# Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 09:29 am GMT

| | | |
|---|---|---|
| PDB ID | : | 5FLM |
| EMDB ID | : | EMD-3218 |
| Title | : | Structure of transcribing mammalian RNA polymerase II |
| Authors | : | Bernecky, C.; Herzog, F.; Baumeister, W.; Plitzko, J.M.; Cramer, P. |
| Deposited on | : | 2015-10-26 |
| Resolution | : | 3.40 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

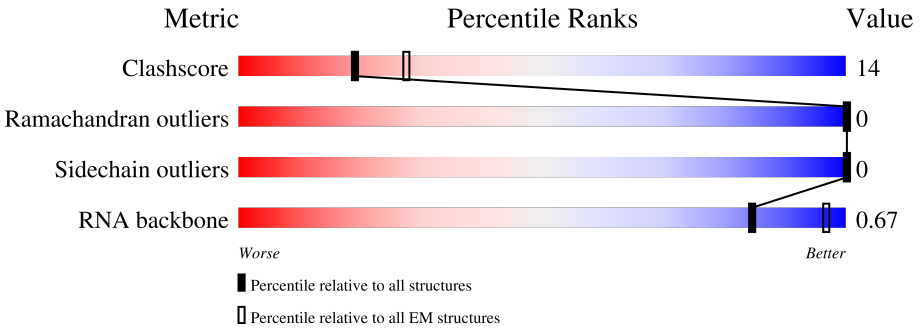
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1970 | 14% 50% 22% 28% |
| 2 | B | 1174 | 15% 63% 33% . |
| 3 | C | 275 | 10% 64% 29% 7% |
| 4 | D | 142 | 90% 47% 43% 10% |
| 5 | E | 210 | 19% 73% 27% |
| 6 | F | 127 | 16% 49% 16% 35% |
| 7 | G | 172 | 97% 53% 46% . |

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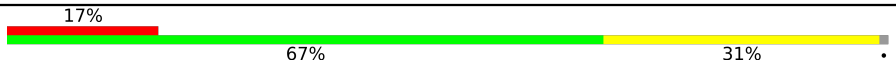
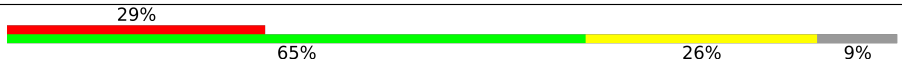
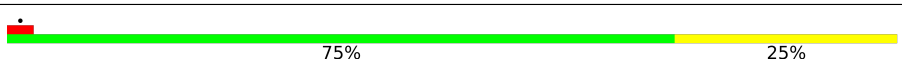
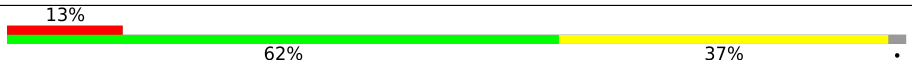
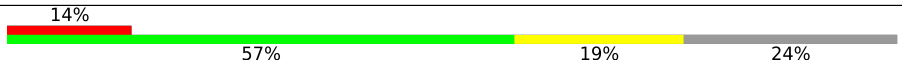
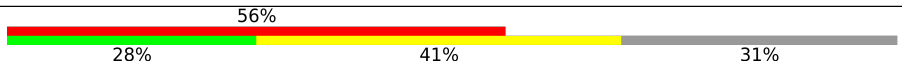
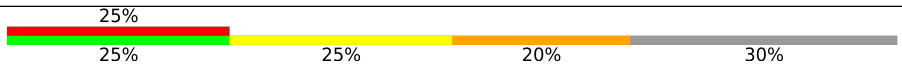
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | H | 150 |   |
| 9 | I | 125 |   |
| 10 | J | 67 |   |
| 11 | K | 117 |   |
| 12 | L | 58 |   |
| 13 | N | 39 |   |
| 14 | P | 20 |   |
| 15 | T | 39 | |

# 2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1427 | 11291 | 7102 | 2021 | 2096 | 72 | 0 | 0 |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1134 | 9062 | 5732 | 1595 | 1671 | 64 | 0 | 0 |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 257 | 2059 | 1294 | 351 | 408 | 6 | 0 | 0 |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 128 | 1005 | 632 | 172 | 197 | 4 | 0 | 0 |

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 209 | 1711 | 1084 | 300 | 319 | 8 | 0 | 0 |

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 419 | 113 | 121 | 5 | | |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1334 | 867 | 216 | 243 | 8 | | |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1186 | 750 | 194 | 237 | 5 | | |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 927 | 571 | 166 | 179 | 11 | | |

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 533 | 345 | 90 | 92 | 6 | | |

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 372 | 231 | 72 | 63 | 6 | | |

- Molecule 13 is a DNA chain called DNA, DNA-RNA ELONGATION SCAFFOLD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | N | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 552 | 266 | 103 | 158 | 25 | | |

- Molecule 14 is a RNA chain called RNA, DNA-RNA ELONGATION SCAFFOLD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | P | 14 | Total | C | N | O | P | 0 | 0 |
| | | | 301 | 135 | 59 | 93 | 14 | | |

- Molecule 15 is a DNA chain called DNA, DNA-RNA ELONGATION SCAFFOLD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | T | 39 | Total | C | N | O | P | 0 | 0 |
| | | | 792 | 380 | 142 | 232 | 38 | | |

- Molecule 16 is ZINC ION (three-letter code: 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 (three-letter code: MG) (formula: Mg).

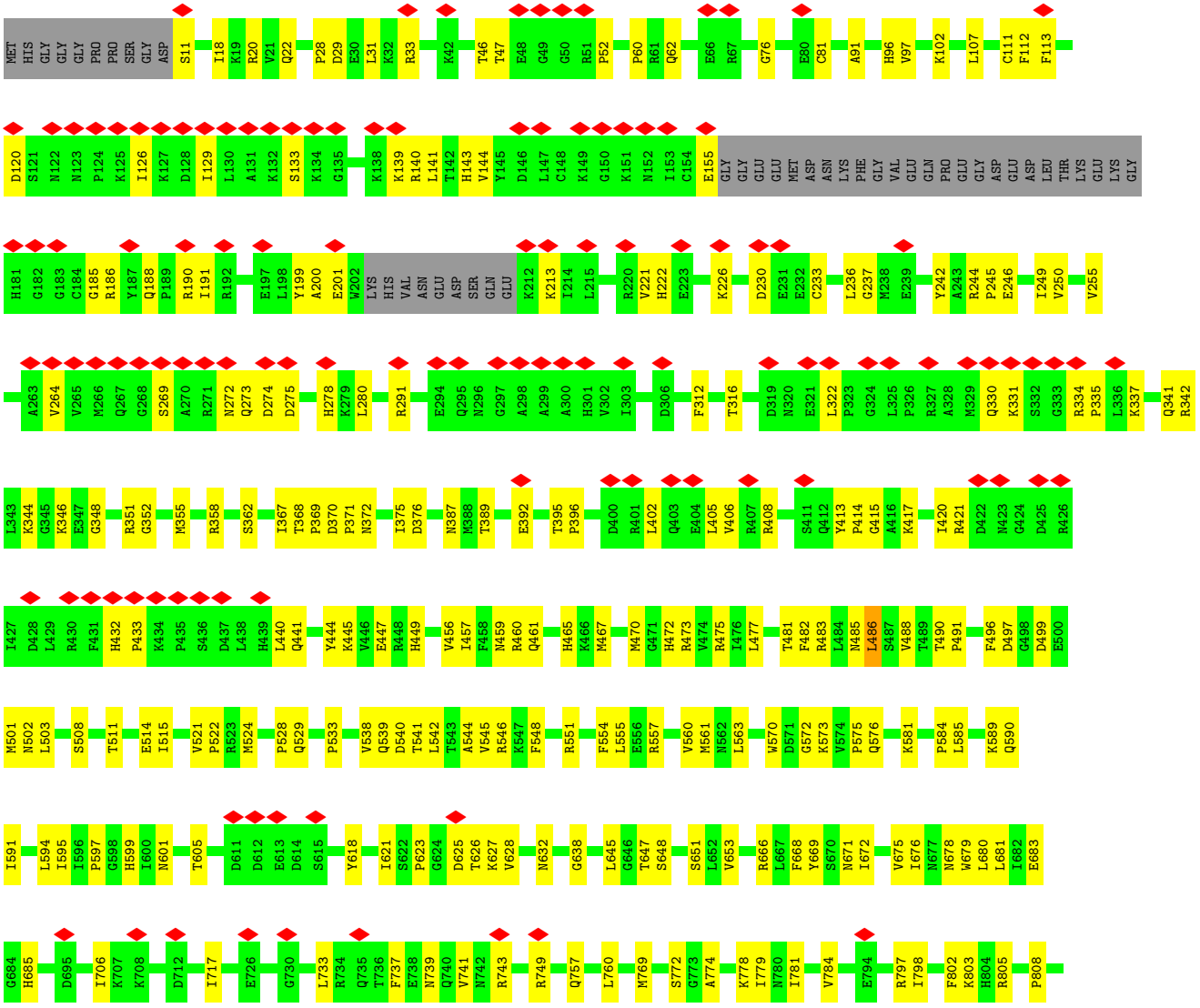
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 17 | A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

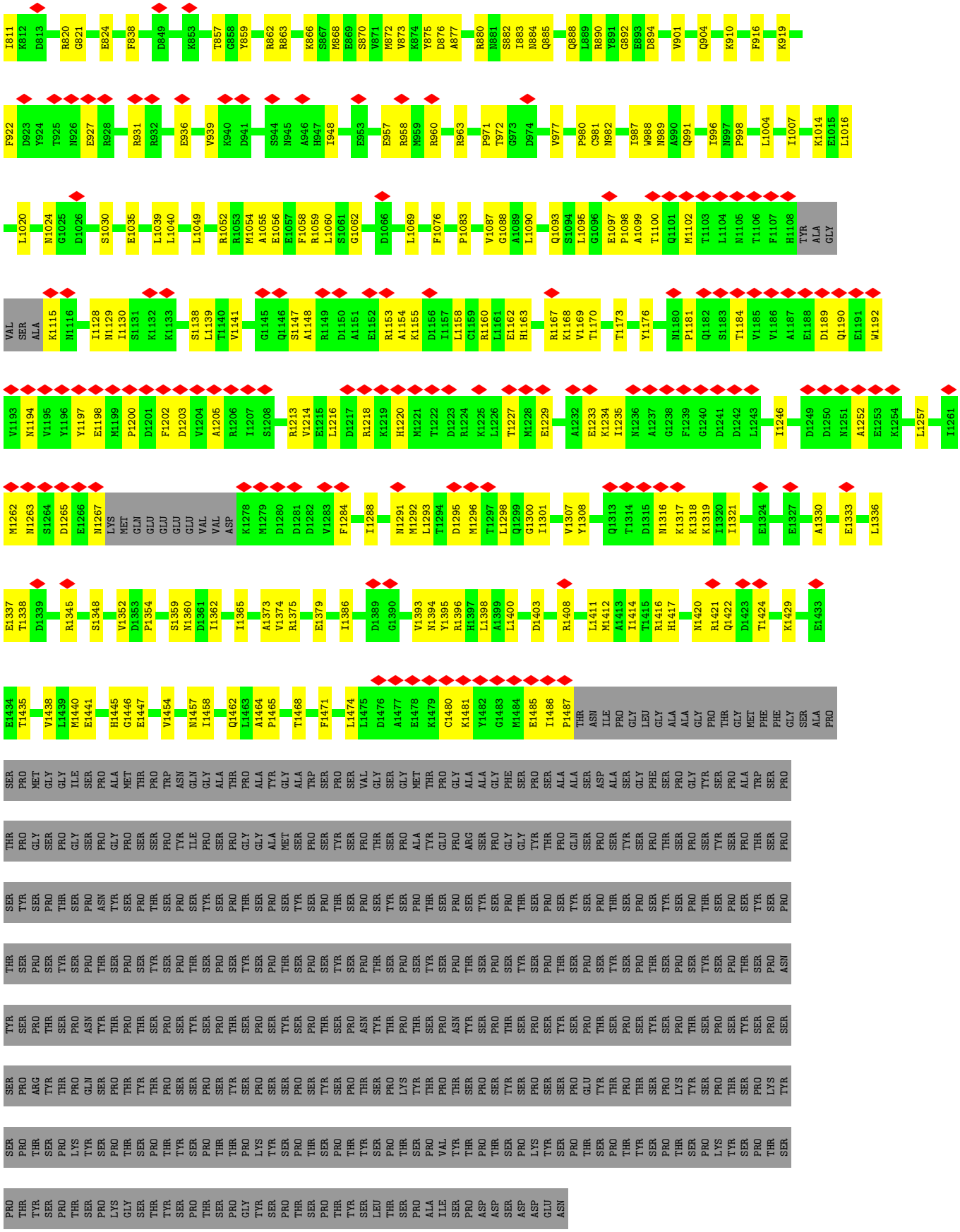
# 3 Residue-property plots (i)

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain A:




I811 K812 D813 R820 G821 E824 F838 D849 K853 T857 G858 Y859 R862 R863 K866 S867 M868 E869 S870 V871 M872 V873 K874 Y875 D876 A877 R880 N881 S882 I883 N884 Q885 Q888 L889 R890 Y891 G892 E893 D894 V901 Q904 K910 F916 K919
F922 D923 Y924 T925 N926 E927 R928 R931 R932 E936 V939 K940 D941 S944 N945 A946 H947 I948 E953 E957 R958 M959 R960 R963 P971 T972 G973 D974 V977 P980 C981 N982 I987 W988 N989 A990 Q991 I996 N997 P998 L1004 I1007 K1014 E1015 L1016
L1020 N1024 G1025 D1026 S1030 E1035 L1039 L1040 L1049 R1052 R1053 M1054 A1055 E1056 E1057 F1058 R1059 L1060 S1061 G1062 D1066 L1069 F1076 P1083 V1087 G1088 A1089 L1090 Q1093 S1094 L1095 G1096 E1097 P1098 A1099 T1100 Q1101 M1102 T1103 L1104 N1105 T1106 F1107 H1108 TYR ALA GLY
VAL SER ALA K1115 N1116 I1128 N1129 I1130 S1131 K1132 K1133 S1138 L1139 T1140 V1141 G1145 Q1146 S1147 A1148 R1149 D1150 A1151 E1152 R1153 A1154 K1155 D1156 I1157 L1158 C1159 R1160 L1161 E1162 H1163 R1167 K1168 V1169 T1170 T1173 Y1176 N1180 P1181 Q1182 S1183 T1184 V1185 V1186 A1187 E1188 D1189 Q1190 E1191 W1192
V1193 N1194 V1195 Y1196 Y1197 E1198 M1199 P1200 D1201 F1202 D1203 V1204 A1205 R1206 I1207 S1208 R1213 V1214 E1215 L1216 D1217 R1218 K1219 H1220 M1221 T1222 D1223 R1224 K1225 L1226 T1227 M1228 E1229 A1232 E1233 K1234 I1235 N1236 A1237 G1238 F1239 G1240 D1241 D1242 L1243 I1246 D1249 D1250 N1251 A1252 E1253 K1254 L1257 I1261
M1262 N1263 S1264 D1265 E1266 N1267 LYS MET GLN GLU GLU GLU VAL VAL ASP K1278 M1279 D1280 D1281 D1282 V1283 F1284 I1288 N1291 M1292 L1293 T1294 D1295 M1296 T1297 L1298 Q1299 G1300 I1301 V1307 Y1308 Q1313 T1314 D1315 N1316 K1317 K1318 K1319 I1320 I1321 E1324 E1327 A1330 E1333 L1336
E1337 T1338 D1339 R1345 S1348 V1352 D1353 P1354 S1359 N1360 D1361 I1362 I1365 A1373 V1374 R1375 E1379 I1386 D1389 G1390 V1393 N1394 Y1395 R1396 H1397 L1398 A1399 L1400 D1403 R1408 L1411 M1412 A1413 I1414 T1415 R1416 H1417 N1420 R1421 Q1422 D1423 T1424 K1429 E1433
E1434 T1435 V1438 L1439 M1440 E1441 H1445 G1446 E1447 V1454 N1457 I1458 Q1462 L1463 A1464 P1465 T1468 F1471 L1474 L1475 D1476 A1477 E1478 K1479 C1480 K1481 Y1482 G1483 M1484 E1485 I1486 P1487 THR ASN ILE PRO GLY LEU GLY ALA ALA GLY PRO THR GLY MET PHE PHE GLY SER ALA PRO
SER PRO MET GLY GLY ILE SER PRO ALA MET THR PRO TRP ASN GLN GLY ALA THR PRO ALA TYR GLY ALA TRP SER PRO SER VAL GLY SER GLY MET THR PRO GLY ALA ALA SER ASP ALA SER GLY PHE SER PRO GLY TYR SER PRO ALA TRP SER PRO
THR PRO GLY SER PRO GLY SER PRO GLY PRO SER SER PRO TYR ILE PRO SER PRO GLY GLY ALA MET THR PRO SER PRO SER PRO THR SER PRO ALA TYR GLU PRO ARG SER PRO GLY GLY TYR THR PRO GLN SER PRO SER TYR SER PRO THR SER PRO PRO SER TYR SER PRO THR SER
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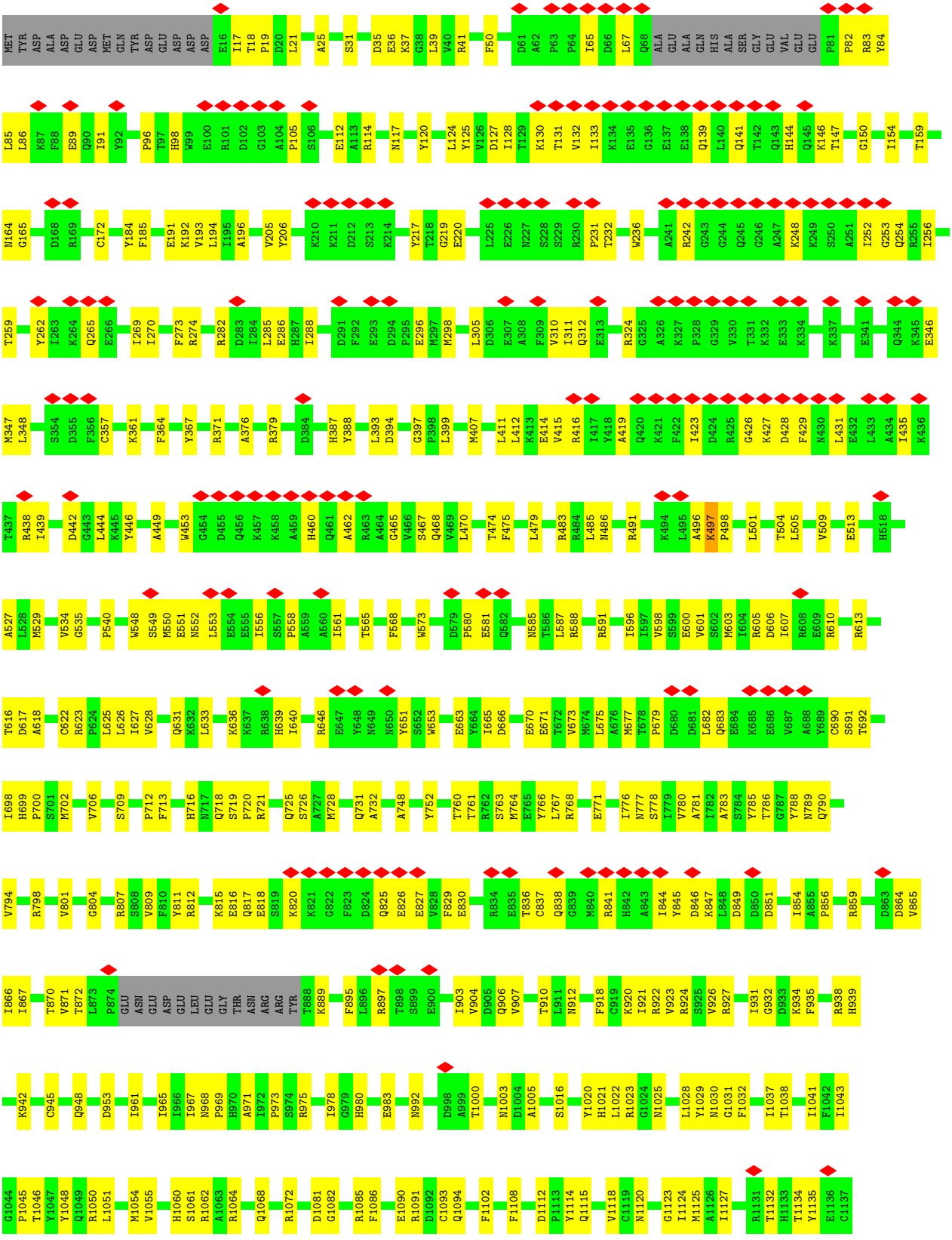
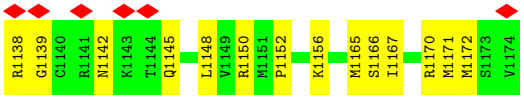
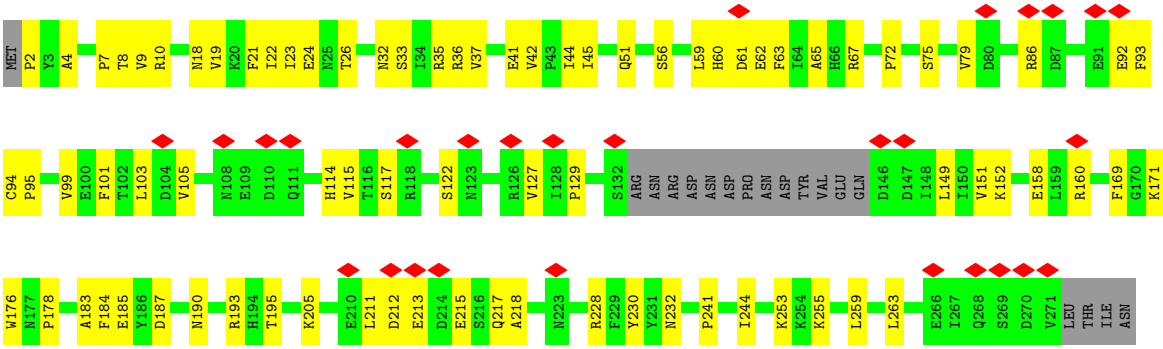
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:

