wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:47 PM GMT

PDB ID	:	2UV8
Title	:	CRYSTAL STRUCTURE OF YEAST FATTY ACID SYNTHASE WITH STALLED ACYL CARRIER PROTEIN AT 3.1 ANGSTROM RESOLUTION
Authors	:	Leibundgut, M.; Jenni, S.; Frick, C.; Ban, N.
Deposited on	:	2007-03-09
Resolution	:	3.10 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:

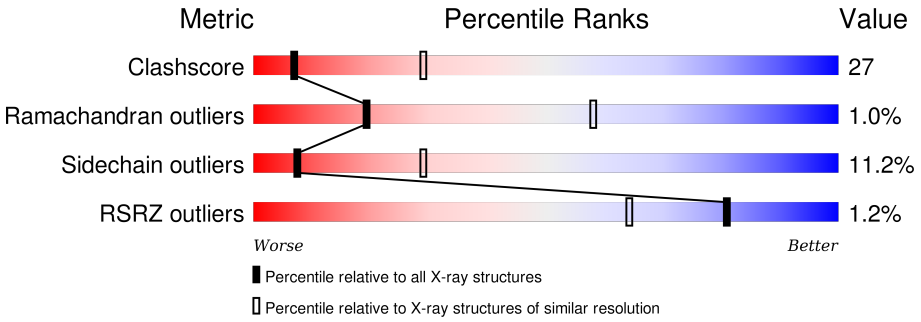
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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% 50% 31% 5% 14%
1	B	1887	2% 51% 30% 5% 14%
1	C	1887	2% 49% 31% 5% 14%
2	G	2051	2% 51% 41% 7%
2	H	2051	2% 52% 40% 7%
2	I	2051	2% 51% 41% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 85962 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.

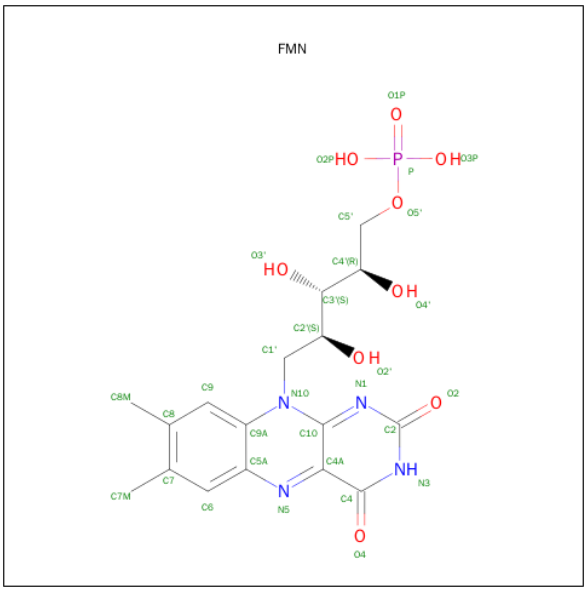
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	B	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	C	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			

- Molecule 2 is a protein called FATTY ACID SYNTHASE SUBUNIT BETA (FAS1).

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



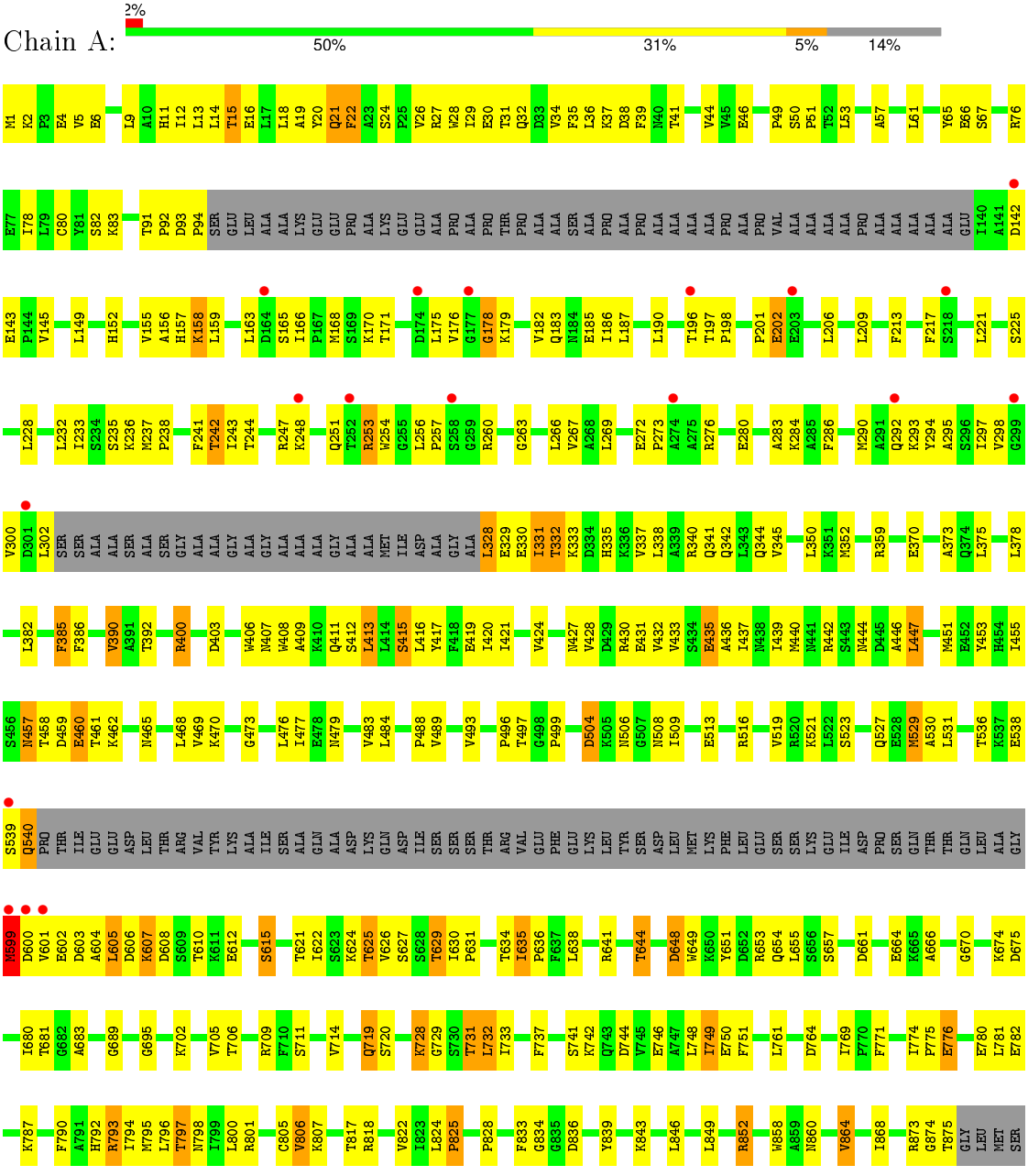
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

