



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:04 PM UTC

PDB ID : 7MKA / pdb\_00007mka  
EMDB ID : EMD-23888  
Title : Structure of EC+EC (leading EC-focused)  
Authors : Yang, C.; Murakami, K.  
Deposited on : 2021-04-22  
Resolution : 3.54 Å(reported)  
Based on initial models : 5C4J, 3PO2, 6GML

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>.

---

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

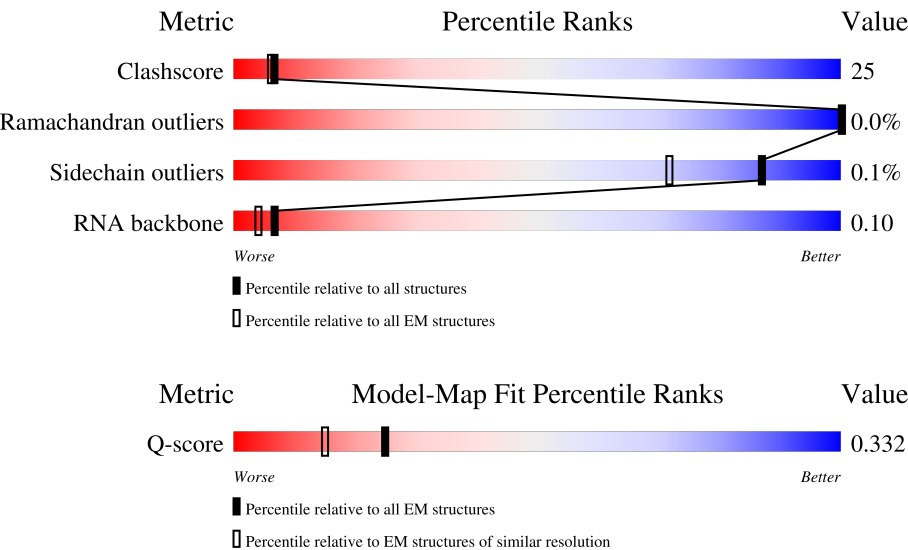
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.54 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.



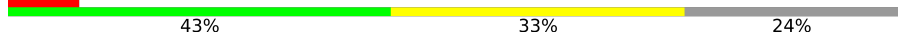
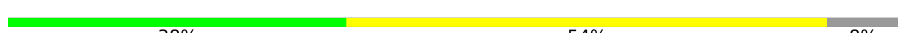
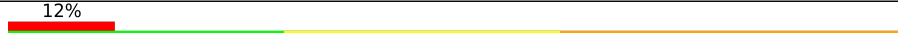
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 12891 ( 3.04 - 4.04 )                                    |

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   | N     | 39     | <div><div></div><div>41%</div><div>59%</div></div>               |
| 2   | O     | 40     | <div><div></div><div>25%</div><div>72%</div><div></div></div>    |
| 3   | a     | 1733   | <div><div></div><div>44%</div><div>38%</div><div>18%</div></div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 4   | b     | 1224   |  |
| 5   | c     | 318    |  |
| 6   | d     | 221    |  |
| 7   | e     | 215    |  |
| 8   | f     | 155    |  |
| 9   | g     | 171    |  |
| 10  | h     | 146    |  |
| 11  | i     | 122    |  |
| 12  | j     | 70     |  |
| 13  | k     | 120    |  |
| 14  | l     | 70     |  |
| 15  | r     | 16     |  |

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33384 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 DNA chain called DNA (40-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | N     | 39       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 798   | 382 | 149 | 228 | 39 |         |       |

- Molecule 2 is a DNA chain called DNA (40-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | O     | 40       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 821   | 394 | 140 | 247 | 40 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | a     | 1425     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11189 | 7046 | 1955 | 2126 | 62 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | b     | 1160     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9197  | 5805 | 1614 | 1723 | 55 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | c     | 265      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2086  | 1312 | 347 | 414 | 13 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | d     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1331  | 822 | 237 | 270 | 2 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | e     | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | f     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 451 | 119 | 132 | 3 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | g     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1339  | 861 | 222 | 248 | 8 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | h     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 679 | 182 | 214 | 5 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11  | i     | 114      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 927   | 571 | 168 | 178 | 10 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | j     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 540   | 345 | 94 | 95 | 6 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | k     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 924   | 593 | 157 | 172 | 2 |         |       |

- Molecule 14 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | l     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 217 | 70 | 61 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 15  | r     | 16       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 333   | 150 | 55 | 112 | 16 |         |       |

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 16  | a     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 16  | b     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | c     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | i     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 16  | j     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | l     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

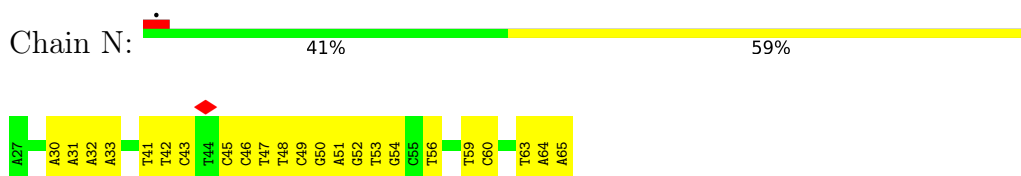
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | a     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

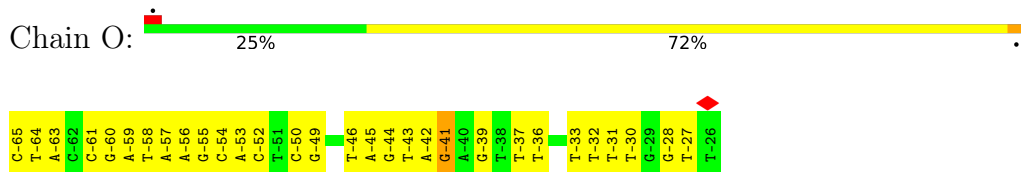
### 3 Residue-property plots

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

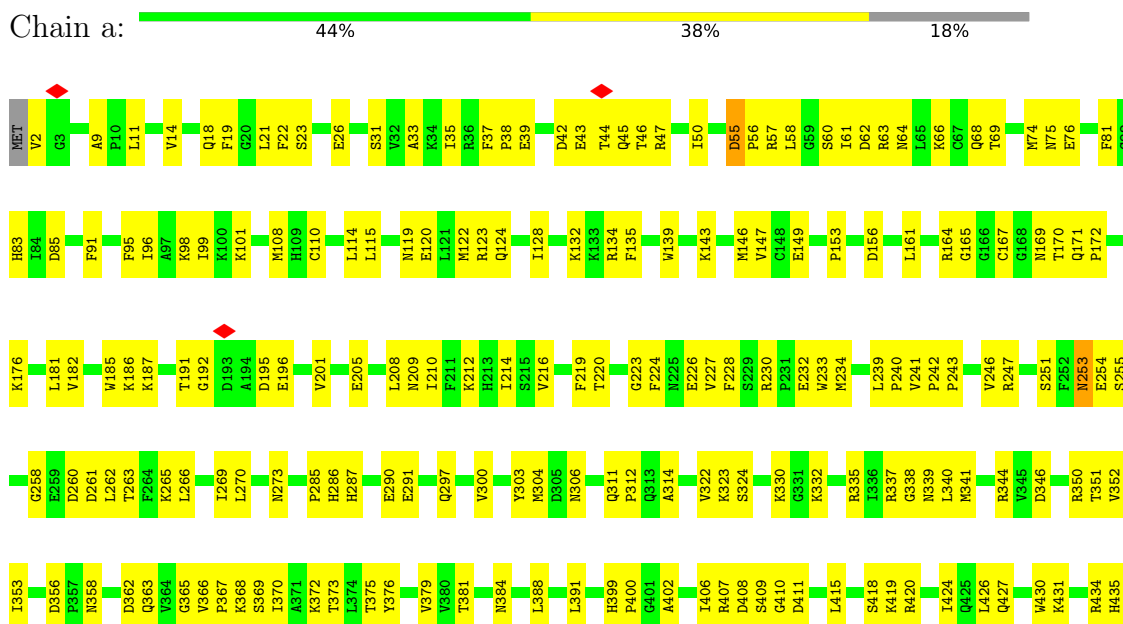
- Molecule 1: DNA (40-MER)



- Molecule 2: DNA (40-MER)



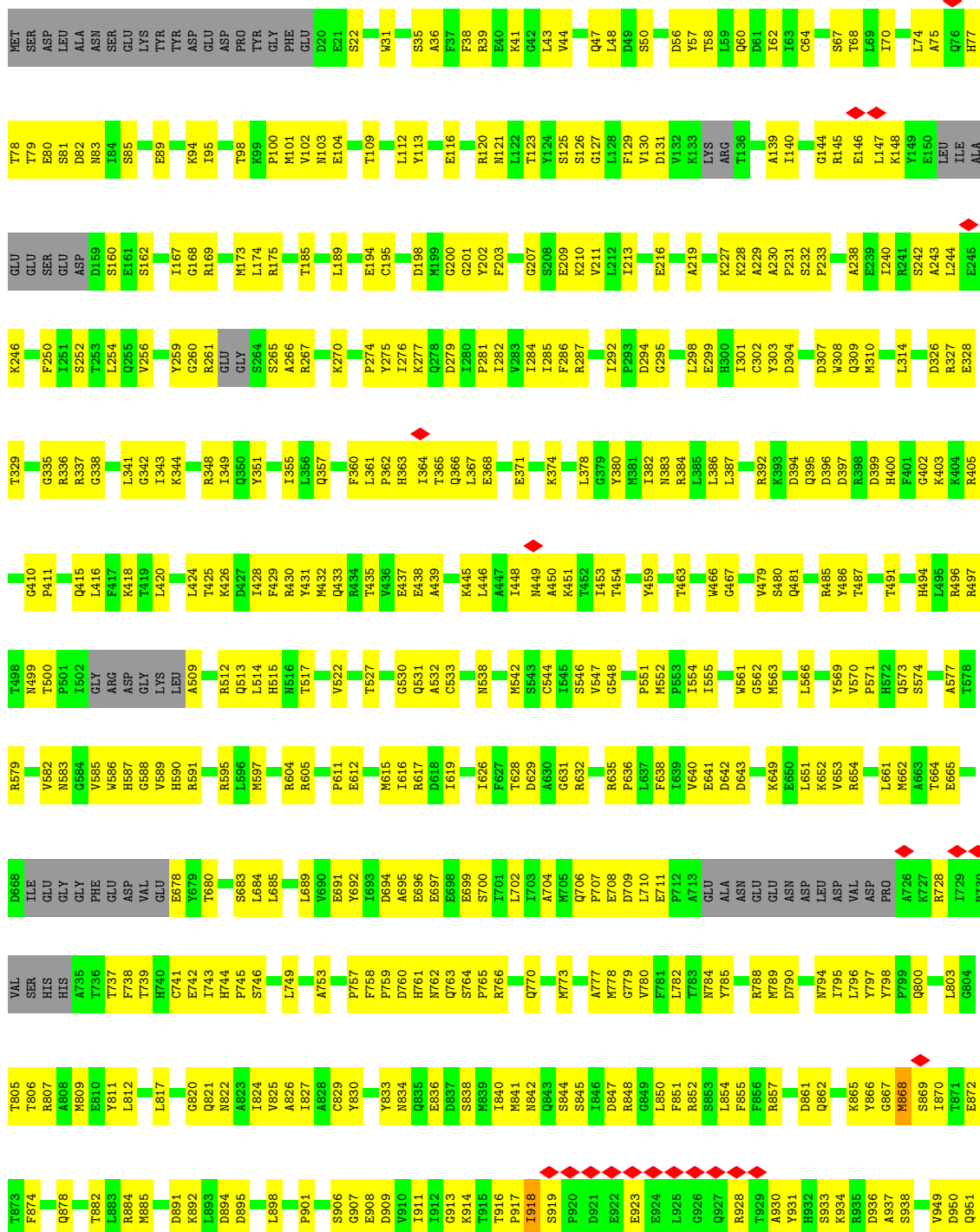
- Molecule 3: DNA-directed RNA polymerase subunit



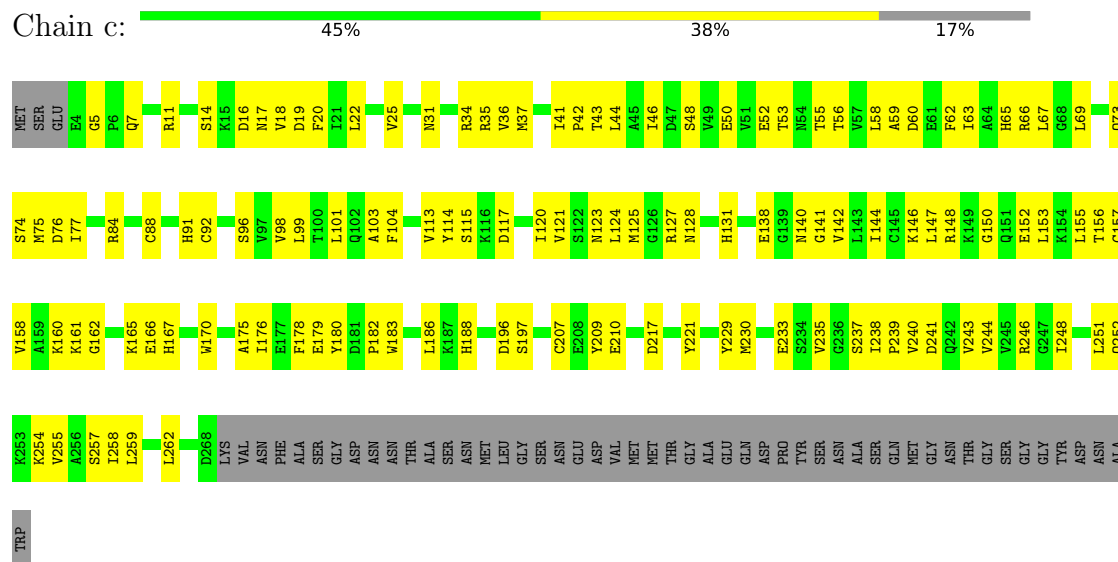
|     |     |     |     |       |       |       |       |       |       |       |      |      |      |      |      |
|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|
| SER | PRO | TYR | ALA | I1445 | R1366 | I1271 | D1198 | P1122 | E1050 | A967  | Y853 | K789 | G574 | S502 | I436 |
| PRO | SER | PRO | GLY | D1446 |       | T1272 | R1199 | G1123 | A1051 | Q968  | I864 | D790 | K575 | Q503 | M437 |
| TYR | PRO | GLY | GLY | E1447 | D1373 | L1273 | A1201 | L1133 | F1053 | Q969  | Q885 | D791 | Q576 | L504 | D438 |
| SER | SER | ALA | ALA | M1454 | T1376 | R1274 | M1202 | S1136 | R1055 | I973  | Y868 | Y792 | I577 | C505 | N439 |
| PRO | PRO | ASP | ASP |       | T1377 |       |       |       | L1054 | D974  | D871 | P794 | L579 | A506 | D440 |
| SER | SER | TYR | TYR |       | G1378 | V1282 | T1208 | T1141 | S1056 | K977  | K872 | E795 | V580 | P508 | P441 |
| TYR | PRO | GLY | GLY |       | G1379 | V1283 | M1209 | T1142 | V1057 | P978  | K873 | S796 |      | I511 | L443 |
| SER | PRO | ALA | ALA |       | T1385 | V1284 | G1210 | T1143 | V1058 | P979  | M874 | G798 | H587 | V512 | P444 |
| TYR | PRO | THR | THR |       | R1386 | M1285 | Q1211 | K1144 | L1059 | S979  | D875 | F799 | Q589 | S513 | N445 |
| SER | SER | GLY | GLY |       | H1387 |       | V1212 | S1145 | P1060 |       | A876 | V800 | L578 | P514 | Q447 |
| PRO | PRO | PRO | PRO |       | G1388 |       | G1213 |       | M1063 | V987  | A877 | H877 | S579 | Q514 | P448 |
| SER | PRO | ILE | ILE |       | E1214 |       | E1214 |       | E1074 |       | H877 | F801 | F591 | Q515 | S449 |
| THR | THR | GLY | PHE |       | R1389 |       | R1215 | T1148 | V1064 | K991  | I878 | N802 |      | P519 | S449 |
| SER | TYR | ASP | GLY |       | M1390 | S1293 | I1216 | T1149 | G1065 | D992  | K879 | N803 | T595 | C520 | L450 |
| PRO | PRO | GLY | ALA |       | R1391 | G1296 | G1217 | S1150 | K880  | L993  | E879 | Y804 | T596 | G529 | H451 |
| SER | SER | GLY | GLY |       |       | E1297 | Q1218 | E1151 | Q1070 | L994  | D874 | L805 | L597 | K452 | M452 |
| TYR | PRO | TYR | TYR |       | L1397 | G1297 | F1220 | I1152 | S1071 | E995  | A875 | G807 | L598 | V524 | M453 |
| SER | SER | GLY | GLY |       |       |       | K1221 | Y1153 |       | N996  | A876 | L808 | D602 | Q525 | S454 |
| PRO | PRO | ALA | ALA |       | C1400 | E1301 |       | Y1154 |       |       | H877 |      | M603 | D526 | M455 |
| THR | THR | VAL | VAL |       | S1401 | P1302 | L1224 | D1155 | T1077 | V999  | I878 | Q811 | M604 | C529 | M456 |
| SER | PRO | THR | THR |       | F1402 | T1308 | F1225 | P1156 | Q1078 | R1001 | E879 | E812 | G604 | A457 | H458 |
| SER | PRO | TYR | TYR |       |       |       |       | D1157 | M1079 | G1002 |      |      | M605 | R459 | V460 |
| PRO | PRO | TYR | PRO |       | T1405 | V1311 | V1226 | S1180 | T1080 | K1003 | N903 | H816 | D609 | I531 | V460 |
| TYR | SER | GLY | GLY |       | V1406 | N1312 | I1227 | T1161 | L1081 | N1004 |      |      |      | R532 | K461 |
| SER | SER | PHE | PHE |       | E1407 | N1313 | W1228 | T1162 | ASN   |       |      | R821 | I612 | K533 | V462 |
| PRO | PRO | GLY | GLY |       | I1408 | S1314 | S1229 | I1163 | THR   | T1007 | L912 | E822 |      | L534 | V462 |
| THR | THR | VAL | VAL |       | L1409 | S1315 | E1230 | I1163 | PHE   | Q1008 | K744 | L913 | V617 | I535 | P464 |
| SER | TYR | GLY | GLY |       | F1410 | V1316 | D1231 | D1166 | HIS   | N1009 | E914 | I825 | M618 | L536 | M465 |
| PRO | PRO | SER | SER |       | E1411 | M1317 | D1232 | E1167 | PHE   | A1010 | E918 | D826 | K619 | R537 | S466 |
| ALA | PRO | VAL | VAL |       | A1412 | T1318 | D1233 | E1168 | ALA   | Q1011 |      | T827 | K620 | F540 | T467 |
| TYR | THR | ASN | ASN |       |       |       |       | I1169 | GLY   | R1012 | L928 |      | T621 | F468 | F468 |
| SER | PRO | ALA | ALA |       | A1416 | T1325 | L1236 | I1170 | VAL   | L1017 | L929 | K830 | V622 | L543 | R469 |
| PRO | PRO | ASP | ASP |       | E1417 |       |       | Q1171 | ALA   | F1018 | D939 | Y836 | L629 | D544 | L470 |
| THR | THR | LEU | LEU |       | L1418 | Y1328 | R1239 | T1172 | ALA   |       |      | I837 | I630 | Q545 | N471 |
| SER | TYR | ASP | ASP |       | D1419 | T1329 | C1240 | L1172 | SER   |       |      |      | V546 | V546 | L472 |
| PRO | PRO | VAL | VAL |       | D1420 | H1173 | R1241 | H1173 | LYS   |       |      |      | H631 | L547 | S473 |
| SER | PRO | LYS | LYS |       | C1421 | N1330 | V1242 | F1174 | K1093 | R1023 | L943 | R839 | V632 | R548 | V474 |
| TYR | THR | ASP | ASP |       |       | S1331 | V1243 | S1175 | V1094 | S1024 | R944 | L841 | V633 | M549 | T475 |
| SER | SER | GLY | GLY |       | V1424 | F1332 | R1244 | LEU   | G1097 | R1025 |      |      | T634 | L550 | S476 |
| PRO | PRO | LEU | LEU |       | S1425 |       | P1245 | LEU   | V1098 |       |      |      | R635 | Y551 | P477 |
| THR | THR | MET | MET |       | E1426 |       | LYS   | ASP   | P1099 | R1029 | G950 | E846 | G638 | W556 | M479 |
| SER | TYR | PHE | PHE |       | N1427 |       | LEU   | GLU   | R1030 | R1030 | D949 |      | P639 | D557 |      |
| SER | PRO | SER | SER |       | V1428 | L1339 | LEU   | GLU   | R1031 | V1031 | G951 | D847 | Q640 | G558 | D483 |
| PRO | PRO | PRO | PRO |       | I1429 |       | ASP   | ALA   | L1032 | L1032 |      | M849 |      | V559 | E486 |
| TYR | TYR | ALA | ALA |       | L1430 | E1342 | ALA   | GLU   | T1104 | Q1033 | A952 | T855 | K644 | I560 | M487 |
| SER | PRO | VAL | VAL |       | G1431 |       | GLU   | GLN   | L1106 | E1034 |      |      | V770 | P563 |      |
| PRO | PRO | ASP | ASP |       | Q1432 | R1345 | THR   | SER   | H1107 | R1035 | N953 |      | E771 | I560 |      |
| THR | THR | SER | SER |       | M1433 |       | GLU   | F1185 | V1107 | R1036 | W954 | Y852 |      | I560 |      |
| SER | PRO | GLY | GLY |       | A1434 | E1351 | A1254 |       | A1108 | L1037 | P955 |      | F646 |      |      |
| PRO | PRO | SER | SER |       | F1435 |       | E1255 | Q1188 | K1109 |       | L956 | D853 | G647 | P563 |      |
| TYR | TYR | ASN | ASN |       | I1436 | A1357 |       | S1189 | M1110 | A1041 | P957 | N854 | N648 |      | H490 |
| TYR | THR | ASP | ASP |       | G1437 | S1358 | M1259 | P1190 | M1111 | F1042 | V958 | T855 | I649 | I566 | V491 |
| SER | SER | ALA | ALA |       | T1438 | D1359 |       | W1191 | M1112 | D1043 | N959 | T856 | Q650 | K567 |      |
| PRO | PRO | MET | MET |       | G1439 | G1360 | I1263 | L1192 | T1113 | V1044 | R857 | R857 | K651 | P568 | E495 |
| ALA | THR | ALA | ALA |       | A1440 | S1361 |       | L1193 | P1114 | V1045 | R961 | N858 | V652 | K569 |      |
| SER | TYR | GLY | GLY |       | F1441 | Y1362 | M1267 | R1194 | S1115 | L1046 | R962 | S859 | V653 | P570 | R498 |
| PRO | PRO | GLY | GLY |       | D1442 | V1363 | L1268 | L1195 | L1116 | S1047 |      | L860 | M654 | L571 | A499 |
| PRO | PRO | PHE | PHE |       | V1443 |       | E1269 | E1196 | L1116 | N1048 | Q965 | G861 | F655 | W572 | E500 |
| TYR | THR | THR | SER |       | M1444 | Y1365 | N1270 | L1197 | E1121 | I1049 | N966 | N862 | W656 | S573 | L501 |



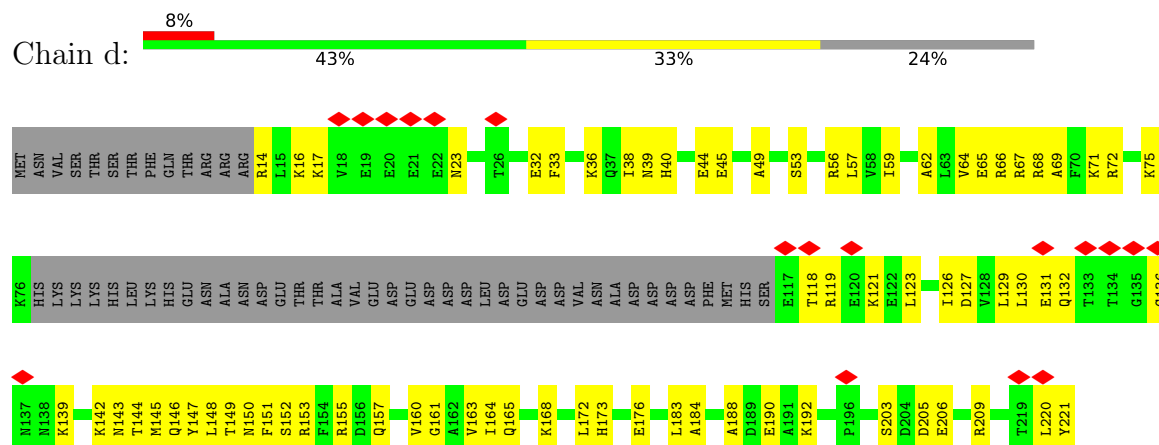
Chain b:



- Molecule 5: DNA-directed RNA polymerase II subunit RPB3

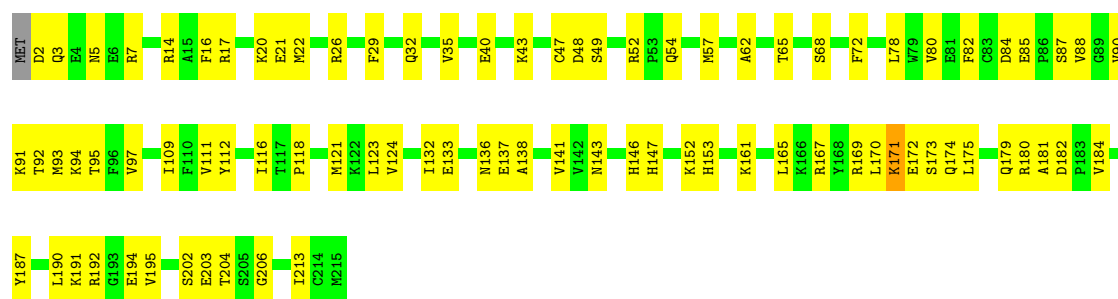


- Molecule 6: DNA-directed RNA polymerase II subunit RPB4

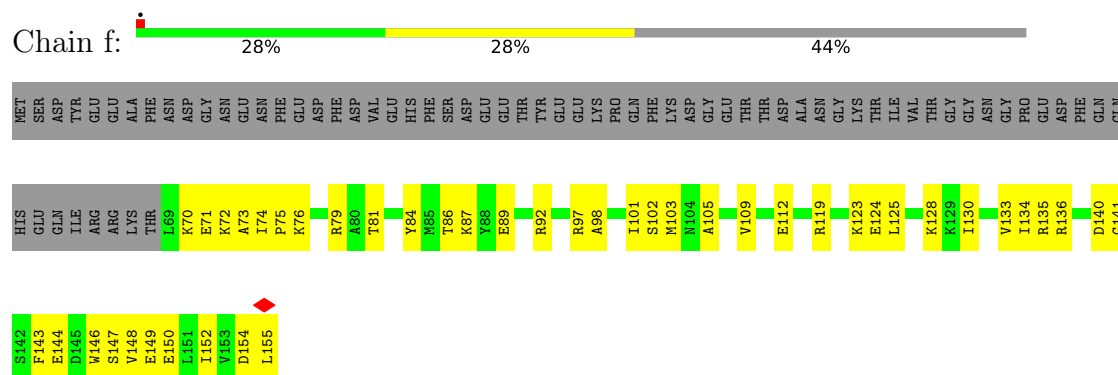


- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

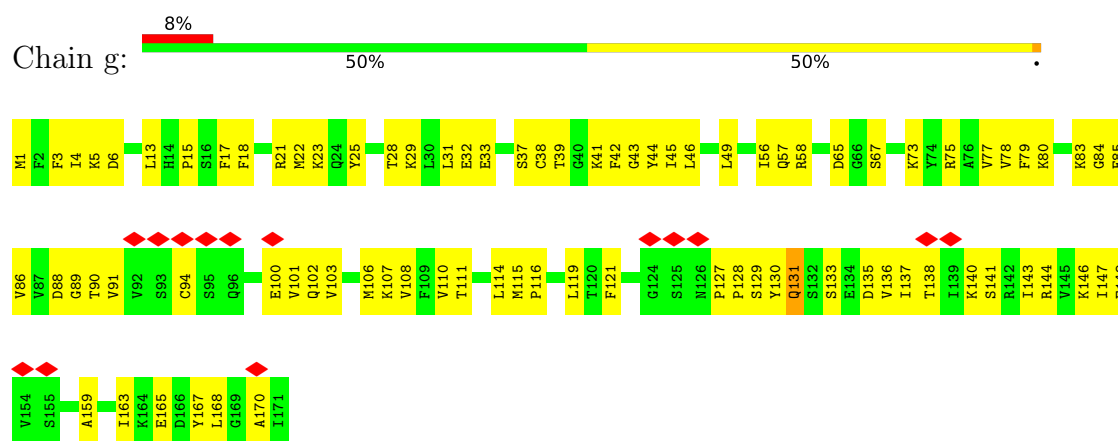




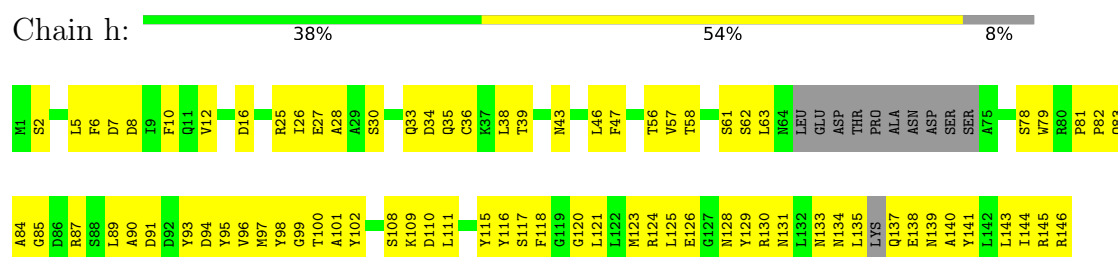
- Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2



- Molecule 9: DNA-directed RNA polymerase II subunit RPB7

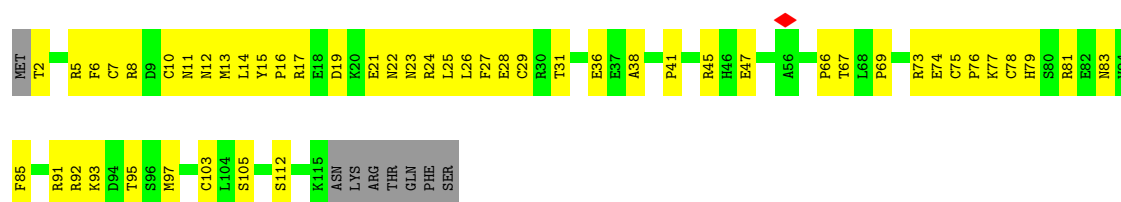


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 11: DNA-directed RNA polymerase II subunit RPB9

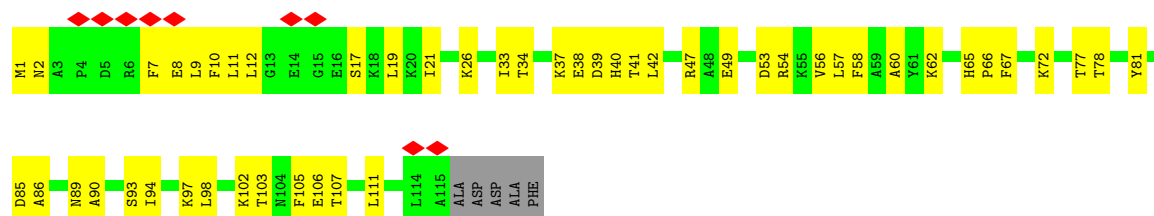




- Molecule 12: DNA-directed RNA polymerases II subunit RPABC5



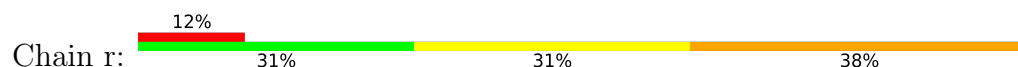
- Molecule 13: DNA-directed RNA polymerase II subunit RPB11



- Molecule 14: DNA-directed RNA polymerases II subunit RPABC4



- Molecule 15: RNA (5'-R(P\*AP\*AP\*CP\*UP\*AP\*GP\*UP\*UP\*AP\*AP\*GP\*AP\*GP\*GP\*UP\*U)-3')



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, C1           | Depositor |
| Number of particles used             | 57690               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.25                | Depositor |
| Minimum defocus (nm)                 | 750                 | Depositor |
| Maximum defocus (nm)                 | 1750                | Depositor |
| Magnification                        | 81000               | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.062               | Depositor |
| Minimum map value                    | -0.030              | Depositor |
| Average map value                    | 0.001               | Depositor |
| Map value standard deviation         | 0.004               | Depositor |
| Recommended contour level            | 0.0101              | Depositor |
| Map size ( $\text{\AA}$ )            | 237.6, 237.6, 237.6 | wwPDB     |
| Map dimensions                       | 220, 220, 220       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.08, 1.08, 1.08    | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | N     | 0.26         | 0/896       | 0.40        | 0/1379          |
| 2   | O     | 0.39         | 0/918       | 0.63        | 2/1416 (0.1%)   |
| 3   | a     | 0.29         | 0/11390     | 0.52        | 4/15408 (0.0%)  |
| 4   | b     | 0.31         | 0/9371      | 0.55        | 3/12636 (0.0%)  |
| 5   | c     | 0.28         | 0/2124      | 0.44        | 0/2879          |
| 6   | d     | 0.16         | 0/1339      | 0.46        | 0/1793          |
| 7   | e     | 0.26         | 0/1788      | 0.48        | 0/2406          |
| 8   | f     | 0.31         | 0/717       | 0.52        | 0/967           |
| 9   | g     | 0.23         | 0/1367      | 0.55        | 0/1844          |
| 10  | h     | 0.25         | 0/1097      | 0.47        | 0/1484          |
| 11  | i     | 0.20         | 0/945       | 0.42        | 0/1273          |
| 12  | j     | 0.35         | 0/549       | 0.54        | 0/738           |
| 13  | k     | 0.26         | 0/942       | 0.43        | 0/1272          |
| 14  | l     | 0.25         | 0/354       | 0.61        | 0/468           |
| 15  | r     | 0.64         | 0/370       | 1.01        | 3/572 (0.5%)    |
| All | All   | 0.29         | 0/34167     | 0.53        | 12/46535 (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 |
|-----|-------|---------------------|---------------------|
| 3   | a     | 0                   | 1                   |
| 4   | b     | 0                   | 1                   |
| 7   | e     | 0                   | 1                   |
| 9   | g     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | r     | 40   | U    | C2'-C3'-O3' | -8.45 | 101.03      | 113.70   |
| 15  | r     | 47   | U    | C1'-C2'-O2' | -8.21 | 96.09       | 108.40   |
| 2   | O     | -39  | DG   | C2'-C3'-O3' | -8.04 | 99.45       | 111.50   |
| 4   | b     | 1210 | MET  | N-CA-C      | -5.71 | 106.30      | 113.20   |
| 3   | a     | 253  | ASN  | CA-C-N      | -5.29 | 115.23      | 121.90   |
| 3   | a     | 253  | ASN  | C-N-CA      | -5.29 | 115.23      | 121.90   |
| 3   | a     | 1107 | VAL  | CA-C-N      | 5.27  | 131.19      | 121.70   |
| 3   | a     | 1107 | VAL  | C-N-CA      | 5.27  | 131.19      | 121.70   |
| 4   | b     | 918  | ILE  | CA-C-N      | 5.19  | 131.04      | 121.70   |
| 4   | b     | 918  | ILE  | C-N-CA      | 5.19  | 131.04      | 121.70   |
| 15  | r     | 40   | U    | C1'-C2'-O2' | 5.14  | 116.10      | 108.40   |
| 2   | O     | -41  | DG   | C4'-C3'-O3' | -5.12 | 102.33      | 110.00   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | a     | 55  | ASP  | Peptide |
| 4   | b     | 868 | MET  | Peptide |
| 7   | e     | 171 | LYS  | Peptide |
| 9   | g     | 131 | GLN  | Peptide |
| 9   | g     | 56  | ILE  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | N     | 798   | 0        | 440      | 31      | 0            |
| 2   | O     | 821   | 0        | 457      | 30      | 0            |
| 3   | a     | 11189 | 0        | 11225    | 602     | 0            |
| 4   | b     | 9197  | 0        | 9180     | 513     | 0            |
| 5   | c     | 2086  | 0        | 2045     | 102     | 0            |
| 6   | d     | 1331  | 0        | 1345     | 62      | 0            |
| 7   | e     | 1752  | 0        | 1776     | 74      | 0            |
| 8   | f     | 705   | 0        | 731      | 40      | 0            |
| 9   | g     | 1339  | 0        | 1357     | 78      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | h     | 1080  | 0        | 1049     | 97      | 0            |
| 11  | i     | 927   | 0        | 880      | 53      | 0            |
| 12  | j     | 540   | 0        | 553      | 42      | 0            |
| 13  | k     | 924   | 0        | 934      | 51      | 0            |
| 14  | l     | 352   | 0        | 374      | 15      | 0            |
| 15  | r     | 333   | 0        | 172      | 8       | 0            |
| 16  | a     | 2     | 0        | 0        | 0       | 0            |
| 16  | b     | 1     | 0        | 0        | 0       | 0            |
| 16  | c     | 1     | 0        | 0        | 0       | 0            |
| 16  | i     | 2     | 0        | 0        | 0       | 0            |
| 16  | j     | 1     | 0        | 0        | 0       | 0            |
| 16  | l     | 1     | 0        | 0        | 0       | 0            |
| 17  | a     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 33384 | 0        | 32518    | 1628    | 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 25.