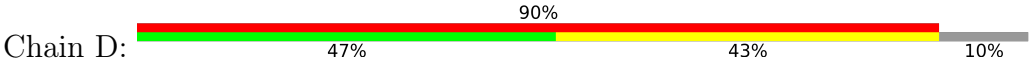


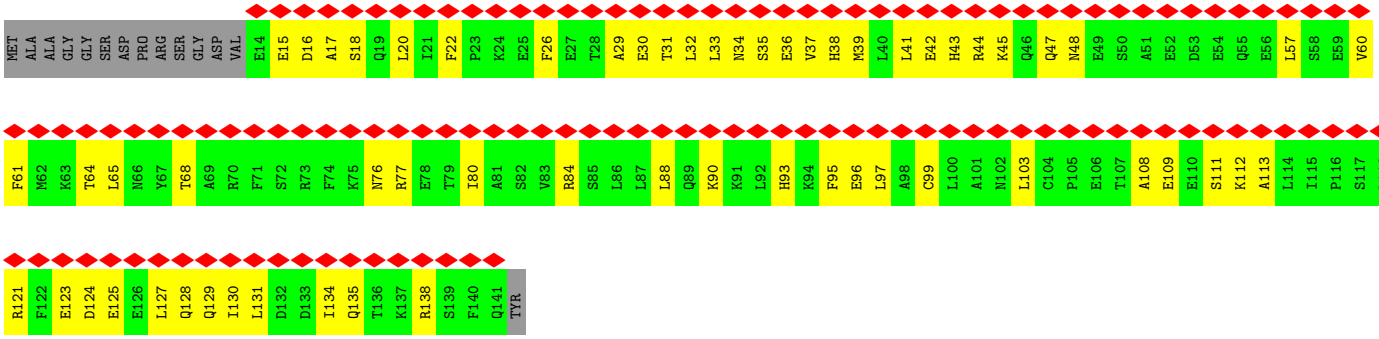



• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

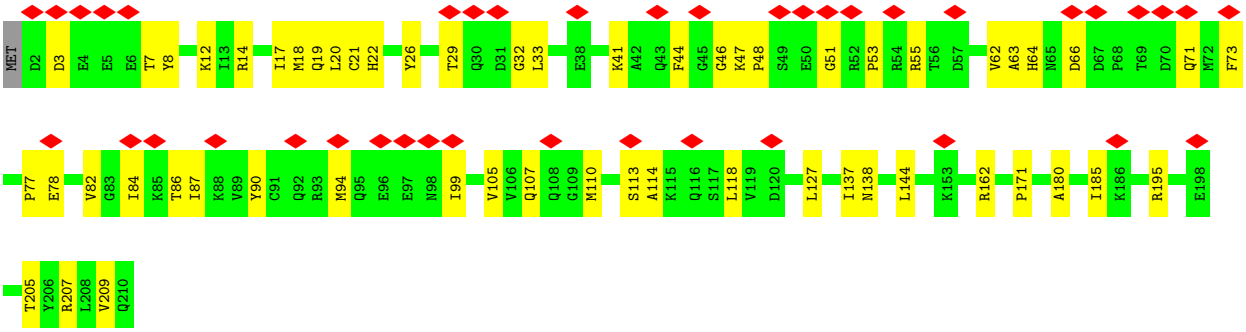



• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

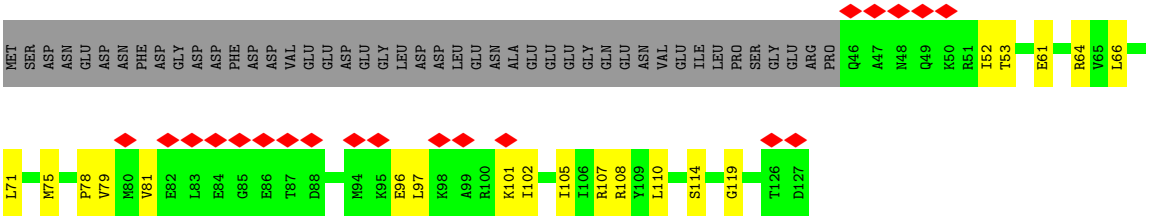


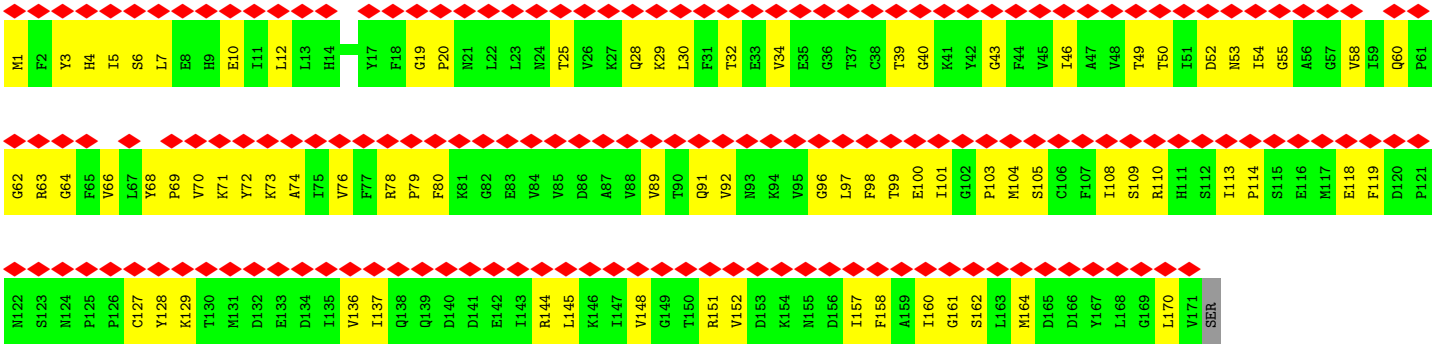

• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1



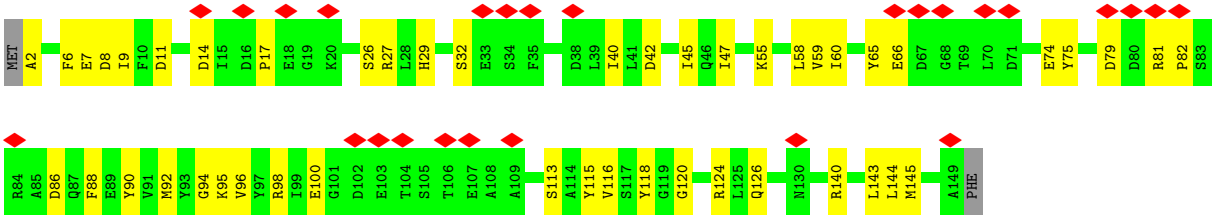

• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



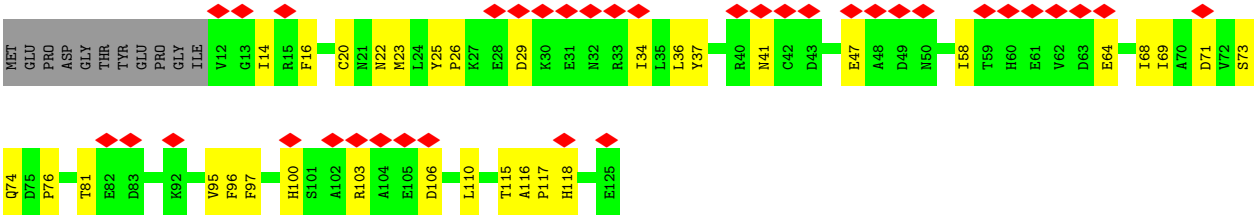

• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



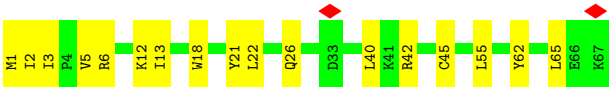

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



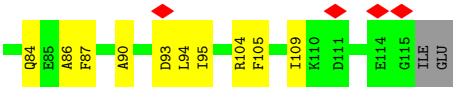

• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



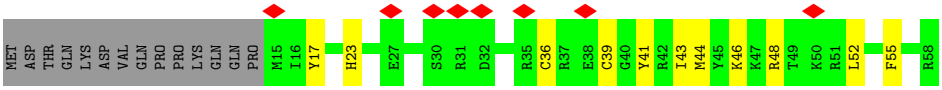

• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



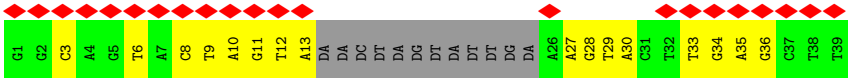

• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



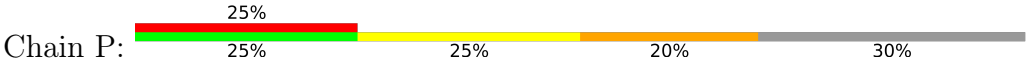

• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

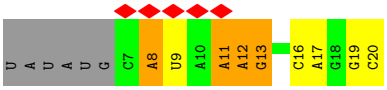



• Molecule 13: DNA, DNA-RNA ELONGATION SCAFFOLD

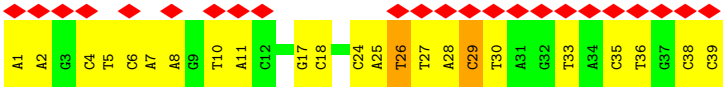



• Molecule 14: RNA, DNA-RNA ELONGATION SCAFFOLD




• Molecule 15: DNA, DNA-RNA ELONGATION SCAFFOLD



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 264134 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | INDIVIDUAL PARTICLES | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 43 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 3100 | Depositor |
| Magnification | 37037 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.500 | Depositor |
| Minimum map value | -0.301 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.018 | Depositor |
| Recommended contour level | 0.07 | Depositor |
| Map size (Å) | 275.4, 275.4, 275.4 | wwPDB |
| Map dimensions | 204, 204, 204 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.35, 1.35, 1.35 | 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 | A | 0.25 | 0/11497 | 0.47 | 1/15521 (0.0%) |
| 2 | B | 0.26 | 0/9243 | 0.47 | 0/12475 |
| 3 | C | 0.26 | 0/2102 | 0.47 | 0/2857 |
| 4 | D | 0.28 | 0/1019 | 0.42 | 0/1374 |
| 5 | E | 0.26 | 0/1742 | 0.46 | 0/2353 |
| 6 | F | 0.53 | 1/668 (0.1%) | 0.51 | 0/903 |
| 7 | G | 0.35 | 0/1365 | 0.50 | 0/1853 |
| 8 | H | 0.26 | 0/1207 | 0.50 | 0/1628 |
| 9 | I | 0.25 | 0/948 | 0.45 | 0/1284 |
| 10 | J | 0.25 | 0/542 | 0.42 | 0/730 |
| 11 | K | 0.26 | 0/939 | 0.46 | 0/1271 |
| 12 | L | 0.27 | 0/377 | 0.52 | 0/500 |
| 13 | N | 0.78 | 4/619 (0.6%) | 1.13 | 0/953 |
| 14 | P | 0.19 | 0/337 | 0.73 | 0/523 |
| 15 | T | 0.93 | 8/887 (0.9%) | 1.13 | 2/1366 (0.1%) |
| All | All | 0.32 | 13/33492 (0.0%) | 0.53 | 3/45591 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 2 | B | 0 | 1 |
| 11 | K | 0 | 1 |
| All | All | 0 | 3 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | T | 26 | DT | O3'-P | -15.93 | 1.42 | 1.61 |
| 6 | F | 102 | ILE | C-N | 11.88 | 1.56 | 1.34 |
| 13 | N | 8 | DC | C1'-N1 | 5.23 | 1.56 | 1.49 |
| 13 | N | 6 | DT | C1'-N1 | 5.23 | 1.56 | 1.49 |
| 13 | N | 9 | DT | C1'-N1 | 5.22 | 1.56 | 1.49 |
| 15 | T | 36 | DT | C1'-N1 | 5.21 | 1.56 | 1.49 |
| 15 | T | 35 | DC | C1'-N1 | 5.20 | 1.56 | 1.49 |
| 15 | T | 33 | DT | C1'-N1 | 5.20 | 1.56 | 1.49 |
| 15 | T | 38 | DC | C1'-N1 | 5.20 | 1.56 | 1.49 |
| 15 | T | 30 | DT | C1'-N1 | 5.16 | 1.55 | 1.49 |
| 13 | N | 3 | DC | C1'-N1 | 5.15 | 1.55 | 1.49 |
| 15 | T | 29 | DC | C1'-N1 | 5.15 | 1.55 | 1.49 |
| 15 | T | 39 | DC | C1'-N1 | 5.08 | 1.55 | 1.49 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | T | 26 | DT | P-O3'-C3' | 11.37 | 133.35 | 119.70 |
| 15 | T | 26 | DT | O3'-P-O5' | 8.16 | 119.51 | 104.00 |
| 1 | A | 486 | LEU | CA-CB-CG | -5.03 | 103.72 | 115.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 910 | LYS | Peptide |
| 2 | B | 497 | LYS | Peptide |
| 11 | K | 7 | PHE | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 11291 | 0 | 11403 | 330 | 0 |
| 2 | B | 9062 | 0 | 9107 | 293 | 0 |
| 3 | C | 2059 | 0 | 2007 | 66 | 0 |
| 4 | D | 1005 | 0 | 964 | 53 | 0 |
| 5 | E | 1711 | 0 | 1733 | 38 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 6 | F | 658 | 0 | 686 | 16 | 0 |
| 7 | G | 1334 | 0 | 1333 | 65 | 0 |
| 8 | H | 1186 | 0 | 1147 | 40 | 0 |
| 9 | I | 927 | 0 | 859 | 30 | 0 |
| 10 | J | 533 | 0 | 554 | 15 | 0 |
| 11 | K | 920 | 0 | 942 | 32 | 0 |
| 12 | L | 372 | 0 | 378 | 13 | 0 |
| 13 | N | 552 | 0 | 309 | 16 | 0 |
| 14 | P | 301 | 0 | 153 | 10 | 0 |
| 15 | T | 792 | 0 | 442 | 16 | 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 | 1 | 0 | 0 | 0 | 0 |
| All | All | 32712 | 0 | 32017 | 916 | 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 14.