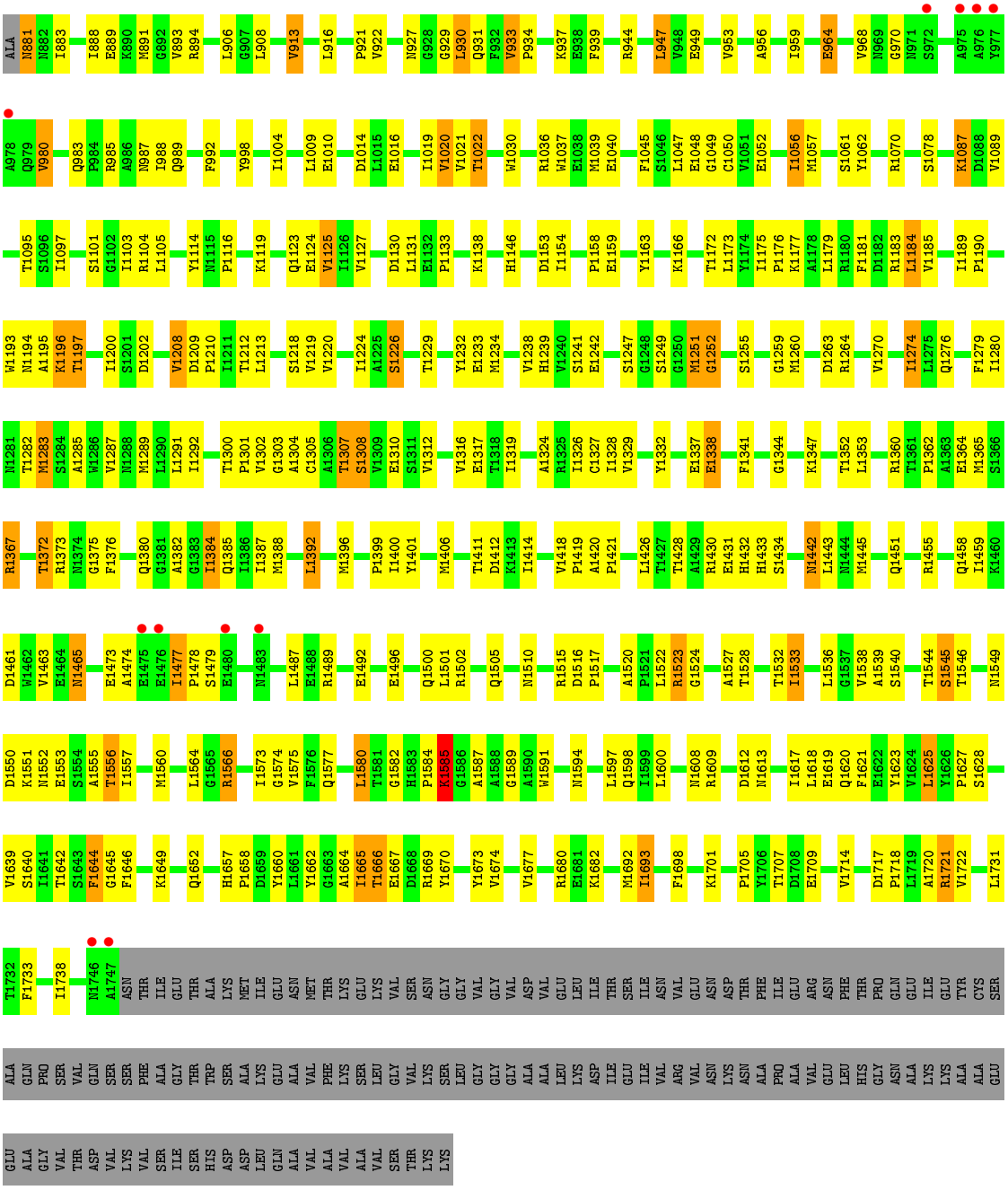
3 Residue-property plots (i)

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 (FAS2)

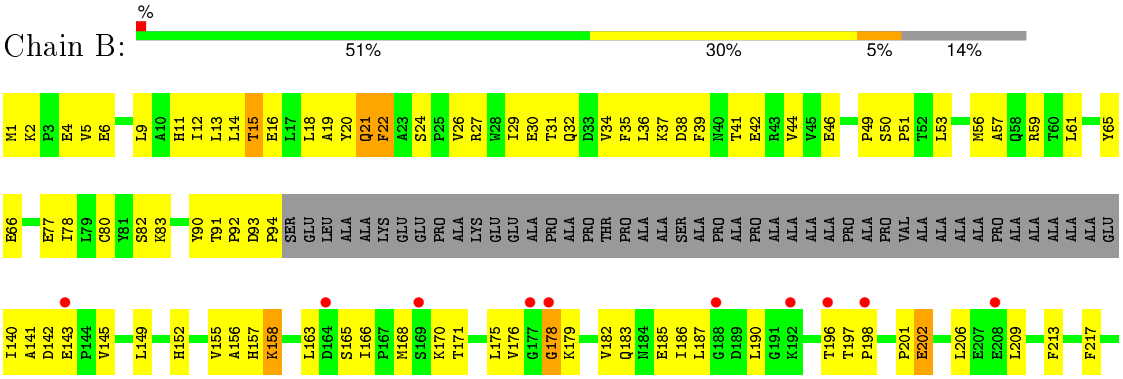
Chain A:

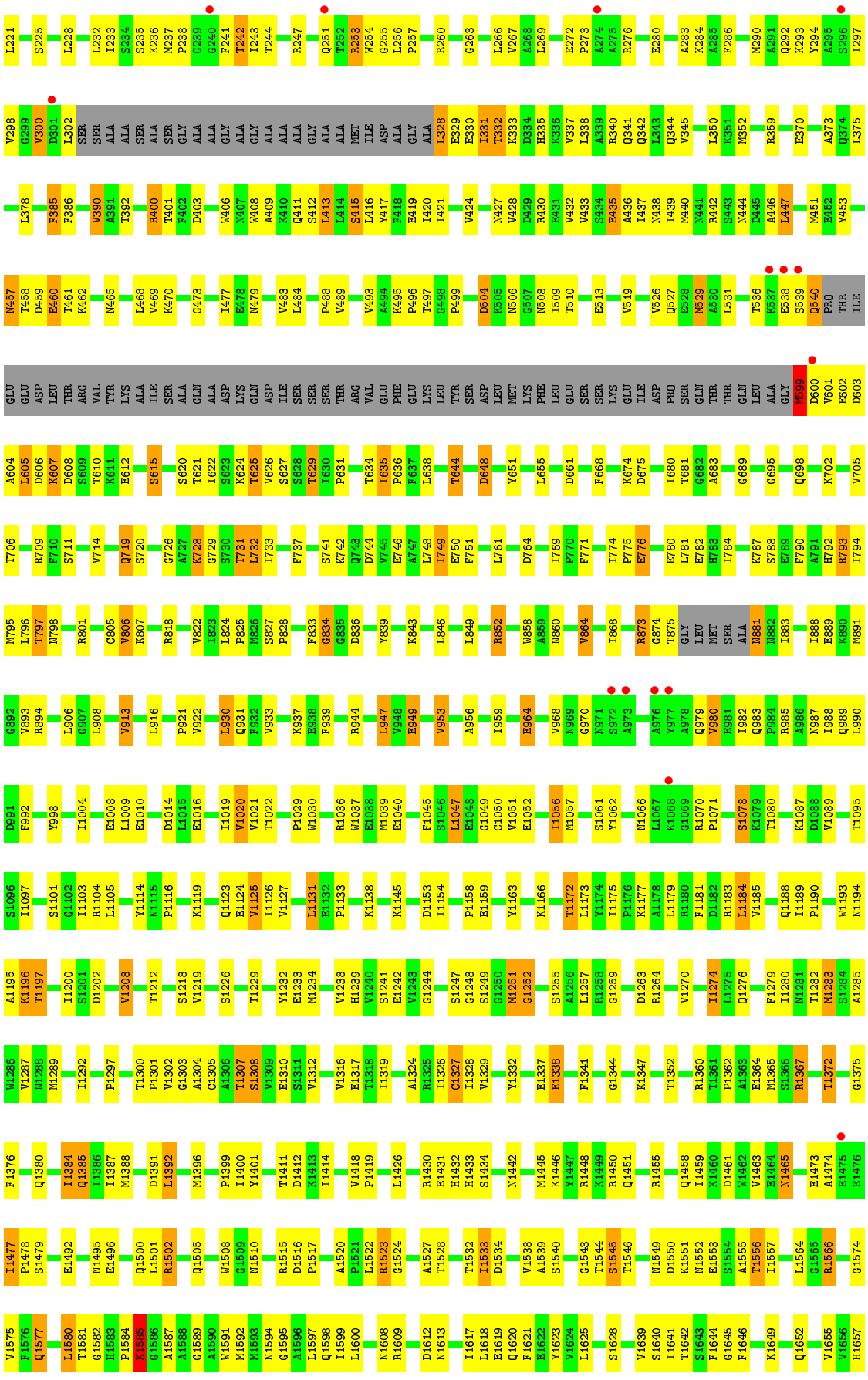


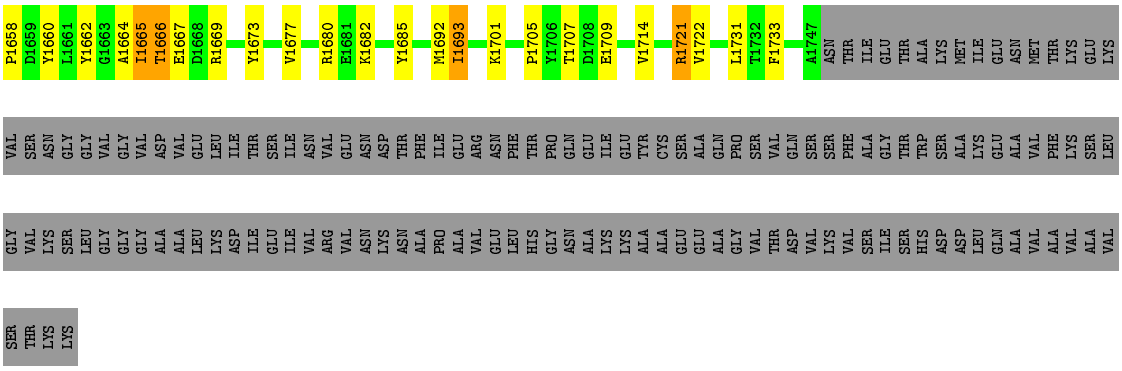


• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2)

Chain B:

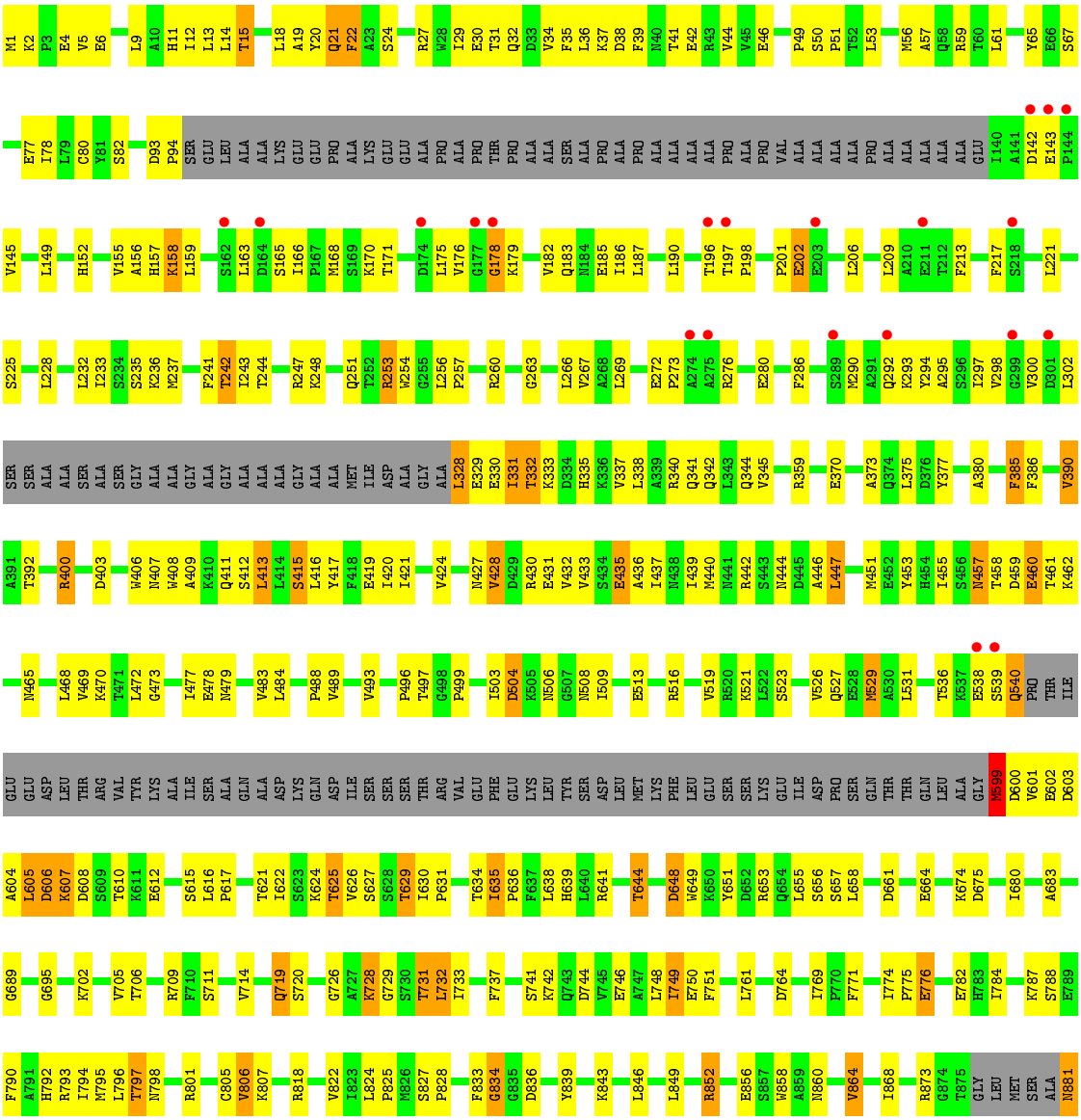


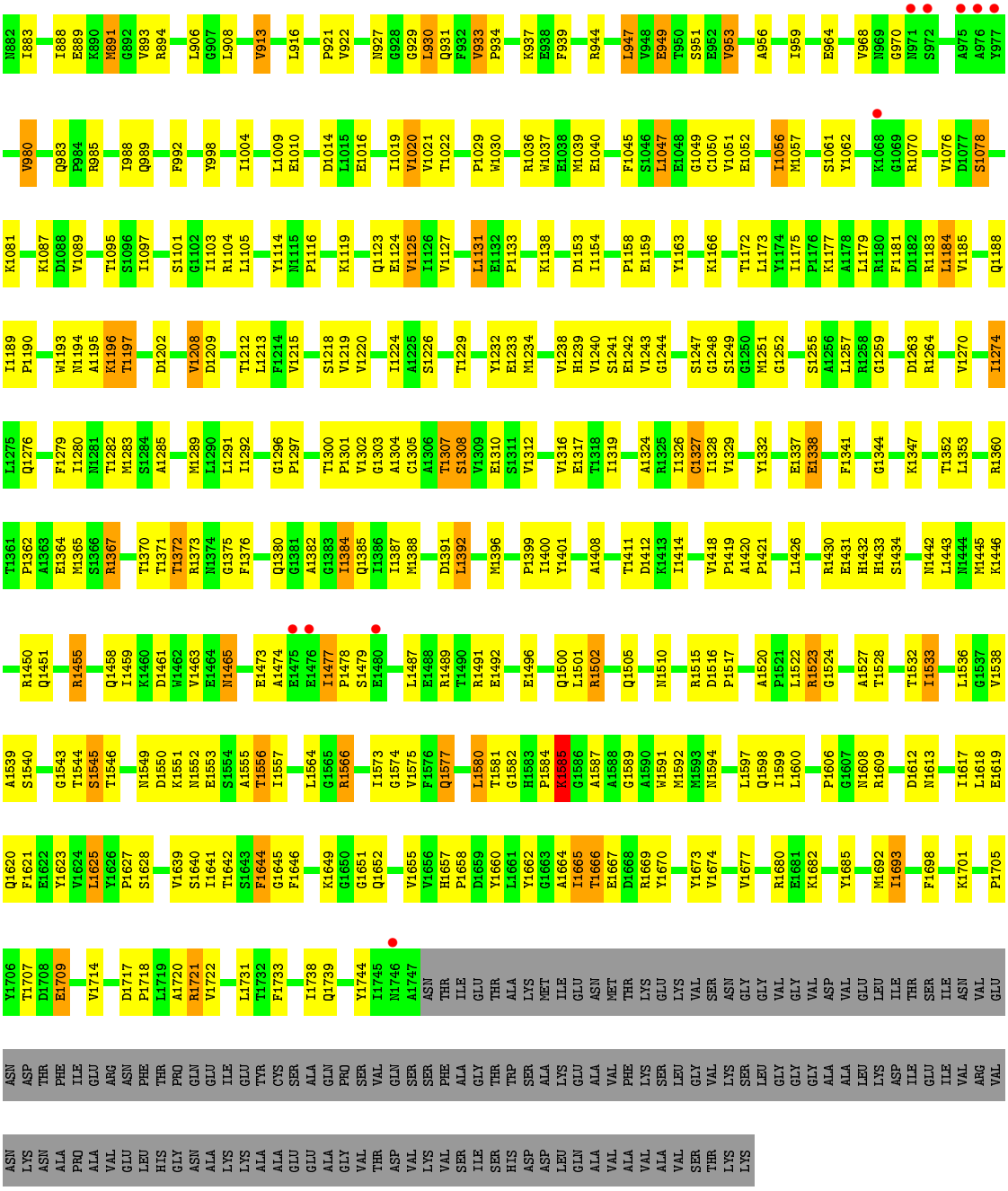

L221 S225 L228 L232 I233 S234 S235 K236 M237 P238 G239 G240 F241 T242 I243 T244 R247 Q251 T252 R253 W254 G255 L256 P257 R260 G263 L266 V267 A268 L269 E272 P273 A274 A275 R276 E280 A283 K284 A285 F286 M290 A291 Q292 K293 Y294 A295 S296 I297
V298 G299 V300 D301 L302 SER SER ALA ALA SER ALA SER GLY ALA ALA GLY ALA GLY ALA ALA 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
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 D504 K505 N506 G507 N508 I509 T510 E513 V519 V526 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 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 S620 T621 I622 S623 K624 T625 V626 S627 S628 T629 I630 P631 T634 I635 P636 F637 L638 T644 D648 Y651 L655 D661 F668 K674 D675 I680 T681 G682 A683 G689 G695 Q698 K702 V705
T706 R709 F710 S711 V714 Q719 S720 G726 A727 K728 G729 S730 T731 I732 I733 F737 S741 K742 Q743 D744 V745 E746 A747 L748 I749 E750 F751 L761 D764 I769 F770 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 Y839 K843 L846 L849 R852 W858 A859 N860 V864 I868 R873 G874 T875 GLY LEU MET SER ALA N881 N882 I883 I888 E889 K890 M891
G892 V893 R894 L906 G907 L908 V913 L916 P921 V922 L930 Q931 F932 V933 K937 E938 F939 R944 L947 V948 E949 V953 A956 I959 E964 V968 N969 G970 N971 S972 A973 A976 Y977 A978 Q979 V980 E981 I982 Q983 P984 R985 A986 N987 I988 Q989 L990
D991 F992 Y998 I1004 E1008 L1009 E1010 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 L1067 K1068 G1069 R1070 P1071 S1078 K1079 T1080 K1087 D1088 V1089 T1095
S1096 I1097 S1101 G1102 I1103 R1104 L1105 Y1114 N1115 P1116 K1119 Q1123 E1124 V1125 I1126 V1127 L1131 E1132 P1133 K1138 K1145 D1153 I1154 P1158 E1159 Y1163 K1166 T1172 L1173 Y1174 I1175 P1176 K1177 A1178 L1179 R1180 F1181 D1182 R1183 L1184 V1185 Q1188 I1189 P1190 W1193 N1194
A1195 K1196 T1197 I1200 S1201 D1202 V1208 T1212 S1218 V1219 S1226 T1229 Y1232 E1233 M1234 V1238 H1239 V1240 S1241 E1242 V1243 G1244 S1247 G1248 S1249 G1250 M1251 G1252 S1255 A1256 L1257 R1258 G1259 D1263 R1264 V1270 I1274 L1275 Q1276 F1279 I1280 N1281 T1282 M1283 S1284 A1285
W1286 V1287 N1288 M1289 I1292 P1297 T1300 P1301 V1302 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 T1372 G1375
F1376 Q1380 I1384 Q1385 I1386 I1387 M1388 D1391 L1392 M1396 P1399 I1400 Y1401 T1411 D1412 K1413 I1414 L1426 R1430 E1431 H1432 H1433 S1434 N1442 M1445 K1446 Y1447 R1448 K1449 R1450 Q1451 R1455 Q1458 I1459 K1460 D1461 W1462 V1463 E1464 N1465 E1473 A1474 E1475 E1476
I1477 P1478 S1479 E1492 N1495 E1496 Q1500 L1501 R1502 Q1505 W1508 G1509 N1510 R1515 D1516 P1517 A1520 P1521 L1522 R1523 G1524 A1527 T1528 T1532 I1533 D1534 V1538 A1539 S1540 G1543 T1544 S1545 T1546 N1549 D1550 K1551 N1552 E1553 S1554 A1555 T1556 I1557 L1564 G1565 R1566 G1574
V1575 F1576 Q1577 L1580 T1581 G1582 H1583 P1584 K1588 G1586 A1587 A1588 G1589 A1590 W1591 M1592 M1593 N1594 G1595 A1596 L1597 Q1598 I1599 L1600 N1608 R1609 D1612 N1613 I1617 L1618 E1619 Q1620 F1621 E1622 Y1623 V1624 L1625 S1628 V1639 S1640 I1641 T1642 S1643 F1644 G1645 F1646 K1649 Q1652 V1655 V1656 H1657



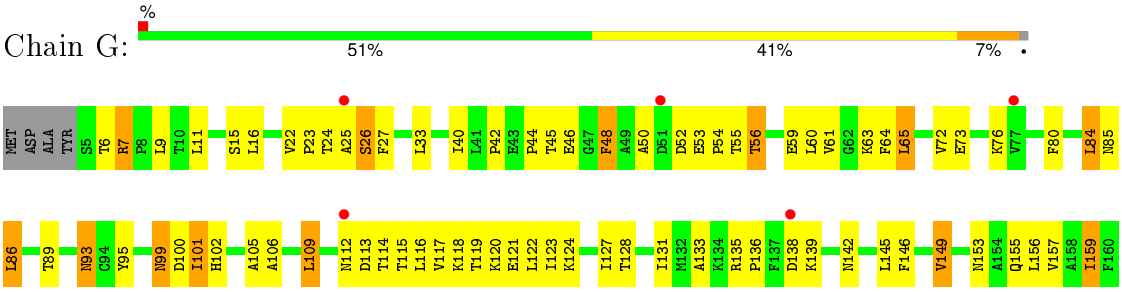
• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2)

