wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 04:26 am BST

PDB ID	:	2VKZ
Title	:	Structure of the cerulenin-inhibited fungal fatty acid synthase type I multienzyme complex
Authors	:	Johansson, P.; Wiltschi, B.; Kumari, P.; Kessler, B.; Vonrhein, C.; Vonck, J.; Oesterhelt, D.; Grininger, M.
Deposited on	:	2008-01-07
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
https://www.wwpdb.org/validation/2017/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:

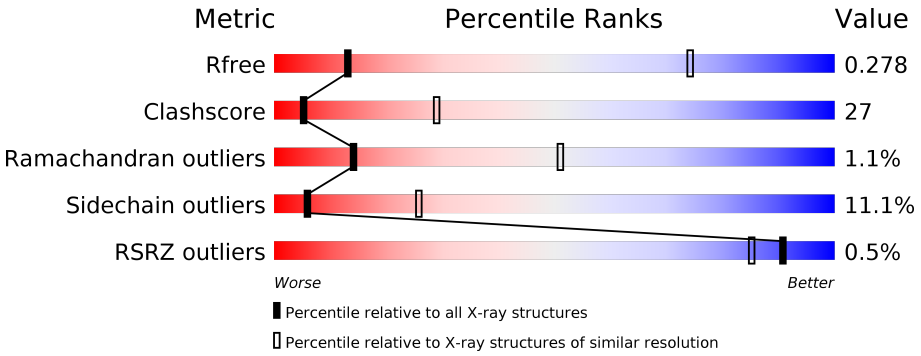
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	% 50% 31% . 14%
1	B	1887	% 50% 30% 5% 14%
1	C	1887	% 49% 32% 5% 14%
2	G	2051	51% 40% 8% .
2	H	2051	% 51% 40% 8% .
2	I	2051	51% 40% 8% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 85959 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.

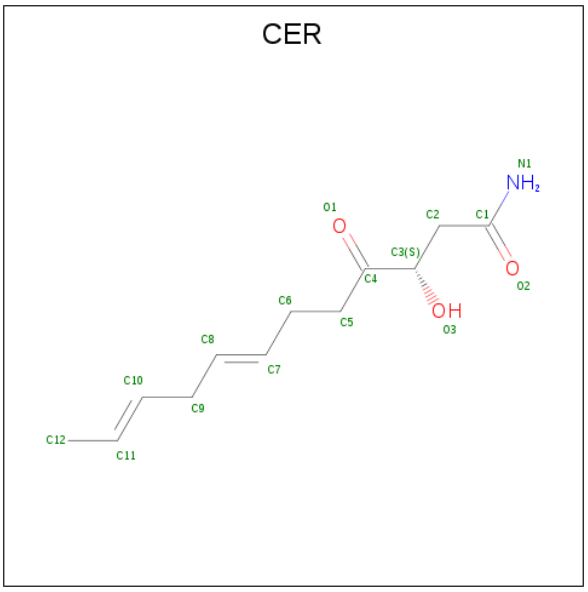
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			
1	B	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			
1	C	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			

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

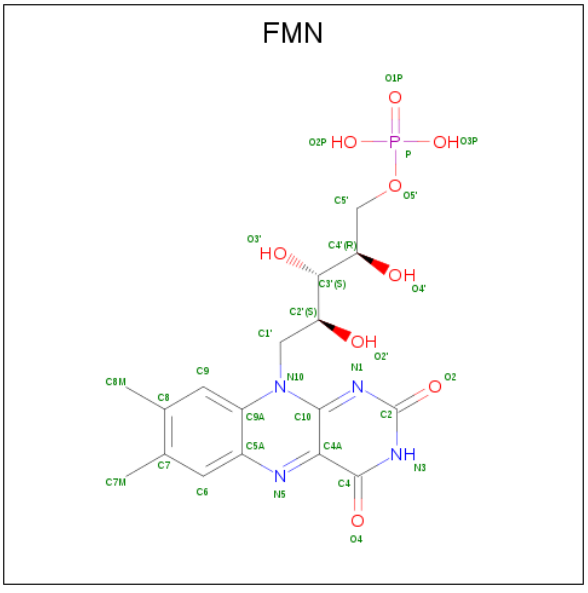
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- 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

Continued on next page...

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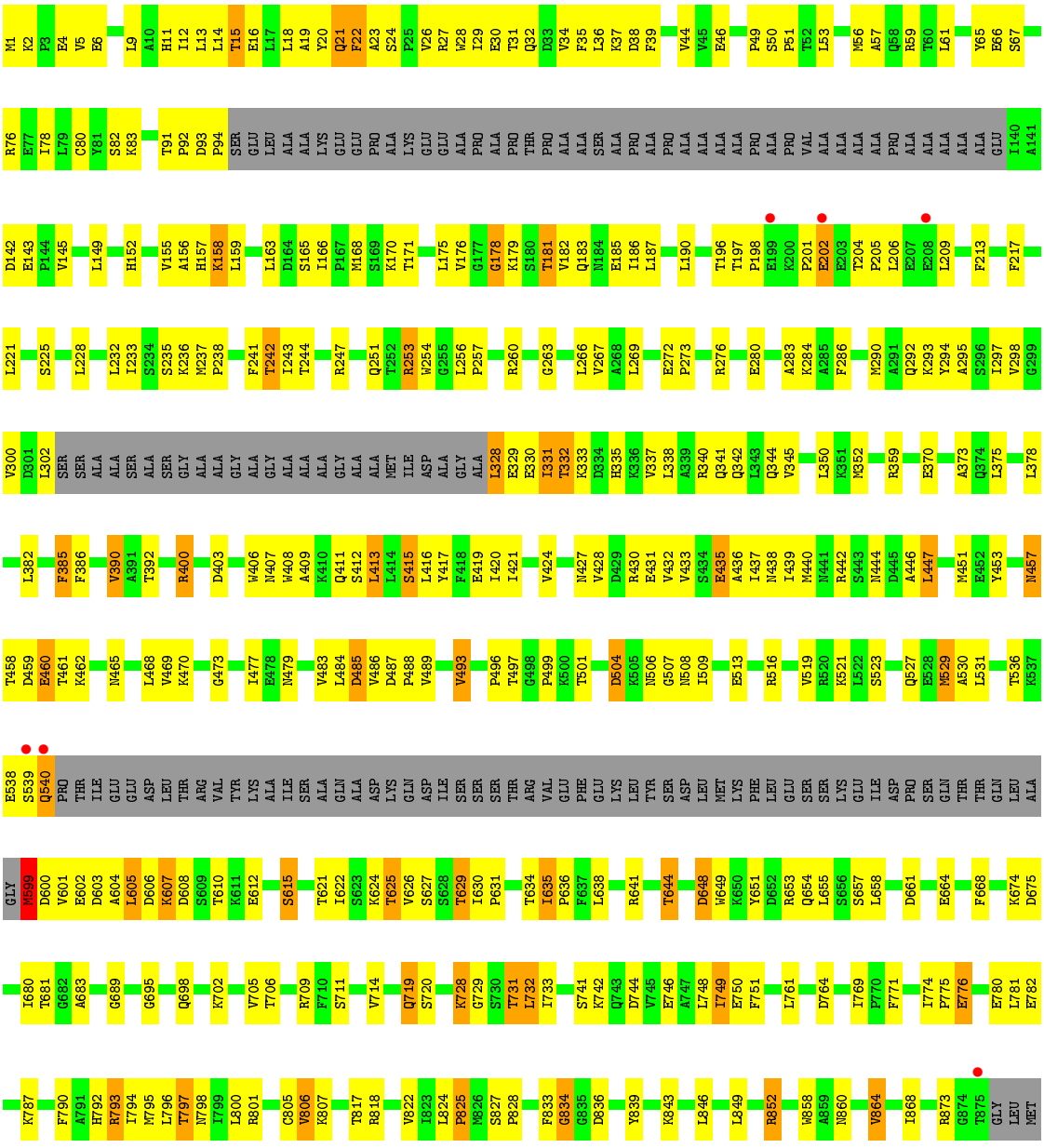
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

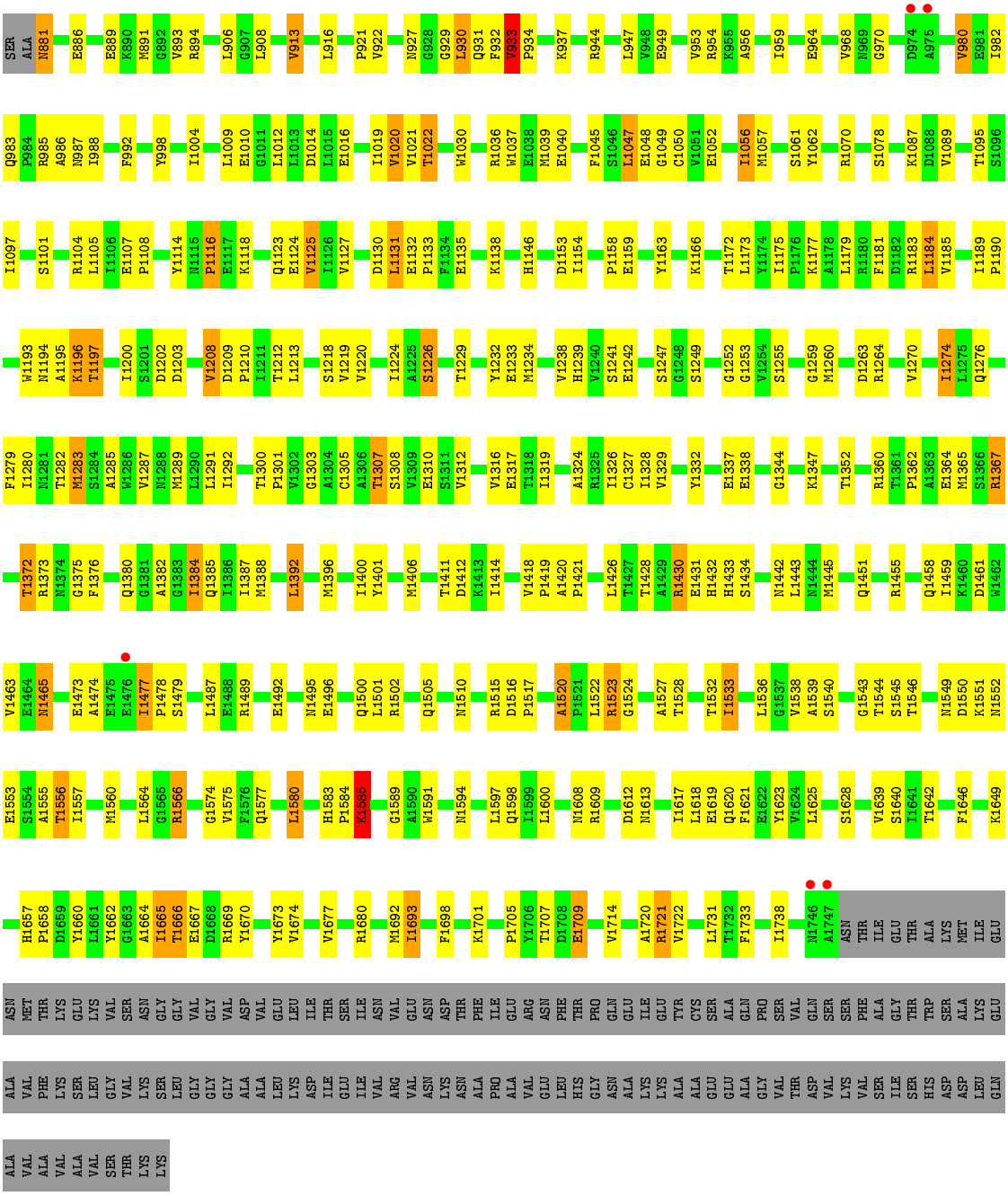
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

