



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:09 PM 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

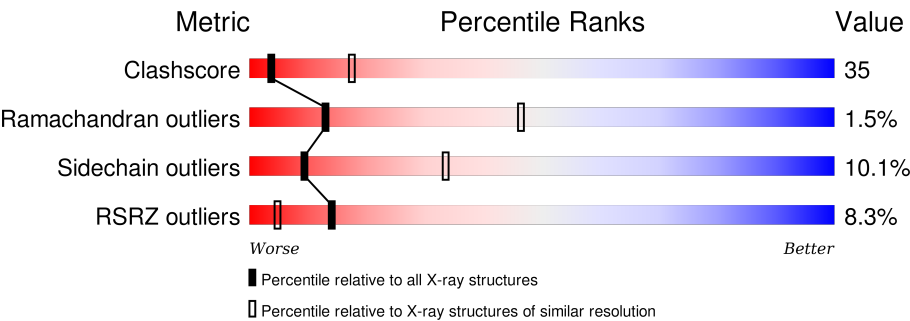
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



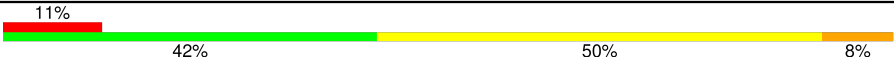

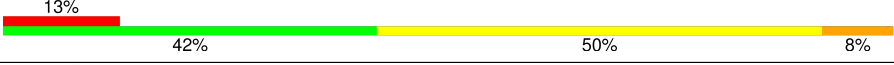
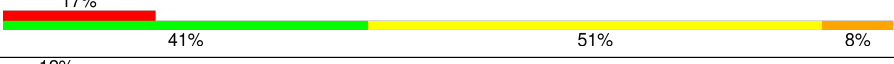
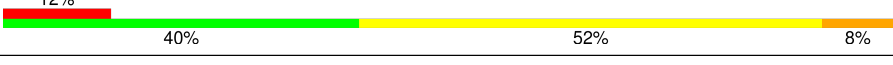
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	<div><div>2%</div><div>39%35%•22%</div></div>
1	B	1878	<div><div>2%</div><div>40%34%•22%</div></div>
1	C	1878	<div><div>2%</div><div>39%34%•22%</div></div>
1	D	1878	<div><div>3%</div><div>39%34%5%22%</div></div>
1	E	1878	<div><div>2%</div><div>38%35%•22%</div></div>
1	F	1878	<div><div>2%</div><div>40%33%•22%</div></div>
2	G	2060	<div><div>8%</div><div>43%49%8%</div></div>

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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.

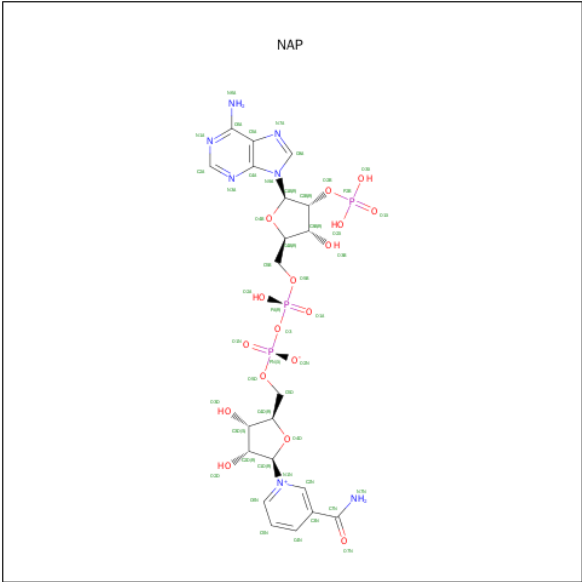
- Molecule 1 is a protein called FATTY ACID SYNTHASE ALPHA SUBUNITS.

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.

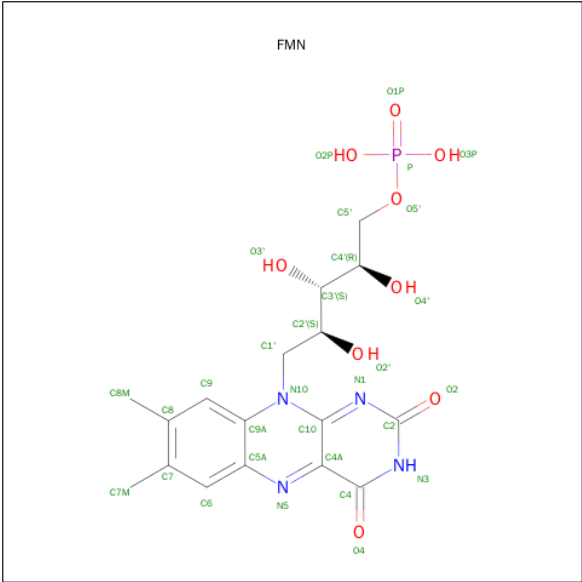
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	H	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	I	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	J	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	K	2060	Total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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