All (1628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:65:DA:H61    | 2:O:-65:DC:N4    | 1.48                     | 1.11              |
| 1:N:65:DA:N6     | 2:O:-65:DC:H42   | 1.48                     | 1.10              |
| 3:a:372:LYS:HD2  | 13:k:2:ASN:HB2   | 1.50                     | 0.94              |
| 4:b:102:VAL:HG12 | 4:b:112:LEU:HD21 | 1.53                     | 0.91              |
| 3:a:208:LEU:HD23 | 3:a:212:LYS:HZ2  | 1.35                     | 0.91              |
| 4:b:47:GLN:HE22  | 4:b:173:MET:HG3  | 1.36                     | 0.91              |
| 10:h:56:THR:HB   | 10:h:145:ARG:HB2 | 1.53                     | 0.90              |
| 4:b:85:SER:HB3   | 4:b:139:ALA:H    | 1.36                     | 0.90              |
| 1:N:50:DG:H1     | 2:O:-50:DC:H5    | 1.19                     | 0.89              |
| 3:a:346:ASP:H    | 4:b:1154:ALA:HB1 | 1.33                     | 0.89              |
| 10:h:144:ILE:O   | 10:h:145:ARG:NH1 | 2.06                     | 0.88              |
| 4:b:842:ASN:HA   | 4:b:999:MET:HE1  | 1.56                     | 0.88              |
| 1:N:49:DC:O2     | 2:O:-49:DG:N2    | 2.06                     | 0.88              |
| 4:b:1117:GLN:NE2 | 4:b:1156:ASP:OD1 | 2.07                     | 0.88              |
| 3:a:353:ILE:HD13 | 3:a:487:MET:HE1  | 1.57                     | 0.87              |
| 3:a:311:GLN:HG2  | 3:a:312:PRO:HD3  | 1.57                     | 0.85              |
| 4:b:829:CYS:HA   | 4:b:834:ASN:HD21 | 1.42                     | 0.82              |
| 4:b:82:ASP:H     | 4:b:83:ASN:HA    | 1.44                     | 0.81              |
| 4:b:260:GLY:HA3  | 4:b:266:ALA:HB3  | 1.63                     | 0.81              |
| 10:h:85:GLY:O    | 10:h:87:ARG:NH1  | 2.13                     | 0.81              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:65:DA:N1     | 2:O:-65:DC:N3     | 2.29                     | 0.80              |
| 7:e:52:ARG:O     | 7:e:54:GLN:NE2    | 2.15                     | 0.80              |
| 11:i:19:ASP:HB3  | 11:i:24:ARG:H     | 1.44                     | 0.80              |
| 3:a:55:ASP:HA    | 3:a:58:LEU:HD23   | 1.64                     | 0.80              |
| 4:b:175:ARG:NH2  | 4:b:198:ASP:O     | 2.12                     | 0.80              |
| 10:h:137:GLN:NE2 | 10:h:139:ASN:OD1  | 2.15                     | 0.80              |
| 12:j:8:PHE:H     | 12:j:49:MET:HE1   | 1.46                     | 0.80              |
| 10:h:39:THR:HB   | 10:h:124:ARG:HB3  | 1.63                     | 0.79              |
| 3:a:961:ARG:HG3  | 3:a:965:GLN:HE22  | 1.45                     | 0.79              |
| 4:b:48:LEU:HD12  | 4:b:173:MET:HE1   | 1.64                     | 0.79              |
| 4:b:448:ILE:HD12 | 4:b:451:LYS:HD3   | 1.65                     | 0.79              |
| 11:i:12:ASN:HD22 | 11:i:31:THR:HG21  | 1.48                     | 0.79              |
| 3:a:353:ILE:HG22 | 3:a:468:PHE:HB2   | 1.65                     | 0.79              |
| 10:h:95:TYR:H    | 10:h:145:ARG:NH1  | 1.80                     | 0.78              |
| 3:a:440:ASP:H    | 3:a:460:VAL:HG12  | 1.47                     | 0.78              |
| 3:a:119:ASN:HB3  | 3:a:122:MET:HE1   | 1.66                     | 0.78              |
| 3:a:635:ARG:NH2  | 3:a:876:ALA:O     | 2.17                     | 0.78              |
| 3:a:1002:GLY:HA3 | 3:a:1007:ILE:HG21 | 1.66                     | 0.77              |
| 4:b:416:LEU:HD21 | 4:b:467:GLY:H     | 1.47                     | 0.77              |
| 5:c:50:GLU:HB2   | 5:c:156:THR:HB    | 1.66                     | 0.77              |
| 9:g:38:CYS:HA    | 9:g:44:TYR:HA     | 1.67                     | 0.77              |
| 3:a:587:HIS:NE2  | 3:a:969:GLN:OE1   | 2.17                     | 0.77              |
| 6:d:206:GLU:OE2  | 6:d:209:ARG:NH2   | 2.17                     | 0.76              |
| 3:a:590:ARG:NH2  | 3:a:620:LYS:O     | 2.18                     | 0.76              |
| 3:a:1407:GLU:OE1 | 3:a:1407:GLU:N    | 2.17                     | 0.76              |
| 4:b:394:ASP:HB2  | 11:i:91:ARG:HH22  | 1.49                     | 0.76              |
| 10:h:82:PRO:O    | 10:h:87:ARG:NH2   | 2.17                     | 0.76              |
| 3:a:346:ASP:OD1  | 4:b:1106:ARG:NH2  | 2.19                     | 0.76              |
| 3:a:251:SER:H    | 3:a:258:GLY:HA3   | 1.49                     | 0.75              |
| 4:b:336:ARG:NH1  | 4:b:351:TYR:OH    | 2.18                     | 0.75              |
| 10:h:83:GLN:O    | 10:h:87:ARG:NH1   | 2.19                     | 0.75              |
| 12:j:7:CYS:HB3   | 12:j:10:CYS:SG    | 2.26                     | 0.75              |
| 3:a:1385:THR:OG1 | 3:a:1388:GLY:N    | 2.19                     | 0.75              |
| 4:b:348:ARG:HG2  | 4:b:351:TYR:H     | 1.52                     | 0.75              |
| 10:h:123:MET:HE1 | 10:h:125:LEU:HB2  | 1.69                     | 0.75              |
| 4:b:416:LEU:HD13 | 4:b:466:TRP:HE3   | 1.48                     | 0.75              |
| 4:b:428:ILE:O    | 4:b:445:LYS:NZ    | 2.19                     | 0.75              |
| 7:e:91:LYS:HD3   | 7:e:94:LYS:HD3    | 1.67                     | 0.75              |
| 4:b:757:PRO:HD3  | 4:b:983:ARG:HE    | 1.50                     | 0.75              |
| 3:a:367:PRO:HG2  | 3:a:370:ILE:HB    | 1.69                     | 0.74              |
| 4:b:209:GLU:OE1  | 4:b:788:ARG:NH2   | 2.19                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:604:ARG:NH2   | 4:b:615:MET:SD    | 2.59                     | 0.74              |
| 4:b:1076:HIS:O    | 5:c:31:ASN:ND2    | 2.20                     | 0.74              |
| 4:b:416:LEU:HD13  | 4:b:466:TRP:CE3   | 2.22                     | 0.74              |
| 4:b:1165:ILE:HD12 | 4:b:1187:ASN:HD22 | 1.52                     | 0.74              |
| 3:a:110:CYS:HB3   | 3:a:167:CYS:SG    | 2.28                     | 0.74              |
| 3:a:120:GLU:HB3   | 3:a:124:GLN:HE22  | 1.53                     | 0.74              |
| 4:b:232:SER:O     | 4:b:261:ARG:NH2   | 2.20                     | 0.74              |
| 4:b:1165:ILE:N    | 4:b:1190:ASP:OD1  | 2.18                     | 0.74              |
| 10:h:99:GLY:HA3   | 10:h:118:PHE:HD1  | 1.52                     | 0.73              |
| 6:d:148:LEU:HA    | 6:d:151:PHE:HD2   | 1.51                     | 0.73              |
| 8:f:89:GLU:OE2    | 8:f:136:ARG:NH2   | 2.21                     | 0.73              |
| 3:a:940:ARG:HH21  | 3:a:944:ARG:HH21  | 1.33                     | 0.73              |
| 4:b:35:SER:HA     | 4:b:811:TYR:HE1   | 1.53                     | 0.73              |
| 9:g:88:ASP:HB3    | 9:g:144:ARG:HG3   | 1.70                     | 0.73              |
| 12:j:7:CYS:SG     | 12:j:9:SER:OG     | 2.46                     | 0.73              |
| 3:a:254:GLU:HG2   | 3:a:255:SER:H     | 1.53                     | 0.73              |
| 3:a:350:ARG:HB2   | 4:b:1128:LEU:HD21 | 1.70                     | 0.73              |
| 4:b:664:THR:HG1   | 4:b:678:GLU:N     | 1.86                     | 0.73              |
| 4:b:1104:HIS:NE2  | 4:b:1126:GLY:O    | 2.20                     | 0.73              |
| 4:b:795:ILE:HB    | 4:b:854:LEU:HB2   | 1.71                     | 0.73              |
| 9:g:165:GLU:HB3   | 9:g:168:LEU:HD12  | 1.70                     | 0.72              |
| 5:c:162:GLY:HA3   | 5:c:170:TRP:CE2   | 2.24                     | 0.72              |
| 3:a:1100:ARG:NH2  | 3:a:1330:ASN:OD1  | 2.21                     | 0.72              |
| 7:e:202:SER:N     | 7:e:206:GLY:O     | 2.22                     | 0.72              |
| 3:a:191:THR:OG1   | 3:a:196:GLU:O     | 2.08                     | 0.72              |
| 3:a:1329:THR:HG22 | 3:a:1331:SER:H    | 1.55                     | 0.72              |
| 4:b:74:LEU:HA     | 4:b:85:SER:HA     | 1.70                     | 0.72              |
| 6:d:149:THR:O     | 6:d:221:TYR:OH    | 2.07                     | 0.72              |
| 10:h:93:TYR:HB3   | 10:h:145:ARG:HH21 | 1.54                     | 0.72              |
| 4:b:763:GLN:HG3   | 4:b:765:PRO:HD2   | 1.71                     | 0.71              |
| 4:b:821:GLN:HE22  | 4:b:851:PHE:HA    | 1.53                     | 0.71              |
| 10:h:57:VAL:HG12  | 10:h:144:ILE:HG22 | 1.72                     | 0.71              |
| 3:a:114:LEU:HD11  | 3:a:171:GLN:HE22  | 1.54                     | 0.71              |
| 4:b:43:LEU:O      | 4:b:496:ARG:NH2   | 2.24                     | 0.71              |
| 4:b:227:LYS:HB3   | 4:b:395:GLN:HE21  | 1.55                     | 0.71              |
| 9:g:4:ILE:HG22    | 9:g:77:VAL:HA     | 1.72                     | 0.71              |
| 13:k:65:HIS:HD2   | 13:k:67:PHE:HB2   | 1.54                     | 0.71              |
| 6:d:32:GLU:HG2    | 9:g:41:LYS:HE3    | 1.71                     | 0.70              |
| 4:b:509:ALA:N     | 4:b:513:GLN:O     | 2.24                     | 0.70              |
| 3:a:1282:VAL:HG12 | 3:a:1308:THR:HA   | 1.73                     | 0.70              |
| 2:O:-50:DC:H2'    | 2:O:-49:DG:C8     | 2.25                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:52:DG:H2'     | 1:N:53:DT:C6      | 2.27                     | 0.70              |
| 3:a:205:GLU:OE1   | 3:a:205:GLU:N     | 2.22                     | 0.70              |
| 3:a:830:LYS:NZ    | 3:a:1079:MET:O    | 2.21                     | 0.70              |
| 4:b:1163:CYS:O    | 4:b:1167:GLY:N    | 2.22                     | 0.70              |
| 8:f:128:LYS:HD2   | 8:f:149:GLU:HA    | 1.74                     | 0.70              |
| 11:i:17:ARG:N     | 11:i:26:LEU:O     | 2.23                     | 0.70              |
| 14:l:47:ARG:NH1   | 14:l:48:CYS:O     | 2.25                     | 0.70              |
| 4:b:809:MET:SD    | 4:b:809:MET:N     | 2.63                     | 0.69              |
| 3:a:862:ASN:HD22  | 7:e:174:GLN:HA    | 1.55                     | 0.69              |
| 1:N:42:DT:H2''    | 1:N:43:DC:H5''    | 1.75                     | 0.69              |
| 3:a:407:ARG:NE    | 3:a:411:ASP:OD2   | 2.24                     | 0.69              |
| 4:b:41:LYS:NZ     | 4:b:544:CYS:SG    | 2.66                     | 0.69              |
| 3:a:551:TYR:O     | 13:k:62:LYS:NZ    | 2.24                     | 0.69              |
| 3:a:1107:VAL:HA   | 3:a:1108:ALA:HB3  | 1.75                     | 0.69              |
| 4:b:357:GLN:NE2   | 4:b:367:LEU:O     | 2.26                     | 0.69              |
| 4:b:1156:ASP:HB3  | 4:b:1198:TYR:H    | 1.57                     | 0.69              |
| 9:g:37:SER:HB3    | 9:g:45:ILE:HB     | 1.75                     | 0.69              |
| 3:a:830:LYS:NZ    | 3:a:1077:THR:O    | 2.23                     | 0.69              |
| 3:a:43:GLU:OE1    | 3:a:43:GLU:N      | 2.25                     | 0.69              |
| 3:a:1255:GLU:HB3  | 3:a:1259:MET:HE1  | 1.72                     | 0.69              |
| 4:b:287:ARG:NH2   | 4:b:292:ILE:O     | 2.26                     | 0.69              |
| 4:b:1033:LYS:NZ   | 4:b:1087:PHE:O    | 2.24                     | 0.69              |
| 3:a:1059:HIS:ND1  | 8:f:86:THR:OG1    | 2.19                     | 0.69              |
| 11:i:78:CYS:SG    | 11:i:105:SER:OG   | 2.51                     | 0.69              |
| 3:a:226:GLU:OE2   | 3:a:230:ARG:NH2   | 2.24                     | 0.68              |
| 5:c:41:ILE:HD12   | 5:c:42:PRO:HD2    | 1.75                     | 0.68              |
| 3:a:85:ASP:O      | 3:a:273:ASN:ND2   | 2.26                     | 0.68              |
| 3:a:265:LYS:HD3   | 3:a:322:VAL:HG21  | 1.75                     | 0.68              |
| 4:b:969:ARG:HH12  | 5:c:60:ASP:H      | 1.41                     | 0.68              |
| 9:g:49:LEU:HD12   | 9:g:75:ARG:HG2    | 1.74                     | 0.68              |
| 3:a:1335:ILE:HG23 | 3:a:1339:LEU:HD12 | 1.74                     | 0.68              |
| 6:d:145:MET:HA    | 6:d:148:LEU:HB2   | 1.75                     | 0.68              |
| 7:e:118:PRO:HA    | 7:e:121:MET:HE2   | 1.76                     | 0.68              |
| 4:b:50:SER:OG     | 4:b:410:GLY:N     | 2.24                     | 0.68              |
| 3:a:330:LYS:HA    | 3:a:1405:THR:HG21 | 1.74                     | 0.68              |
| 9:g:1:MET:N       | 9:g:80:LYS:O      | 2.25                     | 0.68              |
| 3:a:119:ASN:OD1   | 3:a:120:GLU:N     | 2.27                     | 0.68              |
| 3:a:1100:ARG:NH2  | 3:a:1351:GLU:OE1  | 2.27                     | 0.68              |
| 3:a:14:VAL:H      | 3:a:1432:GLN:HE22 | 1.40                     | 0.67              |
| 3:a:1162:VAL:HG11 | 11:i:41:PRO:HG3   | 1.76                     | 0.67              |
| 10:h:135:LEU:HD13 | 10:h:137:GLN:HB3  | 1.77                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:-61:DC:H2''  | 2:O:-60:DG:H5'   | 1.75                     | 0.67              |
| 4:b:430:ARG:NH2  | 4:b:433:GLN:OE1  | 2.27                     | 0.67              |
| 4:b:996:ARG:NH2  | 12:j:10:CYS:O    | 2.26                     | 0.67              |
| 12:j:10:CYS:SG   | 12:j:11:GLY:N    | 2.67                     | 0.67              |
| 8:f:76:LYS:O     | 8:f:79:ARG:NE    | 2.28                     | 0.67              |
| 3:a:717:ASN:OD1  | 3:a:720:ARG:NH2  | 2.27                     | 0.67              |
| 3:a:795:GLU:OE1  | 3:a:795:GLU:N    | 2.22                     | 0.67              |
| 3:a:1110:ASN:O   | 3:a:1112:LYS:NZ  | 2.27                     | 0.67              |
| 7:e:124:VAL:HG23 | 7:e:132:ILE:HB   | 1.76                     | 0.67              |
| 8:f:149:GLU:OE2  | 8:f:149:GLU:N    | 2.21                     | 0.67              |
| 4:b:574:SER:HB3  | 4:b:577:ALA:HB2  | 1.76                     | 0.66              |
| 10:h:33:GLN:HG3  | 10:h:36:CYS:H    | 1.60                     | 0.66              |
| 4:b:244:LEU:HB2  | 4:b:250:PHE:CD2  | 2.30                     | 0.66              |
| 5:c:103:ALA:HB3  | 5:c:153:LEU:HB3  | 1.76                     | 0.66              |
| 3:a:873:MET:O    | 3:a:1366:ARG:NH1 | 2.27                     | 0.66              |
| 4:b:307:ASP:OD1  | 4:b:308:TRP:N    | 2.29                     | 0.66              |
| 4:b:894:ASP:OD1  | 4:b:895:ASP:N    | 2.27                     | 0.66              |
| 3:a:451:HIS:CD2  | 3:a:453:MET:HB2  | 2.31                     | 0.66              |
| 4:b:210:LYS:NZ   | 4:b:481:GLN:O    | 2.29                     | 0.66              |
| 3:a:609:ASP:OD1  | 3:a:969:GLN:NE2  | 2.28                     | 0.66              |
| 4:b:310:MET:SD   | 4:b:310:MET:N    | 2.68                     | 0.66              |
| 4:b:798:TYR:OH   | 5:c:66:ARG:NH2   | 2.27                     | 0.66              |
| 3:a:1229:SER:OG  | 3:a:1233:ASP:OD2 | 2.14                     | 0.65              |
| 8:f:125:LEU:HA   | 8:f:130:ILE:HD11 | 1.76                     | 0.65              |
| 1:N:45:DC:H2'    | 1:N:46:DC:H4'    | 1.78                     | 0.65              |
| 3:a:306:ASN:OD1  | 3:a:324:SER:N    | 2.30                     | 0.65              |
| 3:a:365:GLY:HA3  | 3:a:469:ARG:HB2  | 1.78                     | 0.65              |
| 4:b:357:GLN:HE21 | 4:b:368:GLU:HA   | 1.60                     | 0.65              |
| 3:a:114:LEU:O    | 3:a:164:ARG:NH2  | 2.28                     | 0.65              |
| 3:a:208:LEU:HD23 | 3:a:212:LYS:NZ   | 2.11                     | 0.65              |
| 3:a:567:LYS:HD3  | 10:h:95:TYR:HA   | 1.78                     | 0.65              |
| 3:a:951:GLU:OE2  | 3:a:953:ASN:N    | 2.28                     | 0.65              |
| 4:b:757:PRO:HG3  | 4:b:983:ARG:HH21 | 1.61                     | 0.65              |
| 3:a:513:SER:HB2  | 3:a:520:CYS:HB2  | 1.79                     | 0.65              |
| 3:a:871:ASP:OD2  | 3:a:1366:ARG:NH2 | 2.29                     | 0.65              |
| 4:b:60:GLN:HE22  | 4:b:95:ILE:H     | 1.45                     | 0.65              |
| 9:g:115:MET:HG3  | 9:g:116:PRO:HD2  | 1.79                     | 0.65              |
| 6:d:62:ALA:HB1   | 6:d:66:ARG:HH12  | 1.60                     | 0.65              |
| 6:d:183:LEU:HD21 | 9:g:86:VAL:HG12  | 1.77                     | 0.65              |
| 3:a:1312:ASN:OD1 | 3:a:1313:LEU:N   | 2.29                     | 0.65              |
| 4:b:617:ARG:HE   | 4:b:619:ILE:HG22 | 1.59                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:a:147:VAL:HA   | 3:a:170:THR:HA    | 1.78                     | 0.65              |
| 3:a:186:LYS:HG3  | 3:a:187:LYS:H     | 1.62                     | 0.65              |
| 13:k:8:GLU:OE1   | 13:k:37:LYS:NZ    | 2.30                     | 0.65              |
| 3:a:402:ALA:HA   | 3:a:434:ARG:HA    | 1.79                     | 0.64              |
| 4:b:997:GLU:HB2  | 5:c:35:ARG:HG2    | 1.77                     | 0.64              |
| 13:k:81:TYR:HE2  | 13:k:86:ALA:HB2   | 1.62                     | 0.64              |
| 3:a:56:PRO:O     | 3:a:66:LYS:NZ     | 2.30                     | 0.64              |
| 3:a:209:ASN:HA   | 3:a:212:LYS:HZ3   | 1.60                     | 0.64              |
| 3:a:291:GLU:N    | 3:a:291:GLU:OE1   | 2.28                     | 0.64              |
| 6:d:127:ASP:HA   | 6:d:130:LEU:HD12  | 1.77                     | 0.64              |
| 9:g:37:SER:O     | 9:g:45:ILE:N      | 2.30                     | 0.64              |
| 13:k:12:LEU:HA   | 13:k:37:LYS:HG3   | 1.79                     | 0.64              |
| 3:a:841:LEU:HD11 | 3:a:1105:LEU:HD23 | 1.78                     | 0.64              |
| 3:a:757:ASN:O    | 3:a:761:MET:HG2   | 1.98                     | 0.64              |
| 4:b:424:LEU:O    | 4:b:428:ILE:HG13  | 1.98                     | 0.64              |
| 4:b:635:ARG:NH2  | 4:b:742:GLU:OE2   | 2.30                     | 0.64              |
| 4:b:1024:ALA:HA  | 4:b:1027:ILE:HG22 | 1.80                     | 0.64              |
| 7:e:21:GLU:OE1   | 7:e:146:HIS:NE2   | 2.30                     | 0.64              |
| 10:h:2:SER:HG    | 10:h:61:SER:HG    | 1.46                     | 0.64              |
| 3:a:18:GLN:HB3   | 4:b:1215:ARG:HB2  | 1.79                     | 0.64              |
| 3:a:483:ASP:HA   | 4:b:988:GLY:HA2   | 1.79                     | 0.64              |
| 4:b:230:ALA:HA   | 4:b:261:ARG:HH12  | 1.62                     | 0.64              |
| 9:g:119:LEU:HD22 | 9:g:133:SER:HB2   | 1.79                     | 0.64              |
| 7:e:88:VAL:HB    | 7:e:116:ILE:HG23  | 1.79                     | 0.64              |
| 14:l:30:ILE:O    | 14:l:57:LEU:N     | 2.30                     | 0.64              |
| 3:a:534:LEU:HD12 | 3:a:656:TRP:CD2   | 2.33                     | 0.64              |
| 3:a:1151:GLU:HB2 | 3:a:1194:ARG:HB3  | 1.80                     | 0.64              |
| 4:b:605:ARG:NE   | 4:b:691:GLU:OE2   | 2.31                     | 0.64              |
| 4:b:997:GLU:OE1  | 4:b:997:GLU:N     | 2.30                     | 0.64              |
| 3:a:865:GLN:NE2  | 3:a:1373:ASP:OD2  | 2.31                     | 0.63              |
| 7:e:92:THR:O     | 7:e:95:THR:OG1    | 2.16                     | 0.63              |
| 11:i:29:CYS:SG   | 11:i:31:THR:OG1   | 2.50                     | 0.63              |
| 3:a:1216:ILE:O   | 3:a:1219:THR:OG1  | 2.09                     | 0.63              |
| 4:b:499:ASN:OD1  | 4:b:500:THR:N     | 2.30                     | 0.63              |
| 4:b:577:ALA:HB1  | 4:b:589:VAL:HG11  | 1.80                     | 0.63              |
| 3:a:848:ILE:HD11 | 3:a:856:THR:HG22  | 1.79                     | 0.63              |
| 3:a:857:ARG:HH22 | 7:e:170:LEU:HD21  | 1.63                     | 0.63              |
| 4:b:361:LEU:HG   | 4:b:363:HIS:HD2   | 1.63                     | 0.63              |
| 4:b:573:GLN:N    | 4:b:573:GLN:OE1   | 2.30                     | 0.63              |
| 6:d:53:SER:OG    | 6:d:153:ARG:NH1   | 2.32                     | 0.63              |
| 8:f:97:ARG:NH1   | 8:f:124:GLU:OE2   | 2.32                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:l:61:THR:HG22  | 14:l:63:ARG:H     | 1.64                     | 0.63              |
| 3:a:44:THR:N      | 3:a:45:GLN:HA     | 2.14                     | 0.63              |
| 10:h:63:LEU:HD13  | 10:h:141:TYR:HD2  | 1.63                     | 0.63              |
| 3:a:1079:MET:HE1  | 3:a:1097:GLY:HA2  | 1.80                     | 0.62              |
| 4:b:259:TYR:O     | 4:b:267:ARG:NH2   | 2.31                     | 0.62              |
| 9:g:6:ASP:HA      | 9:g:75:ARG:HA     | 1.81                     | 0.62              |
| 11:i:19:ASP:OD2   | 11:i:24:ARG:NH1   | 2.32                     | 0.62              |
| 3:a:760:GLN:HG2   | 3:a:765:VAL:HA    | 1.80                     | 0.62              |
| 3:a:1209:MET:HA   | 3:a:1212:VAL:HG22 | 1.81                     | 0.62              |
| 4:b:930:ALA:HA    | 4:b:931:TYR:C     | 2.23                     | 0.62              |
| 5:c:148:ARG:NH2   | 12:j:63:TYR:O     | 2.33                     | 0.62              |
| 9:g:84:GLY:N      | 9:g:147:ILE:O     | 2.29                     | 0.62              |
| 3:a:464:PRO:HB2   | 3:a:465:TYR:HD2   | 1.64                     | 0.62              |
| 3:a:1199:ARG:NH1  | 3:a:1231:ASP:O    | 2.28                     | 0.62              |
| 5:c:75:MET:HE1    | 5:c:239:PRO:HD3   | 1.82                     | 0.62              |
| 14:l:42:ARG:HG2   | 14:l:43:THR:HG23  | 1.80                     | 0.62              |
| 3:a:443:LEU:HD21  | 3:a:501:LEU:HG    | 1.81                     | 0.62              |
| 3:a:939:ASP:OD2   | 3:a:1023:ARG:NH1  | 2.32                     | 0.62              |
| 4:b:486:TYR:OH    | 4:b:794:ASN:ND2   | 2.31                     | 0.62              |
| 7:e:171:LYS:O     | 7:e:173:SER:N     | 2.33                     | 0.62              |
| 4:b:824:ILE:N     | 4:b:1009:ASP:OD2  | 2.33                     | 0.62              |
| 4:b:31:TRP:HB3    | 4:b:807:ARG:NH2   | 2.15                     | 0.62              |
| 10:h:83:GLN:OE1   | 10:h:87:ARG:NH1   | 2.33                     | 0.62              |
| 4:b:185:THR:O     | 4:b:189:LEU:N     | 2.30                     | 0.62              |
| 3:a:384:ASN:HB2   | 3:a:388:LEU:HD23  | 1.81                     | 0.62              |
| 3:a:1156:PRO:HA   | 3:a:1190:PRO:HA   | 1.82                     | 0.62              |
| 4:b:227:LYS:HB3   | 4:b:395:GLN:NE2   | 2.15                     | 0.62              |
| 4:b:950:ASP:OD2   | 4:b:969:ARG:NH2   | 2.24                     | 0.62              |
| 9:g:143:ILE:HG23  | 9:g:170:ALA:HB2   | 1.81                     | 0.62              |
| 4:b:44:VAL:HG11   | 4:b:200:GLY:HA2   | 1.81                     | 0.61              |
| 3:a:848:ILE:HD13  | 3:a:864:ILE:HD13  | 1.83                     | 0.61              |
| 5:c:235:VAL:HG21  | 12:j:6:ARG:HH22   | 1.65                     | 0.61              |
| 11:i:76:PRO:HB2   | 11:i:77:LYS:HG3   | 1.81                     | 0.61              |
| 3:a:533:LYS:HE3   | 3:a:662:PHE:HB2   | 1.83                     | 0.61              |
| 3:a:372:LYS:NZ    | 13:k:1:MET:O      | 2.28                     | 0.61              |
| 3:a:1318:THR:HG22 | 7:e:141:VAL:HG11  | 1.83                     | 0.61              |
| 5:c:235:VAL:HG13  | 5:c:237:SER:H     | 1.66                     | 0.61              |
| 3:a:254:GLU:HG2   | 3:a:255:SER:N     | 2.15                     | 0.61              |
| 3:a:1148:ILE:HB   | 3:a:1196:GLU:OE1  | 2.01                     | 0.61              |
| 4:b:906:SER:OG    | 4:b:907:GLY:N     | 2.33                     | 0.61              |
| 4:b:1134:GLU:OE1  | 4:b:1134:GLU:N    | 2.31                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:d:145:MET:HE3  | 6:d:145:MET:O     | 2.00                     | 0.61              |
| 8:f:144:GLU:OE2  | 8:f:146:TRP:NE1   | 2.34                     | 0.61              |
| 3:a:95:PHE:HB3   | 3:a:234:MET:HE3   | 1.82                     | 0.61              |
| 3:a:770:VAL:HG22 | 3:a:771:GLU:OE1   | 2.00                     | 0.61              |
| 3:a:973:ILE:HD11 | 3:a:1036:ARG:HB2  | 1.83                     | 0.61              |
| 12:j:45:CYS:SG   | 12:j:46:CYS:N     | 2.73                     | 0.61              |
| 4:b:882:THR:OG1  | 4:b:885:MET:HB2   | 2.00                     | 0.61              |
| 5:c:14:SER:HB2   | 5:c:17:ASN:H      | 1.64                     | 0.61              |
| 10:h:89:LEU:HD22 | 10:h:91:ASP:HB3   | 1.83                     | 0.61              |
| 3:a:959:ASN:OD1  | 3:a:960:ILE:N     | 2.33                     | 0.61              |
| 4:b:210:LYS:HE3  | 4:b:480:SER:HB2   | 1.83                     | 0.61              |
| 4:b:551:PRO:O    | 4:b:554:ILE:HG12  | 2.01                     | 0.61              |
| 4:b:1096:ARG:O   | 4:b:1097:HIS:ND1  | 2.33                     | 0.61              |
| 6:d:203:SER:OG   | 6:d:205:ASP:OD1   | 2.17                     | 0.61              |
| 14:l:41:SER:N    | 14:l:44:ASP:OD2   | 2.32                     | 0.61              |
| 3:a:247:ARG:HB3  | 3:a:262:LEU:HD11  | 1.81                     | 0.60              |
| 4:b:706:GLN:HB3  | 4:b:709:ASP:HB3   | 1.82                     | 0.60              |
| 5:c:73:GLN:OE1   | 5:c:74:SER:N      | 2.34                     | 0.60              |
| 9:g:86:VAL:HA    | 9:g:146:LYS:HA    | 1.83                     | 0.60              |
| 10:h:56:THR:O    | 10:h:145:ARG:N    | 2.34                     | 0.60              |
| 3:a:42:ASP:HB3   | 3:a:45:GLN:HB2    | 1.83                     | 0.60              |
| 3:a:60:SER:OG    | 3:a:64:ASN:O      | 2.14                     | 0.60              |
| 4:b:31:TRP:HB3   | 4:b:807:ARG:HH22  | 1.64                     | 0.60              |
| 3:a:811:GLN:H    | 3:a:811:GLN:CD    | 2.08                     | 0.60              |
| 3:a:1055:ARG:NE  | 8:f:154:ASP:OD2   | 2.34                     | 0.60              |
| 4:b:1112:GLN:HG2 | 4:b:1115:THR:HG22 | 1.83                     | 0.60              |
| 10:h:101:ALA:HA  | 10:h:116:TYR:HA   | 1.83                     | 0.60              |
| 10:h:137:GLN:NE2 | 10:h:139:ASN:O    | 2.32                     | 0.60              |
| 3:a:765:VAL:HB   | 3:a:800:VAL:HG11  | 1.83                     | 0.60              |
| 3:a:1079:MET:HE2 | 3:a:1098:VAL:HG13 | 1.83                     | 0.60              |
| 4:b:121:ASN:HA   | 4:b:207:GLY:HA3   | 1.83                     | 0.60              |
| 4:b:1045:SER:HG  | 4:b:1048:THR:HG1  | 1.43                     | 0.60              |
| 4:b:923:GLU:O    | 4:b:928:ARG:NH2   | 2.31                     | 0.60              |
| 11:i:10:CYS:SG   | 11:i:31:THR:OG1   | 2.60                     | 0.60              |
| 3:a:444:PHE:O    | 3:a:455:MET:HA    | 2.02                     | 0.60              |
| 4:b:242:SER:OG   | 4:b:252:SER:O     | 2.20                     | 0.60              |
| 9:g:121:PHE:HA   | 9:g:131:GLN:HE21  | 1.67                     | 0.60              |
| 3:a:39:GLU:HG3   | 3:a:50:ILE:HG21   | 1.82                     | 0.60              |
| 5:c:115:SER:HB2  | 5:c:141:GLY:HA3   | 1.83                     | 0.60              |
| 7:e:191:LYS:N    | 7:e:194:GLU:OE2   | 2.34                     | 0.60              |
| 3:a:62:ASP:OD1   | 3:a:63:ARG:NH1    | 2.35                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:b:36:ALA:HA    | 4:b:39:ARG:HG2    | 1.83                     | 0.60              |
| 5:c:75:MET:HE1   | 5:c:239:PRO:CD    | 2.32                     | 0.60              |
| 3:a:557:ASP:OD1  | 3:a:559:VAL:N     | 2.31                     | 0.59              |
| 3:a:576:GLN:O    | 3:a:579:SER:OG    | 2.19                     | 0.59              |
| 4:b:104:GLU:OE2  | 14:l:54:ARG:NH2   | 2.35                     | 0.59              |
| 4:b:661:LEU:HD11 | 4:b:684:LEU:HD11  | 1.82                     | 0.59              |
| 4:b:1065:GLN:OE1 | 4:b:1068:GLY:N    | 2.34                     | 0.59              |
| 9:g:65:ASP:OD1   | 9:g:67:SER:OG     | 2.17                     | 0.59              |
| 14:l:28:LYS:HB2  | 14:l:39:SER:HA    | 1.84                     | 0.59              |
| 3:a:379:VAL:O    | 3:a:384:ASN:ND2   | 2.32                     | 0.59              |
| 3:a:1192:LEU:HB3 | 3:a:1241:ARG:HE   | 1.66                     | 0.59              |
| 3:a:1209:MET:HE1 | 3:a:1228:TRP:HB2  | 1.83                     | 0.59              |
| 13:k:85:ASP:O    | 13:k:89:ASN:ND2   | 2.29                     | 0.59              |
| 3:a:500:GLU:OE2  | 4:b:1146:PHE:N    | 2.35                     | 0.59              |
| 3:a:918:GLU:OE1  | 3:a:918:GLU:N     | 2.34                     | 0.59              |
| 9:g:83:LYS:HE2   | 9:g:150:CYS:HB3   | 1.84                     | 0.59              |
