wwPDB EM Validation Summary Report

Nov 20, 2022 – 04:39 pm GMT

PDB ID	:	5LKI
EMDB ID	:	EMD-4068
Title	:	Cryo-EM structure of the Tc toxin TcdA1 in its pore state
Authors	:	Gatsogiannis, C.; Merino, F.; Prumbaum, D.; Roderer, D.; Leidreiter, F.; Meusch, D.; Raunser, S.
Deposited on	:	2016-07-22
Resolution	:	3.46 Å(reported)

This is a wwPDB EM Validation Summary 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:

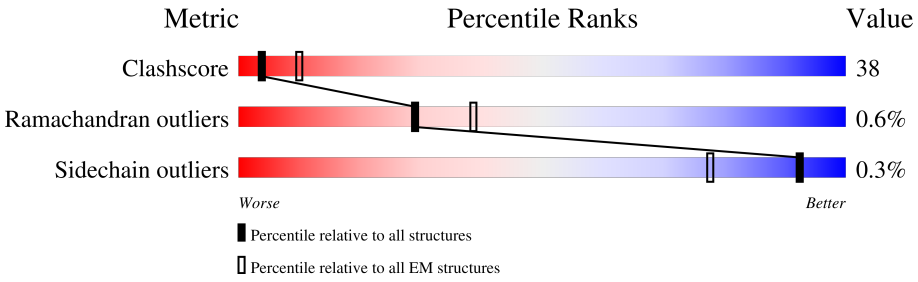
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.46 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	2516	10% 30% 27% · 43%
1	B	2516	10% 30% 27% · 43%
1	C	2516	10% 30% 27% · 43%
1	D	2516	10% 30% 26% · 43%
1	E	2516	10% 29% 27% · 43%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 55415 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.

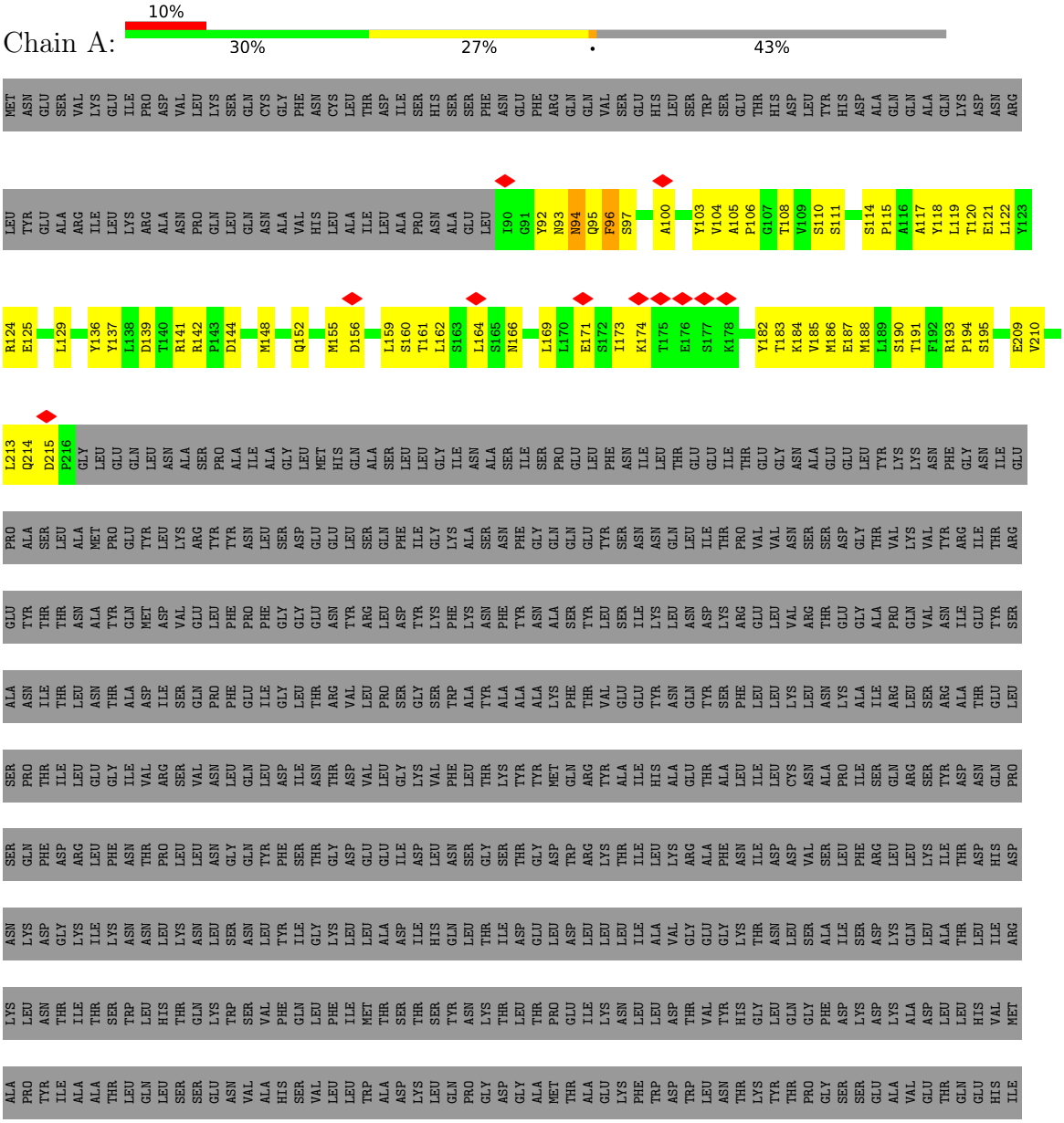
- Molecule 1 is a protein called TcdA1.

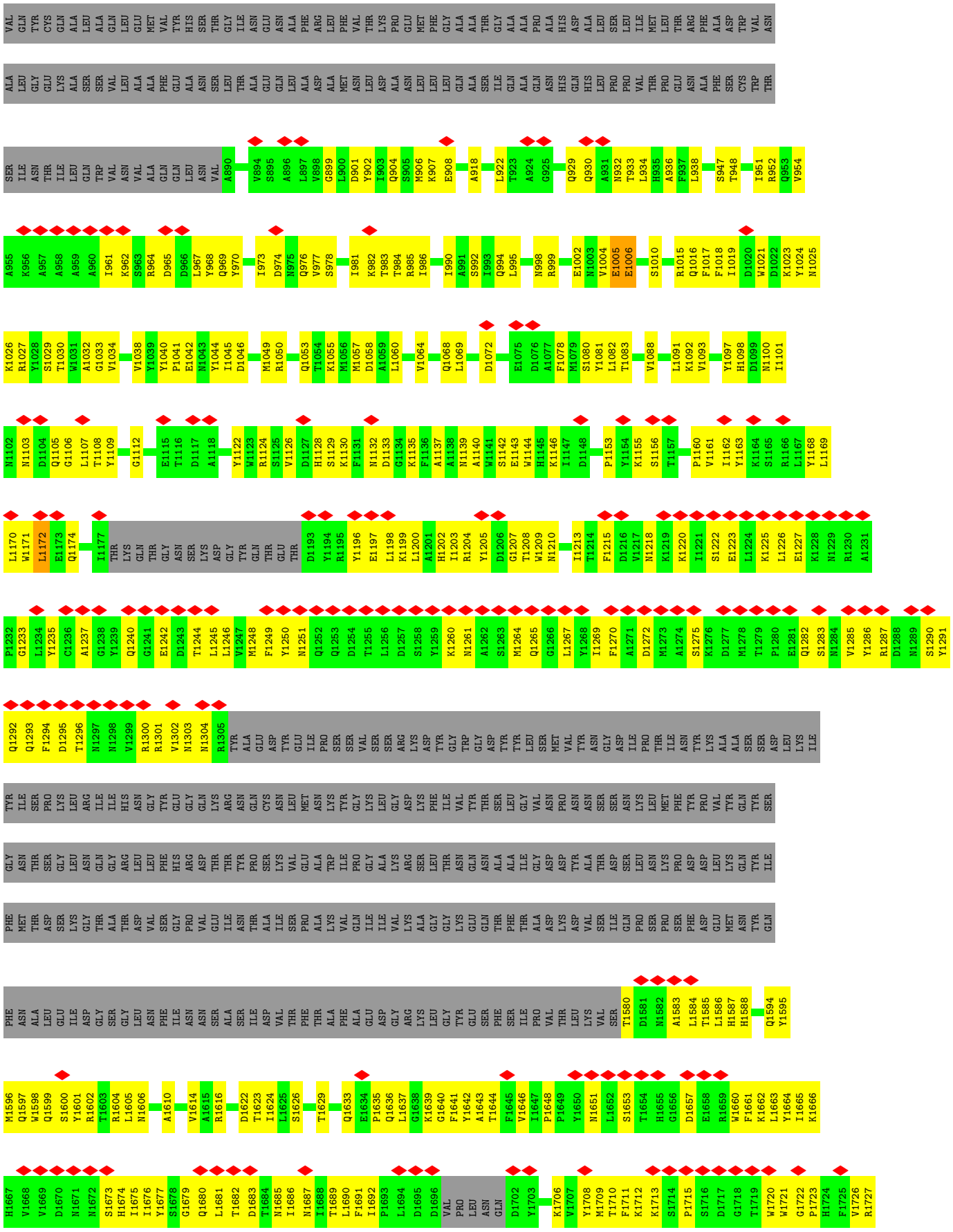
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total	C	N	O	S	0	0
			11083	7001	1914	2130	38		
1	B	1427	Total	C	N	O	S	0	0
			11083	7001	1914	2130	38		
1	C	1427	Total	C	N	O	S	0	0
			11083	7001	1914	2130	38		
1	D	1427	Total	C	N	O	S	0	0
			11083	7001	1914	2130	38		
1	E	1427	Total	C	N	O	S	0	0
			11083	7001	1914	2130	38		

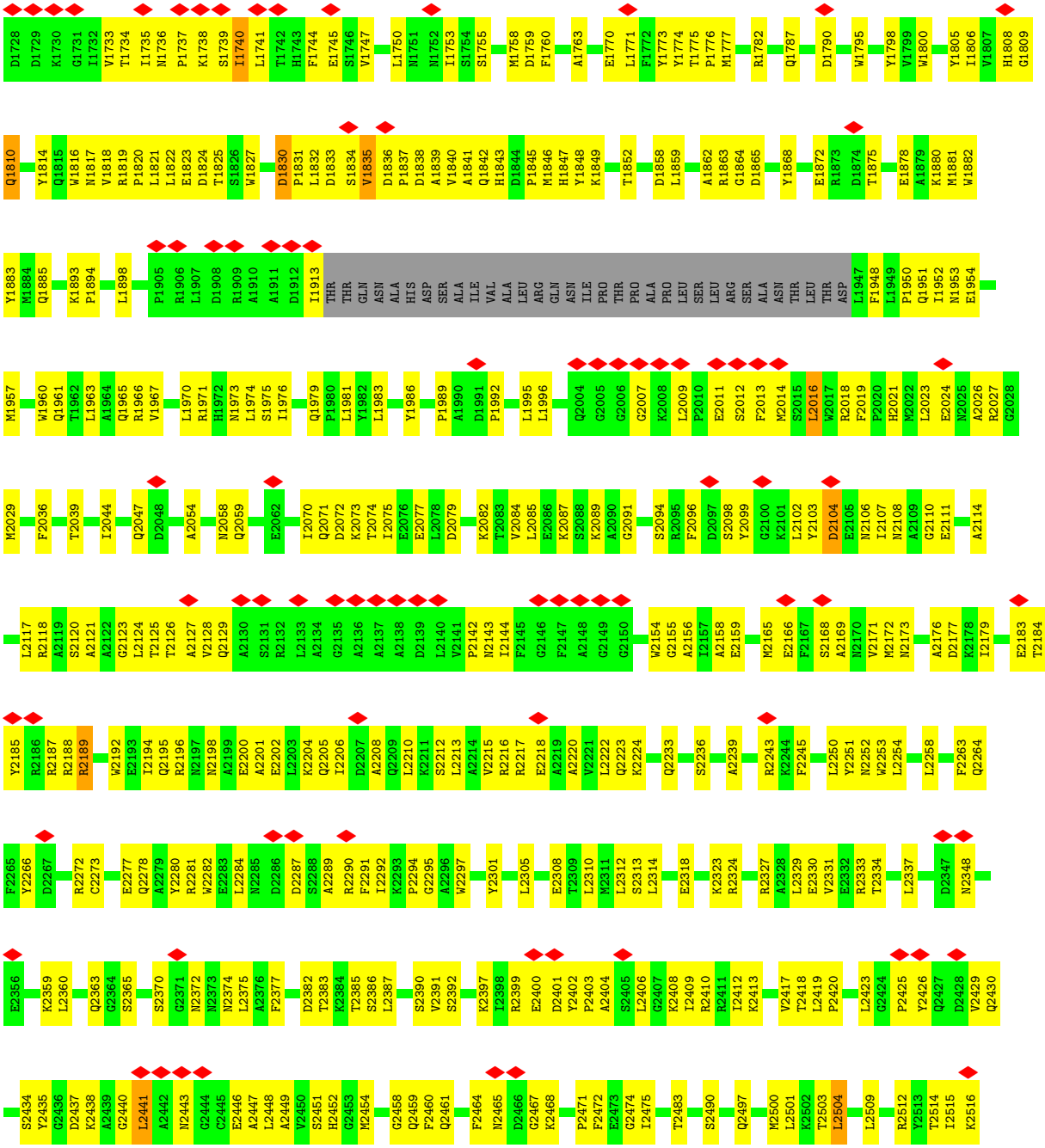
3 Residue-property plots (i)

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.