All (916) 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:A:1481:LYS:HG2 | 7:G:20:PRO:HA | 1.30 | 1.10 |
| 13:N:13:DA:H61 | 15:T:27:DT:H3 | 1.05 | 0.98 |
| 13:N:13:DA:N1 | 15:T:27:DT:O2 | 2.03 | 0.91 |
| 1:A:948:ILE:HG12 | 1:A:1007:ILE:HD11 | 1.52 | 0.89 |
| 1:A:392:GLU:O | 1:A:445:LYS:HA | 1.74 | 0.86 |
| 1:A:1457:ASN:HD22 | 1:A:1465:PRO:HD3 | 1.42 | 0.84 |
| 2:B:718:GLN:HG2 | 2:B:720:PRO:HD2 | 1.58 | 0.83 |
| 3:C:259:LEU:HD11 | 11:K:42:LEU:HD21 | 1.59 | 0.83 |
| 2:B:282:ARG:O | 2:B:286:GLU:HB2 | 1.80 | 0.82 |
| 2:B:159:THR:HA | 2:B:164:ASN:HD22 | 1.45 | 0.81 |
| 2:B:1016:SER:HB2 | 2:B:1022:LEU:HB3 | 1.63 | 0.81 |
| 1:A:111:CYS:SG | 1:A:188:GLN:NE2 | 2.54 | 0.80 |
| 2:B:550:MET:HG2 | 2:B:551:GLU:H | 1.44 | 0.80 |
| 2:B:130:LYS:O | 2:B:141:GLN:HA | 1.81 | 0.79 |
| 1:A:1468:THR:HG23 | 6:F:64:ARG:HB2 | 1.65 | 0.79 |
| 1:A:627:LYS:HG2 | 1:A:628:VAL:H | 1.48 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1031:GLY:O | 3:C:36:ARG:NH2 | 2.18 | 0.77 |
| 15:T:25:DA:H2" | 15:T:26:DT:H5" | 1.65 | 0.76 |
| 1:A:1481:LYS:CG | 7:G:20:PRO:HA | 2.14 | 0.76 |
| 1:A:922:PHE:H | 1:A:1052:ARG:HD2 | 1.51 | 0.76 |
| 1:A:904:GLN:NE2 | 1:A:981:CYS:O | 2.17 | 0.76 |
| 3:C:24:GLU:HG2 | 3:C:228:ARG:HG2 | 1.68 | 0.75 |
| 2:B:1062:ARG:NH1 | 2:B:1081:ASP:O | 2.20 | 0.74 |
| 1:A:129:ILE:O | 1:A:133:SER:HB2 | 1.88 | 0.74 |
| 7:G:89:VAL:HA | 7:G:99:THR:HG22 | 1.68 | 0.74 |
| 13:N:13:DA:N6 | 15:T:27:DT:H3 | 1.83 | 0.74 |
| 1:A:1291:ASN:O | 1:A:1295:ASP:HB3 | 1.88 | 0.73 |
| 2:B:415:VAL:O | 2:B:419:ALA:HB2 | 1.87 | 0.73 |
| 2:B:713:PHE:HB3 | 2:B:716:HIS:HD2 | 1.53 | 0.72 |
| 3:C:7:PRO:O | 11:K:104:ARG:NH1 | 2.22 | 0.72 |
| 4:D:90:LYS:HE2 | 4:D:130:ILE:HD11 | 1.70 | 0.72 |
| 2:B:939:HIS:NE2 | 2:B:983:GLU:OE1 | 2.23 | 0.72 |
| 3:C:99:VAL:HG11 | 3:C:127:VAL:HG21 | 1.72 | 0.71 |
| 13:N:10:DA:H2" | 13:N:11:DG:OP2 | 1.91 | 0.71 |
| 1:A:191:ILE:HA | 1:A:199:TYR:O | 1.90 | 0.71 |
| 1:A:1138:SER:OG | 1:A:1360:ASN:ND2 | 2.23 | 0.71 |
| 2:B:827:GLU:HG2 | 2:B:871:VAL:HG22 | 1.73 | 0.71 |
| 13:N:29:DT:H2' | 13:N:30:DA:C8 | 2.26 | 0.71 |
| 2:B:265:GLN:HE21 | 2:B:324:ARG:HE | 1.36 | 0.71 |
| 2:B:196:ALA:HA | 2:B:394:ASP:O | 1.91 | 0.71 |
| 1:A:18:ILE:H | 1:A:1462:GLN:HE22 | 1.36 | 0.70 |
| 7:G:40:GLY:HA2 | 7:G:157:ILE:HD11 | 1.71 | 0.70 |
| 9:I:115:THR:HG22 | 9:I:116:ALA:H | 1.56 | 0.70 |
| 1:A:264:VAL:HB | 1:A:272:ASN:HB2 | 1.74 | 0.70 |
| 1:A:362:SER:HA | 1:A:503:LEU:O | 1.92 | 0.70 |
| 2:B:760:THR:OG1 | 2:B:764:MET:SD | 2.50 | 0.70 |
| 1:A:904:GLN:HE21 | 1:A:982:ASN:HA | 1.56 | 0.70 |
| 1:A:1087:VAL:HG12 | 1:A:1400:LEU:HD22 | 1.74 | 0.70 |
| 2:B:748:ALA:HB3 | 2:B:811:TYR:HB2 | 1.74 | 0.70 |
| 1:A:1474:LEU:HB2 | 6:F:105:ILE:HG13 | 1.72 | 0.69 |
| 1:A:877:ALA:HB3 | 1:A:890:ARG:HH11 | 1.56 | 0.69 |
| 12:L:17:TYR:HB3 | 12:L:44:MET:HB3 | 1.73 | 0.69 |
| 2:B:1060:HIS:NE2 | 2:B:1082:GLY:O | 2.25 | 0.69 |
| 2:B:415:VAL:O | 2:B:419:ALA:CB | 2.41 | 0.69 |
| 2:B:591:ARG:NH2 | 2:B:663:GLU:OE2 | 2.25 | 0.69 |
| 2:B:924:ARG:NH1 | 3:C:62:GLU:OE2 | 2.25 | 0.69 |
| 7:G:100:GLU:HA | 7:G:105:SER:HA | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:152:VAL:HA | 7:G:157:ILE:HA | 1.76 | 0.68 |
| 1:A:20:ARG:NH2 | 2:B:1172:MET:SD | 2.66 | 0.68 |
| 1:A:538:VAL:HG12 | 1:A:539:GLN:HG2 | 1.75 | 0.68 |
| 2:B:298:MET:HB3 | 9:I:14:ILE:HD12 | 1.76 | 0.68 |
| 2:B:357:CYS:SG | 2:B:361:LYS:NZ | 2.66 | 0.68 |
| 2:B:65:ILE:HB | 2:B:86:LEU:HB2 | 1.75 | 0.68 |
| 2:B:627:ILE:HD11 | 2:B:663:GLU:HB2 | 1.76 | 0.68 |
| 1:A:1348:SER:O | 5:E:12:LYS:NZ | 2.25 | 0.68 |
| 3:C:56:SER:HG | 3:C:158:GLU:H | 1.41 | 0.68 |
| 1:A:372:ASN:ND2 | 2:B:788:TYR:OH | 2.27 | 0.68 |
| 1:A:601:ASN:ND2 | 1:A:989:ASN:OD1 | 2.26 | 0.68 |
| 2:B:438:ARG:O | 2:B:442:ASP:HB2 | 1.93 | 0.68 |
| 4:D:34:ASN:O | 4:D:68:THR:OG1 | 2.11 | 0.67 |
| 7:G:110:ARG:HA | 7:G:113:ILE:HD12 | 1.76 | 0.67 |
| 8:H:58:LEU:HD11 | 8:H:143:LEU:HD11 | 1.75 | 0.67 |
| 2:B:992:ASN:HD21 | 2:B:1020:TYR:HE2 | 1.40 | 0.67 |
| 1:A:811:ILE:HD11 | 2:B:690:CYS:HB2 | 1.77 | 0.67 |
| 3:C:10:ARG:NH1 | 3:C:24:GLU:OE2 | 2.27 | 0.67 |
| 4:D:108:ALA:N | 4:D:128:GLN:OE1 | 2.27 | 0.67 |
| 7:G:148:VAL:N | 7:G:160:ILE:O | 2.27 | 0.67 |
| 1:A:883:ILE:HD11 | 1:A:1424:THR:HG22 | 1.75 | 0.66 |
| 2:B:535:GLY:N | 2:B:600:GLU:OE2 | 2.17 | 0.66 |
| 5:E:63:ALA:HA | 5:E:71:GLN:HA | 1.77 | 0.66 |
| 1:A:461:GLN:HE22 | 1:A:502:ASN:ND2 | 1.94 | 0.66 |
| 2:B:274:ARG:NH1 | 2:B:311:ILE:O | 2.28 | 0.66 |
| 1:A:1416:ARG:O | 1:A:1420:ASN:HB2 | 1.96 | 0.66 |
| 2:B:124:LEU:HB3 | 2:B:150:GLY:O | 1.95 | 0.66 |
| 3:C:59:LEU:HD12 | 3:C:151:VAL:HG23 | 1.77 | 0.66 |
| 2:B:706:VAL:HG13 | 2:B:767:LEU:HD22 | 1.78 | 0.66 |
| 5:E:171:PRO:HB2 | 5:E:207:ARG:HD3 | 1.78 | 0.66 |
| 13:N:11:DG:OP2 | 13:N:11:DG:H8 | 1.78 | 0.66 |
| 5:E:84:ILE:HD11 | 5:E:113:SER:HB3 | 1.78 | 0.66 |
| 1:A:375:ILE:HD11 | 1:A:669:TYR:HB2 | 1.78 | 0.65 |
| 2:B:427:LYS:HG3 | 2:B:428:ASP:H | 1.61 | 0.65 |
| 4:D:34:ASN:O | 4:D:38:HIS:HB2 | 1.96 | 0.65 |
| 1:A:155:GLU:HA | 1:A:185:GLY:HA2 | 1.79 | 0.65 |
| 1:A:885:GLN:HE22 | 1:A:1408:ARG:HH12 | 1.43 | 0.65 |
| 2:B:96:PRO:HG3 | 2:B:154:ILE:HG13 | 1.78 | 0.65 |
| 4:D:48:ASN:HD22 | 4:D:57:LEU:HG | 1.60 | 0.65 |
| 6:F:81:VAL:HG22 | 6:F:101:LYS:HD3 | 1.79 | 0.65 |
| 1:A:894:ASP:OD1 | 1:A:1396:ARG:NH1 | 2.23 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:731:GLN:HE22 | 14:P:19:G:H5' | 1.62 | 0.65 |
| 2:B:778:SER:O | 2:B:1045:PRO:HA | 1.96 | 0.65 |
| 2:B:565:THR:HA | 2:B:610:ARG:HG2 | 1.79 | 0.65 |
| 2:B:816:GLU:HG2 | 2:B:867:ILE:HG21 | 1.77 | 0.65 |
| 1:A:112:PHE:HZ | 1:A:191:ILE:HD11 | 1.62 | 0.64 |
| 1:A:76:GLY:HA2 | 1:A:81:CYS:HB2 | 1.79 | 0.64 |
| 2:B:625:LEU:HD13 | 2:B:675:LEU:HD21 | 1.79 | 0.64 |
| 1:A:1205:ALA:HB1 | 1:A:1267:ASN:HB2 | 1.80 | 0.64 |
| 1:A:581:LYS:NZ | 8:H:86:ASP:O | 2.31 | 0.64 |
| 2:B:364:PHE:O | 2:B:367:TYR:HB3 | 1.97 | 0.64 |
| 2:B:628:VAL:HG22 | 2:B:633:LEU:HD23 | 1.80 | 0.64 |
| 3:C:183:ALA:HB3 | 3:C:232:ASN:HB3 | 1.80 | 0.64 |
| 2:B:217:TYR:OH | 9:I:103:ARG:NH2 | 2.31 | 0.64 |
| 1:A:1184:THR:OG1 | 1:A:1190:GLN:NE2 | 2.31 | 0.63 |
| 2:B:679:PRO:O | 2:B:683:GLN:HB2 | 1.98 | 0.63 |
| 7:G:91:GLN:HB3 | 7:G:98:PHE:HB2 | 1.80 | 0.63 |
| 2:B:636:LYS:H | 2:B:639:HIS:HD2 | 1.47 | 0.63 |
| 1:A:675:VAL:HG23 | 1:A:676:ILE:HG13 | 1.78 | 0.63 |
| 1:A:757:GLN:NE2 | 1:A:778:LYS:HB3 | 2.13 | 0.63 |
| 5:E:195:ARG:NH1 | 5:E:205:THR:OG1 | 2.32 | 0.63 |
| 5:E:62:VAL:O | 5:E:71:GLN:HA | 1.99 | 0.63 |
| 2:B:83:ARG:HB2 | 2:B:133:ILE:HB | 1.81 | 0.62 |
| 2:B:598:VAL:HG12 | 2:B:600:GLU:H | 1.64 | 0.62 |
| 2:B:851:ASP:OD2 | 12:L:17:TYR:OH | 2.16 | 0.62 |
| 3:C:51:GLN:HE21 | 12:L:52:LEU:HB3 | 1.64 | 0.62 |
| 2:B:411:LEU:HD11 | 2:B:435:ILE:HG23 | 1.81 | 0.62 |
| 3:C:205:LYS:NZ | 3:C:212:ASP:O | 2.32 | 0.62 |
| 1:A:1049:LEU:HA | 1:A:1054:MET:HE3 | 1.80 | 0.62 |
| 2:B:194:LEU:HD23 | 2:B:467:SER:HB3 | 1.82 | 0.62 |
| 1:A:653:VAL:HG22 | 1:A:668:PHE:HE2 | 1.62 | 0.62 |
| 1:A:554:PHE:HB3 | 1:A:585:LEU:HD23 | 1.82 | 0.62 |
| 1:A:863:ARG:NH2 | 1:A:1129:ASN:OD1 | 2.30 | 0.62 |
| 1:A:1319:LYS:HE2 | 1:A:1321:ILE:HD11 | 1.82 | 0.62 |
| 2:B:866:ILE:HG22 | 2:B:867:ILE:HG13 | 1.81 | 0.62 |
| 1:A:1485:GLU:HB3 | 6:F:78:PRO:HB3 | 1.81 | 0.62 |
| 2:B:785:TYR:OH | 2:B:953:ASP:O | 2.18 | 0.62 |
| 1:A:375:ILE:HD12 | 1:A:666:ARG:HG3 | 1.82 | 0.61 |
| 1:A:1147:SER:HA | 1:A:1153:ARG:HB2 | 1.82 | 0.61 |
| 2:B:419:ALA:O | 2:B:423:ILE:HG12 | 2.00 | 0.61 |
| 2:B:938:ARG:NH2 | 2:B:983:GLU:OE2 | 2.23 | 0.61 |
| 8:H:26:SER:HB3 | 8:H:45:ILE:HD11 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:10:PHE:HA | 11:K:37:LYS:HB3 | 1.81 | 0.61 |
| 8:H:2:ALA:N | 8:H:66:GLU:O | 2.33 | 0.61 |
| 1:A:605:THR:HA | 1:A:627:LYS:HA | 1.83 | 0.61 |
| 1:A:803:LYS:NZ | 2:B:606:ASP:OD1 | 2.33 | 0.61 |
| 2:B:67:LEU:HD21 | 2:B:423:ILE:HG13 | 1.82 | 0.61 |
| 2:B:387:HIS:NE2 | 2:B:671:GLU:OE2 | 2.33 | 0.61 |
| 1:A:97:VAL:HG21 | 1:A:322:LEU:HD11 | 1.81 | 0.61 |
| 2:B:483:ARG:NH2 | 2:B:527:ALA:O | 2.30 | 0.61 |
| 4:D:26:PHE:CE2 | 7:G:78:ARG:HD3 | 2.35 | 0.61 |
| 1:A:408:ARG:HH11 | 1:A:414:PRO:HB2 | 1.65 | 0.61 |
| 1:A:1417:HIS:O | 1:A:1421:ARG:HG2 | 2.01 | 0.61 |
| 1:A:545:VAL:HG22 | 1:A:676:ILE:HD13 | 1.83 | 0.60 |
| 1:A:483:ARG:HH21 | 2:B:931:ILE:HD11 | 1.66 | 0.60 |
| 1:A:678:ASN:HA | 1:A:681:LEU:HD13 | 1.83 | 0.60 |
| 2:B:1115:GLN:HB3 | 2:B:1148:LEU:HD11 | 1.83 | 0.60 |
| 9:I:29:ASP:CB | 9:I:34:ILE:O | 2.49 | 0.60 |
| 7:G:39:THR:O | 7:G:43:GLY:N | 2.32 | 0.60 |
| 1:A:1115:LYS:HZ3 | 1:A:1337:GLU:HB3 | 1.65 | 0.60 |
| 4:D:95:PHE:O | 4:D:99:CYS:HB2 | 2.02 | 0.60 |
| 5:E:29:THR:HG23 | 5:E:32:GLY:H | 1.66 | 0.60 |
| 2:B:953:ASP:OD1 | 3:C:36:ARG:NH1 | 2.34 | 0.60 |
| 1:A:1412:MET:SD | 1:A:1422:GLN:NE2 | 2.75 | 0.60 |
| 15:T:7:DA:H2' | 15:T:8:DA:C8 | 2.36 | 0.60 |
| 1:A:201:GLU:OE2 | 1:A:213:LYS:NZ | 2.33 | 0.60 |
| 1:A:576:GLN:O | 1:A:590:GLN:NE2 | 2.34 | 0.60 |
| 7:G:55:GLY:HA3 | 7:G:69:PRO:HG2 | 1.84 | 0.60 |
| 2:B:626:LEU:HG | 2:B:698:ILE:HD13 | 1.84 | 0.60 |
| 2:B:809:VAL:HG22 | 2:B:926:VAL:HG12 | 1.84 | 0.60 |
| 2:B:192:LYS:NZ | 2:B:449:ALA:O | 2.34 | 0.60 |
| 13:N:35:DA:H2" | 13:N:36:DG:H8 | 1.66 | 0.60 |
| 1:A:575:PRO:HG3 | 1:A:594:LEU:HD11 | 1.84 | 0.59 |
| 2:B:486:ASN:OD1 | 2:B:491:ARG:NH2 | 2.31 | 0.59 |
| 2:B:474:THR:OG1 | 2:B:732:ALA:O | 2.20 | 0.59 |
| 2:B:856:PRO:HG2 | 12:L:48:ARG:HA | 1.84 | 0.59 |
| 4:D:38:HIS:O | 4:D:42:GLU:HG2 | 2.02 | 0.59 |
| 1:A:1202:PHE:O | 1:A:1263:ASN:ND2 | 2.35 | 0.59 |
| 2:B:407:MET:HE1 | 2:B:444:LEU:N | 2.17 | 0.59 |
| 2:B:580:PRO:HB2 | 2:B:605:ARG:HE | 1.68 | 0.59 |
| 2:B:585:ASN:OD1 | 2:B:588:ARG:NH2 | 2.35 | 0.59 |
| 5:E:55:ARG:HB2 | 5:E:78:GLU:HG2 | 1.84 | 0.59 |
| 1:A:312:PHE:O | 1:A:316:THR:OG1 | 2.10 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:849:ASP:OD2 | 12:L:46:LYS:NZ | 2.34 | 0.59 |
| 4:D:32:LEU:HD11 | 7:G:4:HIS:HB2 | 1.83 | 0.59 |
| 1:A:107:LEU:HD21 | 1:A:221:VAL:HG13 | 1.84 | 0.59 |
| 1:A:733:LEU:HB3 | 9:I:106:ASP:HB2 | 1.83 | 0.59 |
| 2:B:31:SER:HG | 2:B:766:TYR:HH | 1.41 | 0.59 |
| 2:B:131:THR:HG22 | 2:B:141:GLN:HB3 | 1.84 | 0.59 |
| 4:D:41:LEU:HD12 | 4:D:68:THR:HG21 | 1.84 | 0.59 |
| 2:B:296:GLU:OE1 | 2:B:379:ARG:NH2 | 2.33 | 0.59 |
| 2:B:581:GLU:OE2 | 9:I:74:GLN:NE2 | 2.36 | 0.59 |
| 8:H:79:ASP:O | 8:H:82:PRO:HD2 | 2.01 | 0.59 |
| 1:A:102:LYS:HZ1 | 1:A:141:LEU:HD13 | 1.68 | 0.59 |
| 8:H:88:PHE:CD2 | 8:H:144:LEU:HB3 | 2.38 | 0.59 |
| 1:A:1374:VAL:HG11 | 1:A:1411:LEU:HD21 | 1.85 | 0.58 |
| 4:D:111:SER:HB2 | 4:D:131:LEU:HD21 | 1.85 | 0.58 |
| 1:A:648:SER:OG | 1:A:651:SER:OG | 2.20 | 0.58 |
| 1:A:1291:ASN:O | 1:A:1295:ASP:CB | 2.51 | 0.58 |
| 2:B:794:VAL:O | 2:B:945:CYS:HA | 2.04 | 0.58 |
| 2:B:50:PHE:HB2 | 2:B:397:GLY:HA2 | 1.86 | 0.58 |
| 2:B:854:ILE:HD12 | 2:B:866:ILE:HA | 1.85 | 0.58 |
| 4:D:95:PHE:O | 4:D:99:CYS:CB | 2.52 | 0.58 |
| 2:B:164:ASN:OD1 | 2:B:165:GLY:N | 2.36 | 0.58 |
| 1:A:244:ARG:HD3 | 1:A:245:PRO:HD2 | 1.86 | 0.58 |
| 1:A:20:ARG:NH1 | 1:A:22:GLN:OE1 | 2.36 | 0.58 |
| 2:B:39:LEU:HB3 | 2:B:483:ARG:HD2 | 1.86 | 0.58 |
| 3:C:67:ARG:HH12 | 10:J:2:ILE:HD13 | 1.69 | 0.58 |
| 7:G:4:HIS:CE1 | 7:G:73:LYS:HB3 | 2.39 | 0.58 |
| 1:A:870:SER:HB2 | 1:A:882:SER:HB3 | 1.85 | 0.57 |
| 2:B:159:THR:HA | 2:B:164:ASN:ND2 | 2.18 | 0.57 |
| 7:G:129:LYS:HB2 | 7:G:136:VAL:HG22 | 1.84 | 0.57 |
| 1:A:330:GLN:HG3 | 1:A:331:LYS:N | 2.19 | 0.57 |
| 4:D:84:ARG:O | 4:D:88:LEU:HB2 | 2.04 | 0.57 |
| 5:E:87:ILE:HA | 5:E:90:TYR:HD2 | 1.68 | 0.57 |
| 7:G:30:LEU:HD22 | 7:G:70:VAL:HG11 | 1.85 | 0.57 |
| 8:H:59:VAL:O | 8:H:144:LEU:HB2 | 2.04 | 0.57 |
| 1:A:544:ALA:O | 1:A:548:PHE:CB | 2.53 | 0.57 |
| 4:D:16:ASP:OD2 | 4:D:18:SER:OG | 2.17 | 0.57 |
| 4:D:31:THR:HG22 | 7:G:3:TYR:HE1 | 1.69 | 0.57 |
| 3:C:56:SER:OG | 3:C:158:GLU:N | 2.32 | 0.57 |
| 14:P:11:A:N6 | 15:T:25:DA:N1 | 2.53 | 0.57 |
| 1:A:875:TYR:HA | 1:A:1083:PRO:HB3 | 1.86 | 0.57 |
| 2:B:37:LYS:HB3 | 2:B:41:ARG:HG3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:19:VAL:HG23 | 3:C:241:PRO:HB2 | 1.87 | 0.57 |
| 6:F:81:VAL:HG21 | 6:F:96:GLU:HA | 1.86 | 0.57 |
| 5:E:86:THR:HG22 | 5:E:90:TYR:CE2 | 2.40 | 0.57 |
| 8:H:6:PHE:HB3 | 8:H:60:ILE:HB | 1.86 | 0.57 |
| 2:B:206:TYR:O | 2:B:219:GLY:HA2 | 2.05 | 0.56 |
| 1:A:274:ASP:OD2 | 1:A:342:ARG:NH2 | 2.37 | 0.56 |
| 1:A:888:GLN:NE2 | 1:A:1403:ASP:OD2 | 2.31 | 0.56 |
| 1:A:1176:TYR:HE2 | 1:A:1213:ARG:HD3 | 1.69 | 0.56 |
| 1:A:1307:VAL:HG22 | 1:A:1338:THR:HG22 | 1.86 | 0.56 |
| 1:A:1386:ILE:HD12 | 1:A:1398:LEU:HD21 | 1.86 | 0.56 |
| 2:B:617:ASP:OD1 | 2:B:618:ALA:N | 2.38 | 0.56 |
| 4:D:44:ARG:HH12 | 4:D:48:ASN:HB2 | 1.70 | 0.56 |
| 7:G:101:ILE:N | 7:G:104:MET:O | 2.37 | 0.56 |
| 9:I:69:ILE:HG22 | 9:I:71:ASP:H | 1.70 | 0.56 |
| 1:A:1030:SER:HG | 5:E:162:ARG:HE | 1.53 | 0.56 |
| 1:A:1441:GLU:OE2 | 1:A:1445:HIS:NE2 | 2.37 | 0.56 |
| 10:J:18:TRP:O | 10:J:21:TYR:HB3 | 2.06 | 0.56 |
| 1:A:1128:ILE:HG23 | 1:A:1414:ILE:HD12 | 1.86 | 0.56 |
| 13:N:35:DA:H2" | 13:N:36:DG:C8 | 2.41 | 0.56 |
| 4:D:124:ASP:O | 4:D:128:GLN:HB3 | 2.06 | 0.56 |
| 8:H:100:GLU:HB3 | 8:H:113:SER:OG | 2.06 | 0.56 |