| 3:a:563:PRO:HG3  | 3:a:570:PRO:HB3   | 1.84                     | 0.59              |
| 4:b:22:SER:O     | 4:b:654:ARG:NH1   | 2.30                     | 0.59              |
| 11:i:15:TYR:N    | 11:i:28:GLU:O     | 2.35                     | 0.59              |
| 3:a:650:GLN:HA   | 3:a:653:VAL:HG12  | 1.84                     | 0.59              |
| 4:b:548:GLY:N    | 4:b:612:GLU:OE2   | 2.33                     | 0.59              |
| 4:b:969:ARG:NH1  | 5:c:60:ASP:H      | 2.00                     | 0.59              |
| 5:c:182:PRO:HG2  | 5:c:183:TRP:HD1   | 1.67                     | 0.59              |
| 7:e:20:LYS:HB3   | 7:e:35:VAL:HG12   | 1.83                     | 0.59              |
| 4:b:397:ASP:OD2  | 4:b:400:HIS:N     | 2.36                     | 0.59              |
| 1:N:46:DC:H5'    | 1:N:47:DT:H2'     | 1.83                     | 0.59              |
| 3:a:1166:ASP:HA  | 3:a:1169:ILE:HD13 | 1.85                     | 0.59              |
| 4:b:50:SER:HG    | 4:b:410:GLY:H     | 1.49                     | 0.59              |
| 4:b:298:LEU:HA   | 4:b:301:ILE:HG22  | 1.85                     | 0.59              |
| 4:b:360:PHE:HE2  | 4:b:374:LYS:HB3   | 1.68                     | 0.59              |
| 4:b:694:ASP:OD1  | 4:b:696:GLU:N     | 2.32                     | 0.59              |
| 3:a:1277:GLU:OE1 | 3:a:1277:GLU:N    | 2.33                     | 0.59              |
| 4:b:762:ASN:OD1  | 4:b:1023:VAL:N    | 2.35                     | 0.59              |
| 11:i:14:LEU:HB3  | 11:i:27:PHE:HB3   | 1.85                     | 0.59              |
| 3:a:9:ALA:O      | 4:b:1193:GLN:NE2  | 2.36                     | 0.59              |
| 4:b:1076:HIS:HA  | 5:c:35:ARG:HH21   | 1.67                     | 0.59              |
| 3:a:362:ASP:OD2  | 3:a:459:ARG:NE    | 2.33                     | 0.58              |
| 3:a:366:VAL:HG21 | 3:a:460:VAL:HG23  | 1.85                     | 0.58              |
| 4:b:892:LYS:NZ   | 4:b:909:ASP:OD2   | 2.36                     | 0.58              |
| 4:b:1163:CYS:HB3 | 4:b:1166:CYS:HB2  | 1.85                     | 0.58              |
| 4:b:70:ILE:HG22  | 4:b:89:GLU:HA     | 1.83                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:k:17:SER:OG    | 13:k:19:LEU:O     | 2.19                     | 0.58              |
| 4:b:1112:GLN:N    | 4:b:1117:GLN:O    | 2.34                     | 0.58              |
| 5:c:248:ILE:HG21  | 13:k:102:LYS:HB3  | 1.84                     | 0.58              |
| 3:a:1044:TRP:O    | 3:a:1048:ASN:ND2  | 2.34                     | 0.58              |
| 10:h:102:TYR:CZ   | 10:h:115:TYR:HB3  | 2.38                     | 0.58              |
| 3:a:340:LEU:HD21  | 3:a:1429:ILE:HG23 | 1.85                     | 0.58              |
| 3:a:1142:THR:HG23 | 3:a:1145:SER:H    | 1.68                     | 0.58              |
| 3:a:1364:ASN:OD1  | 3:a:1365:TYR:N    | 2.36                     | 0.58              |
| 4:b:891:ASP:OD1   | 4:b:892:LYS:N     | 2.36                     | 0.58              |
| 4:b:1074:ASN:ND2  | 4:b:1077:THR:H    | 2.02                     | 0.58              |
| 11:i:25:LEU:HG    | 11:i:38:ALA:HB3   | 1.86                     | 0.58              |
| 10:h:95:TYR:H     | 10:h:145:ARG:CZ   | 2.17                     | 0.58              |
| 11:i:97:MET:HE3   | 11:i:97:MET:HA    | 1.85                     | 0.58              |
| 3:a:353:ILE:HG21  | 3:a:487:MET:CE    | 2.34                     | 0.58              |
| 4:b:778:MET:HG2   | 4:b:796:LEU:HG    | 1.86                     | 0.58              |
| 4:b:260:GLY:O     | 4:b:267:ARG:NH2   | 2.36                     | 0.58              |
| 11:i:92:ARG:HE    | 11:i:93:LYS:H     | 1.51                     | 0.58              |
| 3:a:185:TRP:HA    | 3:a:187:LYS:HZ1   | 1.68                     | 0.57              |
| 3:a:407:ARG:HB2   | 3:a:430:TRP:CE2   | 2.38                     | 0.57              |
| 3:a:409:SER:OG    | 3:a:411:ASP:OD2   | 2.22                     | 0.57              |
| 3:a:507:VAL:HG23  | 3:a:508:PRO:HD3   | 1.85                     | 0.57              |
| 3:a:1217:LYS:HG2  | 3:a:1221:LYS:HD3  | 1.85                     | 0.57              |
| 3:a:1373:ASP:HA   | 3:a:1376:THR:HG22 | 1.86                     | 0.57              |
| 4:b:842:ASN:CA    | 4:b:999:MET:HE1   | 2.32                     | 0.57              |
| 5:c:165:LYS:HB3   | 13:k:9:LEU:HD13   | 1.85                     | 0.57              |
| 4:b:847:ASP:HB3   | 5:c:167:HIS:CE1   | 2.38                     | 0.57              |
| 5:c:73:GLN:OE1    | 5:c:75:MET:N      | 2.37                     | 0.57              |
| 7:e:143:ASN:HB3   | 7:e:146:HIS:HD2   | 1.69                     | 0.57              |
| 11:i:6:PHE:O      | 11:i:8:ARG:NH1    | 2.36                     | 0.57              |
| 7:e:195:VAL:HG22  | 7:e:213:ILE:HG12  | 1.85                     | 0.57              |
| 9:g:90:THR:O      | 9:g:102:GLN:N     | 2.31                     | 0.57              |
| 9:g:83:LYS:HE2    | 9:g:150:CYS:H     | 1.69                     | 0.57              |
| 1:N:52:DG:H2''    | 1:N:53:DT:H5'     | 1.84                     | 0.57              |
| 3:a:491:VAL:O     | 4:b:1150:ARG:NH2  | 2.37                     | 0.57              |
| 4:b:842:ASN:OD1   | 4:b:844:SER:N     | 2.38                     | 0.57              |
| 6:d:36:LYS:HG2    | 6:d:44:GLU:HG3    | 1.87                     | 0.57              |
| 3:a:848:ILE:HG23  | 3:a:1065:GLY:HA3  | 1.87                     | 0.57              |
| 3:a:881:GLN:NE2   | 3:a:960:ILE:H     | 2.03                     | 0.57              |
| 4:b:308:TRP:CG    | 11:i:2:THR:HG1    | 2.22                     | 0.57              |
| 3:a:961:ARG:HB2   | 3:a:1025:ARG:HH22 | 1.70                     | 0.57              |
| 4:b:301:ILE:HD11  | 4:b:382:ILE:HB    | 1.84                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:277:LYS:N     | 4:b:337:ARG:HH21  | 2.02                     | 0.57              |
| 3:a:208:LEU:CD2   | 3:a:212:LYS:HZ2   | 2.15                     | 0.57              |
| 3:a:232:GLU:N     | 3:a:232:GLU:OE1   | 2.38                     | 0.57              |
| 3:a:261:ASP:OD2   | 3:a:323:LYS:N     | 2.31                     | 0.57              |
| 4:b:542:MET:HE2   | 4:b:636:PRO:HG2   | 1.87                     | 0.57              |
| 4:b:827:ILE:HD11  | 4:b:1014:PRO:HA   | 1.87                     | 0.56              |
| 3:a:1116:LEU:HB3  | 3:a:1329:THR:HG23 | 1.87                     | 0.56              |
| 3:a:1153:TYR:HB2  | 3:a:1192:LEU:HD11 | 1.87                     | 0.56              |
| 5:c:114:TYR:N     | 5:c:117:ASP:OD2   | 2.31                     | 0.56              |
| 10:h:115:TYR:OH   | 10:h:124:ARG:NH1  | 2.38                     | 0.56              |
| 11:i:7:CYS:HB3    | 11:i:10:CYS:O     | 2.05                     | 0.56              |
| 3:a:490:HIS:HB3   | 4:b:1150:ARG:HH12 | 1.69                     | 0.56              |
| 3:a:754:SER:N     | 3:a:757:ASN:OD1   | 2.38                     | 0.56              |
| 3:a:860:LEU:O     | 7:e:174:GLN:NE2   | 2.38                     | 0.56              |
| 4:b:175:ARG:NH2   | 4:b:200:GLY:O     | 2.33                     | 0.56              |
| 5:c:44:LEU:HB2    | 5:c:77:ILE:HD13   | 1.88                     | 0.56              |
| 6:d:152:SER:O     | 6:d:221:TYR:OH    | 2.09                     | 0.56              |
| 7:e:182:ASP:OD1   | 7:e:184:VAL:HG12  | 2.05                     | 0.56              |
| 8:f:98:ALA:O      | 8:f:102:SER:HB2   | 2.06                     | 0.56              |
| 10:h:124:ARG:NE   | 10:h:126:GLU:OE2  | 2.29                     | 0.56              |
| 3:a:537:ARG:NH1   | 3:a:602:ASP:OD2   | 2.39                     | 0.56              |
| 3:a:1063:MET:HE3  | 3:a:1436:ILE:HD13 | 1.88                     | 0.56              |
| 7:e:85:GLU:HG3    | 7:e:87:SER:O      | 2.05                     | 0.56              |
| 3:a:415:LEU:HA    | 3:a:418:SER:HB2   | 1.88                     | 0.56              |
| 3:a:1157:ASP:OD1  | 3:a:1160:SER:N    | 2.38                     | 0.56              |
| 4:b:728:ARG:NH2   | 4:b:1048:THR:O    | 2.37                     | 0.56              |
| 4:b:820:GLY:N     | 4:b:1091:TYR:OH   | 2.39                     | 0.56              |
| 4:b:1050:ILE:HD11 | 4:b:1055:ILE:HD11 | 1.88                     | 0.56              |
| 7:e:94:LYS:HA     | 7:e:97:VAL:HG12   | 1.88                     | 0.56              |
| 12:j:5:VAL:HG12   | 12:j:6:ARG:HG3    | 1.87                     | 0.56              |
| 3:a:170:THR:HB    | 3:a:187:LYS:HD2   | 1.86                     | 0.56              |
| 3:a:745:GLN:O     | 3:a:749:ALA:HB2   | 2.05                     | 0.56              |
| 4:b:486:TYR:HH    | 4:b:1096:ARG:HB3  | 1.70                     | 0.56              |
| 4:b:770:GLN:O     | 4:b:770:GLN:NE2   | 2.39                     | 0.56              |
| 4:b:778:MET:SD    | 4:b:1094:ARG:HB3  | 2.46                     | 0.56              |
| 3:a:471:ASN:OD1   | 3:a:472:LEU:N     | 2.39                     | 0.56              |
| 8:f:86:THR:HG22   | 8:f:89:GLU:CD     | 2.31                     | 0.56              |
| 3:a:443:LEU:HB2   | 3:a:490:HIS:HB2   | 1.88                     | 0.56              |
| 4:b:286:PHE:CE1   | 4:b:378:LEU:HD22  | 2.41                     | 0.56              |
| 4:b:326:ASP:OD1   | 4:b:329:THR:OG1   | 2.14                     | 0.56              |
| 10:h:33:GLN:OE1   | 10:h:34:ASP:N     | 2.38                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:146:MET:O     | 3:a:171:GLN:N     | 2.37                     | 0.56              |
| 3:a:511:ILE:HG21  | 3:a:634:THR:HG21  | 1.87                     | 0.56              |
| 8:f:109:VAL:HG21  | 8:f:124:GLU:HA    | 1.87                     | 0.56              |
| 12:j:21:TYR:HD2   | 12:j:22:LEU:HD22  | 1.71                     | 0.56              |
| 3:a:881:GLN:HE22  | 3:a:960:ILE:H     | 1.54                     | 0.56              |
| 4:b:56:ASP:OD1    | 4:b:57:TYR:N      | 2.39                     | 0.56              |
| 4:b:680:THR:H     | 4:b:683:SER:HB3   | 1.70                     | 0.56              |
| 4:b:861:ASP:N     | 4:b:861:ASP:OD1   | 2.39                     | 0.56              |
| 5:c:142:VAL:HG21  | 12:j:5:VAL:HG22   | 1.87                     | 0.56              |
| 10:h:8:ASP:OD2    | 10:h:30:SER:OG    | 2.12                     | 0.56              |
| 12:j:8:PHE:H      | 12:j:49:MET:CE    | 2.17                     | 0.56              |
| 3:a:959:ASN:OD1   | 3:a:961:ARG:N     | 2.34                     | 0.55              |
| 3:a:1427:ASN:O    | 3:a:1431:GLY:N    | 2.39                     | 0.55              |
| 4:b:466:TRP:CD1   | 4:b:479:VAL:HG21  | 2.41                     | 0.55              |
| 4:b:486:TYR:OH    | 4:b:1096:ARG:HB3  | 2.06                     | 0.55              |
| 3:a:98:LYS:HB3    | 3:a:234:MET:HE1   | 1.89                     | 0.55              |
| 3:a:286:HIS:O     | 3:a:286:HIS:ND1   | 2.36                     | 0.55              |
| 3:a:1220:PHE:HZ   | 3:a:1267:MET:HE1  | 1.71                     | 0.55              |
| 3:a:1325:THR:HA   | 7:e:147:HIS:HA    | 1.88                     | 0.55              |
| 4:b:342:GLY:H     | 4:b:344:LYS:HZ3   | 1.52                     | 0.55              |
| 4:b:342:GLY:N     | 4:b:344:LYS:HZ3   | 2.04                     | 0.55              |
| 4:b:1074:ASN:OD1  | 4:b:1076:HIS:N    | 2.39                     | 0.55              |
| 3:a:1188:GLN:HG3  | 3:a:1243:VAL:HG23 | 1.87                     | 0.55              |
| 4:b:978:ASP:N     | 4:b:989:THR:OG1   | 2.39                     | 0.55              |
| 5:c:251:LEU:HD22  | 13:k:98:LEU:HD21  | 1.87                     | 0.55              |
| 3:a:1361:SER:HB2  | 3:a:1362:TYR:HB3  | 1.88                     | 0.55              |
| 4:b:287:ARG:HE    | 4:b:292:ILE:HA    | 1.71                     | 0.55              |
| 4:b:855:PHE:HB3   | 4:b:970:THR:O     | 2.06                     | 0.55              |
| 5:c:179:GLU:N     | 5:c:229:TYR:O     | 2.37                     | 0.55              |
| 3:a:406:ILE:HB    | 3:a:431:LYS:HB2   | 1.89                     | 0.55              |
| 3:a:563:PRO:HD2   | 10:h:79:TRP:CD1   | 2.41                     | 0.55              |
| 3:a:1009:ASN:HD22 | 3:a:1012:ARG:HH21 | 1.55                     | 0.55              |
| 3:a:362:ASP:O     | 3:a:458:HIS:ND1   | 2.37                     | 0.55              |
| 3:a:961:ARG:HG3   | 3:a:965:GLN:NE2   | 2.18                     | 0.55              |
| 4:b:98:THR:OG1    | 4:b:127:GLY:O     | 2.25                     | 0.55              |
| 6:d:59:ILE:HD13   | 6:d:148:LEU:HD11  | 1.87                     | 0.55              |
| 3:a:857:ARG:NH2   | 7:e:170:LEU:HD21  | 2.21                     | 0.55              |
| 3:a:868:TYR:CZ    | 3:a:1064:VAL:HG21 | 2.42                     | 0.55              |
| 3:a:1293:SER:N    | 3:a:1297:GLU:O    | 2.32                     | 0.55              |
| 3:a:1332:PHE:HA   | 3:a:1335:ILE:HD13 | 1.88                     | 0.55              |
| 3:a:1446:ASP:OD1  | 3:a:1447:GLU:N    | 2.40                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:1037:LEU:O    | 12:j:47:ARG:NH1   | 2.40                     | 0.55              |
| 3:a:1142:THR:O    | 3:a:1145:SER:OG   | 2.22                     | 0.55              |
| 3:a:1169:ILE:HA   | 3:a:1172:LEU:HD12 | 1.88                     | 0.55              |
| 13:k:7:PHE:HB2    | 13:k:11:LEU:HB2   | 1.87                     | 0.55              |
| 13:k:93:SER:O     | 13:k:97:LYS:HG2   | 2.07                     | 0.55              |
| 3:a:768:GLN:NE2   | 3:a:816:HIS:HA    | 2.21                     | 0.55              |
| 4:b:563:MET:HE2   | 4:b:563:MET:HA    | 1.89                     | 0.55              |
| 2:O:-45:DA:H2''   | 3:a:350:ARG:HH12  | 1.71                     | 0.55              |
| 3:a:482:PHE:N     | 4:b:836:GLU:OE1   | 2.40                     | 0.55              |
| 4:b:951:GLN:HB3   | 4:b:967:ARG:HE    | 1.72                     | 0.55              |
| 7:e:40:GLU:N      | 7:e:40:GLU:OE2    | 2.39                     | 0.55              |
| 3:a:825:ILE:HD11  | 4:b:512:ARG:HD3   | 1.88                     | 0.54              |
| 4:b:780:VAL:HG21  | 4:b:817:LEU:HD12  | 1.88                     | 0.54              |
| 7:e:16:PHE:CE2    | 7:e:20:LYS:HD2    | 2.42                     | 0.54              |
| 14:l:38:LEU:HB3   | 14:l:40:LEU:HD23  | 1.89                     | 0.54              |
| 3:a:567:LYS:HE2   | 10:h:47:PHE:HB2   | 1.88                     | 0.54              |
| 3:a:1136:SER:HB2  | 3:a:1274:ARG:HH22 | 1.71                     | 0.54              |
| 4:b:866:TYR:HB2   | 4:b:870:ILE:HG13  | 1.89                     | 0.54              |
| 6:d:62:ALA:HB1    | 6:d:66:ARG:NH1    | 2.22                     | 0.54              |
| 3:a:219:PHE:HB3   | 3:a:224:PHE:HB2   | 1.88                     | 0.54              |
| 3:a:253:ASN:ND2   | 15:r:38:G:N7      | 2.55                     | 0.54              |
| 3:a:438:ASP:HA    | 3:a:460:VAL:HG13  | 1.89                     | 0.54              |
| 3:a:1004:ASN:HD21 | 3:a:1007:ILE:HG12 | 1.72                     | 0.54              |
| 4:b:758:PHE:CZ    | 4:b:1044:ALA:HA   | 2.43                     | 0.54              |
| 3:a:372:LYS:HD3   | 13:k:1:MET:HG3    | 1.90                     | 0.54              |
| 3:a:996:ASN:ND2   | 3:a:1050:GLU:OE1  | 2.27                     | 0.54              |
| 4:b:487:THR:OG1   | 4:b:777:ALA:O     | 2.14                     | 0.54              |
| 4:b:788:ARG:O     | 4:b:789:MET:HE2   | 2.07                     | 0.54              |
| 3:a:549:MET:HE1   | 3:a:655:PHE:CD2   | 2.43                     | 0.54              |
| 3:a:900:ASP:OD1   | 3:a:903:ASN:N     | 2.41                     | 0.54              |
| 3:a:1387:HIS:HB2  | 3:a:1391:ARG:HE   | 1.72                     | 0.54              |
| 4:b:617:ARG:NE    | 4:b:619:ILE:HG22  | 2.23                     | 0.54              |
| 7:e:47:CYS:HA     | 7:e:52:ARG:O      | 2.06                     | 0.54              |
| 10:h:130:ARG:HB2  | 10:h:133:ASN:HB2  | 1.89                     | 0.54              |
| 3:a:577:ILE:O     | 3:a:580:VAL:HG12  | 2.07                     | 0.54              |
| 4:b:302:CYS:SG    | 4:b:303:TYR:N     | 2.81                     | 0.54              |
| 4:b:547:VAL:N     | 4:b:612:GLU:OE2   | 2.40                     | 0.54              |
| 4:b:850:LEU:HG    | 4:b:851:PHE:HD1   | 1.72                     | 0.54              |
| 11:i:5:ARG:NE     | 11:i:6:PHE:H      | 2.05                     | 0.54              |
| 4:b:364:ILE:HG13  | 4:b:365:THR:N     | 2.23                     | 0.54              |
| 4:b:546:SER:OG    | 4:b:632:ARG:N     | 2.32                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:e:112:TYR:CD1   | 7:e:116:ILE:HD11  | 2.42                     | 0.54              |
| 9:g:45:ILE:HA     | 9:g:78:VAL:HG13   | 1.90                     | 0.54              |
| 3:a:808:LEU:HB2   | 4:b:760:ASP:HB2   | 1.89                     | 0.54              |
| 4:b:604:ARG:NH1   | 4:b:692:TYR:O     | 2.41                     | 0.54              |
| 6:d:45:GLU:OE2    | 9:g:5:LYS:NZ      | 2.40                     | 0.54              |
| 4:b:145:ARG:HB3   | 4:b:146:GLU:HB2   | 1.89                     | 0.54              |
| 4:b:842:ASN:ND2   | 4:b:845:SER:OG    | 2.39                     | 0.54              |
| 6:d:67:ARG:NH2    | 6:d:132:GLN:OE1   | 2.41                     | 0.54              |
| 7:e:54:GLN:O      | 7:e:57:MET:HG3    | 2.08                     | 0.54              |
| 10:h:130:ARG:HG3  | 10:h:134:ASN:HB2  | 1.88                     | 0.54              |
| 3:a:568:PRO:HD2   | 3:a:569:LYS:H     | 1.73                     | 0.54              |
| 3:a:741:ASN:HD21  | 3:a:743:VAL:HG12  | 1.73                     | 0.54              |
| 3:a:846:GLU:OE2   | 3:a:846:GLU:N     | 2.39                     | 0.54              |
| 3:a:1315:GLU:OE1  | 3:a:1315:GLU:N    | 2.41                     | 0.54              |
| 3:a:1438:THR:O    | 8:f:92:ARG:NH1    | 2.41                     | 0.54              |
| 3:a:33:ALA:HA     | 3:a:57:ARG:NH2    | 2.23                     | 0.53              |
| 3:a:363:GLN:O     | 3:a:458:HIS:ND1   | 2.40                     | 0.53              |
| 3:a:457:ALA:N     | 3:a:505:CYS:O     | 2.29                     | 0.53              |
| 3:a:654:ASN:OD1   | 3:a:655:PHE:N     | 2.41                     | 0.53              |
| 3:a:791:ASP:OD2   | 3:a:792:TYR:N     | 2.41                     | 0.53              |
| 4:b:749:LEU:HB3   | 4:b:753:ALA:HB3   | 1.89                     | 0.53              |
| 13:k:47:ARG:HD3   | 13:k:60:ALA:HA    | 1.91                     | 0.53              |
| 3:a:368:LYS:HE3   | 13:k:2:ASN:CG     | 2.33                     | 0.53              |
| 3:a:1192:LEU:HD22 | 3:a:1239:ARG:HH21 | 1.72                     | 0.53              |
| 3:a:1325:THR:O    | 7:e:147:HIS:ND1   | 2.41                     | 0.53              |
| 5:c:46:ILE:HD13   | 5:c:67:LEU:HB3    | 1.90                     | 0.53              |
| 10:h:93:TYR:CB    | 10:h:145:ARG:HE   | 2.21                     | 0.53              |
| 3:a:1357:ALA:HA   | 3:a:1361:SER:HB3  | 1.91                     | 0.53              |
| 12:j:19:GLU:O     | 12:j:23:ASN:ND2   | 2.42                     | 0.53              |
| 3:a:852:TYR:CD2   | 8:f:136:ARG:HG3   | 2.43                     | 0.53              |
| 4:b:842:ASN:CG    | 4:b:845:SER:H     | 2.16                     | 0.53              |
| 10:h:63:LEU:HD23  | 10:h:89:LEU:HG    | 1.91                     | 0.53              |
| 9:g:21:ARG:HH11   | 9:g:25:TYR:HB2    | 1.72                     | 0.53              |
| 12:j:23:ASN:OD1   | 12:j:24:LEU:N     | 2.41                     | 0.53              |
| 3:a:424:ILE:HG22  | 3:a:426:LEU:HD12  | 1.90                     | 0.53              |
| 3:a:512:VAL:HA    | 3:a:519:PRO:HA    | 1.90                     | 0.53              |
| 4:b:530:GLY:O     | 4:b:531:GLN:HG3   | 2.08                     | 0.53              |
| 8:f:140:ASP:OD1   | 8:f:141:GLY:N     | 2.41                     | 0.53              |
| 3:a:766:GLY:H     | 3:a:800:VAL:HB    | 1.74                     | 0.53              |
| 4:b:113:TYR:HB2   | 4:b:116:GLU:HB3   | 1.90                     | 0.53              |
| 4:b:129:PHE:HA    | 4:b:167:ILE:HG12  | 1.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:570:VAL:HG13  | 4:b:573:GLN:HB2   | 1.89                     | 0.53              |
| 10:h:83:GLN:HB3   | 10:h:87:ARG:CZ    | 2.39                     | 0.53              |
| 4:b:917:PRO:HA    | 4:b:933:SER:O     | 2.08                     | 0.53              |
| 4:b:1203:LEU:HA   | 4:b:1206:GLU:OE2  | 2.09                     | 0.53              |
| 5:c:101:LEU:HB3   | 5:c:155:LEU:HB2   | 1.91                     | 0.53              |
| 3:a:14:VAL:N      | 3:a:1432:GLN:HE22 | 2.07                     | 0.53              |
| 3:a:849:MET:HE3   | 3:a:1063:MET:HE1  | 1.89                     | 0.53              |
| 4:b:561:TRP:O     | 4:b:595:ARG:NH1   | 2.34                     | 0.53              |
| 4:b:574:SER:OG    | 4:b:591:ARG:NH2   | 2.42                     | 0.53              |
| 4:b:1060:ARG:O    | 4:b:1060:ARG:NH1  | 2.36                     | 0.53              |
| 4:b:1076:HIS:HD2  | 13:k:40:HIS:CD2   | 2.27                     | 0.53              |
| 4:b:1207:LEU:HD22 | 4:b:1214:PRO:HG3  | 1.91                     | 0.53              |
| 4:b:146:GLU:HG2   | 4:b:147:LEU:H     | 1.73                     | 0.52              |
| 5:c:240:VAL:O     | 5:c:243:VAL:HG22  | 2.09                     | 0.52              |
| 3:a:1359:ASP:N    | 3:a:1359:ASP:OD1  | 2.42                     | 0.52              |
| 6:d:33:PHE:CZ     | 9:g:80:LYS:HG2    | 2.44                     | 0.52              |
| 9:g:3:PHE:HB2     | 9:g:80:LYS:NZ     | 2.25                     | 0.52              |
| 11:i:10:CYS:O     | 11:i:12:ASN:N     | 2.42                     | 0.52              |
| 3:a:452:LYS:HZ1   | 4:b:1141:HIS:HA   | 1.73                     | 0.52              |
| 3:a:877:HIS:CD2   | 3:a:1056:SER:HA   | 2.43                     | 0.52              |
| 3:a:1031:VAL:HG12 | 3:a:1032:LEU:HD23 | 1.91                     | 0.52              |
| 3:a:1312:ASN:ND2  | 3:a:1315:GLU:OE2  | 2.43                     | 0.52              |
| 2:O:-37:DT:H1'    | 2:O:-36:DT:H5'    | 1.90                     | 0.52              |
| 3:a:874:ASP:OD1   | 3:a:875:ALA:N     | 2.43                     | 0.52              |
| 4:b:371:GLU:N     | 4:b:371:GLU:OE1   | 2.36                     | 0.52              |
| 5:c:255:VAL:O     | 5:c:258:ILE:HG22  | 2.08                     | 0.52              |
| 11:i:27:PHE:N     | 11:i:36:GLU:O     | 2.34                     | 0.52              |
| 3:a:531:ILE:O     | 3:a:535:THR:HG22  | 2.10                     | 0.52              |
| 3:a:566:ILE:HD13  | 10:h:96:VAL:HG12  | 1.91                     | 0.52              |
| 3:a:1161:THR:HG22 | 3:a:1163:ILE:H    | 1.74                     | 0.52              |
| 4:b:394:ASP:OD1   | 4:b:395:GLN:N     | 2.41                     | 0.52              |
| 5:c:230:MET:N     | 5:c:230:MET:SD    | 2.83                     | 0.52              |
| 9:g:6:ASP:OD2     | 9:g:75:ARG:NE     | 2.41                     | 0.52              |
| 4:b:78:THR:HG23   | 4:b:79:THR:H      | 1.74                     | 0.52              |
| 4:b:210:LYS:HZ3   | 4:b:211:VAL:H     | 1.57                     | 0.52              |
| 4:b:1153:GLU:N    | 4:b:1153:GLU:OE1  | 2.43                     | 0.52              |
| 6:d:139:LYS:NZ    | 6:d:143:ASN:OD1   | 2.42                     | 0.52              |
| 9:g:94:CYS:HB3    | 9:g:127:PRO:HG2   | 1.90                     | 0.52              |
| 12:j:20:SER:HA    | 12:j:23:ASN:HD21  | 1.74                     | 0.52              |
| 3:a:868:TYR:HD2   | 3:a:1058:VAL:HG11 | 1.73                     | 0.52              |
| 4:b:58:THR:O      | 4:b:62:ILE:HG12   | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:b:259:TYR:OH   | 4:b:279:ASP:OD2   | 2.25                     | 0.52              |
| 4:b:304:ASP:OD2  | 4:b:307:ASP:N     | 2.38                     | 0.52              |
| 5:c:196:ASP:OD1  | 5:c:197:SER:N     | 2.43                     | 0.52              |
| 10:h:63:LEU:HD13 | 10:h:141:TYR:CD2  | 2.44                     | 0.52              |
| 3:a:285:PRO:HB2  | 3:a:287:HIS:NE2   | 2.25                     | 0.52              |
| 3:a:1100:ARG:CZ  | 3:a:1104:ILE:HD11 | 2.39                     | 0.52              |
| 4:b:1093:GLN:N   | 4:b:1093:GLN:OE1  | 2.43                     | 0.52              |
| 5:c:76:ASP:OD2   | 5:c:128:ASN:N     | 2.43                     | 0.52              |
| 5:c:162:GLY:HA3  | 5:c:170:TRP:CZ2   | 2.44                     | 0.52              |
| 6:d:40:HIS:CG    | 9:g:73:LYS:HD2    | 2.44                     | 0.52              |
| 7:e:3:GLN:HE21   | 7:e:5:ASN:HB3     | 1.74                     | 0.52              |
| 15:r:35:C:P      | 15:r:35:C:H2'     | 2.50                     | 0.52              |
| 2:O:-42:DA:OP1   | 4:b:857:ARG:NH2   | 2.43                     | 0.52              |
| 3:a:134:ARG:NH2  | 3:a:220:THR:O     | 2.28                     | 0.52              |
| 3:a:367:PRO:HB3  | 3:a:466:SER:HA    | 1.91                     | 0.52              |
| 3:a:644:LYS:O    | 3:a:648:ASN:ND2   | 2.42                     | 0.52              |
| 3:a:1063:MET:HE2 | 3:a:1436:ILE:HA   | 1.92                     | 0.52              |
| 4:b:295:GLY:N    | 11:i:11:ASN:O     | 2.43                     | 0.52              |
| 4:b:1000:PRO:HB2 | 4:b:1072:MET:HE3  | 1.92                     | 0.52              |
| 3:a:176:LYS:HA   | 3:a:181:LEU:HA    | 1.90                     | 0.52              |
| 4:b:611:PRO:HG2  | 4:b:685:LEU:HD21  | 1.91                     | 0.52              |
| 4:b:643:ASP:N    | 4:b:643:ASP:OD1   | 2.41                     | 0.52              |
| 10:h:43:ASN:ND2  | 10:h:46:LEU:HD13  | 2.25                     | 0.52              |
| 10:h:135:LEU:O   | 10:h:137:GLN:N    | 2.43                     | 0.52              |
| 3:a:1297:GLU:N   | 3:a:1297:GLU:OE1  | 2.42                     | 0.51              |
| 4:b:260:GLY:C    | 4:b:267:ARG:HH22  | 2.18                     | 0.51              |
| 4:b:706:GLN:OE1  | 4:b:707:PRO:HD2   | 2.09                     | 0.51              |
| 4:b:1181:GLU:OE2 | 4:b:1187:ASN:N    | 2.44                     | 0.51              |
| 7:e:26:ARG:NH2   | 7:e:187:TYR:O     | 2.37                     | 0.51              |
| 8:f:70:LYS:O     | 8:f:71:GLU:HG3    | 2.10                     | 0.51              |
| 12:j:9:SER:OG    | 12:j:45:CYS:HB2   | 2.10                     | 0.51              |
| 1:N:31:DA:H2''   | 1:N:32:DA:C8      | 2.45                     | 0.51              |
| 3:a:871:ASP:OD1  | 3:a:872:GLY:N     | 2.43                     | 0.51              |
| 4:b:911:ILE:HG21 | 4:b:966:VAL:HG21  | 1.92                     | 0.51              |
| 5:c:254:LYS:O    | 5:c:257:SER:OG    | 2.23                     | 0.51              |
| 6:d:206:GLU:O    | 6:d:209:ARG:HG3   | 2.09                     | 0.51              |
| 5:c:217:ASP:OD1  | 5:c:217:ASP:N     | 2.42                     | 0.51              |
| 10:h:128:ASN:ND2 | 10:h:131:ASN:OD1  | 2.44                     | 0.51              |
| 3:a:482:PHE:O    | 4:b:989:THR:HG22  | 2.10                     | 0.51              |
| 3:a:1053:PHE:O   | 3:a:1056:SER:OG   | 2.24                     | 0.51              |
| 3:a:1373:ASP:O   | 3:a:1377:THR:HG23 | 2.10                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:1438:THR:OG1  | 8:f:92:ARG:NH1    | 2.42                     | 0.51              |
| 3:a:120:GLU:HG3   | 3:a:123:ARG:NH2   | 2.25                     | 0.51              |
| 3:a:169:ASN:OD1   | 3:a:170:THR:N     | 2.36                     | 0.51              |
| 4:b:494:HIS:HA    | 4:b:497:ARG:NH1   | 2.25                     | 0.51              |
| 4:b:1198:TYR:O    | 4:b:1201:LYS:HG3  | 2.09                     | 0.51              |
| 10:h:33:GLN:HG3   | 10:h:35:GLN:H     | 1.74                     | 0.51              |
| 3:a:566:ILE:HB    | 10:h:96:VAL:HB    | 1.93                     | 0.51              |
| 4:b:100:PRO:O     | 4:b:101:MET:HE2   | 2.10                     | 0.51              |
| 4:b:1112:GLN:HG3  | 4:b:1114:LEU:H    | 1.76                     | 0.51              |
| 10:h:93:TYR:HB3   | 10:h:145:ARG:HE   | 1.76                     | 0.51              |
