



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:00 AM UTC

PDB ID : 4V58 / pdb_00004v58
Title : Crystal structure of fatty acid synthase 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

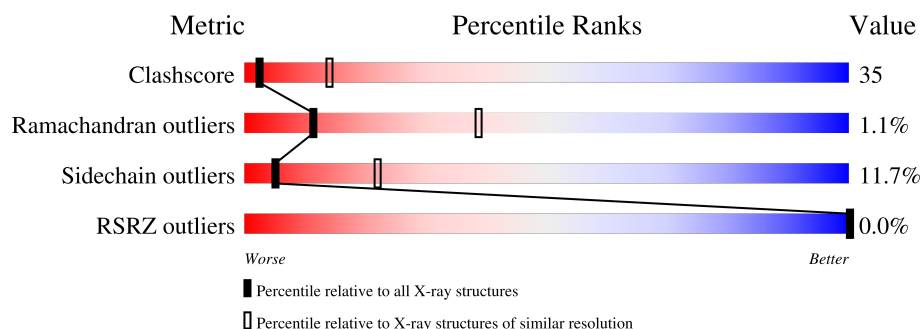
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



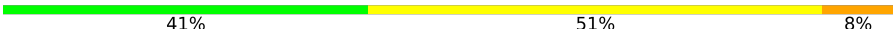
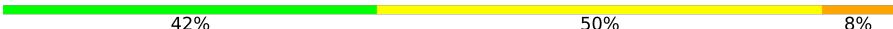
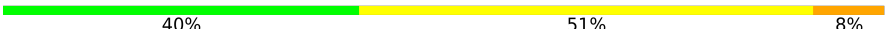
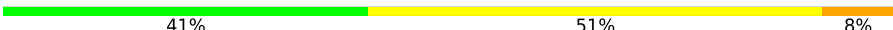
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1878	39% 33% 5% 22%
1	B	1878	40% 32% 5% 22%
1	C	1878	40% 33% 5% 22%
1	D	1878	39% 33% 6% 22%
1	E	1878	39% 33% 5% 22%
1	F	1878	40% 33% 5% 22%
2	G	2060	42% 50% 8%

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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
3	FMN	G	2101	-	-	X	-
3	FMN	H	2101	-	-	X	-
3	FMN	I	2101	-	-	X	-
3	FMN	J	2101	-	-	X	-
3	FMN	K	2101	-	X	X	-
3	FMN	L	2101	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 166671 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 FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

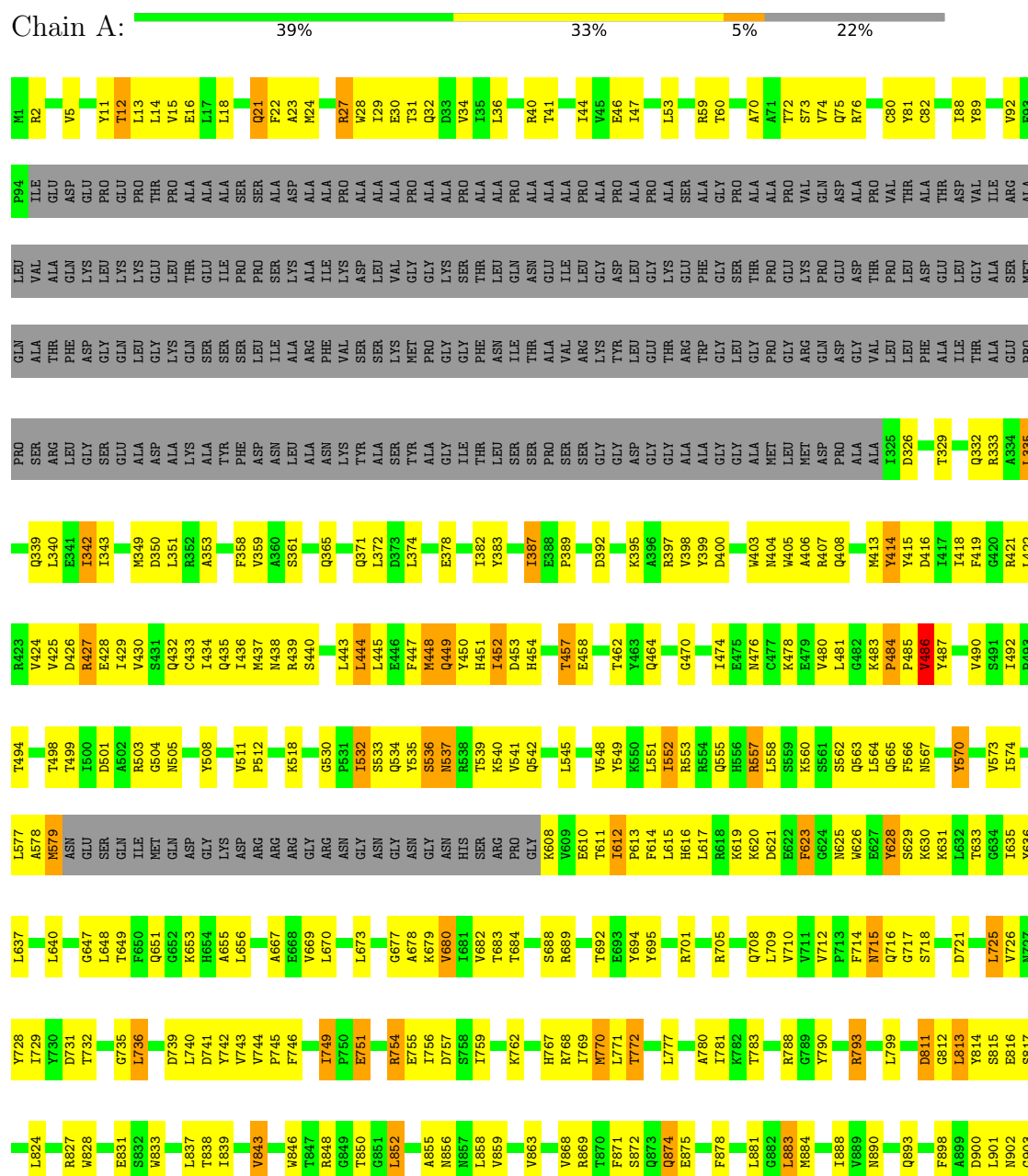


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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]

