wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 02:53 pm GMT

PDB ID	:	4V8V
EMDB ID	:	EMD-2358
Title	:	Structure and conformational variability of the Mycobacterium tuberculosis fatty acid synthase multienzyme complex
Authors	:	Ciccarelli, L.; Connell, S.R.; Enderle, M.; Mills, D.J.; Vonck, J.; Grininger, M.
Deposited on	:	2013-04-18
Resolution	:	20.00 Å(reported)
Based on initial model	:	4B3Y

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 (i) 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 (i)) were used in the production of this report:

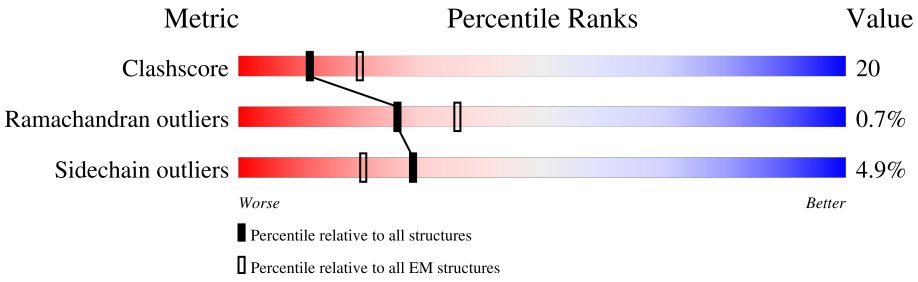
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 20.00 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	3089	57% 31% • 9%
1	B	3089	5% 57% 31% • 9%
1	C	3089	6% 57% 31% • 9%
1	D	3089	5% 57% 31% • 9%
1	E	3089	57% 31% • 9%
1	F	3089	5% 57% 31% • 9%

2 Entry composition (i)

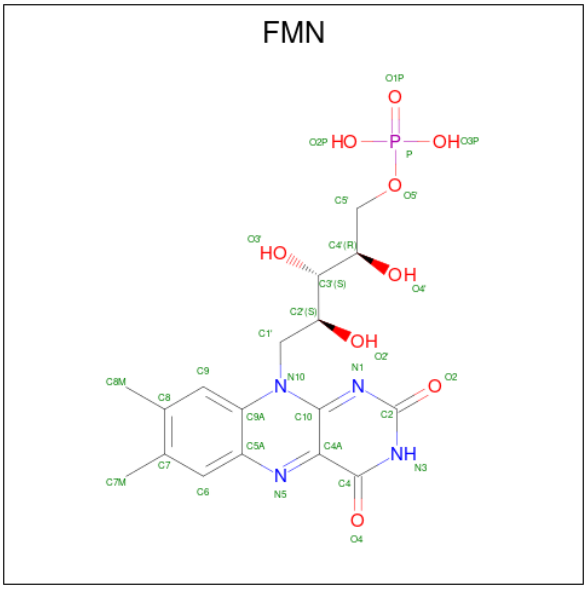
There are 2 unique types of molecules in this entry. The entry contains 125856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYPE-I FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	B	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	C	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	D	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	E	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	F	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

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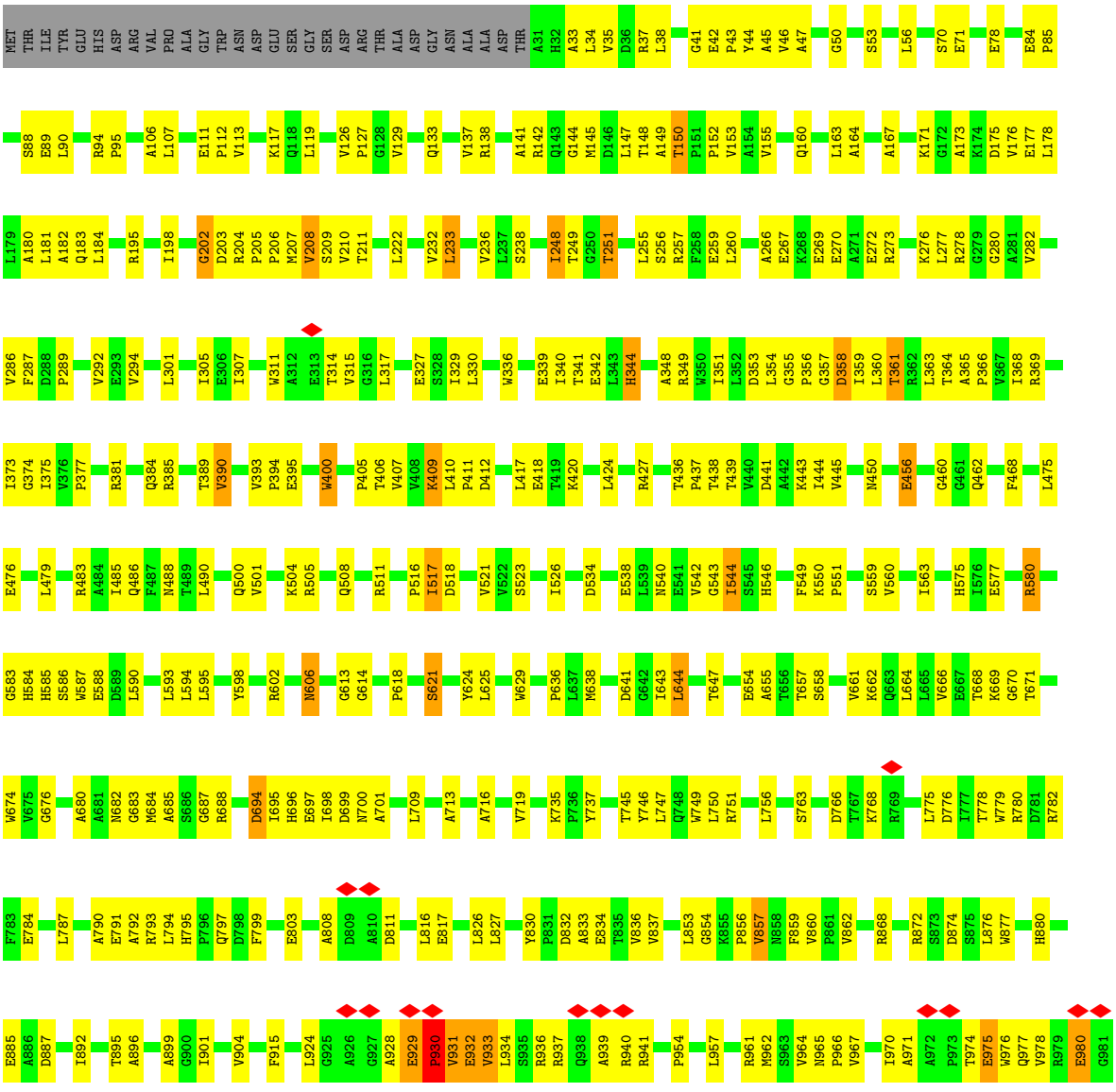
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

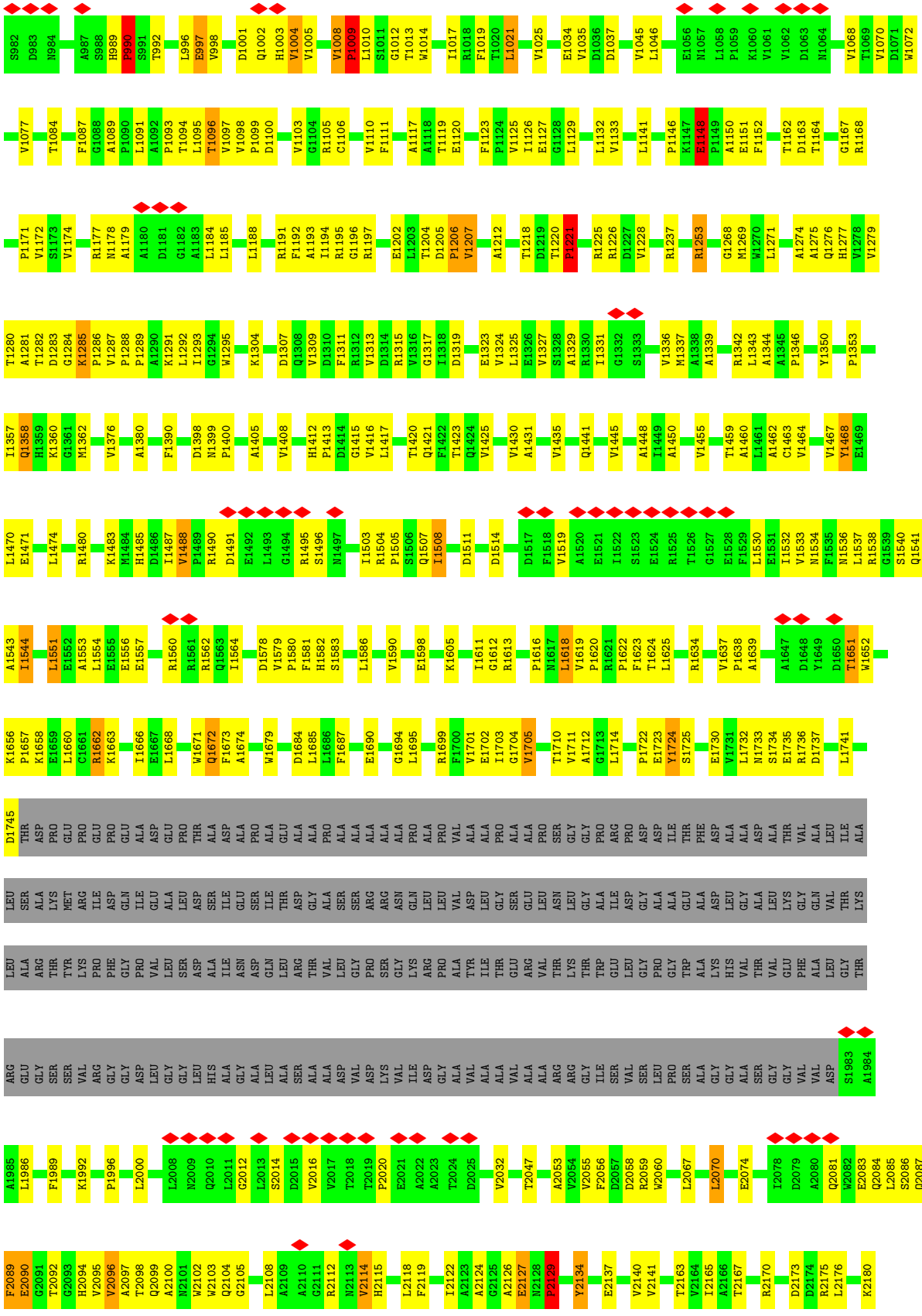
3 Residue-property plots (i)

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: TYPE-I FATTY ACID SYNTHASE

Chain A:

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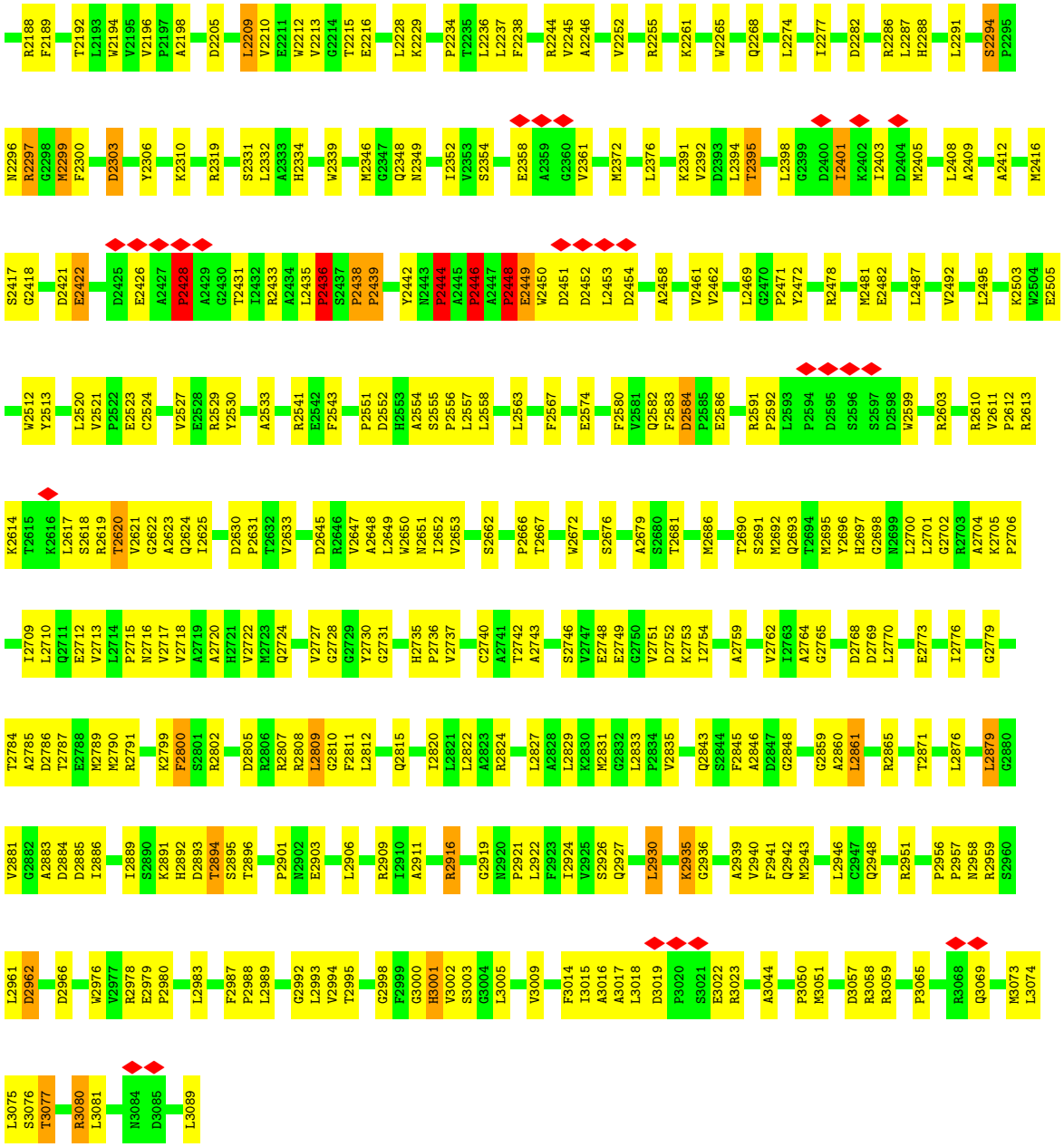
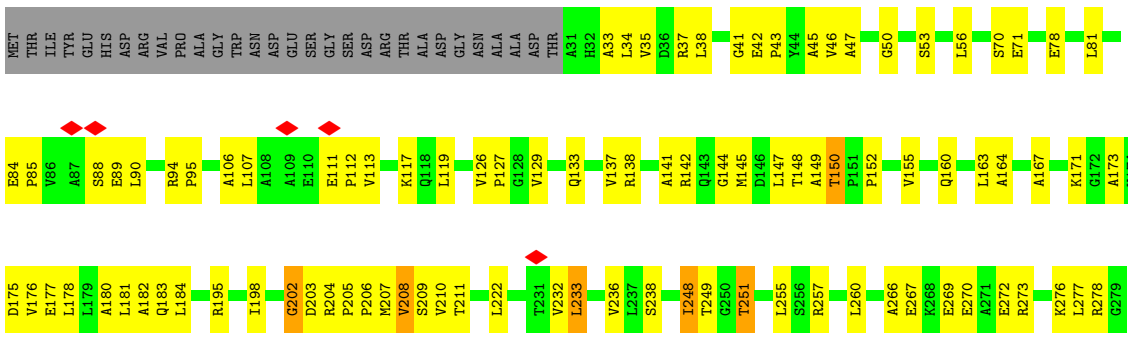
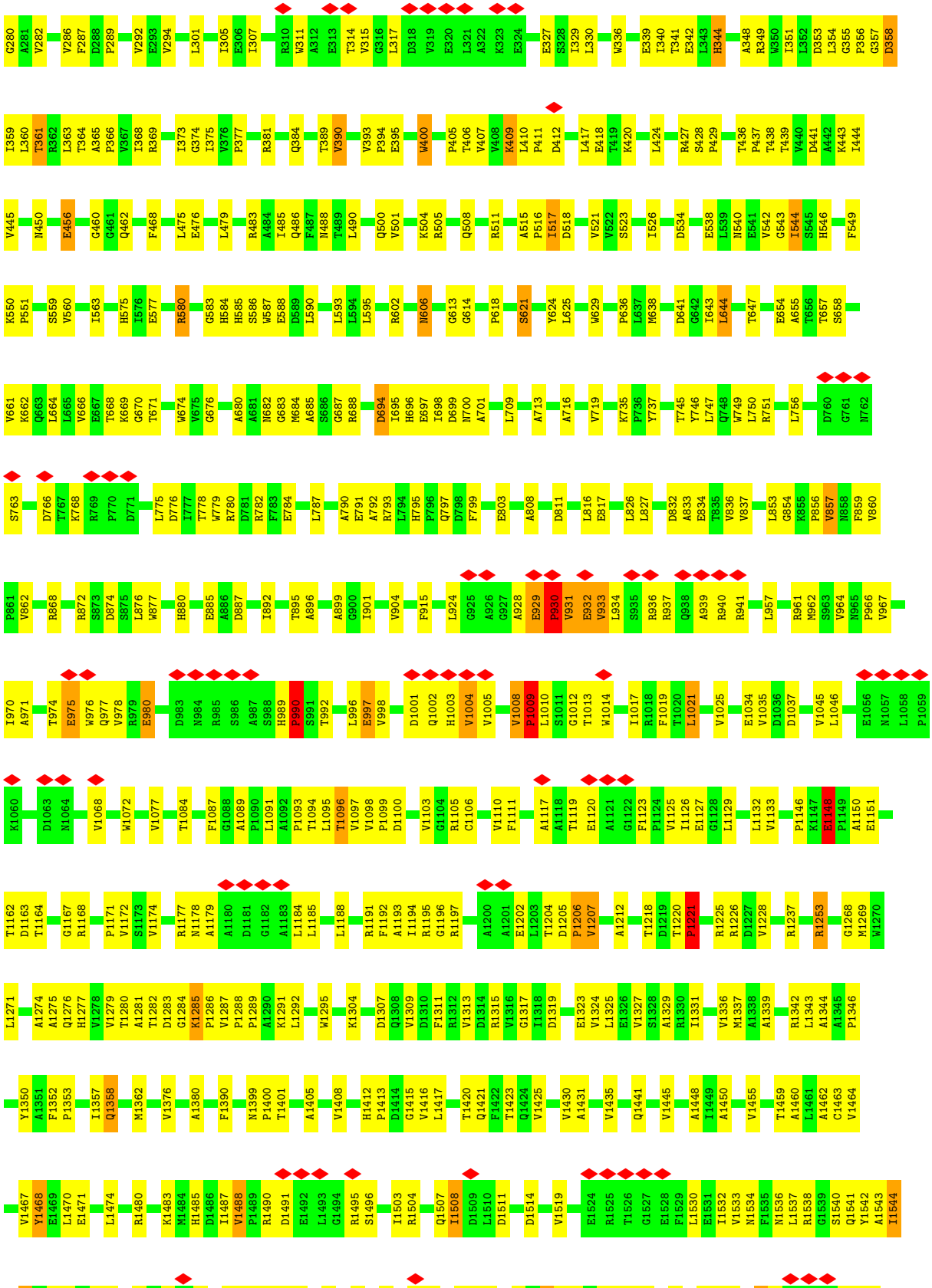
V1077 T1084 F1087 G1088 A1089 P1090 L1091 A1092 P1093 T1094 L1095 T1096 V1097 V1098 P1099 D1100 V1103 G1104 R1105 C1106 V1110 F1111 A1117 A1118 T1119 E1120 F1123 P1124 V1125 I1126 E1127 G1128 L1129 L1132 V1133 L1141 P1146 K1147 E1148 P1149 A1150 E1151 F1152 T1162 D1163 T1164 G1167 R1168
P1171 V1172 S1173 V1174 R1177 N1178 A1179 A1180 D1181 G1182 A1183 L1184 L1185 L1188 R1191 F1192 A1193 I1194 R1195 G1196 R1197 E1202 L1203 T1204 D1205 P1206 V1207 A1212 T1218 D1219 T1220 P1221 R1225 R1226 D1227 V1228 R1237 R1253 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279
T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 I1293 G1294 W1295 K1304 D1307 Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319 E1323 V1324 L1325 E1326 V1327 S1328 A1329 R1330 I1331 G1332 S1333 V1336 M1337 A1338 A1339 R1342 L1343 A1344 A1345 P1346 Y1350 P1353
I1357 Q1358 H1359 K1360 G1361 M1362 V1376 A1380 F1390 D1398 N1399 P1400 A1405 V1408 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425 V1430 A1431 V1435 Q1441 V1445 A1448 I1449 A1450 V1455 T1459 A1460 L1461 A1462 C1463 V1464 V1467 Y1468 E1469
L1470 E1471 L1474 R1480 K1483 M1484 H1485 D1486 I1487 V1488 P1489 R1490 D1491 E1492 L1493 G1494 R1495 S1496 N1497 I1503 R1504 P1505 S1506 Q1507 I1508 D1511 D1514 D1517 F1518 V1519 A1520 E1521 I1522 S1523 E1524 R1525 T1526 G1527 E1528 F1529 L1530 E1531 I1532 V1533 N1534 F1535 N1536 L1537 R1538 G1539 S1540 Q1541 Y1542
A1543 I1544 L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 T1564 D1578 V1579 P1580 F1581 H1582 S1583 L1586 V1590 E1598 K1605 I1611 G1612 R1613 P1616 N1617 L1618 V1619 P1620 R1621 P1622 F1623 T1624 L1625 R1634 V1637 P1638 A1639 A1647 D1648 Y1649 D1650 T1651 W1652
K1656 P1657 K1658 E1659 L1660 C1661 R1662 K1663 I1666 E1667 L1668 W1671 Q1672 F1673 A1674 W1679 D1684 L1685 L1686 F1687 E1690 G1694 L1695 R1699 F1700 V1701 E1702 I1703 G1704 V1705 T1710 V1711 A1712 G1713 L1714 P1722 E1723 Y1724 S1725 E1730 V1731 L1732 N1733 S1734 E1735 R1736 D1737 L1741
D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU GLU ALA ALA PRO ALA ALA ALA ALA ALA PRO ALA PRO ALA ALA ALA ALA PRO VAL ALA ALA ALA PRO ALA ALA PRO SER GLY GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP LEU ILE ALA
LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU GLU SER ILE THR ASP GLY ALA SER SER ARG ASN GLN LEU LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA GLU ALA ASP LEU GLY ALA LEU LYS GLY GLN VAL THR LYS
LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO GLY TRP ALA LYS HIS VAL THR VAL GLU PHE ALA LEU GLY THR
ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU LEU GLY GLY LEU HIS ALA GLY ALA GLY ALA LEU ALA SER ALA ALA ASP VAL ASP LYS VAL ILE ASP GLY ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY VAL VAL ASP S1983 A1984
A1985 L1986 F1989 K1992 P1996 L2000 L2008 N2009 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 V2017 T2018 T2019 P2020 E2021 A2022 A2023 T2024 D2025 V2032 T2047 A2053 V2054 V2055 F2056 D2057 D2058 R2059 W2060 L2067 L2070 E2074 I2078 D2079 A2080 Q2081 W2082 E2083 Q2084 L2085 S2086 Q2087 R2088
F2089 E2090 G2091 T2092 G2093 H2094 V2095 V2096 A2097 T2098 Q2099 A2100 N2101 W2102 W2103 Q2104 G2105 L2108 A2109 A2110 G2111 R2112 N2113 V2114 H2115 L2118 F2119 I2122 A2123 A2124 G2125 A2126 E2127 N2128 P2129 Y2134 E2137 V2140 V2141 T2163 V2164 I2165 A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180



• Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain B:




G280 A281 V282 V286 F287 D288 P289 V292 E293 V294 L301 I305 E306 I307 R310 W311 A312 E313 T314 V315 G316 L317 D318 V319 E320 L321 A322 K323 E324 E327 S328 I329 L330 W336 E339 I340 T341 E342 L343 R344 A348 R349 W350 I351 L352 D353 L354 G355 P356 G357 D358
I359 L360 T361 R362 L363 T364 A365 P366 V367 I368 R369 I373 G374 I375 V376 P377 R381 Q384 T389 V390 V393 P394 E395 W400 P405 T406 V407 V408 K409 L410 P411 D412 L417 E418 T419 K420 L424 R427 S428 P429 T436 P437 T438 T439 V440 D441 A442 K443 T444
V445 N450 E456 G460 G461 Q462 F468 L475 E476 L479 R483 A484 I485 Q486 F487 N488 T489 L490 Q500 V501 K504 R505 Q508 R511 A515 P516 I517 D518 V521 V522 S523 I526 D534 E538 L539 N540 E541 V542 G543 T544 S545 H546 F549
K550 P551 S559 V560 I563 H575 I576 E577 R580 G583 H584 H585 S586 W587 E588 D589 L590 L593 L594 L595 R602 N606 G613 G614 P618 S621 Y624 L625 W629 P636 L637 M638 D641 G642 I643 L644 T647 E654 A655 T656 T657 S658
V661 K662 Q663 L664 L665 V666 E667 T668 K669 G670 T671 W674 V675 G676 A680 A681 N682 G683 M684 A685 S686 G687 R688 D694 I695 H696 E697 I698 D699 N700 A701 L709 A713 A716 V719 K735 P736 Y737 T745 Y746 L747 Q748 W749 L750 R751 L756 D760 G761 N762
S763 D766 T767 K768 R769 P770 D771 L775 D776 I777 T778 W779 R780 D781 R782 F783 E784 L787 A790 E791 A792 R793 L794 H795 P796 Q797 D798 F799 E803 A808 D811 L816 E817 L826 L827 D832 A833 E834 T835 V836 V837 L853 G854 K855 P856 V857 N858 F859 V860
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T1162 D1163 T1164 G1167 R1168 P1171 V1172 S1173 V1174 R1177 N1178 A1179 A1180 D1181 G1162 A1183 L1184 L1185 L1188 R1191 F1192 A1193 I1194 R1195 G1196 R1197 A1200 A1201 E1202 L1203 T1204 D1205 P1206 V1207 A1212 T1218 D1219 T1220 P1221 R1225 R1226 D1227 V1228 R1237 R1253 G1268 M1269 W1270
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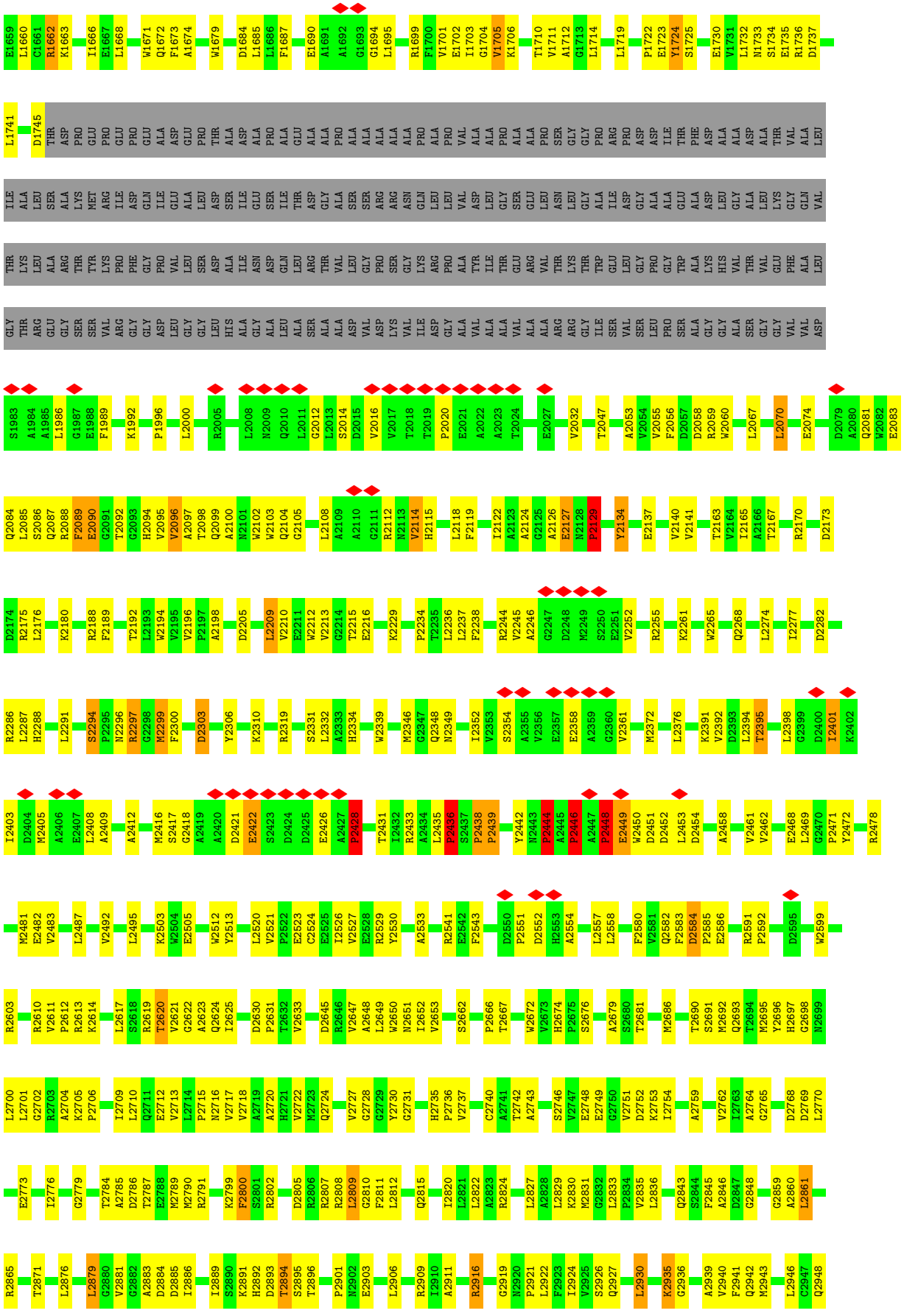
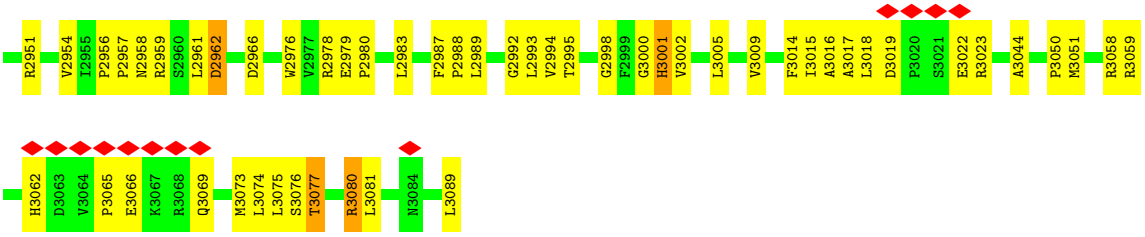
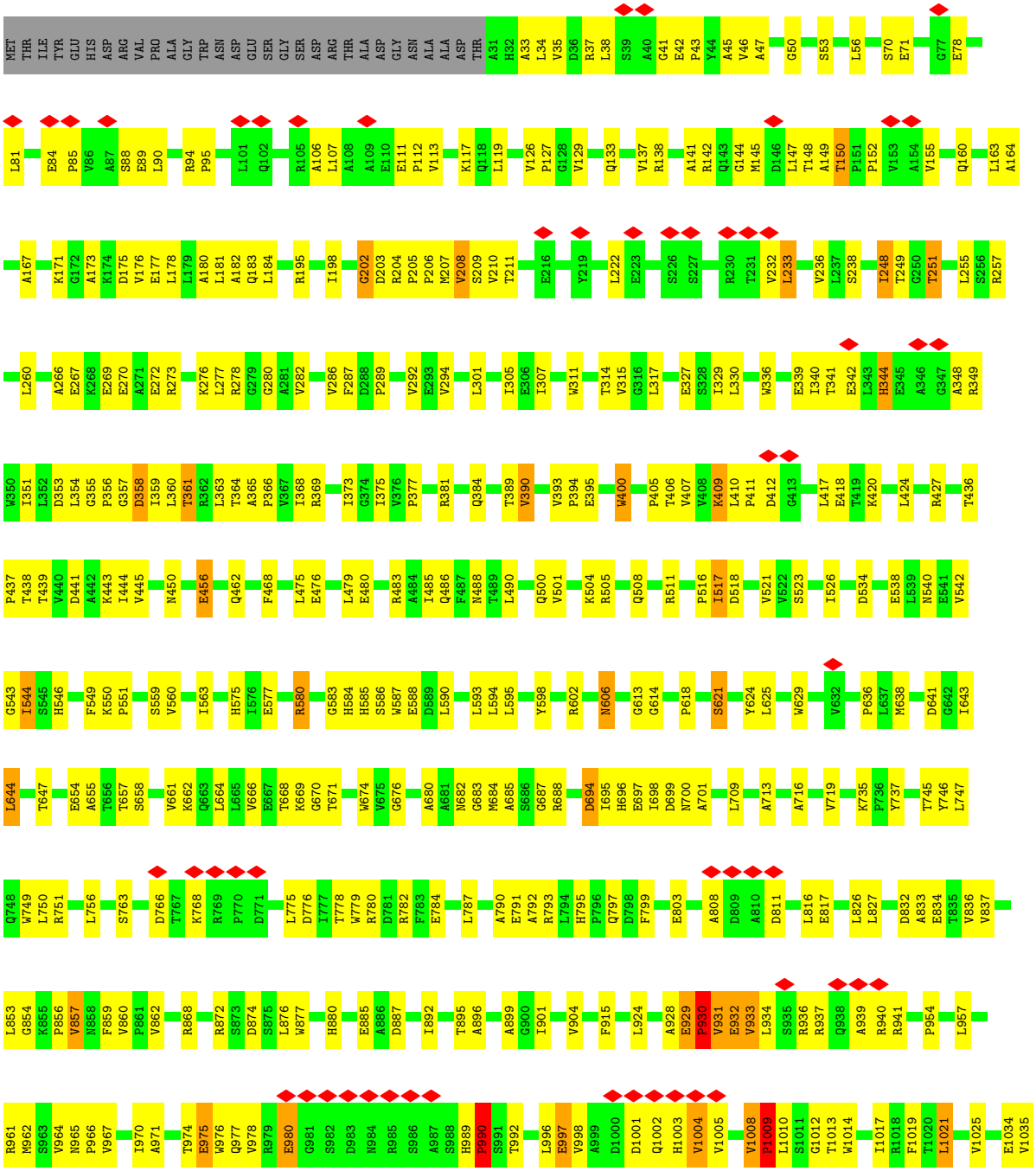
V1467 Y1468 E1469 L1470 E1471 L1474 R1480 K1483 M1484 H1485 D1486 I1487 V1488 P1489 R1490 D1491 E1492 L1493 G1494 R1495 S1496 I1503 R1504 Q1507 I1508 D1509 L1510 D1511 D1514 V1519 E1524 R1525 T1526 G1527 E1528 F1529 L1530 E1531 I1532 V1533 N1534 F1535 N1536 L1537 R1538 S1539 S1540 Q1541 Y1542 A1543 I1544
L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 I1564 D1578 V1579 P1580 F1581 H1582 S1583 L1586 V1590 E1598 D1604 K1605 I1611 G1612 R1613 P1616 N1617 L1618 V1619 P1620 R1621 P1622 F1623 T1624 L1625 R1634 V1637 P1638 A1639 T1651 W1652 R1653 N1654 E1655 K1656 P1657 K1658

