



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 08:28 PM BST

PDB ID : 4V58
Title : Crystal structure of fatty acid synthase from thermomyces lanuginosus at 3.1 angstrom resolution.
Authors : JENNI, S.; LEIBUNDGUT, M.; BOEHRINGER, D.; FRICK, C.; MIKO-LASEK, B.; BAN, N.
Deposited on : 2007-03-09
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

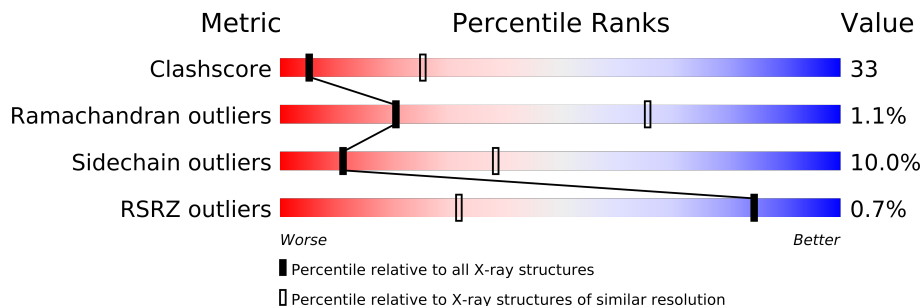
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
2	H	2060	
2	I	2060	
2	J	2060	
2	K	2060	
2	L	2060	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 166671 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

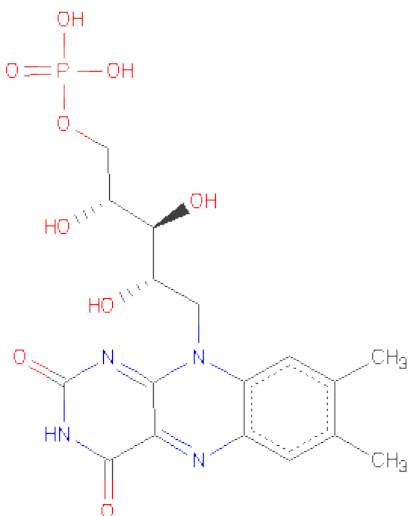
- Molecule 1 is a protein called FATTY ACID SYNTHASE ALPHA SUBUNITS.

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



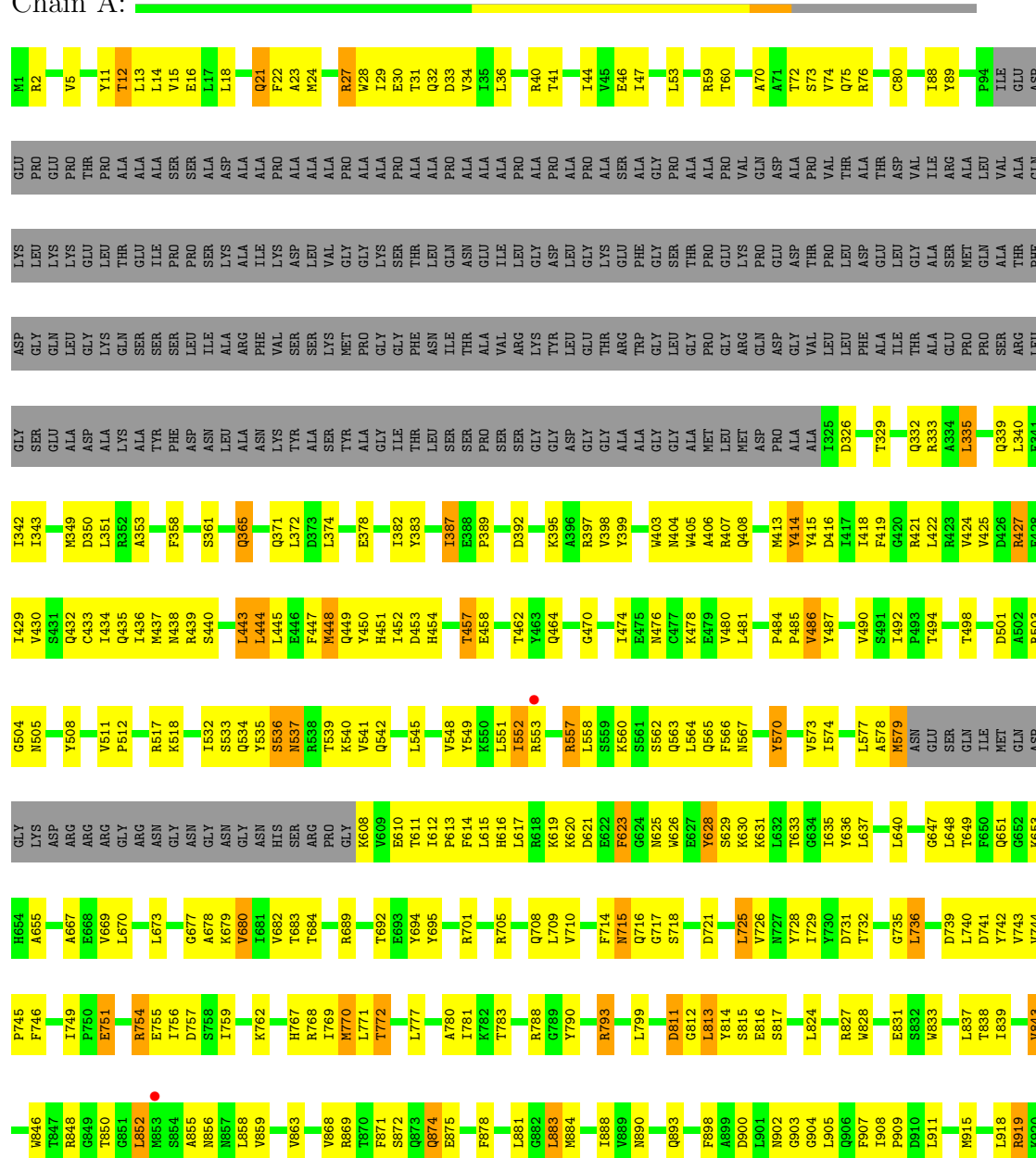
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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.

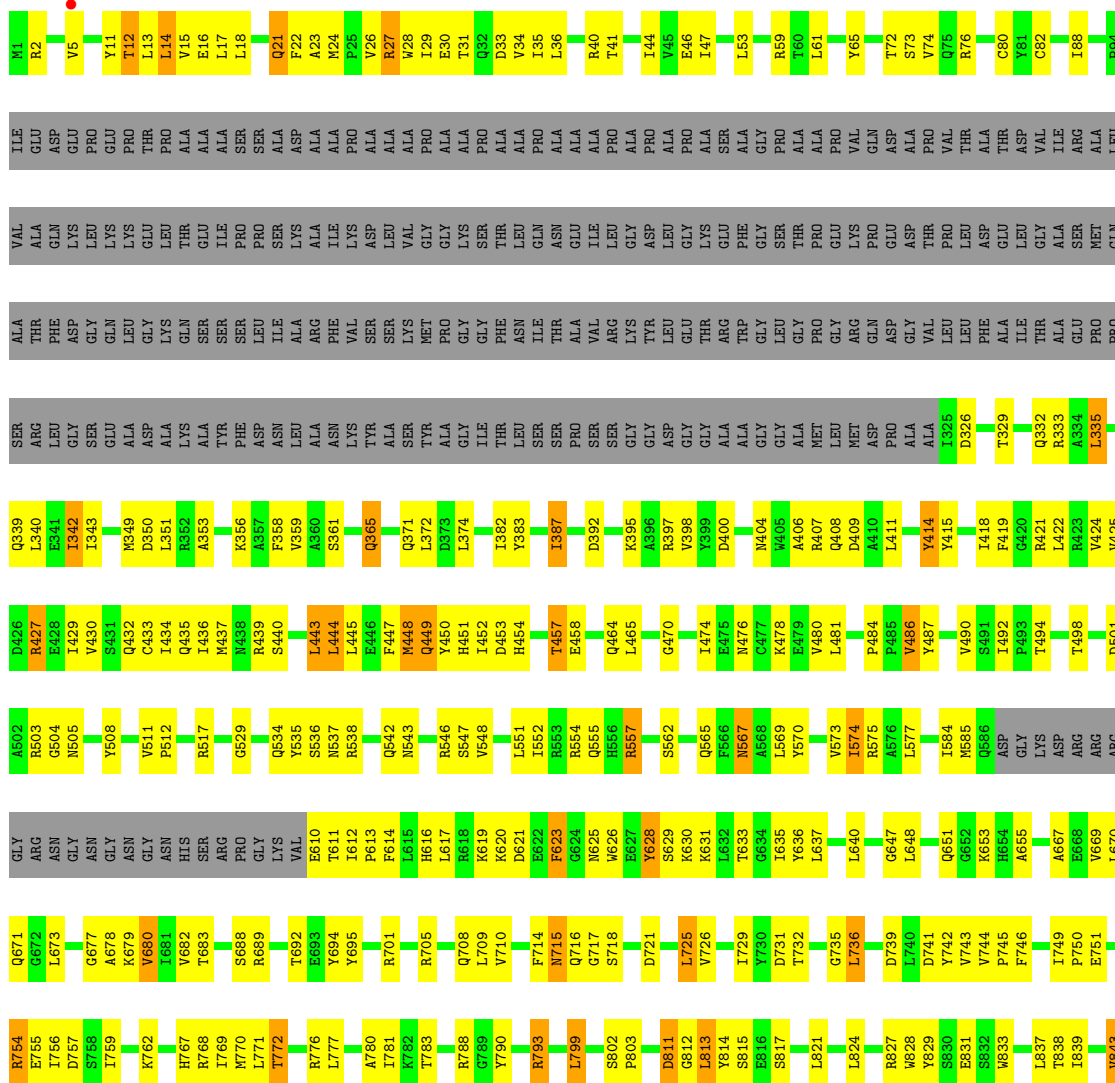
• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS

Chain A:











EL336	FI254	Y1173	FI086	I1002	G910	R827	G735	G647	A578	A502	R427	L347	GLU
PI337	PI176	PI176	Y1089	G1003	L911	W828	G1033	L648	M579	R503	E428	K348	LYS
G1338	T1267	E1177	D1090	P1004	M915	R829	P1004	T649	N580	G504	I429	ASP	GLY
E1339	M1268	D1178	P1091	G1006	R915	R830	D739	F650	E581	M505	V430	ALA	LYS
M1340	G1341	I1179	D1109	N1007	L918	E832	D741	G652	Q582	Y508	C432	L351	GLN
S1341	V1262	I1180	R1093	A1008	R919	R833	D742	K653	I584	Y508	Q433	T329	ALA
R1342	M1263		R1094		E920		V743	A654	M585	V511	I434		THR
P1343	M1264	Y1183	Q1095	R1011	E921	L837	V744	A655	Q586	P512	Q435	ASP	SER
T1344		D1184	L1096	M1014	I922	T838	F745	A667	ASP	R517	I436	ASN	LEU
S1345		P1185	L1097	E1015	S926	R839	F746		GLY	R517	T436	ASN	ILE
T1346	L1267	V1186	Q1098	E1015					LVS			LEU	SER
T1347	S1268	T1187	Q1099						GLY			LEU	ALA
	S1269	T1187	Q1099						GLY			LEU	ALA
	T1270	L1188	V1100	G1018	R929	V843	I749	V669	ARG	K524	R439	S361	PHE
				K1019	Q930	R848	P750	L670	ARG	K524			VAL
		V1192	L1106	F1020	Q930		E751	L671	ARG	M526	S440	Q365	SER
			E1107	F1020	Q930				ARG	A527			ASP
		A1197	P1108	L1022	Q930	T850	R754	L673	GLY	E528	L443	Q371	SER
		L1198			Y942	G851	I756		ASN		L444	T372	LYS
		L1199	K1113	M1028	Y943	R853	D757	G677	ASN	I532	E446	L374	THR
		S1200			N944	R854	S758	K679	ASN	S533	M448	L374	GLY
		S1201	E1117	M1031	E945	A855	I759	V680	GLY	Y535	Q449	I382	ILE
		G1202		M1032	E946	R856		I681	ASN	S536	Y450	Y383	THR
			G1124		D947	R857	K762	V682	ASN	N537	Y450	Y383	LEU
		F1209		M1037	H948	L858	S763	T683	GLY	N537	H451		ASN
		Y1210		H1038	E949		E764		HIS	R538	I452	I387	ILE
		K1211	T1129	N1039	A950	L866		S688	PRO	T539	D453	E388	THR
		E1212	F1130	G1040	L951	G867	H767	R689	PRO	K540		P389	ALA
		Y1213	E1131	P1041	Y952	V868	R768		SER	V541	H454		VAL
		H1214	Q1137	L1042	R953	R869	I769	T692	GLY	Q542		A390	ARG
									ASN				LEU
		L1215	Y1136	P1046	A961	T870	M770	S693	GLY				LEU
		S1216	T1139	Y1047	R962	F871	L771	V694					GLY
		V1217	R1141	Y1047	R962	S872	I772	V695					GLY
		G1218	L1142	M1050	X964	G873	L777	R701					GLY
		G1219	R1143	V1051	Y965	E875							GLY
		N1220		D1052	P966			R705					GLY
			L1148		F967	F878	A780						GLY
		G1223	L1148		F967		I781						GLY
		F1307	S1224	L1149	P968		K782	Q708					GLY
		D1308	G1225	L1150	E969	L881	T783	L709					GLY
		G1225											GLY
		V1226	P1151	E1057	L970	G892		V710					GLY
		G1227	F1310	L883	P1058	M884	R788						GLY
			Q1311	A1153			G789	V712					GLY
		E1312	S1230	L1154	D1061		Y790	P713					GLY
			A1313	Q1155		T888	E791	F714					GLY
		G1313	L1231	F1156	K083		T792	M715					GLY
		G1314	L1232	F1156	K1067		R793	Q716					GLY
		S1315	R1233	D1157	Y1068	P896		E627					GLY
		G1316	R1158		N988	R897		G717					GLY
		E1317	M1235	L1159	Y1071	F898	L799	S718					GLY
			Y1236	V1160	I1072	A899							GLY
		K1321	K1237	A1161		D900	D811	D721					GLY
		D1238	G1162	H1075	Y994	L901	G812						GLY
			Q1163		V994	N902	L813	L725					GLY
		L1241	Q1164	I1078	Y995	G903	Y814	V726					GLY
		D1242	P1165	R1079	V996	G904	S815						GLY
		K1243		I1080	T997	L905		I729					GLY
			W1168	I1081	G998	Q906	L821						GLY
		I1249	D1169	I1082	L999	F907		T730					GLY
		L1250	A1170	P1083	A1000	N908	L824	T732					GLY
		Q1251		E1001		P909							GLY

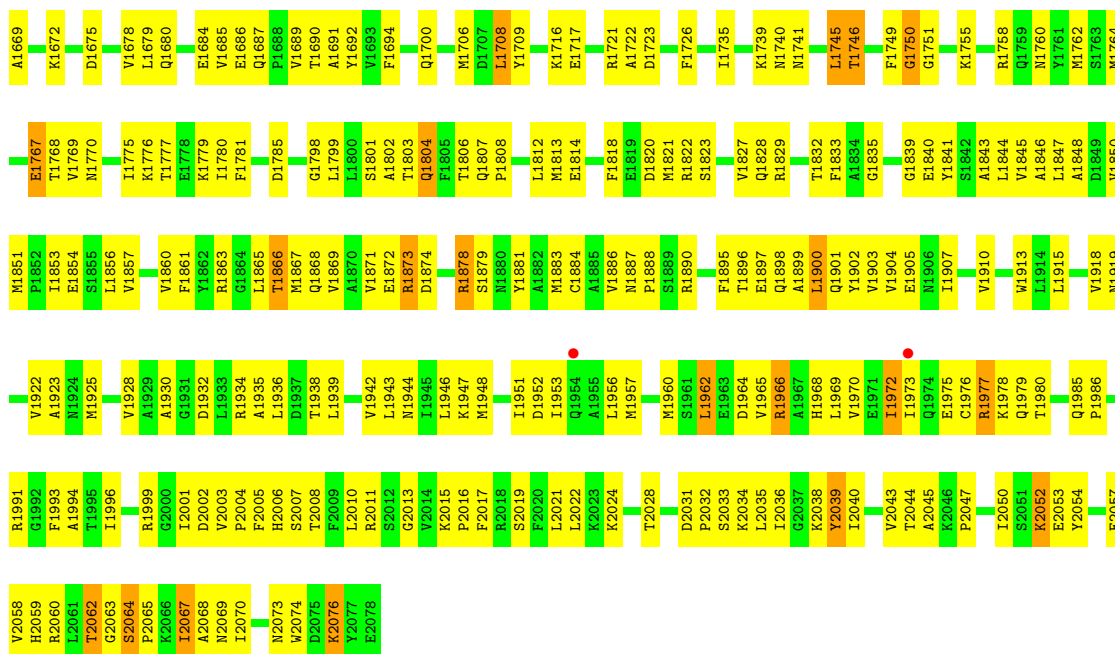
[illegible]

- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS

Chain F:

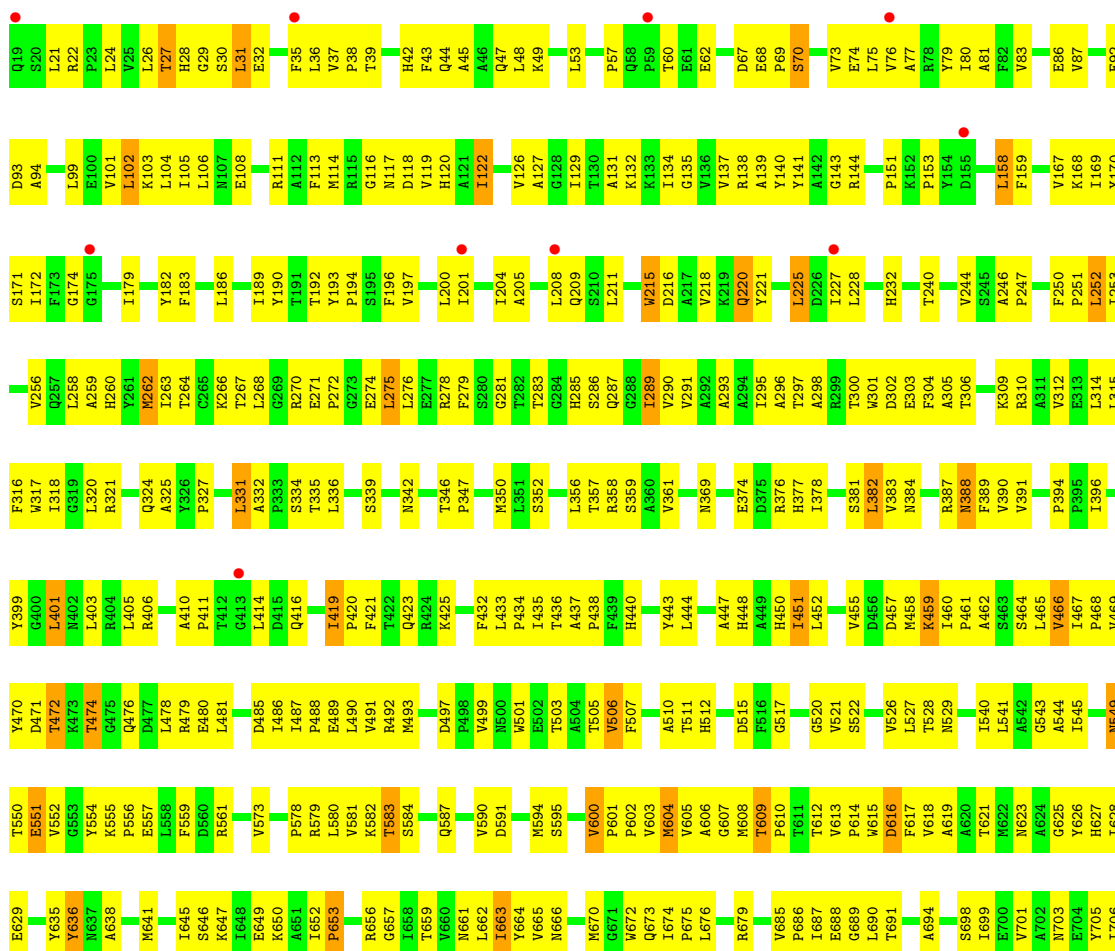
P1185	L1097	G1006	S926	R848	F746	K853	ASP	D501	E498	Q339	SER	ALA	VAL	ILE
V1186	Q1098	M1007	S929	G849	E751	H854	GLY	N505	I429	L940	ARG	THR	ALA	GLU
T1187	E1099	A1008	R929	T850	G851	A855	LYS	N506	V430	E941	LEU	PHE	GLN	ASP
L1188	V1100	R1011	Q930	G851	R754	A857	ASP	Y508	S431	I342	GLY	ASP	LYS	GLY
L1199	D1105	M1014	I333	M852	E755	E868	ARG	Y508	C432	I343	GLU	GLY	LYS	PRO
S1200	L1106	E1015	I333	R854	I756	V869	ARG	V511	I434	M349	ALA	GLY	LYS	PRO
S1201	E1107	P1108	V942	A856	I759	L870	GLY	P512	I436	D350	ASP	GLY	LYS	THR
F1209	K1113	G1018	N944	N857	K762	L873	ASN	R517	M437	R352	LYS	GLN	THR	PRO
K1210	E1117	S1021	E946	V859	K762	L873	GLY	M526	N438	A353	ALA	SER	ALA	ALA
K1211	I1129	F1130	D947	V863	H767	G877	ASN	A527	S440	K356	TYR	SER	ILE	ALA
K1212	V1140	M1028	H948	V868	R768	K879	ASN	A527	S440	K356	PHE	SER	ILE	ALA
K1213	R1141	N1038	H948	M770	I769	V880	GLY	S533	L443	A357	ASP	SER	PRO	SER
K1214	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1215	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1216	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1217	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1218	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1219	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1220	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1221	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1222	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1223	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1224	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1225	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1226	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1227	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1228	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1229	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1230	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1231	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1232	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1233	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1234	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1235	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1236	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
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K1238	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1239	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1240	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1241	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1242	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1243	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1244	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
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K1246	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1247	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1248	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
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K1252	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1253	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1254	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1255	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1256	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1257	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1258	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
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K1260	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1261	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1262	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1263	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
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K1266	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1267	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1268	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1269	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1270	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1271	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1272	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER
K1273	R1141	N1038	H948	M770	I769	V880	GLY	Q534	L444	A357	ASN	ILE	PRO	SER





• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNIT

Chain H:



F1818	V1640	P1568	K1499	V1426	V1351	A1269	A1197	I1120	S1050	S978	Q911	D840	V777	Q707
E1819	G1641	R1572	M1500	M1427	V1352	G1270	P1198	L1121	E1051	L979	K912	D841	A778	T708
D1820	L1644	A1573	Y1504	T1430	G1354	Y1271	T1199	K1122	D1052	L980	V913	Q842	G779	L709
M1821	L1647	P1574	S1505	S1431	K1355	I1275	G1201	A1123	W1053	D985	F915	W843	S780	R712
R1822	D1648	E1578	S1506	Q1432	K1356	R1274	M1202	T1124	Y1057	D986	G916	N845	G781	H713
S1823	L1649	M1579	V1507	F1433	A1356	E1276	Y1203	E1126	Y1061	D987	R917	T846	G783	T714
V1827	T1650				K1359	M1277	V1204		V1062	E988	N918	T847	G784	S715
Q1828	L1653	R1582	G1511	Y1435	P1360	L1278	E1205		G1062	E989	G921	R848	S785	F716
R1829	G1511	G1511		R1436	F1362	T1279	T1206		T1064	Y990		R849	D787	K717
T1832	L1514	L1514	L1514	F1437	R1284	R1284	T1207	L1133	T1064	P991		P850	T788	G719
F1833	E1516	L1515	E1516	Y1439	K1285	K1285	M1208	R1137	I1066	I896	V924	T851	Y789	A723
A1834	L1517	L1517	L1517	T1440	K1364	E1287	P1209	D1138	I1067	L997	L926	W854	P790	A723
G1835	L1518	L1518	L1518	D1441	K1366	F1288	D1211	A1139	Q1068	A998	E927	T855	Y791	T724
	L1519	L1519	L1519	Y1442	I1367	Y1289	P1212	A1139	G1069	A999	D928	T856	L792	Q725
	K1520	L1520	L1520	T1445	G1368	Y1290	K1141	K1141	P1070	Y1000	M929	T793	T793	Q726
	E1521	L1521	L1521		D1369	R1291	T1215	I1142	P1071	P1001	T930	G794	G794	T727
	L1522	L1522	L1522		L1370	V1292	Y1216	S1143	A1072	E1002	Y931	S795	S795	
	L1523	L1523	L1523	E1451	L1371	E1293	I1217		A1073	Q1006	A932	E860	Y796	T730
	Q1524	L1524	L1524	V1452	K1372	F1294	S1218	L1146	K1074	E933	E933	R861	S797	A731
	V1525	L1525	L1525	P1453	L1373	V1219	V1219		Y1075	L1007	E934	G862	T798	A731
	A1526	L1526	L1526	M1454	V1374	R1220	N1153	N1153	S1076	I1008	Y935	E863	K799	N734
	S1527	L1527	L1527	Q1455	H1375		L1154	L1154	K1077	N1009	R936	P864	F800	
	Y1528	L1528	L1528	H1457			P1155	P1155		A1010	R937	T865	G801	F737
	D1529	L1529	L1529		Y1380		Q1224	D1156	D1080	Q1011	M938	R866	Y802	P738
	M1600	L1600	L1600	T1460	R1381	F1301	S1225	V1157	E1081	D1012	V939	K867	P803	T739
	A1601	L1601	L1601	P1461	M1382		A1226	L1158	P1082	P1013	R941	R868	P804	I740
	L1602	L1602	L1602	Q1462	P1388	L1305	K1227	S1159	Q1014	D1014	L941	A869	M805	L741
	P1603	L1603	L1603	L1463			L1228	T1160	K1084	H1015	M942	T870	P806	Q742
	G1604	L1604	L1604	L1464	V1391	V1308	V1229	M1161		F1016	Y943	R871	F807	W743
	T1605	L1605	L1605	A1465	G1392	F1309	K1230		D1088	L1017	V944	G872	D808	W743
	I1606	L1606	L1606	V1466	D1393			I1164	G1089	L1018		G809	G809	G746
		L1607	L1607	L1467	D1394	R1313	I1234		I1090	L1019	K948	R875	C810	R747
		L1608	L1608	L1468	V1394	E1314	L1235	Y1169	H091	C1020	R949	W876	M811	
		L1609	L1609	L1469	L1395	I1315	L1236	W1170	W950	Q1021	W950	K877		G750
		L1610	L1610	S1469	D1396	V1316	V1237	W1171	D1093	R1022	I951	E878	S814	H761
		L1611	L1611	K1470	T1397	H1317	G1238	R1172	H094		D952	L879	R815	H752
		L1612	L1612	E1471	T1398	A1318	D1239	H1173	I1095	K1026	P953	D880	M816	
		L1613	L1613	W1472	A1399		M1240	A1174	K1096	P1027	S954	D881	M817	E755
		L1614	L1614	L1475	Q1400	F1324	T1245	M1175	F1097	V1028	L955	F884	T818	E755
		L1615	L1615	D1476	I1401	V1325	T1246		L1098	P1029	K956	K820	A819	D756
		L1616	L1616	D1477	A1402	M1330	F1247	T1178	L1099	F1030	K957	E888	E821	H758
		L1617	L1617	Q1478	A1403		E1248	E1179		P1031	L958	S889	A822	Q759
		L1618	L1618	H1479	V1404	A1334	G1249	V1180	Y1103	P1032	T959	K890	H823	P760
		L1619	L1619	L1481	I1405	F1335	V1182	F1181	D1104	A1033	G960	R891	T824	L761
		L1620	L1620	E1482	N1406		T1251	Q1183	G1105	L1035	P962	K826	S825	L762
		L1621	L1621	L1483	S1409	R1338	V1256	R1186	K1106	E1036	I963	E894	K826	Y765
		L1622	L1622	L1487	K1410	G1339		F1187	E1107	E1039	R964	L895	Q827	S766
		L1623	L1623	L1488	K1411		L1259	Q1188	E1108	E1039	R965	K896	Q827	R767
		L1624	L1624	V1489	M1412	F1342	T1260	T1189	N1109	Y1040	V966	K897	K829	I768
		L1625	L1625	L1492	V1413	F1343	T1261	M1190	N1109	Y1041	E967	K897	K829	I768
		L1626	L1626	L1492	C1416	A1344	F1261	N1190	P1111	F1042	E968	I903	I832	K770
		L1627	L1627	L1492	G1417	P1345	R1262	P1191	P1112	K1043	R969	K904	W833	C771
		L1628	L1628	L1492	T1418	D1347	Y1265	L1192	I1113	K1044	P970	K905	D834	S772
		L1629	L1629	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1630	L1630	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1631	L1631	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1632	L1632	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1633	L1633	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1634	L1634	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1635	L1635	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1636	L1636	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1637	L1637	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1638	L1638	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1639	L1639	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1640	L1640	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1641	L1641	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1642	L1642	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1643	L1643	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1644	L1644	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1645	L1645	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1646	L1646	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1647	L1647	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1648	L1648	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1649	L1649	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1650	L1650	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1651	L1651	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1652	L1652	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1653	L1653	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1654	L1654	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1655	L1655	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1656	L1656	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1657	L1657	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1658	L1658	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1659	L1659	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1660	L1660	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1661	L1661	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1662	L1662	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1663	L1663	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1664	L1664	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1665	L1665	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1666	L1666	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1667	L1667	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1668	L1668	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1669	L1669	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1670	L1670	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1671	L1671	L1492	T1418	F1348	H1266	K1193	E1114	L1047	T971	L906	A835	N773
		L1672	L1672	L1492	T1418	F1348	H1266	K1193	E1114	L				



● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

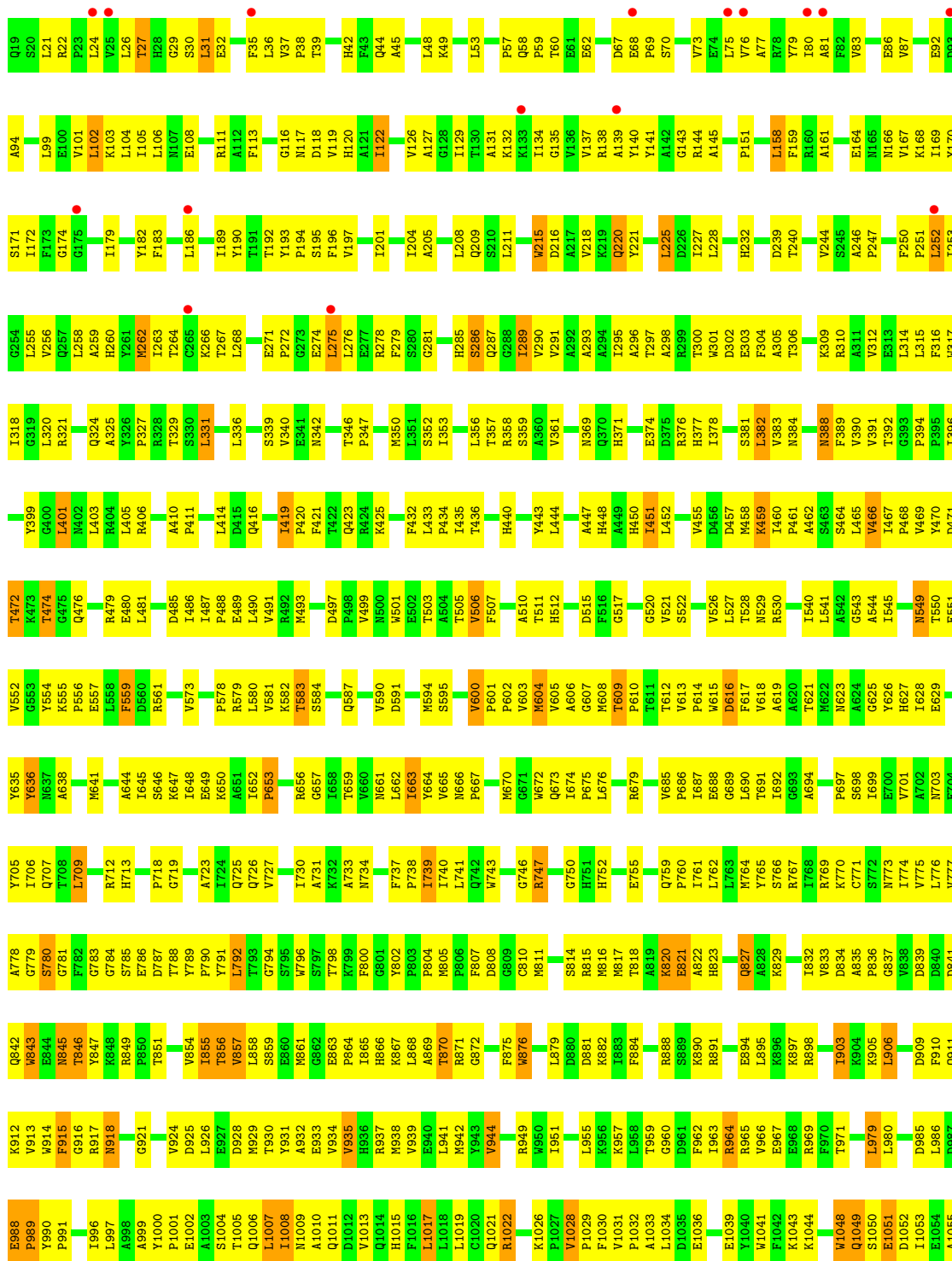
Chain I: █

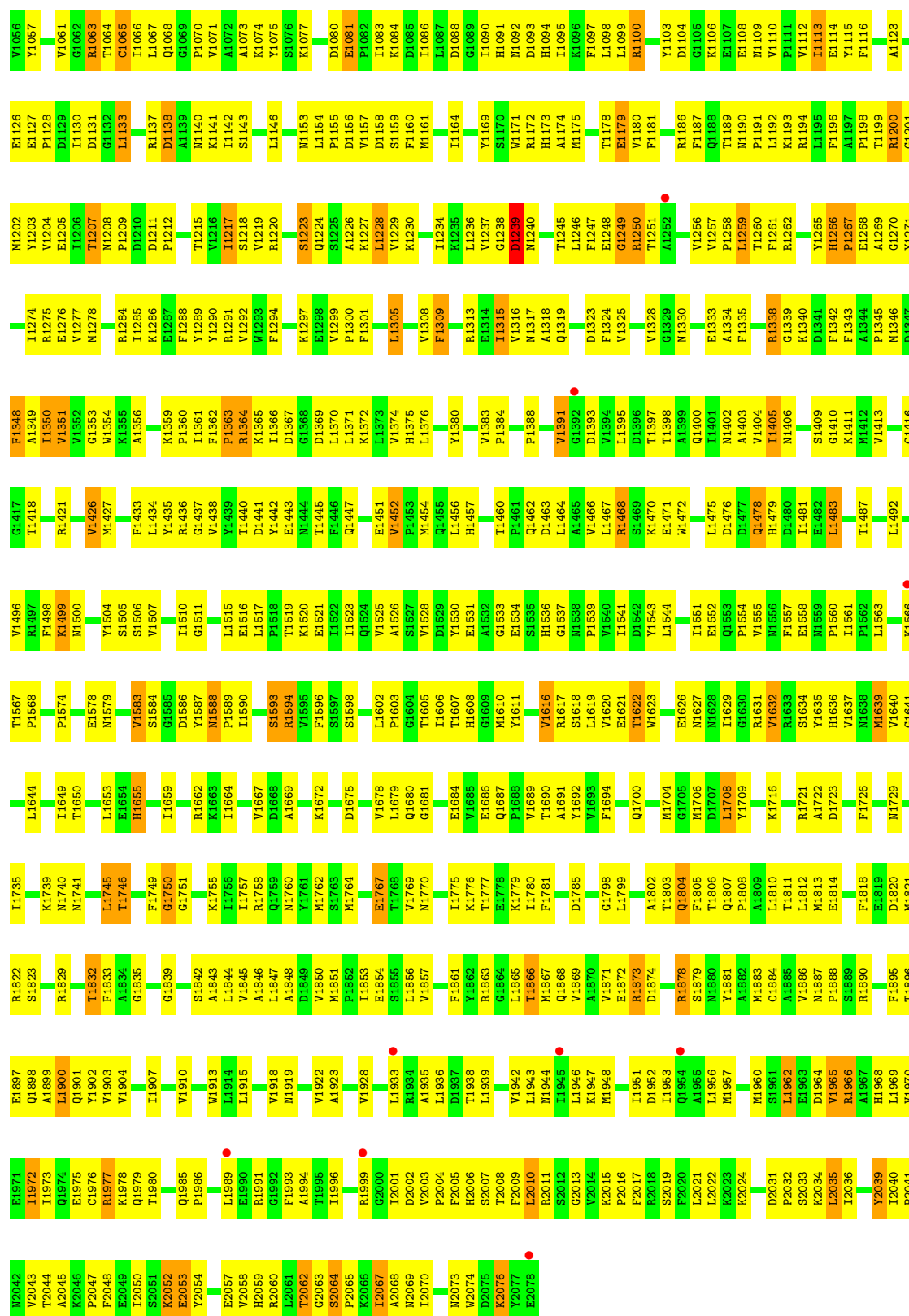




• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain J:

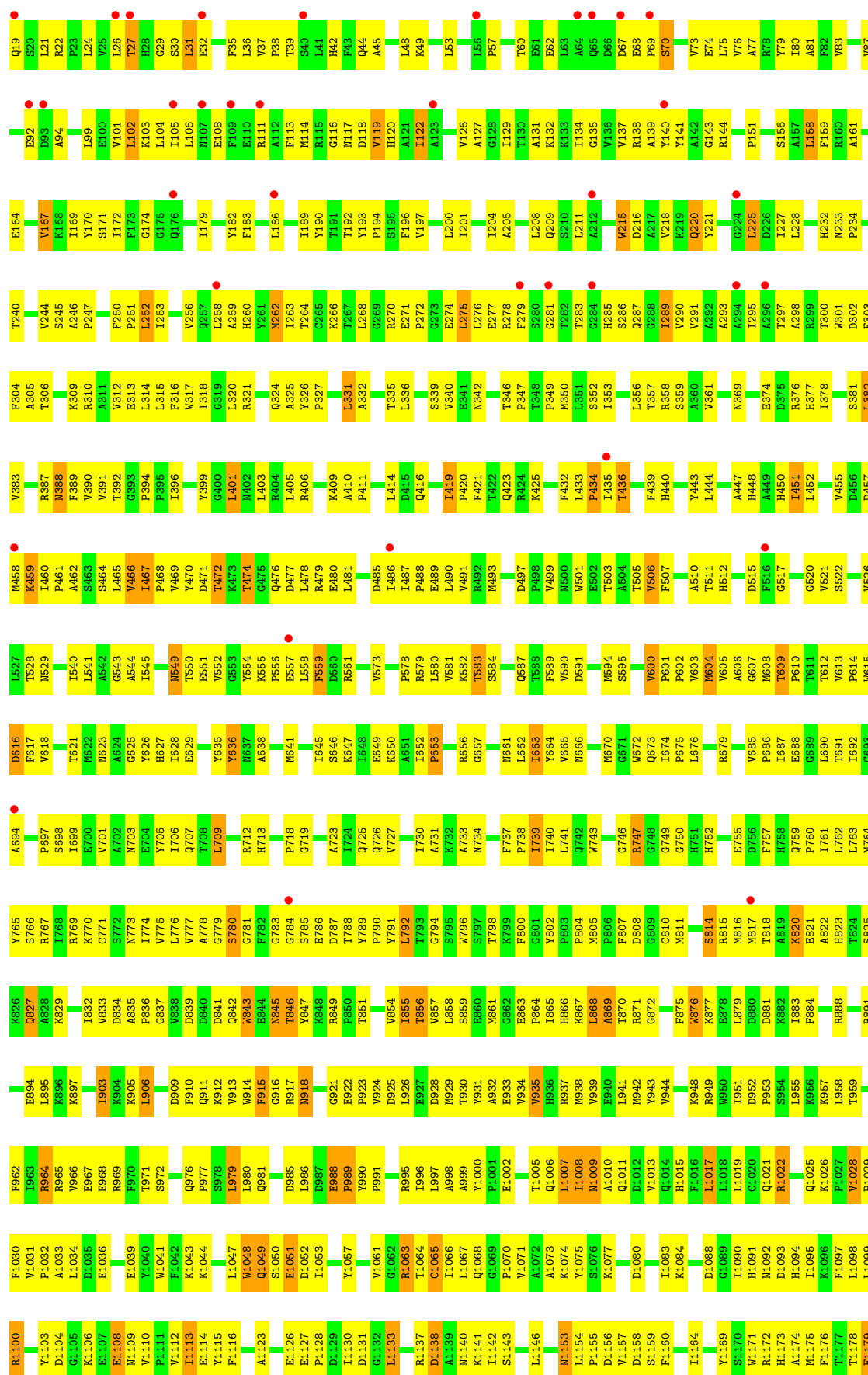


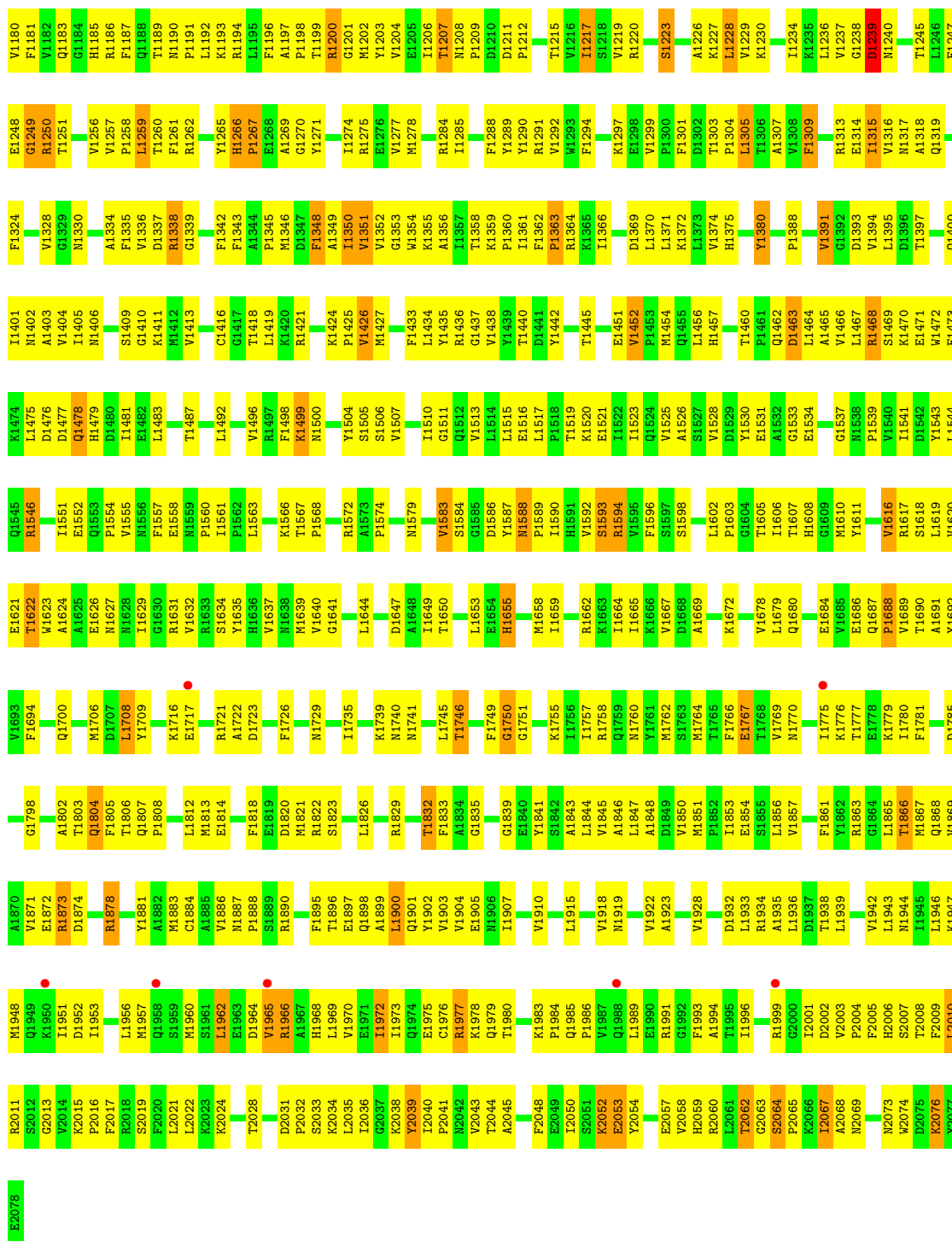


• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain K:

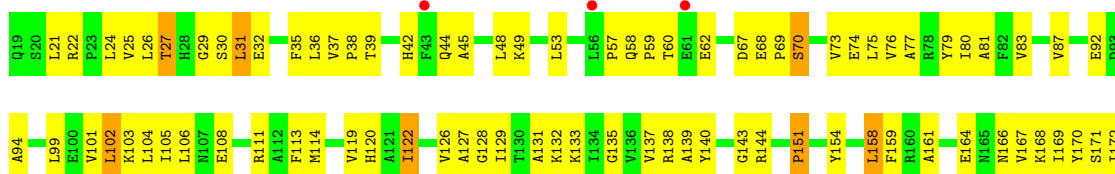






• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain L:



V1277	G1201	D1125	Y1057	L986	W914	E844	S780	L709	Y635	E551	D471	G400	G319	L258	F173
M1278	M1202	E1126	V1061	D987	F915	N845	G781		G636	V552	T472	L401	L320	A259	G174
R1284	Y1203	E1127	G1062	P989	G916	T846	F782	R712	N637	G553	K473	N402	R321	H260	
I1285	V1204	P1128	R1063	Y990	R917	Y847	G783	H713	A638	Y554	T474	L403		Y261	I179
K1286	E1205	R1129	T1064	P991	N918	X848	G784	I714	K555	K555	G475	R404	Q324	M262	
F1287	I1206	I1130	T1064	P991	G821	R849	S785	S715	M641	P566	Q476	L405	A325	I263	Y182
E1287	T1207	D1131	G1065		E922	P850	E786	F716		E557	D477	R406	Y326	F264	F183
F1288	N1208	G1132	L1066	I986	E923	T851	D767	K717	A644		L478	K407	P327	C265	
Y1289	P1209	L1133	L1067	L987	P923		D768	F718	I645		R479			K266	L186
R1291	T1215	R1137	G1069	A999	V924	W854	F789	G719	I646	R561	E480	A410	L331	T267	
R1292	V1216	D1138	V1070	A999	D925	T855	P790		S646		L481	P411	L331	T267	
Y1293	I1217	A1139	V1071	E1002	L926	T856	Y791	A723	I648	V573	D485	T412	S334	L268	I189
F1294	S1218	N1140	A1072		D928	L858	T793	Q725	K650	P578	D485	G413	T335	G269	Y190
	V1219	K1141	A1073	T1005	M929	S859	G794	Q726	A651	R579	I486	L414	L336	R270	T192
	R1220	S1143	K1074	Q1006	Y931	R861	S795	V727	P652	L580	I487	D415		P272	Y193
			Y1075	L1005	T930	E860	H796		P653	V581	P488	Q416	S339	G273	P194
				L1007	A932	X861	S797	I730	R653	K582	E489		V340	E274	S195
				L1008	E933	G862	S797	A731	R566	T583	L490	I419	E341	L275	F196
				L1009	V934	E863	T798		G657	S584	V491	P420	N342	L276	V197
				A1010	H936	P864	K799	N734	G657		R492	F421		E277	
				Q1011	R937	H866	F800	F737	N661	V590	D497	T422	T346	R278	L200
				D1012	M938	L868	G801	P738	L662	D591	P347	Q423	P347	F279	I201
				V1013	V939	A869	P804	I739	I663		V498	K425	P349	G280	
				Q1014	E940	T870	M805	F738	Y664		P496	R424	R350	G281	I204
				H1015	R871	G872	P806	I740	V665	M594	H500	F432	L351	T283	A205
				F1016	M942	G872	F807	L741	N666	S595	W501	L433	S352	G284	L208
				L1018	V943		D808	Q742	P667	R596	E502	P434	I353	H285	Q209
				L1018	Y943		D808	W743	L597	L597	T503	I435		G286	S210
				L1019	V944		G809		M670		A504	T436	L356	Q287	L211
				L1019			G809		G671	V600	T505	A437	T357	G288	
				Q1020			C810	G746	G671	P601	E506	P438	R358	L289	W215
				Q1021	R949		M811	R747	W672	P602	F507	F439	S359	V290	D216
				R1022	Y950		S814		Q673	V603	A510	H440	A360	G291	A217
				K1026	I951	D880	R315	H751	L674	M604	T511		V361	A292	V218
				P1027	L955	D881	M816	H752	P675	V605	H512	L444		A293	K219
				V1028	K956	T883	M817		L676	A606	T513	A447	P373	A294	Q220
				P1029	K957	F884	T818	E755	R679	C607	I513	H448	E374	I295	Y221
				F1030	L958		A319			M608	V514	H448	D375	A296	
				P1031	T959	R888	K820	Q759	V685	T609	D515	A449	R376	T297	L225
				A1032	G960	S889	E821	I761	P886	P610	F516	H450	H377	A298	D226
				L1032	G960	S889	E821	I761	P886	P610	F516	H450	H377	A298	
				A1033	F962	K890	A822	L762	I687	T611	G517	L451	I378	R299	I227
				L1034	I962	R891	H823		E688	V612	G520	L452		T300	L228
				D1034	I963	E894	Q827	W764	L690	P614	G520	V455	S381	W301	
				E1036	R964	E894	Q827	W764	L690	P614	G520	V455	L382	D302	H232
					R965	L895	A828	Y765	T691	M615	V521	D456	N382	E303	
				E1039	V966	K896	K329	S766	A694	D616	S522	D457	N384	F304	T240
				Y1040	E967	K897	R767			F617	V526	M458	A305		
				W1041	E968	R898		I768		V618	L527	K459	R387	T306	V244
				F1042	R969		V833		S698	A619	T528	T460	N388	S245	
				K1043	F970	T903	D834	K770	I699	A620	N529	P461	F389	A246	S245
				K1044	T971	K904	A835	R771	E700	T621		A462	V390	R310	P247
				W1048	Q976	L906	P836	S772	V701	M622	I540	S463	V391	A311	
				Q1049	P977		G837	N773	A702	N623	L541	S464	T392	V312	F250
				S1050	S978	D909	V838	I774	F704	N703	A542	L466	G393	E513	P251
				E1051	L979	F910	D840	L776	Y705		G543	V466	P394	L252	L252
				I1052	L980	Q911	D841	V777	I706	H627	A544	I467	F355	L315	I253
						K912	Q842	V778	Q707	E629		V469	I396	F316	
				I1053		Y913	W843	G779	T708		T550			W317	V256
														Q257	

K1359	R1436	L1583	V1583	L1653	R1758	A1843	V1913	T1980	K2046
P1360	G1437	L1514	S1584	E1654	R1759	L1844	L1913	Q1985	P2047
I1361	I1439	L1515	G1585	H1655	Q1759	V1845	L1914	Q1986	I2050
F1362	Y1439	E1516	D1586	D1586	N1760	A1846	L1915	P1986	S2051
R1363	T1440	L1517	Y1587	I1659	Y1761	A1847	V1916	L1989	K2052
R1364	D1441	P1518	N1588	R1662	M1762	A1848	V1917	E1990	E2053
K1365	Y1442	T1519	P1589	K1663	S1763	V1849	L1918	G1991	Y2054
I1366	T1445	K1520	I1590	I1664	M1764	V1850	V1919	R1991	
D1367		E1521	H1591	K1665	F1765	M1851	Y1920	G1992	
G1368		I1522	V1592	V1667	F1766	P1852	V1921	F1993	
D1369	E1451	I1523	S1593	D1668	E1767	I1853	V1922	A1994	
L1370	V1452	Q1524	S1594	T1668	T1768	E1854	I1995	T1995	
L1371	P1453	Q1525	R1595	A1669	V1769	S1855	Q1926	I1996	
K1372	M1454	A1526	F1596	K1672	N1770	L1856	V1927	F1997	
L1373	Q1455	S1527				V1857	V1928	L1998	
V1374	L1456	V1528	L1602	L1675	I1775			R1999	
H1375	H1457	D1529	P1603	D1676	K1776	F1861	D1932	G2000	
		Y1530	G1604	V1678	T1777	Y1862	L1933	L2001	
Y1380	T1460	E1531	T1605	L1679	E1778	R1863	R1934	I2001	
R1381	P1461	A1532	I1606	L1679	K1779	G1864	A1935	D2002	
M1382	Q1462	G1533	T1607	Q1680	T1780	G1865	L1936	V2003	
	D1463	E1534	H1608	G1681	F1781	T1866	D1937	P2004	
P1388	L1464	S1535	G1609			M1867	T1938	F2005	
	A1465	H1536	M1610	E1684	D1785	Q1868	L1939	H2006	
V1391	V1466	H1537	Y1611	V1685		Q1869		S2007	
G1392	L1467	H1538		E1686	Y1793	A1870	V1942	T2008	
D1393	R1468	P1539	V1616	Q1687	L1799	V1871	L1943	F2009	
V1394	S1469	V1540	R1617	P1688		E1872	M1944	L2010	
L1395	K1470	I1541	S1618	V1689		R1873	L1945	R2011	
D1396	E1471	D1542	L1619	T1690	A1802	T1803	L1946	G2012	
T1397	V1472	V1543	V1620	A1691	L1803	D1874	K1947	S2013	
T1398	E1473	L1544	E1621	V1692	Q1804		M1948	V2014	
A1399	K1474	Q1545	T1622	V1693	F1805	R1878		K2015	
Q1400	L1475	R1546	W1623	F1694	T1806	S1879	T1951	P2016	
I1401	D1476				Q1807	M1880	D1952	F2017	
N1402	D1477				P1808	Y1881	I1953	R2018	
A1403	H1478				L1812	M1882	L1956	S2019	
V1404	H1479				E1813	C1884	M1957	F2020	
I1405	D1480				E1814	V1886		L2021	
M1406	T1481				K1716	P1888	M1960	L2022	
	L1483					P1889	S1961	K2023	
S1409					M1706	S1889	L1962	K2024	
G1410					D1707	S1890	E1963		
K1411	T1487				L1708	L1891	D1964	T2028	
M1412	L1488				Y1709	D1820	V1965	T2029	
V1413	V1489					M1821	R1966	I2030	
C1416	L1492				K1716	S1823	A1967	D2031	
G1417					F1726	Q1828	H1968	P2032	
T1418						R1829	A1969	S2033	
	F1498				N1740	R1829	L1970	K2034	
R1421	K1499				M1741			L2035	
	M1500				P1742			I2036	
K1424						T1832	E1971	T2037	
P1425	Y1504				L1745	F1833	I1972	K2038	
S1505	S1505				T1746	A1834	I1973	Y2039	
V1426	S1506				G1835	V1903	Q1974	I2040	
M1427	V1507				F1749	E1905	C1976	P2041	
					G1750	M1906	R1977	N2042	
					G1751	I1907	K1978	V2043	
						Y1841	T2044	T2044	
						S1842	Q1979	A2045	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	216.37Å 414.43Å 221.51Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 88.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 89.5 (88.45-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.13Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, R_{free}	0.290 , 0.320 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.9	EDS
Estimated twinning fraction	0.280 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Outliers	0 of 629508 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	166671	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/11744	0.55	1/15873 (0.0%)
1	B	0.39	0/11801	0.55	1/15949 (0.0%)
1	C	0.40	0/11785	0.56	0/15928
1	D	0.39	0/11824	0.55	0/15980
1	E	0.39	0/11736	0.55	1/15863 (0.0%)
1	F	0.40	0/11776	0.56	2/15916 (0.0%)
2	G	0.34	0/16573	0.52	0/22516
2	H	0.34	0/16573	0.52	0/22516
2	I	0.34	0/16573	0.52	0/22516
2	J	0.35	0/16573	0.53	0/22516
2	K	0.38	0/16573	0.54	0/22516
2	L	0.35	0/16573	0.53	0/22516
All	All	0.37	0/170104	0.54	5/230605 (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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	585	MET	N-CA-C	9.68	137.14	111.00
1	B	608	LYS	N-CA-C	-7.98	89.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	538	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	579	MET	N-CA-C	5.72	126.45	111.00
1	F	585	MET	CA-C-O	5.45	131.53	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	ALA	Peptide
1	F	584	ILE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11514	0	11476	745	0
1	B	11571	0	11529	706	1
1	C	11555	0	11507	695	0
1	D	11593	0	11552	733	0
1	E	11506	0	11467	745	0
1	F	11546	0	11499	701	0
2	G	16200	0	16081	1178	1
2	H	16200	0	16081	1209	1
2	I	16200	0	16081	1238	0
2	J	16200	0	16081	1213	0
2	K	16200	0	16081	1262	1
2	L	16200	0	16081	1219	0
3	G	31	0	19	10	0
3	H	31	0	19	11	0
3	I	31	0	19	9	0
3	J	31	0	19	9	0
3	K	31	0	19	12	0
3	L	31	0	19	10	0
All	All	166671	0	165630	11004	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 11004 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:43:PHE:HB2	2:I:22:ARG:NH2	1.54	1.21
2:K:1594:ARG:HG2	2:K:1594:ARG:HH11	1.05	1.20
2:H:1594:ARG:HH11	2:H:1594:ARG:HG2	1.02	1.17
1:E:1610:ARG:HH11	1:E:1610:ARG:HG2	1.00	1.16
2:L:1594:ARG:HG2	2:L:1594:ARG:HH11	1.03	1.16