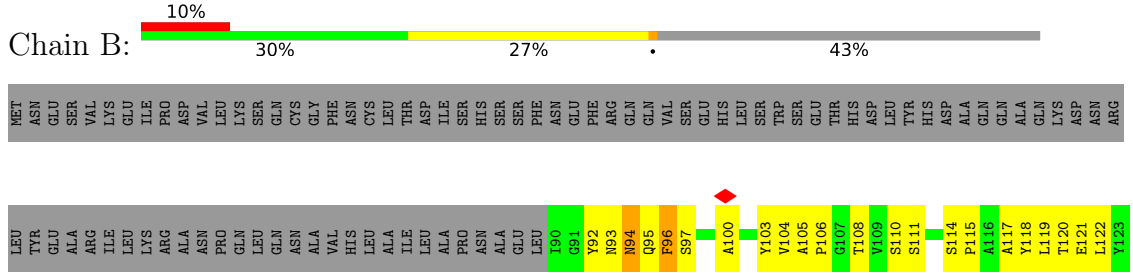
- Molecule 1: TcdA1

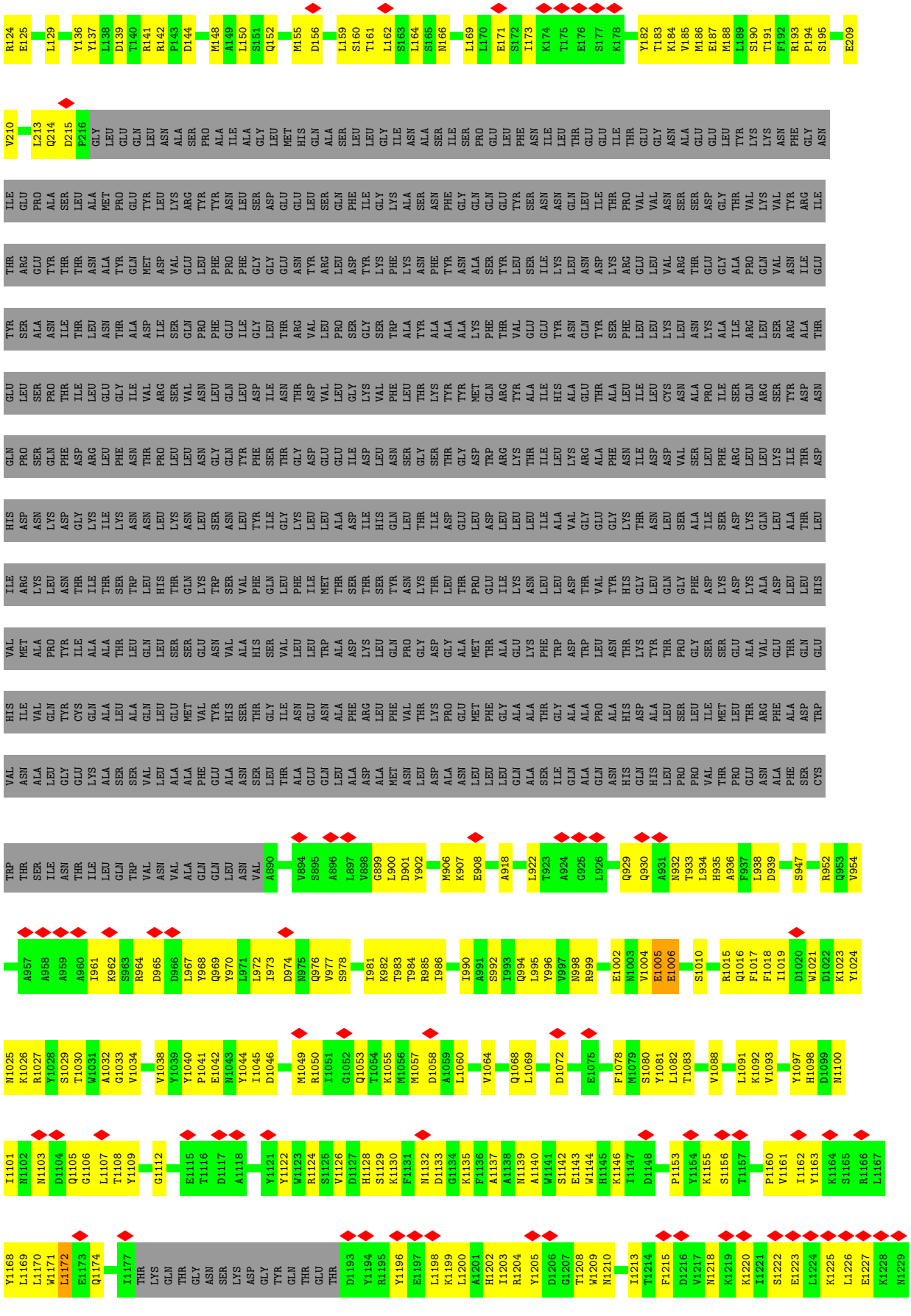






• Molecule 1: TcdA1

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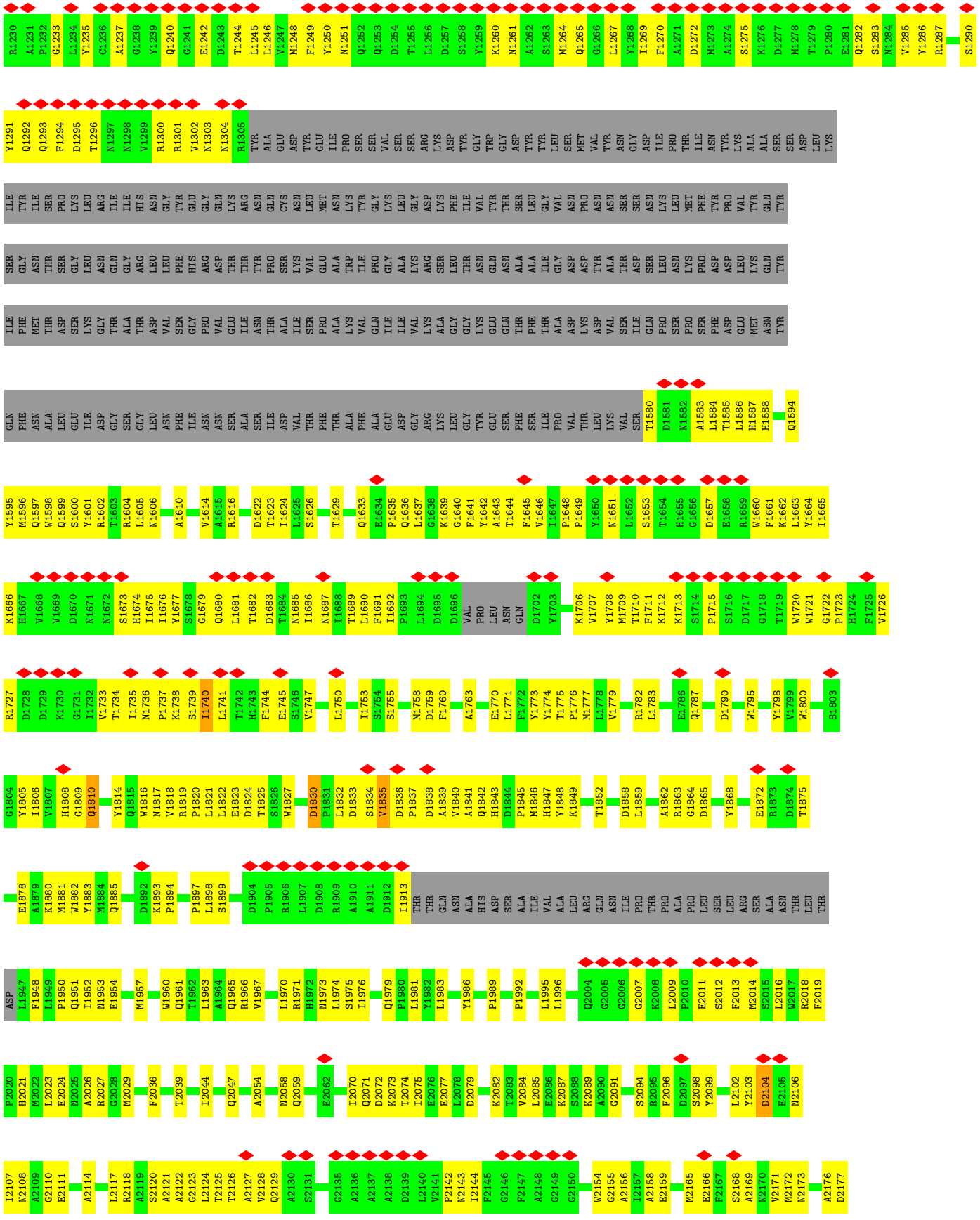
V210 L213 Q214 D215 P216 GLY LEU GLU GLN LEU ASN ALA SER PRO ALA ILE ALA GLY LEU MET HIS GLN ALA SER LEU LEU GLY ILE ASN ALA SER ILE SER PRO GLN GLU LEU PHE ASN ILE LEU THR GLU GLU ILE THR GLU GLY LYS ASN ALA GLU GLU LEU TYR LYS LYS ASN VAL TYR ARG ILE
ILE GLU PRO ALA SER LEU ALA MET PRO GLU TYR LEU LYS ARG TYR TYR ASN LEU SER ASP GLU GLU LEU SER GLN PHE ILE GLY LYS ALA SER ASN PHE ILE GLY GLN GLN GLU LEU PHE SER ASN ASN GLN LEU ILE THR PRO VAL VAL ASN SER SER ASP GLY GLY THR VAL LYS VAL TYR ARG ILE
THR ARG GLU TYR THR THR ASN ALA TYR GLN MET ASP VAL GLU LEU PHE PRO PHE GLY GLY GLU ASN TYR ARG LEU ASP TYR LYS PHE LYS ASN PHE TYR ASN ALA SER GLN GLU TYR LEU LEU SER ILE LYS LEU ASN ASP LYS ARG GLU LEU VAL ARG THR GLU GLY ALA PRO GLN VAL LYS ASN ILE GLU
TYR SER ALA ASN ILE THR LEU ASN THR ASP ILE SER GLN PRO PHE GLU ILE GLY LEU THR ARG VAL LEU PRO SER GLY SER TRP ALA TYR ALA ALA ALA LYS PHE THR VAL GLU GLU TYR ASN GLN TYR SER PHE LEU LEU LYS LEU ASN LYS ALA ILE ARG LEU SER ARG ALA THR
GLU LEU SER PRO THR ILE LEU GLU GLY ILE VAL ARG SER VAL ASN LEU GLN LEU ASP ILE ASN THR ASP VAL LEU GLY LYS VAL PHE LEU THR LYS TYR TYR MET GLN ARG TYR ALA ILE HIS ALA GLU THR ALA LEU LEU ILE LEU CYS ASN ALA PRO ILE SER GLN ARG SER TYR ASP ASN
GLN PRO SER GLN PHE ASP ARG LEU PHE ASN THR PRO LEU LEU ASN GLY GLN TYR PHE SER THR GLY ASP GLU GLU ILE ASP LEU ASN SER GLY SER THR GLY ASP TRP ARG LYS THR ILE LEU LYS ARG ALA PHE ASN ILE ASP ASP VAL SER LEU PHE PHE ARG GLN LEU LEU ARG LEU SER THR ASP
HIS ASP ASN LYS ASP GLY LYS ILE LYS ASN LYS LEU ASN LEU SER ASN LEU TYR ILE GLY LYS LEU LEU ALA ASP ILE HIS GLN LEU THR ILE ASP GLU LEU ASP LEU LEU LEU ILE ALA VAL GLY GLU GLY LYS THR ASN LEU SER ALA ILE SER ASP LYS GLN LEU ALA THR LEU
ILE ARG LYS LEU ASN THR ILE THR SER TRP LEU HIS THR GLN LYS TRP SER VAL PHE GLN LEU PHE ILE MET THR SER THR SER TYR ASN LYS THR PRO GLU ILE LYS ASN LEU LEU ASP THR VAL TYR HIS GLY LEU GLN GLY PHE ASP LYS ASP ALA LYS ALA ASP LEU LEU HIS
VAL MET ALA PRO TYR ILE ALA ALA THR LEU GLN LEU SER SER GLU ASN VAL ALA HIS SER VAL LEU LEU TRP ALA ASP LYS LEU GLN PRO GLY ASP GLY ALA MET THR ALA GLU LYS PHE TRP ASP TRP LEU ASN THR LYS TYR THR PRO GLY GLN GLY PHE ASP LYS ALA ASP LEU GLU GLN
HIS ILE VAL GLN TYR CYS GLN ALA LEU GLN LEU GLU MET VAL TYR HIS SER THR GLY ILE ASN GLU GLN ALA ALA THR GLY ALA ALA PRO ALA HIS ASP ALA LEU SER LEU ILE MET LEU THR ARG PHE ALA ASP TRP
VAL ASN ALA LEU GLY GLU LYS ALA SER SER VAL LEU ALA ASN SER LEU THR ALA GLU GLN LEU ALA ASP ASP MET ASN LEU ASP ALA ASP LEU LEU LEU LEU GLN ILE GLN ALA ASN GLN HIS LEU PRO PRO VAL THR PRO GLU ASN ALA PHE SER CYS
TRP THR SER ILE ASN THR ILE LEU GLN TRP VAL ASN VAL ALA GLN GLN LEU ASN VAL A890 V894 S895 A896 L897 V898 G899 L900 D901 Y902 M906 K907 E908 A918 L922 T923 A924 G925 L926 Q929 Q930 A931 N932 T933 L934 H935 A936 F937 L938 D939 S947 R952 Q953 V954
A957 A958 A959 A960 I961 K962 S963 R964 D965 D966 L967 Y968 Q969 Y970 L971 L972 I973 D974 N975 Q976 V977 S978 I981 K982 T983 Y984 R985 I986 I990 A991 S992 I993 Q994 L995 Y996 W997 N998 R999 E1002 N1003 V1004 E1005 E1006 S1010 R1015 Q1016 F1017 F1018 I1019 D1020 W1021 D1022 K1023 Y1024
N1025 K1026 R1027 Y1028 S1029 T1030 W1031 A1032 G1033 V1034 V1038 Y1039 Y1040 P1041 E1042 N1043 Y1044 I1045 D1046 M1049 R1050 I1051 G1052 Q1053 T1054 K1055 M1056 M1057 D1058 A1059 L1060 V1064 Q1068 L1069 D1072 E1075 F1078 M1079 S1080 Y1081 L1082 T1083 V1088 L1091 K1092 V1093 Y1097 H1098 D1099 N1100