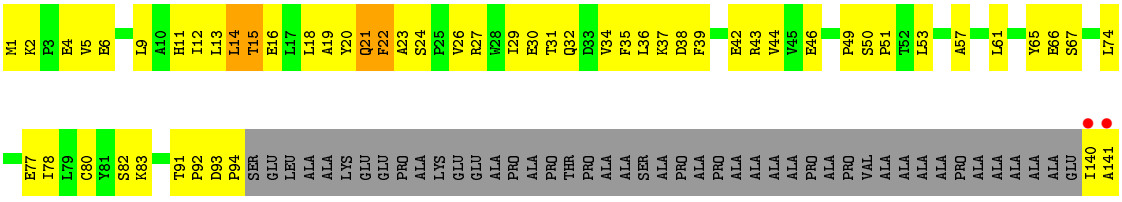
Chain A:

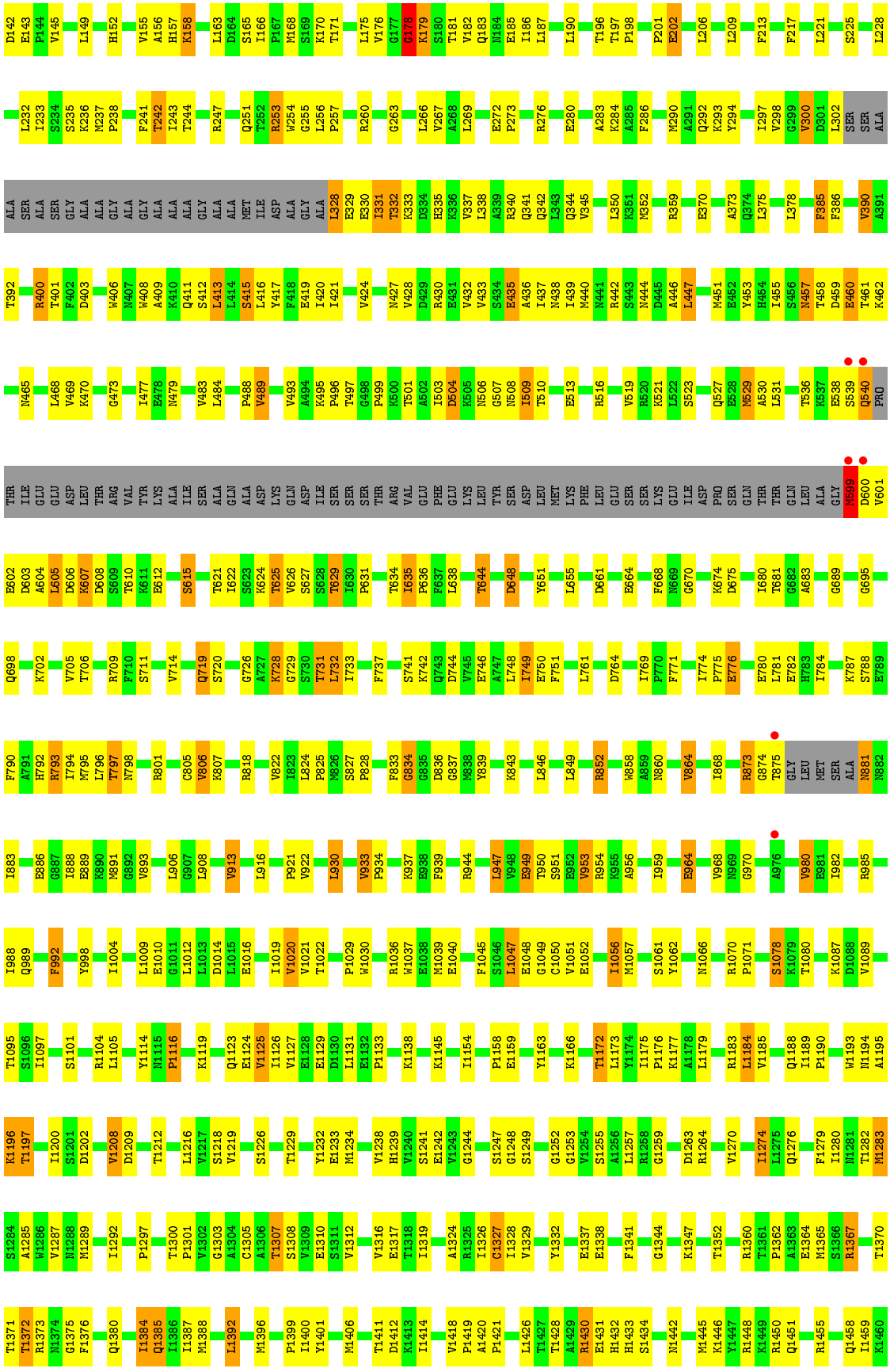


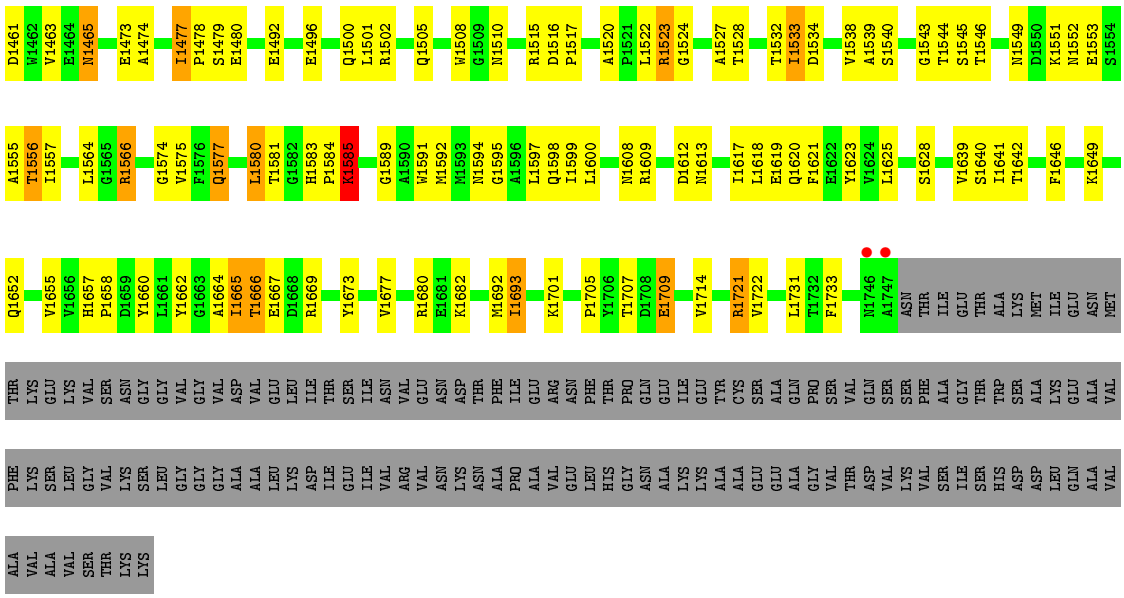


• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA

Chain B:

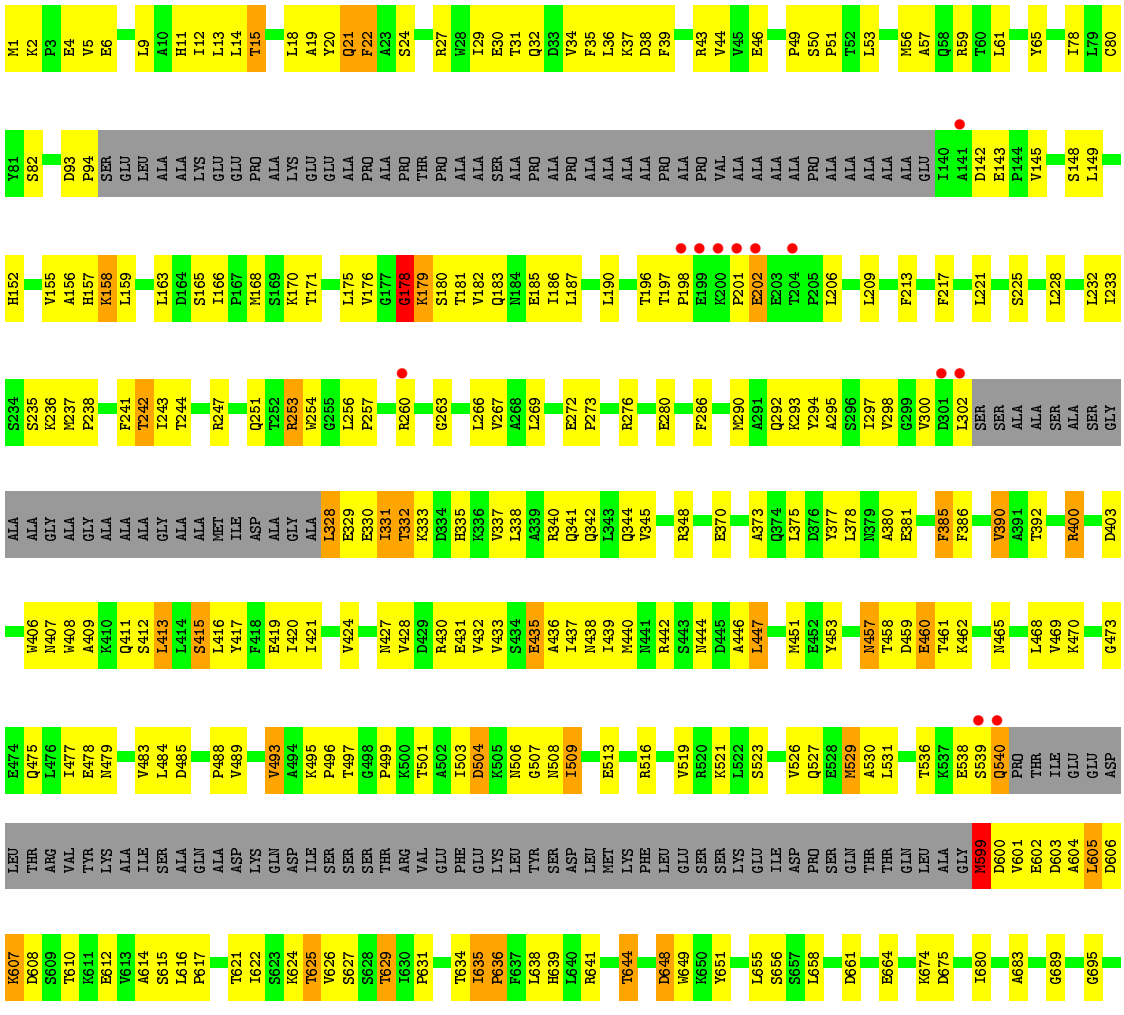


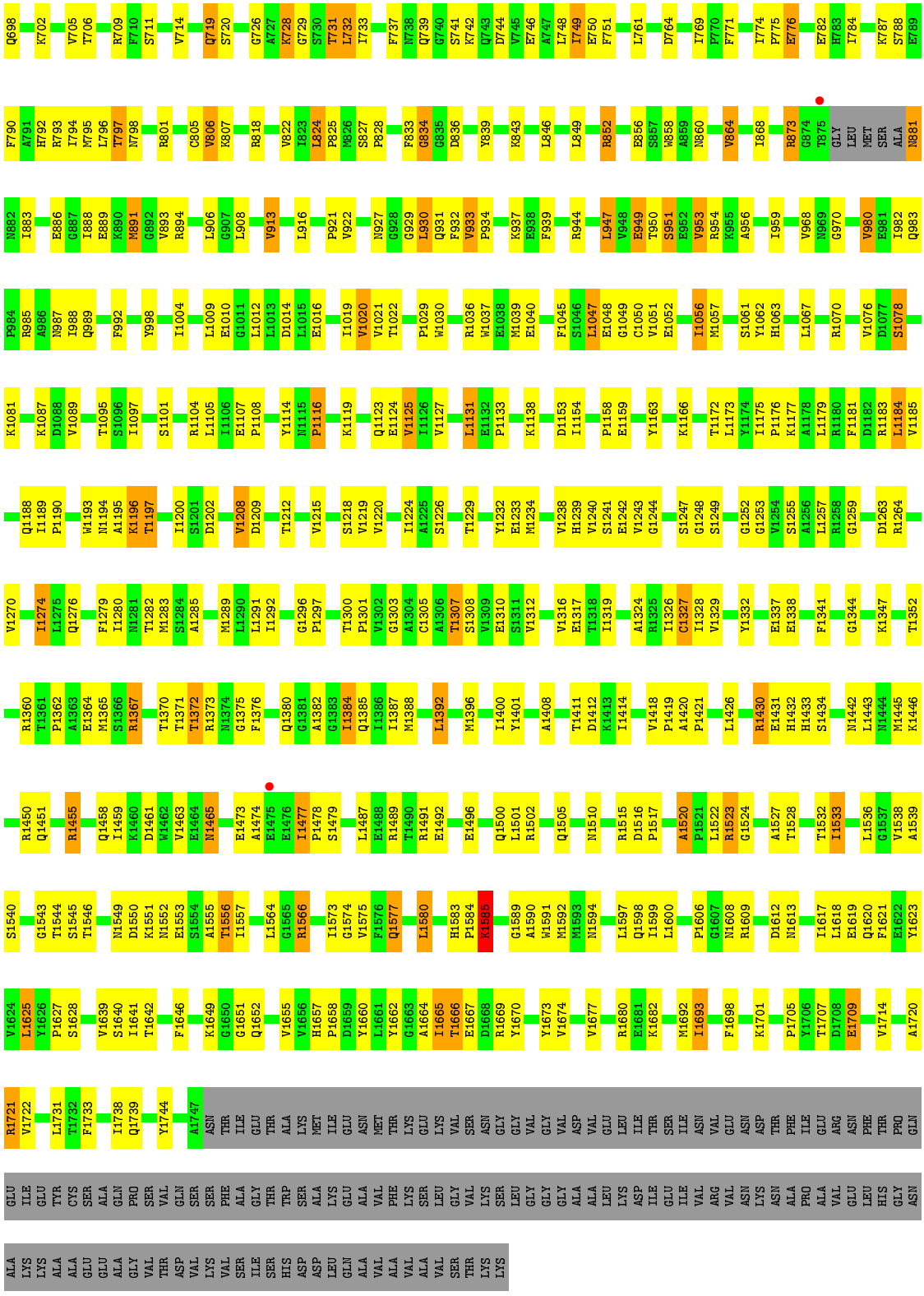




• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA

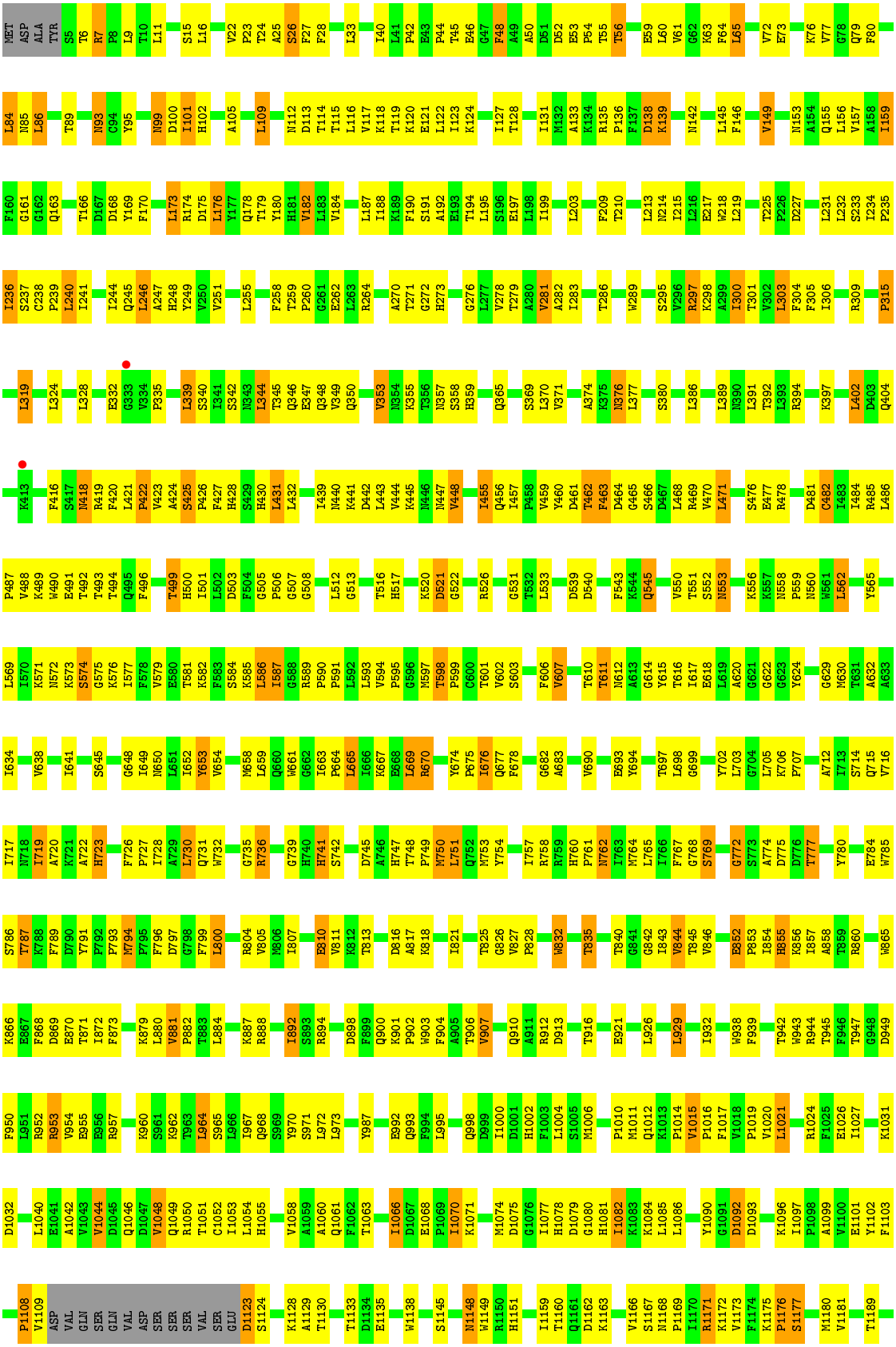
Chain C:

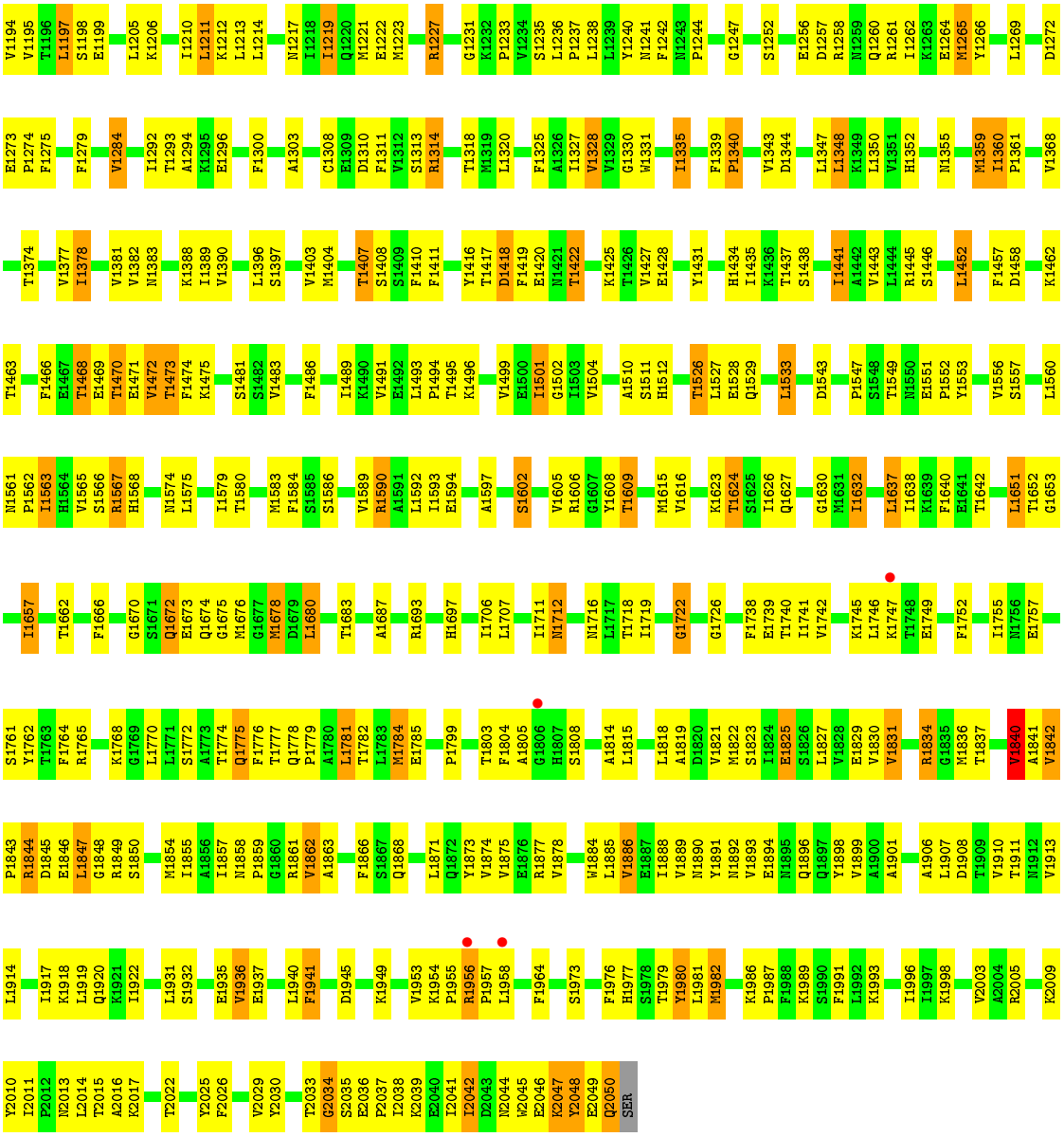




• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA

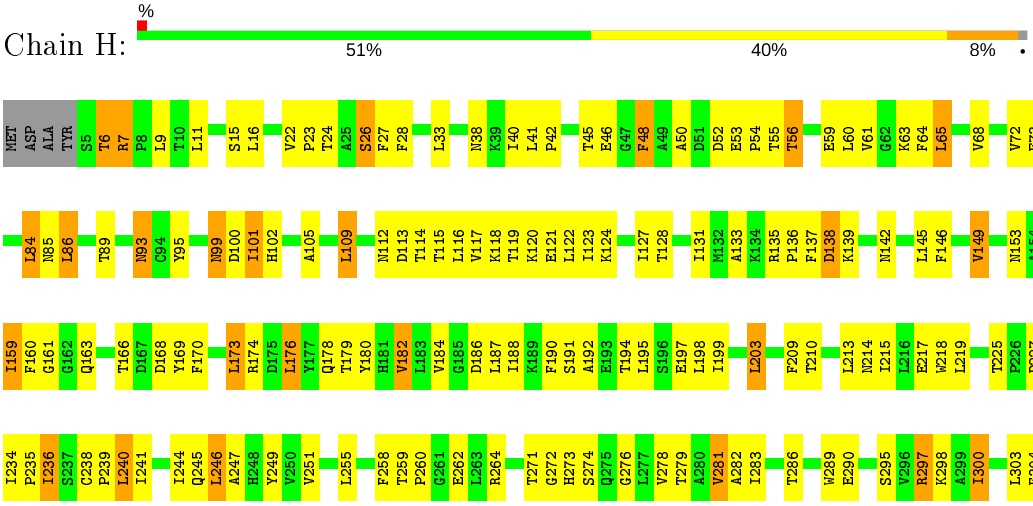
Chain G:

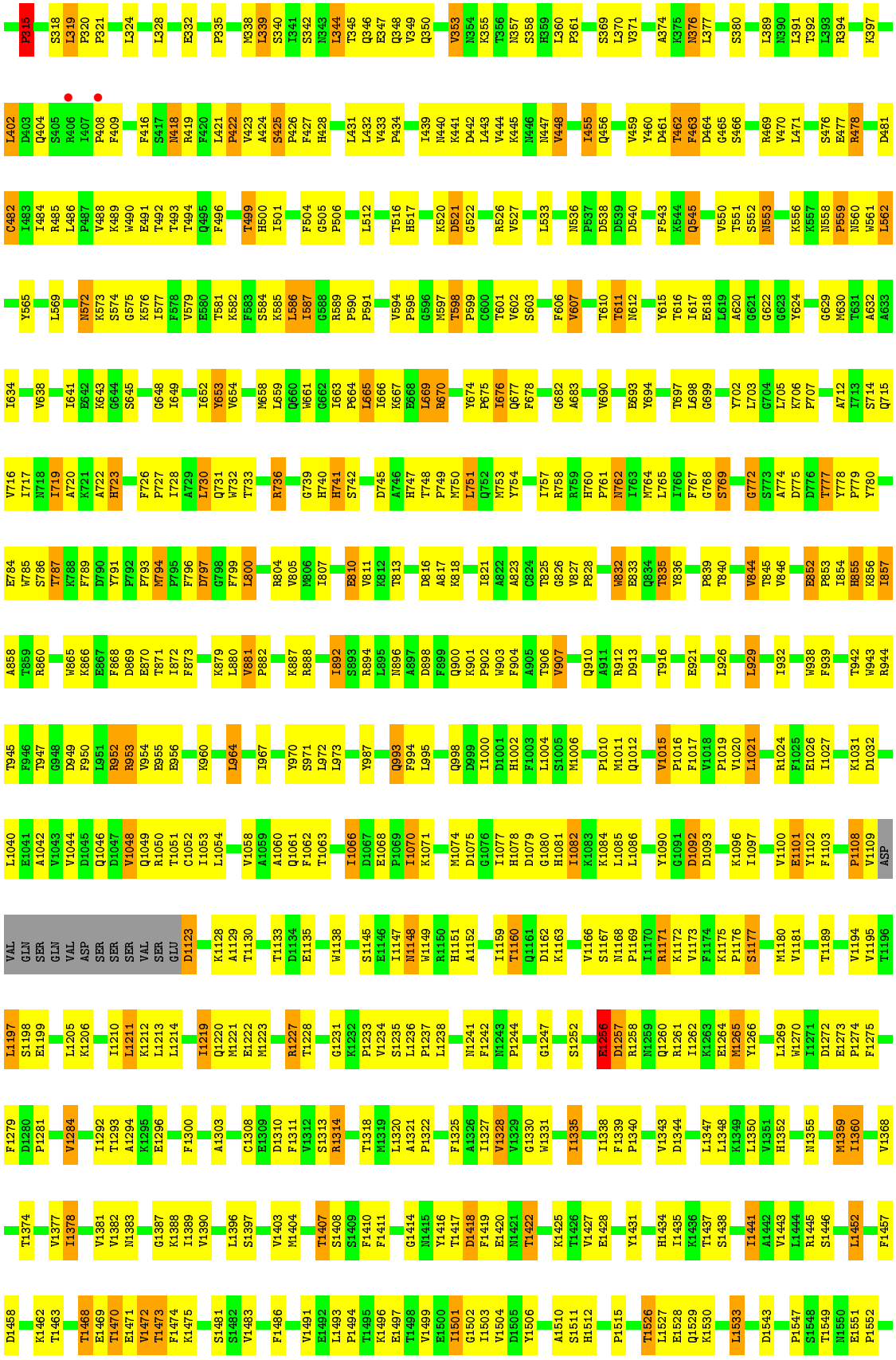




• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA

Chain H:

