wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Jul 24, 2017 – 02:46 PM EDT

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

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

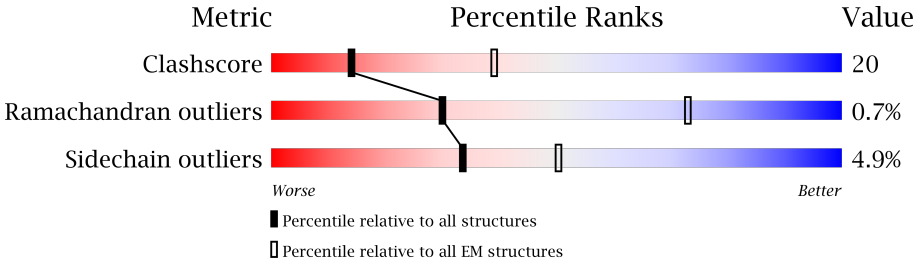
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 20.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	3089	57% 31% • 9%
1	B	3089	57% 31% • 9%
1	C	3089	57% 31% • 9%
1	D	3089	57% 31% • 9%
1	E	3089	57% 31% • 9%
1	F	3089	57% 31% • 9%

2 Entry composition (i)

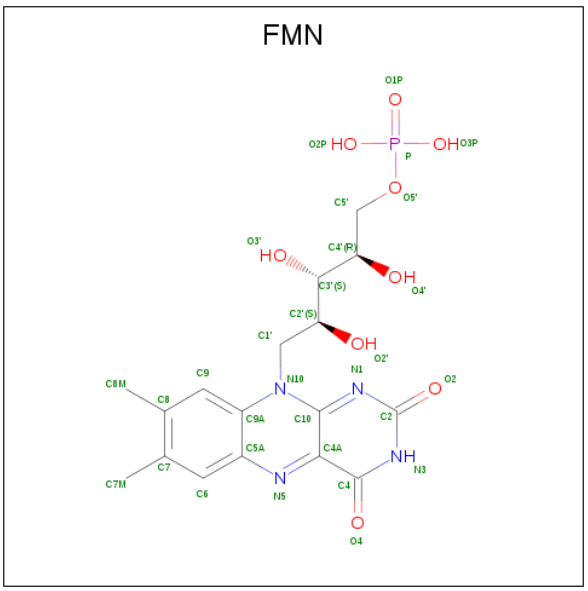
There are 2 unique types of molecules in this entry. The entry contains 125856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TYPE-I FATTY ACID SYNTHASE.

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

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



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

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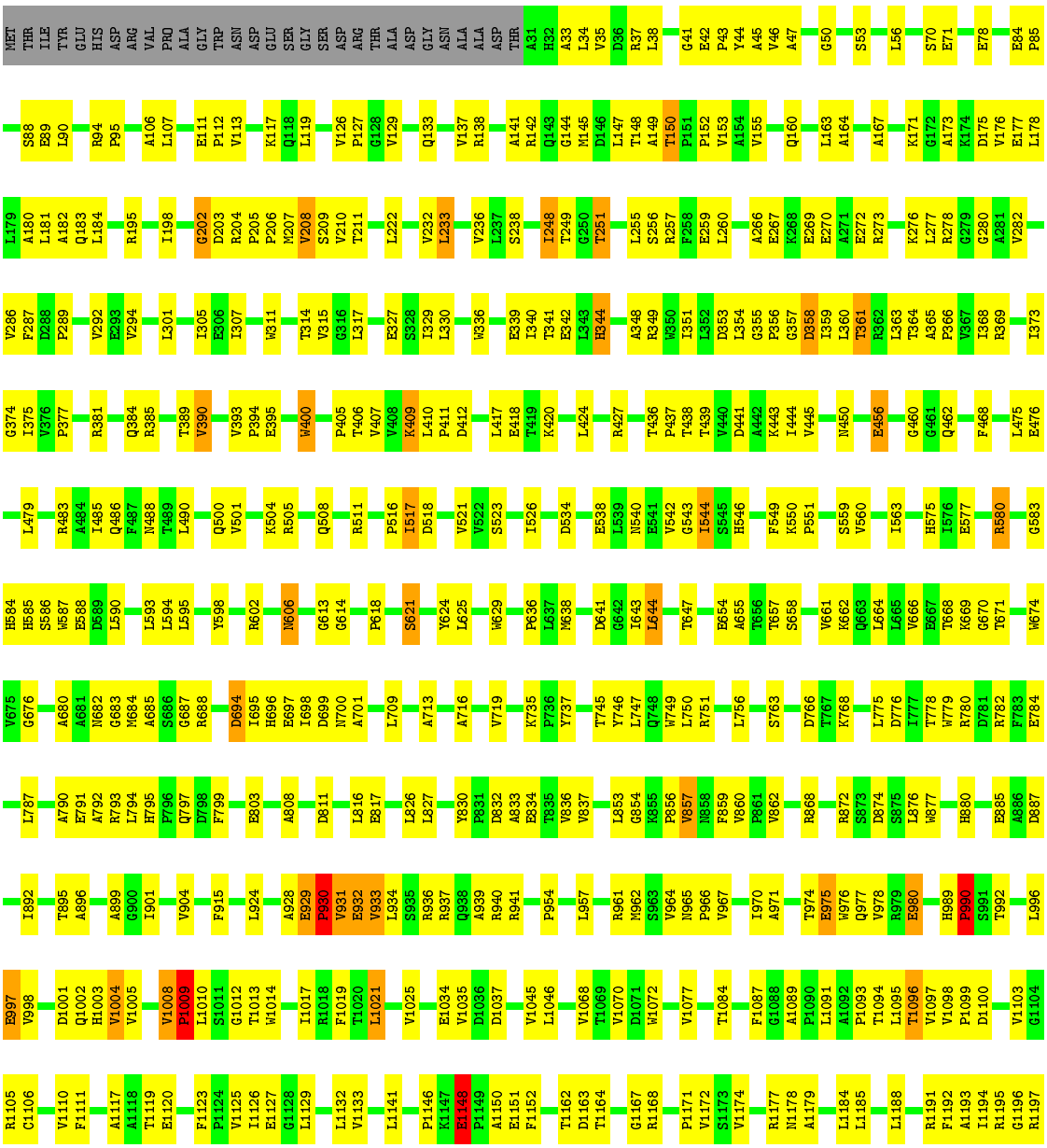
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	C	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	D	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	E	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	F	1	31	17	4	9	1	0

