



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 02:50 PM EDT

PDB ID : 4V8W  
EMDB ID: : EMD-2357  
Title : Structure and conformational variability of the Mycobacterium tuberculosis fatty acid synthase multienzyme complex  
Authors : Ciccarelli, L.; Connell, S.R.; Enderle, M.; Mills, D.J.; Vonck, J.; Grininger, M.  
Deposited on : unknown  
Resolution : 17.50 Å(reported)  
Based on PDB ID : 3ZEN

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

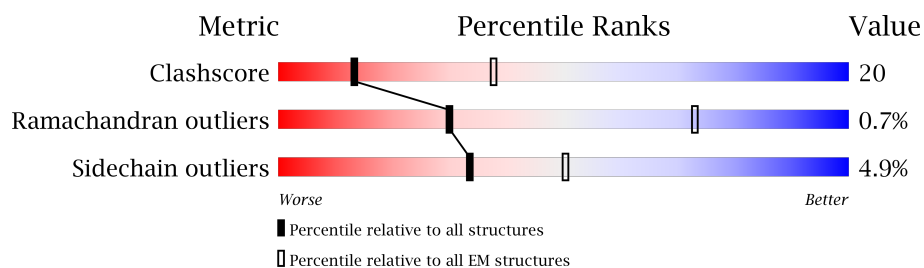
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	3089	
1	B	3089	
1	C	3089	
1	D	3089	
1	E	3089	
1	F	3089	

## 2 Entry composition [i](#)

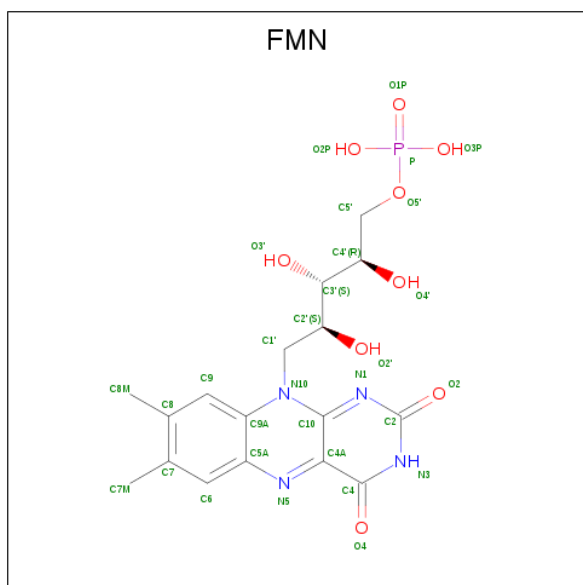
There are 2 unique types of molecules in this entry. The entry contains 123082 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TYPE-I FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	2452	Total	C	N	O	S	0	0
			18171	11459	3176	3473	63		
1	E	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	F	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	A	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	B	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	C	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



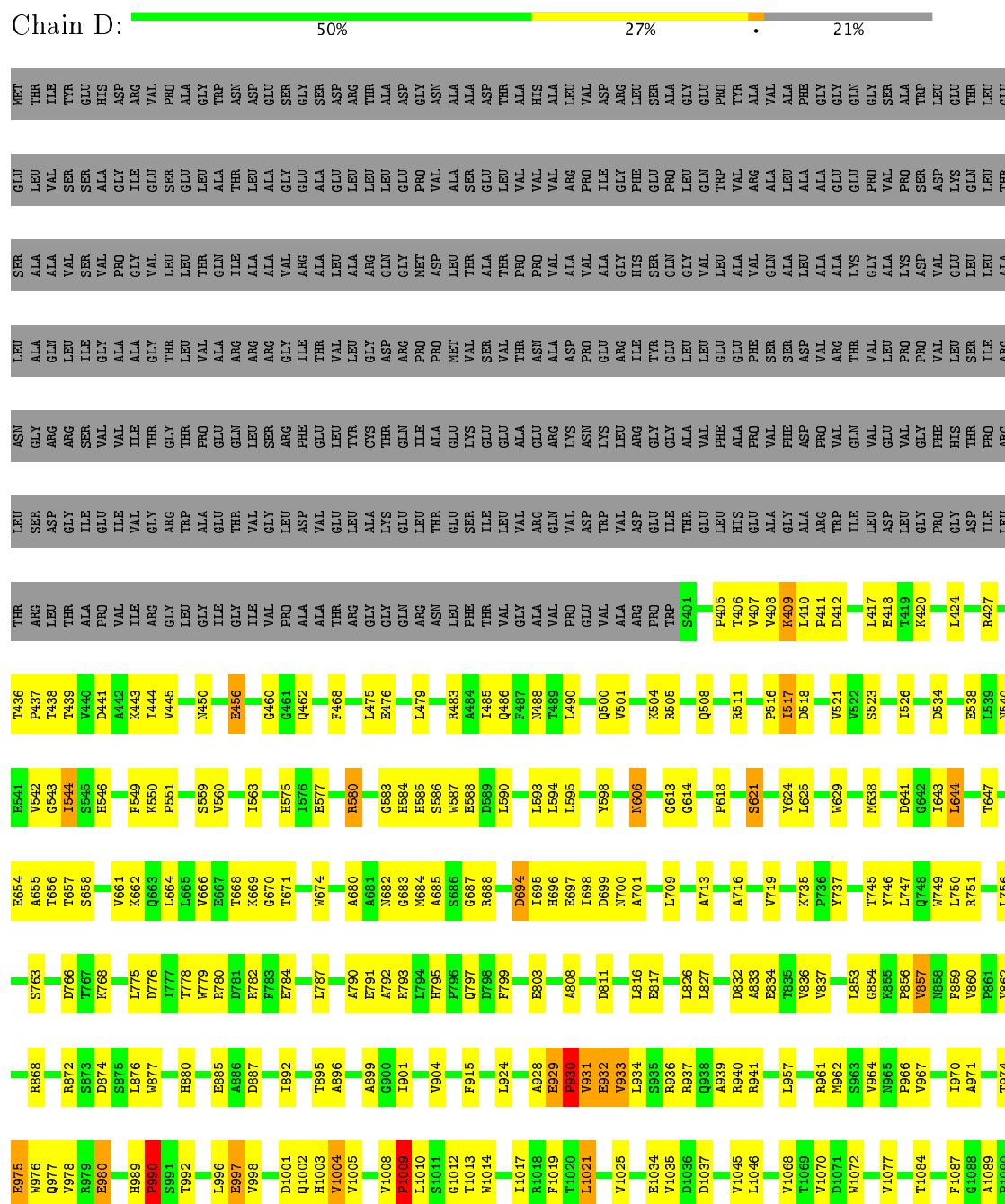
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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: TYPE-I FATTY ACID SYNTHASE

