Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 07:46 PM EST

PDB ID	:	7SID
EMDB ID	:	EMD-25141
Title	:	Human ATM Dimer Bound to Nbs1
Authors	:	Warren, C.; Pavletich, N.P.
Deposited on	:	2021-10-13
Resolution	:	2.53 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:

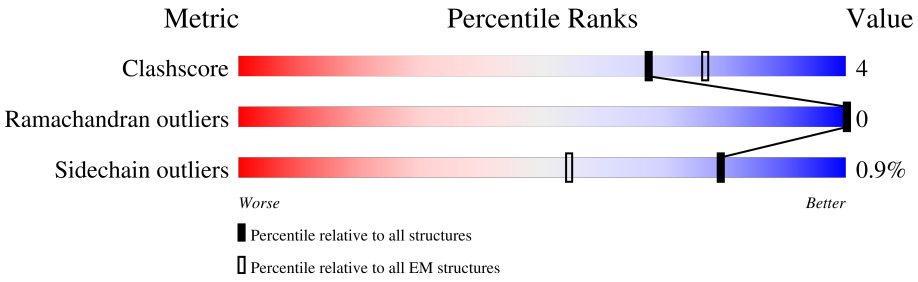
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	3056	39% 80% 10% 9%
1	C	3056	39% 80% 10% 9%
2	B	28	36% 32% · 64%
2	D	28	36% 32% · 64%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44650 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.

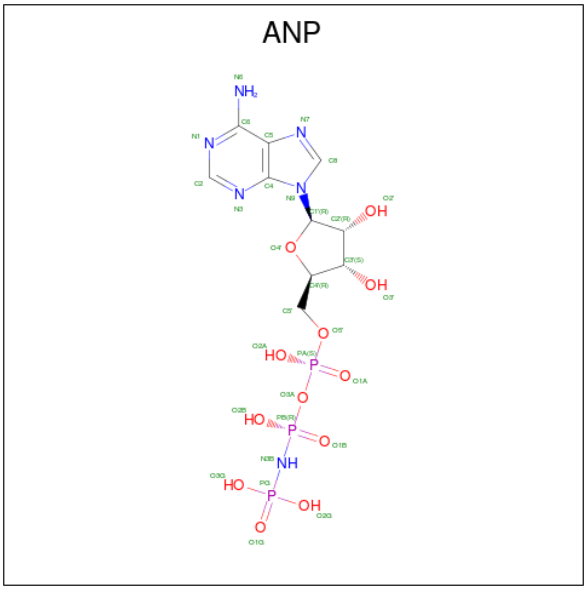
- Molecule 1 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2773	Total 22210	C 14200	N 3774	O 4083	S 153	0	0
1	C	2773	Total 22210	C 14200	N 3774	O 4083	S 153	0	0

- Molecule 2 is a protein called Nibrin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	10	Total 83	C 53	N 14	O 16	0	0
2	D	10	Total 83	C 53	N 14	O 16	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

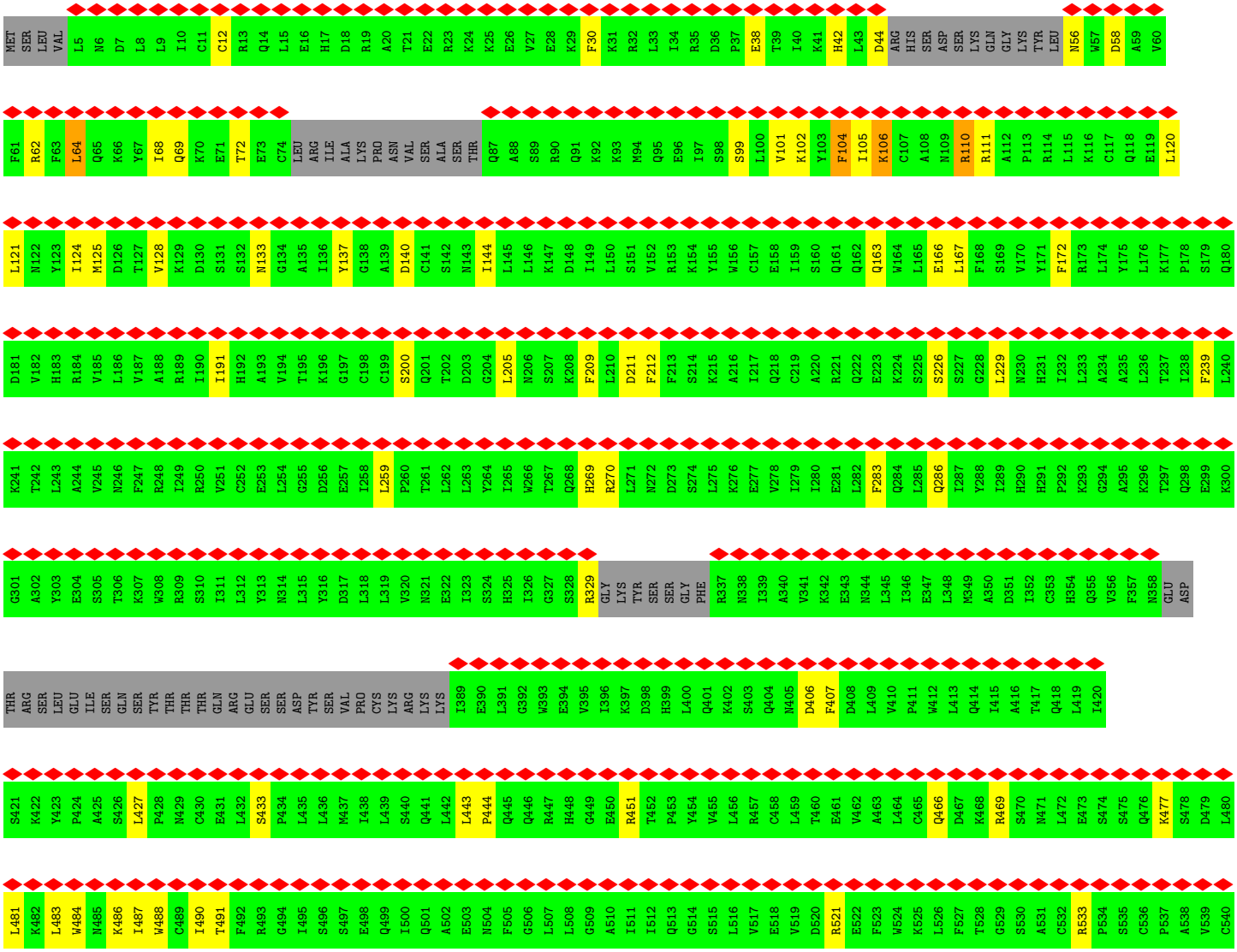
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

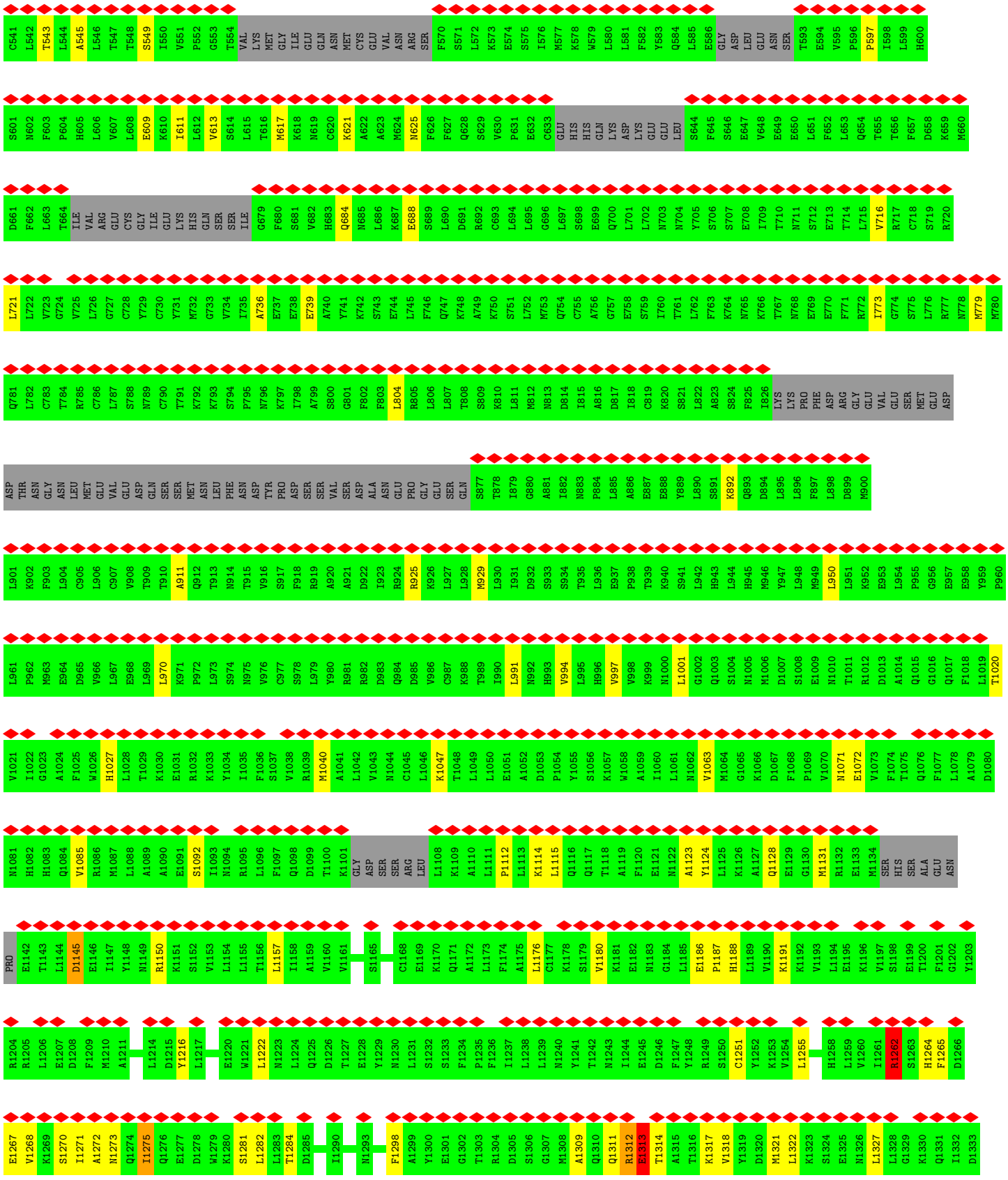
3 Residue-property plots (i)

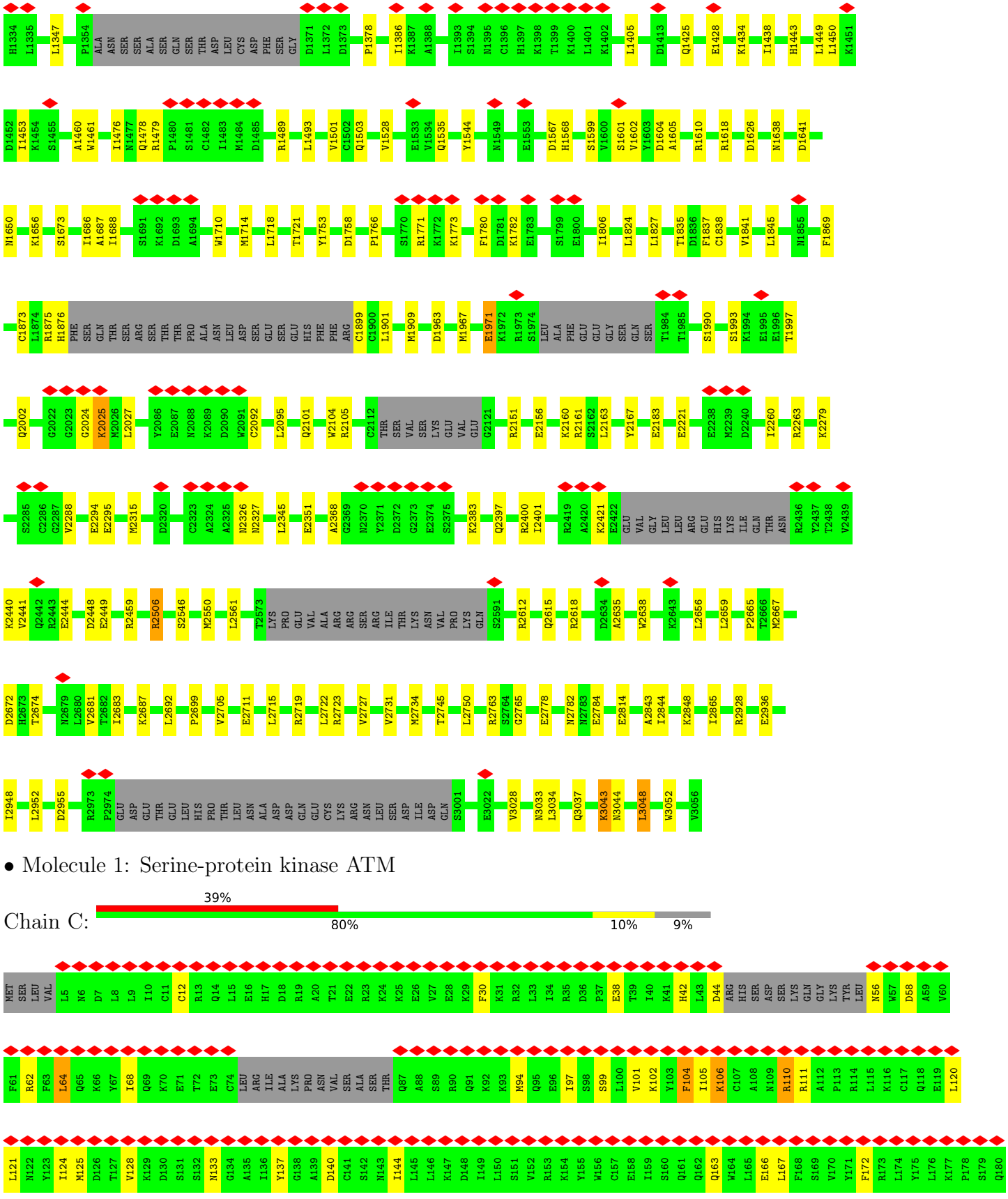
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