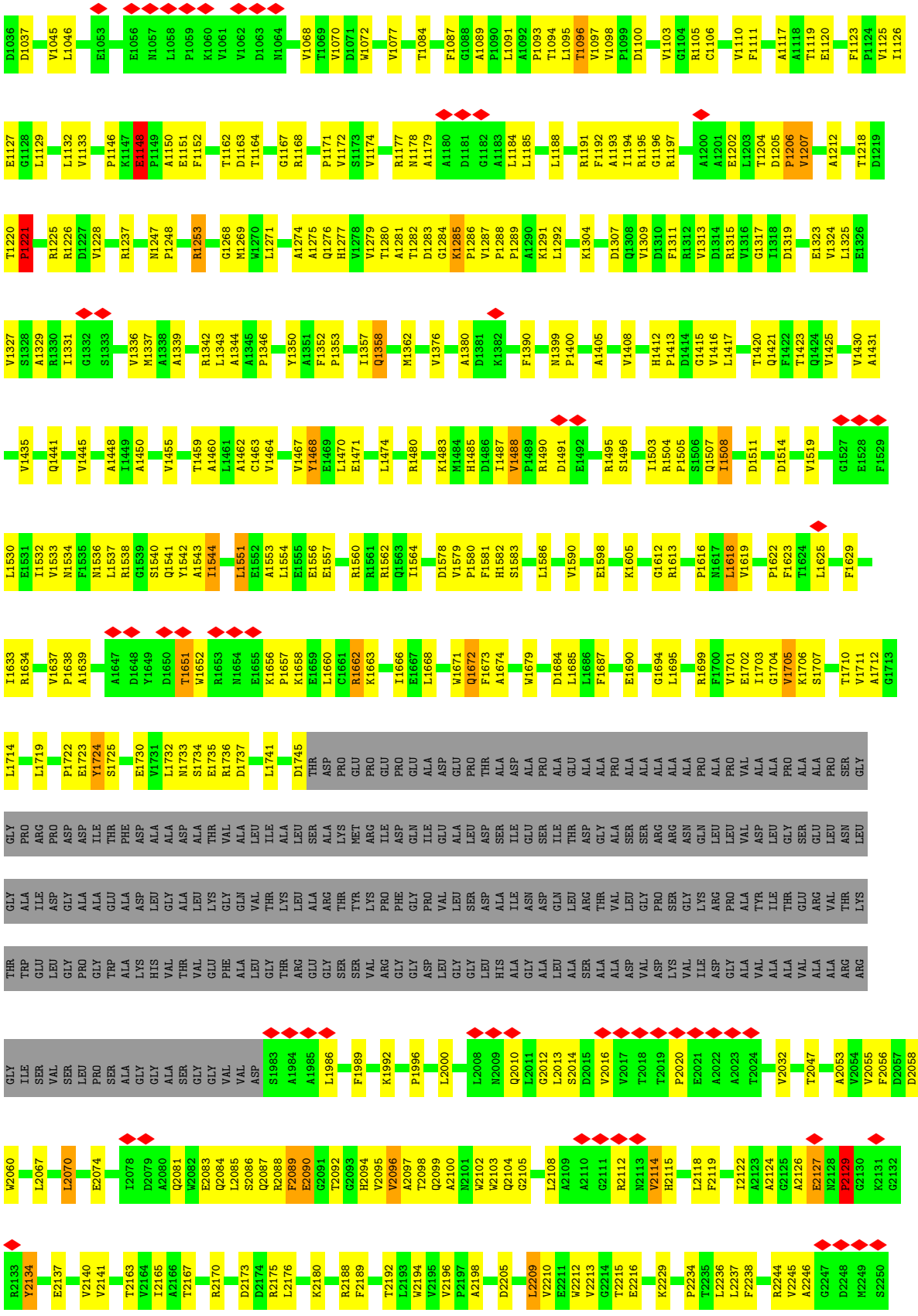




• Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain C:

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E1127 G1128 L1129 L1132 V1133 P1146 K1147 E1148 P1149 A1150 E1151 F1152 T1162 D1163 T1164 G1167 R1168 P1171 V1172 S1173 V1174 R1177 N1178 A1179 A1180 D1181 G1182 A1183 L1184 L1185 L1188 R1191 F1192 A1193 I1194 R1195 G1196 R1197 A1200 A1201 E1202 L1203 T1204 D1205 P1206 V1207 A1212 T1218 D1219
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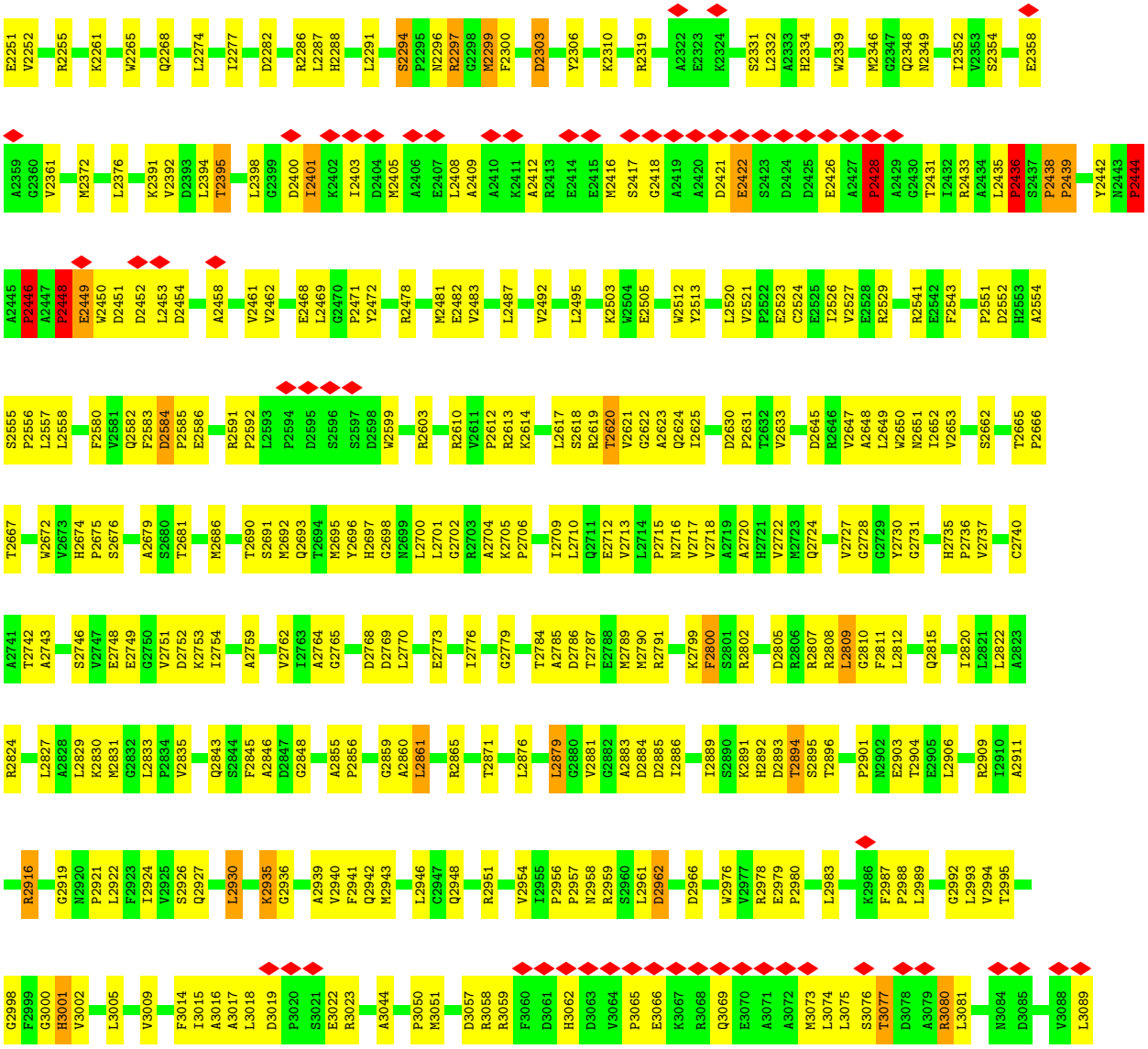
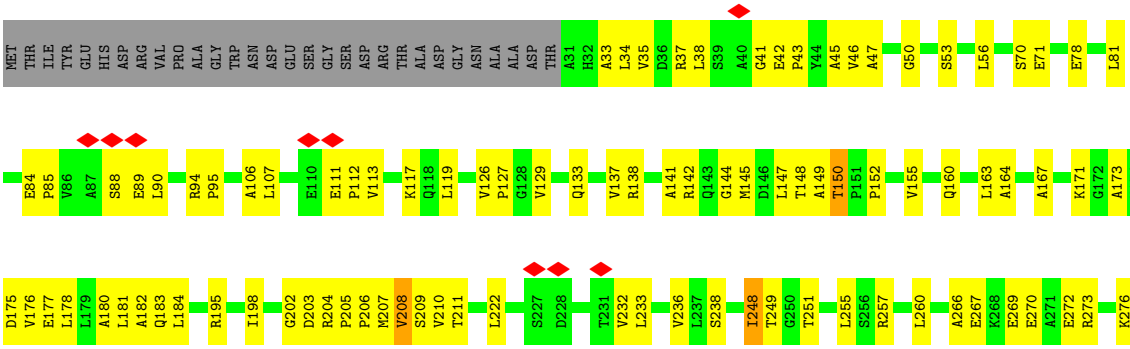
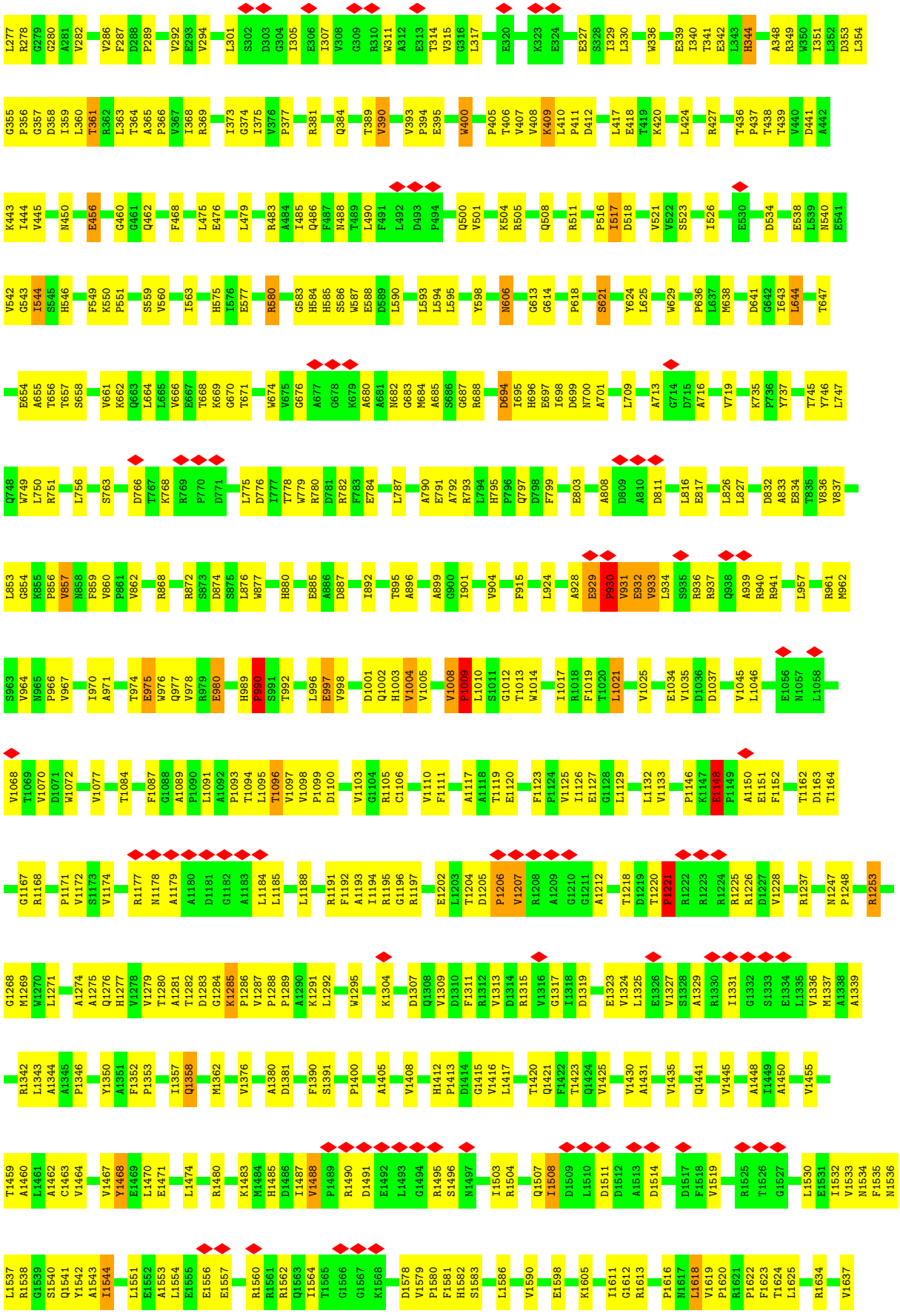
L1714 L1719 P1722 E1723 Y1724 S1725 E1730 V1731 L1732 N1733 S1734 E1735 R1736 D1737 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA ALA ALA ALA ALA PRO ALA PRO VAL ALA ALA PRO ALA ALA PRO SER GLY
GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU
GLY ALA ILE ASP GLY ALA ALA GLU ALA ASP LEU GLY ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LYS
THR TRP GLU LEU GLY PRO GLY TRP ALA LYS HIS VAL THR VAL GLU PHE ALA LEU GLY THR ARG GLU ALA GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY GLY LEU HIS ALA GLY ALA LEU ASP VAL ASP SER VAL ILE ASP GLY VAL ALA ALA ALA VAL ALA ALA VAL THR ARG
GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY GLY ALA SER GLY GLY VAL VAL ASP S1983 A1984 A1985 L1986 F1989 K1992 P1996 L2000 L2008 N2009 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 V2017 T2018 T2019 P2020 E2021 A2022 A2023 T2024 V2032 T2047 A2053 V2054 V2055 F2056 D2057 D2058 R2059
W2060 L2067 L2070 E2074 I2078 D2079 A2080 Q2081 W2082 E2083 Q2084 L2085 S2086 Q2087 R2088 F2089 E2090 G2091 T2092 G2093 H2094 V2095 V2096 A2097 T2098 Q2099 A2100 N2101 W2102 W2103 Q2104 G2105 L2108 A2109 A2110 G2111 R2112 N2113 V2114 H2115 L2118 F2119 I2122 A2123 A2124 G2125 A2126 E2127 N2128 P2129 G2130 K2131 G2132
R2133 Y2134 E2137 V2140 V2141 T2163 V2164 I2165 A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180 R2188 F2189 T2192 L2193 W2194 V2195 V2196 P2197 A2198 D2205 L2209 V2210 E2211 W2212 V2213 G2214 T2215 E2216 K2229 P2234 T2235 L2236 L2237 F2238 R2244 V2245 A2246 G2247 D2248 M2249 S2250



• Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain D:

