



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:34 PM UTC

PDB ID : 7JMF / pdb\_00007jmf  
EMDB ID : EMD-22392  
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots  
- Frame 42 - State 6 (S6)  
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.  
Deposited on : 2020-07-31  
Resolution : 4.50 Å(reported)  
Based on initial model : 5TB4

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

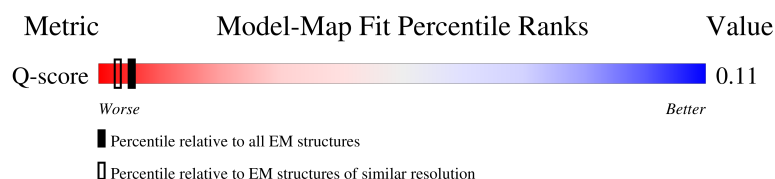
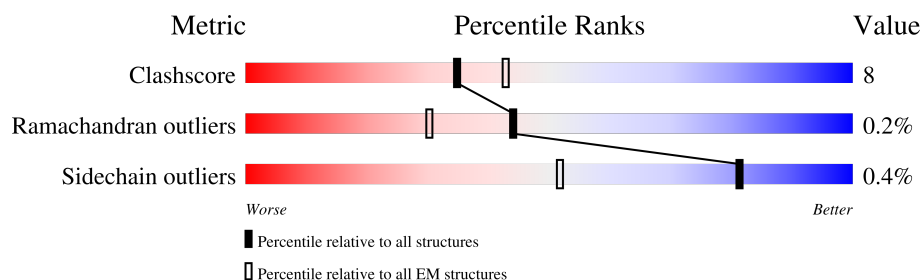
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 2937 ( 4.00 - 5.00 )                                     |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                               |
|-----|-------|--------|------------------------------------------------|
| 1   | A     | 108    | <div> <div>89%</div> <div>67% 32%</div> </div> |
| 1   | F     | 108    | <div> <div>84%</div> <div>69% 31%</div> </div> |
| 1   | H     | 108    | <div> <div>90%</div> <div>69% 31%</div> </div> |
| 1   | J     | 108    | <div> <div>87%</div> <div>69% 31%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                                |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------|
| 2   | B     | 4687   | <div><div>63%</div><div><div></div><div></div><div></div></div><div>73%</div><div>16%</div><div>11%</div></div> |
| 2   | E     | 4687   | <div><div>64%</div><div><div></div><div></div><div></div></div><div>73%</div><div>16%</div><div>11%</div></div> |
| 2   | G     | 4687   | <div><div>69%</div><div><div></div><div></div><div></div></div><div>73%</div><div>16%</div><div>11%</div></div> |
| 2   | I     | 4687   | <div><div>70%</div><div><div></div><div></div><div></div></div><div>73%</div><div>16%</div><div>11%</div></div> |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 120756 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | F     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | J     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |

- Molecule 2 is a protein called ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 2   | B     | 4168     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29369 | 18608 | 5202 | 5402 | 157 |         |       |
| 2   | E     | 4168     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29369 | 18608 | 5202 | 5402 | 157 |         |       |
| 2   | G     | 4168     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29369 | 18608 | 5202 | 5402 | 157 |         |       |
| 2   | I     | 4168     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29369 | 18608 | 5202 | 5402 | 157 |         |       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | I     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest")

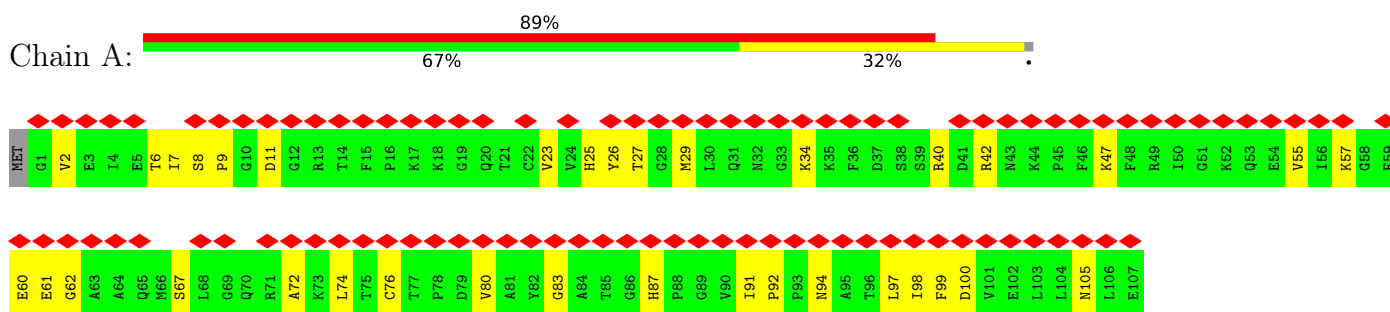
by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | B     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | E     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | G     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | I     | 1        | Total<br>1 | Ca<br>1 | 0       |

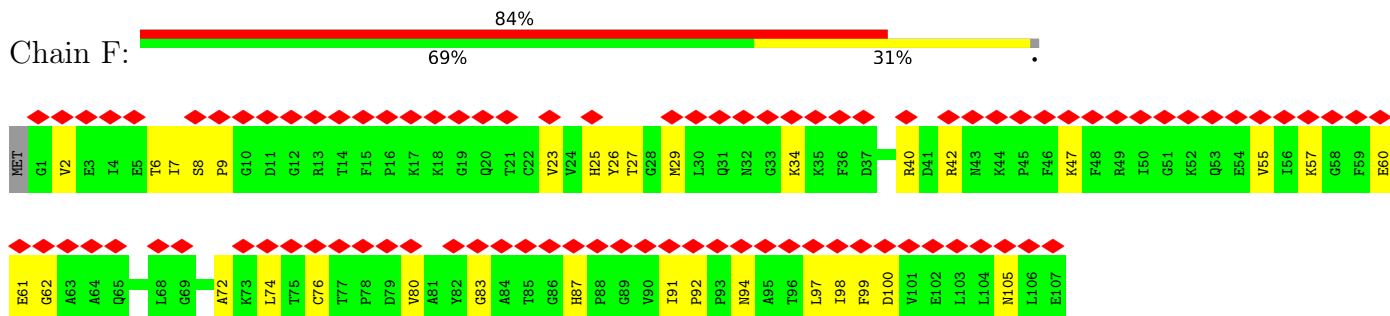
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

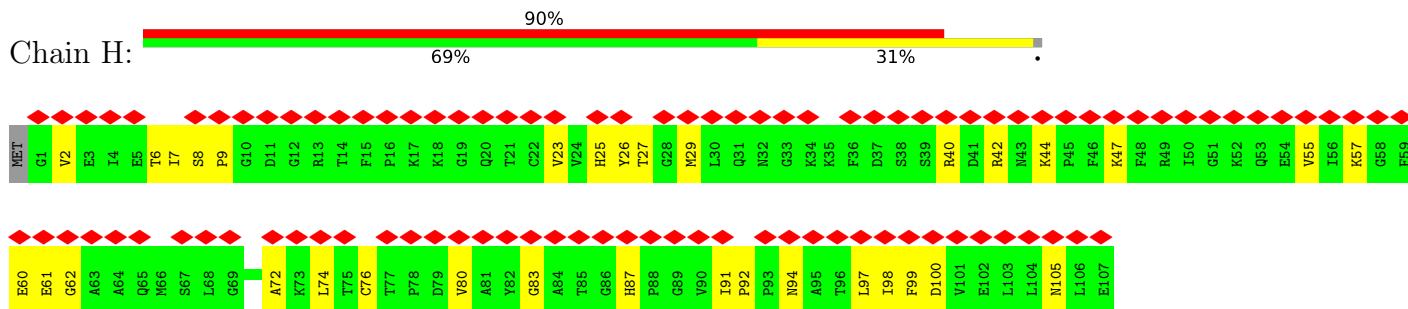
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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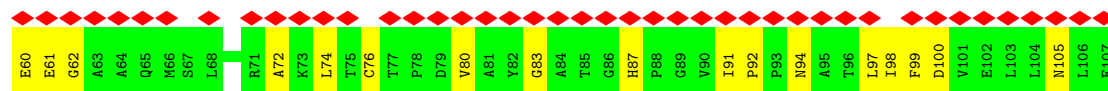
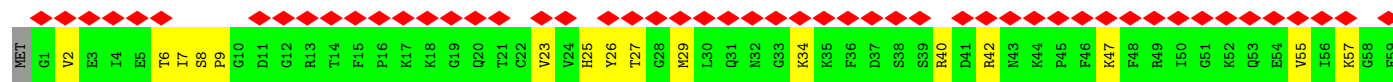


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

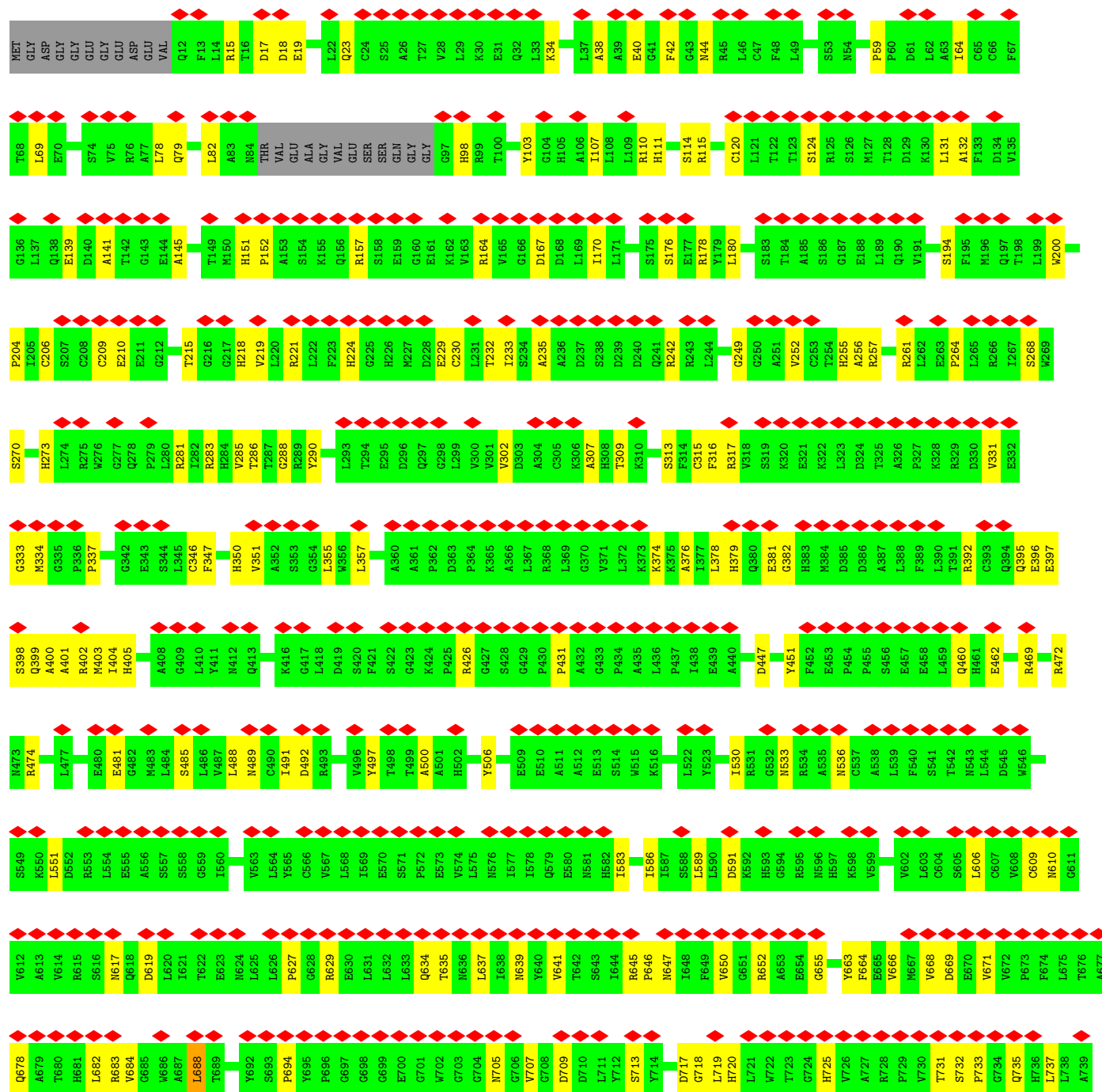
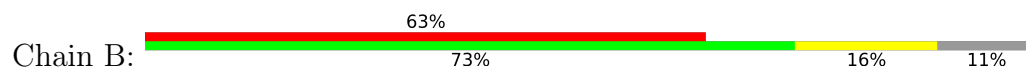


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





# • Molecule 2: ryanodine receptor 1

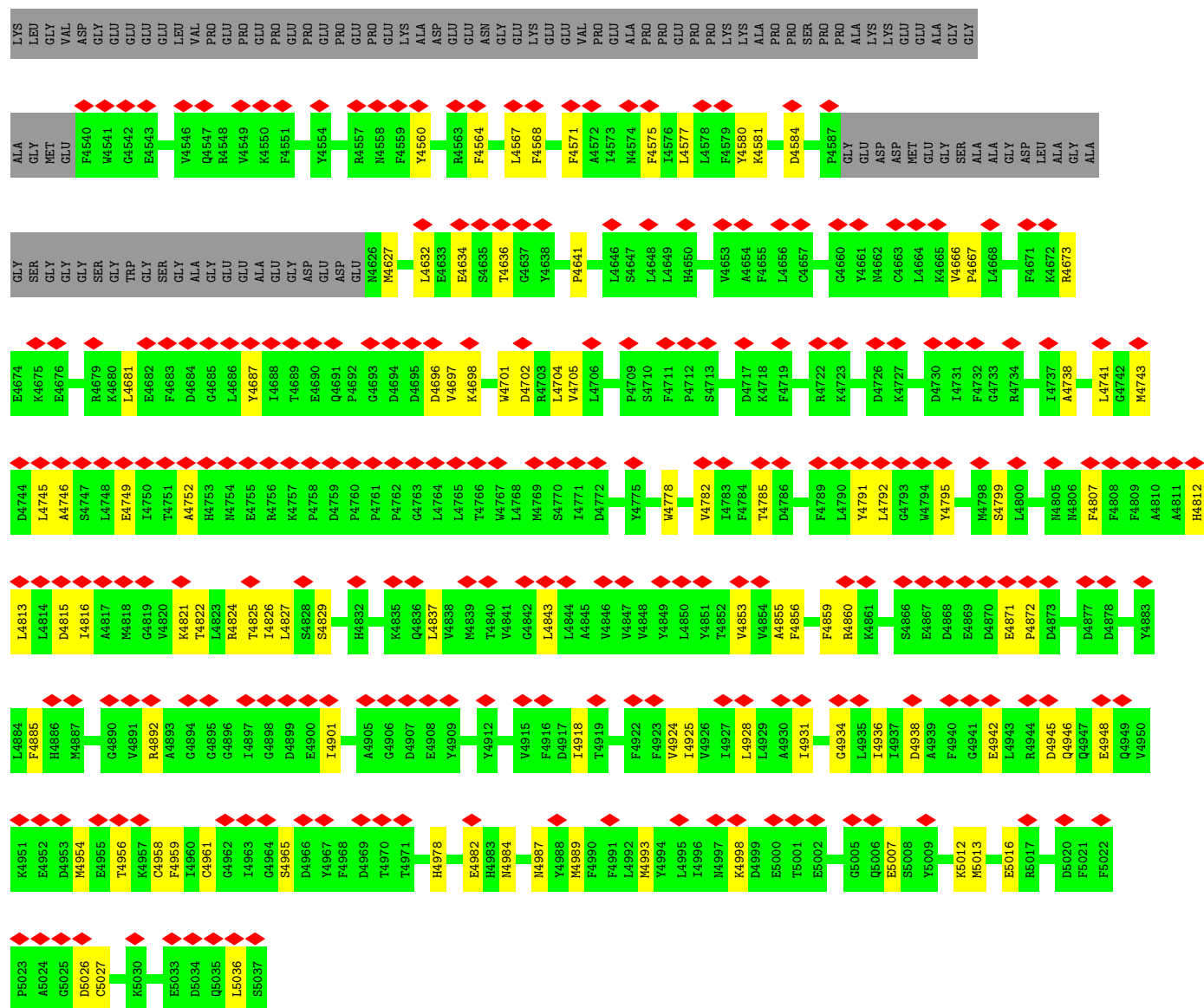


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| M1648 | D1649 | I1650 | L1651 | E1652 | L1653 | R1656 | L1657 | D1658 | L1659 | Q1660 | R1661 | F1662 | H1663 | S1664 | H1665 | T1666 | L1667 | R1668 | L1669 | Y1670 | R1671 | A1672 | A1675 | L1676 | G1677 | M1678 | Q1679 | N1679 | L1680 | V1681 | A1682 | H1683 | A1684 | S1687 | H1688 | L1689 | D1690 | Q1691 | A1692 | V1692 | Q1693 | Q1694 | L1694 | L1695 | H1696 | A1697 | L1698 | E1699 | D1700 | A1701 | H1702 | L1703 | P1704 | G1705 | P1706 | L1707 | A1708 | R1709 | G1710 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X1437 | X1438 | X1439 | X1440 | X1441 | X1442 | X1443 | X1444 | X1445 | X1446 | X1447 | X1448 | X1449 | X1450 | X1451 | X1452 | X1453 | X1454 | X1455 | X1456 | X1459 | X1460 | X1467 | X1468 | X1469 | X1470 | X1471 | X1472 | X1475 | X1476 | X1485 | X1486 | X1487 | X1488 | X1489 | X1490 | X1491 | X1492 | X1493 | X1494 | X1497 | X1498 | X1499 | X1500 | X1501 | X1502 | X1503 | X1504 | X1505 | X1506 | X1507 | X1508 | X1509 | X1510 | X1511 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| Q1244 | F1245 | E1246 | P1247 | V1248 | P1249 | P1250 | E1251 | H1252 | P1253 | H1254 | Y1255 | E1256 | V1257 | A1258 | M1259 | L1260 | D1261 | G1262 | T1263 | V1264 | D1265 | T1266 | P1267 | P1268 | C1269 | L1270 | R1271 | L1272 | L1273 | A1273 | H1274 | L1275 | X1276 | X1277 | X1278 | X1279 | X1280 | X1281 | X1282 | X1283 | X1284 | X1285 | X1286 | X1287 | X1288 | X1289 | X1290 | X1291 | X1292 | X1293 | X1294 | X1295 | X1296 | X1297 | X1298 | X1299 | X1300 | X1301 | X1302 | X1303 | X1304 | X1305 | X1306 | X1307 | X1308 | X1309 | C1310 | Q1311 | A1312 | V1313 | V1314 | T1315 | L1316 | L1317 | L1318 | L1319 | L1320 | L1321 | L1322 | L1323 | L1324 | L1325 | L1326 | L1327 | L1328 | L1329 | L1330 | L1331 | L1332 | L1333 | L1334 | L1335 | L1336 |
| X1512 | X1513 | X1514 | X1515 | X1516 | X1517 | X1518 | X1519 | X1520 | X1521 | X1522 | X1523 | X1524 | X1525 | X1526 | X1527 | X1528 | X1529 | X1530 | X1531 | X1532 | X1533 | X1534 | X1535 | X1536 | X1537 | X1538 | X1539 | X1540 | X1541 | X1542 | X1543 | X1544 | X1545 | X1546 | X1547 | X1548 | X1549 | X1550 | X1551 | X1552 | X1553 | X1554 | X1555 | X1563 | X1564 | X1565 | X1566 | X1567 | X1568 | X1569 | X1570 | X1571 | X1572 | X1573 | X1574 | X1575 | X1576 | X1577 | X1578 | X1579 | X1580 | X1581 | X1582 | X1583 | X1584 | X1585 | X1586 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P1587 | A1588 | P1589 | Q1590 | C1591 | P1592 | P1593 | R1594 | L1595 | E1596 | V1597 | Q1598 | M1599 | L1600 | V1603 | S1604 | W1605 | S1606 | R1607 | M1608 | P1609 | M1610 | H1611 | F1612 | L1613 | Q1614 | GLU   | THR   | ARG   | ALA   | GLY   | E1622 | R1623 | L1624 | G1625 | W1626 | A1627 | V1628 | Q1629 | C1630 | Q1631 | D1632 | L1633 | L1634 | T1635 | M1636 | M1637 | A1638 | L1639 | H1640 | L1641 | P1642 | E1643 | E1644 | M1645 | R1646 | C1647 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P740  | E741  | D742  | S745  | C746  | D749  | L750  | S751  | V752  | P753  | F757  | R758  | I759  | N760  | G761  | C762  | P763  | V764  | Q765  | G766  | V767  | F768  | E769  | A770  | F771  | N772  | L773  | D774  | G775  | L776  | F777  | F778  | P779  | V780  | V781  | S784  | A785  | G786  | V787  | K788  | V789  | R790  | F791  | L792  | L793  | H797  | G798  | E799  | F800  | K801  | F802  | L803  | P804  | P805  | P806  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G807  | Y808  | A809  | P810  | C811  | H812  | E813  | A814  | V815  | L816  | P817  | R818  | E819  | R820  | L821  | R822  | L823  | E824  | P825  | I826  | K827  | E828  | Y829  | R830  | R831  | E832  | G833  | P834  | R835  | G836  | P837  | H838  | G841  | P842  | S843  | R844  | C845  | L846  | S847  | H848  | T849  | D850  | F851  | V852  | P853  | C854  | P855  | V856  | D857  | THR   | VAL   | GLN   | I861  | V862  | L863  | P864  | P865  | H866  | L867  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E868  | R869  | I870  | R871  | E872  | K873  | L874  | A875  | E876  | N877  | I878  | H879  | E880  | L881  | Q882  | A883  | L884  | T885  | R886  | I887  | E888  | Q889  | G890  | W891  | T892  | Y893  | G894  | P895  | V896  | R897  | D898  | D899  | N900  | K901  | R902  | L903  | H904  | P905  | C906  | L907  | V908  | N909  | F910  | H911  | S912  | L913  | P914  | E915  | P916  | E917  | R918  | N919  | Y920  | N921  | L922  | Q923  | M924  | S925  | G926  | E927  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| T928  | L929  | K930  | T931  | L932  | L933  | A934  | L935  | G936  | C937  | H938  | V939  | G940  | M941  | A942  | D943  | E944  | K945  | A946  | E947  | D948  | N949  | L950  | K951  | K952  | T953  | K954  | L955  | P956  | K957  | D958  | Y959  | M960  | N961  | S962  | N963  | G964  | A968  | P969  | L970  | D971  | L972  | S973  | H974  | V975  | R976  | L977  | T978  | P979  | A980  | Q981  | T982  | T983  | L984  | V985  | D986  | L987  | L988  | A989  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G992  | V1001 | A1002 | Q1003 | G1004 | W1005 | S1006 | Y1007 | S1008 | A1009 | VAL   | GLN   | ASP   | ILE   | PRO   | ALA   | ARG   | ARG   | ASN   | PRO   | R1020 | Y1024 | R1025 | L1026 | L1027 | D1028 | E1029 | A1030 | L1031 | K1032 | R1033 | S1034 | N1035 | R1036 | D1037 | S1038 | L1039 | C1040 | Q1041 | A1042 | V1043 | R1044 | T1045 | L1046 | L1047 | G1048 | Y1049 | G1050 | Y1051 | N1052 | I1053 | E1054 | PRO   | PRO   | ASP   | GLN   | GLU   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| PRO   | SER   | GLN   | VAL   | GLU   | ASN   | GLN   | SER   | ARG   | TRP   | D1070 | R1071 | V1072 | I1073 | L1074 | F1075 | R1076 | A1077 | E1078 | K1079 | S1080 | Y1081 | T1082 | V1083 | Q1084 | S1085 | G1086 | R1087 | W1088 | Y1089 | F1090 | E1091 | F1092 | E1093 | A1094 | V1095 | T1096 | T1097 | M1100 | R1101 | V1102 | G1103 | W1104 | A1105 | R1106 | P1107 | E1108 | L1109 | R1110 | P1111 | D1112 | V1113 | E1114 | L1115 | G1116 | A1117 | D1118 | E1119 | L1120 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

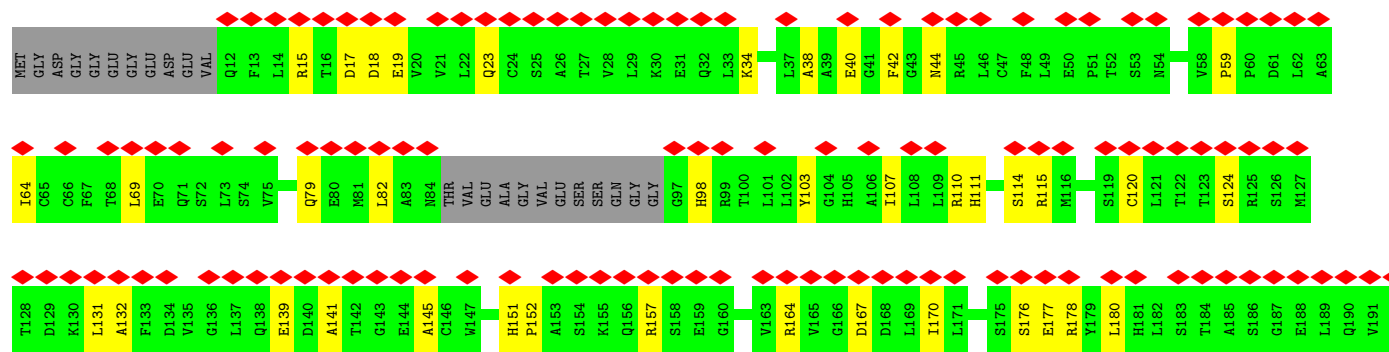
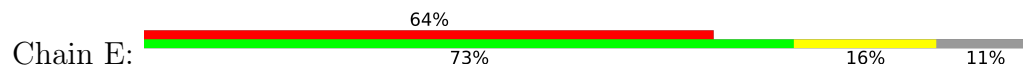


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| X3431 | X3432 | X3433 | X3434 | X3435 | X3436 | X3437 | X3438 | X3439 | X3440 | X3441 | X3442 | X3443 | X3444 | X3445 | X3446 | X3447 | X3448 | X3451 | X3452 | X3453 | X3454 | X3455 | X3456 | X3459 | X3460 | X3461 | X3462 | X3463 | X3464 | X3465 | X3466 | X3467 | X3468 | X3511 | X3512 | X3513 | X3514 | X3515 | X3516 | X3517 | X3518 | X3519 | X3520 | X3521 | X3522 | X3523 | X3524 | X3525 | X3526 | X3527 | X3528 | X3529 | X3530 | X3531 | X3532 | X3533 | X3534 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X3371 | X3372 | X3373 | X3374 | X3375 | X3376 | X3377 | X3378 | X3379 | X3380 | X3381 | X3382 | X3383 | X3384 | X3385 | X3386 | X3387 | X3388 | X3389 | X3390 | X3391 | X3392 | X3393 | X3394 | X3395 | X3396 | X3397 | X3398 | X3399 | X3400 | X3401 | X3402 | X3403 | X3404 | X3405 | X3406 | X3407 | X3408 | X3409 | X3410 | X3411 | X3412 | X3413 | X3414 | X3415 | X3416 | X3417 | X3418 | X3419 | X3420 | X3421 | X3422 | X3423 | X3424 | X3425 | X3426 | X3427 | X3428 | X3429 | X3430 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X3243 | X3244 | X3245 | X3246 | X3247 | X3248 | X3249 | X3250 | X3251 | X3252 | X3253 | X3254 | X3261 | X3262 | X3263 | X3264 | X3265 | X3266 | X3267 | X3268 | X3269 | X3270 | X3271 | X3272 | X3273 | X3274 | X3275 | X3276 | X3277 | X3278 | X3279 | X3280 | X3281 | X3282 | X3283 | X3284 | X3285 | X3286 | X3287 | X3288 | X3289 | X3290 | X3293 | X3294 | X3295 | X3296 | X3297 | X3300 | X3301 | X3302 | X3303 | X3304 | X3305 | X3306 | X3307 | X3308 | X3309 | X3310 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X3311 | X3312 | X3313 | X3314 | X3315 | X3316 | X3317 | X3318 | X3319 | X3320 | X3321 | X3322 | X3323 | X3324 | X3325 | X3326 | X3327 | X3328 | X3329 | X3330 | X3331 | X3332 | X3333 | X3334 | X3335 | X3336 | X3337 | X3338 | X3339 | X3340 | X3341 | X3342 | X3343 | X3344 | X3345 | X3346 | X3347 | X3348 | X3349 | X3350 | X3351 | X3352 | X3353 | X3354 | X3355 | X3356 | X3357 | X3358 | X3359 | X3360 | X3361 | X3362 | X3363 | X3364 | X3365 | X3366 | X3367 | X3368 | X3369 | X3370 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X3177 | X3178 | X3179 | X3182 | X3183 | X3184 | X3185 | X3186 | X3187 | X3188 | X3189 | X3190 | X3191 | X3192 | X3193 | X3194 | X3195 | X3196 | X3197 | X3198 | X3199 | X3200 | X3201 | X3202 | X3203 | X3204 | X3205 | X3206 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 | X3221 | X3222 | X3223 | X3224 | X3225 | X3226 | X3229 | X3230 | X3231 | X3232 | X3233 | X3234 | X3235 | X3236 | X3241 | X3242 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X3036 | X3037 | X3038 | X3039 | X3040 | X3041 | X3042 | X3043 | X3044 | X3045 | X3046 | X3047 | X3048 | X3049 | X3050 | X3053 | X3054 | X3055 | X3056 | X3057 | X3058 | X3059 | X3060 | X3061 | X3062 | X3063 | X3064 | X3065 | X3066 | X3067 | X3068 | X3069 | X3070 | X3073 | X3074 | X3075 | X3076 | X3077 | X3078 | X3079 | X3080 | X3081 | X3082 | X3083 | X3084 | X3085 | X3086 | X3087 | X3088 | X3089 | X3090 | X3091 | X3092 | X3093 | X3094 | X3095 | X3096 | X3097 | X3098 | X3099 | X3100 | X3101 | X3102 | X3103 | X3104 | X3105 | X3106 | X3107 | X3108 | X3109 | X3110 | X3111 | X3112 | X3113 | X3114 | X3115 | X3116 | X3117 | X3118 | X3119 | X3120 | X3121 | X3122 | X3123 | X3124 | X3125 | X3126 | X3127 | X3128 | X3129 | X3130 | X3131 | X3132 | X3133 | X3134 | X3135 | X3136 | X3137 | X3138 | X3139 | X3140 | X3141 | X3142 | X3143 | X3144 | X3145 | X3146 | X3147 | X3148 | X3149 | X3150 | X3153 | X3156 | X3157 | X3160 | X3163 | X3170 | X3171 | X3172 | X3173 | X3174 | X3175 | X3176 |
| X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2962 | X2963 | X2964 | X2965 | X2966 | X2967 | X2968 | X2969 | X2970 | X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X2980 | X2981 | X2982 | X2983 | X2984 | X2985 | X2986 | X2987 | X2988 | X2989 | X2990 | X2991 | X2992 | X2993 | X2994 | X2995 | X2996 | X2997 | X2998 | X2999 | X3000 | X3001 | X3002 | X3003 | X3004 | X3005 | X3006 | X3009 | X3010 | X3011 | X3012 | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 | X3021 | X3022 | X3023 | X3024 | X3025 | X3026 | X3027 | X3028 | X3029 | X3030 | X3031 | X3034 | X3035 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E2893 | L2894 | E2895 | A2896 | E2897 | G2898 | G2899 | G2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | T2912 | A2913 | G2914 | E2915 | P2916 | A2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | L2929 | Q2931 | N2932 | G2933 | G2934 | Y2935 | A2936 | P2937 | T2938 | R2939 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| ARG   | THR   | GLU   | LYS   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SER   | GLN   | THR   | ALA   | GLN   | THR   | TYR   | ASP   | PRO   | ARG   | GLU   | GLY   | Y2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | V2865 | T2866 | L2867 | S2868 | R2869 | E2870 | L2871 | Q2872 | A2873 | M2874 | A2875 | E2876 | L2877 | Q2878 | A2879 | E2880 | N2881 | H2882 | H2883 | N2884 | T2885 | W2886 | G2887 | R2888 | K2889 | K2890 | K2891 | K2892 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| N2773 | N2774 | W2775 | S2776 | L2777 | G2778 | E2779 | N2780 | L2781 | D2782 | E2783 | E2784 | L2785 | K2786 | T2787 | H2788 | P2789 | N2790 | L2791 | R2792 | P2793 | Y2794 | K2795 | T2796 | F2797 | S2798 | E2799 | K2800 | D2801 | K2802 | E2803 | L2804 | Y2805 | R2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | N2816 | L2817 | A2818 | W2819 | E2820 | W2821 | T2822 | L2823 | E2824 | K2825 | A2826 | R2827 | E2828 | G2829 | E2830 | GLU   | GLU   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X2616 | X2617 | X2618 | X2619 | X2620 | X2621 | X2622 | X2623 | X2624 | X2625 | X2626 | X2627 | X2628 | X2629 | X2630 | X2631 | X2632 | X2633 | X2634 | X2635 | X2636 | X2637 | X2638 | X2639 | X2641 | X2642 | X2643 | X2644 | X2645 | X2646 | X2647 | X2648 | X2649 | X2650 | X2651 | X2652 | X2653 | X2654 | X2655 | X2656 | X2657 | X2658 | X2659 | X2662 | X2663 | X2664 | X2665 | X2666 | X2669 | X2670 | X2671 | X2672 | X2673 | X2674 | X2675 | X2676 | X2677 | X2678 | X2679 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X2683 | X2684 | X2685 | X2686 | X2687 | X2688 | X2689 | X2690 | X2691 | X2692 | X2693 | X2694 | X2695 | X2696 | X2697 | X2698 | X2699 | X2700 | X2701 | X2702 | X2703 | X2704 | X2705 | X2706 | X2641 | X2642 | X2643 | X2644 | X2645 | X2646 | X2647 | X2648 | X2649 | X2650 | X2651 | X2652 | X2653 | X2654 | X2655 | X2656 | X2657 | X2658 | X2659 | X2662 | X2663 | X2664 | X2665 | X2666 | X2669 | X2670 | X2671 | X2672 | X2673 | X2674 | X2675 | X2676 | X2677 | X2678 | X2679 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X2541 | X2544 | X2550 | X2551 | X2552 | X2553 | X2554 | X2555 | X2556 | X2557 | X2558 | X2559 | X2560 | X2561 | X2562 | X2563 | X2564 | X2565 | X2566 | X2567 | X2568 | X2569 | X2570 | X2582 | X2583 | X2584 | X2585 | X2586 | X2587 | X2588 | X2589 | X2590 | X2591 | X2592 | X2593 | X2594 | X2595 | X2596 | X2597 | X2598 | X2599 | X2600 | X2601 | X2602 | X2603 | X2604 | X2605 | X2606 | X2607 | X2608 | X2609 | X2610 | X2611 | X2612 | X2613 | X2614 | X2615 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

|     |     |       |       |       |       |       |       |       |       |       |       |
|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| LEU | GLY | E4229 | P4155 | R4085 | K4021 | M9955 | L3888 | K3823 | E3757 | E3685 | X3535 |
| ALA | GLY | K4230 | H4156 | G4086 | D4022 | S3956 | L3889 | K3824 | M3758 | E3686 | X3536 |
| ALA | ASP | F4234 | D4157 | I4087 | M4023 | V9957 | L3890 | E3825 | E3759 | E3687 | X3537 |
| ALA | ASP | F4234 | P4158 | I4088 | V4024 | A3958 | L3890 | V3826 | K3760 | E3688 | X3538 |
| ALA | GLU | E4239 | R4159 | S4089 | L4027 | V9961 | E3893 | F3829 | Q3761 | E3689 | X3539 |
| ARG | VAL | D4240 | L4160 | K4090 | L4030 | N3962 | Q3894 | Q3830 | R3762 | V3690 | X3540 |
| ALA | GLY | T4241 | R4161 | K4091 | L4031 | N3963 | H3895 | S3831 | L3763 | E3691 | X3541 |
| GLY | GLY | I4242 | L4164 | D4092 | E4032 | S9964 | N3896 | I3832 | L3764 | X3602 | X3542 |
| LEU | HIS | I4242 | E4165 | F4093 | G4033 | S9964 | N3897 | I3832 | Y3765 | X3603 | X3543 |
| LEU | GLU | M4245 | E4165 | Q4094 | G4033 | L3965 | D3898 | Q3833 | Q3766 | X3604 | X3544 |
| GLY | ALA | Q4246 | E4168 | K4095 | M4034 | F3966 | F3899 | M3836 | S3768 | Q3767 | X3545 |
| TYR | GLY | Q4246 | E4168 | A4096 | V4035 | Y9966 | Q3900 | Q3837 | R3769 | X3605 | X3546 |
| ARG | GLY | A4249 | E4168 | M4097 | V4036 | G9971 | N3901 | Q3837 | L3770 | X3606 | X3547 |
| ARG | GLY | Q4250 | L4171 | D4098 | M4037 | P9972 | R3904 | S3840 | A3709 | X3607 | X3548 |
| LEU | LYS | I4251 | E4172 | S4099 | Q4038 | C3973 | T3905 | V3841 | L3710 | X3608 | X3549 |
| ARG | VAL | S4252 | Y4173 | Q4100 | M4039 | T3974 | Q3906 | L3842 | T3711 | X3609 | X3550 |
| ARG | VAL | E4253 | F4174 | K4101 | D4046 | G3975 | T3907 | D3843 | E3712 | X3610 | X3551 |
| VAL | THR | P4176 | R4175 | Q4102 | M4047 | N3976 | T3912 | L3844 | K3713 | X3612 | X3552 |
| ARG | ARG | GLY   | P4176 | F4103 | R4042 | Q3977 | Q3908 | L3844 | S3714 | X3613 | X3553 |
| ARG | ARG | GLY   | Y4177 | T4104 | Q4043 | Q3978 | G3909 | N3845 | K3715 | X3613 | X3554 |
| LEU | LEU | GLY   | L4178 | G4105 | M4044 | S9979 | T3910 | A3846 | L3716 | X3613 | X3555 |
| ARG | GLY | GLY   | G4179 | P4106 | V4045 | L3980 | T3911 | F3847 | D3717 | X3613 | X3556 |
| THR | THR | ALA   | R4180 | P4106 | D4046 | L3980 | T3912 | E3848 | E3718 | X3613 | X3557 |
| ALA | ALA | E4182 | I4181 | E4107 | M4047 | A3981 | T3912 | E3848 | D3719 | X3613 | X3558 |
| ASP | ASP | E4182 | E4182 | L4048 | L4048 | H9982 | T3916 | Q3850 | Y3720 | X3613 | X3559 |
| ASP | ASP | A4186 | A4186 | Q4109 | V4049 | S9983 | T3917 | N3851 | C3786 | X3613 | X3560 |
| GLY | GLY | S4187 | S4187 | F4110 | E4050 | R3984 | T3917 | N3852 | Y3722 | X3613 | X3561 |
| GLY | GLY | R4188 | R4188 | F4110 | S4051 | L3985 | T3917 | K3852 | G3788 | X3613 | X3562 |
| GLY | GLY | R4189 | R4189 | S4113 | S4052 | N9986 | V3920 | A3853 | A3724 | X3613 | X3563 |
| ALA | ALA | R4192 | R4192 | E4116 | M4054 | A3988 | D3921 | G3854 | Y3725 | X3613 | X3564 |
| ALA | ALA | R4192 | R4192 | A4117 | V4055 | V3990 | L3924 | G3855 | A3726 | X3613 | X3565 |
| ALA | ALA | R4192 | R4192 | E4117 | V4055 | V3990 | R3925 | G3857 | D3727 | X3613 | X3566 |
| LEU | LEU | R4192 | R4192 | D4118 | V4055 | V3990 | L3926 | M3858 | L3727 | X3613 | X3567 |
| TRP | TRP | R4192 | R4192 | E4119 | L4059 | G3991 | Q3927 | N3859 | M3729 | X3613 | X3568 |
| ALA | ALA | R4192 | R4192 | M4120 | K4060 | F3992 | E3928 | V3859 | K3731 | X3613 | X3569 |
| VAL | VAL | R4192 | R4192 | E4121 | F4061 | H3994 | S3929 | N3860 | A3730 | X3613 | X3570 |
| VAL | VAL | R4192 | R4192 | M4122 | F4062 | V3995 | I3930 | E3861 | K3731 | X3613 | X3571 |
| ALA | ALA | R4192 | R4192 | I4123 | D4063 | F3996 | S3931 | D3862 | S3732 | X3613 | X3572 |
| ALA | ALA | R4192 | R4192 | M4124 | M4064 | A3997 | F3933 | G3863 | C3733 | X3613 | X3573 |
| ALA | ALA | R4192 | R4192 | F4125 | F4065 | H3998 | Y3934 | T3864 | H3734 | X3613 | X3574 |
| ALA | ALA | R4192 | R4192 | E4126 | F4065 | M3999 | Y3935 | V3865 | E3736 | X3613 | X3575 |
| ALA | ALA | R4192 | R4192 | E4127 | L4066 | M4001 | K3935 | V3866 | E3737 | X3613 | X3576 |
| ALA | ALA | R4192 | R4192 | M4129 | L4068 | K4002 | Y3937 | N3867 | E3737 | X3613 | X3577 |
| ALA | ALA | R4192 | R4192 | M4130 | K4069 | L4003 | S3938 | S3803 | G3738 | X3613 | X3578 |
| ALA | ALA | R4192 | R4192 | R4131 | D4070 | A4004 | S3938 | N3805 | G3739 | X3613 | X3579 |
| ALA | ALA | R4192 | R4192 | F4132 | I4071 | Q4005 | Q3939 | G3806 | E3740 | X3613 | X3580 |
| ALA | ALA | R4192 | R4192 | Q4133 | V4072 | Q4005 | K3940 | N3870 | N3741 | X3613 | X3581 |
| ALA | ALA | R4192 | R4192 | Q4133 | G4073 | S4008 | D3941 | G3871 | GLY   | X3613 | X3582 |
| ALA | ALA | R4192 | R4192 | A4136 | S4074 | Q4009 | V3942 | E3872 | GLY   | X3613 | X3583 |
| ALA | ALA | R4192 | R4192 | R4137 | E4075 | Q4009 | I3943 | K3873 | ALA   | X3613 | X3584 |
| ALA | ALA | R4192 | R4192 | D4138 | A4076 | I4010 | I3943 | V3874 | GLU   | X3613 | X3585 |
| ALA | ALA | R4192 | R4192 | T4139 | F4077 | E4011 | Q3946 | M3815 | GLU   | X3613 | X3586 |
| ALA | ALA | R4192 | R4192 | G4140 | F4077 | L4012 | G3947 | M3816 | E3747 | X3613 | X3587 |
| ALA | ALA | R4192 | R4192 | L4146 | Q4078 | L4013 | K3948 | L3818 | D3676 | X3613 | X3588 |
| ALA | ALA | R4192 | R4192 | L4147 | D4079 | L4016 | N3949 | Y3819 | V3749 | X3613 | X3589 |
| ALA | ALA | R4192 | R4192 | E4152 | Y4080 | L4019 | N3950 | L3820 | E3750 | X3613 | X3590 |
| ALA | ALA | R4192 | R4192 | H4153 | V4081 | Q4020 | F3951 | K3821 | V3751 | X3613 | X3591 |
| ALA | ALA | R4192 | R4192 | V4154 | T4082 | Q4020 | A3954 | D3822 | E3752 | X3613 | X3592 |
| ALA | ALA | R4192 | R4192 | V4154 | D4083 | Q4020 | A3954 | E3755 | K3756 | X3613 | X3593 |
| ALA | ALA | R4192 | R4192 | V4154 | P4084 | Q4020 | A3954 | E3755 | K3756 | X3613 | X3594 |



