



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:07 am GMT

PDB ID : 4V59
Title : Crystal structure of fatty acid synthase complexed with nadp+ from thermomyces lanuginosus at 3.1 angstrom resolution.
Authors : JENNI, S.; LEIBUNDGUT, M.; BOEHRINGER, D.; FRICK, C.; MIKOLASEK, B.; BAN, N.
Deposited on : 2007-03-09
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28972

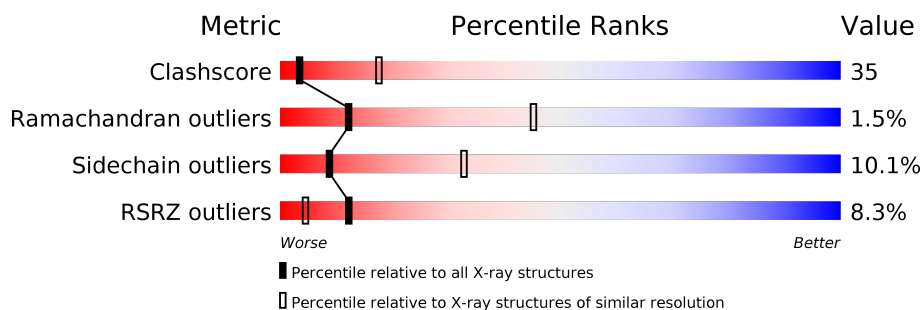
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1878	
1	B	1878	
1	C	1878	
1	D	1878	
1	E	1878	
1	F	1878	
2	G	2060	

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Mol	Chain	Length	Quality of chain
2	H	2060	
2	I	2060	
2	J	2060	
2	K	2060	
2	L	2060	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMN	G	2101	-	-	X	-
4	FMN	H	2101	-	-	X	-
4	FMN	I	2101	-	-	X	-
4	FMN	J	2101	-	-	X	-
4	FMN	K	2101	-	-	X	-
4	FMN	L	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 167247 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 ALPHA SUBUNITS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1457	Total	C	N	O	S	0	0	0
			11514	7290	2005	2170	49			
1	B	1464	Total	C	N	O	S	0	0	0
			11571	7323	2015	2183	50			
1	C	1462	Total	C	N	O	S	0	0	0
			11555	7312	2012	2181	50			
1	D	1467	Total	C	N	O	S	0	0	0
			11593	7336	2021	2186	50			
1	E	1456	Total	C	N	O	S	0	0	0
			11506	7285	2004	2169	48			
1	F	1461	Total	C	N	O	S	0	0	0
			11546	7307	2010	2179	50			

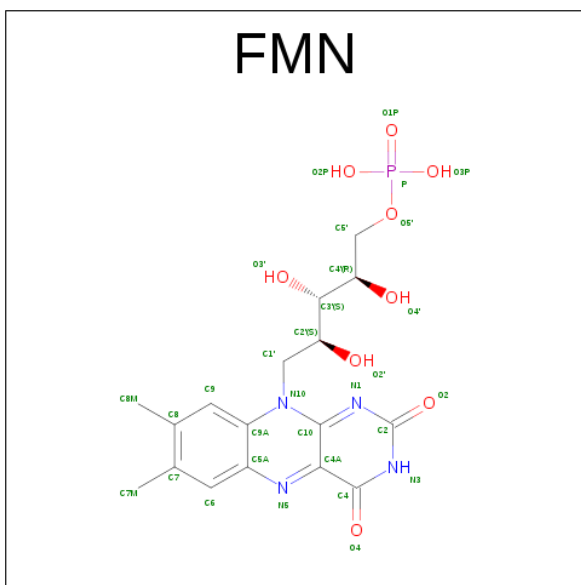
- Molecule 2 is a protein called FATTY ACID SYNTHASE BETA SUBUNITS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	H	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	I	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	J	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	K	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	L	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

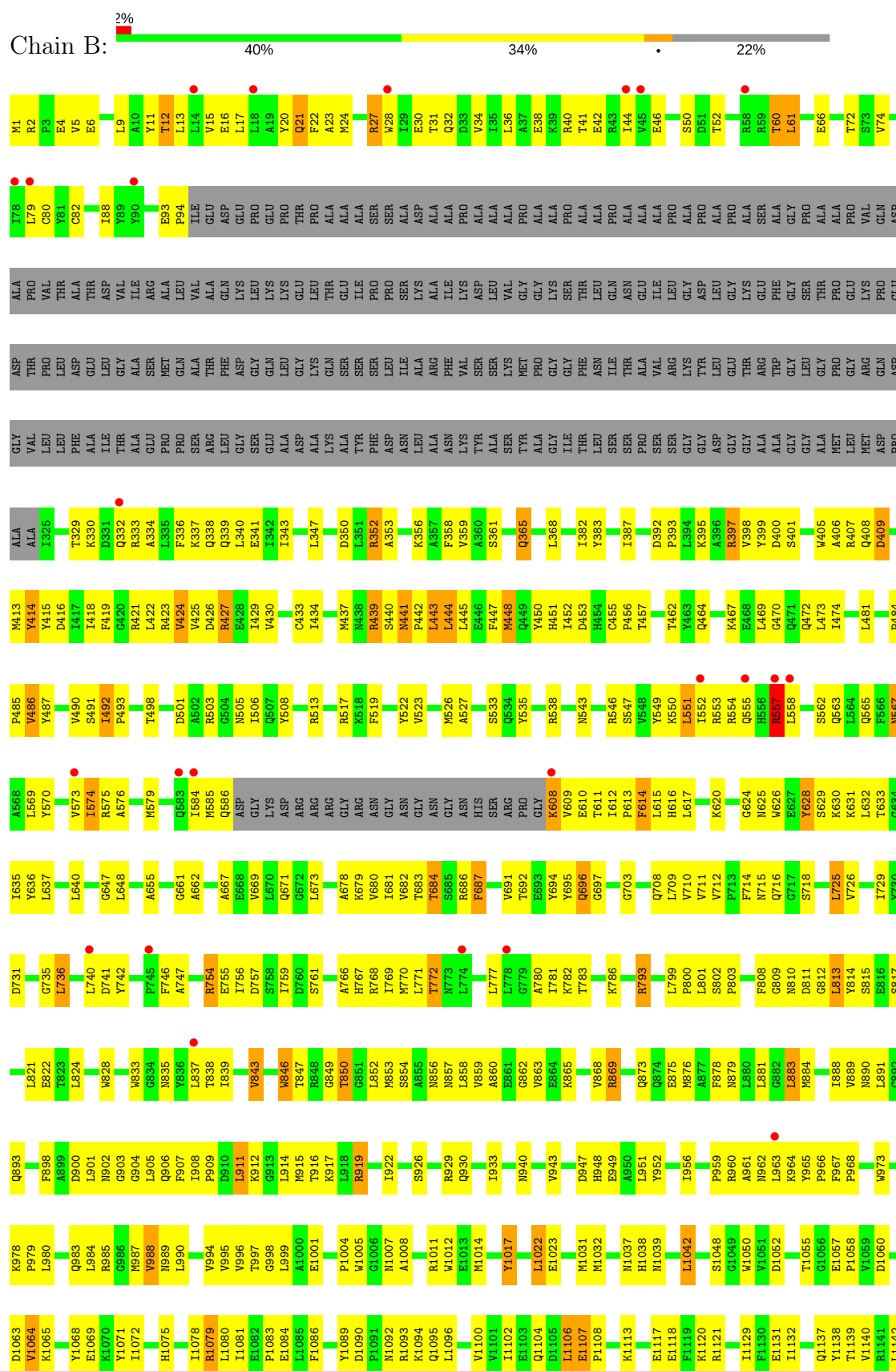


- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

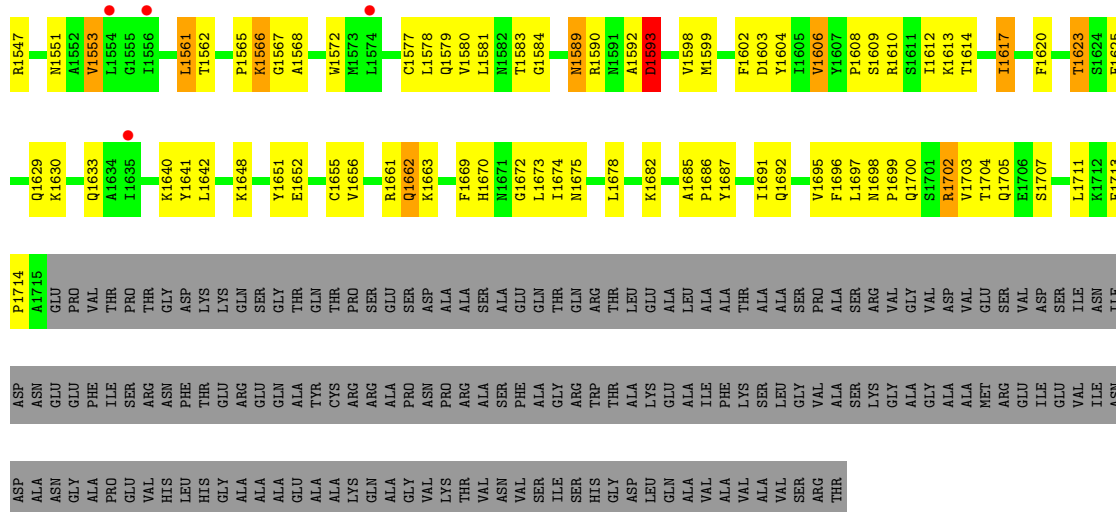


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	K	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	L	1	Total 31	C 17	N 4	O 9	P 1	0	0