| 3:a:682:THR:O     | 3:a:685:GLU:HG3   | 2.10                     | 0.51              |
| 5:c:69:LEU:HG     | 12:j:6:ARG:HD2    | 1.91                     | 0.51              |
| 10:h:93:TYR:HB3   | 10:h:145:ARG:NH2  | 2.22                     | 0.51              |
| 3:a:35:ILE:HD13   | 3:a:241:VAL:HG21  | 1.92                     | 0.51              |
| 3:a:912:LEU:O     | 3:a:979:SER:N     | 2.43                     | 0.51              |
| 8:f:147:SER:O     | 8:f:150:GLU:HG2   | 2.11                     | 0.51              |
| 9:g:21:ARG:NH1    | 9:g:25:TYR:HB2    | 2.26                     | 0.51              |
| 3:a:631:HIS:NE2   | 3:a:879:GLU:OE2   | 2.39                     | 0.51              |
| 3:a:1121:GLU:HG3  | 3:a:1123:GLY:H    | 1.76                     | 0.51              |
| 4:b:420:LEU:HB3   | 4:b:453:ILE:HD12  | 1.93                     | 0.51              |
| 4:b:431:TYR:HD2   | 4:b:445:LYS:HE3   | 1.76                     | 0.51              |
| 4:b:551:PRO:HB3   | 4:b:628:THR:HG21  | 1.93                     | 0.51              |
| 6:d:56:ARG:NE     | 6:d:157:GLN:OE1   | 2.44                     | 0.51              |
| 6:d:126:ILE:HA    | 6:d:129:LEU:HD13  | 1.92                     | 0.51              |
| 10:h:118:PHE:O    | 10:h:120:GLY:N    | 2.44                     | 0.51              |
| 10:h:129:TYR:CZ   | 10:h:130:ARG:HD2  | 2.46                     | 0.51              |
| 1:N:65:DA:H61     | 2:O:-65:DC:H42    | 0.69                     | 0.51              |
| 3:a:242:PRO:C     | 3:a:247:ARG:HH12  | 2.17                     | 0.51              |
| 3:a:852:TYR:HD2   | 8:f:136:ARG:HG3   | 1.76                     | 0.51              |
| 4:b:651:LEU:H     | 4:b:651:LEU:HD23  | 1.75                     | 0.51              |
| 10:h:130:ARG:HD3  | 10:h:130:ARG:H    | 1.75                     | 0.51              |
| 3:a:993:LEU:HG    | 3:a:1046:LEU:HD22 | 1.93                     | 0.50              |
| 3:a:1173:HIS:CE1  | 3:a:1227:ILE:HG23 | 2.45                     | 0.50              |
| 4:b:79:THR:HA     | 4:b:81:SER:H      | 1.75                     | 0.50              |
| 4:b:708:GLU:HA    | 4:b:711:GLU:HG2   | 1.93                     | 0.50              |
| 4:b:1006:ILE:HD12 | 12:j:45:CYS:HB3   | 1.92                     | 0.50              |
| 5:c:22:LEU:HG     | 5:c:25:VAL:HG21   | 1.92                     | 0.50              |
| 3:a:446:ARG:HD2   | 3:a:447:GLN:O     | 2.12                     | 0.50              |
| 4:b:779:GLY:O     | 4:b:795:ILE:HA    | 2.11                     | 0.50              |
| 4:b:867:GLY:HA3   | 4:b:868:MET:C     | 2.36                     | 0.50              |
| 5:c:238:ILE:HD12  | 5:c:239:PRO:HD2   | 1.92                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:d:14:ARG:O     | 6:d:17:LYS:HG2    | 2.11                     | 0.50              |
| 3:a:18:GLN:O     | 4:b:1215:ARG:N    | 2.44                     | 0.50              |
| 3:a:192:GLY:HA3  | 3:a:196:GLU:HB3   | 1.94                     | 0.50              |
| 3:a:543:LEU:O    | 3:a:547:LEU:HG    | 2.12                     | 0.50              |
| 3:a:726:ARG:NH1  | 3:a:765:VAL:O     | 2.41                     | 0.50              |
| 3:a:1329:THR:HB  | 3:a:1335:ILE:HD11 | 1.93                     | 0.50              |
| 4:b:878:GLN:OE1  | 4:b:878:GLN:N     | 2.43                     | 0.50              |
| 7:e:2:ASP:O      | 7:e:7:ARG:NH1     | 2.34                     | 0.50              |
| 9:g:111:THR:HG22 | 9:g:114:LEU:HG    | 1.92                     | 0.50              |
| 3:a:18:GLN:OE1   | 3:a:19:PHE:N      | 2.44                     | 0.50              |
| 4:b:803:LEU:HD22 | 12:j:52:THR:HG21  | 1.93                     | 0.50              |
| 3:a:14:VAL:HB    | 3:a:1430:LEU:HD21 | 1.92                     | 0.50              |
| 3:a:156:ASP:OD1  | 3:a:156:ASP:N     | 2.42                     | 0.50              |
| 3:a:266:LEU:O    | 3:a:269:ILE:HG22  | 2.12                     | 0.50              |
| 3:a:546:VAL:HG23 | 3:a:577:ILE:HD12  | 1.94                     | 0.50              |
| 3:a:1063:MET:CE  | 3:a:1436:ILE:HA   | 2.41                     | 0.50              |
| 4:b:653:VAL:HG22 | 4:b:689:LEU:HD13  | 1.94                     | 0.50              |
| 12:j:36:LEU:HD22 | 12:j:47:ARG:HG3   | 1.94                     | 0.50              |
| 3:a:557:ASP:HA   | 13:k:26:LYS:HE3   | 1.94                     | 0.50              |
| 4:b:38:PHE:CD2   | 4:b:811:TYR:HB3   | 2.46                     | 0.50              |
| 4:b:50:SER:HG    | 4:b:410:GLY:N     | 2.07                     | 0.50              |
| 4:b:1045:SER:O   | 4:b:1047:PHE:N    | 2.45                     | 0.50              |
| 9:g:45:ILE:HG23  | 9:g:78:VAL:HG22   | 1.93                     | 0.50              |
| 3:a:172:PRO:HG3  | 3:a:185:TRP:CZ2   | 2.47                     | 0.50              |
| 5:c:259:LEU:O    | 5:c:262:LEU:HG    | 2.12                     | 0.50              |
| 8:f:112:GLU:HG2  | 8:f:123:LYS:NZ    | 2.27                     | 0.50              |
| 10:h:81:PRO:HB2  | 13:k:54:ARG:HH22  | 1.77                     | 0.50              |
| 11:i:17:ARG:HG3  | 11:i:28:GLU:HB3   | 1.92                     | 0.50              |
| 3:a:335:ARG:HA   | 3:a:339:ASN:HB2   | 1.92                     | 0.50              |
| 3:a:351:THR:OG1  | 3:a:352:VAL:N     | 2.43                     | 0.50              |
| 3:a:827:THR:HA   | 3:a:830:LYS:HG2   | 1.92                     | 0.50              |
| 3:a:1284:MET:C   | 3:a:1285:MET:HE2  | 2.36                     | 0.50              |
| 4:b:428:ILE:O    | 4:b:432:MET:HE3   | 2.12                     | 0.50              |
| 4:b:1110:PRO:O   | 4:b:1111:MET:HE2  | 2.12                     | 0.50              |
| 5:c:66:ARG:HD2   | 12:j:2:ILE:HD11   | 1.94                     | 0.50              |
| 7:e:109:ILE:HG13 | 7:e:133:GLU:OE2   | 2.11                     | 0.50              |
| 3:a:567:LYS:CG   | 3:a:568:PRO:HD3   | 2.42                     | 0.50              |
| 3:a:949:ASP:OD1  | 3:a:950:GLY:N     | 2.45                     | 0.50              |
| 4:b:351:TYR:CE2  | 4:b:355:ILE:HD11  | 2.47                     | 0.50              |
| 4:b:446:LEU:HA   | 4:b:449:ASN:HD22  | 1.77                     | 0.50              |
| 4:b:773:MET:HE1  | 4:b:987:LYS:HD3   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:1065:GLN:NE2  | 4:b:1067:ARG:H    | 2.10                     | 0.50              |
| 6:d:131:GLU:HG3   | 6:d:136:GLY:H     | 1.77                     | 0.50              |
| 11:i:73:ARG:HH12  | 11:i:112:SER:HA   | 1.77                     | 0.50              |
| 11:i:103:CYS:SG   | 11:i:105:SER:OG   | 2.69                     | 0.50              |
| 13:k:81:TYR:CE2   | 13:k:86:ALA:HB2   | 2.45                     | 0.50              |
| 3:a:232:GLU:OE2   | 3:a:233:TRP:NE1   | 2.45                     | 0.49              |
| 3:a:376:TYR:OH    | 3:a:495:GLU:OE2   | 2.26                     | 0.49              |
| 3:a:853:ASP:HB3   | 3:a:855:THR:HG22  | 1.93                     | 0.49              |
| 3:a:311:GLN:CG    | 3:a:312:PRO:HD3   | 2.36                     | 0.49              |
| 3:a:529:CYS:SG    | 3:a:533:LYS:NZ    | 2.83                     | 0.49              |
| 3:a:940:ARG:NH2   | 3:a:944:ARG:HH21  | 2.06                     | 0.49              |
| 11:i:5:ARG:HB3    | 11:i:14:LEU:HB2   | 1.93                     | 0.49              |
| 3:a:91:PHE:N      | 3:a:297:GLN:HE22  | 2.10                     | 0.49              |
| 3:a:119:ASN:O     | 3:a:123:ARG:NH1   | 2.45                     | 0.49              |
| 3:a:185:TRP:CD1   | 3:a:187:LYS:HE2   | 2.46                     | 0.49              |
| 3:a:647:GLY:O     | 3:a:651:LYS:HB2   | 2.12                     | 0.49              |
| 3:a:899:VAL:HG13  | 3:a:929:LEU:HD23  | 1.95                     | 0.49              |
| 5:c:37:MET:HE1    | 5:c:244:VAL:HA    | 1.95                     | 0.49              |
| 10:h:10:PHE:CE2   | 10:h:38:LEU:HB2   | 2.47                     | 0.49              |
| 3:a:43:GLU:HG2    | 3:a:44:THR:N      | 2.27                     | 0.49              |
| 3:a:1094:VAL:HG13 | 3:a:1113:THR:HG21 | 1.94                     | 0.49              |
| 4:b:797:TYR:O     | 12:j:1:MET:HE2    | 2.13                     | 0.49              |
| 4:b:850:LEU:HG    | 4:b:851:PHE:CD1   | 2.48                     | 0.49              |
| 3:a:311:GLN:HG2   | 3:a:312:PRO:CD    | 2.37                     | 0.49              |
| 3:a:591:PHE:HA    | 3:a:595:THR:HG21  | 1.93                     | 0.49              |
| 3:a:1000:LEU:N    | 3:a:1011:GLN:OE1  | 2.44                     | 0.49              |
| 4:b:309:GLN:OE1   | 4:b:392:ARG:NH2   | 2.43                     | 0.49              |
| 4:b:809:MET:O     | 4:b:812:LEU:N     | 2.44                     | 0.49              |
| 4:b:1112:GLN:HB3  | 4:b:1117:GLN:H    | 1.77                     | 0.49              |
| 10:h:100:THR:O    | 10:h:117:SER:N    | 2.32                     | 0.49              |
| 10:h:118:PHE:HB2  | 10:h:121:LEU:HB2  | 1.94                     | 0.49              |
| 3:a:210:ILE:O     | 3:a:214:ILE:HD12  | 2.12                     | 0.49              |
| 3:a:353:ILE:HG21  | 3:a:487:MET:HE1   | 1.93                     | 0.49              |
| 3:a:757:ASN:HB3   | 4:b:1021:MET:HE1  | 1.94                     | 0.49              |
| 5:c:59:ALA:O      | 5:c:63:ILE:HG12   | 2.13                     | 0.49              |
| 9:g:3:PHE:HB2     | 9:g:80:LYS:HZ3    | 1.77                     | 0.49              |
| 10:h:101:ALA:HB2  | 10:h:116:TYR:CE1  | 2.47                     | 0.49              |
| 3:a:46:THR:O      | 3:a:47:ARG:HG2    | 2.12                     | 0.49              |
| 3:a:598:LEU:O     | 10:h:25:ARG:NH2   | 2.45                     | 0.49              |
| 3:a:1004:ASN:ND2  | 7:e:167:ARG:HD2   | 2.27                     | 0.49              |
| 4:b:766:ARG:NH1   | 4:b:1020:ARG:HD3  | 2.28                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:d:144:THR:O     | 6:d:148:LEU:N    | 2.46                     | 0.49              |
| 10:h:94:ASP:H     | 10:h:145:ARG:NE  | 2.10                     | 0.49              |
| 3:a:559:VAL:HA    | 10:h:78:SER:OG   | 2.13                     | 0.49              |
| 3:a:779:PHE:CZ    | 4:b:517:THR:HA   | 2.47                     | 0.49              |
| 3:a:802:ASN:HB3   | 3:a:806:ARG:HD2  | 1.95                     | 0.49              |
| 5:c:175:ALA:HB3   | 5:c:233:GLU:HB3  | 1.95                     | 0.49              |
| 8:f:74:ILE:HD12   | 8:f:75:PRO:HD2   | 1.94                     | 0.49              |
| 8:f:135:ARG:HD2   | 8:f:143:PHE:CD2  | 2.47                     | 0.49              |
| 9:g:110:VAL:HG11  | 9:g:163:ILE:HD11 | 1.95                     | 0.49              |
| 13:k:12:LEU:HD23  | 13:k:12:LEU:H    | 1.77                     | 0.49              |
| 1:N:53:DT:H2''    | 1:N:54:DG:H8     | 1.77                     | 0.49              |
| 2:O:-33:DT:H2''   | 2:O:-32:DT:C6    | 2.47                     | 0.49              |
| 3:a:149:GLU:O     | 3:a:165:GLY:HA3  | 2.12                     | 0.49              |
| 3:a:914:GLU:HG2   | 3:a:979:SER:O    | 2.12                     | 0.49              |
| 3:a:1114:PRO:HB2  | 3:a:1311:VAL:HB  | 1.95                     | 0.49              |
| 9:g:129:SER:O     | 9:g:135:ASP:HB3  | 2.13                     | 0.49              |
| 11:i:74:GLU:OE2   | 11:i:81:ARG:HD3  | 2.12                     | 0.49              |
| 3:a:81:PHE:HE1    | 3:a:243:PRO:HD3  | 1.78                     | 0.49              |
| 3:a:768:GLN:HE21  | 3:a:816:HIS:HA   | 1.77                     | 0.49              |
| 4:b:699:GLU:OE1   | 4:b:699:GLU:N    | 2.43                     | 0.49              |
| 4:b:760:ASP:OD1   | 4:b:761:HIS:N    | 2.46                     | 0.49              |
| 5:c:99:LEU:O      | 5:c:157:CYS:N    | 2.30                     | 0.49              |
| 11:i:5:ARG:HE     | 11:i:6:PHE:H     | 1.58                     | 0.49              |
| 3:a:55:ASP:OD1    | 3:a:58:LEU:N     | 2.46                     | 0.48              |
| 3:a:573:SER:HB3   | 3:a:576:GLN:HB2  | 1.94                     | 0.48              |
| 3:a:666:ILE:HD12  | 3:a:666:ILE:H    | 1.78                     | 0.48              |
| 3:a:862:ASN:HA    | 7:e:174:GLN:HB3  | 1.94                     | 0.48              |
| 3:a:1419:ASP:OD1  | 3:a:1420:ASP:N   | 2.46                     | 0.48              |
| 5:c:241:ASP:OD1   | 5:c:241:ASP:N    | 2.45                     | 0.48              |
| 11:i:75:CYS:SG    | 11:i:79:HIS:N    | 2.85                     | 0.48              |
| 3:a:38:PRO:HA     | 3:a:270:LEU:HD23 | 1.95                     | 0.48              |
| 3:a:81:PHE:CE1    | 3:a:243:PRO:HD3  | 2.48                     | 0.48              |
| 3:a:449:SER:H     | 4:b:1133:MET:HE2 | 1.78                     | 0.48              |
| 4:b:411:PRO:O     | 4:b:415:GLN:HG2  | 2.14                     | 0.48              |
| 4:b:806:THR:HB    | 4:b:1044:ALA:HB3 | 1.95                     | 0.48              |
| 4:b:1106:ARG:NH1  | 4:b:1109:GLY:H   | 2.11                     | 0.48              |
| 4:b:1171:VAL:HG12 | 4:b:1182:CYS:HB2 | 1.95                     | 0.48              |
| 4:b:1205:GLN:HA   | 4:b:1208:MET:SD  | 2.53                     | 0.48              |
| 5:c:161:LYS:O     | 5:c:170:TRP:NE1  | 2.45                     | 0.48              |
| 7:e:29:PHE:CE2    | 7:e:65:THR:HA    | 2.48                     | 0.48              |
| 15:r:35:C:OP1     | 15:r:35:C:H3'    | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:a:96:ILE:O     | 3:a:99:ILE:HG22   | 2.13                     | 0.48              |
| 3:a:567:LYS:HG2  | 3:a:568:PRO:HD3   | 1.95                     | 0.48              |
| 3:a:843:LYS:HD3  | 3:a:846:GLU:OE1   | 2.14                     | 0.48              |
| 4:b:582:VAL:HA   | 4:b:626:ILE:HB    | 1.94                     | 0.48              |
| 4:b:865:LYS:NZ   | 4:b:869:SER:HB2   | 2.28                     | 0.48              |
| 3:a:1270:ASN:OD1 | 3:a:1271:ILE:HD12 | 2.13                     | 0.48              |
| 4:b:336:ARG:HG3  | 4:b:338:GLY:H     | 1.77                     | 0.48              |
| 4:b:805:THR:OG1  | 4:b:809:MET:HE3   | 2.12                     | 0.48              |
| 7:e:40:GLU:HA    | 7:e:43:LYS:HG2    | 1.95                     | 0.48              |
| 3:a:991:LYS:HA   | 3:a:994:GLN:HG2   | 1.94                     | 0.48              |
| 4:b:394:ASP:HB2  | 11:i:91:ARG:NH2   | 2.24                     | 0.48              |
| 4:b:874:PHE:HE1  | 4:b:914:LYS:HE2   | 1.79                     | 0.48              |
| 4:b:901:PRO:HA   | 4:b:949:VAL:HG12  | 1.94                     | 0.48              |
| 5:c:166:GLU:HA   | 13:k:9:LEU:HD21   | 1.94                     | 0.48              |
| 6:d:142:LYS:O    | 6:d:146:GLN:N     | 2.35                     | 0.48              |
| 9:g:147:ILE:HG23 | 9:g:159:ALA:HB1   | 1.94                     | 0.48              |
| 12:j:12:LYS:O    | 12:j:14:VAL:HG23  | 2.14                     | 0.48              |
| 3:a:446:ARG:NH2  | 3:a:478:TYR:O     | 2.47                     | 0.48              |
| 3:a:871:ASP:CG   | 3:a:873:MET:H     | 2.21                     | 0.48              |
| 3:a:1116:LEU:HG  | 3:a:1308:THR:HG21 | 1.96                     | 0.48              |
| 4:b:252:SER:HB3  | 4:b:362:PRO:HG2   | 1.95                     | 0.48              |
| 4:b:1033:LYS:HD3 | 4:b:1059:LEU:HD11 | 1.94                     | 0.48              |
| 7:e:179:GLN:HG3  | 7:e:181:ALA:H     | 1.79                     | 0.48              |
| 2:O:-57:DA:H2''  | 2:O:-56:DA:C8     | 2.49                     | 0.48              |
| 3:a:2:VAL:HG13   | 3:a:410:GLY:HA2   | 1.96                     | 0.48              |
| 4:b:120:ARG:NH2  | 4:b:956:THR:O     | 2.46                     | 0.48              |
| 4:b:702:LEU:HD23 | 4:b:738:PHE:HA    | 1.95                     | 0.48              |
| 4:b:954:VAL:HG23 | 4:b:964:VAL:HG22  | 1.94                     | 0.48              |
| 5:c:55:THR:CG2   | 5:c:152:GLU:H     | 2.27                     | 0.48              |
| 3:a:172:PRO:HG3  | 3:a:185:TRP:CH2   | 2.48                     | 0.48              |
| 3:a:242:PRO:O    | 3:a:247:ARG:NH1   | 2.33                     | 0.48              |
| 3:a:399:HIS:O    | 3:a:435:HIS:ND1   | 2.38                     | 0.48              |
| 3:a:632:VAL:HG13 | 3:a:962:ARG:HD3   | 1.94                     | 0.48              |
| 4:b:276:ILE:HG23 | 4:b:335:GLY:HA3   | 1.96                     | 0.48              |
| 4:b:759:PRO:HD2  | 4:b:1046:PRO:HB3  | 1.95                     | 0.48              |
| 4:b:872:GLU:HG2  | 4:b:916:THR:HA    | 1.94                     | 0.48              |
| 11:i:13:MET:HE1  | 11:i:15:TYR:HA    | 1.96                     | 0.48              |
| 2:O:-45:DA:H4'   | 3:a:350:ARG:NH2   | 2.29                     | 0.48              |
| 3:a:619:LYS:HG3  | 3:a:620:LYS:N     | 2.29                     | 0.48              |
| 3:a:959:ASN:HD21 | 3:a:961:ARG:HB3   | 1.78                     | 0.48              |
| 4:b:209:GLU:OE1  | 4:b:485:ARG:NE    | 2.43                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:546:SER:OG    | 4:b:631:GLY:N     | 2.47                     | 0.48              |
| 8:f:79:ARG:HD2    | 8:f:144:GLU:OE2   | 2.13                     | 0.48              |
| 13:k:21:ILE:HG22  | 13:k:33:ILE:HD12  | 1.95                     | 0.48              |
| 3:a:446:ARG:HB2   | 3:a:487:MET:HG3   | 1.96                     | 0.48              |
| 3:a:525:GLN:HB2   | 4:b:1015:HIS:CG   | 2.49                     | 0.48              |
| 3:a:999:VAL:H     | 3:a:1011:GLN:NE2  | 2.12                     | 0.48              |
| 3:a:1390:ASN:HD22 | 3:a:1402:PHE:HD2  | 1.61                     | 0.48              |
| 4:b:238:ALA:HB3   | 4:b:256:VAL:HB    | 1.95                     | 0.48              |
| 4:b:445:LYS:O     | 4:b:448:ILE:HG22  | 2.13                     | 0.48              |
| 4:b:744:HIS:CG    | 4:b:745:PRO:HD2   | 2.49                     | 0.48              |
| 4:b:865:LYS:HZ3   | 4:b:869:SER:HB2   | 1.78                     | 0.48              |
| 3:a:182:VAL:HG12  | 3:a:201:VAL:HA    | 1.96                     | 0.47              |
| 3:a:185:TRP:HA    | 3:a:187:LYS:NZ    | 2.29                     | 0.47              |
| 3:a:446:ARG:NH2   | 3:a:479:ASN:O     | 2.44                     | 0.47              |
| 3:a:804:TYR:O     | 4:b:761:HIS:ND1   | 2.39                     | 0.47              |
| 5:c:34:ARG:HG2    | 5:c:176:ILE:HD13  | 1.95                     | 0.47              |
| 6:d:69:ALA:HA     | 6:d:72:ARG:HE     | 1.78                     | 0.47              |
| 6:d:139:LYS:HG3   | 6:d:143:ASN:HD21  | 1.78                     | 0.47              |
| 7:e:180:ARG:HH12  | 7:e:192:ARG:HB2   | 1.79                     | 0.47              |
| 13:k:7:PHE:HB2    | 13:k:11:LEU:HD12  | 1.95                     | 0.47              |
| 13:k:65:HIS:CD2   | 13:k:67:PHE:HB2   | 2.44                     | 0.47              |
| 1:N:41:DT:H5"     | 4:b:426:LYS:NZ    | 2.28                     | 0.47              |
| 2:O:-57:DA:H2"    | 2:O:-56:DA:H8     | 1.79                     | 0.47              |
| 3:a:943:LEU:HA    | 3:a:946:VAL:HG12  | 1.95                     | 0.47              |
| 3:a:1041:ALA:O    | 3:a:1045:VAL:HG13 | 2.13                     | 0.47              |
| 3:a:1070:GLN:NE2  | 4:b:1137:CYS:SG   | 2.76                     | 0.47              |
| 4:b:1008:PRO:HB3  | 4:b:1087:PHE:HE1  | 1.78                     | 0.47              |
| 7:e:136:ASN:OD1   | 7:e:137:GLU:N     | 2.47                     | 0.47              |
| 3:a:365:GLY:HA2   | 3:a:463:ILE:HD13  | 1.96                     | 0.47              |
| 3:a:874:ASP:HA    | 3:a:1058:VAL:HG12 | 1.96                     | 0.47              |
| 4:b:298:LEU:HD12  | 11:i:6:PHE:CZ     | 2.50                     | 0.47              |
| 4:b:328:GLU:OE1   | 4:b:328:GLU:N     | 2.35                     | 0.47              |
| 4:b:459:TYR:O     | 4:b:463:THR:HG22  | 2.14                     | 0.47              |
| 4:b:582:VAL:O     | 4:b:585:VAL:HG12  | 2.14                     | 0.47              |
| 4:b:641:GLU:CD    | 4:b:652:LYS:HB2   | 2.40                     | 0.47              |
| 7:e:169:ARG:NH2   | 8:f:140:ASP:OD2   | 2.47                     | 0.47              |
| 10:h:100:THR:N    | 10:h:117:SER:O    | 2.45                     | 0.47              |
| 3:a:367:PRO:HA    | 3:a:463:ILE:O     | 2.14                     | 0.47              |
| 3:a:1059:HIS:CE1  | 8:f:87:LYS:H      | 2.32                     | 0.47              |
| 4:b:82:ASP:HB2    | 4:b:140:ILE:HD11  | 1.96                     | 0.47              |
| 4:b:210:LYS:HD2   | 4:b:210:LYS:HA    | 1.51                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:b:282:ILE:HA   | 4:b:285:ILE:HD13  | 1.97                     | 0.47              |
| 4:b:923:GLU:C    | 4:b:928:ARG:HH22  | 2.22                     | 0.47              |
| 7:e:2:ASP:C      | 7:e:7:ARG:HH12    | 2.20                     | 0.47              |
| 7:e:121:MET:O    | 7:e:124:VAL:HG12  | 2.14                     | 0.47              |
| 8:f:130:ILE:HB   | 8:f:148:VAL:HG11  | 1.96                     | 0.47              |
| 9:g:137:ILE:O    | 9:g:137:ILE:HG13  | 2.14                     | 0.47              |
| 12:j:17:LYS:HB3  | 12:j:39:LEU:HD11  | 1.95                     | 0.47              |
| 3:a:474:VAL:O    | 3:a:477:PRO:HD2   | 2.15                     | 0.47              |
| 3:a:957:PRO:HG2  | 3:a:1018:PHE:CD1  | 2.50                     | 0.47              |
| 3:a:1100:ARG:O   | 3:a:1104:ILE:HD12 | 2.15                     | 0.47              |
| 3:a:1198:ASP:CG  | 3:a:1201:ALA:H    | 2.22                     | 0.47              |
| 3:a:1263:ILE:O   | 3:a:1267:MET:HG2  | 2.14                     | 0.47              |
| 4:b:38:PHE:HD2   | 4:b:811:TYR:HB3   | 1.79                     | 0.47              |
| 4:b:396:ASP:OD1  | 4:b:403:LYS:NZ    | 2.47                     | 0.47              |
| 4:b:466:TRP:NE1  | 4:b:479:VAL:HG11  | 2.29                     | 0.47              |
| 4:b:641:GLU:OE1  | 4:b:641:GLU:N     | 2.47                     | 0.47              |
| 5:c:84:ARG:NE    | 13:k:11:LEU:HD13  | 2.29                     | 0.47              |
| 6:d:165:GLN:O    | 6:d:168:LYS:HG2   | 2.15                     | 0.47              |
| 9:g:46:LEU:HG    | 9:g:77:VAL:O      | 2.14                     | 0.47              |
| 1:N:47:DT:H2"    | 1:N:48:DT:C5      | 2.48                     | 0.47              |
| 2:O:-54:DC:H2"   | 2:O:-53:DA:OP2    | 2.14                     | 0.47              |
| 3:a:14:VAL:H     | 3:a:1432:GLN:NE2  | 2.10                     | 0.47              |
| 3:a:115:LEU:HB3  | 3:a:122:MET:CE    | 2.45                     | 0.47              |
| 3:a:219:PHE:O    | 3:a:223:GLY:N     | 2.47                     | 0.47              |
| 3:a:794:PRO:HB2  | 3:a:799:PHE:HB3   | 1.96                     | 0.47              |
| 3:a:800:VAL:HA   | 3:a:812:GLU:OE1   | 2.15                     | 0.47              |
| 3:a:1149:ALA:HB1 | 11:i:45:ARG:HH21  | 1.79                     | 0.47              |
| 3:a:1342:GLU:O   | 3:a:1345:ARG:HG2  | 2.14                     | 0.47              |
| 4:b:348:ARG:HG2  | 4:b:351:TYR:N     | 2.26                     | 0.47              |
| 7:e:91:LYS:O     | 7:e:94:LYS:HG2    | 2.14                     | 0.47              |
| 10:h:101:ALA:HB2 | 10:h:116:TYR:CZ   | 2.49                     | 0.47              |
| 3:a:101:LYS:HG2  | 3:a:139:TRP:CZ2   | 2.50                     | 0.47              |
| 3:a:114:LEU:HD11 | 3:a:171:GLN:NE2   | 2.27                     | 0.47              |
| 3:a:239:LEU:HD12 | 3:a:240:PRO:HD2   | 1.96                     | 0.47              |
| 3:a:816:HIS:CD2  | 4:b:764:SER:H     | 2.33                     | 0.47              |
| 3:a:1192:LEU:HA  | 3:a:1241:ARG:HG2  | 1.97                     | 0.47              |
| 3:a:1198:ASP:OD2 | 3:a:1201:ALA:N    | 2.46                     | 0.47              |
| 4:b:299:GLU:HB3  | 4:b:571:PRO:HG3   | 1.97                     | 0.47              |
| 4:b:364:ILE:HG23 | 4:b:585:VAL:HG11  | 1.97                     | 0.47              |
| 4:b:800:GLN:OE1  | 4:b:822:ASN:N     | 2.23                     | 0.47              |
| 4:b:806:THR:O    | 4:b:809:MET:HE1   | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:c:114:TYR:CD1   | 5:c:140:ASN:HB3   | 2.49                     | 0.47              |
| 5:c:148:ARG:O     | 5:c:150:GLY:N     | 2.48                     | 0.47              |
| 10:h:126:GLU:C    | 10:h:130:ARG:HH12 | 2.22                     | 0.47              |
| 11:i:22:ASN:ND2   | 11:i:24:ARG:HD3   | 2.30                     | 0.47              |
| 4:b:425:THR:HA    | 4:b:428:ILE:HD12  | 1.97                     | 0.47              |
| 4:b:429:PHE:HD2   | 4:b:430:ARG:HH12  | 1.63                     | 0.47              |
| 4:b:850:LEU:HD13  | 12:j:8:PHE:CD2    | 2.50                     | 0.47              |
| 4:b:1181:GLU:OE1  | 4:b:1188:LYS:HG2  | 2.14                     | 0.47              |
| 5:c:73:GLN:HE22   | 5:c:75:MET:HE3    | 1.79                     | 0.47              |
| 6:d:183:LEU:HD13  | 9:g:144:ARG:HG2   | 1.95                     | 0.47              |
| 3:a:552:TRP:CZ3   | 3:a:651:LYS:HD2   | 2.50                     | 0.47              |
| 3:a:568:PRO:CD    | 3:a:569:LYS:H     | 2.28                     | 0.47              |
| 3:a:1406:VAL:N    | 3:a:1407:GLU:OE1  | 2.47                     | 0.47              |
| 4:b:700:SER:O     | 4:b:700:SER:OG    | 2.28                     | 0.47              |
| 4:b:918:ILE:HA    | 4:b:919:SER:C     | 2.39                     | 0.47              |
| 3:a:455:MET:SD    | 3:a:455:MET:N     | 2.88                     | 0.47              |
| 3:a:635:ARG:HH22  | 3:a:876:ALA:C     | 2.19                     | 0.47              |
| 3:a:1288:ASP:HA   | 3:a:1302:PRO:HA   | 1.95                     | 0.47              |
| 4:b:638:PHE:CD2   | 4:b:743:ILE:HD13  | 2.49                     | 0.47              |
| 8:f:71:GLU:OE1    | 8:f:73:ALA:HB3    | 2.14                     | 0.47              |
| 8:f:119:ARG:HG2   | 8:f:119:ARG:HH21  | 1.80                     | 0.47              |
| 3:a:101:LYS:HE3   | 3:a:139:TRP:CZ3   | 2.50                     | 0.46              |
| 3:a:722:LEU:HD12  | 3:a:799:PHE:CE2   | 2.50                     | 0.46              |
| 3:a:1031:VAL:HA   | 3:a:1035:TYR:HD1  | 1.79                     | 0.46              |
| 4:b:75:ALA:HB1    | 4:b:80:GLU:CD     | 2.40                     | 0.46              |
| 4:b:1025:HIS:O    | 4:b:1028:GLU:HG3  | 2.15                     | 0.46              |
| 5:c:104:PHE:HA    | 5:c:152:GLU:OE1   | 2.16                     | 0.46              |
| 10:h:5:LEU:HD11   | 10:h:61:SER:HB3   | 1.97                     | 0.46              |
| 1:N:50:DG:C2      | 1:N:51:DA:C4      | 3.03                     | 0.46              |
| 3:a:427:GLN:OE1   | 3:a:427:GLN:N     | 2.37                     | 0.46              |
| 3:a:825:ILE:HD11  | 4:b:512:ARG:HH11  | 1.81                     | 0.46              |
| 4:b:530:GLY:C     | 4:b:532:ALA:H     | 2.22                     | 0.46              |
| 4:b:642:ASP:HA    | 4:b:649:LYS:HG2   | 1.97                     | 0.46              |
| 10:h:58:THR:HG22  | 10:h:143:LEU:HB2  | 1.97                     | 0.46              |
| 2:O:-45:DA:H3'    | 2:O:-44:DG:C8     | 2.51                     | 0.46              |
| 3:a:434:ARG:HD2   | 3:a:435:HIS:O     | 2.15                     | 0.46              |
| 3:a:1408:ILE:HG23 | 3:a:1409:LEU:HD12 | 1.96                     | 0.46              |
| 3:a:1441:PHE:CZ   | 8:f:89:GLU:HA     | 2.51                     | 0.46              |
| 4:b:394:ASP:CB    | 11:i:91:ARG:HH22  | 2.25                     | 0.46              |
| 4:b:848:ARG:NH1   | 12:j:8:PHE:O      | 2.47                     | 0.46              |
| 7:e:32:GLN:O      | 7:e:35:VAL:HG22   | 2.15                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:g:146:LYS:HD2  | 9:g:168:LEU:HD11 | 1.98                     | 0.46              |
| 10:h:91:ASP:C    | 10:h:93:TYR:H    | 2.24                     | 0.46              |
| 11:i:21:GLU:HG2  | 11:i:22:ASN:N    | 2.30                     | 0.46              |
| 11:i:91:ARG:HA   | 11:i:95:THR:HG21 | 1.96                     | 0.46              |
| 13:k:65:HIS:CG   | 13:k:66:PRO:HD2  | 2.50                     | 0.46              |
| 2:O:-53:DA:H2''  | 2:O:-52:DC:O5'   | 2.15                     | 0.46              |