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain A: 57% 31% • 9%



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D2630	E2523		M2299		E2090	PRO	GLY	ALA	ILE	Y1724	P1622		T1420	D1314	E1202
P2631	C2524	E2426	F2300	T2192	G2091	SER	TRP	GLU	THR	S1725	F1623	D1514	Q1421	R1315	L1203
T2632		A2427		L2193	T2092	ALA	ALA	ALA	PHE		T1624		F1422	V1316	T1204
V2633	V2527	P2428	D2303	W2194	G2093	GLY	LYS	ASP	ASP	E1730	L1625	V1519	T1423	G1317	D1205
	E2528			V2195	H2094	GLY	HIS	LEU	ALA	V1731			Q1424	I1318	P1206
D2645	R2529	T2431	Y2306	V2196	V2095	ALA	VAL	GLY	ALA	L1732	R1634	L1530	V1425	D1319	V1207
R2646	Y2530	I2432		P2197	V2096	SER	THR	ALA	ASP	N1733		E1531			
V2647		R2433	K2310	A2198	A2097	GLY	VAL	LEU	ALA	S1734	V1637	I1532	V1430	E1323	A1212
A2648	A2533	A2434			T2098	GLY	GLU	LYS	THR	E1735	P1638	V1533	A1431	V1324	
L2649		L2435	R2319	D2205	Q2099	VAL	PHE	GLY	VAL	R1736	A1639	N1534		L1325	T1218
W2650	R2541	P2436			A2100	VAL	ALA	GLN	ALA	D1737		F1535	V1435	E1326	D1219
N2651	E2542	S2437	S2331	L2209	N2101	ASP	LEU	VAL	LEU		T1651	N1536		V1327	T1220
I2652	F2543	P2438	L2332	V2210	W2102	S1983	GLY	THR	ILE	L1741	W1652	L1537	Q1441	S1328	P1221
V2653		P2439	A2333	E2211	W2103		THR	LYS	ALA			R1538		A1329	
	P2551		H2334	W2212	Q2104	L1986	ARG	LEU	LEU	D1745	K1656	G1539	V1445	R1330	R1225
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	H2553	N2443	W2339	G2214		F1989	GLY	ARG	ALA	ASP	K1658	Q1541	A1448		D1227
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W2672	L2557	A2447	Q2348	L2228	N2113	P1996	ARG	PRO	ILE	GLU	R1662		V1455	A1339	
	L2558	P2448	N2349	K2229	V2114		GLY	PHE	ASP	PRO	K1663	L1551			R1253
S2676		E2449			H2115	L2000	GLY	GLY	GLN	GLU		E1552	T1459	R1342	
	L2563	W2450	I2352	P2234			ASP	PRO	ILE	ALA	I1666	A1553	A1460	L1343	G1268
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T2681		L2453		L2237		S2014	GLY	SER	LEU	PRO		E1556	C1463	P1346	L1271
	E2574	D2454	E2358	F2238	I2122	D2015	LEU	ASP	ASP	THR	W1671	E1557	V1464		
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	F2580	A2458	V2361	R2244	A2124		ALA	ILE	ILE	ASP	F1673	R1560	V1467		A1275
T2690	V2581			V2245	G2125	P2020	GLY	ASN	GLU	ALA	A1674	R1561	Y1468	P1353	Q1276
S2691	Q2582	V2461	M2372	A2246	A2126		ALA	ASP	SER	PRO		R1562	E1469		H1277
M2692	F2583	V2462			E2127	V2032	LEU	GLN	ILE	ALA	W1679	Q1563	L1470	I1357	V1278
Q2693	D2584		L2376	V2252	N2128		ALA	LEU	THR	GLU		I1564	E1471	Q1358	V1279
T2694	P2585	L2469			P2129	T2047	SER	ARG	ASP	ALA	D1684			H1359	T1280
M2695	E2586	G2470	K2391	R2255			ALA	THR	GLY	ALA	L1685	D1578	L1474	K1360	A1281
Y2696		P2471	V2392		Y2134	A2053	ALA	VAL	ALA	PRO	L1686	V1579		G1361	T1282
H2697	R2591	Y2472	D2393	K2261		V2054	ASP	LEU	SER	ALA	F1687	P1580	R1480	M1362	D1283
G2698	P2592		L2394		E2137	V2055	VAL	GLY	SER	ALA		F1581			G1284
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L2700	W2599				V2140	D2057	LYS	SER	ARG	ALA		S1583	M1484		P1286
L2701		M2481	L2398	Q2268	V2141	D2058	VAL	GLY	ASN	ALA	G1694		H1485	A1380	V1287
G2702	R2603	E2482				R2059	ILE	LYS	GLN	PRO	L1695	L1586	D1486		P1288
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A2704	R2610	L2487	K2402		V2164		GLY	PRO	LEU	PRO	R1699	V1590	V1488		A1290
K2705	V2611		I2403	I2277	I2165	L2067	ALA	ALA	VAL	VAL	F1700		P1489	D1398	K1291
P2706	P2612	V2492	D2404		A2166		VAL	TYR	ASP	ALA	V1701	E1598	R1490	N1399	L1292
	R2613		M2405	D2282	T2167	L2070	ALA	ILE	LEU	ALA	E1702		D1491	P1400	I1293
I2709	K2614	L2495					ALA	THR	GLY	PRO	I1703	K1605			G1294
L2710			L2408	R2286	R2170	E2074	VAL	GLU	SER	ALA	G1704		R1495	A1405	W1295
Q2711	L2617	K2503	A2409	L2287			ALA	ARG	GLU	ALA	V1705	I1611	S1496		
E2712	S2618	W2504		H2288	D2173	Q2081	ALA	VAL	LEU	PRO		G1612		V1408	K1304
V2713	R2619	E2505	A2412		D2174	W2082	ARG	THR	ASN	SER	T1710	R1613	I1503		
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P2715	V2621	W2512	M2416		L2176	Q2084	GLY	THR	GLY	GLY	A1712	P1616	P1505	P1413	Q1308
N2716	G2622	Y2513	S2417	S2294		L2085	ILE	TRP	ALA	PRO	G1713	N1617	S1506	D1414	V1309
V2717	A2623		G2418	P2295	K2180	S2086	SER	GLU	ILE	ARG	L1714	L1618	Q1507	G1415	D1310
V2718	Q2624	L2520		N2296		Q2087	VAL	LEU	ASP	PRO		V1619	I1508	V1416	F1311
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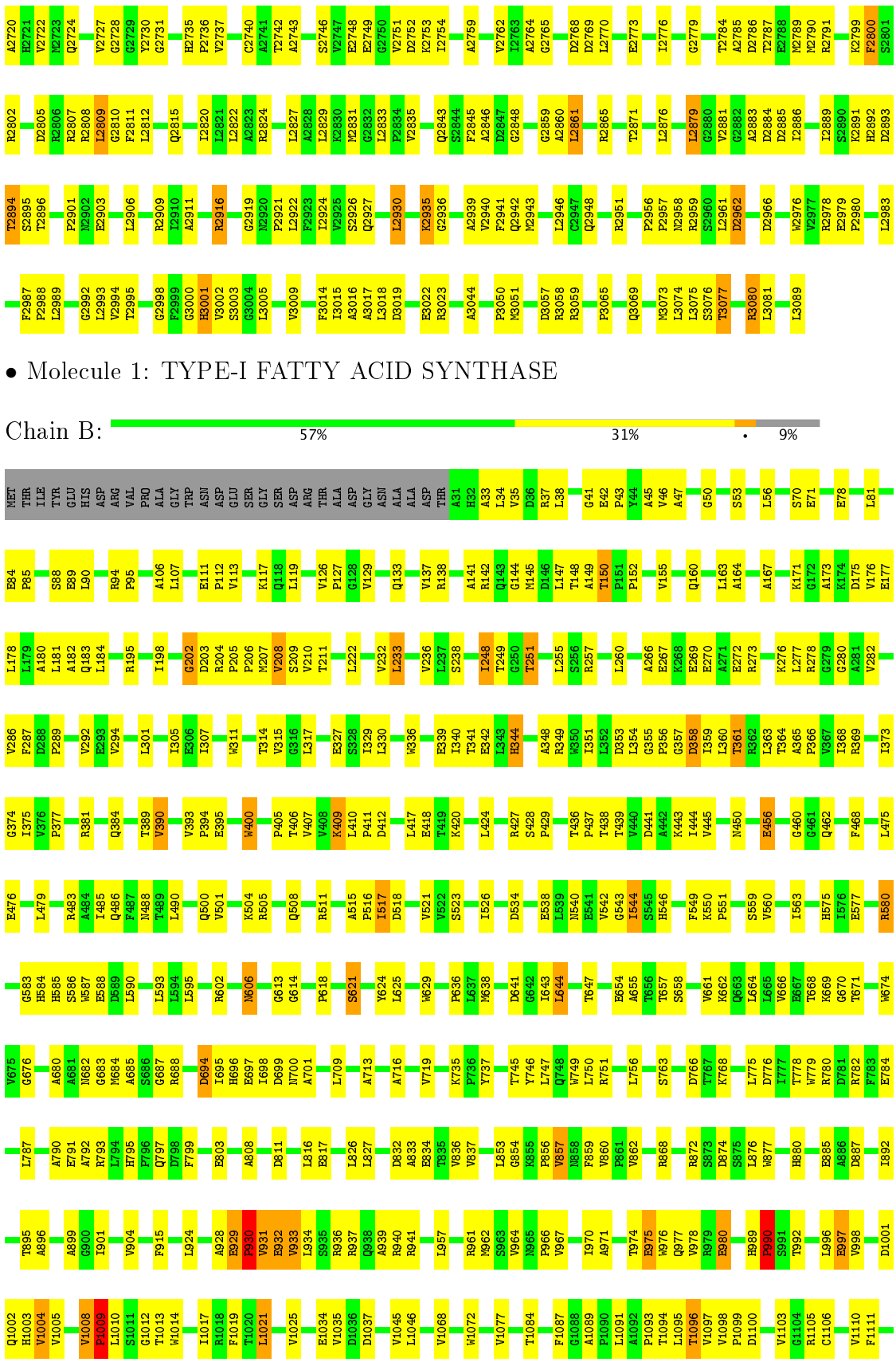
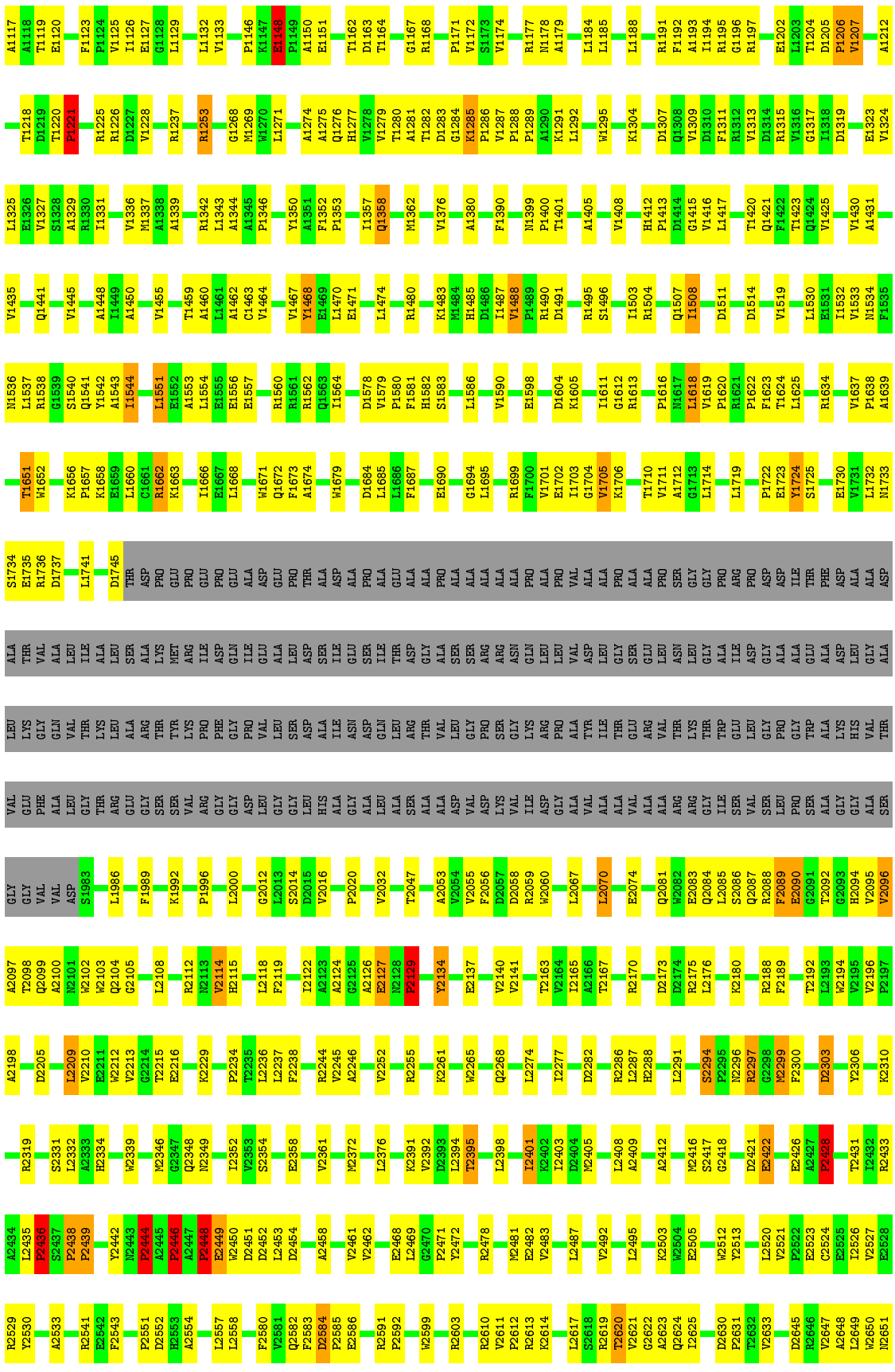


- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain B: 57% 31% • 9%



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T1218 D1219 T1220 P1221 R1225 R1226 D1227 V1228 R1237 R1253 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279 T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 W1295 K1304 D1307 Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319 E1323 V1324

L1325 E1326 V1327 S1328 A1329 R1330 I1331 V1336 M1337 A1338 A1339 R1342 L1343 A1344 A1345 P1346 Y1350 A1351 F1352 P1353 I1357 Q1358 M1362 V1376 A1380 F1390 N1399 P1400 T1401 A1405 V1408 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425 V1430 A1431

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S1734 E1735 R1736 D1737 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA ALA PRO ALA ALA ALA ALA ALA PRO ALA PRO VAL ALA ALA PRO ALA ALA PRO SER GLY GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP

ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA ALA GLU ALA ASP LEU GLY ALA

LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO GLY TRP ALA LYS HIS VAL THR

VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY LEU HIS ALA GLY ALA LEU ALA SER ALA ALA ASP VAL ASP LYS VAL ILE ASP GLY ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY ALA SER

GLY GLY VAL VAL ASP S1983 L1986 F1989 K1992 P1996 L2000 G2012 L2013 S2014 D2015 V2016 P2020 V2032 T2047 A2053 V2054 V2055 F2056 D2057 D2058 R2059 W2060 L2067 L2070 E2074 Q2081 W2082 E2083 Q2084 L2085 S2086 Q2087 R2088 F2089 E2090 G2091 T2092 G2093 H2094 V2095 V2096

A2097 T2098 Q2099 A2100 N2101 W2102 W2103 Q2104 G2105 L2108 R2112 N2113 V2114 H2115 L2118 F2119 I2122 A2123 A2124 G2125 A2126 E2127 N2128 P2129 Y2134 E2137 V2140 V2141 T2163 V2164 I2165 A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180 R2188 F2189 T2192 L2193 W2194 V2195 V2196 P2197

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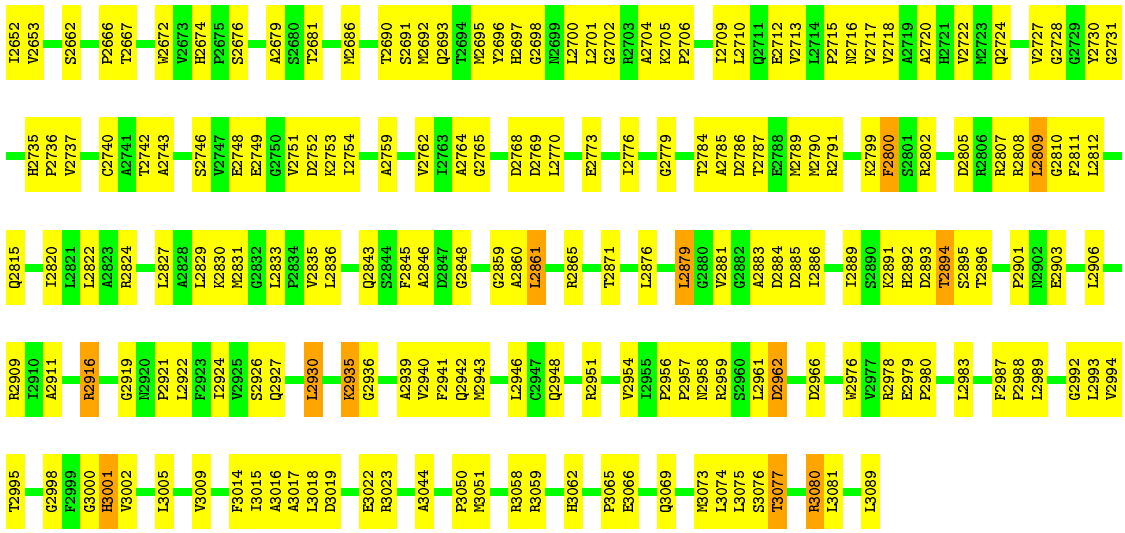
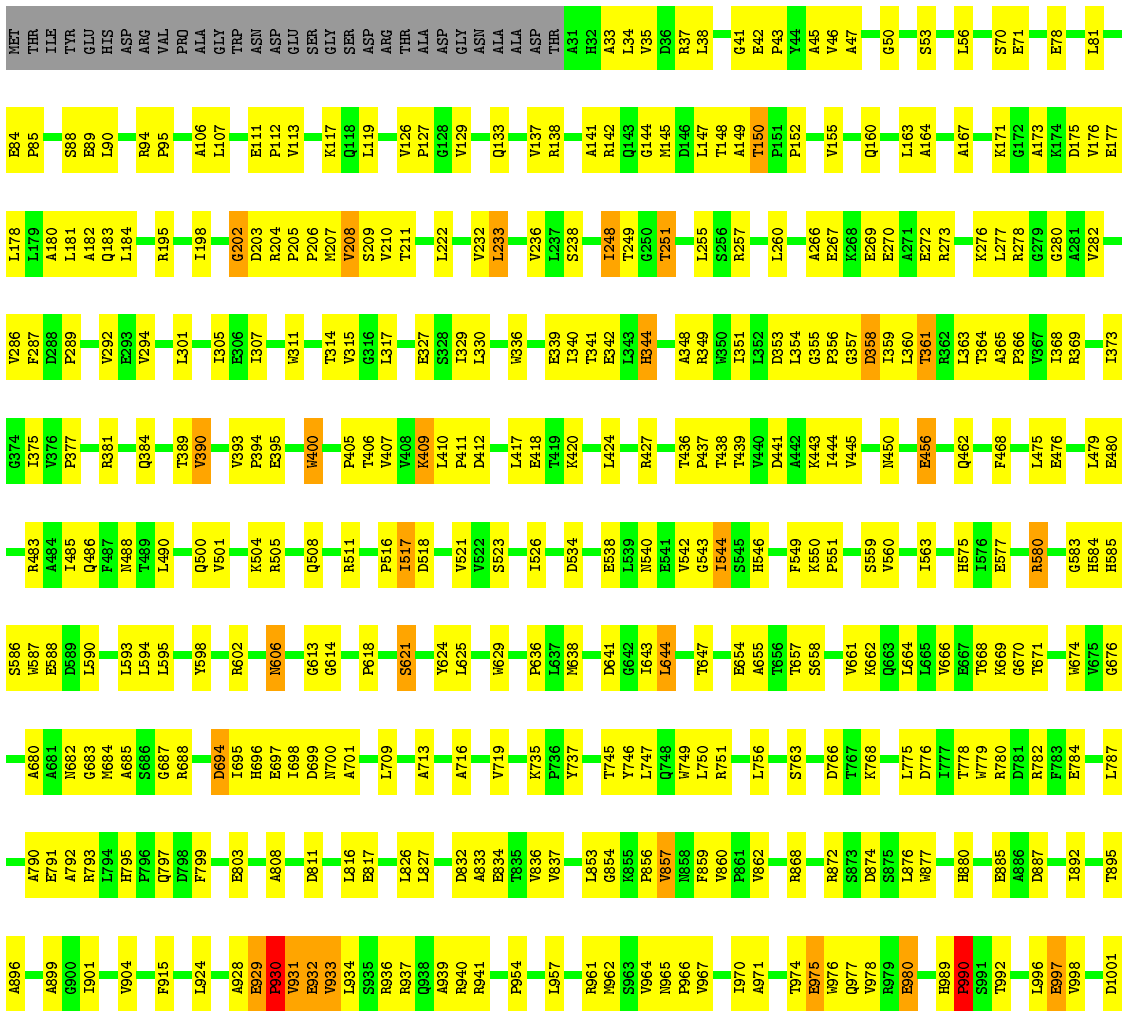
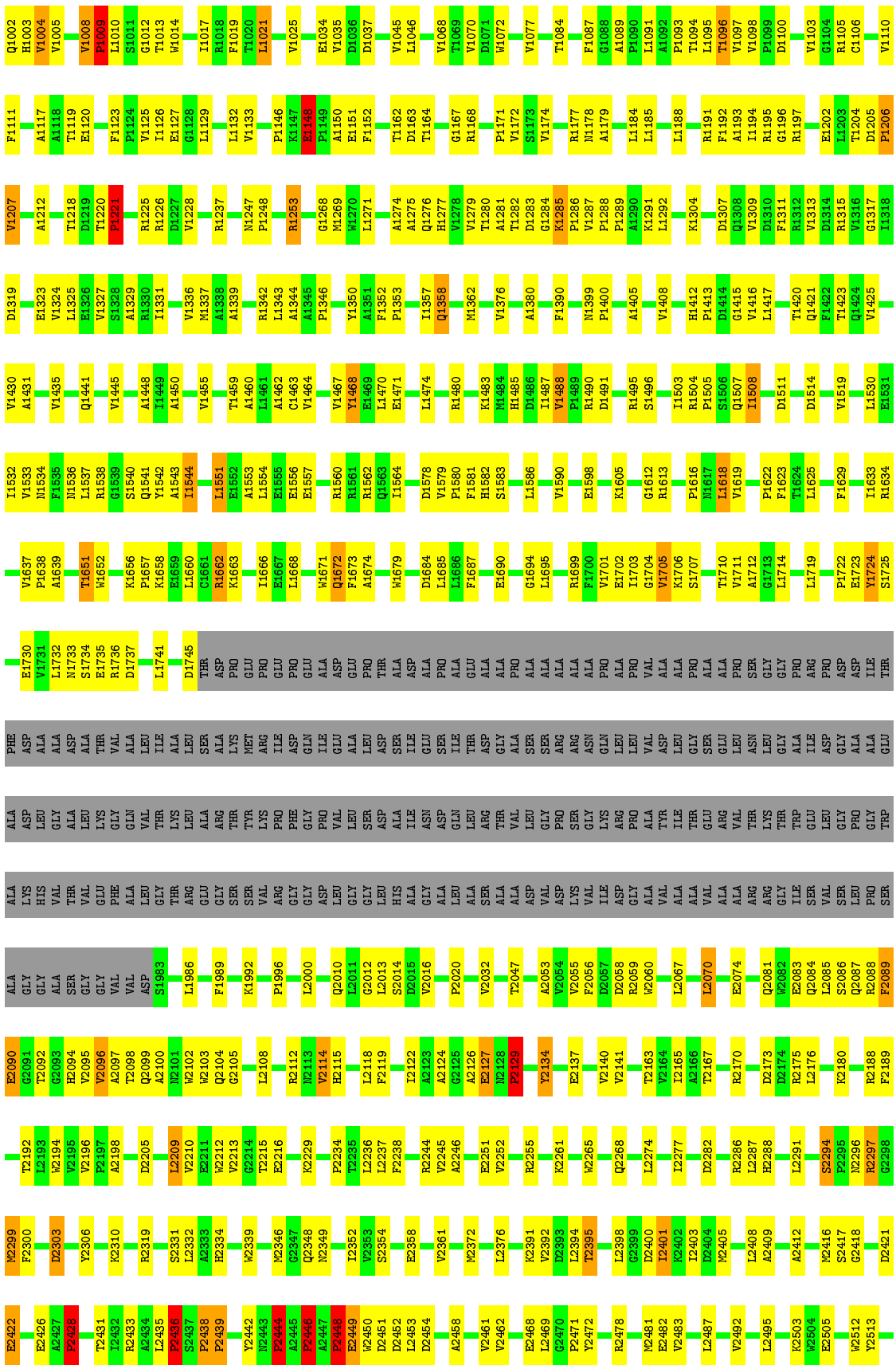
R2529 Y2530 A2533 R2541 E2542 F2543 P2551 D2552 H2553 A2554 L2557 L2558 F2580 V2581 Q2582 F2583 D2584 P2585 E2586 R2591 P2592 W2599 R2603 R2610 V2611 P2612 R2613 K2614 L2617 S2618 R2619 T2620 V2621 G2622 A2623 Q2624 I2625 D2630 P2631 T2632 V2633 D2645 R2646 V2647 A2648 L2649 W2650 N2651



- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain C: 57% 31% • 9%

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M2299 F2300 D2303 Y2306 K2310 R2319 S2331 L2332 A2333 H2334 W2339 M2346 G2347 Q2348 N2349 I2352 V2353 S2354 E2358 V2361 M2372 L2376 K2391 V2392 D2393 L2394 T2395 L2398 G2399 D2400 I2401 K2402 I2403 D2404 M2405 L2408 A2409 A2412 M2416 S2417 G2418 D2421
T2192 K2193 W2194 V2195 V2196 P2197 A2198 D2205 L2209 V2210 E2211 W2212 V2213 G2214 T2215 E2216 K2229 P2234 T2235 L2236 L2237 F2238 R2244 V2245 A2246 E2251 V2252 R2255 K2261 W2265 Q2268 L2274 I2277 D2282 R2286 L2287 H2288 L2291 S2294 P2295 N2296 R2297 G2298
E2090 G2091 T2092 G2093 H2094 V2095 V2096 A2097 T2098 Q2099 A2100 N2101 W2102 W2103 Q2104 G2105 L2108 R2112 N2113 V2114 H2115 L2118 F2119 I2122 A2123 A2124 G2125 A2126 E2127 N2128 P2129 Y2134 E2137 V2140 V2141 T2163 W2164 I2165 A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180 R2188 F2189
ALA GLY GLY ALA SER GLY GLY VAL VAL ASP S1983 L1986 F1989 K1992 P1996 L2000 Q2010 I2011 G2012 L2013 S2014 D2015 V2016 P2020 V2032 T2047 A2053 V2054 V2055 F2056 D2057 D2058 R2059 W2060 L2067 L2070 E2074 Q2081 W2082 E2083 Q2084 L2085 S2086 Q2087 R2088 F2089
ALA LYS HIS VAL THR VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY LEU HIS ALA GLY ALA LEU ALA SER ALA ASP VAL ASP LYS VAL ILE ASP GLY ALA ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER
ALA ASP LEU GLY ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE LEU ASN ASP GLN VAL SER ILE THR ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO GLY TRP
PHE ASP ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA GLU
E1730 V1731 L1732 N1733 S1734 E1735 R1736 D1737 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA ALA GLU ALA PRO ALA GLU ALA ALA ALA ALA PRO ALA PRO ALA PRO VAL ALA ALA PRO SER GLY GLY PRO ASP ASP ILE THR
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I1532 V1533 N1534 F1535 N1536 L1537 R1538 G1539 S1540 Q1541 Y1542 A1543 I1544 L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 I1564 D1578 V1579 P1580 F1581 H1582 S1583 L1586 V1590 E1598 K1605 G1612 R1613 P1616 N1617 L1618 V1619 P1622 F1623 T1624 L1625 F1629 I1633 R1634
V1430 A1431 V1435 Q1441 V1445 A1448 I1449 A1450 V1455 T1459 A1460 L1461 A1462 C1463 V1464 V1467 Y1468 E1469 L1470 E1471 L1474 R1480 K1483 M1484 H1485 D1486 I1487 V1488 P1489 R1490 D1491 R1495 S1496 I1503 R1504 P1505 S1506 Q1507 I1508 D1511 D1514 V1519 L1530 E1531
D1319 E1323 V1324 L1325 E1326 V1327 S1328 A1329 R1330 I1331 V1336 M1337 A1338 A1339 R1342 L1343 A1344 A1345 P1346 Y1350 A1351 F1352 P1353 I1357 Q1358 M1362 V1376 A1380 F1390 N1399 P1400 A1405 V1408 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425
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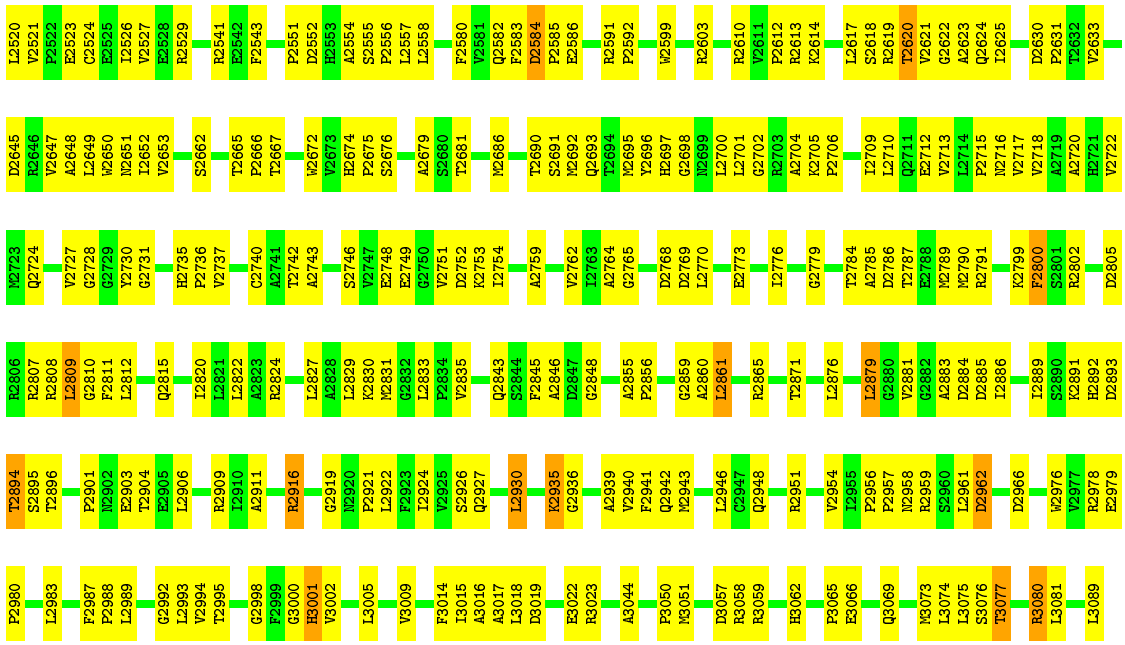
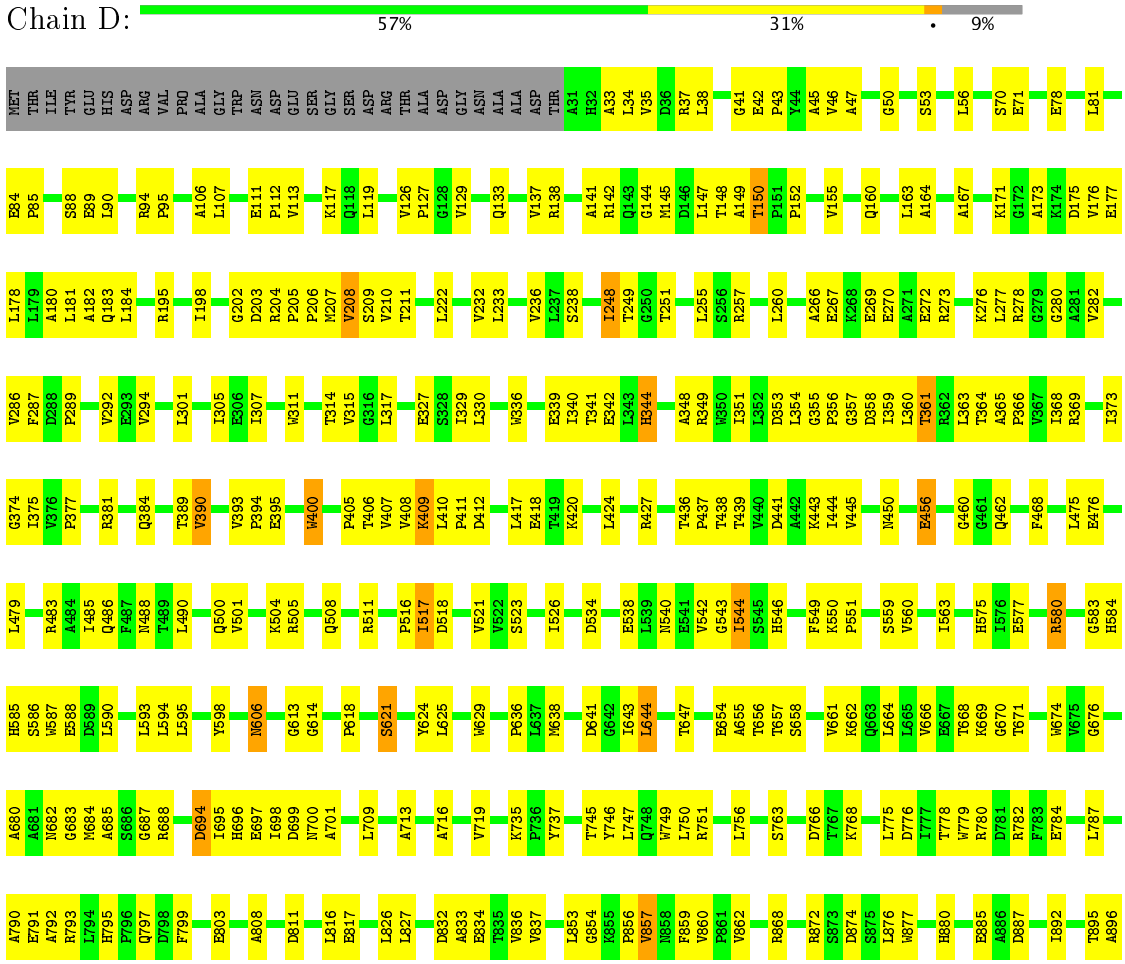
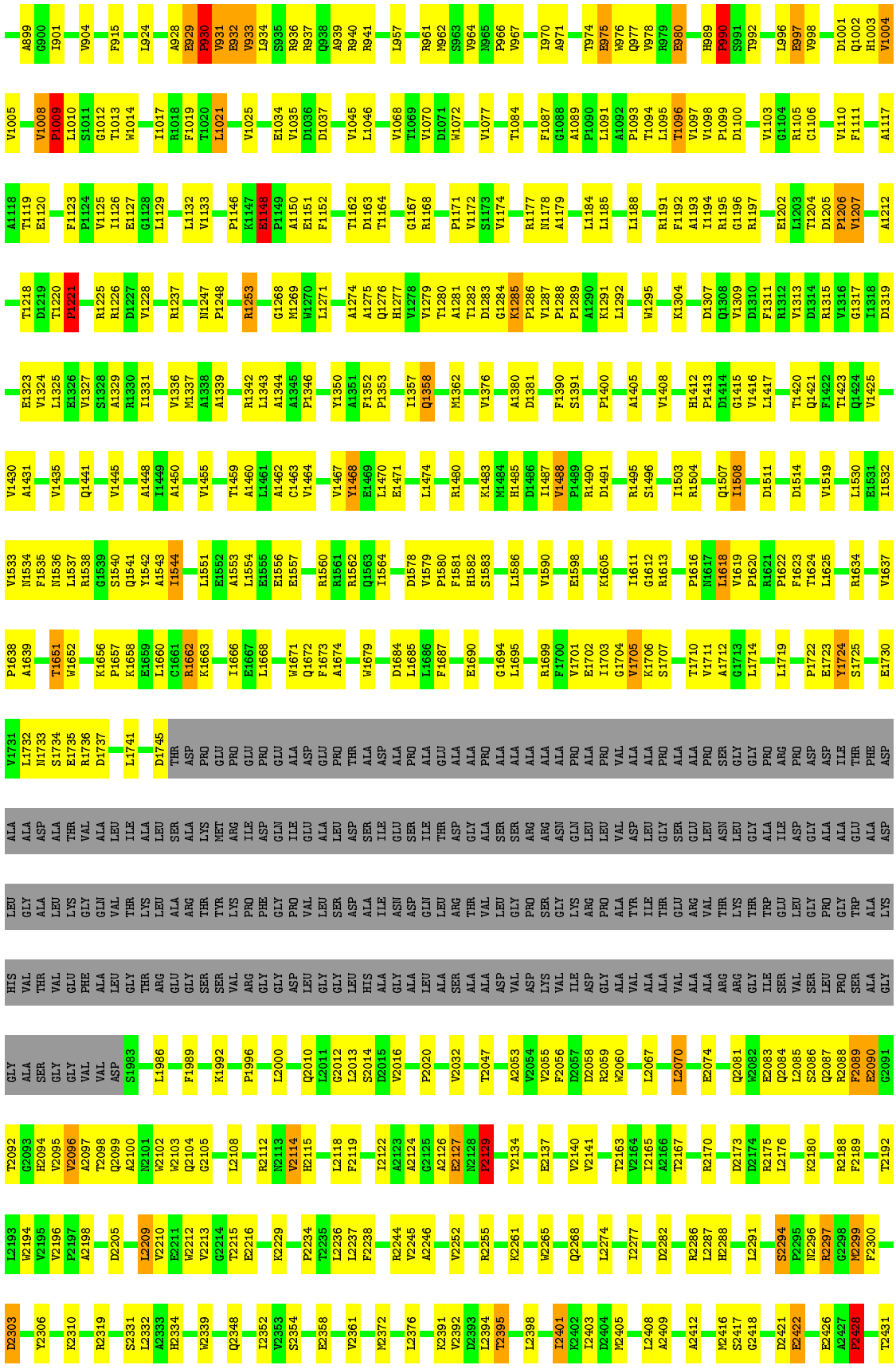


- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain D:

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V1005 V1008 P1009 L1010 S1011 G1012 T1013 W1014 I1017 R1018 F1019 T1020 L1021 V1025 E1034 V1035 D1036 D1037 V1045 L1046 V1068 T1069 V1070 D1071 W1072 V1077 T1084 F1087 G1088 A1089 P1090 L1091 A1092 P1093 T1094 L1095 T1096 V1097 V1098 P1099 D1100 V1103 G1104 R1105 C1106 V1110 F1111 A1117
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T1218 D1219 T1220 P1221 R1225 R1226 D1227 V1228 R1237 N1247 P1248 R1253 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279 T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 W1295 K1304 D1307 Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319
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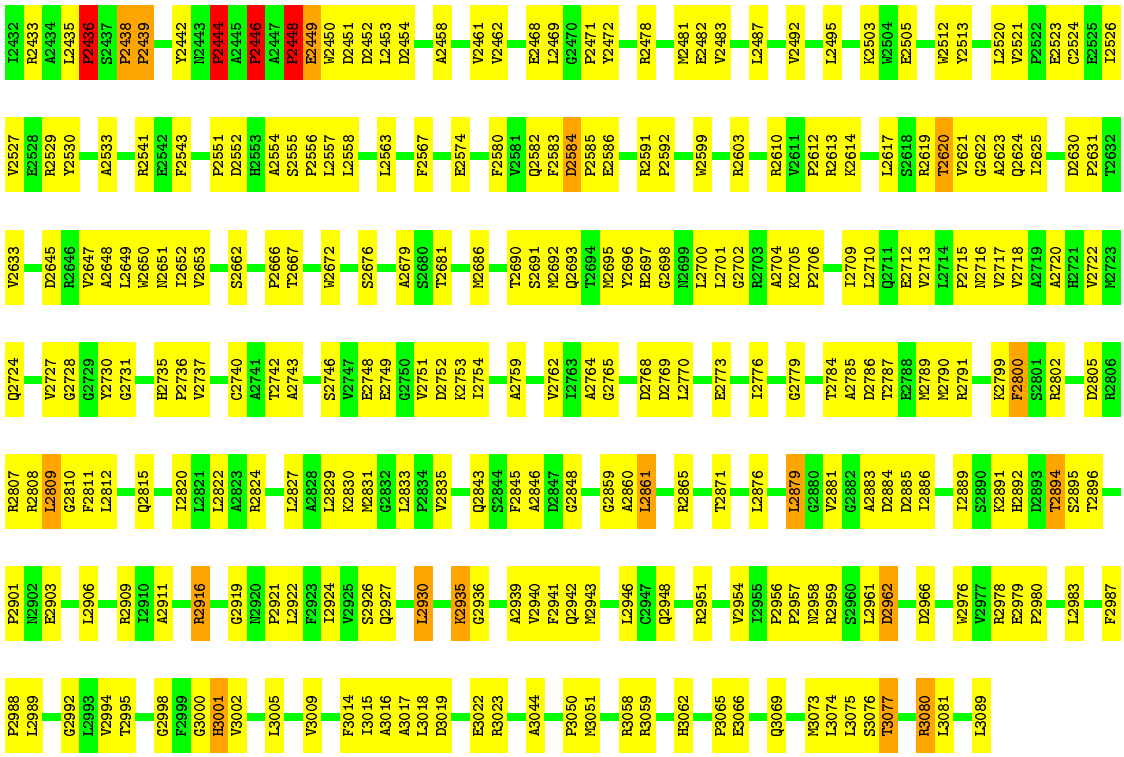
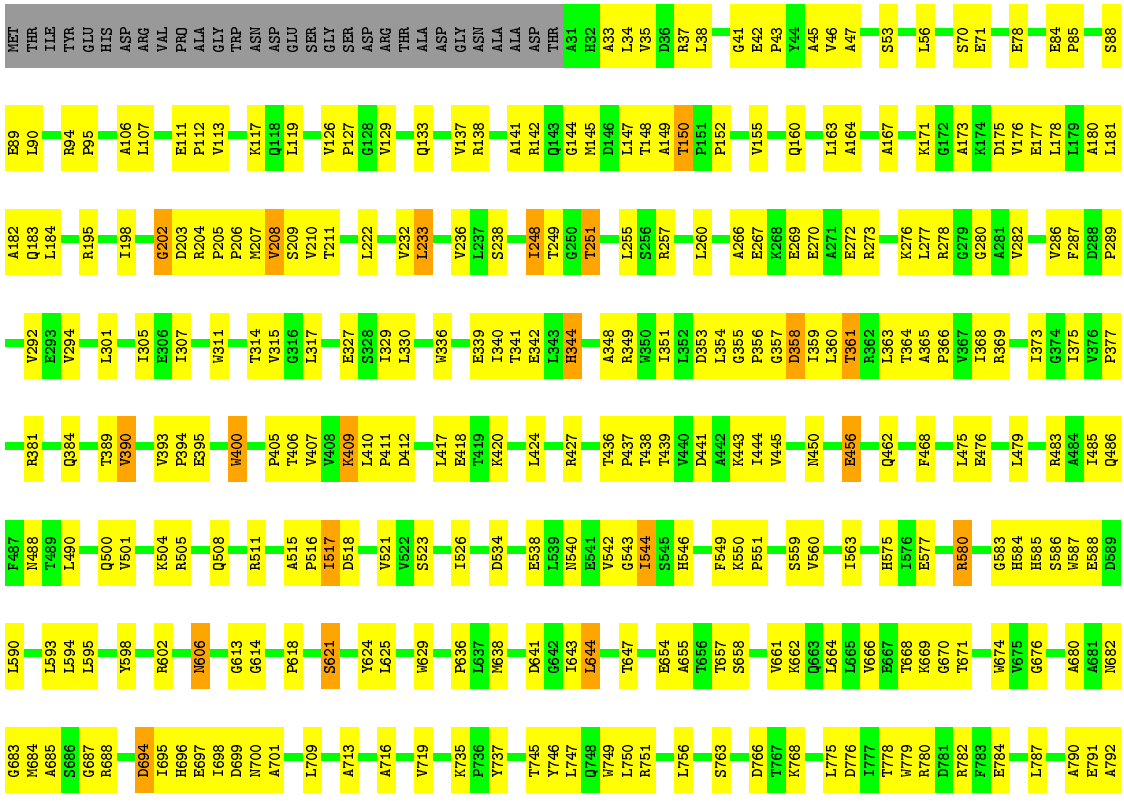
V1731 L1732 N1733 S1734 E1735 R1736 D1737 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA PRO ALA PRO VAL ALA ALA ALA PRO SER SER ALA PRO ALA PRO SER GLY GLY PRO ALA PRO ARG PRO ASP ASP ILE THR PHE ASP
ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU VAL ASP VAL ALA ALA ALA VAL ALA ALA ALA VAL ALA ALA ALA GLU ARG VAL THR LYS THR VAL ASN LEU GLY GLY ASN GLN LYS ARG PRO ALA TYR ILE THR GLU ARG PRO SER GLY ALA ALA ILE ASP GLY ALA ALA GLU ALA ASP
LEU GLY ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA VAL THR LYS THR TRP GLU LEU PRO ARG PRO GLY ALA LYS
HIS VAL THR VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY LEU HIS ALA GLY ALA LEU ALA SER ALA ALA ASP VAL ASP LYS VAL ILE ASP GLY ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ALA ALA ILE SER VAL SER LEU PRO SER ALA GLY
GLY ALA SER GLY GLY VAL VAL ASP S1983 L1986 F1989 K1992 P1996 L2000 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 P2020 V2032 T2047 A2053 W2054 V2055 F2056 D2057 D2058 R2059 W2060 L2067 L2070 E2074 Q2081 W2082 E2083 Q2084 L2085 S2086 Q2087 R2088 F2089 E2090 G2091
T2092 G2093 H2094 V2095 V2096 A2097 T2098 Q2099 A2100 N2101 W2102 W2103 Q2104 G2105 L2108 R2112 N2113 V2114 H2115 L2118 F2119 I2122 A2123 A2124 G2125 A2126 E2127 N2128 P2129 Y2134 E2137 V2140 V2141 T2163 V2164 I2165 A2166 T2167 R2170 D2173 D2174 R2175 L2176 K2180 R2188 F2189 T2192
L2193 W2194 V2195 V2196 P2197 A2198 D2205 L2209 V2210 E2211 W2212 V2213 G2214 T2215 E2216 K2229 P2234 T2235 L2236 L2237 F2238 R2244 V2245 A2246 V2252 R2255 K2261 W2265 Q2268 L2274 I2277 D2282 R2286 L2287 H2288 L2291 S2294 P2295 N2296 R2297 G2298 M2299 F2300
D2303 Y2306 K2310 R2319 S2331 L2332 A2333 H2334 W2339 Q2348 I2352 V2353 S2354 E2358 V2361 M2372 L2376 K2391 V2392 D2393 L2394 T2395 L2398 I2401 K2402 I2403 D2404 M2405 L2408 A2409 A2412 M2416 S2417 G2418 D2421 E2422 E2426 A2427 P2428 T2431



- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain E:



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W2194	G2093	GLY	HIS	LEU	ALA	V1731	R1634	N1536	V1445	V1327		F1123	V1008		L794
V2195	H2094	ALA	VAL	GLY	ALA	L1732		L1537		S1328	R1225	P1124	P1009	V904	H795
V2196	V2095	SER	THR	ALA	ASP	N1733	V1637	R1538	A1448	A1329	R1226	V1125	L1010		P796
P2197	V2096	GLY	VAL	LEU	ALA	S1734	P1638	G1539	I1449	R1330	D1227	I1126	S1011	F915	Q797
A2198	A2097	GLY	GLU	LYS	THR	E1735	A1639	S1540	A1450	I1331	V1228	E1127	G1012		D798
	T2098	VAL	PHE	GLY	VAL	R1736		Q1541				G1128	T1013	L924	F799
D2205	Q2099	VAL	ALA	GLN	ALA	D1737	T1651	Y1542	V1455	V1336	R1237	L1129	W1014		
	A2100	ASP	LEU	VAL	LEU		W1652	A1543	G1456	M1337				A928	E803
L2209	N2101	S1983	GLY	THR	ILE	L1741		I1544	E1457	A1338	N1247	L1132	I1017	E929	
V2210	W2102		THR	LYS	ALA		K1656		Y1458	A1339	P1248	V1133	R1018	P930	A808
E2211	W2103	L1986	ARG	LEU	LEU	D1745	P1657	L1551	T1459				F1019	V931	
W2212	Q2104		GLU	ALA	SER	THR	K1658	E1552	A1460	R1342	R1253	P1146	T1020	E932	D811
V2213	G2105	F1989	GLY	ARG	ALA	ASP	E1659	A1553	L1461	L1343		K1147	L1021	V933	
G2214			SER	THR	LYS	PRO	L1660	L1554	A1462	A1344	G1268	E1148		L934	L816
T2215	L2108	K1992	SER	TYR	MET	GLU	C1661	E1555	C1463	A1345	M1269	P1149	V1025	S935	E817
E2216			VAL	LYS	ARG	PRO	R1662	E1556	V1464	P1346	W1270	A1150		R936	
	R2112	P1996	ARG	PRO	ILE	GLU	K1663	E1557			L1271	E1151	E1034	R937	L826
L2228	N2113		GLY	PHE	ASP	PRO			V1467	Y1350			V1035	Q938	L827
K2229	V2114	L2000	GLY	GLY	GLN	GLU	I1666	R1560	Y1468	A1351	A1274	T1162	D1036	A939	
	H2115		ASP	PRO	ILE	ALA	E1667	R1561	E1469	F1352	A1275	D1163	D1037	R940	D832
P2234		Q2010	LEU	VAL	GLU	ASP	L1668	R1562	L1470	P1353	Q1276	T1164		R941	A833
T2235	L2118	L2011	GLY	LEU	ALA	GLU		Q1563	E1471		H1277		V1045		E834
L2236	F2119	G2012	GLY	SER	LEU	PRO	W1671	I1564		I1357	V1278	G1167	L1046	P954	T835
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F2238	I2122	S2014	HIS	ALA	SER	ALA	F1673	V1574			T1280		V1068	L957	V837
	A2123	D2015	ALA	ILE	ILE	ASP	A1674		R1480	M1362	A1281	P1171			
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V2245	G2125		ALA	ASP	SER	PRO	W1679	V1579	K1483	V1376	D1283	S1173		M962	G854
A2246	A2126	P2020	LEU	GLN	ILE	ALA		P1580	M1484		G1284	V1174	V1077	S963	K855