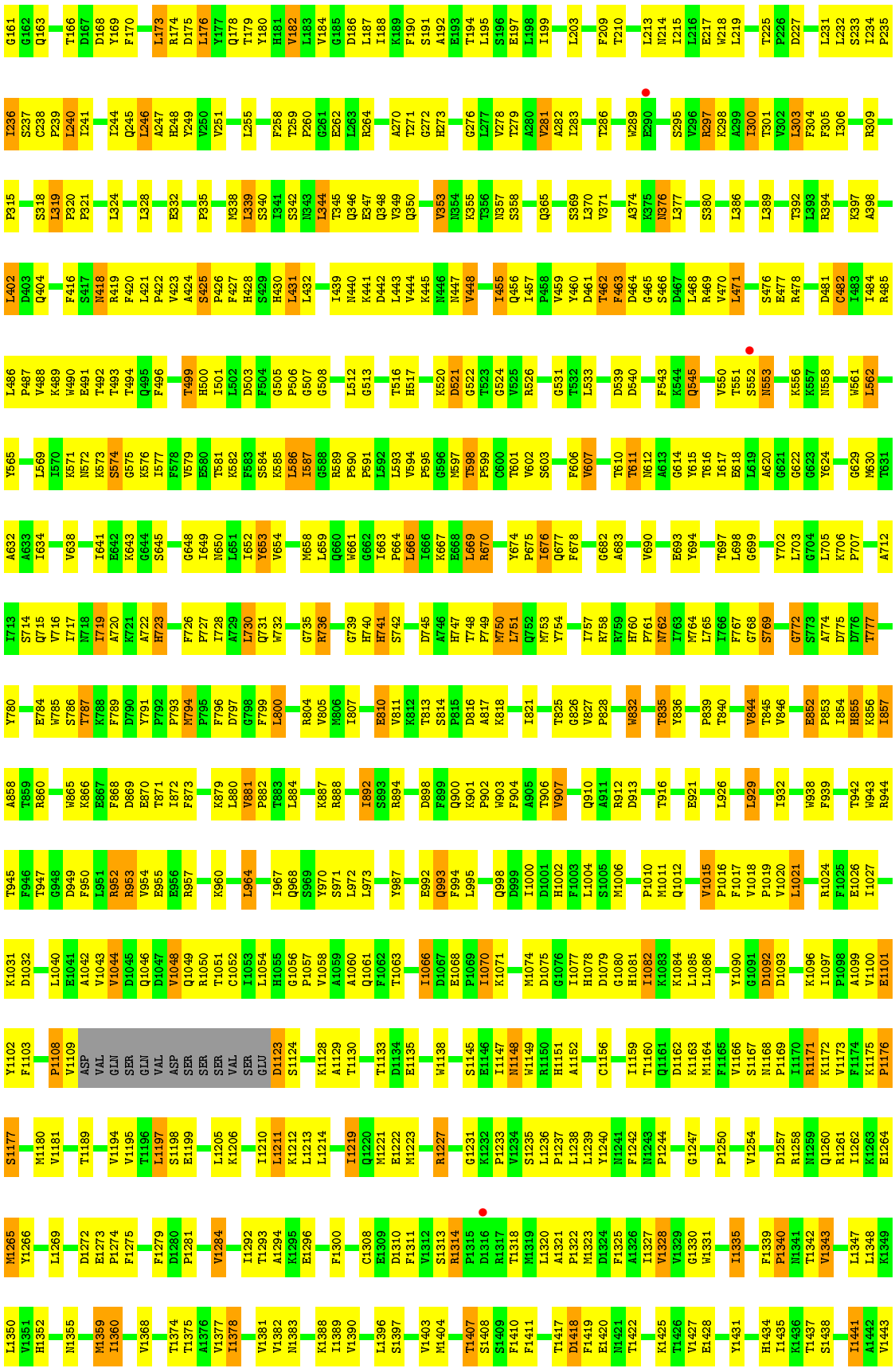
Chain C:

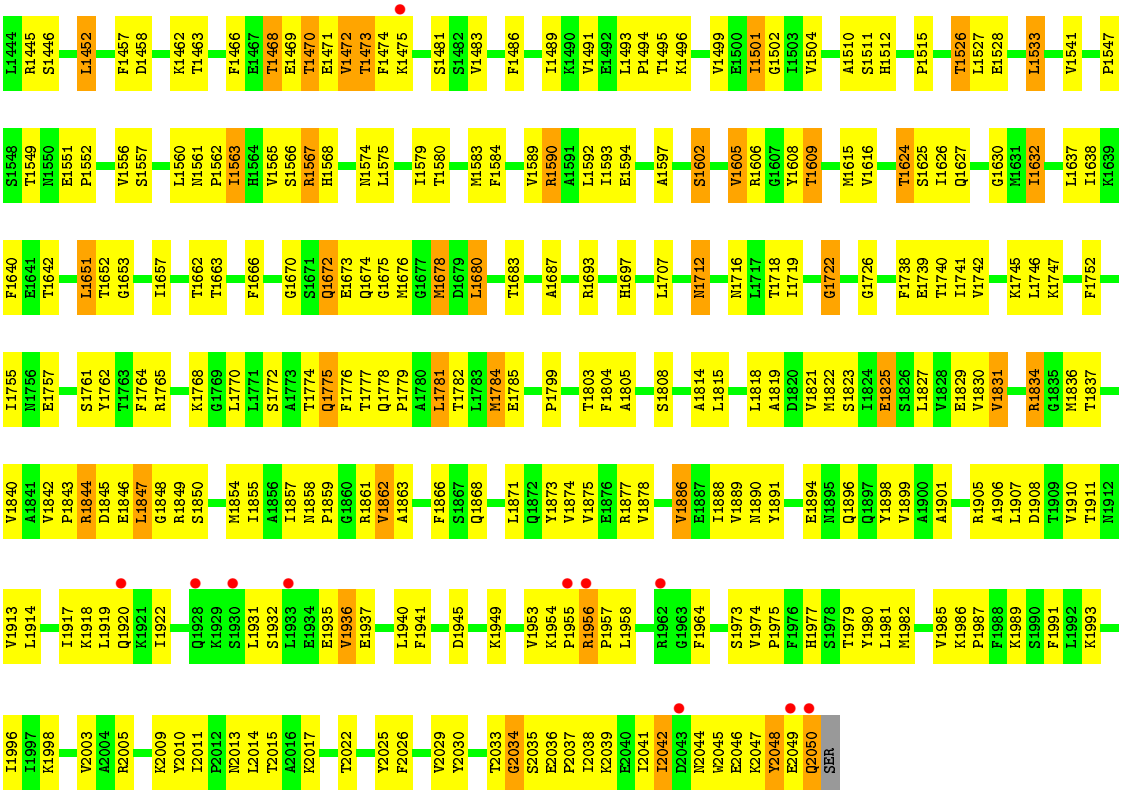




• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)