• Molecule 2: ryanodine receptor 1



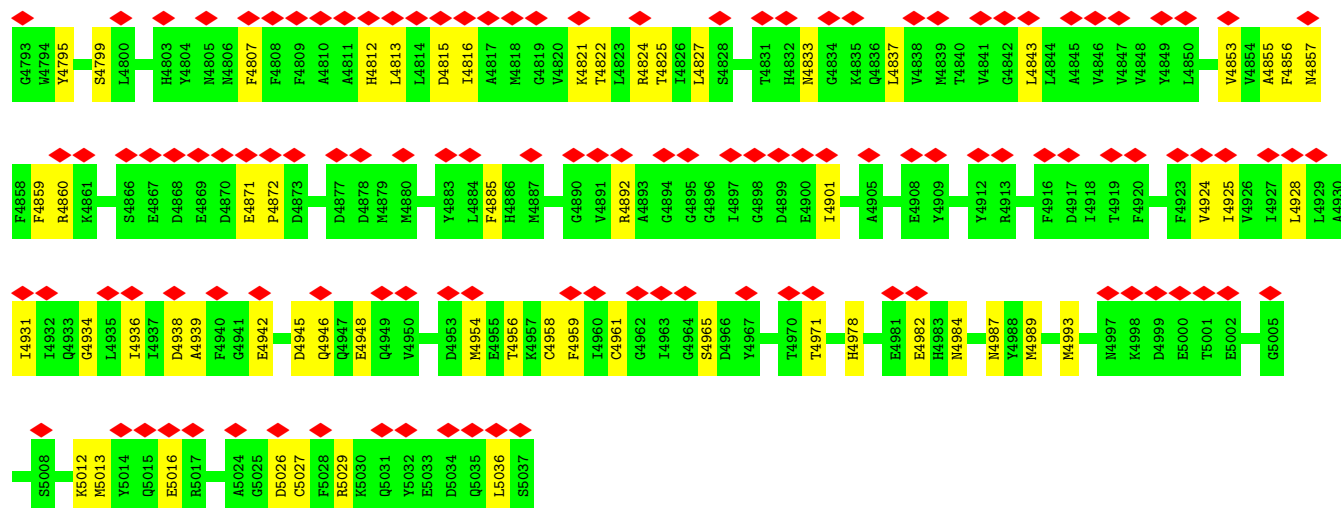




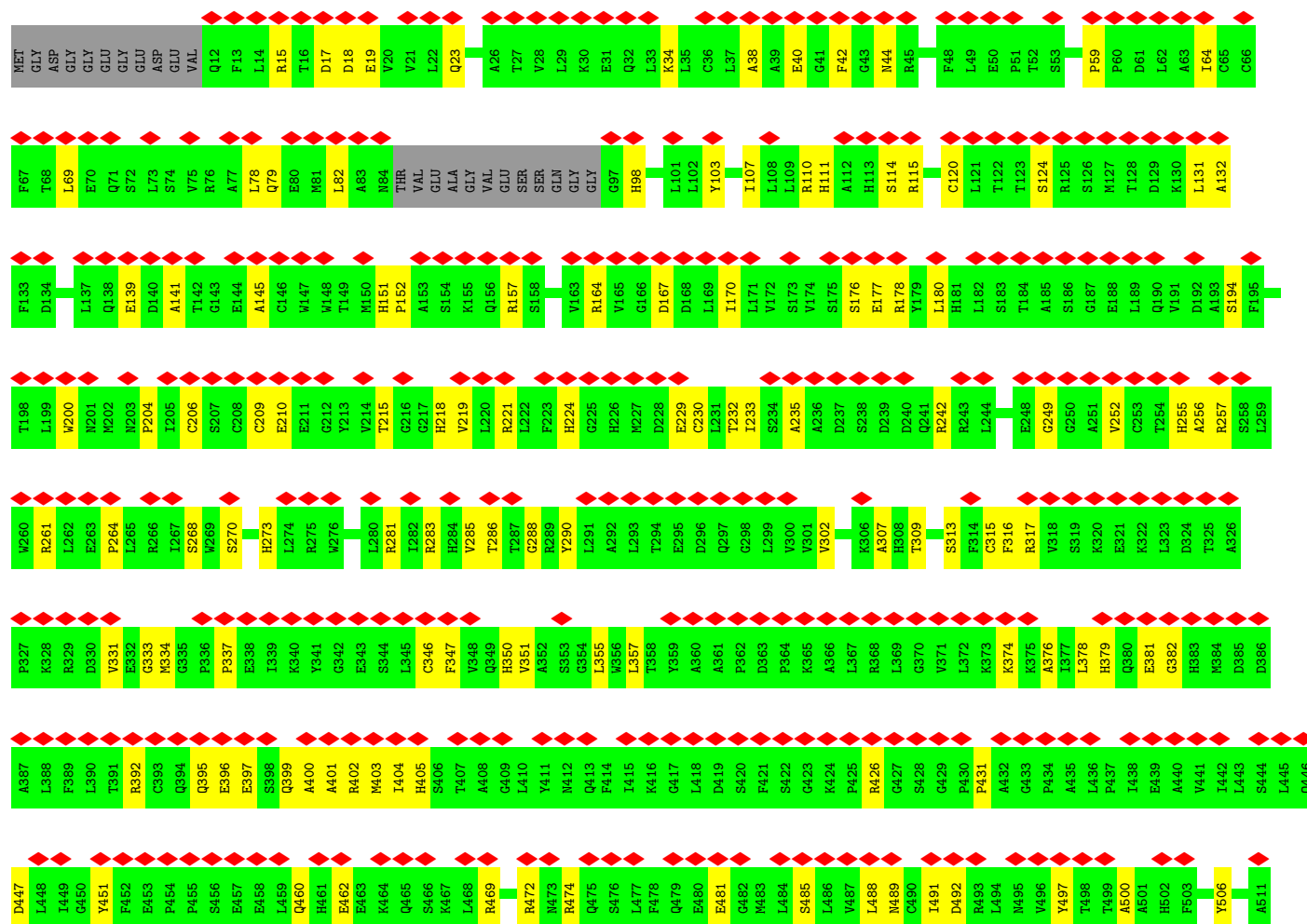
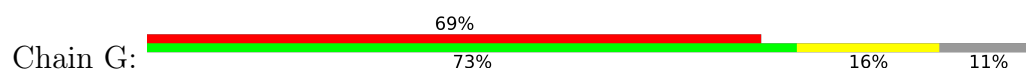
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L2791 | R2792 | P2793 | N2794 | F2795 | D2796 | P2797 | R2798 | E2799 | K2800 | D2801 | K2802 | E2803 | L2804 | Y2805 | R2806 | W2807 | P2808 | L2809 | K2810 | E2811 | L2812 | L2813 | K2814 | L2815 | M2816 | L2817 | A2818 | L2819 | E2820 | W2821 | L2822 | L2823 | E2824 | K2825 | A2826 | K2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | THR   | GLY   | LYS   | LYS   | S2776 | Y2777 | G2778 | E2779 | L2780 | V2781 | D2782 | E2783 | E2784 | L2785 | K2786 | L2787 | P2788 | M2789 | P2790 |
| X2640 | X2641 | X2644 | X2645 | X2646 | X2647 | X2648 | X2649 | X2650 | X2651 | X2652 | X2653 | X2654 | X2655 | X2658 | X2659 | X2660 | X2661 | X2662 | X2663 | X2664 | X2665 | X2666 | X2667 | X2668 | X2669 | X2670 | X2671 | X2672 | X2673 | X2674 | X2675 | X2676 | X2677 | X2678 | X2679 | X2680 | X2681 | X2682 | X2683 | X2684 | X2685 | X2686 | X2687 | X2688 | X2689 | X2690 | X2691 | X2692 | X2693 | X2694 | X2695 | X2696 | X2697 | X2698 | X2699 | X2700 |       |       |       |       |       |       |
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| X2506 | X2507 | X2510 | X2511 | X2512 | X2513 | X2514 | X2515 | X2516 | X2517 | X2518 | X2519 | X2520 | X2521 | X2522 | X2523 | X2524 | X2525 | X2526 | X2527 | X2528 | X2529 | X2530 | X2531 | X2532 | X2533 | X2534 | X2535 | X2536 | X2537 | X2538 | X2541 | X2542 | X2543 | X2544 | X2545 | X2548 | X2552 | X2555 | X2556 | X2557 | X2558 | X2559 | X2560 | X2561 | X2562 | X2563 | X2564 | X2565 | X2566 | X2567 | X2568 | X2569 | X2570 |       |       |       |       |       |       |       |       |       |
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| R2369 | G2370 | E2371 | G2372 | G2373 | S2374 | G2375 | L2376 | L2377 | A2378 | A2379 | I2380 | E2381 | E2382 | A2383 | L2384 | R2385 | I2386 | S2387 | E2388 | D2389 | P2390 | A2391 | R2392 | D2393 | G2394 | P2395 | GLY   | VAL   | ARG   | ASP   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   | PRO   | PRO   | GLU   | N2414 | R2415 | V2416 | S2424 | A2427 | A2428 | L2429 | L2430 | D2431 | L2432 | L2433 | G2434 | R2435 |       |       |       |       |       |       |       |       |       |
| Y2301 | L2302 | A2303 | G2304 | C2305 | G2306 | S2309 | C2310 | P2311 | M2312 | L2313 | L2314 | A2315 | K2316 | P2319 | D2320 | I2321 | C2326 | G2328 | E2329 | R2330 | D2333 | F2334 | L2335 | R2336 | F2340 | V2341 | N2342 | G2343 | E2344 | S2345 | V2346 | E2347 | E2348 | N2349 | A2350 | N2351 | V2352 | V2353 | V2354 | R2355 | L2356 | L2357 | L2358 | R2359 | K2360 | P2361 | E2362 | C2363 | F2364 | G2365 | P2366 | A2367 | L2368 |       |       |       |       |       |       |       |       |       |
| L2236 | C2237 | Y2238 | R2241 | I2242 | S2243 | R2244 | Q2247 | R2248 | F2251 | D2252 | H2253 | L2254 | S2255 | Y2256 | L2257 | L2258 | E2259 | N2260 | S2261 | G2262 | L2263 | G2264 | L2265 | G2266 | M2267 | Q2268 | G2269 | S2270 | T2271 | P2272 | L2273 | D2274 | V2275 | A2276 | A2277 | A2278 | I2281 | D2282 | N2283 | N2284 | E2285 | L2286 | A2287 | L2288 | A2289 | L2290 | Q2291 | E2292 | Q2293 | L2294 | L2295 | V2296 | V2299 | S2300 |       |       |       |       |       |       |       |       |
| Q2173 | W2176 | L2177 | M2178 | I2179 | Q2180 | G2183 | N2184 | L2185 | M2186 | N2187 | N2188 | K2189 | V2190 | F2191 | Y2192 | Q2193 | H2194 | N2196 | L2197 | M2198 | R2199 | A2200 | L2201 | G2202 | M2203 | H2204 | E2205 | T2206 | V2207 | N2208 | E2209 | V2210 | N2211 | V2212 | N2213 | V2214 | L2215 | G2216 | Q2217 | G2218 | E2219 | T2220 | K2221 | E2222 | L2223 | P2226 | K2227 | M2228 | V2229 | T2230 | S2231 | C2232 | G2233 | R2234 | F2235 |       |       |       |       |       |       |       |
| W2105 | A2106 | Q2107 | E2108 | D2109 | Y2110 | Q2111 | Q2112 | S2113 | P2114 | E2115 | L2116 | V2117 | R2118 | A2119 | M2120 | F2121 | S2122 | L2123 | R2126 | Q2127 | Y2128 | D2129 | G2130 | L2131 | G2132 | E2133 | L2134 | L2135 | R2136 | A2137 | L2138 | P2139 | R2140 | A2141 | Y2142 | T2143 | I2144 | S2145 | P2146 | S2147 | S2148 | V2149 | E2150 | D2151 | L2159 | I2162 | R2163 | S2164 | L2165 | L2166 | L2167 | V2168 | Q2169 | M2170 | G2171 | P2172 |       |       |       |       |       |       |
| H2041 | C2042 | G2043 | I2044 | Q2045 | L2046 | E2047 | G2048 | GLU   | GLU   | GLU   | GLU   | PRO   | GLU   | GLU   | THR   | SER   | LEU   | SER   | ARG   | LEU   | ARG   | LEU   | VAL   | ARG   | LEU   | VAL   | LYS   | LYS   | GLU   | GLU   | LYS   | GLU   | GLU   | LEU   | PRO   | ALA   | GLU   | K2089 | K2090 | P2091 | Q2092 | S2093 | L2094 | Q2095 | L2096 | L2097 | V2098 | R2104 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| Q1973 | R1974 | S1975 | R1976 | Y1977 | A1978 | L1979 | L1980 | M1981 | R1982 | A1983 | F1984 | T1985 | M1986 | S1987 | A1988 | A1989 | E1990 | T1991 | A1992 | R1993 | T1995 | R1996 | E1997 | F1998 | S2000 | P2001 | P2002 | Q2003 | E2004 | Q2005 | N2006 | N2007 | M2008 | L2009 | L2010 | H2011 | F2012 | K2013 | A2016 | D2017 | E2018 | E2019 | D2020 | C2021 | P2022 | L2023 | P2024 | E2025 | D2026 | L2027 | R2028 | Q2029 | D2030 | L2039 | A2040 |       |       |       |       |       |       |       |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
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| G3788 | G3789 | T3790 | G3791 | A3792 | M3793 | T3794 | G3795 | S3796 | G3799 |       |       |       | L3800 | G3801 | T3802 | S3803 | L3804 | L3805 | N3806 | G3807 | G3808 | N3809 | V3812 |       |       |       | Q3813 | Q3814 | K3815 | M3816 | L3817 | L3818 | G3819 | L3820 | K3821 | L3822 | K3823 | K3824 | E3825 | V3826 | G3827 | F3828 | F3829 | S3830 | S3831 | L3832 | Q3833 | A3834 | Q3837 |       |       |       | T3838 | C3839 | S3840 | V3841 | L3842 | D3843 | L3844 | N3845 | E3848 |       |       |       | R3849 | G3850 | N3851 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| K3726 | D3727 | L3728 | M3729 | A3730 | S3732 | G3733 | H3734 | L3735 | E3736 | E3737 | D3738 | G3739 | E3740 | GLY   | GLU   | ALA   | GLU   | GLU   | E3747 | E3748 | V3749 | E3750 | V3751 | S3752 | F3753 | E3754 | E3755 | M3758 | E3759 | R3762 | L3763 | L3764 | Y3765 | Q3766 | S3768 | R3769 | L3770 | H3771 | T3772 | R3773 | G3774 | A3775 | A3776 | E3777 | M3778 | V3779 | L3780 | Q3781 | K3782 | L3783 | S3784 | A3785 | C3786 | K3787 | Y3725 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| T3664 | E3665 | D3666 | H3667 | S3668 | F3669 | E3670 | D3671 | R3672 | M3673 | L3674 | D3675 | L3676 | S3677 | G3678 | A3680 | G3681 | E3682 | Q3683 | E3684 | E3685 | E3686 | E3687 | E3688 | E3689 | V3690 | E3691 | E3692 | K3693 | K3694 | P3697 | L3698 | H3699 | Q3700 | L3701 | H3704 | F3705 | S3706 | R3707 | T3708 | A3709 | L3710 | T3711 | E3712 | K3713 | S3714 | K3715 | L3716 | D3717 | E3718 | D3719 | Y3720 | L3721 | Y3722 | M3723 | A3724 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
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| X3511 | X3512 | X3513 | X3514 | X3515 | X3516 | X3517 | X3518 | X3519 | X3520 | X3521 | X3522 | X3523 | X3524 | X3525 | X3526 | X3527 | X3528 | X3529 | X3530 | X3531 | X3532 | X3533 | X3534 | X3535 | X3536 | X3537 | X3538 | X3539 | X3540 | X3543 |       | X3544 | X3545 | X3546 | X3547 | X3548 | X3549 | X3550 | X3551 | X3552 | X3556 |       | X3557 | X3558 | X3559 | X3560 | X3561 | X3562 | X3563 | X3564 | X3565 | X3566 | X3567 | X3568 | X3569 | X3570 | X3571 | X3572 | X3573 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| X3398 | X3399 | X3400 | X3401 | X3402 | X3405 |       | X3406 | X3407 | X3408 | X3409 | X3410 | X3411 | X3412 | X3413 | X3414 | X3415 | X3416 | X3417 | X3418 | X3419 | X3420 | X3421 | X3422 | X3423 | X3424 | X3425 | X3426 | X3427 | X3428 | X3429 | X3430 | X3431 | X3432 | X3433 | X3434 | X3435 | X3436 | X3437 | X3438 | X3439 | X3440 | X3441 | X3442 | X3443 | X3444 | X3447 |       | X3448 | X3458 |       | X3461 | X3462 | X3463 | X3464 | X3465 | X3466 | X3467 | X3468 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| X3337 | X3338 | X3339 | X3340 | X3341 | X3342 | X3343 | X3344 | X3345 | X3346 | X3347 | X3348 | X3349 | X3350 | X3351 | X3352 | X3353 | X3354 | X3355 | X3356 | X3357 | X3358 | X3359 | X3360 | X3361 | X3362 | X3363 | X3366 |       | X3367 | X3368 | X3369 | X3370 | X3371 | X3372 | X3373 | X3374 | X3375 | X3376 | X3377 | X3378 | X3379 | X3380 | X3381 | X3382 | X3383 | X3384 | X3385 | X3386 | X3387 | X3388 | X3389 | X3390 | X3391 | X3392 | X3393 | X3394 | X3395 | X3396 | X3397 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| X3274 | X3275 | X3276 | X3277 | X3278 | X3279 | X3280 | X3281 | X3282 | X3283 | X3284 | X3285 | X3286 | X3287 | X3288 | X3289 | X3290 | X3291 | X3292 | X3295 |       | X3296 | X3297 | X3298 | X3299 | X3300 | X3301 | X3302 | X3303 | X3307 |       | X3308 | X3309 | X3310 | X3311 | X3312 | X3313 | X3314 | X3315 | X3316 | X3317 | X3318 | X3319 | X3320 | X3321 | X3322 | X3323 | X3324 | X3325 | X3326 | X3327 | X3328 | X3329 | X3330 | X3331 | X3332 | X3333 | X3334 | X3335 | X3336 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| X3201 | X3202 | X3203 | X3204 | X3205 | X3206 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 | X3221 | X3222 | X3223 | X3228 |       | X3229 | X3230 | X3231 | X3232 | X3233 | X3234 | X3235 | X3236 | X3237 | X3238 | X3239 | X3240 | X3241 | X3242 | X3243 | X3244 | X3245 | X3246 | X3247 | X3248 | X3249 | X3250 | X3251 | X3252 | X3253 | X3254 | X3255 | X3256 | X3257 | X3258 | X3259 | X3260 | X3261 | X3262 | X3263 | X3264 | X3265 | X3266 | X3267 | X3268 | X3269 | X3270 | X3271 | X3272 | X3273 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| X3052 | X3053 | X3054 | X3055 | X3056 | X3057 | X3058 | X3059 | X3060 | X3061 | X3062 | X3063 | X3064 | X3065 | X3066 | X3067 | X3068 | X3069 | X3070 | X3071 | X3072 | X3073 | X3074 | X3075 | X3076 | X3077 | X3078 | X3079 | X3080 | X3081 | X3082 | X3083 | X3084 | X3085 | X3086 | X3087 | X3088 | X3089 | X3090 | X3091 | X3092 | X3093 | X3094 | X3095 | X3096 | X3097 | X3098 | X3099 | X3100 | X3101 | X3102 | X3103 | X3104 | X3105 | X3106 | X3107 | X3108 | X3109 | X3110 | X3111 | X3112 | X3113 | X3114 | X3115 | X3116 | X3117 | X3118 | X3119 | X3120 | X3121 | X3122 | X3123 | X3124 | X3125 | X3126 | X3127 | X3128 | X3129 | X3130 | X3131 | X3132 | X3133 | X3134 | X3135 | X3136 | X3137 | X3138 | X3139 | X3140 | X3141 | X3142 | X3143 | X3144 | X3145 | X3146 | X3147 | X3148 | X3158 |  |  |  |  |  |
| X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X2980 | X2981 | X2982 | X2983 | X2984 | X2985 | X2986 | X2987 | X2988 | X2989 | X2990 | X2991 | X2992 | X3012 |       | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 | X3021 | X3022 | X3023 | X3024 | X3025 | X3026 | X3027 | X3028 | X3029 | X3030 | X3031 | X3032 | X3033 | X3034 | X3035 | X3036 | X3037 | X3038 | X3039 | X3040 | X3041 | X3042 | X3043 | X3044 | X3045 | X3046 | X3047 | X3048 | X3049 | X3050 | X3051 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| L2911 | T2912 | A2913 | K2914 | E2915 | K2916 | A2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | Q2872 | N2933 | G2934 | Y2935 | A2936 | V2937 | T2938 | R2939 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2962 | X2963 | X2964 | X2965 | X2966 | X2967 | X2968 | X2969 | X2970 | X2971 | X2972 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |
| PRO   | ARG   | GLU   | GLY   | Y2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | T2865 | T2866 | L2867 | S2868 | E2869 | E2870 | L2871 | Q2872 | N2873 | M2874 | A2875 | E2876 | Q2877 | L2878 | A2879 | E2880 | N2881 | T2882 | H2883 | N2884 | T2885 | T2886 | G2887 | R2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | T2897 | G2898 | G2899 | T2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | X2908 | D2909 | T2910 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |

|       |       |       |       |       |       |     |     |     |     |       |       |
|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-------|-------|
| K3852 | K3918 | Y3989 | D4063 | E4126 | K4214 | ALA | ALA | PRO | GLU | I4659 | G4729 |
| A3853 | C3918 | V3990 | M4064 | E4127 | F4217 | ALA | GLY | SER | GLY | I4662 | D4730 |
| G3854 | V3920 | F3991 | F4065 | F4128 | L4218 | GLY | THR | PRO | ALA | M4662 | E4734 |
| L3855 | D3921 | L3993 | L4068 | M4130 | V4221 | GLY | ALA | ALA | GLY | L4663 | E4735 |
| L3856 | Y3922 | H3994 | K4069 | R4131 | W4222 | ALA | GLY | GLY | GLY | L4664 | R4736 |
| L3857 | L3923 | F3995 | D4070 | F4135 | W4223 | GLY | ALA | SER | ASP | K4665 | L4737 |
| L3858 | L3924 | A3997 | G4073 | A4136 | E4224 | ALA | ALA | PRO | GLY | V4666 | A4738 |
| V3859 | R3925 | H3998 | S4074 | A4137 | E4225 | THR | ALA | LYS | ALA | R4673 | E4739 |
| L3860 | L3926 | M3999 | E4075 | D4138 | E4226 | ALA | LEU | ARG | GLY | E4674 | L4740 |
| L3861 | Q3927 | M4000 | S4076 | R4139 | G4227 | LEU | LEU | GLY | GLY | K4675 | L4741 |
| L3862 | E3928 | M4001 | A4076 | N4142 | E4228 | ALA | THR | GLY | ASP | E4676 | G4742 |
| L3863 | L3930 | L4002 | F4077 | L4150 | A4229 | ALA | ALA | GLY | GLY | L4677 | M4743 |
| L3864 | S3931 | M4004 | Q4078 | L4151 | E4230 | ALA | ALA | ASP | GLY | A4678 | D4744 |
| V3865 | D3932 | Q4005 | D4079 | V4154 | E4232 | ALA | ALA | GLY | GLY | L4745 | L4745 |
| L3866 | W3935 | S4008 | Y4080 | P4155 | E4239 | ARG | ALA | GLY | GLY | L4681 | A4746 |
| L3867 | Y3936 | L4017 | Y4081 | H4156 | E4240 | ALA | GLY | GLY | GLY | E4682 | S4747 |
| L3868 | Y3937 | L4018 | T4082 | D4157 | D4241 | GLY | GLY | GLY | GLY | F4683 | L4748 |
| L3869 | S3938 | L4019 | D4083 | P4158 | T4242 | GLY | GLY | GLY | GLY | Y4687 | E4749 |
| L3870 | G3939 | L4016 | F4084 | R4159 | L4243 | VAL | GLY | PRO | GLY | I4688 | L4750 |
| L3871 | K3940 | L4017 | R4085 | F4163 | M4245 | GLY | GLY | GLY | GLY | T4689 | T4751 |
| L3872 | D3941 | L4018 | Y4086 | L4171 | Q4246 | ALA | ALA | PRO | ALA | E4690 | A4752 |
| L3873 | L3942 | L4019 | I4088 | F4175 | E4249 | LYS | VAL | GLY | GLY | Q4691 | H4753 |
| Y3874 | E3944 | L4022 | S4089 | A4176 | A4250 | ALA | THR | GLY | GLY | E4692 | L4754 |
| K3875 | E3945 | M4023 | K4090 | F4177 | T4251 | ALA | VAL | GLY | GLY | G4693 | E4755 |
| A3876 | Q3946 | W4024 | K4091 | A4178 | S4252 | ARG | THR | GLY | GLY | D4694 | R4756 |
| L3877 | G3947 | L4027 | D4092 | R4188 | E4253 | ARG | VAL | GLY | GLY | D4695 | K4757 |
| L3878 | K3948 | L4030 | F4093 | I4189 | PRO   | LEU | ALA | GLY | GLY | Y4696 | D4758 |
| L3879 | E3949 | L4031 | Q4094 | I4190 | GLU   | LEU | ALA | ALA | GLY | V4697 | D4759 |
| L3880 | N3950 | L4032 | K4095 | E4182 | GLY   | GLY | GLY | ASP | GLY | K4698 | P4760 |
| L3881 | M3955 | L4033 | A4096 | G4185 | GLY   | GLY | GLY | GLY | GLY | W4701 | P4761 |
| L3882 | S3956 | L4034 | A4097 | A4186 | GLY   | THR | GLY | GLY | GLY | D4702 | G4763 |
| L3884 | V3957 | Q4033 | D4098 | S4187 | PRO   | PRO | GLY | GLY | GLY | E4703 | L4764 |
| L3885 | N3963 | M4034 | S4099 | R4188 | GLY   | ARG | THR | GLY | GLY | L4704 | L4765 |
| L3886 | Y3968 | W4035 | Q4100 | I4189 | ALA   | GLY | SER | GLY | GLY | W4705 | L4766 |
| L3887 | I3969 | V4036 | K4101 | E4191 | ASP   | ALA | ASP | GLY | GLY | L4706 | T4767 |
| L3888 | Q3970 | M4037 | Q4102 | R4192 | GLY   | THR | GLY | GLY | GLY | M4707 | L4768 |
| L3890 | G3971 | G4038 | F4103 | I4193 | GLY   | GLY | GLY | GLY | GLY | T4708 | M4769 |
| E3893 | P3972 | M4044 | T4104 | Y4194 | GLY   | ALA | GLY | PRO | GLY | P4709 | M4770 |
| F3899 | C3973 | V4045 | G4105 | F4195 | GLY   | ALA | GLY | ALA | GLY | S4710 | L4771 |
| L3900 | T3974 | D4046 | P4106 | E4197 | GLY   | LEU | GLY | GLY | GLY | F4711 | D4772 |
| L3901 | G3975 | M4047 | E4107 | I4197 | ALA   | LEU | GLY | PRO | GLY | P4712 | V4773 |
| L3902 | N3976 | L4048 | T4108 | S4198 | ALA   | TRP | ALA | GLY | GLY | S4713 | K4774 |
| L3903 | Q3977 | V4049 | Q4109 | N4201 | GLY   | ALA | GLY | PRO | GLY | M4714 | Y4775 |
| L3904 | Q3978 | W4050 | F4110 | R4202 | ALA   | VAL | VAL | PRO | GLY | W4715 | W4778 |
| L3905 | S3979 | S4051 | L4111 | A4203 | GLY   | ALA | GLY | LYS | GLY | W4716 | K4779 |
| T3906 | L3980 | S4052 | L4112 | Q4204 | GLY   | ARG | ALA | PRO | GLY | K4718 | F4780 |
| Q3906 | H3981 | S4053 | S4113 | W4205 | GLY   | ALA | GLY | THR | GLY | F4719 | G4781 |
| Q3907 | A3982 | M4054 | E4116 | E4206 | ALA   | ALA | GLY | THR | GLY | W4720 | V4782 |
| G3908 | S3983 | I4058 | A4117 | M4207 | GLY   | GLY | GLY | PRO | GLY | K4721 | L4783 |
| L3909 | R3984 | L4058 | D4118 | P4208 | ALA   | ALA | GLY | PRO | GLY | R4722 | F4784 |
| T3910 | H3986 | F4061 | E4119 | K4211 | GLY   | ASP | ASP | LYS | GLY | L4725 | D4785 |
| T3911 | D3987 | P4062 | M4120 | E4212 | GLY   | GLY | GLY | LYS | GLY | D4726 | T4786 |
| T3912 | A3988 | F4062 | E4121 | S4213 | GLY   | GLY | GLY | PRO | GLY | K4727 | F4789 |
| L3913 |       |       | E4122 |       |       | GLY | GLY | GLY | GLY | H4728 | L4790 |
| L3914 |       |       | M4124 |       |       |     |     |     |     |       | Y4791 |
| L3915 |       |       | F4125 |       |       |     |     |     |     |       | L4792 |



• Molecule 2: ryanodine receptor 1



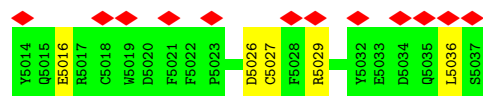
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| Y1255 | G1195 | R1073 | L1133 | H1133 | I1074 | R1073 | ASP | ASP   | D943 | L883 | L823 | F763 | E700 | M636 | V574 | A512 |
| E1256 | P1196 | I1074 | L1134 | L1134 | F1075 | I1074 | ILE | E944  | L884 | L884 | E824 | V764 | G701 | M637 | L575 | E513 |
| V1257 | G1197 | F1075 | G1135 | G1135 | F1076 | F1075 | PRO | K945  | T885 | T885 | P825 | Q765 | W702 | I638 | N576 | S514 |
| A1258 | Q1198 | R1076 | S1136 | S1136 | A1077 | R1076 | ALA | A946  | R886 | R886 | I826 | G766 | G703 | N639 | I577 | W515 |
| R1259 | G1199 | E1078 | E1137 | E1137 | A1077 | E1078 | ARG | E947  | T887 | T887 | K827 | V767 | G704 | Y640 | I578 | K516 |
| M1260 | G1200 | K1079 | P1138 | P1138 | K1079 | K1079 | ASN | D948  | Q888 | Q888 | E828 | F768 | N705 | Y641 | Q579 | E517 |
| D1261 | H1201 | S1080 | F1139 | F1139 | S1080 | S1080 | PRO | N949  | Q889 | Q889 | Y829 | E769 | G706 | N581 | I518 | I518 |
| G1262 | L1202 | Y1081 | G1140 | G1140 | Y1081 | Y1081 |     | L950  | Q890 | Q890 | R830 | A770 | V707 | N581 | V519 | N520 |
| T1263 | N1203 | T1082 | R1141 | R1141 | T1082 | T1082 |     | K951  | K891 | K891 | R831 | F771 | G708 | H844 | H844 | L521 |
| V1264 | L1204 | T1082 | P1142 | P1142 | T1082 | T1082 |     | K952  | T892 | T892 | E832 | N772 | D709 | I583 | I583 | L522 |
| D1265 | G1205 | V1083 | W1143 | W1143 | V1083 | V1083 |     | T953  | Y893 | Y893 | G833 | L773 | D710 | K684 | K684 | Y523 |
| T1266 | Q1206 | Q1084 | S1144 | S1144 | Q1084 | Q1084 |     | K954  | G894 | G894 | P834 | D774 | L711 | N647 | N647 | Y524 |
| P1267 | S1145 | S1085 | G1145 | G1145 | S1085 | S1085 |     | L955  | P895 | P895 | R835 | G775 | W712 | I586 | I586 | E524 |
| P1268 | G1146 | G1086 | D1147 | D1147 | G1086 | G1086 |     | P956  | V896 | V896 | G836 | L776 | S713 | F649 | I587 | L525 |
| G1269 | D1147 | R1087 | V1148 | V1148 | R1087 | R1087 |     | K957  | R897 | R897 | P837 | F777 | Y714 | V650 | S588 | L526 |
| L1270 | S1210 | W1088 | Y1149 | Y1149 | W1088 | W1088 |     | T958  | D898 | D898 | H838 | F778 | G851 | G851 | L589 | A527 |
| R1271 | L1211 | Y1089 | F1090 | F1090 | Y1089 | Y1089 |     | Y959  | D899 | D899 | L839 | P779 | D717 | R652 | L590 | I530 |
| A1272 | F1213 | F1091 | G1150 | G1150 | F1091 | F1091 |     | M960  | N900 | N900 | V840 | W780 | G718 | A653 | D591 | R531 |
| L1273 | F1214 | F1092 | M1152 | M1152 | F1092 | F1092 |     | M961  | K901 | K901 | G841 | W781 | L719 | E654 | K592 | G532 |
| H1274 | A1093 | E1093 | L1155 | L1155 | E1093 | E1093 |     | N963  | L903 | L903 | P842 | S782 | W722 | G655 | G594 | N533 |
| R1275 | A1094 | A1094 | T1156 | T1156 | A1094 | A1094 |     | G964  | H904 | H904 | S843 | F783 | W722 | K661 | R534 | N534 |
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| X1277 | G1218 | T1096 | M1158 | M1158 | T1096 | T1096 |     | P969  | C906 | C906 | L846 | G786 | G724 | Y663 | N536 | N536 |
| X1278 | L1219 | T1097 | L1161 | L1161 | T1097 | T1097 |     | L970  | L907 | L907 | S847 | W787 | W726 | F664 | C537 | C537 |
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| X1282 | F1223 | R1101 | L1164 | L1164 | R1101 | R1101 |     | H974  | H911 | H911 | D850 | F791 | W730 | G604 | F540 | F540 |
| X1284 | E1224 | V1102 | M1165 | M1165 | V1102 | V1102 |     | V975  | S912 | S912 | V852 | L792 | T731 | L606 | S541 | S541 |
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| X1288 | N1229 | R1106 | L1169 | L1169 | R1106 | R1106 |     | A880  | E917 | E917 | V856 | H797 | Q735 | F674 | W546 | W546 |
| X1289 | M1230 | E1108 | M1170 | M1170 | E1108 | E1108 |     | Q981  | E917 | E917 | V857 | G798 | H736 | L675 | V547 | V547 |
| X1290 | Q1231 | L1109 | S1171 | S1171 | L1109 | L1109 |     | T982  | R918 | R918 | THR  | E799 | L738 | T676 | V548 | V548 |
| X1291 | R1232 | P1111 | S1173 | S1173 | P1111 | P1111 |     | N983  | N919 | N919 | GLN  | F900 | A739 | Q678 | S549 | S549 |
| X1292 | P1233 | D1112 | G1174 | G1174 | D1112 | D1112 |     | D986  | Y920 | Y920 | I861 | K901 | P740 | R615 | L551 | L551 |
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| X1430 | S1239 | PRO   | R1179 | R1179 | PRO   | PRO   |     | R998  | G926 | G926 | L867 | G807 | C746 | I621 | S557 | S557 |
| X1431 | K1240 | GLN   | E1178 | E1178 | GLN   | GLN   |     | G998  | E927 | E927 | E868 | Y808 | S745 | L620 | A566 | A566 |
| X1432 | S1241 | VAL   | L1182 | L1182 | VAL   | VAL   |     | V1001 | T928 | T928 | R869 | A809 | T688 | I621 | T622 | I560 |
| X1433 | P1243 | GLU   | A1121 | A1121 | GLU   | GLU   |     | A1002 | L929 | L929 | T870 | P810 | L750 | E823 | L561 | L561 |
| X1434 | Q1244 | ASN   | Y1122 | Y1122 | ASN   | ASN   |     | Q1003 | K930 | K930 | R871 | C811 | S751 | E823 | E562 | E562 |
| X1436 | F1245 | GLN   | W1123 | W1123 | GLN   | GLN   |     | G1004 | T931 | T931 | E872 | E813 | L626 | N624 | V563 | V563 |
| X1437 | F1246 | ARG   | F1124 | F1124 | ARG   | ARG   |     | W1005 | L933 | L933 | L874 | A814 | P753 | L626 | L564 | L564 |
| X1438 | P1247 | TRP   | N1125 | N1125 | TRP   | TRP   |     | S1006 | A934 | A934 | A875 | V815 | S754 | G828 | C566 | C566 |
| X1439 | V1248 | R1071 | G1126 | G1126 | R1071 | R1071 |     | Y1007 | L935 | L935 | E876 | L816 | F757 | R629 | V567 | V567 |
| X1441 | P1249 | Y1072 | H1127 | H1127 | Y1072 | Y1072 |     | S1008 | G936 | G936 | N877 | P817 | R758 | E630 | L568 | L568 |
| X1442 | E1251 | VAL   | A1128 | A1128 | VAL   | VAL   |     | S1009 | C937 | C937 | T878 | E819 | T759 | L631 | I569 | I569 |
| X1443 | P1250 | GLN   | G1129 | G1129 | GLN   | GLN   |     | VAL   | H938 | H938 | H879 | R820 | N760 | L632 | E570 | E570 |
| X1444 | H1252 | R1072 | Q1130 | Q1130 | R1072 | R1072 |     | G980  | V939 | V939 | L881 | L821 | G761 | L633 | S571 | S571 |
| X1445 | P1253 | L1132 | R1131 | R1131 | L1132 | L1132 |     | M941  | G940 | G940 | W882 | R822 | C762 | Q634 | P572 | P572 |
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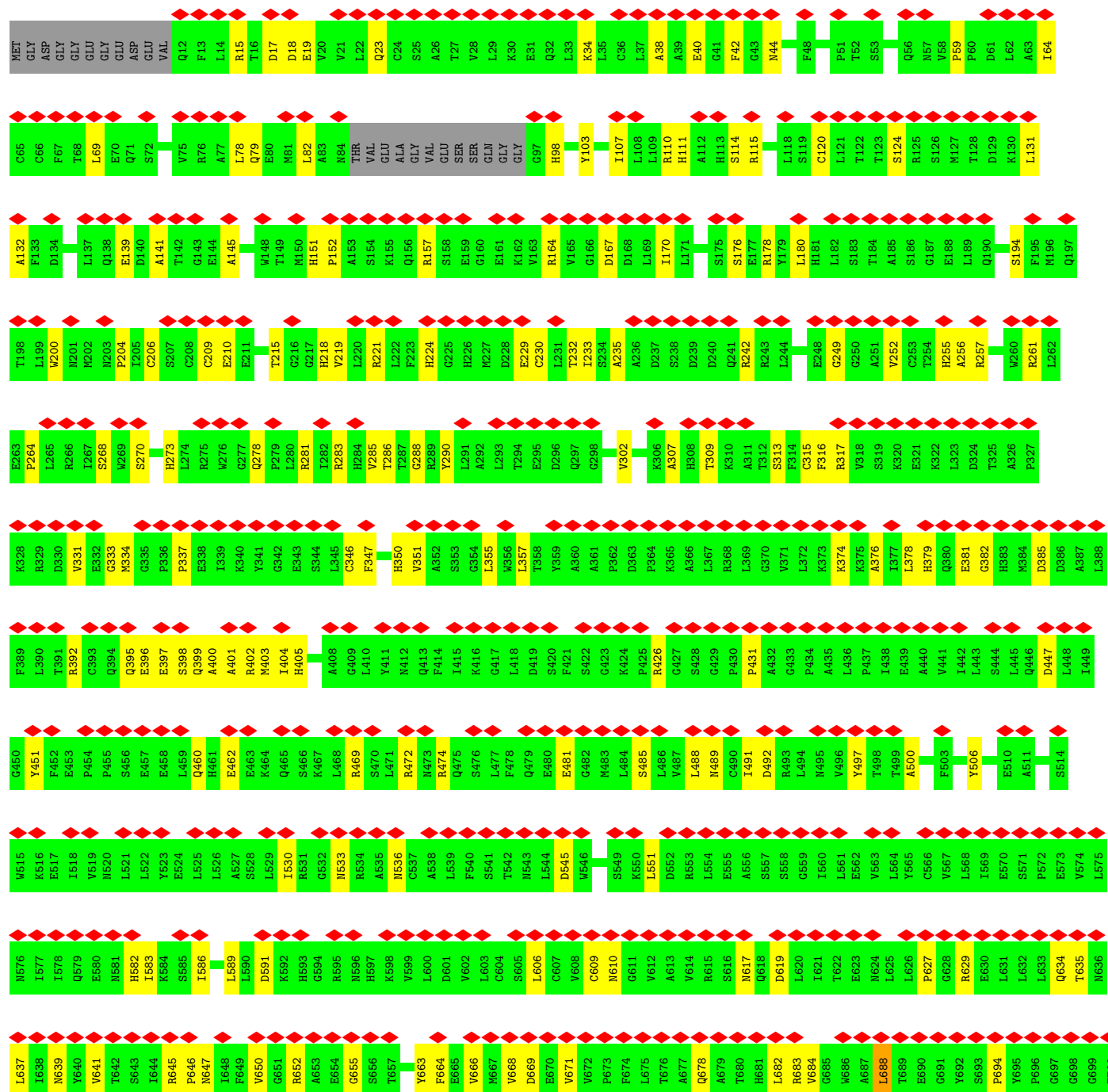
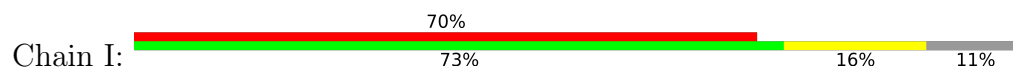
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| X3154 | X3155 | X3158 | X3159 | X3160 | X3161 | X3162 | X3163 | X3170 | X3171 | X3172 | X3173 | X3174 | X3175 | X3176 | X3177 | X3178 | X3181 | X3182 | X3183 | X3184 | X3185 | X3186 | X3187 | X3188 | X3189 | X3190 | X3191 | X3192 | X3193 | X3194 | X3195 | X3196 | X3197 | X3198 | X3199 | X3200 | X3201 | X3202 | X3203 | X3204 | X3205 | X3206 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 |       |       |       |
| R2939 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2964 | X2965 | X2966 | X2967 | X2968 | X2969 | X2970 | X2971 | X2972 | X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X2980 | X3001 | X3002 | X3003 | X3004 | X3005 | X2999 | X3000 | X3009 | X3010 | X3011 | X3012 | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 |       |       |       |
| A2879 | E2880 | N2881 | Y2882 | N2883 | N2884 | T2885 | W2886 | G2887 | R2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | K2897 | G2898 | G2899 | G2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | L2912 | A2913 | E2914 | E2915 | E2916 | E2917 | E2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | N2933 | Q2934 | Y2935 | A2936 | V2937 | T2938 |
| W2819 | E2820 | W2821 | T2822 | T2823 | E2824 | K2825 | A2826 | R2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | GLU   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SPR   | GLN   | ALA   | GLN   | THR   | TVR   | ASP   | ARG   | GLU   | GLY   | N2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | V2865 | T2866 | L2867 | A2868 | E2869 | L2870 | Q2871 | Q2872 | A2873 | N2874 | A2875 | E2876 | Q2877 | L2878 |       |       |       |
| A2759 | E2760 | Y2761 | T2762 | E2763 | E2764 | K2765 | W2766 | A2767 | F2768 | D2769 | K2770 | L2771 | Q2772 | N2773 | L2774 | W2775 | S2776 | Y2777 | G2778 | E2779 | N2780 | V2781 | D2782 | E2783 | L2784 | L2785 | K2786 | T2787 | H2788 | P2789 | W2790 | L2791 | R2792 | P2793 | N2794 | K2795 | T2796 | F2797 | S2798 | E2799 | K2800 | D2801 | T2802 | E2803 | L2804 | Y2805 | R2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | N2816 | L2817 | A2818 |
| W2819 | E2820 | W2821 | T2822 | T2823 | E2824 | K2825 | A2826 | R2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | GLU   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SPR   | GLN   | ALA   | GLN   | THR   | TVR   | ASP   | ARG   | GLU   | GLY   | N2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | V2865 | T2866 | L2867 | A2868 | E2869 | L2870 | Q2871 | Q2872 | A2873 | N2874 | A2875 | E2876 | Q2877 | L2878 |       |       |       |
| A2879 | E2880 | N2881 | Y2882 | N2883 | N2884 | T2885 | W2886 | G2887 | R2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | K2897 | G2898 | G2899 | G2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | L2912 | A2913 | E2914 | E2915 | E2916 | E2917 | E2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | N2933 | Q2934 | Y2935 | A2936 | V2937 | T2938 |
| K2939 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2964 | X2965 | X2966 | X2967 | X2968 | X2969 | X2970 | X2971 | X2972 | X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X2980 | X3001 | X3002 | X3003 | X3004 | X3005 | X2999 | X3000 | X3009 | X3010 | X3011 | X3012 | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 |       |       |       |
| X3021 | X3022 | X3023 | X3024 | X3025 | X3026 | X3027 | X3028 | X3029 | X3030 | X3031 | X3032 | X3033 | X3034 | X3035 | X3036 | X3037 | X3038 | X3039 | X3040 | X3041 | X3042 | X3043 | X3044 | X3045 | X3046 | X3047 | X3048 | X3049 | X3050 | X3051 | X3052 | X3053 | X3054 | X3055 | X3056 | X3057 | X3058 | X3059 | X3060 | X3061 | X3062 | X3063 | X3134 | X3135 | X3136 | X3137 | X3138 | X3139 | X3140 | X3141 | X3142 | X3143 | X3144 | X3145 | X3146 | X3147 | X3148 | X3151 |       |
| X3154 | X3155 | X3158 | X3159 | X3160 | X3161 | X3162 | X3163 | X3170 | X3171 | X3172 | X3173 | X3174 | X3175 | X3176 | X3177 | X3178 | X3181 | X3182 | X3183 | X3184 | X3185 | X3186 | X3187 | X3188 | X3189 | X3190 | X3191 | X3192 | X3193 | X3194 | X3195 | X3196 | X3197 | X3198 | X3199 | X3200 | X3201 | X3202 | X3203 | X3204 | X3205 | X3206 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 |       |       |       |
| E2348 | N2349 | A2350 | N2351 | V2352 | V2353 | V2354 | R2355 | L2356 | L2357 | I2358 | R2359 | K2360 | P2361 | E2362 | C2363 | F2364 | G2365 | V2366 | A2367 | L2368 | R2369 | G2370 | E2371 | G2372 | G2373 | S2374 | G2375 | L2376 | L2377 | A2378 | A2379 | I2380 | E2381 | E2382 | A2383 | I2384 | R2385 | I2386 | G2387 | G2388 | E2389 | P2390 | A2391 | G2394 | P2395 | GLY   | VAL   | ARG   | ASP   | ARG   | ARG   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   |       |
| L2472 | P2473 | L2474 | Q2475 | I2476 | T2477 | T2478 | L2479 | X2487 | X2488 | X2489 | X2490 | X2491 | X2492 | X2493 | X2494 | X2495 | X2500 | X2501 | X2502 | X2503 | X2504 | X2505 | X2506 | X2507 | X2508 | X2509 | X2510 | X2511 | X2512 | X2513 | X2514 | X2515 | X2516 | X2517 | X2518 | X2519 | X2520 | X2521 | X2522 | X2523 | X2524 | X2525 | X2526 | X2527 | X2528 | X2529 | X2530 | X2531 | X2532 | X2533 | X2534 | X2535 | X2536 | X2537 | X2538 |       |       |       |       |
| X2541 | X2542 | X2543 | X2544 | X2545 | X2548 | X2549 | X2550 | X2551 | X2552 | X2555 | X2556 | X2557 | X2558 | X2559 | X2560 | X2561 | X2562 | X2563 | X2564 | X2565 | X2566 | X2567 | X2568 | X2569 | X2570 | X2571 | X2572 | X2573 | X2574 | X2575 | X2576 | X2577 | X2578 | X2579 | X2580 | X2581 | X2582 | X2583 | X2584 | X2585 | X2586 | X2587 | X2588 | X2591 | X2592 | X2593 | X2594 | X2595 | X2598 | X2599 | X2602 | X2603 | X2604 |       |       |       |       |       |       |
| X2605 | X2606 | X2607 | X2608 | X2609 | X2610 | X2611 | X2612 | X2613 | X2614 | X2615 | X2616 | X2617 | X2618 | X2619 | X2620 | X2621 | X2622 | X2623 | X2624 | X2625 | X2626 | X2627 | X2628 | X2629 | X2632 | X2633 | X2636 | X2637 | X2640 | X2641 | X2644 | X2645 | X2646 | X2647 | X2648 | X2649 | X2650 | X2651 | X2652 | X2653 | X2654 | X2655 | X2656 | X2657 | X2658 | X2659 | X2660 | X2661 | X2662 | X2663 | X2664 | X2665 | X2666 | X2668 |       |       |       |       |       |
| X2669 | X2670 | X2671 | X2672 | X2673 | X2674 | X2675 | X2676 | X2677 | X2678 | X2679 | X2680 | X2681 | X2682 | X2683 | X2684 | X2685 | X2686 | X2687 | X2688 | X2689 | X2690 | X2691 | X2692 | X2693 | X2694 | X2695 | X2696 | X2697 | X2698 | X2699 | X2700 | X2701 | X2702 | X2703 | N2734 | F2735 | D2736 | P2737 | R2738 | P2739 | V2740 | E2741 | T2742 | L2743 | N2744 | V2745 | L2746 | I2747 | P2748 | E2749 | K2750 | L2751 | D2752 | S2753 | T2754 | L2755 | N2756 | K2757 | F2758 |
| A2759 | E2760 | Y2761 | T2762 | E2763 | E2764 | K2765 | W2766 | A2767 | F2768 | D2769 | K2770 | L2771 | Q2772 | N2773 | L2774 | W2775 | S2776 | Y2777 | G2778 | E2779 | N2780 | V2781 | D2782 | E2783 | L2784 | L2785 | K2786 | T2787 | H2788 | P2789 | W2790 | L2791 | R2792 | P2793 | N2794 | K2795 | T2796 | F2797 | S2798 | E2799 | K2800 | D2801 | T2802 | E2803 | L2804 | Y2805 | R2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | N2816 | L2817 | A2818 |
| W2819 | E2820 | W2821 | T2822 | T2823 | E2824 | K2825 | A2826 | R2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | GLU   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SPR   | GLN   | ALA   | GLN   | THR   | TVR   | ASP   | ARG   | GLU   | GLY   | N2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | V2865 | T2866 | L2867 | A2868 | E2869 | L2870 | Q2871 | Q2872 | A2873 | N2874 | A2875 | E2876 | Q2877 | L2878 |       |       |       |
| A2879 | E2880 | N2881 | Y2882 | N2883 | N2884 | T2885 | W2886 | G2887 | R2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | K2897 | G2898 | G2899 | G2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | L2912 | A2913 | E2914 | E2915 | E2916 | E2917 | E2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | N2933 | Q2934 | Y2935 | A2936 | V2937 | T2938 |
| K2939 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2964 | X2965 | X2966 | X2967 | X2968 | X2969 | X2970 | X2971 | X2972 | X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X2980 | X3001 | X3002 | X3003 | X3004 | X3005 | X2999 | X3000 | X3009 | X3010 | X3011 | X3012 | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 |       |       |       |
| X3021 | X3022 | X3023 | X3024 | X3025 | X3026 | X3027 | X3028 | X3029 | X3030 | X3031 | X3032 | X3033 | X3034 | X3035 | X3036 | X3037 | X3038 | X3039 | X3040 | X3041 | X3042 | X3043 | X3044 | X3045 | X3046 | X3047 | X3048 | X3049 | X3050 | X3051 | X3052 | X3053 | X3054 | X3055 | X3056 | X3057 | X3058 | X3059 | X3060 | X3061 | X3062 | X3063 | X3134 | X3135 | X3136 | X3137 | X3138 | X3139 | X3140 | X3141 | X3142 | X3143 | X3144 | X3145 | X3146 | X3147 | X3148 | X3151 |       |
| X3154 | X3155 | X3158 | X3159 | X3160 | X3161 | X3162 | X3163 | X3170 | X3171 | X3172 | X3173 | X3174 | X3175 | X3176 | X3177 | X3178 | X3181 | X3182 | X3183 | X3184 | X3185 | X3186 | X3187 | X3188 | X3189 | X3190 | X3191 | X3192 | X3193 | X3194 | X3195 | X3196 | X3197 | X3198 | X3199 | X3200 | X3201 | X3202 | X3203 | X3204 | X3205 | X3206 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 |       |       |       |
| E2348 | N2349 | A2350 | N2351 | V2352 | V2353 | V2354 | R2355 | L2356 | L2357 | I2358 | R2359 | K2360 | P2361 | E2362 | C2363 | F2364 | G2365 | V2366 | A2367 | L2368 | R2369 | G2370 | E2371 | G2372 | G2373 | S2374 | G2375 | L2376 | L2377 | A2378 | A2379 | I2380 | E2381 | E2382 | A2383 | I2384 | R2385 | I2386 | G2387 | G2388 | E2389 | P2390 | A2391 | G2394 | P2395 | GLY   | VAL   | ARG   | ASP   | ARG   | ARG   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   |       |
| L2472 | P2473 | L2474 | Q2475 | I2476 | T2477 | T2478 | L2479 | X2487 | X2488 | X2489 | X2490 | X2491 | X2492 | X2493 | X2494 | X2495 | X2500 | X2501 | X2502 | X2503 | X2504 | X2505 | X2506 | X2507 | X2508 | X2509 | X2510 | X2511 | X2512 | X2513 | X2514 | X2515 | X2516 | X2517 | X2518 | X2519 | X2520 | X2521 | X2522 | X2523 | X2524 | X2525 | X2526 | X2527 | X2528 | X2529 | X2530 | X2531 | X2532 | X2533 | X2534 | X2535 | X2536 | X2537 | X2538 |       |       |       |       |
| X2541 | X2542 | X2543 | X2544 | X2545 | X2548 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