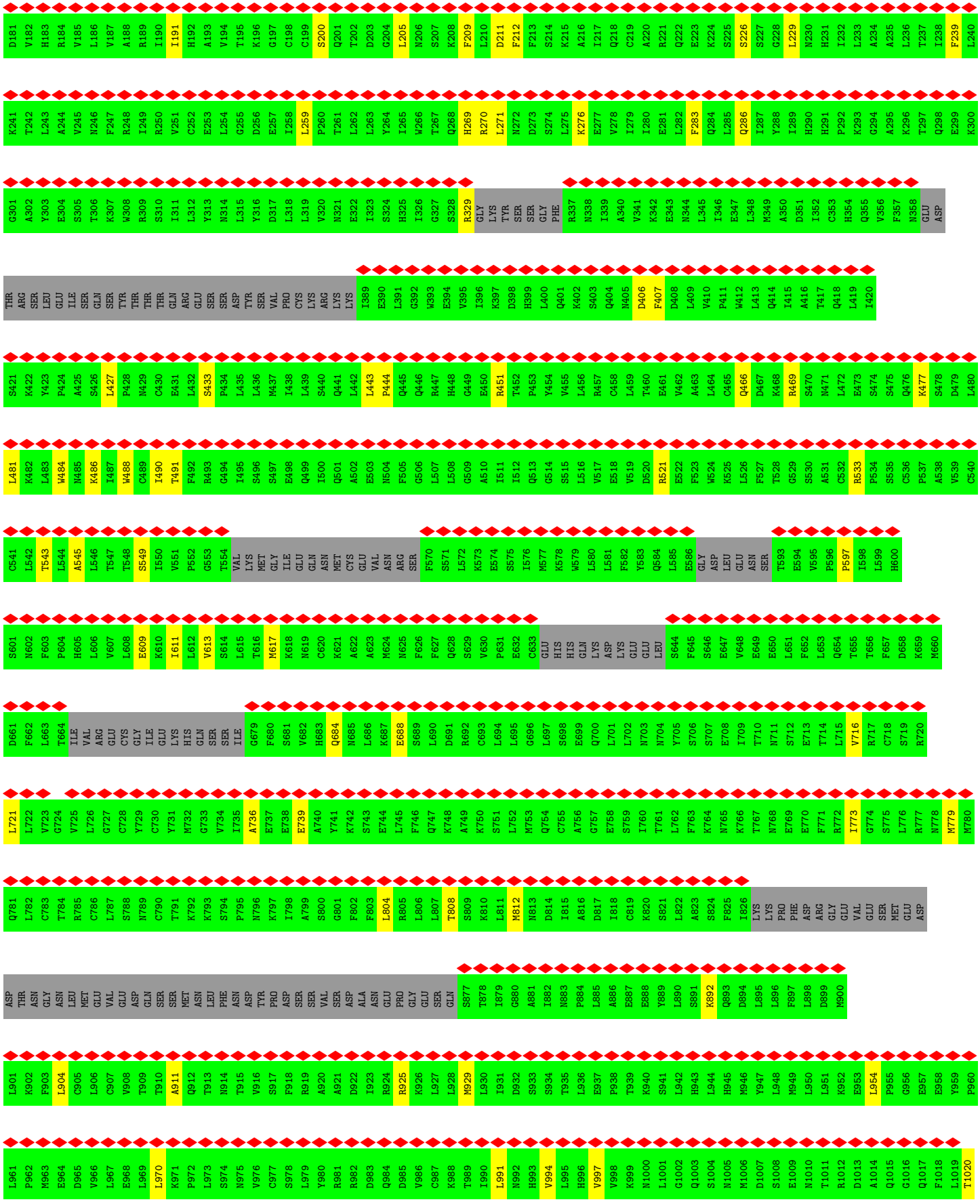


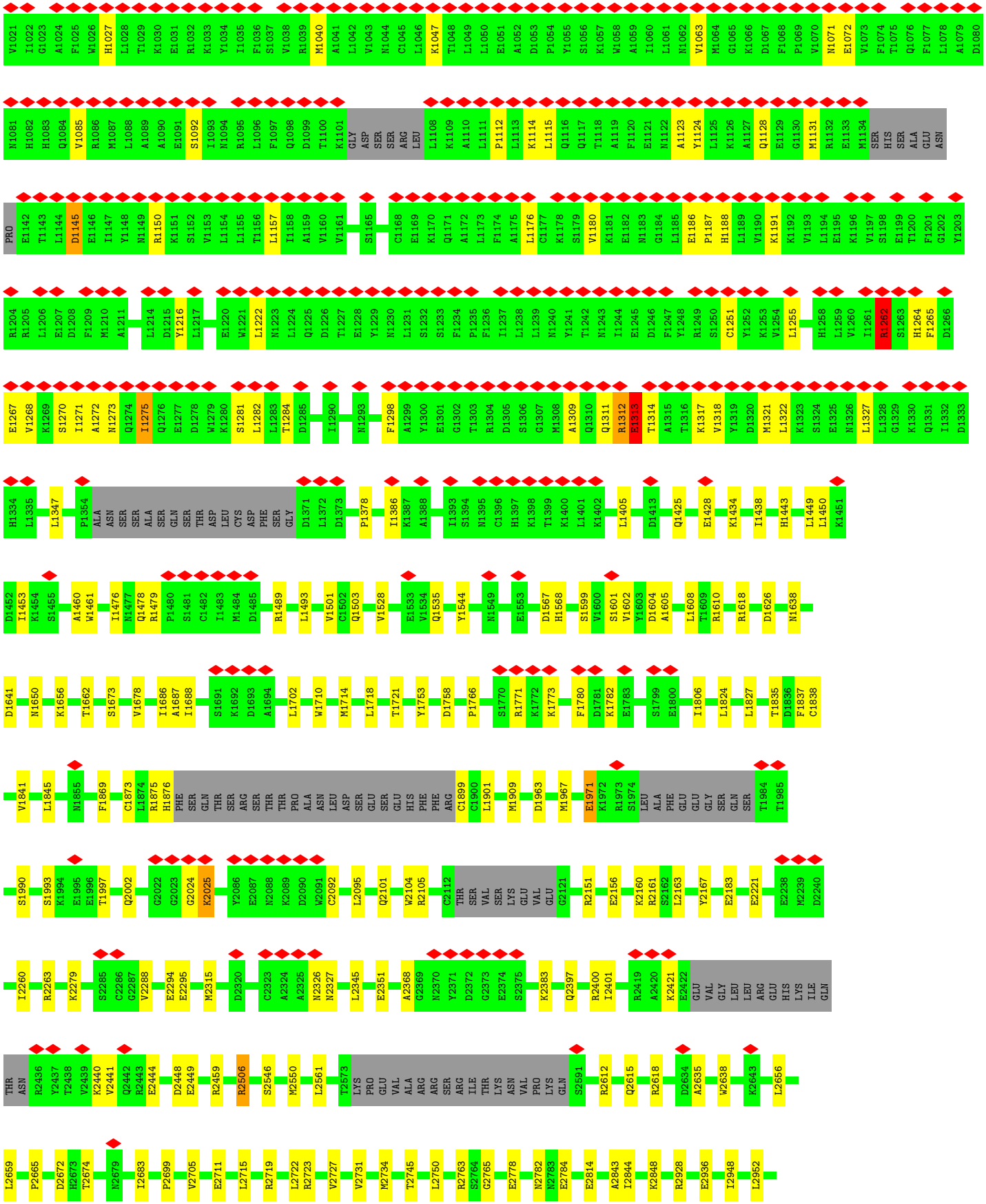

C541 L542 T543 L544 A545 L546 T547 T548 S549 I550 V551 P552 G553 T554 VAL LYS MET GLY ILE GLU GLN ASN MET CYS GLU VAL ASN ARG SER F570 S571 L572 K573 E574 S575 I576 M577 K578 W579 L580 L581 F582 Y583 Q584 L585 E586 GLY ASP LEU GLU ASN SER T593 E594 V595 P596 P597 I598 L599 H600
S601 N602 F603 P604 H605 L606 V607 L608 E609 K610 I611 L612 V613 S614 L615 T616 M617 K618 N619 C620 K621 A622 A623 M624 N625 F626 F627 Q628 S629 V630 P631 E632 C633 GLU HIS HIS GLN LYS ASP LYS GLU GLU LEU S644 F645 S646 E647 V648 E649 E650 L651 F652 L653 Q654 T655 T656 F657 D658 K659 M660
D661 F662 L663 T664 ILE VAL ARG GLU CYS GLY ILE GLU LYS HIS GLN SER SER ILE G679 F680 S681 V682 H683 Q684 N685 L686 K687 E688 S689 L690 D691 R692 C693 L694 L695 G696 L697 S698 E699 Q700 L701 L702 N703 N704 Y705 S706 S707 E708 I709 T710 N711 S712 E713 T714 L715 V716 R717 C718 S719 R720
L721 L722 V723 G724 V725 L726 G727 C728 Y729 C730 Y731 M732 G733 V734 I735 A736 E737 E738 E739 A740 Y741 K742 S743 E744 L745 F746 Q747 K748 A749 K750 S751 L752 M753 Q754 C755 A756 G757 E758 S759 I760 T761 L762 F763 K764 N765 K766 T767 N768 E769 E770 F771 R772 I773 G774 S775 L776 R777 N778 M779 M780
Q781 L782 C783 T784 R785 C786 L787 S788 N789 C790 T791 K792 K793 S794 P795 N796 K797 I798 A799 S800 G801 F802 F803 L804 R805 L806 L807 T808 S809 K810 L811 M812 N813 D814 I815 A816 D817 I818 C819 K820 S821 L822 A823 S824 F825 I826 LYS LYS PRO PHE ASP ARG GLY GLU VAL GLU SER MET GLU ASP
ASP THR ASN GLY ASN LEU MET GLU VAL GLU ASP GLN SER SER MET ASN LEU PHE ASN ASP TYR PRO ASP SER SER VAL SER ASP ALA ASN GLU PRO GLY GLU SER GLN S877 T878 I879 G880 A881 I882 N883 P884 L885 A886 E887 E888 Y889 L890 S891 K892 Q893 D894 L895 L896 F897 L898 D899 M900
L901 K902 F903 L904 C905 L906 C907 V908 T909 T910 A911 Q912 T913 N914 T915 V916 S917 F918 R919 A920 A921 D922 I923 R924 R925 K926 L927 L928 M929 L930 I931 D932 S933 S934 T935 L936 E937 P938 T939 K940 S941 L942 H943 L944 H945 M946 Y947 L948 M949 L950 L951 K952 E953 L954 P955 G956 E957 E958 Y959 P960
L961 P962 M963 E964 D965 V966 L967 E968 L969 L970 K971 P972 L973 S974 N975 V976 C977 S978 L979 Y980 R981 R982 D983 Q984 D985 V986 C987 K988 T989 I990 L991 N992 H993 V994 L995 H996 V997 V998 K999 N1000 L1001 G1002 Q1003 S1004 N1005 M1006 D1007 S1008 E1009 N1010 T1011 R1012 D1013 A1014 Q1015 G1016 Q1017 F1018 L1019 T1020
V1021 I1022 G1023 A1024 F1025 W1026 H1027 L1028 T1029 K1030 E1031 R1032 K1033 Y1034 I1035 F1036 S1037 V1038 R1039 M1040 A1041 L1042 V1043 N1044 C1045 L1046 K1047 T1048 L1049 L1050 E1051 A1052 D1053 P1054 Y1055 S1056 K1057 W1058 A1059 I1060 L1061 N1062 V1063 M1064 G1065 K1066 D1067 F1068 P1069 V1070 N1071 E1072 V1073 F1074 T1075 Q1076 F1077 L1078 A1079 D1080
N1081 H1082 H1083 Q1084 V1085 R1086 M1087 L1088 A1089 A1090 E1091 S1092 I1093 N1094 R1095 L1096 F1097 Q1098 D1099 T1100 K1101 GLY ASP SER SER ARG LEU L1108 K1109 A1110 L1111 P1112 L1113 K1114 L1115 Q1116 Q1117 T1118 A1119 F1120 E1121 N1122 A1123 Y1124 L1125 K1126 A1127 Q1128 E1129 G1130 M1131 R1132 E1133 M1134 SER HIS SER ALA GLU ASN
PRO E1142 T1143 L1144 D1145 E1146 I1147 Y1148 N1149 R1150 K1151 S1152 V1153 L1154 L1155 T1156 L1157 I1158 A1159 V1160 V1161 S1165 C1168 E1169 K1170 Q1171 A1172 L1173 F1174 A1175 L1176 C1177 K1178 S1179 V1180 K1181 E1182 N1183 G1184 L1185 E1186 P1187 H1188 L1189 V1190 K1191 K1192 V1193 L1194 E1195 K1196 V1197 S1198 E1199 T1200 F1201 G1202 Y1203
R1204 R1205 L1206 E1207 D1208 F1209 M1210 A1211 L1214 D1215 Y1216 L1217 E1220 W1221 L1222 N1223 L1224 Q1225 D1226 T1227 E1228 Y1229 N1230 L1231 S1232 S1233 F1234 P1235 F1236 I1237 L1238 L1239 N1240 Y1241 T1242 N1243 I1244 E1245 D1246 F1247 Y1248 R1249 S1250 C1251 Y1252 K1253 V1254 L1255 H1258 L1259 V1260 I1261 R1262 S1263 H1264 F1265 D1266
E1267 V1268 K1269 S1270 I1271 A1272 N1273 Q1274 I1275 Q1276 E1277 D1278 W1279 K1280 S1281 L1282 L1283 T1284 D1285 I1290 N1293 F1298 A1299 Y1300 E1301 G1302 T1303 R1304 D1305 S1306 G1307 M1308 A1309 Q1310 Q1311 R1312 E1313 T1314 A1315 T1316 K1317 V1318 Y1319 D1320 M1321 L1322 K1323 S1324 E1325 N1326 L1327 L1328 G1329 K1330 Q1331 I1332 D1333

