



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 11:52 PM UTC

PDB ID : 6QL7 / pdb\_00006ql7  
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 4.6 angstrom  
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.  
Deposited on : 2019-01-31  
Resolution : 4.60 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](mailto: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  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

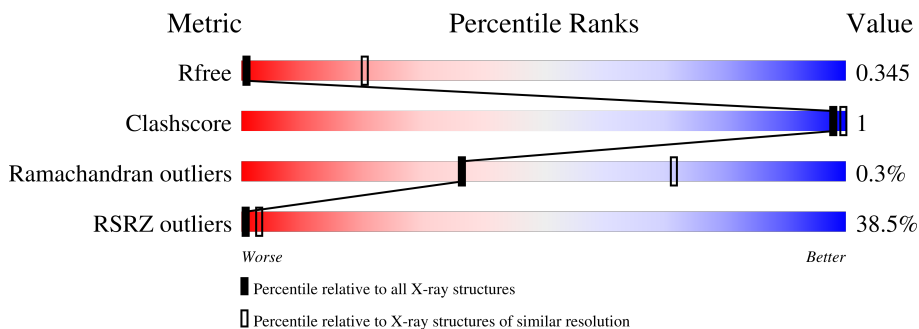
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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))
$R_{free}$	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	1887	
1	C	1887	
1	D	1887	
1	E	1887	
1	F	1887	
1	a	1887	

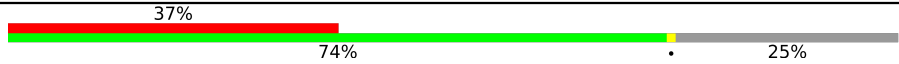
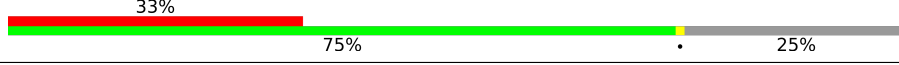
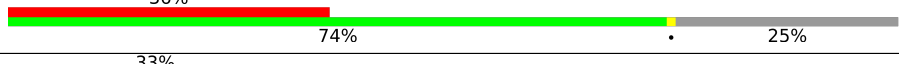

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Mol	Chain	Length	Quality of chain
1	b	1887	35% 92% 7%
1	c	1887	32% 92% 7%
1	d	1887	36% 92% 7%
1	e	1887	37% 92% 7%
1	f	1887	32% 92% 7%
2	G	2051	41% 98% ..
2	H	2051	45% 98% ..
2	I	2051	47% 98% ..
2	J	2051	31% 98% ..
2	K	2051	33% 98% ..
2	L	2051	37% 98% ..
2	g	2051	36% 98% ..
2	h	2051	33% 98% ..
2	i	2051	33% 98% ..
2	j	2051	42% 98% ..
2	k	2051	44% 98% ..
2	l	2051	44% 98% ..
3	M	150	41% 75% 25%
3	N	150	42% 75% 25%
3	O	150	47% 75% 25%
3	P	150	29% 74% 25%
3	Q	150	39% 75% 25%
3	R	150	31% 74% 25%
3	m	150	47% 75% 25%
3	n	150	34% 75% 25%

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Mol	Chain	Length	Quality of chain
3	o	150	
3	p	150	
3	q	150	
3	r	150	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 231252 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	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	B	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	C	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	D	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	E	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	F	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	a	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	b	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	c	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	d	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	e	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			
1	f	1760	Total	C	N	O	0	0	0
			8667	5147	1760	1760			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	H	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	J	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	K	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	L	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	g	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	h	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	i	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	j	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	k	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			
2	l	2036	Total	C	N	O	0	0	0
			10046	5974	2036	2036			

- Molecule 3 is a protein called Translation machinery-associated protein 17.

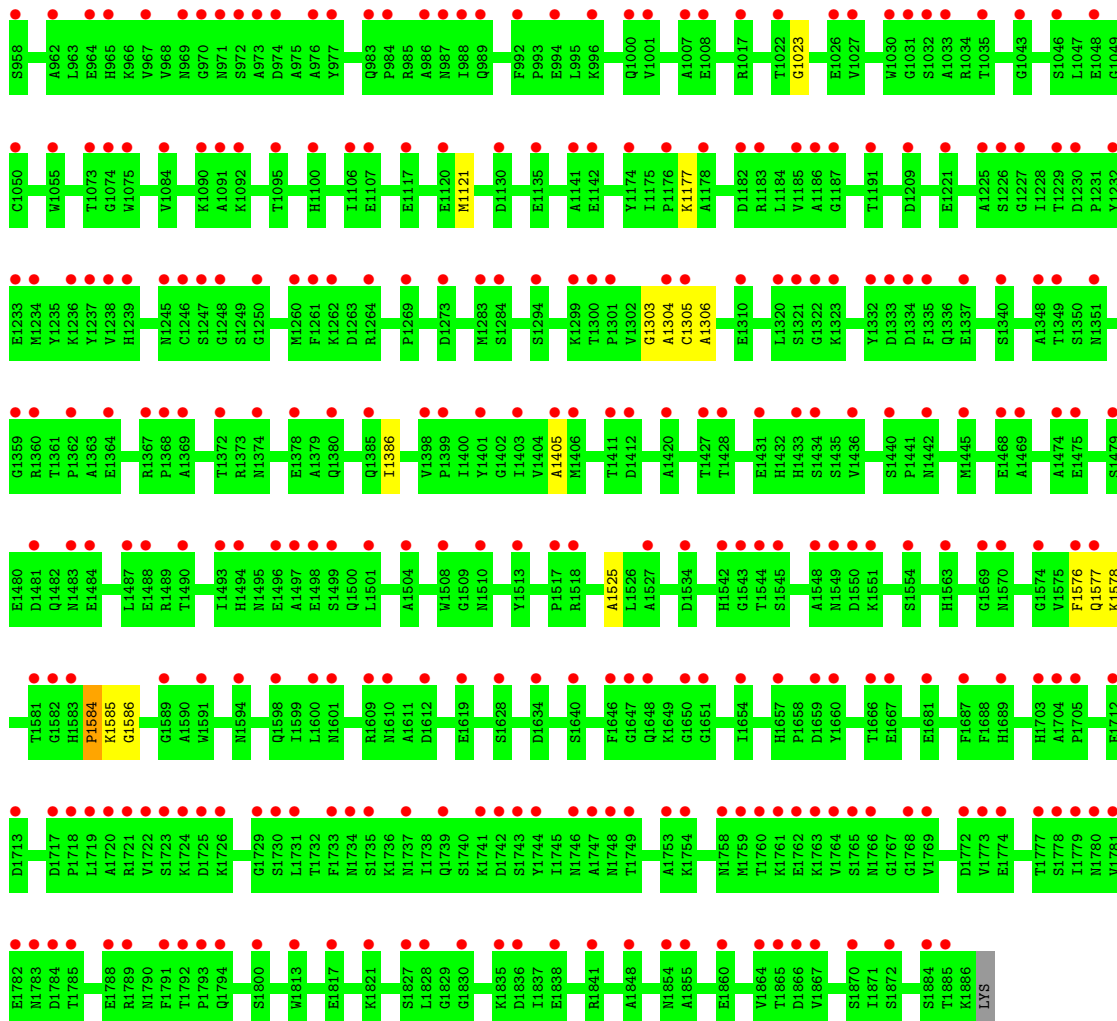
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	N	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	O	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	P	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	Q	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	R	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	m	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	n	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	o	113	Total	C	N	O	0	0	0
			558	332	113	113			

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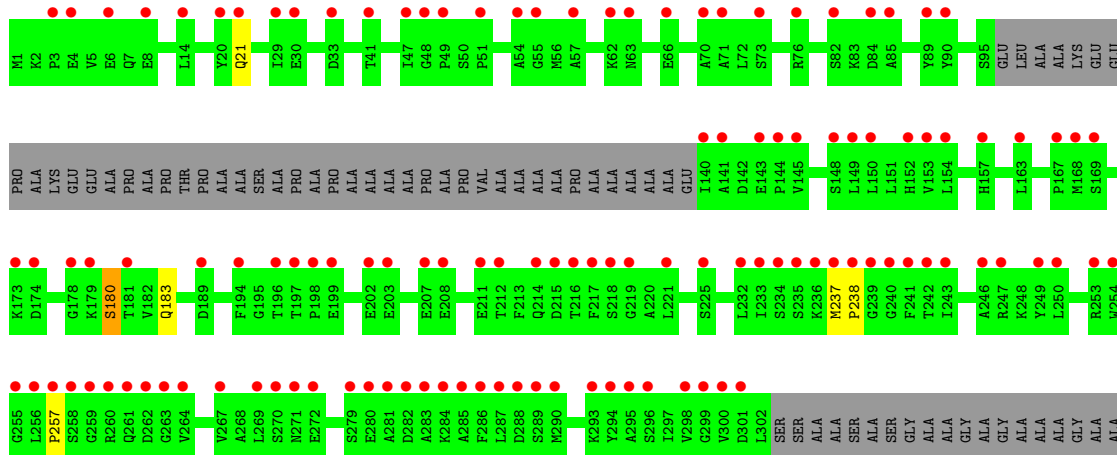
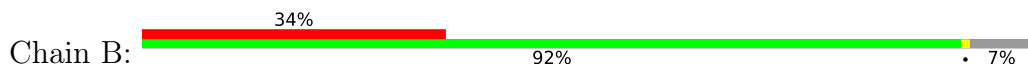
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>	<b>Trace</b>
3	p	113	Total 558	C 332	N 113	O 113	0	0	0
3	q	113	Total 558	C 332	N 113	O 113	0	0	0
3	r	113	Total 558	C 332	N 113	O 113	0	0	0