|       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| E4050 | S3983 | E3854 | G3788 | H3667 | X3581 | X3520 | X3413 | X3353 | X3291 | X3221 |
| S4051 | R3984 | Q3855 | E3789 | S3668 | X3582 | X3621 | X3414 | X3354 | X3292 | X3222 |
| S4052 | L3985 | L3856 | T3790 | F3669 | X3583 | X3622 | X3415 | X3355 | X3293 | X3223 |
| S4053 | W3986 | Q3857 | G3791 | E3670 | X3584 | X3623 | X3416 | X3356 | X3294 | X3224 |
| N4054 | D3987 | M3858 | S3792 | D3671 | X3585 | X3624 | X3417 | X3357 | X3295 | X3225 |
| E4056 | A3988 | V3859 | M3793 | R3672 | X3586 | X3625 | X3418 | X3358 | X3296 | X3226 |
| N4057 | V3989 | N3860 | V3794 | M3673 | X3587 | X3626 | X3419 | X3359 | X3297 | X3227 |
|       | G3991 | E3861 | S3795 | L3674 | X3588 | X3627 | X3420 | X3360 | X3298 | X3228 |
|       | F3992 | D3862 | S3796 | D3675 | X3589 | X3628 | X3421 | X3361 | X3299 | X3229 |
|       | L3993 | Q3863 | T3797 | D3676 | X3590 | X3629 | X3422 | X3362 | X3300 | X3230 |
|       | H3994 | T3798 | G3798 | L3677 | X3591 | X3630 | X3423 | X3363 | X3301 | X3231 |
|       | V3995 | K3799 | K3799 | S3678 | X3592 | X3631 | X3424 | X3364 | X3302 | X3232 |
|       | F3996 | L3800 | L3800 | K3679 | X3593 | X3632 | X3425 | X3365 | X3303 | X3233 |
|       | A3997 | G3801 | G3801 | A3680 | X3594 | X3633 | X3426 | X3366 |       | X3234 |
|       | H3998 | L3802 | L3802 | G3681 | X3595 | X3634 | X3427 | X3367 | X3307 | X3235 |
|       | M3999 | S3803 | S3803 | E3682 | X3596 | X3635 | X3428 | X3368 | X3308 | X3236 |
|       | M4000 | L3804 | L3804 | Q3683 | X3597 | X3636 | X3429 | X3369 | X3309 | X3241 |
|       | M4001 | L3805 | L3805 | E3684 | X3598 | X3637 | X3431 | X3370 | X3310 | X3242 |
|       | K4002 | N3806 | N3806 | E3685 | X3599 | X3638 | X3432 | X3371 | X3311 | X3243 |
|       | L4003 | G3807 | G3807 | E3686 | X3600 | X3639 | X3433 | X3372 | X3312 | X3244 |
|       | A4004 | N3809 | N3809 | E3687 | X3601 | X3640 | X3434 | X3373 | X3313 | X3245 |
|       | Q4005 | V3812 | V3812 | E3688 | X3602 | X3641 | X3435 | X3374 | X3314 | X3246 |
|       | D4006 | Q3813 | Q3813 | E3689 | X3603 | X3642 | X3436 | X3375 | X3315 | X3247 |
|       | S4007 | Q3814 | Q3814 | V3690 | X3604 | X3643 | X3437 | X3376 | X3316 | X3248 |
|       | S4008 | K3815 | K3815 | E3691 | X3605 | X3644 | X3438 | X3377 | X3317 | X3249 |
|       | Q4009 | N3816 | N3816 | E3692 | X3606 | X3645 | X3439 | X3378 | X3318 | X3250 |
|       | L4010 | L3817 | L3817 | K3693 | X3607 | X3646 | X3440 | X3379 | X3319 | X3251 |
|       | E4011 | L3818 | L3818 | K3694 | X3608 | X3647 | X3441 | X3380 | X3320 | X3252 |
|       | L4012 | Q3821 | Q3821 | P3697 | X3609 | X3648 | X3442 | X3381 | X3321 | X3253 |
|       | L4013 | Q3822 | Q3822 | L3698 | X3610 | X3649 | X3443 | X3382 | X3322 | X3254 |
|       | K4014 | S3823 | S3823 | H3699 | X3611 | X3650 | X3444 | X3383 | X3323 | X3261 |
|       | E4015 | L3824 | L3824 | Q3700 | X3612 | X3651 | X3445 | X3384 | X3324 | X3262 |
|       | L4016 | K3825 | K3825 | L3701 | X3613 | X3652 | X3446 | X3385 | X3325 | X3263 |
|       | L4017 | N3826 | N3826 | V3702 | X3614 | X3653 | X3447 | X3386 | X3326 | X3264 |
|       | L4018 | L3827 | L3827 | L3703 | X3615 | X3654 | X3448 | X3387 | X3327 | X3265 |
|       | L4019 | Q3829 | Q3829 | H3704 | X3616 | X3655 | X3449 | X3388 | X3328 | X3266 |
|       | Q4020 | S3830 | S3830 | S3705 | X3617 | X3656 | X3450 | X3389 | X3329 | X3267 |
|       | K4021 | L3831 | L3831 | T3706 | X3618 | X3657 | X3451 | X3390 | X3330 | X3268 |
|       | D4022 | Q3832 | Q3832 | R3707 | X3619 | X3658 | X3452 | X3391 | X3331 | X3269 |
|       | V4023 | Q3833 | Q3833 | T3708 | X3620 | X3659 | X3453 | X3392 | X3332 | X3270 |
|       | V4024 | M3836 | M3836 | L3710 | X3621 | X3660 | X3454 | X3393 | X3333 | X3271 |
|       |       | Q3837 | Q3837 | T3711 | X3622 | X3661 | X3455 | X3394 | X3334 | X3272 |
|       | L4027 | T3838 | T3838 | X3712 | X3623 | X3662 | X3456 | X3395 | X3335 | X3273 |
|       | L4028 | C3839 | C3839 | X3713 | X3624 | X3663 | X3457 | X3396 | X3336 | X3274 |
|       | S4029 | V3840 | V3840 | X3714 | X3625 | X3664 | X3458 | X3397 | X3337 | X3275 |
|       | L4030 | L3841 | L3841 | X3715 | X3626 | X3665 | X3459 | X3398 | X3338 | X3276 |
|       | N4034 | L3842 | L3842 | X3716 | X3627 | X3666 | X3460 | X3399 | X3339 | X3277 |
|       | V4035 | D3843 | D3843 | L3717 | X3628 | X3667 | X3461 | X3400 | X3340 | X3278 |
|       | V4036 | L3844 | L3844 | D3717 | X3629 | X3668 | X3462 | X3401 | X3341 | X3279 |
|       | N4037 | N3845 | N3845 | T3718 | X3630 | X3669 | X3463 | X3402 | X3342 | X3280 |
|       |       | Q3846 | Q3846 | X3719 | X3631 | X3670 | X3464 | X3403 | X3343 | X3281 |
|       | L4042 | F3847 | F3847 | T3720 | X3632 | X3671 | X3465 | X3404 | X3344 | X3282 |
|       | Q4043 | L3848 | L3848 | X3721 | X3633 | X3672 | X3466 | X3405 | X3345 | X3283 |
|       | M4044 | E3849 | E3849 | L3722 | X3634 | X3673 | X3467 | X3406 | X3346 | X3284 |
|       |       | Q3850 | Q3850 | X3723 | X3635 | X3674 | X3468 | X3407 | X3347 | X3285 |
|       |       | L3851 | L3851 | M3723 | X3636 | X3675 | X3469 | X3408 | X3348 | X3286 |
|       |       | N3852 | N3852 | A3724 | X3637 | X3676 | X3470 | X3409 | X3349 | X3287 |
|       |       | K3853 | K3853 | X3725 | X3638 | X3677 | X3471 | X3410 | X3350 | X3288 |
|       |       | A3854 | A3854 | A3726 | X3639 | X3678 | X3472 | X3411 | X3351 | X3289 |
|       |       |       |       | D3727 | X3640 | X3679 | X3473 | X3412 | X3352 | X3290 |





● Molecule 2: ryanodine receptor 1



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| R1584 | K1585 | N1586 | P1587 | P1589 | Q1590 | C1591 | P1592 | P1593 | R1594 | L1595 | E1596 | V1597 | Q1598 | M1599 | L1600 | M1601 | P1602 | V1603 | S1604 | S1606 | R1607 | M1608 | P1609 | M1610 | H1611 | F1612 | Q1614 | V1615 | GLU   | THR   | ARG   | ARG   | ALA   | GLY   | E1622 | R1623 | L1624 | G1625 | W1626 | A1627 | V1628 | Q1629 | C1630 | Q1631 | D1632 | P1633 | L1634 | T1635 | M1636 | M1637 | A1638 | L1639 | H1640 | I1641 | P1642 | E1643 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X1512 | X1513 | X1514 | X1515 | X1516 | X1517 | X1518 | X1519 | X1520 | X1521 | X1522 | X1523 | X1524 | X1525 | X1526 | X1527 | X1528 | X1529 | X1530 | X1531 | X1532 | X1533 | X1534 | X1535 | X1536 | X1537 | X1538 | X1539 | X1540 | X1541 | X1542 | X1543 | X1544 | X1545 | X1546 | X1547 | X1548 | X1549 | X1550 | X1551 | X1552 | X1553 | X1554 |       |       |       |       |       |       |       |       |       |       | X1559 | X1560 | X1561 | X1562 | X1563 | X1564 | X1565 | X1566 | X1567 | X1568 | X1569 | X1570 | X1571 | X1572 | X1573 | X1574 | X1575 | X1576 | X1577 | X1578 | X1579 | F1580 | L1581 | X1582 | E1583 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| X1445 | X1446 | X1449 |       |       | X1450 | X1451 | X1452 | X1453 | X1454 | X1455 | X1456 | X1457 | X1458 | X1459 | X1460 | X1461 | X1462 | X1463 | X1464 | X1465 | X1466 | X1467 | X1468 | X1469 | X1470 | X1471 | X1472 | X1473 | X1474 | X1475 | X1476 | X1477 | X1484 |       |       | X1485 | X1486 | X1487 | X1488 | X1489 | X1490 | X1491 | X1492 | X1493 | X1494 | X1495 | X1496 | X1497 | X1498 | X1499 | X1500 | X1503 |       |       |       | X1504 | X1505 | X1506 | X1507 | X1508 | X1509 | X1510 | X1511 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P1253 | H1254 | Y1255 | E1256 | V1257 | A1258 | R1259 | M1260 | D1261 | G1262 | T1263 | V1264 | D1265 | T1266 | P1267 | P1268 | C1269 | L1270 | R1271 | L1272 | A1273 | L1274 | H1274 | R1275 | X1276 | X1277 | X1278 | X1279 | X1280 | X1281 | X1282 | X1283 | X1284 | X1285 | X1286 | X1287 | X1288 | X1289 | X1290 | X1291 | X1292 | X1293 | X1294 | X1295 | X1296 | X1297 | X1298 | X1299 | X1300 | X1301 | X1302 | X1303 | X1304 | X1305 | X1306 | X1307 | X1308 | X1309 | X1310 | X1311 | X1312 | X1313 | X1314 | X1315 | X1316 | X1317 | X1318 | X1319 | X1320 | X1321 | X1322 | X1323 | X1324 | X1325 | X1326 | X1327 | X1328 | X1329 | X1330 | X1331 | X1332 | X1333 | X1334 | X1335 | X1336 | X1337 | X1338 | X1339 | X1340 | X1341 | X1342 | X1343 | X1344 |
| S1193 | L1194 | P1195 | G1196 | G1197 | Q1198 | V1199 | G1200 | H1201 | L1202 | M1203 | L1204 | G1205 | Q1206 | D1207 | V1208 | S1209 | S1210 | L1211 | R1212 | F1213 | F1214 | A1215 | I1216 | C1217 | G1218 | L1219 | Q1220 | E1221 | G1222 | F1223 | E1224 | P1225 | F1226 | A1227 | I1228 | M1229 | M1230 | Q1231 | R1232 | P1233 | V1234 | T1235 | T1236 | W1237 | F1238 | S1239 | K1240 | S1241 | L1242 | P1243 | Q1244 | F1245 | E1246 | P1247 | V1248 | P1249 | P1250 | E1251 | H1252 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| W1132 | H1133 | L1134 | G1135 | S1136 | F1139 |       | G1140 | R1141 | P1142 | W1143 | Q1144 | S1145 | G1146 | D1147 | V1148 | V1149 | G1150 | C1151 | M1152 | I1153 | D1154 | L1155 | T1156 | E1157 | N1158 | T1159 | I1160 | I1161 | F1162 | T1163 | L1164 | N1165 | G1166 | E1167 | V1168 | L1169 | M1170 | S1171 | D1172 | S1173 | G1174 | S1175 | E1176 | T1177 | A1178 | F1179 | R1180 | E1181 | I1182 | E1183 | I1184 | G1185 | D1186 | G1187 | F1188 | L1189 | P1190 | V1191 | C1192 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| R1071 | V1072 | R1073 | I1074 | F1075 | R1076 | A1077 | E1078 | K1079 | S1080 | Y1081 | T1082 | V1083 | Q1084 | S1085 | Q1086 | R1087 | W1088 | Y1089 | F1090 | E1091 | F1092 | E1093 | A1094 | V1095 | T1096 | E1099 |       | M1100 | V1102 | G1103 | W1104 | A1105 | R1106 | P1107 | E1108 | L1109 | R1110 | P1111 | D1112 | V1113 | E1114 | L1115 | G1116 | A1117 | D1118 | E1119 | L1120 | A1121 | Y1122 | V1123 | F1124 | G1125 | H1127 | G1126 | R1128 | G1129 | Q1130 | R1131 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| GLN   | ASP   | ILE   | PRO   | ALA   | ARG   | ARG   | ASN   | PRO   | R1020 | L1021 | V1022 | P1023 | Y1024 | R1025 | L1026 | L1027 | D1028 | E1029 | A1030 | T1031 | K1032 | R1033 | S1034 | N1035 | R1036 | D1037 | S1038 | L1039 | C1040 | Q1041 | A1042 | V1043 | R1044 | T1045 | L1046 | L1047 | G1048 | Y1049 | G1050 | Y1051 | N1052 | I1053 | E1054 | PRO   | PRO   | ASP   | GLN   | GLU   | PRO   | PRO   | SER   | GLN   | VAL   | GLU   | ASN   | GLN   | SER   | ARG   | THR   | D1070 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| K945  | A946  | E947  | D948  | N949  | L950  | K951  | K952  | T953  | K954  | L955  | P956  | K957  | T958  | Y959  | N960  | N961  | S962  | N963  | G964  | A968  |       | P969  | L970  | D971  | L972  | S973  | H974  | V975  | R976  | L977  | T978  | P979  | A980  | Q981  | T982  | T983  | L984  | V985  | D986  | R987  | L988  | A989  | G992  |       | A997  |       | R998  | D999  | R1000 | V1001 | A1002 | Q1003 | G1004 | W1005 | S1006 | Y1007 | S1008 | A1009 | VAL   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P825  | I826  | K827  | E828  | Y829  | R830  | R831  | E832  | G833  | P834  | R835  | G836  | P837  | H838  | L839  | V840  | G841  | P842  | S843  | R844  | C845  | L846  | S847  | H848  | T849  | D850  | F851  | V852  | P853  | C854  | P855  | V856  | D857  | THR   | VAL   | GLN   | I861  | V862  | L863  | P864  | P865  | H866  | L867  | E868  | R869  | I870  | R871  | E872  | K873  | L874  | A875  | E876  | N877  | I878  | H879  | E880  | L881  | W882  | A883  | L884  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| T885  | R886  | I887  | E888  | Q889  | G890  | K891  | T892  | Y893  | G894  | P895  | V896  | R897  | D898  | D899  | N900  | K901  | L902  | L903  | H904  | P905  | C906  | L907  | V908  | N909  | F910  | H911  | S912  | L913  | P914  | E915  | P916  | E917  | R918  | N919  | Y920  | N921  | L922  | Q923  | N924  | S925  | G926  | E927  | T928  | L929  | K930  | T931  | L932  | L933  | L935  | G936  | C937  | H938  | V939  | G940  | N941  | A942  | D943  | E944  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P763  | V764  | Q765  | G766  | V767  | F768  | E769  | A770  | F771  | N772  | L773  | D774  | G775  | L776  | F777  | F778  | P779  | V780  | W781  | S782  | F783  | S784  | A785  | G786  | V787  | K788  | W789  | R790  | S791  | L792  | L793  |       |       |       | H797  | G798  | E799  | F800  | K801  | F802  | L803  | P804  | P805  | P806  | G807  | Y808  | A809  | P810  | C811  | H812  | E813  | A814  | V815  | L816  | P817  | R818  | E819  | R820  | L821  | R822  | L823  | E824  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G701  | G702  | G703  | N705  | G706  | G707  | G708  | D709  | D710  | L711  | L712  | S713  | Y714  |       |       |       | D717  | G718  | L719  | H720  | L721  | W722  | L723  | G724  | H725  | V726  | A727  | R728  | P729  | V730  | T731  | S732  | P733  | G734  | Q735  | H736  | L737  | L738  | A739  | P740  | E741  | D742  | V743  | V744  | S745  | C746  |       |       | D749  | L750  | S751  | V752  | P753  | T754  | I755  | S756  | F757  | I759  | N760  | G761  | C762  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| E2381 | E2382 | A2383 | T2384 | T2385 | T2386 | S2387 | E2388 | E2389 | P2390 | A2391 | R2392 | D2393 | F2394 | L2395 | F2396 | VAL   | ARG   | ARG   | ASP   | ARG   | ARG   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   | GLU   | PRO   | PRO   | GLU   | GLU   | N2414 | L2418 | I2422 | M2423 | S2424 | F2425 | Y2426 | A2427 | A2428 | L2429 | L2430 | D2431 | L2432 | L2433 | L2434 | R2435 | C2436 | A2437 | F2438 | E2439 | M2440 | H2441 | T2442 | L2443 | Q2444 |       |       |
| P2319 | D2320 | I2321 | G2322 | M2323 | G2327 | G2328 | E2329 | R2330 | Y2331 | L2332 | D2333 | F2334 | L2335 | R2336 | F2337 | A2338 | V2339 | F2340 | V2341 | N2342 | G2343 | E2344 | S2345 | V2346 | E2347 | E2348 | N2349 | A2350 | N2351 | V2352 | V2353 | V2354 | R2355 | L2356 | L2357 | L2358 | R2359 | K2360 | P2361 | E2362 | C2363 | F2364 | G2365 | P2366 | A2367 | L2368 | R2369 | G2370 | E2371 | G2372 | G2373 | S2374 | G2375 | L2376 | L2377 | A2378 | A2379 | I2380 |       |       |
| E2259 | N2260 | S2261 | G2262 | I2263 | G2264 | L2265 | G2266 | M2267 | Q2268 | G2269 | S2270 | T2271 | P2272 | L2273 | D2274 | V2275 | A2276 | A2277 | A2278 | S2279 | V2280 | I2281 | D2282 | N2283 | N2284 | E2285 | L2286 | A2287 | L2288 | A2289 | L2290 | Q2291 | E2292 | Q2293 | D2294 | L2295 | E2296 | K2297 | V2298 | V2299 | S2300 | V2301 | L2302 | A2303 | G2304 | G2305 | G2306 | L2307 | Q2308 | S2309 | F2310 | P2311 | N2312 | L2313 | L2314 | A2315 | K2316 | G2317 | Y2318 |       |
| R2199 | A2200 | L2201 | G2202 | M2203 | H2204 | E2205 | T2206 | V2207 | M2208 | E2209 | V2210 | M2211 | V2212 | M2213 | V2214 | L2215 | G2216 | G2217 | G2218 | E2219 | T2220 | K2221 | E2222 | I2223 | R2224 | F2225 | P2226 | K2227 | M2228 | V2229 | T2230 | S2231 | C2232 | C2233 | R2234 | F2235 | L2236 | C2237 | Y2238 | F2239 | C2240 | R2241 | L2242 | S2243 | R2244 | Q2245 | M2246 | Q2247 | R2248 | S2249 | M2250 | F2251 | F2252 | H2253 | L2254 | S2255 | Y2256 | L2257 | L2258 |       |
| A2137 | L2138 | P2139 | R2140 | M2141 | Y2142 | T2143 | I2144 | S2145 | P2146 | S2147 | V2148 | V2149 | E2150 | D2151 | T2152 | L2155 | L2156 | E2157 | C2158 | L2159 | G2160 | Q2161 | I2162 | R2163 | S2164 | L2165 | L2166 | I2167 | V2168 | Q2169 | M2170 | G2171 | F2172 | E2175 | N2176 | L2177 | M2178 | I2179 | Q2180 | S2181 | I2182 | G2183 | N2184 | I2185 | M2186 | N2187 | N2188 | K2189 | V2190 | F2191 | Y2192 | Q2193 | H2194 | S2195 | Y2196 | L2197 | M2198 |       |       |       |
| LYS   | GLU   | GLU   | LYS   | PRO   | GLU   | GLU   | LEU   | PRO   | ALA   | GLU   | K2089 | K2090 | P2091 | Q2092 | S2093 | L2094 | Q2095 | E2096 | L2097 | V2098 | S2099 | H2100 | M2101 | V2102 | R2103 | R2104 | V2105 | A2106 | Q2107 | E2108 | D2109 | V2110 | V2111 | Q2112 | S2113 | P2114 | E2115 | L2116 | V2117 | R2118 | A2119 | M2120 | F2121 | S2122 | L2123 | L2124 | H2125 | L2126 | Q2127 | Y2128 | D2129 | Q2130 | L2131 | G2132 | L2135 | R2136 |       |       |       |       |
| F2012 | K2013 | D2014 | E2015 | A2016 | D2017 | E2018 | E2019 | D2020 | C2021 | P2022 | L2023 | P2024 | I2027 | R2028 | Q2029 | D2030 | L2031 | F2034 | L2038 | L2039 | A2040 | H2041 | C2042 | G2043 | I2044 | Q2045 | L2046 | E2047 | GLU   | GLU   | GLU   | PRO   | GLU   | GLU   | GLU   | THR   | SER   | LEU   | SER   | SER   | ARG   | LEU   | SER   | THR   | P2001 | Q2002 | Q2003 | E2004 | Q2005 | T2006 | N2007 | M2008 | L2009 | L2010 | H2011 |       |       |       |       |       |
| G1849 | E1850 | L1851 | Q1852 | H1853 | R1854 | V1855 | S1856 | S1857 | L1858 | A1859 | A1860 | F1861 | P1862 | A1863 | V1864 | Y1865 | V1866 | L1869 | Q1870 | Q1873 | R1876 | Y1877 | A1878 | L1879 | L1880 | M1881 | R1882 | A1883 | E1884 | E1885 | E1886 | V1889 | Q1861 | I1862 | L1863 | L1864 | M1865 | I1866 | E1869 | V1870 | F1871 | T1872 | E1873 | E1874 | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   |       |       |
| D1828 | P1829 | V1830 | G1831 | G1832 | S1833 | V1834 | E1835 | F1836 | Q1837 | F1838 | V1839 | P1840 | V1841 | L1842 | L1843 | L1844 | V1845 | S1846 | T1847 | L1848 | L1849 | V1850 | M1851 | G1852 | I1853 | F1854 | G1855 | D1856 | E1857 | L1858 | V1859 | Q1860 | I1861 | T1862 | L1863 | L1864 | M1865 | I1866 | E1869 | V1870 | F1871 | T1872 | E1873 | E1874 | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   |       |       |
| V1767 | T1768 | T1769 | S1770 | L1771 | R1772 | P1773 | P1774 | H1775 | H1776 | F1777 | S1778 | P1779 | P1780 | C1781 | F1782 | V1783 | A1784 | A1785 | T1786 | P1787 | A1788 | ALA   | GLY   | VAL   | ALA   | E1793 | A1794 | P1795 | A1796 | R1797 | D1858 | L1798 | S1799 | I1802 | P1803 | L1804 | E1805 | A1806 | L1807 | R1808 | D1809 | K1810 | G1751 | R1752 | K1753 | M1814 | L1815 | G1755 | N1756 | A1757 | R1758 | V1759 | H1760 | D1821 | G1822 | G1823 | Q1824 | H1825 | A1826 | R1827 |
| E1644 | N1645 | R1646 | C1647 | M1648 | D1649 | I1650 | L1651 | E1652 | L1653 | S1654 | E1655 | R1656 | L1657 | D1658 | L1659 | Q1660 | R1661 | F1662 | H1663 | S1664 | H1665 | T1666 | L1667 | R1668 | L1669 | Y1670 | R1671 | A1672 | A1675 | L1676 | G1677 | N1678 | N1679 | R1680 | V1681 | A1682 | H1683 | A1684 | S1687 | H1688 | V1689 | D1690 | Q1691 | A1692 | Q1693 | L1694 | L1695 | L1696 | A1697 | L1698 | E1699 | D1700 | A1701 | H1702 | L1703 | P1704 | G1705 |       |       |       |
| P1706 | L1707 | R1708 | A1709 | G1710 | Y1711 | Y1712 | D1713 | L1714 | L1715 | L1716 | S1717 | L1718 | H1719 | L1720 | E1721 | S1722 | A1723 | C1724 | R1725 | S1726 | R1727 | R1728 | S1729 | M1730 | L1731 | S1732 | Y1734 | I1735 | L1738 | T1739 | P1740 | E1741 | T1742 | R1743 | A1744 | I1745 | T1746 | L1747 | F1748 | P1749 | P1750 | G1751 | R1752 | K1753 | G1754 | G1755 | A1756 | R1757 | R1758 | H1759 | H1760 | G1761 | L1762 | P1763 | G1764 | V1765 | G1766 |       |       |       |



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| X3392 | X3393 | X3394 | X3395 | X3396 | X3397 | X3398 | X3399 | X3400 | X3401 | X3402 | X3403 | X3404 | X3405 | X3406 | X3407 | X3408 | X3409 | X3410 | X3411 | X3412 | X3413 | X3414 | X3415 | X3416 | X3417 | X3418 | X3419 | X3420 | X3421 | X3422 | X3423 | X3424 | X3425 | X3426 | X3427 | X3428 | X3429 | X3430 | X3431 | X3432 | X3433 | X3434 | X3435 | X3436 | X3437 | X3438 | X3439 | X3440 | X3441 | X3442 | X3443 | X3444 | X3445 | X3446 | X3447 | X3448 | X3449 | X3450 | X3451 |
| X3452 | X3453 | X3454 |       | X3459 | X3460 | X3461 | X3462 | X3463 | X3464 | X3465 | X3466 | X3467 | X3468 | X3469 | X3511 | X3512 | X3513 | X3514 | X3515 | X3516 | X3517 | X3518 | X3519 | X3520 | X3521 | X3522 | X3523 | X3524 | X3525 | X3526 | X3527 | X3528 | X3529 | X3530 | X3531 | X3532 | X3533 | X3534 | X3535 | X3536 | X3537 | X3538 | X3539 | X3540 | X3541 | X3542 | X3543 | X3544 | X3545 | X3546 | X3547 | X3548 | X3549 | X3552 | X3553 | X3554 | X3555 | X3556 | X3557 |
| X3558 | X3559 | X3560 | X3561 | X3562 | X3563 | X3564 | X3565 | X3566 | X3567 | X3568 | X3569 | X3570 | X3571 | X3572 | X3573 | X3574 | X3575 | X3576 | X3577 | X3578 | X3579 | X3580 | X3581 | X3582 | X3583 | X3584 | X3585 | X3586 | X3587 | X3588 | X3589 | X3590 | X3591 | X3592 | X3593 | X3594 | X3595 | X3596 | X3597 | X3598 | X3599 | X3600 | X3601 | X3602 | X3603 | X3604 | X3605 | X3606 | X3607 | X3608 | X3609 | X3610 | X3611 | X3612 | X3613 | T3639 | P3640 | L3641 | Y3642 |
| N3643 | L3644 | P3645 | T3646 | H3647 | R3648 | C3649 | C3650 | N3651 | N3652 | P3653 | L3654 | E3655 | S3656 | Y3657 | K3658 | A3659 | A3660 | V3661 | L3662 | L3663 | T3664 | E3665 | D3666 | H3667 | S3668 | F3669 | E3670 | D3671 | S3672 | N3673 | L3674 | D3675 | D3676 | L3677 | S3678 | C3679 | A3680 | G3681 | E3682 | Q3683 | E3684 | E3685 | E3686 | E3687 | E3688 | E3689 | V3690 | E3691 | E3692 | K3693 | K3694 | L3698 | H3699 | V3702 | F3705 | S3706 |       |       |       |
| R3707 | T3708 | A3709 | L3710 | T3711 | E3712 | K3713 | S3714 | K3715 | L3716 | D3717 | E3718 | D3719 | Y3720 | L3721 | Y3722 | M3723 | A3724 | Y3725 | A3726 | D3727 | L3728 | M3729 | A3730 | K3731 | S3732 | C3733 | H3734 | L3735 | E3736 | E3737 | G3738 | G3739 | E3740 | L3741 | GLY   | GLU   | ALA   | G3681 | E3682 | Q3683 | E3684 | E3685 | E3686 | V3751 | S3752 | F3753 | E3754 | E3755 | K3756 | M3757 | E3759 | K3760 | Q3761 | R3762 | L3763 | L3764 | Y3765 | Q3766 |       |
| Q3767 | S3768 | R3769 | L3770 | H3771 | T3772 | R3773 | G3774 | A3775 | A3776 | E3777 | N3778 | V3779 | L3780 | Q3781 | N3782 | L3783 | S3784 | A3785 | C3786 | K3787 | G3788 | E3789 | G3790 | G3791 | A3792 | N3793 | V3794 | S3795 | L3798 | K3799 | L3800 | G3801 | G3802 | S3803 | L3804 | L3805 | N3806 | G3807 | G3808 | N3809 | A3810 | E3811 | G3812 | Q3813 | Q3814 | K3815 | K3816 | L3817 | D3818 | Y3819 | L3820 | K3821 | D3822 | K3823 | K3824 | E3825 | Y3826 |       |       |
| F3829 | Q3830 | S3831 | L3832 | Q3833 | A3834 | L3835 | N3836 | Q3837 | T3838 | C3839 | S3840 | V3841 | L3842 | D3843 | L3844 | N3845 | A3846 | F3847 | E3848 | R3849 | Q3850 | N3851 | K3852 | A3853 | E3854 | G3855 | L3856 | G3857 | N3858 | V3859 | G3860 | E3861 | G3862 | G3863 | T3864 | V3865 | L3866 | N3867 | R3868 | Q3869 | N3870 | G3871 | E3872 | K3873 | V3874 | A3875 | A3876 | D3877 | L3878 | E3879 | F3880 | N3881 | Q3882 | D3883 | L3884 | F3885 | R3886 | F3887 | L3888 |
| Q3889 | L3890 | L3891 | C3892 | E3893 | G3894 | H3895 | N3896 | N3897 | D3898 | F3899 | Q3900 | N3901 | R3904 | T3905 | Q3906 | T3907 | G3908 | N3909 | T3910 | T3911 | T3912 | L3913 | N3914 | L3915 | L3916 | L3917 | C3918 | T3919 | V3920 | D3921 | Y3922 | L3923 | L3924 | R3925 | L3926 | Q3927 | E3928 | S3929 | L3930 | S3931 | D3932 | F3933 | Y3934 | W3935 | Y3936 | Y3937 | S3938 | C3939 | K3940 | D3941 | V3942 | L3943 | E3944 | E3945 | Q3946 | G3947 | K3948 | R3949 |       |
| N3950 | F3951 | S3952 | K3953 | A3954 | N3955 | S3956 | V3957 | A3958 | K3959 | Q3960 | V3961 | F3962 | S3963 | S3964 | L3965 | T3966 | E3967 | Y3968 | I3969 | Q3970 | C3971 | P3972 | C3973 | S3974 | Q3975 | N3976 | Q3977 | Q3978 | A3981 | H3982 | S3983 | R3984 | L3985 | W3986 | D3987 | A3988 | Y3989 | V3990 | G3991 | F3992 | L3993 | H3994 | V3995 | F3996 | A3997 | H3998 | M3999 | M4000 | M4001 | K4002 | L4003 | A4004 | Q4005 | D4006 | S4007 | S4008 | Q4009 | I4010 |       |
| E4011 | L4012 | L4013 | E4014 | E4015 | L4016 | L4017 | D4018 | L4019 | Q4020 | K4021 | D4022 | M4023 | V4024 | L4027 | L4028 | S4029 | L4030 | L4031 | V4036 | M4037 | G4038 | M4039 | L4040 | A4041 | A4042 | Q4043 | M4044 | V4045 | D4046 | M4047 | L4048 | V4049 | E4050 | S4051 | S4052 | S4053 | M4054 | V4055 | E4056 | M4057 | L4058 | L4059 | K4060 | F4061 | F4062 | D4063 | M4064 | F4065 | L4066 | K4067 | L4068 | D4069 | I4070 | I4071 | A4072 | S4074 |       |       |       |
| E4075 | A4076 | F4077 | Q4078 | D4079 | V4080 | V4081 | T4082 | D4083 | P4084 | R4085 | G4086 | L4087 | L4088 | S4089 | K4090 | K4091 | D4092 | F4093 | Q4094 | K4095 | A4096 | M4097 | D4098 | S4099 | Q4100 | K4101 | Q4102 | F4103 | T4104 | G4105 | P4106 | E4107 | I4108 | Q4109 | L4112 | S4113 | E4116 | A4117 | D4118 | E4119 | N4120 | E4121 | M4122 | I4123 | N4124 | F4125 | E4126 | F4127 | F4128 | A4129 | E4199 | T4200 | N4201 | R4202 | A4203 | A4136 |       |       |       |
| R4137 | D4138 | I4139 | F4140 | F4141 | M4142 | V4143 | A4144 | L4147 | L4150 | S4151 | E4152 | H4153 | V4154 | P4155 | H4156 | D4157 | P4158 | R4159 | L4160 | R4161 | N4162 | E4165 | L4166 | A4167 | E4168 | S4169 | I4170 | L4171 | E4172 | R4175 | P4176 | Y4177 | L4178 | G4179 | R4180 | I4181 | E4182 | S4187 | R4188 | R4189 | I4190 | E4191 | L4192 | I4193 | Y4194 | F4195 | E4196 | I4197 | S4198 | E4199 | T4200 | N4201 | R4202 | A4203 |       |       |       |       |       |
| W4204 | W4205 | E4206 | W4207 | P4208 | K4211 | K4214 | B4215 | L4218 | F4219 | D4220 | V4221 | V4222 | E4224 | G4225 | G4226 | E4227 | A4228 | E4229 | K4230 | M4231 | F4234 | F4237 | C4238 | E4239 | D4240 | T4241 | I4242 | F4243 | E4244 | M4245 | Q4246 | I4247 | A4248 | A4249 | D4250 | I4251 | S4252 | E4253 | PRO   | GLU   | GLY   | GLU   | PRO   | GLU   | ALA   | ASP   | GLU   | ASP   | GLU   | GLY   | GLY   | GLY   | GLY   |       |       |       |       |       |       |



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C4                               | Depositor |
| Number of particles used             | 791956                                  | Depositor |
| Resolution determination method      | OTHER                                   | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.404                                   | Depositor |
| Minimum map value                    | -0.232                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.16                                    | Depositor |
| Map size (Å)                         | 502.0, 502.0, 502.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.255, 1.255, 1.255                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.22         | 0/834       | 0.58        | 1/1123 (0.1%)    |
| 1   | F     | 0.21         | 0/834       | 0.58        | 1/1123 (0.1%)    |
| 1   | H     | 0.21         | 0/834       | 0.58        | 1/1123 (0.1%)    |
| 1   | J     | 0.21         | 0/834       | 0.58        | 1/1123 (0.1%)    |
| 2   | B     | 0.26         | 0/25428     | 0.61        | 2/34534 (0.0%)   |
| 2   | E     | 0.26         | 0/25428     | 0.61        | 2/34534 (0.0%)   |
| 2   | G     | 0.26         | 0/25428     | 0.61        | 2/34534 (0.0%)   |
| 2   | I     | 0.26         | 0/25428     | 0.61        | 2/34534 (0.0%)   |
| All | All   | 0.26         | 0/105048    | 0.61        | 12/142628 (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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 17                  |
| 2   | E     | 0                   | 18                  |
| 2   | G     | 0                   | 17                  |
| 2   | I     | 0                   | 17                  |
| All | All   | 0                   | 69                  |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | E     | 4872 | PRO  | N-CA-C | -6.25 | 105.22      | 113.65   |
| 2   | I     | 4872 | PRO  | N-CA-C | -6.18 | 105.30      | 113.65   |
| 2   | B     | 4872 | PRO  | N-CA-C | -6.17 | 105.32      | 113.65   |
| 2   | G     | 4872 | PRO  | N-CA-C | -5.94 | 105.27      | 113.53   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | B     | 4063 | ASP  | CA-CB-CG | 5.77 | 118.37      | 112.60   |
| 2   | E     | 4063 | ASP  | CA-CB-CG | 5.72 | 118.32      | 112.60   |
| 2   | G     | 4063 | ASP  | CA-CB-CG | 5.66 | 118.26      | 112.60   |
| 2   | I     | 4063 | ASP  | CA-CB-CG | 5.63 | 118.23      | 112.60   |
| 1   | F     | 8    | SER  | N-CA-C   | 5.49 | 120.39      | 113.25   |
| 1   | H     | 8    | SER  | N-CA-C   | 5.47 | 120.36      | 113.25   |
| 1   | J     | 8    | SER  | N-CA-C   | 5.46 | 120.34      | 113.25   |
| 1   | A     | 8    | SER  | N-CA-C   | 5.44 | 120.33      | 113.25   |

There are no chirality outliers.

All (69) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | B     | 1676 | LEU  | Peptide |
| 2   | B     | 1690 | ASP  | Peptide |
| 2   | B     | 1712 | TYR  | Peptide |
| 2   | B     | 1828 | ASP  | Peptide |
| 2   | B     | 1840 | PRO  | Peptide |
| 2   | B     | 2291 | GLN  | Peptide |
| 2   | B     | 2342 | ASN  | Peptide |
| 2   | B     | 2343 | GLY  | Peptide |
| 2   | B     | 2472 | LEU  | Peptide |
| 2   | B     | 2807 | TRP  | Peptide |
| 2   | B     | 3786 | CYS  | Peptide |
| 2   | B     | 3971 | GLY  | Peptide |
| 2   | B     | 4666 | VAL  | Peptide |
| 2   | B     | 4696 | ASP  | Peptide |
| 2   | B     | 4807 | PHE  | Peptide |
| 2   | B     | 694  | PRO  | Peptide |
| 2   | B     | 808  | TYR  | Peptide |
| 2   | E     | 1676 | LEU  | Peptide |
| 2   | E     | 1690 | ASP  | Peptide |
| 2   | E     | 1712 | TYR  | Peptide |
| 2   | E     | 1828 | ASP  | Peptide |
| 2   | E     | 1840 | PRO  | Peptide |
| 2   | E     | 194  | SER  | Peptide |
| 2   | E     | 2291 | GLN  | Peptide |
| 2   | E     | 2342 | ASN  | Peptide |
| 2   | E     | 2343 | GLY  | Peptide |
| 2   | E     | 2472 | LEU  | Peptide |
| 2   | E     | 2807 | TRP  | Peptide |
| 2   | E     | 3786 | CYS  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | E     | 3971 | GLY  | Peptide |
| 2   | E     | 4666 | VAL  | Peptide |
| 2   | E     | 4696 | ASP  | Peptide |
| 2   | E     | 4807 | PHE  | Peptide |
| 2   | E     | 694  | PRO  | Peptide |
| 2   | E     | 808  | TYR  | Peptide |
| 2   | G     | 1676 | LEU  | Peptide |
| 2   | G     | 1690 | ASP  | Peptide |
| 2   | G     | 1712 | TYR  | Peptide |
| 2   | G     | 1828 | ASP  | Peptide |
| 2   | G     | 1840 | PRO  | Peptide |
| 2   | G     | 2291 | GLN  | Peptide |
| 2   | G     | 2342 | ASN  | Peptide |
| 2   | G     | 2343 | GLY  | Peptide |
| 2   | G     | 2472 | LEU  | Peptide |
| 2   | G     | 2807 | TRP  | Peptide |
| 2   | G     | 3786 | CYS  | Peptide |
| 2   | G     | 3971 | GLY  | Peptide |
| 2   | G     | 4666 | VAL  | Peptide |
| 2   | G     | 4696 | ASP  | Peptide |
| 2   | G     | 4807 | PHE  | Peptide |
| 2   | G     | 694  | PRO  | Peptide |
| 2   | G     | 808  | TYR  | Peptide |
| 2   | I     | 1676 | LEU  | Peptide |
| 2   | I     | 1690 | ASP  | Peptide |
| 2   | I     | 1712 | TYR  | Peptide |
| 2   | I     | 1828 | ASP  | Peptide |
| 2   | I     | 1840 | PRO  | Peptide |
| 2   | I     | 2291 | GLN  | Peptide |
| 2   | I     | 2342 | ASN  | Peptide |
| 2   | I     | 2343 | GLY  | Peptide |
| 2   | I     | 2472 | LEU  | Peptide |
| 2   | I     | 2807 | TRP  | Peptide |
| 2   | I     | 3786 | CYS  | Peptide |
| 2   | I     | 3971 | GLY  | Peptide |
| 2   | I     | 4666 | VAL  | Peptide |
| 2   | I     | 4696 | ASP  | Peptide |
| 2   | I     | 4807 | PHE  | Peptide |
| 2   | I     | 694  | PRO  | Peptide |
| 2   | I     | 808  | TYR  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | A     | 818    | 0        | 824      | 20      | 0            |
| 1   | F     | 818    | 0        | 824      | 19      | 0            |
| 1   | H     | 818    | 0        | 824      | 19      | 0            |
| 1   | J     | 818    | 0        | 824      | 20      | 0            |
| 2   | B     | 29369  | 0        | 24710    | 425     | 0            |
| 2   | E     | 29369  | 0        | 24708    | 434     | 0            |
| 2   | G     | 29369  | 0        | 24708    | 436     | 0            |
| 2   | I     | 29369  | 0        | 24711    | 440     | 0            |
| 3   | B     | 1      | 0        | 0        | 0       | 0            |
| 3   | E     | 1      | 0        | 0        | 0       | 0            |
| 3   | G     | 1      | 0        | 0        | 0       | 0            |
| 3   | I     | 1      | 0        | 0        | 0       | 0            |
| 4   | B     | 1      | 0        | 0        | 0       | 0            |
| 4   | E     | 1      | 0        | 0        | 0       | 0            |
| 4   | G     | 1      | 0        | 0        | 0       | 0            |
| 4   | I     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 120756 | 0        | 102133   | 1793    | 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 8.