| 9:I:64:GLU:O | 9:I:68:ILE:HG12 | 2.06 | 0.56 |
| 1:A:485:ASN:OD1 | 1:A:486:LEU:N | 2.38 | 0.56 |
| 2:B:771:GLU:O | 10:J:55:LEU:HD21 | 2.06 | 0.56 |
| 3:C:92:GLU:HG3 | 3:C:93:PHE:H | 1.71 | 0.56 |
| 1:A:459:ASN:OD1 | 1:A:460:ARG:N | 2.38 | 0.55 |
| 1:A:877:ALA:HB3 | 1:A:890:ARG:NH1 | 2.20 | 0.55 |
| 7:G:3:TYR:N | 7:G:76:VAL:O | 2.29 | 0.55 |
| 1:A:599:HIS:ND1 | 1:A:632:ASN:OD1 | 2.39 | 0.55 |
| 1:A:1375:ARG:NE | 1:A:1403:ASP:OD1 | 2.38 | 0.55 |
| 4:D:96:GLU:OE2 | 4:D:121:ARG:NH1 | 2.40 | 0.55 |
| 5:E:55:ARG:NH1 | 5:E:107:GLN:HE21 | 2.04 | 0.55 |
| 15:T:28:DA:H2" | 15:T:29:DC:OP2 | 2.05 | 0.55 |
| 4:D:135:GLN:HA | 4:D:138:ARG:HD3 | 1.87 | 0.55 |
| 9:I:14:ILE:HG21 | 9:I:23:MET:HE2 | 1.89 | 0.55 |
| 1:A:585:LEU:HD22 | 8:H:47:ILE:HD11 | 1.87 | 0.55 |
| 1:A:706:ILE:HG21 | 1:A:824:GLU:HG3 | 1.88 | 0.55 |
| 7:G:60:GLN:OE1 | 7:G:63:ARG:HD2 | 2.07 | 0.55 |
| 1:A:358:ARG:HA | 2:B:1085:ARG:HA | 1.88 | 0.55 |
| 1:A:470:MET:HB3 | 1:A:521:VAL:HG22 | 1.89 | 0.55 |
| 2:B:193:VAL:HG21 | 2:B:470:LEU:HD13 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:118:TYR:CZ | 8:H:143:LEU:HB2 | 2.41 | 0.55 |
| 1:A:544:ALA:HB2 | 1:A:680:LEU:HD13 | 1.89 | 0.55 |
| 2:B:587:LEU:HB3 | 2:B:603:MET:SD | 2.47 | 0.55 |
| 1:A:140:ARG:HD2 | 1:A:237:GLY:HA2 | 1.89 | 0.55 |
| 1:A:542:LEU:HD23 | 1:A:774:ALA:HA | 1.88 | 0.55 |
| 3:C:2:PRO:HB3 | 11:K:54:PRO:HD2 | 1.89 | 0.55 |
| 1:A:1004:LEU:HD13 | 1:A:1062:GLY:HA2 | 1.89 | 0.55 |
| 2:B:85:LEU:HB2 | 2:B:131:THR:OG1 | 2.06 | 0.54 |
| 2:B:961:ILE:HD11 | 10:J:42:ARG:HB2 | 1.88 | 0.54 |
| 2:B:780:VAL:HG21 | 2:B:1048:TYR:CE1 | 2.42 | 0.54 |
| 4:D:48:ASN:ND2 | 4:D:57:LEU:HG | 2.22 | 0.54 |
| 2:B:728:MET:SD | 2:B:942:LYS:HD3 | 2.48 | 0.54 |
| 2:B:812:ARG:HH12 | 2:B:897:ARG:HG3 | 1.72 | 0.54 |
| 2:B:817:GLN:HE22 | 2:B:912:ASN:ND2 | 2.05 | 0.54 |
| 6:F:52:ILE:O | 6:F:53:THR:HG23 | 2.07 | 0.54 |
| 10:J:5:VAL:HG12 | 10:J:6:ARG:HG2 | 1.88 | 0.54 |
| 1:A:540:ASP:HB2 | 2:B:790:GLN:NE2 | 2.22 | 0.54 |
| 2:B:91:ILE:HD11 | 2:B:124:LEU:HD11 | 1.89 | 0.54 |
| 2:B:1032:PHE:O | 3:C:32:ASN:ND2 | 2.40 | 0.54 |
| 1:A:916:PHE:CE1 | 1:A:963:ARG:HD2 | 2.43 | 0.54 |
| 2:B:535:GLY:HA3 | 2:B:618:ALA:HB2 | 1.89 | 0.54 |
| 1:A:420:ILE:HB | 1:A:445:LYS:HB2 | 1.89 | 0.54 |
| 1:A:475:ARG:NH1 | 1:A:477:LEU:HD21 | 2.23 | 0.54 |
| 2:B:534:VAL:N | 2:B:600:GLU:OE2 | 2.41 | 0.54 |
| 4:D:17:ALA:HB2 | 7:G:80:PHE:HB2 | 1.89 | 0.54 |
| 6:F:110:LEU:HD12 | 6:F:114:SER:HB3 | 1.88 | 0.54 |
| 13:N:12:DT:H1' | 13:N:13:DA:N7 | 2.22 | 0.54 |
| 1:A:533:PRO:O | 1:A:647:THR:OG1 | 2.21 | 0.54 |
| 1:A:863:ARG:NH2 | 1:A:1414:ILE:O | 2.30 | 0.54 |
| 2:B:631:GLN:NE2 | 2:B:691:SER:O | 2.33 | 0.54 |
| 2:B:817:GLN:HE22 | 2:B:912:ASN:HD21 | 1.56 | 0.54 |
| 2:B:1115:GLN:HG2 | 2:B:1150:ARG:HG2 | 1.90 | 0.54 |
| 3:C:105:VAL:HG11 | 3:C:115:VAL:HG22 | 1.89 | 0.54 |
| 1:A:546:ARG:HD2 | 1:A:772:SER:HB3 | 1.90 | 0.53 |
| 1:A:996:ILE:HD13 | 1:A:1060:LEU:HA | 1.88 | 0.53 |
| 2:B:1124:ILE:HG22 | 2:B:1125:MET:H | 1.73 | 0.53 |
| 1:A:805:ARG:NH2 | 2:B:673:VAL:O | 2.33 | 0.53 |
| 2:B:185:PHE:O | 2:B:191:GLU:HA | 2.08 | 0.53 |
| 8:H:81:ARG:CG | 8:H:82:PRO:HD3 | 2.39 | 0.53 |
| 11:K:9:SER:HA | 11:K:69:HIS:CG | 2.43 | 0.53 |
| 1:A:358:ARG:NH2 | 2:B:1068:GLN:OE1 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1155:LYS:HD2 | 1:A:1158:LEU:HD23 | 1.90 | 0.53 |
| 1:A:1218:ARG:NH2 | 1:A:1252:ALA:O | 2.42 | 0.53 |
| 4:D:112:LYS:HB3 | 4:D:119:GLU:OE2 | 2.09 | 0.53 |
| 5:E:8:TYR:CE2 | 5:E:12:LYS:HE3 | 2.43 | 0.53 |
| 9:I:29:ASP:HB3 | 9:I:34:ILE:O | 2.08 | 0.53 |
| 15:T:6:DC:H2" | 15:T:7:DA:C8 | 2.43 | 0.53 |
| 2:B:446:TYR:HE1 | 15:T:25:DA:H5" | 1.74 | 0.53 |
| 1:A:112:PHE:CZ | 1:A:191:ILE:HD11 | 2.43 | 0.53 |
| 2:B:725:GLN:HG2 | 2:B:938:ARG:O | 2.08 | 0.53 |
| 3:C:253:LYS:HE3 | 11:K:95:ILE:HG23 | 1.90 | 0.53 |
| 1:A:508:SER:HB3 | 1:A:511:THR:HG22 | 1.91 | 0.53 |
| 2:B:98:HIS:O | 2:B:105:PRO:HA | 2.09 | 0.53 |
| 3:C:62:GLU:HA | 3:C:65:ALA:HB3 | 1.91 | 0.53 |
| 5:E:118:LEU:HD22 | 5:E:127:LEU:HB2 | 1.90 | 0.53 |
| 2:B:89:GLU:HB3 | 2:B:127:ASP:HB2 | 1.91 | 0.52 |
| 3:C:4:ALA:HB2 | 11:K:93:ASP:HB3 | 1.91 | 0.52 |
| 1:A:859:TYR:CE2 | 1:A:863:ARG:HD2 | 2.44 | 0.52 |
| 1:A:1052:ARG:NE | 1:A:1056:GLU:OE2 | 2.42 | 0.52 |
| 3:C:75:SER:HB3 | 3:C:79:VAL:HG21 | 1.91 | 0.52 |
| 5:E:26:TYR:HD1 | 5:E:64:HIS:HA | 1.74 | 0.52 |
| 7:G:108:ILE:HD11 | 7:G:145:LEU:HD22 | 1.92 | 0.52 |
| 11:K:9:SER:HA | 11:K:69:HIS:CD2 | 2.44 | 0.52 |
| 2:B:285:LEU:HD11 | 2:B:305:LEU:HD11 | 1.91 | 0.52 |
| 2:B:910:THR:HG22 | 12:L:43:ILE:HA | 1.91 | 0.52 |
| 1:A:1093:GLN:HE22 | 2:B:1093:CYS:HA | 1.75 | 0.52 |
| 2:B:1123:GLY:HA3 | 2:B:1170:ARG:HB3 | 1.91 | 0.52 |
| 2:B:927:ARG:HD2 | 2:B:1054:MET:SD | 2.49 | 0.52 |
| 2:B:282:ARG:O | 2:B:286:GLU:CB | 2.56 | 0.52 |
| 1:A:1394:ASN:OD1 | 1:A:1395:TYR:N | 2.42 | 0.52 |
| 2:B:752:TYR:HE1 | 3:C:60:HIS:CE1 | 2.28 | 0.52 |
| 11:K:46:ILE:HG21 | 11:K:87:PHE:HE1 | 1.75 | 0.52 |
| 11:K:60:GLY:O | 11:K:73:ILE:HA | 2.09 | 0.52 |
| 1:A:991:GLN:HA | 1:A:996:ILE:HD12 | 1.90 | 0.52 |
| 2:B:605:ARG:NH1 | 2:B:607:ILE:HG12 | 2.25 | 0.52 |
| 3:C:22:ILE:HG12 | 3:C:230:TYR:HD1 | 1.75 | 0.52 |
| 1:A:922:PHE:N | 1:A:1052:ARG:HD2 | 2.22 | 0.52 |
| 1:A:957:GLU:HG2 | 1:A:960:ARG:HH21 | 1.75 | 0.52 |
| 1:A:1375:ARG:NH1 | 1:A:1379:GLU:OE1 | 2.43 | 0.52 |
| 7:G:97:LEU:HB2 | 7:G:108:ILE:HB | 1.92 | 0.52 |
| 8:H:98:ARG:HD2 | 8:H:115:TYR:CD2 | 2.45 | 0.52 |
| 2:B:393:LEU:HD22 | 2:B:485:LEU:HD22 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:96:VAL:HA | 8:H:116:VAL:HA | 1.92 | 0.52 |
| 1:A:573:LYS:NZ | 8:H:74:GLU:OE2 | 2.26 | 0.51 |
| 2:B:625:LEU:HD12 | 2:B:665:ILE:HD12 | 1.92 | 0.51 |
| 2:B:1037:ILE:HG21 | 2:B:1041:ILE:HD11 | 1.92 | 0.51 |
| 7:G:50:THR:O | 7:G:73:LYS:N | 2.39 | 0.51 |
| 2:B:125:TYR:HB3 | 2:B:146:LYS:HA | 1.91 | 0.51 |
| 2:B:918:PHE:HE2 | 2:B:920:LYS:HE3 | 1.76 | 0.51 |
| 1:A:1308:TYR:O | 1:A:1336:LEU:HA | 2.10 | 0.51 |
| 1:A:1458:ILE:HD12 | 2:B:1091:ARG:HH21 | 1.75 | 0.51 |
| 3:C:61:ASP:OD2 | 12:L:48:ARG:NH2 | 2.43 | 0.51 |
| 7:G:79:PRO:HG3 | 7:G:104:MET:SD | 2.50 | 0.51 |
| 7:G:129:LYS:HB3 | 7:G:136:VAL:HG13 | 1.93 | 0.51 |
| 1:A:977:VAL:HG11 | 1:A:1040:LEU:HD21 | 1.92 | 0.51 |
| 1:A:1141:VAL:HG13 | 1:A:1352:VAL:HG13 | 1.92 | 0.51 |
| 2:B:801:VAL:O | 2:B:807:ARG:NH2 | 2.44 | 0.51 |
| 6:F:105:ILE:HG22 | 6:F:119:GLY:HA2 | 1.92 | 0.51 |
| 1:A:1318:LYS:HE2 | 1:A:1330:ALA:HB1 | 1.92 | 0.51 |
| 2:B:114:ARG:NH2 | 2:B:184:TYR:OH | 2.44 | 0.51 |
| 2:B:548:TRP:O | 2:B:549:SER:OG | 2.23 | 0.51 |
| 13:N:33:DT:H2” | 13:N:34:DG:C8 | 2.46 | 0.51 |
| 2:B:529:MET:HG2 | 2:B:702:MET:HB3 | 1.91 | 0.51 |
| 2:B:713:PHE:HB3 | 2:B:716:HIS:CD2 | 2.41 | 0.51 |
| 9:I:29:ASP:HB3 | 9:I:34:ILE:H | 1.75 | 0.51 |
| 2:B:82:PRO:HA | 2:B:133:ILE:O | 2.11 | 0.51 |
| 4:D:124:ASP:O | 4:D:128:GLN:CB | 2.59 | 0.51 |
| 9:I:97:PHE:HB2 | 9:I:100:HIS:HE2 | 1.76 | 0.51 |
| 2:B:84:TYR:CE2 | 2:B:423:ILE:HD12 | 2.45 | 0.51 |
| 2:B:761:THR:HG23 | 2:B:1000:THR:HA | 1.93 | 0.51 |
| 2:B:1038:THR:HA | 3:C:195:THR:HA | 1.93 | 0.51 |
| 5:E:17:ILE:HA | 5:E:20:LEU:HD12 | 1.92 | 0.51 |
| 1:A:802:PHE:HE2 | 1:A:808:PRO:HD3 | 1.76 | 0.51 |
| 3:C:18:ASN:OD1 | 3:C:19:VAL:N | 2.43 | 0.51 |
| 8:H:113:SER:HB3 | 8:H:126:GLN:HG2 | 1.93 | 0.51 |
| 2:B:540:PRO:HB2 | 2:B:596:ILE:HG23 | 1.93 | 0.50 |
| 3:C:67:ARG:NH2 | 3:C:149:LEU:O | 2.44 | 0.50 |
| 4:D:15:GLU:OE1 | 7:G:78:ARG:NH1 | 2.41 | 0.50 |
| 11:K:21:ILE:HG21 | 11:K:84:GLN:HE21 | 1.75 | 0.50 |
| 2:B:1022:LEU:HD12 | 2:B:1023:ARG:HG2 | 1.94 | 0.50 |
| 8:H:98:ARG:HD2 | 8:H:115:TYR:HD2 | 1.76 | 0.50 |
| 1:A:544:ALA:O | 1:A:548:PHE:HB2 | 2.10 | 0.50 |
| 2:B:818:GLU:HB2 | 2:B:829:PHE:CE2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1060:HIS:HE1 | 2:B:1081:ASP:HA | 1.77 | 0.50 |
| 3:C:8:THR:OG1 | 3:C:24:GLU:HB2 | 2.10 | 0.50 |
| 11:K:9:SER:HG | 11:K:10:PHE:HD1 | 1.60 | 0.50 |
| 1:A:52:PRO:HB2 | 1:A:60:PRO:HD3 | 1.93 | 0.50 |
| 1:A:1189:ASP:HA | 1:A:1192:TRP:CZ2 | 2.47 | 0.50 |
| 2:B:622:CYS:HB3 | 2:B:666:ASP:HB3 | 1.93 | 0.50 |
| 2:B:935:PHE:HE1 | 2:B:1050:ARG:HG3 | 1.75 | 0.50 |
| 1:A:355:MET:O | 2:B:1091:ARG:HD2 | 2.11 | 0.50 |
| 1:A:528:PRO:HG2 | 1:A:1090:LEU:HD11 | 1.92 | 0.50 |
| 1:A:563:LEU:HD21 | 1:A:679:TRP:HB2 | 1.94 | 0.50 |
| 2:B:475:PHE:CE2 | 2:B:479:LEU:HD11 | 2.46 | 0.50 |
| 3:C:32:ASN:HA | 3:C:35:ARG:HG2 | 1.93 | 0.50 |
| 5:E:77:PRO:HD2 | 5:E:105:VAL:O | 2.12 | 0.50 |
| 2:B:117:ASN:HD21 | 2:B:815:LYS:NZ | 2.10 | 0.50 |
| 4:D:109:GLU:O | 4:D:113:ALA:CB | 2.60 | 0.50 |
| 4:D:134:ILE:O | 4:D:138:ARG:HG3 | 2.12 | 0.50 |
| 7:G:52:ASP:H | 7:G:72:TYR:HA | 1.76 | 0.50 |
| 2:B:501:LEU:HD12 | 2:B:505:LEU:HD12 | 1.94 | 0.50 |
| 2:B:761:THR:HG22 | 2:B:763:SER:H | 1.77 | 0.50 |
| 4:D:123:GLU:O | 4:D:127:LEU:N | 2.27 | 0.50 |
| 7:G:1:MET:HB3 | 7:G:3:TYR:CZ | 2.47 | 0.50 |
| 11:K:61:TYR:HA | 11:K:72:ILE:O | 2.12 | 0.50 |
| 1:A:387:ASN:ND2 | 2:B:1061:SER:OG | 2.28 | 0.50 |
| 1:A:589:LYS:HZ3 | 1:A:638:GLY:H | 1.58 | 0.50 |
| 1:A:1115:LYS:NZ | 1:A:1337:GLU:HB3 | 2.26 | 0.50 |
| 1:A:1141:VAL:HB | 1:A:1336:LEU:HB2 | 1.93 | 0.50 |
| 7:G:7:LEU:HB2 | 7:G:72:TYR:CZ | 2.47 | 0.50 |
| 7:G:119:PHE:HB2 | 7:G:128:TYR:HE1 | 1.76 | 0.50 |
| 1:A:274:ASP:OD1 | 1:A:275:ASP:N | 2.45 | 0.50 |
| 4:D:125:GLU:O | 4:D:129:GLN:HB2 | 2.12 | 0.50 |
| 1:A:475:ARG:HH12 | 1:A:477:LEU:HD21 | 1.76 | 0.49 |
| 2:B:65:ILE:O | 2:B:85:LEU:HA | 2.12 | 0.49 |
| 9:I:81:THR:HG23 | 9:I:96:PHE:HE1 | 1.77 | 0.49 |
| 1:A:555:LEU:HD12 | 1:A:591:ILE:HD12 | 1.95 | 0.49 |
| 1:A:1139:LEU:HD13 | 1:A:1359:SER:HB3 | 1.94 | 0.49 |
| 2:B:845:TYR:CE1 | 2:B:865:VAL:HG21 | 2.47 | 0.49 |
| 3:C:35:ARG:HD2 | 3:C:184:PHE:CG | 2.47 | 0.49 |
| 4:D:84:ARG:NH1 | 4:D:97:LEU:HD22 | 2.27 | 0.49 |
| 5:E:47:LYS:O | 5:E:51:GLY:HA3 | 2.12 | 0.49 |
| 7:G:151:ARG:O | 7:G:158:PHE:N | 2.28 | 0.49 |
| 1:A:367:ILE:HG22 | 1:A:482:PHE:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1301:ILE:HG12 | 1:A:1345:ARG:HD2 | 1.94 | 0.49 |
| 2:B:1120:ASN:HD22 | 2:B:1145:GLN:HB2 | 1.76 | 0.49 |
| 9:I:29:ASP:HB2 | 9:I:34:ILE:O | 2.12 | 0.49 |
| 1:A:392:GLU:O | 1:A:445:LYS:CA | 2.56 | 0.49 |
| 2:B:785:TYR:CD2 | 2:B:786:THR:HG23 | 2.47 | 0.49 |
| 13:N:11:DG:H2' | 13:N:12:DT:H72 | 1.93 | 0.49 |
| 1:A:255:VAL:HG13 | 1:A:280:LEU:HD13 | 1.94 | 0.49 |
| 1:A:541:THR:O | 1:A:545:VAL:HG23 | 2.12 | 0.49 |
| 3:C:169:PHE:HE1 | 3:C:171:LYS:HD2 | 1.77 | 0.49 |
| 1:A:1194:ASN:O | 1:A:1198:GLU:HG3 | 2.12 | 0.49 |
| 7:G:30:LEU:O | 7:G:34:VAL:HG22 | 2.13 | 0.49 |
| 1:A:375:ILE:HD11 | 1:A:669:TYR:CB | 2.43 | 0.49 |
| 1:A:987:ILE:HG23 | 1:A:1060:LEU:HD11 | 1.93 | 0.49 |
| 8:H:58:LEU:HD12 | 8:H:144:LEU:O | 2.12 | 0.49 |
| 1:A:671:ASN:O | 1:A:675:VAL:HG22 | 2.12 | 0.49 |
| 1:A:958:ARG:HH12 | 1:A:1014:LYS:HZ2 | 1.60 | 0.49 |
| 1:A:1130:ILE:HD13 | 1:A:1411:LEU:HB3 | 1.95 | 0.49 |
| 2:B:646:ARG:HG3 | 2:B:651:TYR:O | 2.12 | 0.49 |
| 2:B:677:MET:H | 2:B:682:LEU:HD22 | 1.78 | 0.49 |
| 5:E:3:ASP:HB3 | 5:E:48:PRO:HD2 | 1.94 | 0.49 |
| 5:E:73:PHE:HB2 | 5:E:99:ILE:HD12 | 1.95 | 0.49 |
| 2:B:907:VAL:HG22 | 2:B:921:ILE:HG12 | 1.95 | 0.49 |
| 11:K:46:ILE:HG21 | 11:K:87:PHE:CE1 | 2.48 | 0.49 |
| 2:B:242:ARG:HB3 | 2:B:254:GLN:HG3 | 1.94 | 0.49 |
| 7:G:97:LEU:HD22 | 7:G:108:ILE:HD12 | 1.95 | 0.49 |
| 10:J:65:LEU:O | 12:L:23:HIS:ND1 | 2.45 | 0.49 |
| 1:A:460:ARG:NH2 | 14:P:20:C:O2' | 2.44 | 0.48 |
| 1:A:560:VAL:HG22 | 1:A:591:ILE:HD11 | 1.93 | 0.48 |
| 1:A:623:PRO:HA | 8:H:27:ARG:HH22 | 1.75 | 0.48 |
| 2:B:820:LYS:HG3 | 2:B:826:GLU:HG2 | 1.94 | 0.48 |
| 9:I:25:TYR:O | 9:I:37:TYR:HA | 2.13 | 0.48 |
| 2:B:1124:ILE:HG22 | 2:B:1125:MET:N | 2.28 | 0.48 |
| 7:G:25:THR:O | 7:G:29:LYS:HG2 | 2.13 | 0.48 |
| 1:A:141:LEU:HD13 | 1:A:1445:HIS:HE1 | 1.79 | 0.48 |
| 1:A:222:HIS:ND1 | 1:A:246:GLU:HB2 | 2.29 | 0.48 |
| 2:B:1003:ASN:C | 2:B:1005:ALA:H | 2.17 | 0.48 |
| 5:E:22:HIS:HB2 | 5:E:33:LEU:HD21 | 1.96 | 0.48 |
| 7:G:52:ASP:N | 7:G:71:LYS:O | 2.46 | 0.48 |
| 7:G:92:VAL:HG11 | 7:G:127:CYS:HA | 1.95 | 0.48 |
| 2:B:553:LEU:HD11 | 2:B:573:TRP:O | 2.13 | 0.48 |
| 10:J:3:ILE:HD13 | 10:J:18:TRP:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:441:GLN:HG2 | 1:A:444:TYR:CE2 | 2.49 | 0.48 |
| 1:A:1160:ARG:O | 1:A:1300:GLY:HA2 | 2.12 | 0.48 |
| 1:A:1148:ALA:HB1 | 1:A:1333:GLU:HB2 | 1.96 | 0.48 |
| 2:B:231:PRO:O | 2:B:232:THR:HG23 | 2.13 | 0.48 |
| 8:H:11:ASP:OD1 | 8:H:55:LYS:HG2 | 2.14 | 0.48 |
| 1:A:461:GLN:HE22 | 1:A:502:ASN:HD22 | 1.60 | 0.48 |
| 1:A:927:GLU:O | 1:A:931:ARG:HG2 | 2.14 | 0.48 |
| 2:B:968:ASN:OD1 | 2:B:969:PRO:HD2 | 2.14 | 0.48 |
| 1:A:370:ASP:OD1 | 11:K:65:HIS:NE2 | 2.46 | 0.48 |
| 1:A:892:GLY:HA3 | 1:A:1396:ARG:HH11 | 1.78 | 0.48 |
| 4:D:76:ASN:OD1 | 4:D:77:ARG:N | 2.47 | 0.48 |
| 6:F:71:LEU:O | 6:F:75:MET:HG3 | 2.14 | 0.48 |
| 1:A:230:ASP:OD1 | 1:A:244:ARG:NH2 | 2.47 | 0.48 |
| 1:A:683:GLU:HA | 2:B:1038:THR:HB | 1.96 | 0.48 |
| 2:B:699:HIS:ND1 | 2:B:700:PRO:HD2 | 2.28 | 0.48 |
| 5:E:185:ILE:HG21 | 5:E:209:VAL:HG21 | 1.96 | 0.48 |
| 1:A:515:ILE:HD11 | 2:B:1102:PHE:CD1 | 2.48 | 0.47 |
| 1:A:628:VAL:HA | 1:A:638:GLY:HA3 | 1.96 | 0.47 |