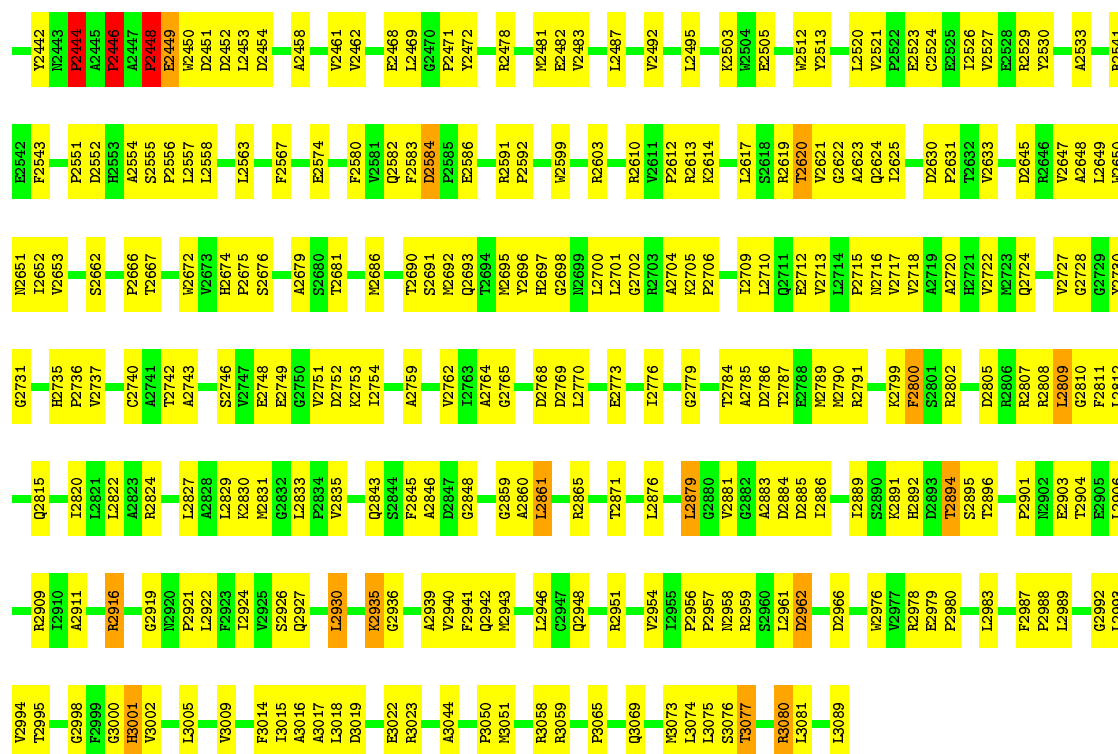


L2495	L2408	D2282	I2165	L2067	ALA	ILE	LEU	ALA	K1706	G1612	I1503	V1408	K1291	L1185	L1091
A2409	A2409	D2282	A2166	L2070	VAL	THR	GLY	PRO	S1707	R1613	I1504	V1408	K1292	L1188	A1092
A2412	A2412	R2286	T2167	E2074	ALA	ARG	GLU	ALA	T1710	P1616	P1505	H1412	K1304	L1188	P1093
M2416	M2416	H2288	R2170	E2074	ARG	THR	ASN	PRO	A1711	R1617	Q1506	D1414	D1307	R1191	L1095
S2417	S2417	L2291	D2173	Q2081	ARG	THR	LEU	GLY	A1712	L1618	Q1507	G1415	Q1308	F1192	T1096
G2418	G2418	L2291	D2174	M2082	GLY	THR	LEU	GLY	G1713	V1619	I1508	V1416	V1309	A1193	V1097
D2421	D2421	L2291	R2175	Q2081	ILE	THR	ALA	PRO	L1714	P1620	D1511	L1417	D1310	I1194	V1098
E2422	E2422	S2294	L2176	Q2084	SER	GLU	ILE	ARG	L1719	F1622	D1514	T1420	F1311	G1196	P1099
V2521	V2521	N2295	R2176	Q2084	VAL	LEU	ASP	PRO	P1722	F1623	D1514	T1420	F1312	G1196	D1100
P2522	P2522	N2296	K2180	S2086	SER	GLY	GLY	ASP	P1723	T1624	V1519	F1422	V1313	V1103	V1103
E2426	E2426	Q2297	R2188	Q2087	LEU	ALA	ALA	ASP	Y1724	L1625	V1519	F1422	D1314	G1104	G1104
A2427	A2427	G2298	F2189	Q2088	PRO	GLY	ALA	ILE	S1725	R1634	I1530	Q1424	R1315	R1105	C1106
P2428	P2428	F2299	F2189	Q2088	SER	THR	GLU	PHE	S1725	R1634	I1530	Q1424	R1315	C1106	C1106
E2525	E2525	E2300	E2090	E2090	ALA	ALA	ALA	ALA	E1730	V1637	E1531	V1425	F1316	V1110	F1110
I2526	I2526	F2300	E2090	E2090	ALA	ALA	ALA	ALA	E1730	V1637	E1531	V1425	F1316	V1110	F1110
V2527	V2527	D2303	L2192	T2092	GLY	LYS	ASP	ALA	E1731	P1638	V1532	V1430	F1317	V1207	V1207
P2528	P2528	K2306	L2193	T2092	GLY	HIS	LEU	GLY	E1732	A1639	N1534	A1431	D1319	V1207	V1207
R2433	R2433	Y2306	K2194	G2093	ALA	VAL	GLY	ALA	L1732	A1639	N1534	A1431	D1319	V1207	V1207
A2434	A2434	Y2306	V2195	H2094	SER	THR	ALA	ASP	N1733	A1639	N1534	A1431	D1319	V1207	V1207
L2435	L2435	K2310	V2196	V2095	GLY	VAL	LEU	ASP	E1734	A1639	N1534	A1431	D1319	V1207	V1207
P2436	P2436	R2319	A2197	V2096	GLY	GLU	LEU	ASP	E1735	A1639	N1534	A1431	D1319	V1207	V1207
S2437	S2437	R2319	A2198	A2097	PHE	THR	GLY	VAL	E1736	A1639	N1534	A1431	D1319	V1207	V1207
P2438	P2438	R2319	A2198	A2097	VAL	THR	GLY	VAL	D1737	A1639	N1534	A1431	D1319	V1207	V1207
P2439	P2439	R2319	D2205	Q2099	ASP	THR	LEU	VAL	L1741	A1639	N1534	A1431	D1319	V1207	V1207
Y2442	Y2442	S2331	L2209	N2101	S1983	GLY	THR	ILE	D1745	A1639	N1534	A1431	D1319	V1207	V1207
N2443	N2443	L2332	V2210	N2102	L1986	THR	LEU	THR	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2444	P2444	H2334	E2211	W2103	L1986	ARG	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
A2445	A2445	H2334	W2212	Q2104	F1989	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2446	P2446	W2339	W2213	G2105	K1989	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
E2447	E2447	W2339	G2214	G2105	K1989	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2448	P2448	Q2348	T2216	L2108	K1992	SER	THR	THR	D1745	A1639	N1534	A1431	D1319	V1207	V1207
W2449	W2449	I2352	E2216	R2112	P1996	VAL	LYS	ARG	D1745	A1639	N1534	A1431	D1319	V1207	V1207
D2451	D2451	V2353	K2229	N2113	P1996	ARG	LYS	ARG	D1745	A1639	N1534	A1431	D1319	V1207	V1207
D2452	D2452	S2354	K2229	N2113	P1996	ARG	LYS	ARG	D1745	A1639	N1534	A1431	D1319	V1207	V1207
L2453	L2453	S2354	K2229	N2113	P1996	ARG	LYS	ARG	D1745	A1639	N1534	A1431	D1319	V1207	V1207
D2454	D2454	E2358	P2234	R2115	L2000	GLY	PRO	ILE	D1745	A1639	N1534	A1431	D1319	V1207	V1207
A2458	A2458	V2361	T2235	L2118	Q2010	LEU	VAL	GLU	D1745	A1639	N1534	A1431	D1319	V1207	V1207
V2461	V2461	M2372	L2236	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
V2462	V2462	L2376	L2236	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
E2468	E2468	K2391	L2237	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
L2469	L2469	V2392	A2246	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
G2470	G2470	V2392	V2252	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2471	P2471	L2394	V2252	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
Y2472	Y2472	T2395	R2255	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
R2478	R2478	L2395	R2255	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
M2481	M2481	L2398	R2261	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
E2482	E2482	T2401	R2261	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
V2483	V2483	L2402	R2261	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
E2586	E2586	I2403	Q2268	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
R2591	R2591	L2403	Q2268	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2592	P2592	M2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
W2599	W2599	L2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
R2603	R2603	L2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
E2610	E2610	L2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
V2611	V2611	L2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207
P2612	P2612	L2405	L2274	F2119	L2011	GLY	LEU	ALA	D1745	A1639	N1534	A1431	D1319	V1207	V1207