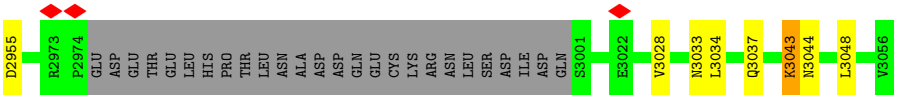


• Molecule 1: Serine-protein kinase ATM

Chain C:

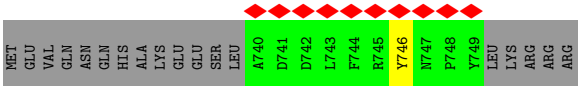

D181 V182 H183 R184 V185 L186 V187 A188 R189 I190 I191 H192 A193 V194 T195 K196 G197 C198 C199 S200 Q201 T202 D203 G204 L205 N206 S207 K208 F209 L210 D211 F212 F213 S214 K215 A216 I217 Q218 C219 A220 R221 Q222 E223 K224 S225 S226 S227 G228 L229 N230 H231 I232 L233 A234 A235 L236 T237 I238 F239 L240
K241 T242 L243 A244 V245 N246 F247 R248 I249 R250 V251 C252 E253 L254 G255 D256 E257 I258 L259 P260 T261 L262 L263 Y264 I265 W266 T267 Q268 H269 R270 L271 N272 D273 S274 L275 K276 E277 V278 I279 I280 E281 L282 F283 Q284 L285 Q286 I287 Y288 I289 H290 H291 P292 K293 G294 A295 K296 T297 Q298 E299 K300
G301 A302 Y303 E304 S305 T306 K307 W308 R309 S310 I311 L312 Y313 N314 L315 Y316 D317 L318 L319 V320 N321 E322 I323 S324 H325 I326 G327 S328 R329 GLY LYS TYR SER SER GLY PHE R337 N338 I339 A340 V341 K342 E343 N344 L345 I346 E347 L348 M349 A350 D351 I352 C353 H354 Q355 V356 F357 N358 GLU ASP
THR ARG SER LEU GLU ILE SER GLN SER TYR THR THR THR GLN ARG GLU SER SER ASP TYR SER VAL PRO CYS LYS ARG LYS LYS I389 E390 L391 G392 W393 E394 V395 I396 K397 D398 H399 L400 Q401 K402 S403 Q404 N405 D406 F407 D408 L409 V410 P411 W412 L413 Q414 I415 A416 T417 Q418 L419 I420
S421 K422 Y423 P424 A425 S426 L427 P428 N429 C430 E431 L432 S433 P434 L435 L436 M437 I438 L439 S440 Q441 L442 L443 P444 Q445 Q446 R447 H448 G449 E450 R451 T452 P453 Y454 V455 L456 R457 C458 L459 T460 E461 V462 A463 L464 C465 Q466 D467 K468 R469 S470 N471 L472 E473 S474 S475 Q476 K477 S478 D479 L480
L481 K482 L483 W484 N485 K486 I487 W488 C489 I490 T491 F492 R493 G494 I495 S496 S497 E498 Q499 I500 Q501 A502 E503 N504 F505 G506 L507 L508 G509 A510 I511 I512 Q513 G514 S515 L516 V517 E518 V519 D520 R521 E522 F523 W524 K525 L526 F527 T528 G529 S530 A531 C532 R533 P534 S535 C536 P537 A538 V539 C540
C541 L542 T543 L544 A545 L546 T547 T548 S549 I550 V551 P552 G553 T554 VAL LYS MET GLY ILE GLU GLN ASN MET CYS GLU VAL ASN ARG SER F570 S571 L572 K573 E574 S575 I576 M577 K578 W579 L580 L581 F582 Y583 Q584 L585 E586 GLY ASP LEU GLU ASN SER T593 E594 V595 P596 P597 I598 L599 H600
S601 N602 F603 P604 H605 L606 V607 L608 E609 K610 I611 L612 V613 S614 L615 T616 M617 K618 N619 C620 K621 A622 A623 M624 N625 F626 F627 Q628 S629 V630 P631 E632 C633 GLU HIS HIS GLN LYS ASP LYS GLU GLU LEU S644 F645 S646 E647 V648 E649 E650 L651 F652 L653 Q654 T655 T656 F657 D658 K659 M660
D661 F662 L663 T664 ILE VAL ARG GLU CYS GLY ILE GLU LYS HIS GLN SER SER ILE G679 F680 S681 V682 H683 Q684 N685 L686 K687 E688 S689 L690 D691 R692 C693 L694 L695 G696 L697 S698 E699 Q700 L701 L702 N703 N704 Y705 S706 S707 E708 I709 T710 N711 S712 E713 T714 L715 V716 R717 C718 S719 R720
L721 L722 V723 G724 V725 L726 G727 C728 Y729 C730 Y731 M732 G733 V734 I735 A736 E737 E738 E739 A740 Y741 K742 S743 E744 L745 F746 Q747 K748 A749 K750 S751 L752 M753 Q754 C755 A756 G757 E758 S759 I760 T761 L762 F763 K764 N765 K766 T767 N768 E769 E770 F771 R772 I773 G774 S775 L776 R777 N778 M779 M780
Q781 L782 C783 T784 R785 C786 L787 S788 N789 C790 T791 K792 K793 S794 P795 N796 K797 I798 A799 S800 G801 F802 F803 L804 R805 L806 L807 T808 S809 K810 L811 M812 N813 D814 I815 A816 D817 I818 C819 K820 S821 L822 A823 S824 F825 I826 LYS LYS PRO PHE ASP ARG GLY GLU VAL GLU SER MET GLU ASP
ASP THR ASN GLY ASN LEU MET GLU VAL GLU ASP GLN SER SER MET ASN LEU PHE ASN ASP TYR PRO ASP SER SER VAL SER ASP ALA ASN GLU PRO GLY GLU SER GLN S877 T878 I879 G880 A881 I882 N883 P884 L885 A886 E887 E888 Y889 L890 S891 K892 Q893 D894 L895 L896 F897 L898 D899 M900
L901 K902 F903 L904 C905 L906 C907 V908 T909 T910 A911 Q912 T913 N914 T915 V916 S917 F918 R919 A920 A921 D922 I923 R924 R925 K926 L927 L928 M929 L930 I931 D932 S933 S934 T935 L936 E937 P938 T939 K940 S941 L942 H943 L944 H945 M946 Y947 L948 M949 L950 L951 K952 E953 L954 P955 G956 E957 E958 Y959 P960
L961 P962 H963 E964 D965 V966 L967 E968 L969 L970 K971 P972 L973 S974 N975 V976 C977 S978 L979 Y980 R981 R982 D983 Q984 D985 V986 C987 K988 T989 I990 L991 N992 H993 V994 L995 H996 V997 V998 K999 N1000 L1001 G1002 Q1003 S1004 N1005 M1006 D1007 S1008 E1009 N1010 T1011 R1012 D1013 A1014 Q1015 G1016 Q1017 F1018 L1019 T1020


V1021 I1022 G1023 A1024 F1025 W1026 H1027 L1028 T1029 K1030 E1031 R1032 K1033 Y1034 I1035 F1036 S1037 V1038 R1039 M1040 A1041 L1042 V1043 N1044 C1045 L1046 K1047 T1048 L1049 L1050 E1051 A1052 D1053 P1054 Y1055 S1056 K1057 W1058 A1059 I1060 L1061 M1062 V1063 M1064 G1065 K1066 D1067 F1068 P1069 V1070 N1071 E1072 V1073 F1074 T1075 Q1076 F1077 L1078 A1079 D1080
N1081 H1082 H1083 Q1084 V1085 R1086 M1087 L1088 A1089 A1090 E1091 S1092 I1093 N1094 R1095 L1096 F1097 Q1098 D1099 T1100 K1101 GLY ASP SER SER ARG LEU L1108 K1109 A1110 L1111 P1112 L1113 K1114 L1115 Q1116 Q1117 T1118 A1119 F1120 E1121 N1122 A1123 Y1124 L1125 K1126 A1127 Q1128 E1129 G1130 M1131 R1132 E1133 M1134 SER HIS SER ALA GLU ASN
PRO E1142 T1143 L1144 D1145 E1146 I1147 Y1148 N1149 R1150 K1151 S1152 V1153 L1154 L1155 T1156 L1157 I1158 A1159 V1160 V1161 S1165 C1168 E1169 K1170 Q1171 A1172 L1173 F1174 A1175 L1176 C1177 K1178 S1179 V1180 K1181 E1182 N1183 G1184 L1185 E1186 P1187 H1188 L1189 V1190 K1191 K1192 V1193 L1194 E1195 K1196 V1197 S1198 E1199 T1200 F1201 G1202 Y1203
R1204 R1205 L1206 E1207 D1208 F1209 M1210 A1211 L1214 D1215 Y1216 L1217 E1220 W1221 L1222 N1223 L1224 Q1225 D1226 T1227 E1228 Y1229 N1230 L1231 S1232 S1233 F1234 P1235 F1236 I1237 L1238 L1239 N1240 Y1241 T1242 N1243 I1244 E1245 D1246 F1247 Y1248 R1249 S1250 C1251 Y1252 K1253 V1254 L1255 H1258 L1259 V1260 I1261 R1262 S1263 H1264 F1265 D1266
E1267 V1268 K1269 S1270 I1271 A1272 N1273 Q1274 I1275 Q1276 E1277 D1278 W1279 K1280 S1281 L1282 L1283 T1284 D1285 I1290 N1293 F1298 A1299 Y1300 E1301 G1302 T1303 R1304 D1305 S1306 G1307 M1308 A1309 Q1310 Q1311 R1312 E1313 T1314 A1315 T1316 K1317 V1318 Y1319 D1320 M1321 L1322 K1323 S1324 E1325 N1326 L1327 L1328 G1329 K1330 Q1331 I1332 D1333
H1334 L1335 L1347 P1354 ALA ASN SER SER ALA SER GLN SER THR ASP LEU CYS ASP PHE SER GLY D1371 L1372 D1373 P1378 I1386 K1387 A1388 I1393 S1394 N1395 C1396 H1397 K1398 T1399 K1400 L1401 K1402 L1405 D1413 Q1425 E1428 K1434 I1438 H1443 L1449 L1450 K1451
D1452 I1453 K1454 S1455 A1460 W1461 I1476 N1477 Q1478 R1479 P1480 S1481 C1482 I1483 M1484 D1485 R1489 L1493 V1501 C1502 Q1503 V1528 E1533 V1534 Q1535 Y1544 N1549 E1553 D1567 H1568 S1599 V1600 S1601 V1602 Y1603 D1604 A1605 L1608 T1609 R1610 R1618 D1626 N1638
D1641 N1650 K1656 T1662 S1673 V1678 I1686 A1687 I1688 S1691 K1692 D1693 A1694 L1702 W1710 M1714 L1718 T1721 Y1753 D1758 P1766 S1770 R1771 K1772 K1773 F1780 D1781 K1782 E1783 S1799 E1800 I1806 L1824 L1827 T1835 D1836 F1837 C1838
V1841 L1845 N1855 F1869 C1873 L1874 R1875 H1876 PHE SER GLN THR SER ARG SER THR THR PRO ALA ASN LEU ASP SER GLU SER GLU HIS PHE PHE ARG C1899 C1900 L1901 M1909 D1963 M1967 E1971 K1972 R1973 S1974 LEU ALA PHE GLU GLU GLY SER GLN SER T1984 T1985
S1990 S1993 K1994 E1995 E1996 T1997 Q2002 G2022 G2023 G2024 K2025 Y2086 E2087 N2088 K2089 D2090 W2091 C2092 L2095 Q2101 W2104 R2105 C2112 THR SER VAL SER LYS GLU VAL GLU G2121 R2151 E2156 K2160 R2161 S2162 L2163 Y2167 E2183 E2221 E2238 M2239 D2240
I2260 R2263 K2279 S2285 C2286 G2287 V2288 E2294 E2295 M2315 D2320 C2323 A2324 A2325 N2326 N2327 L2345 E2351 A2368 G2369 N2370 Y2371 D2372 G2373 E2374 S2375 K2383 Q2397 R2400 I2401 R2419 A2420 K2421 E2422 GLU VAL GLY LEU LEU ARG GLU HIS LYS ILE GLN
THR ASN R2436 Y2437 T2438 V2439 K2440 V2441 Q2442 R2443 E2444 D2448 E2449 R2459 R2506 S2546 M2550 L2561 T2573 LYS PRO GLU VAL ALA ARG ARG SER ARG ILE THR LYS ASN VAL PRO LYS GLN S2591 R2612 Q2615 R2618 D2634 A2635 W2638 K2643 L2656
L2659 P2665 D2672 H2673 T2674 N2679 I2683 P2699 V2705 E2711 L2715 R2719 L2722 R2723 V2727 V2731 M2734 T2745 L2750 R2763 S2764 G2765 E2778 N2782 N2783 E2784 E2814 A2843 I2844 K2848 R2928 E2936 I2948 L2952



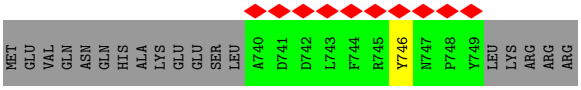
- Molecule 2: Nibrin

Chain B:



- Molecule 2: Nibrin

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	323.4, 323.4, 323.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, 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	0.24	0/22624	0.45	1/30565 (0.0%)
1	C	0.24	0/22624	0.45	1/30565 (0.0%)
2	B	0.28	0/85	0.45	0/115
2	D	0.28	0/85	0.45	0/115
All	All	0.24	0/45418	0.45	2/61360 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1313	GLU	CA-CB-CG	7.62	130.17	113.40
1	C	1313	GLU	CA-CB-CG	7.62	130.17	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1262	ARG	Sidechain
1	C	1262	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22210	0	22392	177	0
1	C	22210	0	22392	174	0
2	B	83	0	69	1	0
2	D	83	0	69	1	0
3	A	31	0	13	0	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	44650	0	44948	350	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (350) 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:C:2506:ARG:HG3	1:C:2506:ARG:HH11	1.27	0.98
1:A:2506:ARG:HG3	1:A:2506:ARG:HH11	1.28	0.97
1:C:1313:GLU:OE1	1:C:1313:GLU:N	2.07	0.87
1:A:1313:GLU:OE1	1:A:1313:GLU:N	2.07	0.87
1:C:1271:ILE:O	1:C:1275:ILE:HB	1.76	0.86
1:A:1271:ILE:O	1:A:1275:ILE:HB	1.76	0.85
1:C:2665:PRO:HD3	1:C:2683:ILE:HD11	1.73	0.71
1:A:2665:PRO:HD3	1:A:2683:ILE:HD11	1.73	0.71
1:A:1309:ALA:O	1:A:1312:ARG:N	2.27	0.68
1:C:1298:PHE:O	1:C:1312:ARG:NH1	2.27	0.68
1:A:1298:PHE:O	1:A:1312:ARG:NH1	2.27	0.68
1:C:1309:ALA:O	1:C:1312:ARG:N	2.27	0.66
1:C:1971:GLU:OE1	1:C:1971:GLU:HA	1.94	0.66
1:A:1971:GLU:HA	1:A:1971:GLU:OE1	1.94	0.66
1:C:1317:LYS:O	1:C:1321:MET:HG2	1.99	0.63
1:A:58:ASP:O	1:A:62:ARG:HG2	1.99	0.62
1:A:1317:LYS:O	1:A:1321:MET:HG2	1.99	0.62
1:A:2506:ARG:HG3	1:A:2506:ARG:NH1	2.04	0.62
1:C:58:ASP:O	1:C:62:ARG:HG2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:O	1:A:469:ARG:NH2	2.28	0.61
1:C:427:LEU:O	1:C:469:ARG:NH2	2.28	0.61
1:C:2745:THR:HG22	1:C:2750:LEU:HD12	1.83	0.60
1:A:466:GLN:OE1	1:A:484:TRP:NE1	2.33	0.60
1:A:2101:GLN:HA	1:A:2104:TRP:CD1	2.37	0.60
1:C:466:GLN:OE1	1:C:484:TRP:NE1	2.33	0.60
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.83	0.59
1:C:1771:ARG:NH1	1:C:1773:LYS:O	2.36	0.59
1:C:2506:ARG:HG3	1:C:2506:ARG:NH1	2.04	0.59
1:A:1771:ARG:NH1	1:A:1773:LYS:O	2.36	0.58
1:C:2101:GLN:HA	1:C:2104:TRP:CD1	2.37	0.58
1:A:1450:LEU:HD11	1:A:1501:VAL:HG22	1.86	0.58
1:C:1450:LEU:HD11	1:C:1501:VAL:HG22	1.86	0.58
1:C:329:ARG:NH2	1:C:407:PHE:O	2.36	0.57
1:C:804:LEU:HD21	1:C:911:ALA:HA	1.85	0.57
1:A:804:LEU:HD21	1:A:911:ALA:HA	1.85	0.57
1:C:2723:ARG:NH1	1:C:2955:ASP:OD2	2.38	0.57
1:A:1963:ASP:O	1:A:1967:MET:HG2	2.05	0.56
1:A:2723:ARG:NH1	1:A:2955:ASP:OD2	2.38	0.56
1:A:44:ASP:OD2	1:A:56:ASN:N	2.38	0.56
1:A:329:ARG:NH2	1:A:407:PHE:O	2.36	0.56
1:A:1827:LEU:HD22	1:A:1837:PHE:HZ	1.70	0.56
1:C:2727:VAL:O	1:C:2731:VAL:HG23	2.06	0.56
1:C:44:ASP:OD2	1:C:56:ASN:N	2.38	0.56
1:A:543:THR:HB	1:A:611:ILE:HD11	1.87	0.56
1:C:1963:ASP:O	1:C:1967:MET:HG2	2.05	0.56
1:A:486:LYS:O	1:A:490:ILE:HD12	2.06	0.56
1:C:1827:LEU:HD22	1:C:1837:PHE:HZ	1.70	0.56
1:C:1309:ALA:O	1:C:1313:GLU:OE1	2.24	0.55
1:C:486:LYS:O	1:C:490:ILE:HD12	2.06	0.55
1:A:1309:ALA:O	1:A:1313:GLU:OE1	2.24	0.55
1:A:2727:VAL:O	1:A:2731:VAL:HG23	2.06	0.55
1:C:1176:LEU:O	1:C:1180:VAL:HG23	2.06	0.55
1:A:1176:LEU:O	1:A:1180:VAL:HG23	2.06	0.54
1:C:1656:LYS:NZ	1:C:2161:ARG:O	2.38	0.54
1:A:1040:MET:HG3	1:A:1085:VAL:HG22	1.89	0.54
1:A:1806:ILE:HG21	1:A:1835:THR:HG23	1.89	0.54
1:C:543:THR:HB	1:C:611:ILE:HD11	1.87	0.54
1:A:1656:LYS:NZ	1:A:2161:ARG:O	2.38	0.54
1:C:2615:GLN:OE1	1:C:2618:ARG:NH1	2.40	0.54
1:C:1040:MET:HG3	1:C:1085:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2151:ARG:NH2	1:C:2183:GLU:OE1	2.38	0.54
1:C:2397:GLN:OE1	1:C:2400:ARG:NH1	2.41	0.54
1:A:2615:GLN:OE1	1:A:2618:ARG:NH1	2.40	0.54
1:C:2731:VAL:HG22	1:C:2952:LEU:HD21	1.90	0.53
1:C:2421:LYS:HA	1:C:2441:VAL:HG11	1.89	0.53
1:A:406:ASP:OD1	1:A:451:ARG:NH1	2.42	0.53
1:A:1688:ILE:HD13	1:A:2163:LEU:HD13	1.91	0.53
1:A:2421:LYS:HA	1:A:2441:VAL:HG11	1.89	0.53
1:C:1806:ILE:HG21	1:C:1835:THR:HG23	1.89	0.53
1:A:2731:VAL:HG22	1:A:2952:LEU:HD21	1.90	0.53
1:A:2105:ARG:NH2	1:A:2221:GLU:OE1	2.42	0.52
1:C:1688:ILE:HD13	1:C:2163:LEU:HD13	1.91	0.52
1:C:406:ASP:OD1	1:C:451:ARG:NH1	2.42	0.52
1:C:773:ILE:HG21	1:C:892:LYS:HB3	1.90	0.52
1:C:2105:ARG:NH2	1:C:2221:GLU:OE1	2.42	0.52
1:A:101:VAL:O	1:A:105:ILE:HG12	2.10	0.52
1:A:970:LEU:HD21	1:A:997:VAL:HG11	1.92	0.52
1:C:101:VAL:O	1:C:105:ILE:HG12	2.10	0.52
1:A:773:ILE:HG21	1:A:892:LYS:HB3	1.90	0.52
1:A:2397:GLN:OE1	1:A:2400:ARG:NH1	2.41	0.52
1:A:716:VAL:HG21	1:A:779:MET:HG3	1.92	0.51
1:C:1275:ILE:HG21	1:C:1282:LEU:HD11	1.92	0.51
1:C:2326:ASN:OD1	1:C:2327:ASN:N	2.42	0.51
1:C:970:LEU:HD21	1:C:997:VAL:HG11	1.92	0.51
1:C:991:LEU:HA	1:C:994:VAL:HG12	1.93	0.51
1:C:1476:ILE:O	1:C:1479:ARG:NH1	2.45	0.50
1:C:2699:PRO:HB2	1:C:2715:LEU:HD11	1.93	0.50
1:A:1753:TYR:OH	1:A:1758:ASP:OD1	2.30	0.50
1:C:1311:GLN:HA	1:C:1314:THR:HG22	1.94	0.50
1:A:38:GLU:O	1:A:42:HIS:ND1	2.45	0.50
1:A:1264:HIS:HB3	1:A:1267:GLU:OE1	2.12	0.50
1:A:1476:ILE:O	1:A:1479:ARG:NH1	2.45	0.50
1:C:716:VAL:HG21	1:C:779:MET:HG3	1.92	0.50
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.45	0.50
1:A:1275:ILE:HG21	1:A:1282:LEU:HD11	1.92	0.50
1:C:1318:VAL:HA	1:C:1321:MET:HE2	1.94	0.50
1:A:2705:VAL:HG22	1:A:2711:GLU:HG2	1.94	0.50
1:A:991:LEU:HA	1:A:994:VAL:HG12	1.93	0.49
1:C:609:GLU:HG3	1:C:721:LEU:HD12	1.94	0.49
1:C:1687:ALA:HB1	1:C:2843:ALA:HB1	1.94	0.49
1:C:1875:ARG:O	1:C:1876:HIS:ND1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1990:SER:OG	1:C:2002:GLN:HG3	2.13	0.49
1:A:259:LEU:HD11	1:A:286:GLN:HG3	1.94	0.49
1:C:2705:VAL:HG22	1:C:2711:GLU:HG2	1.94	0.49
1:C:2722:LEU:HD12	1:C:2765:GLY:HA3	1.95	0.49
1:A:1311:GLN:HA	1:A:1314:THR:HG22	1.94	0.49
1:C:1264:HIS:HB3	1:C:1267:GLU:OE1	2.12	0.49
1:A:1020:THR:HG21	2:B:746:TYR:HB2	1.95	0.49
1:A:2699:PRO:HB2	1:A:2715:LEU:HD11	1.93	0.49
1:A:2722:LEU:HD12	1:A:2765:GLY:HA3	1.95	0.49
1:C:259:LEU:HD11	1:C:286:GLN:HG3	1.94	0.49
1:C:1753:TYR:OH	1:C:1758:ASP:OD1	2.30	0.49
1:C:1993:SER:O	1:C:1997:THR:OG1	2.28	0.49
1:C:38:GLU:O	1:C:42:HIS:ND1	2.45	0.49
1:C:1453:ILE:HD11	1:C:1461:TRP:CD2	2.48	0.49
1:A:1687:ALA:HB1	1:A:2843:ALA:HB1	1.94	0.48
1:A:1718:LEU:HA	1:A:1721:THR:HG22	1.95	0.48
1:A:2326:ASN:OD1	1:A:2327:ASN:N	2.42	0.48
1:C:1145:ASP:OD1	1:C:1145:ASP:N	2.46	0.48
1:A:925:ARG:O	1:A:929:MET:HG2	2.13	0.48
1:A:2260:ILE:HG12	1:A:2263:ARG:HH21	1.78	0.48
1:A:1453:ILE:HD11	1:A:1461:TRP:CD2	2.48	0.48
1:A:2151:ARG:NH2	1:A:2183:GLU:OE1	2.38	0.48
1:A:2546:SER:O	1:A:2550:MET:HG2	2.13	0.48
1:C:925:ARG:O	1:C:929:MET:HG2	2.13	0.48
1:A:609:GLU:HG3	1:A:721:LEU:HD12	1.94	0.48
1:A:1601:SER:HB2	1:A:1610:ARG:HH21	1.78	0.48
1:C:1601:SER:HB2	1:C:1610:ARG:HH21	1.78	0.48
1:C:2260:ILE:HG12	1:C:2263:ARG:HH21	1.78	0.48
1:A:1638:ASN:ND2	1:A:1641:ASP:OD2	2.47	0.48
1:A:2345:LEU:HD13	1:A:2351:GLU:HG3	1.95	0.48
1:A:1990:SER:OG	1:A:2002:GLN:HG3	2.13	0.48
1:A:2279:LYS:NZ	1:A:2295:GLU:OE2	2.45	0.48
1:A:1216:TYR:HD2	1:A:1378:PRO:HG3	1.79	0.48
1:A:2368:ALA:HB1	1:A:2383:LYS:HG2	1.96	0.48
1:C:1020:THR:HG21	2:D:746:TYR:HB2	1.95	0.48
1:C:2156:GLU:O	1:C:2160:LYS:HG3	2.14	0.48
1:C:1216:TYR:HD2	1:C:1378:PRO:HG3	1.79	0.47
1:C:1604:ASP:OD1	1:C:1605:ALA:N	2.47	0.47
1:C:1270:SER:O	1:C:1273:ASN:N	2.47	0.47
1:C:1686:ILE:HG12	1:C:2167:TYR:HE2	1.79	0.47
1:A:1270:SER:O	1:A:1273:ASN:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2156:GLU:O	1:A:2160:LYS:HG3	2.14	0.47
1:C:1638:ASN:ND2	1:C:1641:ASP:OD2	2.47	0.47
1:C:2368:ALA:HB1	1:C:2383:LYS:HG2	1.96	0.47
1:A:1114:LYS:HG3	1:A:1115:LEU:HD12	1.97	0.47
1:A:1272:ALA:O	1:A:1275:ILE:HG22	2.15	0.47
1:A:1993:SER:O	1:A:1997:THR:OG1	2.28	0.47
1:C:1114:LYS:HG3	1:C:1115:LEU:HD12	1.97	0.47
1:C:1123:ALA:HB1	1:C:1157:LEU:HD11	1.97	0.47
1:C:2546:SER:O	1:C:2550:MET:HG2	2.13	0.47
1:A:1145:ASP:OD1	1:A:1145:ASP:N	2.46	0.47
1:A:1604:ASP:OD1	1:A:1605:ALA:N	2.47	0.47
1:C:2288:VAL:HG11	1:C:2315:MET:HG2	1.97	0.47
1:C:736:ALA:HB3	1:C:739:GLU:HG3	1.96	0.47
1:C:1270:SER:HA	1:C:1273:ASN:ND2	2.30	0.47
1:C:2345:LEU:HD13	1:C:2351:GLU:HG3	1.95	0.47
1:A:1824:LEU:HD13	1:A:1845:LEU:HD23	1.96	0.47
1:C:1718:LEU:HA	1:C:1721:THR:HG22	1.95	0.47
1:C:2263:ARG:NE	1:C:2294:GLU:OE2	2.46	0.47
1:A:1123:ALA:HB1	1:A:1157:LEU:HD11	1.97	0.47
1:A:2936:GLU:HG3	1:A:3028:VAL:HG11	1.97	0.47
1:A:1686:ILE:HG12	1:A:2167:TYR:HE2	1.79	0.46
1:C:1528:VAL:O	1:C:1535:GLN:NE2	2.47	0.46
1:A:1270:SER:HA	1:A:1273:ASN:ND2	2.30	0.46
1:C:2928:ARG:NH1	1:C:3033:ASN:OD1	2.48	0.46
1:A:736:ALA:HB3	1:A:739:GLU:HG3	1.96	0.46
1:C:2936:GLU:HG3	1:C:3028:VAL:HG11	1.97	0.46
1:A:1460:ALA:HB2	1:A:1766:PRO:HB3	1.96	0.46
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.48	0.46