| 1:A:222:HIS:CD2 | 1:A:226:LYS:HE3 | 2.50 | 0.47 |
| 1:A:557:ARG:O | 1:A:561:MET:HG2 | 2.14 | 0.47 |
| 1:A:739:ASN:O | 1:A:743:ARG:HG2 | 2.14 | 0.47 |
| 2:B:236:TRP:HB2 | 2:B:259:THR:HB | 1.95 | 0.47 |
| 7:G:162:SER:OG | 7:G:164:MET:HG2 | 2.15 | 0.47 |
| 7:G:114:PRO:HG3 | 7:G:164:MET:HA | 1.96 | 0.47 |
| 1:A:447:GLU:OE1 | 2:B:1064:ARG:NH2 | 2.46 | 0.47 |
| 1:A:798:ILE:O | 1:A:820:ARG:NE | 2.41 | 0.47 |
| 2:B:65:ILE:HD11 | 2:B:412:LEU:HD22 | 1.97 | 0.47 |
| 2:B:388:TYR:HD1 | 2:B:504:THR:OG1 | 1.97 | 0.47 |
| 4:D:42:GLU:OE2 | 4:D:65:LEU:HD11 | 2.14 | 0.47 |
| 7:G:28:GLN:O | 7:G:32:THR:OG1 | 2.26 | 0.47 |
| 1:A:29:ASP:HB3 | 1:A:33:ARG:HH12 | 1.79 | 0.47 |
| 1:A:1167:ARG:HB2 | 1:A:1293:LEU:HB3 | 1.95 | 0.47 |
| 1:A:1184:THR:HB | 1:A:1189:ASP:OD1 | 2.15 | 0.47 |
| 5:E:180:ALA:HA | 5:E:185:ILE:HD12 | 1.96 | 0.47 |
| 1:A:465:HIS:CD2 | 1:A:467:MET:HB2 | 2.50 | 0.47 |
| 1:A:760:LEU:HD11 | 1:A:781:ILE:HG21 | 1.97 | 0.47 |
| 2:B:847:LYS:NZ | 2:B:864:ASP:OD2 | 2.48 | 0.47 |
| 8:H:8:ASP:OD2 | 8:H:32:SER:OG | 2.24 | 0.47 |
| 8:H:8:ASP:OD1 | 8:H:9:ILE:N | 2.47 | 0.47 |
| 14:P:12:A:H2' | 14:P:13:G:O4' | 2.14 | 0.47 |
| 1:A:22:GLN:NE2 | 1:A:1446:GLY:O | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:113:PHE:CE1 | 1:A:186:ARG:HD2 | 2.49 | 0.47 |
| 1:A:389:THR:HG21 | 1:A:417:LYS:HD3 | 1.97 | 0.47 |
| 1:A:472:HIS:CE1 | 1:A:521:VAL:HG21 | 2.50 | 0.47 |
| 1:A:1055:ALA:O | 1:A:1059:ARG:NH1 | 2.47 | 0.47 |
| 2:B:84:TYR:HE2 | 2:B:423:ILE:HG23 | 1.80 | 0.47 |
| 2:B:692:THR:HB | 9:I:76:PRO:HB3 | 1.97 | 0.47 |
| 2:B:841:ARG:HD2 | 2:B:895:PHE:CZ | 2.50 | 0.47 |
| 3:C:117:SER:HB2 | 3:C:129:PRO:HB2 | 1.95 | 0.47 |
| 4:D:33:LEU:O | 4:D:37:VAL:N | 2.37 | 0.47 |
| 7:G:10:GLU:HG2 | 7:G:69:PRO:HA | 1.95 | 0.47 |
| 11:K:105:PHE:CE2 | 11:K:109:ILE:HD11 | 2.50 | 0.47 |
| 1:A:1292:MET:O | 1:A:1296:MET:HG2 | 2.14 | 0.47 |
| 2:B:310:VAL:HG23 | 2:B:311:ILE:HD12 | 1.96 | 0.47 |
| 5:E:62:VAL:O | 5:E:71:GLN:CA | 2.62 | 0.47 |
| 12:L:41:TYR:CE2 | 12:L:43:ILE:HB | 2.50 | 0.47 |
| 1:A:190:ARG:O | 1:A:200:ALA:HA | 2.14 | 0.47 |
| 1:A:570:TRP:CZ3 | 1:A:572:GLY:HA2 | 2.50 | 0.47 |
| 2:B:217:TYR:CE2 | 2:B:376:ALA:HA | 2.50 | 0.47 |
| 2:B:565:THR:HG22 | 2:B:610:ARG:HG3 | 1.97 | 0.47 |
| 7:G:49:THR:H | 7:G:74:ALA:HA | 1.78 | 0.47 |
| 2:B:836:THR:HG23 | 2:B:837:CYS:H | 1.80 | 0.47 |
| 10:J:40:LEU:HD22 | 10:J:45:CYS:HB3 | 1.97 | 0.47 |
| 1:A:348:GLY:O | 1:A:352:GLY:N | 2.41 | 0.46 |
| 1:A:459:ASN:HD21 | 2:B:1090:GLU:HG3 | 1.79 | 0.46 |
| 1:A:618:TYR:HE1 | 8:H:40:ILE:HD13 | 1.79 | 0.46 |
| 1:A:717:ILE:HG12 | 1:A:737:PHE:HZ | 1.79 | 0.46 |
| 1:A:1284:PHE:CE2 | 1:A:1288:ILE:HD11 | 2.50 | 0.46 |
| 2:B:132:VAL:O | 2:B:139:GLN:HA | 2.14 | 0.46 |
| 3:C:44:ILE:HG23 | 3:C:176:TRP:HD1 | 1.80 | 0.46 |
| 7:G:10:GLU:HA | 7:G:68:TYR:O | 2.16 | 0.46 |
| 11:K:29:ASN:ND2 | 11:K:78:THR:O | 2.48 | 0.46 |
| 15:T:4:DC:H2' | 15:T:5:DT:C6 | 2.50 | 0.46 |
| 1:A:415:GLY:H | 1:A:449:HIS:HD2 | 1.63 | 0.46 |
| 1:A:802:PHE:HE2 | 1:A:808:PRO:CD | 2.28 | 0.46 |
| 1:A:1362:ILE:HG23 | 1:A:1374:VAL:HG13 | 1.97 | 0.46 |
| 3:C:72:PRO:HG3 | 10:J:13:ILE:HD11 | 1.97 | 0.46 |
| 1:A:421:ARG:HA | 1:A:444:TYR:CD1 | 2.50 | 0.46 |
| 1:A:467:MET:SD | 1:A:524:MET:HE2 | 2.56 | 0.46 |
| 1:A:499:ASP:OD1 | 14:P:20:C:H4' | 2.16 | 0.46 |
| 1:A:672:ILE:HG23 | 1:A:676:ILE:HD12 | 1.98 | 0.46 |
| 1:A:1169:VAL:HG12 | 1:A:1220:HIS:HB3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1316:ASN:OD1 | 1:A:1317:LYS:N | 2.48 | 0.46 |
| 1:A:1163:HIS:O | 1:A:1168:LYS:NZ | 2.42 | 0.46 |
| 1:A:1454:VAL:HG13 | 1:A:1464:ALA:HB1 | 1.97 | 0.46 |
| 2:B:282:ARG:NH2 | 9:I:16:PHE:HB2 | 2.31 | 0.46 |
| 2:B:1118:VAL:HG11 | 2:B:1171:MET:HB2 | 1.97 | 0.46 |
| 1:A:330:GLN:O | 1:A:331:LYS:HG3 | 2.15 | 0.46 |
| 2:B:84:TYR:CD1 | 2:B:132:VAL:HG12 | 2.50 | 0.46 |
| 2:B:794:VAL:HG22 | 2:B:967:ILE:HG22 | 1.97 | 0.46 |
| 2:B:1072:ARG:O | 2:B:1112:ASP:HB3 | 2.15 | 0.46 |
| 9:I:22:ASN:ND2 | 9:I:41:ASN:HD22 | 2.14 | 0.46 |
| 4:D:125:GLU:O | 4:D:129:GLN:CB | 2.64 | 0.46 |
| 2:B:312:GLN:HE21 | 9:I:41:ASN:HD21 | 1.64 | 0.46 |
| 2:B:429:PHE:HE2 | 2:B:431:LEU:HD23 | 1.81 | 0.46 |
| 2:B:601:VAL:HG22 | 2:B:616:THR:HG23 | 1.97 | 0.46 |
| 2:B:1142:ASN:HD21 | 2:B:1145:GLN:HG3 | 1.81 | 0.46 |
| 3:C:259:LEU:O | 3:C:263:LEU:HB3 | 2.15 | 0.46 |
| 7:G:137:ILE:HG12 | 7:G:170:LEU:HB2 | 1.96 | 0.46 |
| 8:H:58:LEU:HD11 | 8:H:143:LEU:CD1 | 2.44 | 0.46 |
| 13:N:11:DG:C5 | 13:N:12:DT:C4 | 3.04 | 0.46 |
| 1:A:544:ALA:O | 1:A:548:PHE:HB3 | 2.16 | 0.46 |
| 1:A:584:PRO:O | 1:A:585:LEU:HD12 | 2.16 | 0.46 |
| 1:A:931:ARG:HH11 | 1:A:936:GLU:HG3 | 1.79 | 0.46 |
| 2:B:407:MET:HE1 | 2:B:444:LEU:H | 1.81 | 0.46 |
| 7:G:108:ILE:HG12 | 7:G:161:GLY:C | 2.36 | 0.46 |
| 8:H:81:ARG:HG3 | 8:H:82:PRO:HD3 | 1.97 | 0.46 |
| 1:A:432:HIS:HB3 | 1:A:433:PRO:HD2 | 1.97 | 0.46 |
| 1:A:971:PRO:O | 1:A:972:THR:OG1 | 2.24 | 0.46 |
| 1:A:1474:LEU:CD2 | 7:G:58:VAL:HG22 | 2.46 | 0.46 |
| 2:B:465:GLY:O | 2:B:468:GLN:NE2 | 2.48 | 0.46 |
| 2:B:865:VAL:HG22 | 2:B:895:PHE:CE1 | 2.51 | 0.46 |
| 2:B:906:GLN:OE1 | 2:B:922:ARG:NH2 | 2.49 | 0.46 |
| 2:B:939:HIS:CD2 | 2:B:980:HIS:HA | 2.51 | 0.46 |
| 2:B:1108:PHE:HD1 | 2:B:1152:PRO:HG3 | 1.81 | 0.46 |
| 4:D:45:LYS:HB2 | 4:D:61:PHE:HZ | 1.80 | 0.46 |
| 15:T:28:DA:C5 | 15:T:29:DC:N4 | 2.84 | 0.46 |
| 1:A:11:SER:N | 2:B:1135:TYR:HH | 2.13 | 0.46 |
| 1:A:62:GLN:HE22 | 1:A:255:VAL:HG12 | 1.81 | 0.46 |
| 1:A:335:PRO:HD3 | 2:B:460:HIS:CE1 | 2.51 | 0.46 |
| 1:A:595:ILE:HD11 | 1:A:675:VAL:HG21 | 1.98 | 0.46 |
| 2:B:1028:LEU:HD21 | 2:B:1043:ILE:HD11 | 1.97 | 0.46 |
| 3:C:114:HIS:CE1 | 3:C:152:LYS:HE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:781:ALA:HB2 | 2:B:1043:ILE:HG12 | 1.96 | 0.45 |
| 2:B:1030:ASN:OD1 | 2:B:1031:GLY:N | 2.49 | 0.45 |
| 7:G:6:SER:HG | 7:G:73:LYS:HZ3 | 1.55 | 0.45 |
| 4:D:131:LEU:O | 4:D:135:GLN:HG2 | 2.16 | 0.45 |
| 5:E:114:ALA:O | 5:E:118:LEU:HG | 2.16 | 0.45 |
| 9:I:36:LEU:HD23 | 9:I:47:GLU:HA | 1.97 | 0.45 |
| 1:A:1170:THR:HA | 1:A:1216:LEU:HD23 | 1.98 | 0.45 |
| 2:B:1127:ILE:HD11 | 2:B:1138:ARG:HE | 1.82 | 0.45 |
| 3:C:205:LYS:HZ2 | 3:C:213:GLU:HA | 1.82 | 0.45 |
| 5:E:19:GLN:OE1 | 5:E:138:ASN:ND2 | 2.40 | 0.45 |
| 10:J:12:LYS:HG2 | 10:J:13:ILE:N | 2.32 | 0.45 |
| 11:K:20:THR:OG1 | 11:K:34:THR:HB | 2.17 | 0.45 |
| 15:T:10:DT:H2" | 15:T:11:DA:H8 | 1.81 | 0.45 |
| 1:A:880:ARG:HD3 | 1:A:884:ASN:O | 2.17 | 0.45 |
| 1:A:1181:PRO:HB3 | 1:A:1197:TYR:CE2 | 2.51 | 0.45 |
| 2:B:17:ILE:HG22 | 2:B:18:THR:H | 1.81 | 0.45 |
| 2:B:841:ARG:HE | 14:P:8:A:H2 | 1.65 | 0.45 |
| 2:B:859:ARG:HG2 | 2:B:903:ILE:HG12 | 1.98 | 0.45 |
| 4:D:109:GLU:O | 4:D:113:ALA:HB2 | 2.17 | 0.45 |
| 8:H:94:GLY:HA3 | 8:H:118:TYR:HD1 | 1.81 | 0.45 |
| 1:A:868:MET:O | 1:A:1088:GLY:HA3 | 2.17 | 0.45 |
| 2:B:670:GLU:O | 2:B:673:VAL:HG12 | 2.17 | 0.45 |
| 3:C:187:ASP:OD2 | 3:C:190:ASN:HA | 2.17 | 0.45 |
| 1:A:862:ARG:O | 1:A:866:LYS:HG2 | 2.17 | 0.45 |
| 2:B:35:ASP:OD2 | 2:B:646:ARG:NH2 | 2.50 | 0.45 |
| 2:B:830:GLU:OE2 | 2:B:870:THR:OG1 | 2.24 | 0.45 |
| 1:A:931:ARG:HD3 | 1:A:939:VAL:HG11 | 1.98 | 0.45 |
| 1:A:1167:ARG:HG3 | 9:I:58:ILE:HD13 | 1.98 | 0.45 |
| 1:A:1457:ASN:ND2 | 1:A:1465:PRO:HD3 | 2.22 | 0.45 |
| 1:A:1474:LEU:HD11 | 6:F:107:ARG:NE | 2.32 | 0.45 |
| 2:B:193:VAL:O | 2:B:467:SER:HA | 2.16 | 0.45 |
| 2:B:513:GLU:HG3 | 2:B:726:SER:HB3 | 1.97 | 0.45 |
| 2:B:552:ASN:O | 2:B:556:ILE:HG13 | 2.17 | 0.45 |
| 3:C:45:ILE:HG13 | 3:C:79:VAL:HG22 | 1.99 | 0.45 |
| 5:E:14:ARG:O | 5:E:18:MET:HG2 | 2.16 | 0.45 |
| 2:B:838:GLN:N | 2:B:889:LYS:O | 2.46 | 0.45 |
| 4:D:65:LEU:HA | 4:D:68:THR:HG22 | 1.99 | 0.45 |
| 11:K:19:ILE:HG12 | 11:K:35:ILE:HD12 | 1.98 | 0.45 |
| 1:A:545:VAL:HG11 | 1:A:645:LEU:HD12 | 1.99 | 0.45 |
| 1:A:797:ARG:HG2 | 1:A:820:ARG:HB3 | 1.98 | 0.45 |
| 1:A:808:PRO:HB2 | 2:B:675:LEU:HD12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1098:PRO:O | 1:A:1102:MET:HG3 | 2.17 | 0.45 |
| 2:B:144:HIS:ND1 | 2:B:431:LEU:HD12 | 2.32 | 0.45 |
| 2:B:1028:LEU:HD12 | 2:B:1041:ILE:HD13 | 1.98 | 0.45 |
| 5:E:82:VAL:HB | 5:E:110:MET:SD | 2.56 | 0.45 |
| 9:I:81:THR:HG23 | 9:I:96:PHE:CE1 | 2.52 | 0.45 |
| 1:A:369:PRO:HB2 | 1:A:486:LEU:HD11 | 1.99 | 0.45 |
| 1:A:376:ASP:O | 1:A:473:ARG:N | 2.48 | 0.45 |
| 1:A:470:MET:HG2 | 1:A:524:MET:SD | 2.56 | 0.45 |
| 1:A:529:GLN:O | 1:A:1394:ASN:HB2 | 2.17 | 0.45 |
| 5:E:21:CYS:SG | 5:E:62:VAL:HG21 | 2.57 | 0.45 |
| 6:F:61:GLU:OE2 | 6:F:108:ARG:NE | 2.50 | 0.45 |
| 8:H:14:ASP:HB2 | 8:H:29:HIS:HB2 | 1.98 | 0.45 |
| 9:I:97:PHE:HD1 | 9:I:100:HIS:HD2 | 1.65 | 0.45 |
| 1:A:514:GLU:OE2 | 1:A:1468:THR:HG21 | 2.16 | 0.44 |
| 1:A:919:LYS:O | 1:A:1052:ARG:HD3 | 2.16 | 0.44 |
| 1:A:1020:LEU:HD22 | 1:A:1076:PHE:CD2 | 2.52 | 0.44 |
| 2:B:124:LEU:CB | 2:B:150:GLY:O | 2.61 | 0.44 |
| 2:B:1165:MET:O | 2:B:1166:SER:OG | 2.29 | 0.44 |
| 4:D:22:PHE:CE2 | 4:D:93:HIS:HE1 | 2.35 | 0.44 |
| 4:D:93:HIS:HB3 | 4:D:96:GLU:HG3 | 1.98 | 0.44 |
| 11:K:57:LEU:N | 11:K:76:GLN:O | 2.49 | 0.44 |
| 1:A:269:SER:HB3 | 2:B:825:GLN:HE22 | 1.82 | 0.44 |
| 1:A:1417:HIS:CE1 | 13:N:30:DA:H4' | 2.53 | 0.44 |
| 3:C:41:GLU:OE2 | 3:C:255:LYS:NZ | 2.30 | 0.44 |
| 1:A:1359:SER:O | 1:A:1365:ILE:HD11 | 2.17 | 0.44 |
| 2:B:1028:LEU:HD12 | 2:B:1041:ILE:HB | 1.99 | 0.44 |
| 8:H:96:VAL:HB | 8:H:116:VAL:HG22 | 1.99 | 0.44 |
| 11:K:10:PHE:CE2 | 11:K:11:LEU:HG | 2.52 | 0.44 |
| 2:B:83:ARG:HD2 | 2:B:133:ILE:HD12 | 2.00 | 0.44 |
| 2:B:721:ARG:HH21 | 2:B:975:ARG:HG2 | 1.82 | 0.44 |
| 15:T:17:DG:H2' | 15:T:18:DC:C6 | 2.52 | 0.44 |
| 1:A:11:SER:N | 2:B:1135:TYR:OH | 2.50 | 0.44 |
| 1:A:557:ARG:NH1 | 11:K:51:LEU:HD22 | 2.32 | 0.44 |
| 2:B:679:PRO:HA | 2:B:683:GLN:HG2 | 2.00 | 0.44 |
| 2:B:1032:PHE:HA | 3:C:36:ARG:NH2 | 2.33 | 0.44 |
| 1:A:1235:ILE:HA | 1:A:1296:MET:HE1 | 1.99 | 0.44 |
| 2:B:971:ALA:HA | 2:B:975:ARG:NH1 | 2.32 | 0.44 |
| 12:L:36:CYS:HB2 | 12:L:44:MET:CE | 2.48 | 0.44 |
| 1:A:1229:GLU:O | 1:A:1233:GLU:HG2 | 2.17 | 0.44 |
| 2:B:971:ALA:HA | 2:B:975:ARG:HH11 | 1.83 | 0.44 |
| 4:D:29:ALA:HA | 7:G:5:ILE:HG22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:22:LEU:O | 10:J:26:GLN:HG2 | 2.18 | 0.44 |
| 1:A:406:VAL:HG21 | 1:A:440:LEU:HD11 | 2.00 | 0.44 |
| 1:A:1471:PHE:CE2 | 6:F:64:ARG:HD3 | 2.53 | 0.44 |
| 2:B:270:ILE:HG13 | 2:B:305:LEU:HD23 | 1.99 | 0.44 |
| 2:B:427:LYS:HG3 | 2:B:428:ASP:N | 2.30 | 0.44 |
| 4:D:35:SER:O | 4:D:39:MET:HG3 | 2.18 | 0.44 |
| 6:F:66:LEU:HD11 | 6:F:97:LEU:HD22 | 1.99 | 0.44 |
| 9:I:26:PRO:HA | 9:I:36:LEU:O | 2.16 | 0.44 |
| 1:A:576:GLN:HA | 8:H:75:TYR:HB2 | 2.00 | 0.44 |
| 1:A:601:ASN:HB3 | 1:A:988:TRP:CZ3 | 2.53 | 0.44 |
| 1:A:626:THR:OG1 | 1:A:627:LYS:N | 2.47 | 0.44 |
| 1:A:901:VAL:HG12 | 1:A:980:PRO:HA | 1.99 | 0.44 |
| 1:A:991:GLN:NE2 | 1:A:1058:PHE:O | 2.49 | 0.44 |
| 1:A:1139:LEU:HB3 | 1:A:1338:THR:OG1 | 2.18 | 0.44 |
| 2:B:36:GLU:OE1 | 2:B:653:TRP:HB3 | 2.17 | 0.44 |
| 3:C:86:ARG:NE | 11:K:11:LEU:HD21 | 2.32 | 0.44 |
| 4:D:20:LEU:HD22 | 4:D:93:HIS:ND1 | 2.33 | 0.44 |
| 4:D:43:HIS:O | 4:D:47:GLN:HG3 | 2.18 | 0.44 |
| 1:A:312:PHE:O | 1:A:316:THR:CB | 2.66 | 0.43 |
| 1:A:1200:PRO:HB2 | 1:A:1203:ASP:OD2 | 2.17 | 0.43 |
| 7:G:152:VAL:HB | 7:G:157:ILE:HG12 | 1.99 | 0.43 |
| 9:I:73:SER:HA | 9:I:95:VAL:HG11 | 1.99 | 0.43 |
| 11:K:61:TYR:HB3 | 11:K:73:ILE:HG12 | 1.99 | 0.43 |
| 1:A:96:HIS:HB2 | 1:A:250:VAL:HG23 | 2.00 | 0.43 |
| 1:A:337:LYS:HA | 1:A:341:GLN:OE1 | 2.18 | 0.43 |
| 6:F:66:LEU:HD21 | 6:F:97:LEU:HB2 | 2.00 | 0.43 |
| 13:N:11:DG:C8 | 13:N:12:DT:H72 | 2.53 | 0.43 |
| 2:B:19:PRO:C | 2:B:21:LEU:H | 2.21 | 0.43 |
| 2:B:205:VAL:O | 2:B:371:ARG:NH1 | 2.51 | 0.43 |
| 2:B:475:PHE:CE2 | 2:B:768:ARG:HB2 | 2.54 | 0.43 |
| 2:B:719:SER:OG | 2:B:720:PRO:HD3 | 2.17 | 0.43 |
| 3:C:33:SER:O | 3:C:37:VAL:HG23 | 2.19 | 0.43 |
| 9:I:20:CYS:SG | 9:I:22:ASN:ND2 | 2.92 | 0.43 |
| 14:P:16:C:H2' | 14:P:17:A:C8 | 2.53 | 0.43 |
| 1:A:371:PRO:HD2 | 2:B:788:TYR:CE2 | 2.53 | 0.43 |
| 1:A:395:THR:HB | 1:A:396:PRO:HD2 | 1.99 | 0.43 |
| 1:A:749:ARG:NH2 | 1:A:779:ILE:HD11 | 2.34 | 0.43 |
| 2:B:172:CYS:HA | 10:J:62:TYR:HE1 | 1.83 | 0.43 |
| 3:C:37:VAL:HG13 | 3:C:41:GLU:HB2 | 1.99 | 0.43 |
| 1:A:497:ASP:OD1 | 1:A:497:ASP:N | 2.50 | 0.43 |
| 1:A:1375:ARG:HH12 | 1:A:1379:GLU:CD | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1132:THR:HG22 | 2:B:1134:THR:HG23 | 1.99 | 0.43 |
| 3:C:8:THR:O | 3:C:23:ILE:HA | 2.18 | 0.43 |
| 7:G:12:LEU:HA | 7:G:66:VAL:O | 2.18 | 0.43 |
| 8:H:65:TYR:CD1 | 8:H:82:PRO:HB2 | 2.54 | 0.43 |
| 1:A:521:VAL:N | 1:A:522:PRO:HD2 | 2.34 | 0.43 |
| 1:A:1173:THR:HG23 | 1:A:1214:VAL:HG12 | 2.00 | 0.43 |
| 3:C:62:GLU:HB3 | 12:L:55:PHE:CD1 | 2.53 | 0.43 |
| 1:A:589:LYS:NZ | 1:A:625:ASP:OD1 | 2.50 | 0.43 |
| 2:B:812:ARG:NH1 | 2:B:897:ARG:HG3 | 2.33 | 0.43 |
| 5:E:7:THR:OG1 | 5:E:48:PRO:HD3 | 2.18 | 0.43 |
| 7:G:62:GLY:C | 7:G:64:GLY:H | 2.22 | 0.43 |
| 7:G:96:GLY:HA3 | 7:G:109:SER:HA | 2.01 | 0.43 |
| 1:A:1024:ASN:O | 5:E:162:ARG:NH2 | 2.52 | 0.43 |
| 2:B:17:ILE:HG22 | 2:B:18:THR:N | 2.33 | 0.43 |
| 7:G:53:ASN:OD1 | 7:G:54:ILE:N | 2.51 | 0.43 |