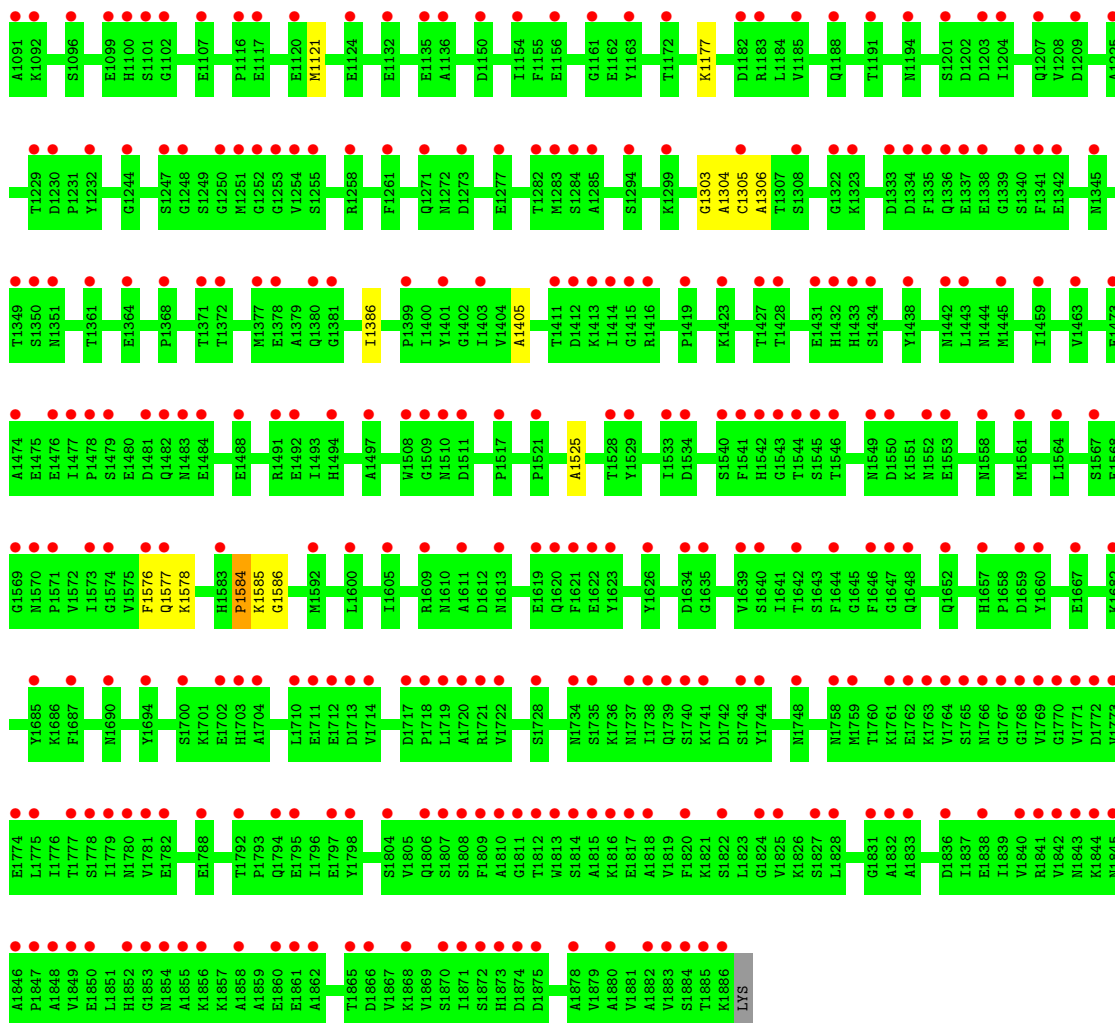


• Molecule 1: Fatty acid synthase subunit alpha



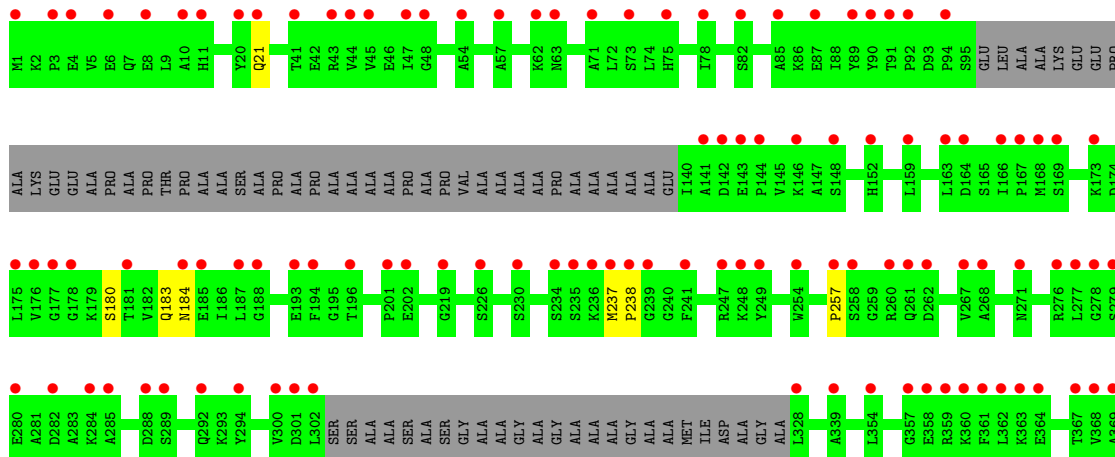


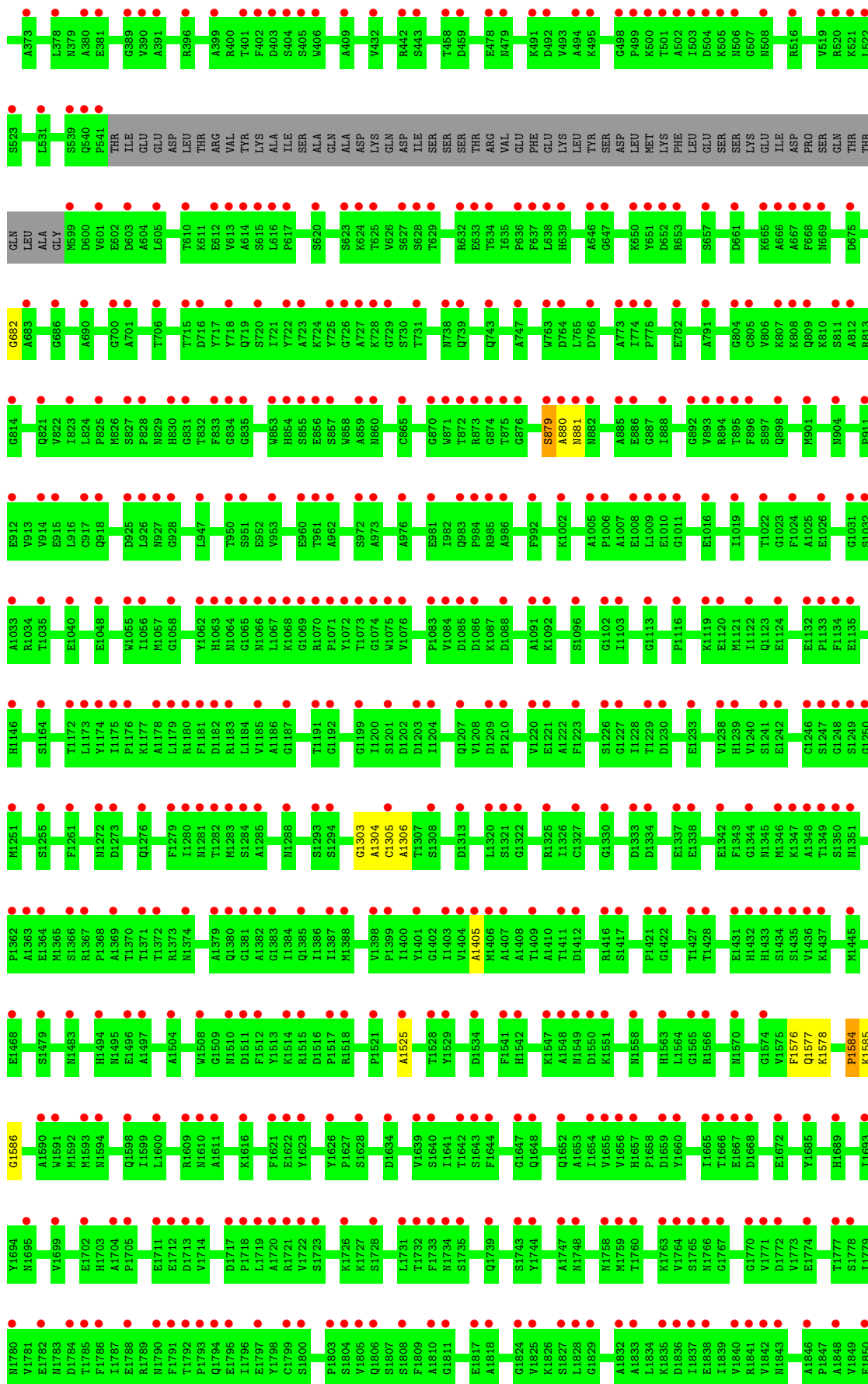




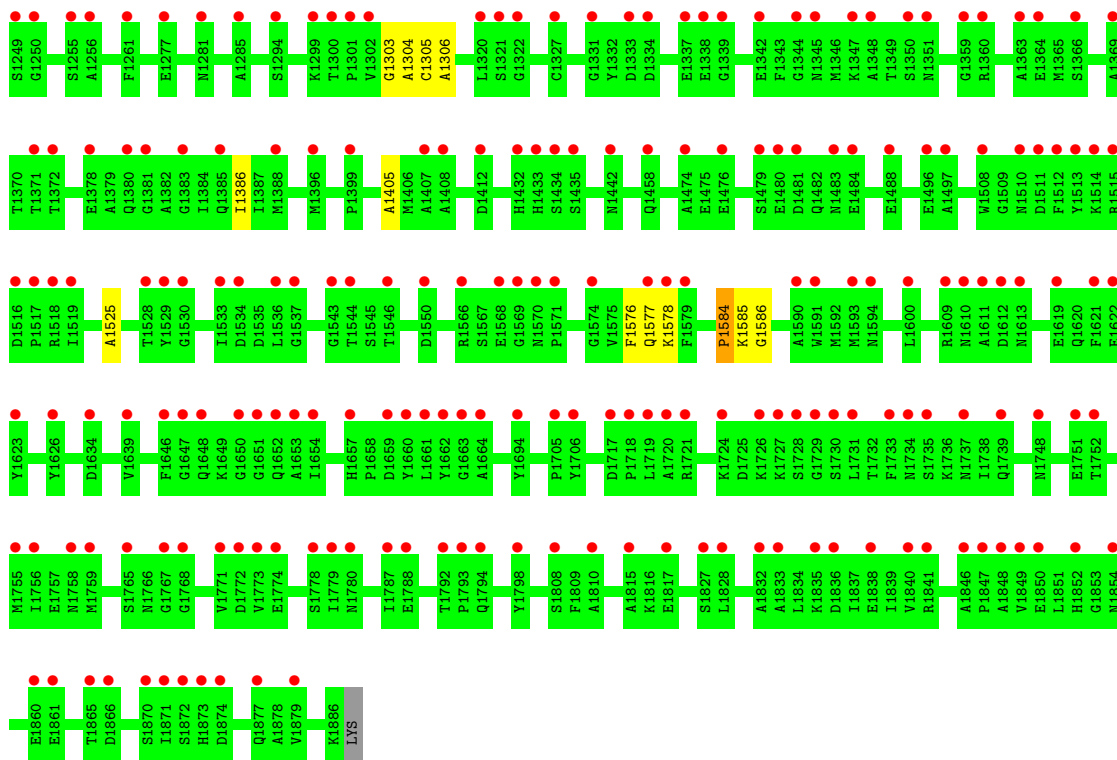
● Molecule 1: Fatty acid synthase subunit alpha

Chain D: 34% 92% 7%

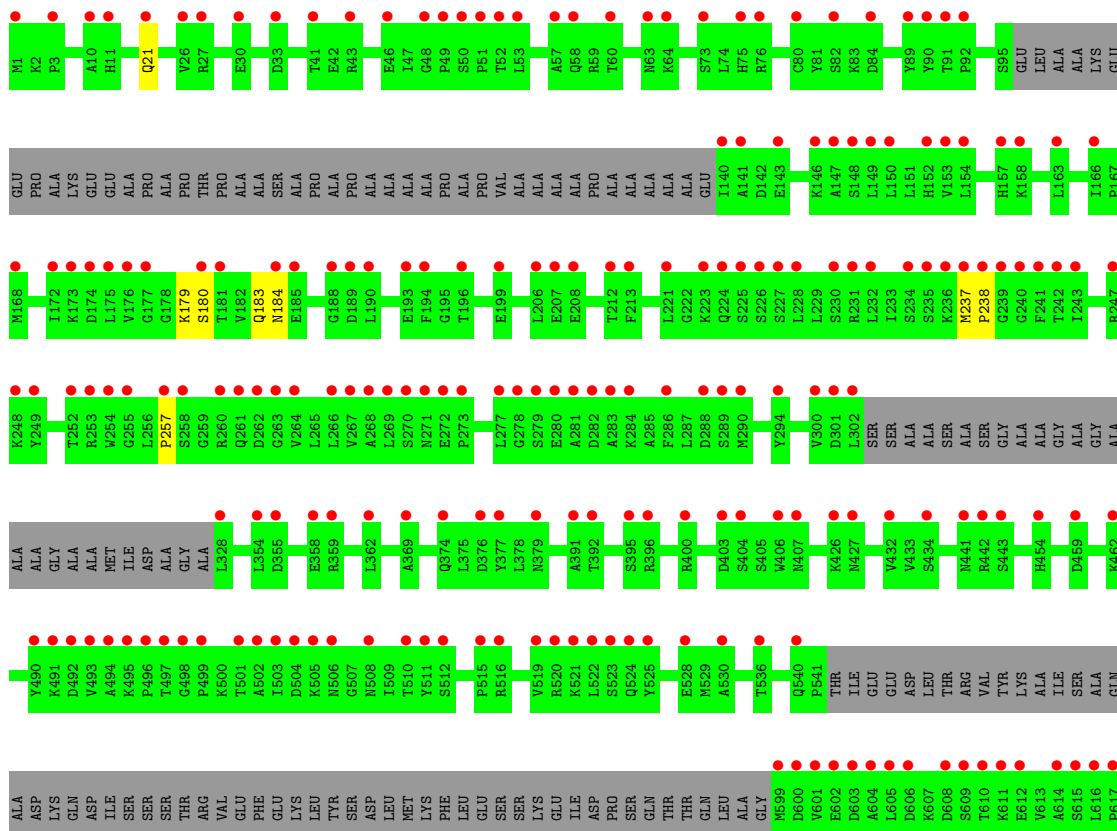
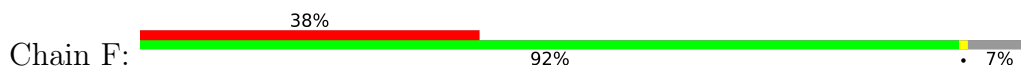