I1101 N1102 N1103 D1104 Q1105 G1106 L1107 T1108 Y1109 G1112 E1115 T1116 D1117 A1118 Y1121 Y1122 W1123 R1124 S1125 V1126 D127 H1128 S1129 K1130 F1131 N1132 D1133 G1134 K1135 F1136 A1137 A1138 N1139 A1140 W1141 S1142 E1143 W1144 H1145 K1146 I1147 D1148 P1153 Y1154 K1155 S1156 T1157 P1160 V1161 I1162 Y1163 K1164 S1165 R1166 L1167
Y1168 L1169 L1170 W1171 L1172 E1173 Q1174 I1177 THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR D1193 Y1194 R1195 Y1196 E1197 L1198 K1199 L1200 A1201 H1202 I1203 R1204 Y1205 D1206 G1207 T1208 W1209 N1210 I1213 T1214 F1215 D1216 V1217 N1218 K1219 K1220 I1221 S1222 E1223 L1224 K1225 L1226 E1227 K1228 N1229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Y1291 Q1292 Q1293 F1294 D1295 T1296 N1297 N1298 V1299 R1300 R1301 V1302 N1303 N1304 R1305 TYR ALA GLU ASP TYR GLU ILE PRO SER SER VAL SER SER ARG LYS ASP TYR GLY TRP GLY ASP TYR TYR LEU SER MET VAL TYR ASN GLY ASP ILE PRO THR ILE ASN TYR LYS ALA ALA SER SER ASP LEU LYS
ILE TYR ILE SER PRO LYS LEU ARG ILE ILE HIS ASN GLY TYR GLU GLY GLN LYS ARG ASN GLN CYS ASN LEU MET ASN LYS TYR GLY LYS LEU GLY ASP LYS PHE ILE VAL TYR THR SER LEU GLY VAL ASN ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL TYR GLN TYR
SER GLY ASN THR SER GLY LEU ASN GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ILE ASN THR ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN GLN THR PHE THR ALA ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LYS GLN TYR
ILE PHE MET THR ASP SER LYS GLY THR GLY PRO VAL GLU ILE ASN THR ALA ILE SER PRO ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN THR PHE THR ALA ASP ASP LYS ASP VAL SER ILE GLN PRO SER PRO SER PHE ASP GLU MET ASN TYR
GLN PHE ASN ALA LEU GLU ILE ASP GLY SER GLY LEU ASN PHE ILE ASN ASN SER ALA SER ILE ASP VAL THR PHE THR ALA PHE ALA GLU ASP GLY ARG LYS LEU GLY TYR GLU SER PHE SER ILE PRO VAL THR LEU LYS VAL SER T1580 D1581 N1582 A1583 L1584 T1585 L1586 H1587 H1588 Q1594
Y1595 M1596 Q1597 W1598 Q1599 S1600 Y1601 R1602 T1603 R1604 L1605 N1606 A1610 V1614 A1615 R1616 D1622 T1623 I1624 L1625 S1626 T1629 Q1633 E1634 P1635 Q1636 L1637 G1638 K1639 G1640 F1641 Y1642 A1643 T1644 F1645 V1646 I1647 P1648 P1649 Y1650 N1651 L1652 S1653 T1654 H1655 G1656 D1657 E1658 R1659 W1660 F1661 K1662 L1663 Y1664 I1665
K1666 H1667 V1668 V1669 D1670 N1671 N1672 S1673 H1674 I1675 I1676 Y1677 S1678 G1679 Q1680 L1681 T1682 D1683 T1684 N1685 I1686 N1687 T1688 T1689 L1690 F1691 I1692 P1693 L1694 D1695 D1696 VAL PRO LEU ASN GLN D1702 Y1703 K1706 V1707 Y1708 M1709 T1710 F1711 K1712 K1713 S1714 P1715 S1716 D1717 G1718 T1719 W1720 W1721 G1722 P1723 H1724 F1725 V1726
R1727 D1728 D1729 K1730 G1731 I1732 V1733 T1734 I1735 N1736 P1737 K1738 S1739 I1740 L1741 T1742 H1743 F1744 E1745 S1746 V1747 L1750 I1753 S1754 S1755 M1758 D1759 F1760 A1763 E1770 L1771 F1772 Y1773 Y1774 T1775 P1776 M1777 L1778 V1779 R1782 L1783 E1786 Q1787 D1790 W1795 Y1798 V1799 W1800 S1803
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E1878 A1879 K1880 M1881 W1882 Y1883 M1884 Q1885 D1892 K1893 P1894 P1897 L1898 S1899 D1904 P1905 R1906 L1907 D1908 R1909 A1910 A1911 D1912 I1913 THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN THR LEU THR
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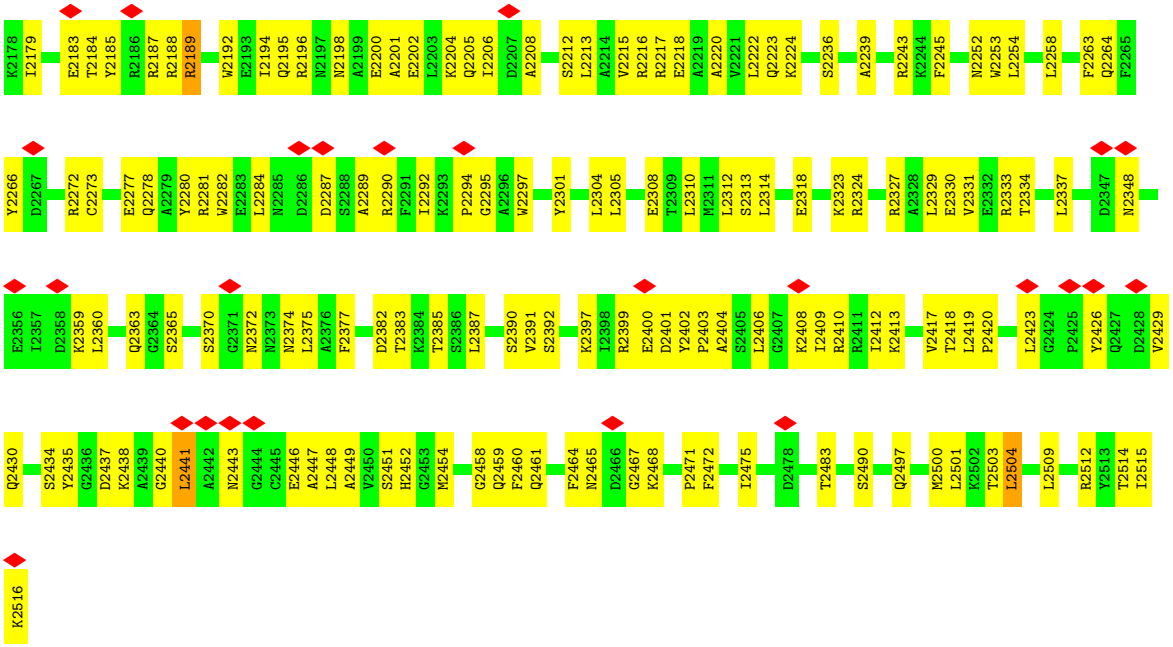
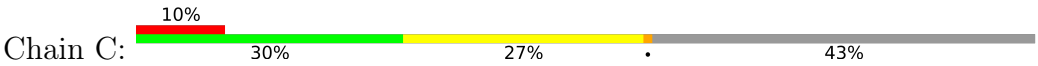
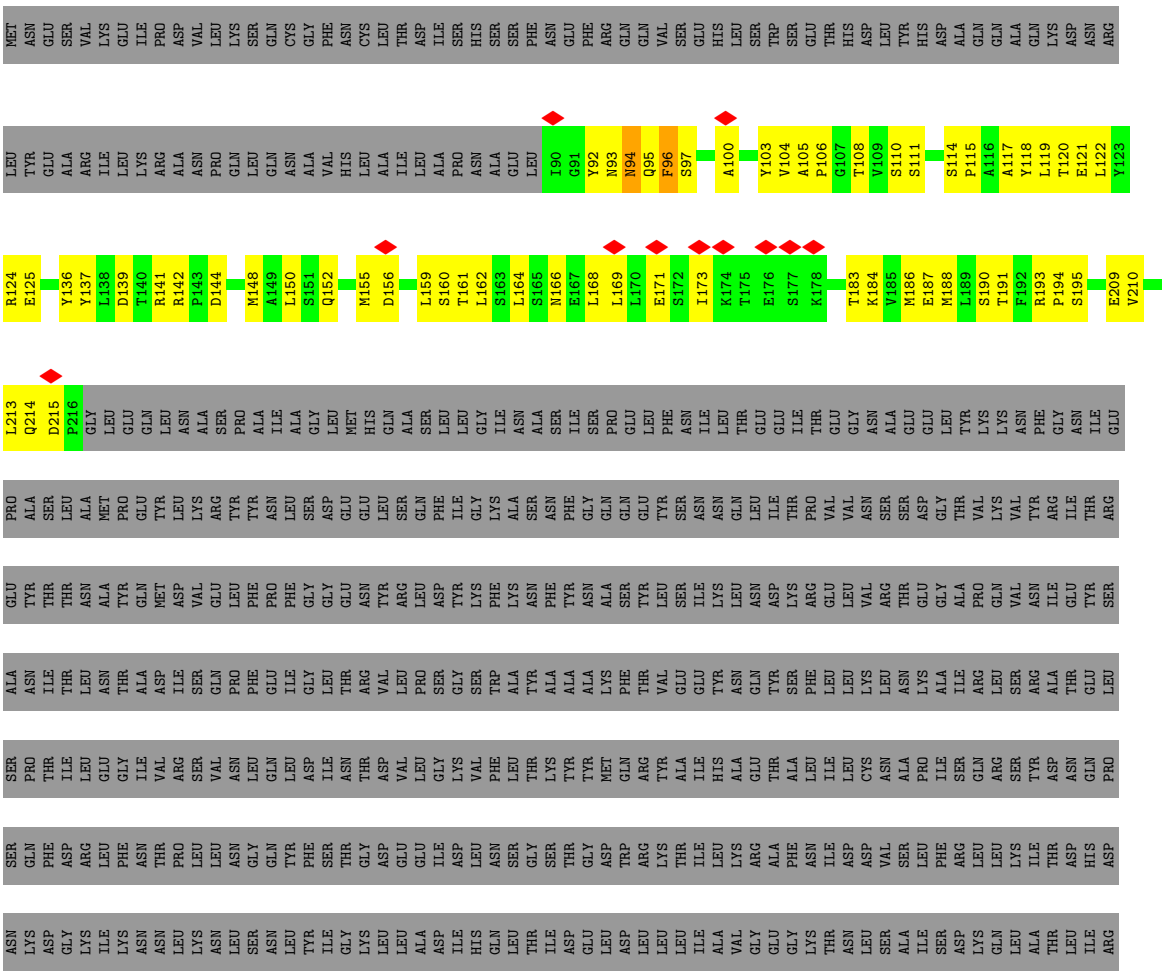
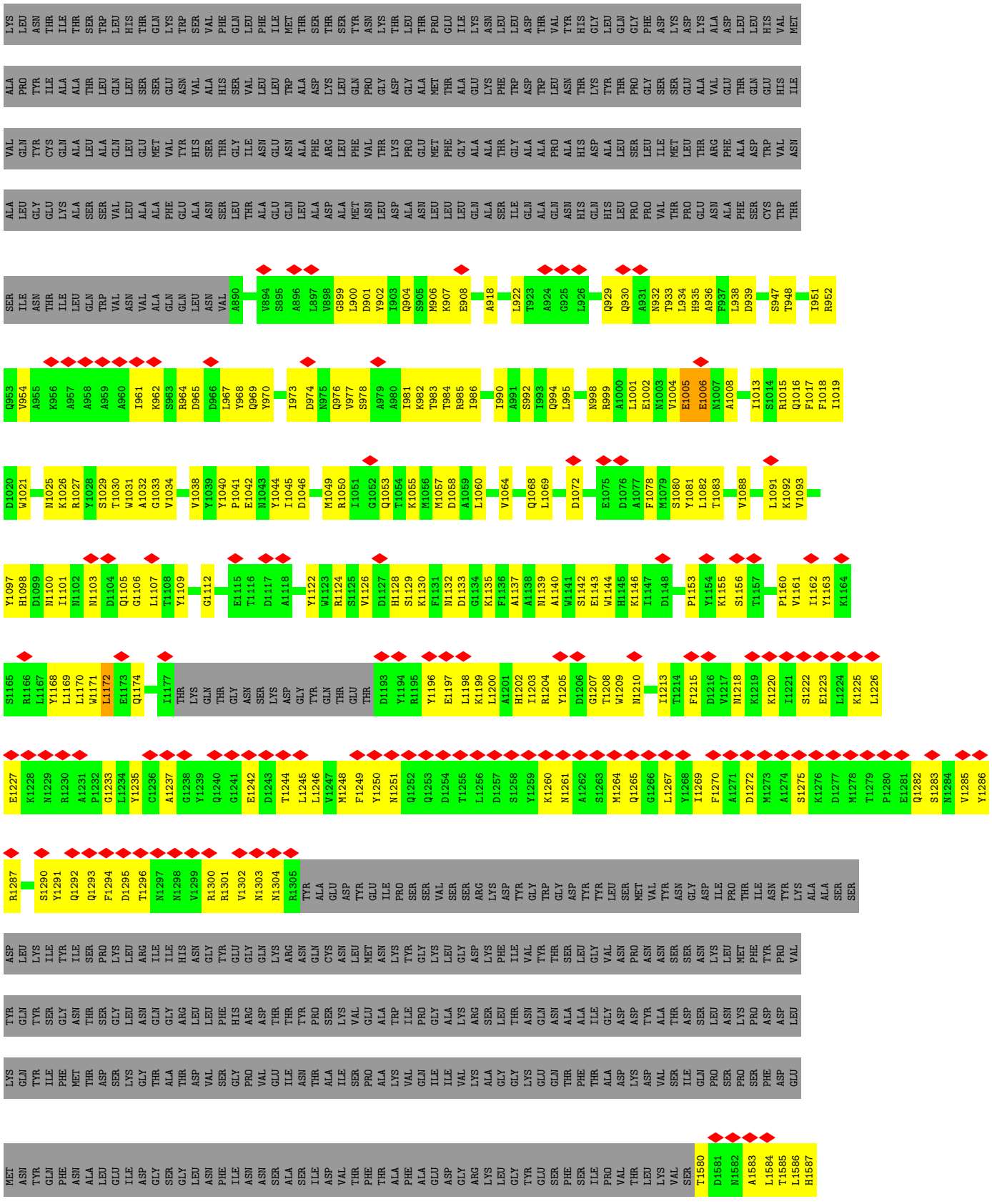