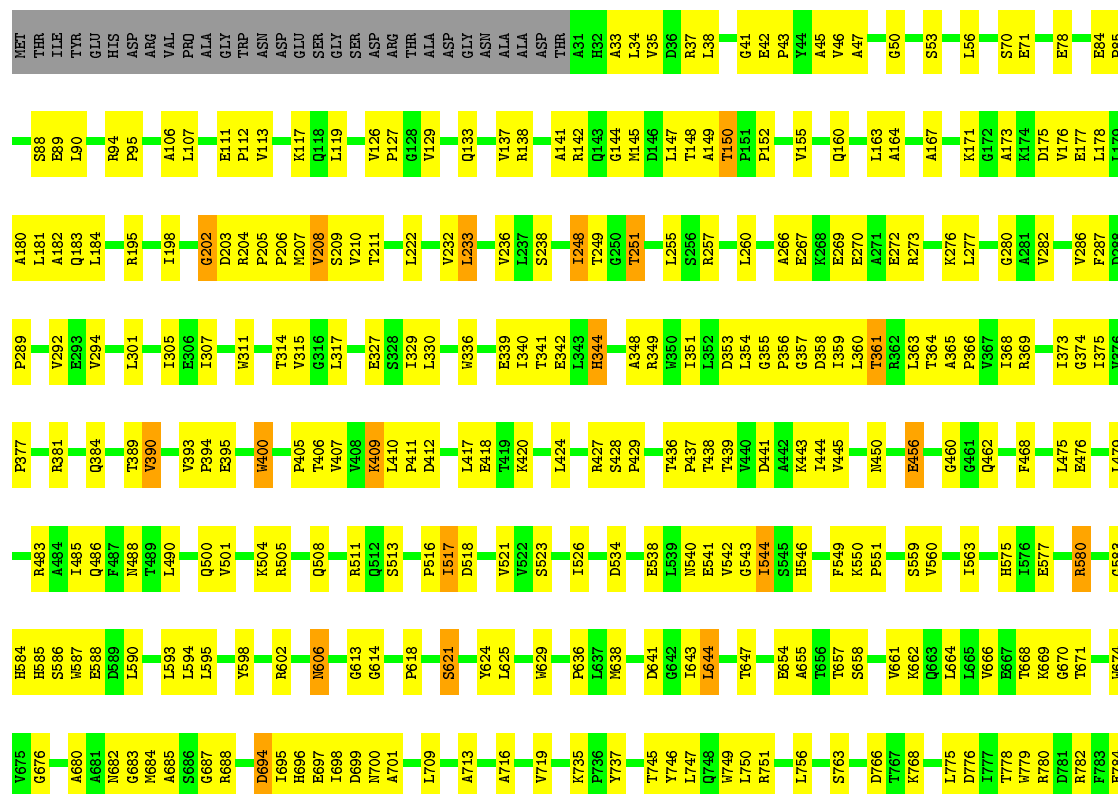
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S2331	L2209	Q2099	ALA	ALA	GLN	VAL	D1737	K1656	S1540	I1449	R1330	R1225	P1124	P1009	G900
L2332	V2210	A2100	GLY	LEU	THR	THR	L1741	P1657	Y1542	A1450	I1331	Q1541	R1226	I1010	I901
A2333	E2211	W2102	LYS	ALA	LYS	ALA	L1745	K1658	A1543	V1455	M1336	D1227	I1126	G1011	V904
E2334	W2212	Q2104	ARG	LEU	LEU	SER	THR	E1659	I1544	G1456	M1337	V1228	E1127	S1011	F915
W2339	G2214	G2105	GLY	ARG	ALA	THR	ASP	L1660	L1551	E1457	A1338	W1237	G1128	T1013	
T2348	K1992	L2108	THR	THR	LYS	ASP	PRQ	C1661	E1552	T1458	A1339	R1253	L1129	W1014	
L2352	P1996	R2112	LYS	VAL	LYS	PRQ	PRQ	K1663	A1553	T1459	R1342	R1253	L1132	I1017	I924
W2353	L2000	W2114	GLY	GLY	LYS	GLU	GLU	E1666	L1554	L1461	L1343	G1268	V1133	R1018	A928
S2354	L2000	R2115	ASP	ASP	THR	GLN	GLU	E1667	E1556	C1463	A1344	M1269	P1146	E929	E930
E2358	Q2010	F2118	LEU	LEU	VAL	ILE	ASP	W1671	R1560	V1464	P1346	W1270	K1147	W931	W931
L2362	L2011	L2118	GLY	GLY	LEU	GLU	GLU	F1672	R1561	E1467	A1351	L1271	P1149	V1025	V932
W2361	G2012	F2119	SER	GLY	LEU	ALA	PRQ	A1674	R1562	E1469	A1150	A1274	E1151	L934	L934
L2372	L2013	L2122	ALA	ALA	ASP	THR	ALA	E1679	Q1563	L1470	E1151	Q1276	E1034	S935	S935
W2372	S2014	A2123	THR	THR	ALA	SER	ALA	F1687	I1564	E1471	A1345	H1277	V1035	R936	R936
L2376	L2015	A2124	ALA	ALA	ILE	SER	ASP	W1679	D1578	L1474	P1346	W1277	D1036	Q938	Q938
K2391	Q2016	A2125	GLY	GLY	ASN	GLU	ALA	D1684	V1579	L1474	Q1358	T1280	D1163	A939	A939
W2392	P2020	A2126	LEU	LEU	GLN	ASP	ALA	L1688	P1580	R1480	M1362	A1281	T1164	R940	R940
D2393	W2082	E2127	ARG	ARG	LEU	THR	ALA	E1690	F1581	R1480	V1376	T1282	G1167	R941	R941
L2401	VAL	W2134	ALA	ALA	THR	GLY	ALA	E1694	H1582	K1483	P1400	D1283	R1168	L957	L957
R2402	ASP	E2137	ASP	ASP	THR	ALA	ALA	F1700	S1583	P1484	A1380	G1284	P1171	R961	R961
L2403	LYS	W2140	SER	SER	GLY	ALA	PRQ	W1701	L1586	H1485	A1172	K1285	V1172	M962	M962
L2408	VAL	V2141	GLY	GLY	LEU	ALA	ALA	E1702	L1586	D1486	P1173	P1286	V1077	S963	S963
A2412	VAL	T2163	THR	THR	PRO	VAL	VAL	G1704	V1590	I1487	F1390	P1287	V1174	W964	W964
M2416	VAL	A2165	ARG	ARG	ASP	ALA	ALA	R1699	E1598	P1488	P1400	P1288	R1177	W965	W965
S2417	VAL	A2166	ASN	ASN	GLY	ALA	ALA	F1700	E1598	R1490	A1405	A1290	N1178	P966	P966
G2418	ILE	T2167	GLN	GLN	LYS	THR	PRQ	W1705	K1605	D1491	D1405	K1291	A1179	V967	V967
D2421	ASP	R2170	PRO	PRO	PRO	LEU	PRQ	E1702	K1606	R1495	V1408	L1292	L1184	I970	I970
E2422	GLY	T2174	VAL	VAL	ALA	VAL	VAL	G1704	P1607	S1496	H1412	W1295	L1185	A971	A971
W2426	ARG	D2173	ALA	ALA	ILE	LEU	ALA	K1706	I1611	I1503	P1413	K1304	L1188	T974	T974
P2428	GLY	E2174	THR	THR	THR	GLY	PRQ	T1710	G1612	R1504	D1414	D1307	A1092	E975	E975
L2431	ILE	R2175	ALA	ALA	GLU	SER	ALA	A1711	R1613	P1505	G1415	Q1308	P1093	W976	W976
W2432	VAL	L2176	VAL	VAL	ARG	LEU	PRQ	V1712	Y1614	S1506	V1416	V1309	T1094	Q977	Q977
T2431	ARG	K2180	ARG	ARG	THR	ASN	SER	A1712	I1615	Q1507	L1417	D1310	T1096	W978	W978
L2432	THR	R2188	THR	THR	LYS	LEU	GLY	G1713	H1617	I1508	T1420	F1311	V1097	R979	R979
W2433	GLY	F2189	GLY	GLY	THR	GLY	GLY	L1714	V1618	D1511	Q1421	R1312	V1098	E980	E980
L2435	VAL	R2192	LEU	LEU	LEU	ASP	PRQ	L1719	V1619	D1514	T1422	D1314	P1099	H989	H989
P2436	LEU	W2196	PRO	PRO	GLY	GLY	ASP	P1722	P1622	V1519	Q1424	R1315	D1100	P990	P990
S2437	THR	T2197	PRO	PRO	GLY	ALA	ASP	E1723	F1623	V1519	V1425	W1316	V1103	S991	S991
W2439	GLY	A2198	GLY	GLY	TRP	ALA	THR	S1725	L1624	L1530	A1431	D1319	G1104	T992	T992
	GLY		GLY	GLY	THR	ALA	PHE	W1730	L1625	E1531	V1431	D1319	R1105	I996	I996
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	E997	E997
	GLY		GLY	GLY	THR	ALA	ASP	W1731	L1626	E1531	V1431	D1319	G1105	V998	V998
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	D1001	D1001
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	Q1002	Q1002
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	H1003	H1003
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	W1004	W1004
	GLY		GLY	GLY	THR	ALA	ASP	E1731	L1626	E1531	V1431	D1319	G1105	V1005	V1005



