wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:12 PM GMT

PDB ID	:	3HMJ
Title	:	Saccharomyces cerevisiae FAS type I
Authors	:	Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.; Grininger, M.
Deposited on	:	2009-05-29
Resolution	:	4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

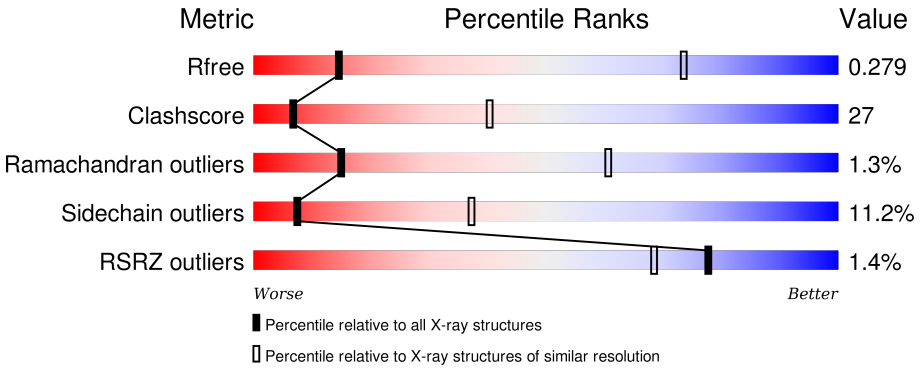
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	2% 55% 32% 5% 7%
1	B	1887	2% 55% 32% 5% 7%
1	C	1887	3% 54% 33% 5% 7%
2	G	2051	51% 40% 8%
2	H	2051	51% 40% 8%

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Mol	Chain	Length	Quality of chain
2	I	2051	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CER	C	2748	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 88830 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

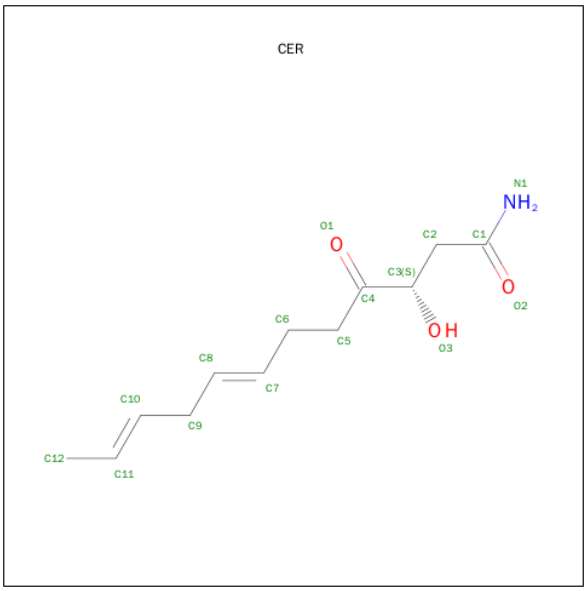
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	B	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	C	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

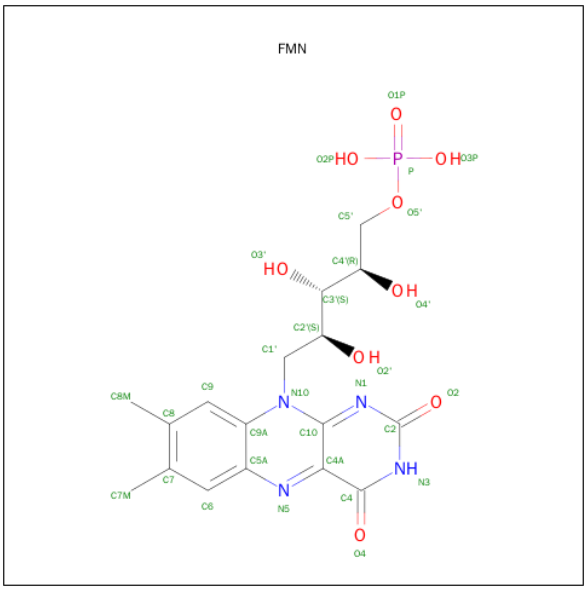
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: $C_{12}H_{19}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 8 1 3	0	0
3	B	1	Total C N O 12 8 1 3	0	0
3	C	1	Total C N O 12 8 1 3	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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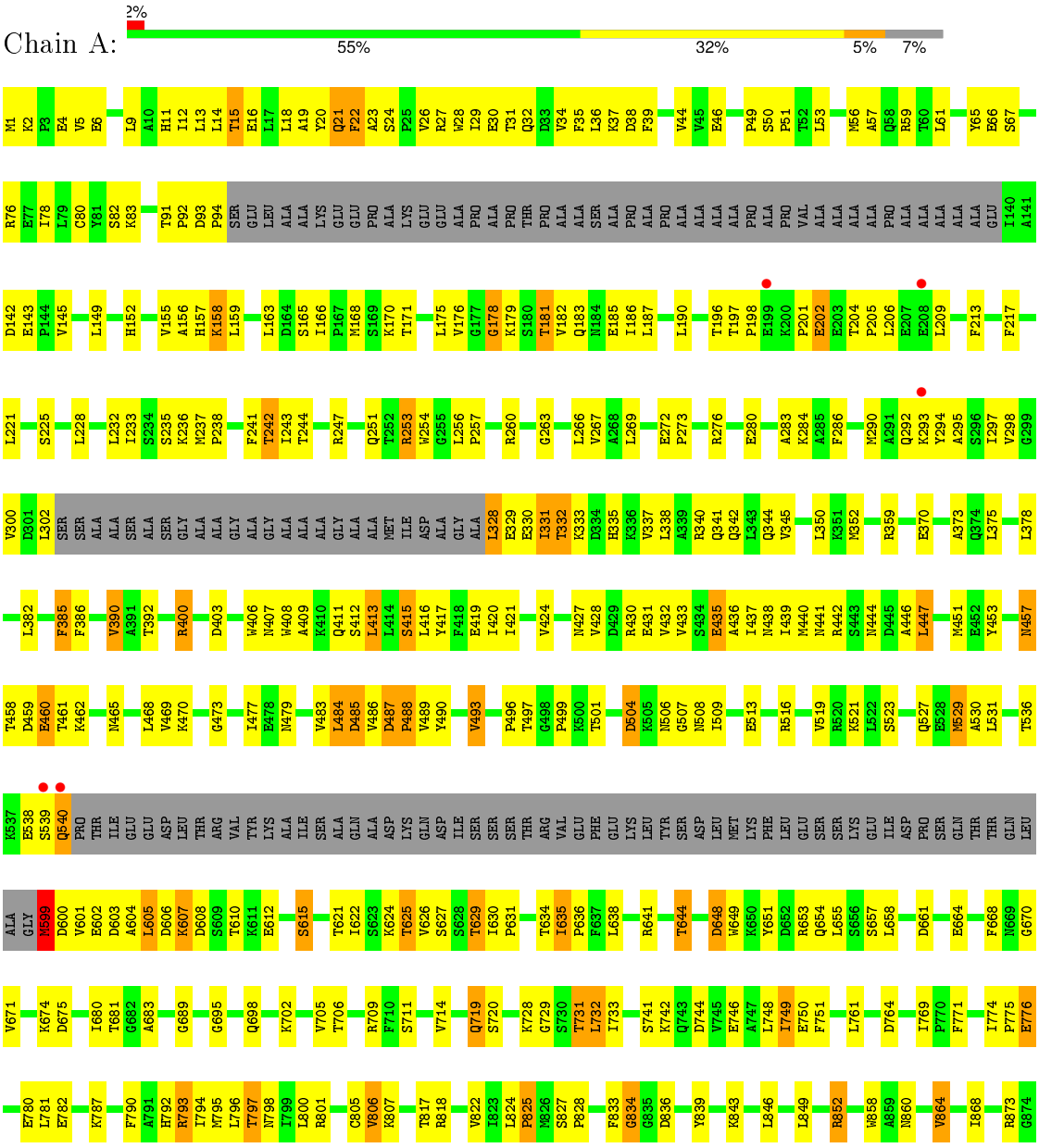
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