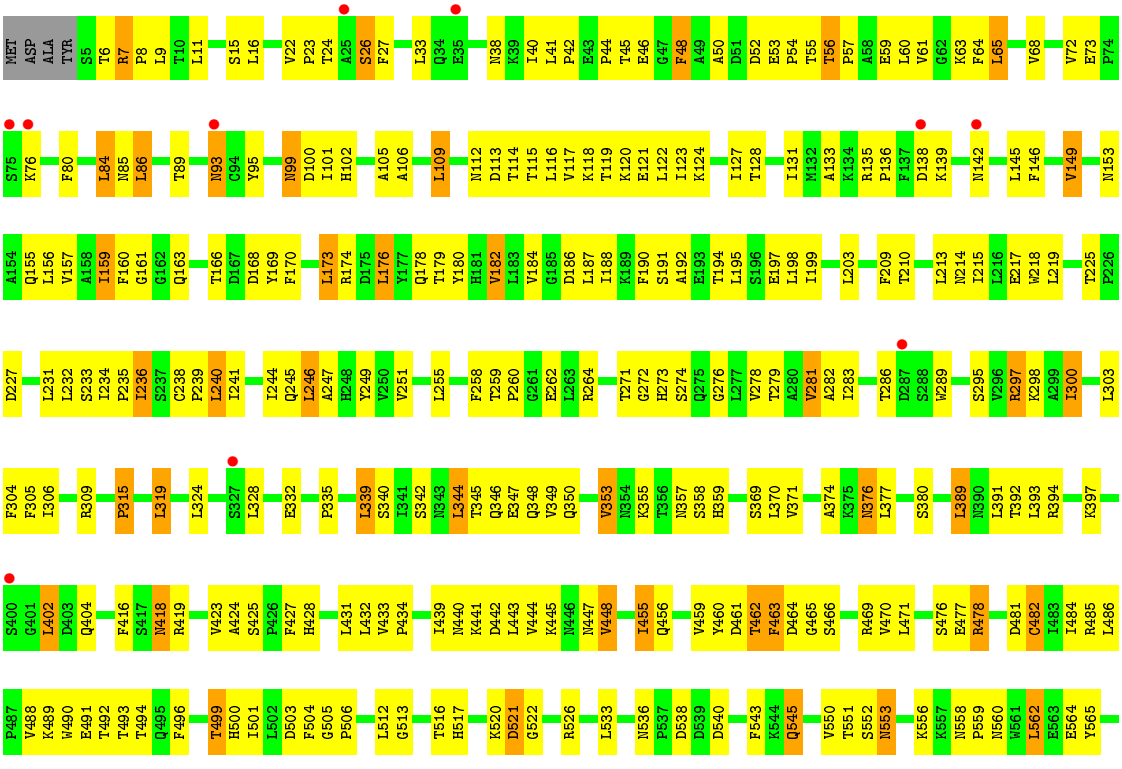


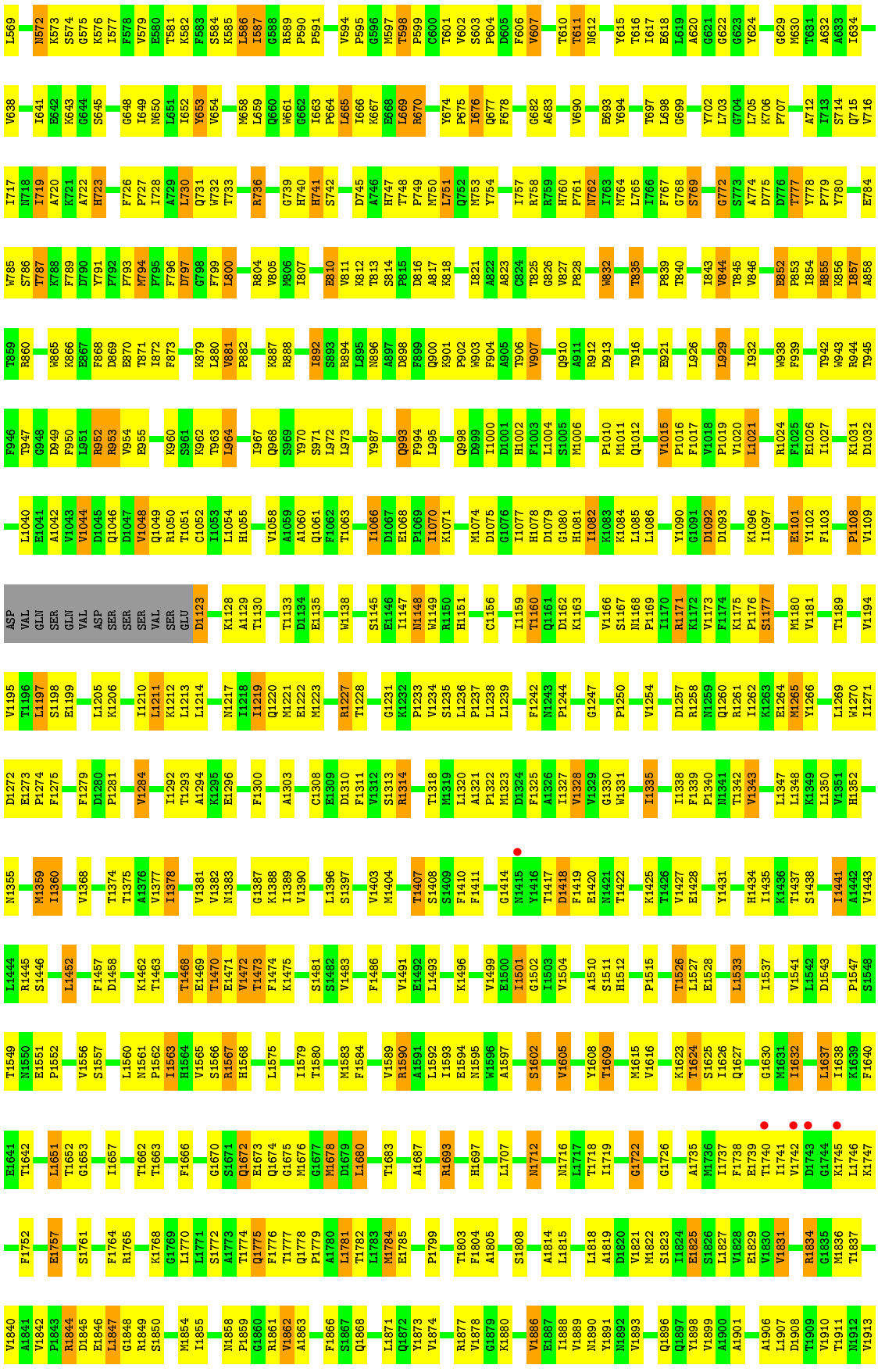


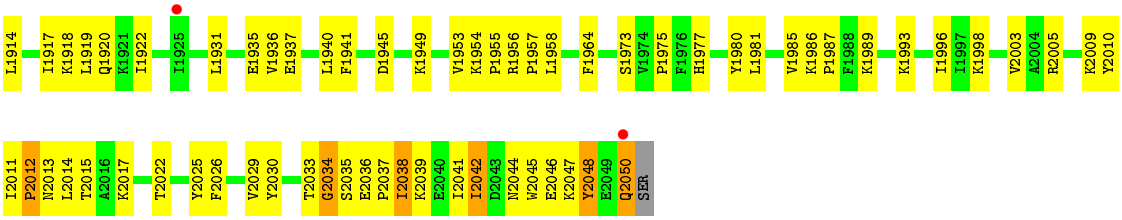


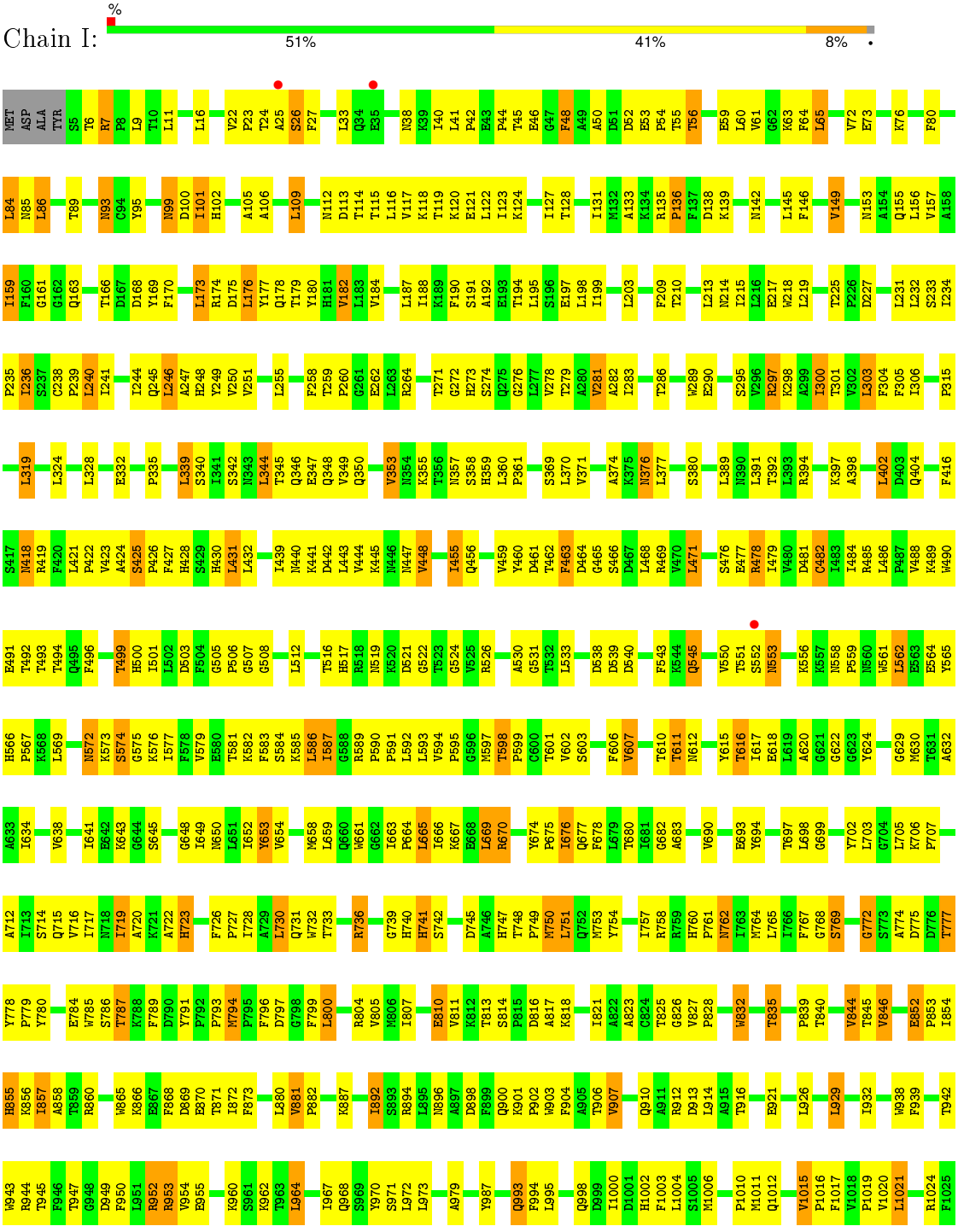
• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)

