wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:28 PM BST

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

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

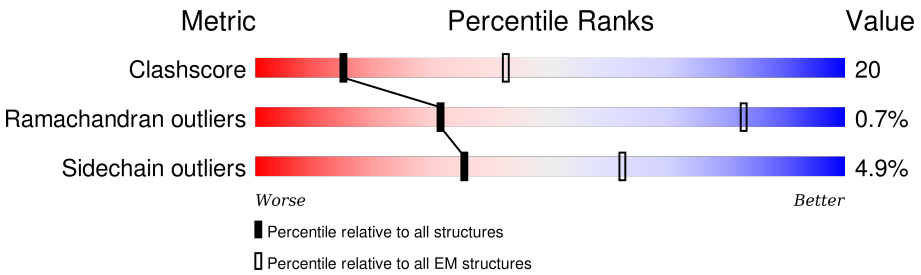
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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)

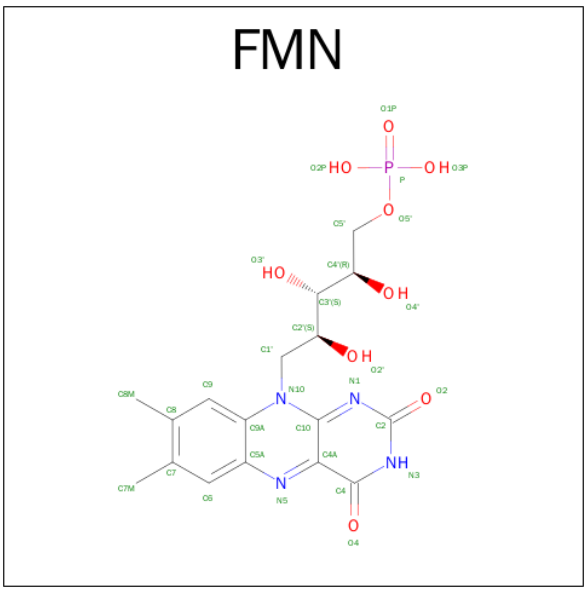
There are 2 unique types of molecules in this entry. The entry contains 125856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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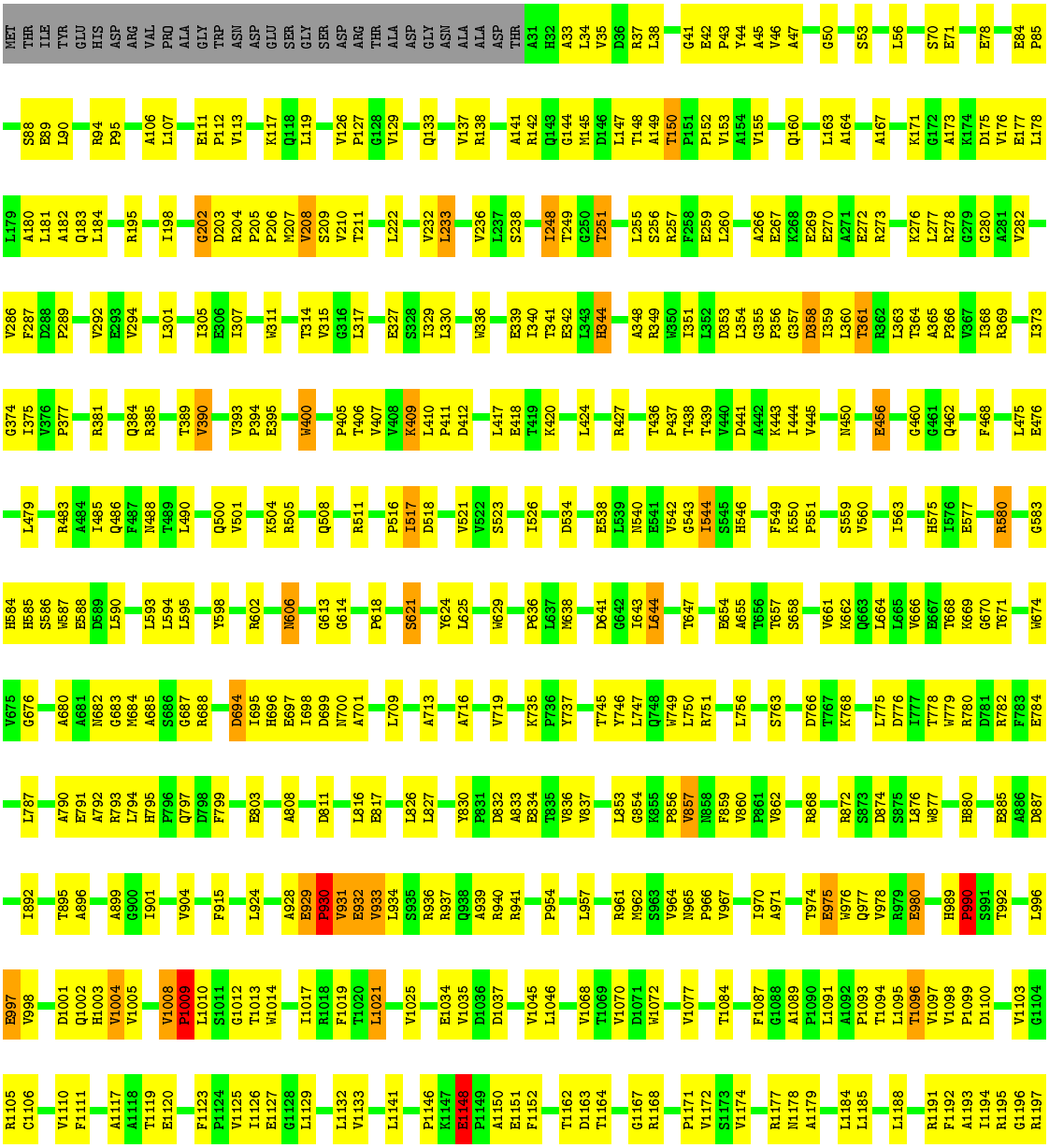
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	C	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	D	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	E	1	31	17	4	9	1	0
			Total	C	N	O	P	
2	F	1	31	17	4	9	1	0