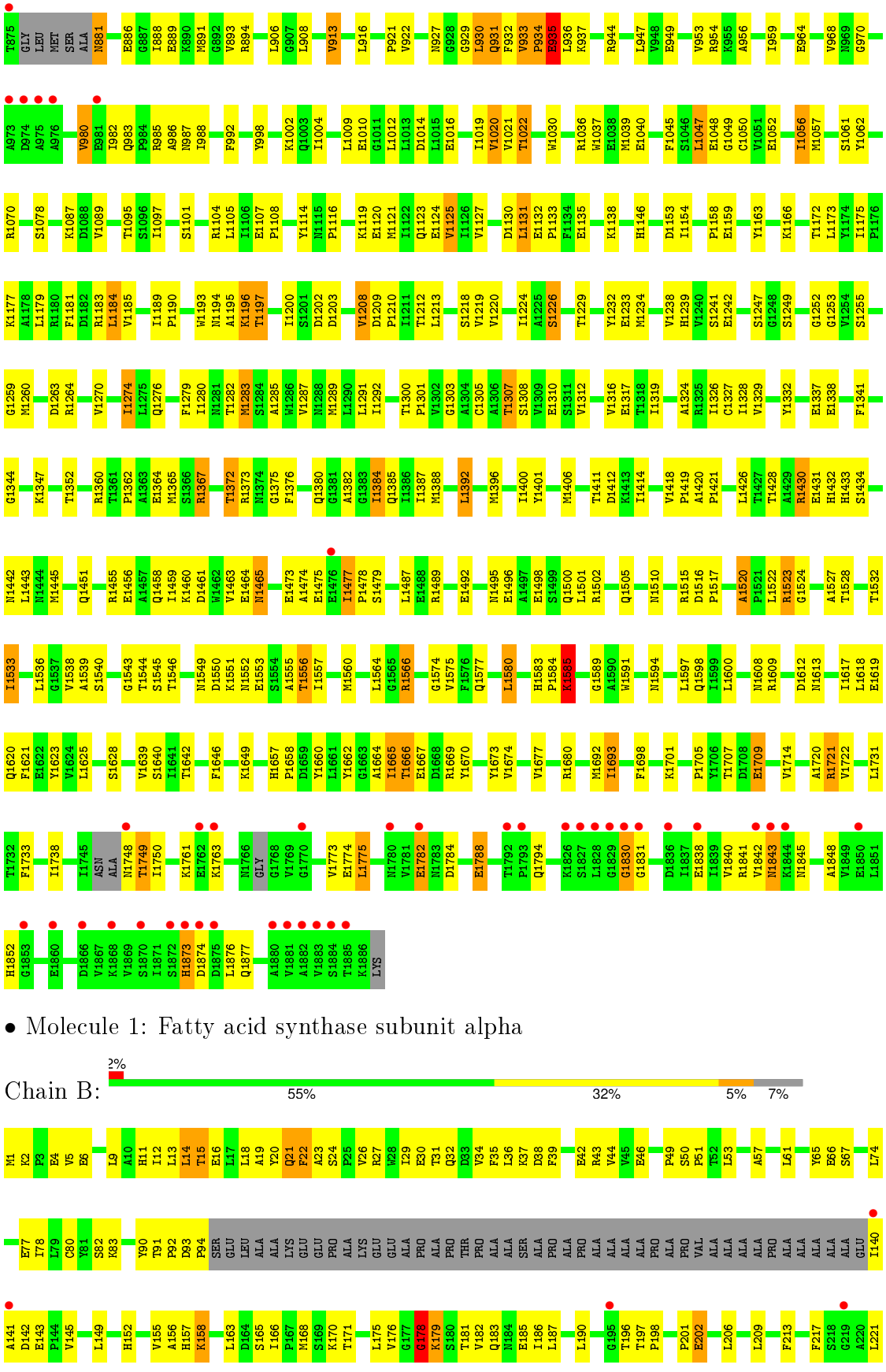
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Fatty acid synthase subunit alpha

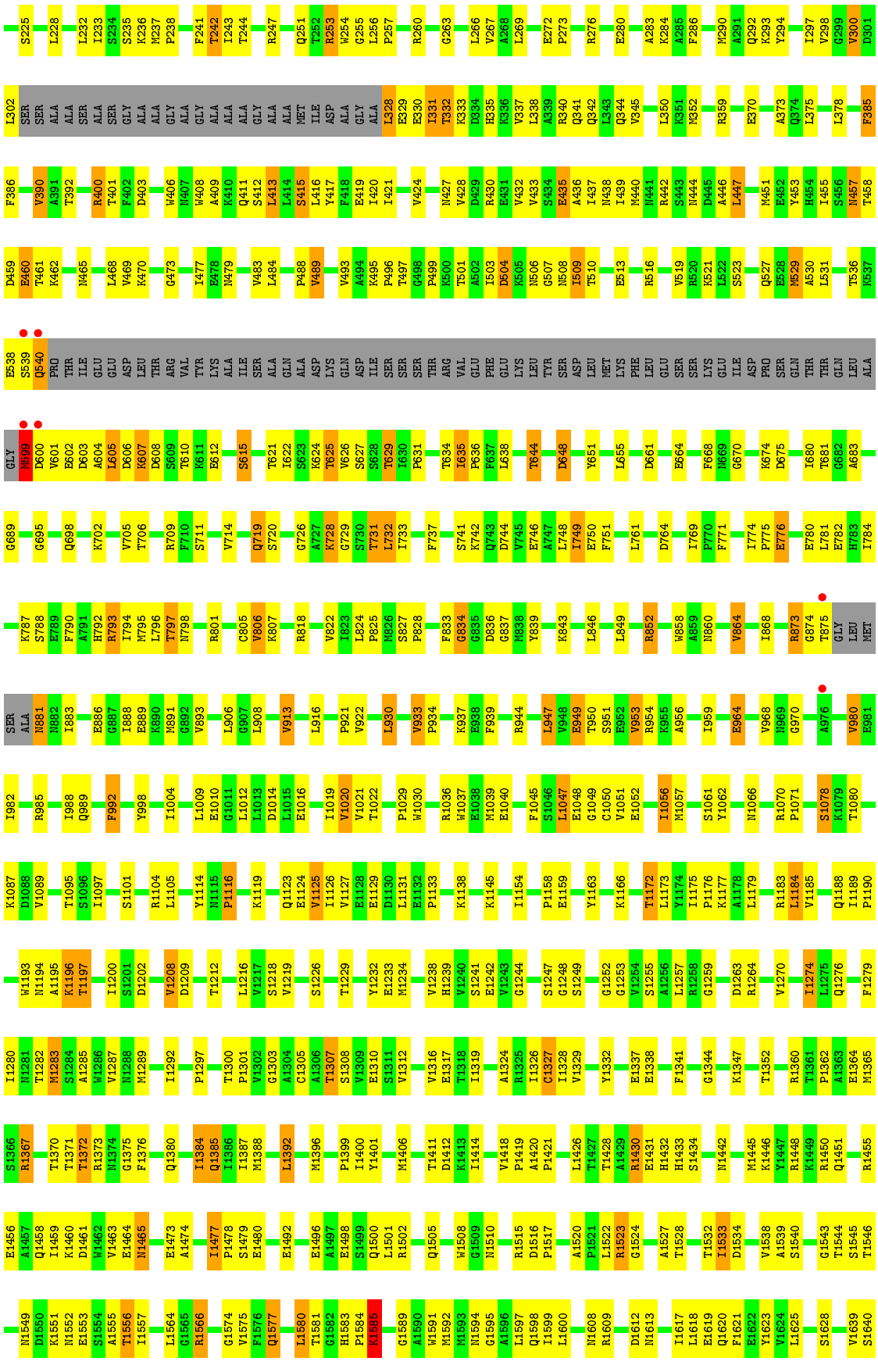
Chain A:





• Molecule 1: Fatty acid synthase subunit alpha

Chain B: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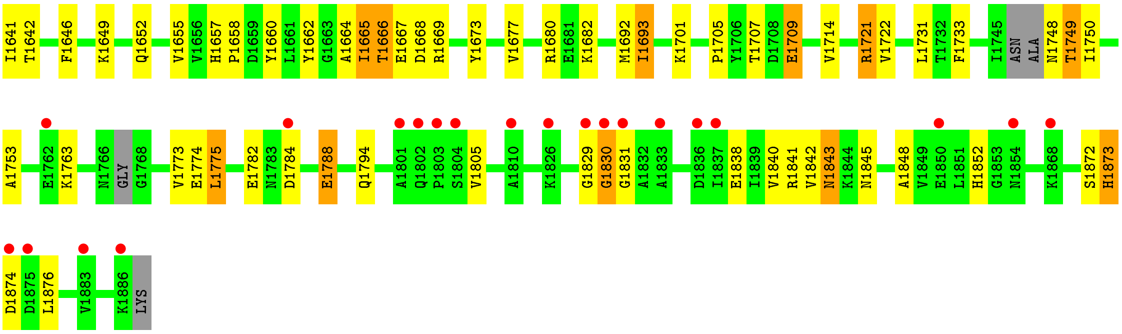
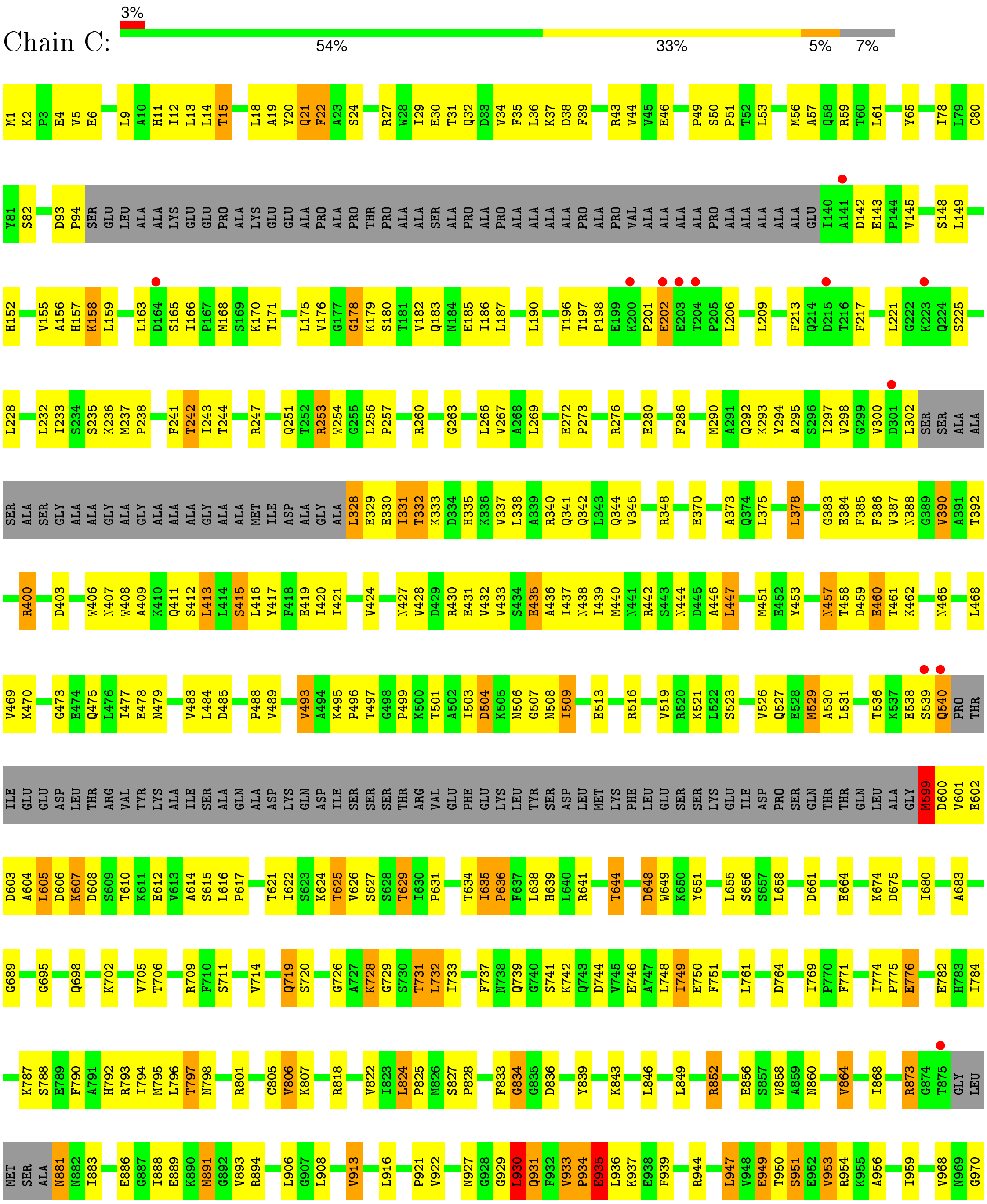
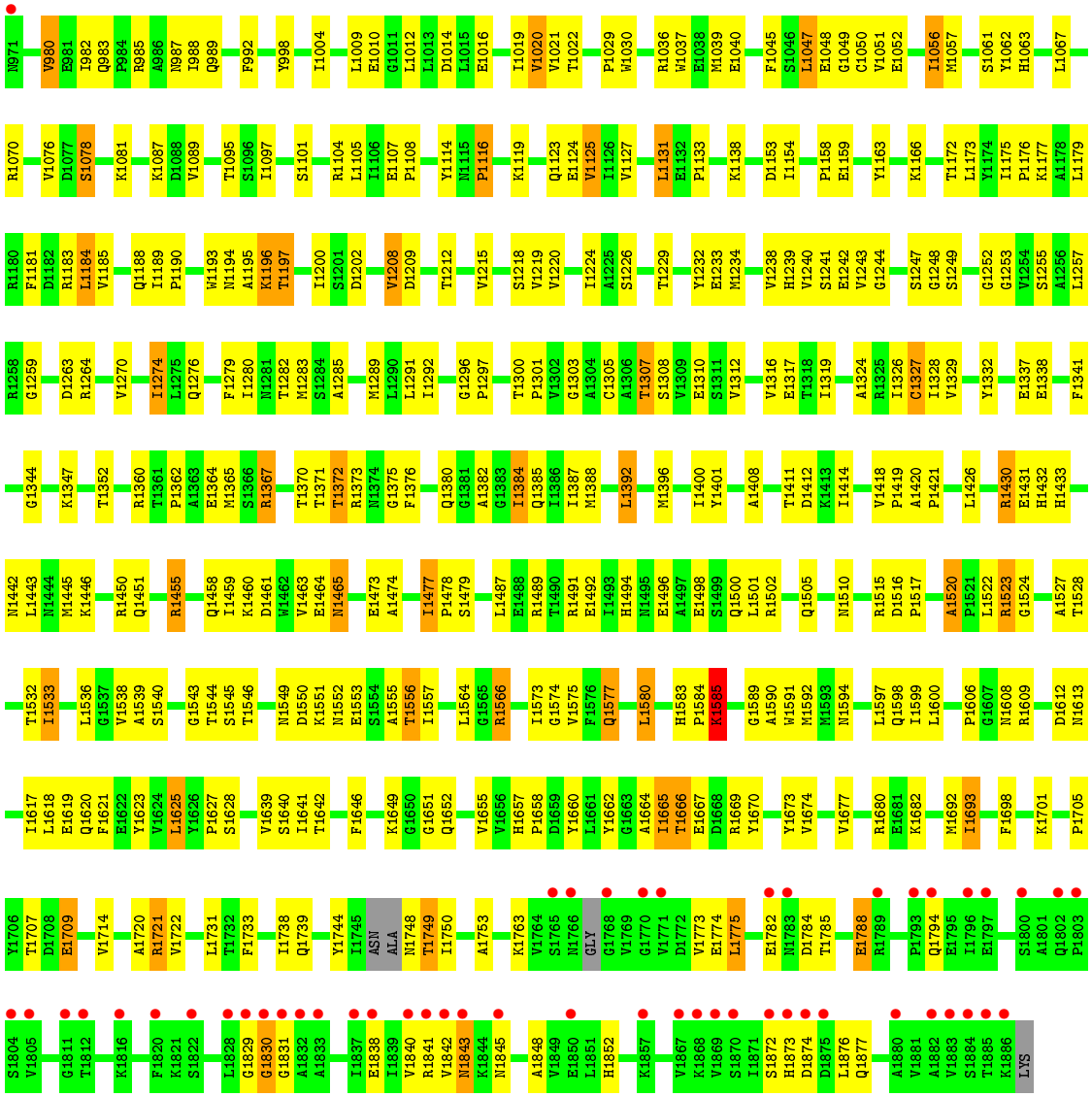
L302 SER SER ALA ALA SER ALA ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA ALA MET ILE ASP ALA GLY ALA L328 E329 E330 I331 T332 K333 D334 H335 K336 V337 L338 A339 R340 Q341 Q342 L343 Q344 V345 L350 K351 M352 R359 E370 A373 Q374 L375 L378 F385
F386 V390 A391 T392 R400 T401 F402 D403 W406 N407 W408 A409 K410 Q411 S412 L413 L414 S415 L416 Y417 F418 E419 I420 I421 V424 N427 V428 D429 R430 E431 V432 V433 S434 E435 A436 I437 N438 I439 M440 N441 R442 S443 N444 D445 A446 L447 M451 E452 Y453 H454 I455 S456 N457 T458
D459 E460 T461 K462 N465 L468 V469 K470 G473 I477 E478 N479 V483 L484 P488 V489 V493 A494 K495 P496 T497 G498 P499 K500 T501 A502 I503 D504 K505 N506 G507 N508 I509 T510 E513 R516 V519 R520 K521 L522 S523 Q527 E528 M529 A530 L531 T536 K537
E538 S539 Q540 PRO THR ILE GLU GLU ASP LEU THR ARG VAL TYR LYS ALA ILE SER ALA GLN ALA ASP LYS GLN ASP ILE SER SER THR ARG VAL GLU PHE GLU LYS LEU TYR SER ASP LEU MET LYS PHE LEU GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA
GLY M599 D600 V601 E602 D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 S615 T621 I622 S623 K624 T625 V626 S627 S628 T629 I630 P631 T634 I635 P636 F637 L638 T644 D648 Y651 L655 D661 E664 F668 N669 G670 K674 D675 I680 T681 G682 A683
G689 G695 Q698 K702 V705 T706 R709 F710 S711 V714 Q719 S720 G726 A727 K728 G729 S730 T731 L732 I733 F737 S741 K742 Q743 D744 V745 E746 A747 L748 I749 E750 F751 L761 D764 I769 P770 F771 I774 P775 E776 E780 L781 E782 H783 I784
K787 S788 E789 F790 A791 H792 R793 I794 M795 L796 T797 N798 R801 C805 V806 K807 R818 V822 I823 L824 P825 M826 S827 P828 F833 G834 G835 D836 G837 M838 Y839 K843 L846 L849 R852 W858 A859 N860 V864 I868 R873 G874 T875 GLY LEU MET
SER ALA N881 N882 I883 E886 G887 I888 E889 K890 M891 G892 V893 L906 G907 L908 V913 L916 P921 V922 L930 V938 P934 K937 E938 F939 R944 I947 V948 E949 T950 S951 E952 Y953 R954 K955 A956 I959 E964 V968 N969 G970 A976 V980 E981
I982 R985 I988 Q989 F992 Y998 I1004 L1009 E1010 G1011 L1012 L1013 D1014 L1015 E1016 I1019 V1020 V1021 T1022 P1029 W1030 R1036 W1037 E1038 M1039 E1040 F1045 S1046 L1047 E1048 G1049 C1050 V1051 E1052 I1056 M1057 S1061 Y1062 N1066 R1070 P1071 S1078 K1079 T1080
K1087 D1088 V1089 T1095 S1096 I1097 S1101 R1104 L1105 Y1114 N1115 P1116 K1119 Q1123 E1124 V1125 I1126 V1127 E1128 E1129 D1130 L1131 E1132 P1133 K1138 K1145 I1154 P1158 E1159 Y1163 K1166 T1172 L1173 Y1174 I1175 P1176 K1177 A1178 L1179 R1183 L1184 V1185 Q1188 I1189 P1190
W1193 N1194 A1195 K1196 T1197 I1200 S1201 D1202 Y1208 D1209 T1212 L1216 Y1217 S1218 V1219 S1226 T1229 Y1232 E1233 M1234 V1238 H1239 Y1240 S1241 E1242 Y1243 G1244 S1247 G1248 S1249 G1252 G1253 Y1254 S1255 A1256 L1257 R1258 G1259 D1263 R1264 V1270 I1274 L1275 Q1276 F1279
I1280 N1281 T1282 M1283 S1284 A1285 W1286 Y1287 N1288 M1289 I1292 P1297 T1300 P1301 Y1302 G1303 A1304 C1305 A1306 T1307 S1308 V1309 E1310 S1311 V1312 V1316 E1317 T1318 I1319 A1324 R1325 I1326 C1327 I1328 V1329 Y1332 E1337 E1338 F1341 G1344 K1347 T1352 R1360 T1361 P1362 A1363 E1364 M1365
S1366 R1367 T1370 T1371 T1372 R1373 N1374 G1375 F1376 Q1380 I1384 Q1385 I1386 I1387 M1388 L1392 M1396 P1399 I1400 Y1401 M1406 T1411 D1412 K1413 I1414 Y1418 P1419 A1420 P1421 L1426 T1427 T1428 A1429 R1430 E1431 H1432 H1433 S1434 N1442 M1445 K1446 Y1447 R1448 K1449 R1450 Q1451 R1455
E1456 A1457 Q1458 I1459 K1460 D1461 W1462 Y1463 E1464 N1465 E1473 A1474 I1477 P1478 S1479 E1480 E1492 E1496 A1497 E1498 S1499 Q1500 L1501 R1502 Q1505 W1508 G1509 N1510 R1515 D1516 P1517 A1520 P1521 L1522 R1523 G1524 A1527 T1528 T1532 I1533 D1534 Y1538 A1539 S1540 G1543 T1544 T1546
N1549 D1550 K1551 N1552 E1553 S1554 A1555 T1556 I1557 L1564 G1565 R1566 G1574 Y1575 F1576 Q1577 L1580 T1581 G1582 H1583 P1584 K1585 G1589 A1590 W1591 M1592 N1593 M1594 G1595 A1596 L1597 Q1598 I1599 L1600 N1608 R1609 D1612 M1613 I1617 L1618 E1619 Q1620 F1621 E1622 Y1623 V1624 L1625 S1628 V1639 S1640