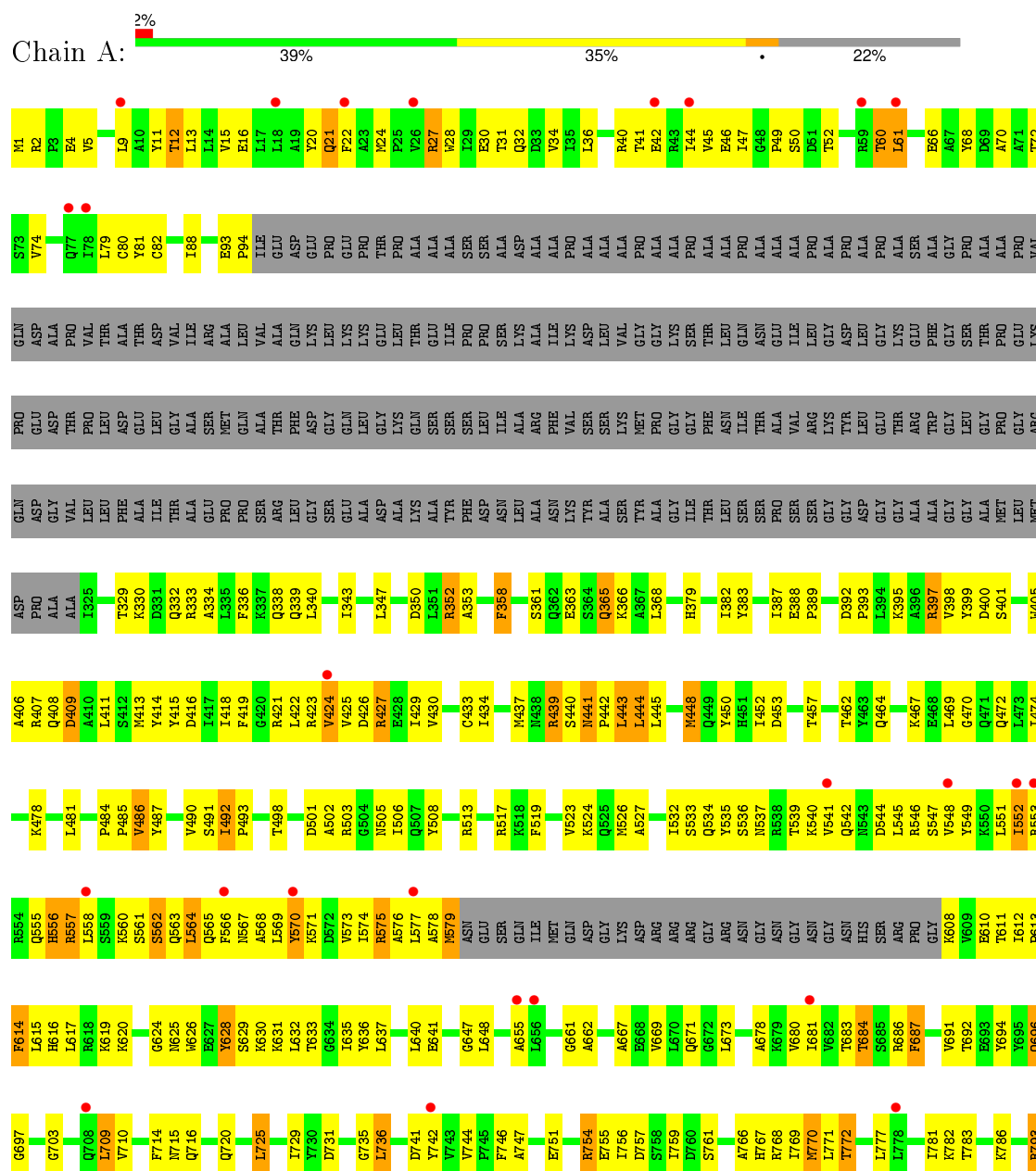


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

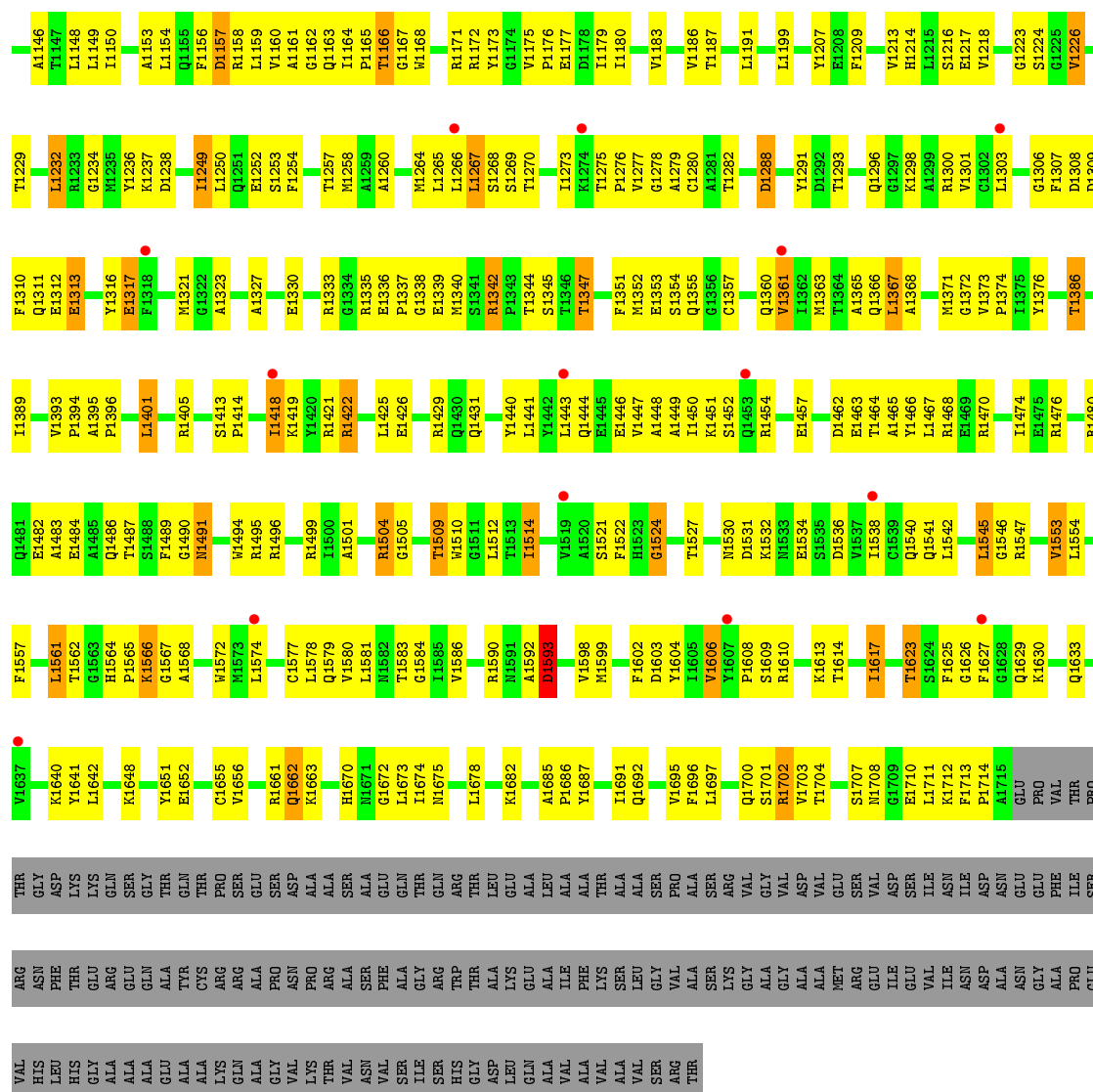
• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



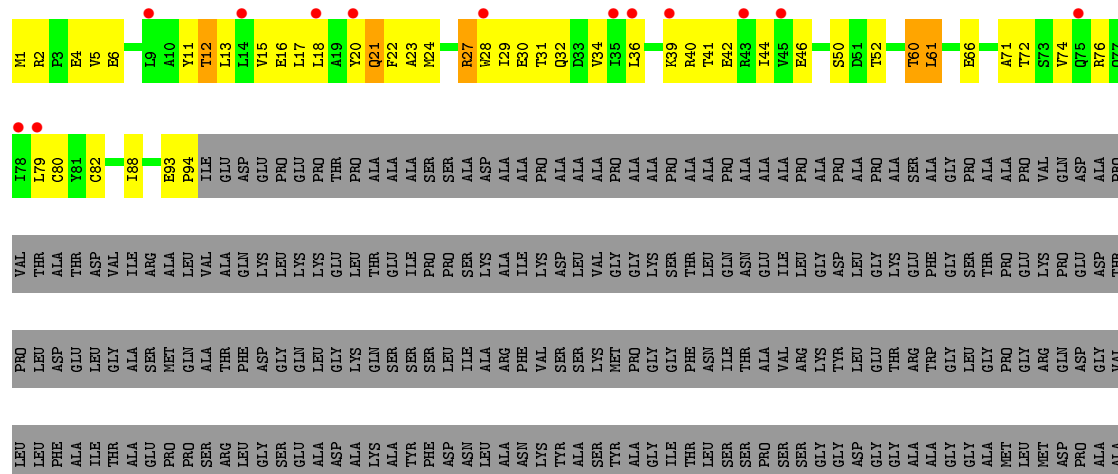
[illegible]

- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS





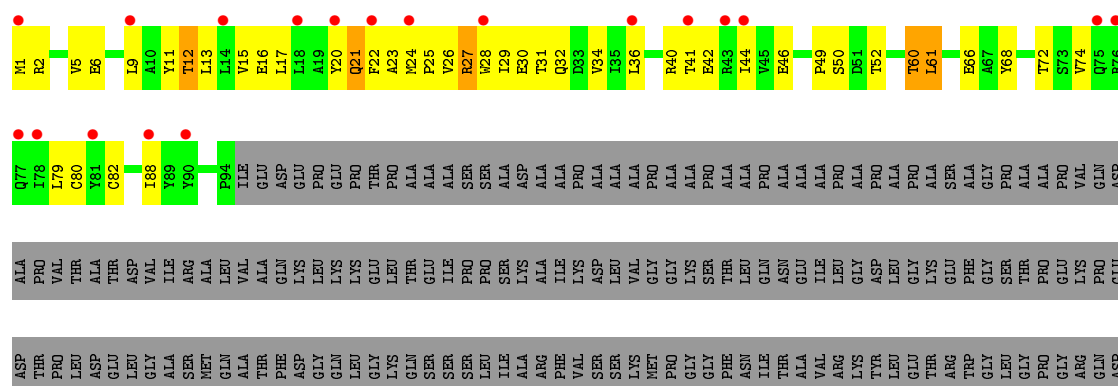
• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