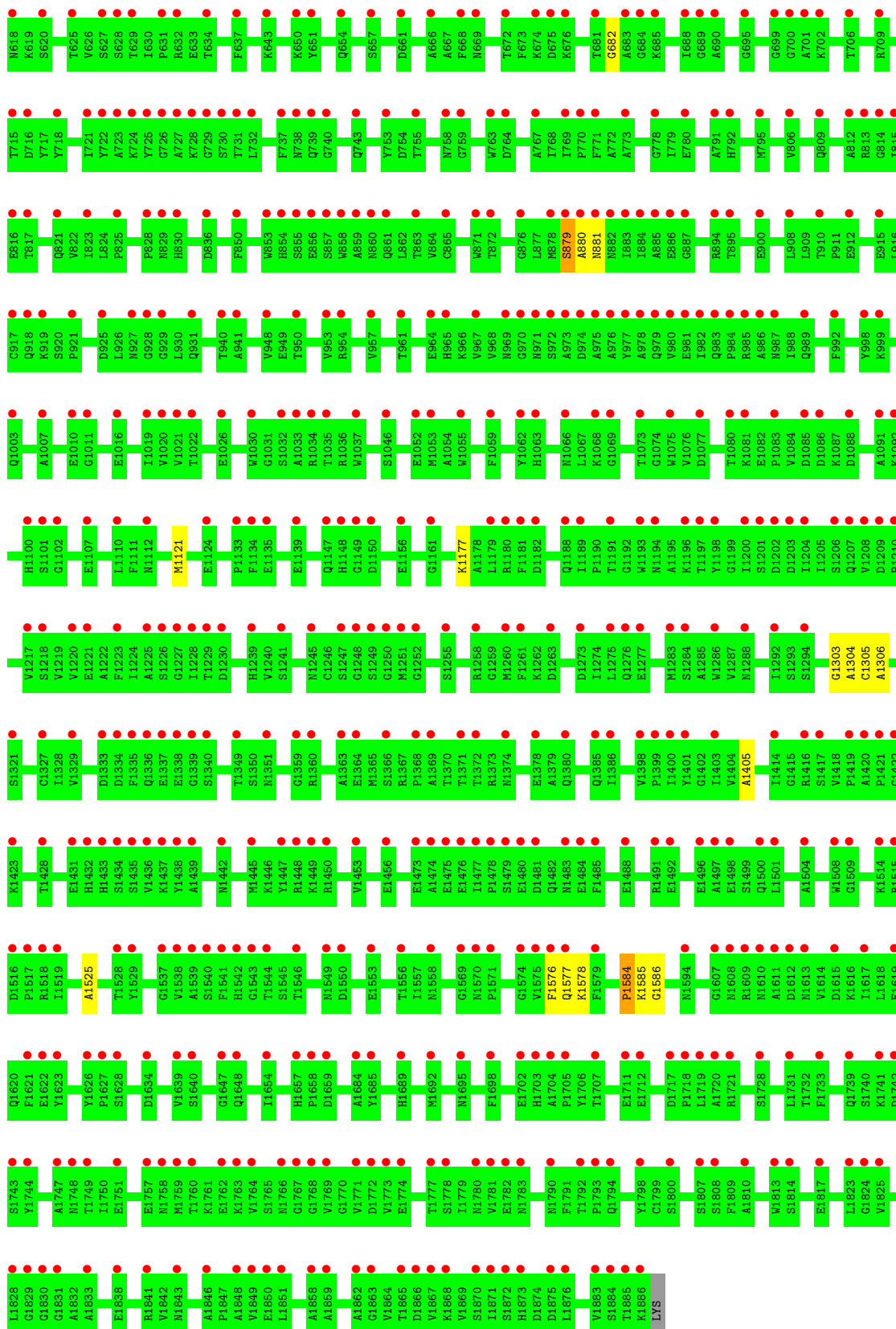




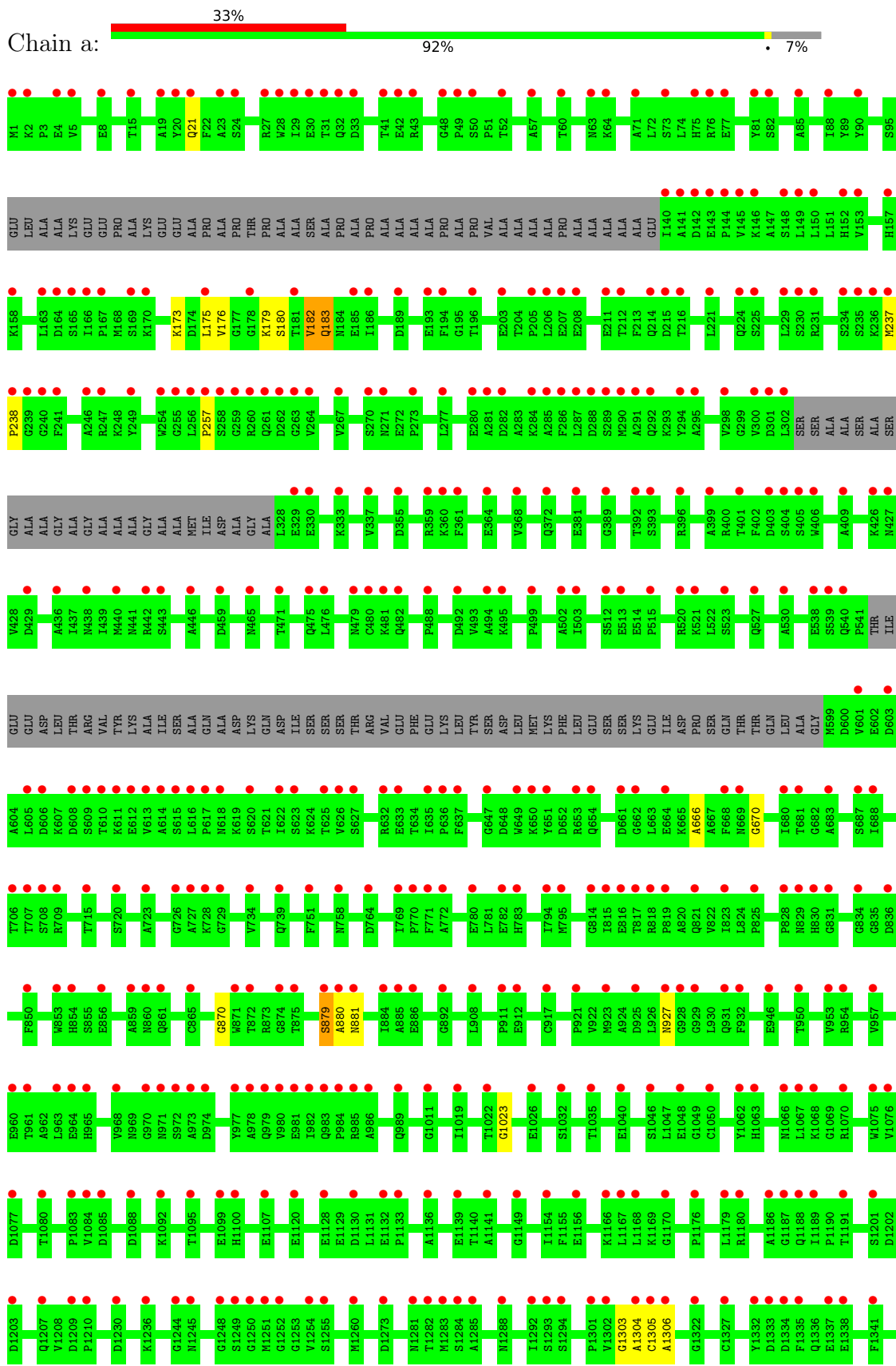


• Molecule 1: Fatty acid synthase subunit alpha

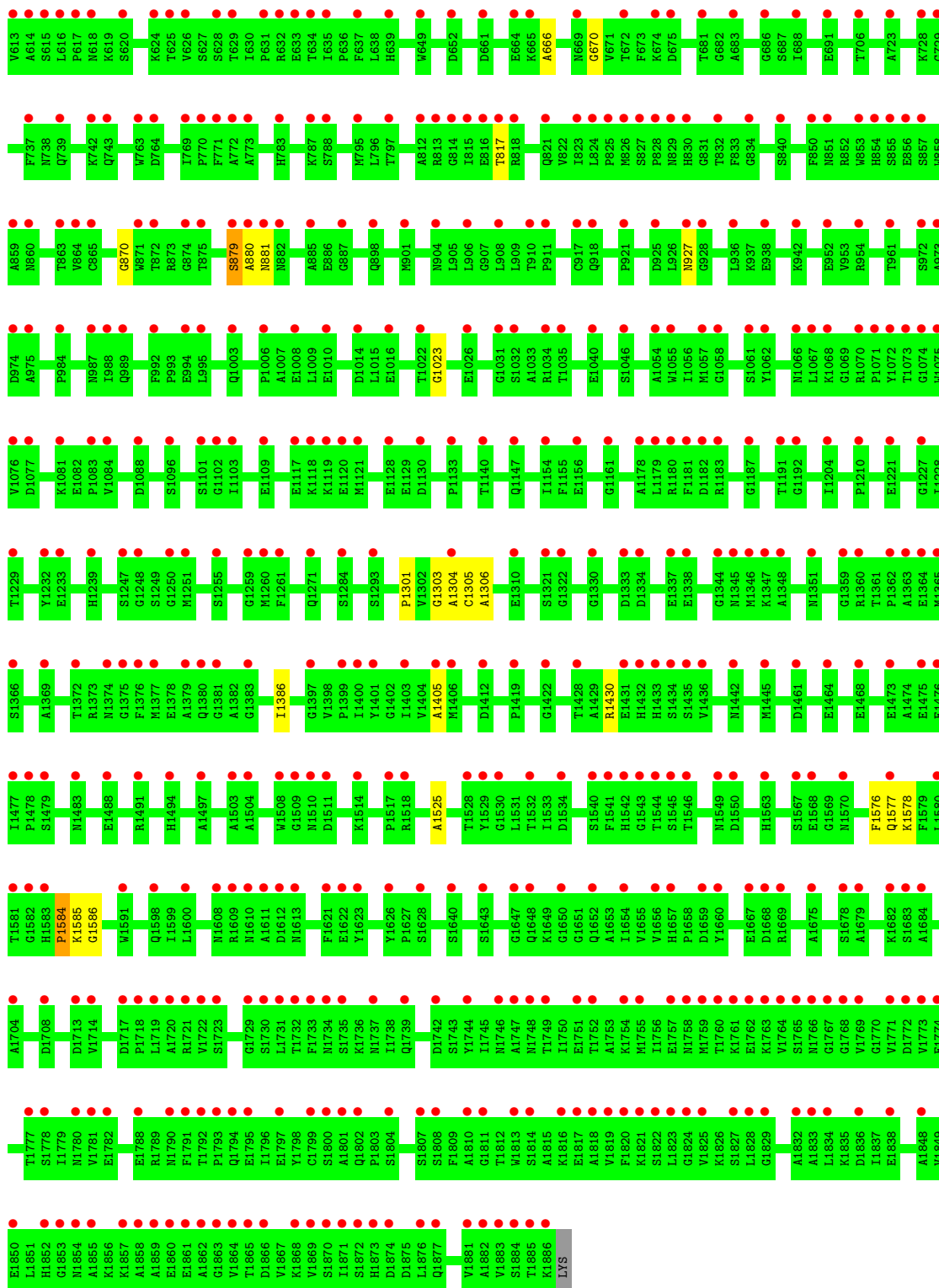




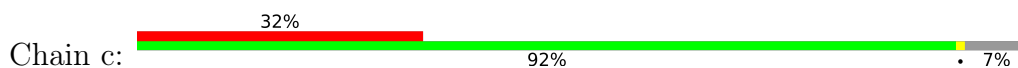
- Molecule 1: Fatty acid synthase subunit alpha