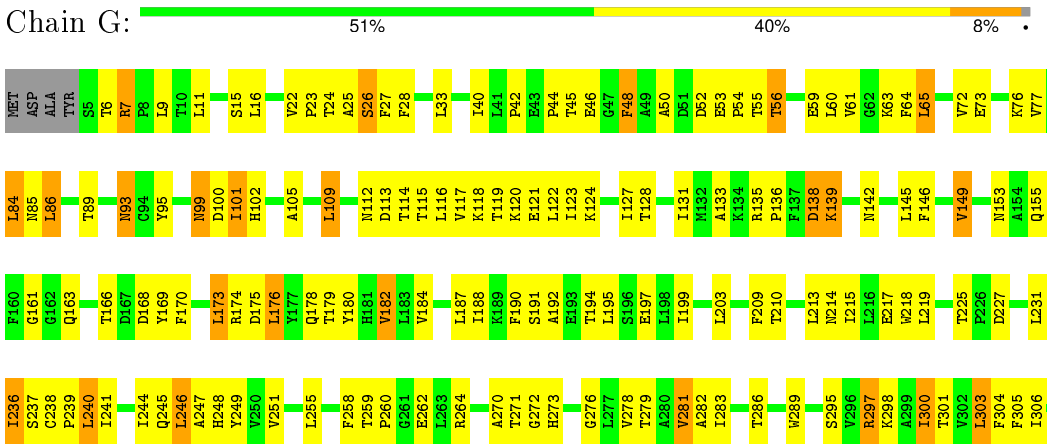
• Molecule 1: Fatty acid synthase subunit alpha