| 1:A:1099:ALA:HA | 1:A:1102:MET:SD | 2.59 | 0.43 |
| 1:A:1445:HIS:HB2 | 1:A:1447:GLU:HG3 | 2.00 | 0.43 |
| 2:B:932:GLY:HA3 | 2:B:1055:VAL:HG11 | 2.00 | 0.43 |
| 2:B:1118:VAL:HG21 | 2:B:1171:MET:SD | 2.59 | 0.43 |
| 3:C:72:PRO:HG3 | 10:J:13:ILE:CD1 | 2.49 | 0.43 |
| 3:C:193:ARG:NH1 | 3:C:217:GLN:OE1 | 2.39 | 0.43 |
| 4:D:39:MET:HE2 | 4:D:39:MET:HB3 | 1.91 | 0.43 |
| 10:J:1:MET:HA | 10:J:55:LEU:HB2 | 2.00 | 0.43 |
| 1:A:344:LYS:O | 1:A:1435:THR:HG21 | 2.19 | 0.43 |
| 1:A:402:LEU:HD23 | 1:A:405:LEU:HD12 | 2.00 | 0.43 |
| 1:A:685:HIS:O | 2:B:783:ALA:HA | 2.19 | 0.43 |
| 1:A:1035:GLU:O | 1:A:1039:LEU:HB2 | 2.18 | 0.43 |
| 2:B:84:TYR:HD1 | 2:B:132:VAL:HG12 | 1.83 | 0.43 |
| 3:C:94:CYS:HB2 | 3:C:95:PRO:HD2 | 2.00 | 0.43 |
| 1:A:141:LEU:HD12 | 1:A:236:LEU:O | 2.19 | 0.42 |
| 2:B:568:PHE:HD2 | 2:B:613:ARG:HG2 | 1.83 | 0.42 |
| 2:B:844:ILE:HG22 | 2:B:846:ASP:H | 1.84 | 0.42 |
| 2:B:1112:ASP:OD1 | 2:B:1112:ASP:N | 2.52 | 0.42 |
| 3:C:205:LYS:NZ | 3:C:215:GLU:O | 2.47 | 0.42 |
| 3:C:211:LEU:HD11 | 3:C:218:ALA:HB2 | 2.01 | 0.42 |
| 4:D:60:VAL:HG13 | 7:G:103:PRO:HB3 | 2.01 | 0.42 |
| 7:G:52:ASP:OD1 | 7:G:73:LYS:HG2 | 2.19 | 0.42 |
| 1:A:1234:LYS:NZ | 1:A:1298:LEU:O | 2.36 | 0.42 |
| 1:A:1440:MET:SD | 2:B:1167:ILE:HD11 | 2.59 | 0.42 |
| 2:B:252:ILE:HG13 | 2:B:253:GLY:N | 2.34 | 0.42 |
| 4:D:30:GLU:O | 7:G:3:TYR:HA | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:90:TYR:HB3 | 8:H:145:MET:HB2 | 2.01 | 0.42 |
| 1:A:668:PHE:CZ | 1:A:672:ILE:HD11 | 2.53 | 0.42 |
| 5:E:44:PHE:O | 5:E:53:PRO:HD3 | 2.20 | 0.42 |
| 11:K:49:GLN:HB2 | 11:K:94:LEU:HD21 | 2.00 | 0.42 |
| 2:B:623:ARG:NH1 | 2:B:625:LEU:HD21 | 2.34 | 0.42 |
| 2:B:836:THR:HG23 | 2:B:837:CYS:N | 2.34 | 0.42 |
| 2:B:904:VAL:HG22 | 2:B:923:VAL:HG22 | 2.01 | 0.42 |
| 2:B:1094:GLN:HE22 | 2:B:1102:PHE:HE2 | 1.67 | 0.42 |
| 3:C:241:PRO:HA | 3:C:244:ILE:HD12 | 2.00 | 0.42 |
| 4:D:84:ARG:O | 4:D:88:LEU:CB | 2.65 | 0.42 |
| 8:H:7:GLU:HG2 | 8:H:59:VAL:HG22 | 2.01 | 0.42 |
| 1:A:998:PRO:HA | 1:A:1059:ARG:HG3 | 2.01 | 0.42 |
| 2:B:248:LYS:O | 2:B:252:ILE:HG12 | 2.20 | 0.42 |
| 2:B:794:VAL:CG1 | 2:B:965:ILE:HG23 | 2.49 | 0.42 |
| 7:G:12:LEU:HD21 | 7:G:60:GLN:HE22 | 1.83 | 0.42 |
| 1:A:46:THR:HG22 | 1:A:47:THR:HG23 | 2.01 | 0.42 |
| 1:A:91:ALA:HB2 | 1:A:291:ARG:HD2 | 2.00 | 0.42 |
| 2:B:220:GLU:OE1 | 2:B:236:TRP:NE1 | 2.52 | 0.42 |
| 2:B:262:TYR:CD2 | 2:B:346:GLU:HG3 | 2.54 | 0.42 |
| 2:B:558:PRO:O | 2:B:561:ILE:HG22 | 2.20 | 0.42 |
| 2:B:712:PRO:O | 2:B:939:HIS:HE1 | 2.03 | 0.42 |
| 2:B:1046:THR:HB | 2:B:1048:TYR:HE1 | 1.85 | 0.42 |
| 3:C:10:ARG:O | 3:C:21:PHE:HA | 2.20 | 0.42 |
| 3:C:42:VAL:HB | 3:C:178:PRO:HG3 | 2.02 | 0.42 |
| 3:C:59:LEU:HD13 | 3:C:63:PHE:CE2 | 2.54 | 0.42 |
| 4:D:64:THR:HG21 | 7:G:46:ILE:HG23 | 2.01 | 0.42 |
| 7:G:62:GLY:O | 7:G:63:ARG:HG2 | 2.20 | 0.42 |
| 9:I:97:PHE:HB2 | 9:I:100:HIS:NE2 | 2.35 | 0.42 |
| 9:I:117:PRO:HB2 | 9:I:118:HIS:CD2 | 2.54 | 0.42 |
| 11:K:81:TYR:HE2 | 11:K:86:ALA:HB2 | 1.85 | 0.42 |
| 2:B:399:LEU:HB3 | 2:B:453:TRP:CZ2 | 2.54 | 0.42 |
| 1:A:230:ASP:HA | 1:A:233:CYS:SG | 2.60 | 0.42 |
| 1:A:749:ARG:HH22 | 1:A:779:ILE:HD11 | 1.84 | 0.42 |
| 2:B:496:ALA:C | 2:B:498:PRO:HD2 | 2.40 | 0.42 |
| 2:B:497:LYS:O | 2:B:497:LYS:HG2 | 2.20 | 0.42 |
| 3:C:259:LEU:O | 3:C:263:LEU:CB | 2.68 | 0.42 |
| 4:D:108:ALA:HB2 | 4:D:128:GLN:HB2 | 2.01 | 0.42 |
| 5:E:41:LYS:HG3 | 5:E:46:GLY:HA2 | 2.02 | 0.42 |
| 9:I:97:PHE:CD1 | 9:I:100:HIS:HD2 | 2.38 | 0.42 |
| 1:A:139:LYS:HG2 | 1:A:143:HIS:CD2 | 2.54 | 0.42 |
| 1:A:264:VAL:HG13 | 14:P:11:A:H1' | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1354:PRO:HB3 | 5:E:137:ILE:HD11 | 2.01 | 0.42 |
| 1:A:1429:LYS:HB2 | 1:A:1438:VAL:HG11 | 2.02 | 0.42 |
| 2:B:130:LYS:NZ | 2:B:429:PHE:O | 2.53 | 0.42 |
| 2:B:776:ILE:HG22 | 2:B:777:ASN:O | 2.19 | 0.42 |
| 1:A:370:ASP:HB2 | 1:A:483:ARG:HB3 | 2.02 | 0.42 |
| 1:A:488:VAL:C | 1:A:491:PRO:HD2 | 2.41 | 0.42 |
| 1:A:904:GLN:NE2 | 1:A:982:ASN:HA | 2.27 | 0.42 |
| 1:A:1471:PHE:CZ | 6:F:61:GLU:HA | 2.55 | 0.42 |
| 4:D:20:LEU:HD12 | 4:D:121:ARG:HH22 | 1.85 | 0.42 |
| 4:D:35:SER:HB3 | 4:D:80:ILE:HD11 | 2.02 | 0.42 |
| 13:N:13:DA:O5' | 13:N:13:DA:H8 | 2.03 | 0.42 |
| 1:A:140:ARG:O | 1:A:144:VAL:HG22 | 2.19 | 0.41 |
| 1:A:369:PRO:HD3 | 1:A:496:PHE:CG | 2.55 | 0.41 |
| 2:B:568:PHE:CD2 | 2:B:613:ARG:HG2 | 2.55 | 0.41 |
| 2:B:709:SER:HB2 | 2:B:767:LEU:HD11 | 2.02 | 0.41 |
| 2:B:826:GLU:H | 2:B:872:THR:HG22 | 1.85 | 0.41 |
| 7:G:62:GLY:O | 7:G:64:GLY:N | 2.50 | 0.41 |
| 8:H:92:MET:HE2 | 8:H:143:LEU:HD23 | 2.01 | 0.41 |
| 2:B:96:PRO:HG2 | 2:B:120:TYR:CZ | 2.56 | 0.41 |
| 2:B:273:PHE:HE2 | 2:B:288:ILE:HD11 | 1.86 | 0.41 |
| 2:B:1032:PHE:CD1 | 11:K:40:HIS:CD2 | 3.08 | 0.41 |
| 3:C:7:PRO:HB3 | 3:C:26:THR:OG1 | 2.20 | 0.41 |
| 10:J:3:ILE:CD1 | 10:J:18:TRP:HB2 | 2.50 | 0.41 |
| 15:T:24:DC:H2" | 15:T:25:DA:C8 | 2.55 | 0.41 |
| 1:A:389:THR:CG2 | 1:A:417:LYS:HD3 | 2.49 | 0.41 |
| 1:A:623:PRO:HA | 8:H:27:ARG:NH2 | 2.35 | 0.41 |
| 4:D:33:LEU:HB2 | 4:D:36:GLU:HG3 | 2.01 | 0.41 |
| 5:E:64:HIS:CD2 | 5:E:66:ASP:HB2 | 2.55 | 0.41 |
| 9:I:96:PHE:HD2 | 9:I:110:LEU:HD22 | 1.86 | 0.41 |
| 13:N:27:DA:H2" | 13:N:28:DG:OP2 | 2.19 | 0.41 |
| 1:A:222:HIS:O | 1:A:226:LYS:HG3 | 2.20 | 0.41 |
| 1:A:1095:LEU:HD23 | 1:A:1393:VAL:HG11 | 2.01 | 0.41 |
| 1:A:1097:GLU:HB3 | 1:A:1098:PRO:HD3 | 2.02 | 0.41 |
| 11:K:56:VAL:HG22 | 11:K:77:THR:HG22 | 2.01 | 0.41 |
| 15:T:1:DA:H2" | 15:T:2:DA:C8 | 2.56 | 0.41 |
| 1:A:28:PRO:HA | 1:A:31:LEU:HD12 | 2.03 | 0.41 |
| 1:A:33:ARG:HD3 | 2:B:1139:GLY:HA2 | 2.02 | 0.41 |
| 1:A:369:PRO:HB3 | 1:A:486:LEU:HD21 | 2.02 | 0.41 |
| 1:A:456:VAL:HG21 | 1:A:503:LEU:HD11 | 2.03 | 0.41 |
| 1:A:551:ARG:NH1 | 8:H:42:ASP:OD2 | 2.53 | 0.41 |
| 1:A:717:ILE:HG12 | 1:A:737:PHE:CZ | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1227:THR:HG22 | 1:A:1229:GLU:H | 1.85 | 0.41 |
| 2:B:934:LYS:HG2 | 2:B:1051:LEU:HD12 | 2.02 | 0.41 |
| 1:A:1262:MET:HG2 | 1:A:1265:ASP:H | 1.84 | 0.41 |
| 2:B:412:LEU:O | 2:B:416:ARG:HG2 | 2.21 | 0.41 |
| 2:B:453:TRP:O | 2:B:462:ALA:HB1 | 2.20 | 0.41 |
| 12:L:36:CYS:HB3 | 12:L:39:CYS:SG | 2.61 | 0.41 |
| 1:A:22:GLN:HG2 | 1:A:242:TYR:CZ | 2.56 | 0.41 |
| 1:A:273:GLN:HB2 | 1:A:278:HIS:NE2 | 2.35 | 0.41 |
| 1:A:481:THR:HG22 | 2:B:1055:VAL:HG21 | 2.03 | 0.41 |
| 2:B:347:MET:SD | 2:B:348:LEU:HD13 | 2.61 | 0.41 |
| 2:B:798:ARG:HB2 | 2:B:948:GLN:HB3 | 2.02 | 0.41 |
| 3:C:37:VAL:O | 3:C:42:VAL:HG23 | 2.21 | 0.41 |
| 7:G:97:LEU:HB3 | 7:G:99:THR:HG23 | 2.03 | 0.41 |
| 8:H:95:LYS:HB2 | 8:H:140:ARG:NH1 | 2.36 | 0.41 |
| 1:A:597:PRO:HD3 | 1:A:668:PHE:CD1 | 2.56 | 0.41 |
| 1:A:621:ILE:HD11 | 8:H:124:ARG:HB2 | 2.02 | 0.41 |
| 1:A:784:VAL:HG13 | 2:B:978:ILE:HD11 | 2.02 | 0.41 |
| 1:A:872:MET:HG2 | 1:A:873:VAL:N | 2.36 | 0.41 |
| 1:A:330:GLN:NE2 | 1:A:334:ARG:HH21 | 2.19 | 0.41 |
| 1:A:346:LYS:HA | 1:A:351:ARG:HD2 | 2.03 | 0.41 |
| 1:A:460:ARG:HB2 | 1:A:501:MET:HG2 | 2.01 | 0.41 |
| 1:A:486:LEU:HD23 | 1:A:486:LEU:HA | 1.71 | 0.41 |
| 1:A:488:VAL:O | 1:A:491:PRO:HD2 | 2.20 | 0.41 |
| 1:A:741:VAL:HG11 | 1:A:797:ARG:NH1 | 2.36 | 0.41 |
| 1:A:857:THR:HG21 | 1:A:1100:THR:HA | 2.01 | 0.41 |
| 1:A:1486:ILE:HG13 | 1:A:1487:PRO:HD3 | 2.02 | 0.41 |
| 2:B:414:GLU:OE1 | 2:B:439:ILE:HD11 | 2.20 | 0.41 |
| 2:B:804:GLY:HA2 | 2:B:807:ARG:HE | 1.85 | 0.41 |
| 2:B:1114:TYR:CE2 | 2:B:1156:LYS:HD3 | 2.56 | 0.41 |
| 5:E:90:TYR:O | 5:E:94:MET:HG2 | 2.20 | 0.41 |
| 8:H:98:ARG:HB3 | 8:H:115:TYR:HB2 | 2.03 | 0.41 |
| 11:K:17:LYS:O | 11:K:36:ASN:ND2 | 2.54 | 0.41 |
| 1:A:457:ILE:HD12 | 2:B:1102:PHE:CZ | 2.55 | 0.41 |
| 2:B:907:VAL:HG13 | 2:B:921:ILE:HG12 | 2.03 | 0.41 |
| 3:C:101:PHE:CE2 | 3:C:122:SER:HB3 | 2.56 | 0.41 |
| 4:D:103:LEU:HB3 | 7:G:144:ARG:HH12 | 1.85 | 0.41 |
| 5:E:8:TYR:CZ | 5:E:12:LYS:HE3 | 2.56 | 0.41 |
| 7:G:118:GLU:HG2 | 7:G:129:LYS:O | 2.20 | 0.41 |
| 8:H:17:PRO:HG3 | 8:H:29:HIS:NE2 | 2.36 | 0.41 |
| 11:K:31:CYS:SG | 11:K:32:LEU:N | 2.94 | 0.41 |
| 11:K:81:TYR:CE2 | 11:K:86:ALA:HB2 | 2.57 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:90:ALA:O | 11:K:94:LEU:HG | 2.21 | 0.41 |
| 1:A:221:VAL:HG12 | 1:A:249:ILE:HD11 | 2.02 | 0.40 |
| 1:A:1373:ALA:HA | 5:E:144:LEU:HB3 | 2.03 | 0.40 |
| 1:A:1480:CYS:HB3 | 7:G:19:GLY:CA | 2.50 | 0.40 |
| 2:B:721:ARG:HD3 | 2:B:721:ARG:HA | 1.90 | 0.40 |
| 2:B:1021:HIS:CD2 | 2:B:1025:ASN:HB2 | 2.56 | 0.40 |
| 3:C:103:LEU:O | 3:C:160:ARG:HA | 2.21 | 0.40 |
| 14:P:16:C:H2' | 14:P:17:A:H8 | 1.85 | 0.40 |
| 1:A:368:THR:O | 1:A:483:ARG:HA | 2.21 | 0.40 |
| 1:A:589:LYS:HD2 | 8:H:120:GLY:HA3 | 2.03 | 0.40 |
| 1:A:1016:LEU:HD22 | 1:A:1069:LEU:HD22 | 2.03 | 0.40 |
| 2:B:25:ALA:HA | 2:B:640:ILE:HD12 | 2.04 | 0.40 |
| 2:B:128:ILE:HD12 | 2:B:147:THR:HG21 | 2.02 | 0.40 |
| 2:B:505:LEU:HD22 | 2:B:509:VAL:HB | 2.03 | 0.40 |
| 2:B:1086:PHE:CZ | 2:B:1090:GLU:HB3 | 2.56 | 0.40 |
| 1:A:821:GLY:HA2 | 1:A:838:PHE:CD2 | 2.56 | 0.40 |
| 1:A:1162:GLU:O | 1:A:1300:GLY:HA3 | 2.22 | 0.40 |
| 2:B:112:GLU:HG3 | 12:L:43:ILE:HD11 | 2.04 | 0.40 |
| 2:B:446:TYR:CE1 | 15:T:25:DA:H5" | 2.54 | 0.40 |
| 2:B:789:ASN:O | 2:B:968:ASN:HB2 | 2.21 | 0.40 |
| 2:B:854:ILE:O | 2:B:907:VAL:HG21 | 2.21 | 0.40 |
| 3:C:205:LYS:NZ | 3:C:213:GLU:HA | 2.36 | 0.40 |
| 1:A:120:ASP:O | 1:A:126:ILE:HD12 | 2.22 | 0.40 |
| 1:A:490:THR:OG1 | 1:A:491:PRO:HD3 | 2.21 | 0.40 |
| 1:A:769:MET:SD | 2:B:973:PRO:HG3 | 2.61 | 0.40 |
| 1:A:876:ASP:O | 1:A:890:ARG:NH1 | 2.55 | 0.40 |
| 1:A:1147:SER:O | 1:A:1154:ALA:HB2 | 2.20 | 0.40 |
| 1:A:1246:ILE:O | 1:A:1257:LEU:HD12 | 2.22 | 0.40 |
| 2:B:423:ILE:O | 2:B:426:GLY:N | 2.41 | 0.40 |
| 2:B:1021:HIS:HD2 | 2:B:1025:ASN:HB2 | 1.87 | 0.40 |
| 3:C:9:VAL:HA | 3:C:22:ILE:O | 2.21 | 0.40 |
| 14:P:8:A:H2' | 14:P:9:U:C6 | 2.57 | 0.40 |
| 1:A:413:TYR:HB3 | 1:A:414:PRO:HD3 | 2.03 | 0.40 |
| 1:A:457:ILE:HD11 | 1:A:515:ILE:HG12 | 2.03 | 0.40 |
| 2:B:256:ILE:O | 2:B:269:ILE:HG12 | 2.21 | 0.40 |
| 2:B:1029:TYR:OH | 3:C:185:GLU:HG3 | 2.21 | 0.40 |
| 2:B:1114:TYR:HE2 | 2:B:1156:LYS:HD3 | 1.86 | 0.40 |
| 6:F:79:VAL:HG13 | 6:F:96:GLU:OE2 | 2.21 | 0.40 |
| 7:G:119:PHE:HA | 7:G:128:TYR:HD1 | 1.85 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1417/1970 (72%) | 1347 (95%) | 70 (5%) | 0 | 100 | 100 |
| 2 | B | 1128/1174 (96%) | 1072 (95%) | 56 (5%) | 0 | 100 | 100 |
| 3 | C | 253/275 (92%) | 238 (94%) | 15 (6%) | 0 | 100 | 100 |
| 4 | D | 126/142 (89%) | 121 (96%) | 5 (4%) | 0 | 100 | 100 |
| 5 | E | 207/210 (99%) | 198 (96%) | 9 (4%) | 0 | 100 | 100 |
| 6 | F | 80/127 (63%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 7 | G | 169/172 (98%) | 164 (97%) | 5 (3%) | 0 | 100 | 100 |
| 8 | H | 146/150 (97%) | 138 (94%) | 8 (6%) | 0 | 100 | 100 |
| 9 | I | 112/125 (90%) | 103 (92%) | 9 (8%) | 0 | 100 | 100 |
| 10 | J | 65/67 (97%) | 59 (91%) | 6 (9%) | 0 | 100 | 100 |
| 11 | K | 113/117 (97%) | 110 (97%) | 3 (3%) | 0 | 100 | 100 |
| 12 | L | 42/58 (72%) | 36 (86%) | 6 (14%) | 0 | 100 | 100 |
| All | All | 3858/4587 (84%) | 3662 (95%) | 196 (5%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 1252/1749 (72%) | 1252 (100%) | 0 | 100 | 100 |
| 2 | B | 993/1027 (97%) | 993 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | C | 234/252 (93%) | 234 (100%) | 0 | 100 | 100 |
| 4 | D | 106/127 (84%) | 106 (100%) | 0 | 100 | 100 |
| 5 | E | 189/190 (100%) | 189 (100%) | 0 | 100 | 100 |
| 6 | F | 71/111 (64%) | 71 (100%) | 0 | 100 | 100 |
| 7 | G | 147/153 (96%) | 147 (100%) | 0 | 100 | 100 |
| 8 | H | 129/131 (98%) | 129 (100%) | 0 | 100 | 100 |
| 9 | I | 103/112 (92%) | 103 (100%) | 0 | 100 | 100 |
| 10 | J | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 11 | K | 104/106 (98%) | 104 (100%) | 0 | 100 | 100 |
| 12 | L | 41/55 (74%) | 41 (100%) | 0 | 100 | 100 |
| All | All | 3425/4069 (84%) | 3425 (100%) | 0 | 100 | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 77 | ASN |
| 1 | A | 330 | GLN |
| 1 | A | 372 | ASN |
| 1 | A | 449 | HIS |
| 1 | A | 502 | ASN |
| 1 | A | 671 | ASN |
| 1 | A | 757 | GLN |
| 1 | A | 791 | GLN |
| 1 | A | 804 | HIS |
| 1 | A | 839 | HIS |
| 1 | A | 1082 | HIS |
| 1 | A | 1093 | GLN |
| 1 | A | 1163 | HIS |
| 1 | A | 1190 | GLN |
| 1 | A | 1220 | HIS |
| 1 | A | 1230 | GLN |
| 1 | A | 1248 | ASN |
| 1 | A | 1360 | ASN |
| 1 | A | 1417 | HIS |
| 1 | A | 1422 | GLN |
| 1 | A | 1457 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1462 | GLN |
| 2 | B | 117 | ASN |
| 2 | B | 245 | GLN |
| 2 | B | 265 | GLN |
| 2 | B | 312 | GLN |
| 2 | B | 370 | HIS |
| 2 | B | 525 | ASN |
| 2 | B | 639 | HIS |
| 2 | B | 699 | HIS |
| 2 | B | 731 | GLN |
| 2 | B | 825 | GLN |
| 2 | B | 1021 | HIS |
| 2 | B | 1097 | HIS |
| 2 | B | 1117 | HIS |
| 3 | C | 51 | GLN |
| 3 | C | 66 | HIS |
| 4 | D | 48 | ASN |
| 4 | D | 93 | HIS |
| 7 | G | 4 | HIS |
| 7 | G | 14 | HIS |
| 8 | H | 126 | GLN |
| 9 | I | 22 | ASN |
| 9 | I | 118 | HIS |
| 10 | J | 52 | HIS |
| 11 | K | 69 | HIS |
| 11 | K | 84 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 14 | P | 13/20 (65%) | 3 (23%) | 1 (7%) |