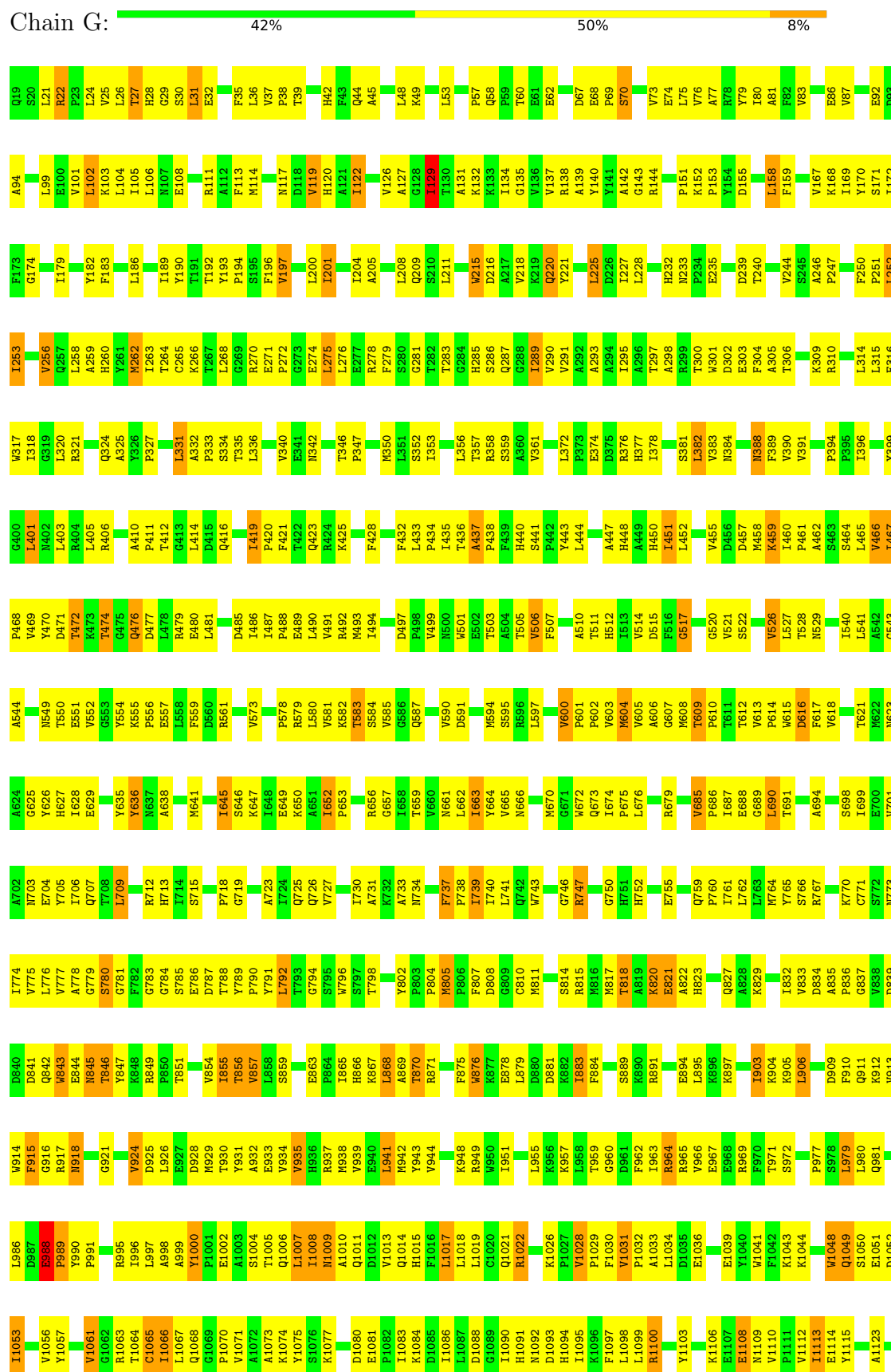
Chain D: 39% 33% 6% 22%



I1378	F1307	G1223	R1141	Y1047	N962	I888	L799	Q716	K630	L569	S491	G420	Q339	SER
M1381	D1308	S1224	L1142	W1050	L963	V899	D811	G717	K631	Y570	I492	R421	L340	ARG
T1382	F1310	G1225	R1143	V1051	K964	N890	G812	S718	L632	K571	P493	L422	E341	LEU
T1386	Q1311	V1226	T1147	D1052	P966	N890	L813	D721	T633	D572	T494	R423	I342	GLY
D1387	E1312	G1228	L1148	T1055	F967	P896	Y814	L725	G634	V573	T498	V424	I343	SER
E1313	E1312	G1228	L1149	T1055	P968	V897	S815	L726	G635	I574	T499	V425		GLU
G1314	G1314	T1229	I1150	G1056	F969	F898	S816	V727	G636	H575	I500	D426	L347	ALA
S1315	P1151	E1057	P1151	L1057	L970	F899	S817	V728	L637	A576	T499	R427	K348	ASP
Y1316	A1152	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	K349	ALA
E1317	A1153	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D350	LYS
	A1154	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	L351	ALA
	A1155	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	R352	TYR
	A1156	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	A353	PHE
	A1157	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	K356	ASP
	A1158	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	A357	ASN
	A1159	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	K357	LEU
	A1160	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	V358	ASN
	A1161	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	V359	ASN
	A1162	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	A360	LYS
	A1163	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	S361	TYR
	A1164	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	S440	ALA
	A1165	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Q365	SER
	A1166	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	E378	SER
	A1167	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Y450	PRO
	A1168	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	H451	PRO
	A1169	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	I452	SER
	A1170	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D453	SER
	A1171	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	H454	GLY
	A1172	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	E388	GLY
	A1173	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	P389	ASP
	A1174	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	E458	GLY
	A1175	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D382	GLY
	A1176	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	T462	ALA
	A1177	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Y463	ALA
	A1178	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Q464	GLY
	A1179	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	G470	GLY
	A1180	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Y399	ALA
	A1181	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D400	MET
	A1182	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	N404	LEU
	A1183	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	W405	PRO
	A1184	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	A406	ASP
	A1185	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	R407	ALA
	A1186	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	E479	ALA
	A1187	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	V480	ALA
	A1188	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	L481	ALA
	A1189	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Q408	ALA
	A1190	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D409	ALA
	A1191	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	M413	ALA
	A1192	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Y414	ALA
	A1193	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	Y415	ALA
	A1194	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	D416	ALA
	A1195	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	I417	ALA
	A1196	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428	I418	ALA
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	A1198	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
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	A1210	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1211	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1212	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1213	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
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	A1216	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
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	A1227	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1228	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
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	A1240	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1241	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1242	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
	A1243	P1058	D900	P1058	D900	F899	S817	V728	L637	A576	I500	E428		
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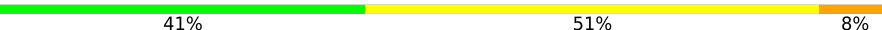
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ALA	GLU	SER	L1642	A1568	S1488	E1330	L1250	D1169	L1080	V994	L911	E831	L740	T649
ALA	GLN	GLY			F1489		Q1251	A1170	I1081	V996	M915	W832	F650	Q651
ALA	THR	ALA	L1646	W1572	G1490	R1333	F1254	Y1173	F1086	G998	L918	L837	V742	G652
ALA	CYS	THR	K1647	M1573	N1491	E1492	T1257	G1174	Y1089	L999	R919	T838	V743	K653
ALA	ARG	PRO	K1648	M1574	F1493	E1493		Y1175	Y1089	A1000	K920	I839	V744	H654
ALA	ARG	PRO	A1649	M1575	W1494	F1493		P1176	Y1089	A1000	E921		P745	A655
GLN	ARG	SER			R1495	G1338	V1262	P1177		G1003	I922	W843	F746	
GLU	GLU	ALA	V1658	L1578	W1495	E1339	M1263	Y1177	R1093	G1003	I922			A657
GLY	PRO	ASN	R1661	Q1579	R1499	E1340	N1264	I1179	Q1094	G1003	I922			E668
VAL	PRO	ALA	Q1662	L1581	R1499	S1341		I1180	L1096	P1004	S926			V669
THR	ARG	ALA	K1663		I1501	R1342	L1267	I1180	L1097	W1005			E751	L670
ALA	SER	ALA		I1585	E1426	P1343	S1268	V1183	Q1098	G1086	R929			
ASN	SER	ALA	H1670	V1586	R1429	T1344	S1268	D1184	Q1099	M1007	Q930		R754	L673
ASN	PHE	GLU	N1671	P1587	Q1430	T1346	S1269	P1185	E1099	A1008			E755	G677
GLN	ALA	GLN	L1672	G1588	Q1431	T1347	T1270	V1186	V1100		I933		D757	K679
THR	GLY	THR	L1673	T1509	I1432		I1273	T1187	D1105	R1011			S758	V680
ARG	ARG	GLN	I1674	W1510	E1437	F1351	T1275	L1188	L1106	M1014	V942		I759	K680
THR	THR	ARG		G1511		M1352	P1276		E1107	E1015	V943			L681
GLY	ALA	LEU	L1678	T1512	L1441	S1355	V1277	V1194	P1108		G945		K762	V682
ASP	LEU	LEU	K1682	I1514	Y1442	G1356	A1279	L1198	K1113	G1018	E946			T683
GLU	GLU	ALA			L1443	C1357	C1280	L1199	E1117	F1020	H948		H767	T684
ALA	ALA	ALA		V1519	Q1444	G1358		S1201		S1021	E949		R768	S688
ALA	ALA	ALA	A1685		E1445		D1288		I1129	L1022	A950		M770	R689
VAL	ILE	ALA	P1686	Q1601	E1446	V1359		F1209	F1139	M1032	L951		T772	T692
ALA	PHE	THR	I1691	F1602	V1447	Q1360	Y1291	Y1210	E1131	M1028	R952		L777	
ALA	ALA	ALA	Q1692	D1603	A1448	V1361		K1211			R953			
VAL	SER	ALA		G1524	A1449	I1362	I1294	V1212	E1134	M1031	R954		L777	Y695
LEU	LEU	ALA		T1525	A1450	M1363	M1295	Y1212		M1032	R955			
GLY	GLY	SER	F1696	S1526	K1451	T1364		V1213	Q1137		R956		A780	R701
SER	VAL	PRO	L1697	T1527		A1365		H1214		M1037	I957		I781	R705
ALA	ALA	ALA		V1528	S1455	Q1366	A1299	L3215	T1139	E1038	E958		T783	
ALA	SER	SER		D1531	E1456	L1367	R1300	S1216	V1140	P959	P959			
GLY	VAL	GLY	S1701	E1534	E1457		V1301	E1217	R1141	P1041	R960		R788	Q708
GLY	GLY	VAL	R1702	S1535	D1462	G1372	C1302	V1218	L1142	L1042	A961		Y790	L709
ASP	ASP	ASP	T1703	D1536	E1463	V1373	C1303	E1218	R1143		L963		G769	L709
ALA	VAL	VAL	T1704	T1537	T1464	P1374	L1303	G1239		P1046	N962		Y790	V710
ALA	MET	GLU	Q1705	V1537	Y1466	I1375	V1304	N1220		Y1047	K964			V711
ARG	ARG	SER	S1707	C1539	Y1466		F1307	G1223	T1147	Y1047	K964			V712
GLU	GLU	VAL	N1708	Y1542	L1467	I1378	D1308	S1224	L1148	W1050	Y965		R793	P713
ILE	ILE	ASP	G1709	L1543			F1309	G1225	L1149	V1051	Y965			F714
GLU	GLU	SER	E1710	K1543	R1470	T1382	D1309	G1226	P1150	D1051	N890		L799	
VAL	VAL	ILE	L1711	H1544	T1471		F1310	V1226	P1151	D1051	P967			Q716
VAL	ILE	ASN	K1712	L1545	E1472		Q1311	G1227	P1152	D1051	P968		D811	S718
ASN	ASN	ILE	F1713	G1546	H1473	T1386	E1312	G1228	A1153	T1055	P969		G812	
ASP	ASP	ASP	F1714	R1547	I1474	D1387	E1313	T1229	L1154	G1056	L970		L813	
ALA	ASN	ALA	A1715		E1475	T1388	S1315	A1231	G1155	E1057	W973		Y814	D721
ASN	ASN	GLU	GLU	N1551	R1476	I1389	Y1316	L1232	F1156	P1058			S815	
GLY	GLU	GLU	PRO	A1552		G1390	E1317	R1233	D1157		I977		E816	L725
GLY	GLU	VAL	VAL	V1553	R1479		M1321	G1234	L1158	Y1064	L901		S817	V726
ALA	ALA	PHE	THR		R1480	V1393	G1322	K1237	L1159	K1067	Q983			N727
PRO	PRO	ILE	THR	Y1560	Q1481	P1394	T1323	D1238	V1160	Y1068	G903		L821	Y728
GLU	GLU	ARG	THR	L1561	E1482		A1324		A1161		G904		I729	
VAL	VAL	ARG	THR		E1483		T1324		G1162	V988	L905		L824	Y730
ASN	ASN	ASN	GLY		A1483		S1325	L1241	Q1163	Y1071	N989			D731
PHE	LEU	PHE	ASP	H1564	A1484	V1400	N1326	D1242	I1164	I1072	L990		R827	T732
THR	THR	THR	LYS	P1565	A1485	T1402	E1485	K1243	P1165	I1078	D991		W828	
GLY	GLY	GLU		K1566	Q1486	T1403	K1328				K992		Y829	G735

● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



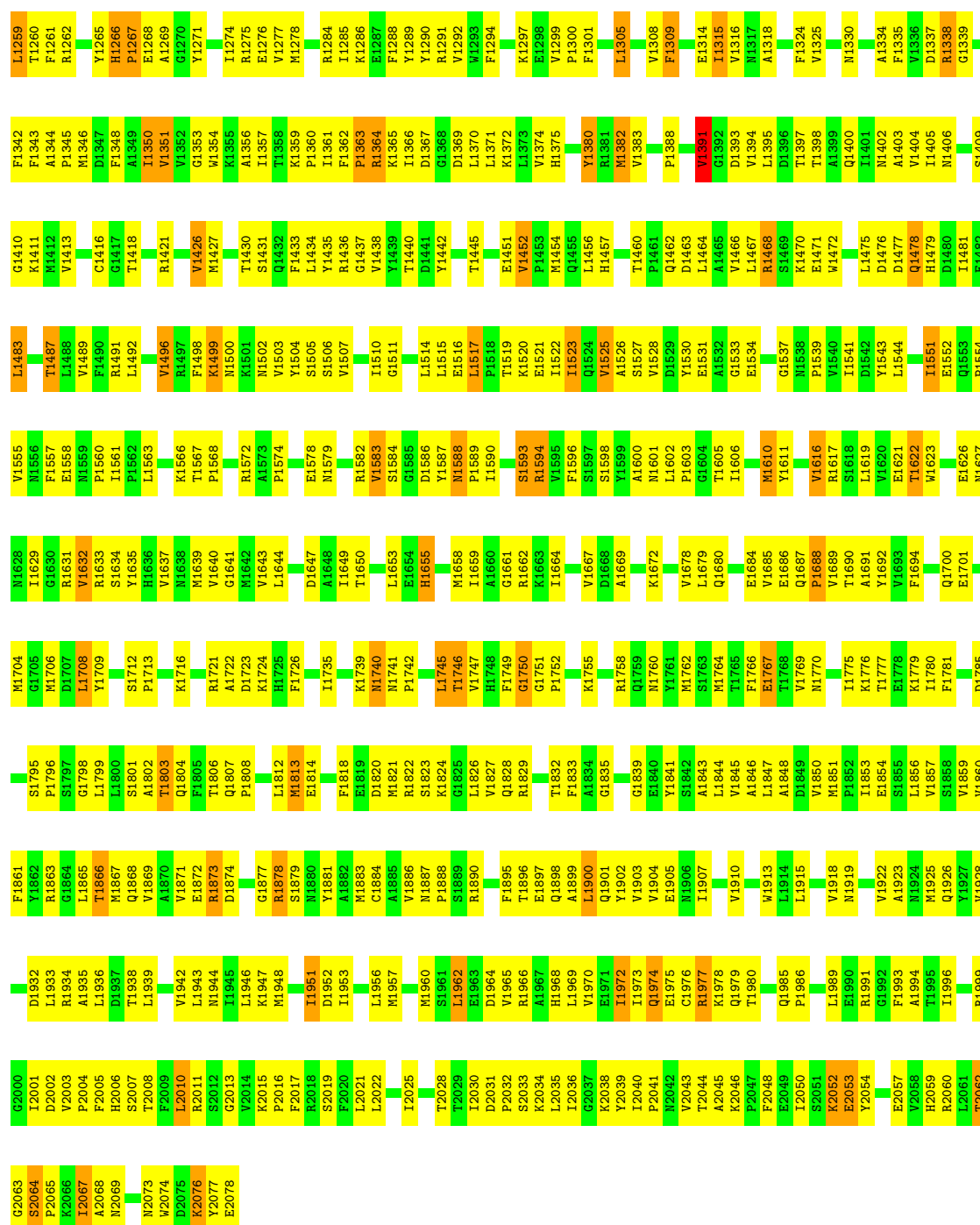
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S1889	R1890	F1895	T1896	L1897	Q1898	L1899	L1900	Q1901	V1902	V1903	V1904	L1905	L1906	L1907	G1839	V1904	E1905	L1906	L1907	V1910	V1913	L1914	L1915	V1918	V1919	L1922	L1923	L1924	L1925	V1928	G2000	L2001	D2002	P2003	P2004	H2006	S2007	T2008	T2009	R2011	G2013	V2014	K2015	P2016	F2017	L2018	L2019	L2020	L2021	L2022	L2025	T2026	L2027	L2028	V2029																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
S1823	K1824	Q1827	T1828	R1829	L1830	T1832	L1833	Q1834	V1835	G1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
I1735	V1637	M1638	M1639	V1640	G1641	M1642	L1643	L1644		H1655		I1659	G1660	S1684	G1681	R1682	K1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	Q1700	E1701	L1801	A1802	T1803	G1804	L1805	T1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
I1735	V1637	M1638	M1639	V1640	G1641	M1642	L1643	L1644		H1655		I1659	G1660	S1684	G1681	R1682	K1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	Q1700	E1701	L1801	A1802	T1803	G1804	L1805	T1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L2030	D2031	P2032	S2033	K2034	L2035	L2036	G2037	L2038	V2039	L2040		V2043	T2044	A2045	K2046	P2047		L2050	S2051	K2052	E2053	V2054		E2057	T2058	H2059	R2060	L2061	T2062	G2063	P2064	L2065	K2066	L2067	A2068	L2069	T2070	N2073	K2074	S2075	K2076	L2077	E2078																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S1351	V1352	L1274	G1353	W1354	K1355	A1356	L1357	T1358	K1359	P1360	I1361	F1362	P1363	R1364	F1365	D1367	G1368	D1369	L1370	K1371	K1372	L1373	V1374	H1375	L1376		Y1380	R1381	M1382	V1383		P1388		Y1391	G1392	L1393	P1394	L1395	D1396	T1397	T1398	A1399	G1400	I1401	N1402	A1403	V1404	I1405	N1406	S1409	F1410	K1411	E1412	L1413	G1416	L1417	T1418	F1419	P1420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain H:  41% 51% 8%