All (1793) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:4860:ARG:HD2 | 2:I:4582:VAL:HG11 | 1.65                     | 0.78              |
| 2:G:177:GLU:HG3  | 2:I:2452:ARG:HH12 | 1.54                     | 0.70              |
| 2:B:646:PRO:HD2  | 2:B:779:PRO:HB2   | 1.72                     | 0.70              |
| 2:G:111:HIS:HD2  | 2:G:114:SER:H     | 1.38                     | 0.70              |
| 2:G:646:PRO:HD2  | 2:G:779:PRO:HB2   | 1.72                     | 0.70              |
| 2:I:646:PRO:HD2  | 2:I:779:PRO:HB2   | 1.72                     | 0.70              |
| 2:G:788:LYS:HG2  | 2:G:1630:CYS:H    | 1.57                     | 0.70              |
| 2:E:788:LYS:HG2  | 2:E:1630:CYS:H    | 1.57                     | 0.70              |
| 2:E:646:PRO:HD2  | 2:E:779:PRO:HB2   | 1.72                     | 0.70              |
| 2:I:788:LYS:HG2  | 2:I:1630:CYS:H    | 1.57                     | 0.70              |
| 2:B:111:HIS:HD2  | 2:B:114:SER:H     | 1.38                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:111:HIS:HD2   | 2:E:114:SER:H     | 1.38                     | 0.69              |
| 2:B:788:LYS:HG2   | 2:B:1630:CYS:H    | 1.57                     | 0.69              |
| 2:I:111:HIS:HD2   | 2:I:114:SER:H     | 1.38                     | 0.69              |
| 2:I:1671:ARG:NH2  | 2:I:1710:GLY:O    | 2.27                     | 0.68              |
| 2:G:1671:ARG:NH2  | 2:G:1710:GLY:O    | 2.27                     | 0.68              |
| 2:B:1671:ARG:NH2  | 2:B:1710:GLY:O    | 2.27                     | 0.68              |
| 2:I:1092:PHE:HB3  | 2:I:1149:VAL:HB   | 1.75                     | 0.68              |
| 2:B:1092:PHE:HB3  | 2:B:1149:VAL:HB   | 1.75                     | 0.68              |
| 2:E:1671:ARG:NH2  | 2:E:1710:GLY:O    | 2.27                     | 0.67              |
| 2:E:4855:ALA:HA   | 2:E:4859:PHE:HB2  | 1.76                     | 0.67              |
| 2:I:4855:ALA:HA   | 2:I:4859:PHE:HB2  | 1.76                     | 0.67              |
| 2:G:1092:PHE:HB3  | 2:G:1149:VAL:HB   | 1.75                     | 0.67              |
| 2:G:1667:LEU:HD23 | 2:G:1671:ARG:HH12 | 1.60                     | 0.67              |
| 2:E:1092:PHE:HB3  | 2:E:1149:VAL:HB   | 1.75                     | 0.67              |
| 2:G:4855:ALA:HA   | 2:G:4859:PHE:HB2  | 1.76                     | 0.67              |
| 2:B:4855:ALA:HA   | 2:B:4859:PHE:HB2  | 1.76                     | 0.66              |
| 2:E:1667:LEU:HD23 | 2:E:1671:ARG:HH12 | 1.60                     | 0.66              |
| 2:I:224:HIS:H     | 2:I:230:CYS:HA    | 1.61                     | 0.66              |
| 2:G:224:HIS:H     | 2:G:230:CYS:HA    | 1.61                     | 0.66              |
| 2:E:4799:SER:HG   | 2:E:4812:HIS:HE2  | 1.43                     | 0.65              |
| 1:H:23:VAL:HG22   | 1:H:47:LYS:HG2    | 1.78                     | 0.65              |
| 2:I:1667:LEU:HD23 | 2:I:1671:ARG:HH12 | 1.60                     | 0.65              |
| 2:E:224:HIS:H     | 2:E:230:CYS:HA    | 1.61                     | 0.65              |
| 1:J:23:VAL:HG22   | 1:J:47:LYS:HG2    | 1.78                     | 0.65              |
| 2:B:219:VAL:HG13  | 2:B:285:VAL:HG21  | 1.78                     | 0.65              |
| 2:B:224:HIS:H     | 2:B:230:CYS:HA    | 1.61                     | 0.65              |
| 2:E:2764:GLU:HG3  | 2:E:2857:PRO:HB2  | 1.79                     | 0.65              |
| 2:B:2764:GLU:HG3  | 2:B:2857:PRO:HB2  | 1.79                     | 0.64              |
| 2:G:219:VAL:HG13  | 2:G:285:VAL:HG21  | 1.78                     | 0.64              |
| 2:G:2764:GLU:HG3  | 2:G:2857:PRO:HB2  | 1.79                     | 0.64              |
| 2:I:4799:SER:HG   | 2:I:4812:HIS:HE2  | 1.43                     | 0.64              |
| 2:I:219:VAL:HG13  | 2:I:285:VAL:HG21  | 1.79                     | 0.64              |
| 1:A:23:VAL:HG22   | 1:A:47:LYS:HG2    | 1.78                     | 0.64              |
| 2:B:3937:TYR:O    | 2:B:4002:LYS:NZ   | 2.30                     | 0.64              |
| 2:B:1667:LEU:HD23 | 2:B:1671:ARG:HH12 | 1.60                     | 0.64              |
| 2:B:3767:GLN:HB3  | 2:B:3772:THR:HG22 | 1.80                     | 0.64              |
| 2:I:3937:TYR:O    | 2:I:4002:LYS:NZ   | 2.30                     | 0.64              |
| 2:G:1247:PRO:HA   | 2:G:1598:GLN:HA   | 1.80                     | 0.64              |
| 2:B:745:SER:HB2   | 2:B:758:ARG:HB3   | 1.80                     | 0.64              |
| 2:E:219:VAL:HG13  | 2:E:285:VAL:HG21  | 1.78                     | 0.64              |
| 2:I:4821:LYS:HA   | 2:I:4824:ARG:HE   | 1.64                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4821:LYS:HA   | 2:B:4824:ARG:HE   | 1.63                     | 0.63              |
| 1:F:23:VAL:HG22   | 1:F:47:LYS:HG2    | 1.78                     | 0.63              |
| 2:I:2764:GLU:HG3  | 2:I:2857:PRO:HB2  | 1.79                     | 0.63              |
| 2:I:3767:GLN:HB3  | 2:I:3772:THR:HG22 | 1.80                     | 0.63              |
| 2:I:1519:UNK:HA   | 2:I:1526:UNK:HA   | 1.81                     | 0.63              |
| 2:B:1700:ASP:OD2  | 2:B:1708:ARG:NH2  | 2.32                     | 0.63              |
| 2:G:1700:ASP:OD2  | 2:G:1708:ARG:NH2  | 2.32                     | 0.63              |
| 2:I:1247:PRO:HA   | 2:I:1598:GLN:HA   | 1.80                     | 0.63              |
| 2:I:1700:ASP:OD2  | 2:I:1708:ARG:NH2  | 2.32                     | 0.63              |
| 2:B:742:ASP:HA    | 2:B:760:ASN:HD21  | 1.63                     | 0.63              |
| 2:E:1700:ASP:OD2  | 2:E:1708:ARG:NH2  | 2.32                     | 0.63              |
| 2:I:745:SER:HB2   | 2:I:758:ARG:HB3   | 1.80                     | 0.63              |
| 2:E:742:ASP:HA    | 2:E:760:ASN:HD21  | 1.63                     | 0.63              |
| 2:E:3937:TYR:O    | 2:E:4002:LYS:NZ   | 2.30                     | 0.63              |
| 2:G:745:SER:HB2   | 2:G:758:ARG:HB3   | 1.80                     | 0.63              |
| 2:G:4821:LYS:HA   | 2:G:4824:ARG:HE   | 1.63                     | 0.63              |
| 2:G:3767:GLN:HB3  | 2:G:3772:THR:HG22 | 1.80                     | 0.63              |
| 2:B:606:LEU:O     | 2:B:617:ASN:ND2   | 2.32                     | 0.63              |
| 2:E:4821:LYS:HA   | 2:E:4824:ARG:HE   | 1.63                     | 0.63              |
| 2:G:3937:TYR:O    | 2:G:4002:LYS:NZ   | 2.30                     | 0.63              |
| 2:E:3767:GLN:HB3  | 2:E:3772:THR:HG22 | 1.80                     | 0.62              |
| 2:E:745:SER:HB2   | 2:E:758:ARG:HB3   | 1.80                     | 0.62              |
| 2:G:742:ASP:HA    | 2:G:760:ASN:HD21  | 1.63                     | 0.62              |
| 2:E:4049:VAL:HG21 | 2:E:4159:ARG:HD2  | 1.82                     | 0.62              |
| 2:G:2755:ILE:HD13 | 2:G:2810:LYS:HG2  | 1.81                     | 0.62              |
| 2:I:742:ASP:HA    | 2:I:760:ASN:HD21  | 1.64                     | 0.62              |
| 2:E:1247:PRO:HA   | 2:E:1598:GLN:HA   | 1.80                     | 0.62              |
| 2:G:606:LEU:O     | 2:G:617:ASN:ND2   | 2.32                     | 0.62              |
| 2:B:4049:VAL:HG21 | 2:B:4159:ARG:HD2  | 1.82                     | 0.62              |
| 2:B:1830:VAL:HB   | 2:B:1837:GLN:HA   | 1.82                     | 0.62              |
| 2:E:281:ARG:NH2   | 2:E:309:THR:OG1   | 2.33                     | 0.62              |
| 2:B:281:ARG:NH2   | 2:B:309:THR:OG1   | 2.33                     | 0.62              |
| 2:E:606:LEU:O     | 2:E:617:ASN:ND2   | 2.32                     | 0.62              |
| 2:E:2755:ILE:HD13 | 2:E:2810:LYS:HG2  | 1.81                     | 0.62              |
| 2:I:606:LEU:O     | 2:I:617:ASN:ND2   | 2.32                     | 0.62              |
| 2:B:1247:PRO:HA   | 2:B:1598:GLN:HA   | 1.81                     | 0.61              |
| 2:B:2003:GLN:O    | 2:B:2007:ASN:ND2  | 2.33                     | 0.61              |
| 2:G:853:PRO:HB3   | 2:G:1024:TYR:H    | 1.65                     | 0.61              |
| 2:G:4049:VAL:HG21 | 2:G:4159:ARG:HD2  | 1.82                     | 0.61              |
| 2:I:281:ARG:NH2   | 2:I:309:THR:OG1   | 2.33                     | 0.61              |
| 2:E:1830:VAL:HB   | 2:E:1837:GLN:HA   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1519:UNK:HA   | 2:G:1526:UNK:HA   | 1.82                     | 0.61              |
| 2:I:853:PRO:HB3   | 2:I:1024:TYR:H    | 1.66                     | 0.61              |
| 2:I:2003:GLN:O    | 2:I:2007:ASN:ND2  | 2.33                     | 0.61              |
| 2:G:2003:GLN:O    | 2:G:2007:ASN:ND2  | 2.33                     | 0.61              |
| 2:I:728:ARG:NH2   | 2:I:1527:UNK:O    | 2.33                     | 0.61              |
| 2:I:1830:VAL:HB   | 2:I:1837:GLN:HA   | 1.82                     | 0.61              |
| 2:I:4049:VAL:HG21 | 2:I:4159:ARG:HD2  | 1.82                     | 0.61              |
| 2:G:281:ARG:NH2   | 2:G:309:THR:OG1   | 2.33                     | 0.61              |
| 2:G:1830:VAL:HB   | 2:G:1837:GLN:HA   | 1.81                     | 0.61              |
| 2:B:2755:ILE:HD13 | 2:B:2810:LYS:HG2  | 1.81                     | 0.61              |
| 2:E:2003:GLN:O    | 2:E:2007:ASN:ND2  | 2.33                     | 0.61              |
| 2:I:2755:ILE:HD13 | 2:I:2810:LYS:HG2  | 1.81                     | 0.61              |
| 2:E:4978:HIS:HA   | 2:E:4982:GLU:HB2  | 1.83                     | 0.60              |
| 2:I:1091:GLU:HB3  | 2:I:1203:ASN:HB3  | 1.83                     | 0.60              |
| 2:I:4978:HIS:HA   | 2:I:4982:GLU:HB2  | 1.83                     | 0.60              |
| 2:B:4978:HIS:HA   | 2:B:4982:GLU:HB2  | 1.83                     | 0.60              |
| 2:E:395:GLN:HG3   | 2:E:397:GLU:H     | 1.67                     | 0.60              |
| 2:G:497:TYR:HB3   | 2:G:500:ALA:HB2   | 1.83                     | 0.60              |
| 2:B:497:TYR:HB3   | 2:B:500:ALA:HB2   | 1.83                     | 0.60              |
| 2:G:1101:ARG:HE   | 2:G:1115:LEU:HB3  | 1.67                     | 0.60              |
| 2:B:853:PRO:HB3   | 2:B:1024:TYR:H    | 1.66                     | 0.60              |
| 2:I:1101:ARG:HE   | 2:I:1115:LEU:HB3  | 1.67                     | 0.60              |
| 2:B:887:ILE:HG21  | 2:B:959:TYR:HA    | 1.84                     | 0.60              |
| 2:E:853:PRO:HB3   | 2:E:1024:TYR:H    | 1.66                     | 0.60              |
| 2:E:4860:ARG:HD2  | 2:G:4582:VAL:HG11 | 1.83                     | 0.60              |
| 2:G:221:ARG:NH2   | 2:G:255:HIS:O     | 2.34                     | 0.60              |
| 2:E:4083:ASP:HA   | 2:E:4085:ARG:HH11 | 1.66                     | 0.60              |
| 2:E:497:TYR:HB3   | 2:E:500:ALA:HB2   | 1.83                     | 0.60              |
| 2:G:4978:HIS:HA   | 2:G:4982:GLU:HB2  | 1.83                     | 0.60              |
| 2:I:887:ILE:HG21  | 2:I:959:TYR:HA    | 1.84                     | 0.60              |
| 1:J:27:THR:HB     | 1:J:100:ASP:HB3   | 1.84                     | 0.60              |
| 2:B:395:GLN:HG3   | 2:B:397:GLU:H     | 1.67                     | 0.59              |
| 2:E:1241:SER:HA   | 2:E:1603:VAL:HA   | 1.84                     | 0.59              |
| 2:G:1241:SER:HA   | 2:G:1603:VAL:HA   | 1.84                     | 0.59              |
| 2:I:1241:SER:HA   | 2:I:1603:VAL:HA   | 1.84                     | 0.59              |
| 2:B:1241:SER:HA   | 2:B:1603:VAL:HA   | 1.84                     | 0.59              |
| 2:E:635:THR:HB    | 2:E:1639:LEU:HD23 | 1.84                     | 0.59              |
| 2:E:1091:GLU:HB3  | 2:E:1203:ASN:HB3  | 1.83                     | 0.59              |
| 1:F:27:THR:HB     | 1:F:100:ASP:HB3   | 1.84                     | 0.59              |
| 2:G:664:PHE:HB2   | 2:G:746:CYS:HB2   | 1.84                     | 0.59              |
| 1:H:27:THR:HB     | 1:H:100:ASP:HB3   | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:395:GLN:HG3   | 2:I:397:GLU:H     | 1.67                     | 0.59              |
| 2:G:972:LEU:O     | 2:G:1044:ARG:NH2  | 2.34                     | 0.59              |
| 2:G:1973:GLN:O    | 2:G:1977:TYR:N    | 2.36                     | 0.59              |
| 2:G:2281:ILE:HG23 | 2:G:2341:VAL:HG11 | 1.85                     | 0.59              |
| 2:I:972:LEU:O     | 2:I:1044:ARG:NH2  | 2.34                     | 0.59              |
| 2:B:1091:GLU:HB3  | 2:B:1203:ASN:HB3  | 1.83                     | 0.59              |
| 2:B:221:ARG:NH2   | 2:B:255:HIS:O     | 2.34                     | 0.59              |
| 2:B:1218:GLY:HA2  | 2:B:1223:PHE:HB2  | 1.84                     | 0.59              |
| 2:E:887:ILE:HG21  | 2:E:959:TYR:HA    | 1.84                     | 0.59              |
| 2:G:395:GLN:HG3   | 2:G:397:GLU:H     | 1.67                     | 0.59              |
| 1:A:6:THR:HA      | 1:A:72:ALA:HA     | 1.85                     | 0.59              |
| 2:B:635:THR:HB    | 2:B:1639:LEU:HD23 | 1.84                     | 0.59              |
| 2:E:972:LEU:O     | 2:E:1044:ARG:NH2  | 2.34                     | 0.59              |
| 2:I:497:TYR:HB3   | 2:I:500:ALA:HB2   | 1.83                     | 0.59              |
| 2:B:4083:ASP:HA   | 2:B:4085:ARG:HH11 | 1.66                     | 0.59              |
| 2:E:18:ASP:HB2    | 2:E:69:LEU:HD12   | 1.84                     | 0.59              |
| 2:E:1973:GLN:O    | 2:E:1977:TYR:N    | 2.36                     | 0.59              |
| 2:G:242:ARG:NH1   | 2:G:481:GLU:OE1   | 2.36                     | 0.59              |
| 2:G:887:ILE:HG21  | 2:G:959:TYR:HA    | 1.84                     | 0.59              |
| 1:H:74:LEU:HB2    | 1:H:99:PHE:HB2    | 1.84                     | 0.59              |
| 1:A:27:THR:HB     | 1:A:100:ASP:HB3   | 1.84                     | 0.59              |
| 2:G:1091:GLU:HB3  | 2:G:1203:ASN:HB3  | 1.83                     | 0.59              |
| 2:G:1096:THR:HG23 | 2:G:1199:VAL:HG22 | 1.84                     | 0.59              |
| 2:I:2281:ILE:HG23 | 2:I:2341:VAL:HG11 | 1.84                     | 0.59              |
| 2:B:972:LEU:O     | 2:B:1044:ARG:NH2  | 2.34                     | 0.59              |
| 2:E:242:ARG:NH1   | 2:E:481:GLU:OE1   | 2.36                     | 0.59              |
| 2:E:472:ARG:NH2   | 2:E:3712:GLU:OE2  | 2.36                     | 0.59              |
| 2:I:1973:GLN:O    | 2:I:1977:TYR:N    | 2.36                     | 0.59              |
| 1:J:74:LEU:HB2    | 1:J:99:PHE:HB2    | 1.84                     | 0.59              |
| 2:E:1101:ARG:HE   | 2:E:1115:LEU:HB3  | 1.67                     | 0.59              |
| 2:I:472:ARG:NH2   | 2:I:3712:GLU:OE2  | 2.36                     | 0.59              |
| 2:I:4083:ASP:HA   | 2:I:4085:ARG:HH11 | 1.67                     | 0.59              |
| 2:B:637:LEU:HD23  | 2:B:1637:MET:HB3  | 1.85                     | 0.58              |
| 2:B:1101:ARG:HE   | 2:B:1115:LEU:HB3  | 1.66                     | 0.58              |
| 2:E:1218:GLY:HA2  | 2:E:1223:PHE:HB2  | 1.84                     | 0.58              |
| 2:G:110:ARG:HH21  | 2:G:115:ARG:HB3   | 1.68                     | 0.58              |
| 2:G:4061:PHE:HA   | 2:G:4065:PHE:HB3  | 1.85                     | 0.58              |
| 2:I:242:ARG:NH1   | 2:I:481:GLU:OE1   | 2.36                     | 0.58              |
| 2:B:18:ASP:HB2    | 2:B:69:LEU:HD12   | 1.85                     | 0.58              |
| 2:B:4892:ARG:NH2  | 2:I:4895:GLY:O    | 2.33                     | 0.58              |
| 2:E:2281:ILE:HG23 | 2:E:2341:VAL:HG11 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4061:PHE:HA   | 2:E:4065:PHE:HB3  | 1.85                     | 0.58              |
| 2:G:18:ASP:HB2    | 2:G:69:LEU:HD12   | 1.84                     | 0.58              |
| 2:G:635:THR:HB    | 2:G:1639:LEU:HD23 | 1.84                     | 0.58              |
| 2:G:1218:GLY:HA2  | 2:G:1223:PHE:HB2  | 1.84                     | 0.58              |
| 2:I:664:PHE:HB2   | 2:I:746:CYS:HB2   | 1.84                     | 0.58              |
| 2:E:591:ASP:O     | 2:E:1594:ARG:NH2  | 2.36                     | 0.58              |
| 2:G:637:LEU:HD23  | 2:G:1637:MET:HB3  | 1.86                     | 0.58              |
| 2:G:4083:ASP:HA   | 2:G:4085:ARG:HH11 | 1.66                     | 0.58              |
| 2:B:650:VAL:HB    | 2:B:777:PHE:HB2   | 1.86                     | 0.58              |
| 2:E:637:LEU:HD23  | 2:E:1637:MET:HB3  | 1.86                     | 0.58              |
| 2:G:591:ASP:O     | 2:G:1594:ARG:NH2  | 2.36                     | 0.58              |
| 2:I:18:ASP:HB2    | 2:I:69:LEU:HD12   | 1.84                     | 0.58              |
| 2:B:242:ARG:NH1   | 2:B:481:GLU:OE1   | 2.36                     | 0.58              |
| 2:E:664:PHE:HB2   | 2:E:746:CYS:HB2   | 1.84                     | 0.58              |
| 2:G:1743:ARG:O    | 2:G:1964:ARG:NH2  | 2.37                     | 0.58              |
| 2:B:472:ARG:NH2   | 2:B:3712:GLU:OE2  | 2.36                     | 0.58              |
| 2:E:1649:ASP:HB3  | 2:E:1652:GLU:HG2  | 1.85                     | 0.58              |
| 2:E:1743:ARG:O    | 2:E:1964:ARG:NH2  | 2.36                     | 0.58              |
| 2:E:2042:CYS:SG   | 2:E:2043:GLY:N    | 2.76                     | 0.58              |
| 1:F:6:THR:HA      | 1:F:72:ALA:HA     | 1.85                     | 0.58              |
| 2:G:1079:LYS:NZ   | 2:G:1107:PRO:O    | 2.37                     | 0.58              |
| 2:I:635:THR:HB    | 2:I:1639:LEU:HD23 | 1.84                     | 0.58              |
| 2:E:650:VAL:HB    | 2:E:777:PHE:HB2   | 1.86                     | 0.58              |
| 2:E:1096:THR:HG23 | 2:E:1199:VAL:HG22 | 1.84                     | 0.58              |
| 2:G:1271:ARG:HA   | 2:G:1471:UNK:HA   | 1.85                     | 0.58              |
| 2:I:379:HIS:HD2   | 2:I:382:GLY:H     | 1.52                     | 0.58              |
| 2:I:637:LEU:HD23  | 2:I:1637:MET:HB3  | 1.86                     | 0.58              |
| 2:I:1096:THR:HG23 | 2:I:1199:VAL:HG22 | 1.84                     | 0.58              |
| 2:I:1743:ARG:O    | 2:I:1964:ARG:NH2  | 2.36                     | 0.58              |
| 2:B:591:ASP:O     | 2:B:1594:ARG:NH2  | 2.36                     | 0.58              |
| 2:B:1519:UNK:HA   | 2:B:1526:UNK:HA   | 1.86                     | 0.58              |
| 2:B:2281:ILE:HG23 | 2:B:2341:VAL:HG11 | 1.84                     | 0.58              |
| 2:E:1079:LYS:NZ   | 2:E:1107:PRO:O    | 2.37                     | 0.58              |
| 2:B:1096:THR:HG23 | 2:B:1199:VAL:HG22 | 1.84                     | 0.58              |
| 2:B:1973:GLN:O    | 2:B:1977:TYR:N    | 2.36                     | 0.58              |
| 2:E:221:ARG:NH2   | 2:E:255:HIS:O     | 2.34                     | 0.58              |
| 2:G:2042:CYS:SG   | 2:G:2043:GLY:N    | 2.76                     | 0.58              |
| 2:I:650:VAL:HB    | 2:I:777:PHE:HB2   | 1.86                     | 0.58              |
| 2:I:2189:LYS:HA   | 2:I:2192:TYR:HD2  | 1.69                     | 0.58              |
| 2:B:1743:ARG:O    | 2:B:1964:ARG:NH2  | 2.36                     | 0.58              |
| 2:B:2440:MET:O    | 2:B:2444:GLN:N    | 2.37                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:110:ARG:HH21  | 2:E:115:ARG:HB3   | 1.68                     | 0.58              |
| 2:E:827:LYS:O     | 2:E:1073:ARG:NH2  | 2.37                     | 0.58              |
| 2:G:472:ARG:NH2   | 2:G:3712:GLU:OE2  | 2.36                     | 0.58              |
| 2:I:110:ARG:HH21  | 2:I:115:ARG:HB3   | 1.68                     | 0.58              |
| 1:A:74:LEU:HB2    | 1:A:99:PHE:HB2    | 1.84                     | 0.57              |
| 2:B:827:LYS:O     | 2:B:1073:ARG:NH2  | 2.37                     | 0.57              |
| 2:E:177:GLU:HG3   | 2:G:2452:ARG:HH12 | 1.69                     | 0.57              |
| 2:I:1218:GLY:HA2  | 2:I:1223:PHE:HB2  | 1.84                     | 0.57              |
| 2:B:2189:LYS:HA   | 2:B:2192:TYR:HD2  | 1.69                     | 0.57              |
| 2:E:3805:LEU:HA   | 2:E:3809:ASN:HD22 | 1.70                     | 0.57              |
| 2:G:650:VAL:HB    | 2:G:777:PHE:HB2   | 1.86                     | 0.57              |
| 2:I:827:LYS:O     | 2:I:1073:ARG:NH2  | 2.37                     | 0.57              |
| 2:B:379:HIS:HD2   | 2:B:382:GLY:H     | 1.51                     | 0.57              |
| 1:F:74:LEU:HB2    | 1:F:99:PHE:HB2    | 1.84                     | 0.57              |
| 2:I:609:CYS:SG    | 2:I:610:ASN:N     | 2.78                     | 0.57              |
| 2:B:664:PHE:HB2   | 2:B:746:CYS:HB2   | 1.84                     | 0.57              |
| 2:B:2862:LEU:HB3  | 2:B:2928:LYS:HB3  | 1.86                     | 0.57              |
| 2:B:4061:PHE:HA   | 2:B:4065:PHE:HB3  | 1.85                     | 0.57              |
| 2:E:1271:ARG:HA   | 2:E:1471:UNK:HA   | 1.85                     | 0.57              |
| 2:I:1232:ARG:HH21 | 2:I:1701:ALA:HB1  | 1.70                     | 0.57              |
| 2:I:2042:CYS:SG   | 2:I:2043:GLY:N    | 2.76                     | 0.57              |
| 2:I:4061:PHE:HA   | 2:I:4065:PHE:HB3  | 1.85                     | 0.57              |
| 2:G:2189:LYS:HA   | 2:G:2192:TYR:HD2  | 1.69                     | 0.57              |
| 2:G:2257:LEU:HD11 | 2:G:2276:ALA:HB2  | 1.86                     | 0.57              |
| 2:G:2440:MET:O    | 2:G:2444:GLN:N    | 2.37                     | 0.57              |
| 2:I:591:ASP:O     | 2:I:1594:ARG:NH2  | 2.36                     | 0.57              |
| 2:B:1649:ASP:HB3  | 2:B:1652:GLU:HG2  | 1.85                     | 0.57              |
| 2:E:1519:UNK:HA   | 2:E:1526:UNK:HA   | 1.87                     | 0.57              |
| 2:E:2257:LEU:HD11 | 2:E:2276:ALA:HB2  | 1.86                     | 0.57              |
| 2:G:639:ASN:H     | 2:G:678:GLN:HE22  | 1.53                     | 0.57              |
| 2:G:2205:GLU:HG2  | 2:G:2253:HIS:HE1  | 1.70                     | 0.57              |
| 1:H:6:THR:HA      | 1:H:72:ALA:HA     | 1.85                     | 0.57              |
| 2:I:2205:GLU:HG2  | 2:I:2253:HIS:HE1  | 1.70                     | 0.57              |
| 2:I:2748:PRO:HD2  | 2:I:2751:LEU:HD12 | 1.87                     | 0.57              |
| 1:J:6:THR:HA      | 1:J:72:ALA:HA     | 1.85                     | 0.57              |
| 2:E:2440:MET:O    | 2:E:2444:GLN:N    | 2.37                     | 0.57              |
| 2:E:4681:LEU:HD21 | 2:E:4687:TYR:HD2  | 1.70                     | 0.57              |
| 2:G:827:LYS:O     | 2:G:1073:ARG:NH2  | 2.37                     | 0.57              |
| 2:G:3904:ARG:NH2  | 2:G:3973:CYS:SG   | 2.78                     | 0.57              |
| 2:I:2862:LEU:HB3  | 2:I:2928:LYS:HB3  | 1.86                     | 0.57              |
| 2:I:3904:ARG:NH2  | 2:I:3973:CYS:SG   | 2.78                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:639:ASN:H     | 2:E:678:GLN:HE22  | 1.53                     | 0.57              |
| 2:E:2862:LEU:HB3  | 2:E:2928:LYS:HB3  | 1.86                     | 0.57              |
| 2:G:379:HIS:HD2   | 2:G:382:GLY:H     | 1.51                     | 0.57              |
| 2:G:1232:ARG:HH21 | 2:G:1701:ALA:HB1  | 1.69                     | 0.57              |
| 2:I:4681:LEU:HD21 | 2:I:4687:TYR:HD2  | 1.69                     | 0.57              |
| 2:B:609:CYS:SG    | 2:B:610:ASN:N     | 2.78                     | 0.57              |
| 2:G:3805:LEU:HA   | 2:G:3809:ASN:HD22 | 1.70                     | 0.57              |
| 2:B:110:ARG:HH21  | 2:B:115:ARG:HB3   | 1.68                     | 0.56              |
| 2:B:451:TYR:O     | 2:B:474:ARG:NH1   | 2.38                     | 0.56              |
| 2:B:813:GLU:OE2   | 2:B:1020:ARG:N    | 2.38                     | 0.56              |
| 2:E:609:CYS:SG    | 2:E:610:ASN:N     | 2.78                     | 0.56              |
| 2:G:2748:PRO:HD2  | 2:G:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:G:4584:ASP:HA   | 2:G:4627:MET:HA   | 1.87                     | 0.56              |
| 2:I:221:ARG:NH2   | 2:I:255:HIS:O     | 2.34                     | 0.56              |
| 2:I:3805:LEU:HA   | 2:I:3809:ASN:HD22 | 1.70                     | 0.56              |
| 2:B:256:ALA:HB1   | 2:B:286:THR:HG21  | 1.87                     | 0.56              |
| 2:B:4749:GLU:HA   | 2:B:4752:ALA:HB3  | 1.88                     | 0.56              |
| 2:E:4584:ASP:HA   | 2:E:4627:MET:HA   | 1.87                     | 0.56              |
| 2:G:1649:ASP:HB3  | 2:G:1652:GLU:HG2  | 1.85                     | 0.56              |
| 2:G:2862:LEU:HB3  | 2:G:2928:LYS:HB3  | 1.86                     | 0.56              |
| 2:B:1079:LYS:NZ   | 2:B:1107:PRO:O    | 2.37                     | 0.56              |
| 2:B:1232:ARG:HH21 | 2:B:1701:ALA:HB1  | 1.70                     | 0.56              |
| 2:E:813:GLU:OE2   | 2:E:1020:ARG:N    | 2.38                     | 0.56              |
| 2:G:813:GLU:OE2   | 2:G:1020:ARG:N    | 2.38                     | 0.56              |
| 2:I:256:ALA:HB1   | 2:I:286:THR:HG21  | 1.87                     | 0.56              |
| 2:I:1079:LYS:NZ   | 2:I:1107:PRO:O    | 2.37                     | 0.56              |
| 2:I:1649:ASP:HB3  | 2:I:1652:GLU:HG2  | 1.85                     | 0.56              |
| 2:I:4581:LYS:HB2  | 2:I:4632:LEU:HB2  | 1.87                     | 0.56              |
| 2:B:639:ASN:H     | 2:B:678:GLN:HE22  | 1.53                     | 0.56              |
| 2:E:2748:PRO:HD2  | 2:E:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:E:3904:ARG:NH2  | 2:E:3973:CYS:SG   | 2.78                     | 0.56              |
| 2:E:4581:LYS:HB2  | 2:E:4632:LEU:HB2  | 1.87                     | 0.56              |
| 2:G:256:ALA:HB1   | 2:G:286:THR:HG21  | 1.87                     | 0.56              |
| 2:I:2440:MET:O    | 2:I:2444:GLN:N    | 2.37                     | 0.56              |
| 2:B:3904:ARG:NH2  | 2:B:3973:CYS:SG   | 2.78                     | 0.56              |
| 2:E:4749:GLU:HA   | 2:E:4752:ALA:HB3  | 1.88                     | 0.56              |
| 2:B:2205:GLU:HG2  | 2:B:2253:HIS:HE1  | 1.70                     | 0.56              |
| 2:B:2257:LEU:HD11 | 2:B:2276:ALA:HB2  | 1.86                     | 0.56              |
| 2:B:4681:LEU:HD21 | 2:B:4687:TYR:HD2  | 1.69                     | 0.56              |
| 2:E:256:ALA:HB1   | 2:E:286:THR:HG21  | 1.87                     | 0.56              |
| 2:E:2205:GLU:HG2  | 2:E:2253:HIS:HE1  | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4843:LEU:HD12 | 2:G:4823:LEU:HD21 | 1.86                     | 0.56              |
| 2:G:619:ASP:OD1   | 2:G:1680:ARG:NH1  | 2.39                     | 0.56              |
| 2:G:4681:LEU:HD21 | 2:G:4687:TYR:HD2  | 1.69                     | 0.56              |
| 2:B:619:ASP:OD1   | 2:B:1680:ARG:NH1  | 2.39                     | 0.56              |
| 2:B:989:ALA:O     | 2:B:1035:ASN:ND2  | 2.39                     | 0.56              |
| 2:B:2927:LEU:HD23 | 2:B:2930:LEU:HD12 | 1.88                     | 0.56              |
| 2:E:157:ARG:NH2   | 2:E:167:ASP:OD1   | 2.38                     | 0.56              |
| 2:E:1764:GLY:HA3  | 2:E:1859:VAL:HG11 | 1.88                     | 0.56              |
| 2:E:2189:LYS:HA   | 2:E:2192:TYR:HD2  | 1.69                     | 0.56              |
| 2:G:1721:GLU:OE2  | 2:G:1725:ARG:NH2  | 2.38                     | 0.56              |
| 2:G:4581:LYS:HB2  | 2:G:4632:LEU:HB2  | 1.87                     | 0.56              |
| 2:G:4749:GLU:HA   | 2:G:4752:ALA:HB3  | 1.88                     | 0.56              |
| 2:I:813:GLU:OE2   | 2:I:1020:ARG:N    | 2.38                     | 0.56              |
| 2:I:989:ALA:O     | 2:I:1035:ASN:ND2  | 2.38                     | 0.56              |
| 2:I:1764:GLY:HA3  | 2:I:1859:VAL:HG11 | 1.88                     | 0.56              |
| 2:B:4918:ILE:HG23 | 2:E:4892:ARG:HD3  | 1.88                     | 0.56              |
| 2:E:379:HIS:HD2   | 2:E:382:GLY:H     | 1.52                     | 0.56              |
| 2:I:639:ASN:H     | 2:I:678:GLN:HE22  | 1.53                     | 0.56              |
| 2:I:1271:ARG:HA   | 2:I:1471:UNK:HA   | 1.87                     | 0.56              |
| 2:I:2257:LEU:HD11 | 2:I:2276:ALA:HB2  | 1.86                     | 0.56              |
| 2:B:157:ARG:NH2   | 2:B:167:ASP:OD1   | 2.38                     | 0.56              |
| 2:B:1211:LEU:HD11 | 2:B:1225:PRO:HB3  | 1.88                     | 0.56              |
| 2:B:3805:LEU:HA   | 2:B:3809:ASN:HD22 | 1.70                     | 0.56              |
| 2:E:989:ALA:O     | 2:E:1035:ASN:ND2  | 2.39                     | 0.56              |
| 2:E:1721:GLU:OE2  | 2:E:1725:ARG:NH2  | 2.38                     | 0.56              |
| 2:G:1764:GLY:HA3  | 2:G:1859:VAL:HG11 | 1.88                     | 0.56              |
| 2:I:4749:GLU:HA   | 2:I:4752:ALA:HB3  | 1.88                     | 0.56              |
| 2:E:1232:ARG:HH21 | 2:E:1701:ALA:HB1  | 1.70                     | 0.56              |
| 2:G:989:ALA:O     | 2:G:1035:ASN:ND2  | 2.39                     | 0.56              |
| 2:E:4984:ASN:OD1  | 2:E:4987:ASN:ND2  | 2.39                     | 0.55              |
| 2:G:609:CYS:SG    | 2:G:610:ASN:N     | 2.78                     | 0.55              |
| 2:E:2927:LEU:HD23 | 2:E:2930:LEU:HD12 | 1.88                     | 0.55              |
| 2:I:619:ASP:OD1   | 2:I:1680:ARG:NH1  | 2.39                     | 0.55              |
| 2:I:1808:ARG:NH1  | 2:I:1853:ILE:O    | 2.39                     | 0.55              |
| 2:B:1838:PHE:HB3  | 2:B:1842:LEU:HD11 | 1.89                     | 0.55              |
| 2:G:1838:PHE:HB3  | 2:G:1842:LEU:HD11 | 1.89                     | 0.55              |
| 2:I:4584:ASP:HA   | 2:I:4627:MET:HA   | 1.87                     | 0.55              |
| 2:B:331:VAL:HG12  | 2:B:333:GLY:H     | 1.71                     | 0.55              |
| 2:B:2748:PRO:HD2  | 2:B:2751:LEU:HD12 | 1.87                     | 0.55              |
| 2:B:3780:LEU:HD11 | 2:B:3816:MET:HG3  | 1.88                     | 0.55              |
| 2:B:4584:ASP:HA   | 2:B:4627:MET:HA   | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1211:LEU:HD11 | 2:E:1225:PRO:HB3  | 1.88                     | 0.55              |
| 2:E:3780:LEU:HD11 | 2:E:3816:MET:HG3  | 1.88                     | 0.55              |
| 2:G:451:TYR:O     | 2:G:474:ARG:NH1   | 2.38                     | 0.55              |
| 2:I:331:VAL:HG12  | 2:I:333:GLY:H     | 1.71                     | 0.55              |
| 2:I:451:TYR:O     | 2:I:474:ARG:NH1   | 2.38                     | 0.55              |
| 2:I:2927:LEU:HD23 | 2:I:2930:LEU:HD12 | 1.88                     | 0.55              |
| 2:I:3780:LEU:HD11 | 2:I:3816:MET:HG3  | 1.88                     | 0.55              |
| 2:B:1764:GLY:HA3  | 2:B:1859:VAL:HG11 | 1.88                     | 0.55              |
| 2:B:4860:ARG:HD2  | 2:E:4582:VAL:HG11 | 1.88                     | 0.55              |
| 2:E:1808:ARG:NH1  | 2:E:1853:ILE:O    | 2.39                     | 0.55              |
| 2:G:426:ARG:HB2   | 2:G:506:TYR:HA    | 1.88                     | 0.55              |
| 2:B:4984:ASN:OD1  | 2:B:4987:ASN:ND2  | 2.40                     | 0.55              |
| 2:G:132:ALA:HA    | 2:G:194:SER:HB2   | 1.89                     | 0.55              |
| 2:I:132:ALA:HA    | 2:I:194:SER:HB2   | 1.89                     | 0.55              |
| 2:B:283:ARG:HH21  | 2:B:402:ARG:HH12  | 1.54                     | 0.55              |
| 2:B:399:GLN:HG2   | 2:B:403:MET:HE3   | 1.89                     | 0.55              |
| 2:E:619:ASP:OD1   | 2:E:1680:ARG:NH1  | 2.39                     | 0.55              |
| 2:E:627:PRO:HB2   | 1:F:92:PRO:HD3    | 1.89                     | 0.55              |
| 2:E:1838:PHE:HB3  | 2:E:1842:LEU:HD11 | 1.89                     | 0.55              |
| 2:B:1636:MET:HE2  | 2:B:1638:ALA:HB2  | 1.89                     | 0.55              |
| 2:B:4581:LYS:HB2  | 2:B:4632:LEU:HB2  | 1.87                     | 0.55              |
| 2:E:451:TYR:O     | 2:E:474:ARG:NH1   | 2.38                     | 0.55              |
| 2:G:1211:LEU:HD11 | 2:G:1225:PRO:HB3  | 1.88                     | 0.55              |
| 2:I:864:PRO:HD2   | 2:I:867:LEU:HD12  | 1.89                     | 0.55              |
| 2:I:1211:LEU:HD11 | 2:I:1225:PRO:HB3  | 1.88                     | 0.55              |
| 2:I:1838:PHE:HB3  | 2:I:1842:LEU:HD11 | 1.89                     | 0.55              |
| 2:I:4984:ASN:OD1  | 2:I:4987:ASN:ND2  | 2.39                     | 0.55              |
| 2:G:3781:GLN:HA   | 2:G:3784:SER:HB3  | 1.89                     | 0.55              |
| 2:B:3767:GLN:NE2  | 2:B:3804:ILE:O    | 2.40                     | 0.55              |
| 2:E:399:GLN:HG2   | 2:E:403:MET:HE3   | 1.89                     | 0.55              |
| 2:E:1636:MET:HE2  | 2:E:1638:ALA:HB2  | 1.89                     | 0.55              |
| 2:G:2927:LEU:HD23 | 2:G:2930:LEU:HD12 | 1.88                     | 0.54              |
| 2:G:3780:LEU:HD11 | 2:G:3816:MET:HG3  | 1.88                     | 0.54              |
| 2:B:4799:SER:OG   | 2:B:4812:HIS:NE2  | 2.41                     | 0.54              |
| 2:G:23:GLN:HE21   | 2:G:34:LYS:HB3    | 1.73                     | 0.54              |
| 2:G:3767:GLN:NE2  | 2:G:3804:ILE:O    | 2.40                     | 0.54              |
| 2:G:4984:ASN:OD1  | 2:G:4987:ASN:ND2  | 2.40                     | 0.54              |
| 2:I:283:ARG:HH21  | 2:I:402:ARG:HH12  | 1.54                     | 0.54              |
| 2:I:3767:GLN:NE2  | 2:I:3804:ILE:O    | 2.40                     | 0.54              |
| 2:B:23:GLN:HE21   | 2:B:34:LYS:HB3    | 1.73                     | 0.54              |
| 2:I:3781:GLN:HA   | 2:I:3784:SER:HB3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:864:PRO:HD2  | 2:B:867:LEU:HD12  | 1.89                     | 0.54              |
| 2:B:2770:LYS:HB3 | 2:B:2775:TRP:HB2  | 1.90                     | 0.54              |
| 2:I:1636:MET:HE2 | 2:I:1638:ALA:HB2  | 1.89                     | 0.54              |
| 2:B:3781:GLN:HA  | 2:B:3784:SER:HB3  | 1.89                     | 0.54              |
| 2:E:331:VAL:HG12 | 2:E:333:GLY:H     | 1.71                     | 0.54              |
| 2:E:647:ASN:ND2  | 2:E:820:ARG:O     | 2.39                     | 0.54              |
| 2:E:2770:LYS:HB3 | 2:E:2775:TRP:HB2  | 1.90                     | 0.54              |
| 2:G:2770:LYS:HB3 | 2:G:2775:TRP:HB2  | 1.90                     | 0.54              |
| 2:I:157:ARG:NH2  | 2:I:167:ASP:OD1   | 2.38                     | 0.54              |
| 2:I:426:ARG:HB2  | 2:I:506:TYR:HA    | 1.88                     | 0.54              |
| 2:I:683:ARG:NH1  | 2:I:707:VAL:O     | 2.40                     | 0.54              |
| 1:A:25:HIS:HB3   | 1:A:40:ARG:HD3    | 1.90                     | 0.54              |
| 2:E:3767:GLN:NE2 | 2:E:3804:ILE:O    | 2.40                     | 0.54              |
| 2:G:157:ARG:NH2  | 2:G:167:ASP:OD1   | 2.38                     | 0.54              |
| 2:G:1667:LEU:O   | 2:G:1671:ARG:NH1  | 2.41                     | 0.54              |
| 2:I:399:GLN:HG2  | 2:I:403:MET:HE3   | 1.89                     | 0.54              |
| 2:B:1667:LEU:O   | 2:B:1671:ARG:NH1  | 2.41                     | 0.54              |
| 2:E:3843:ASP:H   | 2:E:3874:VAL:HG13 | 1.73                     | 0.54              |
| 2:G:283:ARG:HH21 | 2:G:402:ARG:HH12  | 1.54                     | 0.54              |
| 2:B:669:ASP:OD2  | 2:B:790:ARG:NH2   | 2.41                     | 0.54              |
| 2:B:2248:ARG:NH2 | 2:B:2285:GLU:OE1  | 2.41                     | 0.54              |
| 2:G:331:VAL:HG12 | 2:G:333:GLY:H     | 1.71                     | 0.54              |
| 2:G:1636:MET:HE2 | 2:G:1638:ALA:HB2  | 1.89                     | 0.54              |
| 2:B:132:ALA:HA   | 2:B:194:SER:HB2   | 1.89                     | 0.54              |
| 2:B:426:ARG:HB2  | 2:B:506:TYR:HA    | 1.88                     | 0.54              |
| 2:E:283:ARG:HH21 | 2:E:402:ARG:HH12  | 1.54                     | 0.54              |
| 2:G:4799:SER:OG  | 2:G:4812:HIS:NE2  | 2.41                     | 0.54              |
| 2:I:2248:ARG:NH2 | 2:I:2285:GLU:OE1  | 2.41                     | 0.54              |
| 1:A:26:TYR:OH    | 1:A:42:ARG:NH2    | 2.36                     | 0.54              |
| 2:B:229:GLU:HA   | 2:B:249:GLY:HA2   | 1.90                     | 0.54              |
| 2:B:2042:CYS:SG  | 2:B:2043:GLY:N    | 2.76                     | 0.54              |
| 2:E:132:ALA:HA   | 2:E:194:SER:HB2   | 1.89                     | 0.54              |
| 2:G:864:PRO:HD2  | 2:G:867:LEU:HD12  | 1.89                     | 0.54              |
| 2:I:669:ASP:OD2  | 2:I:790:ARG:NH2   | 2.41                     | 0.54              |
| 2:B:396:GLU:O    | 2:B:400:ALA:N     | 2.40                     | 0.53              |
| 2:E:426:ARG:HB2  | 2:E:506:TYR:HA    | 1.88                     | 0.53              |
| 2:I:655:GLY:HA2  | 2:I:1002:ALA:HB2  | 1.90                     | 0.53              |
| 2:I:4155:PRO:HD2 | 2:I:5036:LEU:HD23 | 1.91                     | 0.53              |
| 1:J:25:HIS:HB3   | 1:J:40:ARG:HD3    | 1.90                     | 0.53              |
| 2:B:1808:ARG:NH1 | 2:B:1853:ILE:O    | 2.39                     | 0.53              |
| 2:E:1667:LEU:O   | 2:E:1671:ARG:NH1  | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:399:GLN:HG2   | 2:G:403:MET:HE3   | 1.89                     | 0.53              |
| 2:I:1667:LEU:O    | 2:I:1671:ARG:NH1  | 2.41                     | 0.53              |
| 2:E:655:GLY:HA2   | 2:E:1002:ALA:HB2  | 1.90                     | 0.53              |
| 2:E:683:ARG:NH1   | 2:E:707:VAL:O     | 2.40                     | 0.53              |
| 2:E:3781:GLN:HA   | 2:E:3784:SER:HB3  | 1.89                     | 0.53              |
| 1:F:25:HIS:HB3    | 1:F:40:ARG:HD3    | 1.90                     | 0.53              |
| 2:G:229:GLU:OE2   | 2:G:374:LYS:NZ    | 2.35                     | 0.53              |
| 2:G:669:ASP:OD2   | 2:G:790:ARG:NH2   | 2.41                     | 0.53              |
| 2:I:23:GLN:HE21   | 2:I:34:LYS:HB3    | 1.73                     | 0.53              |
| 2:I:2770:LYS:HB3  | 2:I:2775:TRP:HB2  | 1.90                     | 0.53              |
| 2:B:1721:GLU:OE2  | 2:B:1725:ARG:NH2  | 2.38                     | 0.53              |
| 2:E:2248:ARG:NH2  | 2:E:2285:GLU:OE1  | 2.41                     | 0.53              |
| 2:G:17:ASP:HB2    | 2:G:98:HIS:HE1    | 1.73                     | 0.53              |
| 2:B:1679:ASN:ND2  | 2:B:1798:LEU:O    | 2.41                     | 0.53              |
| 2:B:3843:ASP:H    | 2:B:3874:VAL:HG13 | 1.73                     | 0.53              |
| 2:E:229:GLU:HA    | 2:E:249:GLY:HA2   | 1.91                     | 0.53              |
| 2:G:229:GLU:HA    | 2:G:249:GLY:HA2   | 1.91                     | 0.53              |
| 2:G:551:LEU:HD11  | 2:G:589:LEU:HD13  | 1.90                     | 0.53              |
| 2:G:2248:ARG:NH2  | 2:G:2285:GLU:OE1  | 2.41                     | 0.53              |
| 2:G:3843:ASP:H    | 2:G:3874:VAL:HG13 | 1.73                     | 0.53              |
| 2:I:229:GLU:HA    | 2:I:249:GLY:HA2   | 1.91                     | 0.53              |
| 2:I:1679:ASN:ND2  | 2:I:1798:LEU:O    | 2.41                     | 0.53              |
| 2:E:23:GLN:HE21   | 2:E:34:LYS:HB3    | 1.73                     | 0.53              |
| 2:E:864:PRO:HD2   | 2:E:867:LEU:HD12  | 1.89                     | 0.53              |
| 2:G:4155:PRO:HD2  | 2:G:5036:LEU:HD23 | 1.91                     | 0.53              |
| 1:H:25:HIS:HB3    | 1:H:40:ARG:HD3    | 1.90                     | 0.53              |
| 2:I:17:ASP:HB2    | 2:I:98:HIS:HE1    | 1.73                     | 0.53              |
| 2:I:886:ARG:HB3   | 2:I:891:TRP:HB2   | 1.91                     | 0.53              |
| 2:B:683:ARG:NH1   | 2:B:707:VAL:O     | 2.40                     | 0.53              |
| 2:E:3992:PHE:O    | 2:E:3996:PHE:N    | 2.37                     | 0.53              |
| 2:G:261:ARG:HB3   | 2:G:283:ARG:HB3   | 1.91                     | 0.53              |
| 2:G:647:ASN:ND2   | 2:G:820:ARG:O     | 2.40                     | 0.53              |
| 1:H:26:TYR:OH     | 1:H:42:ARG:NH2    | 2.36                     | 0.53              |
| 2:I:551:LEU:HD11  | 2:I:589:LEU:HD13  | 1.90                     | 0.53              |
| 2:B:647:ASN:ND2   | 2:B:820:ARG:O     | 2.40                     | 0.53              |
| 2:E:4155:PRO:HD2  | 2:E:5036:LEU:HD23 | 1.91                     | 0.53              |
| 2:G:718:GLY:HA3   | 2:G:737:LEU:HA    | 1.90                     | 0.53              |
| 2:G:3992:PHE:O    | 2:G:3996:PHE:N    | 2.38                     | 0.53              |
| 2:G:4924:VAL:HG23 | 2:G:4925:ILE:HG12 | 1.90                     | 0.53              |
| 2:B:17:ASP:HB2    | 2:B:98:HIS:HE1    | 1.73                     | 0.53              |
| 2:B:551:LEU:HD11  | 2:B:589:LEU:HD13  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:645:ARG:N     | 2:E:824:GLU:O     | 2.39                     | 0.53              |
| 2:E:4924:VAL:HG23 | 2:E:4925:ILE:HG12 | 1.90                     | 0.53              |
| 2:G:886:ARG:HB3   | 2:G:891:TRP:HB2   | 1.91                     | 0.53              |
| 2:G:4843:LEU:HD12 | 2:I:4823:LEU:HD21 | 1.91                     | 0.53              |
| 2:B:655:GLY:HA2   | 2:B:1002:ALA:HB2  | 1.90                     | 0.52              |
| 2:B:718:GLY:HA3   | 2:B:737:LEU:HA    | 1.90                     | 0.52              |
| 2:B:886:ARG:HB3   | 2:B:891:TRP:HB2   | 1.91                     | 0.52              |
| 2:E:718:GLY:HA3   | 2:E:737:LEU:HA    | 1.90                     | 0.52              |
| 2:G:655:GLY:HA2   | 2:G:1002:ALA:HB2  | 1.90                     | 0.52              |
| 2:I:718:GLY:HA3   | 2:I:737:LEU:HA    | 1.90                     | 0.52              |
| 2:B:1679:ASN:HA   | 2:B:1682:ALA:HB3  | 1.92                     | 0.52              |
| 2:E:669:ASP:OD2   | 2:E:790:ARG:NH2   | 2.41                     | 0.52              |
| 2:G:4958:CYS:SG   | 2:G:4959:PHE:N    | 2.82                     | 0.52              |
| 2:G:4000:MET:HE2  | 2:G:4061:PHE:HB3  | 1.91                     | 0.52              |
| 2:B:4155:PRO:HD2  | 2:B:5036:LEU:HD23 | 1.91                     | 0.52              |
| 2:E:1196:PRO:O    | 2:E:1198:GLN:NE2  | 2.41                     | 0.52              |
| 2:E:4958:CYS:SG   | 2:E:4959:PHE:N    | 2.82                     | 0.52              |
| 2:G:1679:ASN:ND2  | 2:G:1798:LEU:O    | 2.41                     | 0.52              |
| 2:I:914:PRO:O     | 2:I:918:ARG:N     | 2.42                     | 0.52              |
| 2:I:2803:GLU:OE2  | 2:I:2806:ARG:NH1  | 2.43                     | 0.52              |
| 2:I:3843:ASP:H    | 2:I:3874:VAL:HG13 | 1.73                     | 0.52              |
| 2:B:2803:GLU:OE2  | 2:B:2806:ARG:NH1  | 2.43                     | 0.52              |
| 2:E:261:ARG:HB3   | 2:E:283:ARG:HB3   | 1.91                     | 0.52              |
| 2:E:1679:ASN:ND2  | 2:E:1798:LEU:O    | 2.41                     | 0.52              |
| 2:I:627:PRO:HB2   | 1:J:92:PRO:HD3    | 1.92                     | 0.52              |
| 2:I:1721:GLU:OE2  | 2:I:1725:ARG:NH2  | 2.38                     | 0.52              |