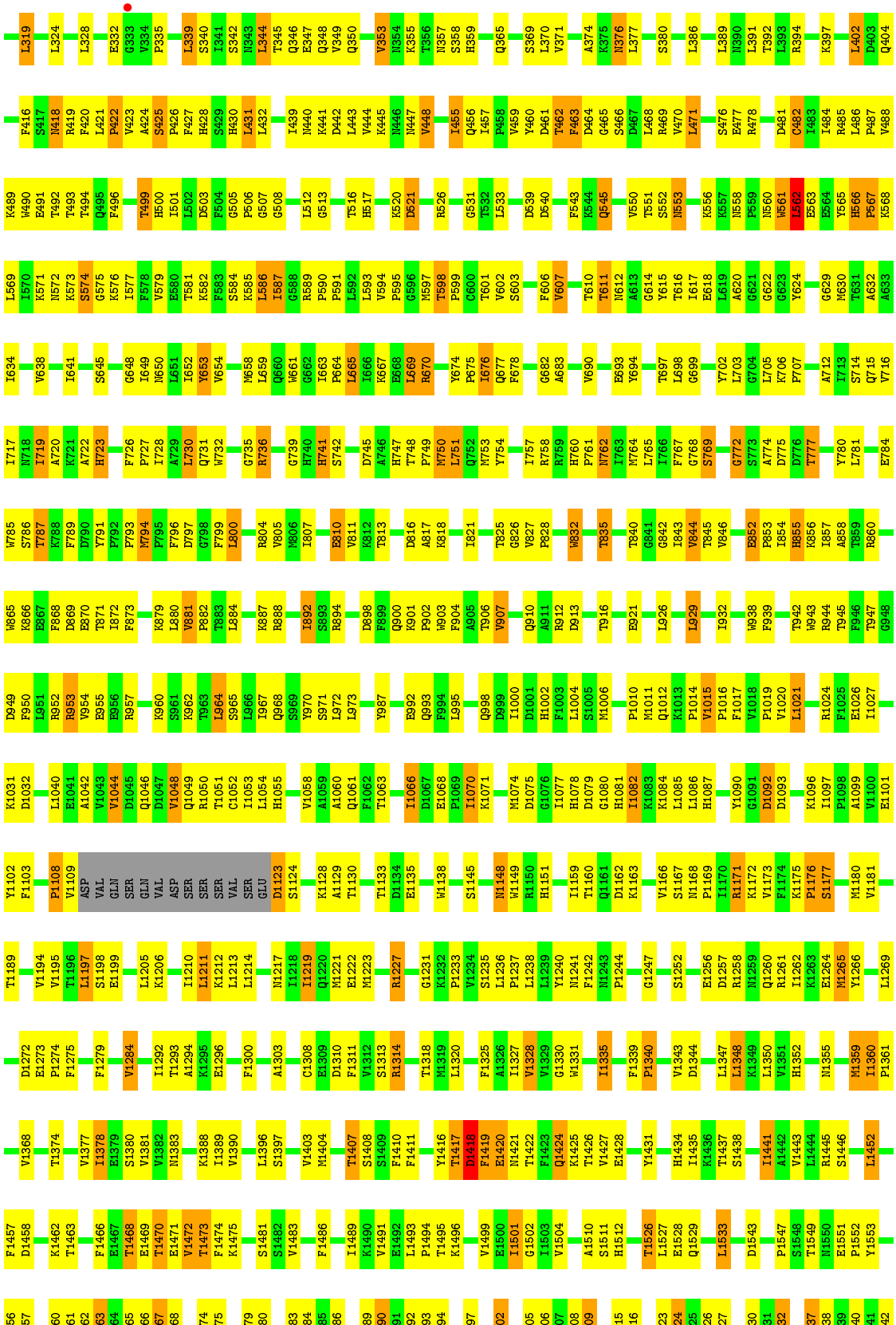




• Molecule 2: Fatty acid synthase subunit beta

Chain G:

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F416 S417 N418 R419 F420 L421 P422 V423 A424 S425 P426 F427 H428 S429 H430 L431 L432 I439 N440 K441 D442 L443 V444 K445 N446 N447 V448 I455 Q456 I457 P458 V459 Y460 D461 T462 F463 D464 G465 S466 D467 L468 R469 V470 L471 S476 E477 R478 D481 C482 I483 I484 R485 L486 P487 V488
K489 W490 E491 T492 T493 T494 Q495 F496 T499 H500 I501 L502 D503 F504 G505 P506 G507 G508 L512 G513 T516 H517 K520 D521 R526 G531 T532 L533 D539 D540 F543 K544 Q545 V550 T551 S552 N553 K556 K557 N558 P559 N560 W561 L562 E563 E564 Y565 H566 P567 K568
L569 I570 K571 N572 K573 S574 G575 K576 I577 F578 V579 E580 T581 K582 F583 S584 K585 L586 I587 G588 R589 P590 P591 L592 L593 V594 P595 G596 M597 T598 P599 G600 T601 V602 S603 F606 V607 T610 T611 N612 A613 G614 Y615 T616 I617 E618 L619 A620 G621 G622 G623 Y624 G629 M630 T631 A632 A633
I634 V638 I641 S645 G648 I649 N650 L651 I652 Y653 V654 M658 L659 Q660 W661 G662 I663 P664 L665 I666 K667 E668 L669 R670 Y674 P675 I676 Q677 F678 G682 A683 V690 E693 Y694 T697 L698 G699 Y702 L703 G704 L705 K706 P707 A712 I713 S714 Q715 V716
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W785 S786 T787 K788 F789 D790 Y791 P792 P793 M794 P795 F796 D797 G798 F799 L800 R804 V805 M806 I807 E810 V811 K812 T813 D816 A817 K818 I821 T825 G826 V827 P828 W832 T835 T840 G841 G842 I843 V844 T845 V846 E852 P853 I854 H855 K856 I857 A858 T859 R860
W865 K866 E867 F868 D869 E870 T871 I872 F873 K879 L880 V881 P882 T883 L884 K887 R888 I892 S893 R894 D898 F899 Q900 K901 P902 W903 F904 A905 T906 V907 Q910 A911 R912 D913 T916 E921 L926 L929 I932 W938 F939 T942 W943 R944 T945 F946 G948
D949 F950 L951 R952 R953 V954 E955 E956 R957 K960 S961 K962 T963 L964 S965 L966 I967 Q968 S969 Y970 S971 L972 L973 Y987 E992 Q993 F994 L995 Q998 D999 I1000 D1001 H1002 F1003 L1004 S1005 M1006 P1010 M1011 Q1012 K1013 P1014 V1015 P1016 F1017 V1018 P1019 V1020 L1021 R1024 F1025 E1026 I1027
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T1189 V1194 V1195 T1196 L1197 S1198 E1199 L1205 K1206 I1210 L1211 K1212 L1213 L1214 N1217 I1218 I1219 Q1220 A1221 E1222 M1223 R1227 G1231 K1232 P1233 V1234 S1235 L1236 P1237 L1238 L1239 Y1240 N1241 F1242 N1243 P1244 G1247 S1252 E1256 D1257 R1258 N1259 Q1260 R1261 I1262 K1263 E1264 M1265 Y1266 L1269
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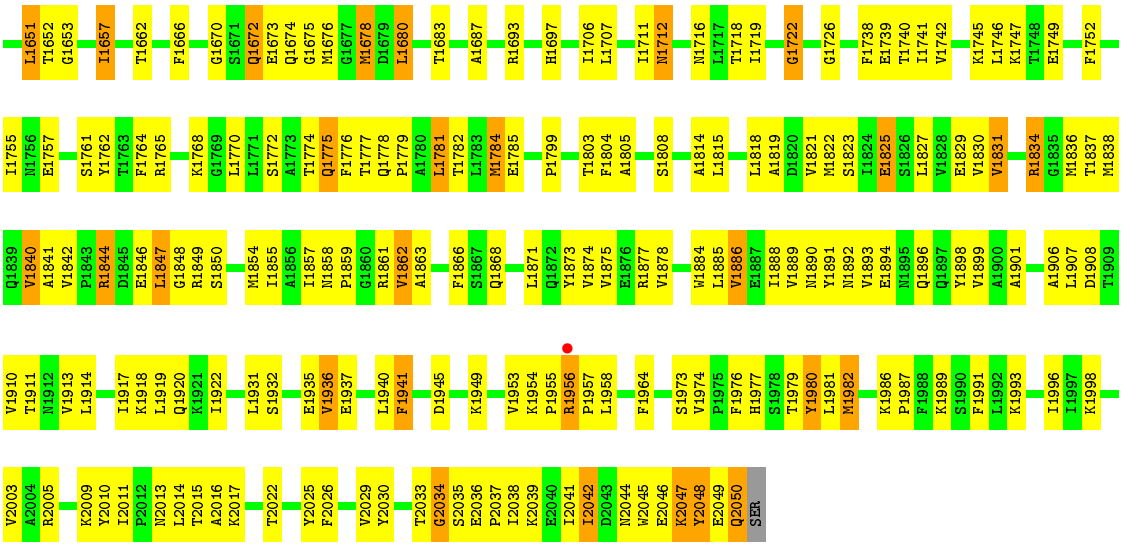
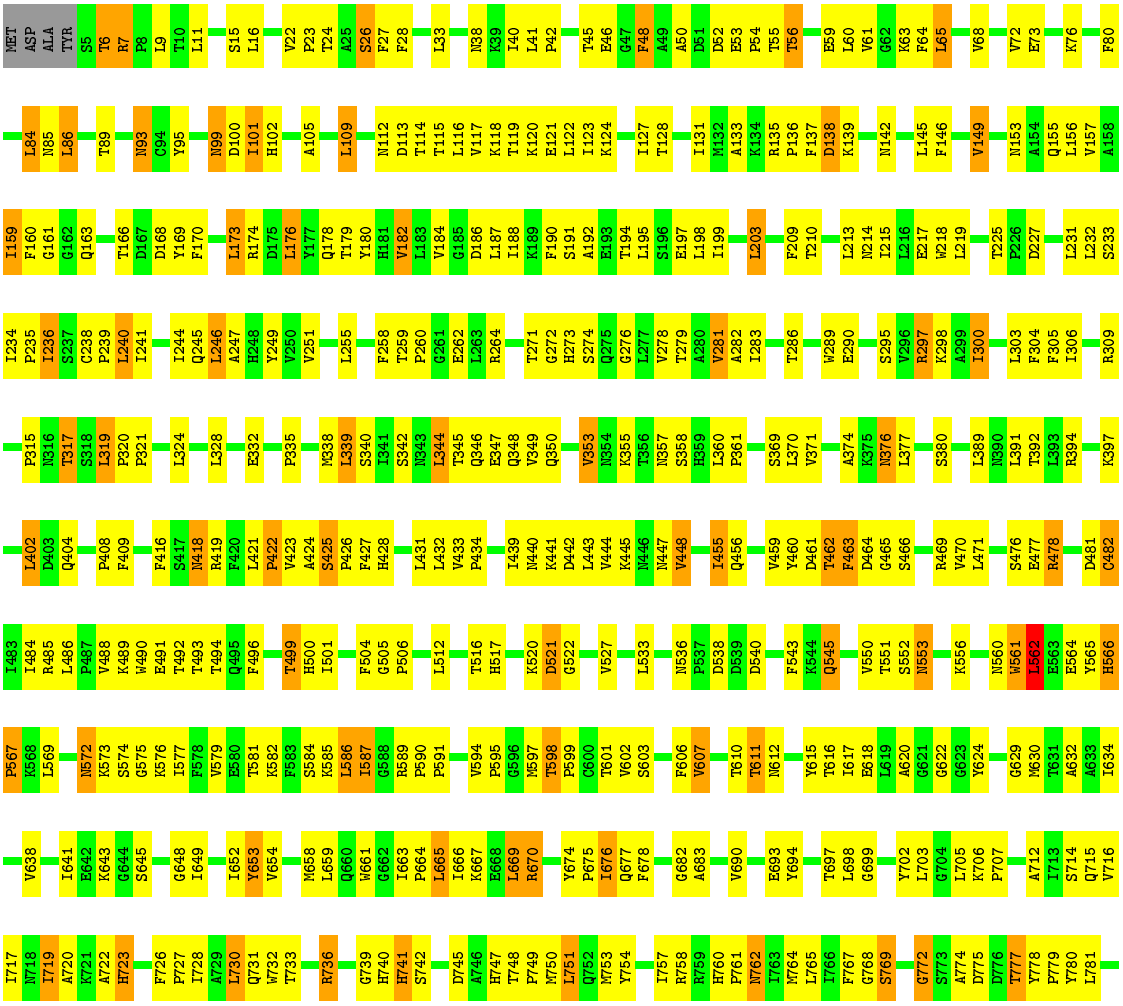
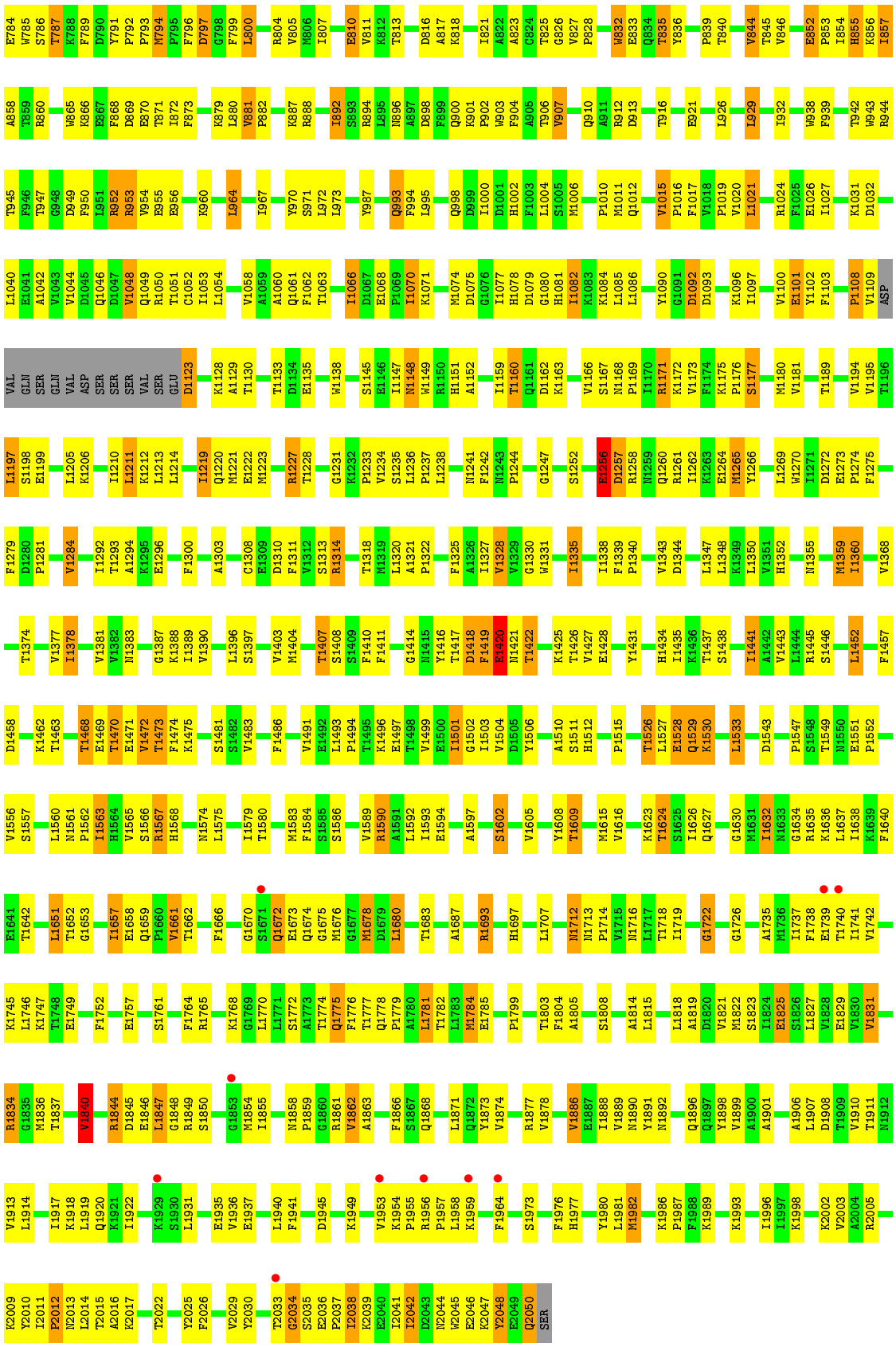