D19	D20	D21	D22	D23	D24	D25	D26	D27	D28	D29	D30	D31	D32	D33	D34	D35	D36	D37	D38	D39	D40	D41	D42	D43	D44	D45	D46	D47	D48	D49	D50	D51	D52	D53	D54	D55	D56	D57	D58	D59	D60	D61	D62	D63	D64	D65	D66	D67	D68	D69	D70	D71	D72	D73	D74	D75	D76	D77	D78	D79	D80	D81	D82	D83	D84	D85	D86	D87	D88	D89	D90	D91	D92	D93
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G1188	T1189	E1108	R965	K996	Q827	S766	T621	A542	L465	P395	F316	V256	G174	A94
L1189	P1190	N1109	V966	K897	A828	R767	H622	G543	V466	I396	W317	Q257	G174	A94
P1191	E968	P1110	E967	I903	K829	I768	H623	A544	P467	L467	G319	Q257	I179	L99
L1192	R969	P1111	E968	K904	I832	R769	A624	T545	P468	L468	G319	Q257	I179	L99
K1193	F970	V1112	K905	K905	I833	K770	G625	N549	V469	G400	L320	A259	Y182	V101
R1194	T971	E1114	K906	L906	D834	C771	H627	T550	D471	M402	R321	H260	F183	L102
L1195	S972	Y1115	S972	D909	A835	S772	H628	E551	T472	L403	Q324	M262	L186	K103
F1196	P977	I1120	P977	F910	H836	N773	E794	V552	K473	R406	A325	T263	L186	L104
P1197	S978	I1121	S978	F911	I839	N774	E795	G553	K474	L405	A325	T263	L186	L104
R1198	L979	A1123	L979	K912	D840	L776	G636	Y554	K475	R406	P327	T264	Y189	N107
T1199	L980	T1124	L980	V913	D841	A778	H637	K555	D476	L410	L331	K266	T191	E108
R1200	L980	T1125	L980	K914	Q842	A778	L709	P556	D477	P411	A332	T267	T192	R111
G1201	F915	E1126	F915	N914	Q842	G779	L709	E557	L478	T412	A332	T267	T192	R111
M1202	F915	E1126	F915	N914	Q842	G779	L709	E557	L478	T412	A332	T267	T192	R111
Y1203	D987	D1130	D987	G916	E844	G781	H713	Y554	K475	R406	P327	T267	T192	R111
E1205	R989	D1131	R989	G916	E844	G781	H713	Y554	K475	R406	P327	T267	T192	R111
E1206	R989	D1131	R989	G916	E844	G781	H713	Y554	K475	R406	P327	T267	T192	R111
I1207	Y990	G1132	Y990	G921	H847	G784	F716	R561	L481	Q416	V340	E274	L200	G116
E1208	P991	L1133	P991	G921	H847	G784	F716	R561	L481	Q416	V340	E274	L200	G116
N1208	I996	R1137	I996	V924	R849	E786	K648	P578	L486	I419	E341	E274	L200	G116
P1209	L997	D1138	L997	D925	T850	D787	K648	P578	L486	I419	E341	E274	L200	G116
C1210	A998	C1139	A998	D925	T850	D787	K648	P578	L486	I419	E341	E274	L200	G116
L1211	A999	N1140	A999	D926	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
P1212	Y1000	K1141	Y1000	D927	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
T1215	P1001	N1142	P1001	D928	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1216	E1002	S1143	E1002	D929	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
S1217	A1003	L1146	A1003	D930	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1218	L1004	N1147	L1004	D931	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1219	L1005	R1148	L1005	D932	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
R1220	Q1006	L1153	Q1006	D933	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
S1223	L1007	L1154	L1007	D934	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
Q1224	H1008	P1155	H1008	D935	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
S1225	N1009	L1156	N1009	D936	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
A1226	A1010	V1157	A1010	D937	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
K1227	Q1011	D1158	Q1011	D938	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
L1228	L1012	S1159	L1012	D939	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1229	V1013	F1160	V1013	D940	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
K1230	H1014	M1161	H1014	D941	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
I1234	Q1015	I1164	Q1015	D942	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
K1235	F1016	Y1169	F1016	D943	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
L1236	L1017	S1170	L1017	D944	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1237	L1018	W1171	L1018	D945	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
G1238	H1019	R1172	G1020	D946	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
D1239	N1091	H1173	C1020	D947	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
N1240	H1092	M1175	Q1021	D948	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
T1245	D1093	T1178	R1022	D949	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
L1246	H1094	E1179	R1022	D950	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
F1247	I1095	I1180	F1027	D951	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
E1248	K1096	V1181	P1028	D952	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
G1249	F1097	F1182	P1029	D953	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
R1250	L1098	Q1183	F1030	D954	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
T1251	L1099	R1186	V1031	D955	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
V1256	R1100	F1187	W1032	D956	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
	Y1103		A1033	D957	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
	K1106		L1034	D958	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
	E1107		D1035	D959	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
			E1036	D960	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D961	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D962	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D963	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D964	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D965	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D966	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D967	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D968	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D969	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D970	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D971	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D972	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D973	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D974	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D975	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D976	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D977	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D978	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D979	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D980	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D981	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D982	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D983	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D984	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D985	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D986	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D987	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D988	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D989	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D990	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D991	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D992	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D993	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D994	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D995	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D996	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D997	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D998	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D999	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1000	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1001	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1002	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1003	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1004	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1005	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1006	T851	D788	K648	P578	L486	I419	E341	E274	L200	G116
				D1007	T851	D788</								



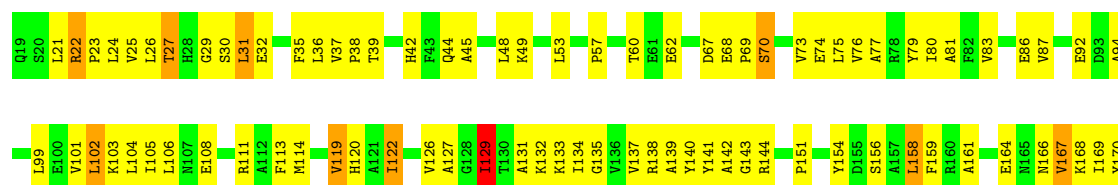
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain I:

41%

51%

8%



P1191	E1107	E1036	F970	K997	L762	T691	V613	T528	A462	V391	L314	F250	S171
L1192	E1108	E1039	T971	T903	L763	L692	P614	N529	S463	T392	L315	F251	I172
R1193	N1109	E1040	E974	A828	M764	G693	W615	N529	S464	G393	F316	P251	F173
R1194	N1110	Y1040	G974	K904	Y765	A694	D616	G534	S465	P394	L252	L252	G174
F1195	P1111	W1041	G975	K905	S766	P697	F617	F540	V466	P395	W317	I253	Q175
F1196	P1112	F1042	Q976	L906	R767	P697	V618	I540	I467	I396	I318	G254	Q176
A1197	P977	K1043	P977	D909	R768	S698	T621	L541	P468	Y399	G319	L255	I179
F1198	S978	K1044	S978	F910	R769	L699	M622	A542	V469	G400	L320	V256	I179
T1199	L979	W1048	L979	F910	K770	E700	M622	G543	Y470	G400	R321	Q257	F182
R1200	L980	Q1049	L980	Q911	C771	W701	M623	A544	D471	L401	Q324	L258	Y183
G1201	Q981	Q1049	Q981	K912	S772	A702	A624	N549	T472	N402	Q324	A259	F183
M1202	W913	S1050	W913	V913	N773	N703	G625	T550	K473	L403	Y326	H260	L186
V1203	L986	E1051	L986	Q914	L774	E704	Y626	E551	T474	R404	Y326	Y651	L186
V1204	D857	D1052	D857	F915	W775	Y705	H627	E551	G475	L405	P327	M262	L186
E1205	E988	I1053	E988	G916	L776	Y706	H627	E552	Q476	R406	L331	L263	I189
I1206	P989	Y1057	P989	R917	L777	Q707	E629	G553	D477	K407	L331	T264	Y190
T1207	Y990	Y1057	Y990	N918	A778	L708	Y635	Y554	L478	A410	S334	C285	T192
G1212	P991	N845	P991	N845	G779	L709	Y636	K555	R479	P411	T335	T267	Y193
L1133	A992	V1061	A992	T846	S780	T709	M637	E557	L481	T412	L336	L268	P194
F1137	V993	T1064	V993	Y847	G781	R712	A638	L558	L481	G413	S339	E271	S195
A1138	D994	C1065	D994	R849	F782	H713	M641	R561	D485	L415	V340	P272	F196
A1139	R995	I1066	R995	P850	G783	T714	L645	W572	I487	D415	E341	G273	V197
S1218	I996	L1067	I996	T851	G784	S715	L646	W573	E488	Q416	N342	L275	L200
K1141	L997	Q1068	L997	T851	S785	S715	L646	W573	E488	Q416	N342	L275	L200
I1142	A998	G1069	A998	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
S1143	A999	G1069	A999	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
S1223	Y1000	P1070	Y1000	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
Q1224	P1001	Y1071	P1001	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
S1225	E1002	A1072	E1002	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
A1226	A1003	L1073	A1003	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
K1227	S1004	K1074	S1004	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
L1228	T1005	Y1075	T1005	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
G1238	Q1006	S1076	Q1006	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
I1234	L1007	K1077	L1007	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
K1235	E1008	D1080	E1008	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
L1236	I1083	P1082	I1083	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
V1237	K1084	K1084	K1084	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
G1238	D1085	D1085	D1085	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
D1239	H1015	L1086	H1015	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
N1240	F1016	L1087	F1016	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
L1244	L1017	D1088	L1017	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
T1245	L1016	G1089	L1016	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
F1247	L1019	H1090	L1019	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
E1248	E878	H1091	E878	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
G1249	Q1021	N1092	Q1021	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
R1250	R1022	L1093	R1022	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
T1251	H1094	H1094	H1094	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
V1256	I1095	I1095	I1095	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
L1259	K1026	K1096	K1026	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
T1260	P1027	K1097	P1027	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
F1261	V1028	F1097	V1028	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
R1262	P1029	L1098	P1029	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
	Q1183	L1099	Q1183	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
	F1187	R1100	F1187	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
	Q1188	Y1103	Q1188	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
	T1189	K1106	T1189	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200
	N1190		N1190	Y854	E786	G719	L646	W573	E488	Q416	N342	L275	L200