| 2:O:-31:DT:H2''  | 2:O:-30:DT:C6    | 2.49                     | 0.46              |
| 4:b:216:GLU:HB3  | 4:b:500:THR:HB   | 1.96                     | 0.46              |
| 4:b:1206:GLU:HA  | 4:b:1209:ALA:HB3 | 1.97                     | 0.46              |
| 5:c:113:VAL:HG12 | 5:c:144:ILE:HD13 | 1.97                     | 0.46              |
| 8:f:84:TYR:CZ    | 8:f:152:ILE:HD11 | 2.51                     | 0.46              |
| 10:h:97:MET:SD   | 10:h:98:TYR:N    | 2.88                     | 0.46              |
| 10:h:98:TYR:CE1  | 10:h:139:ASN:HB2 | 2.51                     | 0.46              |
| 11:i:21:GLU:HG2  | 11:i:22:ASN:H    | 1.80                     | 0.46              |
| 11:i:22:ASN:HB3  | 11:i:24:ARG:HH11 | 1.80                     | 0.46              |
| 4:b:629:ASP:OD2  | 4:b:629:ASP:N    | 2.48                     | 0.46              |
| 2:O:-55:DG:H2''  | 2:O:-54:DC:C6    | 2.51                     | 0.46              |
| 3:a:452:LYS:NZ   | 4:b:1141:HIS:HA  | 2.30                     | 0.46              |
| 3:a:569:LYS:NZ   | 5:c:221:TYR:HB2  | 2.30                     | 0.46              |
| 3:a:788:SER:HB2  | 11:i:69:PRO:HG3  | 1.98                     | 0.46              |
| 3:a:843:LYS:HG2  | 3:a:1402:PHE:HB2 | 1.97                     | 0.46              |
| 4:b:77:HIS:HB3   | 4:b:80:GLU:OE1   | 2.16                     | 0.46              |
| 4:b:79:THR:HA    | 4:b:81:SER:N     | 2.31                     | 0.46              |
| 4:b:85:SER:HB3   | 4:b:139:ALA:N    | 2.18                     | 0.46              |
| 4:b:123:THR:O    | 4:b:125:SER:N    | 2.48                     | 0.46              |
| 4:b:428:ILE:HG22 | 4:b:432:MET:HE3  | 1.97                     | 0.46              |
| 6:d:220:LEU:HG   | 6:d:221:TYR:H    | 1.81                     | 0.46              |
| 7:e:3:GLN:HG2    | 7:e:5:ASN:H      | 1.79                     | 0.46              |
| 7:e:80:VAL:HG12  | 7:e:109:ILE:HB   | 1.96                     | 0.46              |
| 13:k:34:THR:HG22 | 13:k:72:LYS:HG2  | 1.96                     | 0.46              |
| 1:N:31:DA:H2''   | 1:N:32:DA:H8     | 1.81                     | 0.46              |
| 3:a:21:LEU:HD21  | 3:a:95:PHE:HE1   | 1.81                     | 0.46              |
| 3:a:503:GLN:C    | 3:a:504:LEU:HD12 | 2.41                     | 0.46              |
| 4:b:486:TYR:CZ   | 4:b:1096:ARG:HD2 | 2.50                     | 0.46              |
| 4:b:841:MET:SD   | 4:b:990:ILE:HG12 | 2.56                     | 0.46              |
| 6:d:147:TYR:O    | 6:d:151:PHE:N    | 2.45                     | 0.46              |
| 3:a:66:LYS:HG2   | 3:a:69:THR:H     | 1.81                     | 0.46              |
| 3:a:399:HIS:NE2  | 3:a:462:VAL:HG21 | 2.31                     | 0.46              |
| 3:a:506:ALA:HB1  | 3:a:508:PRO:HD2  | 1.98                     | 0.46              |
| 3:a:780:VAL:HG22 | 3:a:781:ASP:CG   | 2.40                     | 0.46              |
| 3:a:804:TYR:OH   | 3:a:816:HIS:NE2  | 2.47                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:a:958:VAL:HG11 | 3:a:1052:GLN:HB3  | 1.97                     | 0.46              |
| 3:a:1035:TYR:HB3 | 3:a:1037:LEU:HD23 | 1.96                     | 0.46              |
| 3:a:1042:PHE:O   | 3:a:1045:VAL:HG22 | 2.15                     | 0.46              |
| 3:a:1208:THR:O   | 3:a:1211:GLN:HG3  | 2.15                     | 0.46              |
| 3:a:1315:GLU:HG2 | 3:a:1316:VAL:N    | 2.31                     | 0.46              |
| 4:b:44:VAL:HG21  | 4:b:200:GLY:HA2   | 1.98                     | 0.46              |
| 4:b:194:GLU:HA   | 4:b:784:ASN:HD22  | 1.80                     | 0.46              |
| 13:k:38:GLU:HG2  | 13:k:42:LEU:HD12  | 1.98                     | 0.46              |
| 3:a:344:ARG:NH2  | 4:b:1120:GLU:OE1  | 2.49                     | 0.46              |
| 3:a:356:ASP:OD1  | 3:a:358:ASN:N     | 2.39                     | 0.46              |
| 3:a:1111:MET:C   | 3:a:1113:THR:H    | 2.24                     | 0.46              |
| 3:a:1202:MET:HE3 | 3:a:1209:MET:HB3  | 1.96                     | 0.46              |
| 4:b:822:ASN:HD22 | 12:j:48:ARG:HB2   | 1.81                     | 0.46              |
| 6:d:172:LEU:HD21 | 6:d:176:GLU:HB2   | 1.97                     | 0.46              |
| 7:e:136:ASN:ND2  | 7:e:138:ALA:HB3   | 2.30                     | 0.46              |
| 9:g:108:VAL:HA   | 9:g:159:ALA:O     | 2.16                     | 0.46              |
| 3:a:545:GLN:O    | 3:a:549:MET:HG2   | 2.16                     | 0.46              |
| 3:a:741:ASN:OD1  | 3:a:743:VAL:N     | 2.49                     | 0.46              |
| 3:a:837:ILE:HD13 | 3:a:840:ARG:HH12  | 1.79                     | 0.46              |
| 3:a:1133:LEU:O   | 3:a:1136:SER:OG   | 2.33                     | 0.46              |
| 4:b:916:THR:N    | 4:b:934:LYS:O     | 2.48                     | 0.46              |
| 4:b:1082:MET:HA  | 4:b:1082:MET:HE2  | 1.97                     | 0.46              |
| 4:b:1202:LEU:HA  | 4:b:1205:GLN:OE1  | 2.16                     | 0.46              |
| 7:e:68:SER:O     | 7:e:72:PHE:N      | 2.42                     | 0.46              |
| 12:j:16:ASP:OD1  | 12:j:16:ASP:N     | 2.46                     | 0.46              |
| 1:N:49:DC:H1'    | 1:N:50:DG:C8      | 2.51                     | 0.45              |
| 3:a:783:THR:O    | 3:a:784:LEU:HD23  | 2.15                     | 0.45              |
| 3:a:1168:GLU:O   | 3:a:1171:GLN:NE2  | 2.50                     | 0.45              |
| 3:a:1259:MET:O   | 3:a:1263:ILE:HG12 | 2.16                     | 0.45              |
| 4:b:281:PRO:HD2  | 4:b:284:ILE:HD13  | 1.98                     | 0.45              |
| 4:b:1099:VAL:O   | 4:b:1103:ILE:HG12 | 2.16                     | 0.45              |
| 5:c:91:HIS:HB2   | 5:c:96:SER:HB3    | 1.97                     | 0.45              |
| 5:c:148:ARG:HH22 | 12:j:64:ASN:HA    | 1.80                     | 0.45              |
| 7:e:167:ARG:HA   | 7:e:167:ARG:HD3   | 1.61                     | 0.45              |
| 9:g:85:GLU:O     | 9:g:147:ILE:N     | 2.48                     | 0.45              |
| 1:N:48:DT:H2''   | 1:N:49:DC:OP2     | 2.14                     | 0.45              |
| 1:N:53:DT:H4'    | 3:a:1387:HIS:CE1  | 2.51                     | 0.45              |
| 3:a:451:HIS:HA   | 3:a:1070:GLN:HG2  | 1.97                     | 0.45              |
| 4:b:233:PRO:O    | 4:b:260:GLY:N     | 2.45                     | 0.45              |
| 7:e:21:GLU:CD    | 7:e:146:HIS:HE2   | 2.23                     | 0.45              |
| 1:N:50:DG:H4'    | 1:N:51:DA:OP1     | 2.15                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:1444:MET:HE2  | 9:g:58:ARG:HB2    | 1.98                     | 0.45              |
| 4:b:428:ILE:HG23  | 4:b:445:LYS:HD2   | 1.98                     | 0.45              |
| 4:b:874:PHE:HA    | 4:b:913:GLY:O     | 2.16                     | 0.45              |
| 4:b:1084:GLN:OE1  | 4:b:1084:GLN:N    | 2.49                     | 0.45              |
| 5:c:210:GLU:OE1   | 5:c:229:TYR:OH    | 2.32                     | 0.45              |
| 5:c:240:VAL:HA    | 5:c:243:VAL:HG22  | 1.98                     | 0.45              |
| 10:h:47:PHE:HZ    | 10:h:146:ARG:HD3  | 1.81                     | 0.45              |
| 10:h:144:ILE:O    | 10:h:144:ILE:HG13 | 2.15                     | 0.45              |
| 12:j:36:LEU:CD2   | 12:j:47:ARG:HG3   | 2.47                     | 0.45              |
| 13:k:9:LEU:HD12   | 13:k:10:PHE:N     | 2.31                     | 0.45              |
| 14:l:49:LYS:C     | 14:l:49:LYS:HD2   | 2.41                     | 0.45              |
| 3:a:556:TRP:CD1   | 3:a:558:GLY:H     | 2.34                     | 0.45              |
| 3:a:1407:GLU:HA   | 3:a:1410:PHE:HD2  | 1.79                     | 0.45              |
| 4:b:1005:GLY:HA3  | 5:c:176:ILE:O     | 2.17                     | 0.45              |
| 7:e:203:GLU:OE1   | 7:e:203:GLU:N     | 2.49                     | 0.45              |
| 9:g:39:THR:N      | 9:g:43:GLY:O      | 2.49                     | 0.45              |
| 13:k:103:THR:HA   | 13:k:106:GLU:OE2  | 2.17                     | 0.45              |
| 3:a:368:LYS:HG2   | 3:a:462:VAL:HG12  | 1.99                     | 0.45              |
| 3:a:665:GLY:HA3   | 4:b:1069:PHE:HE1  | 1.81                     | 0.45              |
| 3:a:1112:LYS:HE2  | 3:a:1112:LYS:HB2  | 1.82                     | 0.45              |
| 3:a:1284:MET:SD   | 3:a:1284:MET:N    | 2.90                     | 0.45              |
| 4:b:144:GLY:HA2   | 4:b:145:ARG:HA    | 1.71                     | 0.45              |
| 4:b:341:LEU:HD23  | 4:b:344:LYS:HG3   | 1.97                     | 0.45              |
| 4:b:530:GLY:O     | 4:b:532:ALA:N     | 2.50                     | 0.45              |
| 4:b:704:ALA:O     | 4:b:741:CYS:HA    | 2.16                     | 0.45              |
| 5:c:44:LEU:HD12   | 5:c:160:LYS:O     | 2.17                     | 0.45              |
| 6:d:118:THR:O     | 6:d:121:LYS:HG3   | 2.17                     | 0.45              |
| 10:h:61:SER:OG    | 10:h:62:SER:N     | 2.49                     | 0.45              |
| 3:a:66:LYS:CG     | 3:a:69:THR:H      | 2.29                     | 0.45              |
| 3:a:344:ARG:HD3   | 4:b:1129:ARG:HA   | 1.99                     | 0.45              |
| 3:a:375:THR:OG1   | 3:a:376:TYR:N     | 2.48                     | 0.45              |
| 3:a:476:SER:OG    | 3:a:477:PRO:HD3   | 2.17                     | 0.45              |
| 4:b:130:VAL:HG23  | 4:b:167:ILE:HG13  | 1.98                     | 0.45              |
| 4:b:357:GLN:O     | 4:b:366:GLN:HB3   | 2.17                     | 0.45              |
| 5:c:60:ASP:O      | 5:c:63:ILE:N      | 2.50                     | 0.45              |
| 7:e:5:ASN:ND2     | 7:e:52:ARG:HH22   | 2.14                     | 0.45              |
| 8:f:133:VAL:HG21  | 9:g:58:ARG:HH21   | 1.81                     | 0.45              |
| 1:N:59:DT:H2"     | 1:N:60:DC:C5      | 2.52                     | 0.45              |
| 3:a:119:ASN:HB3   | 3:a:122:MET:CE    | 2.43                     | 0.45              |
| 4:b:1058:LEU:HD23 | 4:b:1061:GLU:OE1  | 2.17                     | 0.45              |
| 6:d:123:LEU:HD12  | 6:d:145:MET:HG3   | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:g:78:VAL:HB     | 9:g:80:LYS:NZ     | 2.31                     | 0.45              |
| 9:g:78:VAL:HB     | 9:g:80:LYS:HZ1    | 1.82                     | 0.45              |
| 10:h:12:VAL:HG23  | 10:h:26:ILE:HG23  | 1.99                     | 0.45              |
| 3:a:209:ASN:HA    | 3:a:212:LYS:NZ    | 2.30                     | 0.45              |
| 3:a:216:VAL:HA    | 3:a:219:PHE:CE2   | 2.51                     | 0.45              |
| 3:a:243:PRO:O     | 3:a:246:VAL:HG12  | 2.17                     | 0.45              |
| 3:a:372:LYS:HE2   | 13:k:1:MET:HE3    | 1.99                     | 0.45              |
| 3:a:391:LEU:HG    | 3:a:400:PRO:O     | 2.16                     | 0.45              |
| 3:a:575:LYS:HE2   | 10:h:120:GLY:HA2  | 1.99                     | 0.45              |
| 3:a:877:HIS:O     | 3:a:957:PRO:HA    | 2.17                     | 0.45              |
| 4:b:274:PRO:HA    | 4:b:275:TYR:HA    | 1.44                     | 0.45              |
| 4:b:438:GLU:HB3   | 4:b:439:ALA:HB2   | 1.99                     | 0.45              |
| 4:b:486:TYR:CZ    | 4:b:1096:ARG:HB3  | 2.52                     | 0.45              |
| 5:c:88:CYS:HB3    | 5:c:92:CYS:SG     | 2.57                     | 0.45              |
| 6:d:184:ALA:HB3   | 9:g:144:ARG:NH2   | 2.32                     | 0.45              |
| 6:d:206:GLU:HA    | 6:d:209:ARG:HG3   | 1.99                     | 0.45              |
| 7:e:21:GLU:OE1    | 7:e:143:ASN:ND2   | 2.42                     | 0.45              |
| 10:h:10:PHE:HB3   | 10:h:28:ALA:HB1   | 1.98                     | 0.45              |
| 10:h:128:ASN:OD1  | 10:h:131:ASN:ND2  | 2.39                     | 0.45              |
| 10:h:135:LEU:HB3  | 10:h:137:GLN:N    | 2.32                     | 0.45              |
| 1:N:41:DT:H1'     | 1:N:42:DT:H5'     | 1.98                     | 0.45              |
| 3:a:1155:ASP:CG   | 3:a:1162:VAL:HG23 | 2.42                     | 0.45              |
| 3:a:1224:LEU:HA   | 3:a:1243:VAL:HG12 | 1.98                     | 0.45              |
| 4:b:131:ASP:OD1   | 4:b:131:ASP:N     | 2.50                     | 0.45              |
| 4:b:310:MET:HA    | 4:b:386:LEU:HD21  | 1.98                     | 0.45              |
| 4:b:952:VAL:HG13  | 4:b:966:VAL:HG12  | 1.98                     | 0.45              |
| 4:b:243:ALA:HB1   | 4:b:246:LYS:HG3   | 1.99                     | 0.45              |
| 4:b:842:ASN:HD21  | 4:b:844:SER:HB2   | 1.81                     | 0.45              |
| 10:h:108:SER:C    | 10:h:110:ASP:H    | 2.23                     | 0.45              |
| 3:a:23:SER:O      | 3:a:26:GLU:HG3    | 2.16                     | 0.44              |
| 3:a:35:ILE:HD12   | 3:a:35:ILE:H      | 1.81                     | 0.44              |
| 3:a:524:VAL:HB    | 3:a:525:GLN:OE1   | 2.16                     | 0.44              |
| 3:a:549:MET:HE1   | 3:a:655:PHE:HD2   | 1.80                     | 0.44              |
| 3:a:635:ARG:NH2   | 3:a:877:HIS:HA    | 2.32                     | 0.44              |
| 3:a:966:ASN:OD1   | 3:a:967:ALA:N     | 2.49                     | 0.44              |
| 3:a:1419:ASP:CG   | 3:a:1421:CYS:H    | 2.26                     | 0.44              |
| 4:b:94:LYS:O      | 4:b:130:VAL:HG13  | 2.18                     | 0.44              |
| 4:b:708:GLU:OE1   | 4:b:708:GLU:N     | 2.50                     | 0.44              |
| 4:b:737:THR:HB    | 11:i:66:PRO:HB3   | 1.99                     | 0.44              |
| 4:b:842:ASN:ND2   | 4:b:845:SER:H     | 2.14                     | 0.44              |
| 4:b:1160:VAL:HG11 | 4:b:1169:MET:SD   | 2.56                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:c:18:VAL:HG12  | 5:c:20:PHE:HD2   | 1.82                     | 0.44              |
| 8:f:70:LYS:C     | 8:f:71:GLU:HG3   | 2.42                     | 0.44              |
| 1:N:53:DT:H2"    | 1:N:54:DG:C8     | 2.53                     | 0.44              |
| 3:a:22:PHE:HB2   | 4:b:1211:ASN:OD1 | 2.17                     | 0.44              |
| 3:a:42:ASP:OD1   | 3:a:47:ARG:NH2   | 2.51                     | 0.44              |
| 3:a:195:ASP:OD1  | 3:a:196:GLU:N    | 2.50                     | 0.44              |
| 3:a:314:ALA:O    | 3:a:322:VAL:HG12 | 2.17                     | 0.44              |
| 3:a:344:ARG:NE   | 4:b:1129:ARG:HB2 | 2.33                     | 0.44              |
| 3:a:369:SER:OG   | 3:a:370:ILE:HD12 | 2.17                     | 0.44              |
| 3:a:590:ARG:HB3  | 3:a:605:MET:H    | 1.82                     | 0.44              |
| 4:b:67:SER:OG    | 4:b:68:THR:N     | 2.51                     | 0.44              |
| 4:b:173:MET:SD   | 4:b:201:GLY:HA3  | 2.58                     | 0.44              |
| 4:b:566:LEU:HD12 | 4:b:588:GLY:HA2  | 1.99                     | 0.44              |
| 4:b:908:GLU:N    | 4:b:908:GLU:OE1  | 2.51                     | 0.44              |
| 4:b:980:PHE:CZ   | 4:b:1094:ARG:HG3 | 2.52                     | 0.44              |
| 11:i:69:PRO:HB2  | 11:i:85:PHE:CE1  | 2.52                     | 0.44              |
| 3:a:961:ARG:O    | 3:a:965:GLN:NE2  | 2.49                     | 0.44              |
| 3:a:1098:VAL:N   | 3:a:1099:PRO:HD2 | 2.31                     | 0.44              |
| 4:b:79:THR:CA    | 4:b:81:SER:H     | 2.30                     | 0.44              |
| 4:b:402:GLY:O    | 4:b:405:ARG:NH1  | 2.50                     | 0.44              |
| 4:b:569:TYR:OH   | 4:b:571:PRO:HA   | 2.17                     | 0.44              |
| 4:b:762:ASN:ND2  | 4:b:1024:ALA:HB3 | 2.31                     | 0.44              |
| 6:d:64:VAL:HG23  | 6:d:68:ARG:HH12  | 1.83                     | 0.44              |
| 9:g:29:LYS:O     | 9:g:33:GLU:OE1   | 2.34                     | 0.44              |
| 9:g:89:GLY:HA3   | 9:g:103:VAL:HG12 | 1.99                     | 0.44              |
| 9:g:101:VAL:HG12 | 9:g:103:VAL:HG13 | 1.99                     | 0.44              |
| 10:h:99:GLY:HA3  | 10:h:118:PHE:CD1 | 2.43                     | 0.44              |
| 10:h:138:GLU:N   | 10:h:138:GLU:OE1 | 2.51                     | 0.44              |
| 13:k:49:GLU:HG2  | 13:k:94:ILE:HD11 | 1.99                     | 0.44              |
| 4:b:397:ASP:CG   | 4:b:399:ASP:H    | 2.25                     | 0.44              |
| 7:e:48:ASP:OD1   | 7:e:49:SER:N     | 2.46                     | 0.44              |
| 7:e:90:VAL:HA    | 7:e:93:MET:HG3   | 1.99                     | 0.44              |
| 9:g:57:GLN:CD    | 9:g:57:GLN:H     | 2.26                     | 0.44              |
| 11:i:16:PRO:HA   | 11:i:27:PHE:HD1  | 1.81                     | 0.44              |
| 12:j:48:ARG:HG3  | 12:j:49:MET:N    | 2.31                     | 0.44              |
| 3:a:622:VAL:HG23 | 3:a:629:LEU:HD21 | 1.98                     | 0.44              |
| 3:a:878:ILE:HA   | 3:a:956:LEU:O    | 2.16                     | 0.44              |
| 3:a:1373:ASP:O   | 3:a:1376:THR:N   | 2.47                     | 0.44              |
| 4:b:74:LEU:HD12  | 4:b:85:SER:HB2   | 1.99                     | 0.44              |
| 4:b:343:ILE:HB   | 4:b:348:ARG:NH1  | 2.33                     | 0.44              |
| 4:b:898:LEU:HD11 | 4:b:964:VAL:HG11 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:c:73:GLN:OE1   | 5:c:75:MET:HG2    | 2.18                     | 0.44              |
| 6:d:145:MET:HA   | 6:d:148:LEU:CB    | 2.46                     | 0.44              |
| 9:g:28:THR:O     | 9:g:31:LEU:HB2    | 2.18                     | 0.44              |
| 1:n:51:DA:H2'    | 1:n:52:DG:C8      | 2.53                     | 0.44              |
| 3:a:424:ILE:HD12 | 3:a:424:ILE:H     | 1.81                     | 0.44              |
| 4:b:79:THR:HG22  | 4:b:82:ASP:O      | 2.17                     | 0.44              |
| 9:g:130:TYR:CE1  | 9:g:136:VAL:HG12  | 2.53                     | 0.44              |
| 10:h:61:SER:HA   | 10:h:140:ALA:HB1  | 1.98                     | 0.44              |
| 11:i:6:PHE:HA    | 11:i:12:ASN:O     | 2.18                     | 0.44              |
| 3:a:108:MET:C    | 3:a:110:CYS:H     | 2.26                     | 0.44              |
| 3:a:363:GLN:HE21 | 3:a:459:ARG:NH1   | 2.16                     | 0.44              |
| 3:a:368:LYS:HB3  | 13:k:2:ASN:HB3    | 1.99                     | 0.44              |
| 3:a:419:LYS:HG3  | 3:a:420:ARG:HG2   | 1.99                     | 0.44              |
| 3:a:635:ARG:HH22 | 3:a:877:HIS:HA    | 1.83                     | 0.44              |
| 4:b:867:GLY:HA3  | 4:b:868:MET:O     | 2.18                     | 0.44              |
| 5:c:22:LEU:HB2   | 5:c:230:MET:HE1   | 1.99                     | 0.44              |
| 9:g:90:THR:HA    | 9:g:140:LYS:O     | 2.17                     | 0.44              |
| 10:h:6:PHE:CE1   | 10:h:8:ASP:HB2    | 2.52                     | 0.44              |
| 2:O:-43:DT:H2'   | 2:O:-42:DA:C8     | 2.53                     | 0.44              |
| 3:a:843:LYS:NZ   | 4:b:1135:ARG:HH22 | 2.16                     | 0.44              |
| 4:b:48:LEU:HA    | 4:b:173:MET:HE1   | 1.99                     | 0.44              |
| 4:b:641:GLU:HB3  | 4:b:643:ASP:OD1   | 2.17                     | 0.44              |
| 4:b:992:ILE:HD11 | 4:b:994:TYR:CZ    | 2.53                     | 0.44              |
| 7:e:16:PHE:CZ    | 7:e:20:LYS:HD2    | 2.53                     | 0.44              |
| 14:l:44:ASP:OD1  | 14:l:44:ASP:N     | 2.48                     | 0.44              |
| 1:n:56:DT:H5'    | 1:n:56:DT:H6      | 1.83                     | 0.44              |
| 3:a:525:GLN:HB2  | 4:b:1015:HIS:ND1  | 2.33                     | 0.44              |
| 4:b:103:ASN:HB3  | 4:b:109:THR:HA    | 1.99                     | 0.44              |
| 4:b:1045:SER:OG  | 4:b:1048:THR:OG1  | 2.17                     | 0.44              |
| 5:c:123:ASN:OD1  | 5:c:124:LEU:N     | 2.51                     | 0.44              |
| 6:d:67:ARG:HB3   | 6:d:71:LYS:NZ     | 2.32                     | 0.44              |
| 9:g:84:GLY:HA2   | 9:g:146:LYS:HE2   | 1.99                     | 0.44              |
| 3:a:557:ASP:OD1  | 3:a:558:GLY:N     | 2.51                     | 0.43              |
| 3:a:821:ARG:HD3  | 4:b:514:LEU:HB2   | 1.99                     | 0.43              |
| 4:b:100:PRO:HA   | 4:b:126:SER:HB3   | 2.00                     | 0.43              |
| 4:b:579:ARG:HA   | 4:b:589:VAL:HG22  | 1.99                     | 0.43              |
| 4:b:833:TYR:O    | 4:b:838:SER:OG    | 2.22                     | 0.43              |
| 6:d:65:GLU:OE1   | 6:d:68:ARG:NH2    | 2.50                     | 0.43              |
| 6:d:206:GLU:HG2  | 6:d:209:ARG:HE    | 1.83                     | 0.43              |
| 8:f:70:LYS:C     | 8:f:72:LYS:H      | 2.26                     | 0.43              |
| 9:g:1:MET:HA     | 9:g:79:PHE:CE1    | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:k:102:LYS:HG3  | 13:k:103:THR:N    | 2.33                     | 0.43              |
| 13:k:102:LYS:O    | 13:k:105:PHE:N    | 2.50                     | 0.43              |
| 13:k:107:THR:O    | 13:k:111:LEU:HD23 | 2.18                     | 0.43              |
| 2:O:-28:DG:H2'    | 2:O:-27:DT:H71    | 2.00                     | 0.43              |
| 3:a:441:PRO:HG2   | 3:a:498:ARG:HB2   | 2.01                     | 0.43              |
| 3:a:490:HIS:HB3   | 4:b:1150:ARG:NH1  | 2.32                     | 0.43              |
| 4:b:286:PHE:HE1   | 4:b:378:LEU:HD22  | 1.80                     | 0.43              |
| 4:b:344:LYS:HD3   | 4:b:344:LYS:HA    | 1.78                     | 0.43              |
| 4:b:998:ASP:O     | 4:b:1075:GLY:HA3  | 2.17                     | 0.43              |
| 6:d:220:LEU:HG    | 6:d:221:TYR:N     | 2.34                     | 0.43              |
| 13:k:19:LEU:HD23  | 13:k:19:LEU:H     | 1.84                     | 0.43              |
| 4:b:287:ARG:NH2   | 4:b:294:ASP:OD1   | 2.47                     | 0.43              |
| 4:b:287:ARG:NE    | 4:b:292:ILE:HA    | 2.32                     | 0.43              |
| 4:b:428:ILE:HA    | 4:b:445:LYS:HD3   | 1.99                     | 0.43              |
| 4:b:785:TYR:HA    | 4:b:788:ARG:HB3   | 2.00                     | 0.43              |
| 4:b:1074:ASN:HD21 | 4:b:1076:HIS:HB2  | 1.83                     | 0.43              |
| 5:c:99:LEU:HD13   | 5:c:120:ILE:HA    | 1.99                     | 0.43              |
| 12:j:1:MET:O      | 12:j:53:HIS:HE1   | 2.01                     | 0.43              |
| 13:k:53:ASP:OD2   | 13:k:56:VAL:HG13  | 2.18                     | 0.43              |
| 3:a:353:ILE:HG21  | 3:a:487:MET:HE2   | 2.00                     | 0.43              |
| 3:a:363:GLN:HE21  | 3:a:459:ARG:HH12  | 1.66                     | 0.43              |
| 3:a:535:THR:HG21  | 3:a:617:VAL:H     | 1.83                     | 0.43              |
| 4:b:242:SER:O     | 4:b:252:SER:HB2   | 2.18                     | 0.43              |
| 4:b:363:HIS:HB2   | 4:b:585:VAL:HG21  | 2.00                     | 0.43              |
| 4:b:563:MET:SD    | 4:b:588:GLY:HA3   | 2.58                     | 0.43              |
| 4:b:788:ARG:NE    | 4:b:790:ASP:OD2   | 2.52                     | 0.43              |
| 4:b:852:ARG:NH1   | 5:c:65:HIS:HD2    | 2.16                     | 0.43              |
| 4:b:1080:LYS:HG3  | 5:c:180:TYR:CE1   | 2.53                     | 0.43              |
| 5:c:5:GLY:O       | 5:c:7:GLN:NE2     | 2.50                     | 0.43              |
| 6:d:123:LEU:CD1   | 6:d:145:MET:HG3   | 2.48                     | 0.43              |
| 13:k:57:LEU:HB2   | 13:k:77:THR:HA    | 1.99                     | 0.43              |
| 4:b:449:ASN:O     | 4:b:453:ILE:HG12  | 2.19                     | 0.43              |
| 4:b:597:MET:HE2   | 4:b:617:ARG:HB2   | 2.00                     | 0.43              |
| 10:h:7:ASP:OD1    | 10:h:8:ASP:N      | 2.51                     | 0.43              |
| 1:N:63:DT:H2''    | 1:N:64:DA:N7      | 2.34                     | 0.43              |
| 3:a:209:ASN:CA    | 3:a:212:LYS:HZ3   | 2.28                     | 0.43              |
| 3:a:368:LYS:HE3   | 13:k:2:ASN:OD1    | 2.18                     | 0.43              |
| 3:a:604:GLY:O     | 3:a:605:MET:HE2   | 2.18                     | 0.43              |
| 3:a:666:ILE:HD11  | 4:b:1026:LEU:HB3  | 2.01                     | 0.43              |
| 3:a:1169:ILE:HD12 | 3:a:1169:ILE:H    | 1.83                     | 0.43              |
| 4:b:194:GLU:OE1   | 4:b:195:CYS:N     | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:680:THR:H     | 4:b:683:SER:CB    | 2.31                     | 0.43              |
| 4:b:826:ALA:HB3   | 4:b:1011:ILE:HD12 | 1.99                     | 0.43              |
| 4:b:827:ILE:HD12  | 4:b:1012:ILE:HG23 | 2.01                     | 0.43              |
| 4:b:1031:LEU:HD21 | 4:b:1043:ASP:H    | 1.84                     | 0.43              |
| 4:b:1206:GLU:O    | 4:b:1210:MET:N    | 2.52                     | 0.43              |
| 6:d:38:ILE:HG13   | 6:d:39:ASN:H      | 1.84                     | 0.43              |
| 6:d:160:VAL:O     | 6:d:164:ILE:HG13  | 2.19                     | 0.43              |
| 7:e:180:ARG:NH1   | 7:e:192:ARG:HB2   | 2.33                     | 0.43              |
| 9:g:13:LEU:HD11   | 9:g:17:PHE:HB2    | 2.00                     | 0.43              |
| 3:a:434:ARG:NH1   | 3:a:437:MET:HG2   | 2.33                     | 0.43              |
| 3:a:446:ARG:CB    | 3:a:487:MET:HG3   | 2.49                     | 0.43              |
| 3:a:597:LEU:HB3   | 10:h:115:TYR:HE2  | 1.83                     | 0.43              |
| 4:b:438:GLU:OE1   | 4:b:438:GLU:N     | 2.51                     | 0.43              |
| 4:b:758:PHE:CE2   | 4:b:1044:ALA:HA   | 2.54                     | 0.43              |
| 5:c:146:LYS:C     | 5:c:147:LEU:HD12  | 2.44                     | 0.43              |
| 10:h:47:PHE:CZ    | 10:h:146:ARG:HD3  | 2.54                     | 0.43              |
| 11:i:25:LEU:HD23  | 11:i:25:LEU:H     | 1.84                     | 0.43              |
| 3:a:368:LYS:HB3   | 13:k:2:ASN:ND2    | 2.32                     | 0.43              |
| 3:a:368:LYS:HD2   | 3:a:464:PRO:HG3   | 2.01                     | 0.43              |
| 3:a:451:HIS:CD2   | 3:a:453:MET:HE2   | 2.54                     | 0.43              |
| 3:a:483:ASP:OD1   | 3:a:483:ASP:N     | 2.50                     | 0.43              |
| 3:a:744:LYS:O     | 3:a:748:MET:HG2   | 2.18                     | 0.43              |
| 3:a:928:LEU:HD23  | 3:a:987:VAL:HG11  | 1.99                     | 0.43              |
| 3:a:1100:ARG:HH12 | 3:a:1111:MET:HE3  | 1.83                     | 0.43              |
| 3:a:1226:VAL:HG23 | 3:a:1240:CYS:SG   | 2.58                     | 0.43              |
| 3:a:1269:GLU:OE1  | 3:a:1269:GLU:N    | 2.52                     | 0.43              |
| 4:b:604:ARG:HD2   | 4:b:615:MET:HE1   | 2.00                     | 0.43              |
| 4:b:616:ILE:HG22  | 4:b:697:GLU:HA    | 2.00                     | 0.43              |
| 5:c:16:ASP:OD1    | 5:c:16:ASP:N      | 2.48                     | 0.43              |
| 5:c:56:THR:HG22   | 5:c:58:LEU:H      | 1.84                     | 0.43              |
| 12:j:7:CYS:SG     | 12:j:46:CYS:HA    | 2.59                     | 0.43              |
| 2:O:-46:DT:H2"    | 3:a:447:GLN:NE2   | 2.33                     | 0.43              |
| 3:a:132:LYS:O     | 3:a:135:PHE:HB3   | 2.18                     | 0.43              |
| 3:a:871:ASP:OD2   | 3:a:873:MET:HB2   | 2.18                     | 0.43              |
| 3:a:955:PRO:C     | 3:a:956:LEU:HD22  | 2.43                     | 0.43              |
| 3:a:965:GLN:HA    | 3:a:968:GLN:OE1   | 2.19                     | 0.43              |
| 3:a:1154:TYR:CE1  | 3:a:1190:PRO:HB2  | 2.54                     | 0.43              |
| 3:a:1424:VAL:O    | 3:a:1428:VAL:HG23 | 2.18                     | 0.43              |
| 4:b:228:LYS:HG3   | 4:b:229:ALA:H     | 1.84                     | 0.43              |
| 4:b:918:ILE:HA    | 4:b:919:SER:O     | 2.19                     | 0.43              |
| 7:e:17:ARG:NH1    | 7:e:35:VAL:O      | 2.52                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:e:82:PHE:HE1    | 7:e:111:VAL:HG21  | 1.83                     | 0.43              |
| 9:g:28:THR:O      | 9:g:32:GLU:OE1    | 2.37                     | 0.43              |
| 10:h:33:GLN:OE1   | 10:h:35:GLN:N     | 2.52                     | 0.43              |