3 Residue-property plots (i)

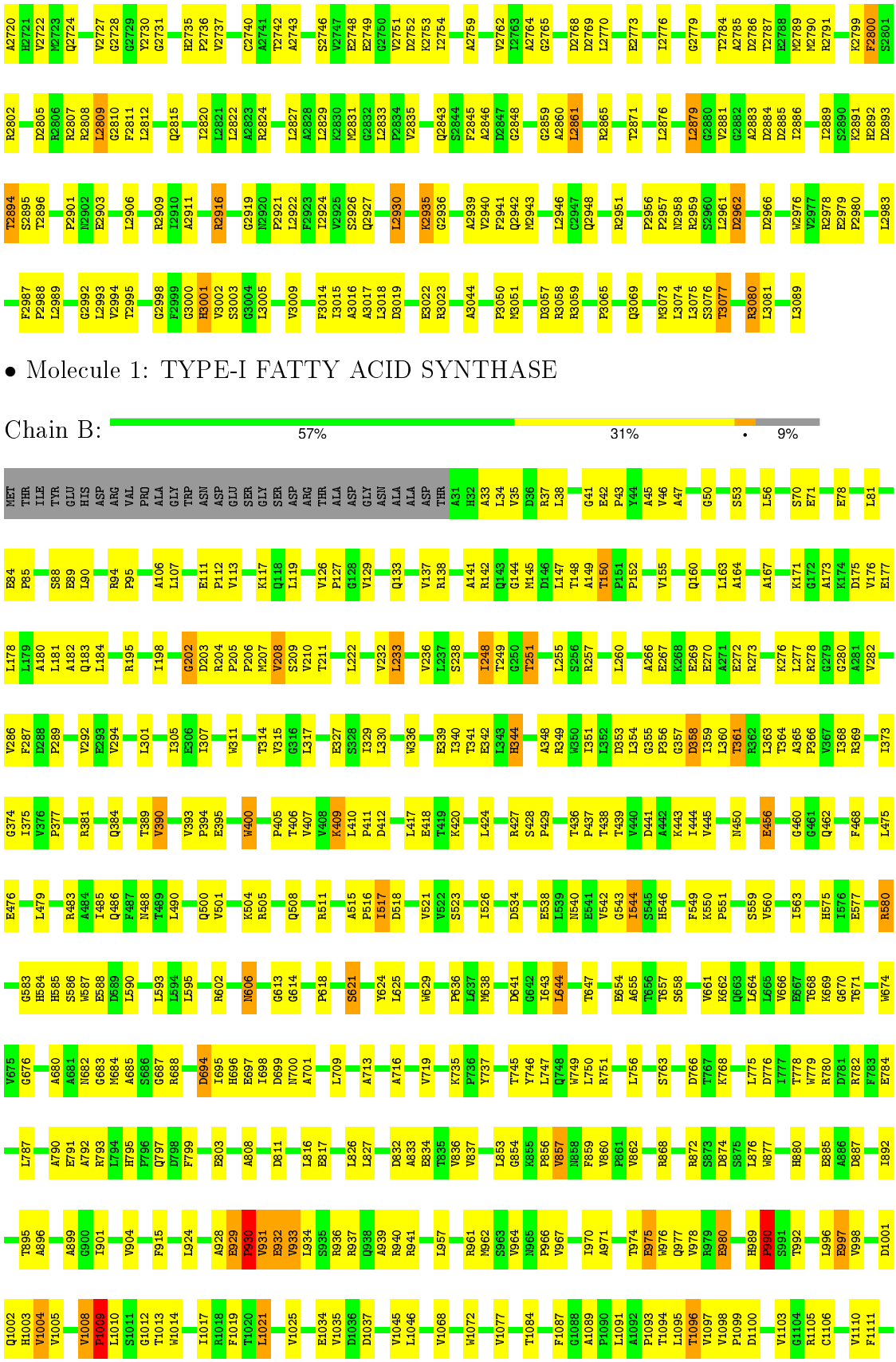
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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%



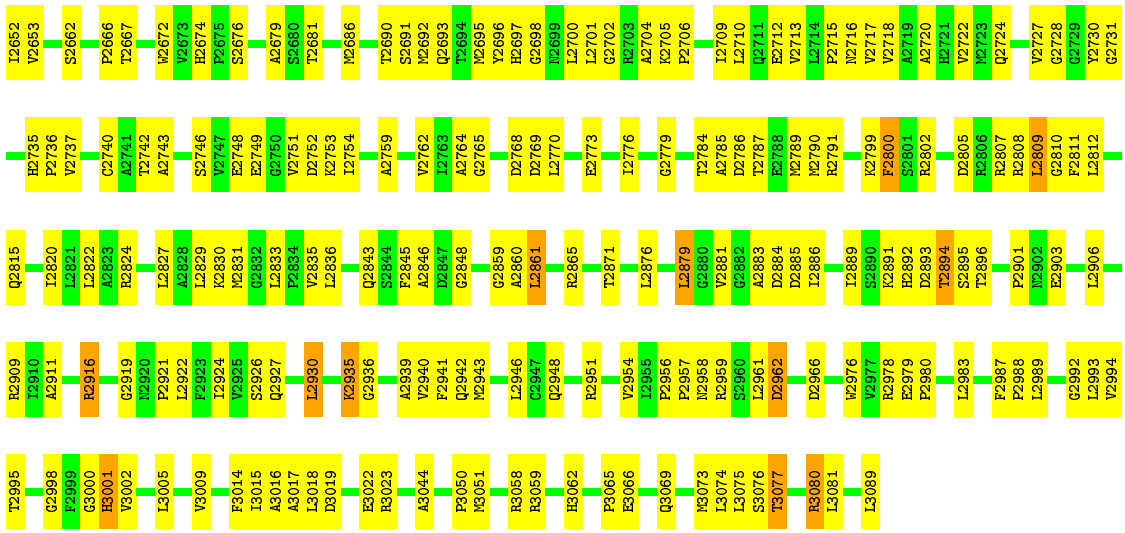
	P2522	E2422	G2298	F2189	F2089	LEU	PRO	ALA	ASP	E1723	R1621	D1511		V1313	
D2630	E2523		M2299		E2090	PRO	GLY	ALA	ILE	Y1724	P1622		T1420	D1314	E1202
P2631	C2524	E2426	F2300	T2192	G2091	SER	TRP	GLU	THR	S1725	F1623	D1514	Q1421	R1315	L1203
T2632		A2427		L2193	T2092	ALA	ALA	ALA	PHE		T1624		F1422	V1316	T1204
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
S2662	D2552	Y2442		V2213	G2105		GLU	ALA	SER	THR	P1657	S1540		I1331	R1226
	H2553	N2443	W2339	G2214		F1989	GLY	ARG	ALA	ASP	K1658	Q1541	A1448		D1227
P2666	A2554	P2444		T2215	L2108		SER	THR	LYS	PRO	E1659	Y1542	I1449	V1336	V1228
T2667	S2555	A2445	M2346	E2216		K1992	SER	TYR	MET	GLU	L1660	A1543	A1450	M1337	
	P2556	P2446	G2347		R2112		VAL	LYS	ARG	PRO	C1661	I1544		A1338	R1237
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
A2679		D2451	V2353	T2235	L2118	G2012	LEU	VAL	GLU	ASP	E1667	L1554	L1461	A1344	M1269
S2680	F2567	D2452	S2354	L2236	F2119	L2013	GLY	LEU	ALA	GLU	L1668	E1555	A1462	A1345	W1270
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		
M2686					A2123	V2016	HIS	ALA	SER	ALA	Q1672			Y1350	A1274
	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
N2699		R2478	T2395	W2265		F2056	ASP	PRO	ARG	ALA	E1690	H1582	K1483	V1376	K1285
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
R2703			I2401	L2274	T2163	W2060	ASP	ARG	LEU	ALA			I1487	F1390	P1289
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		
L2714	T2620			L2291	R2175	E2083	ARG	LYS	LEU	GLY	V1711		R1504	H1412	D1307
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
A2719	I2625	V2521	D2421	R2297	R2188	R2088	SER	GLY	GLY	ASP	P1722	P1620		L1417	R1312