All (3) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | P | 8 | A |
| 14 | P | 11 | A |
| 14 | P | 13 | G |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | P | 12 | A |

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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.

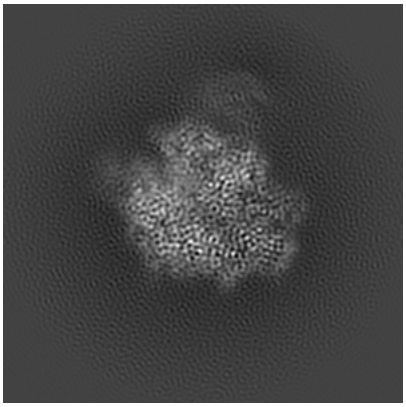
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3218. These allow visual inspection of the internal detail of the map and identification of artifacts.

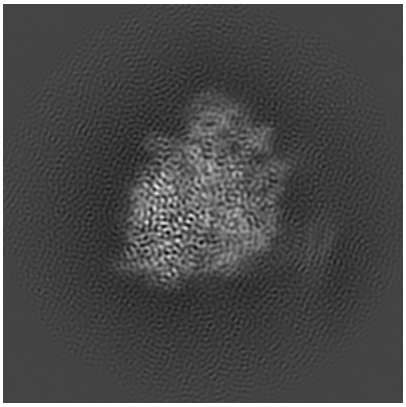
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

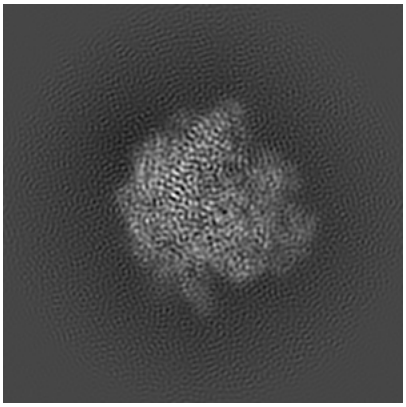
### 6.1.1 Primary map



X



Y

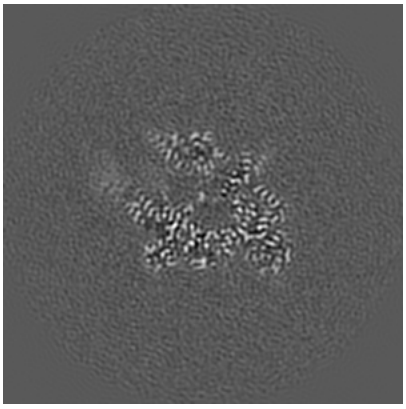


Z

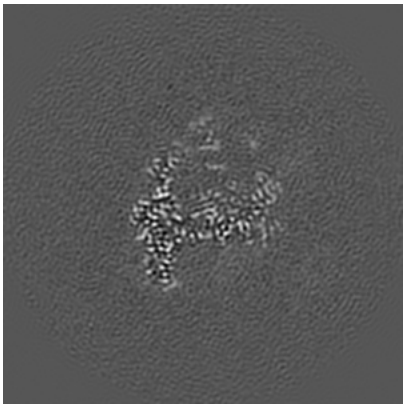
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

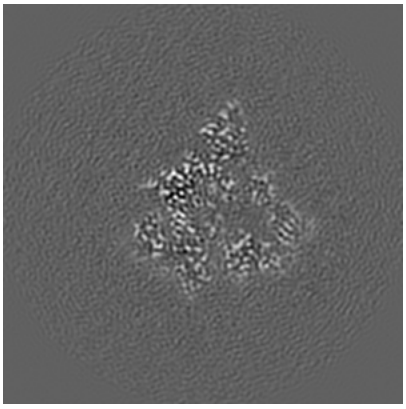
### 6.2.1 Primary map



X Index: 102



Y Index: 102

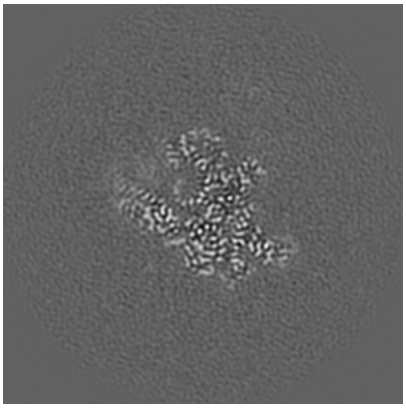


Z Index: 102

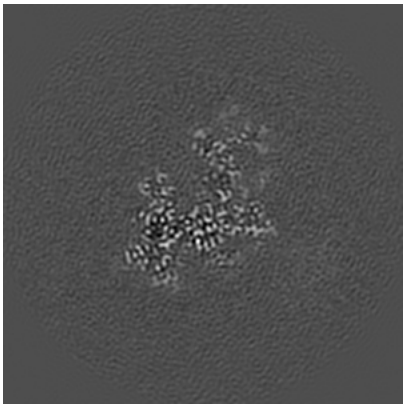
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

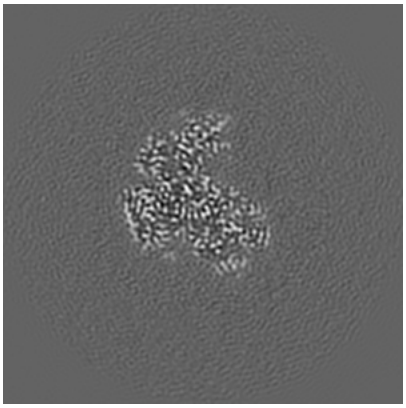
### 6.3.1 Primary map



X Index: 92



Y Index: 109

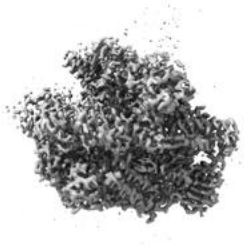


Z Index: 81

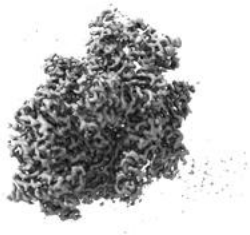
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

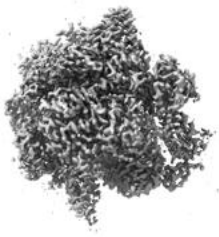
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

