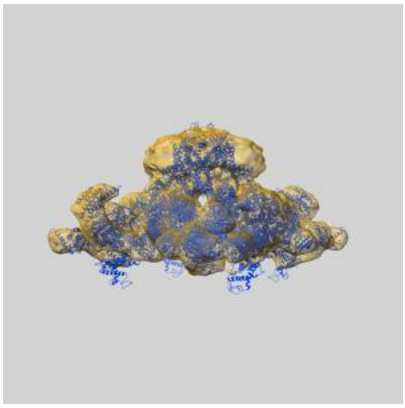
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

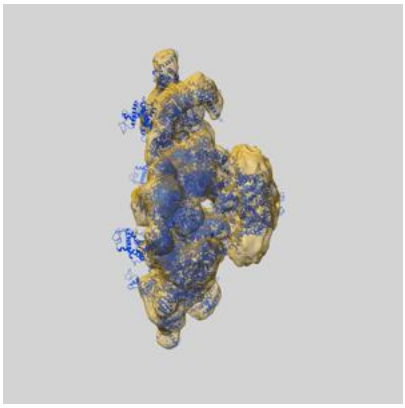
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8303 and PDB model 5L1D. Per-residue inclusion information can be found in section 3 on page 9.

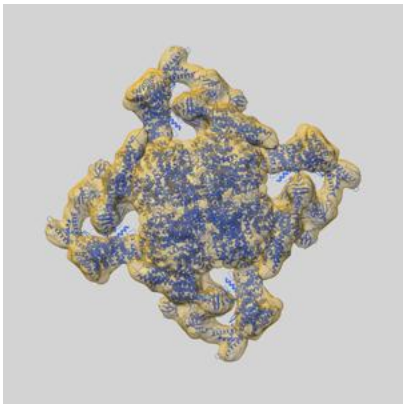
## 9.1 Map-model overlay



X



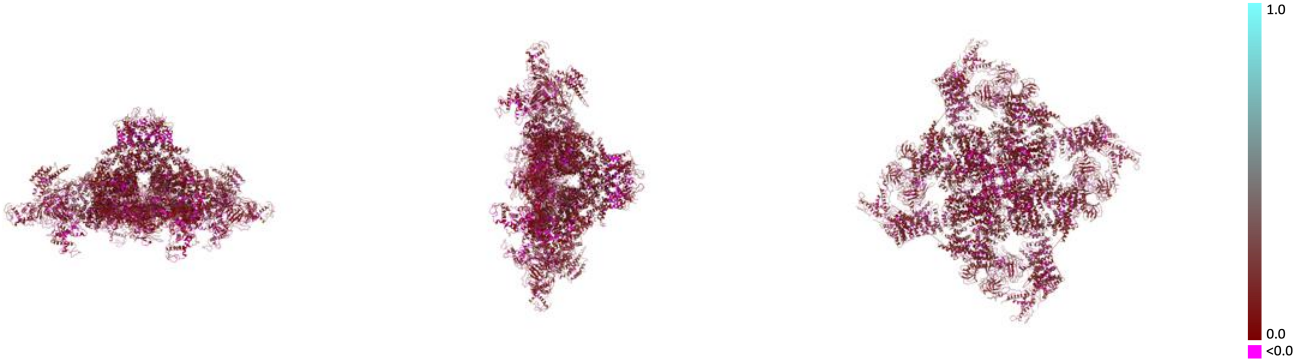
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

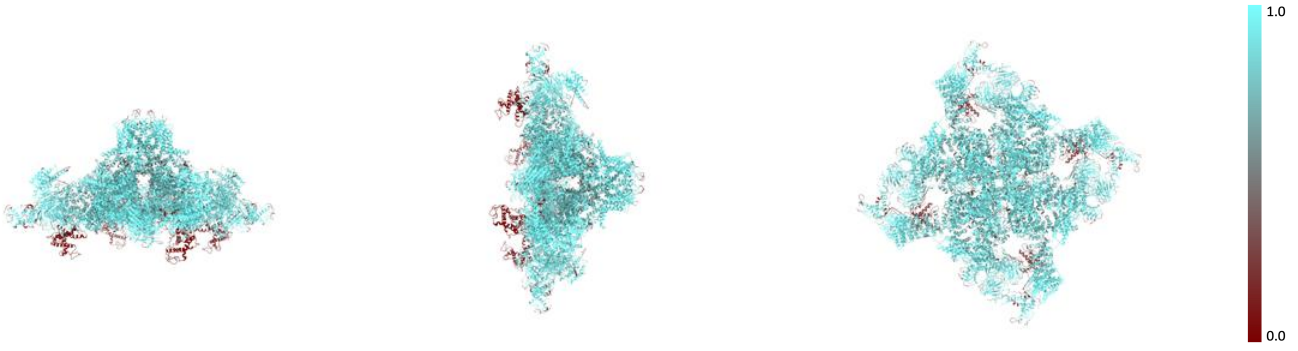
## 9.2 Q-score mapped to coordinate model




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.