Chain H:

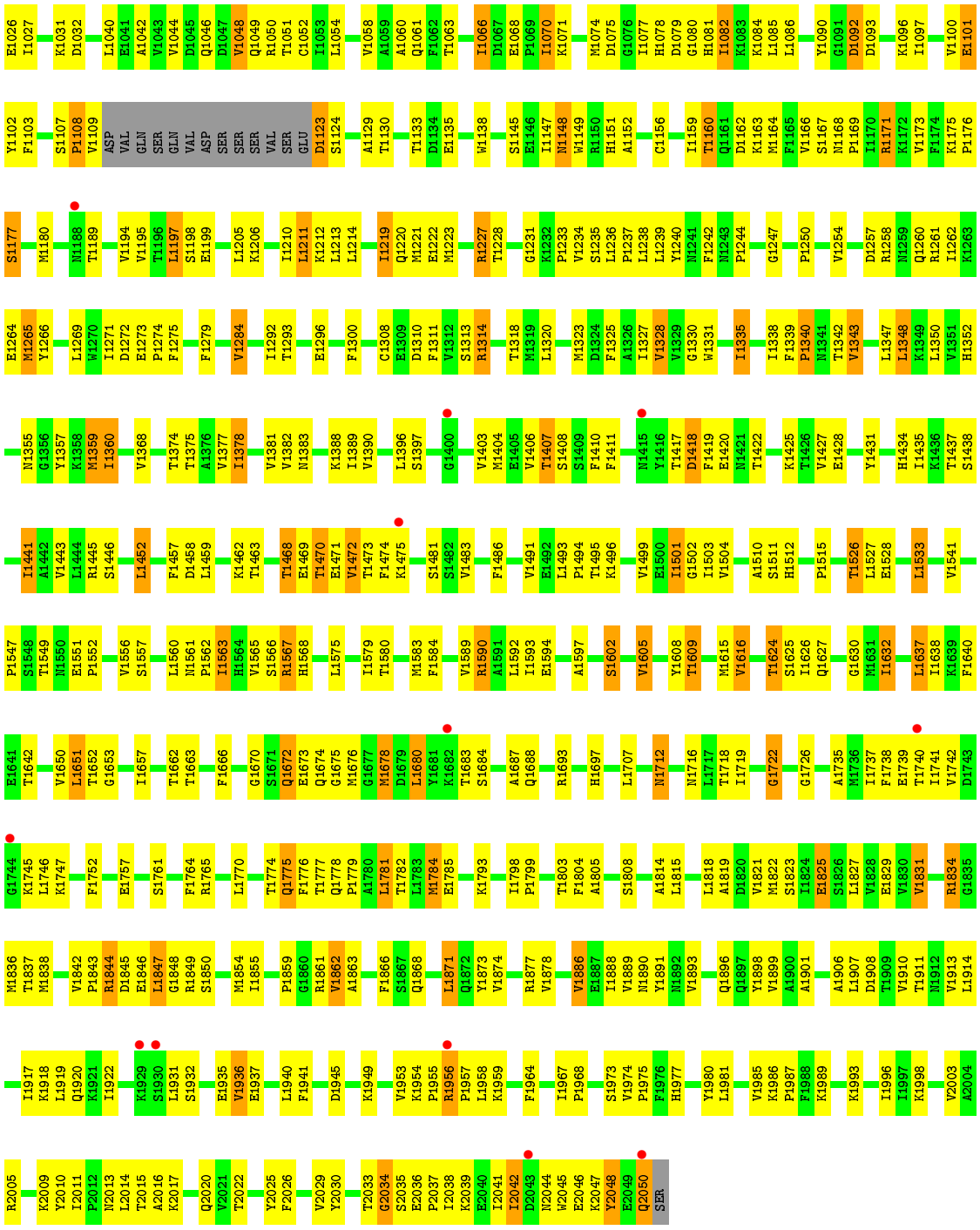








• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)


E1026 I1027 K1031 D1032 L1040 E1041 A1042 V1043 V1044 D1045 Q1046 D1047 V1048 Q1049 R1050 T1051 C1052 I1053 L1054 V1058 A1059 A1060 Q1061 F1062 T1063 I1066 D1067 E1068 P1069 I1070 K1071 M1074 D1075 G1076 I1077 H1078 D1079 G1080 H1081 I1082 K1083 K1084 L1085 L1086 Y1090 G1091 D1092 D1093 K1096 I1097 V1100 E1101
Y1102 F1103 S1107 P1108 V1109 ASP VAL GLN SER GLN VAL ASP SER SER SER VAL SER GLU D1123 S1124 A1129 T1130 T1133 D1134 E1135 W1138 S1145 E1146 I1147 N1148 W1149 R1150 H1151 A1152 C1156 I1159 T1160 Q1161 D1162 K1163 M1164 F1165 V1166 S1167 N1168 P1169 I1170 R1171 K1172 V1173 F1174 K1175 P1176
S1177 M1180 N1188 T1189 V1194 V1195 T1196 L1197 S1198 E1199 L1205 K1206 I1210 L1211 K1212 L1213 L1214 I1219 Q1220 M1221 E1222 M1223 R1227 T1228 G1231 K1232 P1233 V1234 S1235 L1236 P1237 L1238 L1239 Y1240 N1241 F1242 N1243 P1244 G1247 P1250 V1254 D1257 R1258 N1259 Q1260 R1261 I1262 K1263
E1264 M1265 Y1266 L1269 W1270 I1271 D1272 E1273 P1274 F1275 F1279 V1284 I1292 T1293 E1296 F1300 C1308 E1309 D1310 F1311 V1312 S1313 R1314 T1318 M1319 L1320 M1323 D1324 F1325 A1326 I1327 V1328 V1329 G1330 W1331 I1335 I1338 F1339 P1340 N1341 T1342 V1343 L1347 L1348 K1349 L1350 V1351 H1352
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P1547 S1548 T1549 N1550 E1551 P1552 V1556 S1557 L1560 N1561 P1562 I1563 H1564 V1565 S1566 R1567 H1568 L1575 I1579 T1580 M1583 F1584 V1589 R1590 A1591 L1592 I1593 E1594 A1597 S1602 V1605 Y1608 T1609 M1615 V1616 T1624 S1625 I1626 Q1627 G1630 M1631 I1632 L1637 I1638 K1639 F1640
E1641 T1642 V1650 L1651 T1652 G1653 I1657 T1662 T1663 F1666 G1670 S1671 Q1672 E1673 Q1674 G1675 M1676 G1677 M1678 D1679 L1680 Y1681 K1682 T1683 S1684 A1687 Q1688 R1693 H1697 L1707 N1712 N1716 L1717 T1718 I1719 G1722 G1726 A1735 M1736 I1737 F1738 E1739 T1740 I1741 V1742 D1743
G1744 K1745 L1746 K1747 F1752 E1757 S1761 F1764 R1765 L1770 T1774 Q1775 F1776 T1777 Q1778 P1779 A1780 L1781 T1782 L1783 M1784 E1785 K1793 I1798 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 M1838 V1842 P1843 R1844 D1845 E1846 L1847 G1848 R1849 S1850 M1854 I1855 P1859 G1860 R1861 V1862 A1863 F1866 S1867 Q1868 L1871 Q1872 Y1873 V1874 R1877 V1878 V1886 E1887 I1888 V1889 N1890 Y1891 N1892 V1893 Q1896 Q1897 Y1898 V1899 A1900 A1901 A1906 L1907 D1908 T1909 V1910 T1911 N1912 V1913 L1914
I1917 K1918 L1919 Q1920 K1921 I1922 K1929 S1930 L1931 S1932 E1935 V1936 E1937 L1940 F1941 D1945 K1949 V1953 K1954 P1955 R1956 P1957 L1958 K1959 F1964 I1967 P1968 S1973 V1974 P1975 F1976 H1977 Y1980 L1981 V1985 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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	230.60Å 230.60Å 784.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 12.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	86.1 (12.00-3.10) 91.5 (12.00-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.09Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, R_{free}	0.200 , 0.250 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	74.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 341077 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	85962	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.36% 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, GVL