- Molecule 1: TYPE-I FATTY ACID SYNTHASE

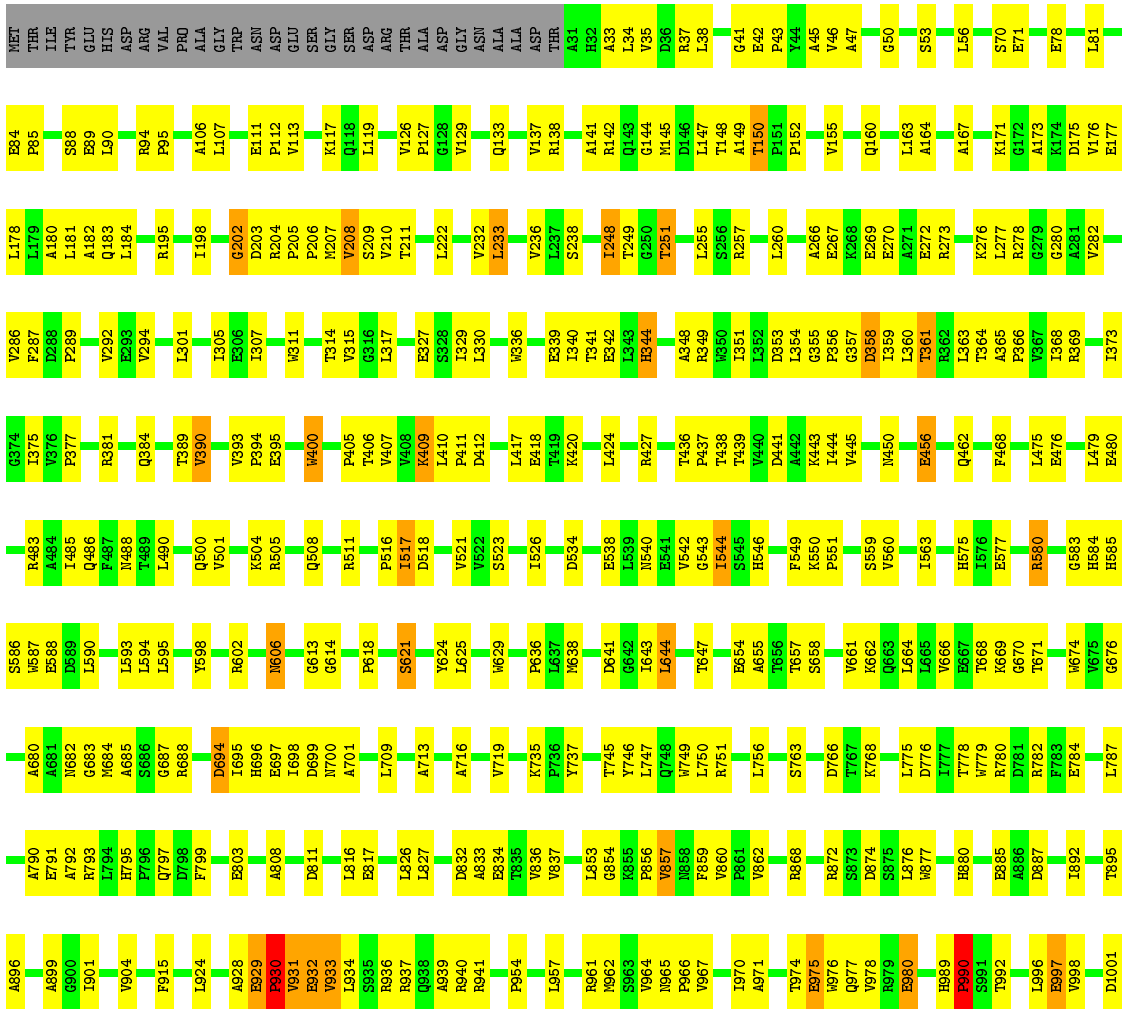
Chain B: 57% 31% • 9%

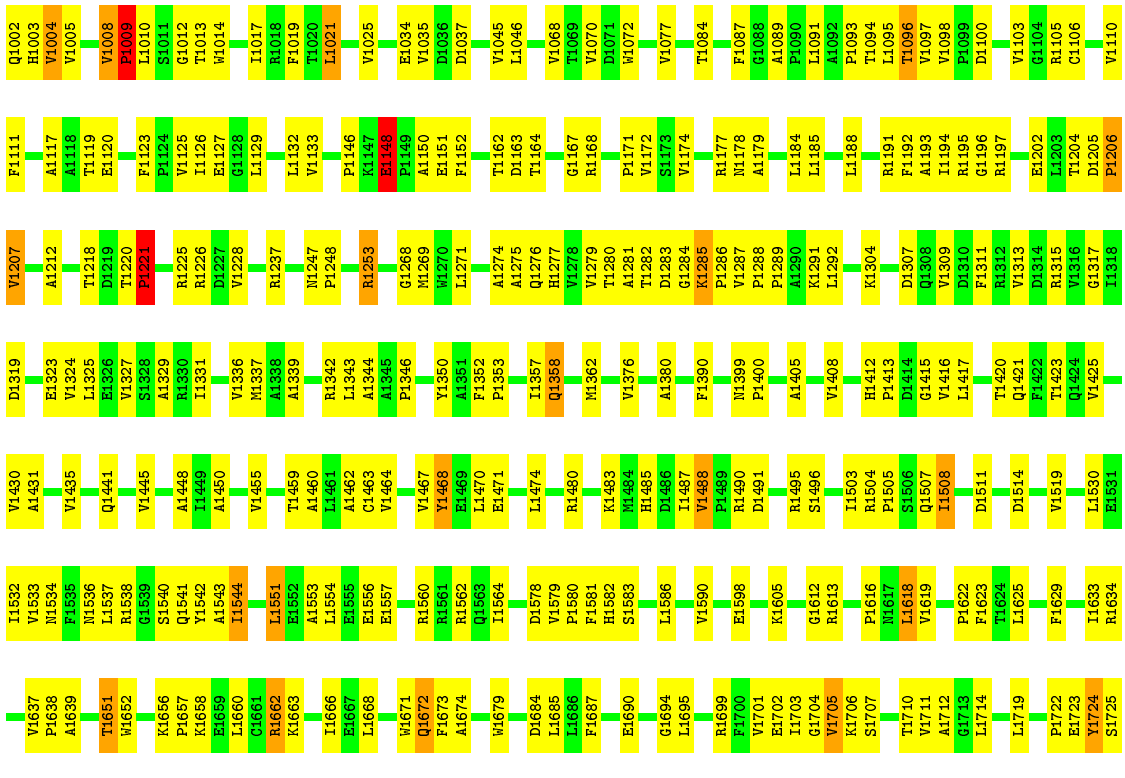
R2529	A2434		A2198	A2097	GLY	VAL	LEU	ALA	S1734		N1536	V1435	L1325			A1117
Y2530	L2435	R2319		T2098	GLY	GLU	LYS	THR	E1735	T1651	L1537		E1326	T1218		A1118
	P2436		D2205	Q2099	VAL	PHE	GLY	VAL	R1736	W1652	R1538	Q1441	V1327	D1219		T1119
A2533	S2437	S2331		A2100	VAL	ALA	GLN	ALA	D1737		G1539		S1328	T1220		E1120
	P2438	L2332	L2209	N2101	ASP	LEU	VAL	LEU		K1656	S1540	V1445	A1329	P1221		
R2541	P2439	A2333	V2210	W2102	S1983	GLY	THR	ILE	L1741	P1657	Q1541		R1330			F1123
E2542		H2334	E2211	W2103		THR	LYS	ALA		K1658	Y1542	A1448	I1331	R1225		P1124
F2543	Y2442		W2212	Q2104	L1986	ARG	LEU	LEU	D1745	E1659	A1543	I1449		R1226		V1125
	N2443	W2339	V2213	G2105		GLU	ALA	SER	THR	L1660	I1544	A1450	V1336	D1227		I1126
P2551	P2444		G2214		F1989	GLY	ARG	ALA	ASP	C1661			M1337	V1228		E1127
D2552	A2445	M2346	T2215	L2108		SER	THR	LYS	PRO	R1662	L1551	V1455	A1338			G1128
H2553	P2446	G2347	E2216		K1992	SER	TYR	MET	GLU	K1663	E1552		A1339	R1237		L1129
A2554	A2447	Q2348		R2112		VAL	LYS	ARG	PRO		A1553	T1459				
	P2448	N2349	K2229	N2113	P1996	ARG	PRO	ILE	GLU	I1666	L1554	A1460	R1342	R1253		L1132
L2557	E2449			V2114		GLY	PHE	ASP	PRO	E1667	E1555	L1461	L1343			V1133
L2558	W2450	I2352	P2234	H2115	L2000	GLY	GLY	GLN	GLU	L1668	E1556	A1462	A1344	G1268		
	D2451	V2353	T2235			ASP	PRO	ILE	ALA		E1557	C1463	A1345	M1269		P1146
F2580	D2452	S2354	L2236	L2118	G2012	LEU	VAL	GLU	ASP	W1671		V1464	P1346	W1270		K1147
V2581	L2453		L2237	F2119	L2013	GLY	LEU	ALA	GLU	Q1672	R1560			L1271		E1148
Q2582	D2454	E2358	F2238		S2014	GLY	SER	LEU	PRO	F1673	R1561	V1467	Y1350			P1149
F2583				I2122	D2015	LEU	ASP	ASP	THR	A1674	R1562	Y1468	A1351	A1274		A1150
D2584	A2458	V2361	R2244	A2123	V2016	HIS	ALA	SER	ALA		Q1563	E1469	F1352	A1275		E1151
P2585			V2245	A2124		ALA	ILE	ILE	ASP	W1679	I1564	L1470	P1353	Q1276		
E2586	V2461	M2372	A2246	G2125	P2020	GLY	ASN	GLU	ALA			E1471		H1277		T1162
	V2462			A2126		ALA	ASP	SER	PRO	D1684	D1578		I1357	V1278		D1163
R2591		L2376	V2252	E2127	V2032	LEU	GLN	ILE	ALA	L1685	V1579	L1474	Q1358	V1279		T1164
P2592	E2468			N2128		ALA	LEU	THR	GLU	L1686	P1580			T1280		
	L2469	K2391	R2255	P2129	T2047	SER	ARG	ASP	ALA	F1687	F1581	R1480	M1362	A1281		G1167
W2599	G2470	V2392				ALA	THR	GLY	ALA		H1582			T1282		R1168