1:C:1272:ALA:O	1:C:1275:ILE:HG22	2.15	0.46
1:A:2288:VAL:HG11	1:A:2315:MET:HG2	1.97	0.46
1:C:64:LEU:O	1:C:68:ILE:HG12	2.16	0.46
1:C:1460:ALA:HB2	1:C:1766:PRO:HB3	1.96	0.46
1:C:1824:LEU:HD13	1:C:1845:LEU:HD23	1.96	0.46
1:C:2672:ASP:OD2	1:C:2674:THR:OG1	2.33	0.46
1:A:209:PHE:O	1:A:212:PHE:HB2	2.16	0.46
1:A:2506:ARG:HH11	1:A:2506:ARG:CG	2.14	0.46
1:C:3034:LEU:HD12	1:C:3037:GLN:HE21	1.81	0.46
1:C:2719:ARG:HG2	1:C:2763:ARG:NH2	2.31	0.46
1:A:99:SER:HA	1:A:102:LYS:HG2	1.98	0.46
1:C:140:ASP:O	1:C:144:ILE:HG12	2.16	0.46
1:A:64:LEU:O	1:A:68:ILE:HG12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:O	1:A:144:ILE:HG12	2.16	0.45
1:A:2687:LYS:NZ	1:A:2711:GLU:OE2	2.39	0.45
1:A:684:GLN:NE2	1:A:688:GLU:OE2	2.50	0.45
1:A:2672:ASP:OD2	1:A:2674:THR:OG1	2.33	0.45
1:C:209:PHE:O	1:C:212:PHE:HB2	2.16	0.45
1:C:443:LEU:N	1:C:444:PRO:HD3	2.31	0.45
1:C:1027:HIS:HB2	1:C:1063:VAL:HG21	1.98	0.45
1:A:1281:SER:HA	1:A:1284:THR:HG22	1.99	0.45
1:A:1405:LEU:HD21	1:A:1449:LEU:HD23	1.99	0.45
1:C:99:SER:HA	1:C:102:LYS:HG2	1.98	0.45
1:A:613:VAL:O	1:A:617:MET:HG2	2.17	0.45
1:A:1047:LYS:HD3	1:A:1092:SER:HB3	1.99	0.45
1:A:1528:VAL:O	1:A:1535:GLN:NE2	2.47	0.45
1:A:2814:GLU:OE1	1:A:2814:GLU:N	2.50	0.45
1:C:1780:PHE:CE2	1:C:1782:LYS:HG3	2.52	0.45
1:C:2279:LYS:NZ	1:C:2295:GLU:OE2	2.45	0.45
1:A:269:HIS:CG	1:A:270:ARG:H	2.35	0.45
1:A:2656:LEU:HD23	1:A:2659:LEU:HD11	1.99	0.45
1:C:684:GLN:NE2	1:C:688:GLU:OE2	2.50	0.45
1:C:1405:LEU:HD21	1:C:1449:LEU:HD23	1.99	0.45
1:A:259:LEU:HG	1:A:283:PHE:HE1	1.82	0.45
1:A:2719:ARG:HG2	1:A:2763:ARG:NH2	2.31	0.45
1:C:259:LEU:HG	1:C:283:PHE:HE1	1.82	0.45
1:C:2448:ASP:OD1	1:C:2449:GLU:N	2.50	0.45
1:C:2814:GLU:N	1:C:2814:GLU:OE1	2.50	0.45
1:A:1780:PHE:CE2	1:A:1782:LYS:HG3	2.52	0.45
1:A:1434:LYS:O	1:A:1438:ILE:HG12	2.17	0.44
1:A:1873:CYS:SG	1:A:1901:LEU:HD22	2.58	0.44
1:A:3034:LEU:HD12	1:A:3037:GLN:HE21	1.81	0.44
1:C:1626:ASP:N	1:C:1626:ASP:OD1	2.50	0.44
1:A:2448:ASP:OD1	1:A:2449:GLU:N	2.50	0.44
1:C:613:VAL:O	1:C:617:MET:HG2	2.17	0.44
1:A:1027:HIS:HB2	1:A:1063:VAL:HG21	1.98	0.44
1:A:443:LEU:N	1:A:444:PRO:HD3	2.31	0.44
1:C:1265:PHE:HA	1:C:1268:VAL:HG12	1.98	0.44
1:A:2263:ARG:NE	1:A:2294:GLU:OE2	2.46	0.44
1:C:1425:GLN:O	1:C:1428:GLU:HG3	2.18	0.44
1:C:1434:LYS:O	1:C:1438:ILE:HG12	2.17	0.44
1:C:172:PHE:HA	1:C:191:ILE:HD11	2.00	0.44
1:C:269:HIS:CG	1:C:270:ARG:H	2.35	0.44
1:C:1112:PRO:HB2	1:C:1115:LEU:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:ALA:HA	1:A:2638:TRP:CZ3	2.53	0.44
1:C:120:LEU:O	1:C:124:ILE:HG12	2.18	0.44
1:C:2844:ILE:O	1:C:2848:LYS:HG2	2.18	0.44
1:C:2948:ILE:O	1:C:2952:LEU:HD13	2.18	0.43
1:A:172:PHE:HA	1:A:191:ILE:HD11	2.00	0.43
1:A:1187:PRO:O	1:A:1191:LYS:HB2	2.18	0.43
1:A:1265:PHE:HA	1:A:1268:VAL:HG12	1.98	0.43
1:A:1626:ASP:OD1	1:A:1626:ASP:N	2.50	0.43
1:A:2667:MET:HE1	1:A:2681:VAL:HB	2.00	0.43
1:C:1131:MET:HG2	1:C:1150:ARG:HB3	2.00	0.43
1:C:1489:ARG:HG3	1:C:1489:ARG:HH11	1.83	0.43
1:A:1425:GLN:O	1:A:1428:GLU:HG3	2.18	0.43
1:A:2844:ILE:O	1:A:2848:LYS:HG2	2.18	0.43
1:C:104:PHE:CD1	1:C:104:PHE:C	2.92	0.43
1:C:2656:LEU:HD23	1:C:2659:LEU:HD11	1.99	0.43
1:A:226:SER:HB2	1:A:229:LEU:HD12	2.01	0.43
1:C:1047:LYS:HD3	1:C:1092:SER:HB3	1.99	0.43
1:C:2778:GLU:O	1:C:2782:ASN:HB2	2.18	0.43
1:A:1489:ARG:HG3	1:A:1489:ARG:HH11	1.83	0.43
1:C:1251:CYS:O	1:C:1255:LEU:HD23	2.18	0.43
1:A:104:PHE:CD1	1:A:104:PHE:C	2.92	0.43
1:A:121:LEU:HD12	1:A:167:LEU:HD11	2.01	0.43
1:C:1281:SER:HA	1:C:1284:THR:HG22	1.99	0.43
1:C:1503:GLN:HG2	1:C:1544:TYR:CE2	2.54	0.43
1:C:1869:PHE:CE1	1:C:1909:MET:HG3	2.53	0.43
1:C:1873:CYS:SG	1:C:1901:LEU:HD22	2.58	0.43
1:C:2506:ARG:HH11	1:C:2506:ARG:CG	2.14	0.43
1:C:2635:ALA:HA	1:C:2638:TRP:CZ3	2.53	0.43
1:A:1251:CYS:O	1:A:1255:LEU:HD23	2.18	0.43
1:A:2948:ILE:O	1:A:2952:LEU:HD13	2.18	0.43
1:C:226:SER:HB2	1:C:229:LEU:HD12	2.01	0.43
1:C:1187:PRO:O	1:C:1191:LYS:HB2	2.18	0.43
1:C:2092:CYS:SG	1:C:2095:LEU:HD13	2.59	0.43
1:A:120:LEU:O	1:A:124:ILE:HG12	2.18	0.43
1:A:125:MET:HA	1:A:128:VAL:HG12	2.01	0.43
1:A:2778:GLU:O	1:A:2782:ASN:HB2	2.18	0.43
1:C:904:LEU:HD23	1:C:904:LEU:HA	1.91	0.43
1:A:1131:MET:HG2	1:A:1150:ARG:HB3	2.00	0.43
1:A:1503:GLN:HG2	1:A:1544:TYR:CE2	2.54	0.43
1:A:2092:CYS:SG	1:A:2095:LEU:HD13	2.59	0.42
1:A:2936:GLU:HG2	1:A:3028:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:HH21	1:A:597:PRO:HB3	1.84	0.42
1:C:121:LEU:HD12	1:C:167:LEU:HD11	2.01	0.42
1:A:205:LEU:HB2	1:A:239:PHE:CE1	2.55	0.42
1:A:545:ALA:O	1:A:549:SER:HB2	2.19	0.42
1:C:2024:GLY:O	1:C:2025:LYS:HG3	2.19	0.42
1:A:1443:HIS:HB2	1:A:1493:LEU:HD21	2.02	0.42
1:A:1838:CYS:HA	1:A:1841:VAL:HG12	2.01	0.42
1:A:1869:PHE:CE1	1:A:1909:MET:HG3	2.53	0.42
1:C:205:LEU:HB2	1:C:239:PHE:CE1	2.55	0.42
1:C:2550:MET:SD	1:C:2612:ARG:HD2	2.59	0.42
1:A:1112:PRO:HB2	1:A:1115:LEU:HD13	2.00	0.42
1:A:1186:GLU:HB3	1:A:1188:HIS:CE1	2.54	0.42
1:C:533:ARG:HH21	1:C:597:PRO:HB3	1.84	0.42
1:C:1186:GLU:HB3	1:C:1188:HIS:CE1	2.54	0.42
1:C:2561:LEU:HD23	1:C:2561:LEU:HA	1.93	0.42
1:C:1124:TYR:O	1:C:1128:GLN:HG2	2.20	0.42
1:C:1222:LEU:HB3	1:C:1262:ARG:HH21	1.84	0.42
1:C:1322:LEU:HA	1:C:1327:LEU:HD12	2.02	0.42
1:A:2550:MET:SD	1:A:2612:ARG:HD2	2.59	0.42
1:C:110:ARG:NH2	1:C:111:ARG:HE	2.18	0.42
1:C:545:ALA:O	1:C:549:SER:HB2	2.19	0.42
1:A:2692:LEU:HA	1:A:2692:LEU:HD23	1.88	0.42
1:C:488:TRP:HA	1:C:491:THR:HG22	2.02	0.42
1:C:2936:GLU:HG2	1:C:3028:VAL:HG21	2.01	0.42
1:C:133:ASN:HB3	1:C:137:TYR:HD2	1.85	0.42
1:C:1702:LEU:HD23	1:C:1702:LEU:HA	1.94	0.42
1:C:3034:LEU:O	1:C:3037:GLN:HG3	2.20	0.42
1:A:621:LYS:O	1:A:625:ASN:ND2	2.49	0.42
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.89	0.42
1:C:125:MET:HA	1:C:128:VAL:HG12	2.01	0.42
1:A:477:LYS:O	1:A:481:LEU:HD23	2.20	0.41
1:A:1124:TYR:O	1:A:1128:GLN:HG2	2.20	0.41
1:A:2024:GLY:O	1:A:2025:LYS:HG3	2.19	0.41
1:C:1567:ASP:O	1:C:1568:HIS:ND1	2.53	0.41
1:A:106:LYS:O	1:A:110:ARG:HB2	2.20	0.41
1:A:163:GLN:HA	1:A:166:GLU:HG2	2.02	0.41
1:A:1567:ASP:O	1:A:1568:HIS:ND1	2.53	0.41
1:A:2440:LYS:O	1:A:2444:GLU:HG2	2.21	0.41
1:A:1318:VAL:HA	1:A:1321:MET:HE2	2.01	0.41
1:A:1322:LEU:HA	1:A:1327:LEU:HD12	2.02	0.41
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:O	1:A:487:ILE:HG23	2.21	0.41
1:A:488:TRP:HA	1:A:491:THR:HG22	2.02	0.41
1:A:1618:ARG:HD2	1:A:1673:SER:HB3	2.01	0.41
1:A:2027:LEU:HD21	1:C:2279:LYS:HZ3	1.85	0.41
1:C:1710:TRP:O	1:C:1714:MET:HG2	2.20	0.41
1:A:133:ASN:HB3	1:A:137:TYR:HD2	1.85	0.41
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.91	0.41
1:A:2561:LEU:HD23	1:A:2561:LEU:HA	1.93	0.41
1:C:163:GLN:HA	1:C:166:GLU:HG2	2.02	0.41
1:C:1443:HIS:HB2	1:C:1493:LEU:HD21	2.02	0.41
1:A:110:ARG:NH2	1:A:111:ARG:HE	2.18	0.41
1:A:1710:TRP:O	1:A:1714:MET:HG2	2.20	0.41
1:A:3034:LEU:O	1:A:3037:GLN:HG3	2.20	0.41
1:C:211:ASP:OD1	1:C:212:PHE:N	2.54	0.41
1:C:954:LEU:HD23	1:C:954:LEU:HA	1.90	0.41
1:A:1071:ASN:OD1	1:A:1072:GLU:N	2.54	0.41
1:C:12:CYS:HA	1:C:30:PHE:HZ	1.85	0.41
1:C:477:LYS:O	1:C:481:LEU:HD23	2.20	0.41
1:A:102:LYS:HE3	1:A:144:ILE:HD11	2.03	0.41
1:C:271:LEU:HB3	1:C:276:LYS:HZ1	1.86	0.41
1:C:1071:ASN:OD1	1:C:1072:GLU:N	2.54	0.41
1:C:1618:ARG:HD2	1:C:1673:SER:HB3	2.01	0.41
1:A:12:CYS:HA	1:A:30:PHE:HZ	1.85	0.41
1:A:1222:LEU:HB3	1:A:1262:ARG:HH21	1.84	0.41
1:A:3043:LYS:HG3	1:A:3044:ASN:N	2.36	0.41
1:C:1838:CYS:HA	1:C:1841:VAL:HG12	2.01	0.41
1:C:2440:LYS:O	1:C:2444:GLU:HG2	2.21	0.41
1:A:2865:ILE:HD13	1:A:2865:ILE:HA	1.94	0.40
1:C:1876:HIS:O	1:C:1899:CYS:N	2.54	0.40
1:C:2401:ILE:HG21	1:C:2459:ARG:HB2	2.03	0.40
1:A:211:ASP:OD1	1:A:212:PHE:N	2.54	0.40
1:A:1599:SER:O	1:A:1602:VAL:HG22	2.21	0.40
1:C:1599:SER:O	1:C:1602:VAL:HG22	2.21	0.40
1:A:1131:MET:HE2	1:A:1131:MET:HB3	1.99	0.40
1:C:94:MET:O	1:C:97:ILE:HG22	2.21	0.40
1:A:69:GLN:HA	1:A:72:THR:HG22	2.04	0.40
1:C:3043:LYS:HG3	1:C:3044:ASN:N	2.36	0.40
1:A:1876:HIS:O	1:A:1899:CYS:N	2.54	0.40
1:A:3048:LEU:HD13	1:A:3052:TRP:CZ3	2.56	0.40
1:C:102:LYS:HE3	1:C:144:ILE:HD11	2.03	0.40
1:C:106:LYS:O	1:C:110:ARG:HB2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:THR:O	1:C:812:MET:HG2	2.22	0.40
1:C:1608:LEU:HD21	1:C:1662:THR:O	2.22	0.40
1:C:1678:VAL:O	1:C:1678:VAL:HG13	2.21	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	2735/3056 (90%)	2688 (98%)	47 (2%)	0	100	100
1	C	2735/3056 (90%)	2688 (98%)	47 (2%)	0	100	100
2	B	8/28 (29%)	8 (100%)	0	0	100	100
2	D	8/28 (29%)	8 (100%)	0	0	100	100
All	All	5486/6168 (89%)	5392 (98%)	94 (2%)	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	2469/2780 (89%)	2446 (99%)	23 (1%)	78	91
1	C	2469/2780 (89%)	2446 (99%)	23 (1%)	78	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	8/26 (31%)	8 (100%)	0	100 100
2	D	8/26 (31%)	8 (100%)	0	100 100
All	All	4954/5612 (88%)	4908 (99%)	46 (1%)	79 91