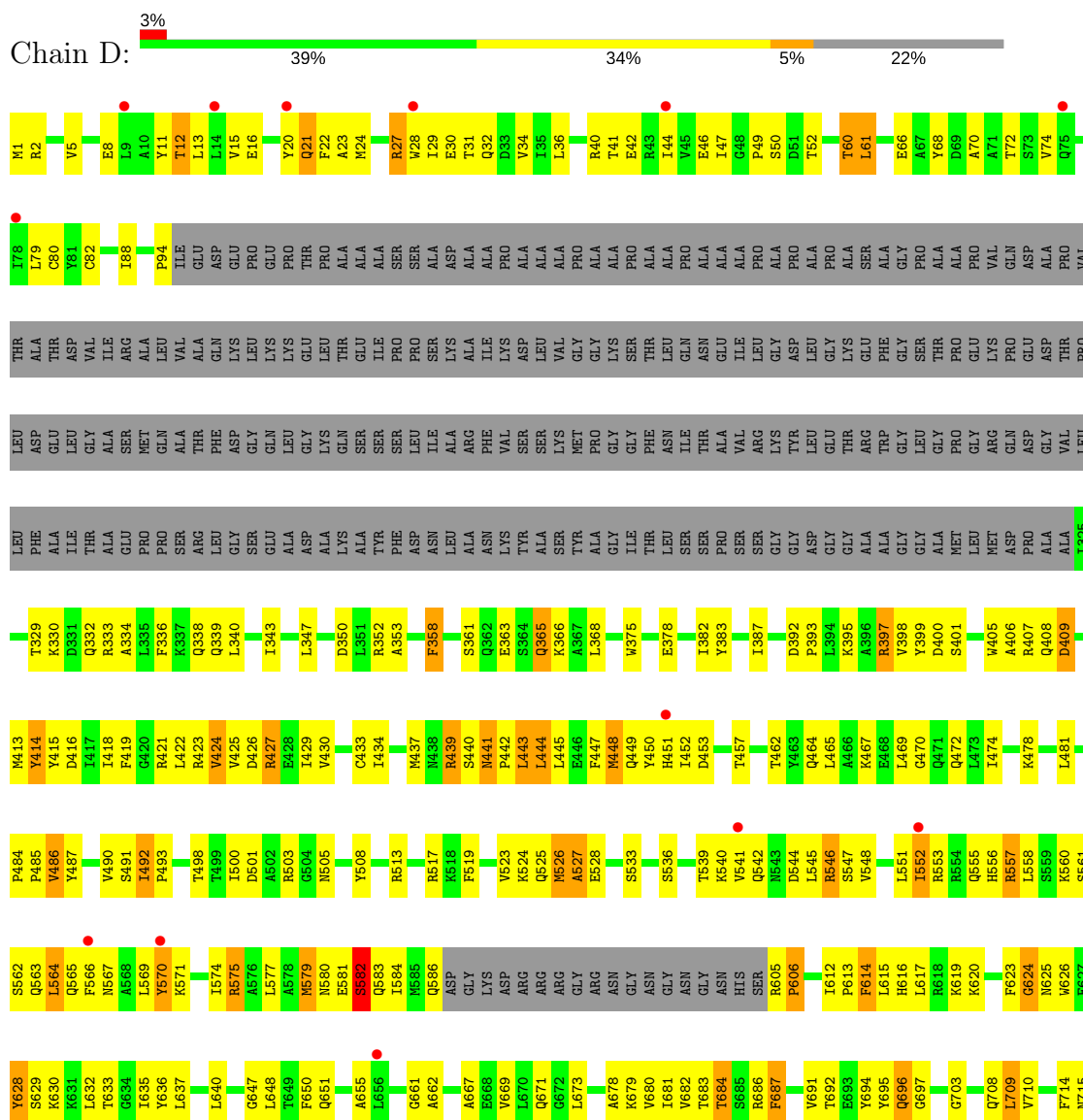
- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



R1468	T1386	G1306	S1216	T1139	V1059	W973	C892	L821	D731	K630	F566	Y487	D416	I325
E1469		F1307	E1217	V1140	D1060	W973	Q893	E822	G735	K631	N567		I417	T329
R1470	I1389	R1308	V1218	R1141	K1061	K978	F898	L824	G736	L632	A568	V490	F418	K330
R1473		D1309	G1223	L1142	K1063	P979	A899		L736	T633	L569		F419	
I1474	V1393	F1310	S1224	A1146	V1064	L980	D900	W828	L740	G634	Y570	P493	R421	Q332
E1475	P1394	Q1311	G1225	T1147	K1065	Q983	N902	E831	D741	L635	W573		L422	R333
R1476	A1395	E1312	W1226	L1148	Y1068	L984	G903	S832	Y742	G636	L574	T498	R423	A334
	P1396	E1313		T1150	E1069	R985	G904	W833	V743	L640	A576	T499	V424	L335
R1480			T1229			G986	L905		P745		L577	I500	V425	F336
Q1481	L1401	Y1316			I1072	W987	Q906	L837	F746	G647	W578	A502	D426	X337
E1482	T1402	E1317	L1232	A1153	H1075	W988	P907	T838	A747	L648	W579	R503	R427	Q338
A1483	T1403	R1233	G1234	L1154		N989	I908	L839			W580	G504	E428	Q339
E1484	A1404	G1323		G1155		L990	P909		E751	A655			I429	
A1485	R1405	W1235		D1157	I1078			W843			Q583	N505	V430	T343
Q1486		Y1236		R1158	R1079	W995	L911	R844	R754	A662		I506		
T1487		L1159		L1159	L1080	W996		R845	E755		L584		C433	D350
A1488	P1414	V1160		V1160	I1081	T997	L914	W846	E756	A667	W585	R513	I434	L351
F1489		A1161		A1161	E1082	Q998	M915	T847	I756		O586		M437	R352
Q1490	I1418	L1249		G1162	P1083	L999	T916	R848	D757	E668	ASP	R517	M438	A353
	K1419	L1250		Q1163	E1084	L999	T916	R848	S758	V669	GLY	K519	M439	
	Y1420	Q1251		Q1163	E1084	L999	T916	R848	I759	V669	LYS	F519	R439	F358
R1491	R1422	E1252		T1164	L1085	E1001	K917	T850	D760	Q671	ASP	S440	S440	
W1494		S1253		P1165	F1086		R919	G851	S761	G672	ARG	Y522	N441	S361
R1495		F1254		T1166		P1004		L852		L673	ARG	Y523	P442	
R1496				G1167	Y1089	W1005		R853	A766		ARG		L443	Q365
	L1425	T1257		W1168	D1090	G1006	I922	S854	H767	A678	GLY	M526	L444	
R1499	E1426	M1258		L1169	P1091	G1006		R854	R768	K679	ARG	A527		L368
I1500	L1427	A1259		L1170	N1092	W1007	S926	R855	I769	V680	ASN	E528	F447	
A1501	R1428	A1260		R1171	K1093	A1008	R929	R856	M770	V681	GLY	G529	M448	W375
	R1429	A1261		R1172	K1094	R1011	Q930	R858	L771	V682	ASN		Q449	
R1504	Q1430	W1264		R1173	K1095	R1012		R859	T772	T683	GLY	S533	Q449	D381
G1505	Q1431			Y1175	L1096	W1013	I933	A860		T684	ASN	Q534	H450	D382
A1506		L1267		G1174	L1097	E1013		R861	L777	S685	GLY	Y535	H451	L382
A1508	W1435	S1268		P1176	L1097	M1014	N940	R862	A780	R686	GLY	S536	I452	Y383
T1509	Y1440	S1269		E1177	V1100	Y1017	V942	R863	I781	F687	HIS	N537	D453	A384
W1510		T1270		L1178	I1102	L1022		R864	K782		SER	E538	T457	L387
G1511	L1443	G1271		L1179	E1103	E1023	E946	R865	I783	V691	ARG		E458	
L1512	Q1444	P1272		L1180	K1104		D947			T692	PRO	N543	T462	D392
I1513	E1446	I1273		V1183	D1105	M1031	H948	W869	K786	E693	GLY	D544	Y463	P393
I1514	E1447	T1274		D1184	L1106	M1032	E949	T870		Y694	LYS	L545	L394	L394
	V1447	P1276		P1185	E1107		A960	R871	R793	Q696	VAL	R546	Q464	X395
	A1448	W1277		V1186	P1108	N1037	L951	S872		G697	E610	S547	L465	A396
A1449		G1278		T1187	K1113	H1038	Y952	Q873	L799		T611	W548	A466	R397
K1451		A1279		L1188	E1117	M1039	R953	R874	P800	Q708	I612	Y549	K457	Y398
		C1280		L1191	E1118		R954	E875	L801	L709	F614	K550	L469	Y399
		A1281		L1192	W1104	K1043	Y955	W876		V710	L615	I552	G470	D400
		T1282		L1193	E1119		I956	R877	N804		H616	R553	Q471	S401
		D1288		L1198	K1120	S1048	P959	F878		F714	L617	R554	Q472	W405
				L1199	R1121	W1049	R960		G809	W715	K620	Q555	Q473	W406
		T1293		Y1207	E1121	G1049	A961	L881	N810	Q716		H556	I474	W407
				E1208	T1129	W1050	A961	G882	D811			R557	L474	Q408
		K1298		F1209	E1130	V1051	N962	L883	G812	Q720	F623		K478	D409
		R1300		E1131	L1132	D1052	L963	W884	L813	L725	G624	K560	L481	A410
		Y1212		L1132		T1055	K964	T888	Y814	W726	R625	S561	L481	L411
		V1213		Q1137		G1056	P966	W889	S815		W626	S562	P464	S412
		H1214		Q1137		E1057	P967	W890	E817	I729	E627	Q563	P464	W413
		L1215		Y1138		P1058	P968	L891	S817	Y730	S629	L564	P465	W414
													V466	Y415