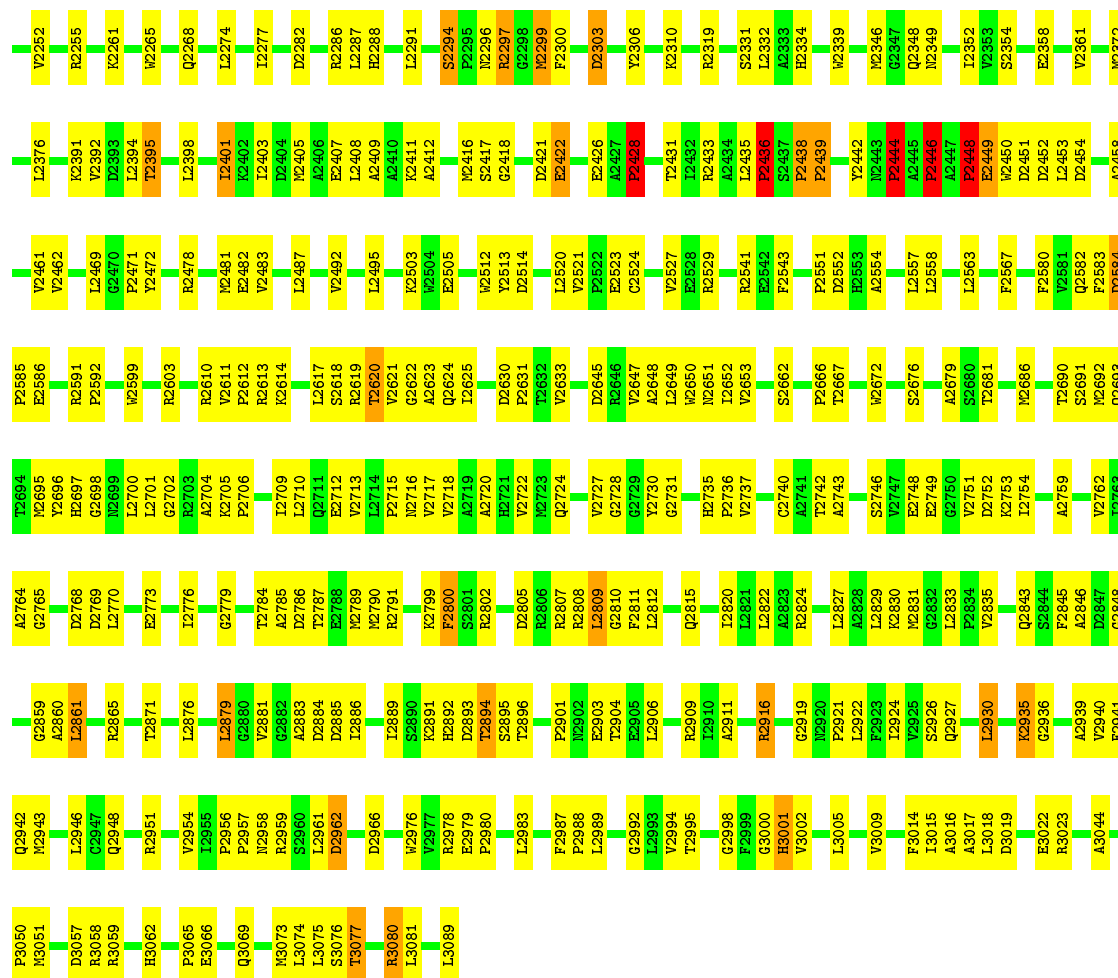


• Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain F: 56% 32% 9%



E2128	V2032	SER	ARG	ASP	ALA	P1580	H4484	H1394	P1288	L1185	L1091	S991	D887	L787
E2129	T2047	ALA	THR	GLY	ALA	F1581	H1485	H1394	A1290	L1188	A1092	T992	I892	A790
Y2134		ASP	VAL	ALA	PRO	H582	D1486	N1399	T1291	L1188	P1093	I996	T895	E791
E2137	A2053	VAL	GLY	SER	ALA	L1586	V1488	P1400	L1292	R1191	T1094	L996	T895	A792
V2140	A2054	ASP	PRO	ARG	ALA	V1590	P1489	T1401	K1304	F1192	T1096	V998	A896	R793
V2141	F2056	LYS	GLY	ARG	ALA		R1490	A1405	D1307	A1193	V1097	D1001	A899	L794
T2163	T2059	ILE	LYS	ASN	ALA	E1598	D1491	A1405	Q1308	I1194	Q1002	Q1002	G900	H795
V2164	W2060	ASP	ARG	LEU	ALA	K1605	S1496	V1408	V1309	R1195	P1099	H1003	I901	P796
A2165	ALA	ALA	VAL	LEU	VAL			V1408	D1310	R1197	D1100	V1004	V797	Q797
A2166	L2067	VAL	TYR	ASP	ALA	I1611	L1500	H1412	F1311		V1103	V1005	V904	D798
T2167		ALA	ILE	LEU	ALA	G1612		P1413	R1312	A1212	G1104	F915	F799	
R2170	E2074	ALA	THR	GLY	PRO	R1613	I1503	D1414	V1313	L1203	R1105	V1008	F915	E803
D2173	Q2081	ARG	LYS	LEU	ALA	F1614	R1504	G1415	D1314	T1204	C1106	P1009	L924	A808
E2175	E2082	GLY	THR	GLY	PRO	R1615	R1504	G1416	D1315	D1205	V1110	S1011	A928	
L2176	Q2084	ILE	TRP	ALA	ALA	I1616	V1507	L1417	V1316	P1206	F1111	G1012	A928	D811
K2180	L2085	ALA	GLY	LEU	ALA	P1616	Q1507	T1420	G1317	V1207	V1111	T1013	E929	
R2188	S2086	VAL	THR	ASN	SER	H1617	I1508	Q1421	I1318		A1117	W1014	P830	
F2189	R2088	LEU	LYS	LEU	GLY	V1619	D1511	F1422	D1319	A1212	A1118		V931	L816
T2192	F2089	PRO	THR	ALA	ILE			T1423	E1323	T1218	A1119	I1017	E932	E817
L2193	E2090	GLY	GLY	GLY	ALA	L1623	D1514	Q1424	V1324	D1219	T1119	R1018	V933	
L2194	G2091	ALA	ALA	THR	ALA	L1625	V1519	V1425	L1325	T1220	E1120	F1019	L934	L826
L2195	L2092	GLY	LYS	ASP	PRO			V1430	E1326	V1228	F1123	T1020	S835	L827
L2196	G2093	ALA	ALA	ASP	ALA			A1431	V1327		F1124	L1021	R836	
L2197	R2094	ALA	VAL	GLY	ALA			A1431	S1328	R1225	V1125	L1021	R937	D832
L2198	V2096	GLY	THR	LEU	ALA			A1448	A1338	R1226	I1126	Q938	E833	A833
L2199	A2097	GLY	LYS	THR	ALA			A1448	A1339	D1227	E1127	A939	E834	
L2200	T2098	VAL	PHE	GLY	VAL			A1449	I1331	V1228	G1128	R940	R835	
D2205	Q2099	ASP	ALA	GLN	ALA			Q1441	V1336	P1233	L1129	G1028	R941	V836
L2209	R2101	S1983	GLY	THR	ILE			V1445	M1337		L1130	G1029	A953	V837
E2210	W2102	L1986	THR	LYS	ALA			V1455	A1337	M1236	S1131	A1030	A953	L838
E2211	Q2104	F1989	GLY	LEU	ALA			G1456	A1344	R1237	L1132	P1031	V956	H839
E2212	G2105	K1989	ARG	LEU	ALA			E1457	P1346	M1269	I1032	V1033	L957	P840
G2214	R2112	P1996	GLY	ASP	ALA			V1460	R1342	R1263	P1146	E1034	W958	L853
E2216	W2114	L2000	GLY	GLY	SER			A1461	L1343	L1268	K1147	V1035	A859	G854
K2229	E2115	Q2010	ASP	PRO	ILE			V1467	A1345	L1271	P1149	D1036	G960	R855
P2234	L2118	L2011	LEU	VAL	GLY			Y1468	F1352	A1274	E1151	A1038	R961	P856
T2235	F2119	G2012	GLY	LEU	ALA			E1469	P1363	Q1275	T1162	T1040	W964	F859
L2236	L2013	L2013	SER	LEU	PRO			A1470	A1462	A1275	D1163	A1041	W965	V860
L2237	I2122	S2014	ASP	ASP	THR			E1471	Q1357	Q1276	T1164	M1042	P866	P861
F2238	I2123	D2015	ALA	GLY	ALA			L1474	Q1358	H1277	G1167	A1044	V967	V862
R2244	A2124	V2016	ILE	ILE	ASP						R1177	V1077	I970	R868
V2245	G2125	W2016	GLY	ASN	GLY						N1178	T1084	A971	
A2246	E2127	P2020	ALA	LEU	ILE						A1179	P1090		
			ALA	LEU	THR						L1184		P990	A886



F2089	LEU	PRO	ALA	ASP	E1723	P1622	F1422	D1314	E1202	V1103	L996	A686	F783	W674	G583
G2090	SER	GLY	GLU	THR	F1623	F1623	T1423	R1315	L1203	G1105	E997	D837	E784	W674	H584
T2092	ALA	TRP	GLU	PHE	T1624	L1625	V1425	V1316	T1204	C1106	V998	I892	L787	G676	S585
G2093	LYS	ALA	ASP	ASP	L1625			I1318	D1205						S586
H2094	GLY	HIS	LEU	ALA	R1634		V1430	D1319	P1206	V1110	D1001	T895	A790	A680	W587