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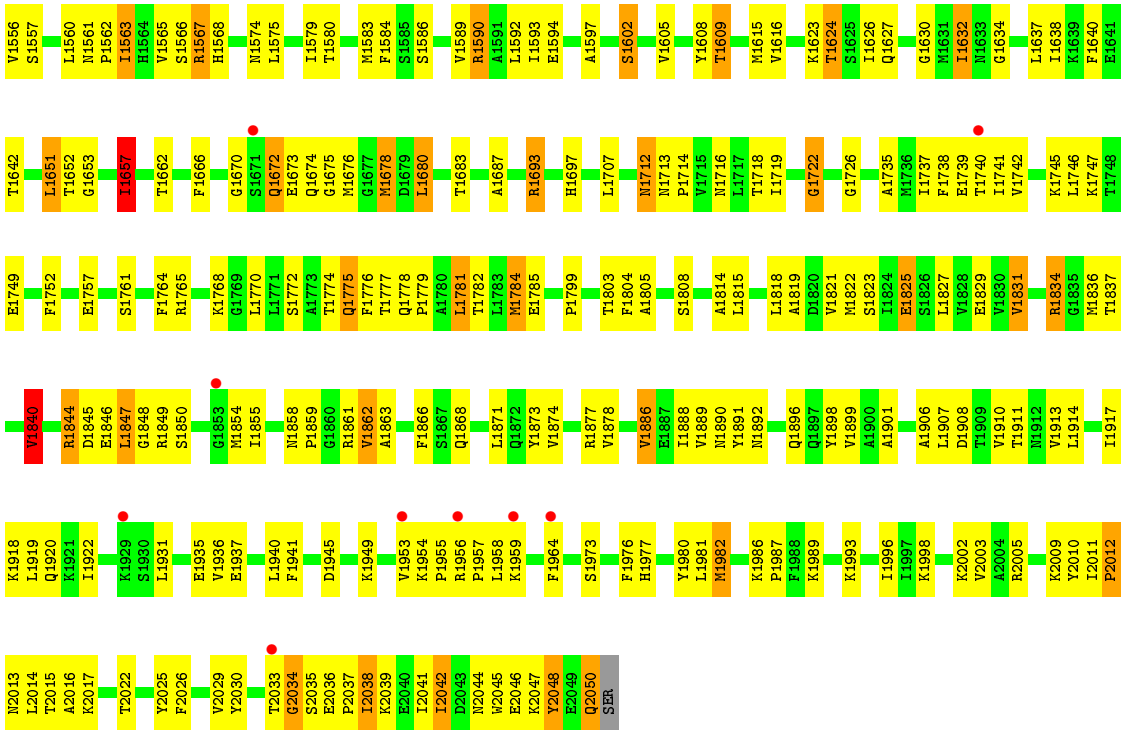
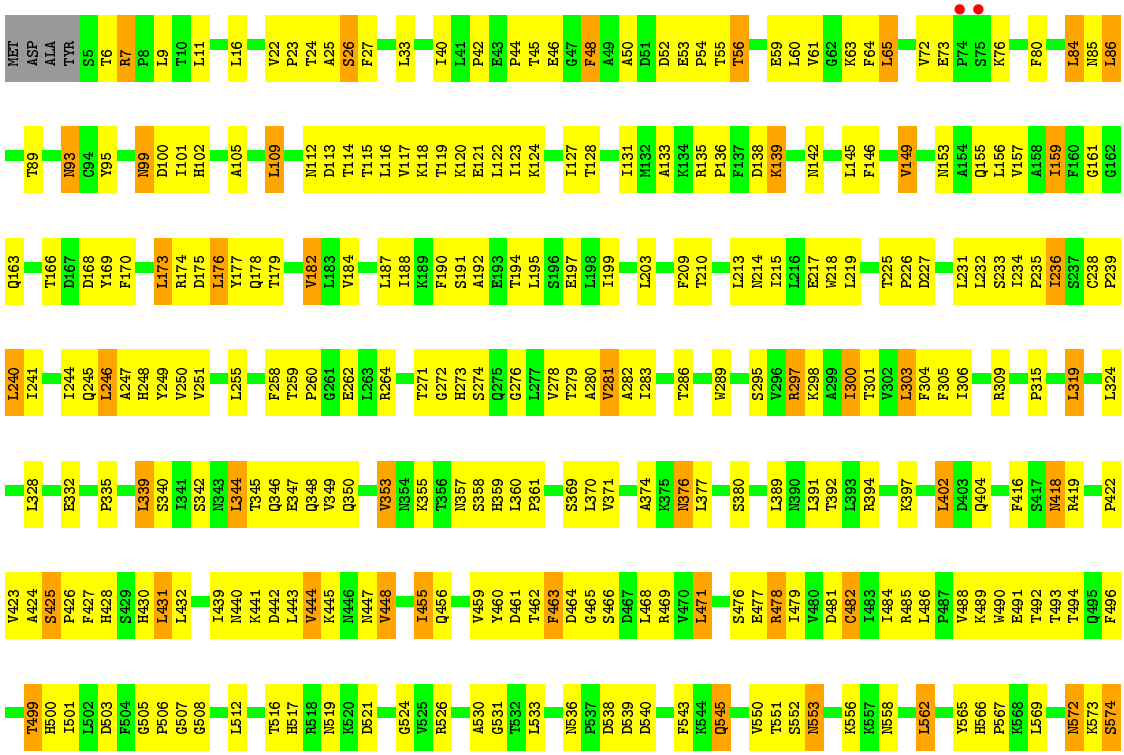
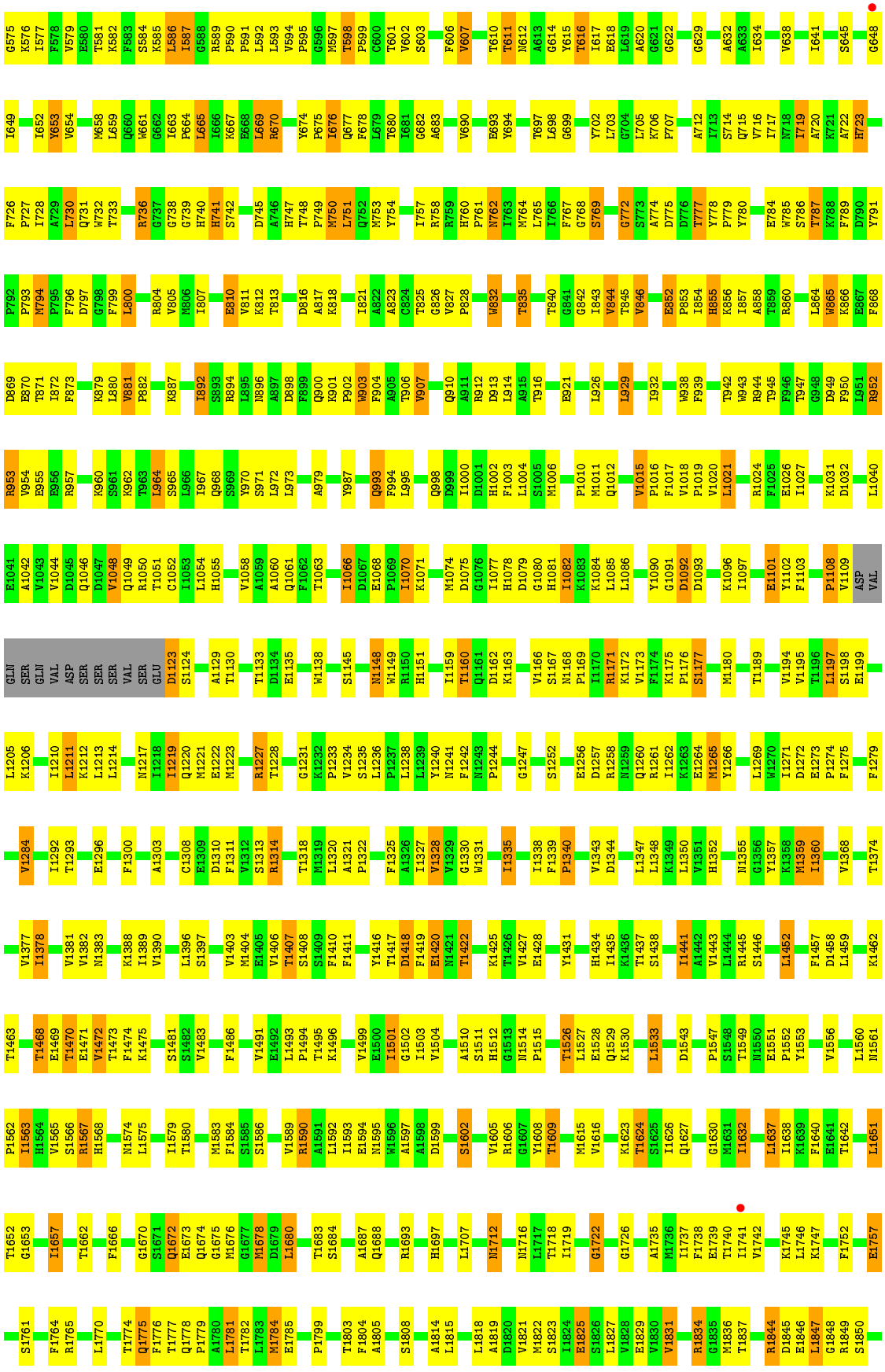
L402 D403 Q404 S405 R406 I407 P408 F409 F416 S417 N418 R419 F420 L421 P422 V423 A424 S425 P426 F427 H428 L431 L432 V433 P434 I439 N440 K441 D442 L443 V444 K445 N446 N447 V448 I455 Q456 V459 Y460 D461 T462 F463 D464 G465 S466 R469 V470 L471 S476 E477 R478 D481
C482 I483 I484 R485 L486 P487 V488 K489 W490 E491 T492 T493 T494 Q495 F496 T499 H500 I501 F504 G505 P506 L512 T516 H517 K520 D521 G522 R526 V527 L533 N536 P537 D538 D539 D540 F543 K544 Q545 V550 T551 S552 N553 K556 K557 N558 P559 N560 W561 L562
Y565 L569 N572 K573 S574 G575 K576 I577 F578 V579 E580 T581 K582 F583 S584 K585 L586 I587 G588 R589 P590 P591 V594 P595 G596 M597 T598 P599 C600 T601 V602 S603 F606 V607 T610 T611 N612 Y615 T616 I617 E618 L619 A620 G621 G622 G623 Y624 G629 M630 T631 A632 A633
I634 V638 I641 E642 K643 G644 S645 G648 I649 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 I717 N718 I719 A720 K721 A722 H723 F726 P727 I728 A729 L730 Q731 W732 T733 R736 G739 H740 H741 S742 D745 A746 H747 T748 P749 M750 L751 Q752 M753 Y754 I757 R758 R759 H760 P761 N762 I763 M764 L765 I766 F767 G768 S769 G772 S773 A774 D775 D776 T777 Y778 P779 Y780
E784 W785 S786 T787 K788 F789 D790 Y791 F792 P793 M794 F795 F796 D797 G798 F799 L800 R804 V805 M806 I807 E810 V811 K812 T813 D816 A817 K818 I821 A822 A823 G824 T825 G826 V827 P828 W832 E833 Q834 T835 Y836 P839 T840 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 K887 R888 I892 S893 R894 L895 N896 A897 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 T947 G948 D949 F950 L951 R952 R953 V954 E955 E956 K960 L964 I967 Y970 S971 L972 L973 Y987 Q993 F994 L995 Q998 D999 I1000 D1001 H1002 F1003 L1004 S1005 M1006 P1010 M1011 Q1012 V1015 P1016 F1017 V1018 P1019 V1020 L1021 R1024 F1025 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 P1108 V1109 ASP
VAL GLN SER GLN VAL ASP SER SER SER VAL SER GLU D1123 K1128 A1129 T1130 T1133 D1134 E1135 W1138 S1145 E1146 I1147 N1148 W1149 R1150 H1151 A1152 I1159 T1160 Q1161 D1162 K1163 V1166 S1167 N1168 P1169 I1170 R1171 K1172 V1173 F1174 K1175 P1176 S1177 M1180 V1181 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 N1241 F1242 N1243 P1244 G1247 S1252 E1256 D1257 R1258 N1259 Q1260 R1261 I1262 K1263 E1264 M1265 Y1266 L1269 W1270 I1271 D1272 E1273 P1274 F1275
F1279 D1280 P1281 V1284 I1292 T1293 A1294 K1296 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 M1359 I1360 V1368
T1374 V1377 I1378 V1381 V1382 N1383 G1387 K1388 I1389 V1390 L1396 S1397 V1403 M1404 T1407 S1408 S1409 F1410 F1411 G1414 N1415 Y1416 T1417 D1418 F1419 E1420 N1421 T1422 K1425 T1426 V1427 E1428 Y1431 H1434 I1435 K1436 T1437 S1438 I1441 A1442 V1443 L1444 R1445 S1446 L1452 F1457
D1458 K1462 T1463 T1468 E1469 T1470 E1471 V1472 T1473 F1474 K1475 S1481 S1482 V1483 F1486 V1491 E1492 L1493 P1494 T1495 K1496 E1497 T1498 V1499 E1500 I1501 G1502 I1503 V1504 D1505 Y1506 A1510 S1511 H1512 P1515 T1526 L1527 E1528 Q1529 K1530 L1533 D1543 P1547 S1548 T1549 M1550 E1551 P1552



• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA

Chain I:

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I649 I652 Y653 V654 M658 L659 Q660 W661 G662 I663 P664 L665 I666 K667 E668 L669 R670 Y674 P675 I676 Q677 F678 L679 T680 I681 G682 A683 V690 E693 Y694 T697 L698 G699 V702 L703 G704 L705 K706 P707 A712 I713 S714 Q715 V716 I717 N718 I719 A720 K721 A722 H723
F726 P727 I728 A729 L730 Q731 W732 T733 R736 G737 G738 G739 H740 H741 S742 D745 A746 H747 T748 P749 M750 L751 Q752 M753 Y754 I757 R758 R759 H760 P761 N762 I763 M764 L765 I766 F767 G768 S769 G772 S773 A774 D775 D776 T777 Y778 P779 Y780 E784 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 A822 A823 C824 T825 G826 V827 P828 W832 T835 T840 G841 G842 I843 V844 T845 V846 E852 P853 I854 H855 K856 I857 A858 T859 R860 L864 W865 K866 E867 F868
D869 E870 T871 I872 F873 K879 L880 V881 P882 K887 I892 S893 R894 L895 N896 A897 D898 F899 Q900 K901 P902 W903 F904 A905 T906 V907 Q910 A911 R912 D913 L914 A915 T916 E921 L926 L929 I932 W938 F939 T942 W943 R944 T945 F946 T947 G948 D949 F950 L951 R952
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GLN SER GLN VAL ASP SER SER SER VAL SER GLU D1123 S1124 A1129 T1130 T1133 D1134 E1135 W1138 S1145 N1148 W1149 R1150 H1151 I1159 T1160 Q1161 D1162 K1163 V1166 S1167 N1168 P1169 I1170 R1171 K1172 V1173 F1174 K1175 P1176 S1177 M1180 T1189 V1194 V1195 T1196 L1197 S1198 E1199
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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 Q1529 K1530 L1533 D1543 P1547 S1548 T1549 N1550 E1551 P1552 Y1553 V1556 L1560 N1561
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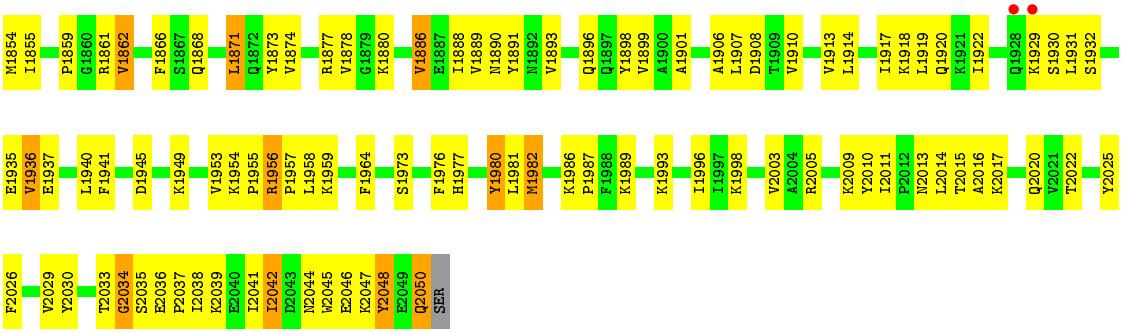
T1652 G1653 I1657 T1662 F1666 G1670 S1671 Q1672 E1673 Q1674 G1675 M1676 G1677 M1678 D1679 L1680 T1683 S1684 A1687 Q1688 R1693 H1697 L1707 N1712 N1716 L1717 T1718 I1719 G1722 G1726 A1735 M1736 I1737 F1738 E1739 T1740 I1741 V1742 K1745 L1746 K1747 F1752 E1757
S1761 F1764 R1765 L1770 T1774 Q1775 F1776 T1777 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 W1890 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 T2042 D2043 M2044 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	231.90Å 231.90Å 756.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 4.00 24.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.99-4.00) 97.3 (24.99-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.97Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.268 , 0.268 0.276 , 0.278	Depositor DCC
R_{free} test set	8547 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 76.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	85959	wwPDB-VP
Average B, all atoms (Å^2)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.50	9/12855 (0.1%)	0.61	8/17369 (0.0%)
1	B	0.44	3/12855 (0.0%)	0.62	9/17369 (0.1%)
1	C	0.48	8/12855 (0.1%)	0.61	7/17369 (0.0%)
2	G	0.42	11/16360 (0.1%)	0.58	7/22198 (0.0%)
2	H	0.55	13/16360 (0.1%)	0.61	9/22198 (0.0%)
2	I	0.42	8/16360 (0.0%)	0.59	12/22198 (0.1%)
All	All	0.47	52/87645 (0.1%)	0.60	52/118701 (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	3
2	I	0	1
All	All	0	5

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1657	ILE	C-N	-32.81	0.58	1.34
2	H	559	PRO	C-N	23.37	1.87	1.34
1	A	485	ASP	C-N	18.89	1.77	1.34
1	C	1430	ARG	C-N	-13.61	1.02	1.34
2	H	1422	THR	C-N	-13.47	1.03	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1657	ILE	O-C-N	-17.23	95.13	122.70
2	H	1657	ILE	CA-C-N	12.14	143.92	117.20
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	H	1657	ILE	C-N-CA	11.19	149.68	121.70
1	C	178	GLY	O-C-N	10.12	138.89	122.70

There are no chirality outliers.

All (5) 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	H	1657	ILE	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	12615	0	12589	601	1
1	B	12615	0	12591	582	6
1	C	12615	0	12587	588	0
2	G	15995	0	15975	998	10
2	H	15995	0	15974	997	7
2	I	15995	0	15976	977	12
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	85959	0	85779	4568	18

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 4568 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:485:ASP:C	1:A:486:VAL:N	1.77	1.36
2:H:559:PRO:C	2:H:560:ASN:N	1.87	1.26
2:H:1956:ARG:HB2	2:H:1957:PRO:HD3	1.24	1.18
2:G:28:PHE:CE2	2:H:7:ARG:HD2	1.80	1.16
2:G:1859:PRO:HG3	2:G:1871:LEU:HD12	1.29	1.15

The worst 5 of 18 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:B:1480:GLU:OE2	2:H:290:GLU:CB[6_555]	0.75	1.45
1:B:1480:GLU:CD	2:H:290:GLU:CB[6_555]	1.29	0.91
2:G:77:VAL:CB	2:I:1929:LYS:CD[6_455]	1.32	0.88
1:B:1480:GLU:OE2	2:H:290:GLU:CG[6_555]	1.43	0.77
2:G:77:VAL:CG2	2:I:1929:LYS:NZ[6_455]	1.47	0.73

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	1604/1887 (85%)	1498 (93%)	92 (6%)	14 (1%)	17	55
1	B	1604/1887 (85%)	1497 (93%)	94 (6%)	13 (1%)	19	58
1	C	1604/1887 (85%)	1499 (94%)	90 (6%)	15 (1%)	17	55
2	G	2029/2051 (99%)	1836 (90%)	167 (8%)	26 (1%)	12	48
2	H	2029/2051 (99%)	1836 (90%)	170 (8%)	23 (1%)	14	51
2	I	2029/2051 (99%)	1833 (90%)	171 (8%)	25 (1%)	13	49
All	All	10899/11814 (92%)	9999 (92%)	784 (7%)	116 (1%)	14	51

5 of 116 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	B	504	ASP

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	1367/1566 (87%)	1224 (90%)	143 (10%)	7	27
1	B	1367/1566 (87%)	1225 (90%)	142 (10%)	7	28
1	C	1367/1566 (87%)	1227 (90%)	140 (10%)	7	28
2	G	1772/1789 (99%)	1567 (88%)	205 (12%)	5	24
2	H	1772/1789 (99%)	1566 (88%)	206 (12%)	5	24
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	5	24
All	All	9417/10065 (94%)	8371 (89%)	1046 (11%)	6	26

5 of 1046 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	431	LEU
2	G	1528	GLU
2	I	1160	THR
2	G	562	LEU
2	G	952	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1063	HIS
2	G	447	ASN
2	I	900	GLN
1	C	1239	HIS

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Mol	Chain	Res	Type
1	C	1563	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	$\#\|Z\| > 2$
4	FMN	G	3051	-	31,33,33	6.88	18 (58%)	40,50,50	1.96	7 (17%)
4	FMN	H	3051	-	31,33,33	6.73	18 (58%)	40,50,50	1.91	8 (20%)
3	CER	A	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.18	3 (33%)
3	CER	B	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.05	3 (33%)
4	FMN	I	3051	-	31,33,33	6.74	21 (67%)	40,50,50	1.81	7 (17%)
3	CER	C	2748	1	10,11,15	4.21	3 (30%)	9,13,17	3.18	3 (33%)

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
4	FMN	G	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
3	CER	A	2748	1	-	5/12/12/16	-
3	CER	B	2748	1	-	5/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	CER	C	2748	1	-	5/12/12/16	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-C10	16.06	1.54	1.38
4	H	3051	FMN	C4A-C10	15.15	1.53	1.38
4	I	3051	FMN	C4A-C10	14.86	1.53	1.38
4	G	3051	FMN	C4A-N5	12.70	1.51	1.33
4	I	3051	FMN	C4A-N5	12.26	1.50	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2748	CER	O1-C4-C5	-7.72	107.97	121.70
3	A	2748	CER	O1-C4-C5	-7.67	108.06	121.70
4	H	3051	FMN	C4-N3-C2	7.46	121.44	115.14
3	B	2748	CER	O1-C4-C5	-7.34	108.64	121.70
4	G	3051	FMN	C4-N3-C2	7.33	121.33	115.14

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C2'-C3'-C4'-C5'
4	G	3051	FMN	O3'-C3'-C4'-C5'
4	H	3051	FMN	C2'-C3'-C4'-C5'
4	H	3051	FMN	O3'-C3'-C4'-C5'
3	A	2748	CER	C2-C3-C4-O1

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	7	0

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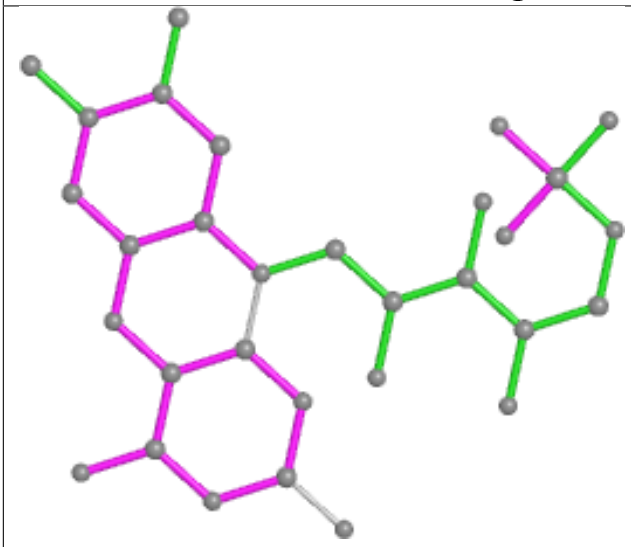
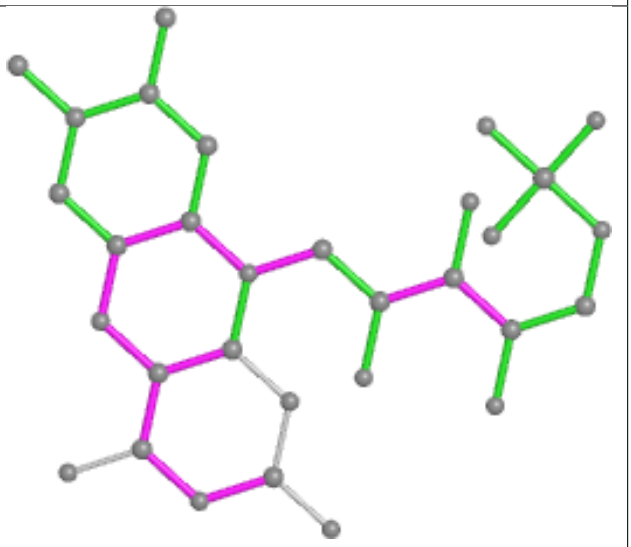
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3051	FMN	6	0
3	A	2748	CER	3	0
3	B	2748	CER	4	0
4	I	3051	FMN	8	0
3	C	2748	CER	4	0

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.