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	104	PHE
1	A	106	LYS
1	A	110	ARG
1	A	200	SER
1	A	433	SER
1	A	521	ARG
1	A	1145	ASP
1	A	1262	ARG
1	A	1275	ILE
1	A	1312	ARG
1	A	1313	GLU
1	A	1347	LEU
1	A	1386	ILE
1	A	1478	GLN
1	A	1650	ASN
1	A	1971	GLU
1	A	2025	LYS
1	A	2506	ARG
1	A	2734	MET
1	A	2784	GLU
1	A	3043	LYS
1	A	3048	LEU
1	C	64	LEU
1	C	104	PHE
1	C	106	LYS
1	C	110	ARG
1	C	200	SER
1	C	433	SER
1	C	521	ARG
1	C	1145	ASP
1	C	1262	ARG
1	C	1275	ILE
1	C	1312	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1313	GLU
1	C	1347	LEU
1	C	1386	ILE
1	C	1478	GLN
1	C	1650	ASN
1	C	1971	GLU
1	C	2025	LYS
1	C	2506	ARG
1	C	2734	MET
1	C	2784	GLU
1	C	3043	LYS
1	C	3048	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1640	GLN
1	C	65	GLN
1	C	1128	GLN
1	C	1640	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	C	3101	-	29,33,33	1.10	4 (13%)	31,52,52	1.07	2 (6%)
3	ANP	A	3101	-	29,33,33	1.10	4 (13%)	31,52,52	1.07	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	3101	-	-	4/14/38/38	0/3/3/3
3	ANP	A	3101	-	-	4/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3101	ANP	PG-N3B	2.44	1.69	1.63
3	C	3101	ANP	PG-N3B	2.44	1.69	1.63
3	A	3101	ANP	PG-O1G	2.44	1.50	1.46
3	C	3101	ANP	PG-O1G	2.44	1.50	1.46
3	A	3101	ANP	PB-O3A	-2.37	1.56	1.59
3	C	3101	ANP	PB-O3A	-2.37	1.56	1.59
3	A	3101	ANP	PB-O1B	2.35	1.49	1.46
3	C	3101	ANP	PB-O1B	2.35	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3101	ANP	PB-O3A-PA	-3.74	119.44	132.62
3	C	3101	ANP	PB-O3A-PA	-3.74	119.44	132.62
3	A	3101	ANP	C5-C6-N6	2.14	123.61	120.35
3	C	3101	ANP	C5-C6-N6	2.14	123.61	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

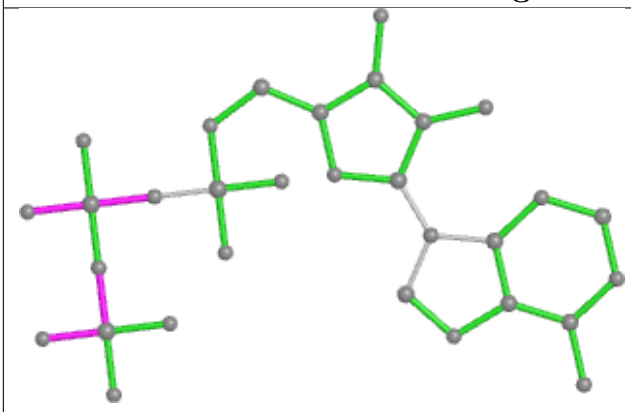
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PG-N3B-PB-O1B
3	C	3101	ANP	PG-N3B-PB-O1B
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	C	3101	ANP	O4'-C4'-C5'-O5'
3	C	3101	ANP	C3'-C4'-C5'-O5'
3	A	3101	ANP	PG-N3B-PB-O3A
3	C	3101	ANP	PG-N3B-PB-O3A

There are no ring outliers.

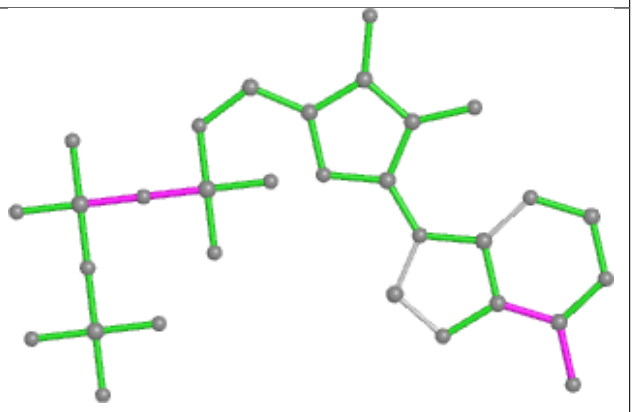
No monomer is involved in short contacts.

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

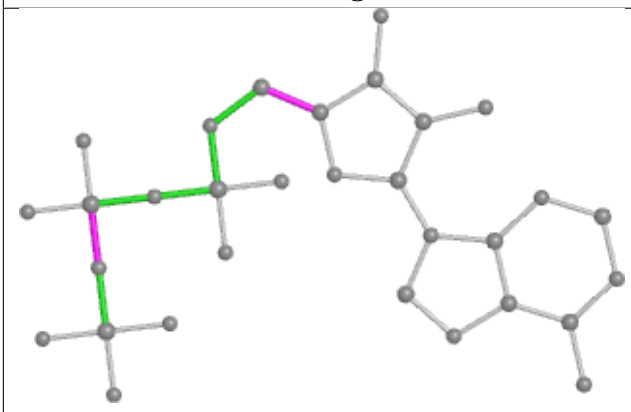
Ligand ANP C 3101



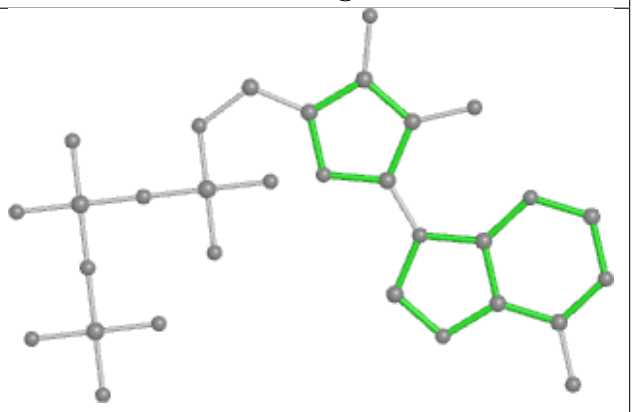
Bond lengths



Bond angles

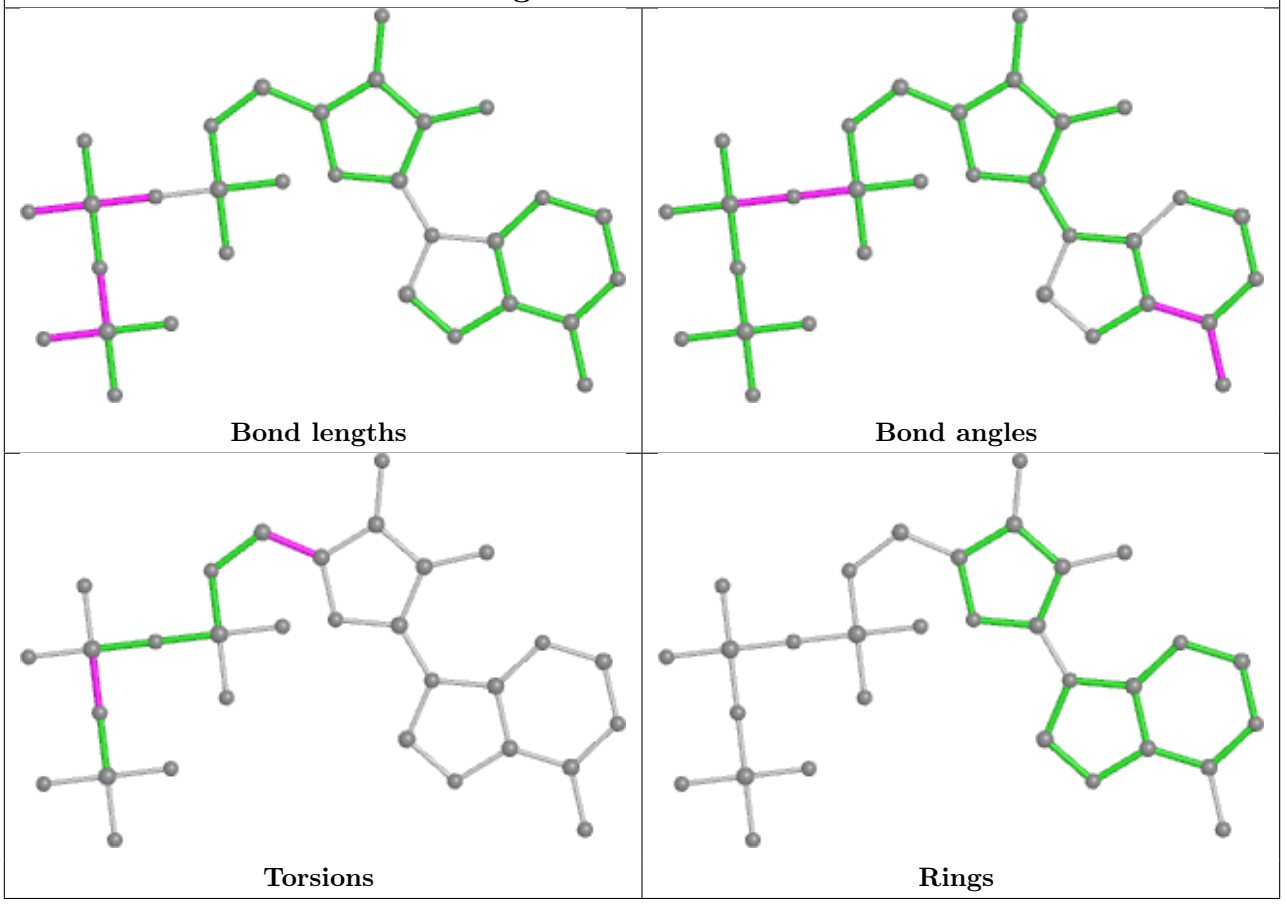


Torsions



Rings

Ligand ANP A 3101



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.

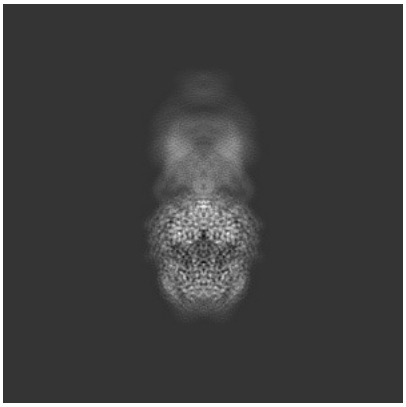
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25141. These allow visual inspection of the internal detail of the map and identification of artifacts.