| 2:I:3674:ILE:HD11 | 2:I:3728:ILE:HG22 | 1.91                     | 0.52              |
| 2:I:4000:MET:HE2  | 2:I:4061:PHE:HB3  | 1.91                     | 0.52              |
| 1:J:26:TYR:OH     | 1:J:42:ARG:NH2    | 2.36                     | 0.52              |
| 2:B:4958:CYS:SG   | 2:B:4959:PHE:N    | 2.82                     | 0.52              |
| 2:E:17:ASP:HB2    | 2:E:98:HIS:HE1    | 1.73                     | 0.52              |
| 2:E:4012:LEU:O    | 2:E:4016:LEU:N    | 2.43                     | 0.52              |
| 2:G:1808:ARG:NH1  | 2:G:1853:ILE:O    | 2.39                     | 0.52              |
| 2:I:2128:TYR:OH   | 2:I:3676:ASP:OD2  | 2.28                     | 0.52              |
| 2:I:4924:VAL:HG23 | 2:I:4925:ILE:HG12 | 1.90                     | 0.52              |
| 2:E:886:ARG:HB3   | 2:E:891:TRP:HB2   | 1.91                     | 0.52              |
| 2:E:2803:GLU:OE2  | 2:E:2806:ARG:NH1  | 2.43                     | 0.52              |
| 2:I:261:ARG:HB3   | 2:I:283:ARG:HB3   | 1.91                     | 0.52              |
| 2:I:488:LEU:O     | 2:I:492:ASP:N     | 2.41                     | 0.52              |
| 2:I:4958:CYS:SG   | 2:I:4959:PHE:N    | 2.82                     | 0.52              |
| 2:E:396:GLU:O     | 2:E:400:ALA:N     | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:551:LEU:HD11  | 2:E:589:LEU:HD13  | 1.90                     | 0.52              |
| 2:E:4704:LEU:HD22 | 2:E:4778:TRP:HB2  | 1.92                     | 0.52              |
| 2:G:3674:ILE:HD11 | 2:G:3728:ILE:HG22 | 1.92                     | 0.52              |
| 2:G:4704:LEU:HD22 | 2:G:4778:TRP:HB2  | 1.92                     | 0.52              |
| 2:I:396:GLU:O     | 2:I:400:ALA:N     | 2.40                     | 0.52              |
| 2:I:1679:ASN:HA   | 2:I:1682:ALA:HB3  | 1.92                     | 0.52              |
| 2:B:3674:ILE:HD11 | 2:B:3728:ILE:HG22 | 1.91                     | 0.52              |
| 2:B:4924:VAL:HG23 | 2:B:4925:ILE:HG12 | 1.90                     | 0.52              |
| 2:G:3772:THR:OG1  | 2:G:3815:LYS:NZ   | 2.43                     | 0.52              |
| 2:I:2751:LEU:HD11 | 2:I:2823:ILE:HG21 | 1.92                     | 0.52              |
| 2:B:1032:LYS:O    | 2:B:1036:ARG:N    | 2.40                     | 0.51              |
| 2:E:2751:LEU:HD11 | 2:E:2823:ILE:HG21 | 1.92                     | 0.51              |
| 2:G:1676:LEU:HD22 | 2:G:2167:ILE:HG13 | 1.93                     | 0.51              |
| 2:I:1865:MET:N    | 2:I:1865:MET:SD   | 2.83                     | 0.51              |
| 2:I:2185:ILE:HA   | 2:I:2188:ASN:HD21 | 1.75                     | 0.51              |
| 2:B:2128:TYR:OH   | 2:B:3676:ASP:OD2  | 2.28                     | 0.51              |
| 2:B:3772:THR:OG1  | 2:B:3815:LYS:NZ   | 2.43                     | 0.51              |
| 2:E:1679:ASN:HA   | 2:E:1682:ALA:HB3  | 1.92                     | 0.51              |
| 2:G:4201:ASN:O    | 2:G:4205:TRP:N    | 2.43                     | 0.51              |
| 2:I:647:ASN:ND2   | 2:I:820:ARG:O     | 2.39                     | 0.51              |
| 2:B:3905:THR:HA   | 2:B:3912:THR:HG23 | 1.93                     | 0.51              |
| 2:E:2128:TYR:OH   | 2:E:3676:ASP:OD2  | 2.28                     | 0.51              |
| 2:G:264:PRO:HG2   | 2:G:270:SER:HB2   | 1.92                     | 0.51              |
| 2:G:2751:LEU:HD11 | 2:G:2823:ILE:HG21 | 1.92                     | 0.51              |
| 2:G:4577:LEU:HG   | 2:G:4580:TYR:HE2  | 1.75                     | 0.51              |
| 2:I:4704:LEU:HD22 | 2:I:4778:TRP:HB2  | 1.92                     | 0.51              |
| 2:B:261:ARG:HB3   | 2:B:283:ARG:HB3   | 1.91                     | 0.51              |
| 2:B:1109:LEU:HA   | 2:B:1120:LEU:HD21 | 1.93                     | 0.51              |
| 2:G:1109:LEU:HA   | 2:G:1120:LEU:HD21 | 1.93                     | 0.51              |
| 2:G:3905:THR:HA   | 2:G:3912:THR:HG23 | 1.93                     | 0.51              |
| 2:I:1196:PRO:O    | 2:I:1198:GLN:NE2  | 2.41                     | 0.51              |
| 2:I:4201:ASN:O    | 2:I:4205:TRP:N    | 2.43                     | 0.51              |
| 2:B:1865:MET:N    | 2:B:1865:MET:SD   | 2.84                     | 0.51              |
| 2:B:2185:ILE:HA   | 2:B:2188:ASN:HD21 | 1.75                     | 0.51              |
| 2:B:3990:VAL:HG13 | 2:B:4051:SER:HB2  | 1.92                     | 0.51              |
| 2:E:707:VAL:HG23  | 2:E:713:SER:HB2   | 1.93                     | 0.51              |
| 2:E:2950:UNK:O    | 2:E:2954:UNK:N    | 2.43                     | 0.51              |
| 2:I:772:ASN:ND2   | 2:I:774:ASP:OD2   | 2.44                     | 0.51              |
| 2:I:2287:ALA:HA   | 2:I:2290:LEU:HD13 | 1.93                     | 0.51              |
| 2:I:2737:PRO:O    | 2:I:2888:ARG:NH2  | 2.44                     | 0.51              |
| 2:I:3990:VAL:HG13 | 2:I:4051:SER:HB2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:877:ASN:HD22  | 2:B:1045:THR:HG23 | 1.76                     | 0.51              |
| 2:B:2751:LEU:HD11 | 2:B:2823:ILE:HG21 | 1.92                     | 0.51              |
| 2:B:4000:MET:HE2  | 2:B:4061:PHE:HB3  | 1.91                     | 0.51              |
| 2:G:1679:ASN:HA   | 2:G:1682:ALA:HB3  | 1.92                     | 0.51              |
| 2:G:1808:ARG:HD3  | 2:G:1853:ILE:HG22 | 1.92                     | 0.51              |
| 2:I:666:VAL:HG21  | 2:I:684:VAL:HG21  | 1.93                     | 0.51              |
| 2:I:877:ASN:HD22  | 2:I:1045:THR:HG23 | 1.76                     | 0.51              |
| 2:I:1240:LYS:O    | 2:I:1604:SER:N    | 2.43                     | 0.51              |
| 2:B:1931:LEU:HB3  | 2:B:1935:VAL:HB   | 1.92                     | 0.51              |
| 2:E:666:VAL:HG21  | 2:E:684:VAL:HG21  | 1.93                     | 0.51              |
| 2:E:831:ARG:HD2   | 2:E:1199:VAL:HG12 | 1.93                     | 0.51              |
| 2:E:2737:PRO:O    | 2:E:2888:ARG:NH2  | 2.44                     | 0.51              |
| 2:E:4000:MET:HE2  | 2:E:4061:PHE:HB3  | 1.91                     | 0.51              |
| 2:G:488:LEU:O     | 2:G:492:ASP:N     | 2.41                     | 0.51              |
| 2:G:831:ARG:HD2   | 2:G:1199:VAL:HG12 | 1.93                     | 0.51              |
| 2:G:1931:LEU:HB3  | 2:G:1935:VAL:HB   | 1.92                     | 0.51              |
| 2:G:2128:TYR:OH   | 2:G:3676:ASP:OD2  | 2.28                     | 0.51              |
| 2:G:4218:ILE:HG23 | 2:G:4954:MET:HE3  | 1.93                     | 0.51              |
| 2:I:4843:LEU:HD22 | 2:I:4928:LEU:HD11 | 1.92                     | 0.51              |
| 2:B:772:ASN:ND2   | 2:B:774:ASP:OD2   | 2.44                     | 0.51              |
| 2:B:3552:UNK:O    | 2:B:3556:UNK:N    | 2.44                     | 0.51              |
| 2:B:4843:LEU:HD22 | 2:B:4928:LEU:HD11 | 1.92                     | 0.51              |
| 2:E:877:ASN:HD22  | 2:E:1045:THR:HG23 | 1.76                     | 0.51              |
| 2:E:3674:ILE:HD11 | 2:E:3728:ILE:HG22 | 1.92                     | 0.51              |
| 2:G:2737:PRO:O    | 2:G:2888:ARG:NH2  | 2.44                     | 0.51              |
| 2:G:2803:GLU:OE2  | 2:G:2806:ARG:NH1  | 2.43                     | 0.51              |
| 2:G:4843:LEU:HD22 | 2:G:4928:LEU:HD11 | 1.92                     | 0.51              |
| 2:I:4218:ILE:HG23 | 2:I:4954:MET:HE3  | 1.93                     | 0.51              |
| 2:E:264:PRO:HG2   | 2:E:270:SER:HB2   | 1.92                     | 0.51              |
| 2:E:1109:LEU:HA   | 2:E:1120:LEU:HD21 | 1.93                     | 0.51              |
| 2:E:3910:THR:HG23 | 2:E:3911:THR:HG23 | 1.93                     | 0.51              |
| 2:G:666:VAL:HG21  | 2:G:684:VAL:HG21  | 1.93                     | 0.51              |
| 2:G:772:ASN:ND2   | 2:G:774:ASP:OD2   | 2.44                     | 0.51              |
| 2:G:1231:GLN:NE2  | 2:G:1821:ASP:O    | 2.44                     | 0.51              |
| 2:G:1258:ALA:HB3  | 2:G:1271:ARG:HB3  | 1.93                     | 0.51              |
| 2:G:4012:LEU:O    | 2:G:4016:LEU:N    | 2.43                     | 0.51              |
| 2:I:1676:LEU:HD22 | 2:I:2167:ILE:HG13 | 1.92                     | 0.51              |
| 2:I:3948:LYS:NZ   | 2:I:4008:SER:O    | 2.44                     | 0.51              |
| 2:I:3992:PHE:O    | 2:I:3996:PHE:N    | 2.37                     | 0.51              |
| 2:I:4577:LEU:HG   | 2:I:4580:TYR:HE2  | 1.75                     | 0.51              |
| 2:B:645:ARG:N     | 2:B:824:GLU:O     | 2.39                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1231:GLN:NE2  | 2:B:1821:ASP:O    | 2.44                     | 0.51              |
| 2:B:2737:PRO:O    | 2:B:2888:ARG:NH2  | 2.44                     | 0.51              |
| 2:B:4704:LEU:HD22 | 2:B:4778:TRP:HB2  | 1.92                     | 0.51              |
| 2:E:1865:MET:N    | 2:E:1865:MET:SD   | 2.84                     | 0.51              |
| 2:E:2185:ILE:HA   | 2:E:2188:ASN:HD21 | 1.75                     | 0.51              |
| 2:E:4024:VAL:HG23 | 2:E:4027:LEU:HD12 | 1.92                     | 0.51              |
| 2:E:4843:LEU:HD22 | 2:E:4928:LEU:HD11 | 1.92                     | 0.51              |
| 2:G:3830:GLN:HA   | 2:G:3833:GLN:HG2  | 1.93                     | 0.51              |
| 2:B:666:VAL:HG21  | 2:B:684:VAL:HG21  | 1.93                     | 0.50              |
| 2:B:1258:ALA:HB3  | 2:B:1271:ARG:HB3  | 1.93                     | 0.50              |
| 2:B:4012:LEU:O    | 2:B:4016:LEU:N    | 2.42                     | 0.50              |
| 2:E:772:ASN:ND2   | 2:E:774:ASP:OD2   | 2.44                     | 0.50              |
| 2:E:1808:ARG:HD3  | 2:E:1853:ILE:HG22 | 1.92                     | 0.50              |
| 2:E:1931:LEU:HB3  | 2:E:1935:VAL:HB   | 1.92                     | 0.50              |
| 2:E:4577:LEU:HG   | 2:E:4580:TYR:HE2  | 1.75                     | 0.50              |
| 2:G:2185:ILE:HA   | 2:G:2188:ASN:HD21 | 1.75                     | 0.50              |
| 2:G:3552:UNK:O    | 2:G:3556:UNK:N    | 2.44                     | 0.50              |
| 2:G:3829:PHE:HA   | 2:G:3832:ILE:HD12 | 1.93                     | 0.50              |
| 2:G:3910:THR:HG23 | 2:G:3911:THR:HG23 | 1.93                     | 0.50              |
| 2:I:1258:ALA:HB3  | 2:I:1271:ARG:HB3  | 1.93                     | 0.50              |
| 2:B:4201:ASN:O    | 2:B:4205:TRP:N    | 2.43                     | 0.50              |
| 2:B:4577:LEU:HG   | 2:B:4580:TYR:HE2  | 1.75                     | 0.50              |
| 2:E:1235:THR:OG1  | 2:E:1607:ARG:NE   | 2.45                     | 0.50              |
| 2:E:1240:LYS:O    | 2:E:1604:SER:N    | 2.43                     | 0.50              |
| 2:G:1865:MET:N    | 2:G:1865:MET:SD   | 2.84                     | 0.50              |
| 2:G:3948:LYS:NZ   | 2:G:4008:SER:O    | 2.44                     | 0.50              |
| 2:I:1109:LEU:HA   | 2:I:1120:LEU:HD21 | 1.93                     | 0.50              |
| 2:I:4813:LEU:HD12 | 2:I:4816:ILE:HD11 | 1.93                     | 0.50              |
| 2:B:15:ARG:HD3    | 2:B:98:HIS:HB3    | 1.93                     | 0.50              |
| 2:B:831:ARG:HD2   | 2:B:1199:VAL:HG12 | 1.93                     | 0.50              |
| 2:B:1240:LYS:O    | 2:B:1604:SER:N    | 2.43                     | 0.50              |
| 2:B:3910:THR:HG23 | 2:B:3911:THR:HG23 | 1.93                     | 0.50              |
| 2:E:3830:GLN:HA   | 2:E:3833:GLN:HG2  | 1.93                     | 0.50              |
| 2:E:3948:LYS:NZ   | 2:E:4008:SER:O    | 2.44                     | 0.50              |
| 2:G:877:ASN:HD22  | 2:G:1045:THR:HG23 | 1.76                     | 0.50              |
| 2:I:3905:THR:HA   | 2:I:3912:THR:HG23 | 1.93                     | 0.50              |
| 2:B:3948:LYS:NZ   | 2:B:4008:SER:O    | 2.44                     | 0.50              |
| 2:E:229:GLU:OE2   | 2:E:374:LYS:NZ    | 2.35                     | 0.50              |
| 2:E:488:LEU:O     | 2:E:492:ASP:N     | 2.41                     | 0.50              |
| 2:G:4241:THR:HG22 | 2:G:4245:MET:HE2  | 1.93                     | 0.50              |
| 2:I:831:ARG:HD2   | 2:I:1199:VAL:HG12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:313:SER:HB3   | 2:B:351:VAL:HB    | 1.94                     | 0.50              |
| 2:B:1676:LEU:HD22 | 2:B:2167:ILE:HG13 | 1.93                     | 0.50              |
| 2:B:3830:GLN:HA   | 2:B:3833:GLN:HG2  | 1.93                     | 0.50              |
| 2:E:1258:ALA:HB3  | 2:E:1271:ARG:HB3  | 1.94                     | 0.50              |
| 2:G:1203:ASN:ND2  | 2:G:1210:SER:O    | 2.44                     | 0.50              |
| 2:G:2287:ALA:HA   | 2:G:2290:LEU:HD13 | 1.93                     | 0.50              |
| 2:I:1032:LYS:O    | 2:I:1036:ARG:N    | 2.40                     | 0.50              |
| 2:I:1808:ARG:HD3  | 2:I:1853:ILE:HG22 | 1.92                     | 0.50              |
| 2:I:1931:LEU:HB3  | 2:I:1935:VAL:HB   | 1.92                     | 0.50              |
| 2:B:914:PRO:O     | 2:B:918:ARG:N     | 2.42                     | 0.50              |
| 2:B:1721:GLU:HG2  | 2:B:1725:ARG:HH12 | 1.77                     | 0.50              |
| 2:B:1808:ARG:HD3  | 2:B:1853:ILE:HG22 | 1.92                     | 0.50              |
| 2:E:313:SER:HB3   | 2:E:351:VAL:HB    | 1.94                     | 0.50              |
| 2:E:3552:UNK:O    | 2:E:3556:UNK:N    | 2.44                     | 0.50              |
| 2:G:15:ARG:HD3    | 2:G:98:HIS:HB3    | 1.93                     | 0.50              |
| 2:G:396:GLU:O     | 2:G:400:ALA:N     | 2.40                     | 0.50              |
| 2:G:683:ARG:NH1   | 2:G:707:VAL:O     | 2.40                     | 0.50              |
| 2:I:1231:GLN:NE2  | 2:I:1821:ASP:O    | 2.44                     | 0.50              |
| 2:I:3829:PHE:HA   | 2:I:3832:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:7:ILE:HG22    | 1:A:9:PRO:HD2     | 1.94                     | 0.50              |
| 2:B:355:LEU:HB3   | 2:B:378:LEU:HB3   | 1.94                     | 0.50              |
| 2:B:460:GLN:HG2   | 2:B:462:GLU:H     | 1.77                     | 0.50              |
| 2:B:1235:THR:OG1  | 2:B:1607:ARG:NE   | 2.45                     | 0.50              |
| 2:B:3955:MET:HG3  | 2:B:4019:LEU:HD22 | 1.94                     | 0.50              |
| 2:E:4088:ILE:HG23 | 2:E:4123:ILE:HB   | 1.94                     | 0.50              |
| 2:E:4241:THR:HG22 | 2:E:4245:MET:HE2  | 1.93                     | 0.50              |
| 2:G:645:ARG:N     | 2:G:824:GLU:O     | 2.39                     | 0.50              |
| 2:G:4088:ILE:HG23 | 2:G:4123:ILE:HB   | 1.94                     | 0.50              |
| 1:H:7:ILE:HG22    | 1:H:9:PRO:HD2     | 1.94                     | 0.50              |
| 2:I:1865:MET:HB3  | 2:I:1926:LEU:HB2  | 1.94                     | 0.50              |
| 2:I:2739:PRO:HB3  | 2:I:2884:ASN:HB3  | 1.94                     | 0.50              |
| 2:I:3910:THR:HG23 | 2:I:3911:THR:HG23 | 1.93                     | 0.50              |
| 2:I:4956:THR:O    | 2:I:4965:SER:N    | 2.42                     | 0.50              |
| 1:J:7:ILE:HG22    | 1:J:9:PRO:HD2     | 1.94                     | 0.50              |
| 2:E:838:HIS:HB3   | 2:E:1200:GLY:H    | 1.77                     | 0.50              |
| 2:E:3990:VAL:HG13 | 2:E:4051:SER:HB2  | 1.93                     | 0.50              |
| 1:F:7:ILE:HG22    | 1:F:9:PRO:HD2     | 1.94                     | 0.50              |
| 2:G:717:ASP:OD1   | 2:G:720:HIS:ND1   | 2.45                     | 0.50              |
| 2:G:1235:THR:OG1  | 2:G:1607:ARG:NE   | 2.44                     | 0.50              |
| 2:I:707:VAL:HG23  | 2:I:713:SER:HB2   | 1.93                     | 0.50              |
| 2:I:3830:GLN:HA   | 2:I:3833:GLN:HG2  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4813:LEU:HD12 | 2:B:4816:ILE:HD11 | 1.93                     | 0.50              |
| 2:E:914:PRO:O     | 2:E:918:ARG:N     | 2.42                     | 0.50              |
| 2:E:2739:PRO:HB3  | 2:E:2884:ASN:HB3  | 1.94                     | 0.50              |
| 2:E:4044:MET:HA   | 2:E:4047:MET:HG2  | 1.94                     | 0.50              |
| 2:G:3674:ILE:HG13 | 2:G:3732:SER:HB3  | 1.94                     | 0.50              |
| 2:G:3955:MET:HG3  | 2:G:4019:LEU:HD22 | 1.94                     | 0.50              |
| 2:G:4813:LEU:HD12 | 2:G:4816:ILE:HD11 | 1.93                     | 0.50              |
| 2:I:3772:THR:OG1  | 2:I:3815:LYS:NZ   | 2.43                     | 0.50              |
| 2:I:4024:VAL:HG23 | 2:I:4027:LEU:HD12 | 1.93                     | 0.50              |
| 2:B:264:PRO:HG2   | 2:B:270:SER:HB2   | 1.92                     | 0.49              |
| 2:B:485:SER:O     | 2:B:489:ASN:N     | 2.44                     | 0.49              |
| 2:B:1196:PRO:O    | 2:B:1198:GLN:NE2  | 2.41                     | 0.49              |
| 2:E:2287:ALA:HA   | 2:E:2290:LEU:HD13 | 1.93                     | 0.49              |
| 2:G:728:ARG:NH2   | 2:G:1527:UNK:O    | 2.45                     | 0.49              |
| 2:G:1196:PRO:O    | 2:G:1198:GLN:NE2  | 2.41                     | 0.49              |
| 2:I:355:LEU:HB3   | 2:I:378:LEU:HB3   | 1.94                     | 0.49              |
| 2:I:3552:UNK:O    | 2:I:3556:UNK:N    | 2.44                     | 0.49              |
| 2:I:4012:LEU:O    | 2:I:4016:LEU:N    | 2.43                     | 0.49              |
| 1:A:76:CYS:HB2    | 1:A:97:LEU:HB2    | 1.94                     | 0.49              |
| 2:B:2287:ALA:HA   | 2:B:2290:LEU:HD13 | 1.93                     | 0.49              |
| 2:B:4088:ILE:HG23 | 2:B:4123:ILE:HB   | 1.94                     | 0.49              |
| 2:E:355:LEU:HB3   | 2:E:378:LEU:HB3   | 1.94                     | 0.49              |
| 2:E:1721:GLU:HG2  | 2:E:1725:ARG:HH12 | 1.77                     | 0.49              |
| 2:E:3905:THR:HA   | 2:E:3912:THR:HG23 | 1.93                     | 0.49              |
| 2:E:4218:ILE:HG23 | 2:E:4954:MET:HE3  | 1.93                     | 0.49              |
| 2:G:707:VAL:HG23  | 2:G:713:SER:HB2   | 1.93                     | 0.49              |
| 2:G:2739:PRO:HB3  | 2:G:2884:ASN:HB3  | 1.94                     | 0.49              |
| 2:I:229:GLU:OE2   | 2:I:374:LYS:NZ    | 2.35                     | 0.49              |
| 2:I:264:PRO:HG2   | 2:I:270:SER:HB2   | 1.92                     | 0.49              |
| 2:I:1235:THR:OG1  | 2:I:1607:ARG:NE   | 2.44                     | 0.49              |
| 2:I:1691:GLN:HG2  | 1:J:42:ARG:HG2    | 1.93                     | 0.49              |
| 2:I:3674:ILE:HG13 | 2:I:3732:SER:HB3  | 1.94                     | 0.49              |
| 2:I:4088:ILE:HG23 | 2:I:4123:ILE:HB   | 1.94                     | 0.49              |
| 2:B:707:VAL:HG23  | 2:B:713:SER:HB2   | 1.93                     | 0.49              |
| 2:B:1865:MET:HB3  | 2:B:1926:LEU:HB2  | 1.94                     | 0.49              |
| 2:B:2868:SER:O    | 2:B:2872:GLN:N    | 2.44                     | 0.49              |
| 2:B:4218:ILE:HG23 | 2:B:4954:MET:HE3  | 1.93                     | 0.49              |
| 2:E:15:ARG:HD3    | 2:E:98:HIS:HB3    | 1.93                     | 0.49              |
| 2:E:139:GLU:O     | 2:E:141:ALA:N     | 2.45                     | 0.49              |
| 2:E:1231:GLN:NE2  | 2:E:1821:ASP:O    | 2.44                     | 0.49              |
| 2:E:1676:LEU:HD22 | 2:E:2167:ILE:HG13 | 1.92                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:3674:ILE:HG13 | 2:E:3732:SER:HB3  | 1.94                     | 0.49              |
| 2:G:139:GLU:O     | 2:G:141:ALA:N     | 2.45                     | 0.49              |
| 2:G:1865:MET:HB3  | 2:G:1926:LEU:HB2  | 1.94                     | 0.49              |
| 2:G:4024:VAL:HG23 | 2:G:4027:LEU:HD12 | 1.92                     | 0.49              |
| 2:I:1269:CYS:HA   | 2:I:1473:UNK:HA   | 1.95                     | 0.49              |
| 2:B:235:ALA:HA    | 2:B:257:ARG:HD3   | 1.95                     | 0.49              |
| 2:B:717:ASP:OD1   | 2:B:720:HIS:ND1   | 2.45                     | 0.49              |
| 2:B:1271:ARG:HA   | 2:B:1471:UNK:HA   | 1.94                     | 0.49              |
| 2:E:913:LEU:HD13  | 2:E:918:ARG:HA    | 1.94                     | 0.49              |
| 2:G:838:HIS:HB3   | 2:G:1200:GLY:H    | 1.77                     | 0.49              |
| 2:G:2336:ARG:HD3  | 2:G:2435:ARG:HD2  | 1.94                     | 0.49              |
| 2:I:717:ASP:OD1   | 2:I:720:HIS:ND1   | 2.45                     | 0.49              |
| 2:I:1163:THR:HA   | 2:I:1168:VAL:HA   | 1.95                     | 0.49              |
| 2:I:2104:ARG:HA   | 2:I:2107:GLN:HB3  | 1.95                     | 0.49              |
| 2:I:4104:THR:HG22 | 2:I:4106:PRO:HD2  | 1.95                     | 0.49              |
| 2:B:2336:ARG:HD3  | 2:B:2435:ARG:HD2  | 1.94                     | 0.49              |
| 2:B:4024:VAL:HG23 | 2:B:4027:LEU:HD12 | 1.93                     | 0.49              |
| 2:B:4104:THR:HG22 | 2:B:4106:PRO:HD2  | 1.95                     | 0.49              |
| 2:E:682:LEU:HD13  | 2:E:787:VAL:HG11  | 1.94                     | 0.49              |
| 2:E:2235:PHE:HA   | 2:E:2238:TYR:HD2  | 1.78                     | 0.49              |
| 2:E:3829:PHE:HA   | 2:E:3832:ILE:HD12 | 1.93                     | 0.49              |
| 2:E:4138:ASP:N    | 2:E:4138:ASP:OD1  | 2.45                     | 0.49              |
| 1:F:76:CYS:HB2    | 1:F:97:LEU:HB2    | 1.94                     | 0.49              |
| 2:I:15:ARG:HD3    | 2:I:98:HIS:HB3    | 1.93                     | 0.49              |
| 2:I:682:LEU:HD13  | 2:I:787:VAL:HG11  | 1.94                     | 0.49              |
| 2:I:2226:PRO:HA   | 2:I:2229:VAL:HG12 | 1.94                     | 0.49              |
| 2:I:2336:ARG:HD3  | 2:I:2435:ARG:HD2  | 1.94                     | 0.49              |
| 2:B:2739:PRO:HB3  | 2:B:2884:ASN:HB3  | 1.94                     | 0.49              |
| 2:B:3829:PHE:HA   | 2:B:3832:ILE:HD12 | 1.93                     | 0.49              |
| 2:B:4738:ALA:HA   | 2:B:4743:MET:HE3  | 1.95                     | 0.49              |
| 2:B:4822:THR:O    | 2:B:4825:THR:OG1  | 2.29                     | 0.49              |
| 2:E:4813:LEU:HD12 | 2:E:4816:ILE:HD11 | 1.93                     | 0.49              |
| 2:G:913:LEU:HD13  | 2:G:918:ARG:HA    | 1.94                     | 0.49              |
| 2:G:914:PRO:O     | 2:G:918:ARG:N     | 2.42                     | 0.49              |
| 2:G:3990:VAL:HG13 | 2:G:4051:SER:HB2  | 1.92                     | 0.49              |
| 2:B:838:HIS:HB3   | 2:B:1200:GLY:H    | 1.77                     | 0.49              |
| 2:B:3674:ILE:HG13 | 2:B:3732:SER:HB3  | 1.94                     | 0.49              |
| 2:E:235:ALA:HA    | 2:E:257:ARG:HD3   | 1.95                     | 0.49              |
| 2:E:460:GLN:HG2   | 2:E:462:GLU:H     | 1.77                     | 0.49              |
| 2:E:4738:ALA:HA   | 2:E:4743:MET:HE3  | 1.95                     | 0.49              |
| 1:F:26:TYR:OH     | 1:F:42:ARG:NH2    | 2.36                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:355:LEU:HB3   | 2:G:378:LEU:HB3   | 1.94                     | 0.49              |
| 2:G:2868:SER:O    | 2:G:2872:GLN:N    | 2.44                     | 0.49              |
| 2:G:4044:MET:HA   | 2:G:4047:MET:HG2  | 1.94                     | 0.49              |
| 2:I:313:SER:HB3   | 2:I:351:VAL:HB    | 1.93                     | 0.49              |
| 2:I:4044:MET:HA   | 2:I:4047:MET:HG2  | 1.94                     | 0.49              |
| 2:I:4241:THR:HG22 | 2:I:4245:MET:HE2  | 1.94                     | 0.49              |
| 2:B:229:GLU:OE2   | 2:B:374:LYS:NZ    | 2.35                     | 0.49              |
| 2:B:1203:ASN:ND2  | 2:B:1210:SER:O    | 2.44                     | 0.49              |
| 2:B:3882:GLN:HB2  | 2:B:3957:VAL:HG22 | 1.95                     | 0.49              |
| 2:E:671:VAL:HG22  | 2:E:740:PRO:HG3   | 1.95                     | 0.49              |
| 2:E:4560:TYR:O    | 2:E:4564:PHE:N    | 2.43                     | 0.49              |
| 2:I:232:THR:HB    | 2:I:252:VAL:HG11  | 1.95                     | 0.49              |
| 2:I:671:VAL:HG22  | 2:I:740:PRO:HG3   | 1.95                     | 0.49              |
| 2:I:1684:ALA:HA   | 2:I:1782:PHE:HZ   | 1.77                     | 0.49              |
| 2:I:4738:ALA:HA   | 2:I:4743:MET:HE3  | 1.95                     | 0.49              |
| 2:E:3772:THR:OG1  | 2:E:3815:LYS:NZ   | 2.43                     | 0.49              |
| 2:G:1240:LYS:O    | 2:G:1604:SER:N    | 2.43                     | 0.49              |
| 2:G:1979:LEU:HA   | 2:G:1983:ALA:HB3  | 1.95                     | 0.49              |
| 2:G:2104:ARG:HA   | 2:G:2107:GLN:HB3  | 1.95                     | 0.49              |
| 2:I:1721:GLU:HG2  | 2:I:1725:ARG:HH12 | 1.77                     | 0.49              |
| 1:A:62:GLY:HA3    | 1:A:74:LEU:HD21   | 1.93                     | 0.49              |
| 2:B:139:GLU:O     | 2:B:141:ALA:N     | 2.45                     | 0.49              |
| 2:B:2104:ARG:HA   | 2:B:2107:GLN:HB3  | 1.95                     | 0.49              |
| 2:B:2257:LEU:O    | 2:B:2261:SER:N    | 2.46                     | 0.49              |
| 2:B:4241:THR:HG22 | 2:B:4245:MET:HE2  | 1.94                     | 0.49              |
| 2:E:1203:ASN:ND2  | 2:E:1210:SER:O    | 2.44                     | 0.49              |
| 2:E:1865:MET:HB3  | 2:E:1926:LEU:HB2  | 1.94                     | 0.49              |
| 2:E:2104:ARG:HA   | 2:E:2107:GLN:HB3  | 1.95                     | 0.49              |
| 2:E:2226:PRO:HA   | 2:E:2229:VAL:HG12 | 1.94                     | 0.49              |
| 2:E:4201:ASN:O    | 2:E:4205:TRP:N    | 2.43                     | 0.49              |
| 2:G:1684:ALA:HA   | 2:G:1782:PHE:HZ   | 1.77                     | 0.49              |
| 2:G:2235:PHE:HA   | 2:G:2238:TYR:HD2  | 1.78                     | 0.49              |
| 2:G:4738:ALA:HA   | 2:G:4743:MET:HE3  | 1.95                     | 0.49              |
| 2:I:139:GLU:O     | 2:I:141:ALA:N     | 2.45                     | 0.49              |
| 2:I:235:ALA:HA    | 2:I:257:ARG:HD3   | 1.95                     | 0.49              |
| 2:B:4044:MET:HA   | 2:B:4047:MET:HG2  | 1.94                     | 0.48              |
| 2:E:3955:MET:HG3  | 2:E:4019:LEU:HD22 | 1.94                     | 0.48              |
| 1:F:62:GLY:HA3    | 1:F:74:LEU:HD21   | 1.94                     | 0.48              |
| 2:G:313:SER:HB3   | 2:G:351:VAL:HB    | 1.93                     | 0.48              |
| 2:G:1721:GLU:HG2  | 2:G:1725:ARG:HH12 | 1.77                     | 0.48              |
| 2:I:793:LEU:HD12  | 2:I:797:HIS:HB2   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:682:LEU:HD13  | 2:B:787:VAL:HG11  | 1.94                     | 0.48              |
| 2:E:1684:ALA:HA   | 2:E:1782:PHE:HZ   | 1.77                     | 0.48              |
| 2:G:1076:ARG:HD3  | 2:G:1237:TRP:HB2  | 1.95                     | 0.48              |
| 2:G:4104:THR:HG22 | 2:G:4106:PRO:HD2  | 1.95                     | 0.48              |
| 1:H:62:GLY:HA3    | 1:H:74:LEU:HD21   | 1.94                     | 0.48              |
| 1:J:62:GLY:HA3    | 1:J:74:LEU:HD21   | 1.94                     | 0.48              |
| 2:E:652:ARG:HB3   | 2:E:773:LEU:HD13  | 1.95                     | 0.48              |
| 2:E:2013:LYS:HA   | 2:E:2028:ARG:HB2  | 1.95                     | 0.48              |
| 2:G:235:ALA:HA    | 2:G:257:ARG:HD3   | 1.95                     | 0.48              |
| 2:G:4795:TYR:HE1  | 2:G:4812:HIS:HA   | 1.79                     | 0.48              |
| 2:I:460:GLN:HG2   | 2:I:462:GLU:H     | 1.77                     | 0.48              |
| 2:I:838:HIS:HB3   | 2:I:1200:GLY:H    | 1.77                     | 0.48              |
| 2:I:1848:LEU:HD22 | 2:I:1853:ILE:HG13 | 1.95                     | 0.48              |
| 2:I:3882:GLN:HB2  | 2:I:3957:VAL:HG22 | 1.95                     | 0.48              |
| 2:B:652:ARG:HB3   | 2:B:773:LEU:HD13  | 1.96                     | 0.48              |
| 2:B:793:LEU:HD12  | 2:B:797:HIS:HB2   | 1.95                     | 0.48              |
| 2:B:1848:LEU:HD22 | 2:B:1853:ILE:HG13 | 1.95                     | 0.48              |
| 2:B:1931:LEU:HD22 | 2:B:1935:VAL:HG11 | 1.96                     | 0.48              |
| 2:B:4795:TYR:HE1  | 2:B:4812:HIS:HA   | 1.79                     | 0.48              |
| 2:E:111:HIS:CD2   | 2:E:114:SER:H     | 2.26                     | 0.48              |
| 2:E:717:ASP:OD1   | 2:E:720:HIS:ND1   | 2.45                     | 0.48              |
| 2:E:4104:THR:HG22 | 2:E:4106:PRO:HD2  | 1.95                     | 0.48              |
| 2:G:232:THR:HB    | 2:G:252:VAL:HG11  | 1.95                     | 0.48              |
| 2:G:460:GLN:HG2   | 2:G:462:GLU:H     | 1.77                     | 0.48              |
| 2:G:652:ARG:HB3   | 2:G:773:LEU:HD13  | 1.96                     | 0.48              |
| 2:G:2226:PRO:HA   | 2:G:2229:VAL:HG12 | 1.94                     | 0.48              |
| 2:G:2257:LEU:O    | 2:G:2261:SER:N    | 2.46                     | 0.48              |
| 2:G:4837:LEU:HD11 | 2:G:4936:ILE:HD11 | 1.96                     | 0.48              |
| 2:G:4849:TYR:OH   | 2:I:4574:ASN:O    | 2.29                     | 0.48              |
| 2:I:652:ARG:HB3   | 2:I:773:LEU:HD13  | 1.96                     | 0.48              |
| 2:I:841:GLY:HA2   | 2:I:1073:ARG:HD2  | 1.95                     | 0.48              |
| 2:B:841:GLY:HA2   | 2:B:1073:ARG:HD2  | 1.95                     | 0.48              |
| 2:B:952:LYS:HB3   | 2:B:968:ALA:HB1   | 1.96                     | 0.48              |
| 2:B:1778:SER:N    | 2:B:1799:SER:O    | 2.46                     | 0.48              |
| 2:E:3994:HIS:O    | 2:E:3998:HIS:ND1  | 2.39                     | 0.48              |
| 2:E:4837:LEU:HD11 | 2:E:4936:ILE:HD11 | 1.96                     | 0.48              |
| 2:G:952:LYS:HB3   | 2:G:968:ALA:HB1   | 1.96                     | 0.48              |
| 2:I:4105:GLY:HA2  | 2:I:4108:ILE:HD12 | 1.95                     | 0.48              |
| 2:I:4837:LEU:HD11 | 2:I:4936:ILE:HD11 | 1.96                     | 0.48              |
| 2:B:1684:ALA:HA   | 2:B:1782:PHE:HZ   | 1.77                     | 0.48              |
| 2:E:880:GLU:OE1   | 2:E:968:ALA:N     | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:682:LEU:HD13  | 2:G:787:VAL:HG11  | 1.94                     | 0.48              |
| 2:G:793:LEU:HD12  | 2:G:797:HIS:HB2   | 1.95                     | 0.48              |
| 2:G:1032:LYS:O    | 2:G:1036:ARG:N    | 2.40                     | 0.48              |
| 2:I:1076:ARG:HD3  | 2:I:1237:TRP:HB2  | 1.95                     | 0.48              |
| 2:I:1713:ASP:O    | 2:I:1717:SER:N    | 2.46                     | 0.48              |
| 2:I:1931:LEU:HD22 | 2:I:1935:VAL:HG11 | 1.96                     | 0.48              |
| 2:I:2235:PHE:HA   | 2:I:2238:TYR:HD2  | 1.78                     | 0.48              |
| 1:A:57:LYS:HB2    | 1:A:80:VAL:HB     | 1.96                     | 0.48              |
| 2:B:215:THR:HG22  | 2:B:273:HIS:HA    | 1.95                     | 0.48              |
| 2:B:1163:THR:HA   | 2:B:1168:VAL:HA   | 1.95                     | 0.48              |
| 2:B:1718:ILE:HG13 | 2:B:1719:HIS:CD2  | 2.49                     | 0.48              |
| 2:B:1979:LEU:HA   | 2:B:1983:ALA:HB3  | 1.95                     | 0.48              |
| 2:B:2235:PHE:HA   | 2:B:2238:TYR:HD2  | 1.78                     | 0.48              |
| 2:E:2336:ARG:HD3  | 2:E:2435:ARG:HD2  | 1.94                     | 0.48              |
| 2:G:1075:PHE:HB2  | 2:G:1192:CYS:HB2  | 1.95                     | 0.48              |
| 2:G:1647:CYS:SG   | 2:G:1648:MET:N    | 2.87                     | 0.48              |
| 2:I:3729:MET:HB3  | 2:I:3770:LEU:HD21 | 1.96                     | 0.48              |
| 1:J:76:CYS:HB2    | 1:J:97:LEU:HB2    | 1.94                     | 0.48              |
| 2:B:1659:LEU:O    | 2:B:1663:HIS:N    | 2.44                     | 0.48              |
| 2:B:1952:GLN:HA   | 2:B:1955:VAL:HG12 | 1.96                     | 0.48              |
| 2:B:4956:THR:O    | 2:B:4965:SER:N    | 2.42                     | 0.48              |
| 2:E:3882:GLN:HB2  | 2:E:3957:VAL:HG22 | 1.95                     | 0.48              |
| 2:G:215:THR:HG22  | 2:G:273:HIS:HA    | 1.95                     | 0.48              |
| 1:H:57:LYS:HB2    | 1:H:80:VAL:HB     | 1.96                     | 0.48              |
| 2:I:1718:ILE:HG13 | 2:I:1719:HIS:CD2  | 2.49                     | 0.48              |
| 1:J:57:LYS:HB2    | 1:J:80:VAL:HB     | 1.96                     | 0.48              |
| 1:J:87:HIS:N      | 1:J:91:ILE:O      | 2.47                     | 0.48              |
| 2:B:2226:PRO:HA   | 2:B:2229:VAL:HG12 | 1.94                     | 0.48              |
| 2:E:1647:CYS:SG   | 2:E:1648:MET:N    | 2.87                     | 0.48              |
| 2:E:1848:LEU:HB3  | 2:E:1853:ILE:HB   | 1.95                     | 0.48              |
| 2:E:1979:LEU:HA   | 2:E:1983:ALA:HB3  | 1.95                     | 0.48              |
| 2:E:4795:TYR:HE1  | 2:E:4812:HIS:HA   | 1.79                     | 0.48              |
| 2:G:988:LEU:O     | 2:G:992:GLY:N     | 2.46                     | 0.48              |
| 2:G:1931:LEU:HD22 | 2:G:1935:VAL:HG11 | 1.96                     | 0.48              |
| 2:G:3817:LEU:HD13 | 2:G:3899:PHE:HD1  | 1.79                     | 0.48              |
| 2:B:913:LEU:HD13  | 2:B:918:ARG:HA    | 1.95                     | 0.48              |
| 2:B:1076:ARG:HD3  | 2:B:1237:TRP:HB2  | 1.95                     | 0.48              |
| 2:B:1854:PHE:HD1  | 2:B:1858:ASP:HB3  | 1.79                     | 0.48              |
| 2:B:3817:LEU:HD13 | 2:B:3899:PHE:HD1  | 1.79                     | 0.48              |
| 2:E:1076:ARG:HD3  | 2:E:1237:TRP:HB2  | 1.95                     | 0.48              |
| 2:E:1163:THR:HA   | 2:E:1168:VAL:HA   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2257:LEU:O    | 2:E:2261:SER:N    | 2.46                     | 0.48              |
| 1:F:57:LYS:HB2    | 1:F:80:VAL:HB     | 1.96                     | 0.48              |
| 2:G:731:THR:OG1   | 2:G:1519:UNK:O    | 2.27                     | 0.48              |
| 2:G:4105:GLY:HA2  | 2:G:4108:ILE:HD12 | 1.95                     | 0.48              |
| 2:G:4956:THR:O    | 2:G:4965:SER:N    | 2.42                     | 0.48              |
| 1:H:76:CYS:HB2    | 1:H:97:LEU:HB2    | 1.94                     | 0.48              |
| 1:H:87:HIS:N      | 1:H:91:ILE:O      | 2.47                     | 0.48              |
| 2:I:1952:GLN:HA   | 2:I:1955:VAL:HG12 | 1.96                     | 0.48              |
| 2:I:2257:LEU:O    | 2:I:2261:SER:N    | 2.46                     | 0.48              |
| 2:I:3955:MET:HG3  | 2:I:4019:LEU:HD22 | 1.94                     | 0.48              |
| 2:B:1848:LEU:HB3  | 2:B:1853:ILE:HB   | 1.95                     | 0.47              |
| 2:B:2950:UNK:O    | 2:B:2954:UNK:N    | 2.47                     | 0.47              |
| 2:E:952:LYS:HB3   | 2:E:968:ALA:HB1   | 1.96                     | 0.47              |
| 2:E:4105:GLY:HA2  | 2:E:4108:ILE:HD12 | 1.95                     | 0.47              |
| 2:G:1653:LEU:HB3  | 2:G:1660:GLN:HB2  | 1.95                     | 0.47              |
| 2:G:3806:ASN:HA   | 2:G:3890:LEU:HD13 | 1.96                     | 0.47              |
| 2:G:3882:GLN:HB2  | 2:G:3957:VAL:HG22 | 1.95                     | 0.47              |
| 2:G:3981:ALA:HA   | 2:G:3986:TRP:HE1  | 1.79                     | 0.47              |
| 2:G:4138:ASP:OD1  | 2:G:4138:ASP:N    | 2.45                     | 0.47              |
| 2:I:641:VAL:HG21  | 2:I:705:ASN:HA    | 1.96                     | 0.47              |
| 2:I:645:ARG:N     | 2:I:824:GLU:O     | 2.39                     | 0.47              |
| 2:I:913:LEU:HD13  | 2:I:918:ARG:HA    | 1.95                     | 0.47              |
| 2:I:3817:LEU:HD13 | 2:I:3899:PHE:HD1  | 1.79                     | 0.47              |
| 2:I:4795:TYR:HE1  | 2:I:4812:HIS:HA   | 1.79                     | 0.47              |
| 2:B:488:LEU:O     | 2:B:492:ASP:N     | 2.41                     | 0.47              |
| 2:B:641:VAL:HG21  | 2:B:705:ASN:HA    | 1.96                     | 0.47              |
| 2:B:671:VAL:HG22  | 2:B:740:PRO:HG3   | 1.95                     | 0.47              |
| 2:B:2013:LYS:HA   | 2:B:2028:ARG:HB2  | 1.95                     | 0.47              |
| 2:E:1931:LEU:HD22 | 2:E:1935:VAL:HG11 | 1.96                     | 0.47              |
| 1:F:87:HIS:N      | 1:F:91:ILE:O      | 2.47                     | 0.47              |
| 2:G:1718:ILE:HG13 | 2:G:1719:HIS:CD2  | 2.49                     | 0.47              |
| 2:G:1848:LEU:HD22 | 2:G:1853:ILE:HG13 | 1.95                     | 0.47              |
| 2:I:952:LYS:HB3   | 2:I:968:ALA:HB1   | 1.96                     | 0.47              |
| 2:I:1647:CYS:SG   | 2:I:1648:MET:N    | 2.87                     | 0.47              |
| 2:B:1647:CYS:SG   | 2:B:1648:MET:N    | 2.87                     | 0.47              |
| 2:E:841:GLY:HA2   | 2:E:1073:ARG:HD2  | 1.96                     | 0.47              |
| 2:E:1232:ARG:HD3  | 2:E:1702:HIS:HB3  | 1.96                     | 0.47              |
| 2:E:1653:LEU:HB3  | 2:E:1660:GLN:HB2  | 1.95                     | 0.47              |
| 2:E:3806:ASN:HA   | 2:E:3890:LEU:HD13 | 1.96                     | 0.47              |
| 2:G:3729:MET:HB3  | 2:G:3770:LEU:HD21 | 1.96                     | 0.47              |
| 2:I:4003:LEU:HB2  | 2:I:4013:LEU:HD13 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:3992:PHE:O    | 2:B:3996:PHE:N    | 2.38                     | 0.47              |
| 2:B:4571:PHE:O    | 2:B:4575:PHE:N    | 2.48                     | 0.47              |
| 2:B:4837:LEU:HD11 | 2:B:4936:ILE:HD11 | 1.96                     | 0.47              |
| 2:E:1848:LEU:HD22 | 2:E:1853:ILE:HG13 | 1.95                     | 0.47              |
| 2:E:4571:PHE:O    | 2:E:4575:PHE:N    | 2.48                     | 0.47              |
| 2:G:841:GLY:HA2   | 2:G:1073:ARG:HD2  | 1.96                     | 0.47              |
| 2:G:1163:THR:HA   | 2:G:1168:VAL:HA   | 1.95                     | 0.47              |
| 2:G:1232:ARG:HD3  | 2:G:1702:HIS:HB3  | 1.96                     | 0.47              |
| 2:G:1848:LEU:HB3  | 2:G:1853:ILE:HB   | 1.95                     | 0.47              |
| 2:I:1232:ARG:HD3  | 2:I:1702:HIS:HB3  | 1.96                     | 0.47              |
| 2:I:1653:LEU:HB3  | 2:I:1660:GLN:HB2  | 1.95                     | 0.47              |
| 2:I:1960:ALA:O    | 2:I:1964:ARG:NE   | 2.48                     | 0.47              |
| 1:A:2:VAL:HG21    | 1:A:61:GLU:HB2    | 1.96                     | 0.47              |
| 2:B:1516:UNK:N    | 2:B:1529:UNK:O    | 2.47                     | 0.47              |
| 2:B:1653:LEU:HB3  | 2:B:1660:GLN:HB2  | 1.95                     | 0.47              |
| 2:B:4003:LEU:HB2  | 2:B:4013:LEU:HD13 | 1.96                     | 0.47              |
| 2:E:232:THR:HB    | 2:E:252:VAL:HG11  | 1.95                     | 0.47              |
| 2:E:1075:PHE:HB2  | 2:E:1192:CYS:HB2  | 1.95                     | 0.47              |
| 2:E:1713:ASP:O    | 2:E:1717:SER:N    | 2.46                     | 0.47              |
| 2:E:2868:SER:O    | 2:E:2872:GLN:N    | 2.44                     | 0.47              |
| 2:E:3840:SER:OG   | 2:E:3875:MET:O    | 2.30                     | 0.47              |
| 2:E:4116:GLU:H    | 2:E:4128:PHE:HZ   | 1.63                     | 0.47              |
| 2:G:637:LEU:HG    | 2:G:1693:GLN:HB3  | 1.96                     | 0.47              |
| 2:G:671:VAL:HG22  | 2:G:740:PRO:HG3   | 1.95                     | 0.47              |
| 2:G:2347:GLU:O    | 2:G:2351:ASN:N    | 2.43                     | 0.47              |
| 2:G:3889:GLN:HE22 | 2:G:3963:ASN:HB3  | 1.80                     | 0.47              |
| 1:A:34:LYS:NZ     | 2:B:635:THR:O     | 2.47                     | 0.47              |
| 2:B:3806:ASN:HA   | 2:B:3890:LEU:HD13 | 1.96                     | 0.47              |
| 2:E:215:THR:HG22  | 2:E:273:HIS:HA    | 1.95                     | 0.47              |
| 2:E:1718:ILE:HG13 | 2:E:1719:HIS:CD2  | 2.49                     | 0.47              |
| 2:E:3920:VAL:O    | 2:E:3924:LEU:N    | 2.44                     | 0.47              |
| 2:I:215:THR:HG22  | 2:I:273:HIS:HA    | 1.95                     | 0.47              |
| 2:I:637:LEU:HG    | 2:I:1693:GLN:HB3  | 1.96                     | 0.47              |
| 2:I:2013:LYS:HA   | 2:I:2028:ARG:HB2  | 1.96                     | 0.47              |
| 2:I:2950:UNK:O    | 2:I:2954:UNK:N    | 2.48                     | 0.47              |
| 2:I:4138:ASP:OD1  | 2:I:4138:ASP:N    | 2.45                     | 0.47              |
| 2:B:988:LEU:O     | 2:B:992:GLY:N     | 2.46                     | 0.47              |
| 2:B:1665:HIS:HA   | 2:B:1668:ARG:HG2  | 1.97                     | 0.47              |
| 2:B:3729:MET:HB3  | 2:B:3770:LEU:HD21 | 1.96                     | 0.47              |
| 2:E:793:LEU:HD12  | 2:E:797:HIS:HB2   | 1.95                     | 0.47              |
| 2:E:988:LEU:O     | 2:E:992:GLY:N     | 2.46                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1032:LYS:O    | 2:E:1036:ARG:N    | 2.40                     | 0.47              |
| 2:E:1778:SER:N    | 2:E:1799:SER:O    | 2.46                     | 0.47              |
| 2:E:1854:PHE:HD1  | 2:E:1858:ASP:HB3  | 1.79                     | 0.47              |
| 2:G:1665:HIS:HA   | 2:G:1668:ARG:HG2  | 1.97                     | 0.47              |
| 2:G:2013:LYS:HA   | 2:G:2028:ARG:HB2  | 1.95                     | 0.47              |
| 2:G:4116:GLU:H    | 2:G:4128:PHE:HZ   | 1.63                     | 0.47              |
| 2:I:379:HIS:CD2   | 2:I:382:GLY:H     | 2.33                     | 0.47              |
| 2:I:880:GLU:OE1   | 2:I:968:ALA:N     | 2.47                     | 0.47              |
| 2:I:1075:PHE:HB2  | 2:I:1192:CYS:HB2  | 1.95                     | 0.47              |
| 2:I:1659:LEU:O    | 2:I:1663:HIS:N    | 2.44                     | 0.47              |
| 2:I:1854:PHE:HD1  | 2:I:1858:ASP:HB3  | 1.79                     | 0.47              |
| 2:I:1979:LEU:HA   | 2:I:1983:ALA:HB3  | 1.95                     | 0.47              |
| 2:I:3889:GLN:HE22 | 2:I:3963:ASN:HB3  | 1.79                     | 0.47              |
| 2:I:3994:HIS:O    | 2:I:3998:HIS:ND1  | 2.39                     | 0.47              |
| 2:I:4824:ARG:HA   | 2:I:4827:LEU:HB3  | 1.97                     | 0.47              |
| 1:A:87:HIS:N      | 1:A:91:ILE:O      | 2.47                     | 0.47              |
| 2:B:1075:PHE:HB2  | 2:B:1192:CYS:HB2  | 1.96                     | 0.47              |
| 2:E:1665:HIS:HA   | 2:E:1668:ARG:HG2  | 1.97                     | 0.47              |
| 2:E:2347:GLU:O    | 2:E:2351:ASN:N    | 2.43                     | 0.47              |
| 1:F:2:VAL:HG21    | 1:F:61:GLU:HB2    | 1.96                     | 0.47              |
| 2:G:120:CYS:H     | 2:G:145:ALA:HB1   | 1.80                     | 0.47              |
| 2:G:485:SER:O     | 2:G:489:ASN:N     | 2.44                     | 0.47              |