	E2127		ALA	LEU	THR	GLU	D1684	F1581	H1485	A1380	K1285			V964	P856
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S2250	P2129		ALA	THR	GLY	ALA	L1686	S1583	I1487	F1390	V1287	N1178		P966	N858
E2251		T2047	ALA	VAL	ALA	PRO	F1687		V1488		P1288	A1179	F1087	V967	F859
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		A2053	VAL	GLY	SER	ALA	E1690		R1490		A1290	L1184	A1089	I970	P861
R2255	E2137	V2054	ASP	PRO	ARG	ALA		V1590	D1491	A1405	K1291	L1185	P1090	A971	V862
		V2055	LYS	SER	ARG	ALA	G1694				L1292		L1091		
K2261	V2140	F2056	VAL	GLY	ASN	ALA	L1695	E1598	R1495	V1408		L1188	A1092	T974	R868
	V2141		ILE	LYS	GLN	PRO			S1496		W1295		P1093	E975	
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	T2163	W2060	GLY	PRO	LEU	PRO	F1700	K1605	L1500	P1413	K1304	F1192	L1095	Q977	S873
Q2268	V2164		ALA	ALA	VAL	VAL	V1701	D1606		D1414		A1193	T1096	V978	D874
	I2165	L2067	VAL	TYR	ASP	ALA	E1702	P1607	I1503	G1415	D1307	I1194	V1097	R979	S875
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	T2167	L2070	ALA	THR	GLY	PRO	G1704	I1611		L1417	V1309	G1196	P1099		W877
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	R2170	E2074	ALA	ARG	GLU	ALA	K1706	R1613	I1508	T1420	F1311			P990	H880
D2282			ALA	VAL	LEU	PRO		Y1614		Q1421	R1312	E1202	V1103	S991	
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R2286	D2174	W2082	ARG	LYS	LEU	GLY	V1711	P1616		T1423	D1314	T1204	R1105		A886
L2287	R2175	E2083	GLY	THR	GLY	GLY	A1712	N1617	D1514	Q1424	R1315	D1205	C1106	L996	D887
H2288	L2176	Q2084	ILE	TRP	ALA	PRO	G1713	L1618		V1425	V1316	P1206		E997	
		L2085	SER	GLU	ILE	ARG	L1714	V1619	V1519		G1317	V1207	V1110	V998	I892
L2291	K2180	S2086	VAL	LEU	ASP	PRO		P1620		V1430	I1318		F1111		
		Q2087	SER	GLY	GLY	ASP	P1722	R1621	L1530	A1431	D1319	A1212		D1001	T895
S2294	R2188	R2088	LEU	PRO	ALA	ASP	E1723	P1622	E1531				A1117	Q1002	A896
P2295	F2189	F2089	PRO	GLY	ALA	ILE	Y1724	F1623	I1532	V1435	E1323	T1218	A1118	H1003	
N2296		E2090	SER	TRP	GLU	THR	S1725	T1624	V1533		V1324	D1219	T1119	V1004	A899
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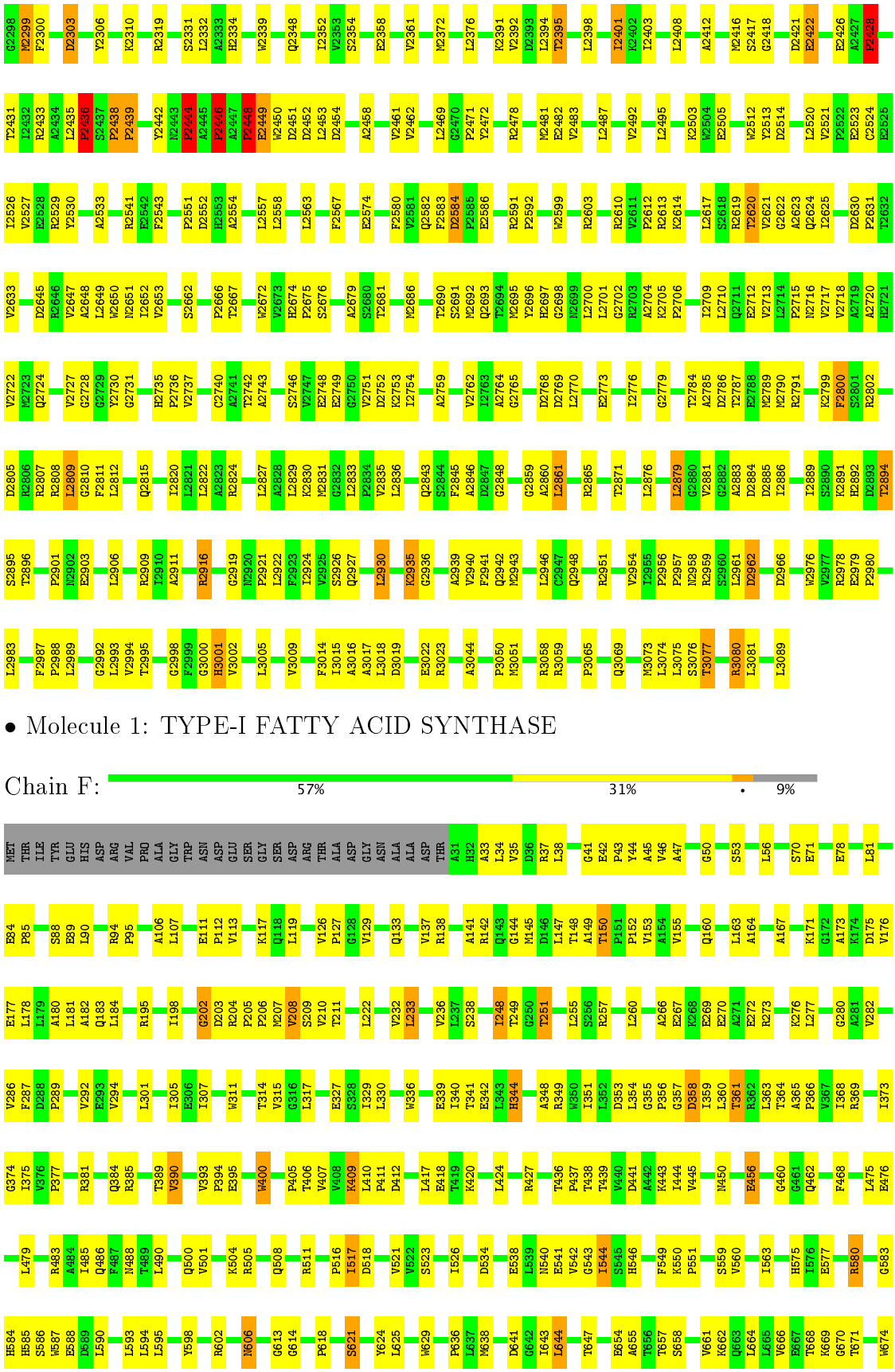
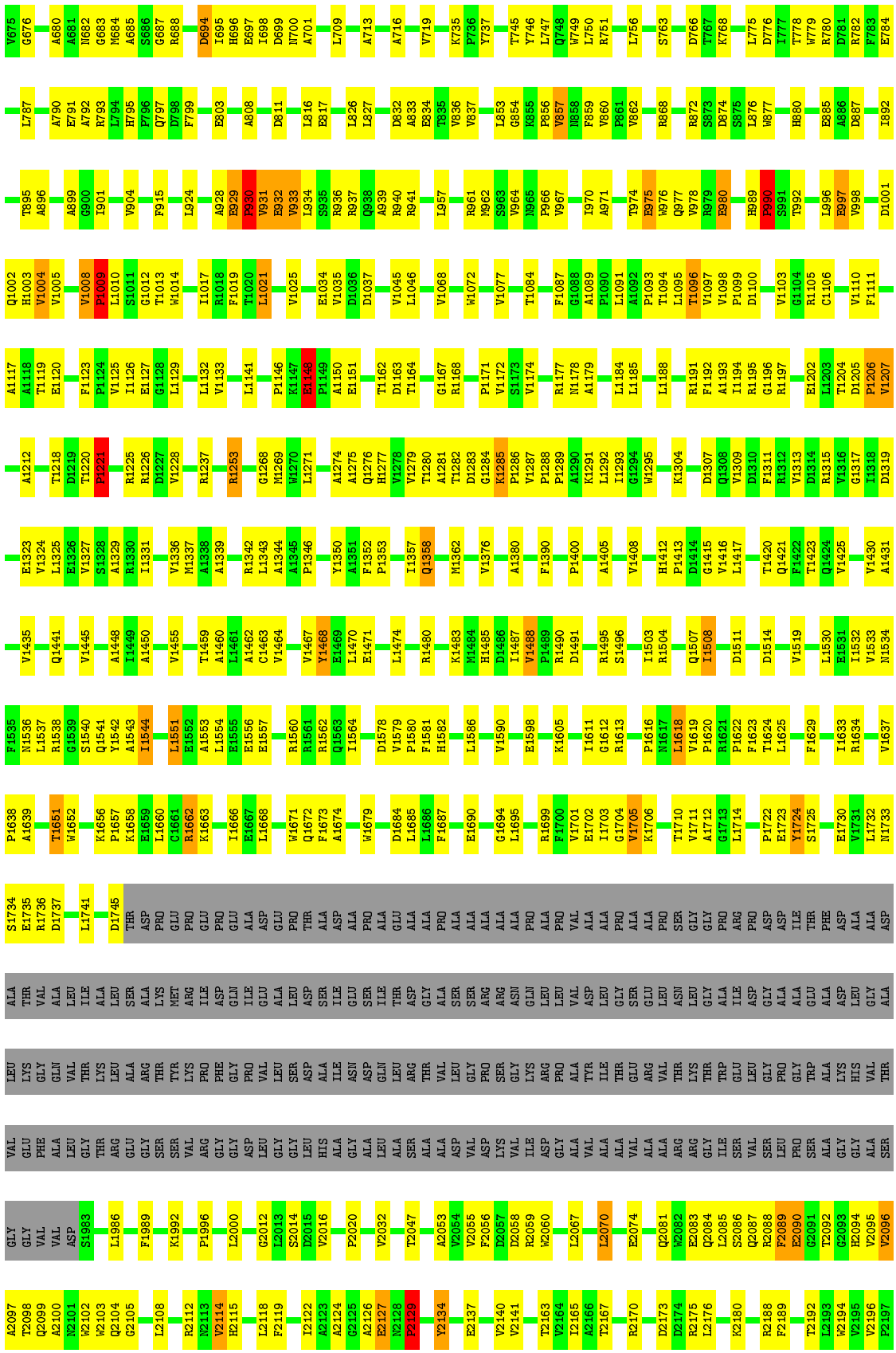


- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain F: 57% 31% • 9%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LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL ALA LYS HIS VAL THR
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A1212 T1218 D1219 T1220 P1221 R1225 R1226 D1227 V1228 R1237 R1253 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279 T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 I1293 G1294 W1295 K1304 D1307 Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319
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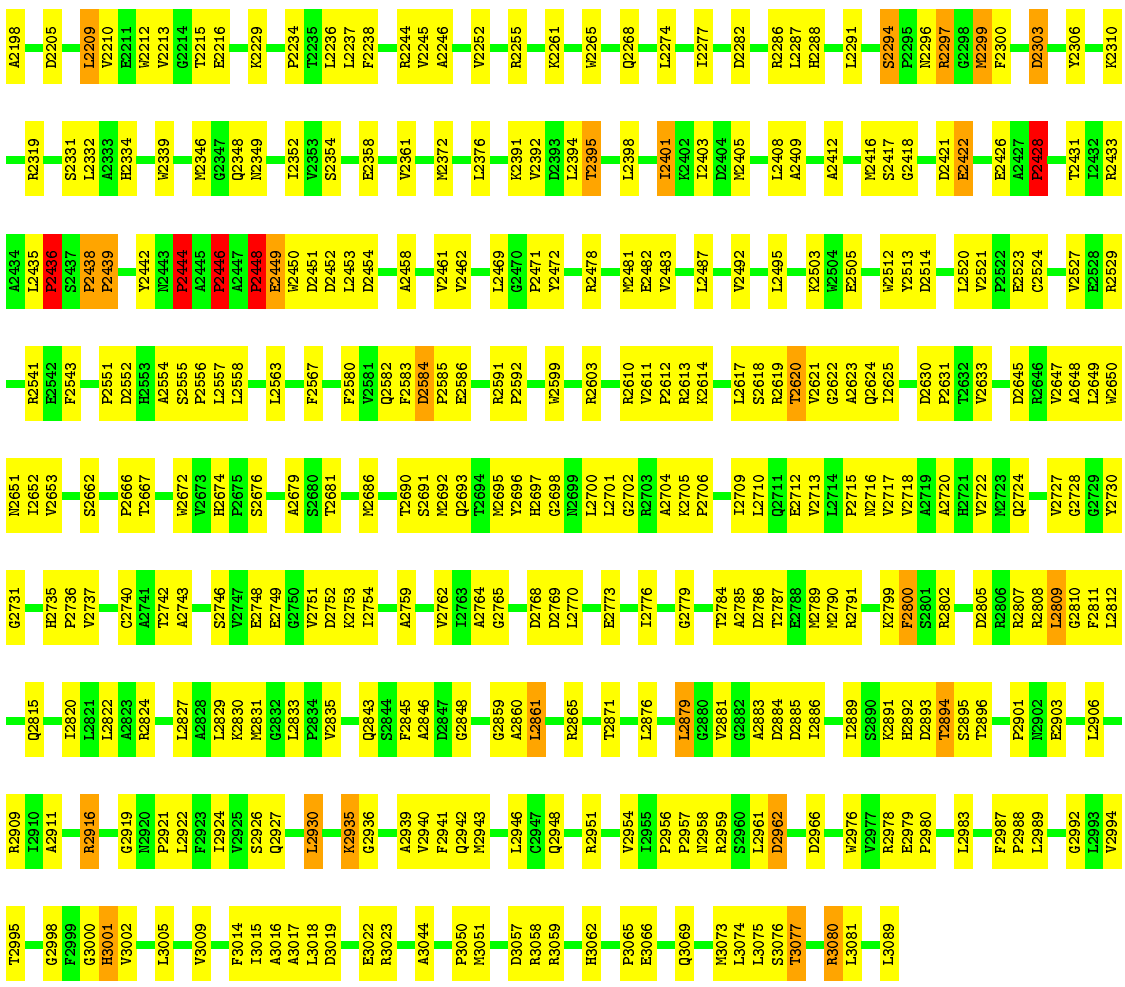
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4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4337	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	B	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	C	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	D	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	E	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	F	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
All	All	0.39	162/128010 (0.1%)	0.51	78/174222 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

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

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

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

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

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1148	GLU	Peptide
1	A	150	THR	Peptide
1	A	202	GLY	Peptide
1	A	2584	ASP	Peptide
1	A	357	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20945	0	20595	881	0
1	B	20945	0	20595	872	0
1	C	20945	0	20595	872	0
1	D	20945	0	20595	873	0
1	E	20945	0	20595	878	0
1	F	20945	0	20595	878	0
2	A	31	0	19	4	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	4	0
2	E	31	0	19	4	0
2	F	31	0	19	5	0
All	All	125856	0	123684	4910	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

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

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	28	71
1	B	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	25	68
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	25	68
1	D	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	25	68
1	E	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	28	71
1	F	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	25	68
All	All	16908/18534 (91%)	15849 (94%)	947 (6%)	112 (1%)	30	68

5 of 112 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2094/2402 (87%)	1992 (95%)	102 (5%)	29	61
1	B	2097/2402 (87%)	1994 (95%)	103 (5%)	29	61
1	C	2094/2402 (87%)	1992 (95%)	102 (5%)	29	61
1	D	2093/2402 (87%)	1991 (95%)	102 (5%)	29	61
1	E	2095/2402 (87%)	1993 (95%)	102 (5%)	29	61
1	F	2094/2402 (87%)	1992 (95%)	102 (5%)	29	61
All	All	12567/14412 (87%)	11954 (95%)	613 (5%)	33	61

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

Mol	Chain	Res	Type
1	C	2395	THR
1	D	1009	PRO
1	F	1651	THR
1	C	2448	PRO
1	D	233	LEU

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

Mol	Chain	Res	Type
1	C	2349	ASN
1	D	1277	HIS
1	F	1617	ASN
1	C	2815	GLN
1	D	486	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMN	A	4000	-	31,33,33	1.33	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	B	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	C	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.51	6 (15%)
2	FMN	D	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.51	6 (15%)
2	FMN	E	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	F	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.48	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	B	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	C	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	D	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	E	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	F	4000	-	-	0/16/18/18	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4000	FMN	C5A-N5	2.27	1.38	1.35
2	A	4000	FMN	C5A-N5	2.29	1.38	1.35
2	B	4000	FMN	C5A-N5	2.29	1.38	1.35
2	F	4000	FMN	C5A-N5	2.32	1.38	1.35
2	C	4000	FMN	C5A-N5	2.36	1.38	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4000	FMN	C4A-C4-N3	-2.59	119.79	123.48
2	E	4000	FMN	C4A-C4-N3	-2.59	119.80	123.48
2	F	4000	FMN	C4A-C4-N3	-2.58	119.81	123.48
2	C	4000	FMN	C4A-C4-N3	-2.58	119.81	123.48
2	D	4000	FMN	C4A-C4-N3	-2.58	119.81	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

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