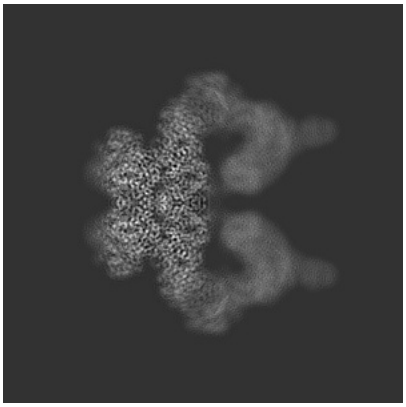
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

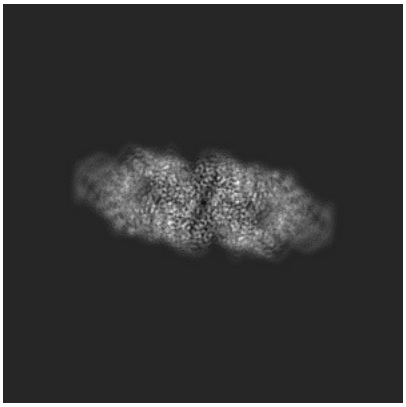
6.1.1 Primary map



X



Y

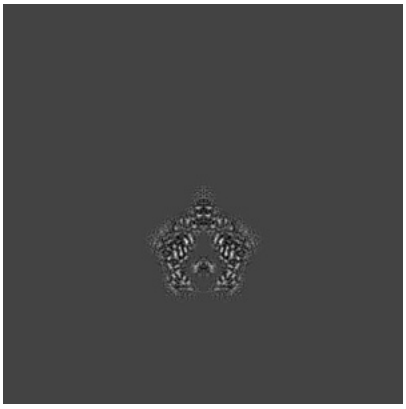


Z

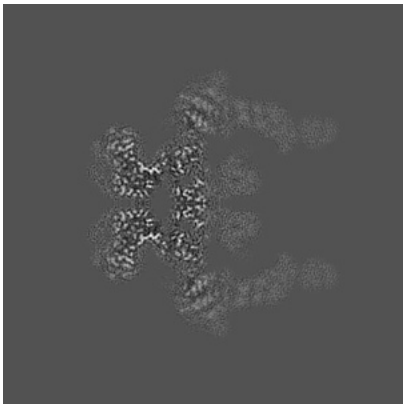
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 150



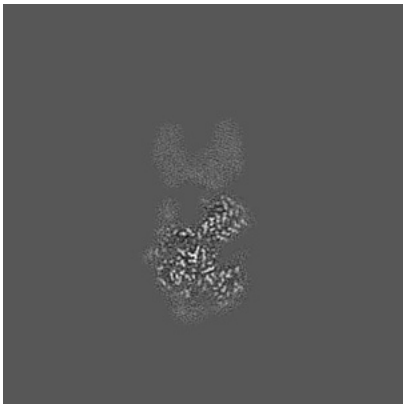
Y Index: 150

Z Index: 150

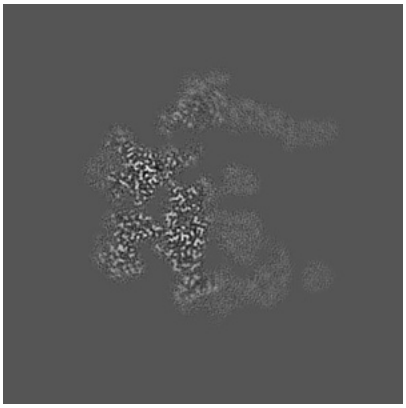
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

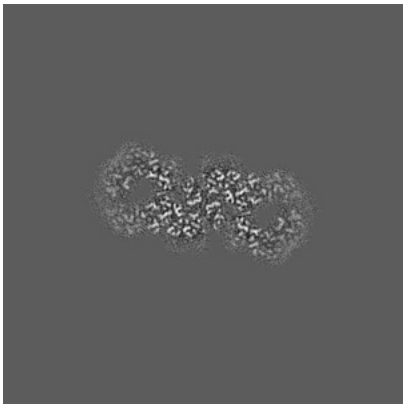
6.3.1 Primary map



X Index: 175



Y Index: 144



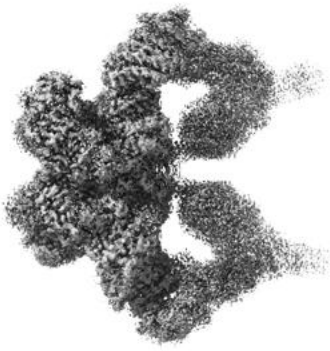
Z Index: 131

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

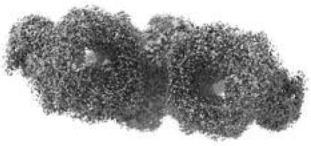
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

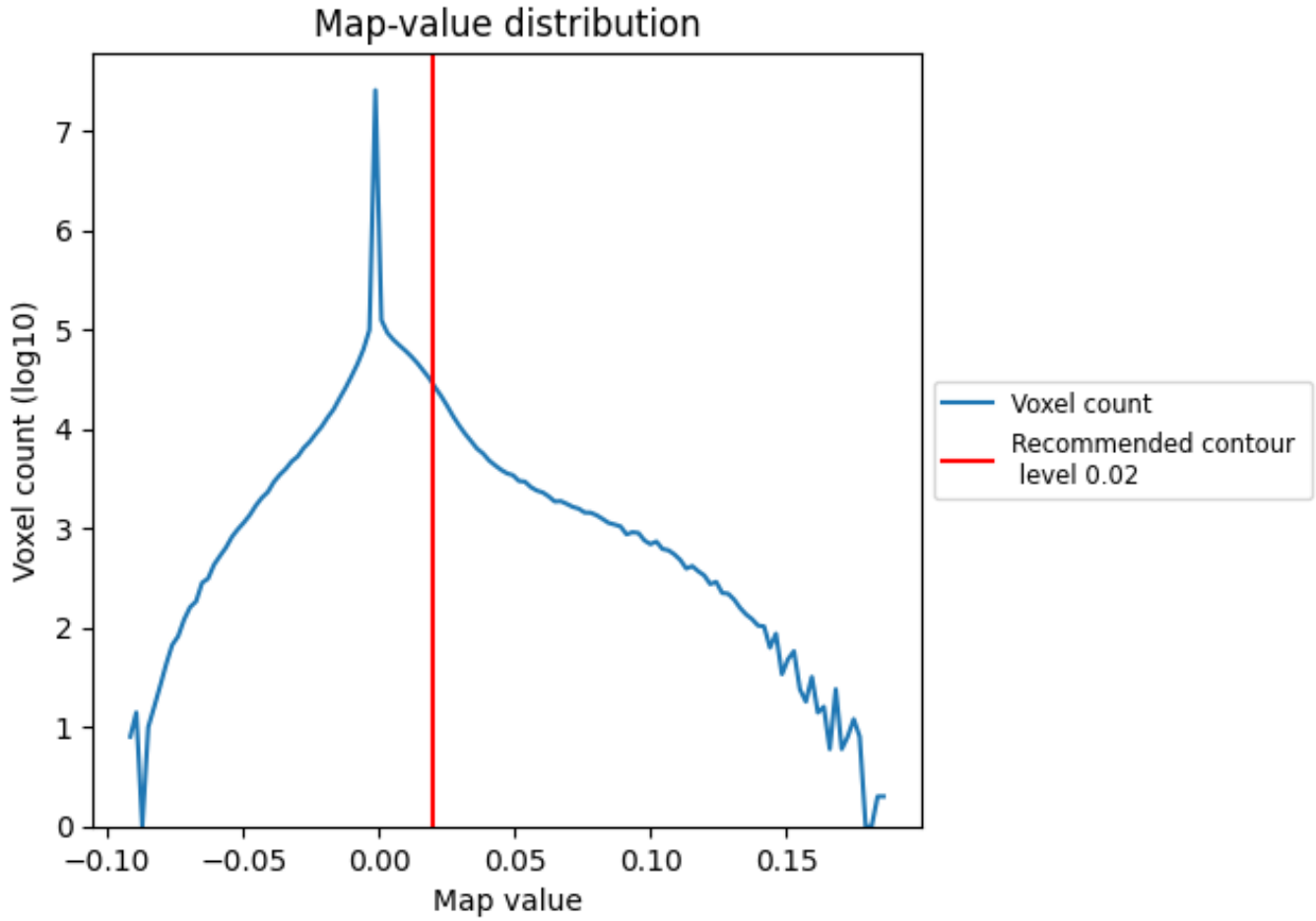
6.5 Mask visualisation (i)

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

7 Map analysis

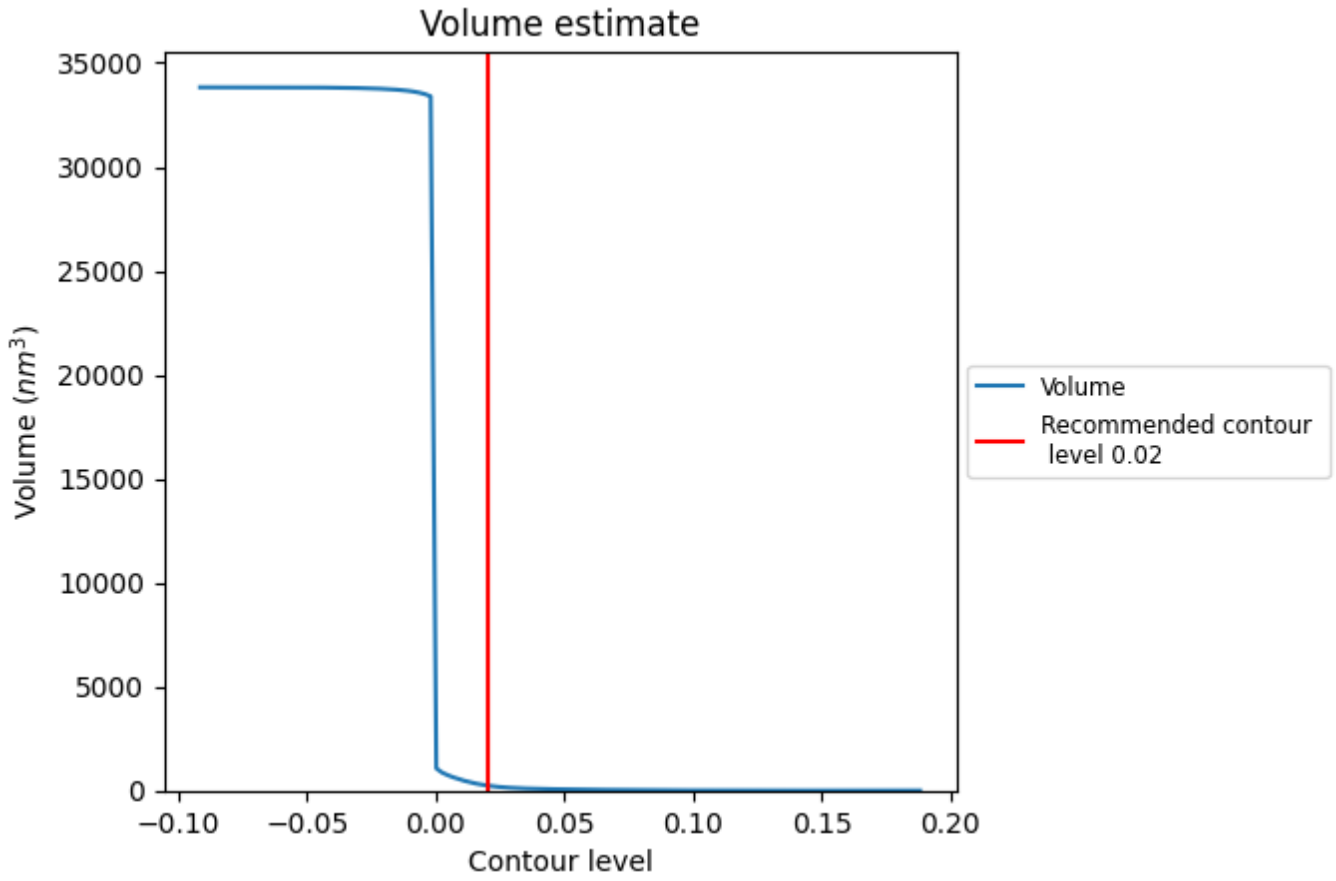
This section contains the results of statistical analysis of the map.

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.

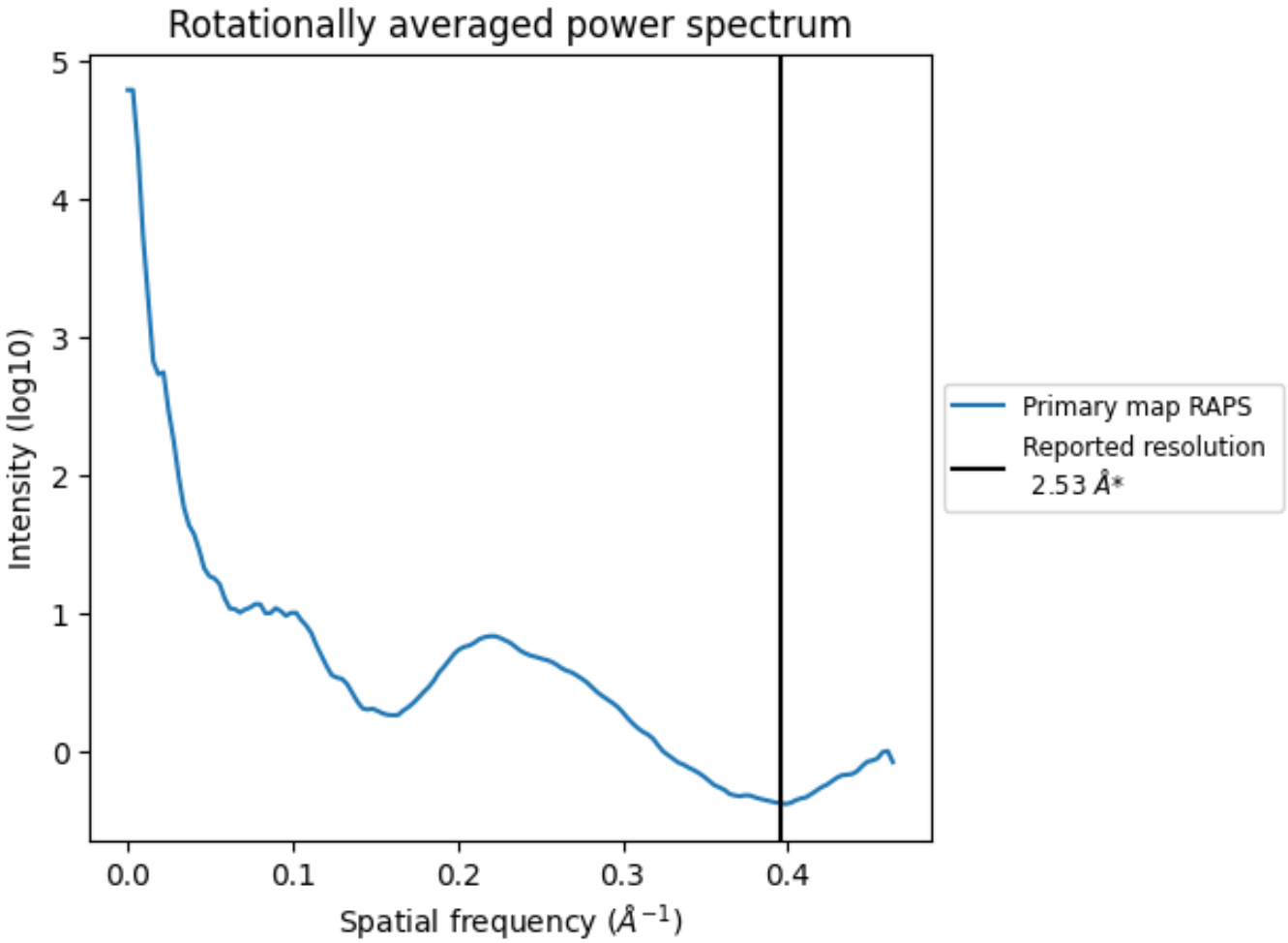
7.2 Volume estimate



The volume at the recommended contour level is 242 nm^3; this corresponds to an approximate mass of 218 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)