| 10:h:145:ARG:HD3  | 10:h:145:ARG:HA   | 1.61                     | 0.43              |
| 11:i:73:ARG:H     | 11:i:83:ASN:HD21  | 1.67                     | 0.43              |
| 3:a:33:ALA:O      | 3:a:83:HIS:ND1    | 2.51                     | 0.43              |
| 3:a:536:LEU:HD23  | 3:a:536:LEU:H     | 1.83                     | 0.43              |
| 3:a:860:LEU:HD22  | 3:a:862:ASN:ND2   | 2.34                     | 0.43              |
| 3:a:1412:ALA:O    | 3:a:1416:ALA:N    | 2.52                     | 0.43              |
| 3:a:1425:SER:O    | 3:a:1428:VAL:N    | 2.52                     | 0.43              |
| 4:b:380:TYR:O     | 4:b:384:ARG:HG2   | 2.19                     | 0.43              |
| 4:b:552:MET:HA    | 4:b:555:ILE:HD13  | 2.01                     | 0.43              |
| 4:b:569:TYR:CZ    | 4:b:571:PRO:HA    | 2.54                     | 0.43              |
| 4:b:694:ASP:OD1   | 4:b:695:ALA:N     | 2.52                     | 0.43              |
| 4:b:744:HIS:CE1   | 4:b:746:SER:HG    | 2.28                     | 0.43              |
| 4:b:809:MET:HB2   | 4:b:809:MET:HE2   | 1.75                     | 0.43              |
| 5:c:182:PRO:HG2   | 5:c:183:TRP:CD1   | 2.51                     | 0.43              |
| 8:f:81:THR:HG21   | 8:f:136:ARG:HD3   | 2.01                     | 0.43              |
| 3:a:648:ASN:O     | 3:a:652:VAL:HG12  | 2.19                     | 0.42              |
| 3:a:1017:LEU:HD12 | 7:e:204:THR:O     | 2.19                     | 0.42              |
| 4:b:74:LEU:HD21   | 4:b:83:ASN:H      | 1.83                     | 0.42              |
| 4:b:1185:CYS:HA   | 6:d:16:LYS:HZ2    | 1.84                     | 0.42              |
| 5:c:99:LEU:HB2    | 5:c:157:CYS:HB2   | 2.01                     | 0.42              |
| 3:a:646:PHE:O     | 3:a:647:GLY:C     | 2.61                     | 0.42              |
| 3:a:1111:MET:SD   | 3:a:1331:SER:HA   | 2.59                     | 0.42              |
| 4:b:246:LYS:H     | 4:b:418:LYS:NZ    | 2.17                     | 0.42              |
| 5:c:62:PHE:CZ     | 12:j:1:MET:HE1    | 2.54                     | 0.42              |
| 10:h:6:PHE:O      | 10:h:58:THR:HA    | 2.20                     | 0.42              |
| 10:h:84:ALA:H     | 13:k:54:ARG:NH1   | 2.17                     | 0.42              |
| 10:h:89:LEU:HD23  | 10:h:90:ALA:N     | 2.34                     | 0.42              |
| 14:l:40:LEU:HD12  | 14:l:44:ASP:HB2   | 2.01                     | 0.42              |
| 3:a:37:PHE:CD2    | 3:a:50:ILE:HG12   | 2.55                     | 0.42              |
| 3:a:1426:GLU:O    | 3:a:1430:LEU:HB2  | 2.20                     | 0.42              |
| 4:b:349:ILE:HD12  | 4:b:349:ILE:H     | 1.83                     | 0.42              |
| 4:b:494:HIS:CD2   | 4:b:497:ARG:HH12  | 2.37                     | 0.42              |
| 4:b:789:MET:HE1   | 4:b:967:ARG:CZ    | 2.50                     | 0.42              |
| 4:b:862:GLN:HB3   | 4:b:963:PHE:HD2   | 1.83                     | 0.42              |
| 4:b:1034:VAL:HG11 | 4:b:1055:ILE:HG23 | 2.00                     | 0.42              |
| 9:g:65:ASP:CG     | 9:g:67:SER:HG     | 2.20                     | 0.42              |
| 11:i:5:ARG:C      | 11:i:14:LEU:HD23  | 2.44                     | 0.42              |
| 2:O:-59:DA:H2"    | 2:O:-58:DT:H71    | 2.00                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:a:495:GLU:HA   | 3:a:498:ARG:HG2  | 2.00                     | 0.42              |
| 3:a:764:CYS:HA   | 3:a:802:ASN:O    | 2.19                     | 0.42              |
| 3:a:913:LEU:HD12 | 3:a:979:SER:O    | 2.19                     | 0.42              |
| 3:a:960:ILE:HB   | 3:a:1025:ARG:NH1 | 2.34                     | 0.42              |
| 4:b:1124:ARG:NH1 | 15:r:38:G:H5'    | 2.35                     | 0.42              |
| 5:c:148:ARG:O    | 5:c:148:ARG:HD2  | 2.19                     | 0.42              |
| 5:c:252:GLN:HA   | 5:c:255:VAL:HG12 | 2.01                     | 0.42              |
| 7:e:202:SER:OG   | 7:e:203:GLU:N    | 2.53                     | 0.42              |
| 11:i:8:ARG:HA    | 11:i:8:ARG:NE    | 2.34                     | 0.42              |
| 11:i:19:ASP:O    | 11:i:23:ASN:HA   | 2.19                     | 0.42              |
| 12:j:1:MET:N     | 12:j:57:ILE:HB   | 2.35                     | 0.42              |
| 3:a:43:GLU:HG2   | 3:a:44:THR:H     | 1.85                     | 0.42              |
| 3:a:66:LYS:HG2   | 3:a:68:GLN:N     | 2.34                     | 0.42              |
| 3:a:597:LEU:HD12 | 3:a:597:LEU:HA   | 1.83                     | 0.42              |
| 3:a:792:TYR:HA   | 3:a:797:LYS:NZ   | 2.34                     | 0.42              |
| 3:a:806:ARG:HD3  | 4:b:728:ARG:HA   | 2.00                     | 0.42              |
| 3:a:993:LEU:HD21 | 3:a:1046:LEU:HB3 | 2.00                     | 0.42              |
| 3:a:1029:ARG:NH2 | 3:a:1033:GLN:OE1 | 2.52                     | 0.42              |
| 4:b:481:GLN:NE2  | 15:r:44:C:OP1    | 2.52                     | 0.42              |
| 4:b:1219:ASP:OD1 | 4:b:1219:ASP:N   | 2.51                     | 0.42              |
| 10:h:99:GLY:HA3  | 10:h:118:PHE:HA  | 2.01                     | 0.42              |
| 10:h:116:TYR:HB2 | 10:h:123:MET:HG3 | 2.02                     | 0.42              |
| 1:N:32:DA:H1'    | 1:N:33:DA:C8     | 2.54                     | 0.42              |
| 3:a:75:ASN:OD1   | 3:a:76:GLU:N     | 2.52                     | 0.42              |
| 3:a:128:ILE:O    | 3:a:134:ARG:HB3  | 2.20                     | 0.42              |
| 3:a:519:PRO:HD3  | 3:a:631:HIS:ND1  | 2.34                     | 0.42              |
| 3:a:570:PRO:C    | 3:a:571:LEU:HD12 | 2.44                     | 0.42              |
| 4:b:169:ARG:H    | 4:b:454:THR:HG1  | 1.65                     | 0.42              |
| 4:b:270:LYS:HD3  | 4:b:279:ASP:HB2  | 2.02                     | 0.42              |
| 4:b:616:ILE:CG2  | 4:b:697:GLU:HA   | 2.50                     | 0.42              |
| 6:d:150:ASN:OD1  | 6:d:155:ARG:NH2  | 2.52                     | 0.42              |
| 9:g:15:PRO:HD3   | 9:g:67:SER:HA    | 2.00                     | 0.42              |
| 9:g:15:PRO:HA    | 9:g:18:PHE:CE1   | 2.55                     | 0.42              |
| 15:r:42:U:H2'    | 15:r:43:A:C8     | 2.55                     | 0.42              |
| 1:N:30:DA:H2''   | 1:N:31:DA:C8     | 2.55                     | 0.42              |
| 3:a:108:MET:SD   | 3:a:171:GLN:HG2  | 2.59                     | 0.42              |
| 3:a:139:TRP:CE2  | 3:a:143:LYS:HE3  | 2.55                     | 0.42              |
| 3:a:370:ILE:HD12 | 3:a:370:ILE:H    | 1.85                     | 0.42              |
| 3:a:399:HIS:HB3  | 3:a:400:PRO:HD3  | 2.01                     | 0.42              |
| 3:a:407:ARG:HB2  | 3:a:430:TRP:CZ2  | 2.54                     | 0.42              |
| 3:a:1379:GLY:O   | 7:e:179:GLN:HB2  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:1397:LEU:HA   | 3:a:1400:CYS:SG   | 2.60                     | 0.42              |
| 4:b:203:PHE:O     | 4:b:210:LYS:N     | 2.52                     | 0.42              |
| 4:b:830:TYR:CE1   | 4:b:1000:PRO:HD3  | 2.54                     | 0.42              |
| 4:b:1001:PHE:HE2  | 5:c:178:PHE:HB3   | 1.84                     | 0.42              |
| 4:b:1196:ILE:HD11 | 4:b:1201:LYS:HB3  | 2.02                     | 0.42              |
| 6:d:72:ARG:O      | 6:d:75:LYS:HG3    | 2.19                     | 0.42              |
| 6:d:172:LEU:HD23  | 6:d:173:HIS:O     | 2.20                     | 0.42              |
| 7:e:152:LYS:NZ    | 7:e:153:HIS:O     | 2.40                     | 0.42              |
| 9:g:83:LYS:HD3    | 9:g:148:GLU:O     | 2.19                     | 0.42              |
| 13:k:65:HIS:CD2   | 13:k:67:PHE:H     | 2.37                     | 0.42              |
| 3:a:567:LYS:HD3   | 10:h:95:TYR:CA    | 2.48                     | 0.42              |
| 3:a:672:ASP:OD1   | 3:a:673:GLY:N     | 2.53                     | 0.42              |
| 3:a:736:ASN:C     | 3:a:736:ASN:HD22  | 2.26                     | 0.42              |
| 4:b:287:ARG:O     | 4:b:327:ARG:HB3   | 2.20                     | 0.42              |
| 4:b:394:ASP:CG    | 4:b:395:GLN:N     | 2.78                     | 0.42              |
| 4:b:445:LYS:HG3   | 4:b:446:LEU:HD23  | 2.01                     | 0.42              |
| 4:b:562:GLY:O     | 4:b:590:HIS:ND1   | 2.52                     | 0.42              |
| 4:b:1104:HIS:ND1  | 4:b:1122:ARG:HG3  | 2.35                     | 0.42              |
| 4:b:1106:ARG:HH12 | 4:b:1109:GLY:H    | 1.66                     | 0.42              |
| 4:b:1194:ILE:HG22 | 4:b:1196:ILE:HG23 | 2.02                     | 0.42              |
| 5:c:52:GLU:HG2    | 5:c:53:THR:HG23   | 2.02                     | 0.42              |
| 6:d:153:ARG:HH12  | 6:d:163:VAL:HG11  | 1.83                     | 0.42              |
| 8:f:101:ILE:HA    | 8:f:105:ALA:HB3   | 2.01                     | 0.42              |
| 10:h:89:LEU:HD23  | 10:h:90:ALA:C     | 2.44                     | 0.42              |
| 13:k:39:ASP:OD1   | 13:k:41:THR:HG22  | 2.20                     | 0.42              |
| 3:a:61:ILE:O      | 3:a:74:MET:HE1    | 2.19                     | 0.42              |
| 3:a:434:ARG:NH1   | 3:a:437:MET:HE3   | 2.35                     | 0.42              |
| 3:a:1136:SER:C    | 3:a:1274:ARG:HH12 | 2.28                     | 0.42              |
| 3:a:1143:LEU:HD12 | 3:a:1143:LEU:H    | 1.85                     | 0.42              |
| 4:b:168:GLY:HA2   | 4:b:450:ALA:HB1   | 2.02                     | 0.42              |
| 4:b:175:ARG:HH22  | 4:b:198:ASP:C     | 2.16                     | 0.42              |
| 4:b:566:LEU:HD11  | 4:b:586:TRP:CD1   | 2.55                     | 0.42              |
| 4:b:852:ARG:NH2   | 14:l:70:ARG:O     | 2.50                     | 0.42              |
| 4:b:917:PRO:O     | 4:b:919:SER:OG    | 2.37                     | 0.42              |
| 7:e:88:VAL:CB     | 7:e:116:ILE:HG23  | 2.49                     | 0.42              |
| 7:e:175:LEU:HD22  | 7:e:213:ILE:HG13  | 2.02                     | 0.42              |
| 10:h:2:SER:HG     | 10:h:62:SER:H     | 1.67                     | 0.42              |
| 14:l:48:CYS:HB3   | 14:l:51:CYS:O     | 2.20                     | 0.42              |
| 1:N:52:DG:H2'     | 1:N:53:DT:H6      | 1.76                     | 0.42              |
| 3:a:99:ILE:HD12   | 3:a:234:MET:HG2   | 2.01                     | 0.42              |
| 3:a:153:PRO:O     | 3:a:161:LEU:HA    | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:574:GLY:O     | 3:a:577:ILE:HG22  | 2.19                     | 0.42              |
| 3:a:974:ASP:OD2   | 3:a:977:LYS:HG2   | 2.19                     | 0.42              |
| 3:a:1328:TYR:CG   | 3:a:1329:THR:N    | 2.88                     | 0.42              |
| 4:b:219:ALA:HB2   | 4:b:405:ARG:HG2   | 2.02                     | 0.42              |
| 4:b:990:ILE:H     | 4:b:990:ILE:HD12  | 1.85                     | 0.42              |
| 6:d:64:VAL:O      | 6:d:67:ARG:HB2    | 2.19                     | 0.42              |
| 12:j:7:CYS:O      | 12:j:11:GLY:N     | 2.53                     | 0.42              |
| 3:a:62:ASP:C      | 3:a:64:ASN:H      | 2.27                     | 0.41              |
| 4:b:147:LEU:C     | 4:b:148:LYS:HG2   | 2.45                     | 0.41              |
| 4:b:361:LEU:HB3   | 4:b:374:LYS:NZ    | 2.35                     | 0.41              |
| 4:b:435:THR:OG1   | 4:b:437:GLU:O     | 2.32                     | 0.41              |
| 4:b:956:THR:CG2   | 4:b:960:GLY:HA2   | 2.50                     | 0.41              |
| 4:b:1185:CYS:HA   | 6:d:16:LYS:NZ     | 2.34                     | 0.41              |
| 5:c:41:ILE:HD11   | 5:c:246:ARG:HB3   | 2.02                     | 0.41              |
| 5:c:43:THR:OG1    | 5:c:44:LEU:N      | 2.52                     | 0.41              |
| 5:c:48:SER:OG     | 5:c:158:VAL:HB    | 2.19                     | 0.41              |
| 5:c:183:TRP:HE1   | 5:c:207:CYS:HA    | 1.85                     | 0.41              |
| 7:e:93:MET:SD     | 7:e:123:LEU:HD23  | 2.60                     | 0.41              |
| 3:a:55:ASP:HA     | 3:a:58:LEU:CD2    | 2.42                     | 0.41              |
| 3:a:341:MET:HE2   | 3:a:341:MET:HB2   | 1.87                     | 0.41              |
| 3:a:341:MET:HE1   | 3:a:1429:ILE:HD11 | 2.02                     | 0.41              |
| 3:a:370:ILE:O     | 3:a:373:THR:OG1   | 2.28                     | 0.41              |
| 3:a:505:CYS:SG    | 4:b:1141:HIS:ND1  | 2.85                     | 0.41              |
| 3:a:1141:THR:OG1  | 3:a:1273:LEU:HB2  | 2.20                     | 0.41              |
| 4:b:126:SER:C     | 4:b:169:ARG:HG3   | 2.45                     | 0.41              |
| 4:b:438:GLU:HA    | 4:b:439:ALA:HA    | 1.70                     | 0.41              |
| 4:b:957:ASN:OD1   | 4:b:960:GLY:N     | 2.52                     | 0.41              |
| 4:b:1085:ILE:HG22 | 4:b:1086:PHE:O    | 2.20                     | 0.41              |
| 4:b:1200:ALA:O    | 4:b:1203:LEU:HB3  | 2.20                     | 0.41              |
| 6:d:49:ALA:HB1    | 9:g:1:MET:HE2     | 2.02                     | 0.41              |
| 10:h:16:ASP:N     | 10:h:16:ASP:OD1   | 2.53                     | 0.41              |
| 3:a:31:SER:HB2    | 3:a:83:HIS:HB3    | 2.01                     | 0.41              |
| 3:a:212:LYS:HE2   | 3:a:212:LYS:HB2   | 1.79                     | 0.41              |
| 3:a:265:LYS:HZ3   | 3:a:303:TYR:N     | 2.19                     | 0.41              |
| 3:a:1301:GLU:HA   | 3:a:1302:PRO:HD3  | 1.89                     | 0.41              |
| 3:a:1329:THR:HG22 | 3:a:1331:SER:N    | 2.30                     | 0.41              |
| 3:a:1436:ILE:O    | 3:a:1439:GLY:N    | 2.38                     | 0.41              |
| 4:b:448:ILE:HA    | 4:b:451:LYS:HG2   | 2.02                     | 0.41              |
| 2:O:-64:DT:H6     | 2:O:-64:DT:H2'    | 1.66                     | 0.41              |
| 3:a:300:VAL:O     | 3:a:304:MET:HG2   | 2.20                     | 0.41              |
| 3:a:567:LYS:HB3   | 10:h:95:TYR:HA    | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:588:LEU:HD12  | 3:a:588:LEU:HA    | 1.85                     | 0.41              |
| 3:a:630:ILE:HG13  | 3:a:631:HIS:N     | 2.35                     | 0.41              |
| 3:a:789:LYS:HE3   | 11:i:67:THR:HB    | 2.03                     | 0.41              |
| 3:a:816:HIS:HE2   | 4:b:763:GLN:HB2   | 1.84                     | 0.41              |
| 3:a:857:ARG:HA    | 3:a:862:ASN:O     | 2.20                     | 0.41              |
| 4:b:428:ILE:HG22  | 4:b:432:MET:CE    | 2.51                     | 0.41              |
| 4:b:662:MET:O     | 4:b:665:GLU:HG3   | 2.20                     | 0.41              |
| 4:b:825:VAL:HG12  | 4:b:1010:LEU:HD21 | 2.02                     | 0.41              |
| 4:b:840:ILE:O     | 4:b:1010:LEU:HA   | 2.20                     | 0.41              |
| 4:b:1155:SER:OG   | 4:b:1156:ASP:N    | 2.47                     | 0.41              |
| 5:c:67:LEU:C      | 5:c:69:LEU:H      | 2.28                     | 0.41              |
| 9:g:22:MET:SD     | 9:g:23:LYS:N      | 2.93                     | 0.41              |
| 9:g:31:LEU:HD23   | 9:g:31:LEU:HA     | 1.91                     | 0.41              |
| 9:g:100:GLU:HB3   | 9:g:107:LYS:HE2   | 2.02                     | 0.41              |
| 3:a:11:LEU:HD23   | 3:a:11:LEU:H      | 1.85                     | 0.41              |
| 3:a:381:THR:HG23  | 3:a:384:ASN:ND2   | 2.35                     | 0.41              |
| 3:a:1054:LEU:HD23 | 3:a:1054:LEU:HA   | 1.85                     | 0.41              |
| 3:a:1434:ALA:O    | 3:a:1436:ILE:N    | 2.53                     | 0.41              |
| 4:b:555:ILE:HD12  | 4:b:555:ILE:H     | 1.85                     | 0.41              |
| 4:b:586:TRP:HD1   | 4:b:588:GLY:H     | 1.67                     | 0.41              |
| 4:b:640:VAL:HB    | 4:b:739:THR:C     | 2.45                     | 0.41              |
| 4:b:936:ASP:OD1   | 4:b:937:ALA:N     | 2.53                     | 0.41              |
| 4:b:1167:GLY:O    | 4:b:1215:ARG:HA   | 2.21                     | 0.41              |
| 5:c:11:ARG:NH2    | 5:c:209:TYR:OH    | 2.53                     | 0.41              |
| 5:c:73:GLN:HB3    | 5:c:131:HIS:H     | 1.85                     | 0.41              |
| 5:c:88:CYS:HB2    | 5:c:92:CYS:HB3    | 2.02                     | 0.41              |
| 6:d:188:ALA:O     | 6:d:192:LYS:HG2   | 2.20                     | 0.41              |
| 9:g:116:PRO:HD3   | 9:g:163:ILE:CG2   | 2.50                     | 0.41              |
| 9:g:128:PRO:HB2   | 9:g:131:GLN:HE22  | 1.85                     | 0.41              |
| 3:a:868:TYR:CE1   | 3:a:1064:VAL:HG21 | 2.55                     | 0.41              |
| 3:a:1035:TYR:HB3  | 3:a:1037:LEU:CD2  | 2.51                     | 0.41              |
| 3:a:1199:ARG:HH22 | 3:a:1231:ASP:CG   | 2.28                     | 0.41              |
| 4:b:174:LEU:HD12  | 4:b:202:TYR:CZ    | 2.56                     | 0.41              |
| 5:c:186:LEU:HB3   | 5:c:188:HIS:NE2   | 2.36                     | 0.41              |
| 5:c:233:GLU:OE1   | 12:j:43:ARG:NH1   | 2.26                     | 0.41              |
| 6:d:184:ALA:HB3   | 9:g:144:ARG:HH21  | 1.86                     | 0.41              |
| 3:a:18:GLN:NE2    | 3:a:1418:LEU:HB3  | 2.36                     | 0.41              |
| 3:a:57:ARG:HA     | 3:a:66:LYS:NZ     | 2.35                     | 0.41              |
| 3:a:311:GLN:H     | 3:a:311:GLN:CD    | 2.29                     | 0.41              |
| 3:a:858:ASN:C     | 3:a:860:LEU:H     | 2.29                     | 0.41              |
| 3:a:861:GLY:HA3   | 7:e:174:GLN:NE2   | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:a:1055:ARG:HD3 | 8:f:155:LEU:HD11  | 2.02                     | 0.41              |
| 4:b:64:CYS:HA    | 4:b:67:SER:HB3    | 2.02                     | 0.41              |
| 4:b:936:ASP:OD1  | 4:b:938:SER:N     | 2.51                     | 0.41              |
| 4:b:959:ASP:OD1  | 4:b:961:LEU:HG    | 2.20                     | 0.41              |
| 4:b:1202:LEU:O   | 4:b:1206:GLU:OE1  | 2.39                     | 0.41              |
| 6:d:57:LEU:HD11  | 6:d:161:GLY:HA2   | 2.02                     | 0.41              |
| 6:d:190:GLU:HB3  | 9:g:167:TYR:CE2   | 2.56                     | 0.41              |
| 7:e:171:LYS:C    | 7:e:173:SER:H     | 2.29                     | 0.41              |
| 2:O:-45:DA:H3'   | 2:O:-44:DG:H8     | 1.85                     | 0.41              |
| 3:a:350:ARG:HD2  | 3:a:486:GLU:CD    | 2.46                     | 0.41              |
| 3:a:525:GLN:HG2  | 3:a:526:ASP:N     | 2.35                     | 0.41              |
| 3:a:560:ILE:HD11 | 13:k:58:PHE:HD1   | 1.86                     | 0.41              |
| 3:a:836:TYR:CZ   | 3:a:840:ARG:HD3   | 2.55                     | 0.41              |
| 3:a:847:ASP:OD1  | 3:a:847:ASP:N     | 2.52                     | 0.41              |
| 3:a:1173:HIS:CD2 | 3:a:1227:ILE:HG23 | 2.55                     | 0.41              |
| 4:b:213:ILE:HD11 | 4:b:481:GLN:HB2   | 2.03                     | 0.41              |
| 4:b:230:ALA:N    | 4:b:231:PRO:HD2   | 2.36                     | 0.41              |
| 4:b:383:ASN:O    | 4:b:387:LEU:HD23  | 2.21                     | 0.41              |
| 5:c:138:GLU:OE1  | 5:c:138:GLU:N     | 2.53                     | 0.41              |
| 6:d:119:ARG:HG3  | 6:d:149:THR:HG21  | 2.03                     | 0.41              |
| 7:e:161:LYS:O    | 7:e:165:LEU:HD23  | 2.20                     | 0.41              |
| 8:f:130:ILE:H    | 8:f:130:ILE:HD12  | 1.85                     | 0.41              |
| 3:a:365:GLY:N    | 3:a:469:ARG:O     | 2.34                     | 0.41              |
| 3:a:434:ARG:HH12 | 3:a:437:MET:HG2   | 1.85                     | 0.41              |
| 3:a:770:VAL:HG23 | 3:a:822:GLU:HG3   | 2.02                     | 0.41              |
| 3:a:852:TYR:CD1  | 3:a:1060:PRO:HB2  | 2.55                     | 0.41              |
| 3:a:860:LEU:O    | 3:a:860:LEU:HD23  | 2.20                     | 0.41              |
| 3:a:890:ASP:CG   | 3:a:1296:GLY:HA3  | 2.46                     | 0.41              |
| 3:a:951:GLU:O    | 3:a:954:TRP:NE1   | 2.53                     | 0.41              |
| 3:a:1154:TYR:HD1 | 3:a:1191:TRP:CD2  | 2.39                     | 0.41              |
| 3:a:1157:ASP:HB3 | 3:a:1160:SER:O    | 2.21                     | 0.41              |
| 3:a:1210:GLY:O   | 3:a:1214:GLU:HG2  | 2.20                     | 0.41              |
| 4:b:160:SER:C    | 4:b:162:SER:H     | 2.29                     | 0.41              |
| 4:b:364:ILE:HG13 | 4:b:365:THR:H     | 1.85                     | 0.41              |
| 4:b:481:GLN:HG2  | 15:r:43:A:O2'     | 2.21                     | 0.41              |
| 4:b:661:LEU:HA   | 4:b:661:LEU:HD23  | 1.82                     | 0.41              |
| 4:b:826:ALA:HB3  | 4:b:1011:ILE:CD1  | 2.50                     | 0.41              |
| 4:b:1000:PRO:C   | 4:b:1072:MET:HE3  | 2.46                     | 0.41              |
| 4:b:1057:LYS:HG2 | 4:b:1061:GLU:OE2  | 2.20                     | 0.41              |
| 4:b:1152:MET:HB3 | 4:b:1153:GLU:OE1  | 2.21                     | 0.41              |
| 5:c:18:VAL:HG12  | 5:c:20:PHE:CD2    | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:c:36:VAL:HG11  | 5:c:251:LEU:HD12  | 2.03                     | 0.41              |
| 5:c:125:MET:CE   | 5:c:127:ARG:HH21  | 2.33                     | 0.41              |
| 8:f:89:GLU:HG2   | 8:f:134:ILE:HD11  | 2.02                     | 0.41              |
| 9:g:49:LEU:HD23  | 9:g:49:LEU:HA     | 1.97                     | 0.41              |
| 10:h:108:SER:HG  | 10:h:111:LEU:H    | 1.68                     | 0.41              |
| 10:h:109:LYS:O   | 10:h:109:LYS:HD3  | 2.21                     | 0.41              |
| 11:i:73:ARG:H    | 11:i:83:ASN:ND2   | 2.18                     | 0.41              |
| 11:i:92:ARG:HG3  | 11:i:93:LYS:N     | 2.35                     | 0.41              |
| 13:k:49:GLU:OE2  | 13:k:90:ALA:HB1   | 2.21                     | 0.41              |
| 14:l:34:CYS:O    | 14:l:36:SER:N     | 2.53                     | 0.41              |
| 3:a:1115:SER:OG  | 3:a:1308:THR:O    | 2.27                     | 0.41              |
| 3:a:1212:VAL:O   | 3:a:1216:ILE:HG12 | 2.21                     | 0.41              |
| 4:b:335:GLY:HA2  | 4:b:337:ARG:HH12  | 1.86                     | 0.41              |
| 4:b:424:LEU:CD1  | 4:b:449:ASN:HB3   | 2.51                     | 0.41              |
| 4:b:485:ARG:NH1  | 4:b:491:THR:HG21  | 2.36                     | 0.41              |
| 4:b:586:TRP:HD1  | 4:b:587:HIS:N     | 2.19                     | 0.41              |
| 4:b:615:MET:N    | 4:b:697:GLU:OE1   | 2.53                     | 0.41              |
| 4:b:1065:GLN:CD  | 4:b:1067:ARG:H    | 2.29                     | 0.41              |
| 4:b:1076:HIS:CD2 | 13:k:40:HIS:CD2   | 3.08                     | 0.41              |
| 4:b:1202:LEU:O   | 4:b:1205:GLN:N    | 2.54                     | 0.41              |
| 6:d:23:ASN:O     | 9:g:83:LYS:HB2    | 2.20                     | 0.41              |
| 7:e:190:LEU:H    | 7:e:190:LEU:HD23  | 1.85                     | 0.41              |
| 9:g:42:PHE:O     | 9:g:80:LYS:HG3    | 2.21                     | 0.41              |
| 12:j:61:LEU:HD12 | 12:j:61:LEU:HA    | 1.91                     | 0.41              |
| 2:O:-64:DT:H2''  | 2:O:-63:DA:C8     | 2.55                     | 0.40              |
| 3:a:22:PHE:CZ    | 4:b:1208:MET:HB2  | 2.56                     | 0.40              |
| 3:a:451:HIS:ND1  | 3:a:1074:GLU:OE2  | 2.54                     | 0.40              |
| 3:a:540:PHE:HB3  | 3:a:571:LEU:HD23  | 2.03                     | 0.40              |
| 3:a:638:GLY:O    | 3:a:640:GLN:N     | 2.53                     | 0.40              |
| 3:a:672:ASP:OD1  | 3:a:674:PRO:HD2   | 2.21                     | 0.40              |
| 3:a:775:ILE:HD12 | 3:a:798:GLY:HA3   | 2.03                     | 0.40              |
| 3:a:1199:ARG:NH2 | 3:a:1236:LEU:HD21 | 2.35                     | 0.40              |
| 4:b:638:PHE:CE2  | 4:b:743:ILE:HA    | 2.56                     | 0.40              |
| 6:d:139:LYS:HG3  | 6:d:143:ASN:ND2   | 2.36                     | 0.40              |
| 9:g:91:VAL:HG22  | 9:g:101:VAL:HG22  | 2.02                     | 0.40              |
| 10:h:10:PHE:CZ   | 10:h:30:SER:HB2   | 2.56                     | 0.40              |
| 10:h:27:GLU:OE2  | 10:h:39:THR:OG1   | 2.24                     | 0.40              |
| 10:h:126:GLU:O   | 10:h:130:ARG:NH1  | 2.53                     | 0.40              |
| 2:O:-42:DA:H4'   | 2:O:-41:DG:OP1    | 2.22                     | 0.40              |
| 3:a:260:ASP:O    | 3:a:263:THR:HG22  | 2.21                     | 0.40              |
| 3:a:515:GLN:HG2  | 3:a:1071:SER:HB2  | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:a:596:THR:HG23 | 3:a:598:LEU:H     | 1.86                     | 0.40              |
| 3:a:889:SER:HA   | 3:a:1296:GLY:O    | 2.21                     | 0.40              |
| 3:a:1009:ASN:ND2 | 3:a:1012:ARG:HH21 | 2.19                     | 0.40              |
| 4:b:884:ARG:NE   | 15:r:36:U:H4'     | 2.37                     | 0.40              |
| 5:c:183:TRP:CE2  | 5:c:207:CYS:HB2   | 2.56                     | 0.40              |
| 7:e:84:ASP:OD1   | 7:e:84:ASP:N      | 2.54                     | 0.40              |
| 9:g:29:LYS:HA    | 9:g:32:GLU:OE1    | 2.21                     | 0.40              |
| 12:j:24:LEU:O    | 12:j:28:ASP:HB2   | 2.22                     | 0.40              |
| 13:k:77:THR:OG1  | 13:k:78:THR:N     | 2.53                     | 0.40              |
| 14:l:47:ARG:NE   | 14:l:52:GLY:HA2   | 2.36                     | 0.40              |
| 2:O:-55:DG:H2''  | 2:O:-54:DC:H6     | 1.86                     | 0.40              |
| 3:a:227:VAL:HG13 | 3:a:228:PHE:CD1   | 2.56                     | 0.40              |
| 3:a:332:LYS:H    | 3:a:337:ARG:NE    | 2.19                     | 0.40              |
| 3:a:746:MET:HE1  | 4:b:1015:HIS:HA   | 2.03                     | 0.40              |
| 3:a:1025:ARG:HA  | 3:a:1030:ARG:NH1  | 2.36                     | 0.40              |
| 4:b:416:LEU:HD11 | 4:b:466:TRP:HB3   | 2.04                     | 0.40              |
| 4:b:709:ASP:OD1  | 4:b:710:LEU:N     | 2.54                     | 0.40              |
| 4:b:798:TYR:CE2  | 12:j:4:PRO:HB3    | 2.57                     | 0.40              |
| 4:b:882:THR:HG22 | 4:b:934:LYS:CA    | 2.52                     | 0.40              |
| 9:g:138:THR:H    | 9:g:141:SER:HB3   | 1.86                     | 0.40              |
| 3:a:306:ASN:ND2  | 3:a:322:VAL:HG13  | 2.36                     | 0.40              |
| 3:a:337:ARG:CD   | 3:a:839:ARG:HH22  | 2.35                     | 0.40              |
| 3:a:338:GLY:HA2  | 4:b:1129:ARG:HH22 | 1.85                     | 0.40              |
| 3:a:535:THR:CG2  | 3:a:617:VAL:H     | 2.34                     | 0.40              |
| 3:a:1268:LEU:HB3 | 3:a:1269:GLU:OE1  | 2.21                     | 0.40              |
| 4:b:116:GLU:O    | 4:b:120:ARG:HB2   | 2.21                     | 0.40              |
| 4:b:310:MET:O    | 4:b:314:LEU:HG    | 2.22                     | 0.40              |
| 5:c:98:VAL:HG12  | 5:c:121:VAL:HB    | 2.04                     | 0.40              |
| 7:e:22:MET:HB2   | 7:e:187:TYR:HE1   | 1.86                     | 0.40              |
| 7:e:62:ALA:HB3   | 7:e:78:LEU:HB3    | 2.04                     | 0.40              |
| 1:N:54:DG:C2     | 2:O:-53:DA:C2     | 3.10                     | 0.40              |
| 3:a:290:GLU:H    | 3:a:290:GLU:CD    | 2.24                     | 0.40              |
| 3:a:408:ASP:OD1  | 3:a:408:ASP:N     | 2.54                     | 0.40              |
| 3:a:434:ARG:CZ   | 3:a:437:MET:HE3   | 2.52                     | 0.40              |
| 3:a:532:ARG:NH1  | 3:a:745:GLN:HB2   | 2.37                     | 0.40              |
| 3:a:575:LYS:O    | 3:a:612:ILE:HD12  | 2.22                     | 0.40              |
| 3:a:1442:ASP:HB2 | 8:f:135:ARG:HB3   | 2.03                     | 0.40              |
| 4:b:240:ILE:HG23 | 4:b:254:LEU:HB3   | 2.03                     | 0.40              |
| 4:b:485:ARG:CZ   | 4:b:782:LEU:HD11  | 2.52                     | 0.40              |
| 4:b:515:HIS:ND1  | 4:b:517:THR:HG22  | 2.37                     | 0.40              |
| 4:b:522:VAL:HG23 | 4:b:538:ASN:O     | 2.22                     | 0.40              |