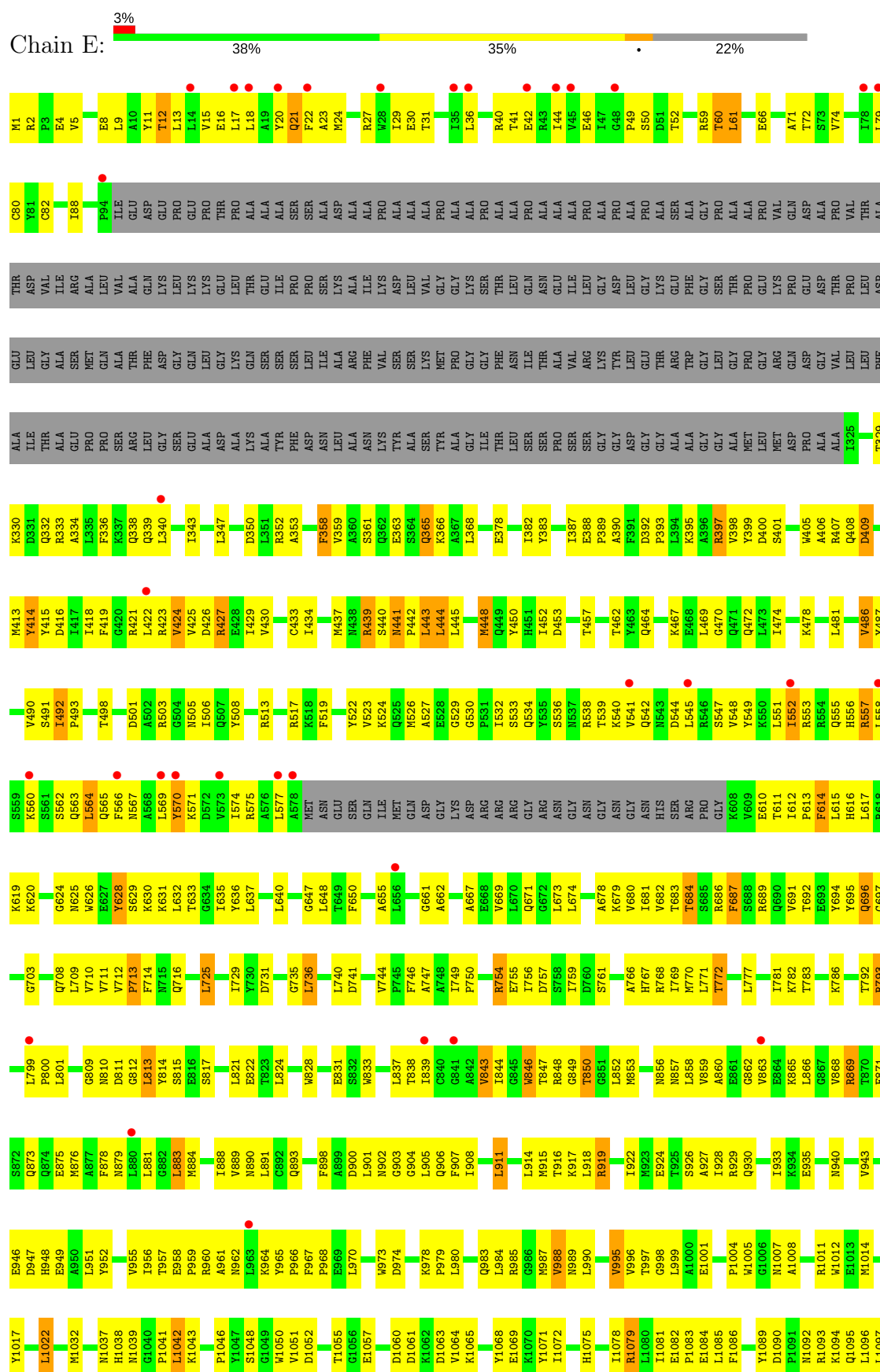


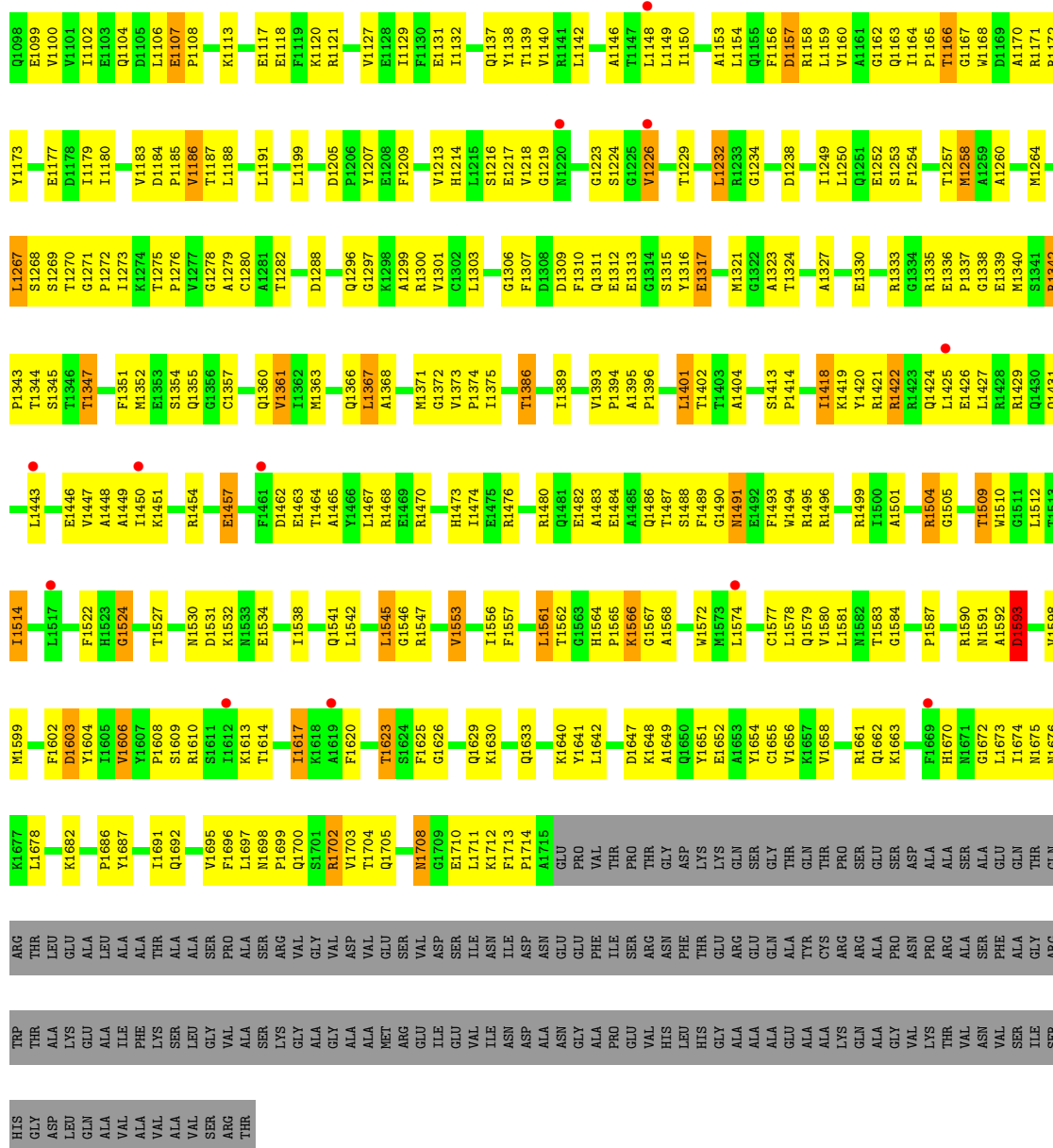
● Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



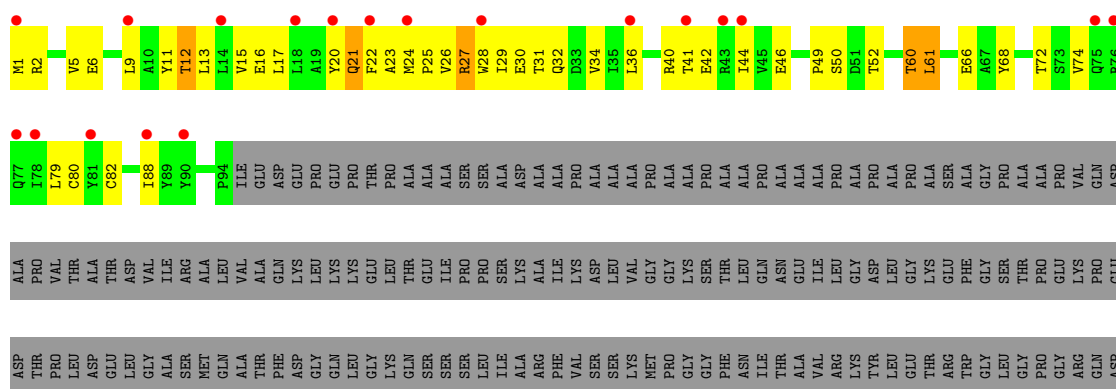
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GLY	VAL	S1701	I1617	N1533	D1462	I1362	D1288	Y1207	R1121	K1043	Y956	M876	P803	L725
ALA	ASP	R1702	I1617	E1534	T1463	M1363	T1293	E1208	R1121	K1043	I956	A877	P803	L725
MET	VAL	T1703	F1620	I1538	T1464	Q1366	T1293	E1209	E1129	S1048	P959	F878	G809	V726
ARG	VAL	Q1705	F1620	I1538	T1466	Q1367	Q1296	F1209	I1129	G1049	P959	F878	G809	V726
GLU	VAL	Q1705	F1620	I1538	T1466	Q1367	Q1296	F1209	I1129	G1049	P959	F878	G809	V726
GLU	VAL	Q1705	F1620	I1538	T1466	Q1367	Q1296	F1209	I1129	G1049	P959	F878	G809	V726
ILE	ASP	Q1708	T1623	Q1541	Y1466	A1368	Q1297	K1211	E1131	W1050	R960	L881	D811	I729
ILE	ASP	Q1708	T1623	Q1541	Y1466	A1368	Q1297	K1211	E1131	W1050	R960	L881	D811	I729
VAL	ASP	Q1708	T1623	Q1541	Y1466	A1368	Q1297	K1211	E1131	W1050	R960	L881	D811	I729
VAL	ASP	Q1708	T1623	Q1541	Y1466	A1368	Q1297	K1211	E1131	W1050	R960	L881	D811	I729
ILE	ASP	Q1711	S1624	L1545	R1467	L1369	Q1298	K1212	E1132	W1051	N962	L883	C812	I730
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ASN	ASN	F1713	G1626	L1545	R1469	M1371	R1300	H1214	Q1138	T1056	L963	M884	K964	S815
ASN	ASN	F1713	G1626	L1545	R1469	M1371	R1300	H1214	Q1138	T1056	L963	M884	K964	S815
ASN	ASN	F1713	G1626	L1545	R1469	M1371	R1300	H1214	Q1138	T1056	L963	M884	K964	S815
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ASP	ASP	P1714	K1630	R1547	R1470	G1372	C1302	S1216	T1139	E1057	P967	E887	E816	L736
ASN	ASN	A1715	G1631	V1553	H1473	P1374	L1303	E1217	V1140	P1058	P968	I888	S817	
ASN	ASN	A1715	G1631	V1553	H1473	P1374	L1303	E1217	V1140	P1058	P968	I888	S817	
ASN	ASN	A1715	G1631	V1553	H1473	P1374	L1303	E1217	V1140	P1058	P968	I888	S817	
GLY	GLU	Q1716	Q1633	G1556	R1476	D1387	F1307	G1223	L1142	D1061	W973	N890	E822	V742
GLY	GLU	Q1716	Q1633	G1556	R1476	D1387	F1307	G1223	L1142	D1061	W973	N890	E822	V742
ALA	PHE	THR	THR	L1556	R1480	I1388	D1308	G1226	T1147	D1063	K978	C892	L824	V744
ALA	PHE	THR	THR	L1556	R1480	I1388	D1308	G1226	T1147	D1063	K978	C892	L824	V744
PRO	THR	THR	THR	L1561	R1481	I1389	D1309	W1226	L1148	V1064	P979	Q893		V745
PRO	THR	THR	THR	L1561	R1481	I1389	D1309	W1226	L1148	V1064	P979	Q893		V745
GLU	THR	THR	THR	L1562	E1482	F1393	F1310	V1226	L1148	V1064	P979	Q893		V745
VAL	ARG	THR	THR	L1562	E1482	F1393	F1310	V1226	L1148	V1064	P979	Q893		V745
HIS	ASN	THR	THR	L1563	E1483	P1394	Q1311	W1226	L1148	V1064	P979	Q893		V745
LEU	PHE	ASP	ASP	G1564	E1484	P1394	Q1311	W1226	L1148	V1064	P979	Q893		V745
HIS	THR	LYS	THR	P1565	L1485	T1401	G1314	L1232	A1153	H1075	M987	G903		V745
GLY	GLU	LYS	THR	P1565	L1485	T1401	G1314	L1232	A1153	H1075	M987	G903		V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
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ALA	GLU	LYS	THR	P1566	Q1486	L1402	S1315	R1233	L1154					V745
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ALA	GLU													

- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS

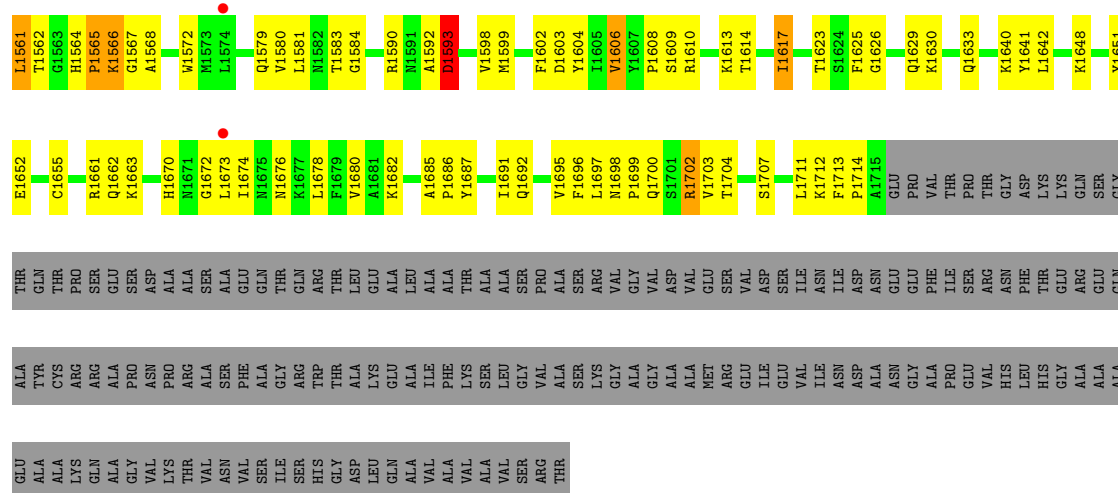




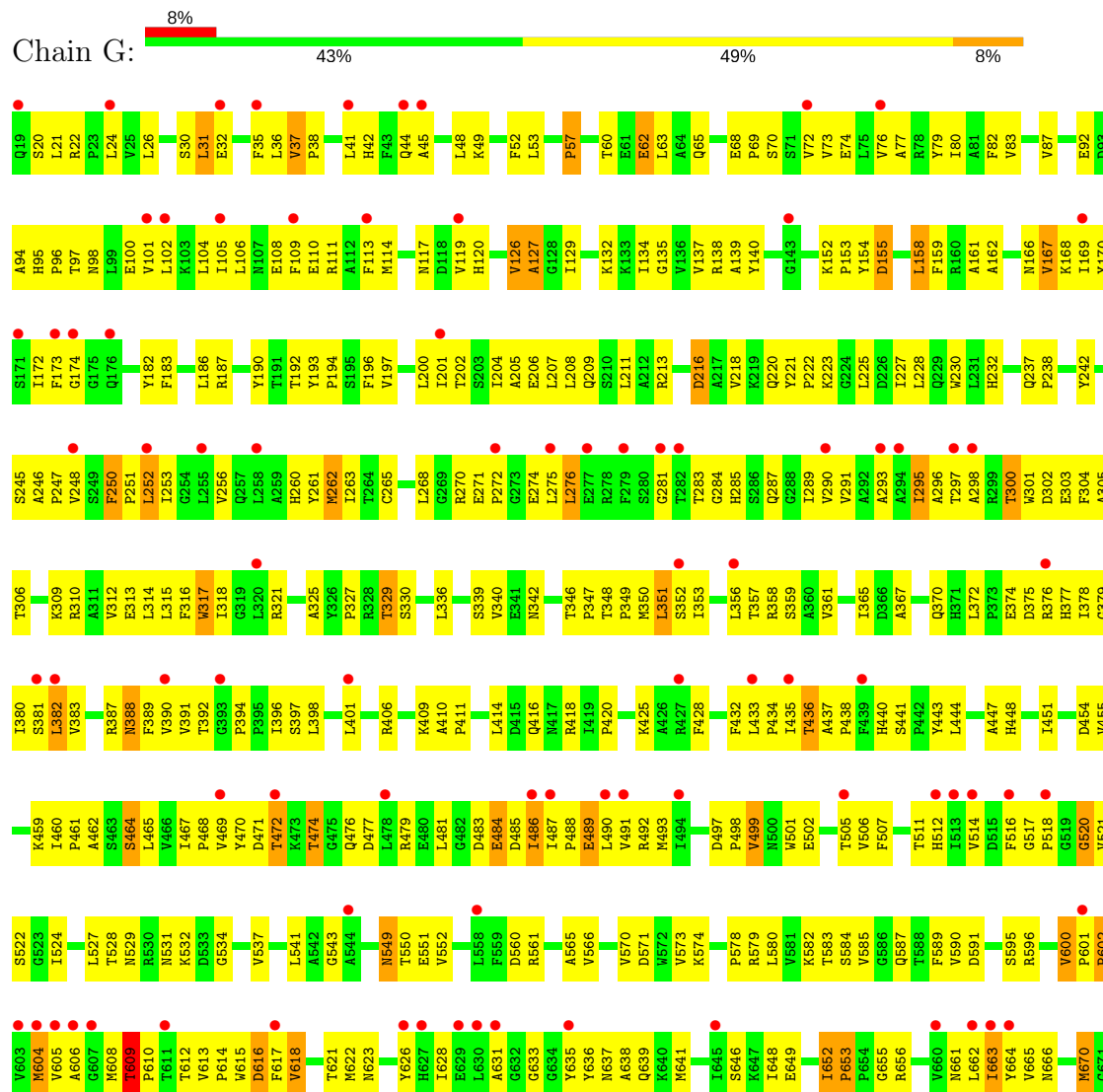
• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