• Molecule 2: Fatty acid synthase subunit beta

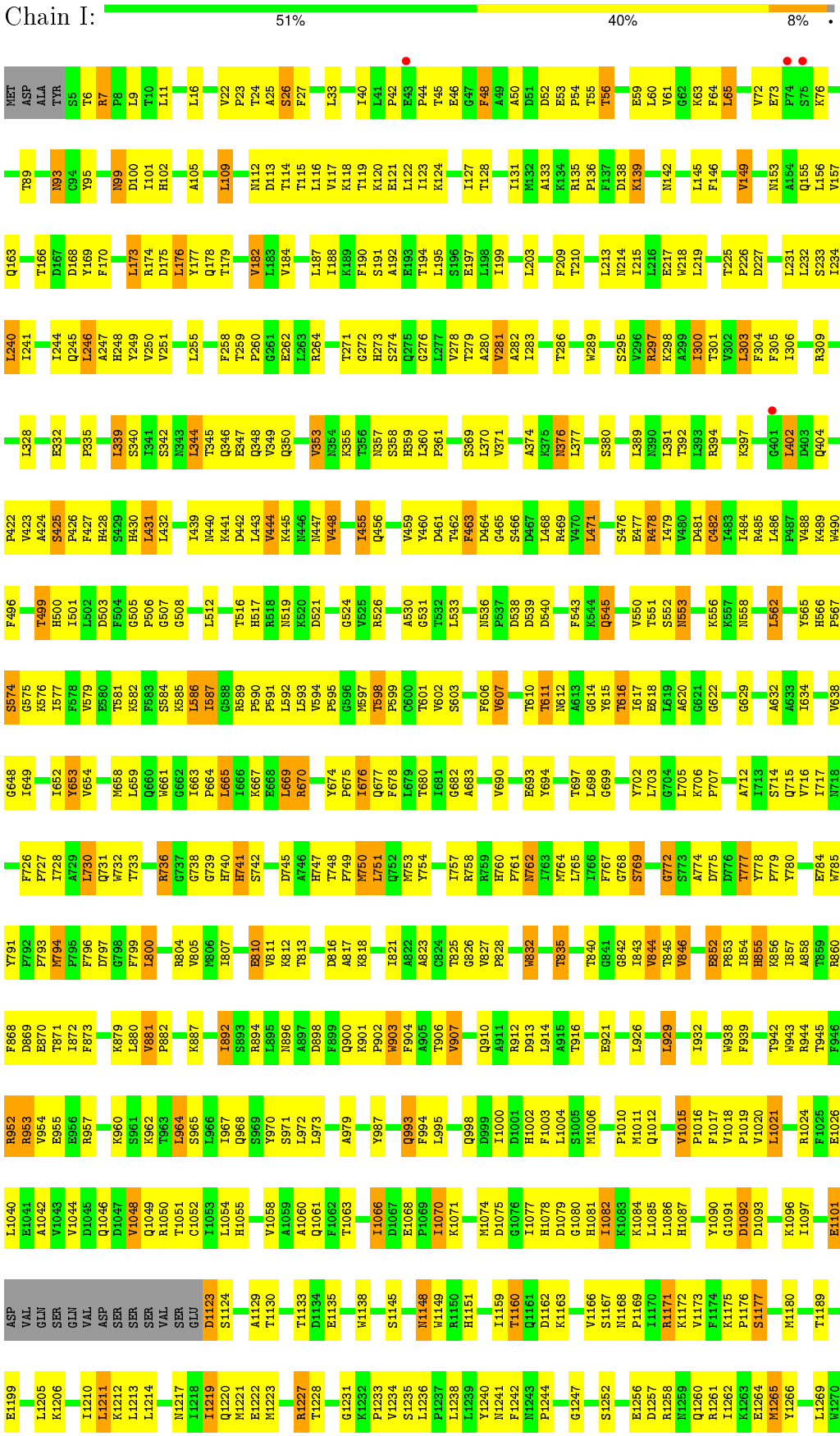
Chain H:

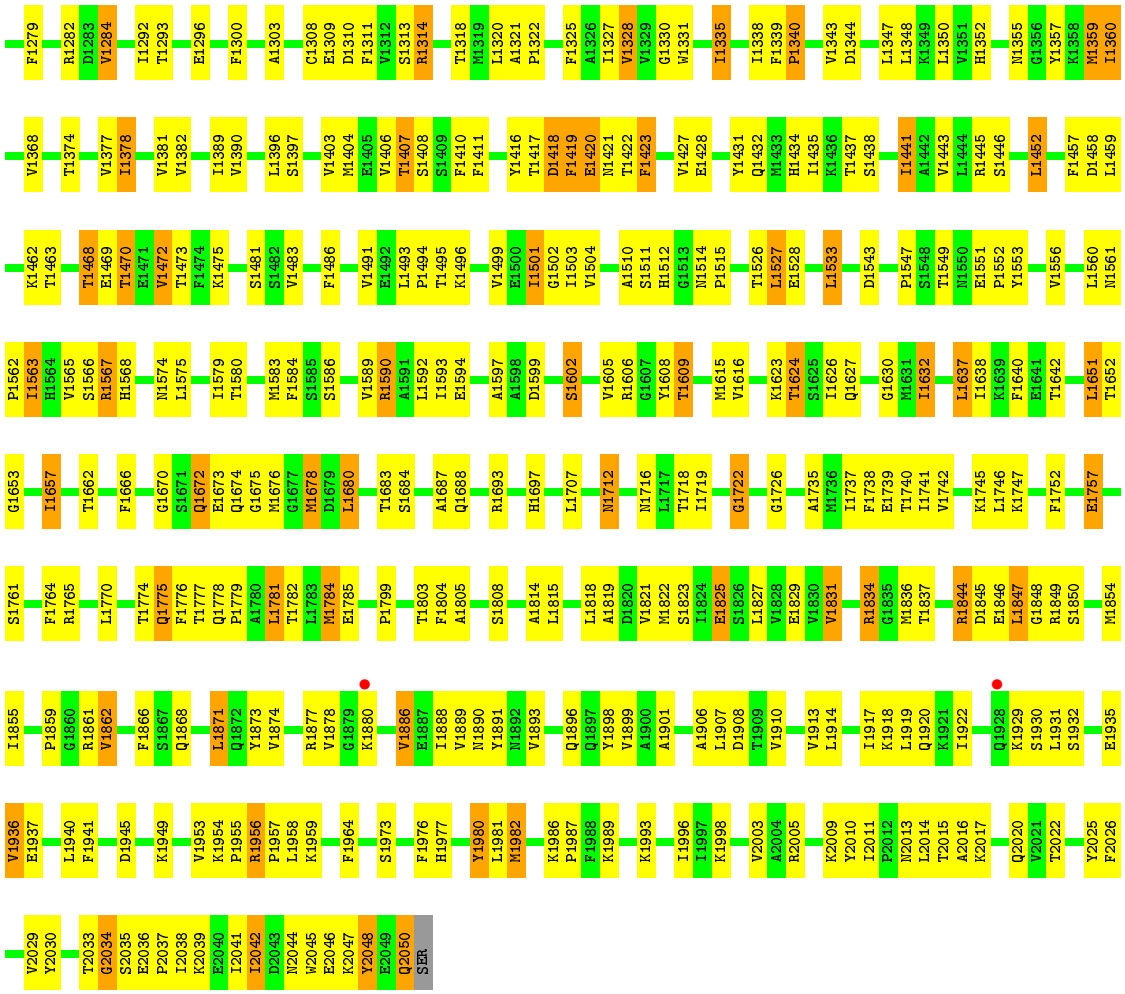




- Molecule 2: Fatty acid synthase subunit beta

Chain I:




F1279 R1282 D1283 V1284 I1292 T1293 E1296 F1300 A1303 C1308 E1309 D1310 F1311 V1312 S1313 R1314 T1318 M1319 L1320 A1321 P1322 F1325 A1326 I1327 V1328 V1329 G1330 W1331 I1335 I1338 F1339 P1340 V1343 D1344 L1347 L1348 K1349 L1350 V1351 H1352 N1355 G1356 Y1357 K1358 M1359 I1360
V1368 T1374 V1377 I1378 V1381 V1382 I1389 V1390 L1396 S1397 V1403 M1404 E1405 V1406 T1407 S1408 S1409 F1410 F1411 Y1416 T1417 D1418 F1419 E1420 N1421 T1422 F1423 V1427 E1428 Y1431 Q1432 M1433 H1434 I1435 K1436 T1437 S1438 I1441 A1442 V1443 L1444 R1445 S1446 L1452 F1457 D1458 L1459
K1462 T1463 T1468 E1469 T1470 E1471 V1472 T1473 F1474 K1475 S1481 S1482 V1483 F1486 V1491 E1492 L1493 P1494 T1495 K1496 V1499 E1500 I1501 G1502 I1503 V1504 A1510 S1511 H1512 G1513 N1514 P1515 T1526 L1527 E1528 L1533 D1543 P1547 S1548 T1549 N1550 E1551 P1552 Y1553 V1556 L1560 N1561
P1562 I1563 H1564 V1565 S1566 R1567 H1568 N1574 L1575 I1579 T1580 M1583 F1584 S1585 S1586 V1589 R1590 A1591 L1592 I1593 E1594 A1597 A1598 D1599 S1602 V1605 R1606 G1607 Y1608 T1609 M1615 V1616 K1623 T1624 S1625 I1626 Q1627 G1630 M1631 I1632 L1637 I1638 K1639 F1640 E1641 T1642 L1651 T1652
G1653 I1657 T1662 F1666 G1670 S1671 Q1672 E1673 Q1674 G1675 M1676 G1677 M1678 D1679 L1680 T1683 S1684 A1687 Q1688 R1693 H1697 L1707 N1712 N1716 L1717 T1718 I1719 G1722 G1726 A1735 M1736 I1737 F1738 E1739 T1740 I1741 V1742 K1745 L1746 K1747 F1752 E1757
S1761 F1764 R1765 L1770 T1774 Q1775 F1776 T1777 Q1778 P1779 A1780 L1781 T1782 L1783 M1784 E1785 P1799 T1803 F1804 A1805 S1808 A1814 L1815 L1818 A1819 D1820 V1821 M1822 S1823 I1824 E1825 S1826 L1827 V1828 E1829 V1830 V1831 R1834 G1835 M1836 T1837 R1844 D1845 E1846 L1847 G1848 R1849 S1850 M1854
I1855 P1859 G1860 R1861 V1862 F1866 S1867 Q1868 L1871 Q1872 Y1873 V1874 R1877 V1878 G1879 K1880 V1886 E1887 I1888 V1889 N1890 Y1891 N1892 V1893 Q1896 Q1897 Y1898 V1899 A1900 A1901 A1906 L1907 D1908 T1909 V1910 V1913 L1914 I1917 K1918 L1919 Q1920 K1921 I1922 Q1928 K1929 S1930 L1931 S1932 E1935
V1936 E1937 L1940 F1941 D1945 K1949 V1953 K1954 P1955 R1956 P1957 L1958 K1959 F1964 S1973 F1976 H1977 Y1980 L1981 M1982 K1986 P1987 F1988 K1989 K1993 I1996 I1997 K1998 V2003 A2004 R2005 K2009 Y2010 I2011 P2012 N2013 L2014 T2015 A2016 K2017 Q2020 V2021 T2022 Y2025 F2026
V2029 Y2030 T2033 G2034 S2035 E2036 P2037 I2038 K2039 E2040 I2041 I2042 D2043 N2044 W2045 E2046 K2047 Y2048 E2049 Q2050 SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	231.88Å 231.88Å 756.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-4.00) 97.3 (20.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.267 0.275 , 0.279	Depositor DCC
R_{free} test set	8521 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 75.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 168120 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	88830	wwPDB-VP
Average B, all atoms (Å^2)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	5/13822 (0.0%)	0.59	6/18682 (0.0%)
1	B	0.43	3/13822 (0.0%)	0.61	9/18682 (0.0%)
1	C	0.43	4/13822 (0.0%)	0.59	4/18682 (0.0%)
2	G	0.41	7/16360 (0.0%)	0.58	6/22198 (0.0%)
2	H	0.40	7/16360 (0.0%)	0.57	3/22198 (0.0%)
2	I	0.40	5/16360 (0.0%)	0.58	10/22198 (0.0%)
All	All	0.42	31/90546 (0.0%)	0.59	38/122640 (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
2	G	0	1
2	H	0	2
2	I	0	1
All	All	0	4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	PHE	C-N	13.35	1.59	1.34
1	C	992	PHE	C-N	13.18	1.59	1.34
2	I	842	GLY	C-N	11.12	1.59	1.34
2	G	315	PRO	C-N	10.45	1.58	1.34
1	C	485	ASP	C-N	9.61	1.56	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	I	1982	MET	O-C-N	-9.44	107.59	122.70
2	G	842	GLY	O-C-N	-8.86	108.52	122.70
2	G	1053	ILE	O-C-N	-8.58	108.97	122.70
1	B	992	PHE	O-C-N	8.47	137.19	121.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
2	H	1256	GLU	Mainchain
2	I	1108	PRO	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	13572	0	13489	663	15
1	B	13572	0	13490	618	6
1	C	13572	0	13490	638	22
2	G	15995	0	15978	1026	32
2	H	15995	0	15978	1023	7
2	I	15995	0	15977	983	26
3	A	12	0	10	3	0
3	B	12	0	10	4	0
3	C	12	0	10	4	0
4	G	31	0	19	7	0
4	H	31	0	19	6	0
4	I	31	0	19	8	0
All	All	88830	0	88489	4773	54