| 2:G:880:GLU:OE1   | 2:G:968:ALA:N     | 2.47                     | 0.47              |
| 2:G:2950:UNK:O    | 2:G:2954:UNK:N    | 2.48                     | 0.47              |
| 2:I:1665:HIS:HA   | 2:I:1668:ARG:HG2  | 1.97                     | 0.47              |
| 2:I:3981:ALA:HA   | 2:I:3986:TRP:HE1  | 1.79                     | 0.47              |
| 2:B:232:THR:HB    | 2:B:252:VAL:HG11  | 1.95                     | 0.47              |
| 2:B:4105:GLY:HA2  | 2:B:4108:ILE:HD12 | 1.95                     | 0.47              |
| 2:E:1952:GLN:HA   | 2:E:1955:VAL:HG12 | 1.96                     | 0.47              |
| 2:G:1713:ASP:O    | 2:G:1717:SER:N    | 2.46                     | 0.47              |
| 2:I:1848:LEU:HB3  | 2:I:1853:ILE:HB   | 1.95                     | 0.47              |
| 2:E:120:CYS:H     | 2:E:145:ALA:HB1   | 1.80                     | 0.47              |
| 2:E:2871:LEU:HD22 | 2:E:2927:LEU:HD22 | 1.97                     | 0.47              |
| 2:I:485:SER:O     | 2:I:489:ASN:N     | 2.44                     | 0.47              |
| 2:I:1286:UNK:HA   | 2:I:1461:UNK:HA   | 1.96                     | 0.47              |
| 2:B:4560:TYR:O    | 2:B:4564:PHE:N    | 2.43                     | 0.46              |
| 2:B:4824:ARG:HA   | 2:B:4827:LEU:HB3  | 1.97                     | 0.46              |
| 2:G:4822:THR:O    | 2:G:4825:THR:OG1  | 2.29                     | 0.46              |
| 2:I:731:THR:OG1   | 2:I:1519:UNK:O    | 2.28                     | 0.46              |
| 2:I:4634:GLU:HG3  | 2:I:4636:THR:H    | 1.81                     | 0.46              |
| 2:I:5012:LYS:O    | 2:I:5016:GLU:N    | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:2:VAL:HG21    | 1:J:61:GLU:HB2    | 1.96                     | 0.46              |
| 2:B:379:HIS:CD2   | 2:B:382:GLY:H     | 2.33                     | 0.46              |
| 2:B:1232:ARG:HD3  | 2:B:1702:HIS:HB3  | 1.97                     | 0.46              |
| 2:B:2231:SER:HA   | 2:B:2234:ARG:HG2  | 1.98                     | 0.46              |
| 2:B:4634:GLU:HG3  | 2:B:4636:THR:H    | 1.80                     | 0.46              |
| 2:B:5012:LYS:O    | 2:B:5016:GLU:N    | 2.43                     | 0.46              |
| 2:E:3729:MET:HB3  | 2:E:3770:LEU:HD21 | 1.96                     | 0.46              |
| 2:E:3817:LEU:HD13 | 2:E:3899:PHE:HD1  | 1.79                     | 0.46              |
| 2:E:3889:GLN:HE22 | 2:E:3963:ASN:HB3  | 1.80                     | 0.46              |
| 2:E:3981:ALA:HA   | 2:E:3986:TRP:HE1  | 1.79                     | 0.46              |
| 2:E:4003:LEU:HB2  | 2:E:4013:LEU:HD13 | 1.96                     | 0.46              |
| 2:G:733:PRO:HD2   | 2:G:763:PRO:HD2   | 1.97                     | 0.46              |
| 2:G:1854:PHE:HD1  | 2:G:1858:ASP:HB3  | 1.79                     | 0.46              |
| 2:G:1952:GLN:HA   | 2:G:1955:VAL:HG12 | 1.96                     | 0.46              |
| 2:G:2871:LEU:HD22 | 2:G:2927:LEU:HD22 | 1.97                     | 0.46              |
| 2:G:4003:LEU:HB2  | 2:G:4013:LEU:HD13 | 1.96                     | 0.46              |
| 2:I:1778:SER:N    | 2:I:1799:SER:O    | 2.46                     | 0.46              |
| 2:I:4571:PHE:O    | 2:I:4575:PHE:N    | 2.48                     | 0.46              |
| 2:B:4116:GLU:H    | 2:B:4128:PHE:HZ   | 1.63                     | 0.46              |
| 2:E:733:PRO:HD2   | 2:E:763:PRO:HD2   | 1.97                     | 0.46              |
| 2:G:641:VAL:HG21  | 2:G:705:ASN:HA    | 1.96                     | 0.46              |
| 2:G:4560:TYR:O    | 2:G:4564:PHE:N    | 2.43                     | 0.46              |
| 2:G:4571:PHE:O    | 2:G:4575:PHE:N    | 2.48                     | 0.46              |
| 2:I:865:PRO:O     | 2:I:869:ARG:N     | 2.49                     | 0.46              |
| 2:I:1855:GLY:O    | 2:I:1859:VAL:N    | 2.45                     | 0.46              |
| 2:B:637:LEU:HG    | 2:B:1693:GLN:HB3  | 1.96                     | 0.46              |
| 2:E:164:ARG:N     | 2:E:167:ASP:OD2   | 2.48                     | 0.46              |
| 2:E:641:VAL:HG21  | 2:E:705:ASN:HA    | 1.96                     | 0.46              |
| 2:E:2231:SER:HA   | 2:E:2234:ARG:HG2  | 1.98                     | 0.46              |
| 2:G:164:ARG:N     | 2:G:167:ASP:OD2   | 2.48                     | 0.46              |
| 2:G:1778:SER:N    | 2:G:1799:SER:O    | 2.46                     | 0.46              |
| 1:H:2:VAL:HG21    | 1:H:61:GLU:HB2    | 1.96                     | 0.46              |
| 2:I:120:CYS:H     | 2:I:145:ALA:HB1   | 1.80                     | 0.46              |
| 2:I:2231:SER:HA   | 2:I:2234:ARG:HG2  | 1.98                     | 0.46              |
| 2:I:3806:ASN:HA   | 2:I:3890:LEU:HD13 | 1.96                     | 0.46              |
| 2:I:4826:ILE:O    | 2:I:4829:SER:OG   | 2.33                     | 0.46              |
| 2:B:120:CYS:H     | 2:B:145:ALA:HB1   | 1.80                     | 0.46              |
| 2:B:731:THR:OG1   | 2:B:1519:UNK:O    | 2.27                     | 0.46              |
| 2:E:637:LEU:HG    | 2:E:1693:GLN:HB3  | 1.96                     | 0.46              |
| 2:E:1229:ASN:O    | 2:E:1827:ARG:N    | 2.43                     | 0.46              |
| 2:E:1729:SER:O    | 2:E:2163:ARG:NH1  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1779:PRO:HG2  | 1:H:44:LYS:HE3    | 1.98                     | 0.46              |
| 2:G:2231:SER:HA   | 2:G:2234:ARG:HG2  | 1.98                     | 0.46              |
| 2:G:4634:GLU:HG3  | 2:G:4636:THR:H    | 1.81                     | 0.46              |
| 2:I:69:LEU:HD22   | 2:I:107:ILE:HD11  | 1.98                     | 0.46              |
| 2:B:38:ALA:HB1    | 2:B:64:ILE:HG13   | 1.97                     | 0.46              |
| 2:B:880:GLU:OE1   | 2:B:968:ALA:N     | 2.47                     | 0.46              |
| 2:E:1152:MET:HB2  | 2:E:1161:ILE:HB   | 1.97                     | 0.46              |
| 2:E:1960:ALA:O    | 2:E:1964:ARG:NE   | 2.48                     | 0.46              |
| 2:G:1229:ASN:O    | 2:G:1827:ARG:N    | 2.43                     | 0.46              |
| 2:G:4824:ARG:HA   | 2:G:4827:LEU:HB3  | 1.97                     | 0.46              |
| 2:I:4782:VAL:O    | 2:I:4785:THR:OG1  | 2.34                     | 0.46              |
| 2:B:69:LEU:HD22   | 2:B:107:ILE:HD11  | 1.98                     | 0.46              |
| 2:B:103:TYR:HB3   | 2:B:152:PRO:HD3   | 1.98                     | 0.46              |
| 2:B:1713:ASP:O    | 2:B:1717:SER:N    | 2.46                     | 0.46              |
| 2:B:3981:ALA:HA   | 2:B:3986:TRP:HE1  | 1.79                     | 0.46              |
| 2:E:379:HIS:CD2   | 2:E:382:GLY:H     | 2.33                     | 0.46              |
| 2:E:4824:ARG:HA   | 2:E:4827:LEU:HB3  | 1.97                     | 0.46              |
| 2:G:1729:SER:O    | 2:G:2163:ARG:NH1  | 2.49                     | 0.46              |
| 2:I:838:HIS:CE1   | 2:I:1201:HIS:HD2  | 2.34                     | 0.46              |
| 2:I:1152:MET:HB2  | 2:I:1161:ILE:HB   | 1.97                     | 0.46              |
| 2:B:838:HIS:CE1   | 2:B:1201:HIS:HD2  | 2.34                     | 0.46              |
| 2:B:3758:MET:O    | 2:B:3762:ARG:NE   | 2.46                     | 0.46              |
| 2:I:103:TYR:HB3   | 2:I:152:PRO:HD3   | 1.98                     | 0.46              |
| 2:I:733:PRO:HD2   | 2:I:763:PRO:HD2   | 1.97                     | 0.46              |
| 1:A:83:GLY:O      | 1:A:94:ASN:N      | 2.48                     | 0.46              |
| 2:E:3927:GLN:O    | 2:E:3931:SER:N    | 2.45                     | 0.46              |
| 2:E:4634:GLU:HG3  | 2:E:4636:THR:H    | 1.81                     | 0.46              |
| 2:I:4942:GLU:O    | 2:I:4946:GLN:N    | 2.44                     | 0.46              |
| 2:B:629:ARG:HB3   | 2:B:634:GLN:NE2   | 2.32                     | 0.45              |
| 2:B:733:PRO:HD2   | 2:B:763:PRO:HD2   | 1.97                     | 0.45              |
| 2:B:3889:GLN:HE22 | 2:B:3963:ASN:HB3  | 1.80                     | 0.45              |
| 2:B:4697:VAL:O    | 2:B:4701:TRP:N    | 2.49                     | 0.45              |
| 2:G:629:ARG:HB3   | 2:G:634:GLN:NE2   | 2.32                     | 0.45              |
| 2:G:4998:LYS:NZ   | 2:G:5007:GLU:OE1  | 2.42                     | 0.45              |
| 2:I:1203:ASN:ND2  | 2:I:1210:SER:O    | 2.44                     | 0.45              |
| 2:I:2871:LEU:HD22 | 2:I:2927:LEU:HD22 | 1.97                     | 0.45              |
| 2:I:4116:GLU:H    | 2:I:4128:PHE:HZ   | 1.63                     | 0.45              |
| 1:J:83:GLY:O      | 1:J:94:ASN:N      | 2.48                     | 0.45              |
| 2:B:1729:SER:O    | 2:B:2163:ARG:NH1  | 2.49                     | 0.45              |
| 2:B:2336:ARG:NH2  | 2:B:2428:ALA:O    | 2.49                     | 0.45              |
| 2:E:709:ASP:HB3   | 2:E:725:HIS:CE1   | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4934:GLY:O    | 2:E:4938:ASP:N    | 2.47                     | 0.45              |
| 1:F:23:VAL:HB     | 1:F:105:ASN:HA    | 1.99                     | 0.45              |
| 2:I:38:ALA:HB1    | 2:I:64:ILE:HG13   | 1.97                     | 0.45              |
| 2:I:1729:SER:O    | 2:I:2163:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:23:VAL:HB     | 1:A:105:ASN:HA    | 1.99                     | 0.45              |
| 2:B:4942:GLU:O    | 2:B:4946:GLN:N    | 2.43                     | 0.45              |
| 2:E:719:LEU:HD22  | 2:E:735:GLN:HG2   | 1.98                     | 0.45              |
| 2:G:38:ALA:HB1    | 2:G:64:ILE:HG13   | 1.97                     | 0.45              |
| 2:G:865:PRO:O     | 2:G:869:ARG:N     | 2.49                     | 0.45              |
| 2:G:1152:MET:HB2  | 2:G:1161:ILE:HB   | 1.97                     | 0.45              |
| 2:I:2868:SER:O    | 2:I:2872:GLN:N    | 2.44                     | 0.45              |
| 2:I:2880:GLU:O    | 2:I:2884:ASN:N    | 2.45                     | 0.45              |
| 2:B:124:SER:HA    | 2:B:132:ALA:HB3   | 1.99                     | 0.45              |
| 2:B:709:ASP:HB3   | 2:B:725:HIS:CE1   | 2.52                     | 0.45              |
| 2:E:38:ALA:HB1    | 2:E:64:ILE:HG13   | 1.97                     | 0.45              |
| 2:E:2286:LEU:HA   | 2:E:2289:ALA:HB3  | 1.99                     | 0.45              |
| 2:E:4697:VAL:O    | 2:E:4701:TRP:N    | 2.49                     | 0.45              |
| 2:G:838:HIS:CE1   | 2:G:1201:HIS:HD2  | 2.34                     | 0.45              |
| 2:G:4791:TYR:HD2  | 2:G:4792:LEU:HD22 | 1.82                     | 0.45              |
| 2:I:709:ASP:HB3   | 2:I:725:HIS:CE1   | 2.52                     | 0.45              |
| 2:B:210:GLU:HG3   | 2:B:337:PRO:HG3   | 1.98                     | 0.45              |
| 2:B:1152:MET:HB2  | 2:B:1161:ILE:HB   | 1.97                     | 0.45              |
| 2:B:2871:LEU:HD22 | 2:B:2927:LEU:HD22 | 1.97                     | 0.45              |
| 2:B:2880:GLU:O    | 2:B:2884:ASN:N    | 2.45                     | 0.45              |
| 2:E:124:SER:HA    | 2:E:132:ALA:HB3   | 1.99                     | 0.45              |
| 2:E:629:ARG:HB3   | 2:E:634:GLN:NE2   | 2.32                     | 0.45              |
| 2:E:838:HIS:CE1   | 2:E:1201:HIS:HD2  | 2.34                     | 0.45              |
| 2:E:4741:LEU:HB2  | 2:E:4743:MET:HE2  | 1.98                     | 0.45              |
| 2:G:709:ASP:HB3   | 2:G:725:HIS:CE1   | 2.52                     | 0.45              |
| 2:G:4741:LEU:HB2  | 2:G:4743:MET:HE2  | 1.99                     | 0.45              |
| 1:H:23:VAL:HB     | 1:H:105:ASN:HA    | 1.99                     | 0.45              |
| 2:I:210:GLU:HG3   | 2:I:337:PRO:HG3   | 1.98                     | 0.45              |
| 2:I:2347:GLU:O    | 2:I:2351:ASN:N    | 2.43                     | 0.45              |
| 1:J:23:VAL:HB     | 1:J:105:ASN:HA    | 1.99                     | 0.45              |
| 1:A:11:ASP:OD1    | 1:A:67:SER:OG     | 2.31                     | 0.45              |
| 2:B:2132:GLY:O    | 2:B:2136:ARG:N    | 2.50                     | 0.45              |
| 2:E:40:GLU:HB3    | 2:E:44:ASN:HB3    | 1.99                     | 0.45              |
| 2:E:210:GLU:HG3   | 2:E:337:PRO:HG3   | 1.98                     | 0.45              |
| 2:E:1659:LEU:O    | 2:E:1663:HIS:N    | 2.44                     | 0.45              |
| 2:G:103:TYR:HB3   | 2:G:152:PRO:HD3   | 1.98                     | 0.45              |
| 2:G:124:SER:HA    | 2:G:132:ALA:HB3   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:4109:GLN:O    | 2:G:4113:SER:N   | 2.45                     | 0.45              |
| 2:I:2869:ARG:HA   | 2:I:2872:GLN:HB3 | 1.99                     | 0.45              |
| 2:B:19:GLU:HB2    | 2:B:206:CYS:HB3  | 1.99                     | 0.45              |
| 2:B:719:LEU:HD22  | 2:B:735:GLN:HG2  | 1.98                     | 0.45              |
| 2:B:4138:ASP:OD1  | 2:B:4138:ASP:N   | 2.45                     | 0.45              |
| 2:B:4961:CYS:SG   | 2:B:4978:HIS:NE2 | 2.90                     | 0.45              |
| 2:E:209:CYS:HA    | 2:E:334:MET:HE2  | 1.99                     | 0.45              |
| 2:E:1577:ALA:HB1  | 2:E:1584:ARG:HA  | 1.99                     | 0.45              |
| 2:E:4782:VAL:O    | 2:E:4785:THR:OG1 | 2.34                     | 0.45              |
| 2:G:69:LEU:HD22   | 2:G:107:ILE:HD11 | 1.98                     | 0.45              |
| 2:G:2286:LEU:HA   | 2:G:2289:ALA:HB3 | 1.99                     | 0.45              |
| 2:G:4705:VAL:HB   | 2:G:4778:TRP:CG  | 2.52                     | 0.45              |
| 1:H:83:GLY:O      | 1:H:94:ASN:N     | 2.48                     | 0.45              |
| 2:I:40:GLU:HB3    | 2:I:44:ASN:HB3   | 1.99                     | 0.45              |
| 2:I:124:SER:HA    | 2:I:132:ALA:HB3  | 1.99                     | 0.45              |
| 2:B:2208:MET:HE1  | 2:B:2253:HIS:HB3 | 1.98                     | 0.45              |
| 2:B:2286:LEU:HA   | 2:B:2289:ALA:HB3 | 1.99                     | 0.45              |
| 2:B:2869:ARG:HA   | 2:B:2872:GLN:HB3 | 1.98                     | 0.45              |
| 2:B:4853:VAL:HA   | 2:B:4856:PHE:HB3 | 1.98                     | 0.45              |
| 2:E:69:LEU:HD22   | 2:E:107:ILE:HD11 | 1.98                     | 0.45              |
| 2:E:485:SER:O     | 2:E:489:ASN:N    | 2.44                     | 0.45              |
| 2:E:1041:GLN:O    | 2:E:1045:THR:OG1 | 2.29                     | 0.45              |
| 1:F:83:GLY:O      | 1:F:94:ASN:N     | 2.48                     | 0.45              |
| 2:G:2430:ILE:HG21 | 2:G:2502:UNK:HA  | 1.97                     | 0.45              |
| 2:I:629:ARG:HB3   | 2:I:634:GLN:NE2  | 2.31                     | 0.45              |
| 2:I:683:ARG:HG2   | 2:I:717:ASP:HB3  | 1.99                     | 0.45              |
| 2:I:3920:VAL:O    | 2:I:3924:LEU:N   | 2.44                     | 0.45              |
| 2:I:4961:CYS:SG   | 2:I:4978:HIS:NE2 | 2.90                     | 0.45              |
| 2:B:683:ARG:HG2   | 2:B:717:ASP:HB3  | 1.99                     | 0.45              |
| 2:B:1960:ALA:O    | 2:B:1964:ARG:NE  | 2.48                     | 0.45              |
| 2:B:4741:LEU:HB2  | 2:B:4743:MET:HE2 | 1.98                     | 0.45              |
| 2:E:732:SER:HB3   | 2:E:764:VAL:HA   | 1.99                     | 0.45              |
| 2:G:732:SER:HB3   | 2:G:764:VAL:HA   | 1.99                     | 0.45              |
| 2:G:2132:GLY:O    | 2:G:2136:ARG:N   | 2.50                     | 0.45              |
| 2:G:2758:PHE:O    | 2:G:2762:THR:N   | 2.47                     | 0.45              |
| 2:G:4853:VAL:HA   | 2:G:4856:PHE:HB3 | 1.98                     | 0.45              |
| 2:I:180:LEU:HD22  | 2:I:200:TRP:NE1  | 2.32                     | 0.45              |
| 2:I:233:ILE:HD12  | 2:I:242:ARG:HB3  | 1.99                     | 0.45              |
| 2:I:2132:GLY:O    | 2:I:2136:ARG:N   | 2.50                     | 0.45              |
| 2:I:3758:MET:O    | 2:I:3762:ARG:NE  | 2.46                     | 0.45              |
| 1:J:29:MET:HB3    | 1:J:98:ILE:HB    | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:40:GLU:HB3    | 2:B:44:ASN:HB3    | 1.99                     | 0.45              |
| 2:B:865:PRO:O     | 2:B:869:ARG:N     | 2.49                     | 0.45              |
| 2:B:2247:GLN:NE2  | 2:B:2285:GLU:OE2  | 2.50                     | 0.45              |
| 2:B:4998:LYS:NZ   | 2:B:5007:GLU:OE1  | 2.42                     | 0.45              |
| 2:E:4791:TYR:HD2  | 2:E:4792:LEU:HD22 | 1.81                     | 0.45              |
| 2:G:40:GLU:HB3    | 2:G:44:ASN:HB3    | 1.99                     | 0.45              |
| 2:G:233:ILE:HD12  | 2:G:242:ARG:HB3   | 1.99                     | 0.45              |
| 2:G:683:ARG:HG2   | 2:G:717:ASP:HB3   | 1.99                     | 0.45              |
| 2:G:1577:ALA:HB1  | 2:G:1584:ARG:HA   | 1.99                     | 0.45              |
| 2:G:1960:ALA:O    | 2:G:1964:ARG:NE   | 2.48                     | 0.45              |
| 2:G:2869:ARG:HH12 | 2:G:2945:UNK:C    | 2.30                     | 0.45              |
| 2:G:3773:ARG:HG2  | 2:G:3815:LYS:HD3  | 1.99                     | 0.45              |
| 2:I:4560:TYR:O    | 2:I:4564:PHE:N    | 2.43                     | 0.45              |
| 2:I:4791:TYR:HD2  | 2:I:4792:LEU:HD22 | 1.82                     | 0.45              |
| 2:I:4989:MET:O    | 2:I:4993:MET:N    | 2.42                     | 0.45              |
| 2:B:1294:UNK:HA   | 2:B:1455:UNK:HA   | 1.99                     | 0.44              |
| 2:B:4791:TYR:HD2  | 2:B:4792:LEU:HD22 | 1.82                     | 0.44              |
| 2:E:103:TYR:HB3   | 2:E:152:PRO:HD3   | 1.98                     | 0.44              |
| 1:F:29:MET:HB3    | 1:F:98:ILE:HB     | 1.99                     | 0.44              |
| 2:G:4885:PHE:HE2  | 2:G:4901:ILE:HD11 | 1.82                     | 0.44              |
| 2:G:4961:CYS:SG   | 2:G:4978:HIS:NE2  | 2.90                     | 0.44              |
| 2:I:2286:LEU:HA   | 2:I:2289:ALA:HB3  | 1.99                     | 0.44              |
| 2:I:4853:VAL:HA   | 2:I:4856:PHE:HB3  | 1.98                     | 0.44              |
| 2:B:3765:TYR:O    | 2:B:3769:ARG:N    | 2.48                     | 0.44              |
| 2:E:2271:THR:HG22 | 2:E:2273:LEU:H    | 1.83                     | 0.44              |
| 2:E:4705:VAL:HB   | 2:E:4778:TRP:CG   | 2.52                     | 0.44              |
| 2:E:5012:LYS:O    | 2:E:5016:GLU:N    | 2.43                     | 0.44              |
| 2:G:2869:ARG:HA   | 2:G:2872:GLN:HB3  | 1.98                     | 0.44              |
| 2:G:4710:SER:OG   | 2:G:4772:ASP:OD2  | 2.31                     | 0.44              |
| 2:I:19:GLU:HB2    | 2:I:206:CYS:HB3   | 1.99                     | 0.44              |
| 2:I:1497:UNK:HA   | 2:I:1535:UNK:HA   | 1.98                     | 0.44              |
| 2:I:4799:SER:OG   | 2:I:4812:HIS:NE2  | 2.40                     | 0.44              |
| 2:I:4885:PHE:HE2  | 2:I:4901:ILE:HD11 | 1.82                     | 0.44              |
| 2:B:1229:ASN:O    | 2:B:1827:ARG:N    | 2.43                     | 0.44              |
| 2:E:59:PRO:HG3    | 2:E:307:ALA:HB3   | 1.99                     | 0.44              |
| 2:E:233:ILE:HD12  | 2:E:242:ARG:HB3   | 1.99                     | 0.44              |
| 2:E:488:LEU:HD23  | 2:E:491:ILE:HD12  | 1.99                     | 0.44              |
| 2:G:78:LEU:O      | 2:G:82:LEU:N      | 2.49                     | 0.44              |
| 2:G:379:HIS:CD2   | 2:G:382:GLY:H     | 2.33                     | 0.44              |
| 2:G:978:THR:HB    | 2:G:980:ALA:H     | 1.83                     | 0.44              |
| 2:G:2105:TRP:HE3  | 2:G:2120:MET:HE3  | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:2107:GLN:O    | 2:G:3694:LYS:NZ   | 2.45                     | 0.44              |
| 2:G:2208:MET:HE1  | 2:G:2253:HIS:HB3  | 1.99                     | 0.44              |
| 2:G:2247:GLN:NE2  | 2:G:2285:GLU:OE2  | 2.50                     | 0.44              |
| 2:I:164:ARG:N     | 2:I:167:ASP:OD2   | 2.48                     | 0.44              |
| 2:I:2208:MET:HE1  | 2:I:2253:HIS:HB3  | 1.98                     | 0.44              |
| 2:I:2271:THR:HG22 | 2:I:2273:LEU:H    | 1.83                     | 0.44              |
| 2:B:59:PRO:HG3    | 2:B:307:ALA:HB3   | 1.99                     | 0.44              |
| 2:B:233:ILE:HD12  | 2:B:242:ARG:HB3   | 1.99                     | 0.44              |
| 2:B:2105:TRP:HE3  | 2:B:2120:MET:HE3  | 1.83                     | 0.44              |
| 2:E:639:ASN:HD22  | 2:E:1635:THR:HA   | 1.83                     | 0.44              |
| 2:G:1659:LEU:O    | 2:G:1663:HIS:N    | 2.44                     | 0.44              |
| 2:G:2142:TYR:CG   | 2:G:2197:LEU:HD13 | 2.53                     | 0.44              |
| 2:G:3649:ALA:O    | 2:G:3653:PHE:N    | 2.46                     | 0.44              |
| 2:I:59:PRO:HG3    | 2:I:307:ALA:HB3   | 2.00                     | 0.44              |
| 2:I:4705:VAL:HB   | 2:I:4778:TRP:CG   | 2.52                     | 0.44              |
| 1:A:29:MET:HB3    | 1:A:98:ILE:HB     | 1.99                     | 0.44              |
| 2:B:2271:THR:HG22 | 2:B:2273:LEU:H    | 1.83                     | 0.44              |
| 2:B:3713:LYS:HG2  | 2:B:3715:LYS:H    | 1.83                     | 0.44              |
| 2:B:4109:GLN:O    | 2:B:4113:SER:N    | 2.45                     | 0.44              |
| 2:B:4885:PHE:HE2  | 2:B:4901:ILE:HD11 | 1.82                     | 0.44              |
| 2:E:870:ILE:HD11  | 2:E:1049:TYR:CG   | 2.53                     | 0.44              |
| 2:E:1817:GLU:O    | 2:E:1821:ASP:N    | 2.44                     | 0.44              |
| 2:E:2105:TRP:HE3  | 2:E:2120:MET:HE3  | 1.83                     | 0.44              |
| 2:G:488:LEU:HD23  | 2:G:491:ILE:HD12  | 1.99                     | 0.44              |
| 2:G:3927:GLN:O    | 2:G:3931:SER:N    | 2.45                     | 0.44              |
| 2:G:5012:LYS:O    | 2:G:5016:GLU:N    | 2.43                     | 0.44              |
| 2:I:357:LEU:HD21  | 2:I:376:ALA:HB1   | 1.99                     | 0.44              |
| 2:I:1649:ASP:OD1  | 2:I:1650:ILE:N    | 2.51                     | 0.44              |
| 2:I:3773:ARG:HG2  | 2:I:3815:LYS:HD3  | 2.00                     | 0.44              |
| 2:B:639:ASN:HD22  | 2:B:1635:THR:HA   | 1.83                     | 0.44              |
| 2:B:870:ILE:HD11  | 2:B:1049:TYR:CG   | 2.53                     | 0.44              |
| 2:B:1577:ALA:HB1  | 2:B:1584:ARG:HA   | 1.99                     | 0.44              |
| 2:B:4705:VAL:HB   | 2:B:4778:TRP:CG   | 2.52                     | 0.44              |
| 2:E:19:GLU:HB2    | 2:E:206:CYS:HB3   | 1.99                     | 0.44              |
| 2:E:2208:MET:HE1  | 2:E:2253:HIS:HB3  | 1.98                     | 0.44              |
| 2:E:3773:ARG:HG2  | 2:E:3815:LYS:HD3  | 1.99                     | 0.44              |
| 2:E:4885:PHE:HE2  | 2:E:4901:ILE:HD11 | 1.82                     | 0.44              |
| 2:E:4961:CYS:SG   | 2:E:4978:HIS:NE2  | 2.90                     | 0.44              |
| 2:G:1991:THR:O    | 2:G:1995:THR:OG1  | 2.30                     | 0.44              |
| 2:I:1516:UNK:N    | 2:I:1529:UNK:O    | 2.51                     | 0.44              |
| 2:I:1577:ALA:HB1  | 2:I:1584:ARG:HA   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:2105:TRP:HE3  | 2:I:2120:MET:HE3  | 1.83                     | 0.44              |
| 2:I:3927:GLN:NE2  | 2:I:3988:ALA:O    | 2.47                     | 0.44              |
| 2:E:683:ARG:HG2   | 2:E:717:ASP:HB3   | 1.99                     | 0.44              |
| 2:E:3998:HIS:CE1  | 2:E:4054:ASN:HD21 | 2.36                     | 0.44              |
| 2:G:180:LEU:HD22  | 2:G:200:TRP:NE1   | 2.32                     | 0.44              |
| 2:G:639:ASN:HD22  | 2:G:1635:THR:HA   | 1.83                     | 0.44              |
| 2:G:719:LEU:HD22  | 2:G:735:GLN:HG2   | 1.98                     | 0.44              |
| 2:G:3880:PHE:O    | 2:G:3884:LEU:N    | 2.51                     | 0.44              |
| 2:G:4702:ASP:HA   | 2:G:4778:TRP:HE1  | 1.83                     | 0.44              |
| 2:I:639:ASN:HD22  | 2:I:1635:THR:HA   | 1.83                     | 0.44              |
| 2:I:978:THR:HB    | 2:I:980:ALA:H     | 1.83                     | 0.44              |
| 2:I:2142:TYR:CG   | 2:I:2197:LEU:HD13 | 2.53                     | 0.44              |
| 2:B:732:SER:HB3   | 2:B:764:VAL:HA    | 1.99                     | 0.44              |
| 2:E:316:PHE:HB3   | 2:E:346:CYS:HB3   | 2.00                     | 0.44              |
| 2:E:2247:GLN:NE2  | 2:E:2285:GLU:OE2  | 2.50                     | 0.44              |
| 2:E:4853:VAL:HA   | 2:E:4856:PHE:HB3  | 1.98                     | 0.44              |
| 2:G:19:GLU:HB2    | 2:G:206:CYS:HB3   | 1.99                     | 0.44              |
| 2:G:210:GLU:HG3   | 2:G:337:PRO:HG3   | 1.98                     | 0.44              |
| 2:G:867:LEU:HD22  | 2:G:929:LEU:HD22  | 2.00                     | 0.44              |
| 2:I:719:LEU:HD22  | 2:I:735:GLN:HG2   | 1.98                     | 0.44              |
| 2:I:2758:PHE:O    | 2:I:2762:THR:N    | 2.47                     | 0.44              |
| 2:I:4741:LEU:HB2  | 2:I:4743:MET:HE2  | 1.99                     | 0.44              |
| 2:B:17:ASP:HB2    | 2:B:98:HIS:CE1    | 2.53                     | 0.44              |
| 2:B:180:LEU:HD22  | 2:B:200:TRP:NE1   | 2.32                     | 0.44              |
| 2:B:2347:GLU:O    | 2:B:2351:ASN:N    | 2.43                     | 0.44              |
| 2:E:865:PRO:O     | 2:E:869:ARG:N     | 2.49                     | 0.44              |
| 2:E:1516:UNK:N    | 2:E:1529:UNK:O    | 2.51                     | 0.44              |
| 2:G:209:CYS:HA    | 2:G:334:MET:HE2   | 1.99                     | 0.44              |
| 2:G:663:TYR:HB2   | 2:G:808:TYR:HB3   | 2.00                     | 0.44              |
| 2:G:1245:PHE:HE1  | 2:G:1600:LEU:HD23 | 1.83                     | 0.44              |
| 2:G:2271:THR:HG22 | 2:G:2273:LEU:H    | 1.83                     | 0.44              |
| 1:H:29:MET:HB3    | 1:H:98:ILE:HB     | 2.00                     | 0.44              |
| 2:I:709:ASP:O     | 2:I:725:HIS:ND1   | 2.51                     | 0.44              |
| 2:I:3713:LYS:HG2  | 2:I:3715:LYS:H    | 1.83                     | 0.44              |
| 2:B:111:HIS:CD2   | 2:B:114:SER:H     | 2.26                     | 0.43              |
| 2:B:2004:GLU:HA   | 2:B:2007:ASN:HD22 | 1.83                     | 0.43              |
| 2:B:4826:ILE:O    | 2:B:4829:SER:OG   | 2.33                     | 0.43              |
| 2:E:663:TYR:HB2   | 2:E:808:TYR:HB3   | 2.00                     | 0.43              |
| 2:E:829:TYR:HB3   | 2:E:1073:ARG:HH11 | 1.83                     | 0.43              |
| 2:E:3880:PHE:O    | 2:E:3884:LEU:N    | 2.51                     | 0.43              |
| 2:E:4109:GLN:O    | 2:E:4113:SER:N    | 2.45                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:59:PRO:HG3    | 2:G:307:ALA:HB3   | 2.00                     | 0.43              |
| 2:G:2004:GLU:HA   | 2:G:2007:ASN:HD22 | 1.83                     | 0.43              |
| 2:I:488:LEU:HD23  | 2:I:491:ILE:HD12  | 1.99                     | 0.43              |
| 2:I:1663:HIS:O    | 2:I:1667:LEU:N    | 2.50                     | 0.43              |
| 2:B:209:CYS:HA    | 2:B:334:MET:HE2   | 1.99                     | 0.43              |
| 2:B:316:PHE:HB3   | 2:B:346:CYS:HB3   | 2.00                     | 0.43              |
| 2:B:488:LEU:HD23  | 2:B:491:ILE:HD12  | 1.99                     | 0.43              |
| 2:B:867:LEU:HD22  | 2:B:929:LEU:HD22  | 2.00                     | 0.43              |
| 2:B:3880:PHE:O    | 2:B:3884:LEU:N    | 2.51                     | 0.43              |
| 2:E:357:LEU:HD21  | 2:E:376:ALA:HB1   | 2.00                     | 0.43              |
| 2:E:709:ASP:O     | 2:E:725:HIS:ND1   | 2.51                     | 0.43              |
| 2:E:1245:PHE:HE1  | 2:E:1600:LEU:HD23 | 1.83                     | 0.43              |
| 2:E:1649:ASP:OD1  | 2:E:1650:ILE:N    | 2.51                     | 0.43              |
| 2:E:2142:TYR:CG   | 2:E:2197:LEU:HD13 | 2.53                     | 0.43              |
| 2:E:2327:GLY:HA2  | 2:E:2330:ARG:HD3  | 2.00                     | 0.43              |
| 2:G:357:LEU:HD21  | 2:G:376:ALA:HB1   | 1.99                     | 0.43              |
| 2:G:1817:GLU:O    | 2:G:1821:ASP:N    | 2.44                     | 0.43              |
| 2:G:3974:THR:HA   | 2:G:3977:GLN:HB2  | 2.00                     | 0.43              |
| 2:G:4782:VAL:O    | 2:G:4785:THR:OG1  | 2.34                     | 0.43              |
| 2:I:78:LEU:O      | 2:I:82:LEU:N      | 2.49                     | 0.43              |
| 2:B:709:ASP:O     | 2:B:725:HIS:ND1   | 2.51                     | 0.43              |
| 2:B:1991:THR:O    | 2:B:1995:THR:OG1  | 2.30                     | 0.43              |
| 2:B:2142:TYR:CG   | 2:B:2197:LEU:HD13 | 2.53                     | 0.43              |
| 2:B:2758:PHE:O    | 2:B:2762:THR:N    | 2.47                     | 0.43              |
| 2:E:3974:THR:HA   | 2:E:3977:GLN:HB2  | 2.00                     | 0.43              |
| 2:E:4745:LEU:O    | 2:E:4749:GLU:N    | 2.50                     | 0.43              |
| 2:G:1663:HIS:O    | 2:G:1667:LEU:N    | 2.50                     | 0.43              |
| 2:G:3758:MET:O    | 2:G:3762:ARG:NE   | 2.46                     | 0.43              |
| 2:G:4989:MET:O    | 2:G:4993:MET:N    | 2.42                     | 0.43              |
| 2:I:209:CYS:HA    | 2:I:334:MET:HE2   | 1.99                     | 0.43              |
| 2:I:870:ILE:HD11  | 2:I:1049:TYR:CG   | 2.53                     | 0.43              |
| 2:I:1077:ALA:HB3  | 2:I:1189:LEU:HD11 | 2.01                     | 0.43              |
| 2:I:2207:VAL:HG13 | 2:I:2232:CYS:HB2  | 2.00                     | 0.43              |
| 2:I:4697:VAL:O    | 2:I:4701:TRP:N    | 2.49                     | 0.43              |
| 2:B:164:ARG:N     | 2:B:167:ASP:OD2   | 2.48                     | 0.43              |
| 2:B:2361:PRO:HA   | 2:B:2364:PHE:HD2  | 1.83                     | 0.43              |
| 2:B:4782:VAL:O    | 2:B:4785:THR:OG1  | 2.34                     | 0.43              |
| 2:E:978:THR:HB    | 2:E:980:ALA:H     | 1.83                     | 0.43              |
| 2:G:1649:ASP:OD1  | 2:G:1650:ILE:N    | 2.51                     | 0.43              |
| 2:G:2361:PRO:HA   | 2:G:2364:PHE:HD2  | 1.83                     | 0.43              |
| 2:I:732:SER:HB3   | 2:I:764:VAL:HA    | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:3676:ASP:N    | 2:I:3676:ASP:OD1  | 2.51                     | 0.43              |
| 2:B:709:ASP:HA    | 2:B:725:HIS:H     | 1.84                     | 0.43              |
| 2:B:1649:ASP:OD1  | 2:B:1650:ILE:N    | 2.51                     | 0.43              |
| 2:B:1679:ASN:O    | 2:B:1683:HIS:ND1  | 2.38                     | 0.43              |
| 2:B:2207:VAL:HG13 | 2:B:2232:CYS:HB2  | 2.00                     | 0.43              |
| 2:B:3773:ARG:HG2  | 2:B:3815:LYS:HD3  | 1.99                     | 0.43              |
| 2:B:3974:THR:HA   | 2:B:3977:GLN:HB2  | 2.00                     | 0.43              |
| 2:B:3998:HIS:CE1  | 2:B:4054:ASN:HD21 | 2.36                     | 0.43              |
| 2:E:180:LEU:HD22  | 2:E:200:TRP:NE1   | 2.32                     | 0.43              |
| 2:E:867:LEU:HD22  | 2:E:929:LEU:HD22  | 2.00                     | 0.43              |
| 2:E:1077:ALA:HB3  | 2:E:1189:LEU:HD11 | 2.01                     | 0.43              |
| 2:E:2869:ARG:HA   | 2:E:2872:GLN:HB3  | 1.99                     | 0.43              |
| 2:I:709:ASP:HA    | 2:I:725:HIS:H     | 1.84                     | 0.43              |
| 2:I:765:GLN:NE2   | 2:I:1522:UNK:O    | 2.51                     | 0.43              |
| 2:I:1095:VAL:HA   | 2:I:1146:GLY:H    | 1.84                     | 0.43              |
| 2:I:2247:GLN:NE2  | 2:I:2285:GLU:OE2  | 2.50                     | 0.43              |
| 2:I:4957:LYS:HB3  | 2:I:4957:LYS:HE3  | 1.83                     | 0.43              |
| 2:B:151:HIS:HB2   | 2:B:170:ILE:HB    | 2.01                     | 0.43              |
| 2:B:2466:LEU:HA   | 2:B:2469:ILE:HD12 | 2.01                     | 0.43              |
| 2:B:3676:ASP:OD1  | 2:B:3676:ASP:N    | 2.51                     | 0.43              |
| 2:B:4702:ASP:HA   | 2:B:4778:TRP:HE1  | 1.83                     | 0.43              |
| 2:E:1092:PHE:O    | 2:E:1149:VAL:N    | 2.48                     | 0.43              |
| 2:E:2004:GLU:HA   | 2:E:2007:ASN:HD22 | 1.83                     | 0.43              |
| 2:E:2144:ILE:H    | 2:E:2144:ILE:HG13 | 1.75                     | 0.43              |
| 2:E:3713:LYS:HG2  | 2:E:3715:LYS:H    | 1.83                     | 0.43              |
| 2:G:252:VAL:HA    | 2:G:255:HIS:CG    | 2.54                     | 0.43              |
| 2:G:1095:VAL:HA   | 2:G:1146:GLY:H    | 1.84                     | 0.43              |
| 2:G:4697:VAL:O    | 2:G:4701:TRP:N    | 2.49                     | 0.43              |
| 2:I:2004:GLU:HA   | 2:I:2007:ASN:HD22 | 1.83                     | 0.43              |
| 2:I:2361:PRO:HA   | 2:I:2364:PHE:HD2  | 1.83                     | 0.43              |
| 2:I:3880:PHE:O    | 2:I:3884:LEU:N    | 2.51                     | 0.43              |
| 2:I:4702:ASP:HA   | 2:I:4778:TRP:HE1  | 1.83                     | 0.43              |
| 2:B:357:LEU:HD21  | 2:B:376:ALA:HB1   | 1.99                     | 0.43              |
| 2:B:4745:LEU:O    | 2:B:4749:GLU:N    | 2.50                     | 0.43              |
| 2:E:809:ALA:O     | 2:E:811:CYS:N     | 2.50                     | 0.43              |
| 2:E:2207:VAL:HG13 | 2:E:2232:CYS:HB2  | 2.00                     | 0.43              |
| 2:E:4702:ASP:HA   | 2:E:4778:TRP:HE1  | 1.83                     | 0.43              |
| 2:G:316:PHE:HB3   | 2:G:346:CYS:HB3   | 2.00                     | 0.43              |
| 2:B:79:GLN:HA     | 2:B:82:LEU:HB2    | 2.01                     | 0.43              |
| 2:B:1077:ALA:HB3  | 2:B:1189:LEU:HD11 | 2.01                     | 0.43              |
| 2:B:1111:PRO:HD3  | 2:B:1605:TRP:HE1  | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2869:ARG:HH12 | 2:B:2945:UNK:C    | 2.32                     | 0.43              |
| 2:B:4934:GLY:O    | 2:B:4938:ASP:N    | 2.47                     | 0.43              |
| 2:E:79:GLN:HA     | 2:E:82:LEU:HB2    | 2.01                     | 0.43              |
| 2:E:1812:LEU:HD21 | 2:E:1861:GLN:HG2  | 2.01                     | 0.43              |
| 2:E:3765:TYR:O    | 2:E:3769:ARG:N    | 2.48                     | 0.43              |
| 2:G:685:GLY:N     | 2:G:780:VAL:O     | 2.39                     | 0.43              |
| 2:G:709:ASP:O     | 2:G:725:HIS:ND1   | 2.51                     | 0.43              |
| 2:G:829:TYR:HB3   | 2:G:1073:ARG:HH11 | 1.84                     | 0.43              |
| 2:G:1077:ALA:HB3  | 2:G:1189:LEU:HD11 | 2.01                     | 0.43              |
| 2:G:1105:ALA:O    | 2:G:1189:LEU:N    | 2.52                     | 0.43              |
| 2:G:1516:UNK:N    | 2:G:1529:UNK:O    | 2.51                     | 0.43              |
| 2:G:3998:HIS:CE1  | 2:G:4054:ASN:HD21 | 2.36                     | 0.43              |
| 2:I:401:ALA:HA    | 2:I:404:ILE:HD12  | 2.01                     | 0.43              |
| 2:I:3840:SER:OG   | 2:I:3875:MET:O    | 2.30                     | 0.43              |
| 2:I:3974:THR:HA   | 2:I:3977:GLN:HB2  | 2.00                     | 0.43              |
| 2:B:583:ILE:HA    | 2:B:586:ILE:HD12  | 2.01                     | 0.43              |
| 2:B:1497:UNK:HA   | 2:B:1535:UNK:HA   | 2.01                     | 0.43              |
| 2:B:2327:GLY:HA2  | 2:B:2330:ARG:HD3  | 2.00                     | 0.43              |
| 2:B:3927:GLN:O    | 2:B:3931:SER:N    | 2.45                     | 0.43              |
| 2:E:151:HIS:HB2   | 2:E:170:ILE:HB    | 2.00                     | 0.43              |
| 2:E:583:ILE:HA    | 2:E:586:ILE:HD12  | 2.01                     | 0.43              |
| 2:E:4857:ASN:HB2  | 2:G:4807:PHE:CE1  | 2.53                     | 0.43              |
| 2:G:533:ASN:HB3   | 2:G:536:ASN:HB2   | 2.01                     | 0.43              |
| 2:G:870:ILE:HD11  | 2:G:1049:TYR:CG   | 2.53                     | 0.43              |
| 2:G:1866:ILE:HG13 | 2:G:1926:LEU:HB3  | 2.01                     | 0.43              |
| 2:I:379:HIS:CD2   | 2:I:381:GLU:H     | 2.37                     | 0.43              |
| 2:I:829:TYR:HB3   | 2:I:1073:ARG:HH11 | 1.84                     | 0.43              |
| 2:I:867:LEU:HD22  | 2:I:929:LEU:HD22  | 2.00                     | 0.43              |
| 2:I:1111:PRO:HD3  | 2:I:1605:TRP:HE1  | 1.84                     | 0.43              |
| 2:I:1268:PRO:HB2  | 2:I:1591:CYS:HB2  | 2.01                     | 0.43              |
| 2:I:2430:ILE:HG21 | 2:I:2502:UNK:HA   | 2.00                     | 0.43              |
| 2:I:4822:THR:O    | 2:I:4825:THR:OG1  | 2.29                     | 0.43              |
| 2:B:469:ARG:HH21  | 2:B:3712:GLU:HB3  | 1.84                     | 0.43              |
| 2:B:663:TYR:HB2   | 2:B:808:TYR:HB3   | 2.00                     | 0.43              |
| 2:B:1095:VAL:HA   | 2:B:1146:GLY:H    | 1.84                     | 0.43              |
| 2:B:3927:GLN:NE2  | 2:B:3988:ALA:O    | 2.48                     | 0.43              |
| 2:E:2880:GLU:O    | 2:E:2884:ASN:N    | 2.45                     | 0.43              |
| 2:E:4822:THR:O    | 2:E:4825:THR:OG1  | 2.29                     | 0.43              |
| 2:G:709:ASP:HA    | 2:G:725:HIS:H     | 1.84                     | 0.43              |
| 2:G:731:THR:OG1   | 2:G:1520:UNK:O    | 2.37                     | 0.43              |
| 2:G:1149:VAL:HG22 | 2:G:1164:LEU:HD13 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:3713:LYS:HG2  | 2:G:3715:LYS:H    | 1.83                     | 0.43              |
| 2:I:1046:LEU:HB3  | 2:I:1051:TYR:HB2  | 2.01                     | 0.43              |
| 2:I:1092:PHE:O    | 2:I:1149:VAL:N    | 2.48                     | 0.43              |
| 2:I:1777:PHE:HA   | 2:I:1799:SER:HB2  | 2.01                     | 0.43              |
| 2:I:2021:CYS:HA   | 2:I:2022:PRO:HD3  | 1.91                     | 0.43              |
| 2:I:2327:GLY:HA2  | 2:I:2330:ARG:HD3  | 2.00                     | 0.43              |
| 2:E:2132:GLY:O    | 2:E:2136:ARG:N    | 2.50                     | 0.42              |
| 2:E:4956:THR:O    | 2:E:4965:SER:N    | 2.42                     | 0.42              |
| 2:E:5026:ASP:OD1  | 2:E:5027:CYS:N    | 2.52                     | 0.42              |
| 2:G:176:SER:HB2   | 2:G:178:ARG:HH21  | 1.84                     | 0.42              |
| 2:I:533:ASN:ND2   | 2:I:536:ASN:OD1   | 2.45                     | 0.42              |
| 2:I:663:TYR:HB2   | 2:I:808:TYR:HB3   | 2.00                     | 0.42              |
| 2:I:2185:ILE:HA   | 2:I:2188:ASN:ND2  | 2.34                     | 0.42              |
| 2:I:3842:LEU:O    | 2:I:3929:SER:OG   | 2.37                     | 0.42              |
| 2:I:3850:GLN:HA   | 2:I:3853:ALA:HB3  | 2.01                     | 0.42              |
| 2:I:4791:TYR:OH   | 2:I:4815:ASP:HB2  | 2.19                     | 0.42              |
| 2:B:379:HIS:CD2   | 2:B:381:GLU:H     | 2.37                     | 0.42              |
| 2:B:684:VAL:HA    | 2:B:781:VAL:HA    | 2.01                     | 0.42              |
| 2:B:978:THR:HB    | 2:B:980:ALA:H     | 1.83                     | 0.42              |
| 2:B:4208:PRO:HA   | 2:B:4211:LYS:HB3  | 2.02                     | 0.42              |
| 2:E:17:ASP:HB2    | 2:E:98:HIS:CE1    | 2.53                     | 0.42              |
| 2:E:401:ALA:HA    | 2:E:404:ILE:HD12  | 2.01                     | 0.42              |
| 2:G:809:ALA:O     | 2:G:811:CYS:N     | 2.50                     | 0.42              |
| 2:G:932:LEU:HD23  | 2:G:935:LEU:HD12  | 2.02                     | 0.42              |
| 2:G:1812:LEU:HD21 | 2:G:1861:GLN:HG2  | 2.01                     | 0.42              |
| 2:G:3663:LEU:H    | 2:G:3663:LEU:HG   | 1.64                     | 0.42              |
| 2:G:4208:PRO:HA   | 2:G:4211:LYS:HB3  | 2.01                     | 0.42              |
| 2:G:4673:ARG:HH22 | 2:G:4698:LYS:HB2  | 1.84                     | 0.42              |
| 2:I:176:SER:HB2   | 2:I:178:ARG:HH21  | 1.84                     | 0.42              |
| 2:I:2466:LEU:HA   | 2:I:2469:ILE:HD12 | 2.01                     | 0.42              |
| 2:I:4567:LEU:HD12 | 2:I:4816:ILE:HD12 | 2.01                     | 0.42              |
| 2:I:4998:LYS:NZ   | 2:I:5007:GLU:OE1  | 2.42                     | 0.42              |
| 2:B:1268:PRO:HB2  | 2:B:1591:CYS:HB2  | 2.01                     | 0.42              |
| 2:E:932:LEU:HD23  | 2:E:935:LEU:HD12  | 2.02                     | 0.42              |
| 2:E:1095:VAL:HA   | 2:E:1146:GLY:H    | 1.84                     | 0.42              |
| 2:E:1663:HIS:O    | 2:E:1667:LEU:N    | 2.50                     | 0.42              |
| 2:G:1777:PHE:HA   | 2:G:1799:SER:HB2  | 2.01                     | 0.42              |
| 2:G:3676:ASP:OD1  | 2:G:3676:ASP:N    | 2.51                     | 0.42              |
| 2:I:316:PHE:HB3   | 2:I:346:CYS:HB3   | 2.00                     | 0.42              |
| 2:I:684:VAL:HA    | 2:I:781:VAL:HA    | 2.01                     | 0.42              |
| 2:I:4934:GLY:O    | 2:I:4938:ASP:N    | 2.47                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:91:ILE:HD12   | 1:A:97:LEU:HD11   | 2.02                     | 0.42              |
| 2:B:252:VAL:HA    | 2:B:255:HIS:CG    | 2.54                     | 0.42              |
| 2:B:3842:LEU:O    | 2:B:3929:SER:OG   | 2.37                     | 0.42              |
| 2:B:4791:TYR:OH   | 2:B:4815:ASP:HB2  | 2.19                     | 0.42              |
| 2:E:252:VAL:HA    | 2:E:255:HIS:CG    | 2.54                     | 0.42              |
| 2:E:315:CYS:SG    | 2:E:316:PHE:N     | 2.93                     | 0.42              |
| 2:E:1149:VAL:HG22 | 2:E:1164:LEU:HD13 | 2.01                     | 0.42              |
| 2:E:2361:PRO:HA   | 2:E:2364:PHE:HD2  | 1.83                     | 0.42              |
| 2:E:4928:LEU:HA   | 2:E:4931:ILE:HD12 | 2.01                     | 0.42              |
| 2:G:79:GLN:HA     | 2:G:82:LEU:HB2    | 2.01                     | 0.42              |
| 2:G:379:HIS:CD2   | 2:G:381:GLU:H     | 2.37                     | 0.42              |
| 2:G:583:ILE:HA    | 2:G:586:ILE:HD12  | 2.01                     | 0.42              |
| 2:G:2265:LEU:HD22 | 2:G:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:G:2327:GLY:HA2  | 2:G:2330:ARG:HD3  | 2.00                     | 0.42              |
| 2:G:3850:GLN:HA   | 2:G:3853:ALA:HB3  | 2.01                     | 0.42              |
| 2:G:3927:GLN:NE2  | 2:G:3988:ALA:O    | 2.48                     | 0.42              |
| 2:I:426:ARG:HG2   | 2:I:431:PRO:HA    | 2.02                     | 0.42              |
| 2:I:3765:TYR:O    | 2:I:3769:ARG:N    | 2.48                     | 0.42              |
| 2:I:4208:PRO:HA   | 2:I:4211:LYS:HB3  | 2.01                     | 0.42              |