	P2471	D2393	K2261	Y2134	A2053	ALA	VAL	ALA	PRO	E1690	S1583	K1483	V1376	D1283		
R2603	Y2472	L2394			V2054	ASP	LEU	SER	ALA			M1484		G1284		P1171
		T2395	W2265	E2137	V2055	VAL	GLY	SER	ALA	G1694	L1586	H1485	A1380	K1285		V1172
R2610	R2478				F2056	ASP	PRO	ARG	ALA	L1695		D1486		P1286		S1173
V2611		L2398	Q2268	V2140	D2057	LYS	SER	ARG	ALA		V1590	I1487	F1390	V1287		V1174
P2612	M2481			V2141	D2058	VAL	GLY	ASN	ALA	R1699		V1488		P1288		
R2613	E2482	I2401	L2274		R2059	ILE	LYS	GLN	PRO	F1700	E1598	P1489	N1399	P1289		R1177
K2614	V2483	K2402		T2163	W2060	ASP	ARG	LEU	ALA	V1701		R1490	P1400	A1290		N1178
		I2403	I2277	V2164		GLY	PRO	LEU	PRO	E1702	D1604	D1491	T1401	K1291		A1179
L2617	L2487	D2404		I2165	L2067	ALA	ALA	VAL	VAL	I1703	K1605			L1292		
S2618		M2405	D2282	A2166		VAL	TYR	ASP	ALA	G1704		R1495	A1405			L1184
R2619	V2492			T2167	L2070	ALA	ILE	LEU	ALA	V1705	I1611	S1496		W1295		L1185
T2620		L2408	R2286			ALA	THR	GLY	PRO	K1706	G1612		V1408			
V2621	L2495	A2409	L2287	R2170	E2074	VAL	GLU	SER	ALA		R1613	I1503		K1304		L1188
G2622			H2288			ALA	ARG	GLU	ALA	T1710		R1504	H1412			
A2623	K2503	A2412		D2173	Q2081	ALA	VAL	LEU	PRO	V1711	P1616		P1413	D1307		R1191
Q2624	W2504		L2291	D2174	W2082	ARG	THR	ASN	SER	A1712	N1617	Q1507	D1414	Q1308		F1192
I2625	E2505	M2416		R2175	E2083	ARG	LYS	LEU	GLY	G1713	L1618	I1508	G1415	V1309		A1193
		S2417	S2294	L2176	Q2084	GLY	THR	GLY	GLY	L1714	V1619		V1416	D1310		I1194
D2630	W2512	G2418	P2295		L2085	ILE	TRP	ALA	PRO		P1620	D1511	L1417	F1311		R1195
P2631	Y2513		N2296	K2180	S2086	SER	GLU	ILE	ARG	L1719	R1621			R1312		G1196
T2632		D2421	R2297		Q2087	VAL	LEU	ASP	PRO		P1622	D1514	T1420	V1313		R1197
V2633	L2520	E2422	G2298	R2188	R2088	SER	GLY	GLY	ASP	P1722	F1623		Q1421	D1314		
	V2521		M2299	F2189	F2089	LEU	PRO	ALA	ASP	E1723	T1624	V1519	F1422	R1315		E1202
D2645	P2522	E2426	F2300		E2090	PRO	GLY	ALA	ILE	Y1724	L1625		T1423	V1316		L1203
R2646	E2523	A2427		T2192	G2091	SER	TRP	GLU	THR	S1725		L1530	Q1424	G1317		T1204
V2647	C2524	P2428	D2303	L2193	T2092	ALA	ALA	ALA	PHE		R1634	E1531	V1425	I1318		D1205
A2648	E2525			W2194	G2093	GLY	LYS	ASP	ASP	E1730		I1532		D1319		P1206
L2649	I2526	T2431	Y2306	V2195	H2094	GLY	HIS	LEU	ALA	V1731	V1637	V1533	V1430			V1207
W2650	V2527	I2432		V2196	V2095	ALA	VAL	GLY	ALA	L1732	P1638	N1534	A1431	E1323		
N2651	E2528	R2433	K2310	P2197	V2096	SER	THR	ALA	ASP	N1733	A1639	F1535		V1324		A1212



- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain C:

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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 VAL ILE ASP GLY ALA ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER
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 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
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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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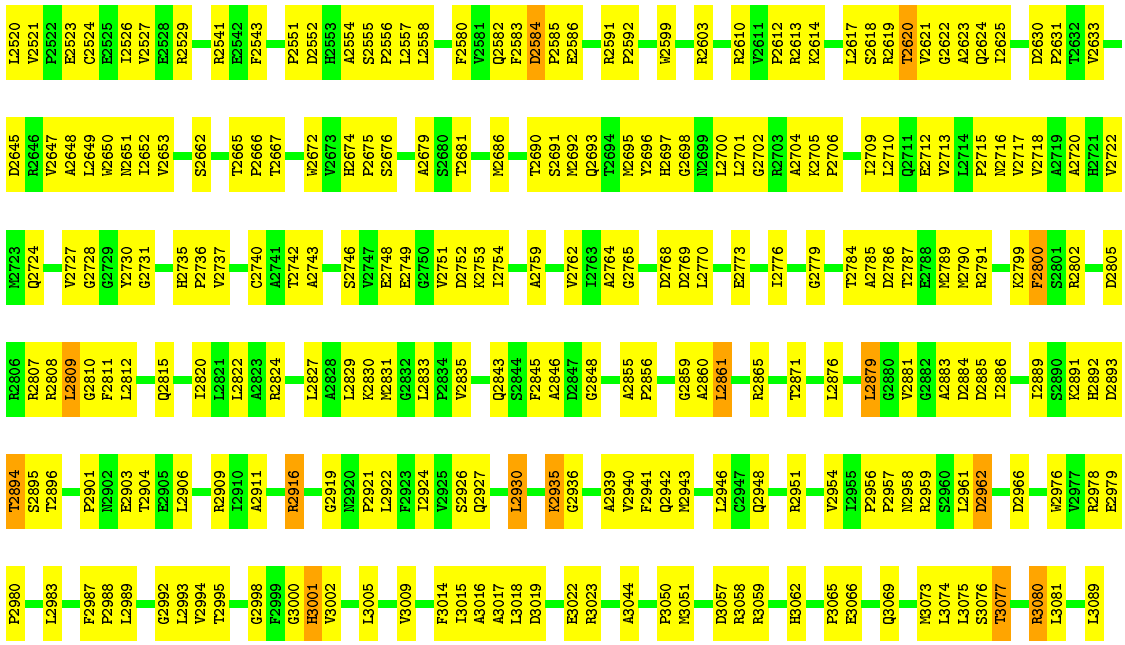
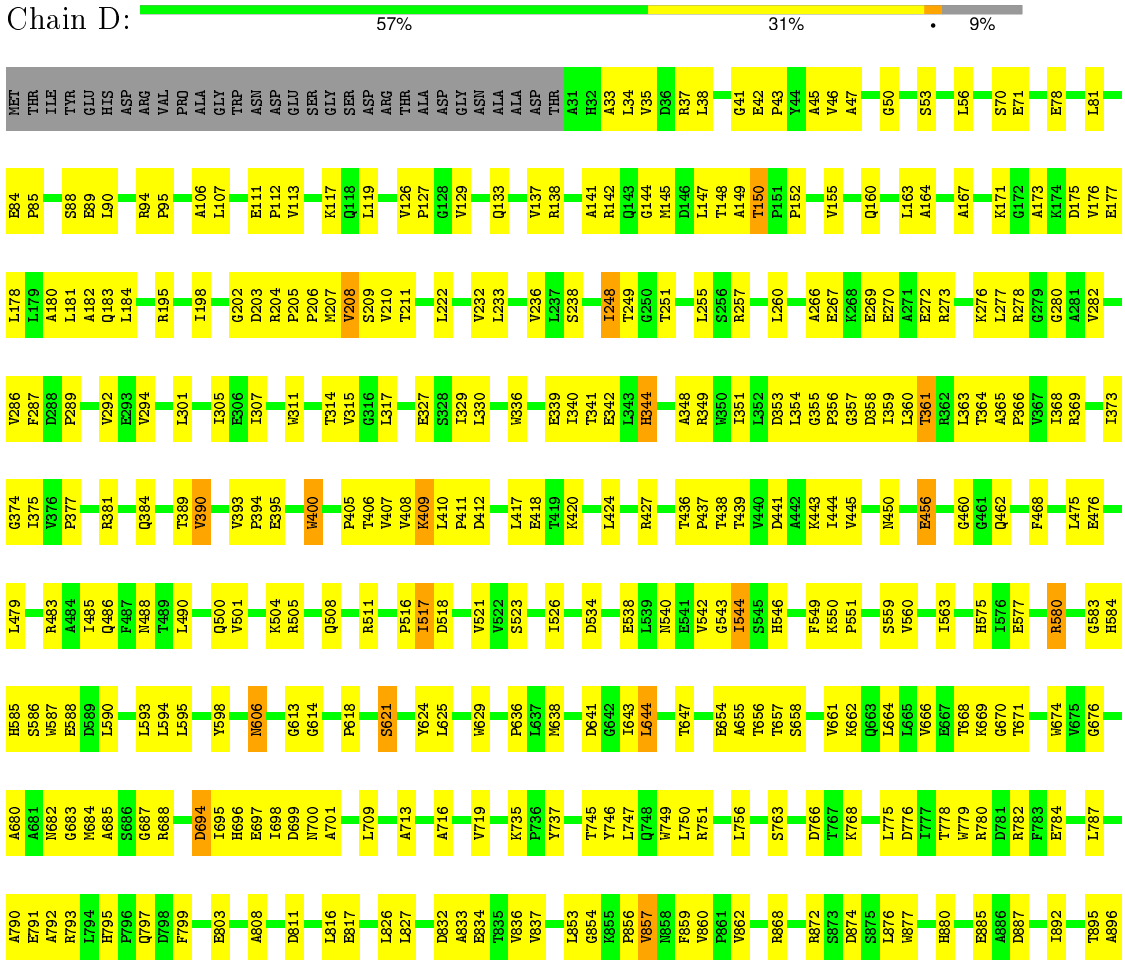
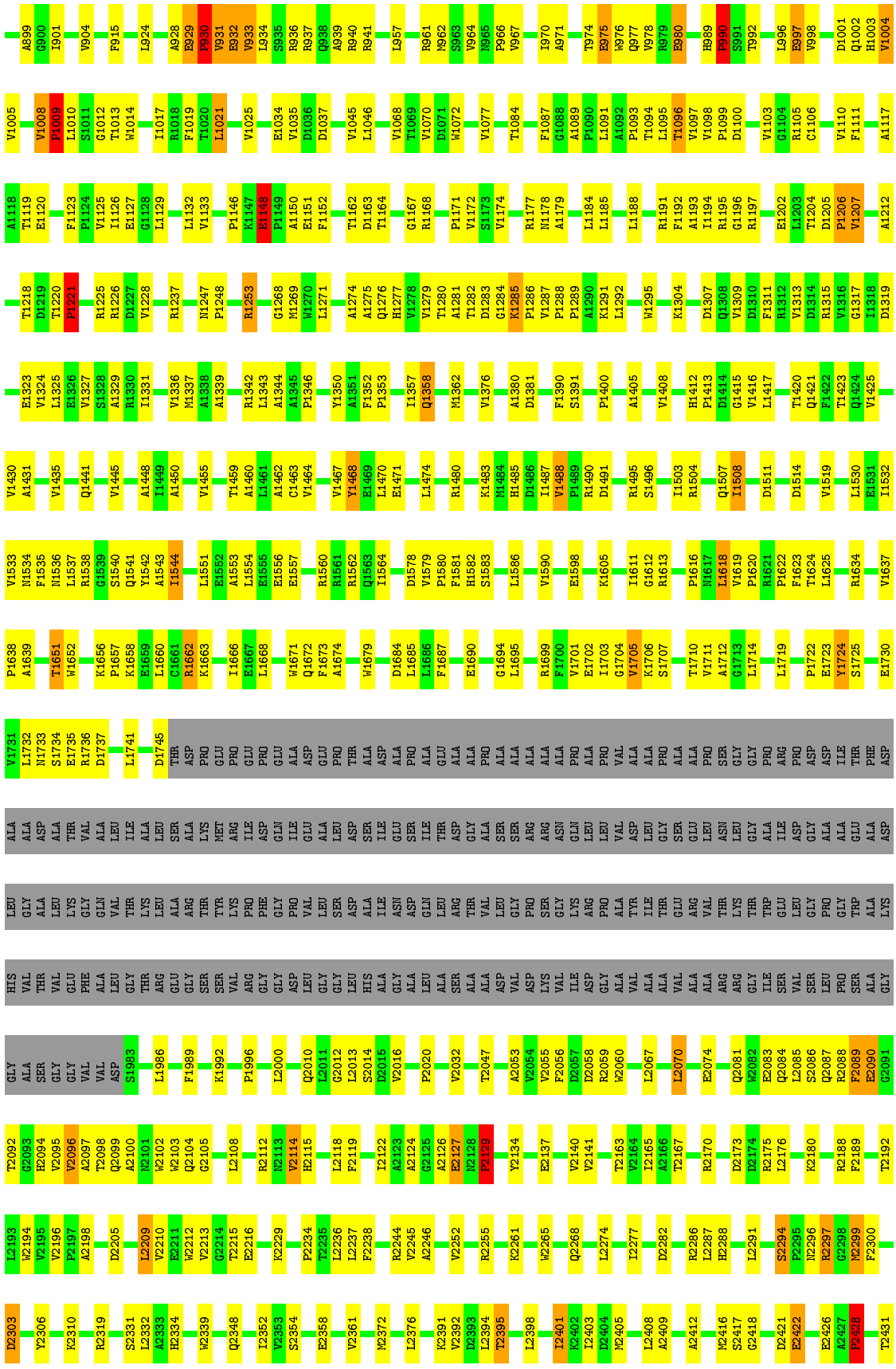


- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain D:

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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 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 Q2010 L2011 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
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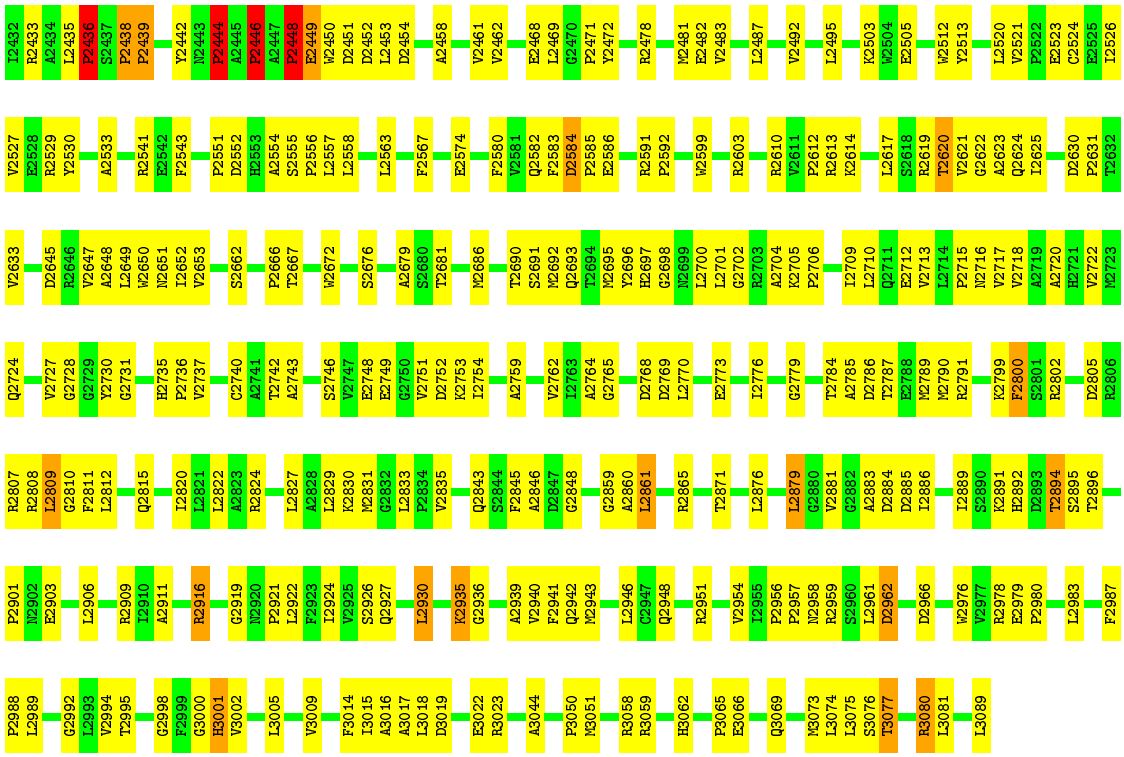
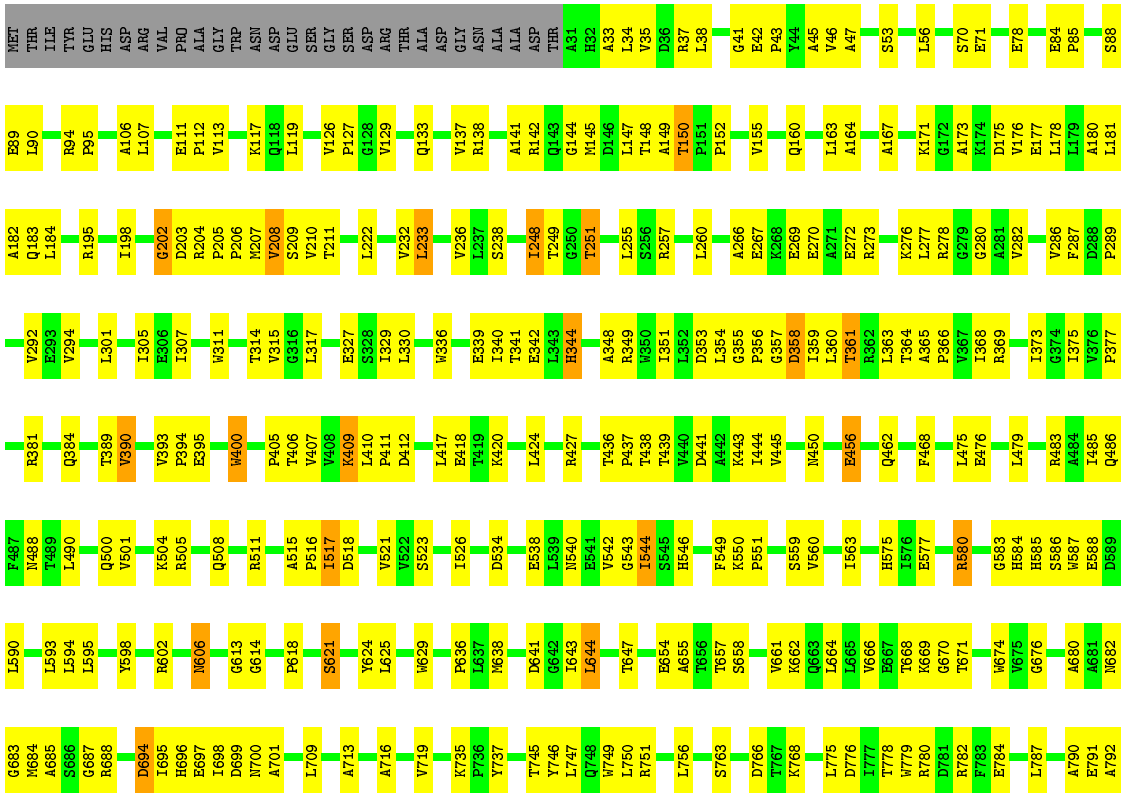


- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain E:



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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	
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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
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	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	
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P2234		Q2010	LEU	VAL	GLU	ASP	L1668	R1562	L1470	P1353	Q1276	T1164		R941	A833
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	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
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		V2055	LYS	SER	ARG	ALA	G1694				L1292		L1091		
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	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
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	R2170	E2074	ALA	ARG	GLU	ALA	K1706	R1613	I1508	T1420	F1311			P990	H880
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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
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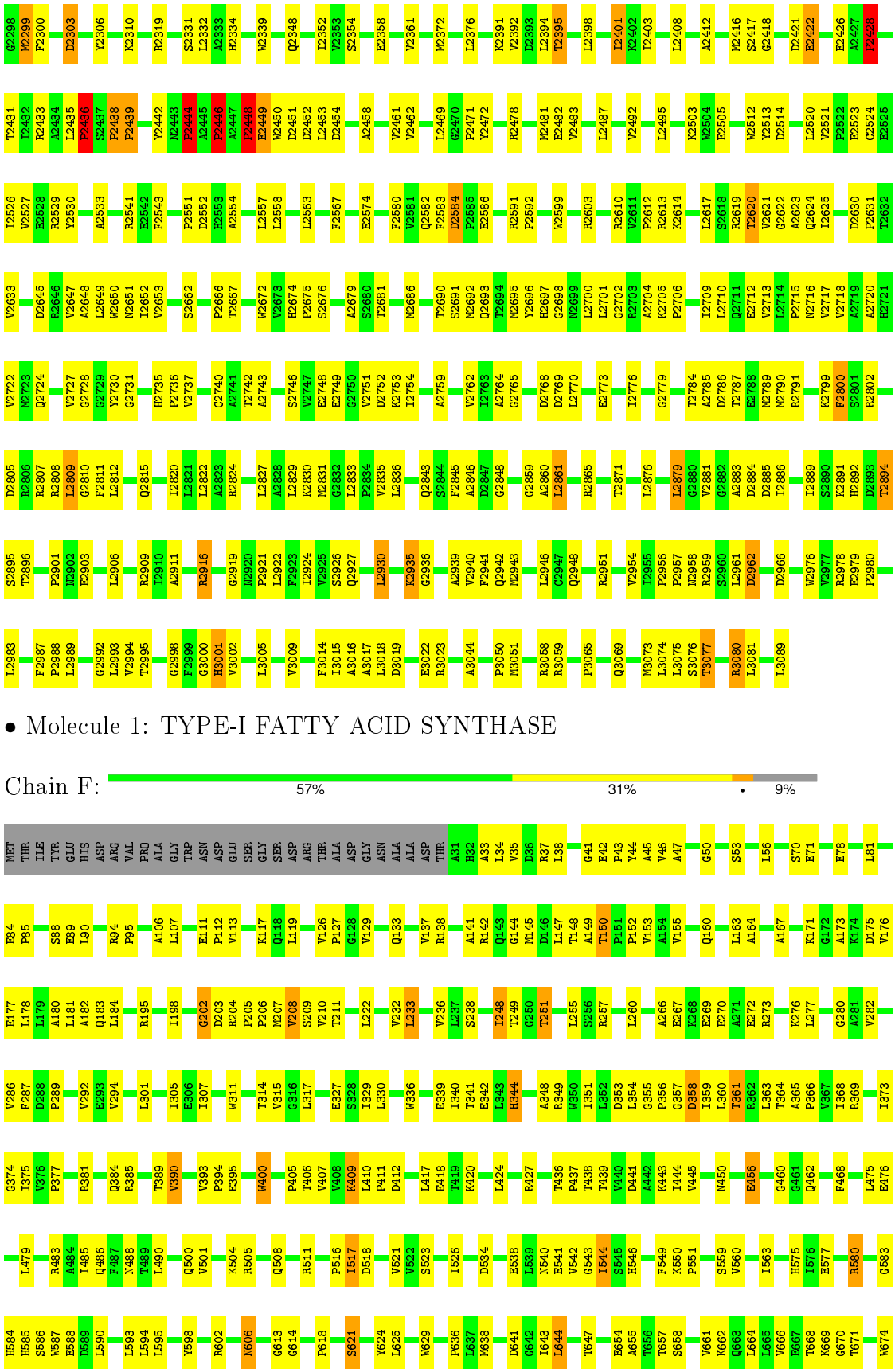
N2296		E2090	SER	TRP	GLU	THR	S1725	T1624	V1533		V1324	D1219	T1119	V1004	A899
R2297	T2192	G2091	ALA	ALA	ALA	PHE		L1625	N1534	Q1441	L1325	T1220	E1120	V1005	G900



- Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain F: 57% 31% • 9%

A2097	GLY	VAL	LEU	ALA	S1734	P1638	F1535				A1117	Q1002				V675
T2098	GLY	GLU	LYS	THR	E1735	A1639	N1536	V1435	E1323	A1212	A1118	H1003	T895	L787		G676
Q2099	VAL	PHE	GLY	VAL	R1736		L1537		V1324		T1119	V1004	A896			
A2100	VAL	ALA	GLN	ALA	D1737	T1651	R1538	Q1441	L1325	T1218	E1120	V1005		A790		A680
N2101	ASP	LEU	VAL	LEU		W1652	G1539		E1326	D1219			A899	E791		A681
W2102	S1983	GLY	THR	ILE	L1741		S1540	V1445	V1327	T1220	F1123	V1008	G900	A792		N682
W2103		THR	LYS	ALA		K1656	Q1541		S1328	P1221	P1124	P1009	I901	R793		G683
Q2104	L1986	ARG	LEU	LEU	D1745	P1657	Y1542	A1448	A1329		V1125	L1010		L794		M684
G2105		GLU	ALA	SER	THR	K1658	A1543	I1449	R1330	R1225	I1126	S1011	V904	H795		A685
	F1989	GLY	ARG	ALA	ASP	E1659	I1544	A1450	I1331	R1226	E1127	G1012		P796		S686
L2108		SER	THR	LYS	PRO	L1660				D1227	G1128	T1013	F915	Q797		G687
	K1992	SER	TYR	MET	GLU	C1661	L1551	V1455	V1336	V1228	L1129	W1014		D798		R688
R2112		VAL	LYS	ARG	PRO	R1662	E1552		M1337				L924	F799		
N2113	P1996	ARG	PRO	ILE	GLU	K1663	A1553	T1459	A1338	R1237	L1132	I1017				D694
V2114		GLY	PHE	ASP	PRO		L1554	A1460	A1339		V1133	R1018	A928	E803		I695
H2115	L2000	GLY	GLY	GLN	GLU	I1666	E1555	L1461		R1253		F1019	E929			H696
		ASP	PRO	ILE	ALA	E1667	E1556	A1462	R1342		L1141	T1020	P930	A808		E697
L2118	G2012	LEU	VAL	GLU	ASP	L1668	E1557	C1463	L1343	G1268		L1021	V931			I698
F2119	L2013	GLY	LEU	ALA	GLU			V1464	A1344	M1269	P1146		E932	D811		D699
	S2014	GLY	SER	LEU	PRO	W1671	R1560		A1345	W1270	K1147	V1025	V933			N700
I2122	D2015	LEU	ASP	ASP	THR	Q1672	R1561	V1467	P1346	L1271	E1148		L934	L816		A701
A2123	V2016	HIS	ALA	SER	ALA	F1673	R1562	Y1468			P1149	E1034	S935	E817		
A2124		ALA	ILE	ILE	ASP	A1674	Q1563	E1469	Y1350	A1274	A1150	V1035	R936			L709
G2125	P2020	GLY	ASN	GLU	ALA		I1564	L1470	A1351	A1275	E1151	D1036	R937	L826		
A2126		ALA	ASP	SER	PRO	W1679		E1471	F1352	Q1276		D1037	Q938	L827		A713
E2127	V2032	LEU	GLN	ILE	ALA		D1578		P1353	H1277	T1162		A939			
N2128		ALA	LEU	THR	GLU	D1684	V1579	L1474		V1278	D1163	V1045	R940	D832		A716
P2129	T2047	SER	ARG	ASP	ALA	L1685	P1580		I1357	V1279	T1164	L1046	R941	A833		
		ALA	THR	GLY	ALA	L1686	F1581	R1480	Q1358	T1280				E834		V719
Y2134	A2053	ALA	VAL	ALA	PRO	F1687	H1582			A1281	G1167	V1068	L957	T835		
	V2054	ASP	LEU	SER	ALA			K1483	M1362	T1282	R1168			V836		K735
E2137	V2055	VAL	GLY	SER	ALA	E1690	L1586	M1484		D1283		W1072	R961	V837		P736
	F2056	ASP	PRO	ARG	ALA			H1485	V1376	G1284	P1171		M962			Y737
V2140	D2057	LYS	SER	ARG	ALA	G1694	V1590	D1486		K1285	V1172	V1077	S963	L853		
V2141	D2058	VAL	GLY	ASN	ALA	L1695		I1487	A1380	P1286	S1173		V964	G854		T745
	R2059	ILE	LYS	GLN	PRO		E1598	V1488		V1287	V1174	T1084	N965	K855		Y746
T2163	W2060	ASP	ARG	LEU	ALA	R1699		P1489	F1390	P1288			P966	P856		L747
V2164		GLY	PRO	LEU	PRO	F1700	K1605	R1490		P1289	R1177	F1087	V967	V857		Q748
I2165	L2067	ALA	ALA	VAL	VAL	V1701		D1491	P1400	A1290	N1178	G1088		N858		W749
A2166		VAL	TYR	ASP	ALA	E1702	I1611			K1291	A1179	A1089	I970	F859		L750
T2167	L2070	ALA	ILE	LEU	ALA	I1703	G1612	R1495	A1405	L1292		P1090	A971	V860		R751
		ALA	THR	GLY	PRO	G1704	R1613	S1496		I1293	L1184	L1091		P861		
R2170	E2074	VAL	GLU	SER	ALA	V1705			V1408	G1294	L1185	A1092	T974	V862		L756
		ALA	ARG	GLU	ALA	K1706	P1616	I1503		W1295		P1093	E975			
D2173	Q2081	ALA	VAL	LEU	PRO		N1617	R1504	H1412		L1188	T1094	W976	R868		S763
D2174	W2082	ARG	THR	ASN	SER	T1710	L1618		P1413	K1304		L1095	Q977			
R2175	E2083	ARG	LYS	LEU	GLY	V1711	V1619	Q1507	D1414		R1191	T1096	V978	R872		D766
L2176	Q2084	GLY	THR	GLY	GLY	A1712	P1620	I1508	G1415	D1307	F1192	V1097	R979	S873		T767
	L2085	ILE	TRP	ALA	PRO	G1713	R1621		V1416	Q1308	A1193	V1098	E980	D874		K768
K2180	S2086	SER	GLU	ILE	ARG	L1714	P1622	D1511	L1417	V1309	I1194	P1099		S875		
	Q2087	VAL	LEU	ASP	PRO		F1623			D1310	R1195	D1100	H989	L876		L775
R2188	R2088	SER	GLY	GLY	ASP	P1722	T1624	D1514	T1420	F1311	G1196		P990	W877		D776
F2189	F2089	LEU	PRO	ALA	ASP	E1723	L1625		Q1421	R1312	R1197	V1103	S991			I777
	E2090	PRO	GLY	ALA	ILE	Y1724		V1519	F1422	V1313		G1104	T992	H880		T778
T2192	G2091	SER	TRP	GLU	THR	S1725	F1629		T1423	D1314	E1202	R1105				W779
L2193	T2092	ALA	ALA	ALA	PHE			L1530	Q1424	R1315	L1203	C1106	L996	E885		R780
W2194	G2093	GLY	LYS	ASP	ASP	E1730	I1633	E1531	V1425	V1316	T1204		E997	A886		D781
V2195	H2094	GLY	HIS	LEU	ALA	V1731	R1634	I1532		G1317	D1205	V1110	V998	D887		R782
V2196	V2095	ALA	VAL	GLY	ALA	L1732		V1533	V1430	I1318	P1206	F1111				F783
P2197	V2096	SER	THR	ALA	ASP	N1733	V1637	N1534	A1431	D1319	V1207		D1001	I892		E784