V2095	ALA	VAL	GLY	ALA	W1731		A1431	I1318	V1207	F1111	Q1002	A896	E791	A681	E588
V2096	SER	VAL	ALA	ASP	L1732		V1532	E1323	A1212	A1117	H1003	M882	A792	N682	D589
A2097	GLY	VAL	GLY	THR	S1734		V1435	V1324	A1212	A1118	V1004	A899	R793	G683	L590
T2098	GLY	LYS	LYS	THR	A1639		N1534	L1325	T1218	T1119	V1005	G900	L794	N684	L593
Q2099	VAL	PHE	GLY	VAL	R1736		F1535	E1326	T1219	E1120	I901	I901	H795	A685	L594
A2100	VAL	ALA	GLN	ALA	D1737		M1651	V1327	T1218		Y1008	S686	F796	S686	L594
W2101	ASP	LEU	VAL	LEU	W1652		V1445	S1328	T1220		P1009	W904	Q797	G687	L595
W2102	S1983	GLY	THR	ILE	L1741		V1445	V1328	P1221	F1123	L1010	F915	F799	R688	Y598
W2103	L1986	THR	LYS	ALA	D1745		A1448	R1330	R1225	P1124	S1011	F915	F799	D694	Y598
Q2104	L1986	ARG	LEU	LEU	P1657		S1540	I1449	R1226	V1125	G1012		E803	I695	R602
G2105	F1989	GLY	ALA	SER	K1658		Q1541	I1331	D1226	T1013	T1013	L924		H696	
		GLY	ARG	ALA	ASP		Y1542	V1336	D1227	E1127	W1014				
L2108	K1992	SER	THR	LYS	E1659		V1455	M1337	V1228	G1128	I1017	A928	A808		W606
R2112	P1996	VAL	LYS	ARG	G1661		G1456	A1338		L1129	F1018	E929		I698	
W2113		ARG	PRO	ILE	R1662		E1457	A1339	R1237		R1018	P930	D811		G613
V2114	L2000	GLY	PHE	ASP	K1663		Y1458	I1342	R1253	L1132	F1019	V931	L816	N700	G614
H2115		GLY	GLY	ASP	E1665		A1460	L1343		L1133	T1020	V932	E817	A701	P618
L2118	G2012	LEU	VAL	ILE	E1667		I1461	A1344	G1268	P1146	V1025	S935	L826		S621
G2125	L2013	GLY	GLY	GLU	L1668		E1555	A1345	M1269	E1148	E1035	R936	L827	A713	Y624
S2014	S2014	GLY	LEU	ALA			C1463	P1346	W1270	P1149	E1034	R937		A716	L625
L2122	P2015	SER	LEU	SER	W1671		V1464	A1350	D1271		Y1035	Q938	Y830		W629
A2123	V2016	LEU	ASP	ASP	F1672		E1557		V1279	E1151	D1036	R939	D832	V719	
L2124		HIS	ALA	SER	Q1673		V1467	P1353	A1274	F1152	D1037	R940	A833	K735	P636
G2125	A2124	ALA	ILE	ASP	R1561		Y1468		Q1276					P736	L637
A2126	P2020	GLY	ASN	GLU	R1562		E1469	L1357	Q1277	T1162	V1045	P954	D835	Y737	W638
E2127	A2126	ALA	ASP	SER	W1679		L1470	Q1358	H1277	D1163	L1046				
W2128	V2032	LEU	GLN	ILE	L1564		E1471		V1278	T1164	V1068	L957		T745	D641
L2128		ALA	LEU	THR	D1684		L1474	M1362	T1280	G1167	T1069			Y746	G642
A2123	T2047	SER	ARG	ASP	L1685				A1281	R1168	V1070	R961	L853	L747	L643
L2124		ALA	VAL	GLY	L1686		V1579	V1376	T1282		W1072	M962	G854	Q748	L644
E2137	V2054	ASP	LEU	SER	F1687		P1580	A1380	D1283	P1171	W1072	S963	R855	W749	
V2140	V2065	VAL	GLY	SER	E1690		H1582	D1381	G1284	P1172	V1077	N965	N857	L750	T647
V2141	D2057	LYS	SER	ARG			L1586		P1286	S1173		P966	N858	R751	
T2163	D2058	VAL	GLY	ASN	L1695		D1486	F1390	V1287	V1174	T1084	P967	F853		E654
W2163	R2059	ILE	LYS	GLY			T1487	S1391	P1288	R1177		I970	W860	L756	A655
L2164	W2060	ASP	ARG	LEU			P1488	P1400	P1289	N1178	G1088	A971		S763	T656
A2165	L2067	ALA	VAL	VAL	E1701		R1490	P1400	K1291	A1179	G1088		W862		T657
E2166		ALA	TTR	ASP	E1702		D1491	A1405	L1292	A1089	A1089				S658
T2167	L2070	ALA	ILE	ALA	I1703		K1605			L1184	P1090	T974	R868	D766	V661
R2170	E2074	VAL	THR	GLY	G1704		R1495	V1408	W1295	L1185	L1091	E975		T767	K662
Q2081		ALA	ARG	LEU	V1705		S1496		K1304		A1092	W976	R872	K768	G663
D2173	Q2081	ALA	VAL	LEU	K1706		R1613	P1413		L1188	P1093	Q977	S873	L775	L664
E2174	W2082	ARG	THR	ASN			L1615	D1414	D1307	R1191	L1095	N978	D874	D776	L665
L2176	Q2083	ARG	LYS	LEU	V1711		P1616	Q1308		F1192	T1096	E980	R875	I777	V666
L2176	Q2084	GLY	GLY	GLY	A1712		W1617	V1416	V1309	A1193	V1097		L876	T778	G667
K2180	S2085	ILE	TRP	ALA	G1713		L1618	L1618	D1310	I1194	V1098	H989	H877	W779	T668
	S2086	SER	GLU	ILE	L1714		V1619	L1417	F1311	R1195	P1099	P990	H880	W780	R669
Q2087	Q2087	LEU	LEU	ASP	L1714		P1620	T1420	R1312	G1196	D1100			D781	G670
R2088	E2088	SER	GLY	GLY	P1722		R1621	Q1421	V1313	R1197		T992	E885	R782	T671