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	Distance(Å)	Clash(Å)
2:H:1527:SER:O	2:K:19:GLN:NE2[2_646]	2.09	0.11
1:B:1452:SER:O	2:G:1092:ASN:ND2[1_556]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	1291 (89%)	148 (10%)	12 (1%)	27	74
1	B	1458/1878 (78%)	1295 (89%)	151 (10%)	12 (1%)	27	74
1	C	1456/1878 (78%)	1293 (89%)	151 (10%)	12 (1%)	27	74
1	D	1461/1878 (78%)	1290 (88%)	155 (11%)	16 (1%)	21	65
1	E	1450/1878 (77%)	1292 (89%)	146 (10%)	12 (1%)	27	74
1	F	1455/1878 (78%)	1300 (89%)	140 (10%)	15 (1%)	22	68
2	G	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	18	60
2	H	2058/2060 (100%)	1786 (87%)	244 (12%)	28 (1%)	16	58
2	I	2058/2060 (100%)	1799 (87%)	233 (11%)	26 (1%)	18	60
2	J	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	18	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	2058/2060 (100%)	1772 (86%)	258 (12%)	28 (1%)	16	58
2	L	2058/2060 (100%)	1777 (86%)	253 (12%)	28 (1%)	16	58
All	All	21079/23628 (89%)	18479 (88%)	2359 (11%)	241 (1%)	21	65

5 of 241 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1227	GLY
1	A	1566	LYS
1	A	1593	ASP
1	B	614	PHE
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%)	1101 (90%)	119 (10%)	12	40
1	B	1227/1527 (80%)	1111 (90%)	116 (10%)	12	42
1	C	1225/1527 (80%)	1102 (90%)	123 (10%)	11	38
1	D	1229/1527 (80%)	1110 (90%)	119 (10%)	12	41
1	E	1219/1527 (80%)	1101 (90%)	118 (10%)	12	41
1	F	1224/1527 (80%)	1109 (91%)	115 (9%)	13	43
2	G	1752/1752 (100%)	1571 (90%)	181 (10%)	10	36
2	H	1752/1752 (100%)	1579 (90%)	173 (10%)	11	39
2	I	1752/1752 (100%)	1571 (90%)	181 (10%)	10	36
2	J	1752/1752 (100%)	1573 (90%)	179 (10%)	11	37
2	K	1752/1752 (100%)	1575 (90%)	177 (10%)	11	38
2	L	1752/1752 (100%)	1576 (90%)	176 (10%)	11	38
All	All	17856/19674 (91%)	16079 (90%)	1777 (10%)	11	38

5 of 1777 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1108	GLU
2	H	1266	HIS
2	L	609	THR
2	G	1348	PHE
2	H	215	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 470 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1375	HIS
2	H	1462	GLN
2	L	512	HIS
2	G	1608	HIS
2	H	416	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMN	G	2101	-	33,33,33	6.27	23 (69%)	46,50,50	1.84	9 (19%)
3	FMN	H	2101	-	33,33,33	6.22	22 (66%)	46,50,50	1.78	10 (21%)
3	FMN	I	2101	-	33,33,33	6.24	21 (63%)	46,50,50	1.85	10 (21%)
3	FMN	J	2101	-	33,33,33	6.41	23 (69%)	46,50,50	1.83	11 (23%)
3	FMN	K	2101	-	33,33,33	6.47	24 (72%)	46,50,50	1.93	13 (28%)
3	FMN	L	2101	-	33,33,33	6.21	20 (60%)	46,50,50	1.78	10 (21%)

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	FMN	G	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	H	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	I	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	J	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	K	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	L	2101	-	-	0/18/18/18	0/3/3/3

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2101	FMN	O2-C2	15.43	1.41	1.21
3	K	2101	FMN	O2-C2	15.41	1.41	1.21
3	L	2101	FMN	O2-C2	14.92	1.41	1.21
3	J	2101	FMN	O2-C2	14.86	1.40	1.21
3	I	2101	FMN	O2-C2	14.81	1.40	1.21

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2101	FMN	C2-N1-C10	6.64	121.35	114.95
3	G	2101	FMN	C2-N1-C10	6.41	121.12	114.95
3	I	2101	FMN	C2-N1-C10	5.59	120.33	114.95
3	L	2101	FMN	C2-N1-C10	5.59	120.33	114.95
3	H	2101	FMN	C2-N1-C10	5.52	120.27	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.12	2 (0%) 93 70	17, 54, 105, 150	0
1	B	1464/1878 (77%)	-0.13	3 (0%) 93 61	16, 52, 111, 158	0
1	C	1462/1878 (77%)	-0.11	3 (0%) 93 61	15, 51, 111, 159	0
1	D	1467/1878 (78%)	-0.14	2 (0%) 93 70	17, 54, 108, 158	0
1	E	1456/1878 (77%)	-0.12	2 (0%) 93 70	15, 54, 110, 157	0
1	F	1461/1878 (77%)	-0.12	2 (0%) 93 70	16, 51, 108, 159	0
2	G	2060/2060 (100%)	0.00	9 (0%) 90 45	27, 83, 129, 169	0
2	H	2060/2060 (100%)	0.06	19 (0%) 81 25	24, 86, 132, 167	0
2	I	2060/2060 (100%)	0.06	22 (1%) 77 22	23, 86, 132, 167	0
2	J	2060/2060 (100%)	0.08	25 (1%) 75 20	28, 89, 133, 172	0
2	K	2060/2060 (100%)	0.19	43 (2%) 60 11	27, 91, 136, 172	0
2	L	2060/2060 (100%)	0.08	13 (0%) 86 36	23, 87, 133, 172	0
All	All	21127/23628 (89%)	-0.00	145 (0%) 84 32	15, 75, 127, 172	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	93	ASP	7.4
2	K	27	THR	4.7
2	I	1773	GLY	4.6
2	K	26	LEU	4.4
2	I	1123	ALA	4.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FMN	G	2101	31/31	0.28	0.50	19,64,105,124	0
3	FMN	H	2101	31/31	0.25	0.03	21,53,91,110	0
3	FMN	I	2101	31/31	0.22	-0.25	23,54,85,115	0
3	FMN	L	2101	31/31	0.23	-0.26	15,51,89,119	0
3	FMN	J	2101	31/31	0.18	-0.64	19,56,106,122	0
3	FMN	K	2101	31/31	0.17	-1.07	24,63,111,122	0

6.5 Other polymers

There are no such residues in this entry.