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 27.

The worst 5 of 4773 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:1749:THR:CB	1:A:1874:ASP:HB3	1.53	1.37
1:B:1749:THR:CB	1:B:1874:ASP:HB3	1.56	1.34
1:B:1749:THR:CB	1:B:1873:HIS:O	1.75	1.32
1:A:1464:GLU:HG3	1:A:1773:VAL:CG1	1.58	1.32
1:C:1749:THR:CB	1:C:1874:ASP:HB3	1.62	1.29

The worst 5 of 54 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1784:ASP:CA	2:G:1087:HIS:CE1[7_655]	0.16	2.04
1:A:1784:ASP:CG	2:I:1087:HIS:CE1[7_545]	0.52	1.68
1:C:1784:ASP:C	2:G:1087:HIS:NE2[7_655]	0.54	1.66
1:C:1784:ASP:CB	2:G:1087:HIS:ND1[7_655]	0.56	1.64
1:A:1784:ASP:OD2	2:I:1087:HIS:ND1[7_545]	0.58	1.62

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1736/1887 (92%)	1614 (93%)	100 (6%)	22 (1%)	15	60
1	B	1736/1887 (92%)	1619 (93%)	100 (6%)	17 (1%)	19	65
1	C	1736/1887 (92%)	1618 (93%)	96 (6%)	22 (1%)	15	60
2	G	2029/2051 (99%)	1825 (90%)	173 (8%)	31 (2%)	13	58
2	H	2029/2051 (99%)	1826 (90%)	173 (8%)	30 (2%)	13	58
2	I	2029/2051 (99%)	1829 (90%)	174 (9%)	26 (1%)	15	60
All	All	11295/11814 (96%)	10331 (92%)	816 (7%)	148 (1%)	15	60

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1460/1566 (93%)	1308 (90%)	152 (10%)	9	40
1	B	1460/1566 (93%)	1312 (90%)	148 (10%)	9	41
1	C	1460/1566 (93%)	1310 (90%)	150 (10%)	9	40
2	G	1772/1789 (99%)	1563 (88%)	209 (12%)	6	35
2	H	1772/1789 (99%)	1560 (88%)	212 (12%)	6	33
2	I	1772/1789 (99%)	1561 (88%)	211 (12%)	6	34
All	All	9696/10065 (96%)	8614 (89%)	1082 (11%)	7	37

5 of 1082 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	344	LEU
2	G	1452	LEU
2	I	1145	SER
2	G	471	LEU
2	G	857	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 294 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	989	GLN
2	G	418	ASN
2	I	900	GLN
1	C	1064	ASN

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Mol	Chain	Res	Type
1	C	1542	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	CER	A	2748	-	10,11,15	4.07	3 (30%)	9,13,17	3.23	2 (22%)
3	CER	B	2748	-	10,11,15	4.07	3 (30%)	9,13,17	3.11	2 (22%)
3	CER	C	2748	-	10,11,15	4.09	3 (30%)	9,13,17	3.24	2 (22%)
4	FMN	G	3051	-	32,33,33	6.16	19 (59%)	34,50,50	1.96	6 (17%)
4	FMN	H	3051	-	32,33,33	6.07	19 (59%)	34,50,50	1.97	6 (17%)
4	FMN	I	3051	-	32,33,33	6.11	21 (65%)	34,50,50	1.87	6 (17%)

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	CER	A	2748	-	-	0/12/12/16	0/0/0/0
3	CER	B	2748	-	-	0/12/12/16	0/0/0/0
3	CER	C	2748	-	-	0/12/12/16	0/0/0/0
4	FMN	G	3051	-	-	0/18/18/18	0/3/3/3
4	FMN	H	3051	-	-	0/18/18/18	0/3/3/3
4	FMN	I	3051	-	-	0/18/18/18	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3051	FMN	C7M-C7	2.12	1.55	1.51
4	I	3051	FMN	C8M-C8	2.28	1.55	1.51
4	G	3051	FMN	P-O3P	2.92	1.64	1.54
3	A	2748	CER	C5-C4	3.14	1.55	1.51
4	H	3051	FMN	P-O3P	3.16	1.65	1.54

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2748	CER	O1-C4-C3	-6.71	108.66	120.03
3	C	2748	CER	O1-C4-C3	-6.69	108.69	120.03
3	C	2748	CER	O1-C4-C5	-6.55	107.97	121.70
3	A	2748	CER	O1-C4-C5	-6.51	108.06	121.70
3	B	2748	CER	O1-C4-C3	-6.48	109.06	120.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2748	CER	3	0
3	B	2748	CER	4	0
3	C	2748	CER	4	0
4	G	3051	FMN	7	0
4	H	3051	FMN	6	0
4	I	3051	FMN	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1750/1887 (92%)	-0.30	47 (2%) 58 46	95, 134, 347, 457	0
1	B	1750/1887 (92%)	-0.34	31 (1%) 71 61	96, 133, 302, 419	0
1	C	1750/1887 (92%)	-0.26	64 (3%) 45 34	98, 135, 423, 568	0
2	G	2033/2051 (99%)	-0.45	2 (0%) 95 95	131, 169, 218, 267	0
2	H	2033/2051 (99%)	-0.36	10 (0%) 91 88	130, 170, 215, 265	0
2	I	2033/2051 (99%)	-0.43	6 (0%) 94 92	131, 171, 215, 261	0
All	All	11349/11814 (96%)	-0.36	160 (1%) 78 68	95, 162, 239, 568	0

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1882	ALA	10.5
1	C	1831	GLY	9.3
1	A	1829	GLY	8.0
1	C	1830	GLY	7.8
1	C	1870	SER	7.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CER	C	2748	12/16	0.90	0.34	2.51	67,131,249,250	0
3	CER	A	2748	12/16	0.84	0.30	1.87	67,131,240,249	0
4	FMN	H	3051	31/31	0.80	0.32	0.09	131,157,181,186	0
4	FMN	G	3051	31/31	0.82	0.27	-0.19	135,158,184,203	0
4	FMN	I	3051	31/31	0.82	0.26	-0.23	129,161,178,201	0
3	CER	B	2748	12/16	0.91	0.20	-0.50	67,131,249,250	0

6.5 Other polymers

There are no such residues in this entry.