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G355 P356 G357 D358 I359 L360 T361 R362 L363 T364 A365 P366 V367 I368 R369 I373 G374 I375 V376 P377 R381 Q384 T389 V390 V393 P394 E395 W400 P405 T406 V407 V408 K409 L410 P411 D412 L417 E418 T419 K420 L424 R427 T436 P437 T438 T439 V440 D441 A442
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L853 G854 K855 P856 V857 N858 F859 V860 P861 V862 R868 R872 S873 D874 S875 L876 W877 H880 E885 A886 D887 I892 T895 A896 A899 G900 I901 V904 F915 L924 A928 E929 P930 V931 E932 V933 L934 S935 R936 R937 Q938 A939 R940 R941 L957 R961 M962
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V1068 T1069 V1070 D1071 W1072 V1077 T1084 F1087 G1088 A1089 P1090 L1091 A1092 P1093 T1094 L1095 T1096 V1097 V1098 P1099 D1100 V1103 G1104 R1105 C1106 V1110 F1111 A1117 A1118 E1120 F1123 P1124 V1125 I1126 E1127 G1128 L1129 L1132 V1133 P1146 K1147 E1148 P1149 A1150 E1151 F1152 T1162 D1163 T1164
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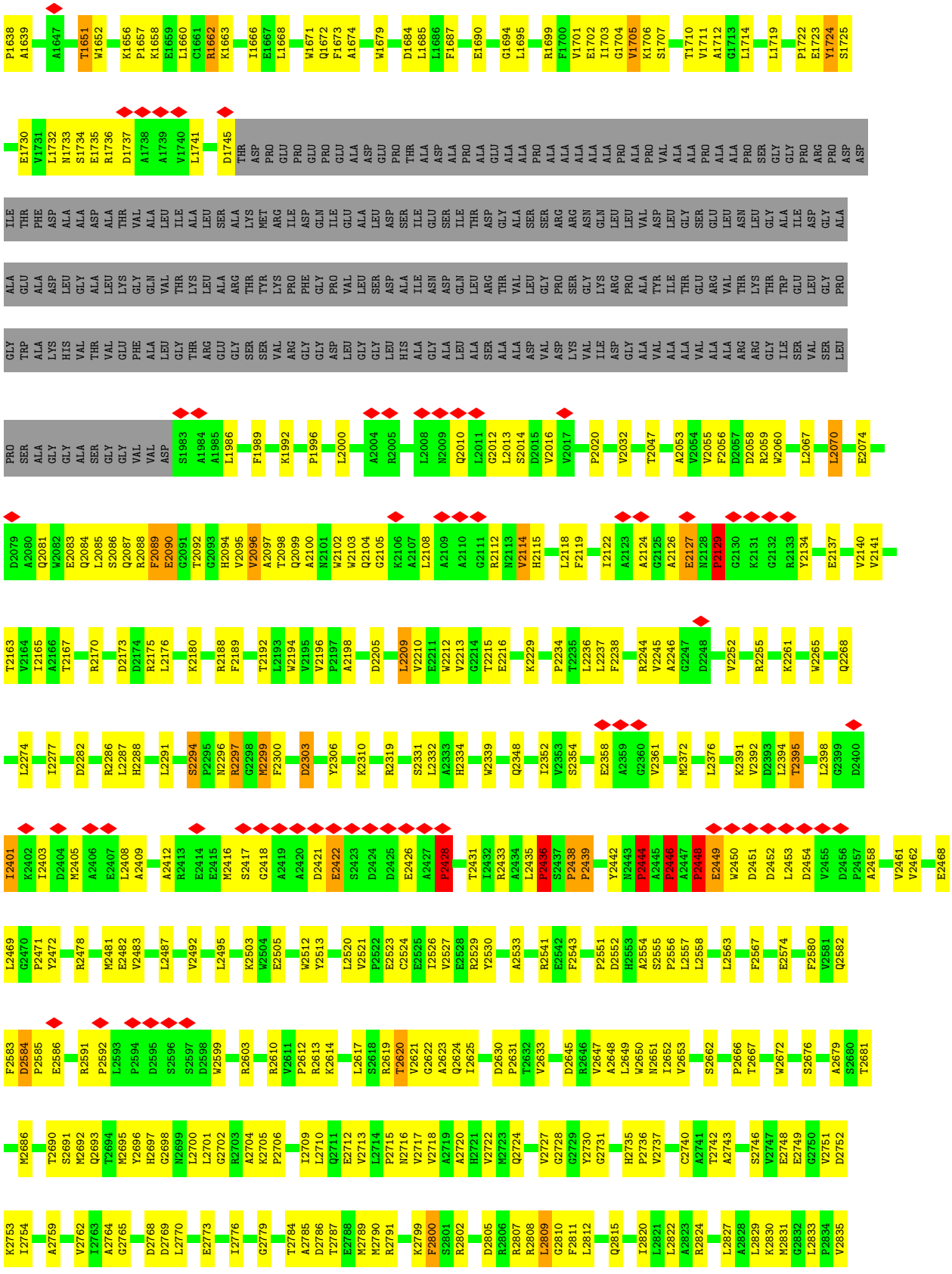
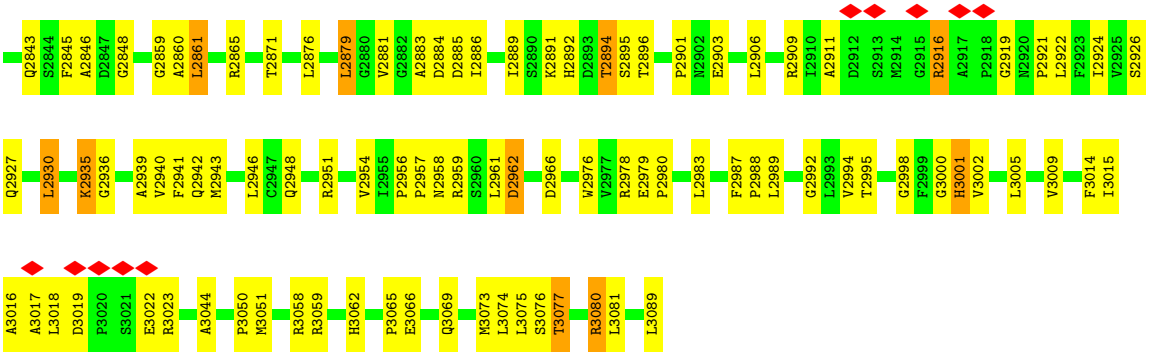
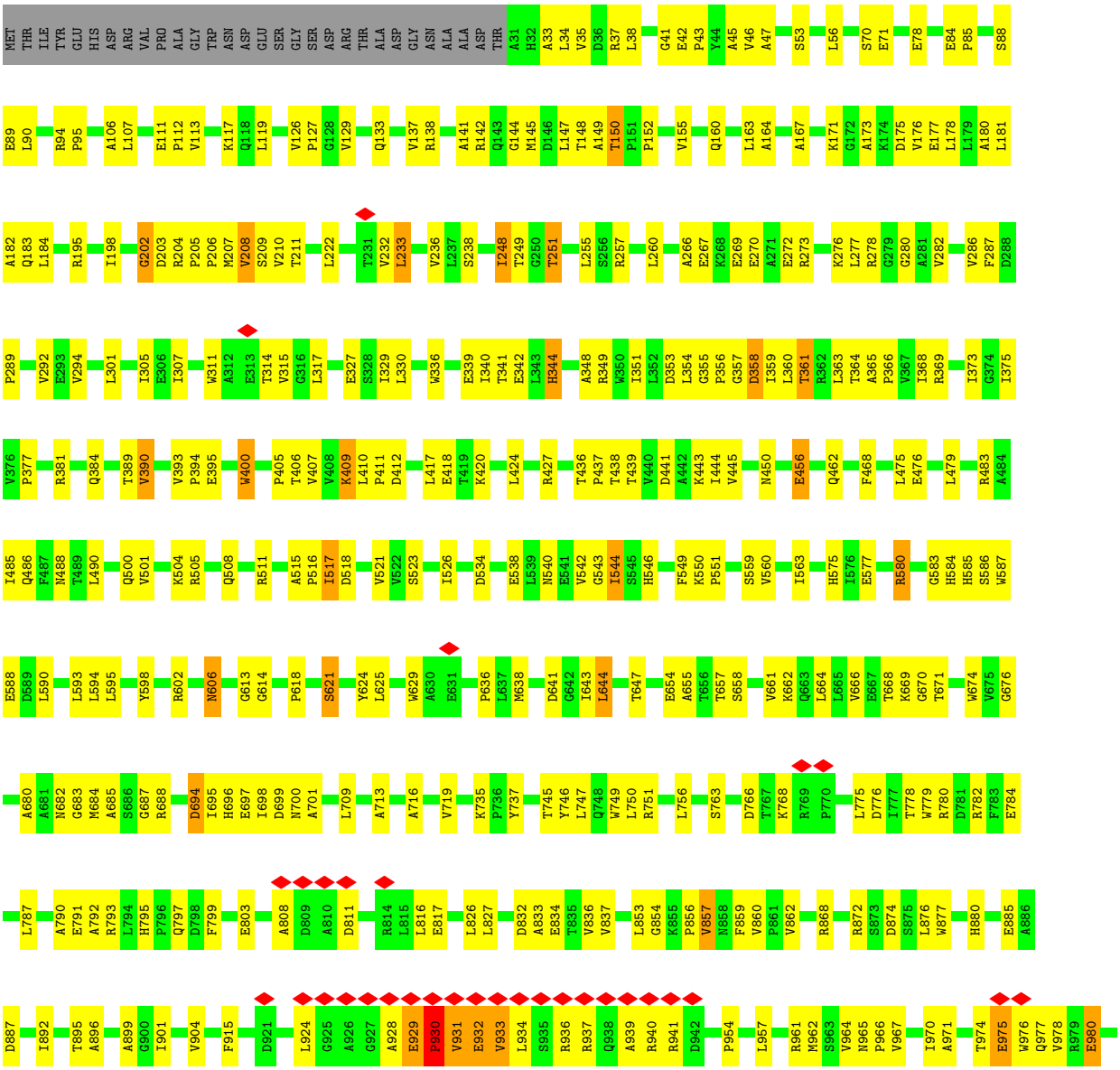
R1342 L1343 A1344 A1345 P1346 Y1350 A1351 F1352 P1353 I1357 Q1358 M1362 V1376 A1380 D1381 F1390 S1391 P1400 A1405 V1408 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425 V1430 A1431 V1435 Q1441 V1445 A1448 I1449 A1450 V1455
T1459 A1460 L1461 A1462 C1463 V1464 V1467 Y1468 E1469 L1470 E1471 L1474 R1480 K1483 M1484 H1485 D1486 I1487 V1488 P1489 R1490 D1491 E1492 L1493 G1494 R1495 S1496 N1497 I1503 R1504 Q1507 I1508 D1509 L1510 D1511 D1512 A1513 D1514 D1517 F1518 V1519 R1525 T1526 G1527 L1530 E1531 I1532 V1533 N1534 F1535 N1536
L1537 R1538 G1539 S1540 Q1541 Y1542 A1543 I1544 L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 I1564 T1565 G1566 G1567 K1568 D1578 V1579 P1580 F1581 H1582 S1583 L1586 V1590 E1598 K1605 I1611 G1612 R1613 P1616 N1617 L1618 V1619 P1620 R1621 P1622 F1623 T1624 L1625 R1634 V1637

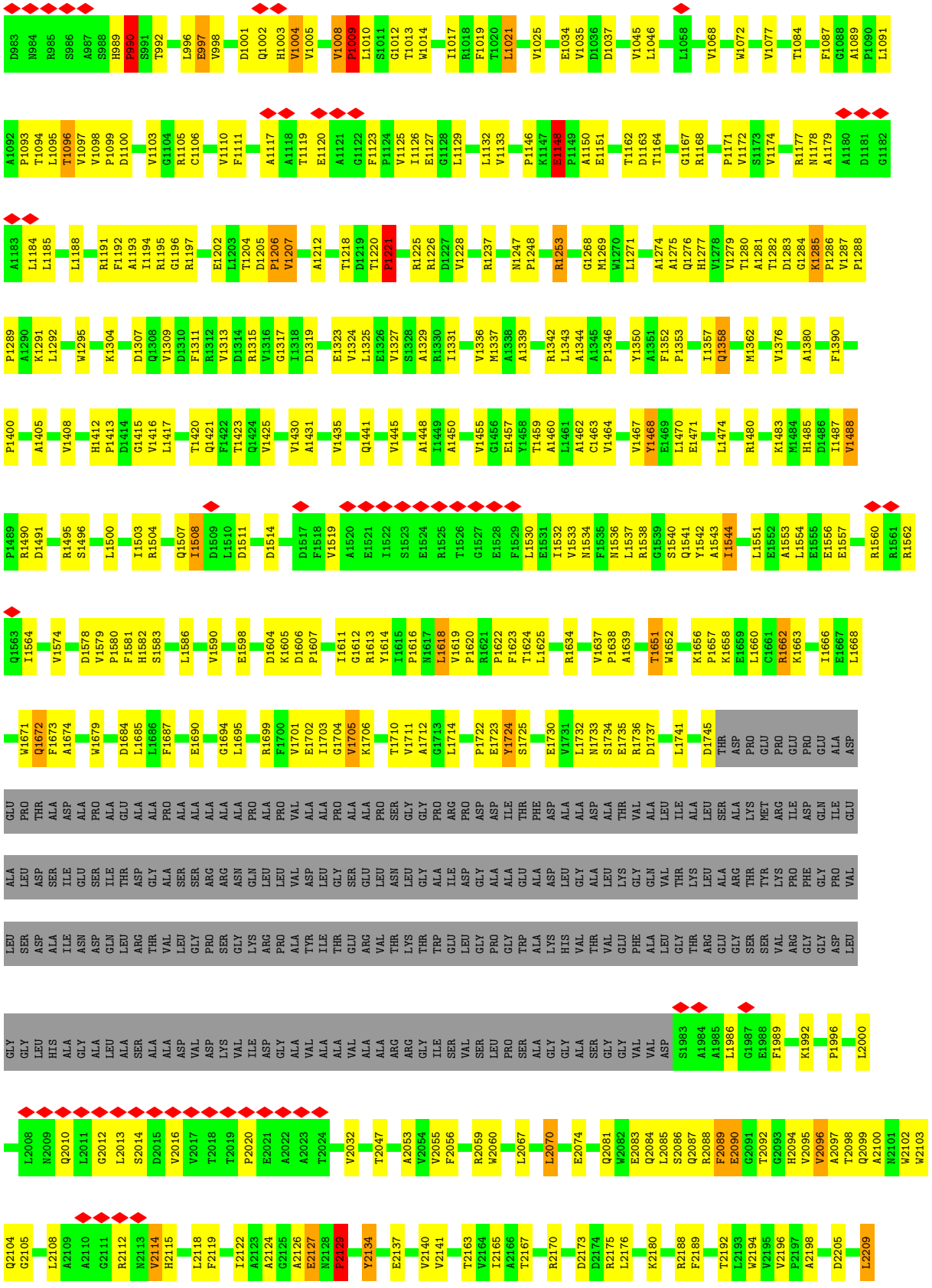


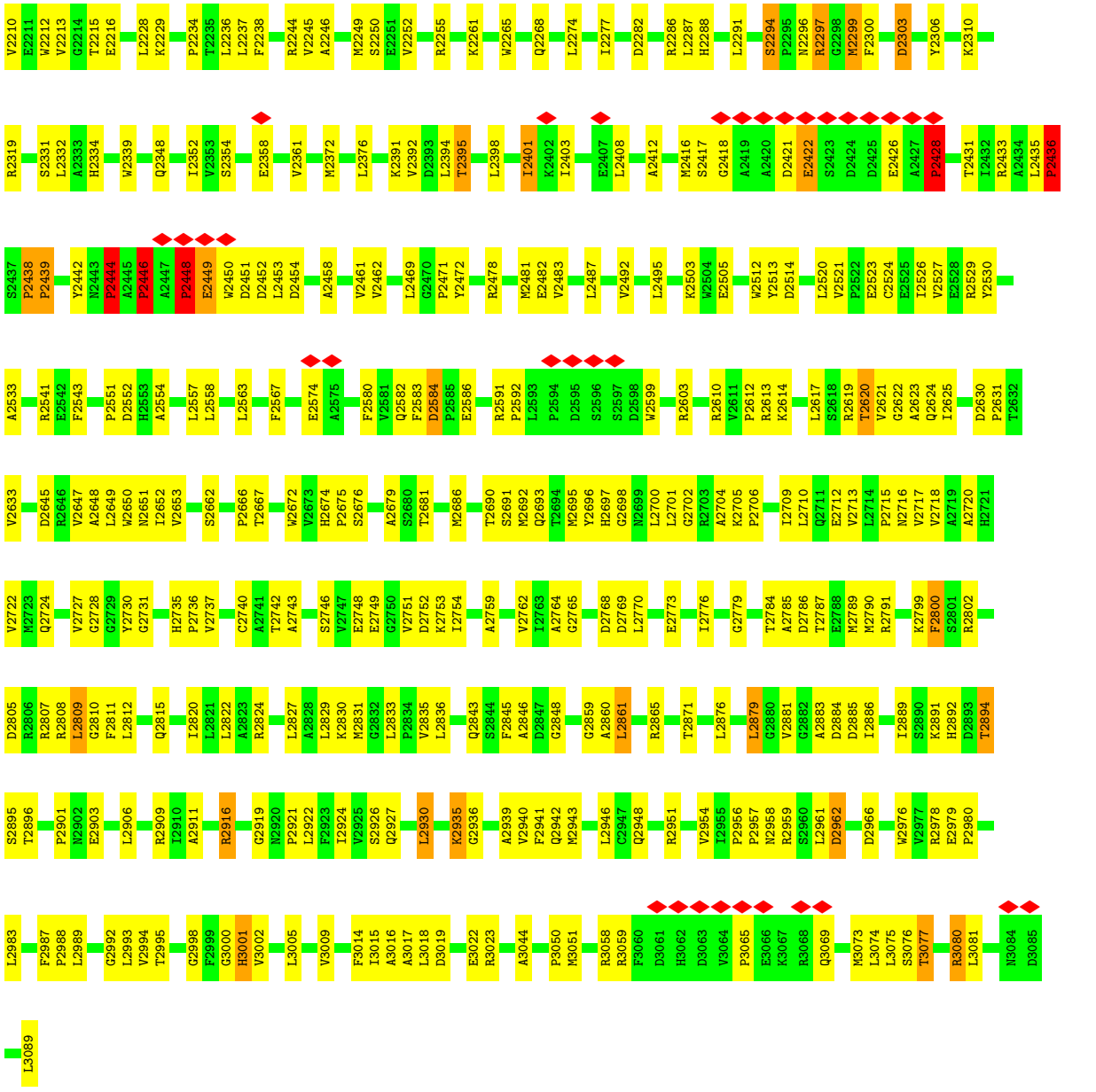


• Molecule 1: TYPE-I FATTY ACID SYNTHASE

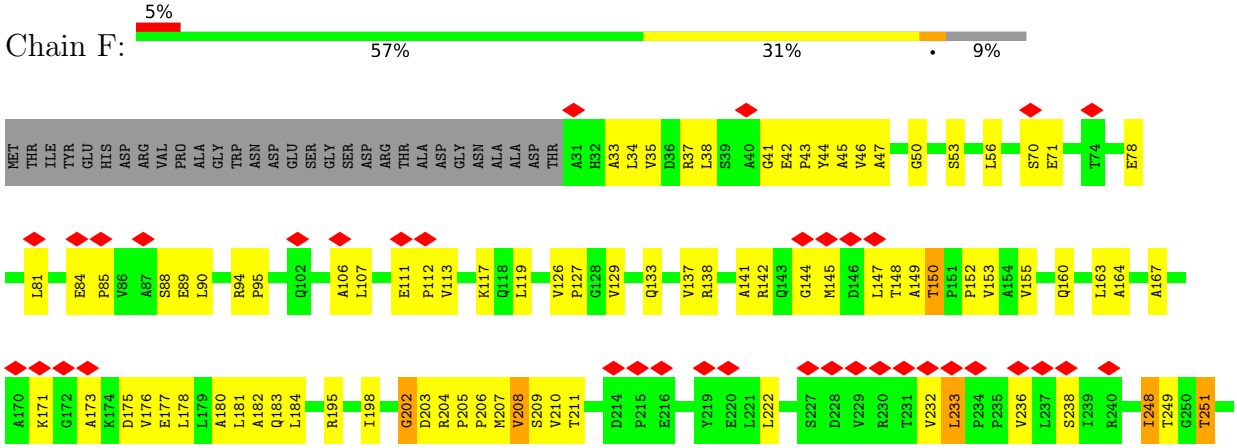
Chain E:

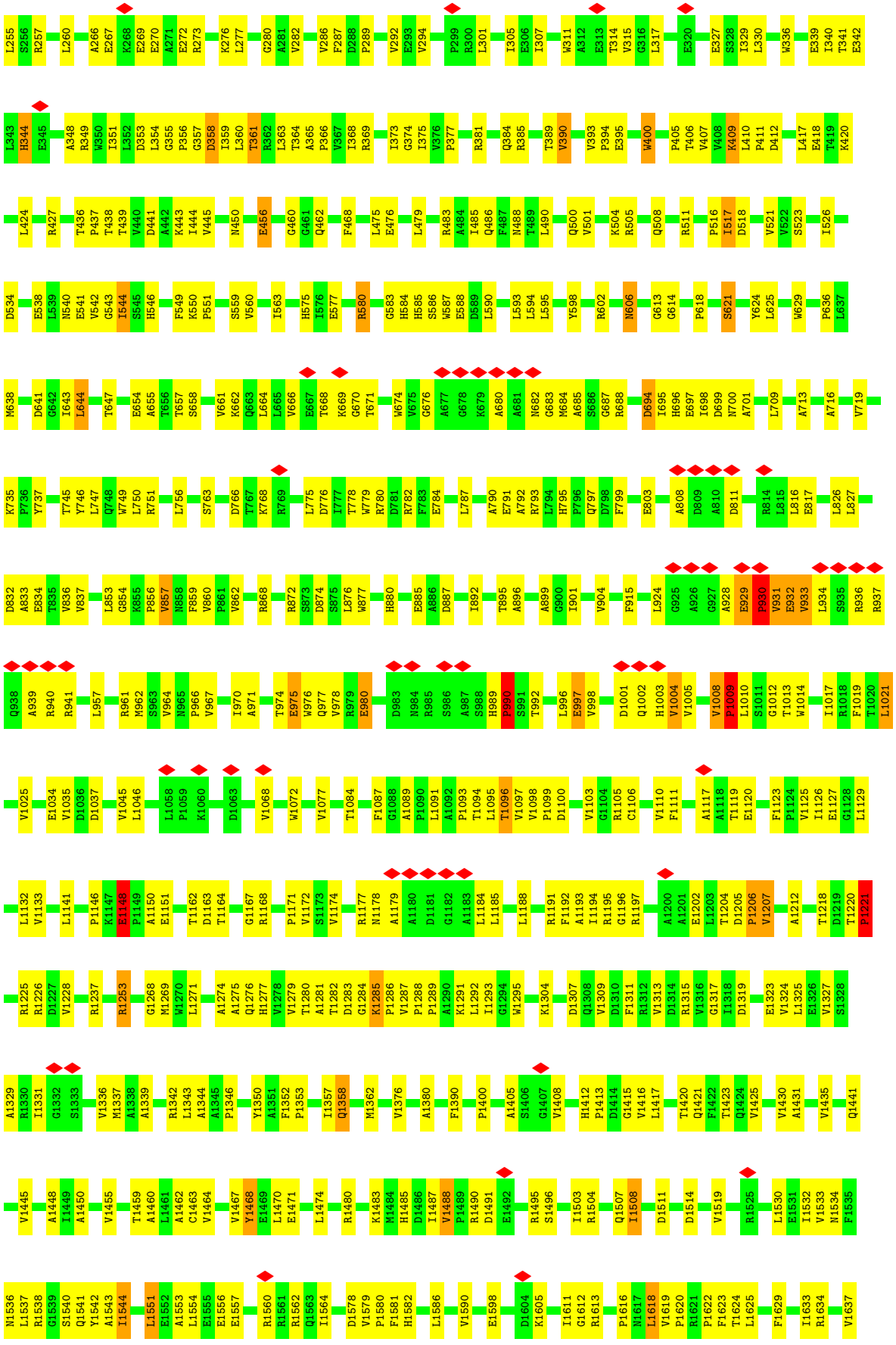


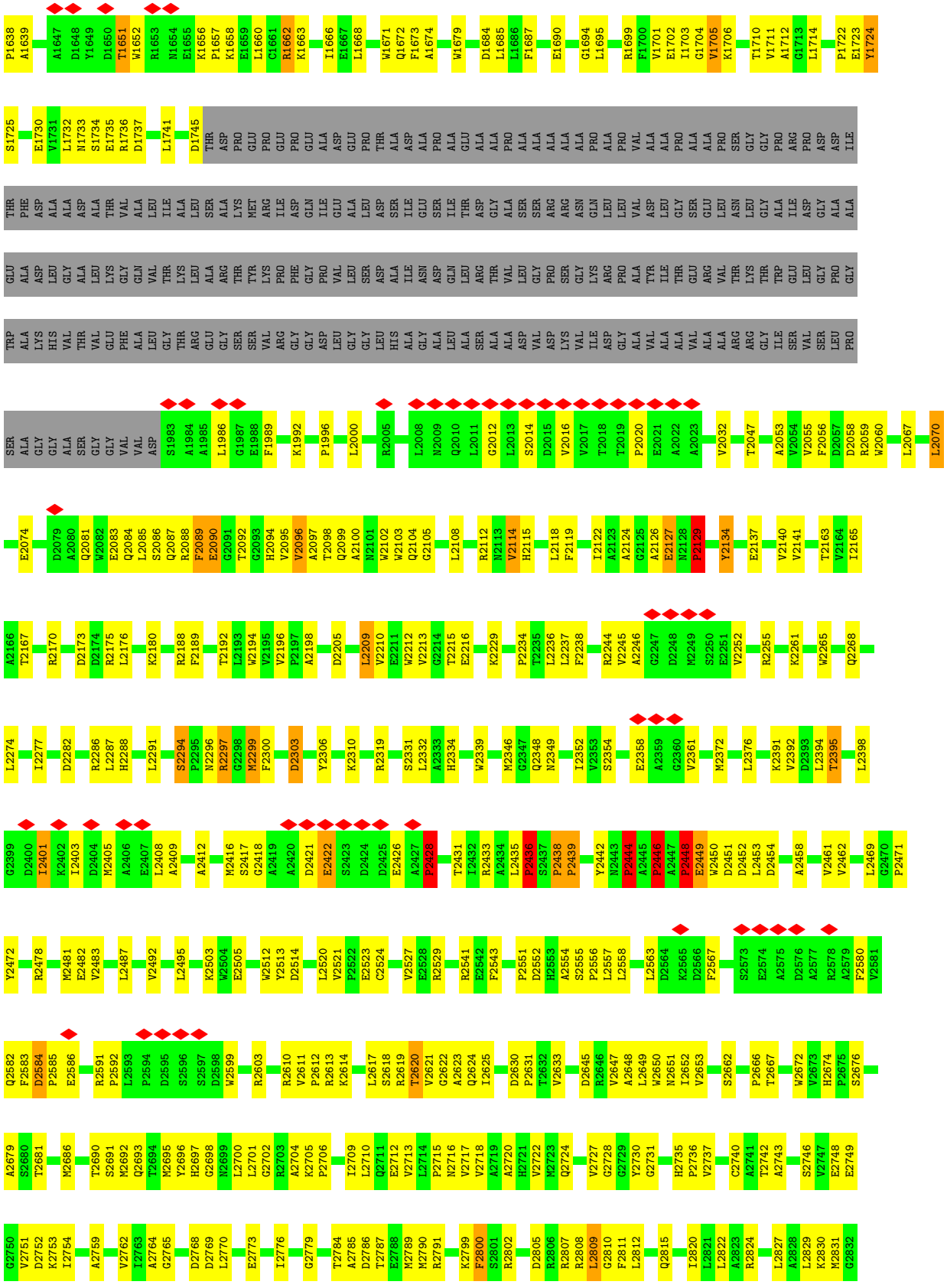




• Molecule 1: TYPE-I FATTY ACID SYNTHASE



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S1725 E1730 V1731 L1732 N1733 S1734 E1735 R1736 D1737 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA ALA PRO GLU ALA ALA ALA ALA PRO ALA PRO GLU GLY GLY PRO ARG PRO ASP
THR PHE ASP ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER GLN LEU ARG THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU GLU ARG VAL THR LEU GLY GLY ALA ILE ASP GLY ALA
GLU ALA ASP LEU GLY ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP SER ALA ILE ASN GLN ARG LEU GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LEU GLU LEU GLY PRO
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A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180 R2188 F2189 T2192 L2193 W2194 V2195 V2196 P2197 A2198 D2205 L2209 V2210 E2211 W2212 V2213 G2214 T2215 E2216 K2229 P2234 T2235 L2236 L2237 F2238 R2244 V2245 A2246 G2247 D2248 M2249 S2250 E2251 V2252 R2255 K2261 W2265 Q2268
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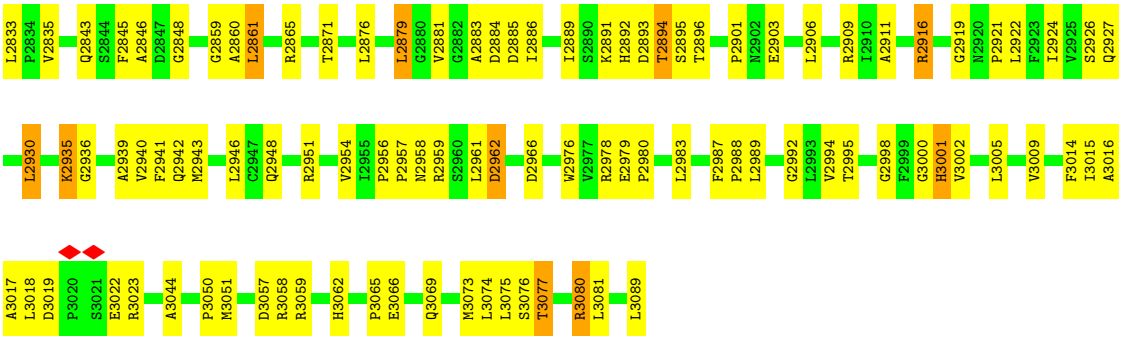
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4337	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	10.361	Depositor
Minimum map value	-2.852	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.8	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.28, 2.28, 2.28	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	B	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	C	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	D	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	E	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	F	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
All	All	0.39	162/128010 (0.1%)	0.51	78/174222 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2442	TYR	CB-CG	-6.38	1.42	1.51
1	A	2442	TYR	CB-CG	-6.36	1.42	1.51
1	B	2442	TYR	CB-CG	-6.35	1.42	1.51
1	F	2442	TYR	CB-CG	-6.33	1.42	1.51
1	D	2442	TYR	CB-CG	-6.31	1.42	1.51

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	930	PRO	N-CA-CB	7.04	111.75	103.30
1	B	930	PRO	N-CA-CB	7.01	111.71	103.30
1	D	930	PRO	N-CA-CB	6.99	111.69	103.30
1	E	930	PRO	N-CA-CB	6.98	111.68	103.30
1	A	930	PRO	N-CA-CB	6.97	111.66	103.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1148	GLU	Peptide
1	A	150	THR	Peptide
1	A	202	GLY	Peptide
1	A	2584	ASP	Peptide
1	A	357	GLY	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	20945	0	20595	881	0
1	B	20945	0	20595	872	0
1	C	20945	0	20595	872	0
1	D	20945	0	20595	873	0
1	E	20945	0	20595	878	0
1	F	20945	0	20595	878	0
2	A	31	0	19	4	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	4	0
2	E	31	0	19	4	0
2	F	31	0	19	5	0
All	All	125856	0	123684	4910	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 20.

The worst 5 of 4910 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:THR:HG23	1:A:1014:TRP:H	1.15	1.10
1:E:1013:THR:HG23	1:E:1014:TRP:H	1.15	1.09
1:A:2112:ARG:H	1:A:2115:HIS:CG	1.73	1.07
1:C:2094:HIS:CG	1:C:2096:VAL:HG22	1.90	1.06
1:D:1013:THR:HG23	1:D:1014:TRP:H	1.15	1.06

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	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	25	66
1	B	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	22	63
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	22	63
1	D	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	22	63
1	E	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	25	66
1	F	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	22	63
All	All	16908/18534 (91%)	15849 (94%)	947 (6%)	112 (1%)	26	63

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	930	PRO
1	A	1148	GLU
1	A	2428	PRO
1	A	2436	PRO
1	A	2446	PRO

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	2094/2402 (87%)	1992 (95%)	102 (5%)	25	50
1	B	2097/2402 (87%)	1994 (95%)	103 (5%)	25	50
1	C	2094/2402 (87%)	1992 (95%)	102 (5%)	25	50
1	D	2093/2402 (87%)	1991 (95%)	102 (5%)	25	50
1	E	2095/2402 (87%)	1993 (95%)	102 (5%)	25	50
1	F	2094/2402 (87%)	1992 (95%)	102 (5%)	25	50
All	All	12567/14412 (87%)	11954 (95%)	613 (5%)	29	50

5 of 613 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1618	LEU
1	F	2070	LEU
1	E	2294	SER
1	E	1564	ILE
1	F	358	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2942	GLN
1	F	540	ASN
1	F	1672	GLN
1	C	486	GLN
1	C	386	ASN

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)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	FMN	F	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
2	FMN	E	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
2	FMN	D	4000	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	B	4000	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	A	4000	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	C	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)

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
2	FMN	F	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	E	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	D	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	A	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	5/18/18/18	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	4.14	1.38	1.30
2	F	4000	FMN	C4A-N5	4.12	1.38	1.30
2	E	4000	FMN	C4A-N5	4.10	1.38	1.30
2	A	4000	FMN	C4A-N5	4.09	1.38	1.30
2	D	4000	FMN	C4A-N5	4.08	1.38	1.30

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4000	FMN	C4-N3-C2	-3.02	120.06	125.64
2	C	4000	FMN	C4-N3-C2	-2.99	120.12	125.64
2	E	4000	FMN	C4-N3-C2	-2.98	120.13	125.64
2	D	4000	FMN	C4-N3-C2	-2.98	120.13	125.64
2	B	4000	FMN	C4-N3-C2	-2.97	120.15	125.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4000	FMN	O3'-C3'-C4'-C5'
2	B	4000	FMN	O3'-C3'-C4'-C5'
2	C	4000	FMN	O3'-C3'-C4'-C5'
2	D	4000	FMN	O3'-C3'-C4'-C5'
2	E	4000	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

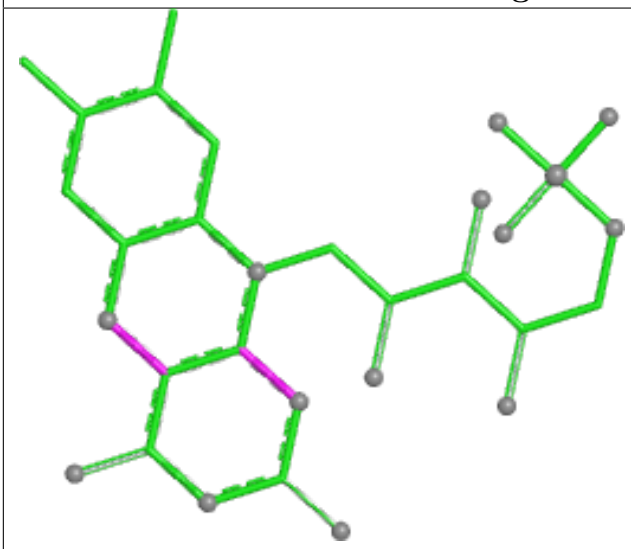
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4000	FMN	5	0
2	E	4000	FMN	4	0
2	D	4000	FMN	4	0
2	B	4000	FMN	5	0
2	A	4000	FMN	4	0
2	C	4000	FMN	4	0