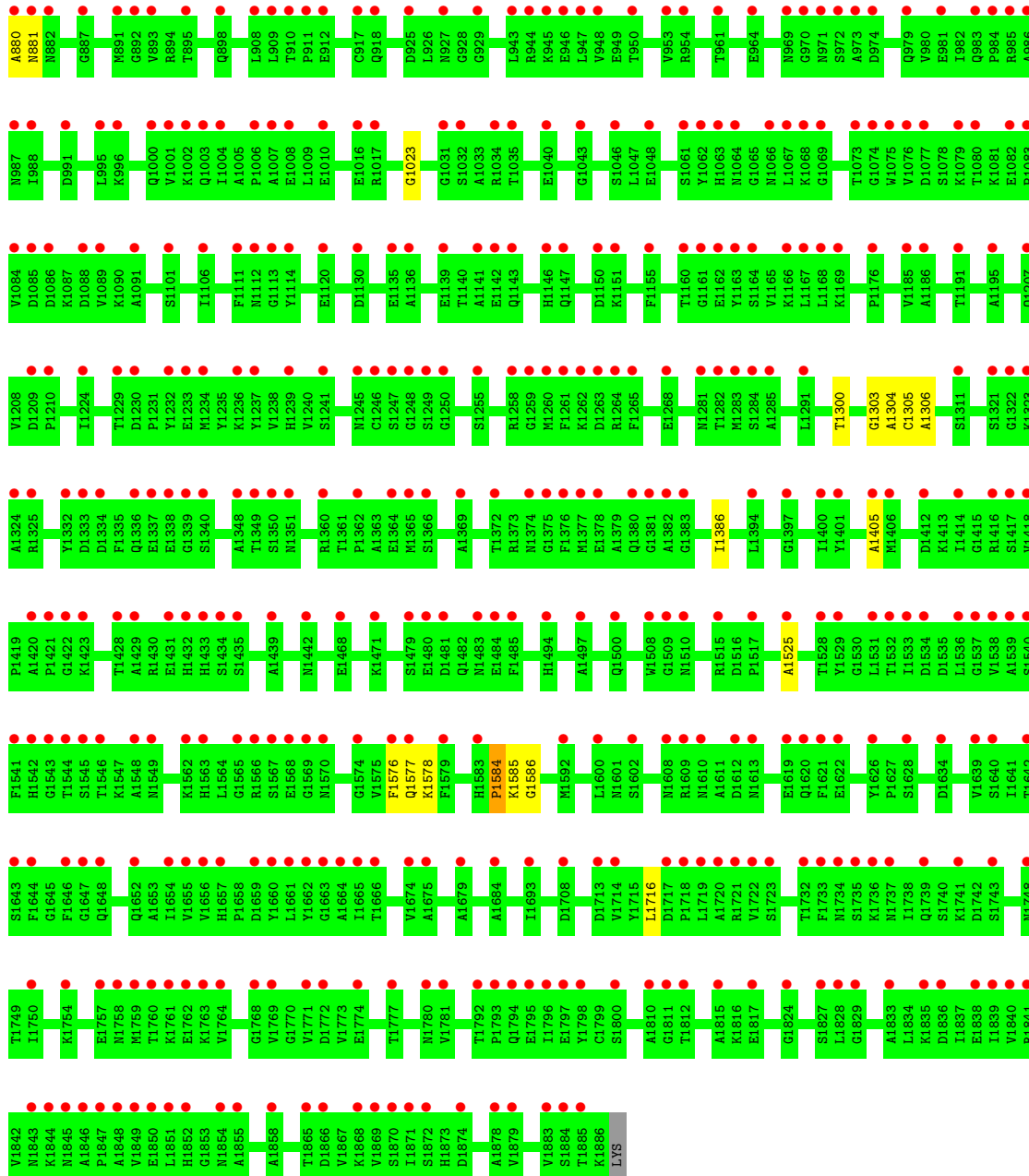


• Molecule 1: Fatty acid synthase subunit alpha

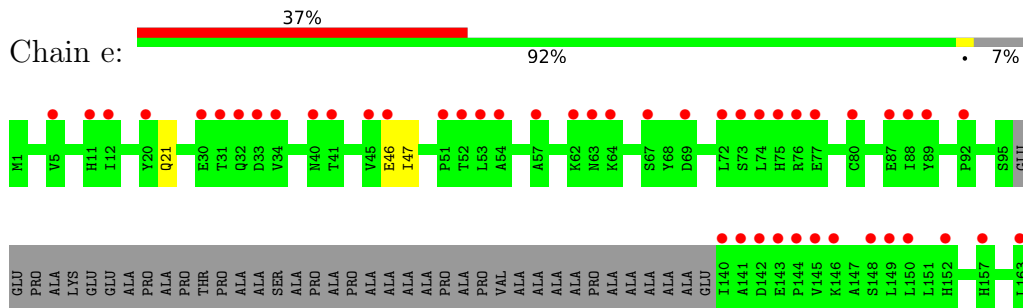






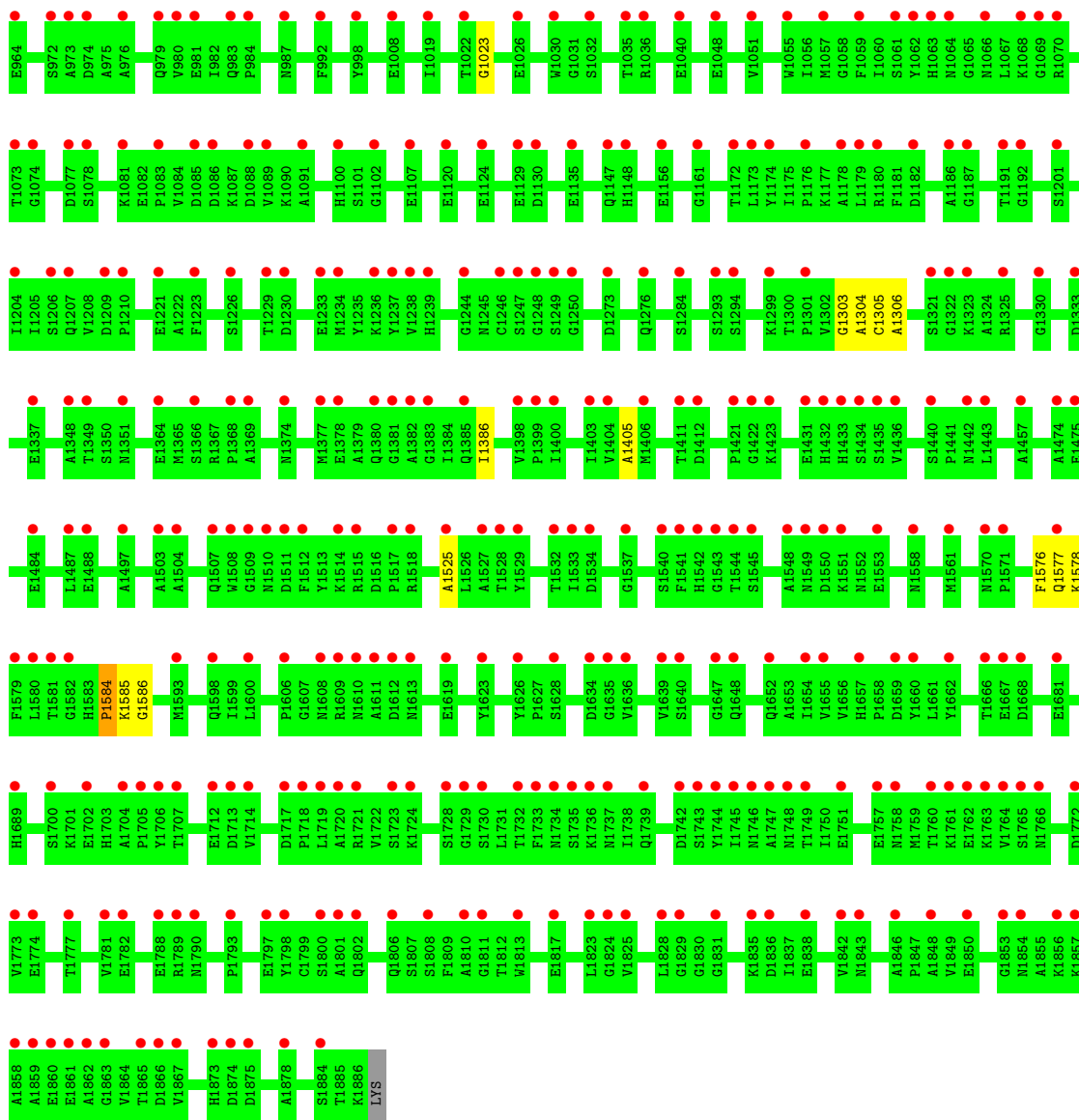


● Molecule 1: Fatty acid synthase subunit alpha

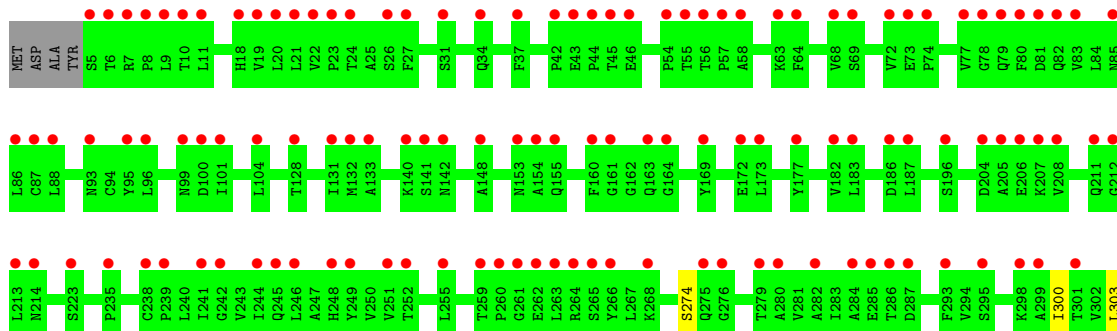




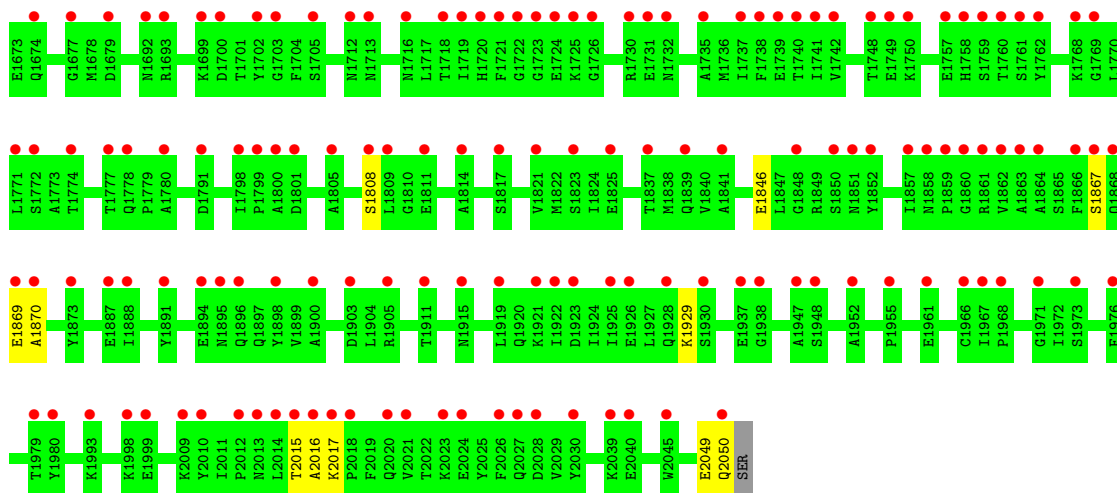




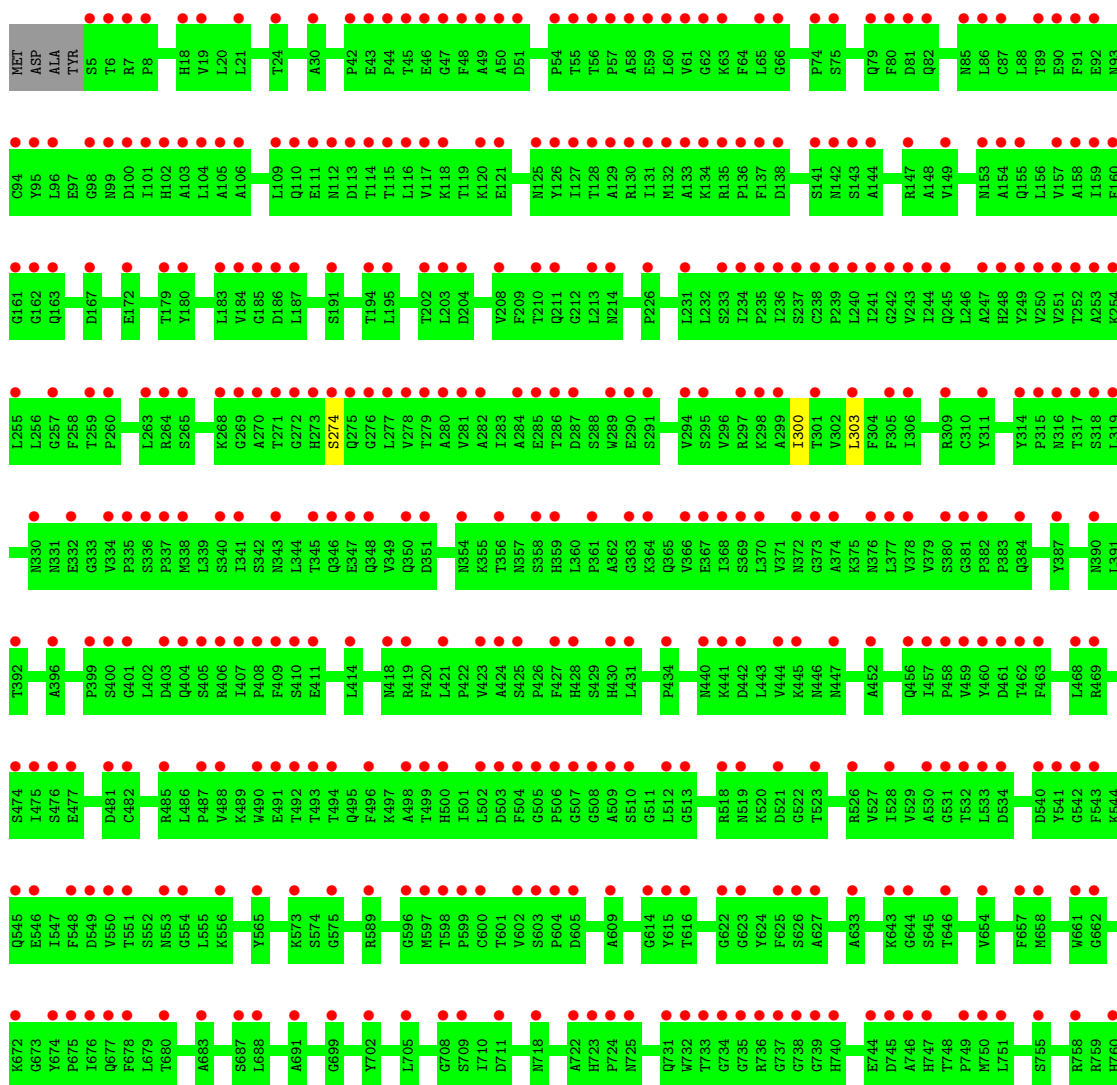
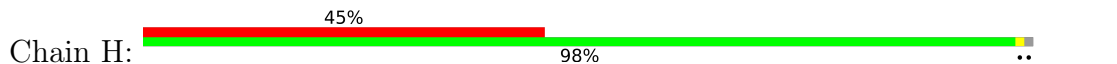
• Molecule 2: Fatty acid synthase subunit beta

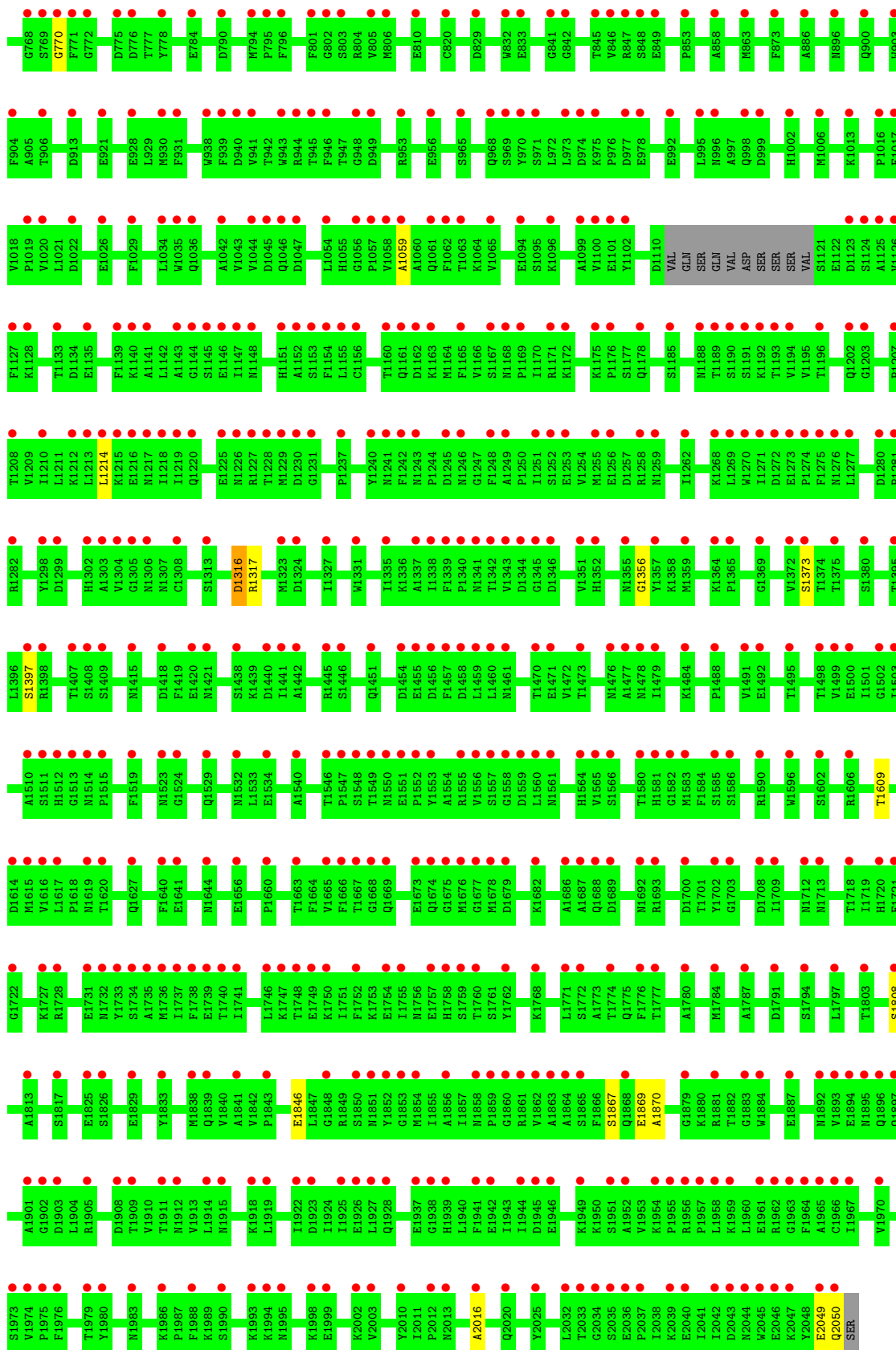






● Molecule 2: Fatty acid synthase subunit beta

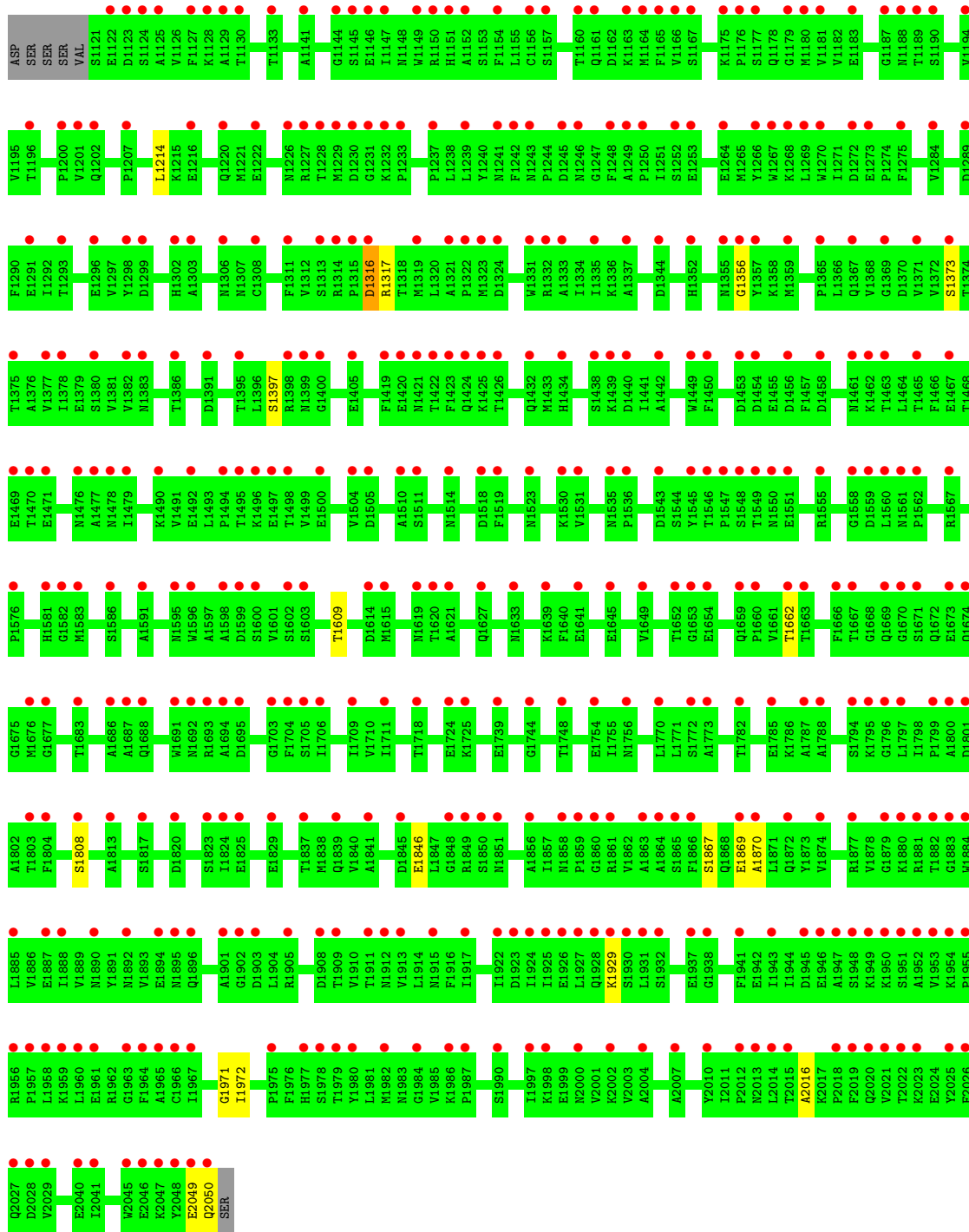




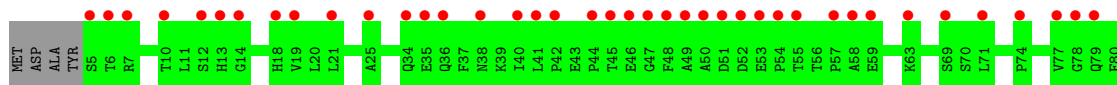
• Molecule 2: Fatty acid synthase subunit beta