| 2:I:4945:ASP:HA   | 2:I:4948:GLU:HB2  | 2.02                     | 0.42              |
| 2:B:176:SER:HB2   | 2:B:178:ARG:HH21  | 1.84                     | 0.42              |
| 2:B:876:GLU:O     | 2:B:880:GLU:N     | 2.48                     | 0.42              |
| 2:B:1105:ALA:O    | 2:B:1189:LEU:N    | 2.52                     | 0.42              |
| 2:B:4945:ASP:HA   | 2:B:4948:GLU:HB2  | 2.02                     | 0.42              |
| 2:B:5026:ASP:OD1  | 2:B:5027:CYS:N    | 2.52                     | 0.42              |
| 2:E:469:ARG:HH21  | 2:E:3712:GLU:HB3  | 1.84                     | 0.42              |
| 2:E:4673:ARG:HH22 | 2:E:4698:LYS:HB2  | 1.84                     | 0.42              |
| 2:G:627:PRO:HB2   | 1:H:92:PRO:HD3    | 2.02                     | 0.42              |
| 2:G:684:VAL:HA    | 2:G:781:VAL:HA    | 2.01                     | 0.42              |
| 2:G:1268:PRO:HB2  | 2:G:1591:CYS:HB2  | 2.01                     | 0.42              |
| 2:G:2207:VAL:HG13 | 2:G:2232:CYS:HB2  | 2.00                     | 0.42              |
| 2:G:3842:LEU:O    | 2:G:3929:SER:OG   | 2.38                     | 0.42              |
| 2:G:4568:PHE:HA   | 2:G:4571:PHE:HD2  | 1.85                     | 0.42              |
| 2:I:79:GLN:HA     | 2:I:82:LEU:HB2    | 2.01                     | 0.42              |
| 2:I:469:ARG:HH21  | 2:I:3712:GLU:HB3  | 1.84                     | 0.42              |
| 2:I:3779:VAL:HG23 | 2:I:3780:LEU:HD12 | 2.01                     | 0.42              |
| 2:I:3998:HIS:CE1  | 2:I:4054:ASN:HD21 | 2.36                     | 0.42              |
| 2:B:1046:LEU:HB3  | 2:B:1051:TYR:HB2  | 2.01                     | 0.42              |
| 2:B:1703:LEU:HD21 | 2:B:1830:VAL:HG13 | 2.01                     | 0.42              |
| 2:B:1812:LEU:HD21 | 2:B:1861:GLN:HG2  | 2.01                     | 0.42              |
| 2:B:1866:ILE:HG13 | 2:B:1926:LEU:HB3  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:426:ARG:HG2   | 2:E:431:PRO:HA    | 2.02                     | 0.42              |
| 2:E:1111:PRO:HD3  | 2:E:1605:TRP:HE1  | 1.84                     | 0.42              |
| 2:E:2466:LEU:HA   | 2:E:2469:ILE:HD12 | 2.01                     | 0.42              |
| 2:E:4208:PRO:HA   | 2:E:4211:LYS:HB3  | 2.01                     | 0.42              |
| 2:E:4799:SER:OG   | 2:E:4812:HIS:NE2  | 2.40                     | 0.42              |
| 2:G:426:ARG:HG2   | 2:G:431:PRO:HA    | 2.02                     | 0.42              |
| 2:G:1111:PRO:HD3  | 2:G:1605:TRP:HE1  | 1.84                     | 0.42              |
| 2:G:2466:LEU:HA   | 2:G:2469:ILE:HD12 | 2.01                     | 0.42              |
| 2:G:4063:ASP:HB3  | 2:G:4170:ILE:HG13 | 2.02                     | 0.42              |
| 2:G:5026:ASP:OD1  | 2:G:5027:CYS:N    | 2.52                     | 0.42              |
| 2:I:288:GLY:HA3   | 2:I:405:HIS:CE1   | 2.55                     | 0.42              |
| 2:I:583:ILE:HA    | 2:I:586:ILE:HD12  | 2.01                     | 0.42              |
| 2:I:3915:ILE:O    | 2:I:3919:THR:N    | 2.51                     | 0.42              |
| 2:I:4673:ARG:HH22 | 2:I:4698:LYS:HB2  | 1.84                     | 0.42              |
| 2:B:426:ARG:HG2   | 2:B:431:PRO:HA    | 2.02                     | 0.42              |
| 2:B:533:ASN:HB3   | 2:B:536:ASN:HB2   | 2.01                     | 0.42              |
| 2:B:1092:PHE:O    | 2:B:1149:VAL:N    | 2.48                     | 0.42              |
| 2:B:2185:ILE:HA   | 2:B:2188:ASN:ND2  | 2.34                     | 0.42              |
| 2:B:2265:LEU:HD22 | 2:B:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:E:684:VAL:HA    | 2:E:781:VAL:HA    | 2.01                     | 0.42              |
| 2:E:3842:LEU:O    | 2:E:3929:SER:OG   | 2.37                     | 0.42              |
| 1:F:91:ILE:HD12   | 1:F:97:LEU:HD11   | 2.02                     | 0.42              |
| 2:G:488:LEU:HA    | 2:G:491:ILE:HB    | 2.02                     | 0.42              |
| 2:G:2185:ILE:HA   | 2:G:2188:ASN:ND2  | 2.34                     | 0.42              |
| 2:G:4567:LEU:HD12 | 2:G:4816:ILE:HD12 | 2.01                     | 0.42              |
| 2:G:4743:MET:HB3  | 2:G:4746:ALA:HB3  | 2.02                     | 0.42              |
| 2:I:533:ASN:HB3   | 2:I:536:ASN:HB2   | 2.01                     | 0.42              |
| 2:I:1105:ALA:O    | 2:I:1189:LEU:N    | 2.52                     | 0.42              |
| 2:I:1970:GLN:HB2  | 2:I:3642:TYR:HA   | 2.01                     | 0.42              |
| 2:B:317:ARG:N     | 2:B:347:PHE:O     | 2.52                     | 0.42              |
| 2:B:1149:VAL:HG22 | 2:B:1164:LEU:HD13 | 2.01                     | 0.42              |
| 2:E:379:HIS:CD2   | 2:E:381:GLU:H     | 2.37                     | 0.42              |
| 2:E:2265:LEU:HD22 | 2:E:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:E:3649:ALA:O    | 2:E:3653:PHE:N    | 2.46                     | 0.42              |
| 2:G:315:CYS:SG    | 2:G:316:PHE:N     | 2.93                     | 0.42              |
| 2:G:4928:LEU:HA   | 2:G:4931:ILE:HD12 | 2.01                     | 0.42              |
| 2:I:278:GLN:N     | 2:I:315:CYS:SG    | 2.90                     | 0.42              |
| 2:I:932:LEU:HD23  | 2:I:935:LEU:HD12  | 2.02                     | 0.42              |
| 2:I:1245:PHE:HE1  | 2:I:1600:LEU:HD23 | 1.83                     | 0.42              |
| 2:I:1951:LEU:HD13 | 2:I:2126:ARG:HH21 | 1.85                     | 0.42              |
| 2:B:932:LEU:HD23  | 2:B:935:LEU:HD12  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1245:PHE:HE1  | 2:B:1600:LEU:HD23 | 1.83                     | 0.42              |
| 2:B:4567:LEU:HD12 | 2:B:4816:ILE:HD12 | 2.01                     | 0.42              |
| 2:E:709:ASP:HA    | 2:E:725:HIS:H     | 1.83                     | 0.42              |
| 2:E:1777:PHE:HA   | 2:E:1799:SER:HB2  | 2.01                     | 0.42              |
| 2:E:1970:GLN:HB2  | 2:E:3642:TYR:HA   | 2.01                     | 0.42              |
| 2:E:4743:MET:HB3  | 2:E:4746:ALA:HB3  | 2.02                     | 0.42              |
| 2:G:401:ALA:HA    | 2:G:404:ILE:HD12  | 2.01                     | 0.42              |
| 2:G:469:ARG:HH21  | 2:G:3712:GLU:HB3  | 1.84                     | 0.42              |
| 2:G:4942:GLU:O    | 2:G:4946:GLN:N    | 2.44                     | 0.42              |
| 2:I:151:HIS:HB2   | 2:I:170:ILE:HB    | 2.01                     | 0.42              |
| 2:I:634:GLN:HB3   | 1:J:34:LYS:NZ     | 2.35                     | 0.42              |
| 2:I:809:ALA:O     | 2:I:811:CYS:N     | 2.50                     | 0.42              |
| 2:I:2265:LEU:HD22 | 2:I:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:I:4182:GLU:HA   | 2:I:4192:ARG:HA   | 2.02                     | 0.42              |
| 2:I:4568:PHE:HA   | 2:I:4571:PHE:HD2  | 1.85                     | 0.42              |
| 2:I:4743:MET:HB3  | 2:I:4746:ALA:HB3  | 2.02                     | 0.42              |
| 2:B:313:SER:HB2   | 2:B:350:HIS:CE1   | 2.55                     | 0.42              |
| 2:B:315:CYS:SG    | 2:B:316:PHE:N     | 2.93                     | 0.42              |
| 2:B:401:ALA:HA    | 2:B:404:ILE:HD12  | 2.01                     | 0.42              |
| 2:E:176:SER:HB2   | 2:E:178:ARG:HH21  | 1.84                     | 0.42              |
| 2:E:288:GLY:HA3   | 2:E:405:HIS:CE1   | 2.55                     | 0.42              |
| 2:E:2185:ILE:HA   | 2:E:2188:ASN:ND2  | 2.34                     | 0.42              |
| 2:G:151:HIS:HB2   | 2:G:170:ILE:HB    | 2.01                     | 0.42              |
| 2:G:288:GLY:HA3   | 2:G:405:HIS:CE1   | 2.55                     | 0.42              |
| 2:G:2829:GLY:HA3  | 2:G:2933:ASN:H    | 1.85                     | 0.42              |
| 2:G:2880:GLU:O    | 2:G:2884:ASN:N    | 2.45                     | 0.42              |
| 2:I:17:ASP:HB2    | 2:I:98:HIS:CE1    | 2.53                     | 0.42              |
| 2:I:1812:LEU:HD21 | 2:I:1861:GLN:HG2  | 2.01                     | 0.42              |
| 2:I:3927:GLN:O    | 2:I:3931:SER:N    | 2.45                     | 0.42              |
| 2:B:204:PRO:HG2   | 2:B:268:SER:HB3   | 2.02                     | 0.41              |
| 2:B:947:GLU:HG3   | 2:B:1049:TYR:HD1  | 1.85                     | 0.41              |
| 2:B:4743:MET:HB3  | 2:B:4746:ALA:HB3  | 2.02                     | 0.41              |
| 2:E:317:ARG:N     | 2:E:347:PHE:O     | 2.52                     | 0.41              |
| 2:E:1268:PRO:HB2  | 2:E:1591:CYS:HB2  | 2.01                     | 0.41              |
| 2:E:1693:GLN:HA   | 2:E:1696:HIS:HB3  | 2.02                     | 0.41              |
| 2:E:4567:LEU:HD12 | 2:E:4816:ILE:HD12 | 2.00                     | 0.41              |
| 2:E:4945:ASP:HA   | 2:E:4948:GLU:HB2  | 2.02                     | 0.41              |
| 2:G:3779:VAL:HG23 | 2:G:3780:LEU:HD12 | 2.02                     | 0.41              |
| 2:G:3932:ASP:HA   | 2:G:3935:TRP:HD1  | 1.85                     | 0.41              |
| 2:I:252:VAL:HA    | 2:I:255:HIS:CG    | 2.54                     | 0.41              |
| 2:I:313:SER:HB2   | 2:I:350:HIS:CE1   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:947:GLU:HG3   | 2:I:1049:TYR:HD1  | 1.85                     | 0.41              |
| 2:E:1866:ILE:HG13 | 2:E:1926:LEU:HB3  | 2.01                     | 0.41              |
| 2:E:2869:ARG:HH12 | 2:E:2945:UNK:C    | 2.33                     | 0.41              |
| 2:E:4942:GLU:O    | 2:E:4946:GLN:N    | 2.43                     | 0.41              |
| 2:G:1046:LEU:HB3  | 2:G:1051:TYR:HB2  | 2.01                     | 0.41              |
| 2:G:1693:GLN:HA   | 2:G:1696:HIS:HB3  | 2.02                     | 0.41              |
| 2:G:4791:TYR:OH   | 2:G:4815:ASP:HB2  | 2.19                     | 0.41              |
| 2:G:4945:ASP:HA   | 2:G:4948:GLU:HB2  | 2.02                     | 0.41              |
| 2:I:204:PRO:HG2   | 2:I:268:SER:HB3   | 2.02                     | 0.41              |
| 2:I:1866:ILE:HG13 | 2:I:1926:LEU:HB3  | 2.01                     | 0.41              |
| 2:I:2002:PRO:HA   | 2:I:2005:GLN:HB3  | 2.03                     | 0.41              |
| 2:B:288:GLY:HA3   | 2:B:405:HIS:CE1   | 2.55                     | 0.41              |
| 2:B:4182:GLU:HA   | 2:B:4192:ARG:HA   | 2.02                     | 0.41              |
| 2:B:4673:ARG:HH22 | 2:B:4698:LYS:HB2  | 1.84                     | 0.41              |
| 2:E:1046:LEU:HB3  | 2:E:1051:TYR:HB2  | 2.01                     | 0.41              |
| 2:E:1105:ALA:O    | 2:E:1189:LEU:N    | 2.52                     | 0.41              |
| 2:E:3779:VAL:HG23 | 2:E:3780:LEU:HD12 | 2.02                     | 0.41              |
| 2:E:4568:PHE:HA   | 2:E:4571:PHE:HD2  | 1.85                     | 0.41              |
| 2:E:4989:MET:O    | 2:E:4993:MET:N    | 2.42                     | 0.41              |
| 2:G:317:ARG:N     | 2:G:347:PHE:O     | 2.52                     | 0.41              |
| 2:G:1703:LEU:HD21 | 2:G:1830:VAL:HG13 | 2.01                     | 0.41              |
| 2:G:2002:PRO:HA   | 2:G:2005:GLN:HB3  | 2.02                     | 0.41              |
| 2:G:2336:ARG:NH2  | 2:G:2428:ALA:O    | 2.49                     | 0.41              |
| 2:G:4176:PRO:O    | 2:G:4202:ARG:NH1  | 2.54                     | 0.41              |
| 2:G:4826:ILE:O    | 2:G:4829:SER:OG   | 2.33                     | 0.41              |
| 2:I:1708:ARG:HG2  | 2:I:1711:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:55:VAL:HG23   | 1:A:60:GLU:HB2    | 2.03                     | 0.41              |
| 2:B:668:VAL:HG22  | 2:B:789:VAL:HG23  | 2.03                     | 0.41              |
| 2:B:790:ARG:HG2   | 2:B:1627:ALA:HA   | 2.01                     | 0.41              |
| 2:B:3662:ILE:H    | 2:B:3662:ILE:HG13 | 1.71                     | 0.41              |
| 2:E:204:PRO:HG2   | 2:E:268:SER:HB3   | 2.02                     | 0.41              |
| 2:E:2829:GLY:HA3  | 2:E:2933:ASN:H    | 1.85                     | 0.41              |
| 2:E:3663:LEU:H    | 2:E:3663:LEU:HG   | 1.64                     | 0.41              |
| 2:E:5013:MET:HA   | 2:E:5016:GLU:HB3  | 2.02                     | 0.41              |
| 2:G:1951:LEU:HD13 | 2:G:2126:ARG:HH21 | 1.85                     | 0.41              |
| 2:I:1149:VAL:HG22 | 2:I:1164:LEU:HD13 | 2.01                     | 0.41              |
| 2:I:1679:ASN:O    | 2:I:1683:HIS:ND1  | 2.38                     | 0.41              |
| 2:I:2874:MET:HA   | 2:I:2877:GLN:HB3  | 2.03                     | 0.41              |
| 2:B:1951:LEU:HD13 | 2:B:2126:ARG:HH21 | 1.85                     | 0.41              |
| 2:B:4568:PHE:HA   | 2:B:4571:PHE:HD2  | 1.85                     | 0.41              |
| 2:B:4928:LEU:HA   | 2:B:4931:ILE:HD12 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:790:ARG:HG2   | 2:E:1627:ALA:HA   | 2.01                     | 0.41              |
| 2:E:1703:LEU:HD21 | 2:E:1830:VAL:HG13 | 2.01                     | 0.41              |
| 2:E:3676:ASP:OD1  | 2:E:3676:ASP:N    | 2.51                     | 0.41              |
| 2:E:3850:GLN:HA   | 2:E:3853:ALA:HB3  | 2.01                     | 0.41              |
| 2:E:4791:TYR:OH   | 2:E:4815:ASP:HB2  | 2.19                     | 0.41              |
| 2:G:17:ASP:HB2    | 2:G:98:HIS:CE1    | 2.53                     | 0.41              |
| 2:G:204:PRO:HG2   | 2:G:268:SER:HB3   | 2.02                     | 0.41              |
| 2:G:290:TYR:O     | 2:G:302:VAL:N     | 2.53                     | 0.41              |
| 2:G:790:ARG:HG2   | 2:G:1627:ALA:HA   | 2.01                     | 0.41              |
| 2:G:2022:PRO:HB2  | 2:G:2024:PRO:HD2  | 2.02                     | 0.41              |
| 2:G:4182:GLU:HA   | 2:G:4192:ARG:HA   | 2.02                     | 0.41              |
| 2:I:315:CYS:SG    | 2:I:316:PHE:N     | 2.93                     | 0.41              |
| 2:I:488:LEU:HA    | 2:I:491:ILE:HB    | 2.02                     | 0.41              |
| 2:I:668:VAL:HG22  | 2:I:789:VAL:HG23  | 2.03                     | 0.41              |
| 2:I:1703:LEU:HD21 | 2:I:1830:VAL:HG13 | 2.01                     | 0.41              |
| 2:I:4928:LEU:HA   | 2:I:4931:ILE:HD12 | 2.01                     | 0.41              |
| 1:J:91:ILE:HD12   | 1:J:97:LEU:HD11   | 2.02                     | 0.41              |
| 2:B:404:ILE:HG21  | 2:B:481:GLU:HG3   | 2.03                     | 0.41              |
| 2:B:792:LEU:HD22  | 2:B:799:GLU:H     | 1.85                     | 0.41              |
| 2:B:809:ALA:O     | 2:B:811:CYS:N     | 2.50                     | 0.41              |
| 2:B:829:TYR:HB3   | 2:B:1073:ARG:HH11 | 1.84                     | 0.41              |
| 2:B:1777:PHE:HA   | 2:B:1799:SER:HB2  | 2.01                     | 0.41              |
| 2:B:2002:PRO:HA   | 2:B:2005:GLN:HB3  | 2.02                     | 0.41              |
| 2:B:3850:GLN:HA   | 2:B:3853:ALA:HB3  | 2.01                     | 0.41              |
| 2:E:3927:GLN:NE2  | 2:E:3988:ALA:O    | 2.47                     | 0.41              |
| 2:E:4182:GLU:HA   | 2:E:4192:ARG:HA   | 2.02                     | 0.41              |
| 2:G:530:ILE:HA    | 2:G:536:ASN:HB3   | 2.02                     | 0.41              |
| 2:G:1970:GLN:HB2  | 2:G:3642:TYR:HA   | 2.01                     | 0.41              |
| 2:I:942:ALA:HB2   | 2:I:1052:ASN:HB2  | 2.03                     | 0.41              |
| 1:J:55:VAL:HG23   | 1:J:60:GLU:HB2    | 2.03                     | 0.41              |
| 1:A:92:PRO:HD3    | 2:B:627:PRO:HB2   | 2.02                     | 0.41              |
| 2:B:42:PHE:HD1    | 2:B:447:ASP:HB3   | 1.86                     | 0.41              |
| 2:B:2874:MET:HA   | 2:B:2877:GLN:HB3  | 2.03                     | 0.41              |
| 2:E:947:GLU:HG3   | 2:E:1049:TYR:HD1  | 1.85                     | 0.41              |
| 2:E:3932:ASP:HA   | 2:E:3935:TRP:HD1  | 1.85                     | 0.41              |
| 1:F:55:VAL:HG23   | 1:F:60:GLU:HB2    | 2.03                     | 0.41              |
| 2:G:313:SER:HB2   | 2:G:350:HIS:CE1   | 2.55                     | 0.41              |
| 2:I:2022:PRO:HB2  | 2:I:2024:PRO:HD2  | 2.02                     | 0.41              |
| 2:I:3663:LEU:H    | 2:I:3663:LEU:HG   | 1.64                     | 0.41              |
| 2:I:4745:LEU:O    | 2:I:4749:GLU:N    | 2.50                     | 0.41              |
| 2:I:5026:ASP:OD1  | 2:I:5027:CYS:N    | 2.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:218:HIS:HB3   | 2:B:392:ARG:HD3   | 2.03                     | 0.41              |
| 2:B:942:ALA:HB2   | 2:B:1052:ASN:HB2  | 2.03                     | 0.41              |
| 2:B:2032:GLN:O    | 2:B:2036:GLN:N    | 2.49                     | 0.41              |
| 2:B:4176:PRO:O    | 2:B:4202:ARG:NH1  | 2.54                     | 0.41              |
| 2:B:5013:MET:HA   | 2:B:5016:GLU:HB3  | 2.02                     | 0.41              |
| 2:E:313:SER:HB2   | 2:E:350:HIS:CE1   | 2.55                     | 0.41              |
| 2:E:533:ASN:ND2   | 2:E:536:ASN:OD1   | 2.45                     | 0.41              |
| 2:E:731:THR:OG1   | 2:E:1520:UNK:O    | 2.39                     | 0.41              |
| 2:E:1708:ARG:HG2  | 2:E:1711:TYR:CE2  | 2.56                     | 0.41              |
| 2:E:2022:PRO:HB2  | 2:E:2024:PRO:HD2  | 2.02                     | 0.41              |
| 2:E:3758:MET:O    | 2:E:3762:ARG:NE   | 2.46                     | 0.41              |
| 2:E:4710:SER:OG   | 2:E:4772:ASP:OD2  | 2.31                     | 0.41              |
| 2:G:4843:LEU:HA   | 2:G:4846:VAL:HG12 | 2.03                     | 0.41              |
| 1:H:91:ILE:HD12   | 1:H:97:LEU:HD11   | 2.02                     | 0.41              |
| 2:I:218:HIS:HB3   | 2:I:392:ARG:HD3   | 2.03                     | 0.41              |
| 2:I:988:LEU:O     | 2:I:992:GLY:N     | 2.47                     | 0.41              |
| 2:B:290:TYR:O     | 2:B:302:VAL:N     | 2.53                     | 0.41              |
| 2:B:530:ILE:HA    | 2:B:536:ASN:HB3   | 2.02                     | 0.41              |
| 2:B:688:LEU:HB3   | 2:B:777:PHE:CE1   | 2.56                     | 0.41              |
| 2:B:1189:LEU:HD12 | 2:B:1190:PRO:HD2  | 2.03                     | 0.41              |
| 2:B:1694:LEU:HD23 | 2:B:1715:LEU:HD13 | 2.03                     | 0.41              |
| 2:B:1708:ARG:HG2  | 2:B:1711:TYR:CE2  | 2.56                     | 0.41              |
| 2:B:1721:GLU:O    | 2:B:1725:ARG:NH2  | 2.54                     | 0.41              |
| 2:B:2437:ALA:HA   | 2:B:2438:PRO:HD3  | 1.94                     | 0.41              |
| 2:B:3779:VAL:HG23 | 2:B:3780:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:3932:ASP:HA   | 2:B:3935:TRP:HD1  | 1.85                     | 0.41              |
| 2:E:42:PHE:HD1    | 2:E:447:ASP:HB3   | 1.86                     | 0.41              |
| 2:E:290:TYR:O     | 2:E:302:VAL:N     | 2.53                     | 0.41              |
| 2:E:379:HIS:NE2   | 2:E:381:GLU:OE1   | 2.54                     | 0.41              |
| 2:E:392:ARG:HH12  | 2:E:398:SER:HB2   | 1.86                     | 0.41              |
| 2:E:488:LEU:HA    | 2:E:491:ILE:HB    | 2.02                     | 0.41              |
| 2:E:533:ASN:HB3   | 2:E:536:ASN:HB2   | 2.01                     | 0.41              |
| 2:E:1679:ASN:O    | 2:E:1683:HIS:ND1  | 2.38                     | 0.41              |
| 2:E:2002:PRO:HA   | 2:E:2005:GLN:HB3  | 2.03                     | 0.41              |
| 2:E:2255:SER:HA   | 2:E:2258:LEU:HB3  | 2.03                     | 0.41              |
| 2:E:2874:MET:HA   | 2:E:2877:GLN:HB3  | 2.03                     | 0.41              |
| 2:E:4176:PRO:O    | 2:E:4202:ARG:NH1  | 2.54                     | 0.41              |
| 2:E:4833:ASN:HD22 | 2:E:4936:ILE:HD13 | 1.86                     | 0.41              |
| 2:G:218:HIS:HB3   | 2:G:392:ARG:HD3   | 2.03                     | 0.41              |
| 2:G:379:HIS:NE2   | 2:G:381:GLU:OE1   | 2.54                     | 0.41              |
| 2:G:533:ASN:ND2   | 2:G:536:ASN:OD1   | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:668:VAL:HG22  | 2:G:789:VAL:HG23  | 2.03                     | 0.41              |
| 2:G:876:GLU:O     | 2:G:880:GLU:N     | 2.48                     | 0.41              |
| 2:G:1708:ARG:HG2  | 2:G:1711:TYR:CE2  | 2.56                     | 0.41              |
| 2:G:1721:GLU:O    | 2:G:1725:ARG:NH2  | 2.54                     | 0.41              |
| 2:G:3920:VAL:O    | 2:G:3924:LEU:N    | 2.44                     | 0.41              |
| 2:G:3994:HIS:O    | 2:G:3998:HIS:ND1  | 2.39                     | 0.41              |
| 2:G:5013:MET:HA   | 2:G:5016:GLU:HB3  | 2.02                     | 0.41              |
| 1:H:55:VAL:HG23   | 1:H:60:GLU:HB2    | 2.03                     | 0.41              |
| 2:I:379:HIS:NE2   | 2:I:381:GLU:OE1   | 2.54                     | 0.41              |
| 2:I:404:ILE:HG21  | 2:I:481:GLU:HG3   | 2.03                     | 0.41              |
| 2:I:1739:THR:H    | 2:I:1742:THR:HB   | 1.86                     | 0.41              |
| 2:I:3901:ASN:OD1  | 2:I:3904:ARG:NH1  | 2.43                     | 0.41              |
| 2:I:3932:ASP:HA   | 2:I:3935:TRP:HD1  | 1.85                     | 0.41              |
| 2:I:4558:ASN:OD1  | 2:I:4558:ASN:N    | 2.52                     | 0.41              |
| 2:B:758:ARG:NH2   | 2:B:803:LEU:O     | 2.54                     | 0.41              |
| 2:B:2318:TYR:HA   | 2:B:2319:PRO:HD3  | 1.89                     | 0.41              |
| 2:B:4126:GLU:O    | 2:B:4130:ASN:ND2  | 2.54                     | 0.41              |
| 2:E:792:LEU:HD22  | 2:E:799:GLU:H     | 1.85                     | 0.41              |
| 2:E:3901:ASN:OD1  | 2:E:3904:ARG:NH1  | 2.43                     | 0.41              |
| 2:E:4126:GLU:O    | 2:E:4130:ASN:ND2  | 2.54                     | 0.41              |
| 2:G:792:LEU:HD22  | 2:G:799:GLU:H     | 1.85                     | 0.41              |
| 2:G:4126:GLU:O    | 2:G:4130:ASN:ND2  | 2.54                     | 0.41              |
| 2:G:4833:ASN:HD21 | 2:G:4939:ALA:HB2  | 1.86                     | 0.41              |
| 2:G:4934:GLY:O    | 2:G:4938:ASP:N    | 2.48                     | 0.41              |
| 2:I:42:PHE:HD1    | 2:I:447:ASP:HB3   | 1.86                     | 0.41              |
| 2:I:758:ARG:NH2   | 2:I:803:LEU:O     | 2.54                     | 0.41              |
| 2:I:2336:ARG:NH2  | 2:I:2428:ALA:O    | 2.49                     | 0.41              |
| 2:I:2829:GLY:HA3  | 2:I:2933:ASN:H    | 1.85                     | 0.41              |
| 2:I:4126:GLU:O    | 2:I:4130:ASN:ND2  | 2.54                     | 0.41              |
| 2:I:4971:THR:HG21 | 2:I:5029:ARG:HH12 | 1.86                     | 0.41              |
| 2:I:5013:MET:HA   | 2:I:5016:GLU:HB3  | 2.02                     | 0.41              |
| 2:B:2430:ILE:HG21 | 2:B:2502:UNK:HA   | 2.03                     | 0.40              |
| 2:B:4989:MET:O    | 2:B:4993:MET:N    | 2.42                     | 0.40              |
| 2:E:241:GLN:O     | 2:E:289:ARG:NH1   | 2.49                     | 0.40              |
| 2:E:758:ARG:NH2   | 2:E:803:LEU:O     | 2.54                     | 0.40              |
| 2:E:1721:GLU:O    | 2:E:1725:ARG:NH2  | 2.54                     | 0.40              |
| 2:E:1950:GLU:OE2  | 2:E:1954:ARG:NH2  | 2.54                     | 0.40              |
| 2:E:1951:LEU:HD13 | 2:E:2126:ARG:HH21 | 1.85                     | 0.40              |
| 2:G:42:PHE:HD1    | 2:G:447:ASP:HB3   | 1.86                     | 0.40              |
| 2:G:1497:UNK:HA   | 2:G:1535:UNK:HA   | 2.03                     | 0.40              |
| 2:I:290:TYR:O     | 2:I:302:VAL:N     | 2.53                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:545:ASP:HA    | 2:I:582:HIS:CE1   | 2.56                     | 0.40              |
| 2:I:688:LEU:HB3   | 2:I:777:PHE:CE1   | 2.56                     | 0.40              |
| 2:I:2039:LEU:HA   | 2:I:2042:CYS:HB3  | 2.03                     | 0.40              |
| 2:I:4097:MET:HB3  | 2:I:4108:ILE:HG12 | 2.03                     | 0.40              |
| 2:B:392:ARG:HH12  | 2:B:398:SER:HB2   | 1.86                     | 0.40              |
| 2:E:218:HIS:HB3   | 2:E:392:ARG:HD3   | 2.03                     | 0.40              |
| 2:E:688:LEU:HB3   | 2:E:777:PHE:CE1   | 2.56                     | 0.40              |
| 2:E:2758:PHE:O    | 2:E:2762:THR:N    | 2.47                     | 0.40              |
| 2:E:4833:ASN:HD21 | 2:E:4939:ALA:HB2  | 1.87                     | 0.40              |
| 2:G:545:ASP:HA    | 2:G:582:HIS:CE1   | 2.56                     | 0.40              |
| 2:G:758:ARG:NH2   | 2:G:803:LEU:O     | 2.54                     | 0.40              |
| 2:G:1071:ARG:HD3  | 2:G:1241:SER:HB3  | 2.03                     | 0.40              |
| 2:I:317:ARG:N     | 2:I:347:PHE:O     | 2.52                     | 0.40              |
| 2:I:385:ASP:OD1   | 2:I:385:ASP:N     | 2.54                     | 0.40              |
| 2:I:1694:LEU:HD23 | 2:I:1715:LEU:HD13 | 2.03                     | 0.40              |
| 2:I:1950:GLU:OE2  | 2:I:1954:ARG:NH2  | 2.54                     | 0.40              |
| 2:I:2199:ARG:NH2  | 2:I:2246:ASN:OD1  | 2.55                     | 0.40              |
| 2:B:78:LEU:O      | 2:B:82:LEU:N      | 2.49                     | 0.40              |
| 2:B:1663:HIS:O    | 2:B:1667:LEU:N    | 2.50                     | 0.40              |
| 2:B:1691:GLN:HE22 | 2:B:1802:ILE:HG12 | 1.86                     | 0.40              |
| 2:B:2587:UNK:O    | 2:B:2591:UNK:N    | 2.55                     | 0.40              |
| 2:E:404:ILE:HG21  | 2:E:481:GLU:HG3   | 2.03                     | 0.40              |
| 2:E:2336:ARG:NH2  | 2:E:2428:ALA:O    | 2.49                     | 0.40              |
| 2:E:4971:THR:HG21 | 2:E:5029:ARG:HH12 | 1.86                     | 0.40              |
| 2:G:688:LEU:HB3   | 2:G:777:PHE:CE1   | 2.56                     | 0.40              |
| 2:G:947:GLU:HG3   | 2:G:1049:TYR:HD1  | 1.85                     | 0.40              |
| 2:G:3765:TYR:O    | 2:G:3769:ARG:N    | 2.48                     | 0.40              |
| 2:G:4833:ASN:HD22 | 2:G:4936:ILE:HD13 | 1.86                     | 0.40              |
| 2:I:790:ARG:HG2   | 2:I:1627:ALA:HA   | 2.02                     | 0.40              |
| 2:I:2144:ILE:H    | 2:I:2144:ILE:HG13 | 1.76                     | 0.40              |
| 2:I:4176:PRO:O    | 2:I:4202:ARG:NH1  | 2.54                     | 0.40              |
| 2:I:4833:ASN:HD21 | 2:I:4939:ALA:HB2  | 1.86                     | 0.40              |
| 2:B:379:HIS:NE2   | 2:B:381:GLU:OE1   | 2.54                     | 0.40              |
| 2:B:1693:GLN:HA   | 2:B:1696:HIS:HB3  | 2.02                     | 0.40              |
| 2:B:3229:UNK:HA   | 2:B:3302:UNK:HA   | 2.03                     | 0.40              |
| 2:B:4192:ARG:HH12 | 2:B:4982:GLU:HG2  | 1.87                     | 0.40              |
| 2:E:530:ILE:HA    | 2:E:536:ASN:HB3   | 2.02                     | 0.40              |
| 2:E:668:VAL:HG22  | 2:E:789:VAL:HG23  | 2.03                     | 0.40              |
| 2:E:2039:LEU:HA   | 2:E:2042:CYS:HB3  | 2.04                     | 0.40              |
| 2:E:2212:VAL:O    | 2:E:2216:GLY:N    | 2.53                     | 0.40              |
| 2:G:404:ILE:HG21  | 2:G:481:GLU:HG3   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:2255:SER:HA   | 2:G:2258:LEU:HB3  | 2.03                     | 0.40              |
| 2:G:2874:MET:HA   | 2:G:2877:GLN:HB3  | 2.03                     | 0.40              |
| 2:G:3361:UNK:O    | 2:G:3365:UNK:N    | 2.55                     | 0.40              |
| 2:G:3915:ILE:O    | 2:G:3919:THR:N    | 2.51                     | 0.40              |
| 2:G:4192:ARG:HH12 | 2:G:4982:GLU:HG2  | 1.87                     | 0.40              |
| 2:I:530:ILE:HA    | 2:I:536:ASN:HB3   | 2.02                     | 0.40              |
| 2:I:792:LEU:HD22  | 2:I:799:GLU:H     | 1.85                     | 0.40              |
| 2:I:1693:GLN:HA   | 2:I:1696:HIS:HB3  | 2.02                     | 0.40              |
| 2:I:4833:ASN:HD22 | 2:I:4936:ILE:HD13 | 1.86                     | 0.40              |
| 2:B:1829:PRO:HB2  | 2:B:1837:GLN:HB2  | 2.04                     | 0.40              |
| 2:B:1970:GLN:HB2  | 2:B:3642:TYR:HA   | 2.01                     | 0.40              |
| 2:B:3649:ALA:O    | 2:B:3653:PHE:N    | 2.46                     | 0.40              |
| 2:E:176:SER:HB2   | 2:E:178:ARG:HD3   | 2.04                     | 0.40              |
| 2:E:635:THR:O     | 1:F:34:LYS:NZ     | 2.51                     | 0.40              |
| 2:E:870:ILE:HD12  | 2:E:870:ILE:HA    | 1.89                     | 0.40              |
| 2:E:1189:LEU:HD12 | 2:E:1190:PRO:HD2  | 2.04                     | 0.40              |
| 2:E:4978:HIS:ND1  | 2:E:4982:GLU:OE1  | 2.43                     | 0.40              |
| 2:G:4971:THR:HG21 | 2:G:5029:ARG:HH12 | 1.86                     | 0.40              |
| 2:I:392:ARG:HH12  | 2:I:398:SER:HB2   | 1.86                     | 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     | 105/108 (97%)   | 96 (91%)   | 9 (9%)    | 0        | 100         | 100 |
| 1   | F     | 105/108 (97%)   | 96 (91%)   | 9 (9%)    | 0        | 100         | 100 |
| 1   | H     | 105/108 (97%)   | 96 (91%)   | 9 (9%)    | 0        | 100         | 100 |
| 1   | J     | 105/108 (97%)   | 96 (91%)   | 9 (9%)    | 0        | 100         | 100 |
| 2   | B     | 3235/4687 (69%) | 2862 (88%) | 367 (11%) | 6 (0%)   | 43          | 77  |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 2   | E     | 3235/4687 (69%)   | 2861 (88%)  | 367 (11%)  | 7 (0%)   | 43          | 77 |
| 2   | G     | 3235/4687 (69%)   | 2863 (88%)  | 365 (11%)  | 7 (0%)   | 43          | 77 |
| 2   | I     | 3235/4687 (69%)   | 2863 (88%)  | 365 (11%)  | 7 (0%)   | 43          | 77 |
| All | All   | 13360/19180 (70%) | 11833 (89%) | 1500 (11%) | 27 (0%)  | 44          | 77 |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1829 | PRO  |
| 2   | B     | 1932 | PRO  |
| 2   | E     | 1829 | PRO  |
| 2   | G     | 1829 | PRO  |
| 2   | I     | 1829 | PRO  |
| 2   | B     | 1708 | ARG  |
| 2   | B     | 4667 | PRO  |
| 2   | E     | 1708 | ARG  |
| 2   | E     | 1932 | PRO  |
| 2   | E     | 4667 | PRO  |
| 2   | G     | 1708 | ARG  |
| 2   | G     | 1932 | PRO  |
| 2   | G     | 4667 | PRO  |
| 2   | I     | 1708 | ARG  |
| 2   | I     | 1932 | PRO  |
| 2   | I     | 4667 | PRO  |
| 2   | B     | 2343 | GLY  |
| 2   | E     | 2343 | GLY  |
| 2   | I     | 2343 | GLY  |
| 2   | G     | 2343 | GLY  |
| 2   | B     | 4641 | PRO  |
| 2   | E     | 1840 | PRO  |
| 2   | E     | 4641 | PRO  |
| 2   | G     | 1840 | PRO  |
| 2   | G     | 4641 | PRO  |
| 2   | I     | 1840 | PRO  |
| 2   | I     | 4641 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 1   | A     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 1   | F     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 1   | H     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 1   | J     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 2   | B     | 2493/3209 (78%)   | 2485 (100%)  | 8 (0%)   | 86          | 84  |
| 2   | E     | 2493/3209 (78%)   | 2484 (100%)  | 9 (0%)   | 84          | 82  |
| 2   | G     | 2493/3209 (78%)   | 2483 (100%)  | 10 (0%)  | 84          | 82  |
| 2   | I     | 2493/3209 (78%)   | 2483 (100%)  | 10 (0%)  | 84          | 82  |
| All | All   | 10324/13192 (78%) | 10287 (100%) | 37 (0%)  | 81          | 82  |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 131  | LEU  |
| 2   | B     | 688  | LEU  |
| 2   | B     | 978  | THR  |
| 2   | B     | 3663 | LEU  |
| 2   | B     | 3805 | LEU  |
| 2   | B     | 4036 | VAL  |
| 2   | B     | 4154 | VAL  |
| 2   | B     | 4871 | GLU  |
| 2   | E     | 131  | LEU  |
| 2   | E     | 688  | LEU  |
| 2   | E     | 978  | THR  |
| 2   | E     | 2144 | ILE  |
| 2   | E     | 3663 | LEU  |
| 2   | E     | 3805 | LEU  |
| 2   | E     | 4036 | VAL  |
| 2   | E     | 4154 | VAL  |
| 2   | E     | 4871 | GLU  |
| 2   | G     | 131  | LEU  |
| 2   | G     | 688  | LEU  |
| 2   | G     | 815  | VAL  |
| 2   | G     | 978  | THR  |
| 2   | G     | 2144 | ILE  |
| 2   | G     | 3663 | LEU  |
| 2   | G     | 3805 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 4036 | VAL  |
| 2   | G     | 4154 | VAL  |
| 2   | G     | 4871 | GLU  |
| 2   | I     | 131  | LEU  |
| 2   | I     | 688  | LEU  |
| 2   | I     | 815  | VAL  |
| 2   | I     | 978  | THR  |
| 2   | I     | 1123 | VAL  |
| 2   | I     | 3663 | LEU  |
| 2   | I     | 3805 | LEU  |
| 2   | I     | 4036 | VAL  |
| 2   | I     | 4154 | VAL  |
| 2   | I     | 4871 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (220) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 25   | HIS  |
| 1   | A     | 87   | HIS  |
| 2   | B     | 23   | GLN  |
| 2   | B     | 111  | HIS  |
| 2   | B     | 113  | HIS  |
| 2   | B     | 151  | HIS  |
| 2   | B     | 190  | GLN  |
| 2   | B     | 201  | ASN  |
| 2   | B     | 203  | ASN  |
| 2   | B     | 224  | HIS  |
| 2   | B     | 273  | HIS  |
| 2   | B     | 379  | HIS  |
| 2   | B     | 405  | HIS  |
| 2   | B     | 639  | ASN  |
| 2   | B     | 678  | GLN  |
| 2   | B     | 797  | HIS  |
| 2   | B     | 838  | HIS  |
| 2   | B     | 877  | ASN  |
| 2   | B     | 1035 | ASN  |
| 2   | B     | 1041 | GLN  |
| 2   | B     | 1679 | ASN  |
| 2   | B     | 1691 | GLN  |
| 2   | B     | 1696 | HIS  |
| 2   | B     | 1719 | HIS  |
| 2   | B     | 1775 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1837 | GLN  |
| 2   | B     | 1861 | GLN  |
| 2   | B     | 1949 | GLN  |
| 2   | B     | 1970 | GLN  |
| 2   | B     | 2005 | GLN  |
| 2   | B     | 2127 | GLN  |
| 2   | B     | 2188 | ASN  |
| 2   | B     | 2194 | HIS  |
| 2   | B     | 2763 | HIS  |
| 2   | B     | 3761 | GLN  |
| 2   | B     | 3766 | GLN  |
| 2   | B     | 3809 | ASN  |
| 2   | B     | 3814 | GLN  |
| 2   | B     | 3882 | GLN  |
| 2   | B     | 3895 | HIS  |
| 2   | B     | 3896 | ASN  |
| 2   | B     | 3960 | GLN  |
| 2   | B     | 4034 | ASN  |
| 2   | B     | 4054 | ASN  |
| 2   | B     | 4109 | GLN  |
| 2   | B     | 4120 | ASN  |
| 2   | B     | 4142 | ASN  |
| 2   | B     | 4246 | GLN  |
| 2   | B     | 4691 | GLN  |
| 2   | B     | 4833 | ASN  |
| 2   | B     | 4947 | GLN  |
| 2   | B     | 4984 | ASN  |
| 2   | B     | 4987 | ASN  |
| 2   | B     | 5031 | GLN  |
| 2   | E     | 23   | GLN  |
| 2   | E     | 111  | HIS  |
| 2   | E     | 113  | HIS  |
| 2   | E     | 151  | HIS  |
| 2   | E     | 190  | GLN  |
| 2   | E     | 201  | ASN  |
| 2   | E     | 203  | ASN  |
| 2   | E     | 224  | HIS  |
| 2   | E     | 273  | HIS  |
| 2   | E     | 308  | HIS  |
| 2   | E     | 379  | HIS  |
| 2   | E     | 405  | HIS  |
| 2   | E     | 639  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 678  | GLN  |
| 2   | E     | 797  | HIS  |
| 2   | E     | 838  | HIS  |
| 2   | E     | 877  | ASN  |
| 2   | E     | 1035 | ASN  |
| 2   | E     | 1041 | GLN  |
| 2   | E     | 1220 | GLN  |
| 2   | E     | 1598 | GLN  |
| 2   | E     | 1679 | ASN  |
| 2   | E     | 1691 | GLN  |
| 2   | E     | 1696 | HIS  |
| 2   | E     | 1719 | HIS  |
| 2   | E     | 1775 | HIS  |
| 2   | E     | 1837 | GLN  |
| 2   | E     | 1861 | GLN  |
| 2   | E     | 1949 | GLN  |
| 2   | E     | 1970 | GLN  |
| 2   | E     | 2005 | GLN  |
| 2   | E     | 2127 | GLN  |
| 2   | E     | 2188 | ASN  |
| 2   | E     | 2194 | HIS  |
| 2   | E     | 2763 | HIS  |
| 2   | E     | 2858 | GLN  |
| 2   | E     | 3761 | GLN  |
| 2   | E     | 3809 | ASN  |
| 2   | E     | 3814 | GLN  |
| 2   | E     | 3850 | GLN  |
| 2   | E     | 3882 | GLN  |
| 2   | E     | 3895 | HIS  |
| 2   | E     | 3896 | ASN  |
| 2   | E     | 3960 | GLN  |
| 2   | E     | 4034 | ASN  |
| 2   | E     | 4054 | ASN  |
| 2   | E     | 4109 | GLN  |
| 2   | E     | 4120 | ASN  |
| 2   | E     | 4130 | ASN  |
| 2   | E     | 4142 | ASN  |
| 2   | E     | 4246 | GLN  |
| 2   | E     | 4691 | GLN  |
| 2   | E     | 4833 | ASN  |
| 2   | E     | 4886 | HIS  |
| 2   | E     | 4947 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 4984 | ASN  |
| 2   | E     | 4987 | ASN  |
| 2   | E     | 5031 | GLN  |
| 1   | F     | 25   | HIS  |
| 2   | G     | 23   | GLN  |
| 2   | G     | 111  | HIS  |
| 2   | G     | 113  | HIS  |
| 2   | G     | 151  | HIS  |
| 2   | G     | 190  | GLN  |
| 2   | G     | 201  | ASN  |
| 2   | G     | 203  | ASN  |
| 2   | G     | 224  | HIS  |
| 2   | G     | 273  | HIS  |
| 2   | G     | 379  | HIS  |
| 2   | G     | 405  | HIS  |
| 2   | G     | 639  | ASN  |
| 2   | G     | 678  | GLN  |
| 2   | G     | 797  | HIS  |
| 2   | G     | 838  | HIS  |
| 2   | G     | 877  | ASN  |
| 2   | G     | 1035 | ASN  |
| 2   | G     | 1041 | GLN  |
| 2   | G     | 1598 | GLN  |
| 2   | G     | 1679 | ASN  |
| 2   | G     | 1691 | GLN  |
| 2   | G     | 1719 | HIS  |
| 2   | G     | 1775 | HIS  |
| 2   | G     | 1837 | GLN  |
| 2   | G     | 1861 | GLN  |
| 2   | G     | 1949 | GLN  |
| 2   | G     | 2005 | GLN  |
| 2   | G     | 2127 | GLN  |
| 2   | G     | 2188 | ASN  |
| 2   | G     | 2194 | HIS  |
| 2   | G     | 2858 | GLN  |
| 2   | G     | 3761 | GLN  |
| 2   | G     | 3766 | GLN  |
| 2   | G     | 3809 | ASN  |
| 2   | G     | 3814 | GLN  |
| 2   | G     | 3882 | GLN  |
| 2   | G     | 3895 | HIS  |
| 2   | G     | 3896 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 3960 | GLN  |
| 2   | G     | 4034 | ASN  |
| 2   | G     | 4054 | ASN  |
| 2   | G     | 4109 | GLN  |
| 2   | G     | 4120 | ASN  |
| 2   | G     | 4130 | ASN  |
| 2   | G     | 4142 | ASN  |
| 2   | G     | 4246 | GLN  |
| 2   | G     | 4691 | GLN  |
| 2   | G     | 4833 | ASN  |
| 2   | G     | 4984 | ASN  |
| 2   | G     | 4987 | ASN  |
| 2   | G     | 5031 | GLN  |
| 1   | H     | 25   | HIS  |
| 2   | I     | 23   | GLN  |
| 2   | I     | 111  | HIS  |
| 2   | I     | 113  | HIS  |
| 2   | I     | 151  | HIS  |
| 2   | I     | 190  | GLN  |
| 2   | I     | 201  | ASN  |
| 2   | I     | 203  | ASN  |
| 2   | I     | 224  | HIS  |
| 2   | I     | 273  | HIS  |
| 2   | I     | 379  | HIS  |
| 2   | I     | 405  | HIS  |
| 2   | I     | 639  | ASN  |
| 2   | I     | 678  | GLN  |
| 2   | I     | 765  | GLN  |
| 2   | I     | 797  | HIS  |
| 2   | I     | 838  | HIS  |
| 2   | I     | 877  | ASN  |
| 2   | I     | 1035 | ASN  |
| 2   | I     | 1041 | GLN  |
| 2   | I     | 1598 | GLN  |
| 2   | I     | 1679 | ASN  |
| 2   | I     | 1691 | GLN  |
| 2   | I     | 1719 | HIS  |
| 2   | I     | 1775 | HIS  |
| 2   | I     | 1837 | GLN  |
| 2   | I     | 1861 | GLN  |
| 2   | I     | 1949 | GLN  |
| 2   | I     | 2005 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 2127 | GLN  |
| 2   | I     | 2161 | GLN  |
| 2   | I     | 2188 | ASN  |
| 2   | I     | 2194 | HIS  |
| 2   | I     | 2763 | HIS  |
| 2   | I     | 3761 | GLN  |
| 2   | I     | 3809 | ASN  |
| 2   | I     | 3814 | GLN  |
| 2   | I     | 3882 | GLN  |
| 2   | I     | 3889 | GLN  |
| 2   | I     | 3895 | HIS  |
| 2   | I     | 3896 | ASN  |
| 2   | I     | 3960 | GLN  |
| 2   | I     | 4034 | ASN  |
| 2   | I     | 4054 | ASN  |
| 2   | I     | 4109 | GLN  |
| 2   | I     | 4120 | ASN  |
| 2   | I     | 4130 | ASN  |
| 2   | I     | 4142 | ASN  |
| 2   | I     | 4246 | GLN  |
| 2   | I     | 4691 | GLN  |
| 2   | I     | 4833 | ASN  |
| 2   | I     | 4886 | HIS  |
| 2   | I     | 4947 | GLN  |
| 2   | I     | 4984 | ASN  |
| 2   | I     | 4987 | ASN  |
| 2   | I     | 5031 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | I     | 12               |
| 2   | B     | 12               |
| 2   | G     | 12               |
| 2   | E     | 12               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I     | 3613:UNK  | C      | 3639:THR  | N      | 43.91        |
| 1     | B     | 3613:UNK  | C      | 3639:THR  | N      | 43.68        |
| 1     | G     | 3613:UNK  | C      | 3639:THR  | N      | 43.62        |
| 1     | E     | 3613:UNK  | C      | 3639:THR  | N      | 43.61        |
| 1     | I     | 3163:UNK  | C      | 3170:UNK  | N      | 16.30        |
| 1     | B     | 3163:UNK  | C      | 3170:UNK  | N      | 16.29        |
| 1     | E     | 3163:UNK  | C      | 3170:UNK  | N      | 16.26        |
| 1     | G     | 3163:UNK  | C      | 3170:UNK  | N      | 16.24        |
| 1     | G     | 3468:UNK  | C      | 3511:UNK  | N      | 15.09        |
| 1     | I     | 3468:UNK  | C      | 3511:UNK  | N      | 15.04        |
| 1     | E     | 3468:UNK  | C      | 3511:UNK  | N      | 15.02        |
| 1     | B     | 3468:UNK  | C      | 3511:UNK  | N      | 15.00        |
| 1     | I     | 2703:UNK  | C      | 2734:ASN  | N      | 14.81        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | E     | 2703:UNK  | C      | 2734:ASN  | N      | 14.71        |
| 1     | B     | 2703:UNK  | C      | 2734:ASN  | N      | 14.67        |
| 1     | G     | 2703:UNK  | C      | 2734:ASN  | N      | 14.61        |
| 1     | I     | 3063:UNK  | C      | 3134:UNK  | N      | 14.51        |
| 1     | G     | 3063:UNK  | C      | 3134:UNK  | N      | 14.50        |
| 1     | E     | 3063:UNK  | C      | 3134:UNK  | N      | 14.48        |
| 1     | B     | 3063:UNK  | C      | 3134:UNK  | N      | 14.47        |
| 1     | I     | 3236:UNK  | C      | 3241:UNK  | N      | 13.17        |
| 1     | G     | 3236:UNK  | C      | 3241:UNK  | N      | 13.16        |
| 1     | E     | 3236:UNK  | C      | 3241:UNK  | N      | 13.07        |
| 1     | B     | 3236:UNK  | C      | 3241:UNK  | N      | 13.05        |
| 1     | B     | 1564:UNK  | C      | 1573:MET  | N      | 12.84        |
| 1     | E     | 1564:UNK  | C      | 1573:MET  | N      | 12.81        |
| 1     | I     | 1564:UNK  | C      | 1573:MET  | N      | 12.73        |
| 1     | G     | 1564:UNK  | C      | 1573:MET  | N      | 12.72        |
| 1     | B     | 2976:UNK  | C      | 2995:UNK  | N      | 12.10        |
| 1     | E     | 2976:UNK  | C      | 2995:UNK  | N      | 12.09        |
| 1     | G     | 2976:UNK  | C      | 2995:UNK  | N      | 12.09        |
| 1     | I     | 2976:UNK  | C      | 2995:UNK  | N      | 12.07        |
| 1     | G     | 3254:UNK  | C      | 3261:UNK  | N      | 8.66         |
| 1     | E     | 3254:UNK  | C      | 3261:UNK  | N      | 8.62         |
| 1     | I     | 3254:UNK  | C      | 3261:UNK  | N      | 8.62         |
| 1     | B     | 3254:UNK  | C      | 3261:UNK  | N      | 8.56         |
| 1     | B     | 1297:UNK  | C      | 1430:UNK  | N      | 5.73         |
| 1     | G     | 1297:UNK  | C      | 1430:UNK  | N      | 5.70         |
| 1     | E     | 1297:UNK  | C      | 1430:UNK  | N      | 5.67         |
| 1     | I     | 1297:UNK  | C      | 1430:UNK  | N      | 5.44         |
| 1     | B     | 2939:ARG  | C      | 2942:UNK  | N      | 3.59         |
| 1     | I     | 2939:ARG  | C      | 2942:UNK  | N      | 3.56         |
| 1     | G     | 2479:LEU  | C      | 2487:UNK  | N      | 3.55         |
| 1     | I     | 2479:LEU  | C      | 2487:UNK  | N      | 3.55         |
| 1     | E     | 2479:LEU  | C      | 2487:UNK  | N      | 3.47         |
| 1     | G     | 2939:ARG  | C      | 2942:UNK  | N      | 3.46         |
| 1     | B     | 2479:LEU  | C      | 2487:UNK  | N      | 3.45         |
| 1     | E     | 2939:ARG  | C      | 2942:UNK  | N      | 3.34         |