*Continued on next page...*



Continued from previous page...

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:b:527:THR:CG2  | 4:b:533:CYS:HA  | 2.52                     | 0.40              |
| 4:b:583:ASN:N    | 4:b:626:ILE:O   | 2.51                     | 0.40              |
| 5:c:11:ARG:N     | 5:c:19:ASP:O    | 2.49                     | 0.40              |
| 7:e:14:ARG:HG2   | 7:e:141:VAL:O   | 2.22                     | 0.40              |
| 8:f:103:MET:HE2  | 8:f:103:MET:O   | 2.22                     | 0.40              |
| 9:g:103:VAL:HG23 | 9:g:106:MET:SD  | 2.61                     | 0.40              |
| 10:h:81:PRO:HB2  | 13:k:54:ARG:NH2 | 2.37                     | 0.40              |
| 11:i:45:ARG:HB3  | 11:i:47:GLU:OE1 | 2.21                     | 0.40              |
| 12:j:32:GLU:OE2  | 12:j:32:GLU:N   | 2.35                     | 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 |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3   | a     | 1417/1733 (82%) | 1235 (87%) | 182 (13%) | 0        | 100         | 100 |
| 4   | b     | 1142/1224 (93%) | 983 (86%)  | 159 (14%) | 0        | 100         | 100 |
| 5   | c     | 263/318 (83%)   | 225 (86%)  | 38 (14%)  | 0        | 100         | 100 |
| 6   | d     | 164/221 (74%)   | 156 (95%)  | 8 (5%)    | 0        | 100         | 100 |
| 7   | e     | 212/215 (99%)   | 193 (91%)  | 18 (8%)   | 1 (0%)   | 24          | 58  |
| 8   | f     | 85/155 (55%)    | 77 (91%)   | 8 (9%)    | 0        | 100         | 100 |
| 9   | g     | 169/171 (99%)   | 152 (90%)  | 17 (10%)  | 0        | 100         | 100 |
| 10  | h     | 129/146 (88%)   | 111 (86%)  | 18 (14%)  | 0        | 100         | 100 |
| 11  | i     | 112/122 (92%)   | 104 (93%)  | 8 (7%)    | 0        | 100         | 100 |
| 12  | j     | 64/70 (91%)     | 54 (84%)   | 10 (16%)  | 0        | 100         | 100 |
| 13  | k     | 113/120 (94%)   | 106 (94%)  | 7 (6%)    | 0        | 100         | 100 |
| 14  | l     | 42/70 (60%)     | 30 (71%)   | 12 (29%)  | 0        | 100         | 100 |
| All | All   | 3912/4565 (86%) | 3426 (88%) | 485 (12%) | 1 (0%)   | 100         | 100 |



All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | e     | 172 | GLU  |

### 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 |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3   | a     | 1240/1520 (82%) | 1239 (100%) | 1 (0%)   | 88          | 87  |
| 4   | b     | 999/1061 (94%)  | 998 (100%)  | 1 (0%)   | 88          | 87  |
| 5   | c     | 233/274 (85%)   | 233 (100%)  | 0        | 100         | 100 |
| 6   | d     | 146/200 (73%)   | 146 (100%)  | 0        | 100         | 100 |
| 7   | e     | 196/197 (100%)  | 196 (100%)  | 0        | 100         | 100 |
| 8   | f     | 77/137 (56%)    | 77 (100%)   | 0        | 100         | 100 |
| 9   | g     | 152/152 (100%)  | 152 (100%)  | 0        | 100         | 100 |
| 10  | h     | 118/128 (92%)   | 118 (100%)  | 0        | 100         | 100 |
| 11  | i     | 108/116 (93%)   | 108 (100%)  | 0        | 100         | 100 |
| 12  | j     | 61/65 (94%)     | 61 (100%)   | 0        | 100         | 100 |
| 13  | k     | 99/102 (97%)    | 99 (100%)   | 0        | 100         | 100 |
| 14  | l     | 39/57 (68%)     | 39 (100%)   | 0        | 100         | 100 |
| All | All   | 3468/4009 (86%) | 3466 (100%) | 2 (0%)   | 87          | 87  |

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | a     | 1211 | GLN  |
| 4   | b     | 265  | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | a     | 209 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | a     | 358  | ASN  |
| 3   | a     | 447  | GLN  |
| 3   | a     | 548  | ASN  |
| 3   | a     | 576  | GLN  |
| 3   | a     | 768  | GLN  |
| 3   | a     | 881  | GLN  |
| 3   | a     | 965  | GLN  |
| 3   | a     | 1009 | ASN  |
| 3   | a     | 1211 | GLN  |
| 3   | a     | 1432 | GLN  |
| 4   | b     | 47   | GLN  |
| 4   | b     | 278  | GLN  |
| 4   | b     | 325  | GLN  |
| 4   | b     | 357  | GLN  |
| 4   | b     | 383  | ASN  |
| 4   | b     | 395  | GLN  |
| 4   | b     | 449  | ASN  |
| 4   | b     | 794  | ASN  |
| 4   | b     | 821  | GLN  |
| 4   | b     | 822  | ASN  |
| 4   | b     | 834  | ASN  |
| 4   | b     | 1062 | HIS  |
| 4   | b     | 1076 | HIS  |
| 4   | b     | 1179 | GLN  |
| 4   | b     | 1187 | ASN  |
| 5   | c     | 65   | HIS  |
| 5   | c     | 242  | GLN  |
| 5   | c     | 267  | GLN  |
| 6   | d     | 23   | ASN  |
| 7   | e     | 5    | ASN  |
| 7   | e     | 63   | ASN  |
| 7   | e     | 106  | GLN  |
| 9   | g     | 113  | HIS  |
| 10  | h     | 52   | GLN  |
| 11  | i     | 79   | HIS  |
| 13  | k     | 65   | HIS  |
| 13  | k     | 76   | GLN  |

### 5.3.3 RNA ⓘ

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 15  | r     | 15/16 (93%) | 9 (60%)           | 0               |

All (9) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | r     | 35  | C    |
| 15  | r     | 36  | U    |
| 15  | r     | 38  | G    |
| 15  | r     | 41  | C    |
| 15  | r     | 42  | U    |
| 15  | r     | 43  | A    |
| 15  | r     | 45  | U    |
| 15  | r     | 47  | U    |
| 15  | r     | 48  | C    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

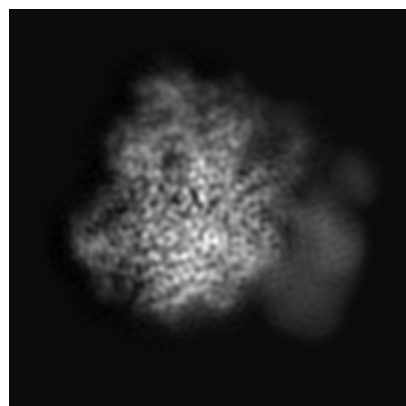
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23888. These allow visual inspection of the internal detail of the map and identification of artifacts.

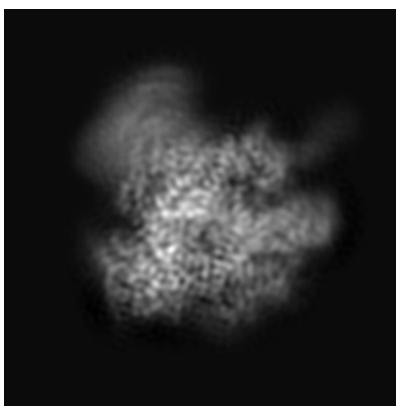
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

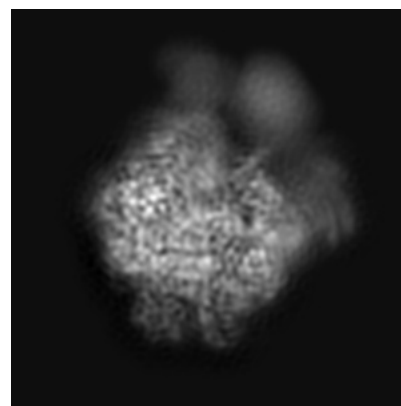
#### 6.1.1 Primary map



X

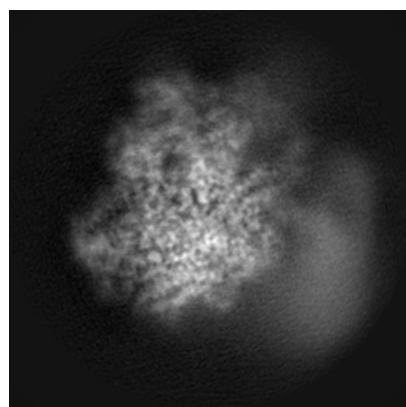


Y

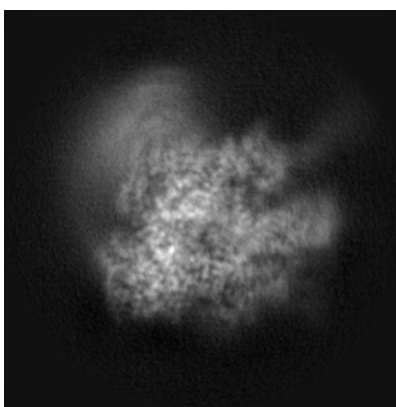


Z

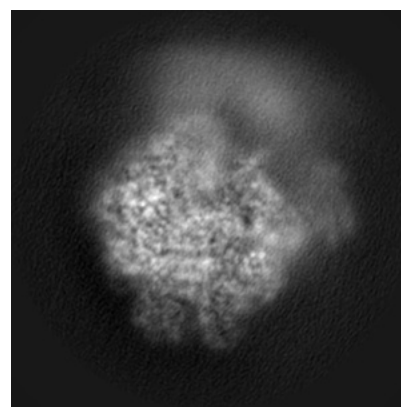
#### 6.1.2 Raw map



X



Y

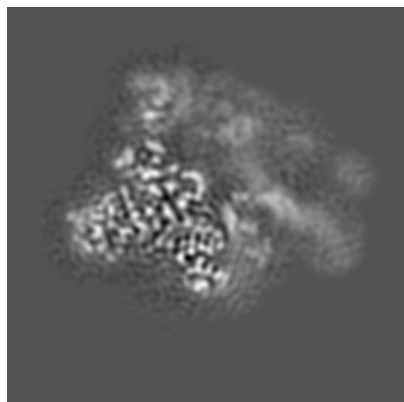


Z

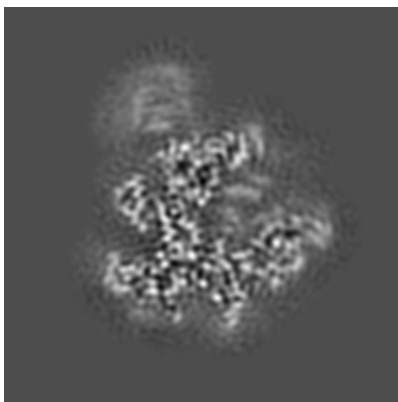
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

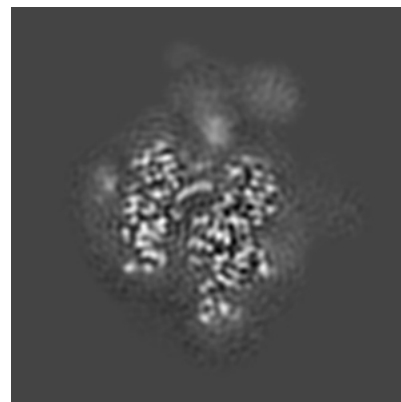
### 6.2.1 Primary map



X Index: 110

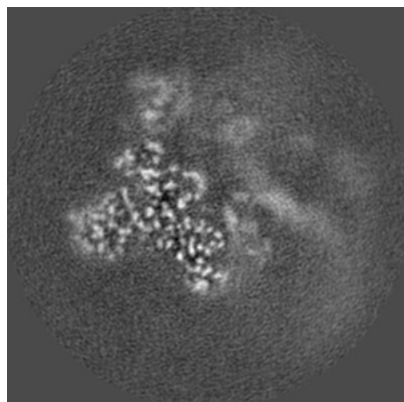


Y Index: 110

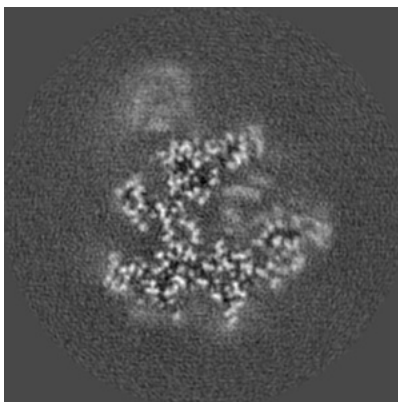


Z Index: 110

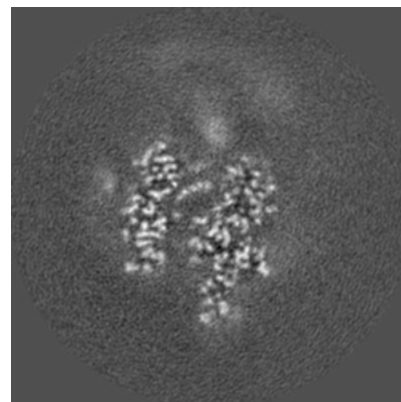
### 6.2.2 Raw map



X Index: 110



Y Index: 110

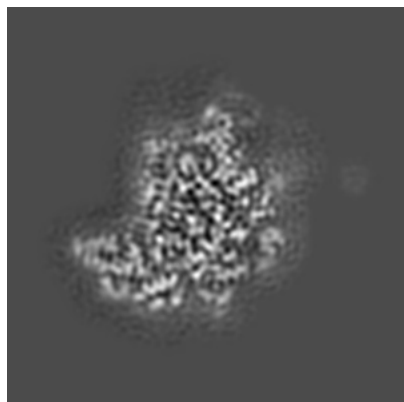


Z Index: 110

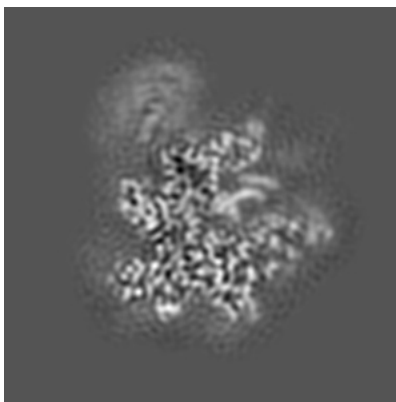
The images above show central slices of the map in three orthogonal directions.