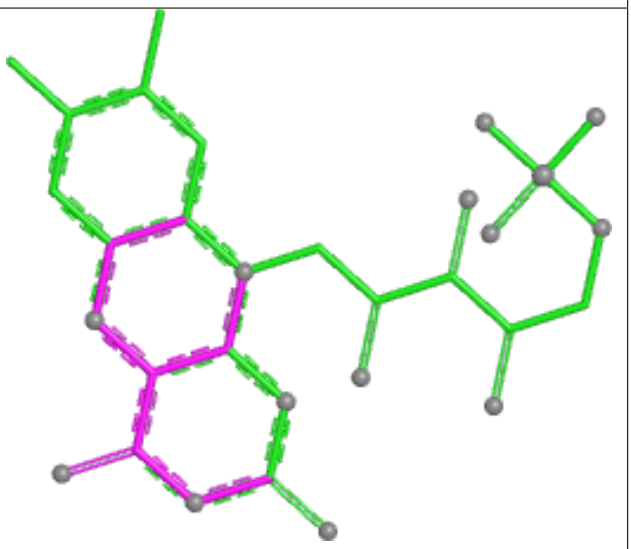
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

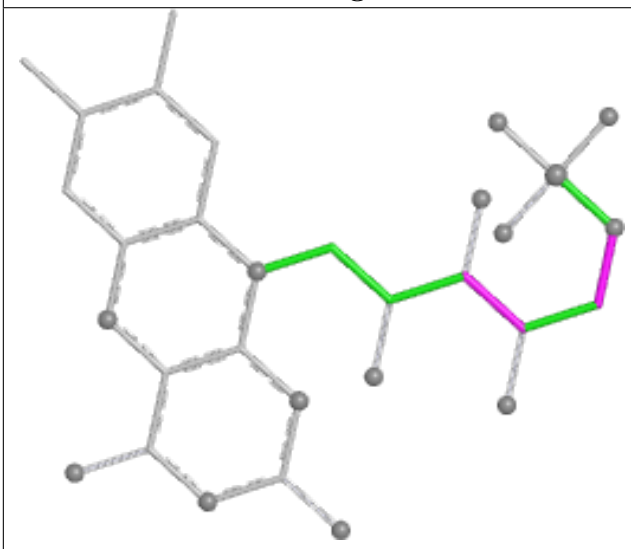
Ligand FMN F 4000



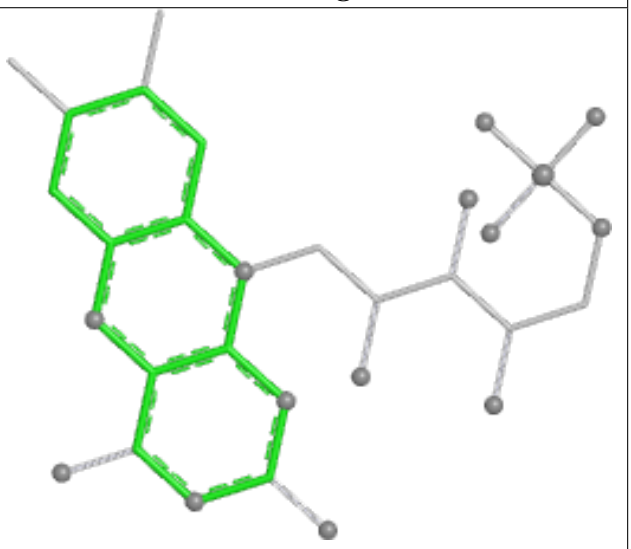
Bond lengths



Bond angles

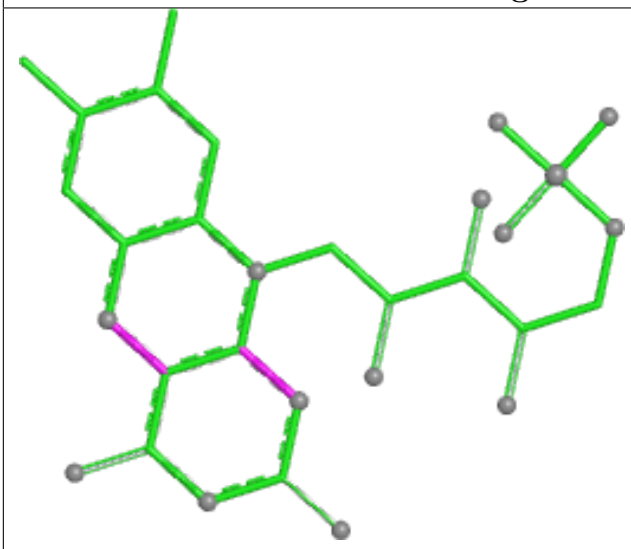


Torsions

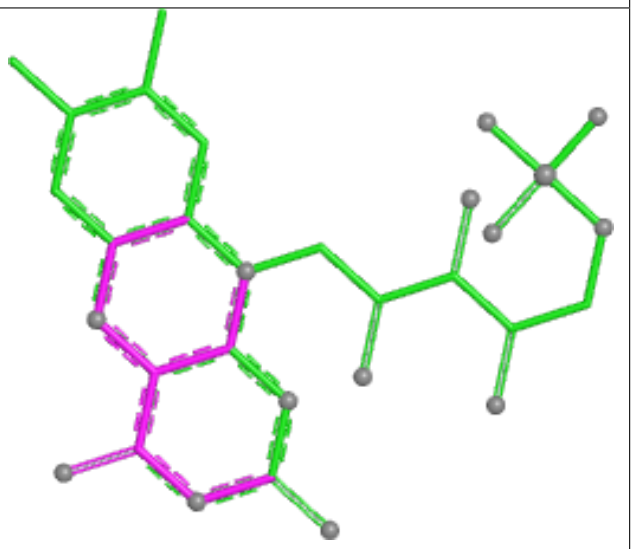


Rings

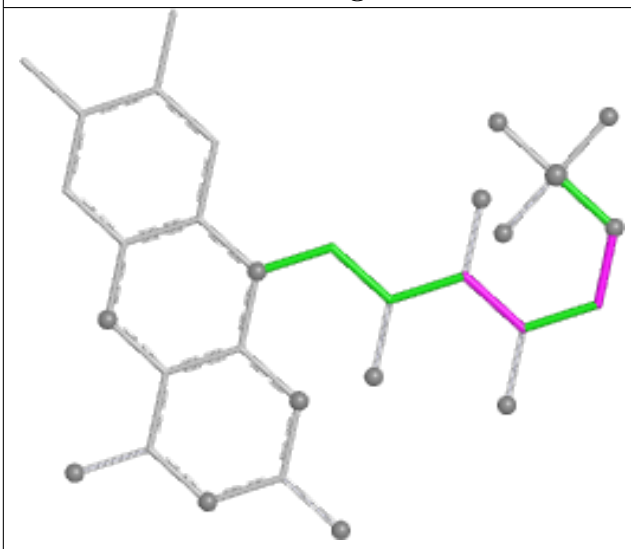
Ligand FMN E 4000



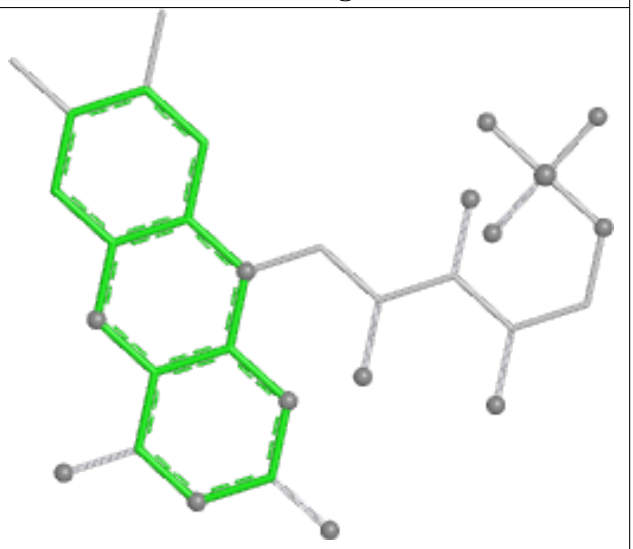
Bond lengths



Bond angles

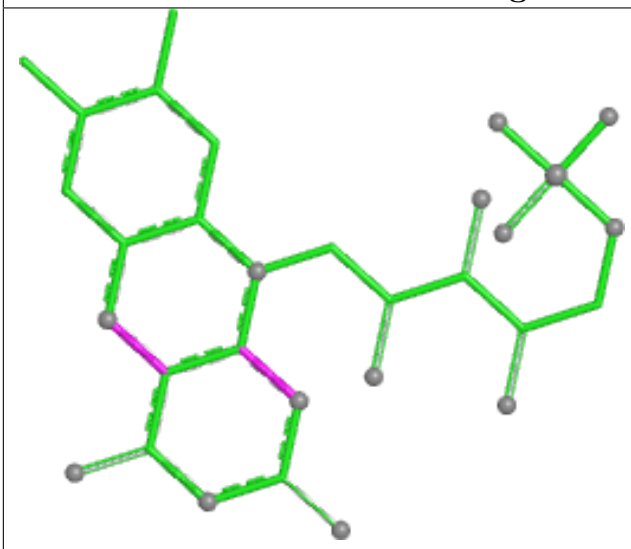


Torsions

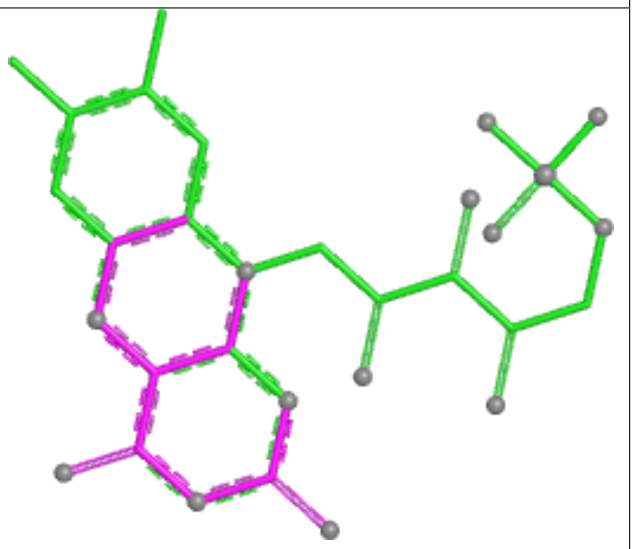


Rings

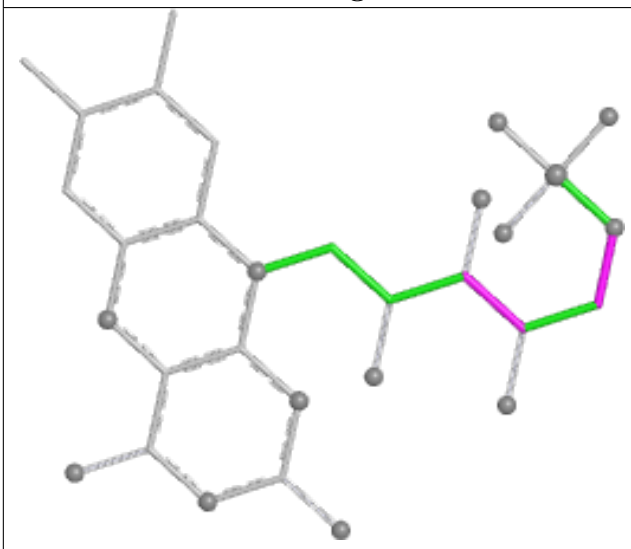
Ligand FMN D 4000



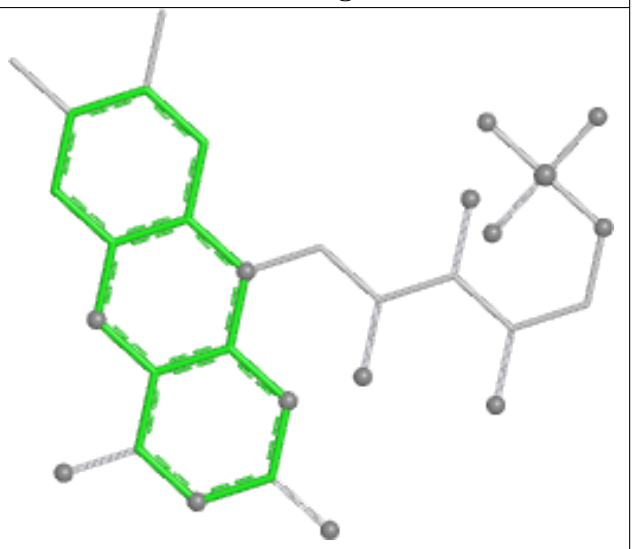
Bond lengths



Bond angles

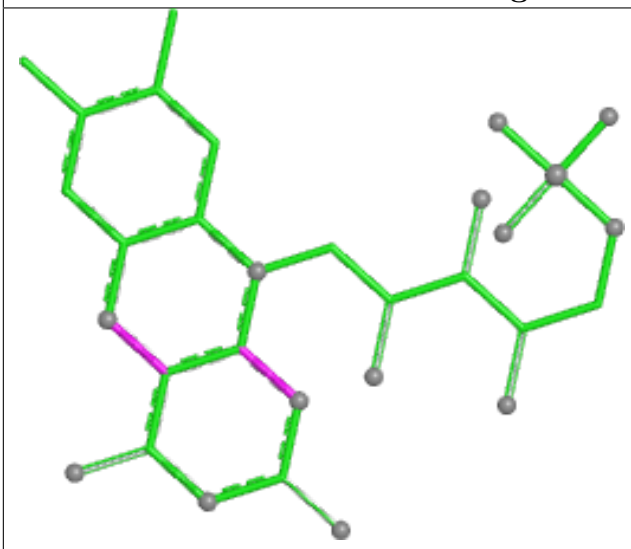


Torsions

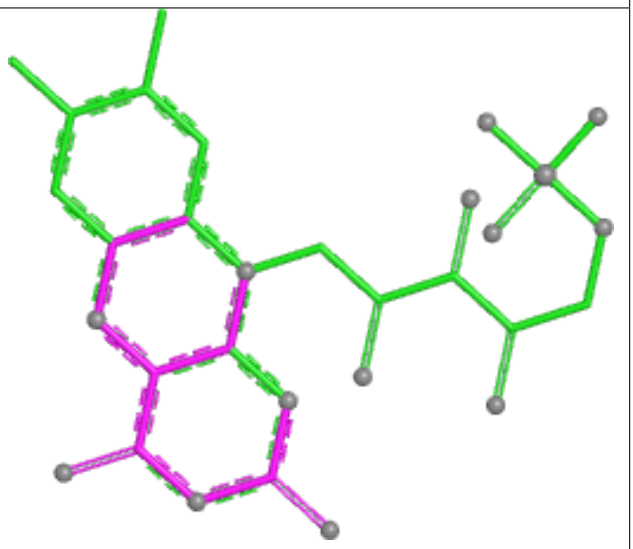


Rings

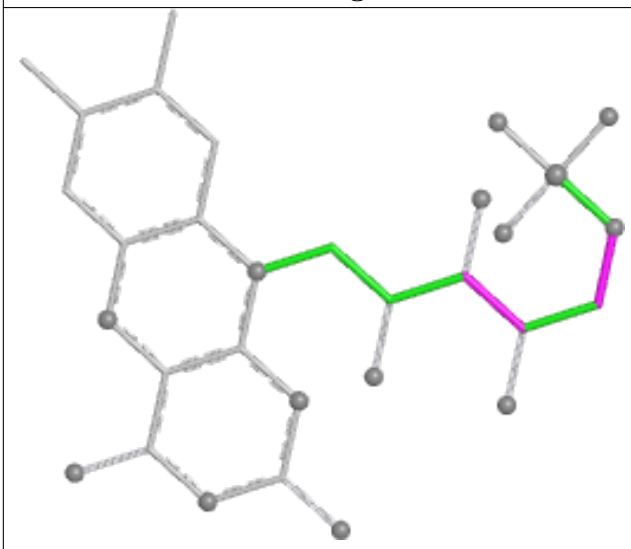
Ligand FMN B 4000



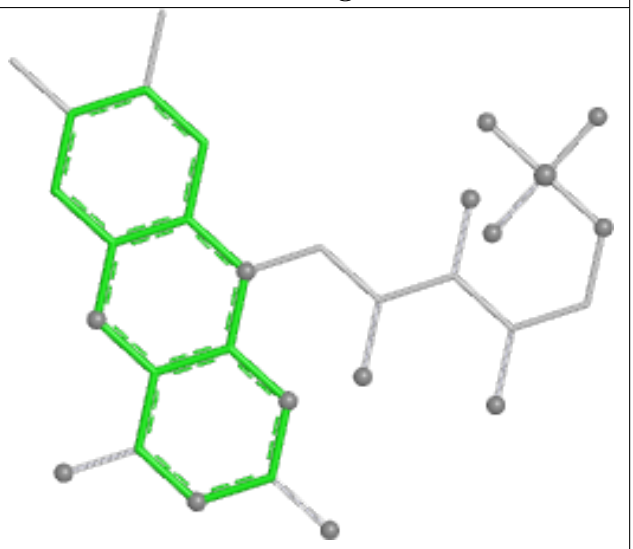
Bond lengths



Bond angles

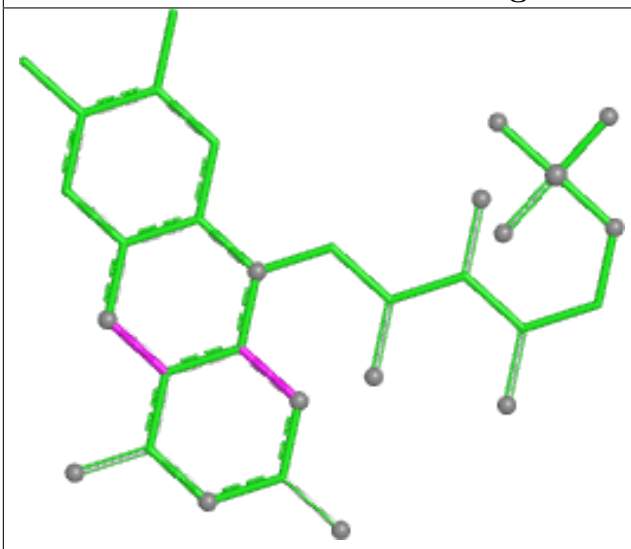


Torsions

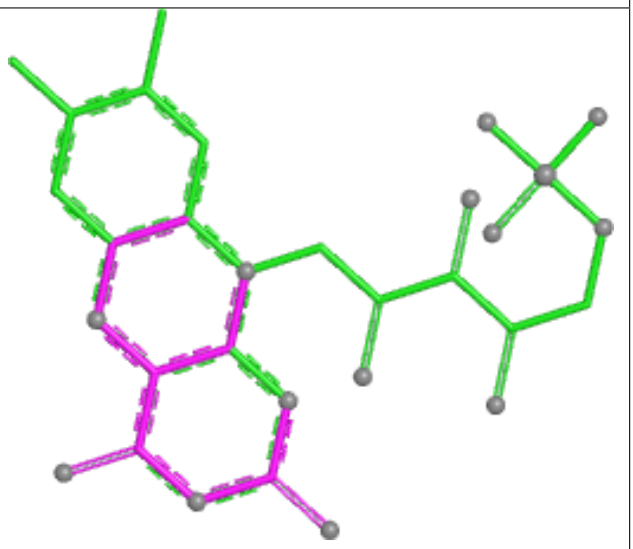


Rings

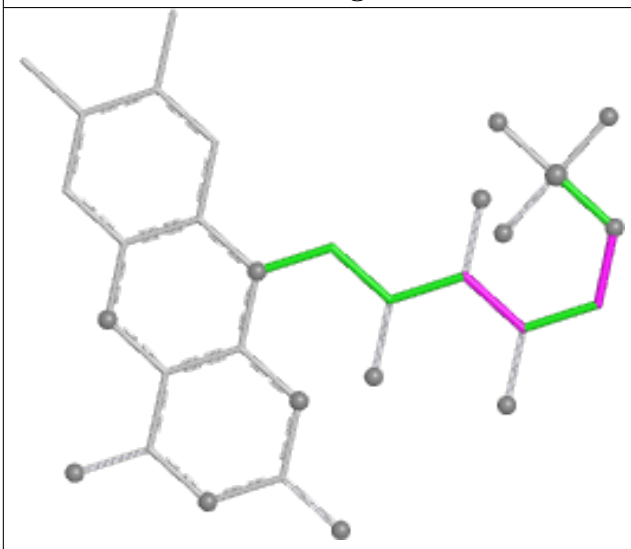
Ligand FMN A 4000



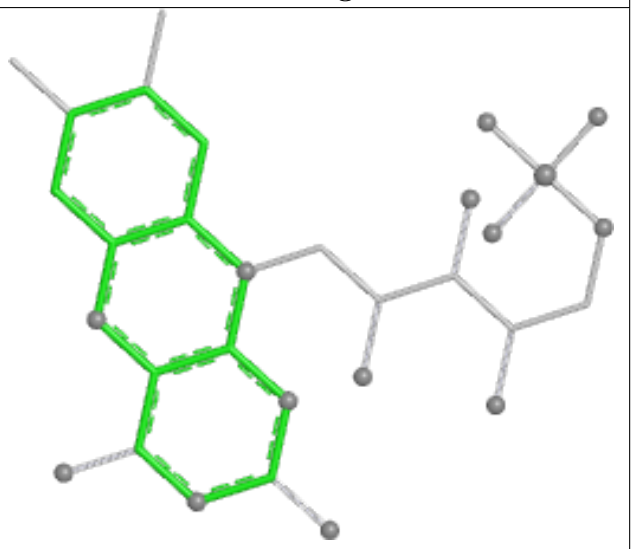
Bond lengths



Bond angles

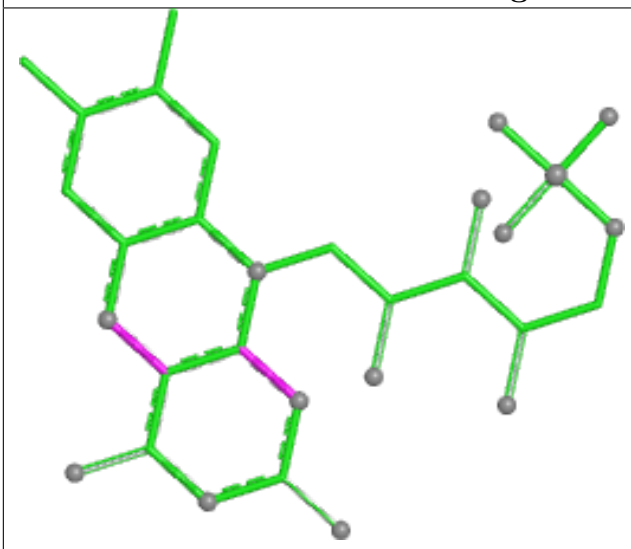


Torsions

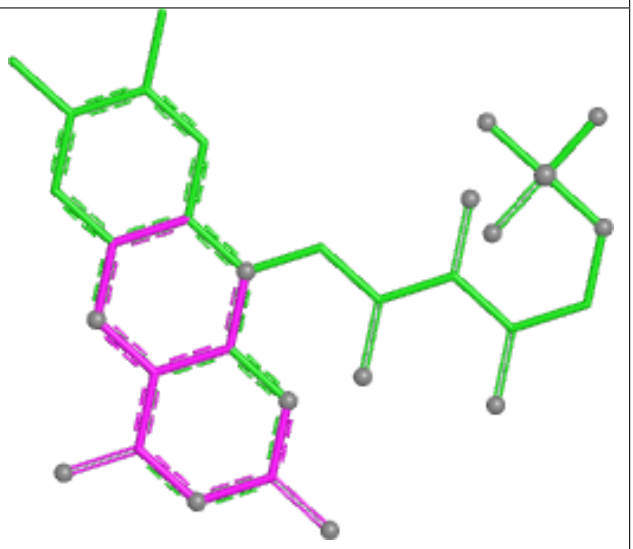


Rings

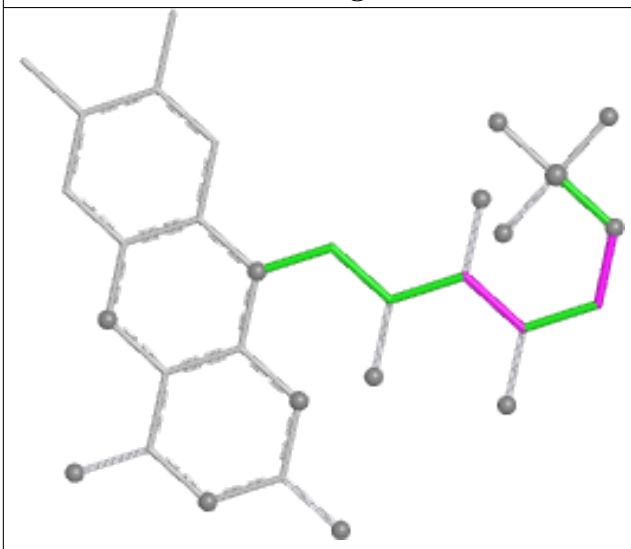