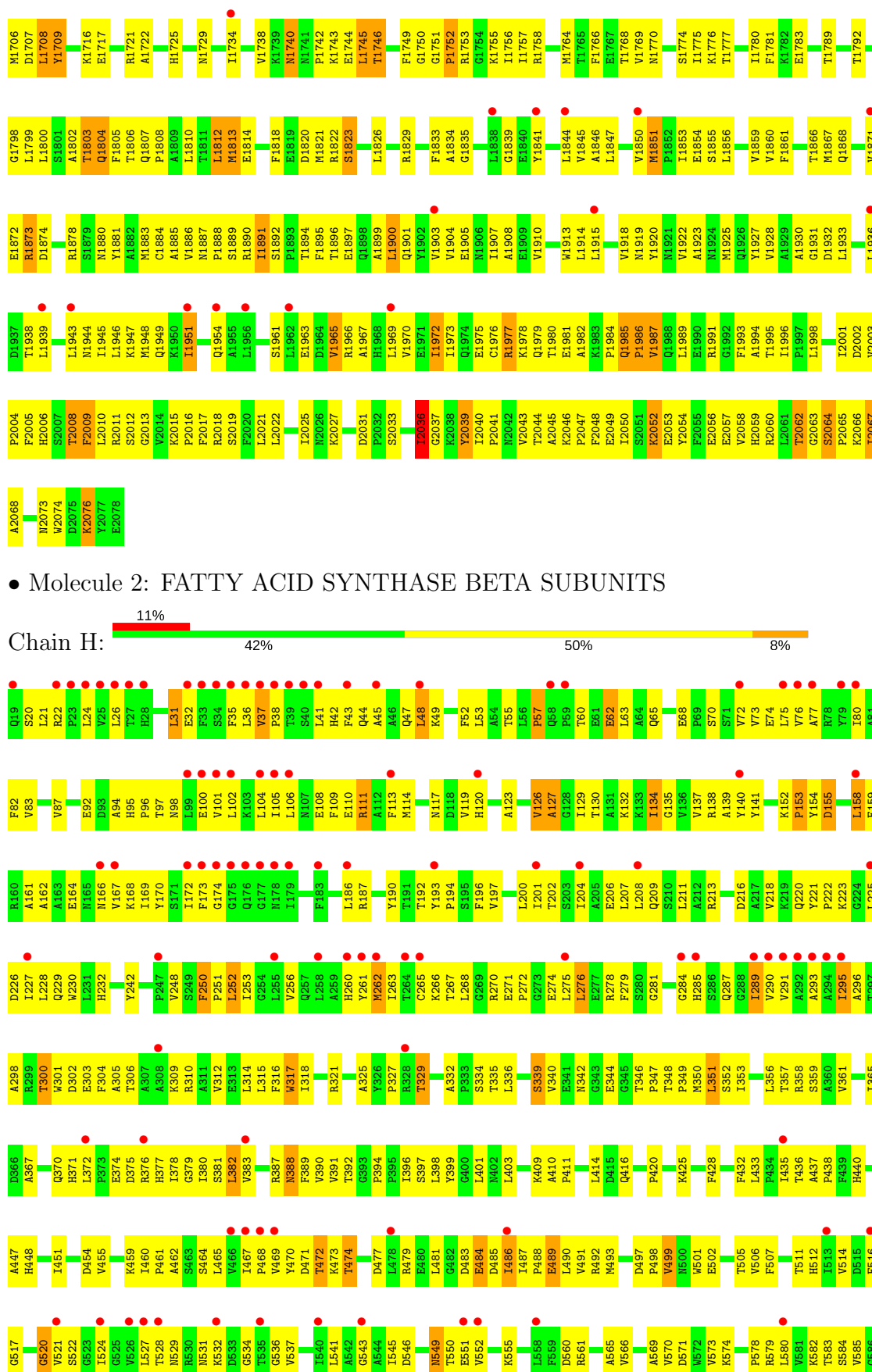
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F1540	L1196	L1271	L1196	L1110	M1041	A961	T876	D787	V702	GLY	R557	R455	ALA	GLY
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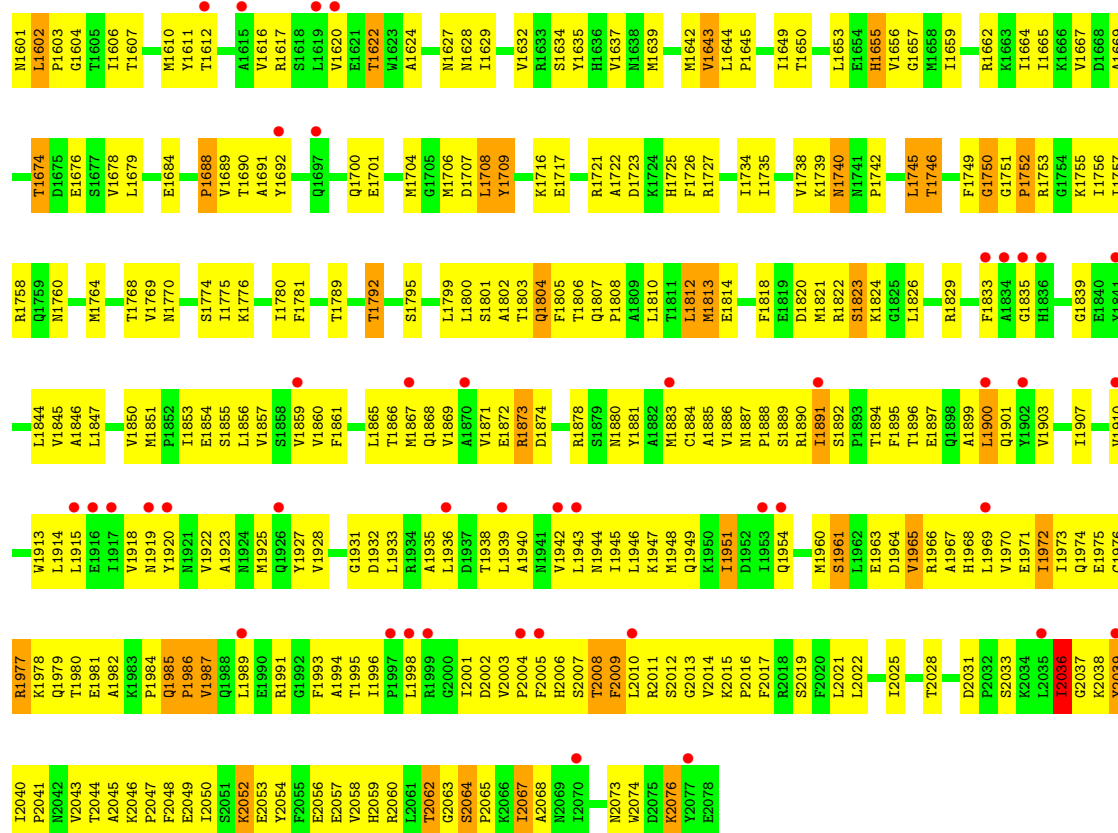
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



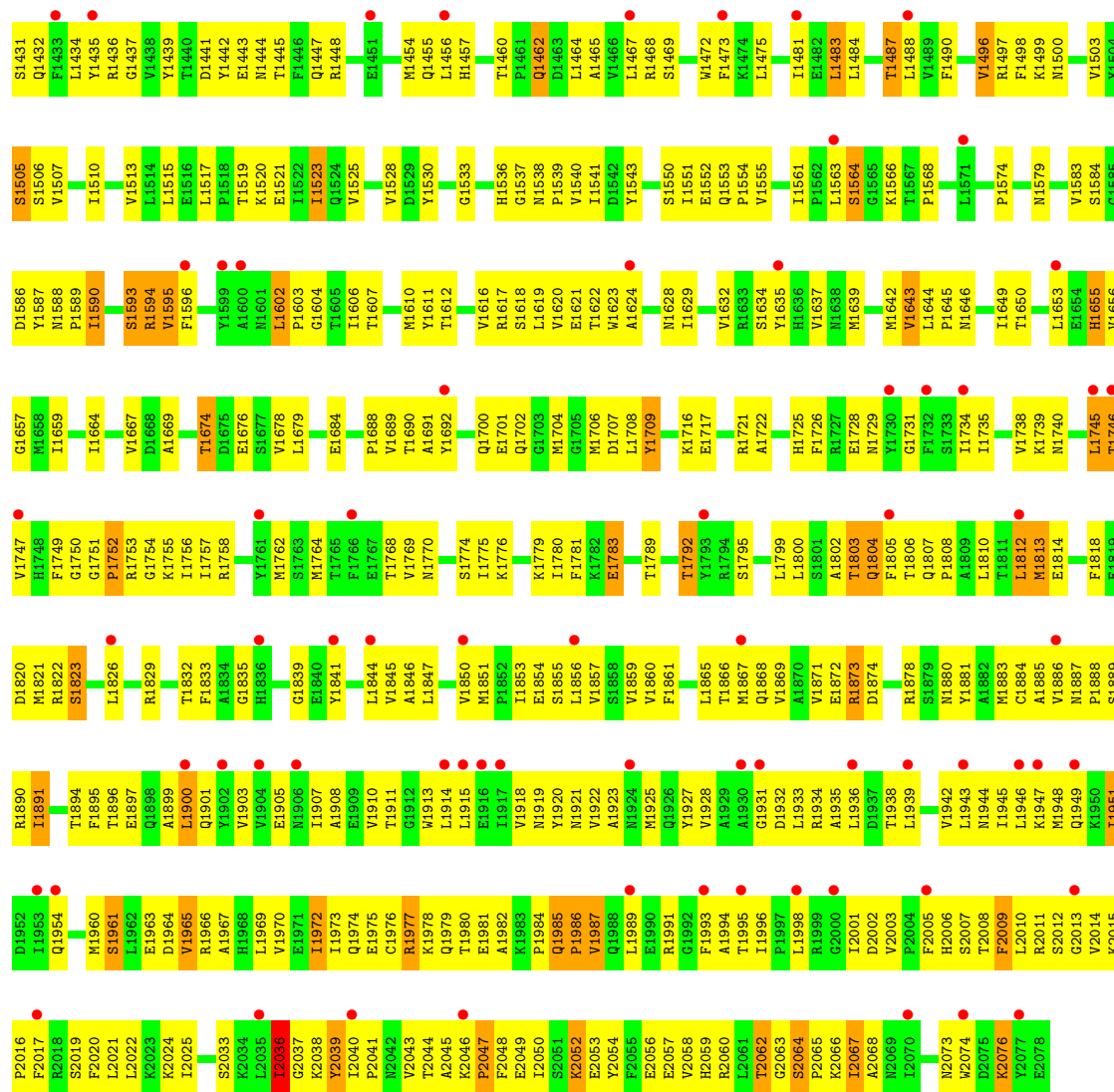
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	Q1447		N1378	T1378	N1240	N1240	W1171	P1082	Q1011	M938	K867	I736	
Q1700	R1448		G1379	A1318	L1242	L1242	I1083	K1084	Q1012		L868	P738	
E1701			Y1380	Q1319	A1243	A1243	K1084	D1085	Q1013	L941	A869	P738	
	M1454		Q1455	A1320	L1244	L1244	D1085	Q1014	Q1014	N942	T870	I739	
M1704	S1535		V1383	V1321	T1245	T1245	I1086	H1015	F806	Y943	R871	I740	
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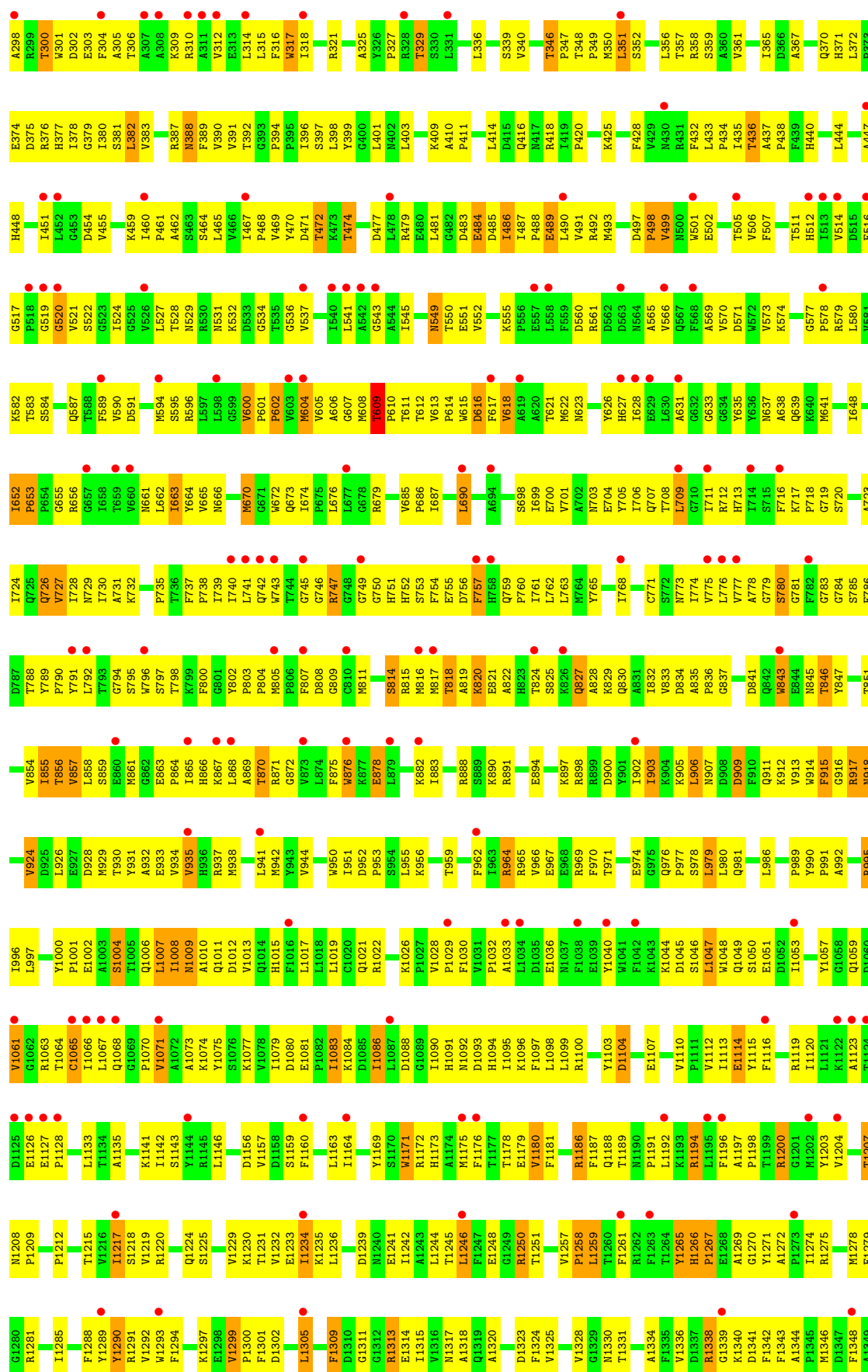