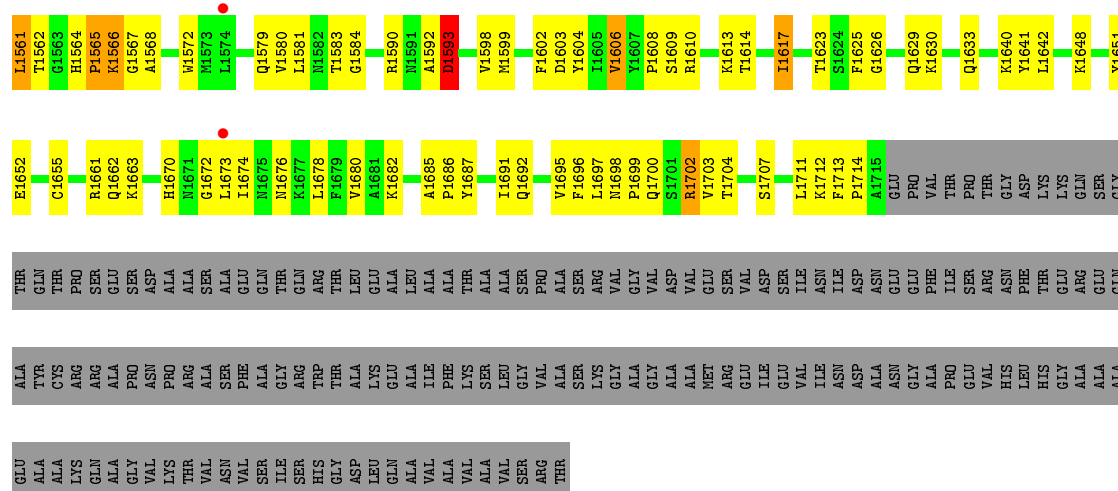


- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS

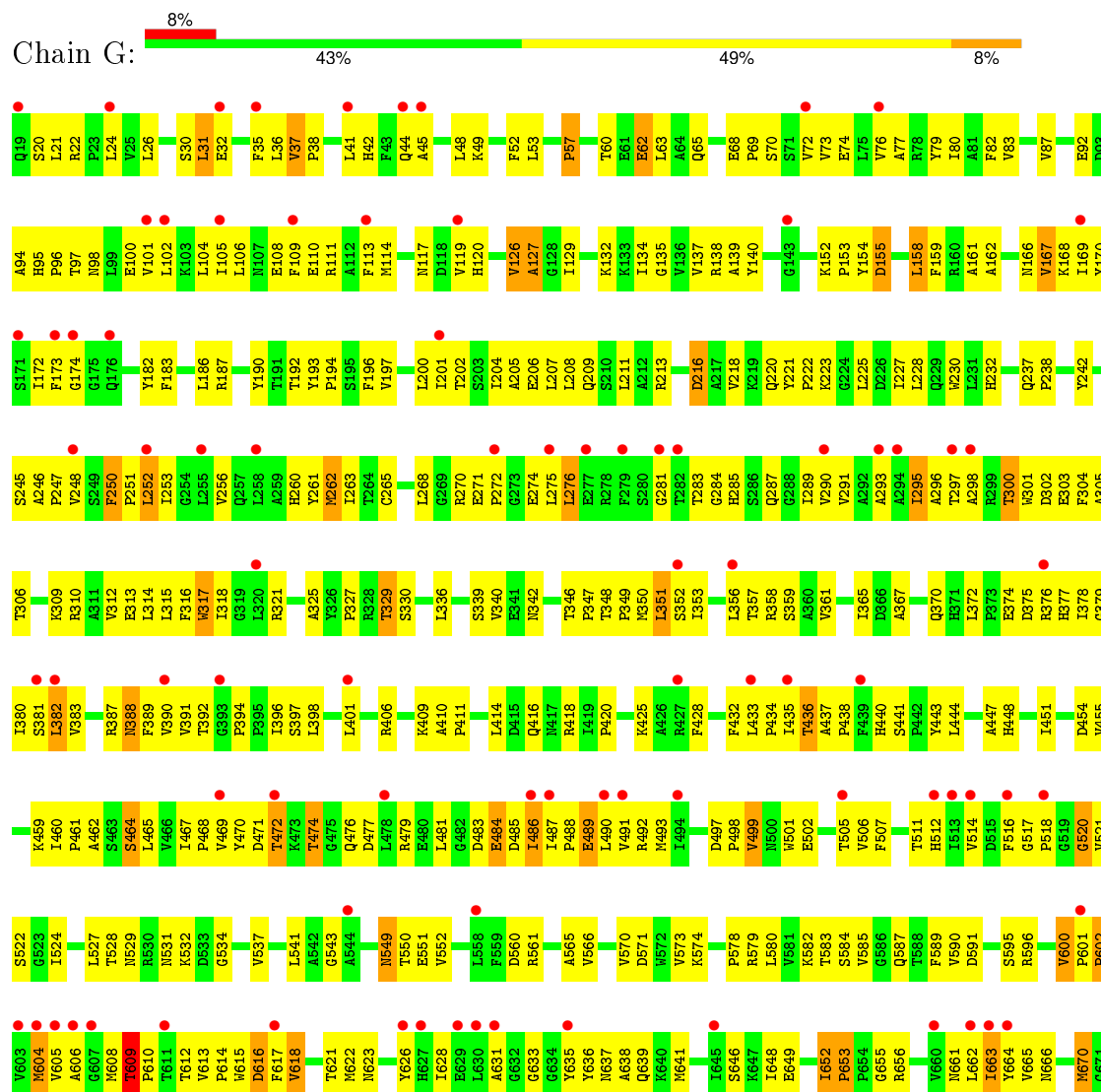




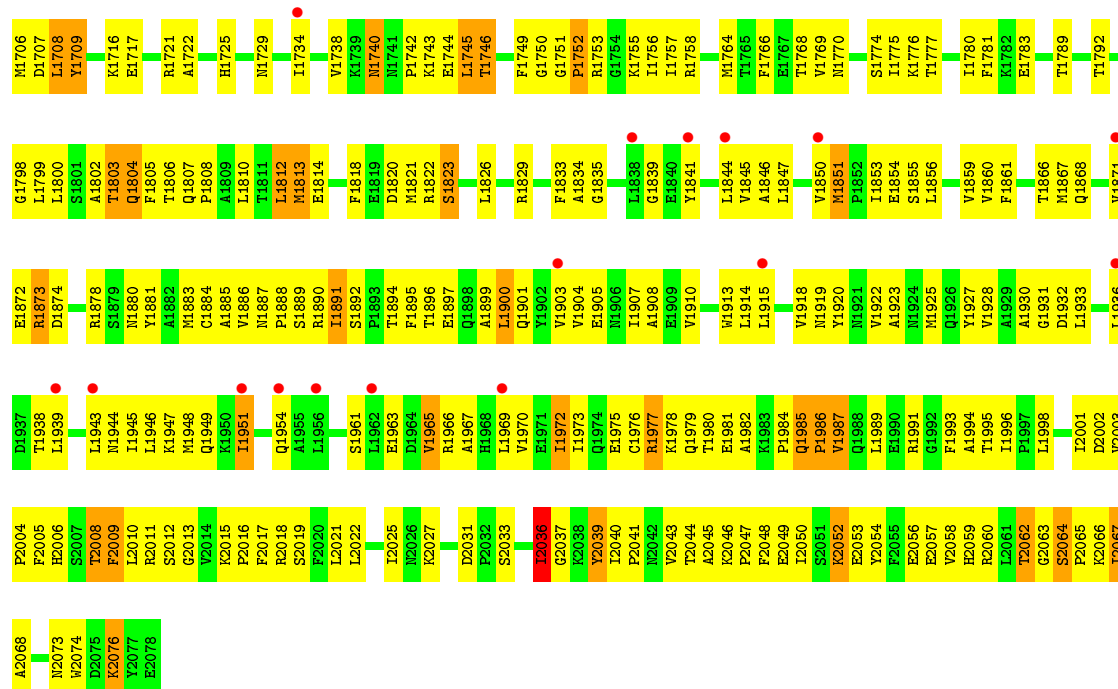
H1473	G1306	S1224	R1141	V1064	K978	A899	E831	Y742	L640	V573	Y414	GLY
I1474	F1307	G1225	L1142	K1065	P979	D900	S832	Y743	G647	I574	Y415	VAL
E1475	D1308	V1226	A1146	Y1068	L980	L901	N902	P744	L648	A575	D416	LEU
R1480	I1389	T1229	T1147	E1069	Q983	G903	G834	P745	L649	A576	I417	PHE
A1483	F1309	F1310	L1148	K1070	Q984	G904	N935	F746	H654	L577	I418	ALA
E1484	Q1311	L1232	L1149	Y1071	R985	L905	Y836	A747	A655	A578	G420	ILE
E1485	A1395	G1233	I1150	I1072	G986	F906	T838	E751	G661	M579	R421	THR
Q1486	E1312	R1234	A1153	H1075	V988	F907	T838	Y751	G662	M580	R422	ALA
T1487	E1317	K1237	L1154	I1078	N989	F908	I839	R754	A662	A502	R423	GLU
S1488	M1321	D1237	Q1155	I1079	N989	P909	V843	E755	A667	G504	R424	PRO
F1489	G1322	K1237	D1157	L1080	V995	G912	N846	D756	F668	N505	V425	PRO
A1495	A1327	L1241	L1158	I1081	V996	G913	T847	D757	F669	N506	D426	SER
R1496	G1322	I1249	L1159	E1082	T997	L914	R848	D758	L670	Y508	E428	ARG
R1499	A1327	I1250	V1160	P1083	G998	N915	G849	D759	L671	L340	I429	LEU
I1500	E1330	Q1251	A1161	E1084	I999	T916	T850	S761	L673	R513	V430	SER
L1503	G1334	G1252	Q1162	L1085	A1000	K917	G851	A766	L674	R517	C433	ALA
R1504	R1333	S1253	I1164	F1086	E1001	L918	L852	H767	A678	R518	I434	ASP
E1505	R1334	F1254	T1166	D1090	P1004	R919	R853	R768	K679	F519	Q435	ALA
L1506	R1335	T1257	G1167	P1091	M1006	I922	S854	I769	V680	N523	D350	LYS
A1507	E1336	M1258	V1168	N1092	G1006	S826	N856	M770	I681	V623	M437	ALA
L1507	P1337	A1259	D1169	R1093	N1007	S827	N857	L771	V682	V626	N438	TYR
Q1508	G1338	I1260	A1170	K1094	A1008	S828	L858	L772	T683	A527	R439	PHE
T1509	R1342	M1261	I1171	Q1095	M1012	R929	R859	L777	T684	M441	S440	ASP
W1510	E1343	L1262	V1175	E1100	Y1017	Q930	R860	L778	V691	S533	N442	ASN
G1511	T1344	S1268	P1176	V1101	E1012	Q930	R861	L779	T692	P442	M443	ALA
L1512	S1345	T1270	E1177	E1103	W1013	G1095	E861	G780	V693	Q362	L444	ASN
I1514	T1346	G1271	I1180	Q1104	E1014	I933	R863	I781	T694	Q363	E363	LYS
V1519	T1347	P1272	I1183	D1105	M1014	N940	E864	I782	V695	Q364	L445	TYR
F1522	F1351	L1273	V1183	L1106	Y1017	E1017	R865	K783	Q696	M448	M448	ALA
H1523	M1352	K1274	V1186	E1107	M1032	A950	R869	R793	Q697	Q449	Q449	TYR
G1524	E1353	P1275	T1187	P1108	N1037	L951	S872	L799	L801	Y450	Y450	SER
T1525	S1354	P1276	L1188	P1108	H1038	Y952	Q874	P800	L801	H451	H451	TYR
S1526	Q1355	G1278	L1188	K1113	E1038	E875	E875	L801	L709	D452	D452	ALA
D1531	C1357	A1279	L1191	E1117	M1039	I956	A877	F808	V710	S547	T462	PRO
K1532	Q1360	C1280	L1199	E1118	L1042	P959	F878	G809	N810	R554	Y463	SER
E1533	V1361	A1281	L1199	F1119	S1048	R960	N879	N810	F714	Q555	Q464	GLY
E1534	I1362	T1282	Y1207	K1120	G1049	A961	L880	G812	N715	R556	K467	GLY
T1538	M1363	F1209	F1208	R1121	W1050	N962	L881	L813	Q716	R557	E468	ASP
Q1541	Q1366	V1289	F1208	V1127	V1051	L963	G882	Y814	L725	K560	L469	GLY
L1545	L1367	D1288	V1213	E1128	D1082	Y965	N884	S815	V726	S561	G470	GLY
G1546	E1463	L1287	L1214	F1130	T1055	P966	I888	E816	I729	S662	Q471	ALA
R1547	T1461	D1289	L1215	E1131	G1056	P967	R889	S817	D731	Q563	Q472	ALA
V1553	D1462	V1289	L1216	I1132	E1057	P968	N890	E822	L731	Q565	I474	GLY
	E1469	K1298	L1217	I1132	P1058	L970	N890	T823	G735	F566	L481	ALA
	R1470	A1299	E1217	I1132	P1058	L971	N890	L824	L736	N567	V486	GLY
		R1300	V1218	Q1137	D1061	P971	C882	L824	L736	A568	R407	ALA
		V1301	G1219	T1138	K1062	N972	Q893	L824	L736	L569	Q408	LEU
		C1302	G1223	V1140	N973	N973	F898	R827	L740	Y570	D409	ASP
		L1303						W828	D741		N413	PRO