8%





R1338	A1403	D1477	L1551	V1628	M1706	Q1804	V1871	L1946	Z2014	Q19	D83	I169	F250
G1339	V1404	Q1478	E1552	I1629	D1707	F1805	E1872	K1947	K2015	S20	A94	Y170	P251
K1340	N1405	H1479	Q1553	G1630	Y1708	T1806	D1873	M1948	P2016	L21	L99	S171	L252
D1341	N1406	D1480	P1554	P1631	Y1709	T1807	D1874	F2017	F2017	R22	G174	I172	I253
F1342	S1409	I1481	V1555	V1632	K1716	P1808	R1878	I1951	R2018	P23	V101	G174	V256
F1343	G1410	E1482	E1558	S1634	R1721	L1810	S1879	L1952	S2019	L24	L102	I179	Q257
A1344	G1411	L1483	H1559	Y1635	A1722	T1811	M1880	I1953	F2020	V25	K103	I179	L258
M1345	K1411	A1346	P1560	H1636	A1723	L1812	Y1881	L1956	L2021	L26	L104	Y182	A259
M1346	M1412	M1347	S1561	V1637	D1723	M1813	A1882	M1957	L2022	H28	L106	F183	H280
D1347	V1413	D1348	P1562	M1638	K1724	E1814	M1883	M1957	I2025	G29	M107	L186	G261
F1348	R1491	F1349	L1492	M1639	H1725	F1726	C1884	M1960	S1961	S30	E108	L186	M262
A1350	G1417	I1350	V1496	G1640	F1726	F1818	A1885	M1960	S1961	L31	E108	L186	M262
V1351	T1413	V1352	T1497	G1641	M1729	E1819	V1886	L1962	L1962	E32	R111	I189	I263
W1354	R1421	G1353	F1497	M1642	M1729	D1820	M1887	E1963	S2033	F35	R111	I189	T264
K1355	P1568	K1499	F1499	V1643	I1735	M1821	P1888	E1963	K2034	L36	F113	Y190	C285
A1356	V1426	N1500	N1501	L1644	I1735	R1822	S1899	V1965	L2035	V37	M114	T192	K266
I1357	M1427	V1502	V1503	T1649	K1739	S1823	R1966	V1966	I2036	P38	G116	Y193	L268
T1358	F1433	V1503	V1504	T1650	M1741	G1825	F1895	A1967	Y2039	T39	G116	P194	G269
K1359	L1434	Y1504	S1505	L1653	M1741	L1826	T1896	L1969	I2040	H42	M117	S195	R270
P1360	Y1435	S1505	S1506	E1654	L1745	L1653	Q1898	V1970	P2041	D118	D118	F196	E271
T1361	R1436	S1506	S1507	H1655	T1746	H1655	Q1899	E1971	N2042	F43	V119	V197	P272
F1362	G1437	V1507	G1585	M1658	V1747	H1748	A1999	I1972	V2043	Q44	H120	L200	G273
P1363	V1438	Y1439	D1586	M1659	H1748	F1833	Q1901	Q1974	A2045	A45	A121	I201	L275
R1364	T1440	M1588	V1587	T1659	F1749	A1839	Y1902	C1976	R2046	L48	V126	I204	L276
K1365	D1441	P1589	P1589	K1662	G1750	G1835	V1903	P2047	F2048	K49	A127	A205	E277
D1367	Y1442	I1590	I1590	K1663	G1751	G1839	V1904	R1977	E2049	D50	G128	L208	F279
G1368	E1443	E1516	E1516	I1664	K1755	S1842	I1907	Q1979	T1980	L53	I129	Q209	S280
D1369	M1443	L1517	P1518	V1667	I1756	A1843	V1910	T1980	S2851	P57	A131	S210	G281
L1370	T1445	T1519	T1519	D1688	R1758	L1844	W1913	Q1985	K2052	T60	K133	L211	L282
K1372	Q1447	K1520	K1520	A1669	Q1759	V1845	L1914	P1986	Y2054	E61	G135	W215	G284
L1373	E1451	E1521	E1521	K1672	M1761	A1846	L1915	L1989	E2057	E62	V136	D216	H285
V1374	V1452	I1523	I1523	V1678	M1762	A1848	L1915	E1990	V2058	D67	V137	V218	S286
H1375	P1453	Q1524	Q1524	L1679	M1764	D1849	V1918	R1991	R2059	E68	R138	K219	I289
L1376	M1454	A1526	A1526	Q1681	M1764	M1851	N1919	G1992	R2060	P69	A139	Q220	V290
Y1380	Q1455	L1456	L1456	G1681	E1767	P1852	V1922	F1993	L2061	S70	Y141	Y221	V291
R1381	H1457	H1457	H1457	E1684	T1768	I1853	M1924	A1994	G2063	V73	A142	L225	A292
M1382	T1460	D1528	D1528	V1685	V1769	E1854	M1925	I1996	S2064	E74	G143	D226	A293
V1383	P1461	Y1530	Y1530	E1686	M1770	S1855	M1925	I1996	P2065	E75	R144	I227	A294
P1384	Q1462	E1531	E1531	Q1687	I1775	L1856	V1928	R1999	K2066	L75	P151	L228	A296
Y1388	D1463	A1533	A1533	Y1611	K1776	V1857	V1928	G2000	I2067	V76	P151	L228	A298
V1391	L1464	E1534	E1534	V1616	T1777	S1858	L1933	I2001	A2068	A77	S156	H232	P299
G1392	A1465	S1535	S1535	V1616	E1778	V1859	R1934	V2003	I2070	R78	A157	N233	P300
D1393	V1466	H1536	H1536	S1617	K1779	T1690	A1935	P2004	N2073	Y79	L158	P234	W301
V1394	L1467	H1537	H1537	S1618	I1780	Y1692	L1936	F2005	W2074	I80	F159	E235	D302
L1395	R1468	N1538	N1538	L1619	F1781	G1693	D1937	H2006	D2075	A81	R160	D239	E303
D1396	S1469	V1620	V1620	F1694	G1798	G1864	L1938	T2008	Z2076	F82	G160	T240	F304
S1469	K1470	E1621	E1621	Q1700	L1799	T1866	L1939	F2009	Y2077	V83	A161	T240	A305
T1397	E1471	T1541	T1541	E1701	L1800	M1867	V1942	L2010	Z2077	E86	E164	V244	T306
T1398	A1399	D1542	D1542	E1701	S1801	Q1868	L1943	R2011	E2078	V87	V167	S245	K309
Q1400	L1475	L1544	L1544	M1704	A1802	V1869	N1944	S2012		E92	K168	A246	R310
N1402	D1476			N1627	T1803	A1870	I1945	G2013				P247	

● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

Chain K:



Q19	D83	I169	F250	Q19	D83	I169	F250
L21	A94	Y170	P251	L21	A94	Y170	P251
R22	L99	S171	L252	R22	L99	S171	L252
P23	V101	G174	I253	P23	V101	G174	I253
L24	L102	I179	V256	L24	L102	I179	V256
V25	K103	Y182	Q257	V25	K103	Y182	Q257
L26	L104	F183	L258	L26	L104	F183	L258
T27	L106	L186	A259	T27	L106	L186	A259
H28	M107	L186	H280	H28	M107	L186	H280
S30	E108	L186	S30	S30	E108	L186	S30
L31	R111	I189	L261	L31	R111	I189	L261
E32	F113	Y190	I263	E32	F113	Y190	I263
F35	M114	T192	T264	F35	M114	T192	T264
L36	G116	S195	K266	L36	G116	S195	K266
V37	H120	F196	L268	V37	H120	F196	L268
P38	A121	V197	G269	P38	A121	V197	G269
T39	I122	L200	L270	T39	I122	L200	L270
Q44	V126	I201	T271	Q44	V126	I201	T271
A45	A127	L204	E272	A45	A127	L204	E272
A46	G128	A205	L273	A46	G128	A205	L273
Q47	I129	L208	G274	Q47	I129	L208	G274
L48	L130	Q209	L275	L48	L130	Q209	L275
K49	K133	S210	E276	K49	K133	S210	E276
D50	T134	L211	L277	D50	T134	L211	L277
L53	G135	W215	E278	L53	G135	W215	E278
P57	V136	D216	G281	P57	V136	D216	G281
T60	V137	I218	L282	T60	V137	I218	L282
E61	R138	K219	G284	E61	R138	K219	G284
E62	A139	Q220	H285	E62	A139	Q220	H285
D67	Y140	Y221	S286	D67	Y140	Y221	S286
E68	Y141	L225	G287	E68	Y141	L225	G287
P69	A142	D226	S288	P69	A142	D226	S288
S70	R144	I227	I289	S70	R144	I227	I289
V73	P151	L228	G290	V73	P151	L228	G290
E74	S156	H232	L291	E74	S156	H232	L291
L75	A157	N233	L292	L75	A157	N233	L292
V76	L158	P234	L293	V76	L158	P234	L293
A77	F159	E235	L294	A77	F159	E235	L294
R78	R160	D302	A295	R78	R160	D302	A295
Y79	G161	F303	A305	Y79	G161	F303	A305
I80	E164	T306		I80	E164	T306	
A81	V167			A81	V167		
F82	K168			F82	K168		
V83				V83			
E86				E86			
V87				V87			
E92				E92			