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	0.41	0/12848	0.59	2/17358 (0.0%)
1	B	0.42	0/12848	0.59	2/17358 (0.0%)
1	C	0.41	0/12848	0.59	2/17358 (0.0%)
2	G	0.37	0/16360	0.56	0/22198
2	H	0.37	0/16360	0.57	0/22198
2	I	0.37	0/16360	0.56	0/22198
All	All	0.39	0/87624	0.58	6/118668 (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	1
2	I	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	599	MET	N-CA-C	-6.92	92.32	111.00
1	B	599	MET	N-CA-C	-6.91	92.36	111.00
1	C	599	MET	N-CA-C	-6.90	92.36	111.00
1	B	540	GLN	N-CA-C	-5.67	95.69	111.00
1	C	540	GLN	N-CA-C	-5.63	95.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
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	12628	0	12603	572	0
1	B	12628	0	12603	587	0
1	C	12628	0	12603	584	0
2	G	15995	0	15978	984	0
2	H	15995	0	15978	995	0
2	I	15995	0	15978	996	0
3	G	31	0	19	7	0
3	H	31	0	19	6	0
3	I	31	0	19	6	0
All	All	85962	0	85800	4562	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 27.

The worst 5 of 4562 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)
2:I:1956:ARG:HB2	2:I:1957:PRO:HD3	1.23	1.21
2:G:499:THR:HB	2:G:500:HIS:HD2	1.07	1.16
2:G:1956:ARG:HB2	2:G:1957:PRO:HD3	1.23	1.14
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.11	1.13
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.12	1.13

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 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	1603/1887 (85%)	1498 (93%)	91 (6%)	14 (1%)	21	61
1	B	1603/1887 (85%)	1495 (93%)	95 (6%)	13 (1%)	24	63
1	C	1603/1887 (85%)	1498 (93%)	90 (6%)	15 (1%)	21	61
2	G	2029/2051 (99%)	1841 (91%)	163 (8%)	25 (1%)	16	52
2	H	2029/2051 (99%)	1841 (91%)	166 (8%)	22 (1%)	17	55
2	I	2029/2051 (99%)	1837 (90%)	168 (8%)	24 (1%)	16	52
All	All	10896/11814 (92%)	10010 (92%)	773 (7%)	113 (1%)	19	58

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY
1	A	1252	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	1366/1565 (87%)	1220 (89%)	146 (11%)	8	31
1	B	1366/1565 (87%)	1222 (90%)	144 (10%)	8	31
1	C	1366/1565 (87%)	1224 (90%)	142 (10%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	1772/1789 (99%)	1564 (88%)	208 (12%)	7 26
2	H	1772/1789 (99%)	1564 (88%)	208 (12%)	7 26
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	6 25
All	All	9414/10062 (94%)	8356 (89%)	1058 (11%)	7 29

5 of 1058 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	402	LEU
2	G	1501	ILE
2	I	1171	ARG
2	G	539	ASP
2	G	929	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 276 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1000	GLN
2	G	440	ASN
2	I	910	GLN
1	C	1066	ASN
1	C	1563	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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	GVL	A	180	1	13,18,19	0.82	1 (7%)	16,26,28	1.10	2 (12%)
1	GVL	B	180	1	13,18,19	0.74	0	16,26,28	1.18	2 (12%)
1	GVL	C	180	1	13,18,19	0.85	1 (7%)	16,26,28	1.24	3 (18%)

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
1	GVL	A	180	1	-	0/21/25/27	0/0/0/0
1	GVL	B	180	1	-	0/21/25/27	0/0/0/0
1	GVL	C	180	1	-	0/21/25/27	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	GVL	P24-O23	2.07	1.63	1.55
1	A	180	GVL	P24-O23	2.20	1.64	1.55

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	180	GVL	C32-C34-N36	-2.13	115.95	117.45
1	A	180	GVL	C32-C34-N36	-2.12	115.96	117.45
1	B	180	GVL	O-C-CA	-2.03	120.29	125.72
1	C	180	GVL	C30-C29-C32	2.16	113.10	109.17
1	A	180	GVL	O35-C34-C32	2.31	120.60	118.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	FMN	G	3051	-	32,33,33	6.17	19 (59%)	34,50,50	1.95	6 (17%)
3	FMN	H	3051	-	32,33,33	6.06	19 (59%)	34,50,50	1.97	6 (17%)
3	FMN	I	3051	-	32,33,33	6.11	21 (65%)	34,50,50	1.88	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	FMN	G	3051	-	-	0/18/18/18	0/3/3/3
3	FMN	H	3051	-	-	0/18/18/18	0/3/3/3
3	FMN	I	3051	-	-	0/18/18/18	0/3/3/3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3051	FMN	C7M-C7	2.11	1.55	1.51
3	I	3051	FMN	C8M-C8	2.29	1.55	1.51
3	G	3051	FMN	P-O3P	2.92	1.64	1.54
3	H	3051	FMN	P-O3P	3.12	1.65	1.54
3	I	3051	FMN	P-O3P	3.21	1.65	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	3051	FMN	N3-C2-N1	-4.81	119.59	127.69
3	I	3051	FMN	N3-C2-N1	-4.53	120.06	127.69
3	G	3051	FMN	N3-C2-N1	-4.25	120.53	127.69
3	H	3051	FMN	C4A-C4-N3	-4.19	118.04	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3051	FMN	C4A-C4-N3	-4.15	118.10	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3051	FMN	7	0
3	H	3051	FMN	6	0
3	I	3051	FMN	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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	1613/1887 (85%)	-0.60	29 (1%)	71	50	28, 59, 126, 166	0
1	B	1613/1887 (85%)	-0.59	25 (1%)	76	58	30, 59, 127, 170	0
1	C	1613/1887 (85%)	-0.59	31 (1%)	70	48	29, 61, 126, 170	0
2	G	2033/2051 (99%)	-0.52	19 (0%)	85	72	39, 73, 114, 151	0
2	H	2033/2051 (99%)	-0.54	17 (0%)	87	75	41, 73, 113, 152	0
2	I	2033/2051 (99%)	-0.53	15 (0%)	89	78	42, 74, 113, 150	0
All	All	10938/11814 (92%)	-0.56	136 (1%)	81	64	28, 69, 119, 170	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	977	TYR	5.7
1	C	976	ALA	5.3
1	C	975	ALA	5.2
2	H	35	GLU	5.2
1	C	1475	GLU	4.7

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

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
1	GVL	C	180	19/20	0.76	0.38	-	49,130,161,187	0
1	GVL	B	180	19/20	0.82	0.30	-	48,119,172,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	GVL	A	180	19/20	0.86	0.26	-	44,125,164,189	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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	FMN	G	3051	31/31	0.96	0.14	0.27	31,55,81,100	0
3	FMN	H	3051	31/31	0.97	0.14	0.03	27,54,78,82	0
3	FMN	I	3051	31/31	0.96	0.13	-0.19	26,57,75,97	0

6.5 Other polymers (i)

There are no such residues in this entry.