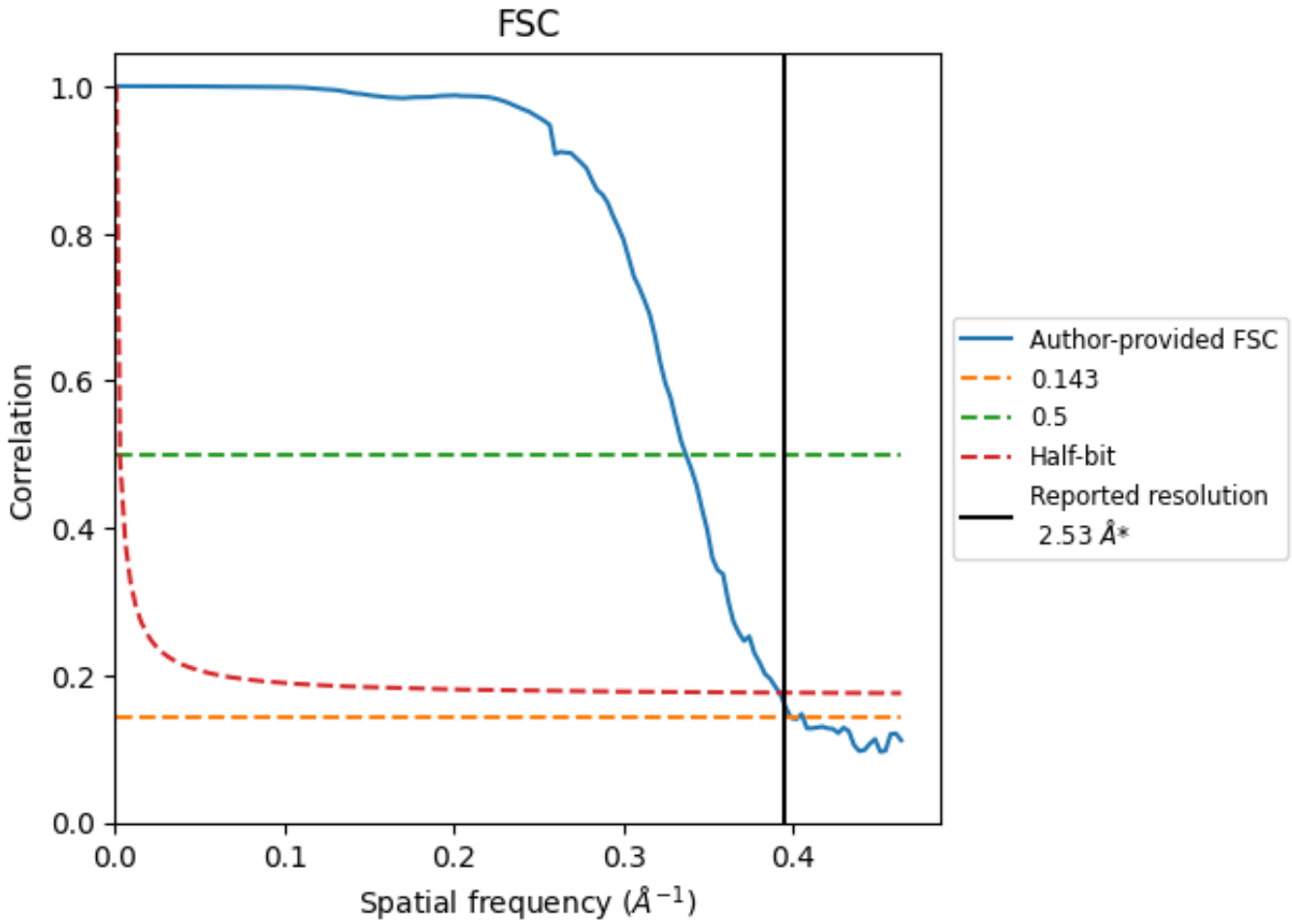


*Reported resolution corresponds to spatial frequency of 0.395 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

8.2 Resolution estimates (i)

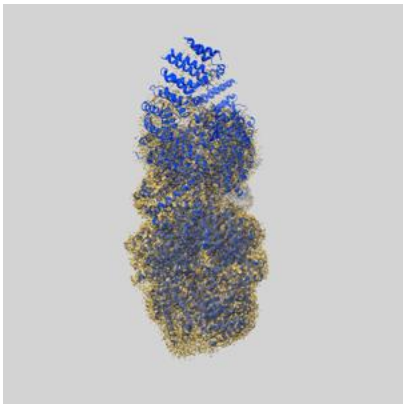
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.51	2.97	2.55
Unmasked-calculated*	-	-	-

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

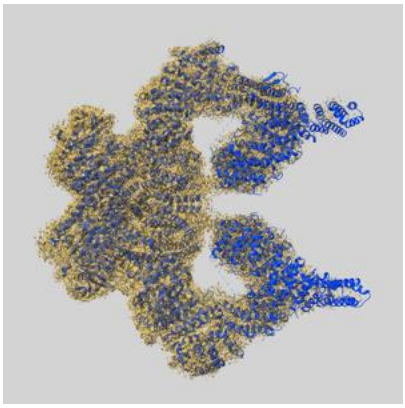
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25141 and PDB model 7SID. Per-residue inclusion information can be found in section 3 on page 5.

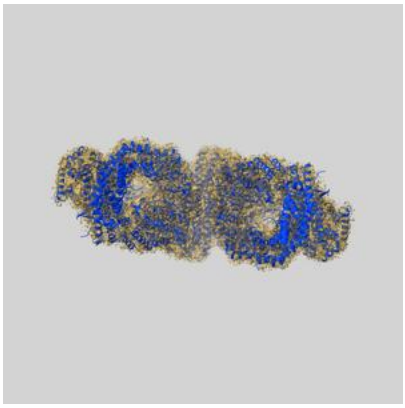
9.1 Map-model overlay



X



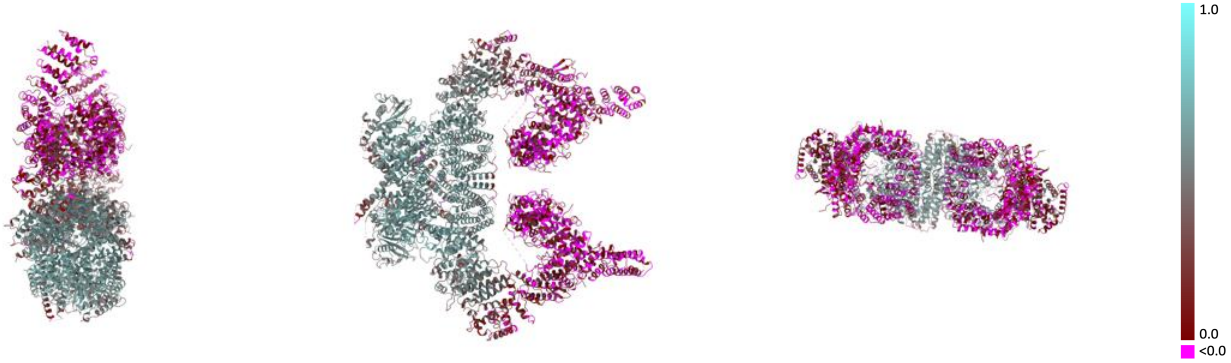
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

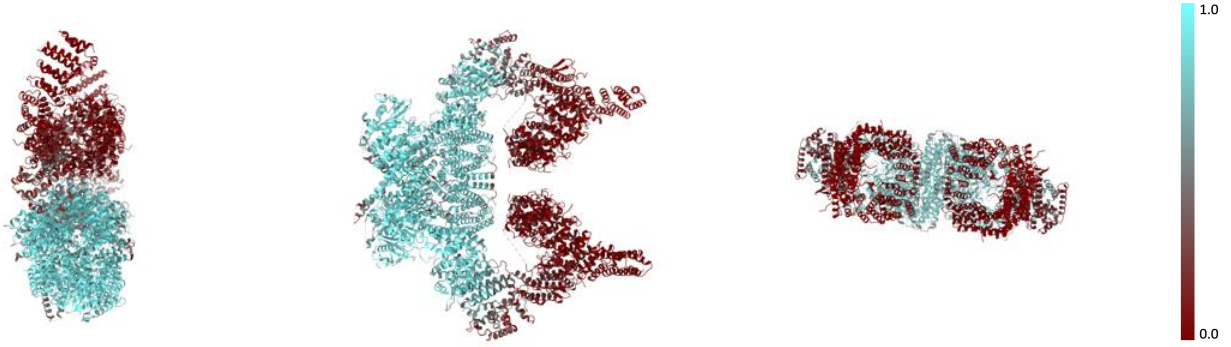
9.2 Q-score mapped to coordinate model



X Y Z

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

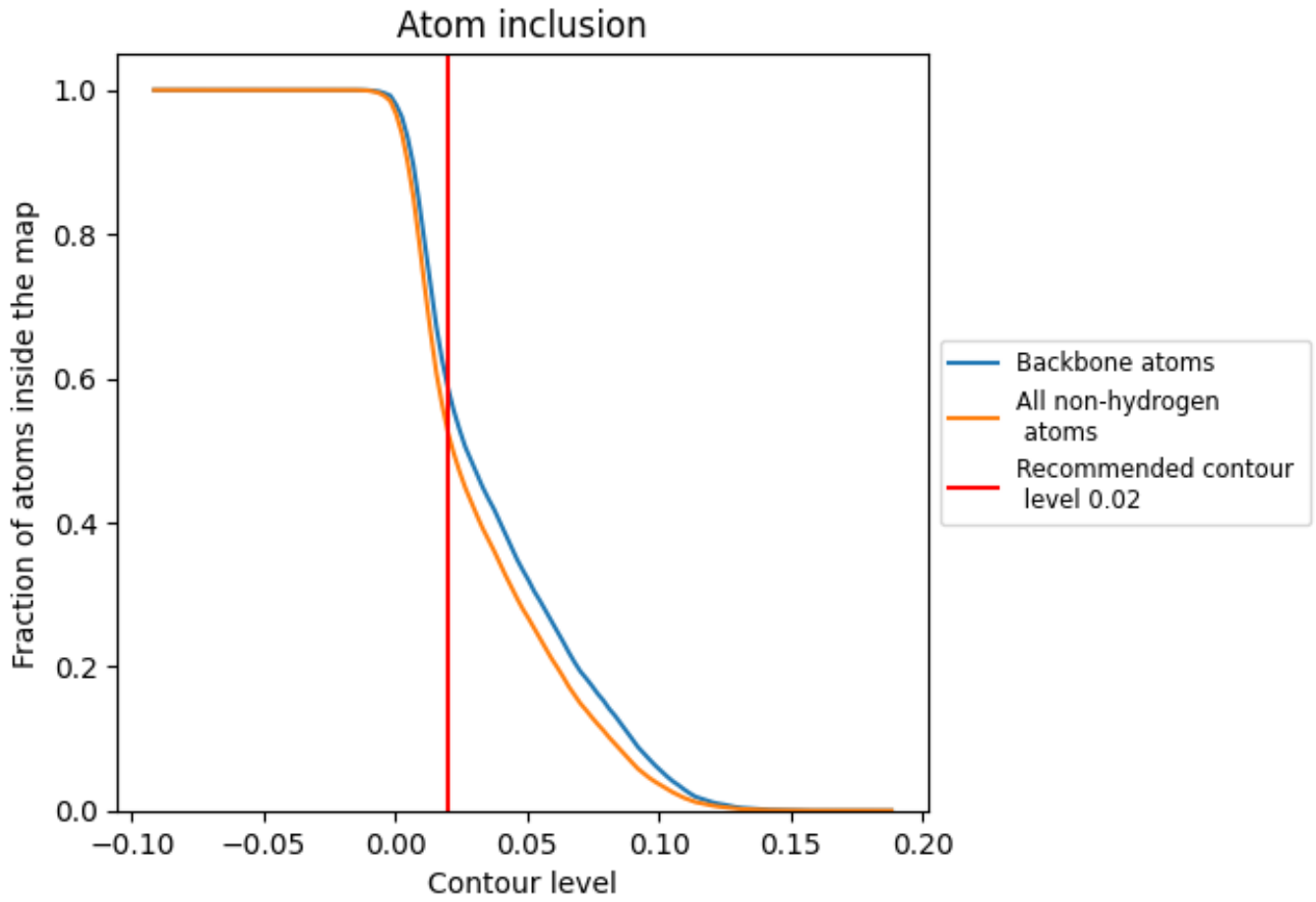
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 52% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5243	0.3360
A	0.5261	0.3370
B	0.0250	0.0430
C	0.5261	0.3380
D	0.0250	0.0470