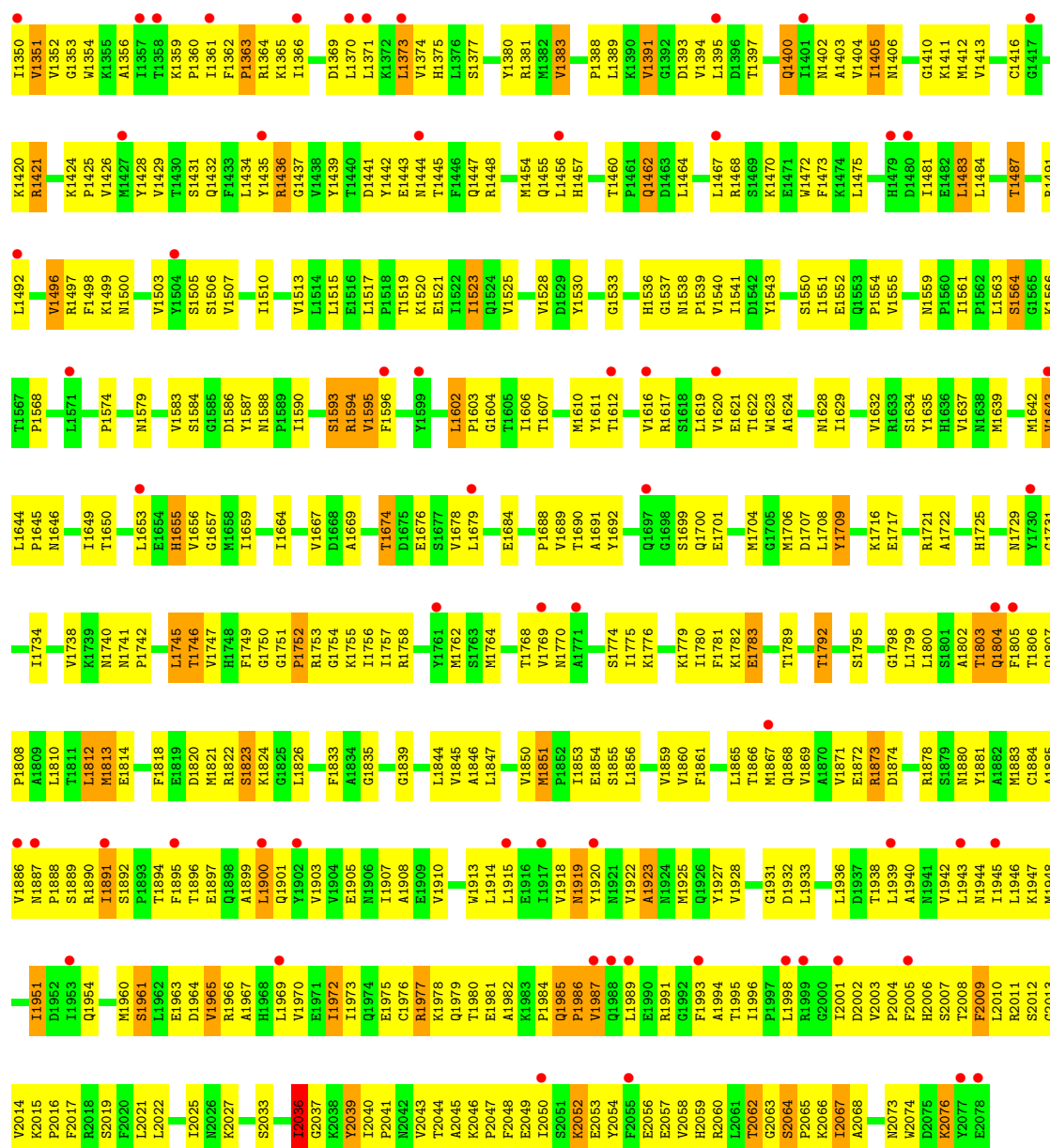




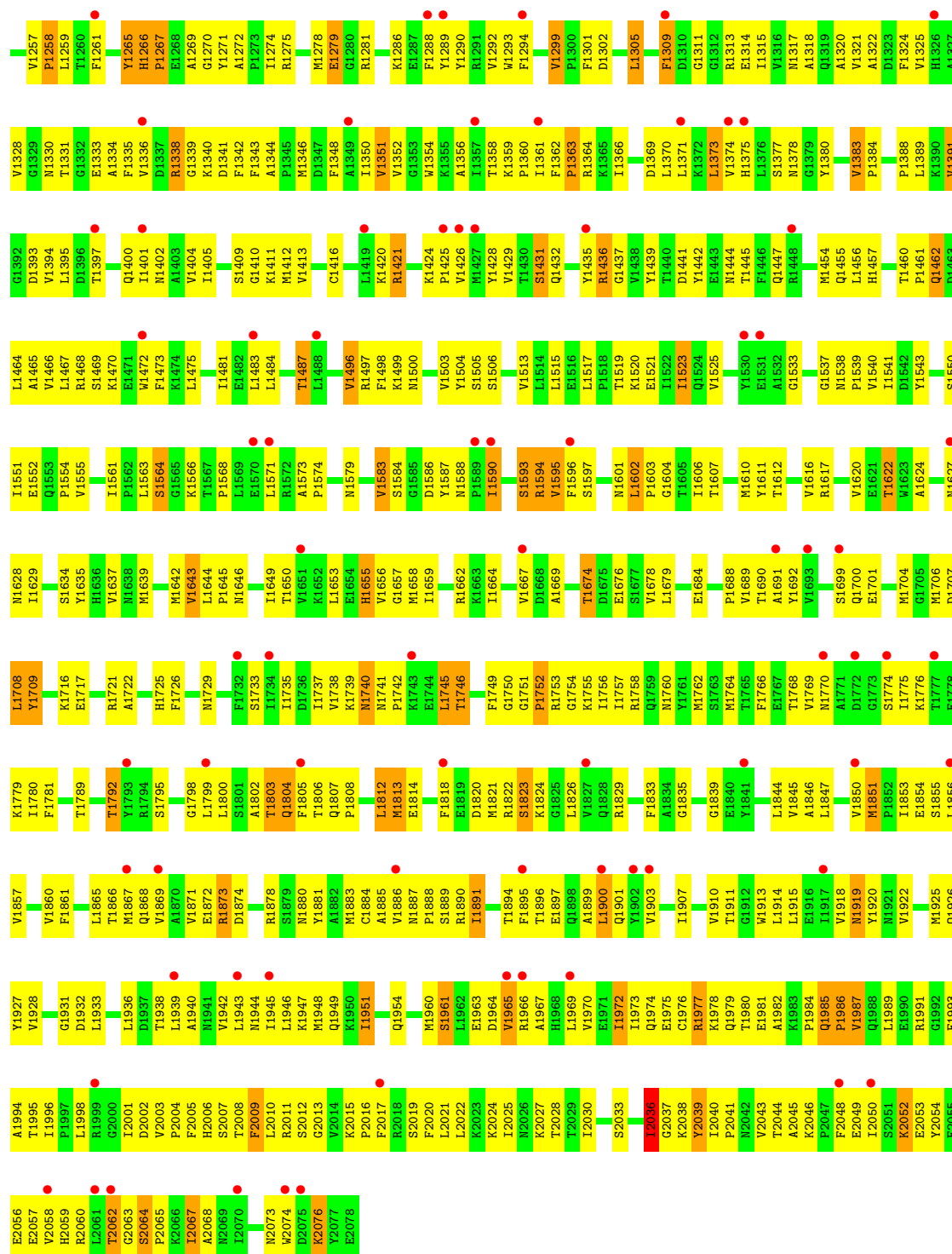
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L1368	L1305	E1232	M1161	E1081	V1013	L941	T870	P806	T739	P666	M595	G521	D454
G1369	Q1162	E1233	Q1162	V1082	G1014	M942	R871	R807	I740	P667	S592	G522	V455
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G1373	V1169	V1237	Y1169	L1086	L1018	W950	K877	M811	G745	G672	P601	L527	I460
L1374	S1170	G1238	S1170	L1087	L1019	I951	K877	R812	G745	W672	P602	T528	P461
L1375	W1171	D1239	W1171	D1088	G1020	D952	E978	R815	G746	Q673	M603	N529	A462
H1376	R1172	E1240	R1172	G1089	Q1021	P953	K882	M816	R747	I674	M604	S463	S463
S1377	H1173	E1241	H1173	I1090	A1022	S954	I883	M818		P875	V605	K532	S464
	A1174	I1242	A1174	H1091	R1023	K956	I883	T818	G750	L876	A606	D533	L465
Y1380	M1175	A1243	M1175	N1092	K1026	T959	R888	R819	H751	R679	M608	G534	V466
V1383	F1176	L1244	F1176	D1093	P1027		S889	A819	H752		T609	V537	I467
P1384	T1177	L1245	T1177	H1094	V1028		K890	R820	S753	P685	M609	V537	P468
	L1246	F1247	L1246	I1095	P1029		R891	E821	F754	P686	T611	R538	V469
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L1389	V1190	F1097	V1190	F1097	P1031		E894	H823	D756	I541	P614	I541	D471
K1390	F1181	L1098	F1181	L1098	P1032		R897	T824	F757	E688	V613	L541	T472
V1391		R1250		R1109	A1033		R897	S825		G689	P614	A542	K473
G1392	R1186	T1251	R1186	D1101	K1044		K897	K326	I761	L690	W615	G543	T474
A1397	F1187	K1257	F1187	E1101	D1045		R898	Q827	L762	T691	D616	A544	
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G1399	T1189	P1258	T1189	Y1103	L1047		D900	K829	W764	N549	V618	I545	L478
P1394	N1190	L1259	N1190	D1104	F1038		Y901	Q830	W765	T550	T621	E551	E480
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Q1400	L1193	F1262	L1193	V1110	S1046		L906	D834	I774	Y705	Y626	K555	E484
I1401	L1196	F1263	L1196	P1111	L1047		N907	A835	W775	I706	I628	P556	I486
A1402	A1197	H1265	A1197	V1112	Q1048		D908	P836	L776	Q707	I628	P556	I486
V1404	P1198	P1198	P1198	I1113	Q1049		D909	R838	W777	L558	F559	L558	I487
I1405	T1199	E1114	T1199	E1114	S1050		F910	D839	A778	T708	A631	F559	P488
N1406	R1200	V1115	R1200	Y1115	E1051		Q911	D840	G779	L709	G632	D580	E489
		F1116		F1116	D1052		Q912	D841	S780	G710	G633	R561	L490
S1409	Y1203	I1120	Y1203	I1120	L1053		V913	Q842	I711	I711	G634	A565	V491
G1410	V1204	L1121	V1204	L1121	Y1057		W914	W843	F782	R712	Y635	A565	R492
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M1412	I1206	A1122	I1206	A1122	Q1059		G916	N845	G784	R713	N637		
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E1414	N1208	D1125	N1208	D1125	V1061		N918	Y847	E786	K717	Q639	D571	P498
C1416	P1209	E1126	P1209	E1126	G1062		G921		D787	P718	R640	W573	V499
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T1418	T1215	P1128	T1215	P1128	G1065		D926	W854	P790	S720	S646		E502
L1419	V1216	V1130	V1216	V1130	L1066		L926	I855	I791	A723	K647	P578	T505
K1420	I1217	A1135	I1217	A1135	L1067		E927	T866	L792	I724	I648	R579	V506
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	V1219	P1070	V1219	P1070	G1069		P1001	L858	G794	T726	V581		
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P1425	V1292	K1141	V1292	K1141	V1071		Y931	E860	W796	I728	P653	T583	T511
V1426	W1293	S1142	V1293	S1142	A1003		A932	M861	S797	N729	P654	S584	H512
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V1429	A1226	P1226	V1429	P1226	K1074		V934	E863	F800	A731	V514	V514	V514
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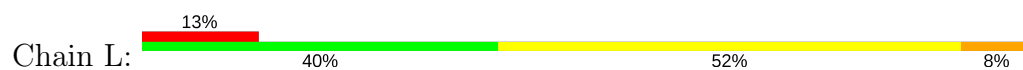








• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



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Y1075	A1010	L941	L867	P804	I740	Y664	M594	G519	I451	R376	F304	P234	S171	T97
S1076	Q1011	M805	L868	M805	I741	V665	S595	G520	V455	R377	F305	Y242	I172	N98
K1077	D1012	N942	L869	P806	Q742	P667	S596	S521	V455	G379	A306	Y242	F173	L99
Y1078	Y433	Y443	T870	P807	Q743	R668	S597	G523	K459	I380	T305	S245	G175	E100
I1079	Q1013	Y944	R871	D808	T744	R669	L597	G523	K459	S381	K309	S245	Q176	V101
D1080	H1015	K945	F875	Q809	G745	M670	L598	I524	P461	S382	R310	A246	Q177	L102
P1082	L1016	E947	H876	M811	G746	G671	G599	I524	A462	V383	A311	P247	G178	K103
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K1084	L1018	E947	E878	G813	G748	Q673	P602	T528	S464	V383	K309	S245	I180	E105
D1085	C1020	N951	L879	N814	Q749	Q674	N603	H530	L465	R388	K314	F250	E181	L106
I1086	Q1021	D852	R879	R815	H751	P675	N604	N531	Y466	F389	L315	P251	I182	N107
L1087	R1022	P953	R882	M816	H752	L676	V605	D533	I467	V390	L316	L253	E182	E108
D1088	R1023	L955	T818	N817	F754	L677	G607	D533	P468	V391	W317	G254	E183	F109
G1089	R1024	L955	G608	G607	F755	L677	N608	T535	V469	T392	I318	L255	E184	E110
I1090	K1026	K956	R888	A819	F756	P686	T609	G536	Y470	G393	R321	V256	L186	A112
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A1123	V1061	L996	L926	T855	Y791	Q726	V647	K574	E502	F432	T357	S286	A217	P153
D1125	G1062	L997	E927	T856	L792	V727	V648	K574	E502	F432	T357	S286	A217	P153
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I1127	C1064	L997	E929	T858	L794	V729	V650	K574	E502	F432	T357	S286	A217	P153
P1128	C1065	L997	E930	T859	L795	V730	V651	K574	E502	F432	T357	S286	A217	P153
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T1134	G1069	L997	E934	T863	L799	V734	V655	K574	E502	F432	T357	S286	A217	P153
A1135	Q1070	L997	E935	T864	L800	V735	V656	K574	E502	F432	T357	S286	A217	P153
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	T2008	L1943	N1881	T1811	N1740	V1656	Y1588	L1510	L1434	R1366	W1293		
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		V1965			Q1759	Q1880	T1607	Y1530		P1388		I1243	M1175
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Y2039		E1975			V1769	F1693	L1619	D1542	R1468	A1399		V1257	
P2041		V1910			M1770	F1694	V1620	Y1543	S1469	A1334		P1258	
		W1913					E1621	S1550		F1335		L1259	
N2042		L1914			S1774	Q1700	T1622	I1551	W1472	I1401		T1260	
V2043		L1915			I1775	E1701	W1623	E1552	F1473	N1402		F1261	
T2044		E1916			K1776		A1624	P1563	K1474	G1339		R1263	
A2045		V1918			K1779	M1704		S1564	L1475	D1341		L1195	
K2046		N1918			I1780	G1705	N1627	P1560		F1342		T1264	
P2047		N1919			F1781	M1706	I1628	I1561		F1343		T1265	
F2048		Y1920			E1782	D1707	I1629	L1562		A1344		H1266	
E2049		N1921			E1783	L1708		L1563		P1345		E1268	
I2050		V1922				Y1709	V1632	S1564		M1346		R1200	
S2051		A1923					R1633	S1564		D1347		G1201	
K2052		N1924			T1789	E1717	Y1635	G1565		F1348		M1202	
E2053		M1925					H1636	K1566		A1349		Y1271	
Y2054		Q1926			T1792		V1637	T1567		I1350		A1272	
P2055		Y1927			S1795		M1638	P1569		V1351		P1273	
E2056		V1928					M1639			K1420		R1275	
E2057		A1929						P1574		R1421		R1276	
V2058		A1930			G1798	H1724	M1642			W1354		M1278	
H2059		G1931			L1799	H1725	V1643			P1425		E1279	
R2060		D1932			L1800	F1726	L1644	M1577		K1424			
		L1933			S1801	R1727	P1645	E1576		P1426			
L2061		V1869					P1646			M1427			
T2062		A1870			A1802	E1728							
G2063		V1871			T1803	M1729							
S2064		E1872			Q1804	Y1730		Y1580					
P2065		R1873			F1805								

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	215.78Å 412.67Å 220.90Å 90.00° 111.57° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 96.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.10) 92.6 (96.48-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, R_{free}	0.270 , 0.300 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.078 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	167247	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/11744	0.60	1/15873 (0.0%)
1	B	0.43	0/11801	0.60	1/15949 (0.0%)
1	C	0.44	0/11785	0.59	0/15928
1	D	0.43	0/11824	0.60	0/15980
1	E	0.42	0/11736	0.59	0/15863
1	F	0.44	0/11776	0.60	5/15916 (0.0%)
2	G	0.36	0/16573	0.53	0/22516
2	H	0.35	0/16573	0.53	0/22516
2	I	0.35	0/16573	0.53	0/22516
2	J	0.36	0/16573	0.54	0/22516
2	K	0.39	0/16573	0.55	0/22516
2	L	0.36	0/16573	0.54	0/22516
All	All	0.39	0/170104	0.56	7/230605 (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	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	585	MET	N-CA-C	9.44	136.48	111.00
1	B	608	LYS	N-CA-C	-8.94	86.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	614	PHE	N-CA-C	6.04	127.30	111.00
1	F	613	PRO	CA-C-N	5.57	129.46	117.20
1	A	579	MET	N-CA-C	5.39	125.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	ALA	Peptide
1	F	613	PRO	Peptide

5.2 Too-close contacts ⓘ

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	11514	0	11476	746	1
1	B	11571	0	11529	708	1
1	C	11555	0	11507	717	0
1	D	11593	0	11552	725	0
1	E	11506	0	11467	754	0
1	F	11546	0	11499	701	0
2	G	16200	0	16081	1290	1
2	H	16200	0	16081	1326	1
2	I	16200	0	16081	1344	0
2	J	16200	0	16081	1326	0
2	K	16200	0	16081	1391	0
2	L	16200	0	16081	1366	0
3	A	48	0	25	5	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0
3	D	48	0	25	6	0
3	E	48	0	25	4	0
3	F	48	0	25	4	0
3	G	48	0	25	4	0
3	H	48	0	25	5	0
3	I	48	0	25	4	0
3	J	48	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	48	0	25	4	0
3	L	48	0	25	4	0
4	G	31	0	19	17	0
4	H	31	0	19	16	0
4	I	31	0	19	16	0
4	J	31	0	19	15	0
4	K	31	0	19	15	0
4	L	31	0	19	15	0
All	All	167247	0	165930	11767	2

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 35.