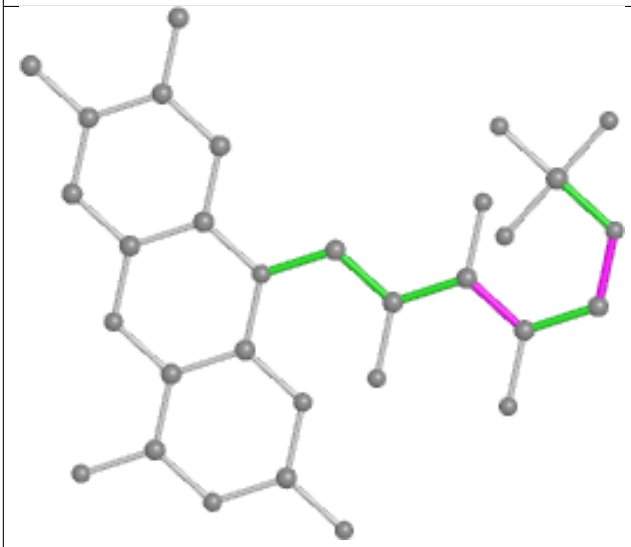
Ligand FMN G 3051



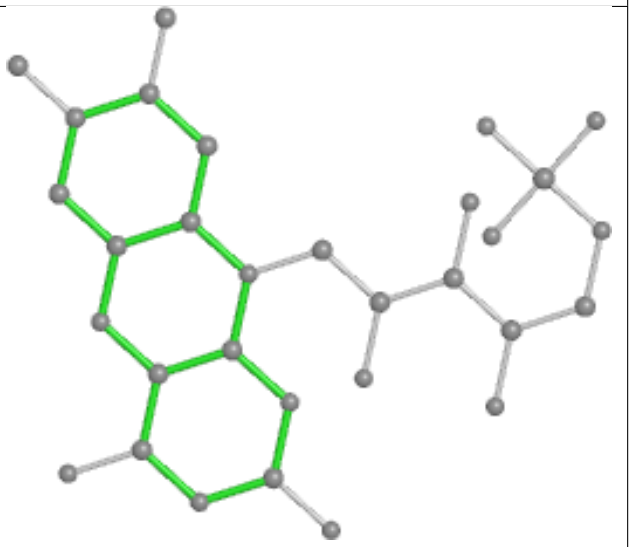
Bond lengths



Bond angles

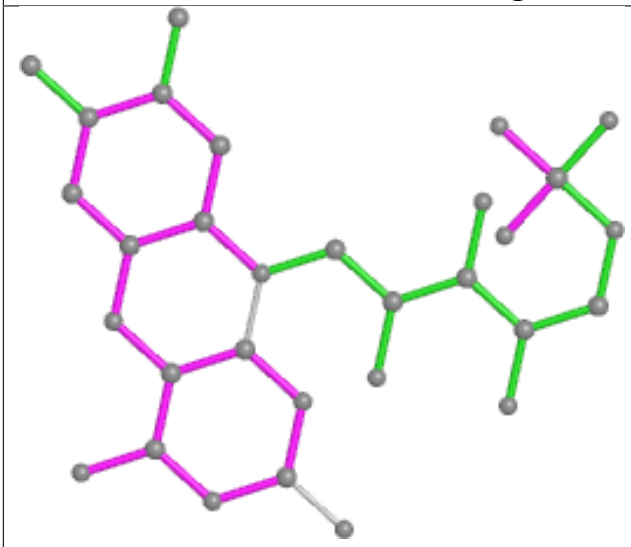


Torsions

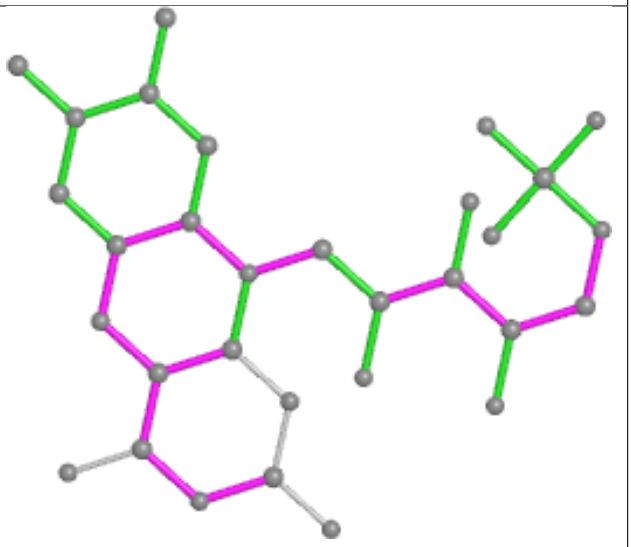


Rings

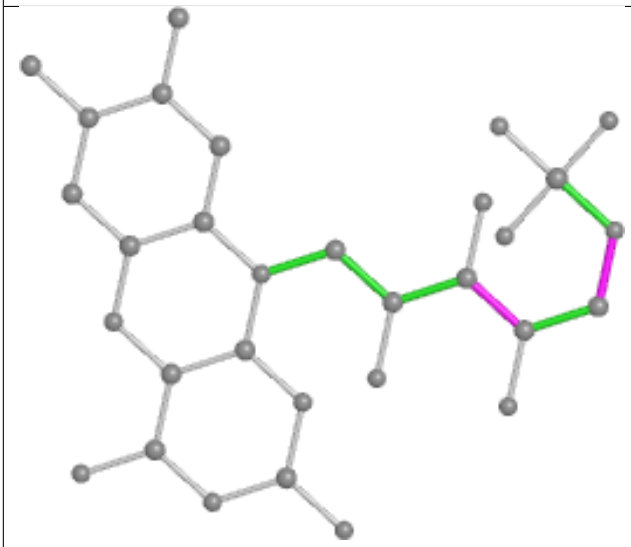
Ligand FMN H 3051



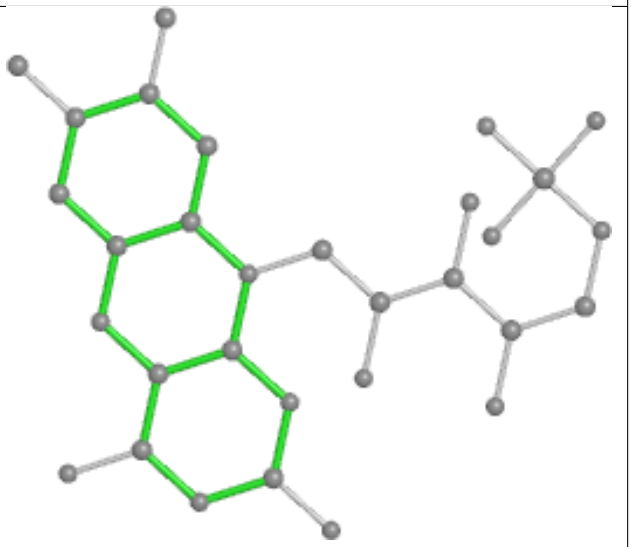
Bond lengths



Bond angles

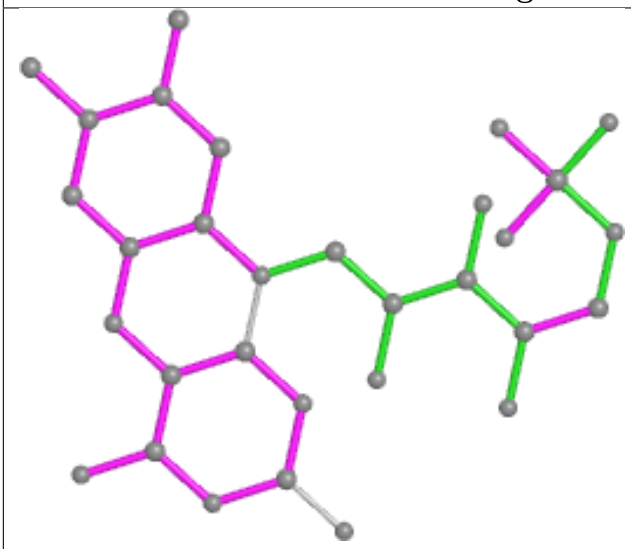


Torsions

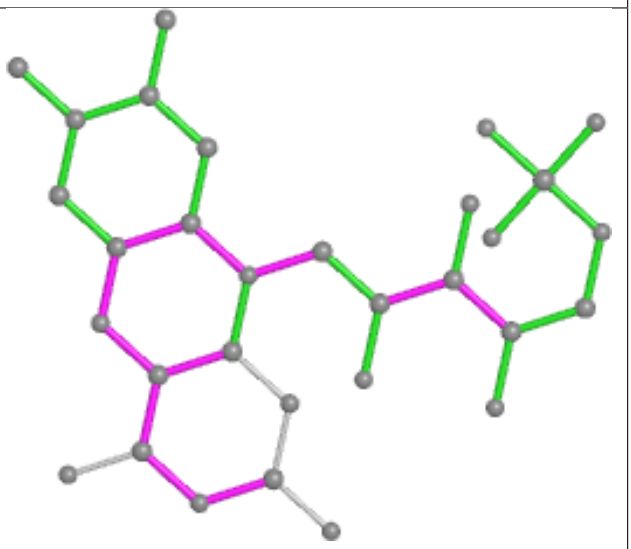


Rings

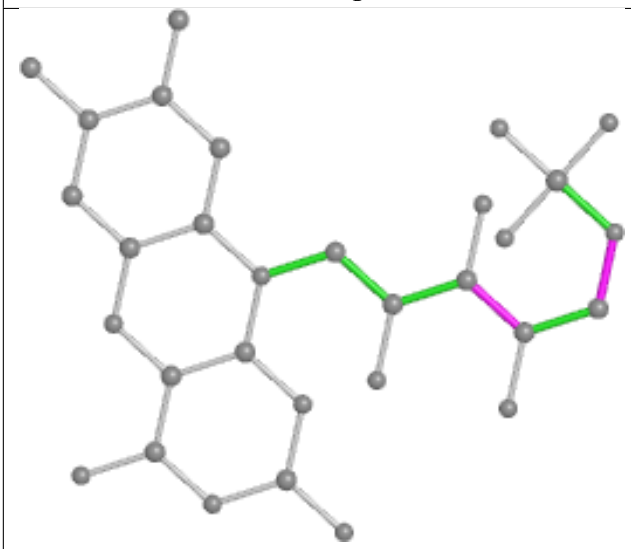
Ligand FMN I 3051



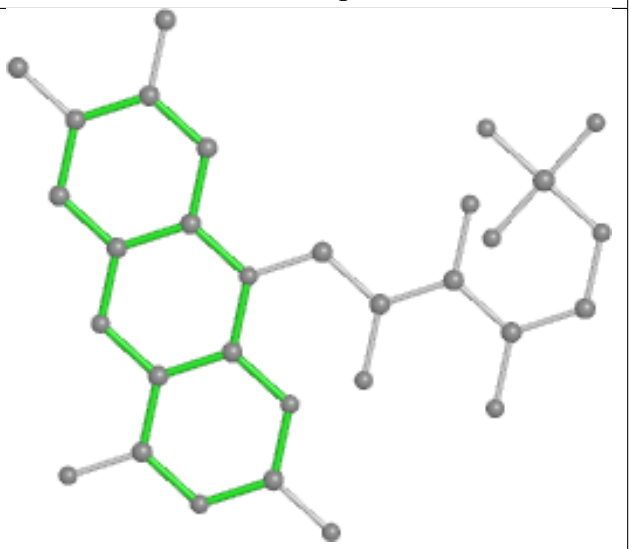
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	6
1	C	4
2	G	3

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Mol	Chain	Number of breaks
1	A	3
2	I	2

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	559:PRO	C	560:ASN	N	1.87
1	A	485:ASP	C	486:VAL	N	1.77
1	H	315:PRO	C	316:ASN	N	1.64
1	H	1530:LYS	C	1531:VAL	N	1.60
1	C	932:PHE	C	933:VAL	N	1.19

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	1614/1887 (85%)	-0.42	11 (0%)	87	82	98, 134, 233, 288	0
1	B	1614/1887 (85%)	-0.42	10 (0%)	89	84	99, 133, 233, 296	0
1	C	1614/1887 (85%)	-0.41	14 (0%)	84	77	100, 135, 233, 294	0
2	G	2033/2051 (99%)	-0.42	6 (0%)	94	90	134, 172, 221, 270	0
2	H	2033/2051 (99%)	-0.31	11 (0%)	91	85	133, 173, 218, 268	0