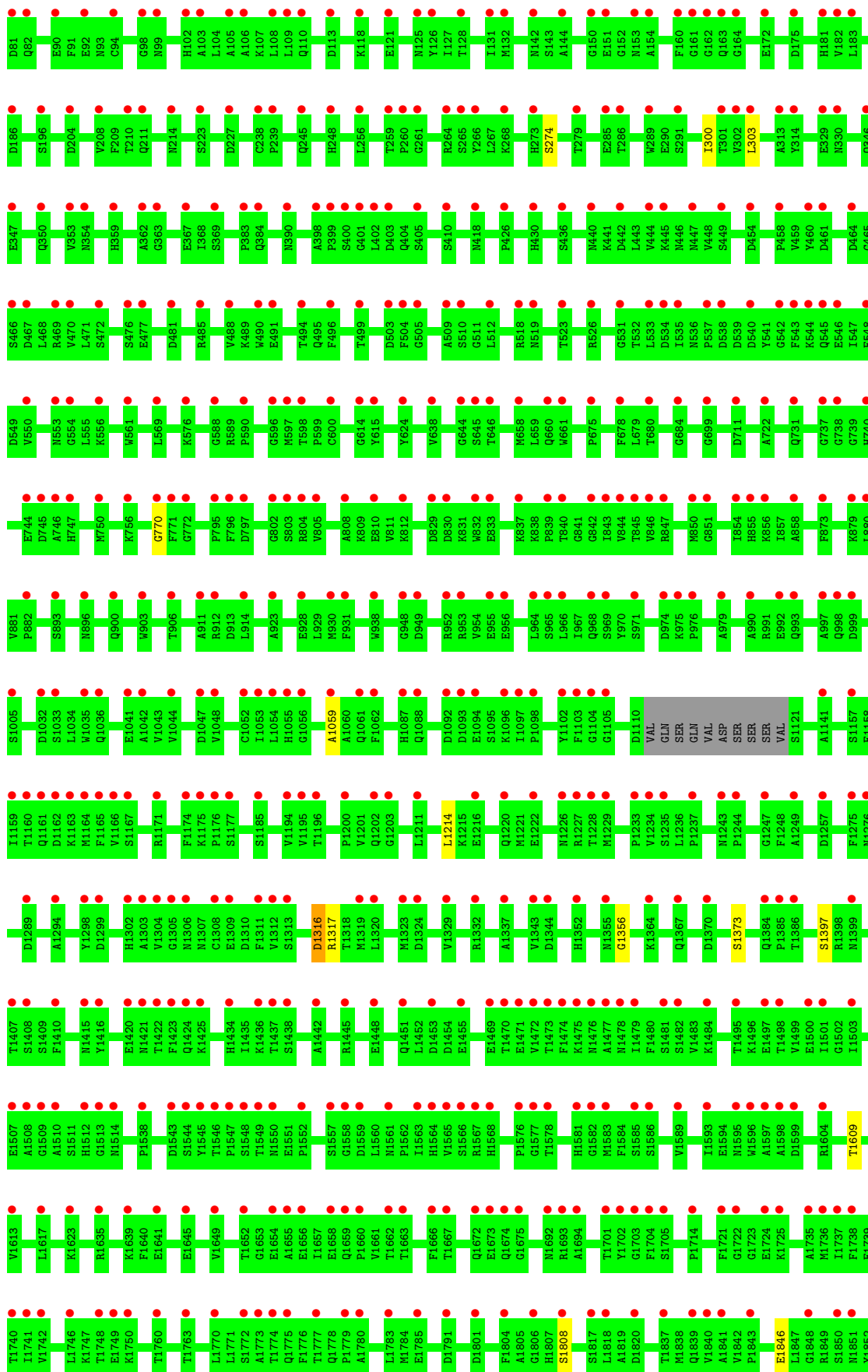


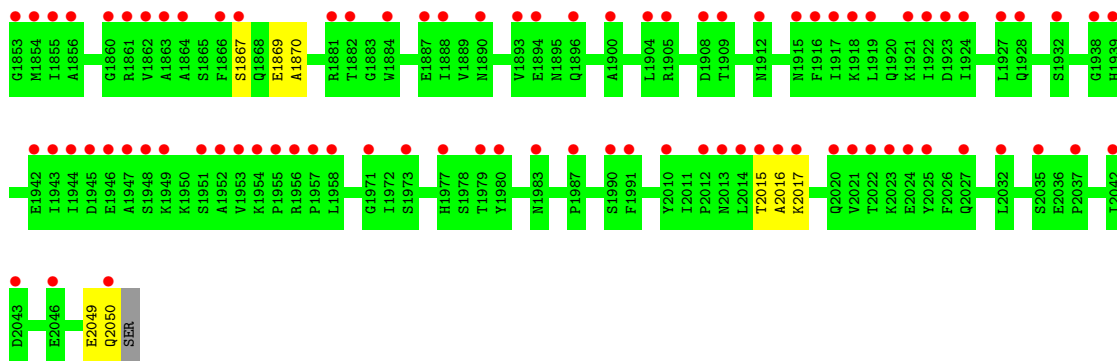
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H99	D100	H101	H102	A103	L104	A105	D113	T114	L115	L116	E121	N125	T128	I131	M132	A133	K134	R135	P136	F137	D138	K139	S140	T141	N142	A148	V149	G150	E151	G152	N153	A154	Q155	L156	V157	A158	I159	F160	G161	G162	Q163	A164	N165	D168	Y169	F170	E171	E172	T259	Q261					
Y180	H181	L182	L183	G184	V185	D186	L187	T194	L195	E196	L198	I199	D204	A205	E206	T210	Q211	G212	L213	N214	P222	F223	N224	T225	P226	D227	Y230	L231	L232	S233	S237	C238	P239	L240	S400	I241	G242	V243	I244	Q245	L246	A247	H248	Y249	V250	V251	K254	L255	L259	P260	G261				
Y266	L267	K268	G269	A270	T271	G272	H273	S274	Q275	G276	L277	V278	T279	A280	V281	A282	I283	A284	E285	S288	W289	E290	S291	F292	F293	N294	S295	K298	A299	I300	V302	L303	Y311	E312	A313	Y314	P315	N316	T317	S318	L319	P320	A247	S322	I323	N330	N331	E332	C333	V334	P335	S336	P337		
K338	L339	S340	T345	L343	E347	Q348	V349	Q350	G363	K364	Q365	V366	E367	V368	L369	S369	L370	V371	K372	A373	A374	W375	K376	L377	S380	G381	P382	P383	Q384	S385	D386	L387	L388	L389	P389	S400	G401	S405	R406	S410	E411	R412	F416	R419	E422	V423	A424	S425	P426						
F427	H428	S429	H430	L431	L432	S436	L438	L439	N440	K441	D442	L443	V444	K445	N446	N447	V448	S449	F450	G373	N451	A452	K453	D454	L455	Q456	L457	P458	V459	Y460	D461	T462	F463	D464	G465	S466	D467	L468	R469	V470	S474	L475	E477	C482	L483	V488	K489	N490	T491	T492	T493	F496	K497		
L498	T499	L502	D503	F504	G505	F506	G507	A508	F509	S510	G511	L512	G513	V514	L515	T516	H517	R518	N519	K520	D521	G522	T523	R526	V527	L528	V529	A530	G531	T532	L533	D534	I535	D538	D539	D540	Y541	G542	K543	Q544	E545	E546	L547	F548	D549	V550	N553	K556	K557	N558	P559	N560	W561	L562	
E563	P567	K568	L569	W661	I570	S574	I577	F578	V579	E580	T581	K582	F583	P590	F591	L592	P595	G596	M597	T598	P599	C600	T601	V602	S603	F606	A613	G614	Y615	T616	G621	G622	G623	Y624	F625	S626	A627	M630	T631	K643	G644	T646	M650	K653	V654	M655	P656								
F657	M658	L659	W661	W662	I663	P664	L665	Y674	P675	I676	Q677	F678	L679	T680	A683	P686	S687	L688	E689	S692	E693	Y694	L695	E696	E697	L698	G699	L700	K701	Y702	K706	F707	G708	D711	G724	F725	S726	N718	H723	P724	N725	Q731	W732	T733	G734	G735	R736	G737	G738						
G739	H740	H741	S742	F743	E744	D745	A746	H747	R758	F761	R764	S769	F771	G772	S773	D776	T782	W785	D790	Y791	F792	F793	R794	F795	F796	D797	L800	F801	G802	S803	R804	W805	R806	L807	E810	V811	K812	T813	S814	F815	D816	A817	G820	D829	D830	R831									
H832	E833	Q834	T835	H836	K837	G842	T845	L846	W846	R847	S848	E849	L854	H855	A858	T859	R860	D869	W881	L884	E885	H896	Q890	W903	T906	V907	N908	G909	Q910	A911	R912	D913	T916	E928	L929	N930	F931	D940	N943	F946	D949	N953													
E956	R957	F958	T959	K960	S961	K962	T963	L964	S965	L966	I967	Q968	S969	Y970	S971	D974	D977	E978	F981	F984	N985	A986	Y987	P988	A989	A990	R991	E992	Q993	F994	L995	N996	A997	Q998	D999	H1002	N1006	C1007	F1010	V1015	P1016	F1017	V1020	D1110	L1021	D1022	R1023	K1031	D1032						
W1035	Q1036	S1037	H1038	H1039	L1040	E1041	A1042	V1043	L1044	Q1045	Q1046	D1047	V1048	Q1049	C1052	I1053	L1054	H1055	P1057	A1059	A1060	Q1061	V1065	I1066	D1067	T1082	K1083	K1084	L1085	L1086	H1087	Q1088	Y1089	G1091	D1092	D1093	P1098	A1099	V1100	E1101	Y1102	F1103	G1104	V1109	VAL	GLN	SER	GLN	GLM	VAL					



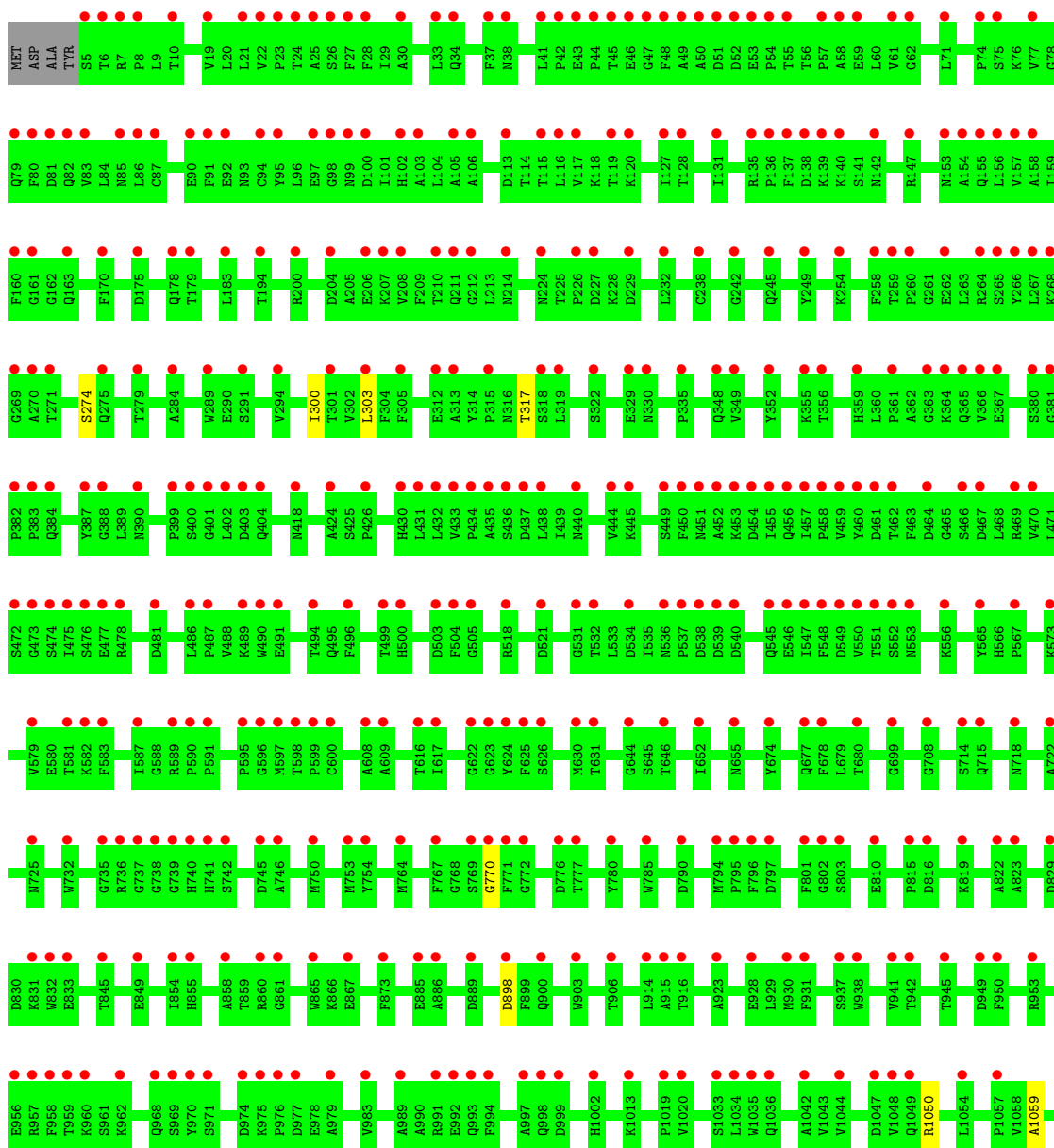
● Molecule 2: Fatty acid synthase subunit beta

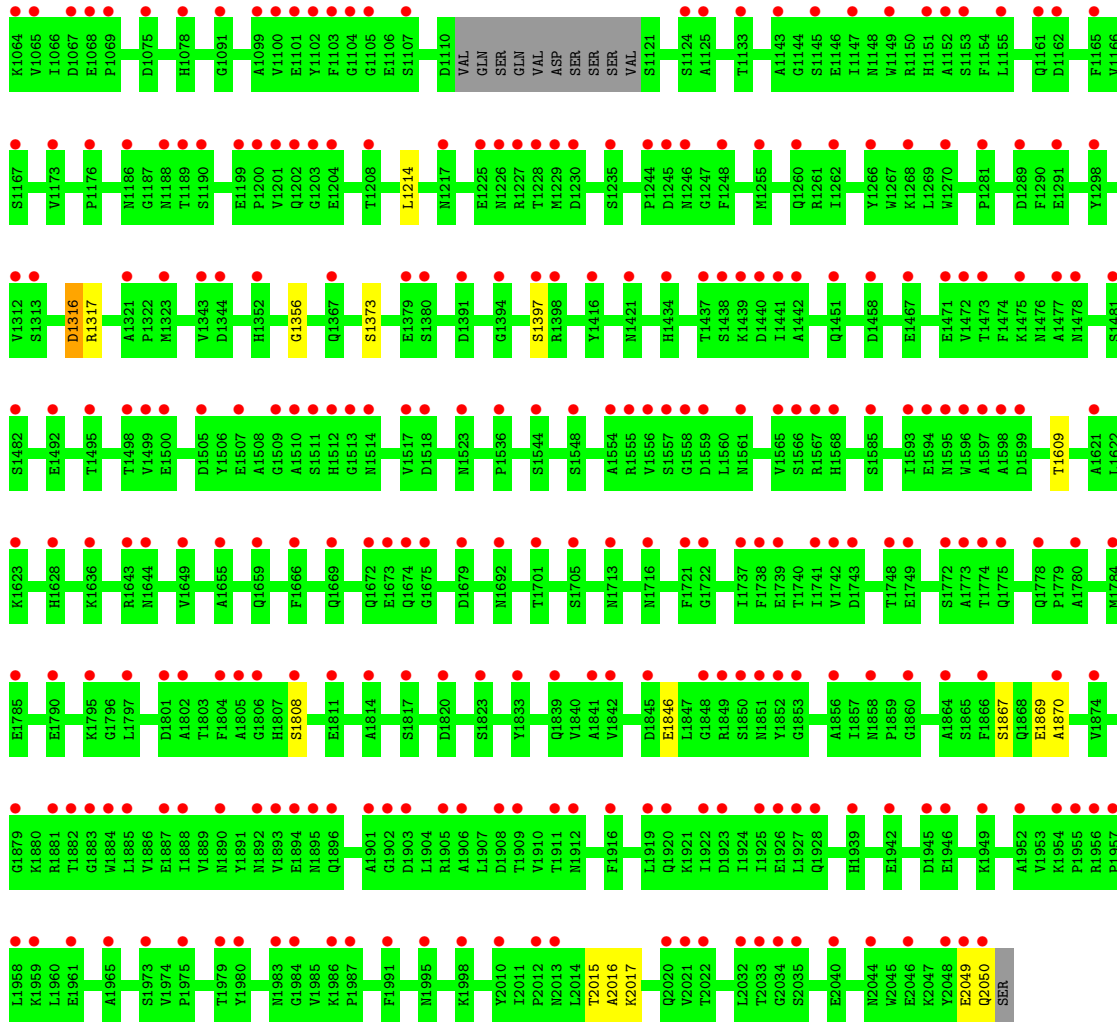




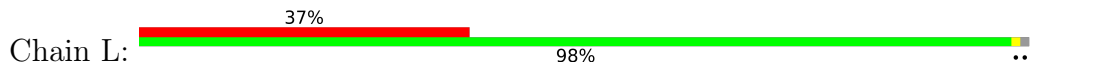


● Molecule 2: Fatty acid synthase subunit beta

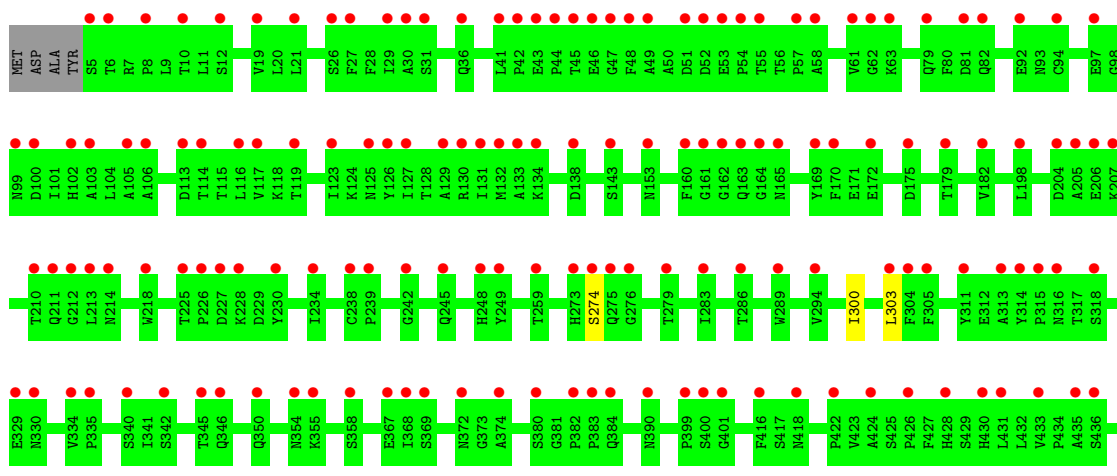




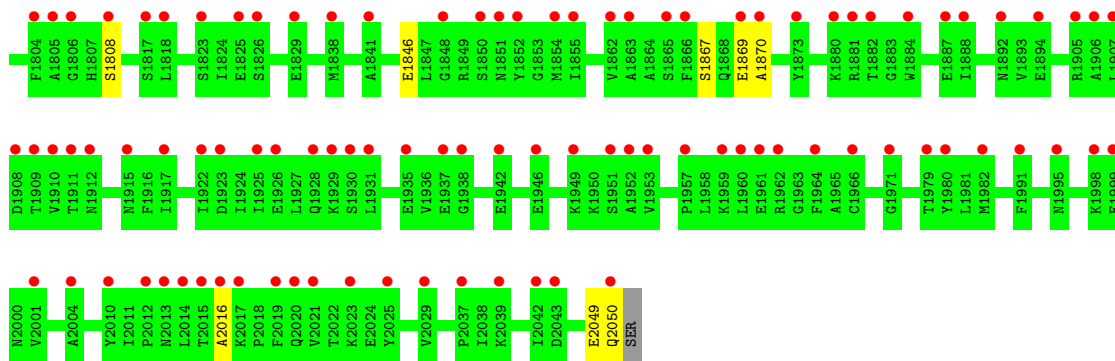
• Molecule 2: Fatty acid synthase subunit beta