WORLDWIDE
PDB
PROTEIN DATA BANK

E2057	E2058	H2059	R2060	L2061	T2062	G2063	S2064	P2065	K2066	L2067	A2068	N2069	N2073	W2074	L2075	K2076	Y2077	E2078																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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V2014	K1947	R1878	P1808	K1716	H1636	P1560	R1491	C1416
K2015	M1948	S1879	L1812	K1716	V1637	I1561	L1492	G1417
P2016	I1951	M1880	M1813	R1721	M1639	P1562	L1492	T1418
F2017	D1952	Y1881	E1814	A1722	V1640	V1496	V1496	R1421
R2018	L1953	A1882	F1818	F1726	G1641	K1566	F1498	K1424
S2019	F2020	M1883	E1819	I1735	M1642	T1567	K1499	P1425
F2020	L1956	C1884	D1820	K1739	V1643	P1568	M1500	M1427
L2021	M1957	A1885	M1821	K1739	P1645	R1572	N1502	L1434
L2022	M1960	M1887	R1822	K1739	P1646	A1573	V1503	Y1435
I2025	S1961	P1888	S1823	N1740	D1647	P1574	Y1504	R1436
T2028	L1962	S1889	K1824	N1741	A1648	N1579	S1505	G1437
T2029	E1963	R1890	G1825	P1742	I1649	V1583	S1506	V1507
I2030	D1964	F1895	L1826	L1745	T1650	S1584	I1510	G1511
D2031	V1965	T1896	V1827	T1746	L1653	G1585	G1511	Y1439
P2032	R1966	E1897	Q1828	V1747	E1654	H1585	T1440	T1440
S2033	A1967	E1897	R1829	H1748	H1655	D1586	D1441	D1441
K2034	H1968	Q1898	T1832	F1749	V1656	Y1587	Y1442	Y1442
L2035	L1969	A1899	F1833	G1750	G1657	N1588	L1514	L1514
L2036	V1970	L1900	F1834	G1751	M1658	P1589	L1515	L1515
G2037	E1971	Q1901	G1835	K1755	I1659	T1590	E1516	E1516
K2038	L1972	Y1902	G1835	K1755	R1662	H1591	L1517	T1445
Y2039	I1973	V1903	G1839	R1768	K1663	T1592	E1451	E1451
L2040	Q1974	V1904	E1840	Q1768	K1663	S1593	T1452	T1452
P2041	E1975	E1905	Y1841	Q1769	I1664	R1594	F1453	F1453
N2042	C1976	M1906	S1842	M1760	H1664	F1596	M1454	M1454
V2043	R1977	I1907	A1843	Y1761	V1667	F1596	I1522	Q1485
T2044	K1978	V1910	L1844	M1762	D1668	L1602	I1523	L1456
A2045	Q1979	V1910	V1845	S1763	A1669	P1603	Q1524	H1457
K2046	T1980	V1913	A1846	M1764	K1672	G1604	V1525	V1525
P2047	Q1985	L1914	L1847	T1765	K1672	T1605	A1526	A1526
I2050	P1986	L1915	A1848	F1766	K1672	T1606	F1461	F1461
S2051	L1989	V1918	D1849	E1767	V1678	T1607	V1528	V1528
K2052	F1990	M1919	M1850	T1768	L1679	Y1530	D1463	D1463
E2053	R1991	Y1920	M1851	V1769	Q1680	H1608	L1464	L1464
Y2054	G1992	M1921	P1852	M1770	G1681	G1609	A1465	A1465
E2057	F1993	Y1922	L1853	I1775	E1684	M1610	V1466	V1466
V2058	A1994	A1923	E1854	K1776	V1685	Y1611	L1467	L1467
H2059	T1995	L1856	S1855	T1777	E1686	V1616	R1468	R1468
R2060	I1996	V1857	L1856	K1778	Q1687	S1617	S1469	S1469
L2061	P1997	Q1926	V1857	E1778	P1688	R1617	K1470	K1470
T2062	L1998	V1928	S1858	K1779	V1689	S1618	E1471	E1471
G2063	R1999	D1932	V1860	I1780	L1619	L1619	V1472	V1472
S2064	P2001	L1933	F1861	F1781	V1620	V1620	F1473	F1473
K2066	D2002	R1934	Y1862	D1785	A1691	E1621	K1474	K1474
I2067	V2003	A1935	R1863	D1785	A1691	T1622	L1475	L1475
A2068	P2004	L1936	G1864	Y1793	V1693	W1623	D1476	D1476
N2069	P2005	D1937	L1865	Y1793	F1694	E1626	Q1477	Q1477
N2073	H2006	T1938	T1866	L1799	Q1700	N1627	Q1478	Q1478
V2074	S2007	L1939	M1867	L1800	E1701	N1628	H1479	H1479
D2075	T2008	V1942	Q1868	S1801	M1704	I1629	D1480	D1480
K2076	F2009	L1943	V1869	A1802	G1705	G1630	E1552	E1552
Y2077	L2010	L1943	V1871	Q1804	M1706	V1632	Q1563	Q1563
E2078	S2012	M1944	R1872	Q1805	D1707	R1633	P1554	P1554
			L1873	T1806	L1708	S1634	P1555	P1555
			D1874	Q1807	Y1709	V1635	M1556	M1556
							F1557	F1557
							V1488	V1488
							L1489	L1489
							F1490	F1490

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 12.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 89.5 (12.00-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.290 , 0.320 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.276 for l,k,h	Xtriage
F_o, F_c correlation	0.83	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.

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

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	0.49	0/11744	0.90	24/15873 (0.2%)
1	B	0.50	1/11801 (0.0%)	0.89	25/15949 (0.2%)
1	C	0.51	0/11785	0.90	19/15928 (0.1%)
1	D	0.49	0/11824	0.90	22/15980 (0.1%)
1	E	0.49	0/11736	0.90	25/15863 (0.2%)
1	F	0.52	1/11776 (0.0%)	0.91	24/15916 (0.2%)
2	G	0.44	0/16573	0.87	31/22516 (0.1%)
2	H	0.44	0/16573	0.88	28/22516 (0.1%)
2	I	0.44	0/16573	0.88	34/22516 (0.2%)
2	J	0.44	0/16573	0.89	29/22516 (0.1%)
2	K	0.48	0/16573	0.90	34/22516 (0.2%)
2	L	0.45	0/16573	0.88	39/22516 (0.2%)
All	All	0.47	2/170104 (0.0%)	0.89	334/230605 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1564	HIS	CG-ND1	5.12	1.43	1.38
1	B	1373	VAL	CA-CB	-5.05	1.50	1.55

The worst 5 of 334 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	612	ILE	CA-C-N	14.66	138.17	119.84
1	F	612	ILE	C-N-CA	14.66	138.17	119.84
1	A	484	PRO	CA-C-N	9.57	130.28	120.14
1	A	484	PRO	C-N-CA	9.57	130.28	120.14
1	E	484	PRO	CA-C-N	9.34	130.04	120.14

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 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	778	0
1	B	11571	0	11529	745	1
1	C	11555	0	11507	727	0
1	D	11593	0	11552	762	0
1	E	11506	0	11467	775	0
1	F	11546	0	11499	737	0
2	G	16200	0	16081	1237	1
2	H	16200	0	16081	1270	1
2	I	16200	0	16081	1293	0
2	J	16200	0	16081	1262	0
2	K	16200	0	16081	1318	1
2	L	16200	0	16081	1273	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	9	0
All	All	166671	0	165630	11515	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 11515 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)
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:HG2	2:H:1594:ARG:HH11	1.02	1.17
1:E:1610:ARG:HG2	1:E:1610:ARG:HH11	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	Interatomic distance (Å)	Clash overlap (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 [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%)	1291 (89%)	148 (10%)	12 (1%)	16	47
1	B	1458/1878 (78%)	1295 (89%)	151 (10%)	12 (1%)	16	47
1	C	1456/1878 (78%)	1293 (89%)	151 (10%)	12 (1%)	16	47
1	D	1461/1878 (78%)	1290 (88%)	155 (11%)	16 (1%)	11	39
1	E	1450/1878 (77%)	1292 (89%)	146 (10%)	12 (1%)	16	47
1	F	1455/1878 (78%)	1300 (89%)	140 (10%)	15 (1%)	12	41
2	G	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	9	35
2	H	2058/2060 (100%)	1786 (87%)	244 (12%)	28 (1%)	9	34
2	I	2058/2060 (100%)	1799 (87%)	233 (11%)	26 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	9	35
2	K	2058/2060 (100%)	1772 (86%)	258 (12%)	28 (1%)	9	34
2	L	2058/2060 (100%)	1777 (86%)	253 (12%)	28 (1%)	9	34
All	All	21079/23628 (89%)	18479 (88%)	2359 (11%)	241 (1%)	11	39

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%)	1085 (89%)	135 (11%)	6	24
1	B	1227/1527 (80%)	1097 (89%)	130 (11%)	6	26
1	C	1225/1527 (80%)	1089 (89%)	136 (11%)	6	24
1	D	1229/1527 (80%)	1091 (89%)	138 (11%)	6	24
1	E	1219/1527 (80%)	1084 (89%)	135 (11%)	6	24
1	F	1224/1527 (80%)	1089 (89%)	135 (11%)	6	24
2	G	1752/1752 (100%)	1538 (88%)	214 (12%)	5	20
2	H	1752/1752 (100%)	1539 (88%)	213 (12%)	5	20
2	I	1752/1752 (100%)	1537 (88%)	215 (12%)	4	20
2	J	1752/1752 (100%)	1540 (88%)	212 (12%)	5	20
2	K	1752/1752 (100%)	1537 (88%)	215 (12%)	4	20
2	L	1752/1752 (100%)	1538 (88%)	214 (12%)	5	20
All	All	17856/19674 (91%)	15764 (88%)	2092 (12%)	5	22

5 of 2092 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	1785	ASP
2	L	340	VAL
2	K	1767	GLU
2	L	1974	GLN
1	F	1422	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 536 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	1185	HIS
2	K	1702	GLN
2	K	1173	HIS
2	L	1462	GLN
1	F	1098	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMN	H	2101	-	33,33,33	6.41	23 (69%)	48,50,50	1.35	7 (14%)
3	FMN	J	2101	-	33,33,33	6.62	24 (72%)	48,50,50	1.40	11 (22%)
3	FMN	K	2101	-	33,33,33	6.65	25 (75%)	48,50,50	1.46	12 (25%)
3	FMN	L	2101	-	33,33,33	6.35	22 (66%)	48,50,50	1.36	9 (18%)
3	FMN	I	2101	-	33,33,33	6.41	23 (69%)	48,50,50	1.43	8 (16%)
3	FMN	G	2101	-	33,33,33	6.42	24 (72%)	48,50,50	1.40	8 (16%)

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	H	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	K	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	L	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	I	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	G	2101	-	-	5/18/18/18	0/3/3/3

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2101	FMN	C6-C7	13.67	1.58	1.39
3	J	2101	FMN	C6-C7	13.45	1.57	1.39
3	H	2101	FMN	C6-C7	13.39	1.57	1.39
3	G	2101	FMN	C6-C7	13.28	1.57	1.39
3	I	2101	FMN	C6-C7	12.95	1.57	1.39

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2101	FMN	C9A-C5A-N5	-3.32	118.93	122.45
3	I	2101	FMN	C5A-C9A-N10	3.30	120.95	117.97
3	K	2101	FMN	C4-N3-C2	-3.23	119.90	125.64
3	I	2101	FMN	C9A-C5A-N5	-3.21	119.05	122.45
3	L	2101	FMN	C9A-C5A-N5	-3.18	119.08	122.45

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2101	FMN	C2'-C3'-C4'-C5'
3	G	2101	FMN	O3'-C3'-C4'-C5'
3	H	2101	FMN	C2'-C3'-C4'-C5'
3	H	2101	FMN	O3'-C3'-C4'-C5'
3	I	2101	FMN	C2'-C3'-C4'-C5'