Ligand FMN C 4000



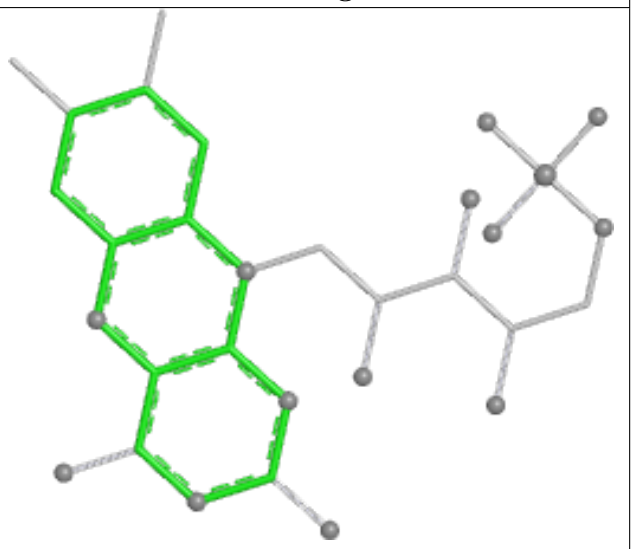
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

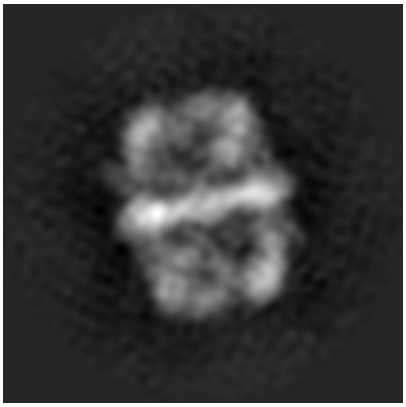
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2358. These allow visual inspection of the internal detail of the map and identification of artifacts.

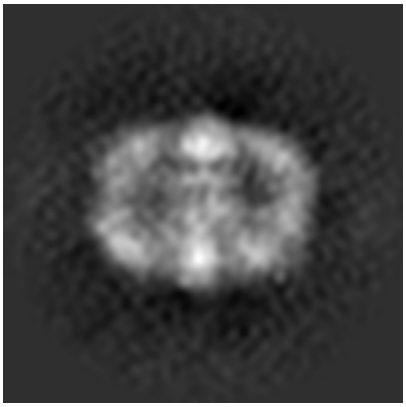
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

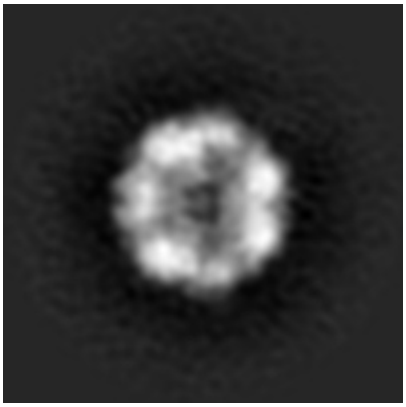
6.1.1 Primary map



X



Y

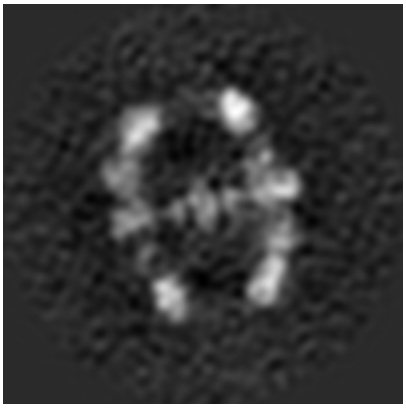


Z

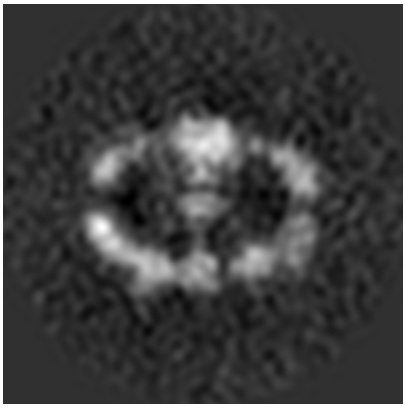
The images above show the map projected in three orthogonal directions.

6.2 Central slices

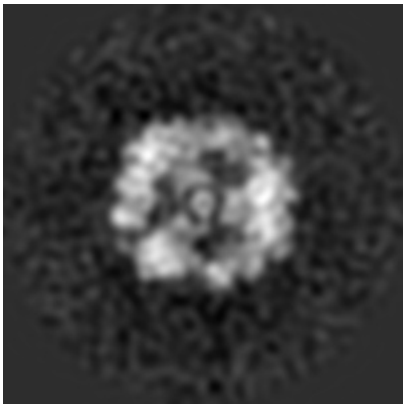
6.2.1 Primary map



X Index: 100



Y Index: 100

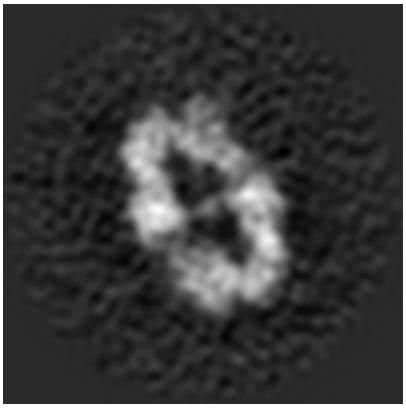


Z Index: 100

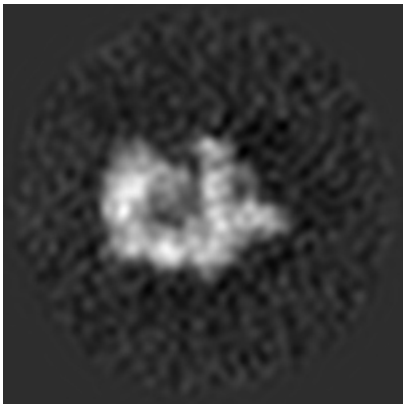
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

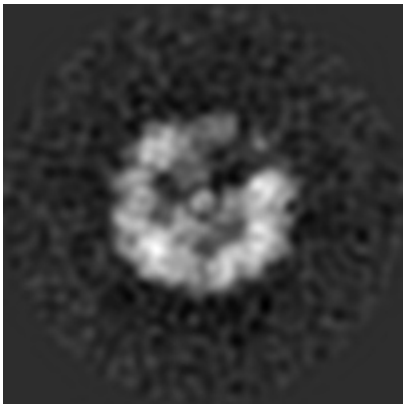
6.3.1 Primary map



X Index: 76



Y Index: 131

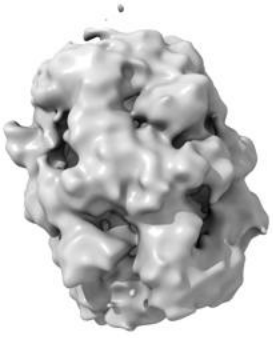


Z Index: 96

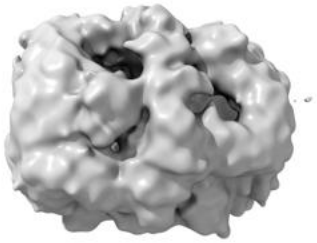
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

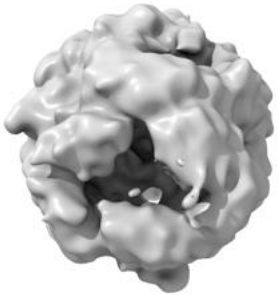
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

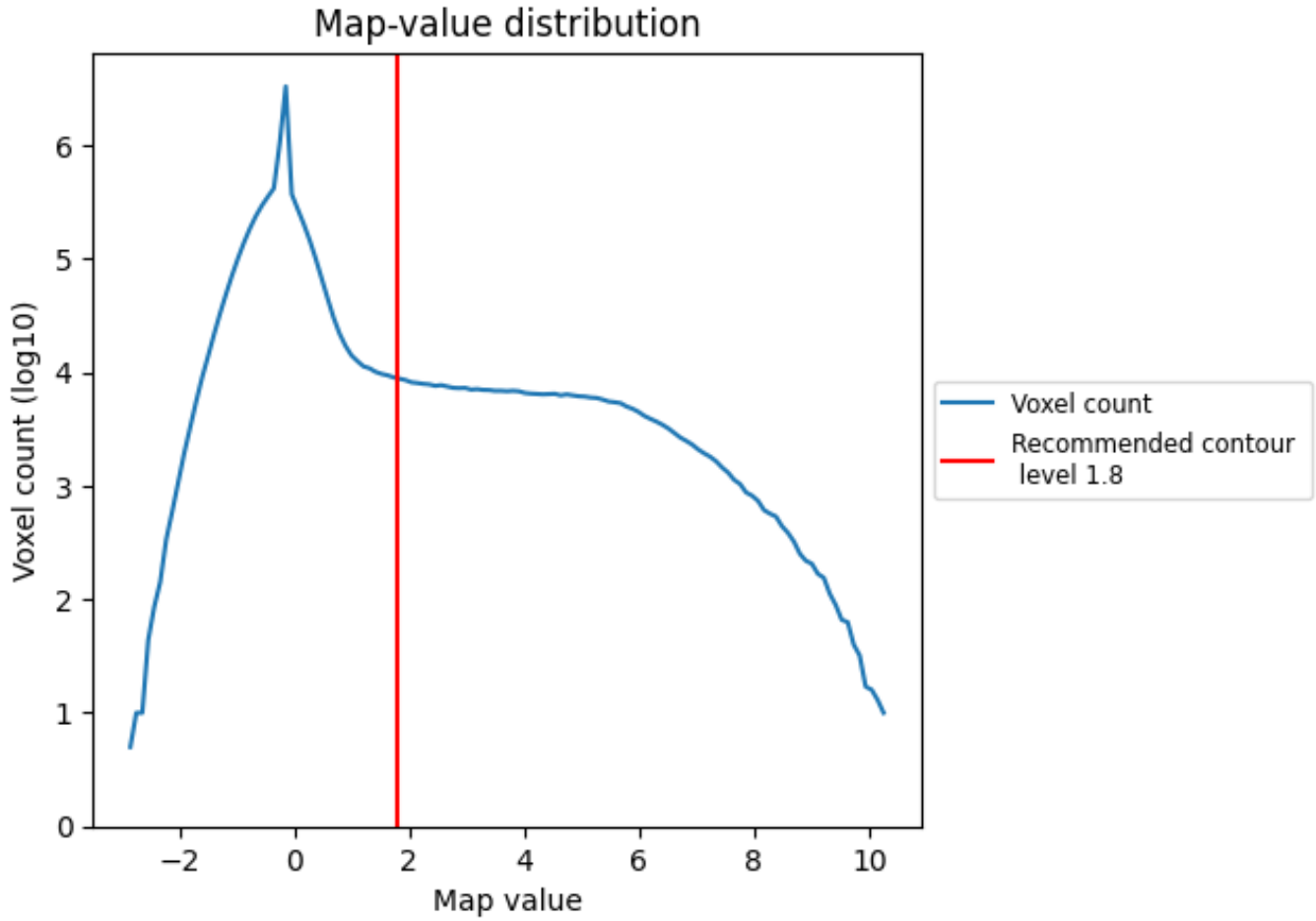
6.5 Mask visualisation (i)