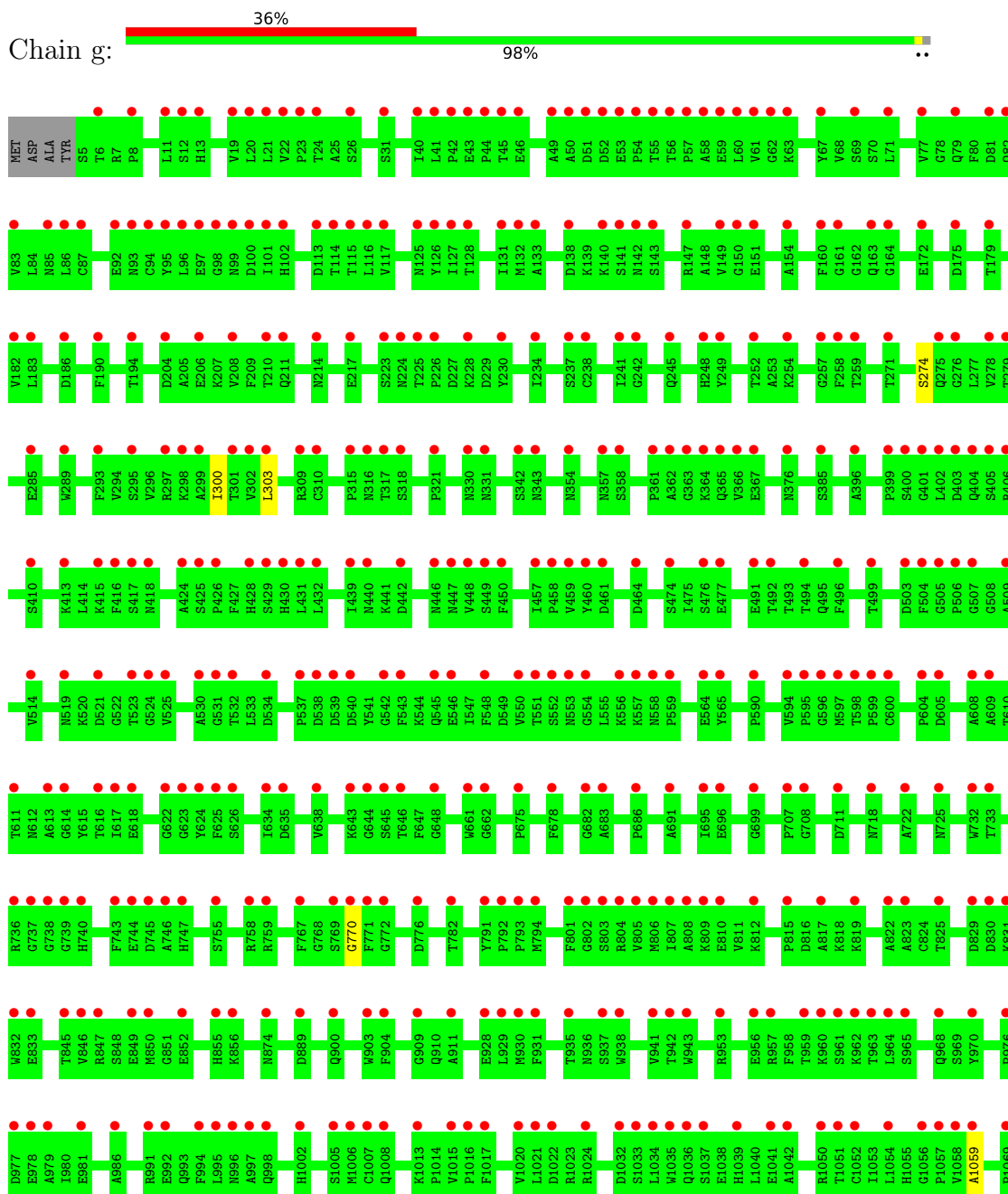
Chain L:





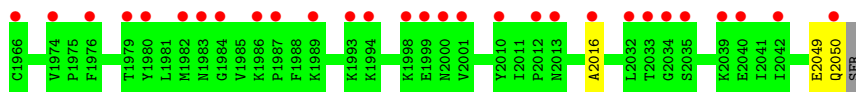


● Molecule 2: Fatty acid synthase subunit beta

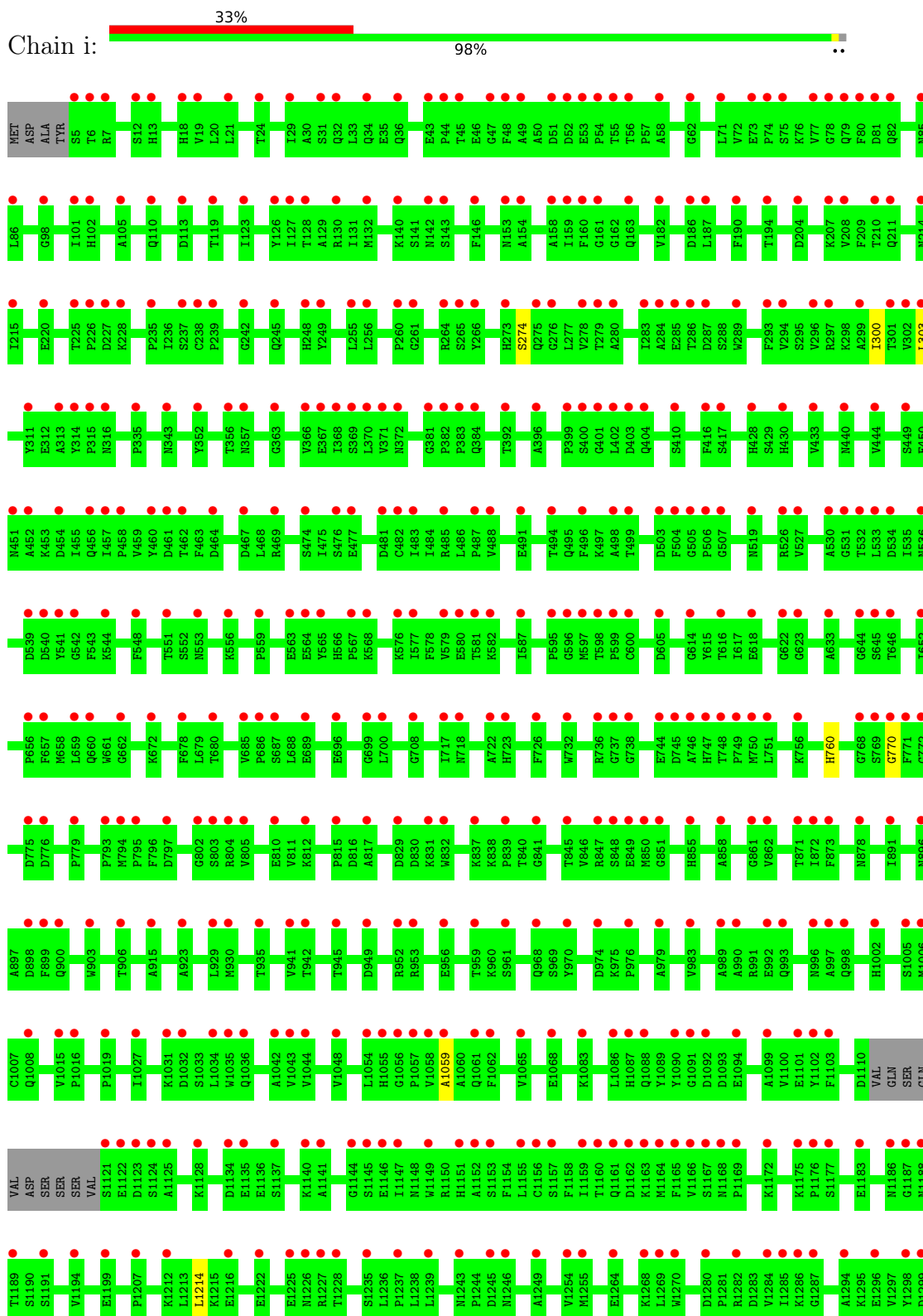


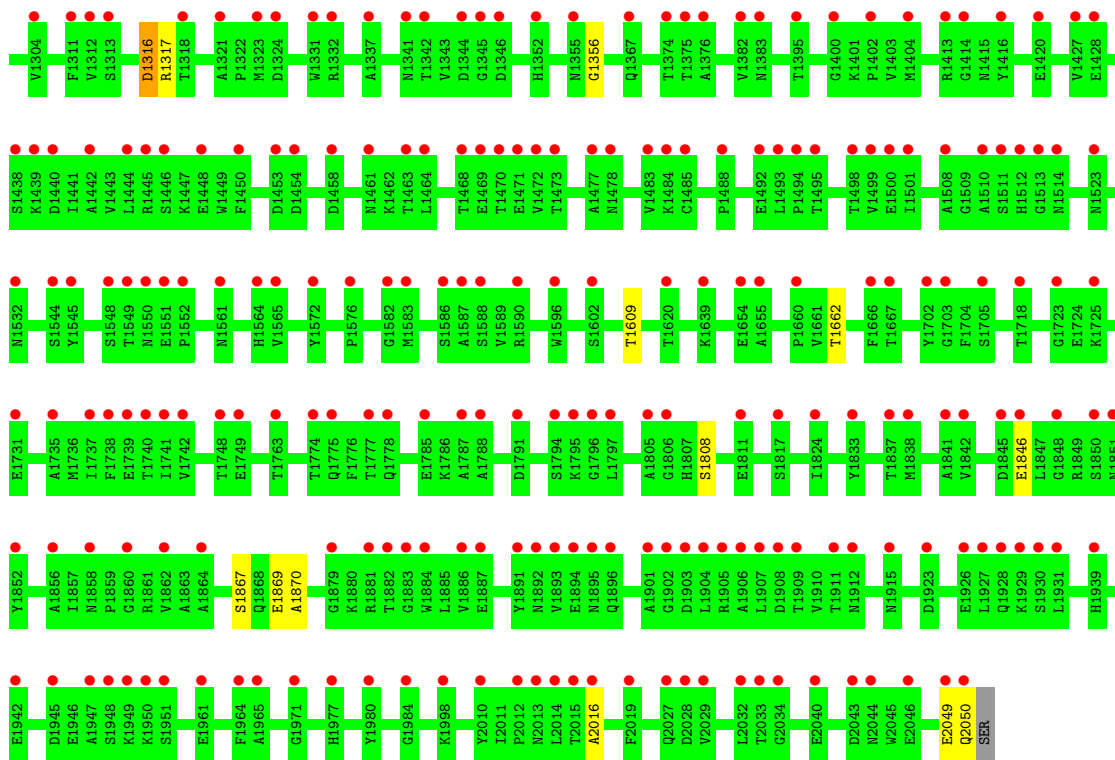


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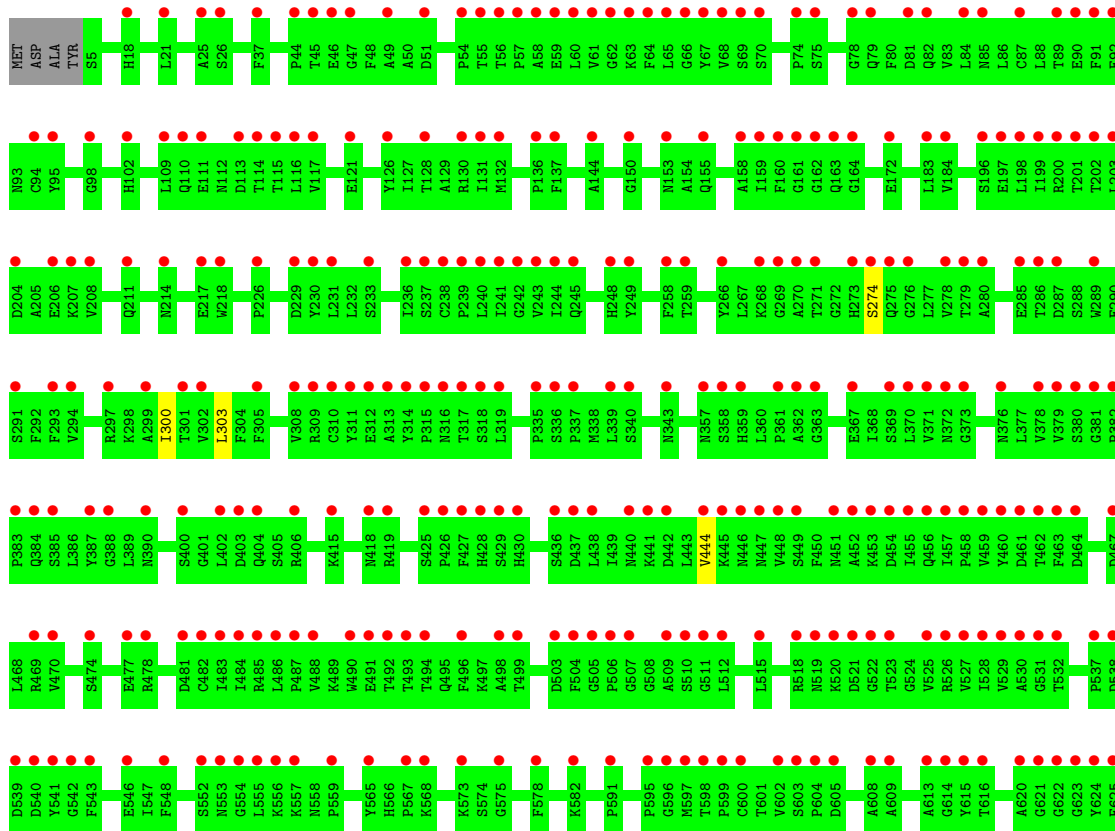
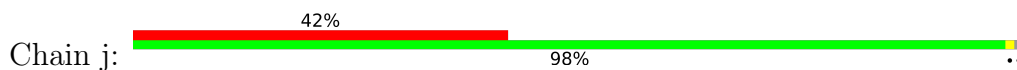