• Molecule 1: TcdA1



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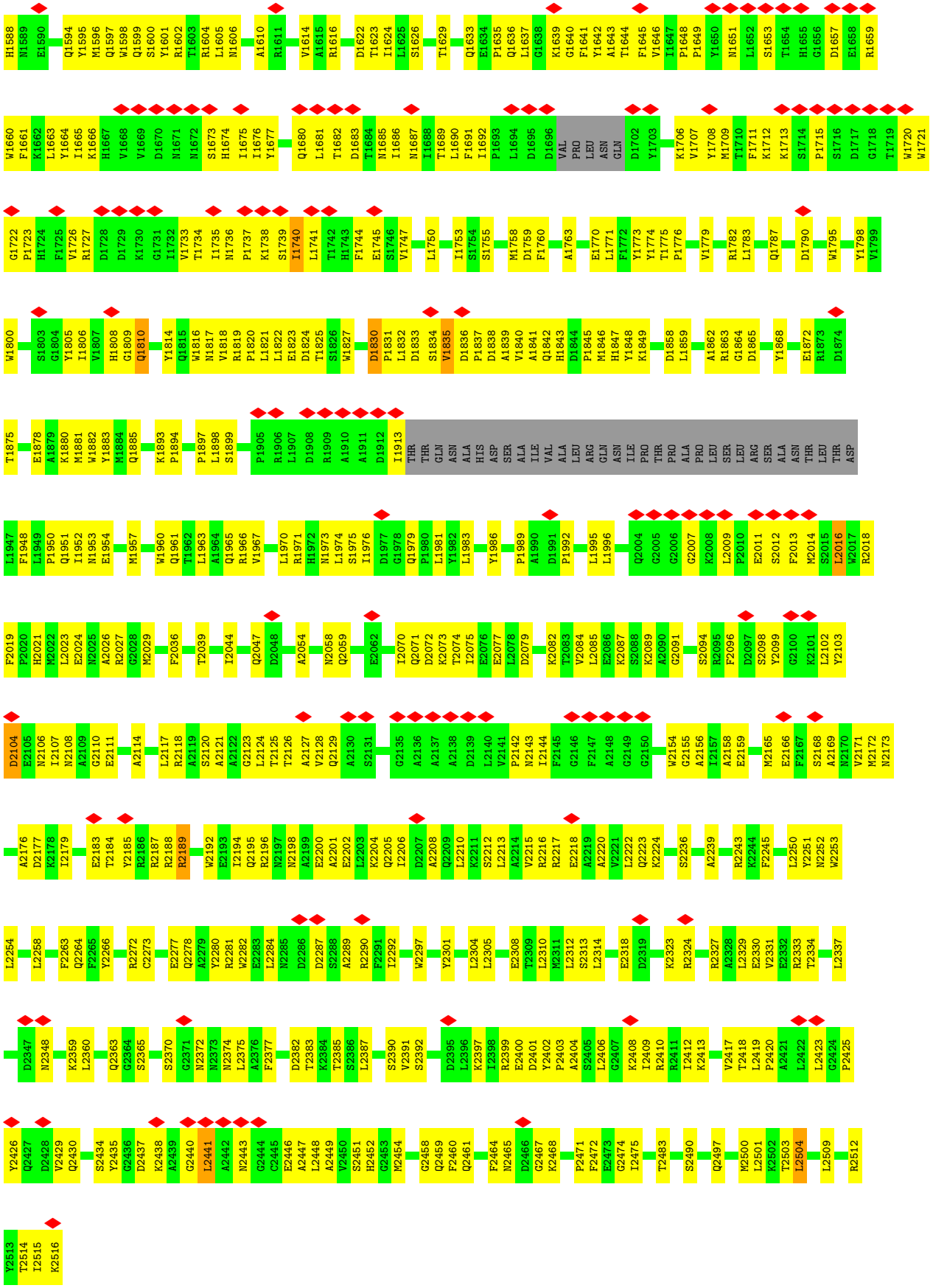
ALA PRO TYR ILE ALA ALA THR LEU GLN LEU SER SER GLU ASN VAL ALA HIS SER VAL LEU PHE ASN GLU ASN ALA ASP LYS LEU GLN LEU LEU TRP ASP THR ALA ASP LYS LEU GLN LEU LEU ASP GLY ASP GLY ALA MET THR ALA GLU LYS PHE TRP ASP TRP LEU ASN THR LYS TYR THR PRO GLY SER SER GLU ALA VAL GLU THR GLN ARG PHE ALA ASP TRP VAL ILE
VAL GLN TYR CYS GLN ALA LEU ALA GLN LEU GLU MET VAL TYR HIS SER THR GLY ILE ASN GLU ASN ALA PHE ARG LEU PHE VAL THR LYS PRO GLU MET PHE GLY ALA ALA THR GLY ALA ALA PRO ALA HIS ASP ALA LEU SER LEU ILE MET LEU THR ARG PHE ALA ASP TRP VAL ASN
ALA LEU GLY GLU LYS ALA SER SER VAL LEU GLU ALA ALA PHE GLU GLN ALA ASN SER LEU THR ALA GLU GLN LEU ALA ASP ALA MET ASN LEU ASP ALA GLN ALA GLN ASN HIS GLN HIS LEU PRO VAL THR PRO GLU GLN ASN ALA PHE SER CYS TRP THR
SER ILE ASN THR ILE LEU GLN TRP VAL ASN VAL ALA GLN LEU ASN VAL A890 V894 S895 A896 L897 V898 G899 L900 D901 Y902 I903 Q904 S905 M906 K907 E908 A918 L922 T923 A924 G925 L926 Q929 Q930 A931 N932 T933 L934 H935 A936 F937 L938 D939 S947 T948 I951 R952
Q953 V954 A955 K956 A957 A958 A959 A960 I961 K962 S963 R964 D965 D966 L967 Y968 Q969 Y970 I973 D974 N975 Q976 V977 S978 A979 A980 I981 K982 T983 T984 R985 I986 I990 A991 S992 I993 Q994 L995 N998 R999 A1000 L1001 E1002 N1003 V1004 E1005 E1006 N1007 A1008 I1013 S1014 R1015 Q1016 F1017 F1018 I1019
D1020 W1021 N1025 K1026 R1027 Y1028 S1029 T1030 W1031 A1032 G1033 V1034 V1038 Y1039 Y1040 P1041 E1042 N1043 Y1044 I1045 D1046 M1049 R1050 I1051 G1052 Q1053 T1054 K1055 M1056 M1057 D1058 A1059 L1060 V1064 Q1068 L1069 D1072 E1075 D1076 A1077 F1078 M1079 S1080 Y1081 L1082 T1083 V1088 L1091 K1092 V1093
Y1097 H1098 D1099 N1100 I1101 N1102 N1103 D1104 Q1105 G1106 L1107 T1108 Y1109 G1112 E1115 T1116 D1117 A1118 Y1122 W1123 R1124 S1125 V1126 D1127 H1128 S1129 K1130 F1131 N1132 D1133 C1134 K1135 F1136 A1137 A1138 N1139 A1140 W1141 S1142 E1143 W1144 H1145 K1146 I1147 D1148 P1153 Y1154 K1155 S1156 T1157 P1160 V1161 I1162 Y1163 K1164
S1165 R1166 L1167 Y1168 L1169 L1170 W1171 L1172 E1173 Q1174 I1177 THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR D1193 Y1194 R1195 Y1196 E1197 L1198 K1199 L1200 A1201 H1202 I1203 R1204 Y1205 D1206 G1207 T1208 W1209 N1210 I1213 T1214 F1215 D1216 V1217 N1218 K1219 K1220 I1221 S1222 E1223 L1224 K1225 L1226
E1227 K1228 N1229 R1230 A1231 P1232 G1233 L1234 Y1235 C1236 A1237 G1238 Y1239 Q1240 G1241 E1242 D1243 T1244 L1245 L1246 V1247 M1248 F1249 Y1250 N1251 Q1252 Q1253 D1254 T1255 L1256 D1257 S1258 Y1259 K1260 N1261 A1262 S1263 M1264 Q1265 G1266 L1267 Y1268 I1269 F1270 A1271 D1272 M1273 A1274 S1275 K1276 D1277 M1278 T1279 P1280 E1281 Q1282 S1283 N1284 V1285 Y1286
R1287 S1290 Y1291 Q1292 Q1293 F1294 D1295 T1296 N1297 N1298 V1299 R1300 R1301 V1302 N1303 N1304 R1305 TYR ALA GLU ASP TYR GLU ILE PRO SER SER VAL SER SER ARG LYS ASP TYR GLY TRP GLY ASP TYR LEU SER MET VAL TYR ASN GLY ASP ILE PRO THR ILE ASN TYR LYS ALA ALA SER SER
ASP LEU LYS ILE TYR ILE SER PRO LYS LEU ARG ILE ILE HIS ASN GLY TYR GLU GLY GLN LYS ARG ASN GLN CYS ASN LEU MET ASN LYS TYR GLY LYS LEU GLY ASP LYS PHE ILE VAL TYR THR SER LEU GLY VAL ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL
TYR GLN TYR SER GLY LEU ASN THR SER GLY GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ALA TRP ILE PRO GLY LEU ALA LYS ARG SER LEU THR ASN GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU
LYS GLN TYR ILE PHE MET THR ASP SER LYS GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR ALA PRO ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN THR PHE THR ALA ASP LYS ASP VAL SER ILE GLN PRO SER PRO SER PHE ASP GLU
MET ASN TYR GLN PHE ASN ALA LEU GLU ILE ASP GLY SER GLY LEU ASN PHE ILE ASN ASN SER ALA SER ILE ASP VAL THR PHE THR ALA PHE ALA GLU ASP GLY ARG LYS LEU GLY TYR GLU SER PHE SER ILE PRO VAL THR LEU LYS VAL SER T1580 D1581 N1582 A1583 L1584 T1585 L1586 H1587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G1722 P1723 H1724 F1725 V1726 R1727 D1728 D1729 K1730 G1731 I1732 V1733 T1734 I1735 N1736 P1737 K1738 S1739 I1740 L1741 T1742 H1743 F1744 E1745 S1746 V1747 L1750 I1753 S1754 S1755 M1758 D1759 F1760 A1763 E1770 L1771 F1772 Y1773 Y1774 T1775 P1776 V1779 R1782 L1783 Q1787 D1790 W1795 Y1798 V1799
W1800 S1803 G1804 Y1805 I1806 V1807 H1808 G1809 Q1810 Y1814 Q1815 W1816 N1817 V1818 R1819 P1820 L1821 L1822 E1823 D1824 T1825 S1826 W1827 D1830 P1831 L1832 D1833 S1834 V1835 D1836 P1837 D1838 A1839 V1840 A1841 Q1842 H1843 D1844 P1845 M1846 H1847 Y1848 K1849 D1858 L1859 A1862 R1863 G1864 D1865 Y1868 E1872 R1873 D1874
T1875 E1878 A1879 K1880 M1881 W1882 Y1883 M1884 Q1885 K1893 P1894 P1897 L1898 S1899 P1905 R1906 L1907 D1908 R1909 A1910 A1911 D1912 I1913 THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN THR LEU THR ASP
L1947 F1948 L1949 P1950 Q1951 I1952 N1953 E1954 M1957 W1960 Q1961 T1962 L1963 A1964 Q1965 R1966 V1967 L1970 R1971 H1972 N1973 L1974 S1975 I1976 D1977 G1978 Q1979 P1980 L1981 Y1982 L1983 Y1986 P1989 A1990 D1991 P1992 L1995 L1996 Q2004 G2005 G2006 G2007 K2008 L2009 P2010 E2011 S2012 P2013 M2014 S2015 L2016 W2017 R2018
F2019 P2020 H2021 M2022 L2023 E2024 N2025 A2026 R2027 G2028 M2029 F2036 T2039 I2044 Q2047 D2048 A2054 N2058 Q2059 E2062 I2070 Q2071 D2072 K2073 T2074 I2075 E2076 E2077 L2078 D2079 K2082 T2083 V2084 L2085 E2086 K2087 S2088 K2089 A2090 G2091 S2094 R2095 F2096 D2097 S2098 Y2099 G2100 K2101 L2102 Y2103
D2104 E2105 N2106 I2107 N2108 A2109 G2110 E2111 A2114 L2117 R2118 A2119 S2120 A2121 A2122 G2123 L2124 T2125 T2126 A2127 V2128 Q2129 A2130 S2131 G2135 A2136 A2137 A2138 D2139 L2140 Y2141 P2142 N2143 I2144 F2145 G2146 F2147 A2148 G2149 G2150 W2154 G2155 A2156 I2157 A2158 E2159 M2165 E2166 F2167 S2168 A2169 N2170 V2171 M2172 N2173
A2176 D2177 K2178 I2179 E2183 T2184 Y2185 R2186 R2187 R2188 R2189 W2192 E2193 I2194 Q2195 R2196 N2197 W2198 A2199 E2200 A2201 E2202 L2203 K2204 Q2205 I2206 D2207 A2208 Q2209 L2210 K2211 S2212 L2213 A2214 V2215 R2216 R2217 E2218 A2219 A2220 V2221 L2222 Q2223 K2224 S2236 A2239 R2243 K2244 F2245 L2250 Y2251 N2252 W2253
L2254 L2258 F2263 Q2264 F2265 Y2266 R2272 C2273 E2277 Q2278 A2279 Y2280 R2281 W2282 E2283 L2284 N2285 D2286 D2287 S2288 A2289 R2290 F2291 I2292 W2297 Y2301 L2304 L2305 E2308 T2309 L2310 M2311 L2312 S2313 L2314 E2318 D2319 K2323 R2324 R2327 A2328 L2329 E2330 V2331 E2332 R2333 T2334 L2337
D2347 N2348 K2359 L2360 Q2363 G2364 S2365 S2370 G2371 N2372 N2373 N2374 L2375 A2376 F2377 D2382 T2383 K2384 T2385 S2386 L2387 S2390 V2391 S2392 D2395 L2396 K2397 I2398 R2399 E2400 D2401 Y2402 P2403 A2404 S2405 L2406 G2407 K2408 I2409 R2410 R2411 I2412 K2413 V2417 T2418 L2419 P2420 A2421 L2422 L2423 G2424 P2425
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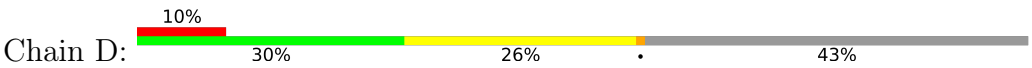
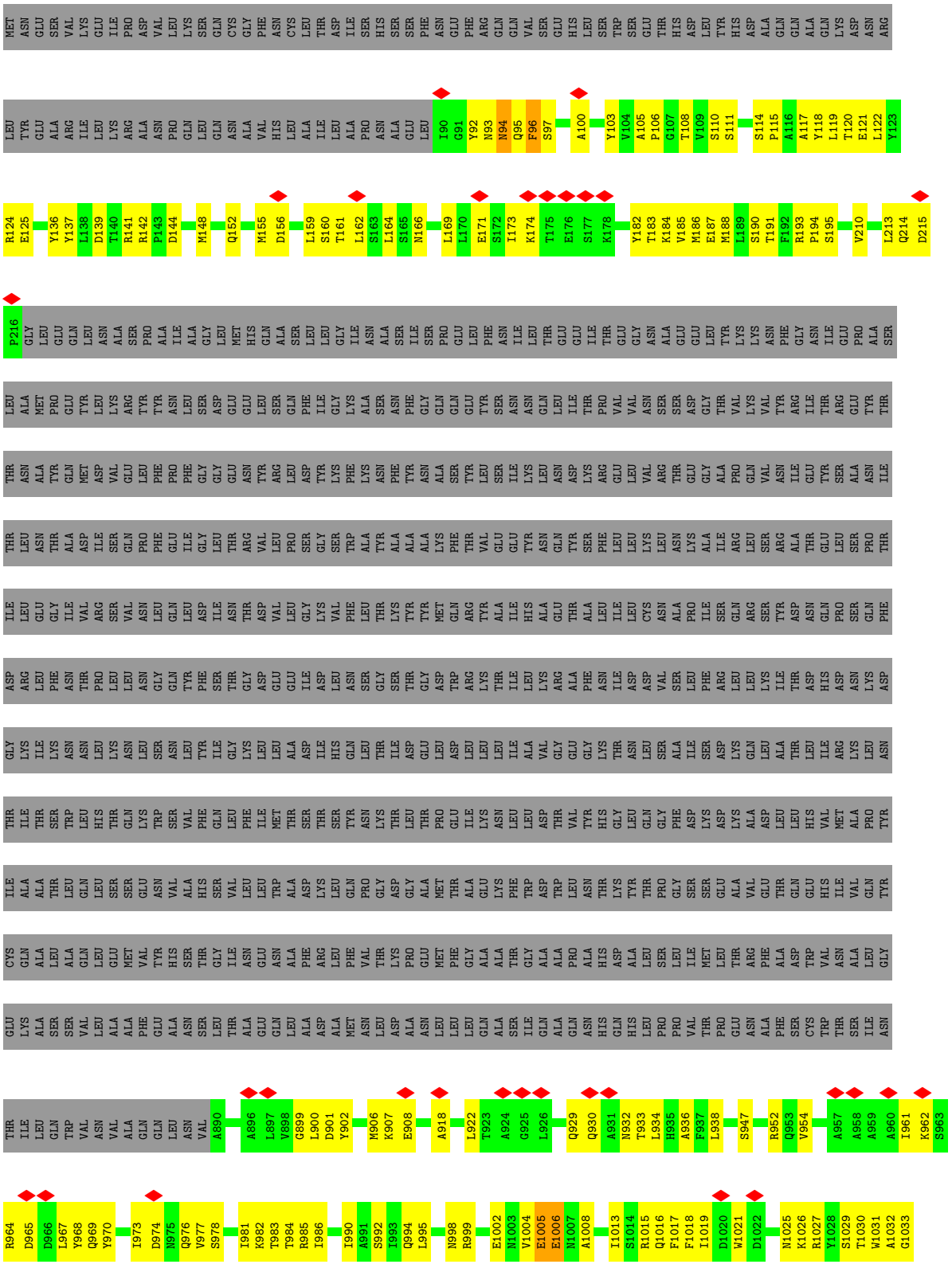
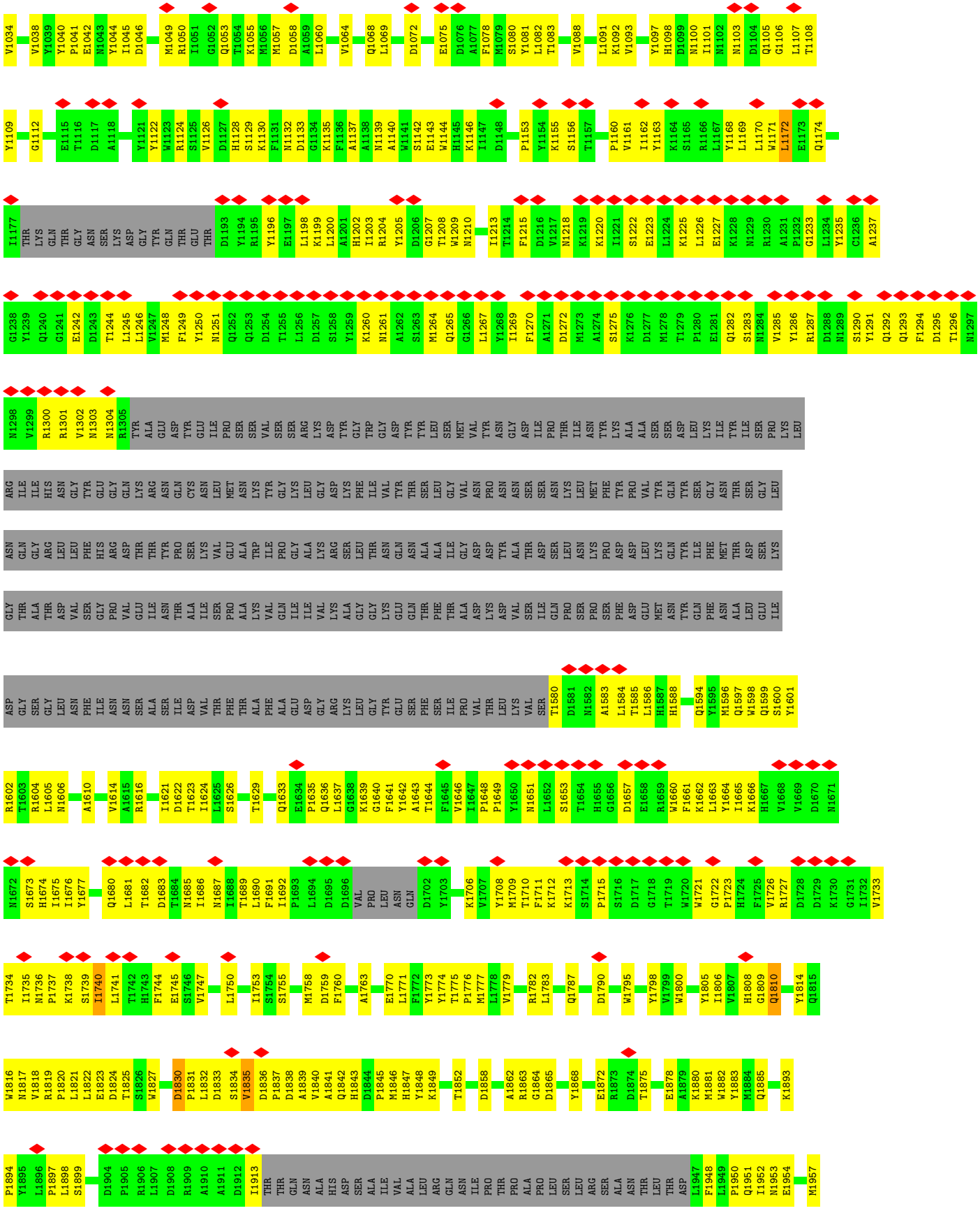
• Molecule 1: TcdA1