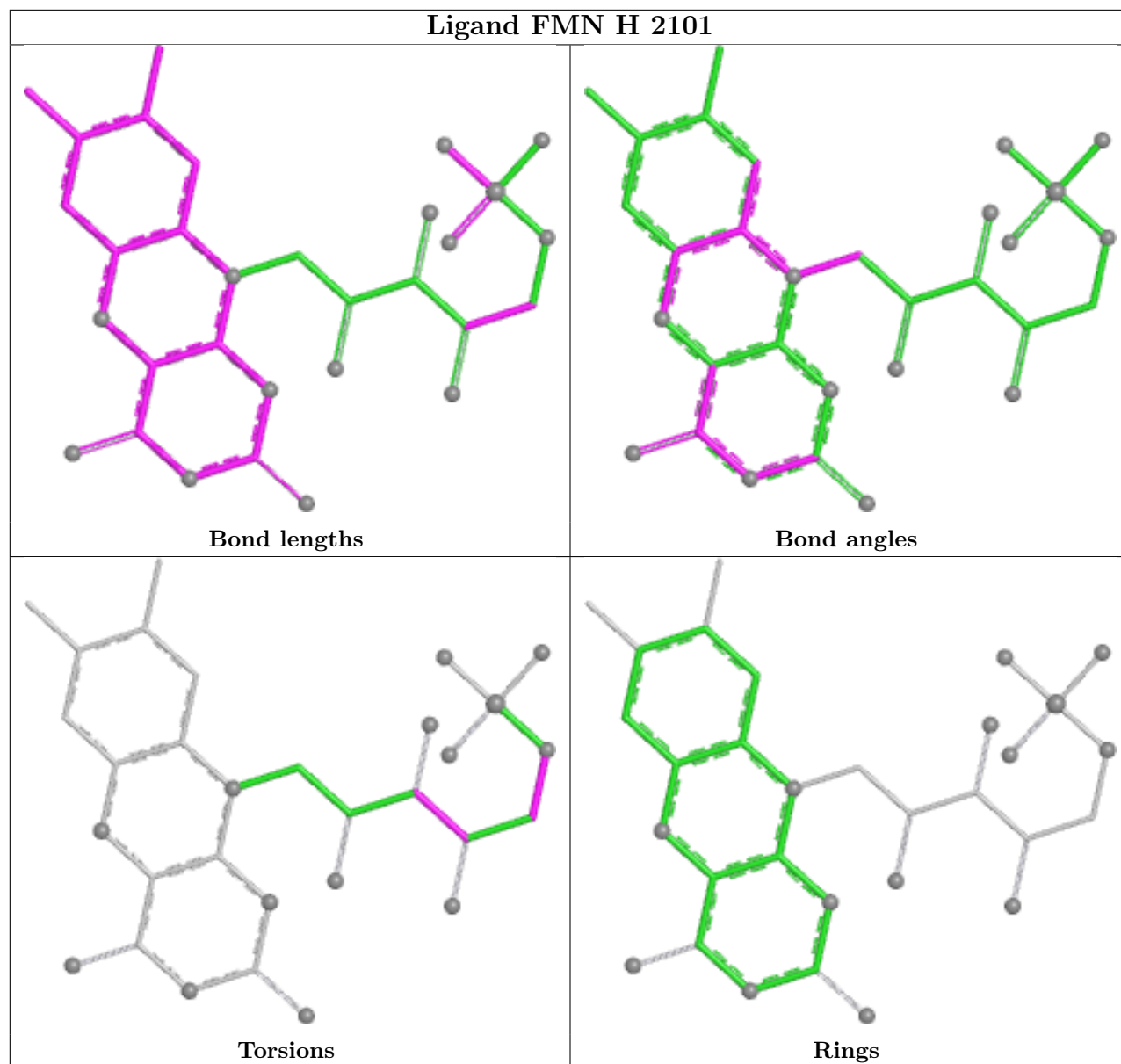
There are no ring outliers.

6 monomers are involved in 60 short contacts:

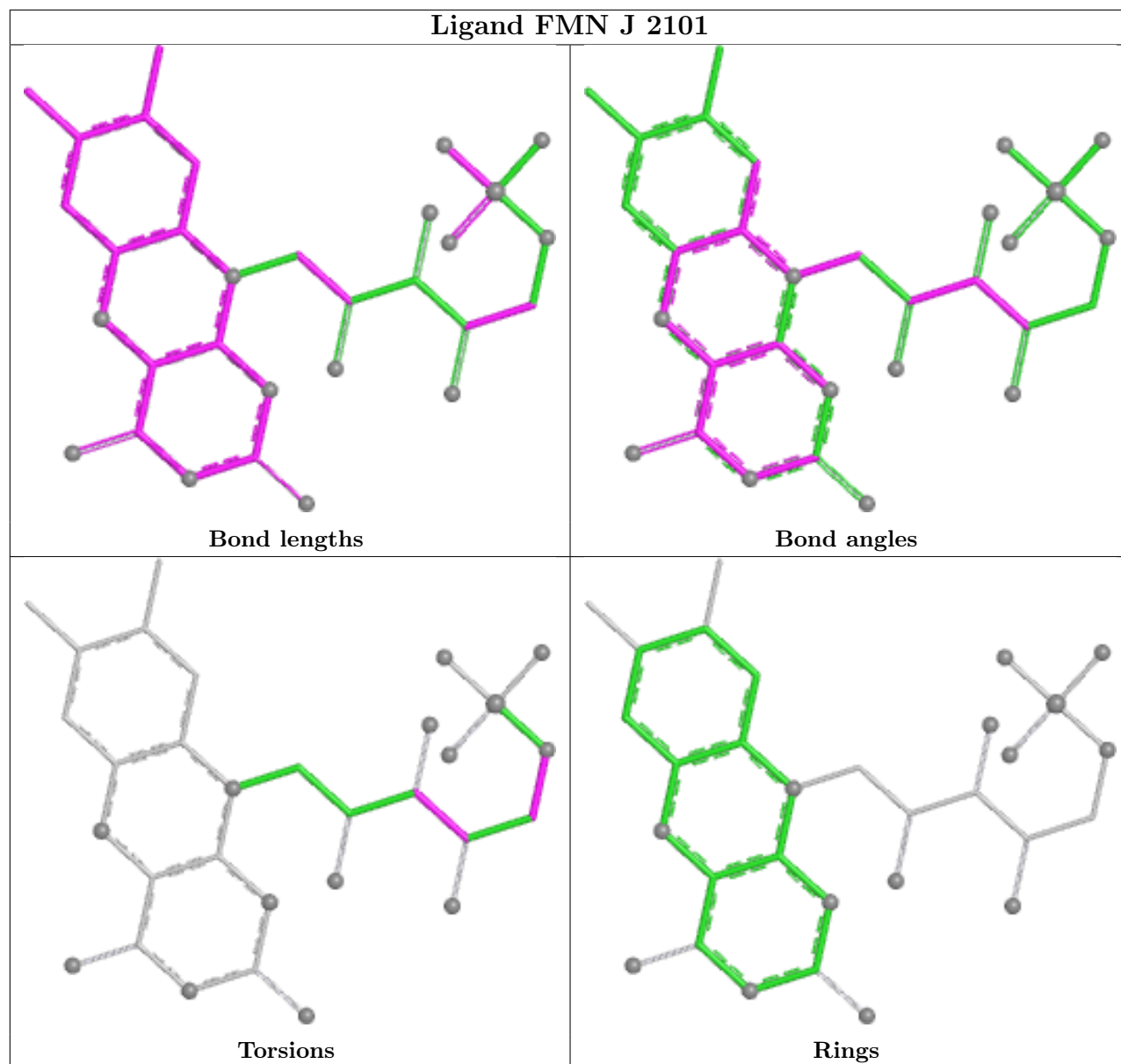
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2101	FMN	11	0
3	J	2101	FMN	9	0
3	K	2101	FMN	12	0
3	L	2101	FMN	9	0
3	I	2101	FMN	9	0
3	G	2101	FMN	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