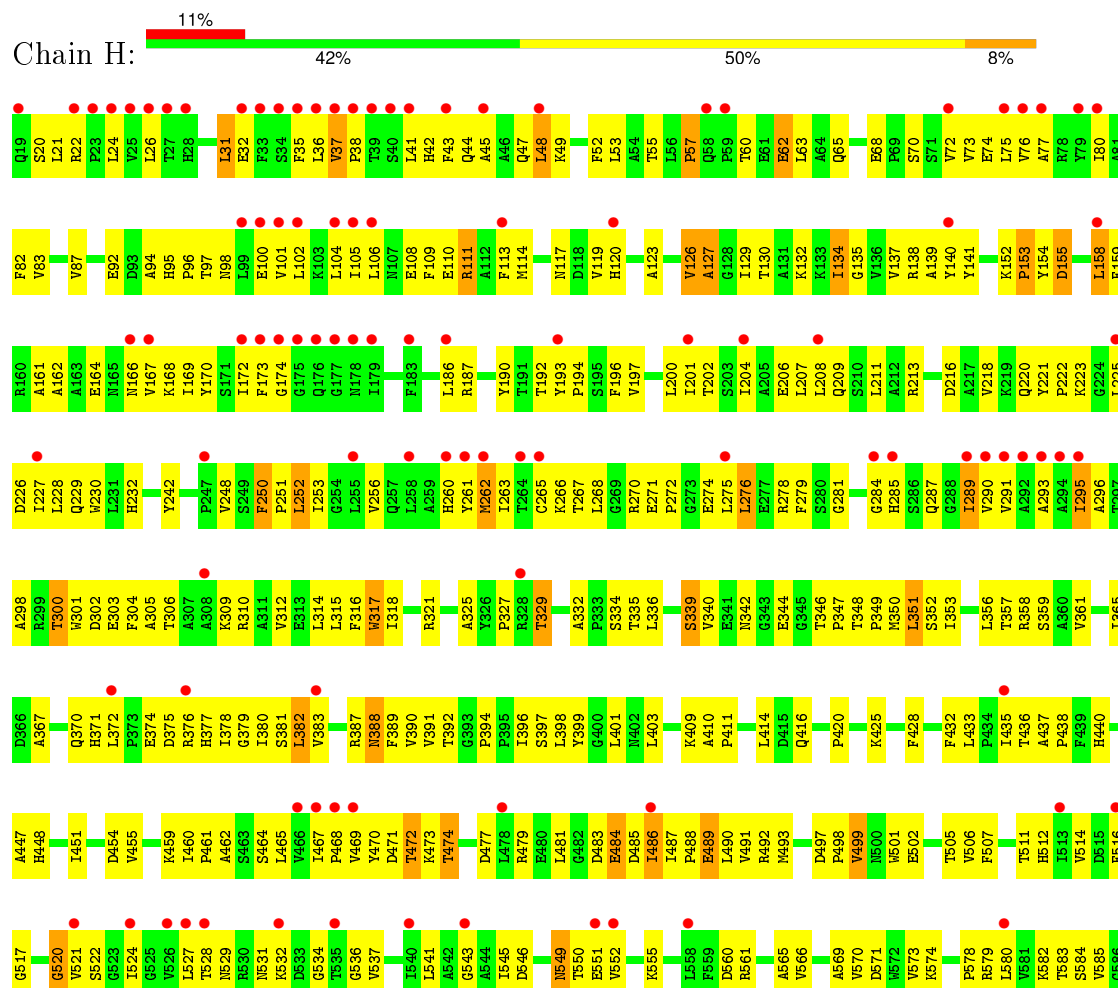
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



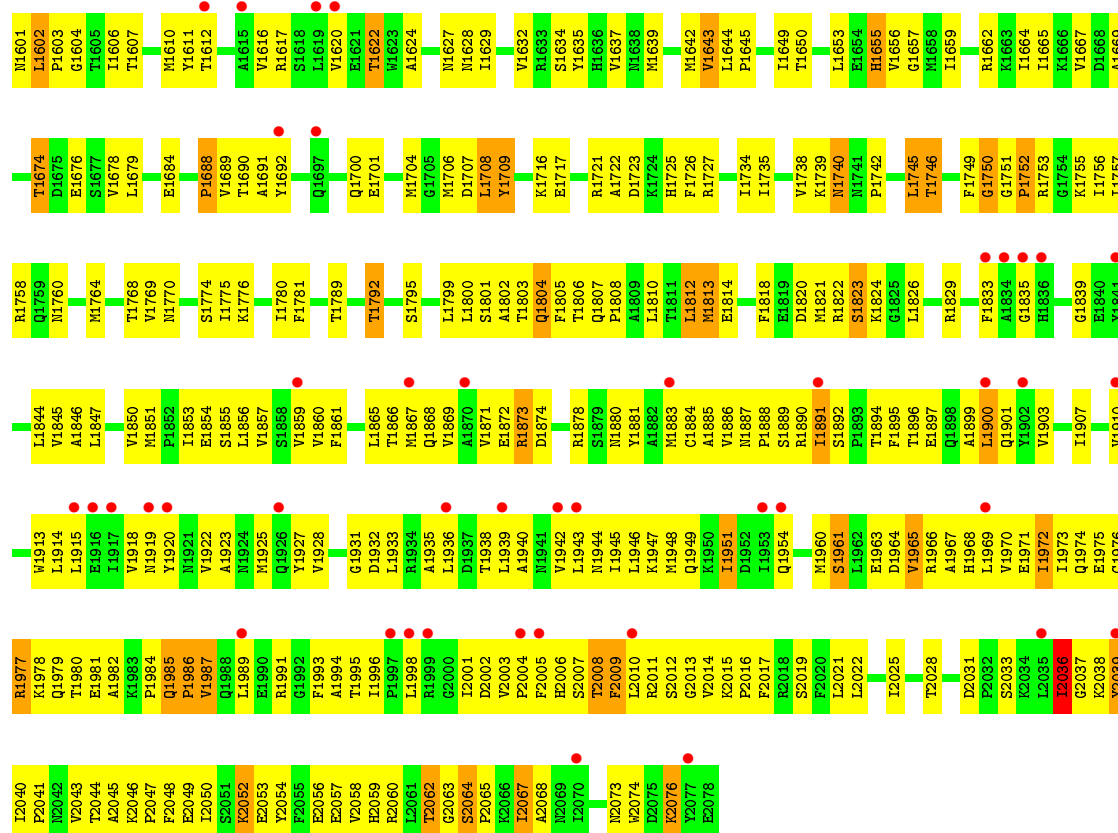
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A1624	L1540	P1461	V1325	G1249	H1090	L1019	E947	K877	M811	W744	L674
M1627	D1542	Q1463	V1329	T1251	M1091	C1020	W950	E878	S814	G746	P675
N1629	Y1543	L1464	G1329	E1252	D1092	Q1021	I951	K882	R815	L676	L676
	S1550	D1393	N1330	E1253	H1094	R1022	D952	I883	M816	G748	
	L1551	L1394	T1331	P1258	K1095	K1026	P954	F884	R817	V685	
V1632	L1467	R1468	E1332	L1259	K1096	P1027	S954	D887	T818	P686	
R1633	R1468	E1332	E1333	L1259	F1097	P1028	S954	K888	A819	H751	
Q1634	T1397	E1333	E1334	L1260	L1098	P1029	K956	K888	K820	H752	
V1635	W1472	F1335	F1336	F1261	L1099	V1030	T959	S889	E821	S753	
H1636	F1473	F1336	D1337	F1262	L1100	V1031		K890	A822	S753	
V1637	K1474	D1337	F1337	F1263	D1101	P1032		R891	H823	T691	
M1638	L1475	R1338	R1338	F1264	L1102	A1033	F962	E894	T824	G693	
M1639	A1403	R1338	R1339	T1265	Y1103	E1036	I963		S825	A694	
	V1403	K1340	F1340	H1266	D1104	K1044	R965	K897	K826	G695	
M1642	L1481	K1341	D1341	H1266	G1105	D1045	V966	K898	Q827	S698	
V1643	L1483	F1342	F1342	P1267	K1106	D1046	E967	R899	A828	L699	
L1644	L1484	F1343	F1343	E1268	E1107	W1047	R969	D900	K829	L762	
P1645	S1409	A1344	A1344	A1269	V1110	L1047	E968	N907	W764	L763	
	G1410	P1345	P1345	Y1271	P1111	W1048	R969	D908	Y901	W765	
	K1411	M1346	F1347	A1272	V1112	Q1049	F970	D909	V832	A702	
	M1412	K1411	F1348	L1273	I1113	S1050	T971	K905	D834	N703	
	V1413	F1348	A1349	R1275	E1114	E1051		K905	A835	E704	
	C1416	I1350	I1350	E1279	F1115	D1052		L906	P836	V705	
	K1420	V1352	V1352	E1279	F1116	I1053		N907	G837	I706	
	R1421	K1420	K1353	K1286	R1119	Y1057		D908	B837	Q707	
	K1424	K1354	K1354	E1287	I1120	Y1057		L776	D839	L776	
	P1425	K1355	K1355	F1288	I1121	Q1058		D909	D840	L709	
	Y1426	K1357	K1357	Y1289	K1122	Q1059		Q911	Q842	G710	
	M1427	L1358	L1358	L1290	V1216	D1060		K912	W843	I711	
	Y1428	K1359	K1359	R1291	E1123	V1061		W914	E844	H713	
S1505	Y1429	P1360	P1360	V1292	T1124	R1062		F915	N845	I714	
S1506	V1429	W1293	W1293	Y1292	P1128	R1063		G916	T846	S715	
	T1430	L1361	L1361	F1294		T1064		R917	Y847	F716	
	S1431	F1362	F1362		A1135	G1065		N918	T851	K717	
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	L1434	K1364	K1364	P1300	I1142	Q1068		I854	G853	G719	
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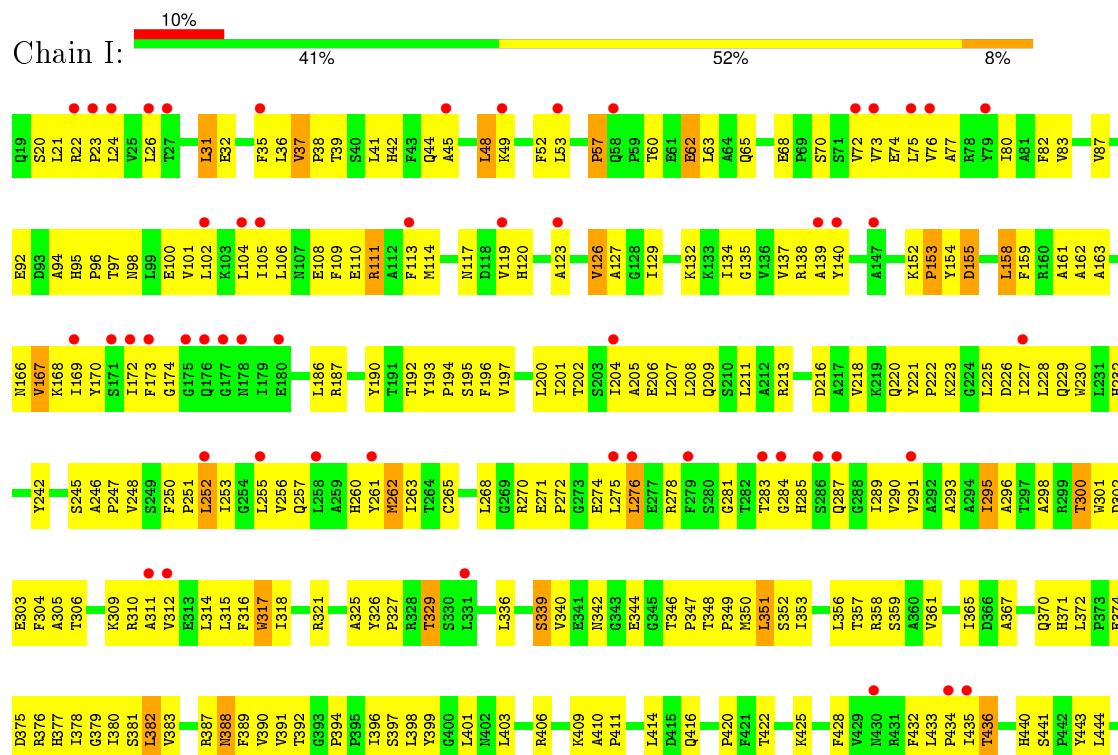
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