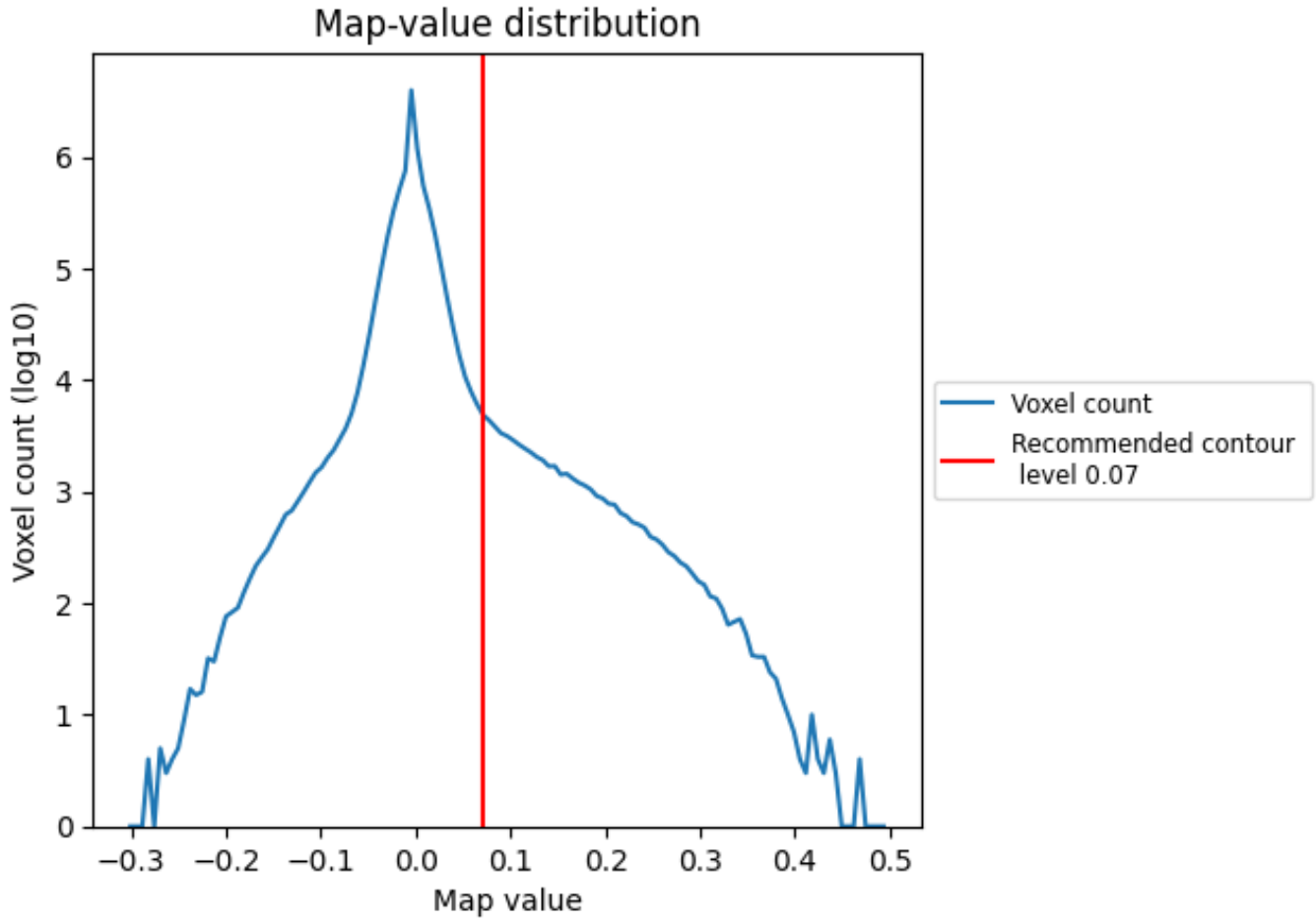
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

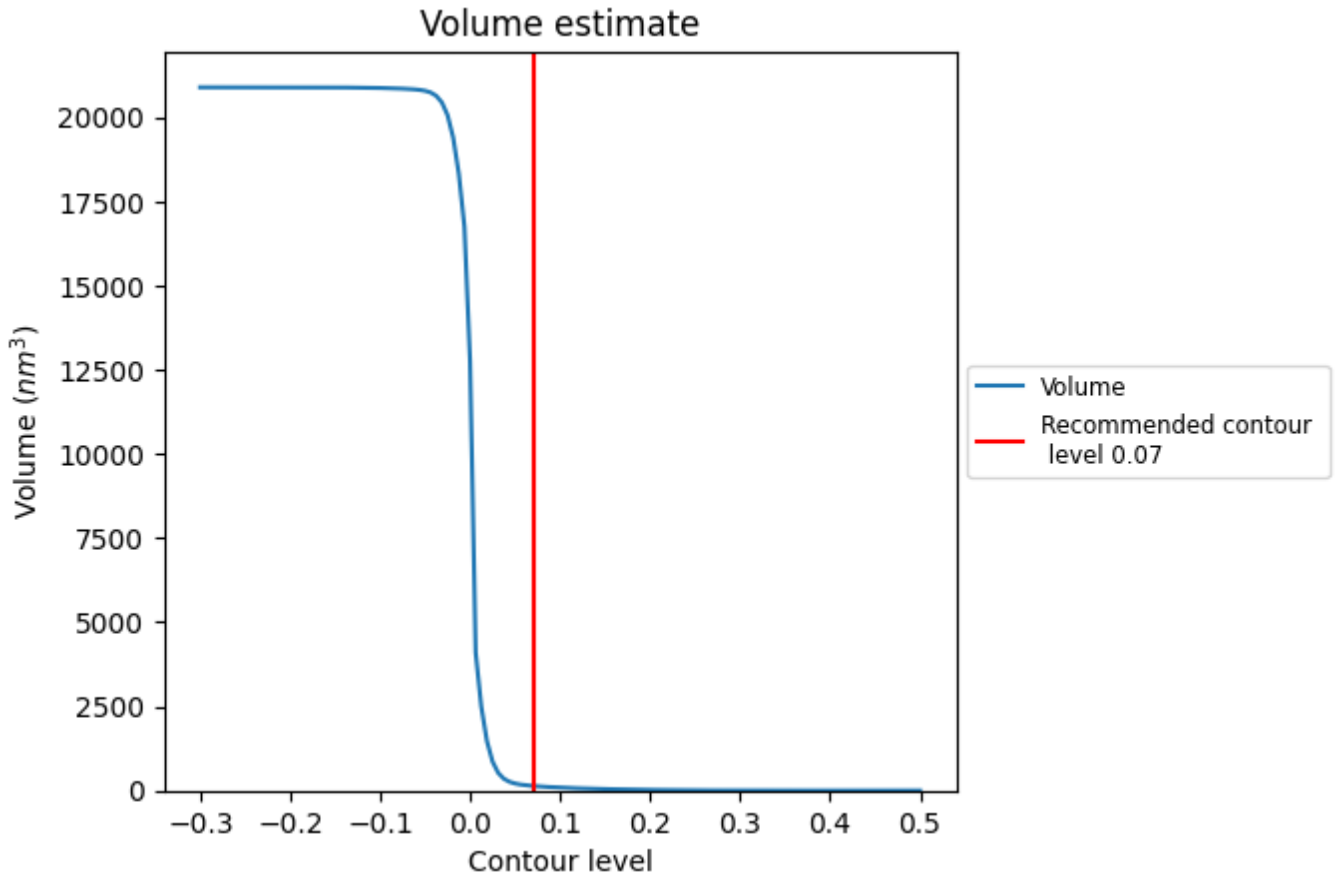
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

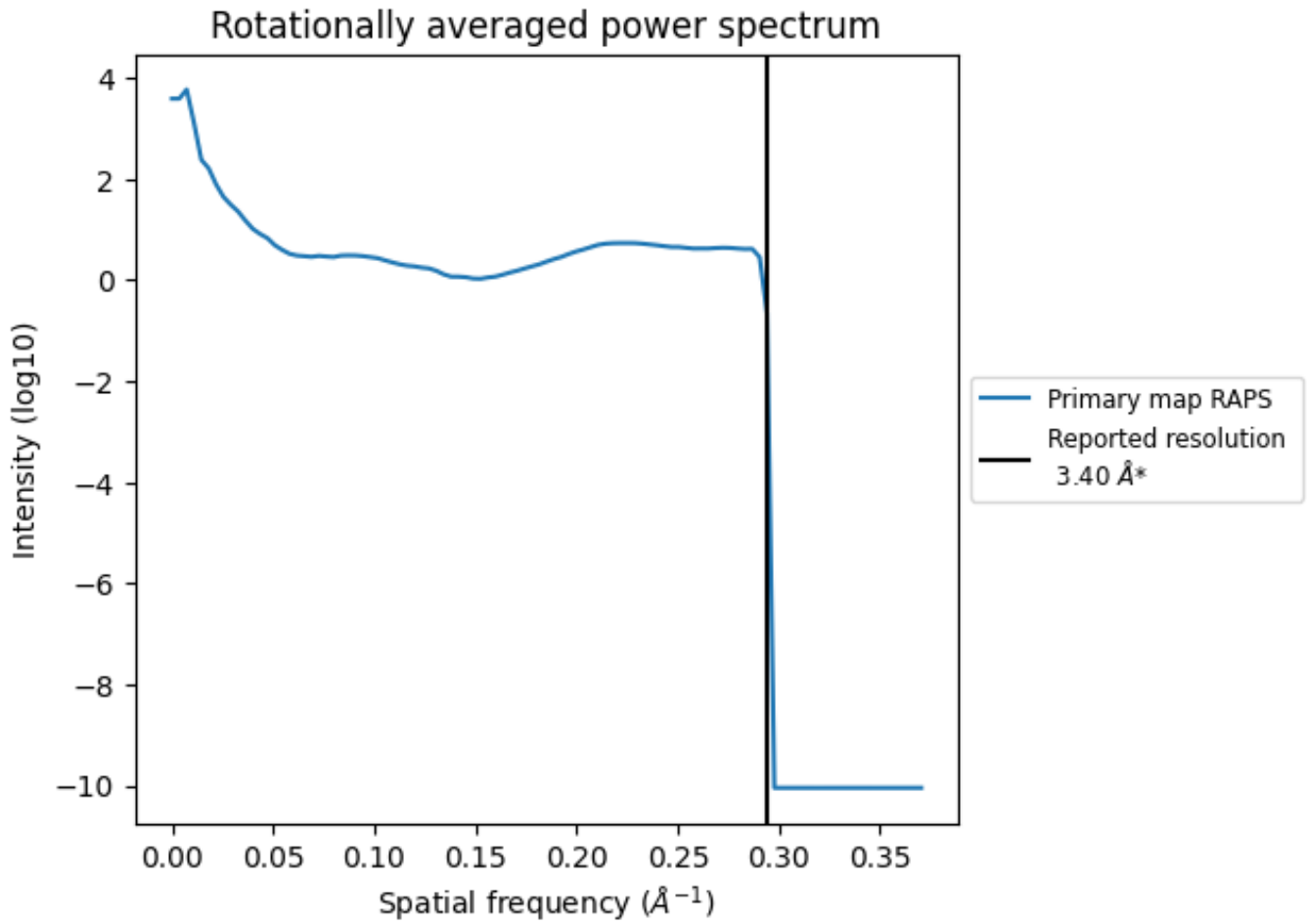
## 7.2 Volume estimate




The volume at the recommended contour level is 135 $nm^3$; this corresponds to an approximate mass of 122 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.294 Å$^{-1}$

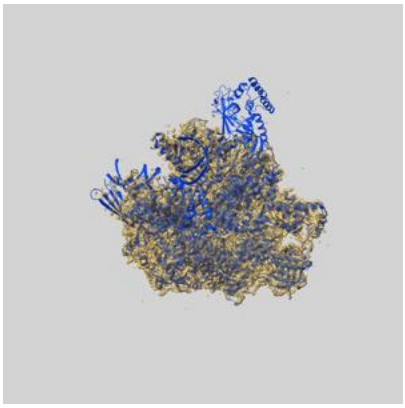
# 8 Fourier-Shell correlation

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

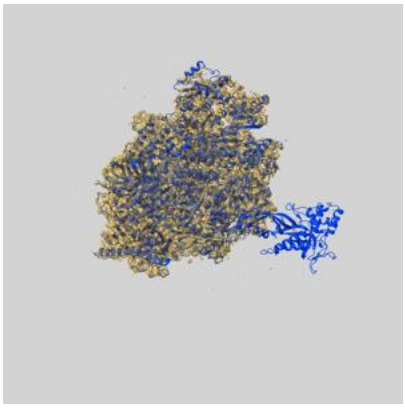
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3218 and PDB model 5FLM. Per-residue inclusion information can be found in section 3 on page 7.

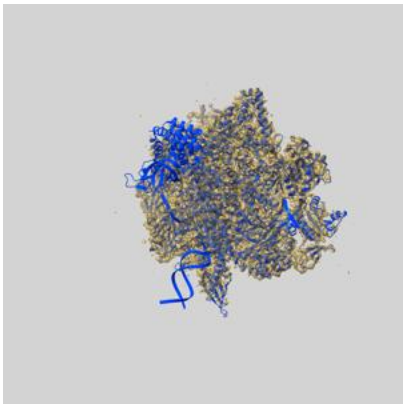
## 9.1 Map-model overlay



X



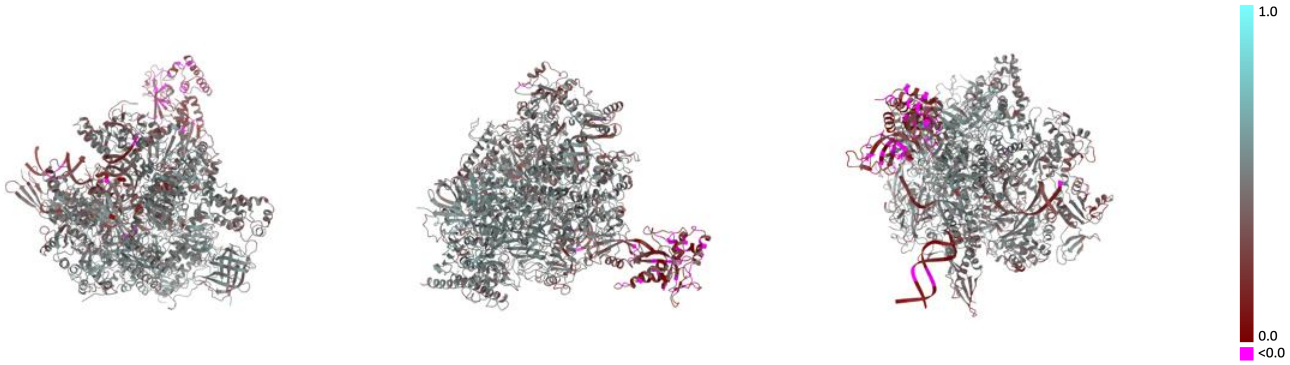
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

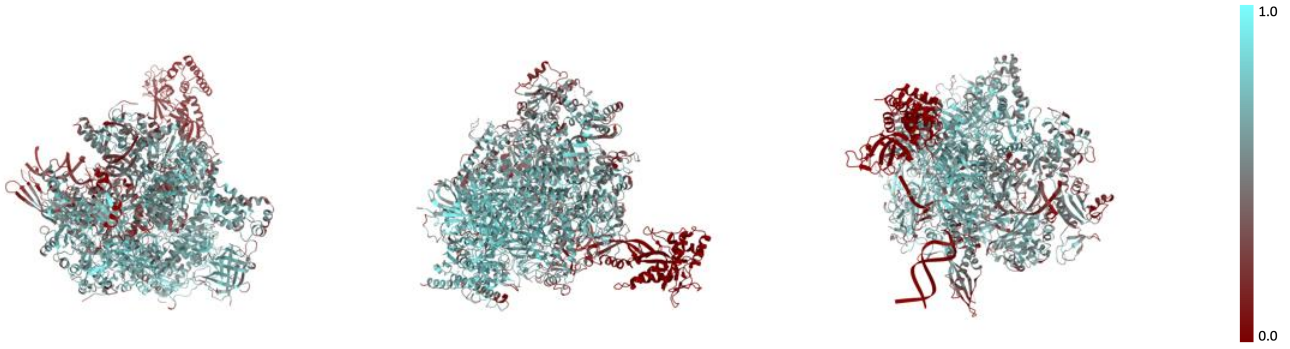
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

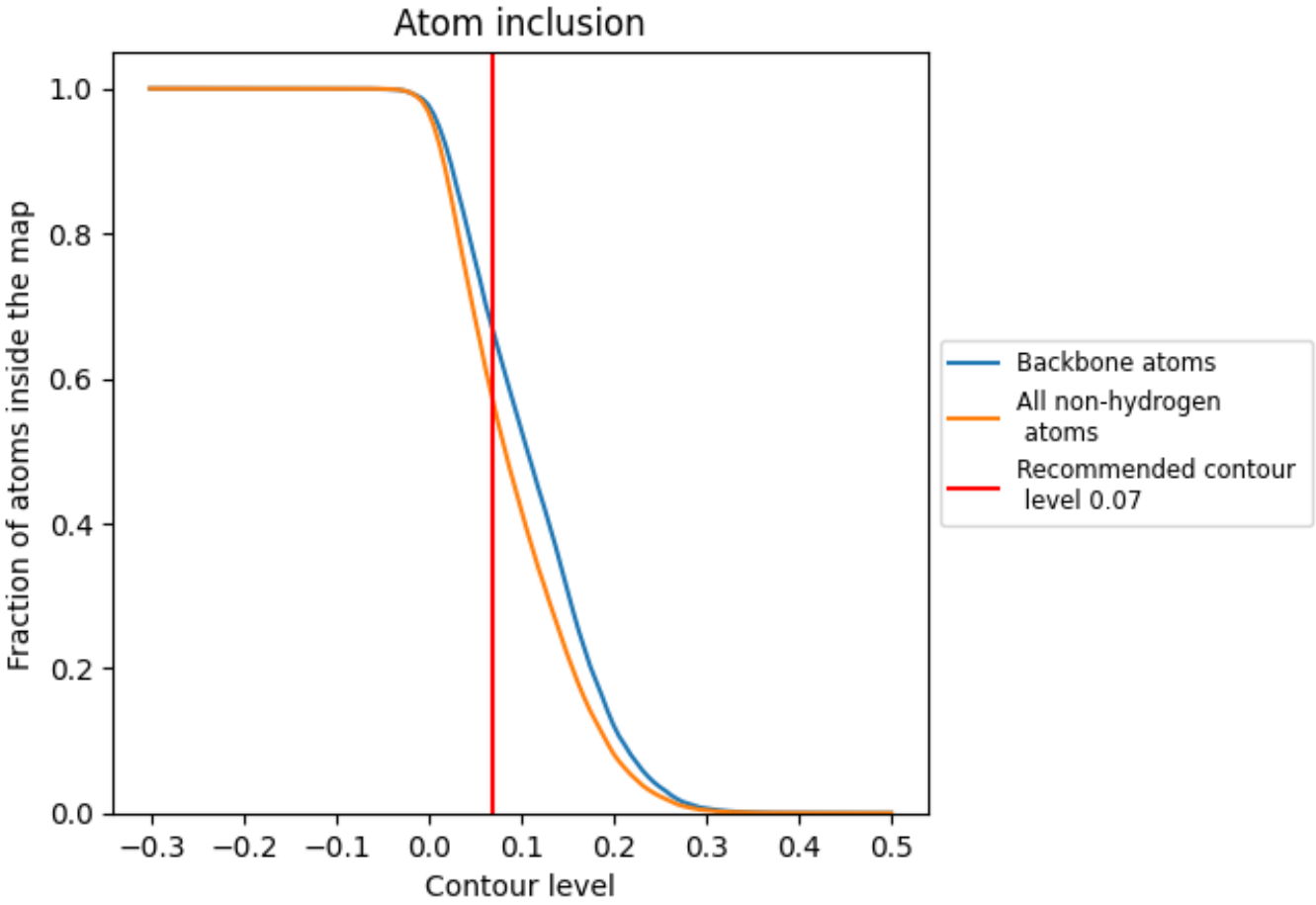
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

## 9.4 Atom inclusion (i)




At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5664 | 0.4420 |
| A | 0.6029 | 0.4690 |
| B | 0.6474 | 0.4790 |
| C | 0.6843 | 0.4900 |
| D | 0.0010 | 0.1330 |
| E | 0.5940 | 0.4570 |
| F | 0.5806 | 0.4640 |
| G | 0.0608 | 0.2020 |
| H | 0.6195 | 0.4680 |
| I | 0.5165 | 0.4490 |
| J | 0.7505 | 0.5160 |
| K | 0.6458 | 0.4900 |
| L | 0.6180 | 0.4570 |
| N | 0.1757 | 0.1710 |
| P | 0.5083 | 0.3920 |
| T | 0.3649 | 0.3080 |