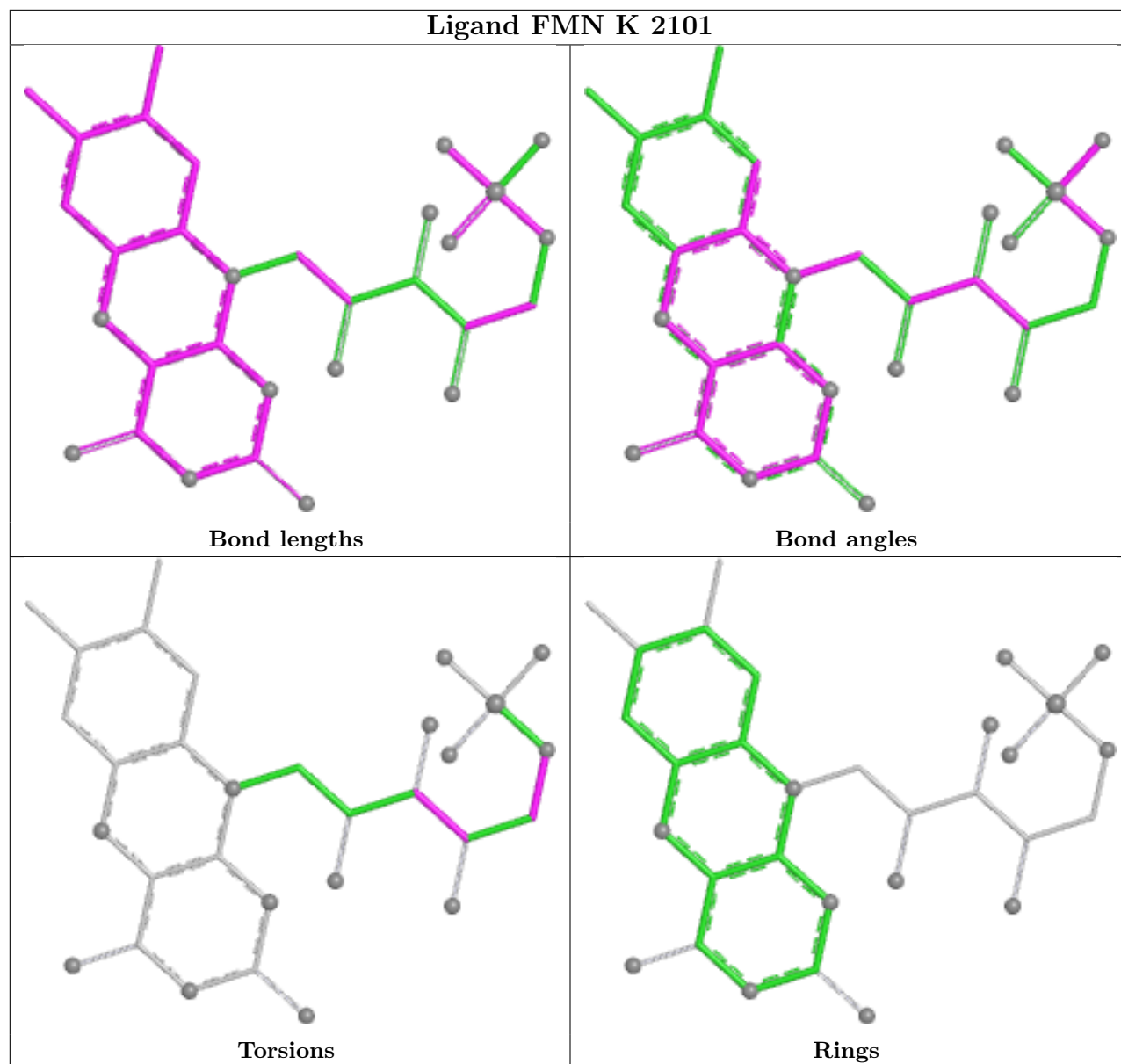
Ligand FMN H 2101



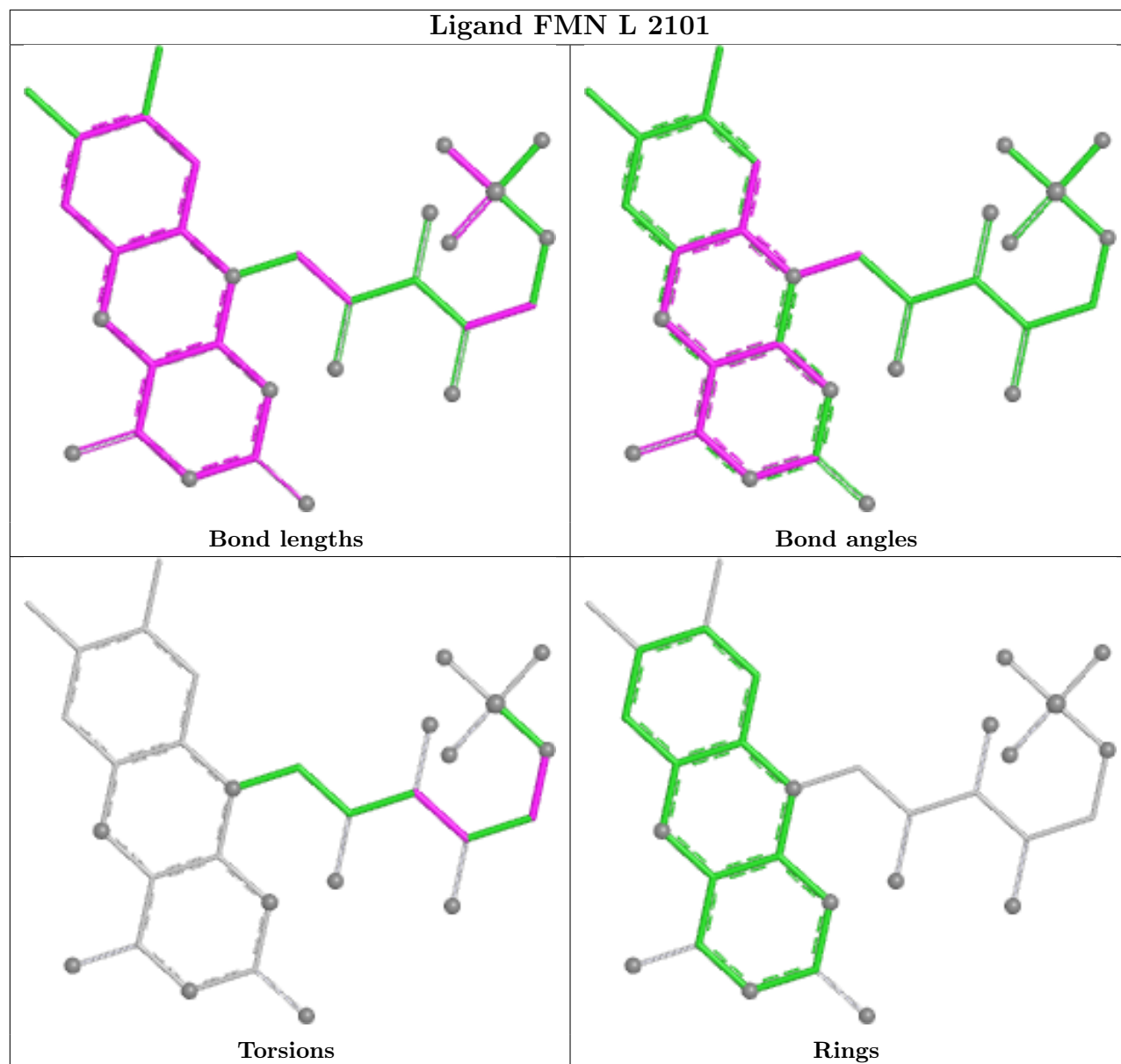
Ligand FMN J 2101

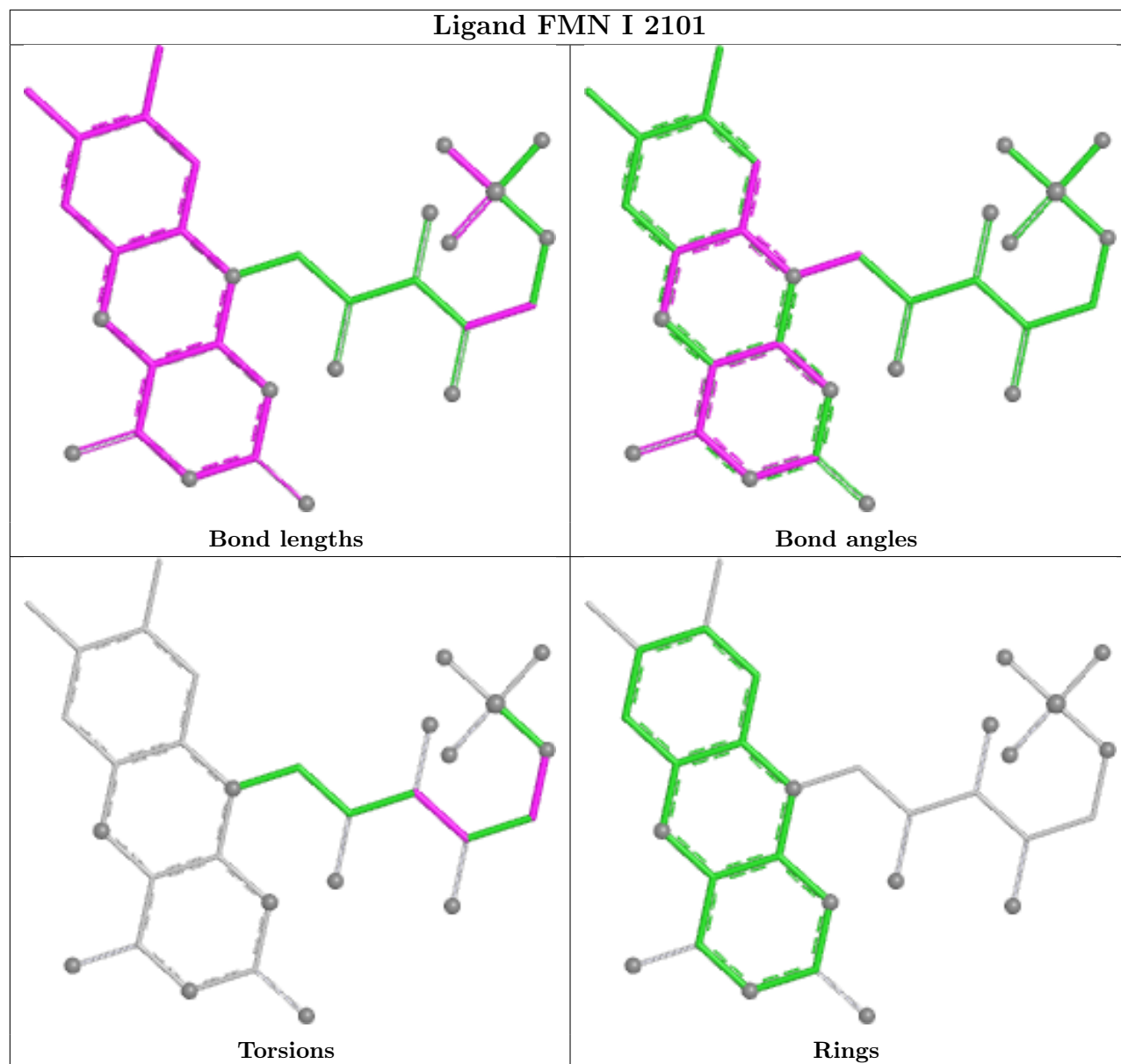


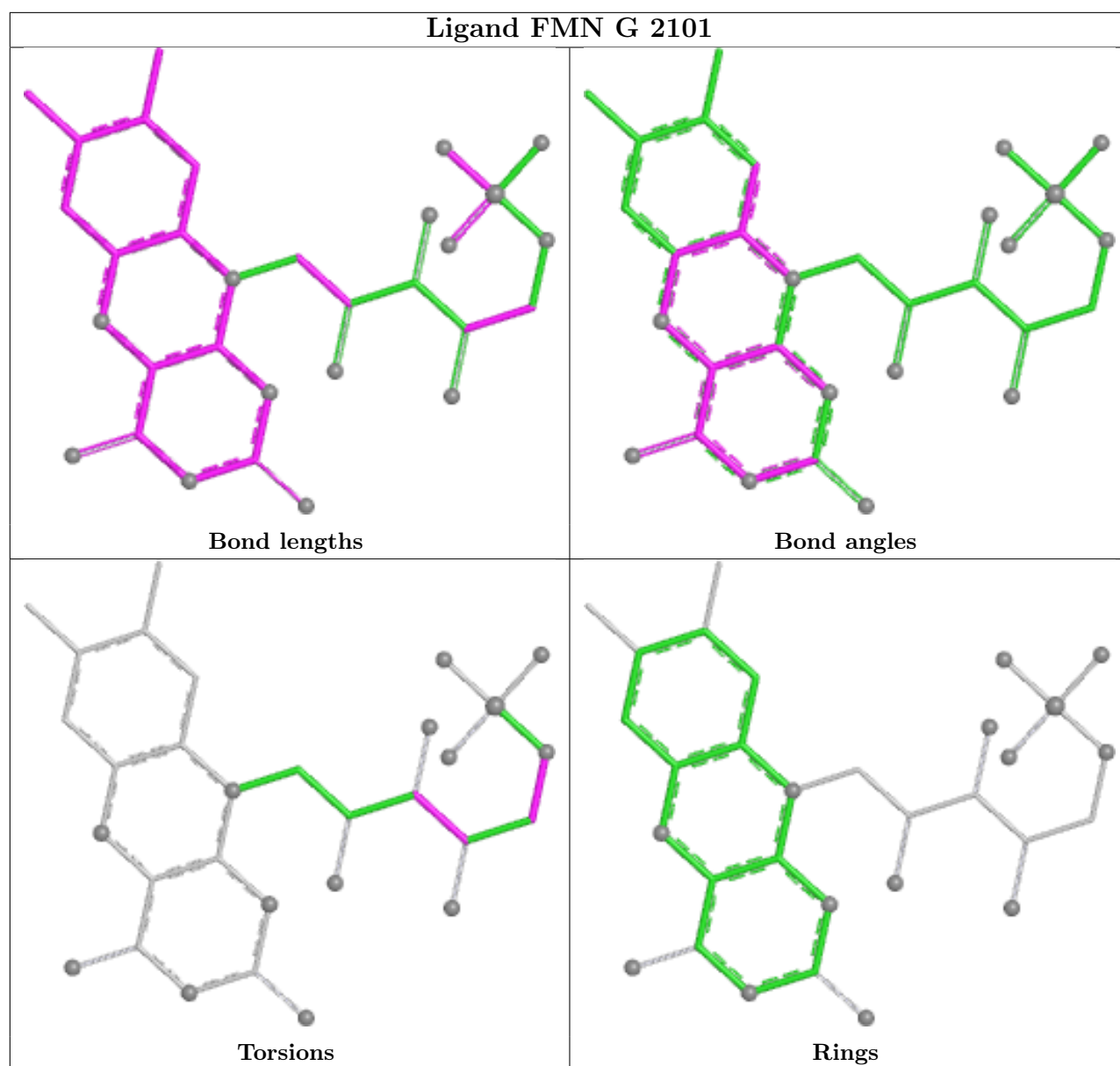
Ligand FMN K 2101



Ligand FMN L 2101







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 ⓘ

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%)	-1.47	0 100 100	17, 54, 105, 150	0
1	B	1464/1878 (77%)	-1.47	0 100 100	16, 52, 111, 158	0
1	C	1462/1878 (77%)	-1.48	0 100 100	15, 51, 111, 159	0
1	D	1467/1878 (78%)	-1.47	0 100 100	16, 54, 108, 158	0
1	E	1456/1878 (77%)	-1.46	0 100 100	15, 54, 110, 157	0
1	F	1461/1878 (77%)	-1.49	0 100 100	16, 51, 108, 159	0
2	G	2060/2060 (100%)	-1.28	0 100 100	27, 83, 129, 169	0
2	H	2060/2060 (100%)	-1.24	0 100 100	24, 86, 132, 167	0
2	I	2060/2060 (100%)	-1.24	0 100 100	23, 86, 132, 167	0
2	J	2060/2060 (100%)	-1.20	1 (0%) 100 100	28, 89, 133, 172	0
2	K	2060/2060 (100%)	-1.16	0 100 100	27, 91, 136, 172	0
2	L	2060/2060 (100%)	-1.20	0 100 100	23, 87, 133, 172	0
All	All	21127/23628 (89%)	-1.32	1 (0%) 100 100	15, 75, 127, 172	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	93	ASP	2.0

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 oligosaccharides in this entry.