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

7 Map analysis

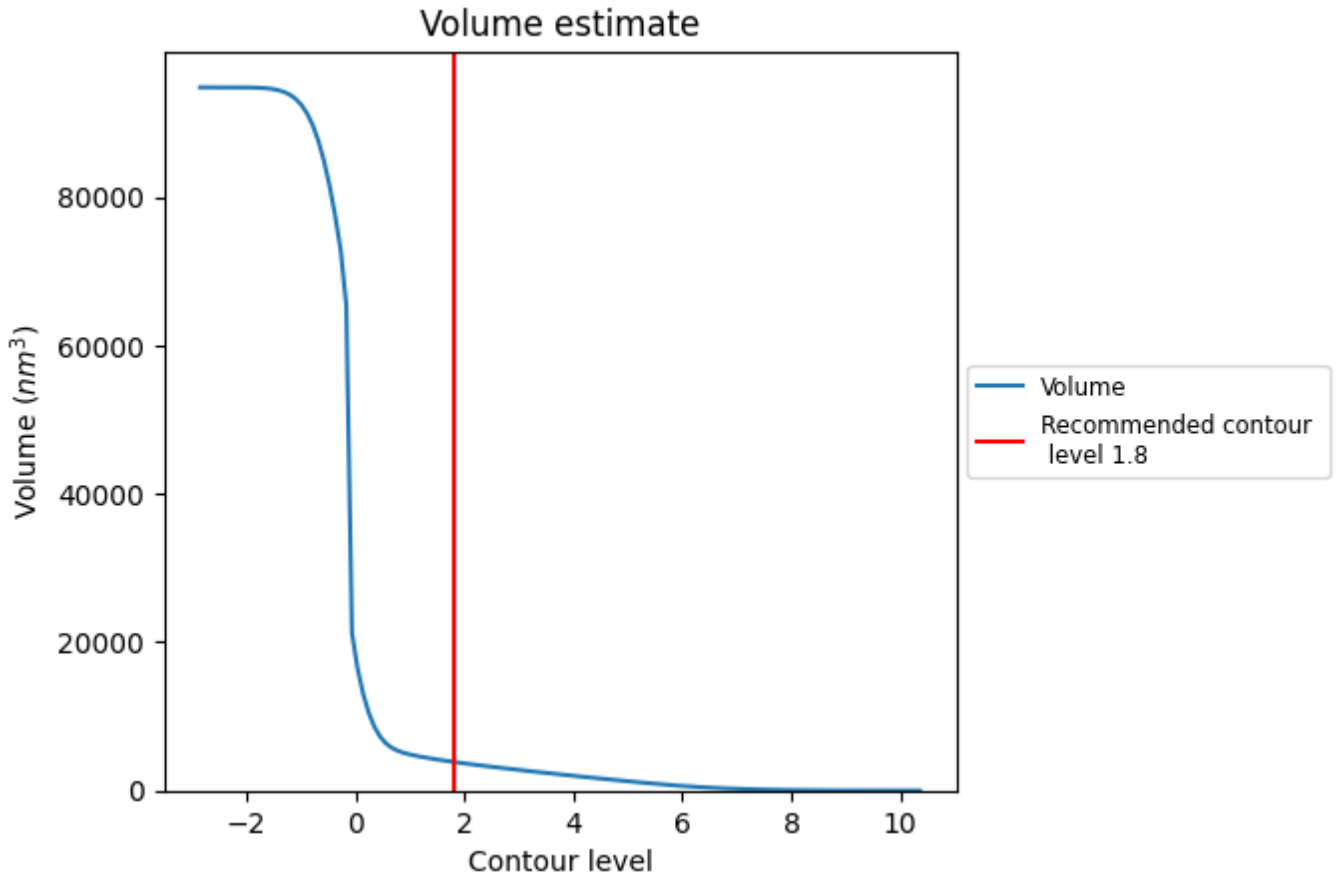
This section contains the results of statistical analysis of the map.

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.

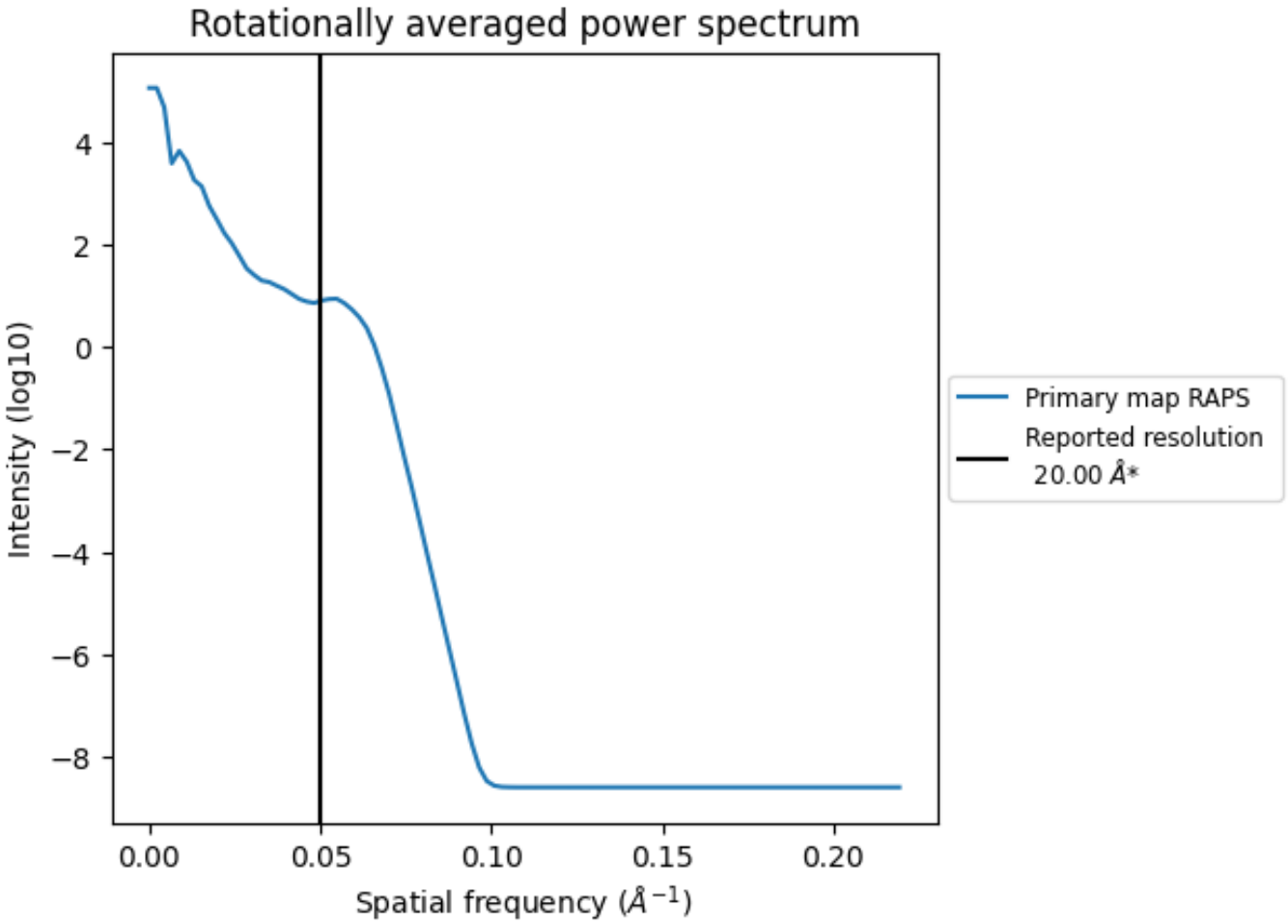
7.2 Volume estimate (i)



The volume at the recommended contour level is 3860 nm^3; this corresponds to an approximate mass of 3487 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 0.050 Å^{-1}

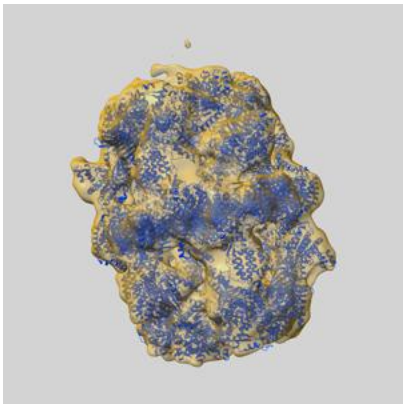
8 Fourier-Shell correlation (i)

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

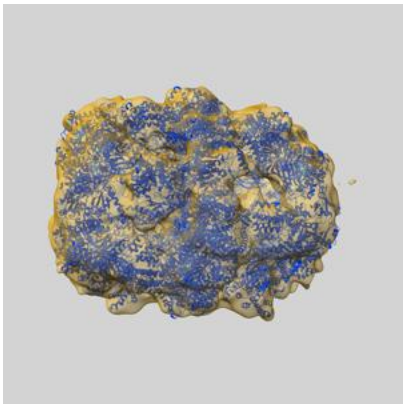
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2358 and PDB model 4V8V. Per-residue inclusion information can be found in section 3 on page 5.

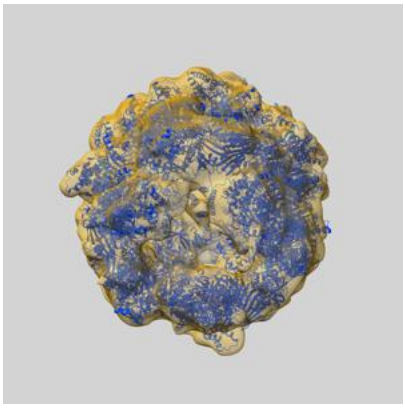
9.1 Map-model overlay



X



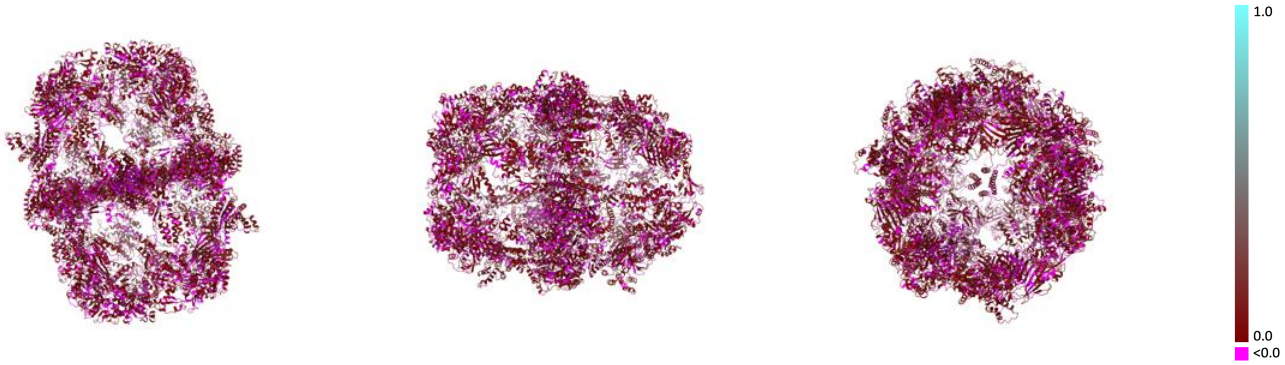
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8 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.

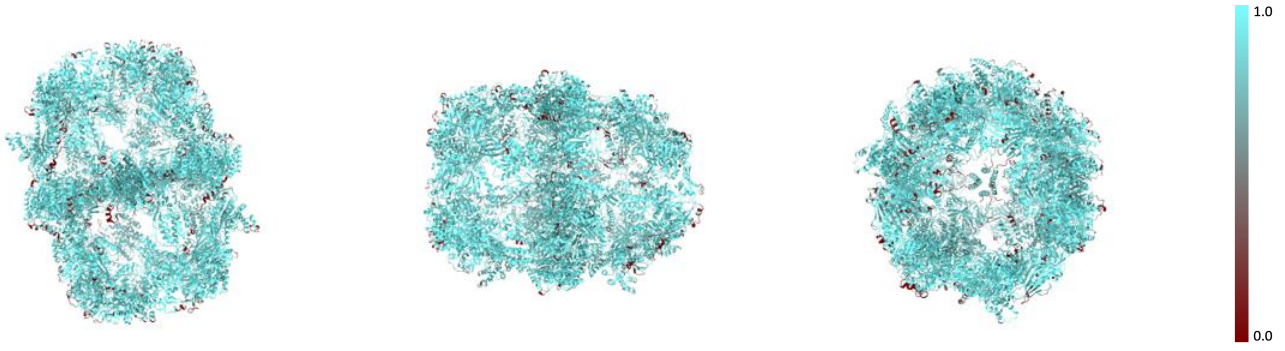
9.2 Q-score mapped to coordinate model



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.

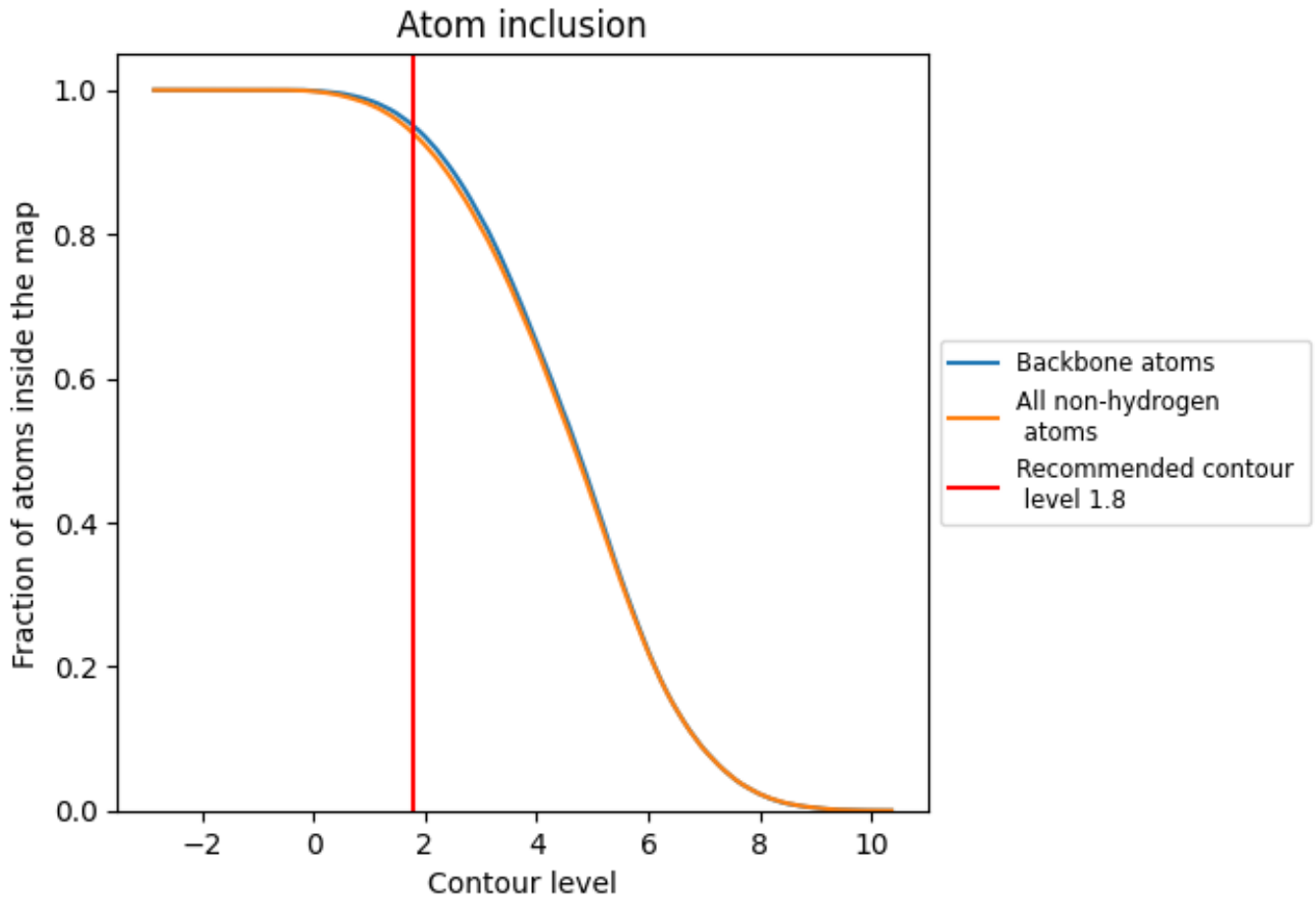
9.3 Atom inclusion mapped to coordinate model



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 (1.8).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9391	0.0500
A	0.9573	0.0520
B	0.9363	0.0450
C	0.9278	0.0440
D	0.9312	0.0490
E	0.9485	0.0560
F	0.9336	0.0520