Chain D:



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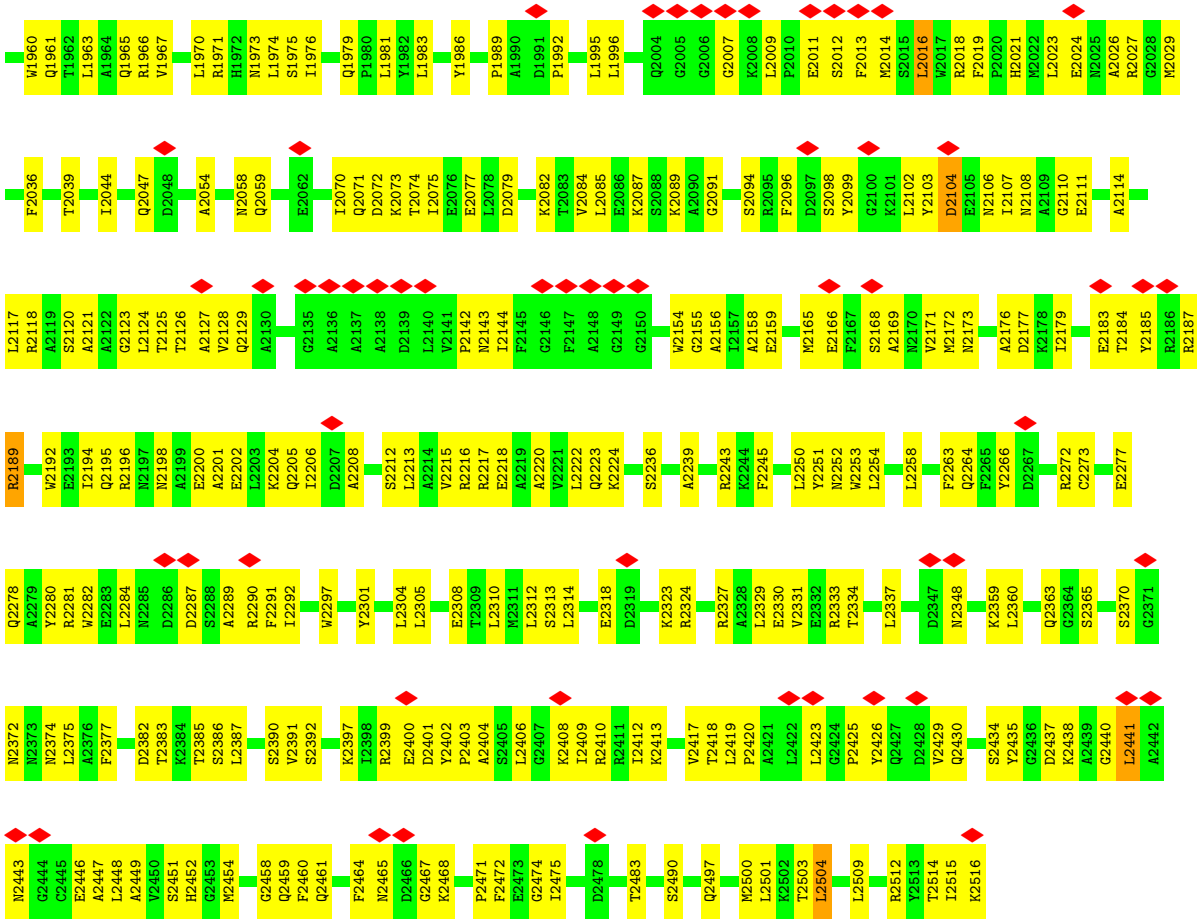
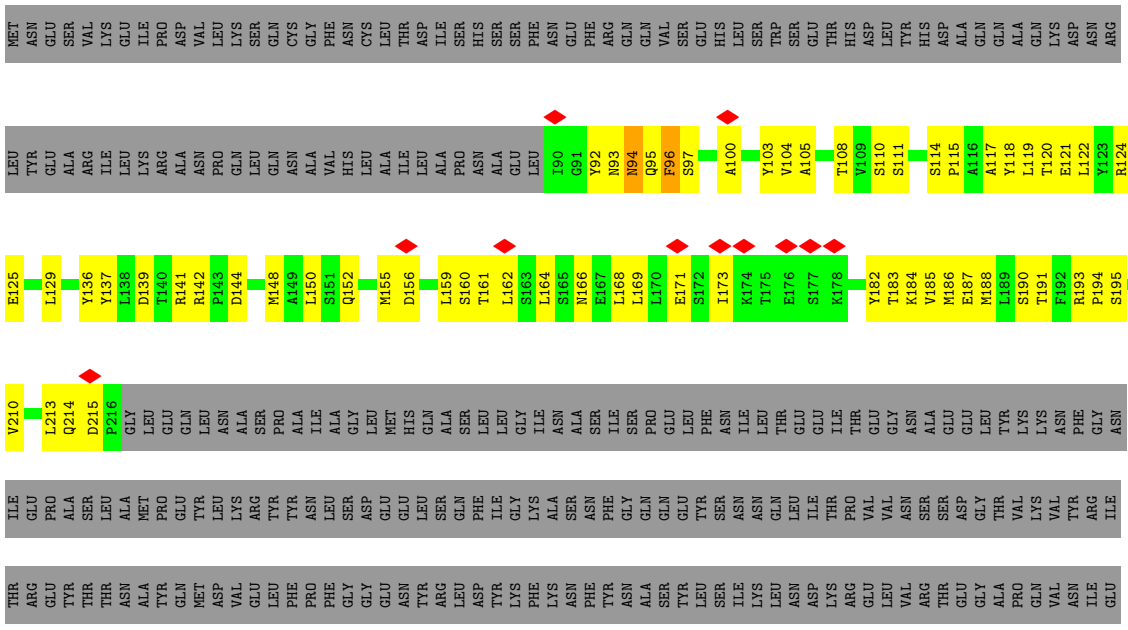
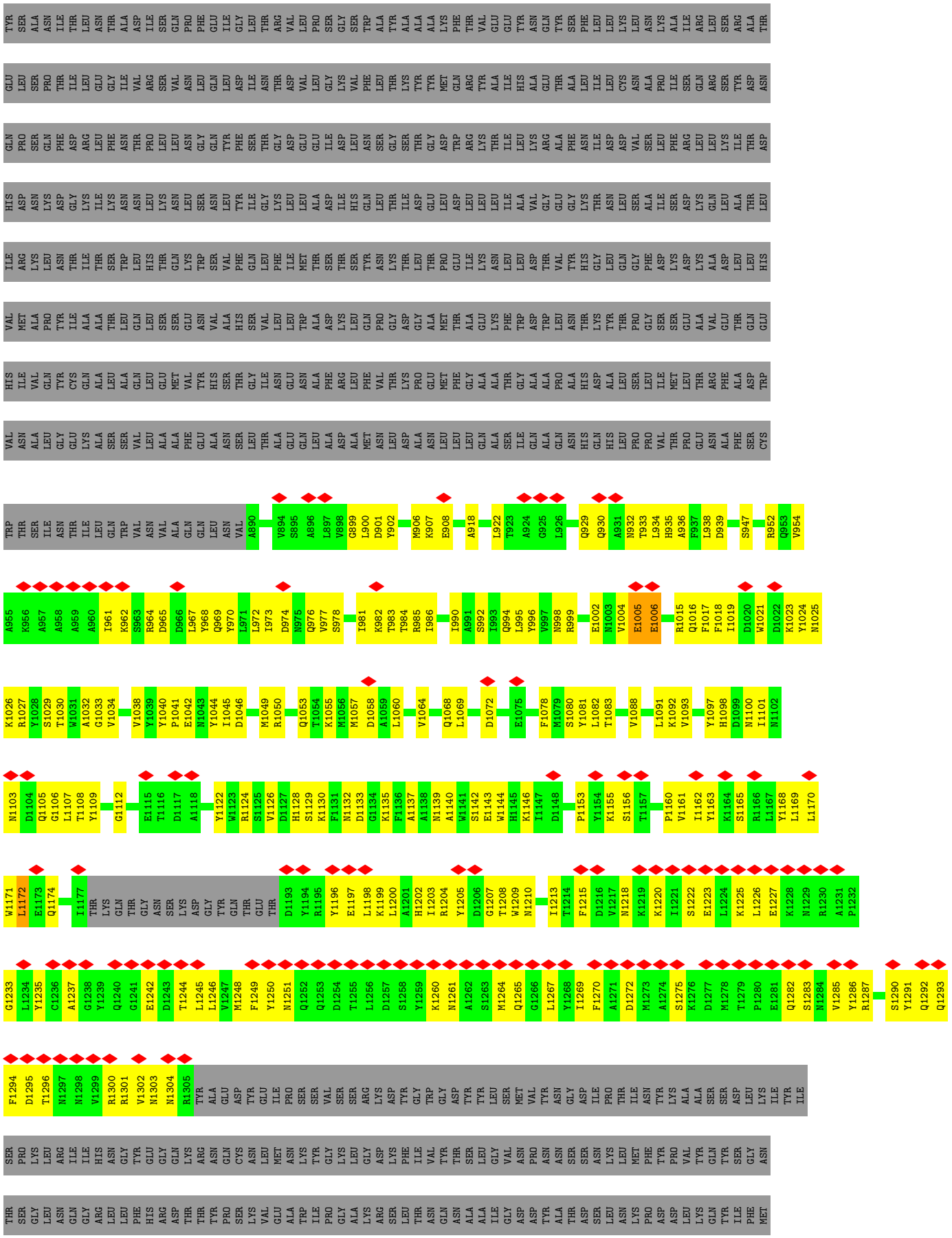
I1177 THR LYS GLN THR GLY ASN SER LYS ASP GLY TYR GLN THR GLU THR D1193 Y1194 R1195 Y1196 E1197 L1198 K1199 L1200 A1201 H1202 I1203 R1204 Y1205 D1206 G1207 T1208 W1209 N1210 I1213 T1214 F1215 D1216 V1217 N1218 K1219 K1220 I1221 S1222 E1223 L1224 K1225 L1226 E1227 K1228 N1229 R1230 A1231 P1232 G1233 L1234 Y1235 C1236 A1237
G1238 Y1239 Q1240 G1241 E1242 D1243 T1244 L1245 L1246 V1247 M1248 F1249 Y1250 N1251 Q1252 Q1253 D1254 T1255 L1256 D1257 S1258 Y1259 K1260 N1261 A1262 S1263 M1264 Q1265 G1266 L1267 Y1268 I1269 F1270 A1271 D1272 M1273 A1274 S1275 K1276 D1277 M1278 T1279 P1280 E1281 Q1282 S1283 N1284 V1285 Y1286 R1287 D1288 N1289 S1290 Y1291 Q1292 Q1293 F1294 D1295 T1296 N1297
N1298 V1299 R1300 R1301 V1302 N1303 N1304 R1305 TYR ALA GLU ASP TYR GLU ILE PRO SER SER VAL SER SER ARG LYS ASP TYR GLY TRP GLY ASP TYR TYR TYR LEU SER MET VAL TYR ASN GLY ASP ILE PRO THR ILE ASN TYR LYS ALA ALA SER SER ASP LEU LYS ILE TYR ILE SER PRO LYS LEU
ARG ILE ILE HIS ASN GLY TYR GLU GLY GLN LYS LYS ARG ASN GLN CYS ASN LEU MET ASN LYS TYR GLY LYS LEU GLY ASP LYS PHE ILE VAL TYR THR SER LEU SER GLY VAL ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE PHE TYR PRO VAL TYR GLN TYR SER GLY ASN THR SER GLY GLU
ASN GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ALA TRP ILE PRO GLY ALA LYS ARG SER LEU THR ASN GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LYS GLN TYR ILE PHE MET THR ASP SER LYS
GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR ALA ILE SER PRO ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN THR PHE THR ALA ASP LYS ASP VAL SER ILE GLN PRO SER PRO SER PHE ASP GLU MET ASN TYR GLN PHE ASN ALA LEU GLU ILE
ASP GLY SER GLY LEU ASN PHE ILE ASN ASN SER ALA SER ILE ASP VAL THR PHE THR ALA PHE ALA GLU ASP GLY ARG LYS LEU GLY TYR GLU SER PHE SER ILE PRO VAL THR LEU LYS VAL SER T1580 D1581 N1582 A1583 L1584 T1585 L1586 H1587 H1588 Q1594 Y1595 M1596 Q1597 W1598 Q1599 S1600 Y1601
R1602 T1603 R1604 L1605 N1606 A1610 V1614 A1615 R1616 I1621 D1622 T1623 I1624 L1625 S1626 T1629 Q1633 E1634 P1635 Q1636 L1637 G1638 K1639 G1640 F1641 Y1642 A1643 T1644 F1645 V1646 I1647 P1648 P1649 Y1650 N1651 L1652 S1653 T1654 H1655 G1656 D1657 E1658 R1659 W1660 F1661 K1662 L1663 Y1664 I1665 K1666 H1667 V1668 V1669 D1670 N1671
N1672 S1673 H1674 I1675 I1676 Y1677 Q1680 L1681 T1682 D1683 T1684 N1685 I1686 N1687 I1688 T1689 L1690 F1691 I1692 P1693 L1694 D1695 D1696 VAL PRO LEU ASN GLN D1702 Y1703 K1706 V1707 Y1708 M1709 T1710 F1711 K1712 K1713 S1714 P1715 S1716 D1717 G1718 T1719 W1720 W1721 G1722 P1723 H1724 F1725 V1726 R1727 D1728 D1729 K1730 G1731 I1732 V1733
T1734 I1735 N1736 P1737 K1738 S1739 I1740 L1741 T1742 H1743 F1744 E1745 S1746 V1747 L1750 I1753 S1754 S1755 M1758 D1759 F1760 A1763 E1770 L1771 F1772 Y1773 Y1774 T1775 P1776 M1777 L1778 V1779 R1782 L1783 Q1787 D1790 W1795 Y1798 V1799 W1800 Y1805 I1806 V1807 H1808 G1809 Q1810 Y1814 Q1815
W1816 N1817 V1818 R1819 P1820 L1821 L1822 E1823 D1824 T1825 S1826 W1827 D1830 P1831 L1832 D1833 S1834 V1835 D1836 P1837 D1838 A1839 V1840 A1841 Q1842 H1843 D1844 P1845 M1846 H1847 Y1848 K1849 T1852 D1858 A1862 R1863 G1864 D1865 Y1868 E1872 R1873 D1874 T1875 E1878 A1879 K1880 M1881 W1882 Y1883 M1884 Q1885 K1893
P1894 Y1895 L1896 P1897 L1898 S1899 D1904 P1905 R1906 L1907 D1908 R1909 A1910 A1911 D1912 I1913 THR THR GLN ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN THR LEU THR ASP L1947 F1948 L1949 P1950 Q1951 I1952 N1953 E1954 M1957

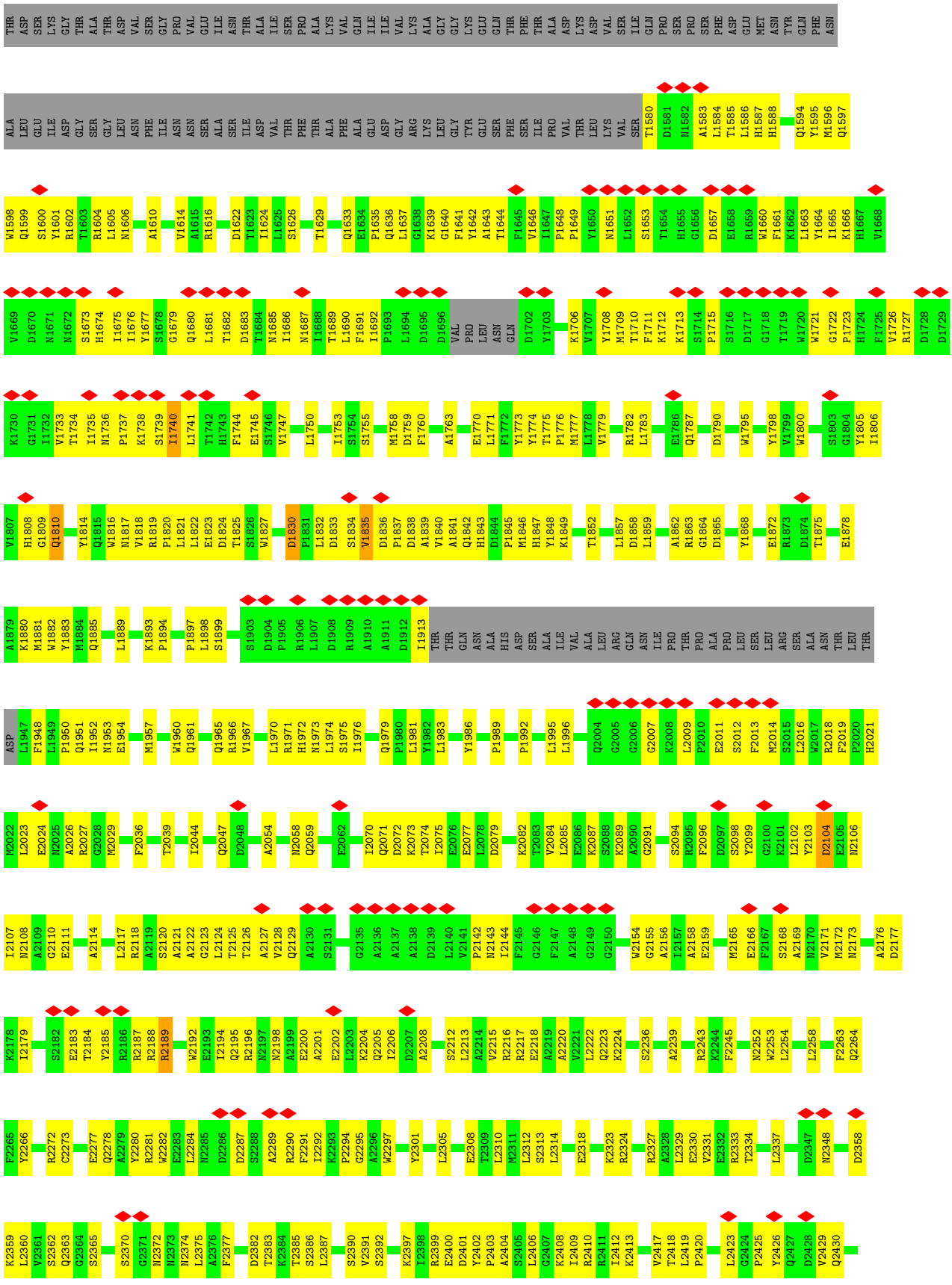


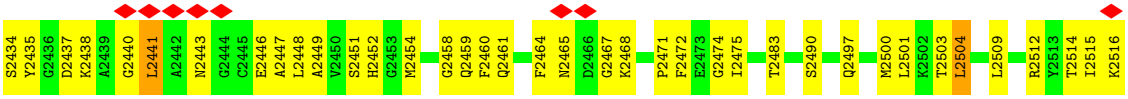
• Molecule 1: TcdA1

Chain E:





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K2438
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L2448
A2449
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M2454
G2458
Q2459
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F2464
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D2466
G2467
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S2490
Q2497
M2500
L2501
K2502
T2503
L2504
L2509
R2512
Y2513
T2514
I2515
K2516

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13000	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 ($e^-/Å^2$)	15.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	29.239	Depositor
Minimum map value	-15.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.75	Depositor
Map size (Å)	442.74002, 442.74002, 442.74002	wwPDB
Map dimensions	282, 282, 282	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.66	1/11313 (0.0%)	0.65	4/15367 (0.0%)
1	B	0.66	1/11313 (0.0%)	0.65	3/15367 (0.0%)
1	C	0.66	1/11313 (0.0%)	0.65	5/15367 (0.0%)
1	D	0.66	1/11313 (0.0%)	0.65	4/15367 (0.0%)
1	E	0.66	1/11313 (0.0%)	0.65	3/15367 (0.0%)
All	All	0.66	5/56565 (0.0%)	0.65	19/76835 (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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1830	ASP	C-N	-16.99	1.01	1.34
1	D	1830	ASP	C-N	-16.98	1.01	1.34
1	C	1830	ASP	C-N	-16.96	1.02	1.34
1	B	1830	ASP	C-N	-16.95	1.02	1.34
1	A	1830	ASP	C-N	-16.92	1.02	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2441	LEU	CA-CB-CG	5.75	128.53	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2441	LEU	CA-CB-CG	5.75	128.51	115.30
1	B	2441	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	2441	LEU	CA-CB-CG	5.74	128.50	115.30
1	E	2441	LEU	CA-CB-CG	5.73	128.48	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1005	GLU	Peptide
1	B	1005	GLU	Peptide
1	C	1005	GLU	Peptide
1	D	1005	GLU	Peptide
1	E	1005	GLU	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	11083	0	10580	1079	0
1	B	11083	0	10579	1079	0
1	C	11083	0	10579	1084	0
1	D	11083	0	10580	1096	0
1	E	11083	0	10579	1092	0
All	All	55415	0	52897	4117	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 38.