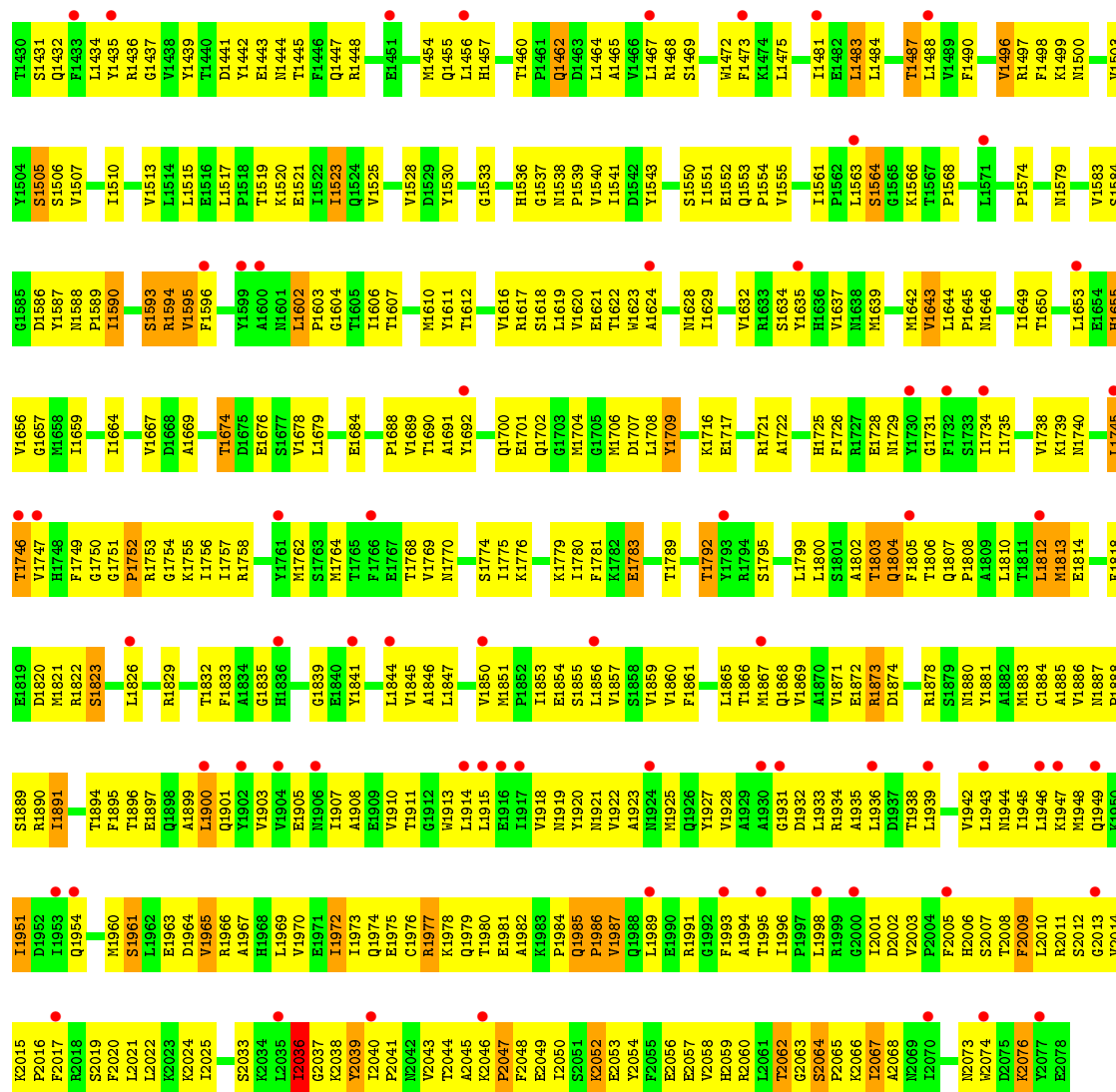
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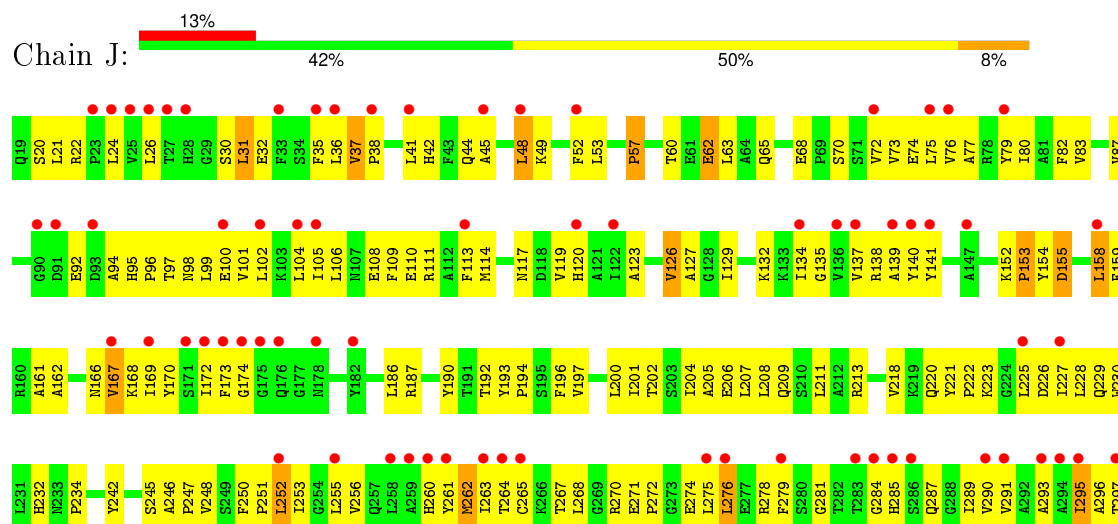
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