The worst 5 of 11767 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:D:542:GLN:HB3	1:D:579:MET:HE2	1.25	1.17
1:F:1443:LEU:HD21	1:F:1470:ARG:HB3	1.18	1.17
1:B:1268:SER:HB3	1:D:1389:ILE:HG13	1.23	1.16
1:F:1504:ARG:HH11	1:F:1504:ARG:HG3	1.04	1.15
1:D:1504:ARG:HH11	1:D:1504:ARG:HG3	1.02	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:NH1	2:H:164:GLU:O[2_555]	2.01	0.19
1:B:1452:SER:O	2:G:1092:ASN:ND2[1_556]	2.18	0.02

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	1451/1878 (77%)	1270 (88%)	164 (11%)	17 (1%)	15	51
1	B	1458/1878 (78%)	1278 (88%)	160 (11%)	20 (1%)	13	47
1	C	1456/1878 (78%)	1283 (88%)	156 (11%)	17 (1%)	15	51
1	D	1461/1878 (78%)	1276 (87%)	161 (11%)	24 (2%)	11	43
1	E	1450/1878 (77%)	1276 (88%)	155 (11%)	19 (1%)	14	48
1	F	1455/1878 (78%)	1282 (88%)	153 (10%)	20 (1%)	13	47
2	G	2058/2060 (100%)	1789 (87%)	237 (12%)	32 (2%)	11	43
2	H	2058/2060 (100%)	1791 (87%)	230 (11%)	37 (2%)	10	40
2	I	2058/2060 (100%)	1787 (87%)	238 (12%)	33 (2%)	11	43
2	J	2058/2060 (100%)	1784 (87%)	240 (12%)	34 (2%)	11	42
2	K	2058/2060 (100%)	1785 (87%)	239 (12%)	34 (2%)	11	42
2	L	2058/2060 (100%)	1780 (86%)	241 (12%)	37 (2%)	10	40
All	All	21079/23628 (89%)	18381 (87%)	2374 (11%)	324 (2%)	12	45

5 of 324 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	PHE
1	A	1566	LYS
1	B	614	PHE
1	B	624	GLY
1	B	1566	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1220/1527 (80%)	1107 (91%)	113 (9%)	10	38
1	B	1227/1527 (80%)	1117 (91%)	110 (9%)	11	40
1	C	1225/1527 (80%)	1110 (91%)	115 (9%)	10	38
1	D	1229/1527 (80%)	1107 (90%)	122 (10%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1219/1527 (80%)	1106 (91%)	113 (9%)	10	38
1	F	1224/1527 (80%)	1111 (91%)	113 (9%)	11	39
2	G	1752/1752 (100%)	1569 (90%)	183 (10%)	8	31
2	H	1752/1752 (100%)	1569 (90%)	183 (10%)	8	31
2	I	1752/1752 (100%)	1565 (89%)	187 (11%)	8	30
2	J	1752/1752 (100%)	1567 (89%)	185 (11%)	8	30
2	K	1752/1752 (100%)	1566 (89%)	186 (11%)	8	30
2	L	1752/1752 (100%)	1563 (89%)	189 (11%)	7	30
All	All	17856/19674 (91%)	16057 (90%)	1799 (10%)	9	33

5 of 1799 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1436	ARG
2	H	1564	SER
2	L	726	GLN
2	G	1707	ASP
2	H	616	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 492 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1500	ASN
2	H	1655	HIS
2	L	448	HIS
2	G	1725	HIS
2	H	388	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAP	A	1901	-	44,52,52	1.05	2 (4%)	51,80,80	1.54	2 (3%)
3	NAP	B	1901	-	44,52,52	1.02	2 (4%)	51,80,80	1.53	4 (7%)
3	NAP	C	1901	-	44,52,52	1.08	2 (4%)	51,80,80	1.60	2 (3%)
3	NAP	D	1901	-	44,52,52	1.12	2 (4%)	51,80,80	1.71	2 (3%)
3	NAP	E	1901	-	44,52,52	1.08	2 (4%)	51,80,80	1.68	4 (7%)
3	NAP	F	1901	-	44,52,52	1.06	2 (4%)	51,80,80	1.64	2 (3%)
4	FMN	G	2101	-	31,33,33	6.07	20 (64%)	38,50,50	1.81	6 (15%)
3	NAP	G	2102	-	44,52,52	1.04	3 (6%)	51,80,80	1.68	1 (1%)
4	FMN	H	2101	-	31,33,33	6.09	19 (61%)	38,50,50	1.69	6 (15%)
3	NAP	H	2102	-	44,52,52	1.06	3 (6%)	51,80,80	1.69	2 (3%)
4	FMN	I	2101	-	31,33,33	6.08	18 (58%)	38,50,50	1.71	6 (15%)
3	NAP	I	2102	-	44,52,52	1.00	2 (4%)	51,80,80	1.72	1 (1%)
4	FMN	J	2101	-	31,33,33	6.33	21 (67%)	38,50,50	1.84	4 (10%)
3	NAP	J	2102	-	44,52,52	1.07	3 (6%)	51,80,80	1.70	2 (3%)
4	FMN	K	2101	-	31,33,33	6.31	20 (64%)	38,50,50	1.65	4 (10%)
3	NAP	K	2102	-	44,52,52	0.99	3 (6%)	51,80,80	1.61	2 (3%)
4	FMN	L	2101	-	31,33,33	6.10	19 (61%)	38,50,50	1.71	5 (13%)
3	NAP	L	2102	-	44,52,52	1.05	3 (6%)	51,80,80	1.66	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	1901	-	-	0/27/67/67	0/5/5/5
3	NAP	B	1901	-	-	0/27/67/67	0/5/5/5
3	NAP	C	1901	-	-	0/27/67/67	0/5/5/5
3	NAP	D	1901	-	-	0/27/67/67	0/5/5/5
3	NAP	E	1901	-	-	0/27/67/67	0/5/5/5
3	NAP	F	1901	-	-	0/27/67/67	0/5/5/5
4	FMN	G	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	G	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	H	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	H	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	I	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	I	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	J	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	J	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	K	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	K	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	L	2101	-	-	0/16/18/18	0/3/3/3
3	NAP	L	2102	-	-	0/27/67/67	0/5/5/5

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2101	FMN	C1'-N10	-2.01	1.46	1.48
4	G	2101	FMN	C8M-C8	2.02	1.55	1.51
3	L	2102	NAP	C6N-N1N	2.15	1.41	1.35
3	G	2102	NAP	C6N-N1N	2.22	1.41	1.35
3	I	2102	NAP	C2A-N1A	2.23	1.38	1.33

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2102	NAP	N3A-C2A-N1A	-10.85	119.41	128.86
3	D	1901	NAP	N3A-C2A-N1A	-10.80	119.45	128.86
3	G	2102	NAP	N3A-C2A-N1A	-10.42	119.78	128.86
3	J	2102	NAP	N3A-C2A-N1A	-10.40	119.80	128.86
3	L	2102	NAP	N3A-C2A-N1A	-10.31	119.88	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	NAP	5	0
3	B	1901	NAP	5	0
3	C	1901	NAP	4	0
3	D	1901	NAP	6	0
3	E	1901	NAP	4	0
3	F	1901	NAP	4	0
4	G	2101	FMN	17	0
3	G	2102	NAP	4	0
4	H	2101	FMN	16	0
3	H	2102	NAP	5	0
4	I	2101	FMN	16	0
3	I	2102	NAP	4	0
4	J	2101	FMN	15	0
3	J	2102	NAP	4	0
4	K	2101	FMN	15	0
3	K	2102	NAP	4	0
4	L	2101	FMN	15	0
3	L	2102	NAP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1457/1878 (77%)	0.30	44 (3%)	51	27	16, 50, 103, 146	0
1	B	1464/1878 (77%)	0.31	38 (2%)	56	33	17, 50, 106, 157	0
1	C	1462/1878 (77%)	0.33	44 (3%)	51	27	15, 48, 107, 155	0
1	D	1467/1878 (78%)	0.29	47 (3%)	48	25	17, 52, 106, 151	0
1	E	1456/1878 (77%)	0.31	47 (3%)	48	25	17, 50, 106, 152	0
1	F	1461/1878 (77%)	0.34	37 (2%)	58	35	17, 47, 106, 156	0
2	G	2060/2060 (100%)	0.48	170 (8%)	12	4	24, 83, 128, 156	0
2	H	2060/2060 (100%)	0.57	222 (10%)	6	2	24, 85, 129, 155	0
2	I	2060/2060 (100%)	0.51	212 (10%)	7	2	20, 85, 129, 158	0
2	J	2060/2060 (100%)	0.61	275 (13%)	4	1	27, 88, 132, 157	0
2	K	2060/2060 (100%)	0.85	353 (17%)	2	1	25, 90, 133, 157	0
2	L	2060/2060 (100%)	0.58	259 (12%)	4	2	22, 86, 131, 158	0
All	All	21127/23628 (89%)	0.48	1748 (8%)	12	4	15, 74, 125, 158	0

The worst 5 of 1748 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	176	GLN	16.8
2	H	178	ASN	14.1
2	K	178	ASN	14.0
2	K	175	GLY	12.8
2	K	516	PHE	12.5

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAP	B	1901	48/48	0.92	0.32	0.43	23,78,115,145	0
3	NAP	A	1901	48/48	0.90	0.32	0.34	19,76,121,169	0
3	NAP	F	1901	48/48	0.87	0.31	0.30	19,78,125,159	0
3	NAP	C	1901	48/48	0.87	0.34	0.17	23,81,130,171	0
3	NAP	D	1901	48/48	0.87	0.34	0.14	21,83,127,174	0
3	NAP	L	2102	48/48	0.93	0.31	-0.06	37,84,116,120	0
3	NAP	K	2102	48/48	0.90	0.29	-0.33	43,94,127,131	0
3	NAP	E	1901	48/48	0.93	0.26	-0.39	24,77,123,157	0
4	FMN	J	2101	31/31	0.94	0.32	-0.41	23,61,101,113	0
3	NAP	H	2102	48/48	0.92	0.25	-0.43	37,85,113,122	0
3	NAP	I	2102	48/48	0.95	0.26	-0.43	29,80,104,116	0
4	FMN	L	2101	31/31	0.96	0.29	-0.54	19,59,102,114	0
4	FMN	I	2101	31/31	0.97	0.30	-0.55	22,56,87,103	0
4	FMN	G	2101	31/31	0.95	0.31	-0.58	26,63,101,111	0
3	NAP	G	2102	48/48	0.92	0.24	-0.60	42,87,119,128	0
4	FMN	H	2101	31/31	0.96	0.32	-0.63	25,49,105,113	0
4	FMN	K	2101	31/31	0.92	0.36	-0.67	27,66,110,123	0
3	NAP	J	2102	48/48	0.89	0.21	-0.78	35,88,118,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.