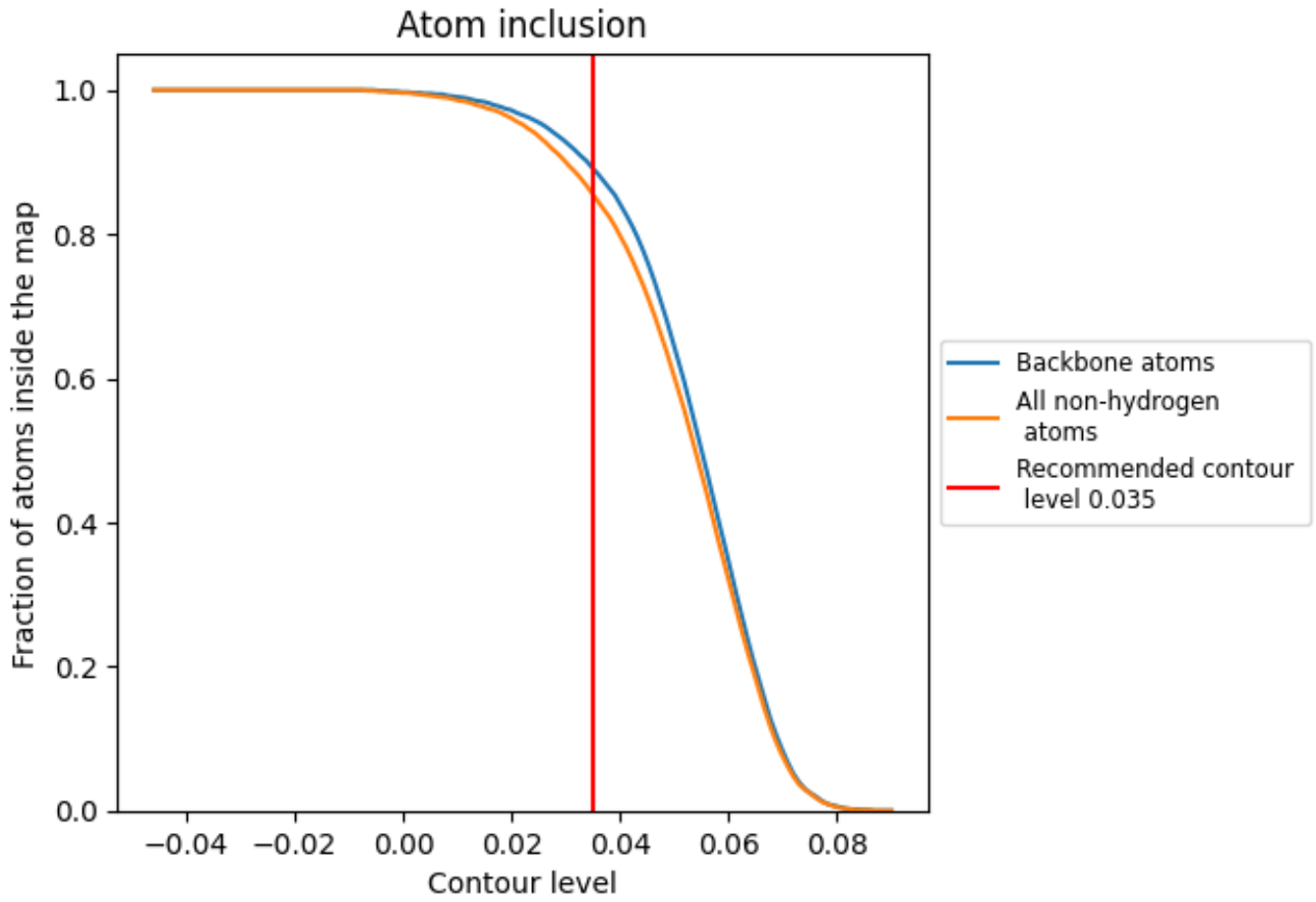
## 9.3 Atom inclusion mapped to coordinate model




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 (0.035).

## 9.4 Atom inclusion (i)




At the recommended contour level, 89% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8550 | 0.0820 |
| A | 0.8560 | 0.0820 |
| B | 0.8470 | 0.0660 |
| C | 0.8560 | 0.0820 |
| D | 0.8460 | 0.0720 |
| E | 0.8550 | 0.0820 |
| F | 0.8440 | 0.0750 |
| G | 0.8560 | 0.0830 |
| H | 0.8380 | 0.0700 |