F2189	M2299	E2426	V2521	D2630	A2719	S2801	H2892	E2979
F2192	F2300	E2427	P2522	P2631	A2720	R2802	D2893	P2980
L2193	D2303	P2428	E2523	V2632	E2721	D2805	T2894	L2983
V2194	C2524	P2428	E2524	V2633	V2722	D2806	S2895	L2983
V2195	Y2306	T2431	E2525	D2645	M2723	R2807	T2896	F2987
V2196	K2310	L2432	L2526	E2646	Q2724	R2808	P2901	P2988
F2197	K2319	L2433	V2527	V2647	V2727	L2809	E2902	G2992
A2198	R2319	L2435	E2528	A2648	G2728	G2810	E2903	L2993
D2205	S2331	P2436	Y2530	L2649	G2729	F2811	L2906	V2994
L2209	S2332	S2437	A2533	M2650	G2730	L2812	T2995	T2995
V2210	L2332	P2438	L2534	L2651	G2731	Q2815	R2909	G2998
E2211	A2333	P2439	R2541	V2652	H2735	I2820	I2910	F2999
V2212	H2334	Y2442	E2542	V2653	P2736	L2821	A2911	G3000
V2213	V2339	R2443	P2543	S2662	V2737	L2822	R2916	H3001
G2214	V2339	P2444	P2551	P2666	C2740	A2823	G2919	V3002
T2215	M2346	L2445	D2552	T2667	A2741	R2824	V3019	G3003
E2216	G2347	P2446	H2553	V2672	T2742	L2827	H2920	G3004
K2229	Q2348	P2448	A2554	V2673	A2743	A2828	P2921	L3005
P2234	M2349	E2449	L2557	H2674	S2746	L2829	L2922	V3009
T2235	I2352	D2450	L2558	S2675	V2747	K2830	I2924	F3014
L2236	S2354	D2451	L2563	S2676	E2748	M2831	V2925	I3015
L2237	E2358	D2452	L2567	A2679	G2750	L2833	S2926	A3016
F2238	E2358	D2454	F2567	S2680	V2751	P2834	Q2927	A3017
R2244	V2361	A2458	F2580	T2681	K2752	L2835	L2930	L3018
V2245	M2372	V2461	V2581	M2686	I2754	Q2843	K2935	D3019
A2246	L2376	V2462	Q2582	T2690	A2759	S2844	G2936	E3022
V2252	L2376	L2469	P2583	S2691	V2762	F2845	A2939	R3023
R2255	K2391	G2470	D2585	M2692	I2763	A2846	V2940	A3044
K2261	V2392	P2471	E2586	Q2693	A2764	D2847	F2941	P3050
V2265	D2393	Y2472	R2591	M2695	G2765	G2848	Q2942	M3051
Q2268	L2394	R2478	P2592	L2696	D2768	G2859	L2946	R3058
L2274	T2395	M2481	V2599	H2697	D2769	A2860	C2947	R3059
I2277	L2401	E2482	R2603	G2698	L2770	L2861	Q2948	P3065
D2282	R2402	V2483	R2610	I2700	E2773	R2865	R2951	Q3069
R2286	A2408	L2495	G2611	L2701	I2776	T2871	V2954	M3073
L2287	A2409	K2503	V2612	G2702	I2779	L2876	I2955	L3074
H2288	A2412	M2504	R2613	A2704	G2779	L2879	P2956	L3075
L2291	M2416	E2505	R2619	P2706	T2784	G2880	N2957	S3076
S2294	S2417	G2512	T2620	I2709	A2785	V2881	N2958	T3077
P2295	G2418	G2622	V2621	L2710	T2786	G2882	S2959	R3080
N2296	D2421	Q2624	G2622	L2711	T2787	A2883	S2960	L3081
R2297	E2422	D2514	A2623	E2712	M2789	D2885	D2962	L3089
G2298		L2520	Q2625	L2713	R2791	I2886	D2966	
				P2715	K2799	I2889	W2976	
				N2716	F2800	S2890	V2977	
				L2625		K2891	R2978	

• Molecule 1: TYPE-I FATTY ACID SYNTHASE

Chain B:  57% 31% 9%

MET	S88	A180	D288	V376	I485
THR	E89	L181	P289	F377	Q486
ILE	L90	A182	V292	R381	F487
GLU	R94	Q183	V293	Q384	N488
ASP	P95	L194	E294	R389	T489
ARG	A106	R195	L301	V390	L490
VAL	L107	I198	I305	V393	Q500
PRO	E111	G202	D203	V394	K504
GLY	P112	R204	R204	E395	R505
TRP	V113	P205	P205	W400	Q508
ASN	K117	P206	W311	P405	R511
ASP	Q118	M207	T314	P405	A515
SER	L119	V208	V315	T406	P516
SER	V126	S209	G316	V407	I517
ASP	P127	V210	L317	V408	D518
ARG	V129	T211	E327	L410	V521
THR	Q133	L222	I328	P411	V522
ALA	V137	V232	L330	D412	S523
ASP	R138	L233	W336	L417	I526
ASN	A141	V236	E339	T419	D534
ALA	R142	L237	T341	K420	
ALA	Q143	S238	T342	L424	
GLY	G144	I248	E342	E338	I539
ASN	M145	T249	R343	N540	E541
ASP	D146	G250	H344	V542	G543
ASP	L147	T251	A348	I544	S545
ASP	T148	L255	R349	H546	
L38	A149	S256	I351	P436	F549
	T150	R257	L352	P437	K550
	P151	L260	D353	T438	P551
	P152	A266	L354	V440	S559
	V155	E267	G355	D441	V560
	Q160	K268	P356	E456	I563
	L163	E269	G357	Q462	H575
	A164	E270	L360	F468	I576
	A167	E272	R361	L475	R580
	S53	R273	R362	E476	G583
	L56	K276	L363	L479	H584
	K171	L277	T364		H585
	G172	R278	A365		S586
	A173	G279	P366		W587
	E71	G280	V367		
	K174	I368	K369		
	D175	A281	R369		
	V176	V282	I373		
	E177	V286	G374		
	E84	F287	I375		
P85	L479	A484			