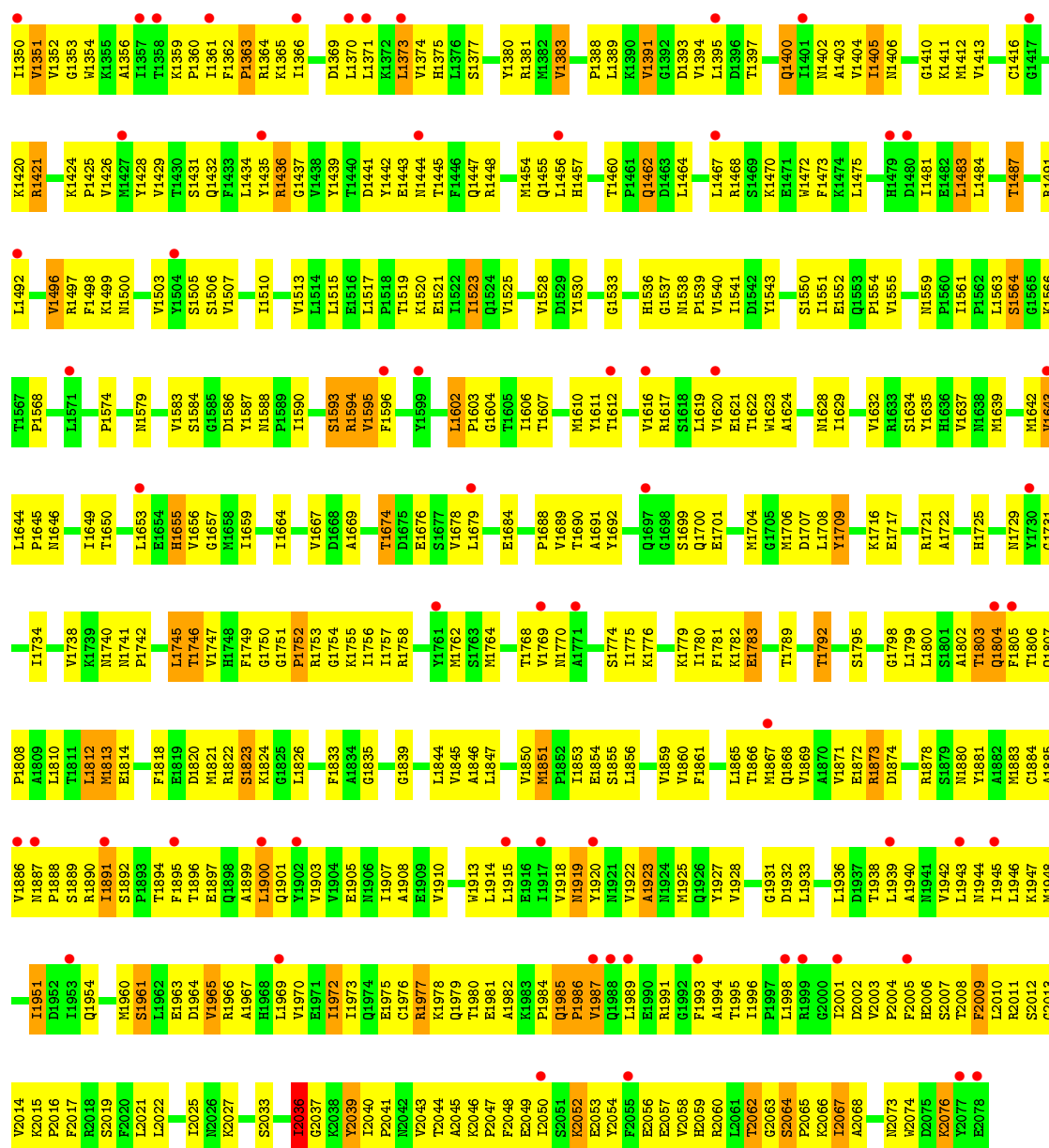
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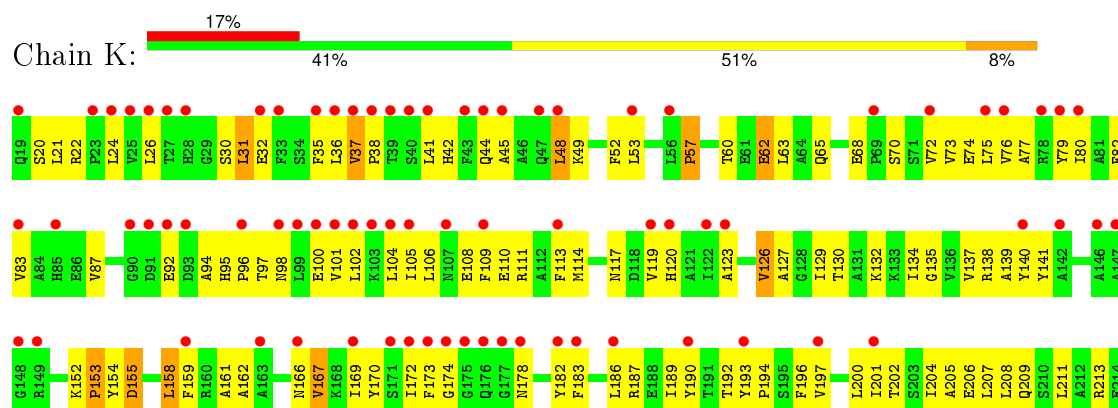
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



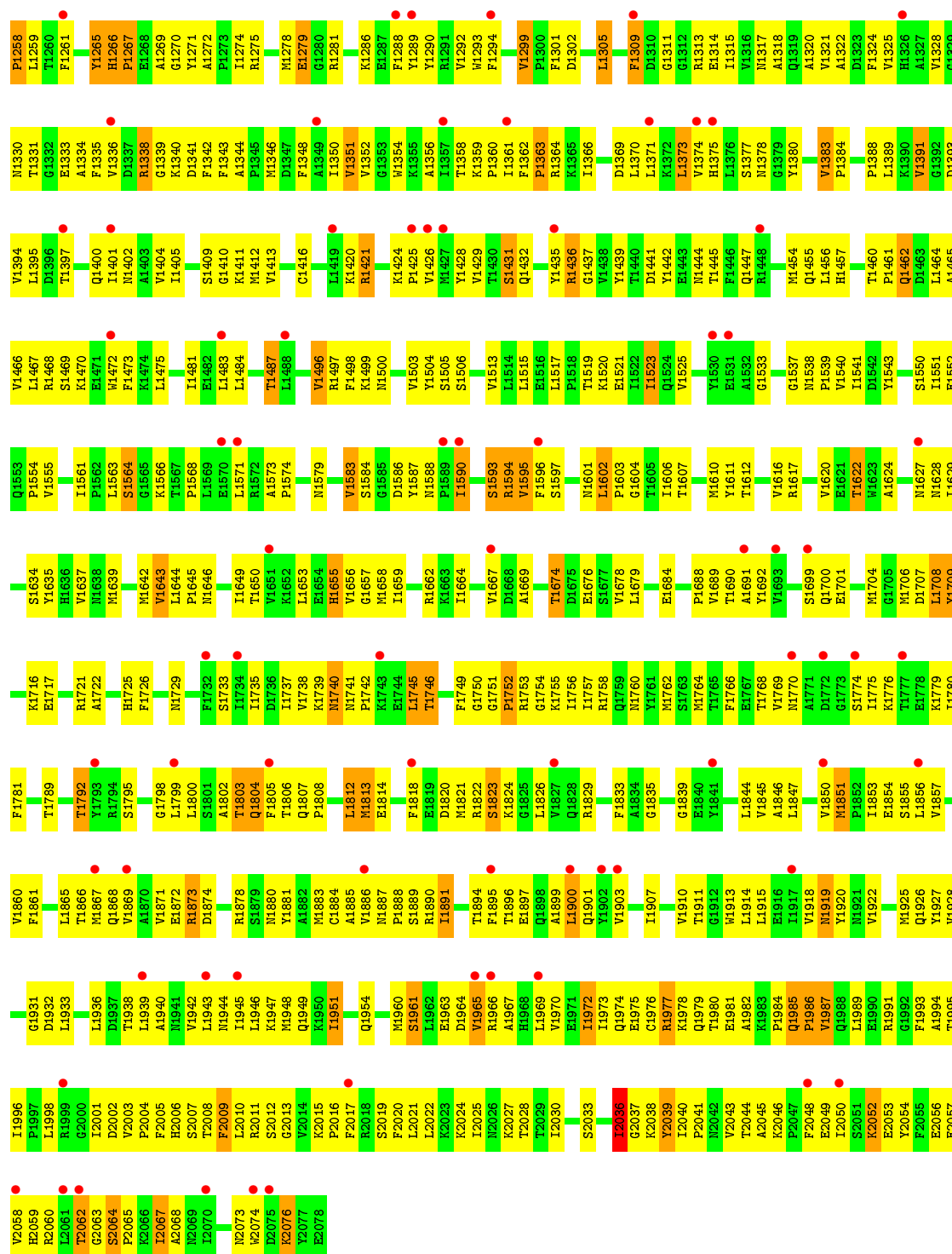
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E1339	E1268	F1196	V1112	L1047	L979	N907	P836	V775	I711	L433	A569	E502	L433	S359
K1340	A1269	A1197	E1113	W1043	L980	D908	G837	L776	R712	P434	V570	E502	P434	A360
D1341	G1270	P1198	V1115	Q1049	Q981	D909	G837	V777	H713	I435	D571	T505	I435	V361
F1342	F1271	T1199	F1116	S1050	L986	F910	D841	A778	I714	T436	W572	V506	T436	I365
F1343	A1272	D1200	D1052	E1051	P989	Q911	Q842	G779	S715	F507	V573	F507	F507	I366
P1345	P1273	G1201	L1053	I1053	Y989	V913	E844	S780	K717	P438	K574	F439	P438	A367
M1346	R1275	Y1203	Y1057	Y1057	P991	W914	R845	F782	P718	H440	G577	T511	H440	Q370
D1347	M1278	V1204	G1058	G1058	P991	F915	R846	G783	G719	L444	P578	I513	L444	H371
A1349	E1279	T1207	D1060	D1060	A992	G916	T847	S785	S720	L580	R579	V514	L580	L372
					R995	N918	T851	E786	A723		V581	F516	A447	P373