T2995	R2909		G2731	N2651		A2434		A2198
	I2910	Q2815		I2652	R2541	L2435	R2319	
G2998	A2911		H2735	V2653	E2542	P2436		D2205
F2999		I2820	P2736		F2543	S2437	S2331	
G3000	R2916	L2821	V2737	S2662		P2438	L2332	L2209
H3001		L2822			P2551	P2439	A2333	V2210
V3002	G2919	A2823	C2740	P2666	D2552		H2334	E2211
	N2920	R2824	A2741	T2667	H2553	Y2442		W2212
L3005	P2921		T2742		A2554	N2443	W2339	V2213
	L2922	L2827	A2743	W2672	S2555	P2444		G2214
V3009	F2923	A2828		V2673	P2556	A2445	M2346	T2215
	I2924	L2829	S2746	H2674	L2557	P2446	G2347	E2216
F3014	V2925	K2830	V2747	P2675	L2558	A2447	Q2348	
I3015	S2926	M2831	E2748	S2676		P2448	N2349	K2229
A3016	Q2927	G2832	E2749		L2563	E2449		
A3017		L2833	G2750	A2679		W2450	I2352	P2234
L3018	L2930	P2834	V2751	S2680	F2567	D2451	V2353	T2235
D3019		V2835	D2752	T2681		D2452	S2354	L2236
	K2935		K2753		F2580	L2453		L2237
E3022	G2936	Q2843	I2754	M2686	V2581	D2454	E2358	F2238
R3023		S2844			Q2582			
	A2939	F2845	A2759	T2690	F2583	A2458	V2361	R2244
A3044	V2940	A2846		S2691	D2584			V2245
	F2941	D2847	V2762	M2692	P2585	V2461	M2372	A2246
P3050	Q2942	G2848	I2763	Q2693	E2586	V2462		
M3051	M2943		A2764	T2694			L2376	V2252
		G2859	G2765	M2695	R2591	L2469		
D3057	L2946	A2860		Y2696	P2592	G2470	K2391	R2255
R3058	C2947	L2861	D2768	H2697		P2471	V2392	
R3059	Q2948		D2769	G2698	W2599	Y2472	D2393	K2261
		R2865	L2770	N2699			L2394	
H3062	R2951			L2700	R2603	R2478	T2395	W2265
		T2871	E2773	L2701				
P3065	V2954			G2702	R2610	M2481	L2398	Q2268
E3066	I2955	L2876	I2776	R2703	V2611	E2482		
	P2956			A2704	P2612	V2483	I2401	L2274
Q3069	P2957	L2879	G2779	K2705	R2613		K2402	
	N2958	G2880		P2706	K2614	L2487	I2403	I2277
M3073	R2959	V2881	T2784				D2404	
L3074	S2960	G2882	A2785	I2709	L2617	V2492	M2405	D2282
L3075	L2961	A2883	D2786	L2710	S2618			
S3076	D2962	D2884	T2787	Q2711	R2619	L2495	L2408	R2286
T3077		D2885	E2788	E2712	T2620		A2409	L2287
	D2966	I2886	M2789	V2713	V2621	K2503		H2288
R3080			M2790	L2714	G2622	W2504	A2412	
L3081	W2976	I2889	R2791	P2715	A2623	E2505		L2291
	V2977	S2890		N2716	Q2624		M2416	
L3089	R2978	K2891	K2799	V2717	I2625	W2512	S2417	S2294
	E2979	H2892	F2800	V2718		Y2513	G2418	P2295
	P2980	D2893	S2801	A2719	D2630	D2514		N2296
		T2894	R2802	A2720	P2631		D2421	R2297
	L2983	S2895		H2721	T2632	L2520	E2422	G2298
		T2896	D2805	V2722	V2633	V2521		M2299
	F2987		R2806	M2723		P2522	E2426	F2300
	P2988	P2901	R2807	Q2724	D2645	E2523	A2427	
	L2989	N2902	R2808		R2646	C2524	P2428	D2303
		E2903	L2809	V2727	V2647			
	G2992		G2810	G2728	A2648	V2527	T2431	Y2306
	L2993	L2906	F2811	G2729	L2649	E2528	I2432	
	V2994		L2812	Y2730	W2650	R2529	R2433	K2310

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO163 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:HG12	1.90	1.06
1:F:1013:THR:HG23	1:F: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%)	30	74
1	B	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	26	71
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	26	71
1	D	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	26	71
1	E	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	30	74
1	F	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	26	71
All	All	16908/18534 (91%)	15849 (94%)	947 (6%)	112 (1%)	31	71

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	2099/2402 (87%)	1997 (95%)	102 (5%)	31	67
1	B	2100/2402 (87%)	1997 (95%)	103 (5%)	31	67
1	C	2100/2402 (87%)	1998 (95%)	102 (5%)	31	67
1	D	2100/2402 (87%)	1998 (95%)	102 (5%)	31	67
1	E	2100/2402 (87%)	1998 (95%)	102 (5%)	31	67
1	F	2100/2402 (87%)	1998 (95%)	102 (5%)	31	67
All	All	12599/14412 (87%)	11986 (95%)	613 (5%)	35	67

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	-	32,33,33	1.20	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	B	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	C	4000	-	32,33,33	1.22	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	D	4000	-	32,33,33	1.22	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	E	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	F	4000	-	32,33,33	1.22	3 (9%)	34,50,50	1.69	7 (20%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4000	FMN	C5A-N5	2.21	1.38	1.35
2	A	4000	FMN	C5A-N5	2.23	1.38	1.35
2	B	4000	FMN	C5A-N5	2.23	1.38	1.35
2	F	4000	FMN	C5A-N5	2.26	1.38	1.35
2	C	4000	FMN	C5A-N5	2.30	1.38	1.35

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4000	FMN	N3-C2-N1	-4.48	120.15	127.69
2	B	4000	FMN	N3-C2-N1	-4.48	120.15	127.69
2	E	4000	FMN	N3-C2-N1	-4.46	120.17	127.69
2	D	4000	FMN	N3-C2-N1	-4.45	120.20	127.69
2	C	4000	FMN	N3-C2-N1	-4.44	120.21	127.69

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.