LEU	PRO	ALA	ASP	LEU723	TI624	LI530	VI430	DI319	AI212	AI117	VI004	A899	E791	A681	E588
PRO	GLY	ALA	ILE	YI724	LI625	LI531	AI431	EL323	TI218	AI118	VI005	G900	A792	M652	D699
ALA	ALA	ALA	PRE	SI725	LI634	LI532	AI431	EL324	DI219	TI119	VI008	I901	L794	G683	L590
GLY	LYS	ASP	ASP	EL730	VI637	LI533	VI435	LI325	LI220	EL120	P1009	V904	H795	A685	L593
LYS	GLY	LEU	ALA	VI731	VI638	LI534	Q1441	EL326	P1221	F1123	S1011	F915	P796	S686	L594
VAL	THR	ALA	ASP	LI732	LI639	LI535	VI445	VI327	LI225	VI125	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	MI733	LI639	LI536	VI445	LI328	LI226	LI126	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	SI734	LI639	LI537	VI445	LI329	LI227	LI127	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	EL735	LI639	LI538	VI445	LI330	LI228	LI128	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	RI736	LI639	LI539	VI445	LI331	LI229	LI129	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	DI737	LI639	LI540	VI445	LI332	LI230	LI130	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	LI741	LI639	LI541	VI445	LI333	LI231	LI131	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	DI745	LI639	LI542	VI445	LI334	LI232	LI132	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	THR	LI640	LI543	VI445	LI335	LI233	LI133	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ASP	LI641	LI544	VI445	LI336	LI234	LI134	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	PRO	LI642	LI545	VI445	LI337	LI235	LI135	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	GLY	LI643	LI546	VI445	LI338	LI236	LI136	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	THR	LI644	LI547	VI445	LI339	LI237	LI137	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI645	LI548	VI445	LI340	LI238	LI138	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI646	LI549	VI445	LI341	LI239	LI139	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI647	LI550	VI445	LI342	LI240	LI140	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI648	LI551	VI445	LI343	LI241	LI141	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI649	LI552	VI445	LI344	LI242	LI142	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI650	LI553	VI445	LI345	LI243	LI143	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI651	LI554	VI445	LI346	LI244	LI144	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI652	LI555	VI445	LI347	LI245	LI145	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI653	LI556	VI445	LI348	LI246	LI146	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI654	LI557	VI445	LI349	LI247	LI147	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI655	LI558	VI445	LI350	LI248	LI148	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI656	LI559	VI445	LI351	LI249	LI149	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI657	LI560	VI445	LI352	LI250	LI150	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI658	LI561	VI445	LI353	LI251	LI151	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI659	LI562	VI445	LI354	LI252	LI152	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI660	LI563	VI445	LI355	LI253	LI153	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI661	LI564	VI445	LI356	LI254	LI154	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI662	LI565	VI445	LI357	LI255	LI155	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI663	LI566	VI445	LI358	LI256	LI156	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI664	LI567	VI445	LI359	LI257	LI157	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI665	LI568	VI445	LI360	LI258	LI158	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI666	LI569	VI445	LI361	LI259	LI159	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI667	LI570	VI445	LI362	LI260	LI160	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI668	LI571	VI445	LI363	LI261	LI161	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI669	LI572	VI445	LI364	LI262	LI162	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI670	LI573	VI445	LI365	LI263	LI163	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI671	LI574	VI445	LI366	LI264	LI164	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI672	LI575	VI445	LI367	LI265	LI165	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI673	LI576	VI445	LI368	LI266	LI166	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI674	LI577	VI445	LI369	LI267	LI167	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI675	LI578	VI445	LI370	LI268	LI168	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI676	LI579	VI445	LI371	LI269	LI169	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI677	LI580	VI445	LI372	LI270	LI170	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI678	LI581	VI445	LI373	LI271	LI171	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI679	LI582	VI445	LI374	LI272	LI172	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI680	LI583	VI445	LI375	LI273	LI173	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI681	LI584	VI445	LI376	LI274	LI174	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI682	LI585	VI445	LI377	LI275	LI175	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI683	LI586	VI445	LI378	LI276	LI176	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI684	LI587	VI445	LI379	LI277	LI177	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI685	LI588	VI445	LI380	LI278	LI178	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI686	LI589	VI445	LI381	LI279	LI179	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI687	LI590	VI445	LI382	LI280	LI180	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI688	LI591	VI445	LI383	LI281	LI181	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI689	LI592	VI445	LI384	LI282	LI182	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI690	LI593	VI445	LI385	LI283	LI183	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI691	LI594	VI445	LI386	LI284	LI184	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI692	LI595	VI445	LI387	LI285	LI185	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI693	LI596	VI445	LI388	LI286	LI186	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI694	LI597	VI445	LI389	LI287	LI187	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI695	LI598	VI445	LI390	LI288	LI188	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI696	LI599	VI445	LI391	LI289	LI189	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI697	LI600	VI445	LI392	LI290	LI190	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI698	LI601	VI445	LI393	LI291	LI191	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI699	LI602	VI445	LI394	LI292	LI192	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI700	LI603	VI445	LI395	LI293	LI193	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI701	LI604	VI445	LI396	LI294	LI194	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI702	LI605	VI445	LI397	LI295	LI195	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI703	LI606	VI445	LI398	LI296	LI196	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI704	LI607	VI445	LI399	LI297	LI197	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI705	LI608	VI445	LI400	LI298	LI198	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI706	LI609	VI445	LI401	LI299	LI199	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI707	LI610	VI445	LI402	LI300	LI200	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI708	LI611	VI445	LI403	LI301	LI201	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI709	LI612	VI445	LI404	LI302	LI202	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI710	LI613	VI445	LI405	LI303	LI203	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI711	LI614	VI445	LI406	LI304	LI204	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI712	LI615	VI445	LI407	LI305	LI205	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI713	LI616	VI445	LI408	LI306	LI206	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI714	LI617	VI445	LI409	LI307	LI207	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI715	LI618	VI445	LI410	LI308	LI208	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI716	LI619	VI445	LI411	LI309	LI209	G1012	I915	Q797	G687	L595
GLY	ALA	LEU	ASP	ALA	LI717	LI620	VI445	LI412	LI310	LI210	G1012	I915	Q797	G687	L595
GLY	ALA	LEU													