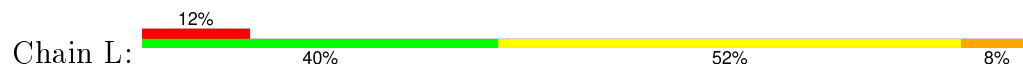
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



Q1188	D1104	W1041	Q830	I768	W703	Y626	L558	V491	I419	S352	T283	V215
TI189	G1105	K1106	A831	I788	E704	H627	F589	R492	P420	I353	G284	D216
M1190	F1102	F1042	I832		I705	E629	R561	R493	K425	L356	H285	A217
L1192	E1107	T971	V833	N773	T706	E628	R561	L494		T357	V218	K219
K1193	V1110	K1044	D834	T774	Q707	L430	A565	T496	F428	R358	Q287	Q220
R1194	P1113	L1045	A835	T775	T708	A631	V566	T496		S359	G288	Y221
L1195	P1112	S1046	P836	L776	L709	G632	D497	D497	F432	A360	I289	P222
F1196	V1113	L1047	G837	T777	G710	G633	A569	P498	L433	V361	V291	K223
A1197	I1113	W1048	R838	T778	H712	G634	V570	V499	A292		G224	G224
P1198	E1114	Q1049	D839	G779	H713	Y635	D571	W501	A293		L226	L226
T1199	F1115	S1050	H840	S780	H714	A638	W572	E502	T436		I295	I227
R1200	F1116	D1052	Q842	G781	T715		W573		A437		A296	L228
	R1119	I1063	W843	G783	S716	W641	W574	T505	P438		T297	Q229
Y1203	I1120	Y1057	E844	G784	K717	S642		V506	F439	Q370	W230	W230
W1204	T1121	G1058	N845	S785	P718	A644	P578	F507	S441	H371	R299	H231
T1207	T1124	Q1059	T846	S786	G719	A644	R579		S441	H372	H232	H232
N1208	P1205	D1060	Y847	D787	S720		L580		P442	P373	W301	N233
P1209	E1127	P091	T851	T788		I648	W581	H512	Y443	E374	D302	P234
P1212	Y1203	V993		T789	A723	E649	K582	H513		I380	A308	
T1215	A1135	R995	V854	T790	Q726	K650	T583	H514	A447	S381	R309	S249
V1216		I996	I855	T791	W727		S584	D515	H448	R376	R310	F250
I1217	K1141	L997	T856	T792	I728	I652	W585	F516		H377	F304	A305
S1218	I1142	Y1000	L858	G794	W729	P653	G586	G517	I451	I378	A305	
V1219	S1143	P1001	S859	S795	I730	G655	Q587	P518		G379	T306	S245
R1220	E1002	E1002	E860	T796	A731	R656	F589	G520	D454	I380	A307	
	E1071	E1002	M861	T798	K732		D591	S522	V455	S381	R309	
Q1224	A1072	A1003	G862	T799	P735	T659	D591	S522	K458	R384	V312	L252
S1225	S1004	R933	E863	F800	T736	N661	M594	T524	I460	R384	E313	L253
A1226	K1074	V934	P864	G801	F737	L662	S595	G525	P461	A386	L314	G254
K1227	Y1075	V935	L865	F802	P738	I663	A596	V526	A462	R387	L255	L255
L1228	S1076	H936	H866	P803	I739	Y664	L587	L527	S463	N388	F316	Q257
V1229	K1077	R937	K867	P804	I740	V665	L588	T528	S464	F389	W317	V256
N1009	V1078	N938	L868	M805	L741	N666	G593	N529	L465	V390	I318	L258
K1230	I1079		A869	P806	Q742		W600	N530	V466	V391	A259	
T1231	D1080	L941	T870	F807	W743	W670	P601	N531	I467	T392	H260	
V1232	E1081	R942	R871	D808	T744	G671	P602	K532	P468	G393	Y261	
E1233	P1082	Y943	G872	G809	G745	W672	W603	D533	V469	P394	M262	
I1234	K1083	V944	V873	C810	G746	Q673	W604	G534	Y470	P395	V326	I263
K1235	K1084	K945	L874	M811	I674	I674	W605	T535	D471	I396	P327	T264
L1236	D1085	H946	F875	H812	G748	P675	A606	G536	T472	S397	R328	C265
V1237	L1017		W876	G813	G749	L676	G607	V537	K473	L398	T329	K266
G1238	L1018	W950	K877	S814	G750		W608		T474	V399	S330	T267
D1239	L1019	P951	E878	R815	H751	V685	T609	L541	D477	G400	L331	L268
N1240	C1020	D952	R871	M816	H752	P686	P610	A542	L477	L401	L336	G269
E1241	Q1021	P953	I883	M817	S753	I687	T611	G543	R479	R406	E271	E271
I1242	R1022	S954	I883	T818	F754		T612	A544	E490	K407	P272	P272
A1243	K1026	D887	D887	K820	E755	L690	W613	I545	L481	V408	G273	G273
T1244	P1027	R888	R888	E821	D756	T691	W615	D546	G482	K409	E274	E274
L1245	V1028	S889	K889	A822	H758	I692	D616	N549	E483	E341	N342	L275
F1247	P1029	K990	K990	H823	Q759	G693	F617	T550	E484	P411	L276	L276
E1248	F1030	R824	R891	H823	Q759	A694	W618	E551	G481	T346	E277	E277
L1249	V1031	T963	R891	S825	I761	S698		V562	I485	P347	R278	R278
R1250	P1032	R964	E894	K826	I762	I699	T621	V562	I487	D415	F279	F279
T1251	A1033	R965	E894	Q827	L763	E700	W622	R555	I487	Q416	S280	S280
	E1036	V966	K897	K828	W764	V701	N623	P566	E489	N417	N350	G281
V1257		E967	R898	K829	Y765	A702		E557	L490	R418	L351	T282



Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



Chain L:





K2066	V2003	T1938	D1874	T1806	I1734	T1850	V1583	Y1504	V1429	P1360	F1288	Y1216	K1141
I2067	P2004	L1939	R1878	Q1807	I1735	L1853	S1584	S1505	T1430	I1361	Y1289	I1217	I1142
A2068	F2005	A1940	R1879	A1809		E1854	G1585	S1506	S1431	P1362	Y1290	S1218	S1143
	H2006	N1941	S1879	A1808	V1738	E1853	D1586	V1507	Q1432	P1363		V1219	Y1144
	S2007	L1943	N1880	T1811	K1739	H1655	V1587	Q1508	K1364	K1365	W1292	R1220	L1146
	T2008	L1942	Y1881	L1812	N1740	V1656	M1588	T1509	L1434	K1365	W1293		
	F2009	N1944	A1882	L1813	N1741	G1657	P1589	I1510	Y1435	I1366	F1294	Q1224	
	L2010	I1945	M1883	M1814	P1742	H1658	I1590		R1436			S1225	D1156
	R2011	L1946	C1884		K1743	I1659	H1591	V1513	D1437	D1369	V1299	S1226	V1157
	S2012	K1947	A1885	F1818	L1744	R1662	V1592	L1514	V1438	L1370	P1300	K1227	V1157
	G2013	M1948	V1886	F1819	L1745	K1663	S1593	L1515	L1371	F1301	S1159	L1228	S1159
		Q1949	N1887	E1820	T1746	I1664	R1594	E1516	T1440	D1302	F1160	V1229	M1160
	K2015	K1950	P1887	D1820			V1595	L1517	D1441			K1230	M1161
	P2016	I1951	S1888	M1821	F1749	V1667	F1596	F1516	Y1442	L1305		T1231	
	F2017	D1952	R1890	R1822	G1750	D1668	S1597	T1519	E1443	F1309		V1232	
	R2018	I1953	I1891	K1824	P1752	A1669	S1598	K1520	N1444	D1310		V1233	
	S2019	Q1954		G1825	R1753		V1599	I1521	T1445	S1377		L1234	
				L1826	G1754	T1674	A1600	I1522	F1446	G1311		K1235	
	L2021	M1960	F1895		K1755	D1675	M1601	I1523	Q1447	G1379		L1236	
	L2022	S1961	T1896	R1829	K1756	E1676	L1602	V1525	R1448	R1313		V1237	
	I2025	E1963	Q1898		I1757	D1677	P1603	T1519		E1314		V1238	
	N2026	D1964	A1899	F1833	R1758	S1677	G1604	K1528	M1454	I1315		D1239	
	K2027	V1965	L1900	A1834	V1759	V1678	T1605	I1529	Q1455	V1316		M1240	
		R1966	Q1901	G1835	N1760	L1679	L1606	D1530	H1456	N1317		E1241	
	I2030	A1967	Y1902	H1836	I1761	Q1680	T1607	Y1530	H1457	A1318		I1242	
			V1903		M1762	E1684	M1610	G1533	T1460	L1389		A1243	
	S2033	L1969	V1904	G1839	S1763	P1688	V1611	G1537	P1461	A1320		T1244	
	K2034	E1970	E1905	E1840	T1765	P1689	T1612	D1537	Q1462	F1324		T1245	
	L2035	E1971	N1906	Y1841	K1765	T1689	V1616	K1538	D1463	K1325		F1247	
	I2036	I1972	I1907	Y1842	F1766	T1690	R1617	N1539	L1464	V1394		L1246	
	G2037	L1973	A1908	A1843	E1767	A1691	S1613	V1540	L1465	H1326		E1248	
	R2038	Q1974	E1909	L1844	T1768	V1692	L1617	I1541	V1466	T1331		G1249	
	Y2039	E1975	V1910	V1845	V1769	F1693	S1619	D1542	L1467	D1395		A1250	
	P2041	R1977		A1846	N1770	F1694	V1620	Y1543	R1468	T1397		T1251	
	N2042	L1914	L1913	L1847	S1774	Q1700	E1621	S1550	S1469	A1399		V1257	
	V2043	L1915	L1915	D1849	I1775	E1701	H1623	I1551	W1472	I1401		P1258	
	T2044	E1916	E1916	V1850	K1776		A1624	E1552	F1473	D1337		L1259	
	A2045	I1917	I1917	M1851	M1704			Q1553	K1474	G1338		F1260	
	K2046	V1918	V1918	P1852	G1705	M1706	M1627	P1554	R1475	A1403		L1261	
	P2047	N1919	N1919	I1853	I1780	D1707	N1628	P1554	V1404	D1341		F1262	
	F2048	P1984	P1984	E1854	F1781	L1708	I1629	V1555		I1405		R1263	
	E2049	Q1985	P1985	S1855	K1782	Y1709			I1481	N1406		T1264	
	I2050	P1986	V1922	L1856	E1783		V1632	P1560	E1482	F1343		T1265	
	S2051	N1923	A1923	S1857		K1716	R1633	I1561	L1483	A1344		R1266	
	K2052	Q1988	N1924	S1858	T1789	E1717	S1634	L1563	L1484	P1345		P1267	
	E2053	L1989	M1925	V1859			Y1635	S1564		M1346		E1268	
	Y2054	Q1926	Q1926	V1860	T1792		H1636	G1565	T1487	D1347		A1269	
	F2055	Y1927	Y1927	F1861		R1721	V1637	K1566	L1488	F1348		G1270	
	E2056	V1928	V1928		S1795	A1722	M1638	T1567	R1491	A1349		Y1271	
	E2057	F1993	A1929	L1865		D1723	M1639		L1492	I1350		A1272	
	V2058	A1930	G1931	G1798	G1798	K1724		P1574	K1420	V1352		P1273	
	H2059	T1995	G1931	L1799	L1799	H1725	M1642		V1496	R1421		R1275	
	R2060	I1996	D1932	L1800	L1800	F1726	V1643	M1577	R1497	G1353		P1276	
	P1997	Q1997	V1869	S1801	S1801	R1727	L1644	E1576	K1498	W1354		M1278	
	L1998	A1997	A1870	A1802	A1802	E1728	P1645	E1576	K1499	A1355		E1279	
	G2063	S2064	E1871	T1803	T1803	M1729	M1646	E1576	N1500	I1357		R1281	
	P2065	D2002	E1872	Q1804	Q1804	Y1730		Y1580	M1427	T1358		P1212	
			R1873	F1805	F1805		I1649		V1503	K1359		T1215	