• Molecule 2: Fatty acid synthase subunit beta



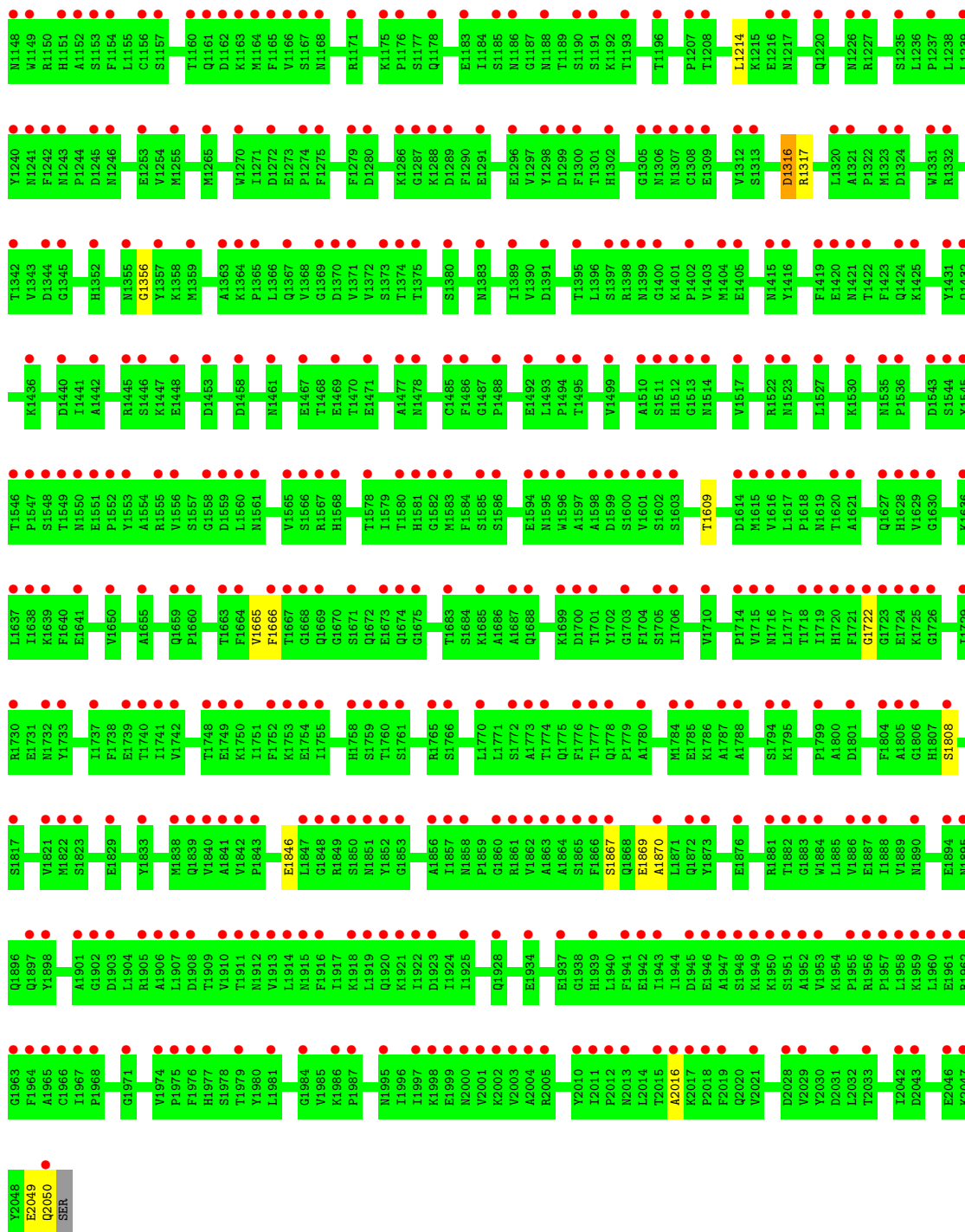


• Molecule 2: Fatty acid synthase subunit beta

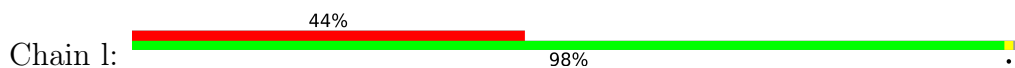


S626	M630	A633	I634	D635	E642	K643	T646	F647	G648	I652	V653	M655	P656	F657	M658	L659	O660	W661	G662	S671	Y674	P675	I676	Q677	F678	L679	T680	A683	G684	V685	P686	S687	L688	E689	V690	G699	Y702	L703	G704	P707	G708	G709	N718	A722	H723	P724																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
W725	W732	G734	G735	R736	G737	H740	E744	D745	A746	H747	T748	W753	Y754	S755	W756	L757	R758	H759	G769	S768	G770	G771	G772	A774	D775	D776	F777	W782	F785	W786	W787	W788	W794	F795	F796	D797	F801	G802	S803	R806	L807	R808	F810	H811	K812	A817																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C820	D829	W832	E833	Q834	R835	Y836	P839	T840	W844	R845	W846	E849	E852	P853	L854	H855	K856	R860	R868	S869	Y870	S871	L872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000	R1001	R1002	R1003	R1004	R1005	R1006	R1007	R1008	R1009	R1010	R1011	R1012	R1013	R1014	R1015	R1016	R1017	R1018	R1019	R1020	R1021	R1022	R1023	R1024	R1025	R1026	R1027	R1028	R1029	R1030	R1031	R1032	R1033	R1034	R1035	R1036	R1037	R1038	R1039	R1040	R1041	R1042	R1043	R1044	R1045	R1046	R1047	R1048	R1049	R1050	R1051	R1052	R1053	R1054	R1055	R1056	R1057	R1058	R1059	R1060	R1061	R1062	R1063	R1064	R1065	R1066	R1067	R1068	R1069	R1070	R1071	R1072	R1073	R1074	R1075	R1076	R1077	R1078	R1079	R1080	R1081	R1082	R1083	R1084	R1085	R1086	R1087	R1088	R1089	R1090	R1091	R1092	R1093	R1094	R1095	R1096	R1097	R1098	R1099	R1100	R1101	R1102	R1103	R1104	R1105	R1106	R1107	R1108	R1109	R1110	R1111	R1112	R1113	R1114	R1115	R1116	R1117	R1118	R1119	R1120	R1121	R1122	R1123	R1124	R1125	R1126	R1127	R1128	R1129	R1130	R1131	R1132	R1133	R1134	R1135	R1136	R1137	R1138	R1139	R1140	R1141	R1142	R1143	R1144	R1145	R1146	R1147	R1148	R1149	R1150	R1151	R1152	R1153	R1154	R1155	R1156	R1157	R1158	R1159	R1160	R1161	R1162	R1163	R1164	R1165	R1166	R1167	R1168	R1169	R1170	R1171	R1172	R1173	R1174	R1175	R1176	R1177	R1178	R1179	R1180	R1181	R1182	R1183	R1184	R1185	R1186	R1187	R1188	R1189	R1190	R1191	R1192	R1193	R1194	R1195	R1196	R1197	R1198	R1199	R1200	R1201	R1202	R1203	R1204	R1205	R1206	R1207	R1208	R1209	R1210	R1211	R1212	R1213	R1214	R1215	R1216	R1217	R1218	R1219	R1220	R1221	R1222	R1223	R1224	R1225	R1226	R1227	R1228	R1229	R1230	R1231	R1232	R1233	R1234	R1235	R1236	R1237	R1238	R1239	R1240	R1241	R1242	R1243	R1244	R1245	R1246	R1247	R1248	R1249	R1250	R1251	R1252	R1253	R1254	R1255	R1256	R1257	R1258	R1259	R1260	R1261	R1262	R1263	R1264	R1265	R1266	R1267	R1268	R1269	R1270	R1271	R1272	R1273	R1274	R1275	R1276	R1277	R1278	R1279	R1280	R1281	R1282	R1283	R1284	R1285	R1286	R1287	R1288	R1289	R1290	R1291	R1292	R1293	R1294	R1295	R1296	R1297	R1298	R1299	R1300	R1301	R1302	R1303	R1304	R1305	R1306	R1307	R1308	R1309	R1310	R1311	R1312	R1313	R1314	R1315	R1316	R1317	R1318	R1319	R1320	R1321	R1322	R1323	R1324	R1325	R1326	R1327	R1328	R1329	R1330	R1331	R1332	R1333	R1334	R1335	R1336	R1337	R1338	R1339	R1340	R1341	R1342	R1343	R1344	R1345	R1346	R1347	R1348	R1349	R1350	R1351	R1352	R1353	R1354	R1355	R1356	R1357	R1358	R1359	R1360	R1361	R1362	R1363	R1364	R1365	R1366	R1367	R1368	R1369	R1370	R1371	R1372	R1373	R1374	R1375	R1376	R1377	R1378	R1379	R1380	R1381	R1382	R1383	R1384	R1385	R1386	R1387	R1388	R1389	R1390	R1391	R1392	R1393	R1394	R1395	R1396	R1397	R1398	R1399	R1400	R1401	R1402	R1403	R1404	R1405	R1406	R1407	R1408	R1409	R1410	R1411	R1412	R1413	R1414	R1415	R1416	R1417	R1418	R1419	R1420	R1421	R1422	R1423	R1424	R1425	R1426	R1427	R1428	R1429	R1430	R1431	R1432	R1433	R1434	R1435	R1436	R1437	R1438	R1439	R1440	R1441	R1442	R1443	R1444	R1445	R1446	R1447	R1448	R1449	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460	R1461	R1462	R1463	R1464	R1465	R1466	R1467	R1468	R1469	R1470	R1471	R1472	R1473	R1474	R1475	R1476	R1477	R1478	R1479	R1480	R1481	R1482	R1483	R1484	R1485	R1486	R1487	R1488	R1489	R1490	R1491	R1492	R1493	R1494	R1495	R1496	R1497	R1498	R1499	R1500	R1501	R1502	R1503	R1504	R1505	R1506	R1507	R1508	R1509	R1510	R1511	R1512	R1513	R1514	R1515	R1516	R1517	R1518	R1519	R1520	R1521	R1522	R1523	R1524	R1525	R1526	R1527	R1528	R1529	R1530	R1531	R1532	R1533	R1534	R1535	R1536	R1537	R1538	R1539	R1540	R1541	R1542	R1543	R1544	R1545	R1546	R1547	R1548	R1549	R1550	R1551	R1552	R1553	R1554	R1555	R1556	R1557	R1558	R1559	R1560	R1561	R1562	R1563	R1564	R1565	R1566	R1567	R1568	R1569	R1570	R1571	R1572	R1573	R1574	R1575	R1576	R1577	R1578	R1579	R1580	R1581	R1582	R1583	R1584	R1585	R1586	R1587	R1588	R1589	R1590	R1591	R1592	R1593	R1594	R1595	R1596	R1597	R1598	R1599	R1600	R1601	R1602	R1603	R1604	R1605	R1606	R1607	R1608	R1609	R1610	R1611	R1612	R1613	R1614	R1615	R1616	R1617	R1618	R1619	R1620	R1621	R1622	R1623	R1624	R1625	R1626	R1627	R1628	R1629	R1630	R1631	R1632	R1633	R1634	R1635	R1636	R1637	R1638	R1639	R1640	R1641	R1642	R1643	R1644	R1645	R1646	R1647	R1648	R1649	R1650	R1651	R1652	R1653	R1654	R1655	R1656	R1657	R1658	R1659	R1660	R1661	R1662	R1663	R1664	R1665	R1666	R1667	R1668	R1669	R1670	R1671	R1672	R1673	R1674	R1675	R1676	R1677	R1678	R1679	R1680	R1681	R1682	R1683	R1684	R1685	R1686	R1687	R1688	R1689	R1690	R1691	R1692	R1693	R1694	R1695	R1696	R1697	R1698	R1699	R1700	R1701	R1702	R1703	R1704	R1705	R1706	R1707	R1708	R1709	R1710	R1711	R1712	R1713	R1714	R1715	R1716	R1717	R1718	R1719	R1720	R1721	R1722	R1723	R1724	R1725	R1726	R1727	R1728	R1729	R1730	R1731	R1732	R1733	R1734	R1735	R1736	R1737	R1738	R1739	R1740	R1741	R1742	R1743	R1744	R1745	R1746	R1747	R1748	R1749	R1750	R1751	R1752	R1753	R1754	R1755	R1756	R1757	R1758	R1759	R1760	R1761	R1762	R1763	R1764	R1765	R1766	R1767	R1768	R1769	R1770	R1771	R1772	R1773	R1774	R1775	R1776	R1777	R1778	R1779	R1780	R1781	R1782	R1783	R1784	R1785	R1786	R1787	R1788	R1789	R1790	R1791	R1792	R1793	R1794	R1795	R1796	R1797	R1798	R1799	R1800	R1801	R1802	R1803	R1804	R1805	R1806	R1807	R1808	R1809	R1810	R1811	R1812	R1813	R1814	R1815	R1816	R1817	R1818	R1819	R1820	R1821	R1822	R1823	R1824	R1825	R1826	R1827	R1828	R1829	R1830	R1831	R1832	R1833	R1834	R1835	R1836	R1837	R1838	R1839	R1840	R1841	R1842	R1843	R1844	R1845	R1846	R1847	R1848	R1849	R1850	R1851	R1852	R1853	R1854	R1855	R1856	R1857	R1858	R1859	R1860	R1861	R1862	R1863	R1864	R1865	R1866	R1867	R1868	R1869	R1870	R1871	R1872	R1873	R1874	R1875	R1876	R1877	R1878	R1879	R1880	R1881	R1882	R1883	R1884	R1885	R1886	R1887	R1888	R1889	R1890	R1891	R1892	R1893	R1894	R1895	R1896	R1897	R1898	R1899	R1900	R1901	R1902	R1903	R1904	R1905	R1906	R1907	R1908	R1909	R1910	R1911	R1912	R1913	R1914	R1915	R1916	R1917	R1918	R1919	R1920	R1921	R1922	R1923	R1924	R1925	R1926	R1927	R1928	R1929	R1930	R1931	R1932	R1933	R1934	R1935	R1936	R1937	R1938	R1939	R1940	R1941	R1942	R1943	R1944	R1945	R1946	R1947	R1948	R1949	R1950	R1951	R1952	R1953	R1954	R1955	R1956	R1957	R1958	R1959	R1960	R1961	R1962	R1963	R1964	R1965	R1966	R1967	R1968	R1969	R1970	R1971	R1972	R1973	R1974	R1975	R1976	R1977	R1978	R1979	R1980	R1981	R1982	R1983	R1984	R1985	R1986	R1987	R1988	R1989	R1990	R1991	R1992	R1993	R1994	R1995	R1996	R1997	R1998	R1999	R2000

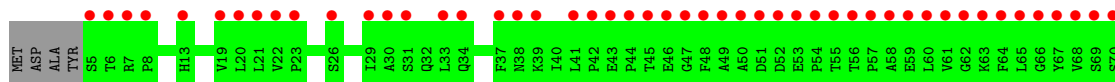




• Molecule 2: Fatty acid synthase subunit beta



Chain 1:



L171	V72	E73	F74	V77	G78	Q79	F80	D81	Q82	V83	L84	N85	L86	C87	L88	T89	E90	F91	C94	E95	N98	D100	H101	I102	A103	L104	A105	A106	A107	L108	L109	Q110	E111	N112	D113	T114	T115	L116	V117	K118	T119	K120	E121	L122	I123	I124	N125	Y126	I127	T128	A129	R130	I131	M132	A133	K134							
R135	F136	F137	K140	S141	N142	S143	L144	L145	A148	G149	N153	C154	D155	D156	A158	I159	F160	G161	G162	G163	G164	N165	T166	D167	D168	Y169	F170	R174	Y177	Q178	T179	Y180	H181	V182	L183	V184	G185	D186	L187	I188	E189	L190	V191	F192	F193	S194	H195	S196	E197	R198	D199	D200	D204	A205									
Q211	N214	L215	E217	W218	L219	N224	P225	D227	N153	D229	Y230	L231	L232	S233	L236	S237	G161	C162	P238	L240	L241	T166	G242	Q245	L246	A247	H248	Y249	V250	V251	W254	L255	L256	H181	V182	G257	F258	T259	P260	L263	R264	K355	L188	R264	T356	N357	F190	S191	A192	E193	S196	E197	T279	T283	A284	E285	T286	D287					
S288	W289	E290	F293	I300	T301	V302	L303	F305	R309	C310	K228	Y311	D229	Y230	L231	L232	S233	L236	S237	G161	C162	P238	L240	L241	T166	G242	Q245	L246	A247	H248	Y249	V250	V251	W254	L255	L256	H181	V182	G257	F258	T259	P260	L263	R264	K355	L188	R264	T356	N357	F190	S191	A192	E193	S196	E197	T279	T283	A284	E285	T286	D287		
S369	L370	V371	N372	G373	A374	K375	N376	L377	V380	F305	R309	C310	K228	Y311	D229	Y230	L231	L232	S233	L236	S237	G161	C162	P238	L240	L241	T166	G242	Q245	L246	A247	H248	Y249	V250	V251	W254	L255	L256	H181	V182	G257	F258	T259	P260	L263	R264	K355	L188	R264	T356	N357	F190	S191	A192	E193	S196	E197	T279	T283	A284	E285	T286	D287
N447	V448	S449	F450	M451	G455	I457	P458	D461	T462	F305	R309	C310	K228	Y311	D229	Y230	L231	L232	S233	L236	S237	G161	C162	P238	L240	L241	T166	G242	Q245	L246	A247	H248	Y249	V250	V251	W254	L255	L256	H181	V182	G257	F258	T259	P260	L263	R264	K355	L188	R264	T356	N357	F190	S191	A192	E193	S196	E197	T279	T283	A284	E285	T286	D287
V497	V498	S499	F500	M501	G505	I507	P508	D512	T513	F305	R309	C310	K228	Y311	D229	Y230	L231	L232	S233	L236	S237	G161	C162	P238	L240	L241	T166	G242	Q245	L246	A247	H248	Y249	V250	V251	W254	L255	L256	H181	V182	G257	F258	T259	P260	L263	R264	K355	L188	R264	T356	N357	F190	S191	A192	E193	S196	E197	T279	T283	A284	E285	T286	D287
R514	N519	K520	D521	G522	T523	R526	V527	S528	L533	D534	L535	N536	P537	D538	D539	D540	Y541	G542	F543	K544	K545	E546	F547	F548	D549	V550	T551	S552	V553	G554	L555	K556	K557	N558	P559	N560	Y561	L562	E563	E564	Y565	H566	L567	F568	F569	K568	L569	L570	K576	G588	R589	P590	F591	G708									
L592	P595	G596	M597	T598	P599	C600	T601	V602	S603	P604	D605	A608	A609	L533	D534	L535	N536	P537	D538	D539	D540	Y541	G542	F543	K544	K545	E546	F547	F548	D549	V550	T551	S552	V553	G554	L555	K556	K557	N558	P559	N560	Y561	L562	E563	E564	Y565	H566	L567	F568	F569	K568	L569	L570	K576	G588	R589	P590	F591	G708				
Q715	K721	A722	T732	T733	G734	R735	R736	G737	P738	G739	H740	F743	E744	D745	A746	H747	T748	Q752	M753	Y754	S755	G756	A757	R759	W762	G770	S771	F771	G772	S773	A774	D775	D776	T782	W785	P792	G684	V685	K901	P902	M903	G909	Q910	A911	S923	M930	I907																
A808	K809	E810	V811	K812	T813	S814	P815	D816	A817	K818	K819	C820	A823	D829	W832	E833	G841	G842	T845	V846	R847	S848	E849	T854	H855	A858	F873	K879	L880	V881	P882	S883	A887	D888	F889	Q900	K901	P902	M903	G909	Q910	A911	S923	M930	I907																		
R833	S834	W838	V841	T842	V858	E856	K962	S865	Q868	D874	D877	E878	E881	F884	R891	E892	Q893	N896	A897	Q898	D899	H1002	P1016	V1020	L1021	D1022	E1026	D1032	S1033	L1034	W1035	Q1036	E1041	A1042	V1043	V1044	D1047	V1048	Q1049	T1051																							
G1052	T1053	L1054	H1055	G1056	P1057	V1058	A1059	A1060	Q1061	F1062	E1068	P1069	I1073	M1074	D1075	H1078	D1079	K1083	H1087	Q1088	V1089	Y1090	G1091	M1091	D1092	D1093	E1094	E1101	G1104	G1105	E1106	S1107	D1110	VAL	GLN	SER	GLN	VAL	ASP	SER	SER	SER	VAL	S1121	K1128	S1132	T1133	D1134	E1135	E1136													
A1141	L1142	A1143	G1144	S1145	V1149	L1155	Q1156	S1157	Q1161	F1165	V1166	S1167	M1168	P1169	K1172	V1173	F1174	K1175	P1176	S1177	Q1178	G1179	M1180	V1181	G1187	K1192	T1193	E1199	P1200	V1201	Q1202	G1203	E1204	P1207	T1208	L1214	N1217	M1226	R1227	M1241	D1245	A1249	V1368																				
M1255	Y1266	L1269	M1270	N1276	L1277	D1278	P1281	K1288	D1289	A1294	S1167	M1168	P1169	H1078	D1079	K1083	H1087	Q1088	V1089	Y1090	G1091	M1091	D1092	D1093	E1094	E1101	G1104	G1105	E1106	S1107	D1110	VAL	GLN	SER	GLN	VAL	ASP	SER	SER	VAL	S1121	K1128	S1132	T1133	D1134	E1135	E1136																









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.92Å 430.31Å 422.61Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	192.50 – 4.60 192.50 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (192.50-4.60) 99.6 (192.50-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 4.66Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.252 , 0.310 0.328 , 0.345	Depositor DCC
$R_{free}$ test set	22715 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	218.0	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	231252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	256.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	1.22	1/8663 (0.0%)	1.73	6/12042 (0.0%)
1	B	1.23	1/8663 (0.0%)	1.73	6/12042 (0.0%)
1	C	1.23	1/8663 (0.0%)	1.73	6/12042 (0.0%)
1	D	1.22	0/8663	1.73	6/12042 (0.0%)
1	E	1.23	1/8663 (0.0%)	1.73	8/12042 (0.1%)
1	F	1.23	0/8663	1.73	6/12042 (0.0%)
1	a	1.23	0/8663	1.74	10/12042 (0.1%)
1	b	1.23	1/8663 (0.0%)	1.74	7/12042 (0.1%)
1	c	1.23	0/8663	1.74	6/12042 (0.0%)
1	d	1.23	0/8663	1.74	4/12042 (0.0%)
1	e	1.23	1/8663 (0.0%)	1.74	4/12042 (0.0%)
1	f	1.22	0/8663	1.73	7/12042 (0.1%)
2	G	1.25	0/10042	1.69	0/13972
2	H	1.25	0/10042	1.69	0/13972
2	I	1.25	0/10041	1.70	0/13969
2	J	1.24	0/10042	1.69	0/13972
2	K	1.24	0/10042	1.69	0/13972
2	L	1.24	0/10042	1.69	0/13972
2	g	1.24	0/10042	1.70	0/13972
2	h	1.24	0/10042	1.69	0/13972
2	i	1.25	0/10042	1.69	1/13972 (0.0%)
2	j	1.25	0/10042	1.69	0/13972
2	k	1.25	0/10042	1.69	0/13972
2	l	1.25	0/10042	1.69	0/13972
3	M	1.28	0/555	1.83	0/768
3	N	1.28	0/555	1.83	0/768
3	O	1.29	0/555	1.83	0/768
3	P	1.29	0/555	1.83	0/768
3	Q	1.28	0/555	1.83	0/768
3	R	1.29	0/555	1.83	0/768
3	m	1.28	0/555	1.82	0/768
3	n	1.28	0/555	1.83	0/768
3	o	1.28	0/555	1.83	0/768
3	p	1.28	0/555	1.82	0/768

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	q	1.28	0/555	1.82	0/768
3	r	1.29	0/555	1.83	0/768
All	All	1.24	6/231119 (0.0%)	1.72	77/321381 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	a	0	3
1	b	0	3
1	c	0	3
1	d	0	3
1	e	0	3
1	f	0	3
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
2	k	0	1
2	l	0	1
All	All	0	48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	180	SER	C-O	7.44	1.33	1.24
1	e	180	SER	C-O	6.07	1.31	1.24
1	B	180	SER	CA-CB	5.76	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	180	SER	C-O	5.57	1.30	1.24
1	A	180	SER	C-O	5.55	1.30	1.24

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	179	LYS	CB-CA-C	-10.09	104.93	116.63
1	E	178	GLY	CA-C-N	7.34	135.56	121.54
1	E	178	GLY	C-N-CA	7.34	135.56	121.54
1	a	175	LEU	CA-C-N	6.53	131.85	122.45
1	a	175	LEU	C-N-CA	6.53	131.85	122.45

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1584	PRO	Peptide
1	A	237	MET	Peptide
1	A	879	SER	Peptide
1	B	237	MET	Peptide
1	B	879	SER	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	8667	0	4008	12	0
1	B	8667	0	4008	12	0
1	C	8667	0	4008	12	0
1	D	8667	0	4008	14	0
1	E	8667	0	4008	9	0
1	F	8667	0	4008	16	0
1	a	8667	0	4008	11	0
1	b	8667	0	4008	14	0
1	c	8667	0	4008	12	0
1	d	8667	0	4008	14	0
1	e	8667	0	4008	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	8667	0	4008	11	0
2	G	10046	0	4474	8	1
2	H	10046	0	4474	6	0
2	I	10046	0	4473	10	3
2	J	10046	0	4474	7	0
2	K	10046	0	4474	9	0
2	L	10046	0	4474	7	0
2	g	10046	0	4474	6	0
2	h	10046	0	4474	10	1
2	i	10046	0	4474	6	0
2	j	10046	0	4474	6	3
2	k	10046	0	4474	8	0
2	l	10046	0	4474	8	0
3	M	558	0	252	0	0
3	N	558	0	252	0	0
3	O	558	0	252	0	0
3	P	558	0	252	1	0
3	Q	558	0	252	0	0
3	R	558	0	252	1	0
3	m	558	0	252	0	0
3	n	558	0	252	0	0
3	o	558	0	252	1	0
3	p	558	0	252	0	0
3	q	558	0	252	1	0
3	r	558	0	252	0	0
All	All	231252	0	104807	223	4

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 1.

The worst 5 of 223 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:F:180:SER:HA	1:F:183:GLN:CB	1.69	1.19
2:I:1971:GLY:C	2:I:1972:ILE:N	2.00	1.19
1:F:180:SER:O	1:F:184:ASN:N	1.87	1.07
1:B:180:SER:HA	1:B:183:GLN:CB	1.94	0.97
1:D:180:SER:HA	1:D:183:GLN:CB	1.99	0.93

All (4) 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)
2:G:1929:LYS:CB	2:h:1399:ASN:O[2_645]	1.63	0.57
2:I:1929:LYS:O	2:j:444:VAL:CB[1_655]	1.72	0.48
2:I:1929:LYS:O	2:j:444:VAL:CA[1_655]	2.16	0.04
2:I:1929:LYS:C	2:j:444:VAL:CB[1_655]	2.17	0.03

## 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	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	43 77
1	B	1752/1887 (93%)	1647 (94%)	101 (6%)	4 (0%)	43 77
1	C	1752/1887 (93%)	1651 (94%)	97 (6%)	4 (0%)	43 77
1	D	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	43 77
1	E	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	36 71
1	F	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	36 71
1	a	1752/1887 (93%)	1647 (94%)	99 (6%)	6 (0%)	36 71
1	b	1752/1887 (93%)	1649 (94%)	99 (6%)	4 (0%)	43 77
1	c	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	36 71
1	d	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	43 77
1	e	1752/1887 (93%)	1650 (94%)	97 (6%)	5 (0%)	36 71
1	f	1752/1887 (93%)	1649 (94%)	99 (6%)	4 (0%)	43 77
2	G	2029/2051 (99%)	1901 (94%)	120 (6%)	8 (0%)	30 67
2	H	2029/2051 (99%)	1900 (94%)	121 (6%)	8 (0%)	30 67
2	I	2027/2051 (99%)	1902 (94%)	117 (6%)	8 (0%)	30 67
2	J	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	30 67
2	K	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	30 67
2	L	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	30 67
2	g	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	2029/2051 (99%)	1900 (94%)	121 (6%)	8 (0%)	30	67
2	i	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	30	67
2	j	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	30	67
2	k	2029/2051 (99%)	1901 (94%)	120 (6%)	8 (0%)	30	67
2	l	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	30	67
3	M	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	N	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	O	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	P	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	Q	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	R	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	m	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	n	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	o	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	p	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	q	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
3	r	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	14	49
All	All	46654/49056 (95%)	43793 (94%)	2699 (6%)	162 (0%)	36	71

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1304	ALA
1	B	1304	ALA
1	C	1304	ALA
1	D	1304	ALA
1	E	179	LYS

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	3
2	G	2
2	i	2
2	j	2
2	H	2
2	J	2
2	K	2
2	L	2
2	g	2
2	h	2
2	k	2
2	l	2

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	299:ALA	C	300:ILE	N	4.56
1	I	299:ALA	C	300:ILE	N	4.56
1	i	299:ALA	C	300:ILE	N	4.56
1	j	299:ALA	C	300:ILE	N	4.56
1	H	299:ALA	C	300:ILE	N	4.55

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1760/1887 (93%)	1.72	620 (35%) 1 3	111, 211, 438, 635	0
1	B	1760/1887 (93%)	1.78	640 (36%) 1 3	107, 216, 435, 651	0
1	C	1760/1887 (93%)	1.99	715 (40%) 0 2	122, 236, 466, 673	0
1	D	1760/1887 (93%)	1.79	648 (36%) 1 3	109, 208, 394, 609	0
1	E	1760/1887 (93%)	1.67	598 (33%) 1 4	115, 206, 386, 636	0
1	F	1760/1887 (93%)	1.97	717 (40%) 0 2	130, 229, 422, 813	0
1	a	1760/1887 (93%)	1.70	628 (35%) 1 3	110, 216, 416, 637	0
1	b	1760/1887 (93%)	1.92	668 (37%) 1 3	116, 216, 423, 674	0
1	c	1760/1887 (93%)	1.73	602 (34%) 1 4	116, 216, 398, 624	0
1	d	1760/1887 (93%)	1.91	685 (38%) 1 3	126, 226, 466, 854	0
1	e	1760/1887 (93%)	1.91	705 (40%) 0 2	120, 221, 442, 771	0
1	f	1760/1887 (93%)	1.69	600 (34%) 1 4	117, 207, 427, 597	0
2	G	2036/2051 (99%)	1.95	839 (41%) 0 2	49, 279, 395, 567	0
2	H	2036/2051 (99%)	2.15	918 (45%) 0 2	55, 284, 406, 514	0
2	I	2036/2051 (99%)	2.26	972 (47%) 0 2	51, 295, 399, 627	0
2	J	2036/2051 (99%)	1.63	646 (31%) 1 4	37, 219, 306, 450	0
2	K	2036/2051 (99%)	1.76	683 (33%) 1 4	48, 243, 350, 531	0
2	L	2036/2051 (99%)	1.83	757 (37%) 1 3	34, 252, 335, 519	0
2	g	2036/2051 (99%)	1.86	748 (36%) 1 3	39, 252, 359, 448	0
2	h	2036/2051 (99%)	1.72	687 (33%) 1 4	38, 229, 318, 416	0
2	i	2036/2051 (99%)	1.69	678 (33%) 1 4	43, 256, 340, 447	0
2	j	2036/2051 (99%)	2.03	853 (41%) 0 2	39, 265, 377, 499	0
2	k	2036/2051 (99%)	2.09	908 (44%) 0 2	40, 274, 383, 525	0
2	l	2036/2051 (99%)	2.20	894 (43%) 0 2	45, 240, 421, 717	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	M	113/150 (75%)	2.62	61 (53%) 0 1	275, 371, 473, 531	0
3	N	113/150 (75%)	2.48	63 (55%) 0 1	219, 329, 521, 654	0
3	O	113/150 (75%)	3.13	71 (62%) 0 1	278, 384, 520, 573	0
3	P	113/150 (75%)	1.95	43 (38%) 1 3	221, 299, 420, 523	0
3	Q	113/150 (75%)	2.36	59 (52%) 0 1	219, 342, 501, 595	0
3	R	113/150 (75%)	2.15	46 (40%) 0 2	258, 354, 440, 475	0
3	m	113/150 (75%)	2.62	70 (61%) 0 1	230, 335, 505, 561	0
3	n	113/150 (75%)	1.94	51 (45%) 0 2	198, 287, 476, 589	0
3	o	113/150 (75%)	2.33	56 (49%) 0 2	209, 341, 439, 549	0
3	p	113/150 (75%)	2.14	49 (43%) 0 2	216, 316, 430, 481	0
3	q	113/150 (75%)	2.41	54 (47%) 0 2	224, 349, 493, 560	0
3	r	113/150 (75%)	2.42	49 (43%) 0 2	220, 337, 511, 527	0
All	All	46908/49056 (95%)	1.89	18081 (38%) 1 3	34, 243, 401, 854	0

The worst 5 of 18081 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	f	141	ALA	21.2
1	C	140	ILE	19.6
2	I	1952	ALA	18.2
1	c	972	SER	16.8
1	C	141	ALA	16.4

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.