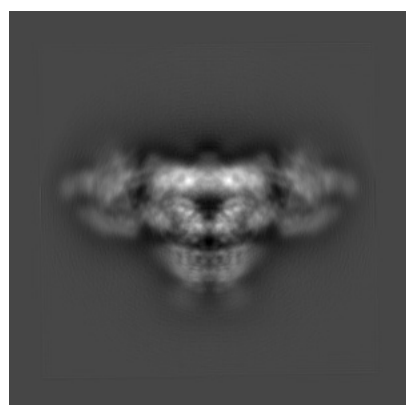
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22392. These allow visual inspection of the internal detail of the map and identification of artifacts.

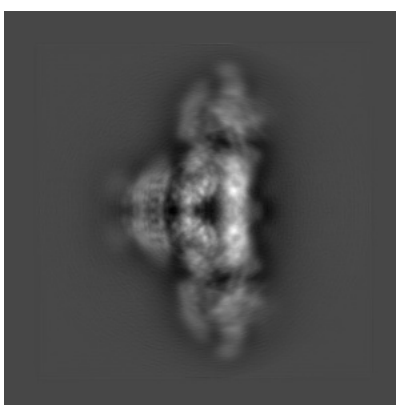
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

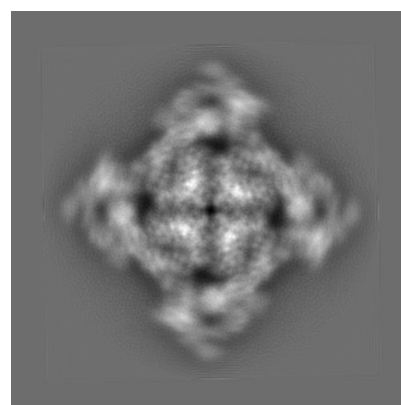
#### 6.1.1 Primary map



X



Y

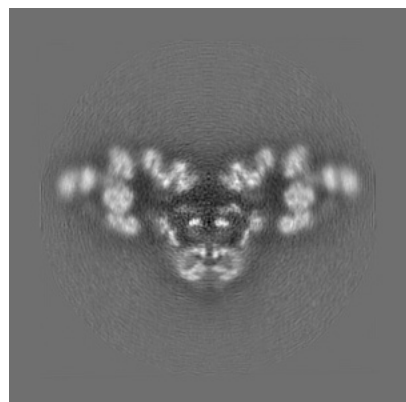


Z

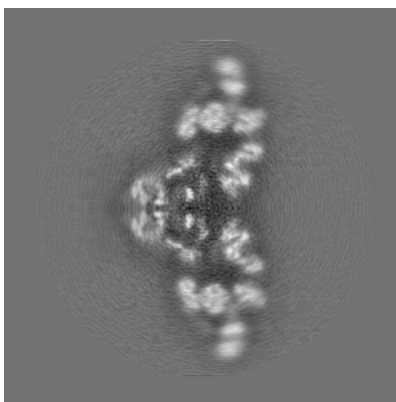
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

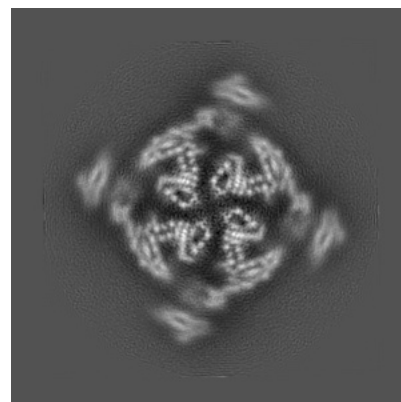
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

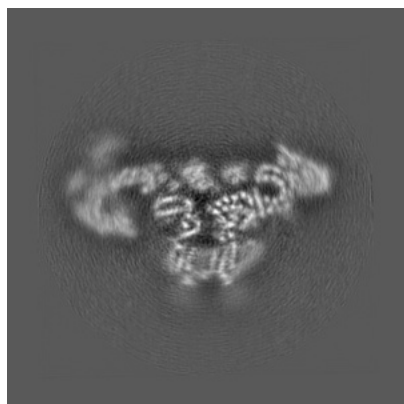


Z Index: 200

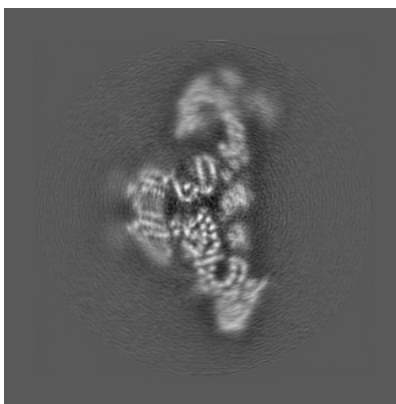
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

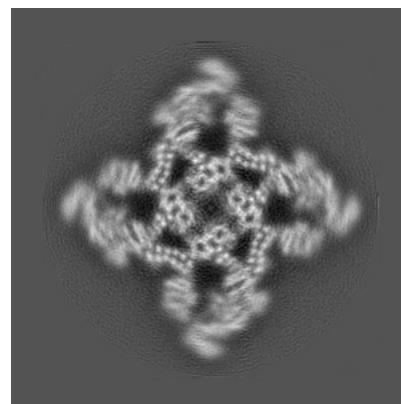
### 6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 226

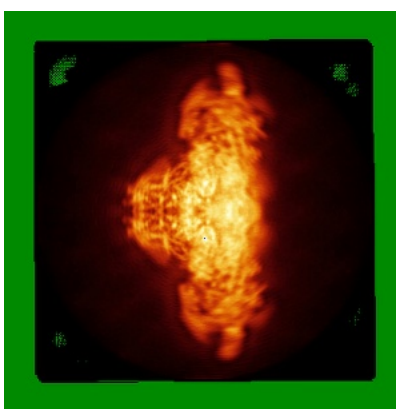
The images above show the largest variance slices of the map in three orthogonal directions.

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

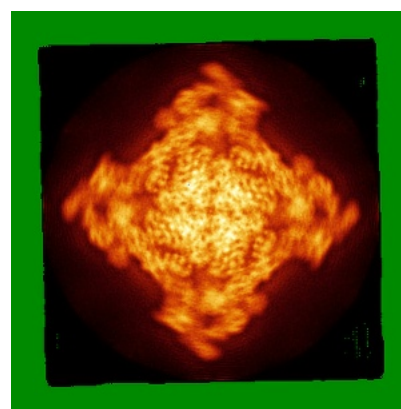
### 6.4.1 Primary map



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

This section was not generated.

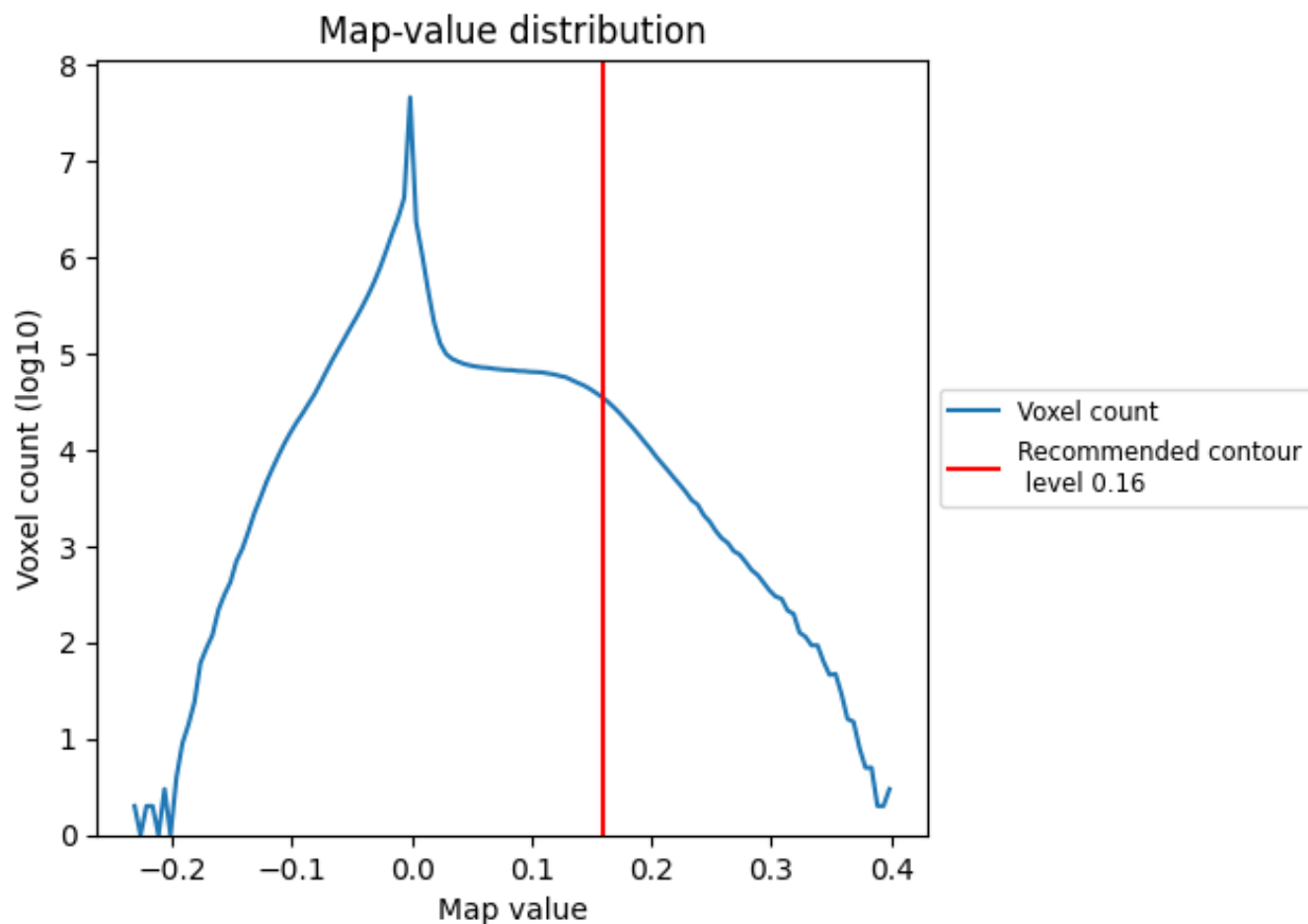
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

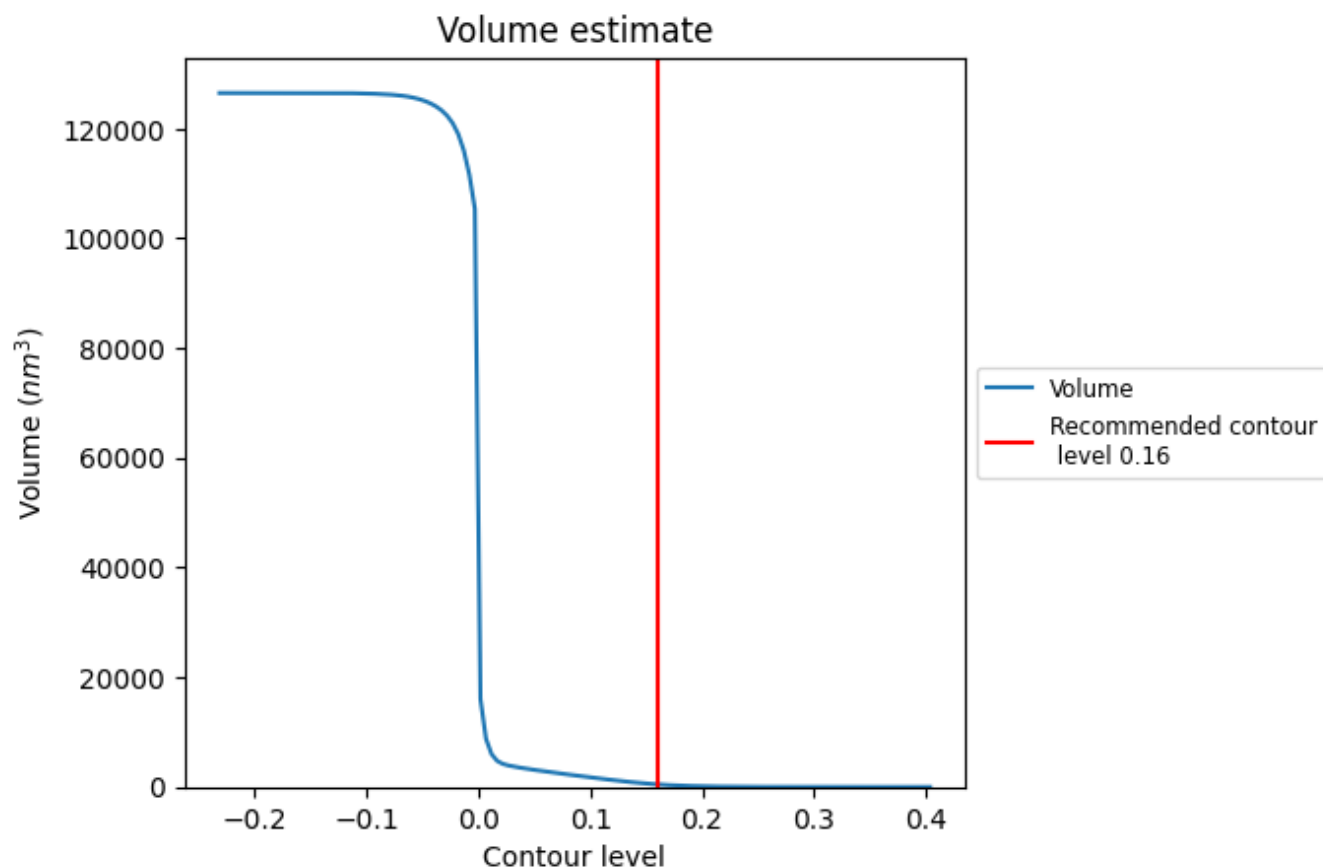
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

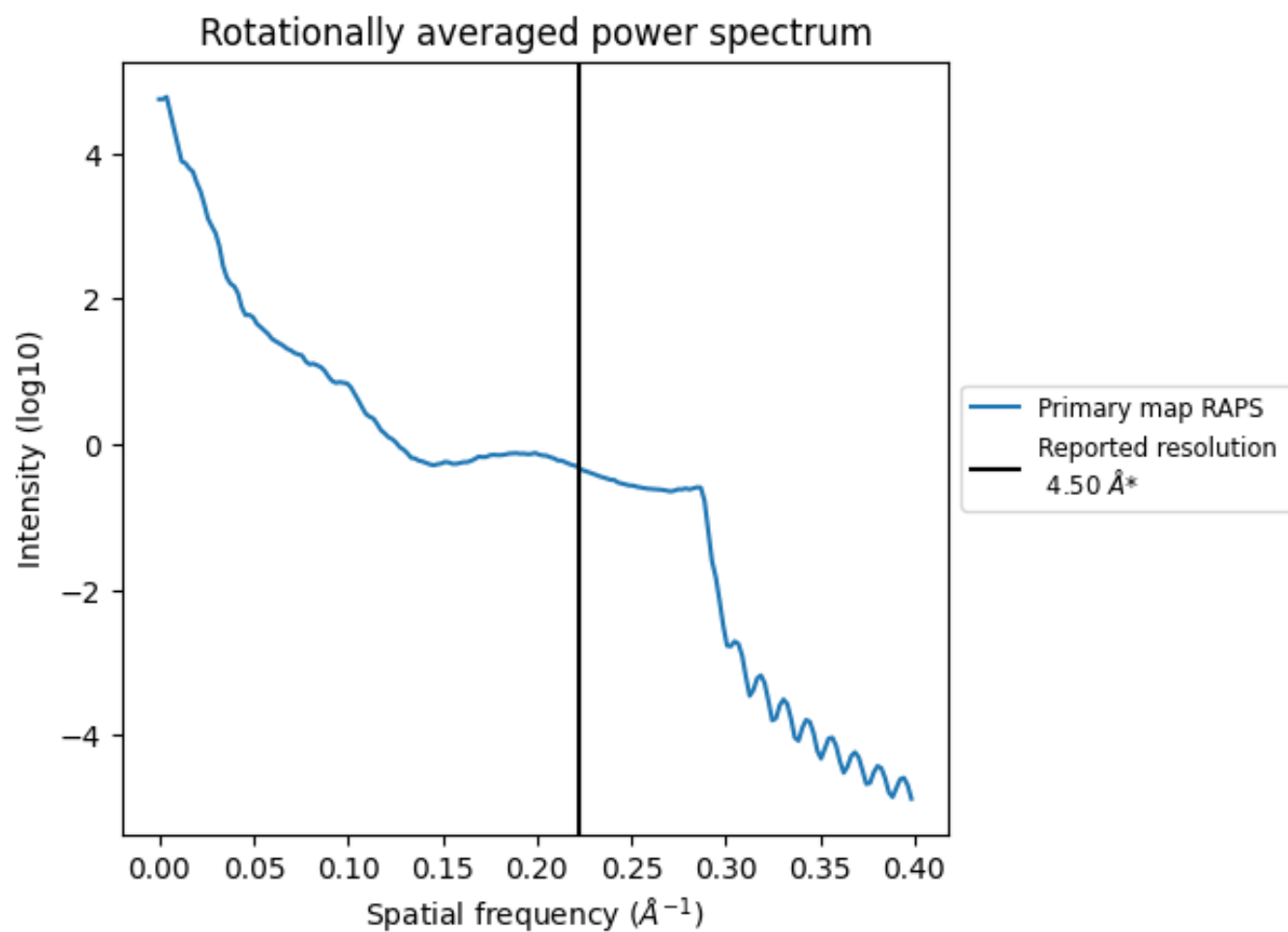
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm<sup>3</sup>; this corresponds to an approximate mass of 423 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

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

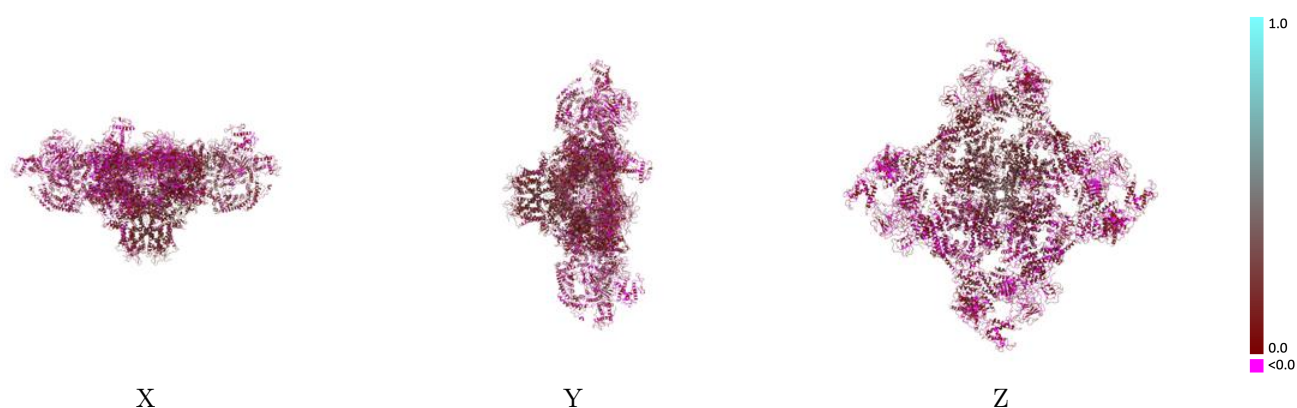
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22392 and PDB model 7JMF. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)

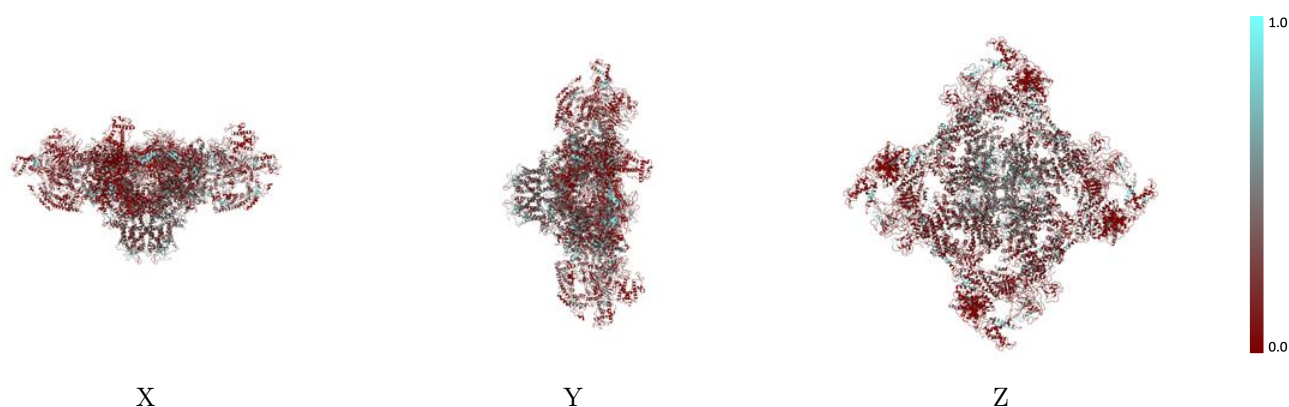
This section was not generated.

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



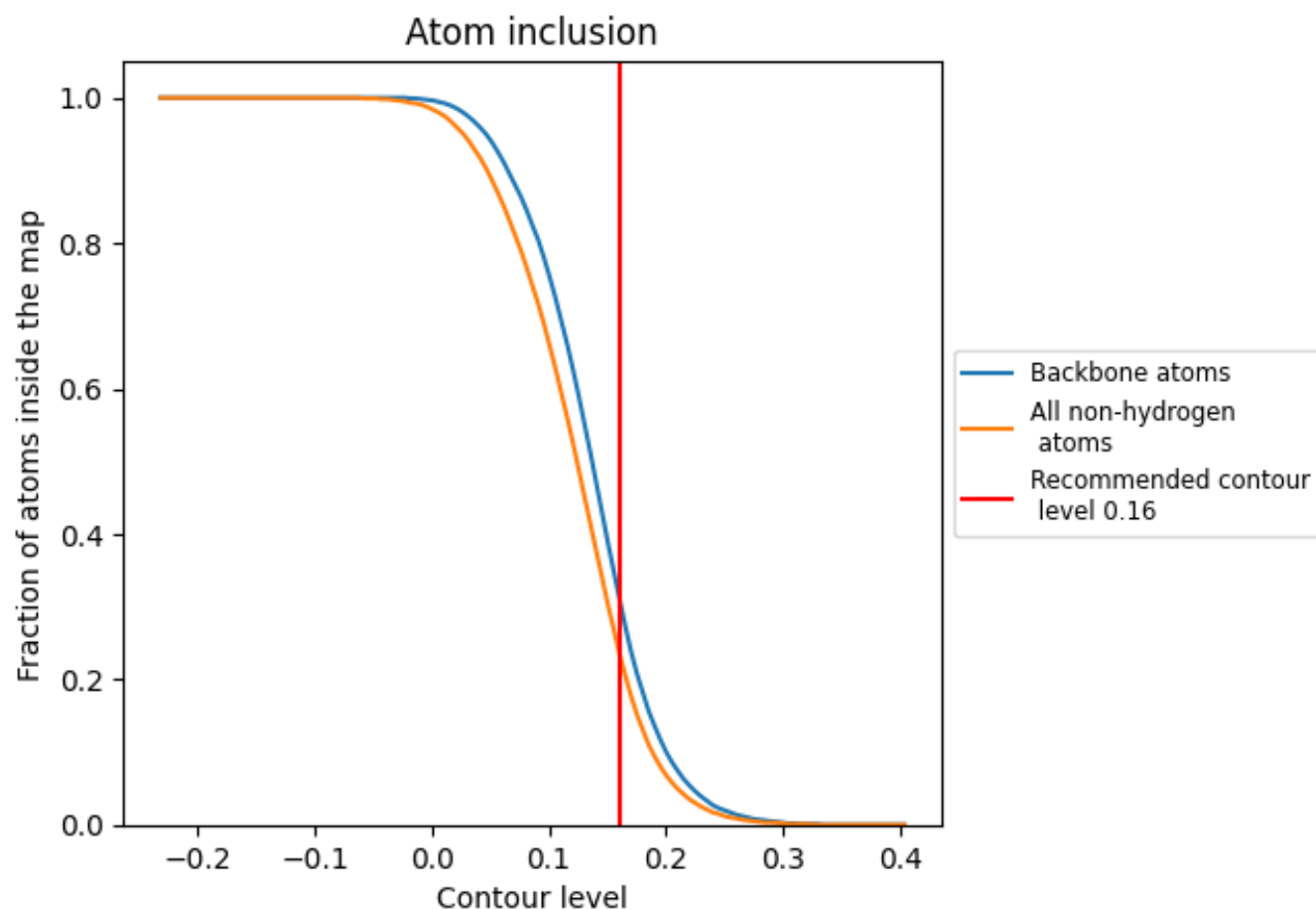
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 31% of all backbone atoms, 24% 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 (0.16) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.2380 | <div></div> 0.1100 |
| A     | <div></div> 0.1450 | <div></div> 0.1330 |
| B     | <div></div> 0.2720 | <div></div> 0.1490 |
| E     | <div></div> 0.2580 | <div></div> 0.1200 |
| F     | <div></div> 0.1430 | <div></div> 0.0750 |
| G     | <div></div> 0.2200 | <div></div> 0.0820 |
| H     | <div></div> 0.1090 | <div></div> 0.0850 |
| I     | <div></div> 0.2150 | <div></div> 0.0890 |
| J     | <div></div> 0.1250 | <div></div> 0.0820 |