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 0.269 , (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
Estimated twinning fraction	0.078 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 645017 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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($^{\circ}$)	Ideal($^{\circ}$)
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%)	16	52
1	B	1458/1878 (78%)	1278 (88%)	160 (11%)	20 (1%)	14	48
1	C	1456/1878 (78%)	1283 (88%)	156 (11%)	17 (1%)	16	52
1	D	1461/1878 (78%)	1276 (87%)	161 (11%)	24 (2%)	12	44
1	E	1450/1878 (77%)	1276 (88%)	155 (11%)	19 (1%)	15	50
1	F	1455/1878 (78%)	1282 (88%)	153 (10%)	20 (1%)	14	48
2	G	2058/2060 (100%)	1789 (87%)	237 (12%)	32 (2%)	12	44
2	H	2058/2060 (100%)	1791 (87%)	230 (11%)	37 (2%)	11	42
2	I	2058/2060 (100%)	1787 (87%)	238 (12%)	33 (2%)	12	44
2	J	2058/2060 (100%)	1784 (87%)	240 (12%)	34 (2%)	11	43
2	K	2058/2060 (100%)	1785 (87%)	239 (12%)	34 (2%)	11	43
2	L	2058/2060 (100%)	1780 (86%)	241 (12%)	37 (2%)	11	42
All	All	21079/23628 (89%)	18381 (87%)	2374 (11%)	324 (2%)	13	46

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%)	11	39
1	B	1227/1527 (80%)	1117 (91%)	110 (9%)	12	41
1	C	1225/1527 (80%)	1110 (91%)	115 (9%)	11	39
1	D	1229/1527 (80%)	1107 (90%)	122 (10%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1219/1527 (80%)	1106 (91%)	113 (9%)	11	39
1	F	1224/1527 (80%)	1111 (91%)	113 (9%)	11	40
2	G	1752/1752 (100%)	1569 (90%)	183 (10%)	9	32
2	H	1752/1752 (100%)	1569 (90%)	183 (10%)	9	32
2	I	1752/1752 (100%)	1565 (89%)	187 (11%)	8	31
2	J	1752/1752 (100%)	1567 (89%)	185 (11%)	8	31
2	K	1752/1752 (100%)	1566 (89%)	186 (11%)	8	31
2	L	1752/1752 (100%)	1563 (89%)	189 (11%)	8	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	-	45,52,52	1.16	3 (6%)	55,80,80	1.82	4 (7%)
3	NAP	B	1901	-	45,52,52	1.16	3 (6%)	55,80,80	1.78	5 (9%)
3	NAP	C	1901	-	45,52,52	1.20	3 (6%)	55,80,80	1.83	4 (7%)
3	NAP	D	1901	-	45,52,52	1.31	3 (6%)	55,80,80	1.97	4 (7%)
3	NAP	E	1901	-	45,52,52	1.18	3 (6%)	55,80,80	1.92	6 (10%)
3	NAP	F	1901	-	45,52,52	1.19	3 (6%)	55,80,80	1.93	5 (9%)
4	FMN	G	2101	-	32,33,33	5.94	21 (65%)	34,50,50	2.05	6 (17%)
3	NAP	G	2102	-	45,52,52	1.12	4 (8%)	55,80,80	1.88	5 (9%)
4	FMN	H	2101	-	32,33,33	5.95	21 (65%)	34,50,50	1.90	6 (17%)
3	NAP	H	2102	-	45,52,52	1.13	4 (8%)	55,80,80	1.90	4 (7%)
4	FMN	I	2101	-	32,33,33	5.96	19 (59%)	34,50,50	1.91	6 (17%)
3	NAP	I	2102	-	45,52,52	1.08	3 (6%)	55,80,80	1.91	3 (5%)
4	FMN	J	2101	-	32,33,33	6.20	22 (68%)	34,50,50	2.00	4 (11%)
3	NAP	J	2102	-	45,52,52	1.16	4 (8%)	55,80,80	1.90	6 (10%)
4	FMN	K	2101	-	32,33,33	6.21	21 (65%)	34,50,50	1.83	5 (14%)
3	NAP	K	2102	-	45,52,52	1.09	4 (8%)	55,80,80	1.79	5 (9%)
4	FMN	L	2101	-	32,33,33	6.01	21 (65%)	34,50,50	1.91	5 (14%)
3	NAP	L	2102	-	45,52,52	1.12	3 (6%)	55,80,80	1.84	4 (7%)

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	-	-	0/18/18/18	0/3/3/3
3	NAP	G	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	H	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	H	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	I	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	I	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	J	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	J	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	K	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	K	2102	-	-	0/27/67/67	0/5/5/5
4	FMN	L	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	L	2102	-	-	0/27/67/67	0/5/5/5

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2101	FMN	C8M-C8	2.00	1.55	1.51
3	G	2102	NAP	C6N-N1N	2.01	1.41	1.35
4	H	2101	FMN	P-O5'	2.09	1.65	1.59
3	K	2102	NAP	C6N-N1N	2.15	1.41	1.35
3	I	2102	NAP	C2A-N1A	2.17	1.38	1.33

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2102	NAP	N3A-C2A-N1A	-12.04	119.41	128.87
3	D	1901	NAP	N3A-C2A-N1A	-11.99	119.45	128.87
3	G	2102	NAP	N3A-C2A-N1A	-11.57	119.78	128.87
3	J	2102	NAP	N3A-C2A-N1A	-11.55	119.80	128.87
3	L	2102	NAP	N3A-C2A-N1A	-11.45	119.88	128.87

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(Å²)	Q<0.9
1	A	1457/1878 (77%)	0.29	44 (3%)	54	29	16, 50, 103, 146	0
1	B	1464/1878 (77%)	0.31	38 (2%)	59	35	17, 50, 106, 157	0
1	C	1462/1878 (77%)	0.33	43 (2%)	55	31	15, 48, 107, 155	0
1	D	1467/1878 (78%)	0.29	48 (3%)	50	26	17, 52, 106, 151	0
1	E	1456/1878 (77%)	0.31	46 (3%)	51	27	17, 50, 106, 152	0
1	F	1461/1878 (77%)	0.34	37 (2%)	61	37	17, 47, 106, 156	0
2	G	2060/2060 (100%)	0.48	170 (8%)	14	5	24, 83, 128, 156	0
2	H	2060/2060 (100%)	0.57	222 (10%)	8	2	24, 85, 129, 155	0
2	I	2060/2060 (100%)	0.51	212 (10%)	9	3	20, 85, 129, 158	0
2	J	2060/2060 (100%)	0.61	274 (13%)	4	2	27, 88, 132, 157	0
2	K	2060/2060 (100%)	0.84	352 (17%)	2	1	25, 90, 133, 157	0
2	L	2060/2060 (100%)	0.58	257 (12%)	5	2	22, 86, 131, 158	0
All	All	21127/23628 (89%)	0.48	1743 (8%)	14	5	15, 74, 125, 158	0

The worst 5 of 1743 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	0.15	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	-0.57	26,63,101,111	0
3	NAP	G	2102	48/48	0.92	0.24	-0.61	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.