2	I	2033/2051 (99%)	-0.39	6 (0%)	94	90	134, 173, 218, 264	0
All	All	10941/11814 (92%)	-0.39	58 (0%)	91	85	98, 164, 226, 296	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	SER	6.2
1	C	875	THR	5.8
1	B	875	THR	5.3
1	B	1747	ALA	5.3
1	A	540	GLN	4.1

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

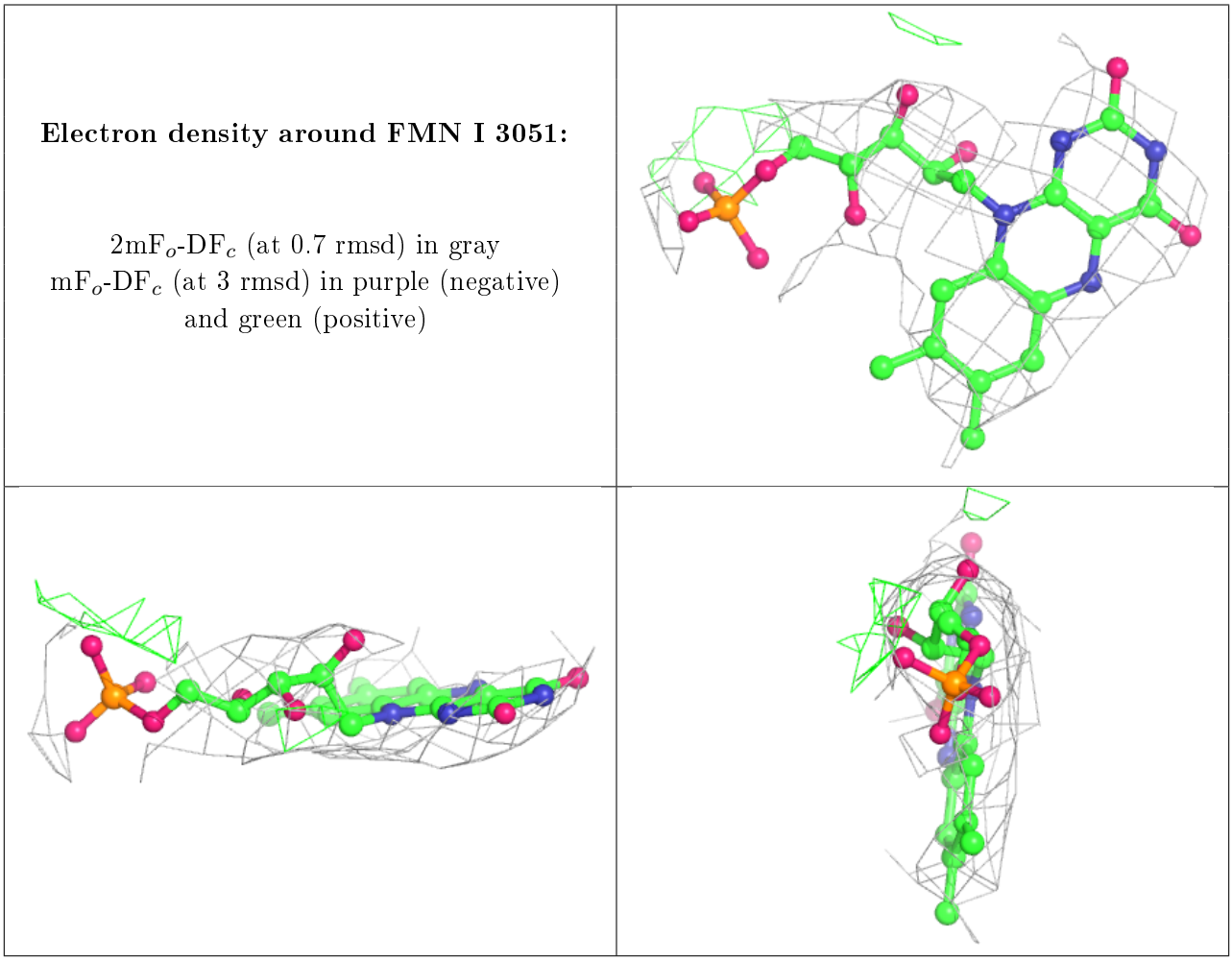
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CER	A	2748	12/16	0.81	0.32	70,134,243,252	0
4	FMN	I	3051	31/31	0.85	0.41	132,164,181,204	0
4	FMN	G	3051	31/31	0.87	0.33	137,161,187,206	0
4	FMN	H	3051	31/31	0.88	0.26	133,160,184,188	0
3	CER	C	2748	12/16	0.90	0.37	70,134,252,253	0
3	CER	B	2748	12/16	0.91	0.21	70,134,252,253	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

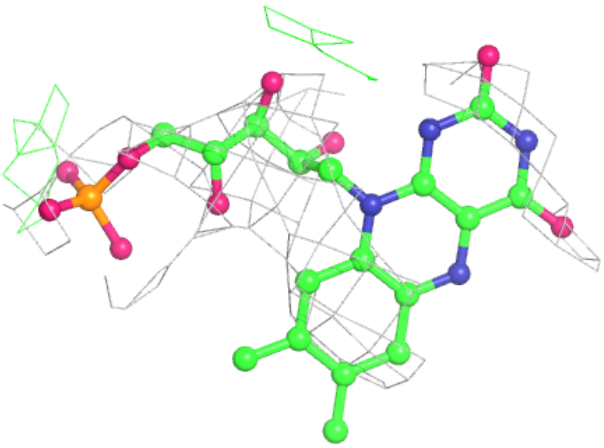
Electron density around FMN I 3051:

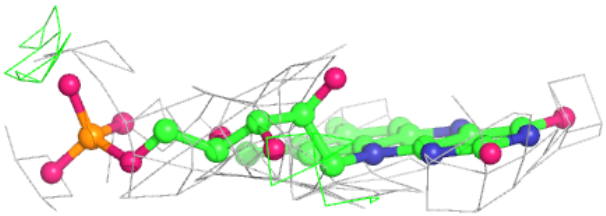
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

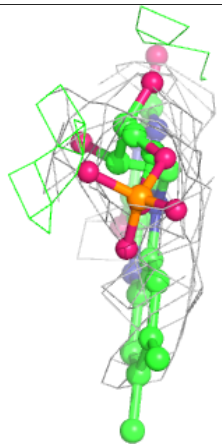


Electron density around FMN G 3051:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

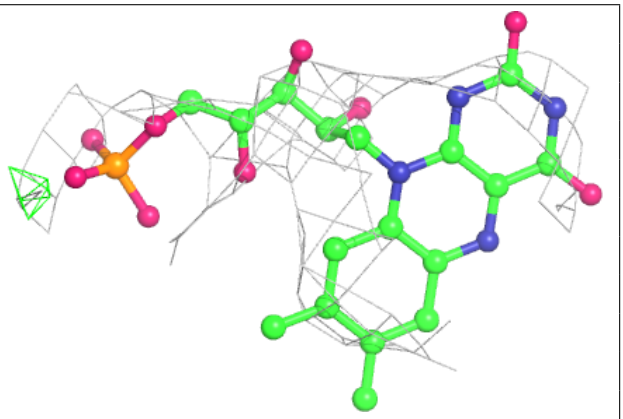


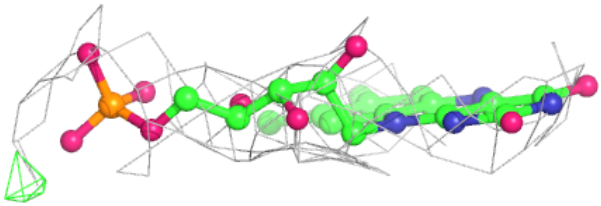


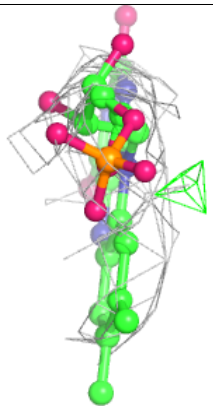


Electron density around FMN H 3051:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.