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

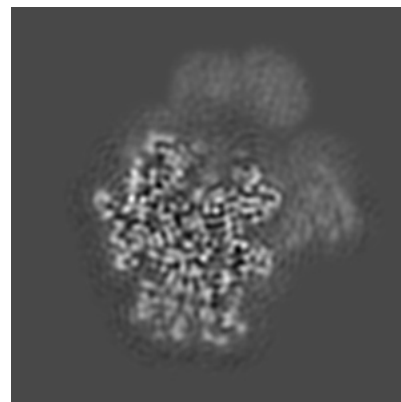
### 6.3.1 Primary map



X Index: 78

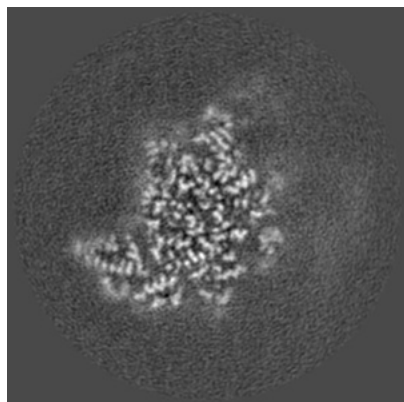


Y Index: 106

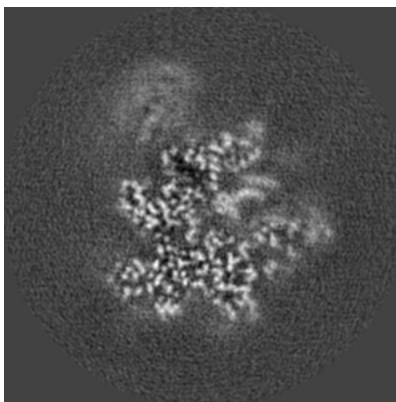


Z Index: 93

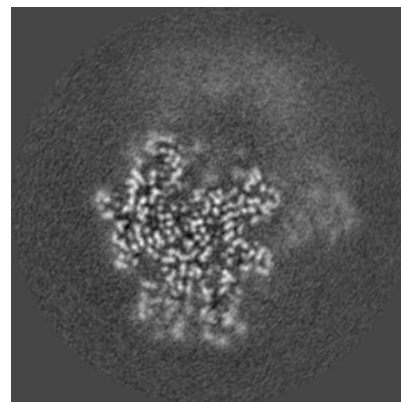
### 6.3.2 Raw map



X Index: 78



Y Index: 106

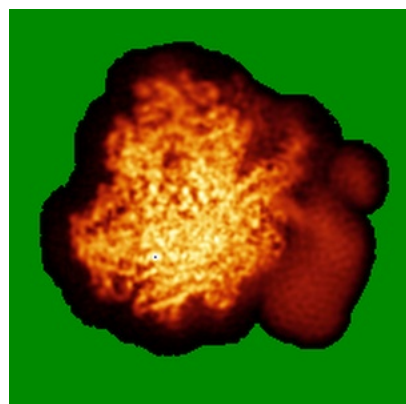


Z Index: 93

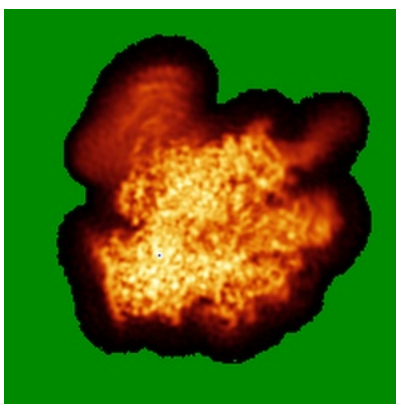
The images above show the largest variance slices of the map in three orthogonal directions.

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

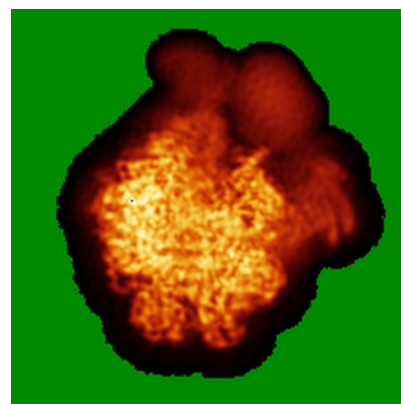
### 6.4.1 Primary map



X

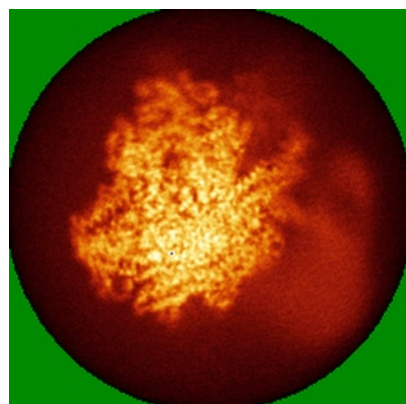


Y

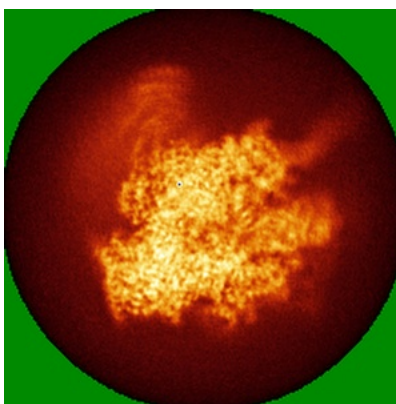


Z

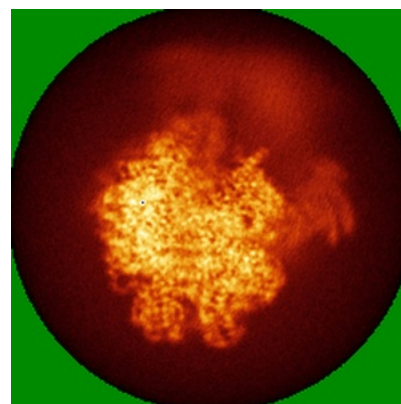
### 6.4.2 Raw map



X



Y



Z

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



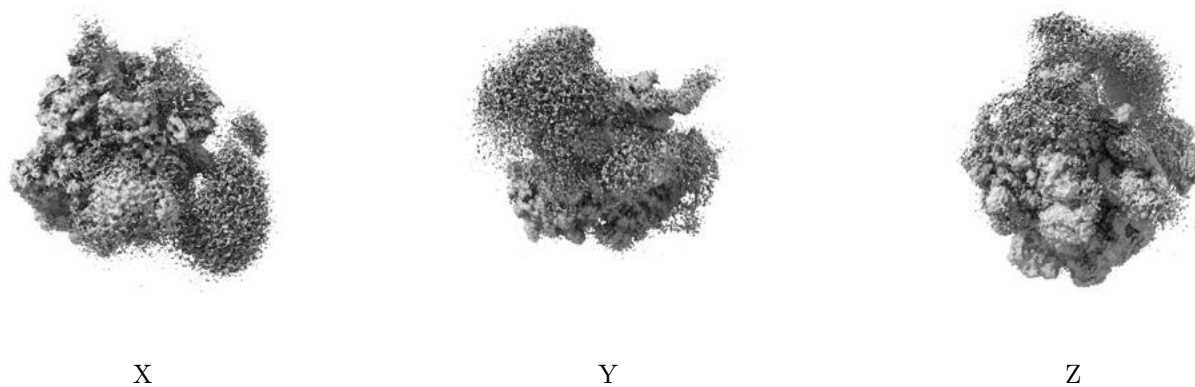
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0101. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

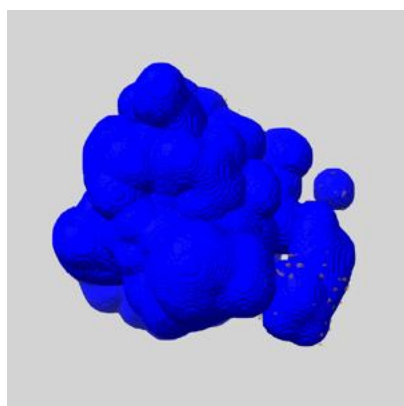
## 6.6 Mask visualisation [i](#)

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

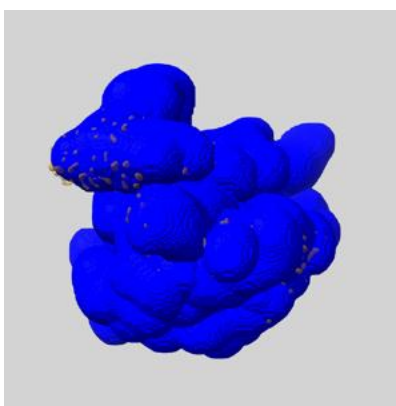
A mask typically either:

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

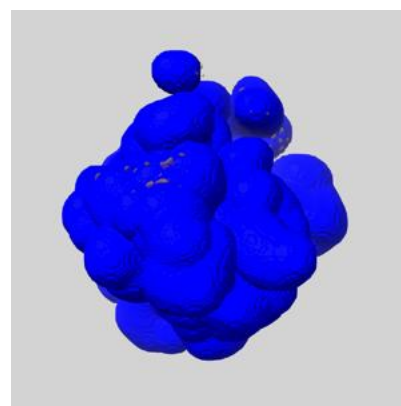
### 6.6.1 emd\_23888\_msk\_1.map [i](#)



X



Y

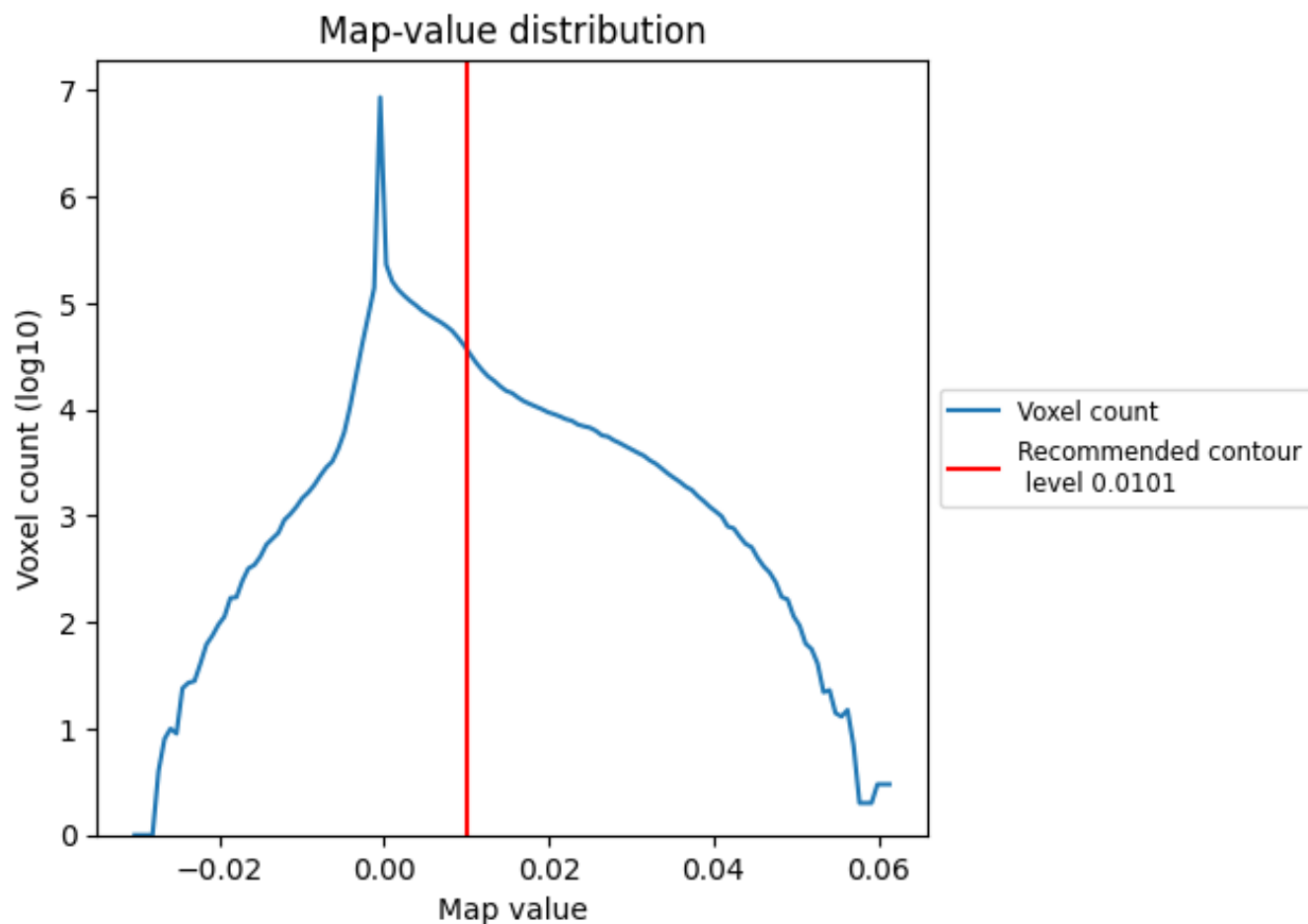


Z

## 7 Map analysis [i](#)

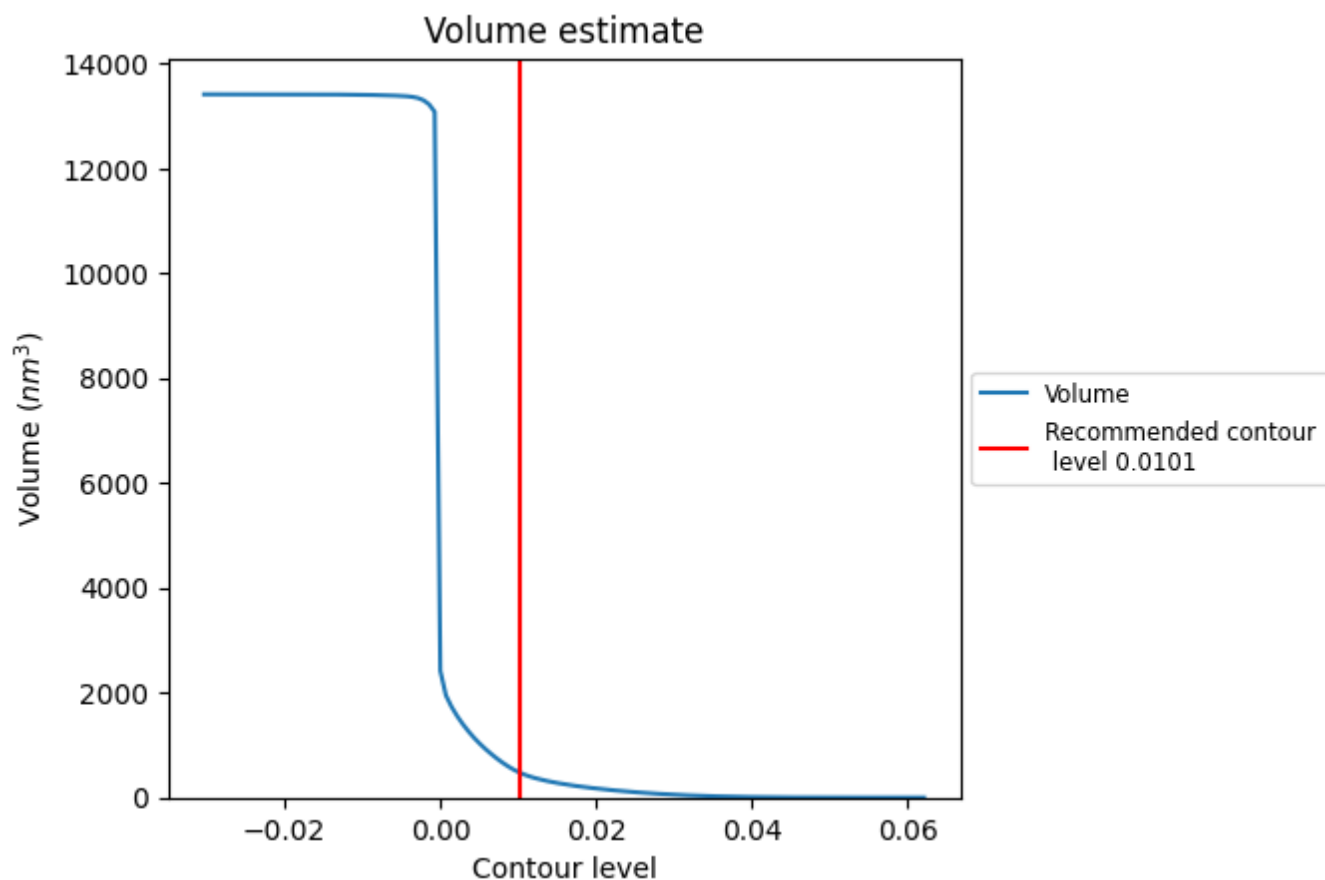
This section contains the results of statistical analysis of the map.

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



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

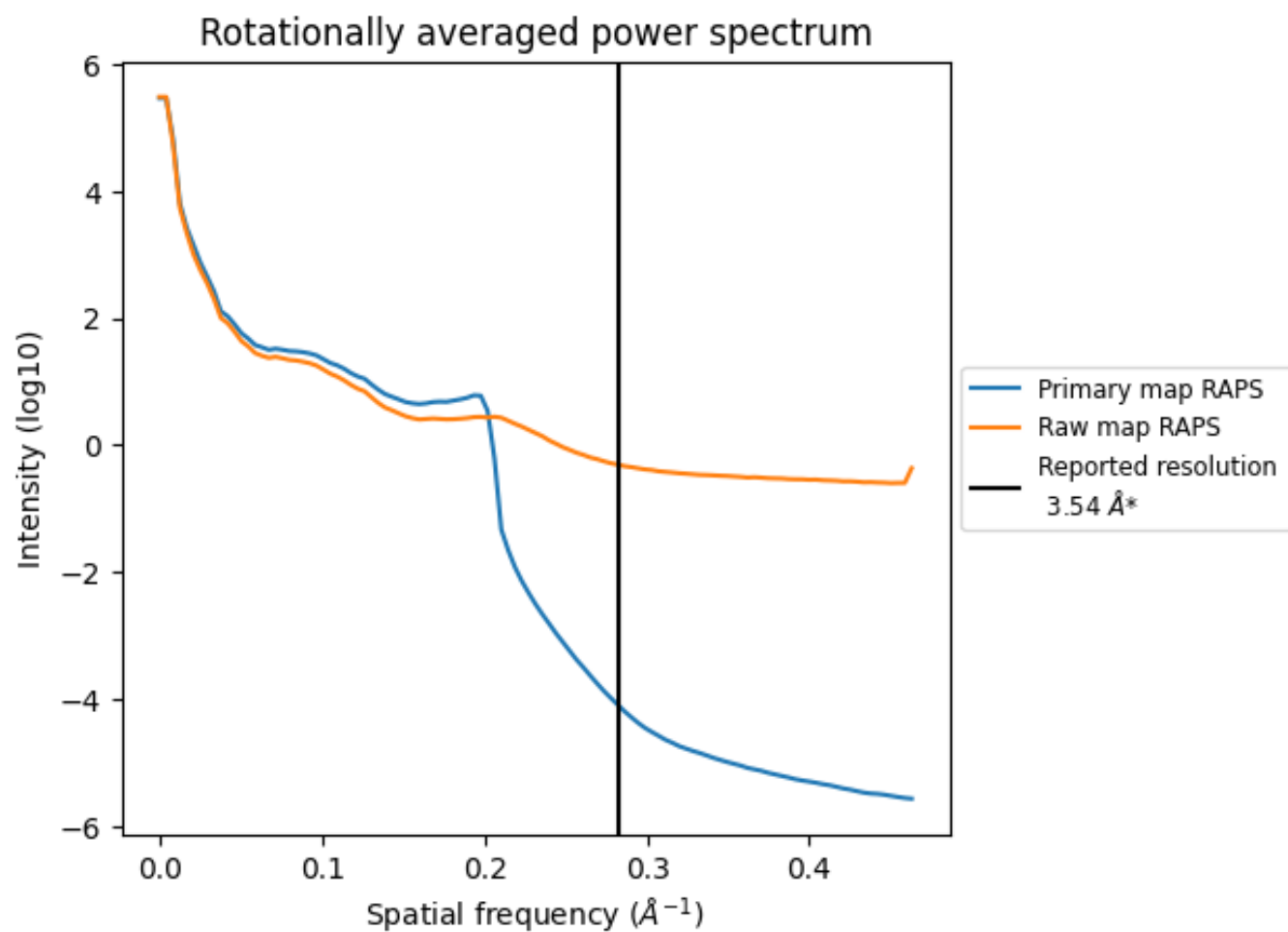
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm<sup>3</sup>; this corresponds to an approximate mass of 435 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 ⓘ

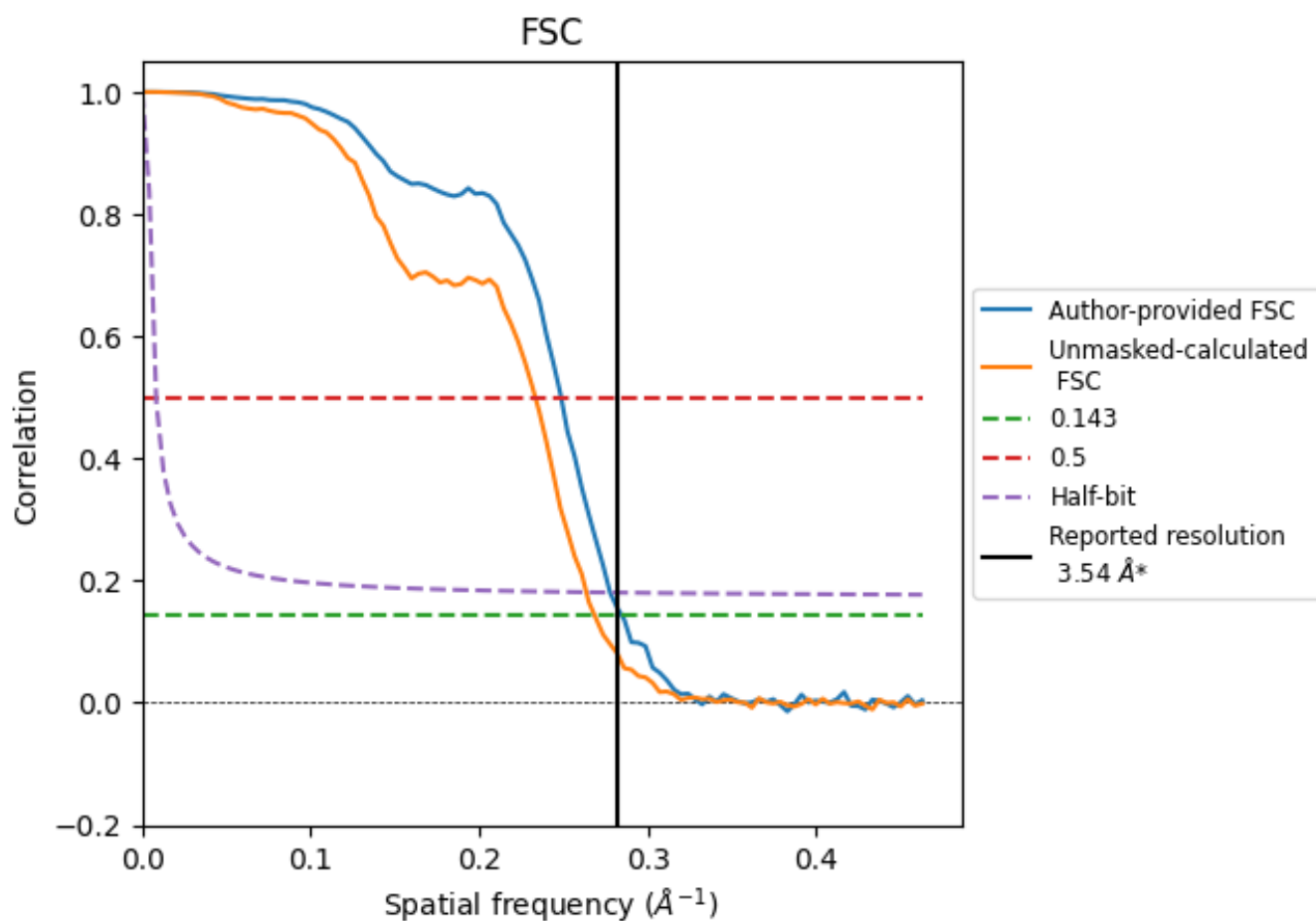


\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.282  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

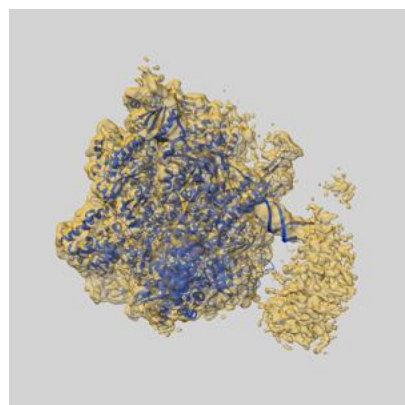
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.54                               | -    | -        |
| Author-provided FSC curve | 3.51                               | 4.02 | 3.60     |
| Unmasked-calculated*      | 3.72                               | 4.29 | 3.79     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

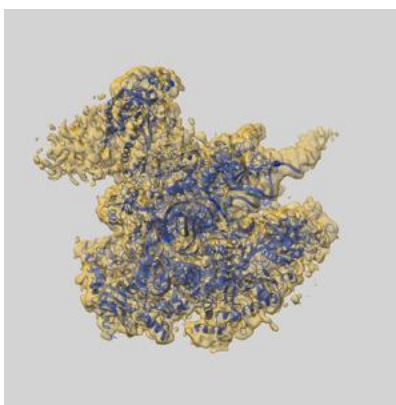
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23888 and PDB model 7MKA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

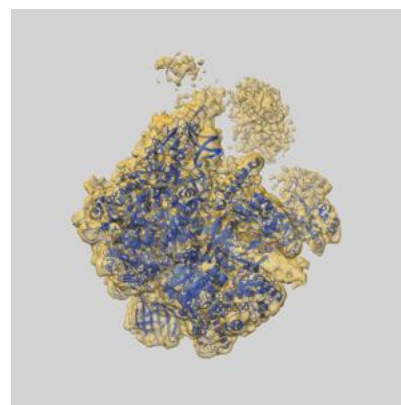
### 9.1 Map-model overlay [i](#)



X



Y

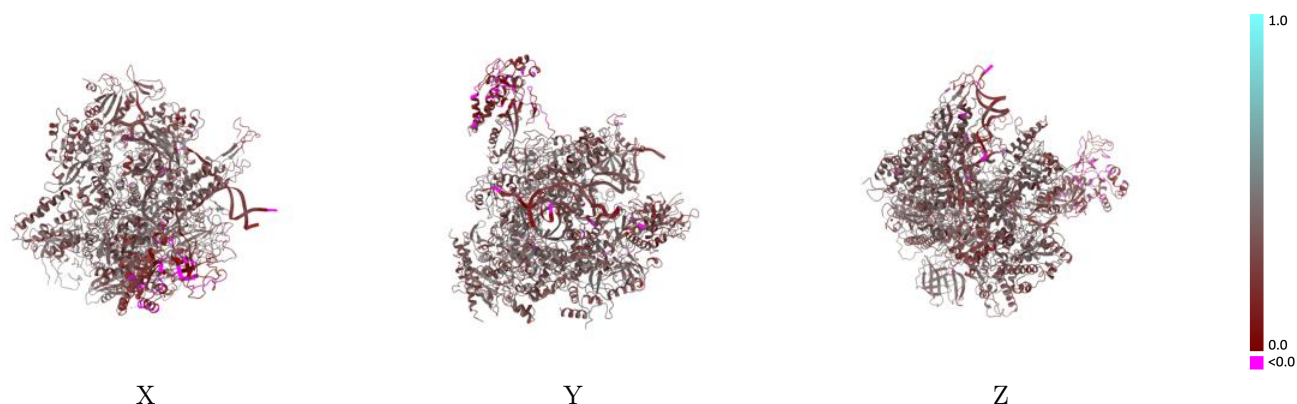


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

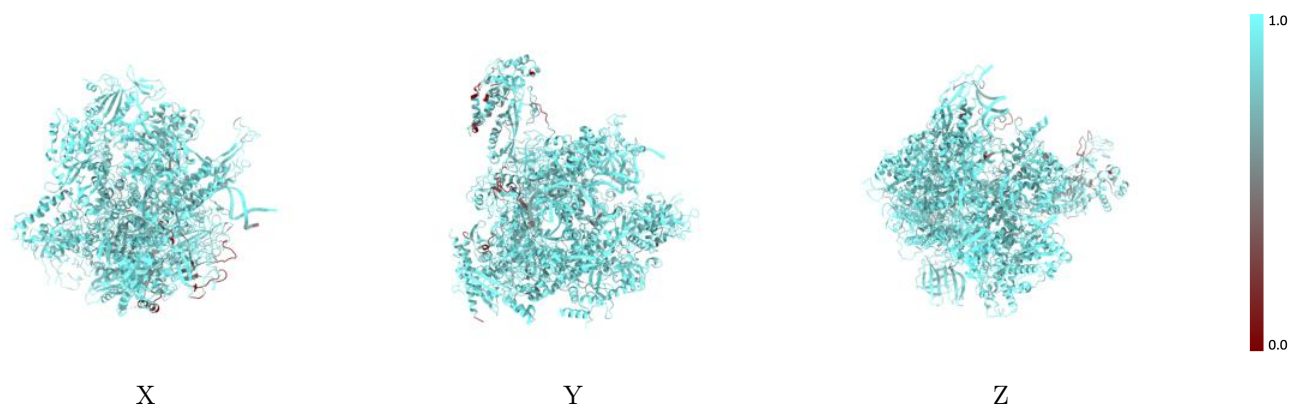


## 9.2 Q-score mapped to coordinate model [i](#)



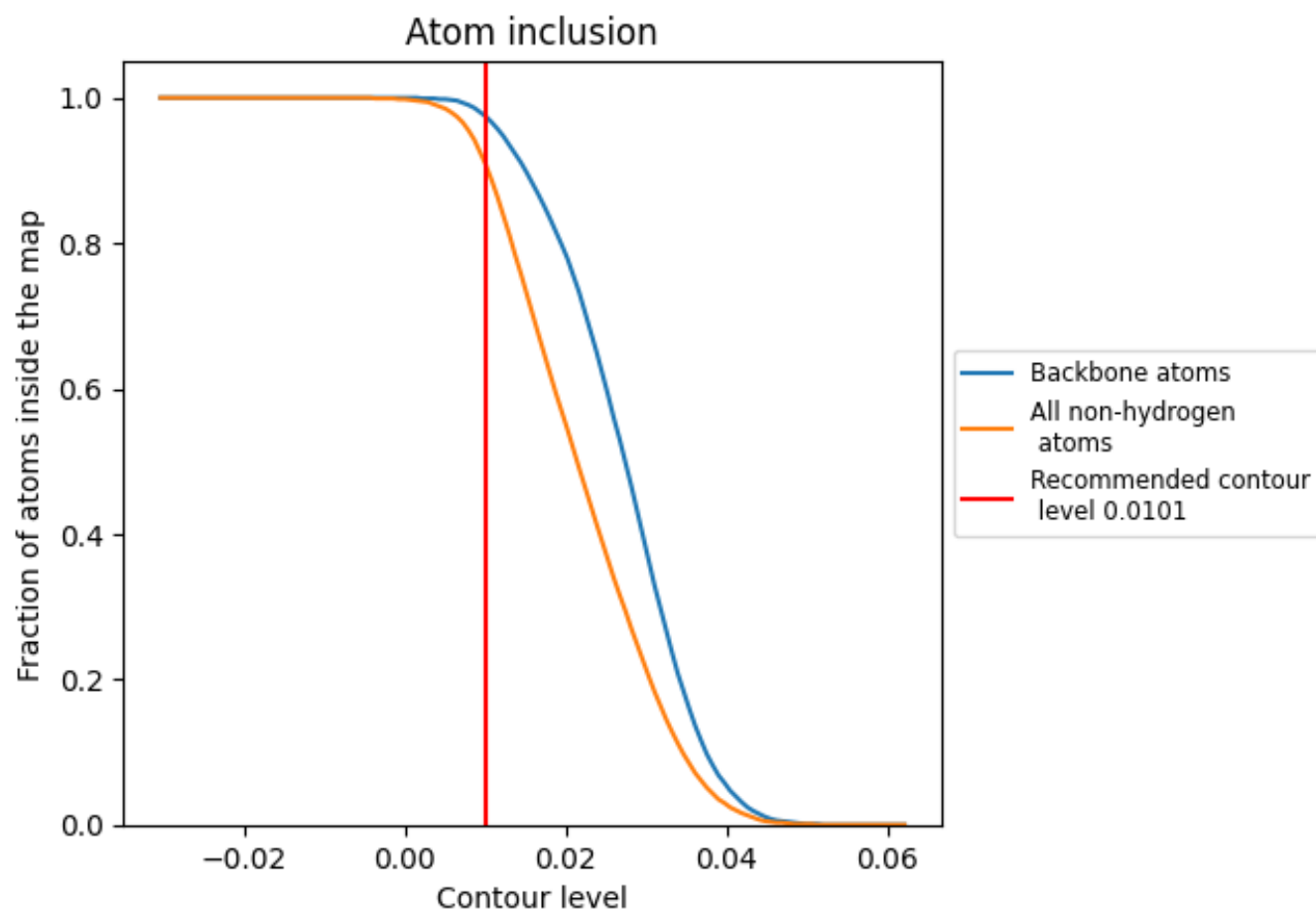
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0101).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.0101) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9070 | <div></div> 0.3320 |
| N     | <div></div> 0.8730 | <div></div> 0.2180 |
| O     | <div></div> 0.9400 | <div></div> 0.2870 |
| a     | <div></div> 0.9280 | <div></div> 0.3500 |
| b     | <div></div> 0.9020 | <div></div> 0.3530 |
| c     | <div></div> 0.9290 | <div></div> 0.3660 |
| d     | <div></div> 0.7680 | <div></div> 0.1610 |
| e     | <div></div> 0.9500 | <div></div> 0.3510 |
| f     | <div></div> 0.9180 | <div></div> 0.3540 |
| g     | <div></div> 0.8030 | <div></div> 0.2110 |
| h     | <div></div> 0.9440 | <div></div> 0.3470 |
| i     | <div></div> 0.9230 | <div></div> 0.3220 |
| j     | <div></div> 0.9510 | <div></div> 0.3650 |
| k     | <div></div> 0.8560 | <div></div> 0.3400 |
| l     | <div></div> 0.9230 | <div></div> 0.3510 |
| r     | <div></div> 0.8380 | <div></div> 0.2540 |

1.0

0.0

<0.0