6.4 Ligands

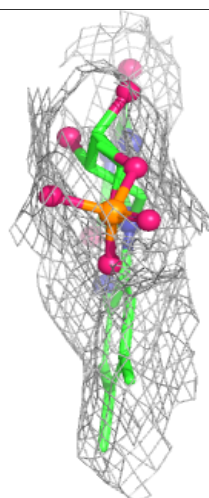
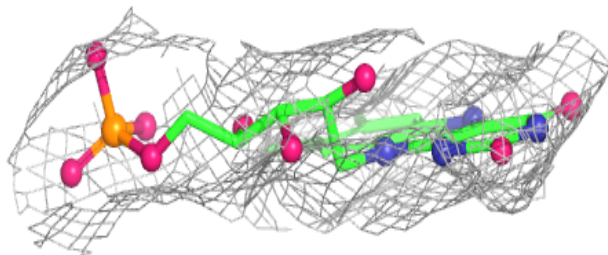
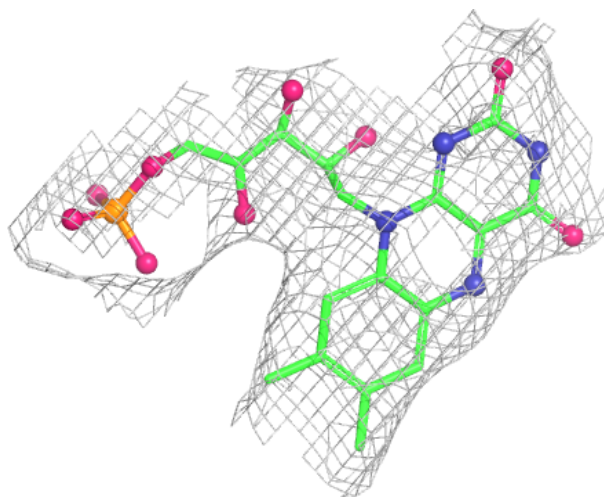
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMN	K	2101	31/31	0.99	0.04	24,63,111,122	0
3	FMN	H	2101	31/31	1.00	0.04	21,53,91,110	0
3	FMN	I	2101	31/31	1.00	0.04	23,54,85,115	0
3	FMN	J	2101	31/31	1.00	0.03	19,56,106,122	0
3	FMN	G	2101	31/31	1.00	0.04	19,64,105,124	0
3	FMN	L	2101	31/31	1.00	0.05	15,51,89,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

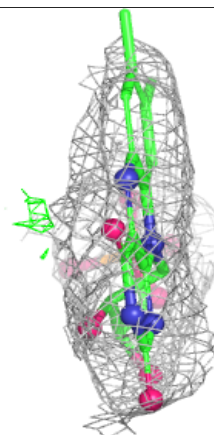
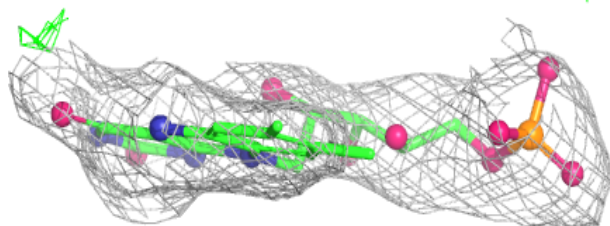
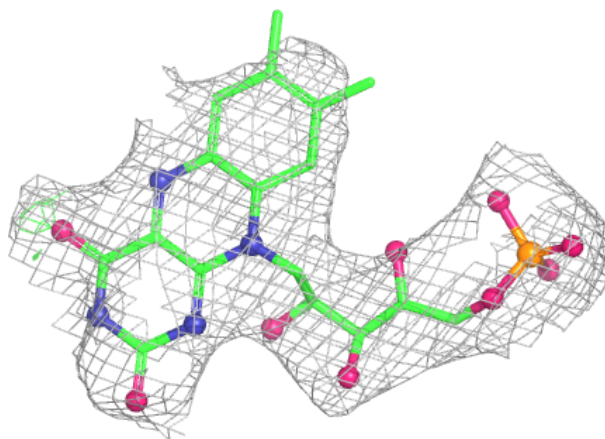
Electron density around FMN K 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



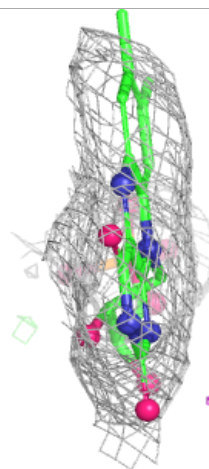
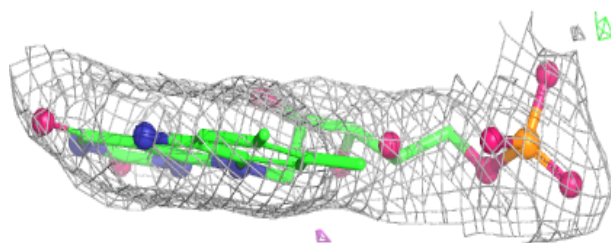
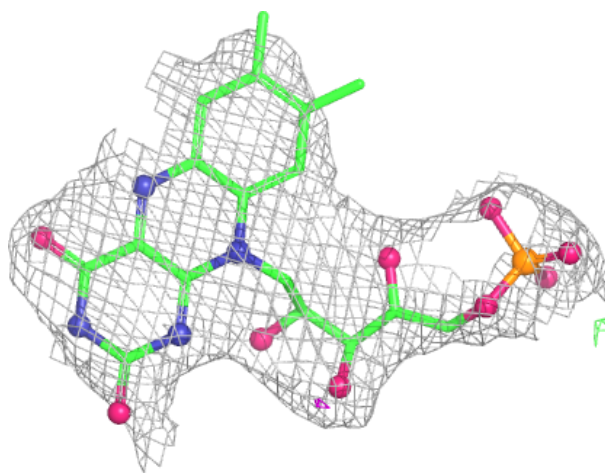
Electron density around FMN H 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



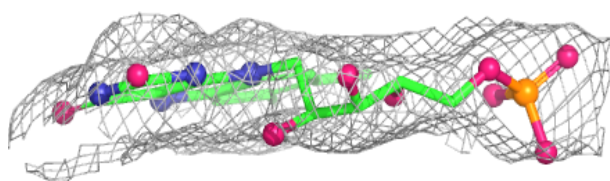
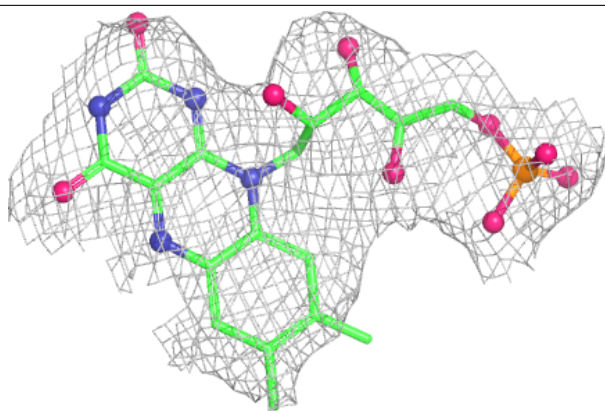
Electron density around FMN I 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



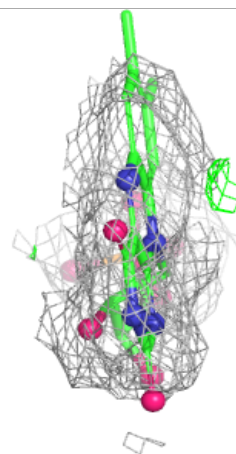
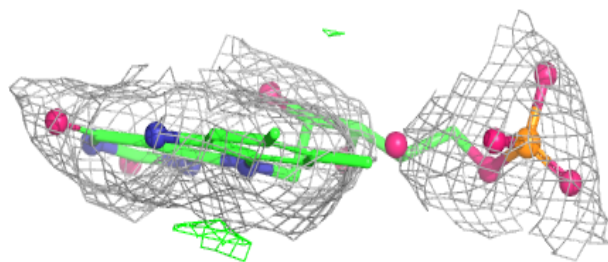
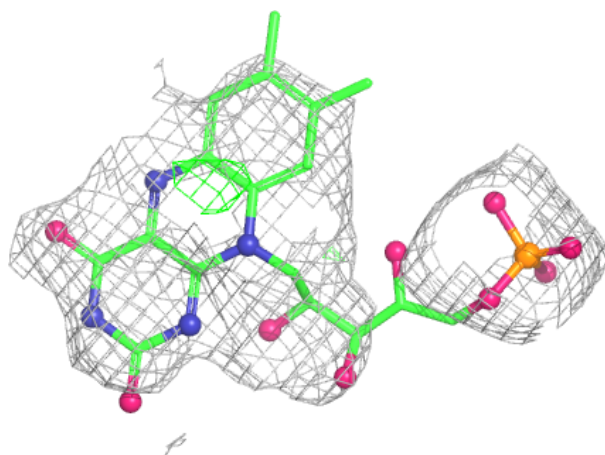
Electron density around FMN J 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



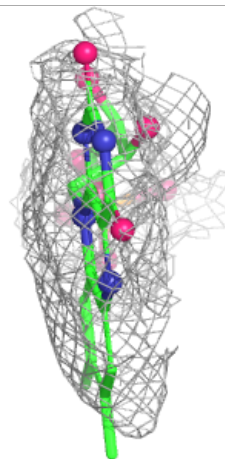
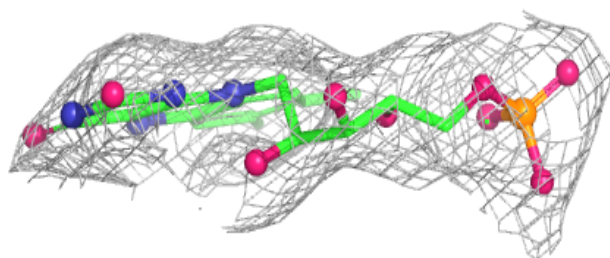
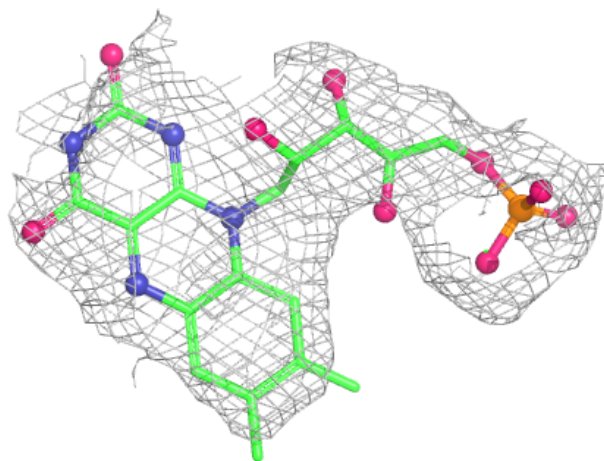
Electron density around FMN G 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN L 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.