The worst 5 of 4117 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:2176:ALA:CB	1:D:2117:LEU:HD22	1.13	1.59
1:D:2176:ALA:CB	1:E:2117:LEU:HD22	1.13	1.59
1:D:2169:ALA:CB	1:E:2124:LEU:HD22	1.29	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2169:ALA:HB2	1:B:2124:LEU:CD2	1.14	1.58
1:A:2117:LEU:HD22	1:E:2176:ALA:CB	1.16	1.58

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	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	25	62
1	B	1415/2516 (56%)	1297 (92%)	110 (8%)	8 (1%)	25	62
1	C	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	25	62
1	D	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	25	62
1	E	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	25	62
All	All	7075/12580 (56%)	6489 (92%)	546 (8%)	40 (1%)	29	62

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	954	VAL
1	A	1810	GLN
1	A	2144	ILE
1	B	96	PHE

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	1135/2157 (53%)	1132 (100%)	3 (0%)	92 98
1	B	1135/2157 (53%)	1132 (100%)	3 (0%)	92 98
1	C	1135/2157 (53%)	1132 (100%)	3 (0%)	92 98
1	D	1135/2157 (53%)	1132 (100%)	3 (0%)	92 98
1	E	1135/2157 (53%)	1132 (100%)	3 (0%)	92 98
All	All	5675/10785 (53%)	5660 (100%)	15 (0%)	92 98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2104	ASP
1	E	2104	ASP
1	C	2189	ARG
1	E	2189	ARG
1	D	2189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1202	HIS
1	D	2497	GLN
1	D	1265	GLN
1	D	1972	HIS
1	E	1202	HIS

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1830:ASP	C	1831:PRO	N	1.02
1	B	1830:ASP	C	1831:PRO	N	1.02
1	C	1830:ASP	C	1831:PRO	N	1.02
1	D	1830:ASP	C	1831:PRO	N	1.02
1	E	1830:ASP	C	1831:PRO	N	1.02

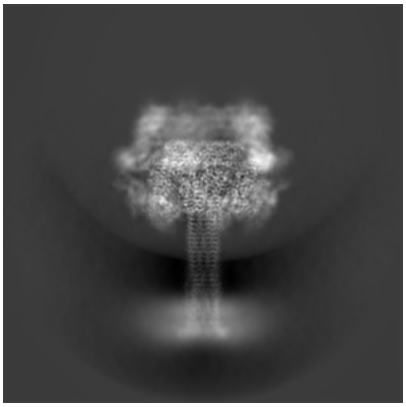
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4068. These allow visual inspection of the internal detail of the map and identification of artifacts.

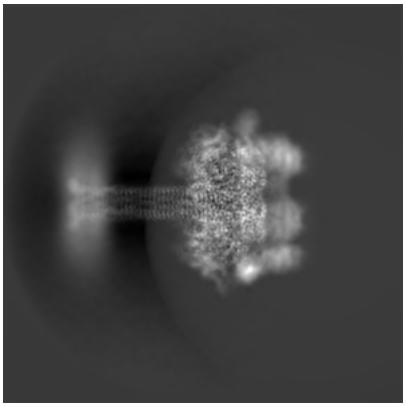
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

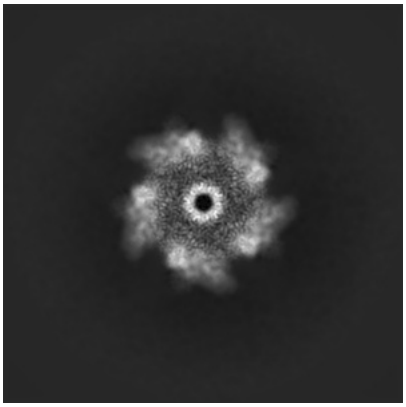
6.1.1 Primary map



X



Y



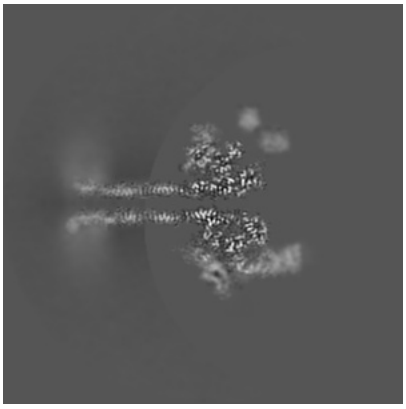
Z

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

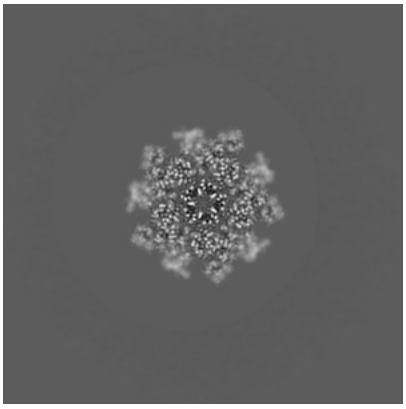
6.2 Central slices

6.2.1 Primary map

X Index: 141



Y Index: 141

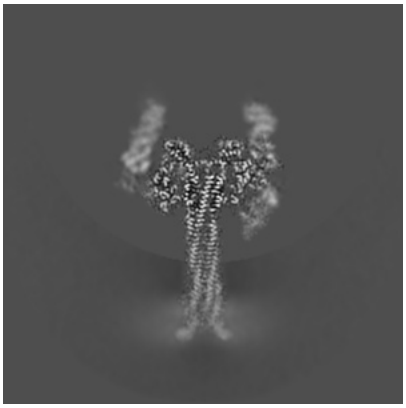


Z Index: 141

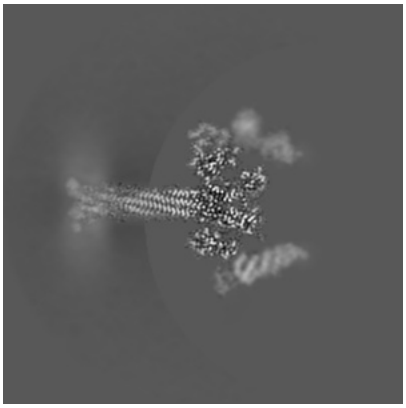
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

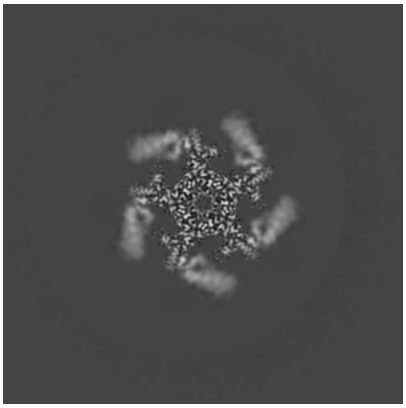
6.3.1 Primary map



X Index: 134



Y Index: 132



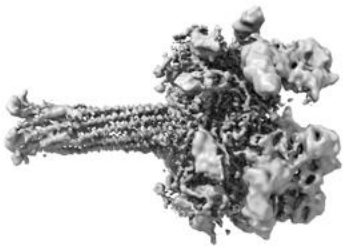
Z Index: 169

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

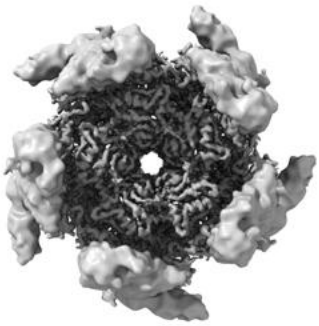
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

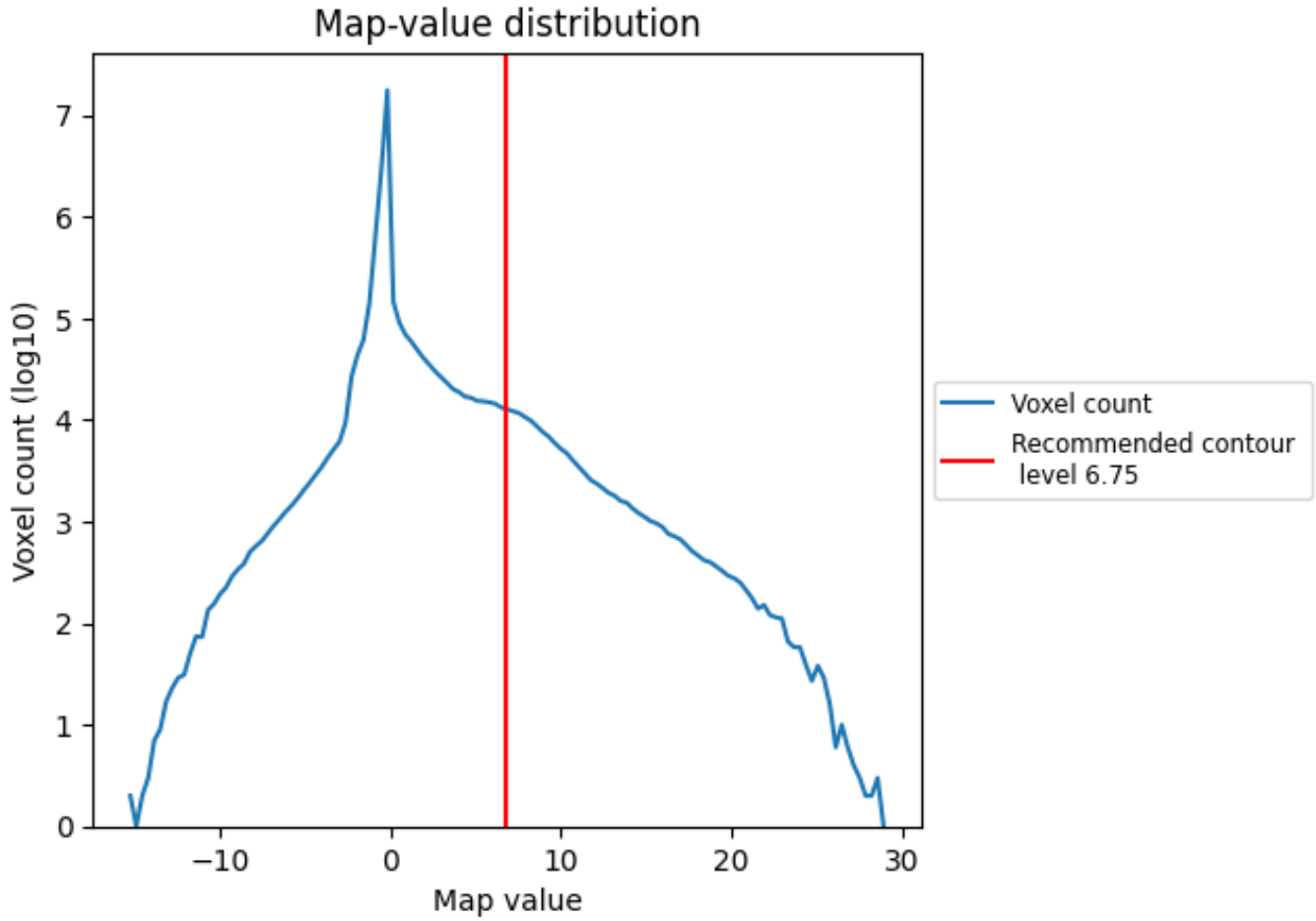
6.5 Mask visualisation (i)

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

7 Map analysis

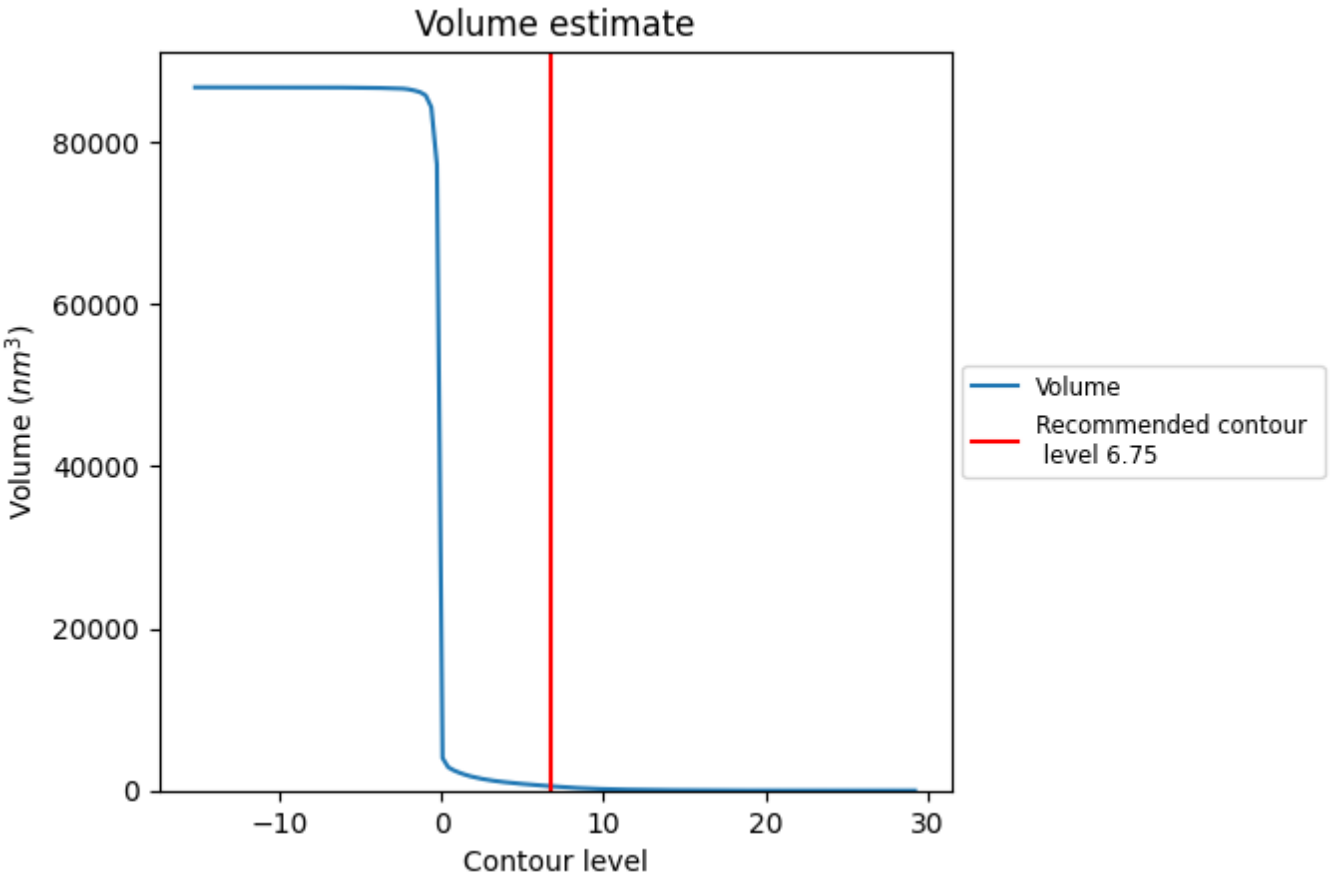
This section contains the results of statistical analysis of the map.

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.

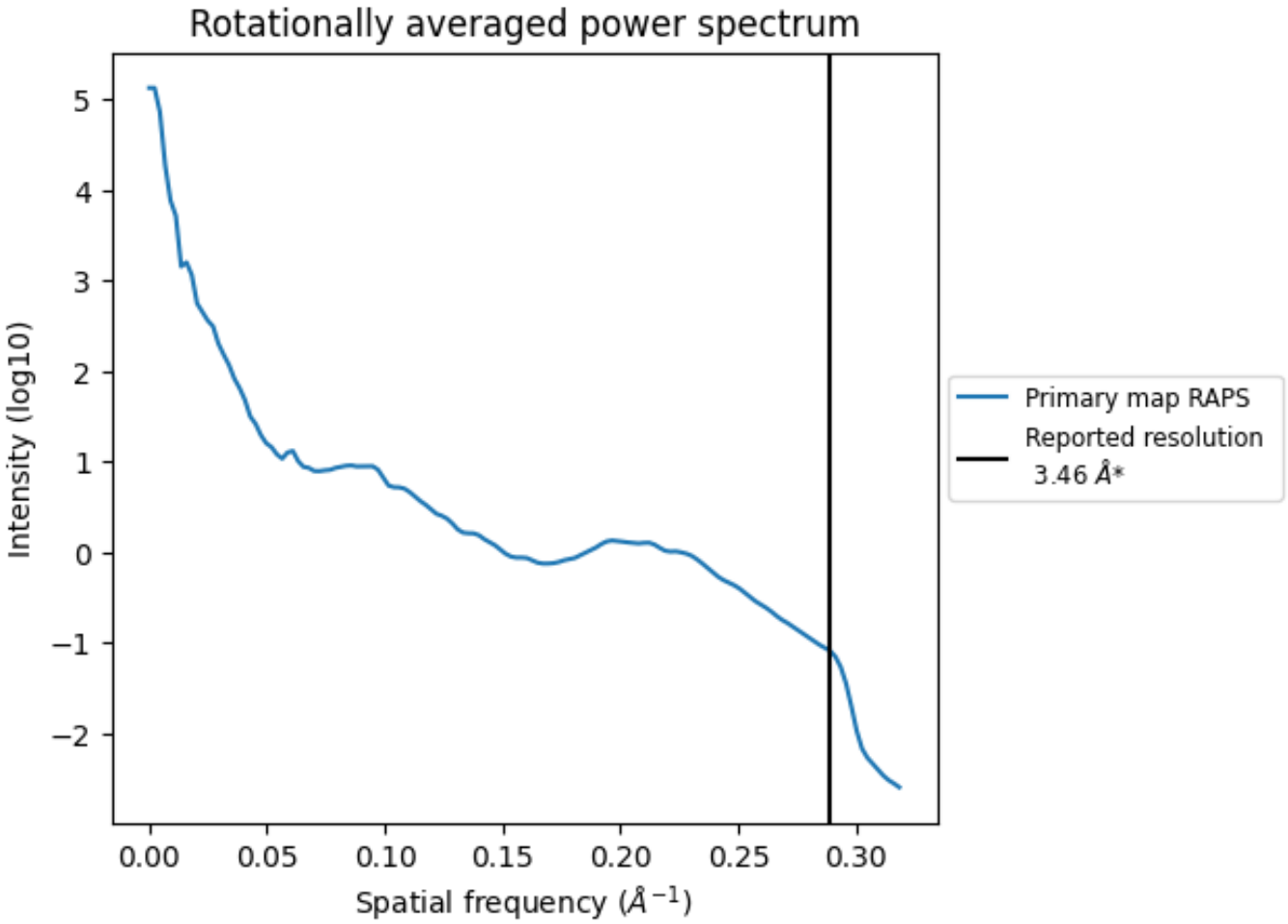
7.2 Volume estimate (i)



The volume at the recommended contour level is 535 nm^3; this corresponds to an approximate mass of 483 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 0.289 Å^{-1}

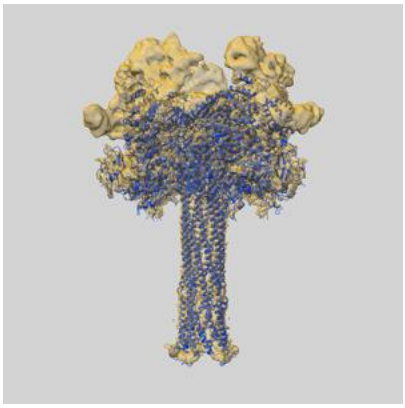
8 Fourier-Shell correlation (i)

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

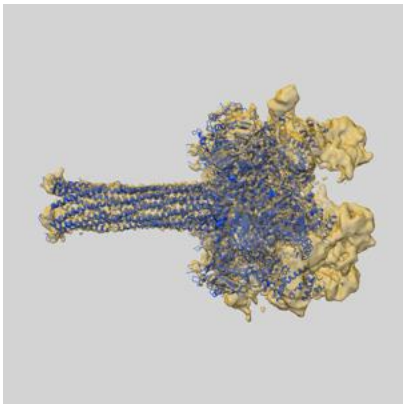
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4068 and PDB model 5LKI. Per-residue inclusion information can be found in section 3 on page 4.

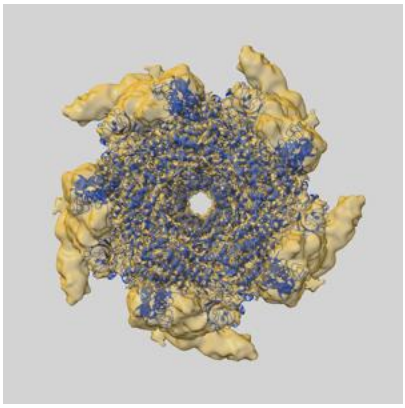
9.1 Map-model overlay



X



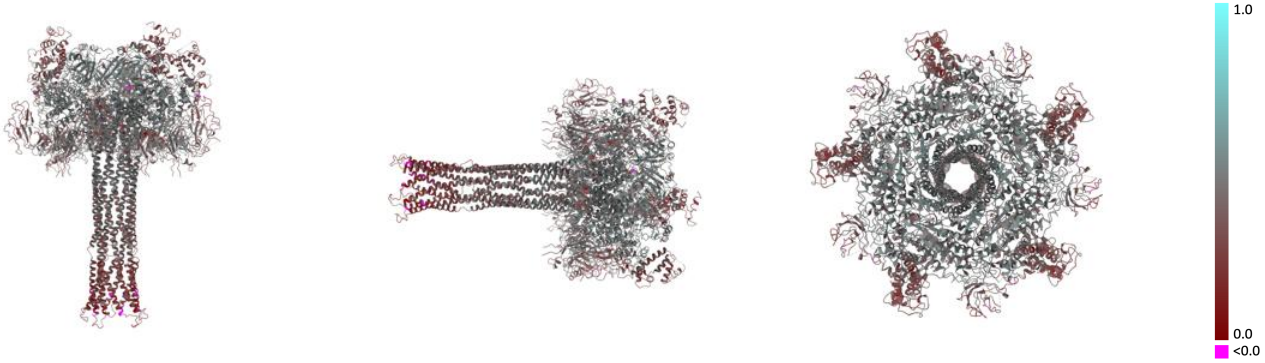
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.75 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.

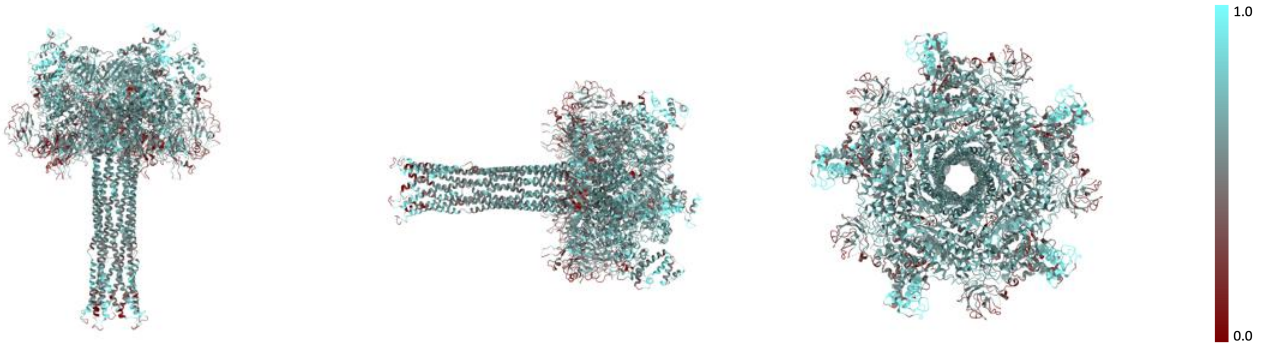
9.2 Q-score mapped to coordinate model (i)



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.

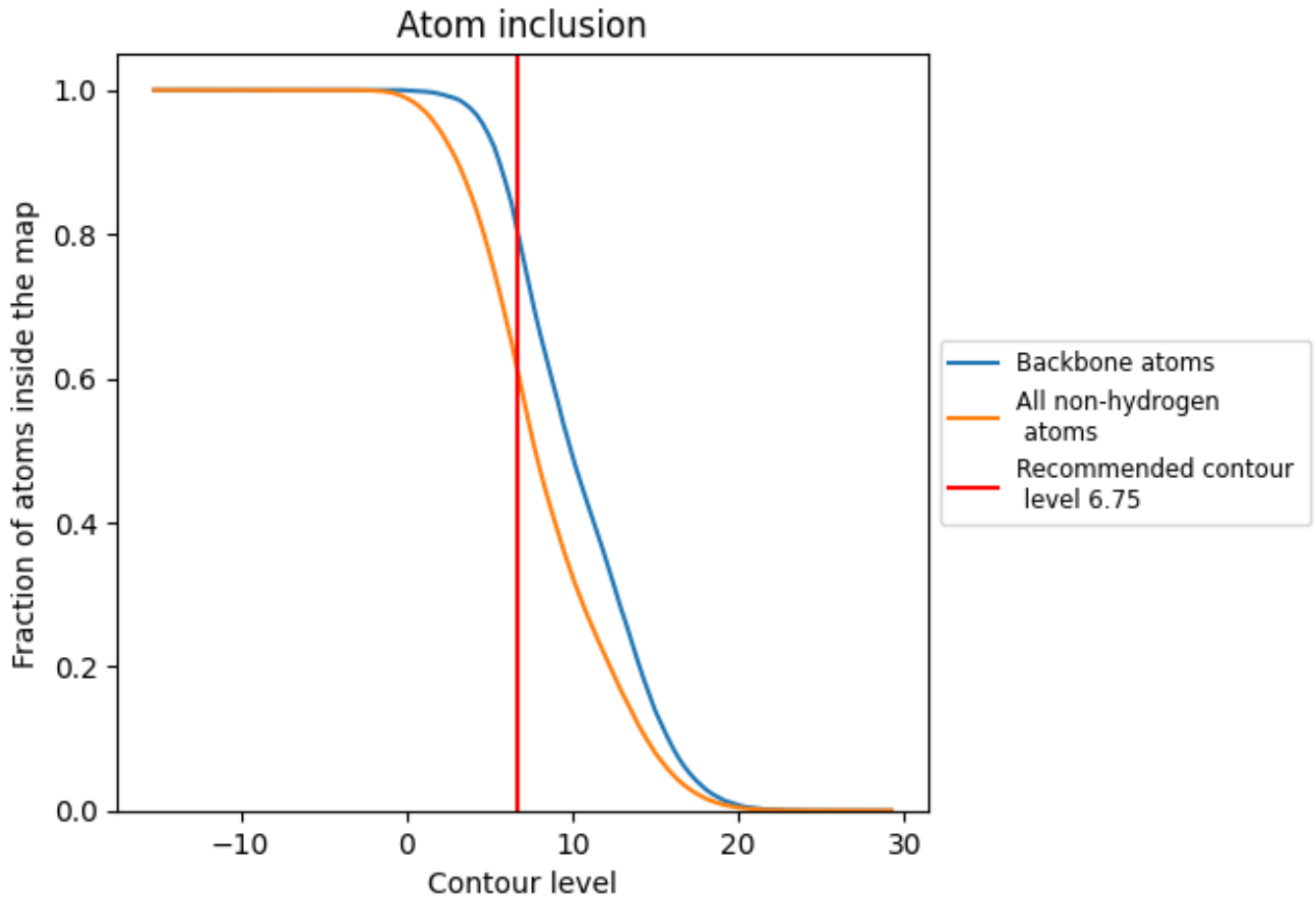
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.75).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 61% 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 (6.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6053	0.4300
A	0.6124	0.4380
B	0.6015	0.4270
C	0.6021	0.4270
D	0.6046	0.4280
E	0.6059	0.4300