SER	VAL	GLU	ILE	ARG	L1719	L14625	L1530	V1425	E1323	A1212	A1117	H1003	A899	A790	A680	W587	R483
VAL	SER	LEU	ASP	PRO	P1722	F1629	E1531	V1430	E1324	T1218	A1118	V1004	A898	E791	A681	E588	A484
SER	LEU	PRO	ALA	ASP	E1723	F1629	V1532	V1431	V1325	T1219	A1119	V1005	A899	A792	B682	D589	I485
SER	TRP	GLY	ALA	ILE	Y1724	I1633	N1533	A1431	L1325	D1219	E1120	V1008	I901	R793	G683	L590	I486
ALA	ALA	ALA	ALA	THR	S1725	R1634	N1534	V1435	E1326	T1220	E1121	P1009	W04	H794	B684	L593	F487
ALA	LYS	ALA	ALA	PHE	E1730	V1637	N1536	Q1441	E1328	D1221	F1123	L1010	F915	H795	A685	L594	I488
GLY	GLY	HIS	LEU	ASP	V1731	P1638	L1537	Q1442	A1329	R1225	F1124	S1011	F915	P796	S686	L595	I489
SER	ALA	VAL	ALA	ALA	L1732	A1639	G1539	V1445	R1330	D1226	V1125	G1012	L924	D797	G687	L596	L490
GLY	GLY	VAL	LEU	ALA	N1733	A1639	G1539	V1445	I1331	D1227	V1126	T1013	L924	F799	B688	L596	
GLY	GLY	VAL	LEU	THR	S1734	T1651	Q1541	A1448	V1336	V1228	G1128	W1014	L924	F799	B688	L596	
VAL	VAL	PHE	GLY	VAL	E1735	W1652	Y1542	T1449	M1337	R1237	E1127	W1014	L924	F799	B688	L596	
VAL	VAL	ALA	GLN	LEU	R1736	K1656	A1543	A1450	A1338	R1237	G1129	L1017	L924	F799	B688	L596	
ASP	ASP	LEU	VAL	LEU	D1737	P1657	I1544	V1455	A1339	R1237	E1129	L1017	L924	F799	B688	L596	
S1983		GLY	THR	ILE	L1741	K1658	E1551	V1455	A1339	R1237	E1129	L1017	L924	F799	B688	L596	
L1986		THR	LYS	ALA	D1745	E1659	E1552	T1459	R1342	R1237	E1129	L1017	L924	F799	B688	L596	
F1989		GLU	LEU	LEU	THR	K1660	A1553	T1459	L1343	R1237	E1129	L1017	L924	F799	B688	L596	
K1992		ARG	ALA	SER	ASP	G1661	E1554	A1460	A1344	R1237	E1129	L1017	L924	F799	B688	L596	
P1996		THR	ALA	ALA	THR	K1663	E1556	A1462	A1346	R1237	E1129	L1017	L924	F799	B688	L596	
		VAL	LYS	MET	GLU	E1557	E1557	V1464	Y1350	R1237	E1129	L1017	L924	F799	B688	L596	
		ARG	PRO	ARG	PRO	I1666	R1560	V1467	A1351	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	GLU	ASP	GLU	E1667	E1561	Y1468	F1352	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	PHE	ASP	PRO	L1668	E1562	E1469	P1353	R1237	E1129	L1017	L924	F799	B688	L596	
		ASP	GLY	GLN	GLU	W1671	R1562	E1469	L1357	R1237	E1129	L1017	L924	F799	B688	L596	
		LEU	PRO	ILE	ALA	A1672	Q1563	L1470	I1358	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	VAL	GLU	ASP	F1673	I1564	E1471	Q1358	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	LEU	ALA	GLU	A1674	D1578	L1474	H1359	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	SER	LEU	PRO		D1579	L1474	K1360	R1237	E1129	L1017	L924	F799	B688	L596	
		LEU	THR	ASP	THR		F1579	L1474	K1361	R1237	E1129	L1017	L924	F799	B688	L596	
		HIS	ALA	SER	ALA		P1580	R1480	M1362	R1237	E1129	L1017	L924	F799	B688	L596	
		ALA	ILE	ILE	ASP		F1581	K1483	V1376	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	ASN	GLY	ALA		H1582	M1484	A1380	R1237	E1129	L1017	L924	F799	B688	L596	
		LEU	ASP	ALA	PRO		S1583	H1485	A1380	R1237	E1129	L1017	L924	F799	B688	L596	
		LEU	GLN	ILE	ALA		L1586	H1485	A1380	R1237	E1129	L1017	L924	F799	B688	L596	
		ALA	LEU	THR	GLU		F1687	D1488	P1286	R1237	E1129	L1017	L924	F799	B688	L596	
		SER	ARG	ASP	ALA		V1590	I1487	F1390	R1237	E1129	L1017	L924	F799	B688	L596	
		ALA	THR	GLY	ALA		E1690	E1488	D1398	R1237	E1129	L1017	L924	F799	B688	L596	
		VAL	VAL	ALA	PRO		E1598	P1489	N1399	R1237	E1129	L1017	L924	F799	B688	L596	
		ASP	LEU	SER	ALA		G1694	R1490	P1400	R1237	E1129	L1017	L924	F799	B688	L596	
		VAL	ALA	ALA	ALA		L1695	D1491	P1400	R1237	E1129	L1017	L924	F799	B688	L596	
		ASP	PRO	ARG	ALA		K1605	R1495	A1405	R1237	E1129	L1017	L924	F799	B688	L596	
		LYS	SER	ARG	ALA		D1606	S1496	V1408	R1237	E1129	L1017	L924	F799	B688	L596	
		VAL	GLY	ASN	ALA		P1607	S1496	V1408	R1237	E1129	L1017	L924	F799	B688	L596	
		ILE	LYS	GLN	PRO		I1611	I1503	D1307	R1237	E1129	L1017	L924	F799	B688	L596	
		ASP	ARG	LEU	ALA		G1612	R1504	Q1308	R1237	E1129	L1017	L924	F799	B688	L596	
		GLY	PRO	LEU	PRO		P1505	P1505	V1309	R1237	E1129	L1017	L924	F799	B688	L596	
		ALA	ALA	VAL	VAL		S1506	S1506	D1310	R1237	E1129	L1017	L924	F799	B688	L596	
		TYR	ALA	ASP	ALA		P1616	Q1507	D1414	R1237	E1129	L1017	L924	F799	B688	L596	
		ILE	LEU	LEU	ALA		N1617	Q1507	F1311	R1237	E1129	L1017	L924	F799	B688	L596	
		THR	GLY	GLY	PRO		L1618	I1508	R1312	R1237	E1129	L1017	L924	F799	B688	L596	
		ARG	LEU	SER	ALA		V1619	V1508	L1417	R1237	E1129	L1017	L924	F799	B688	L596	
		ALA	GLY	LEU	ALA		P1620	D1511	L1417	R1237	E1129	L1017	L924	F799	B688	L596	
		VAL	LEU	LEU	ALA		R1621	D1511	T1420	R1237	E1129	L1017	L924	F799	B688	L596	
		ARG	THR	ASN	PRO		F1622	D1514	Q1421	R1237	E1129	L1017	L924	F799	B688	L596	
		LYS	THR	LEU	SER		F1622	D1514	Q1421	R1237	E1129	L1017	L924	F799	B688	L596	
		THR	GLY	GLY	GLY		F1622	D1514	Q1421	R1237	E1129	L1017	L924	F799	B688	L596	
		THR	GLY	GLY	GLY		F1622	D1514	Q1421	R1237	E1129	L1017	L924	F799	B688	L596	
		TRP	ALA	ALA	PRO		T1624	D1519	Q1424	R1237	E1129	L1017	L924	F799	B688	L596	



M3073	M3074	L3075	S3076	T3077	R3080	L3081	L3089	N2958	R2959	S2960	L2961	D2962	D2966	V2976	V2977	R2978	E2979	P2980	L2983	F2987	P2988	L2989	G2992	L2993	V2994	T2995	G2998	F2999	G3000	H3001	V3002	L3005	V3009	F3014	I3015	A3016	A3017	L3018	D3019	E3022	R3023	A3044	P3050	M3051	D3057	R3058	R3059	H3062	P3065	E3066	Q3069	D2786	T2787	E2788	M2789	M2790	R2791	K2799	F2800	S2801	R2802	D2805	R2806	R2807	T2808	P2901	V2902	E2903	L2906	R2909	I2910	A2911	R2916	G2919	N2920	P2921	L2922	I2924	V2925	S2926	Q2927	L2930	K2935	G2936	A2939	V2940	F2941	Q2942	M2943	L2946	C2947	Q2948	R2951	V2954	I2955	P2957	D2776	T2777	E2778	M2779	G2780	A2855	P2856	G2859	A2860	L2861	R2865	T2871	L2876	L2879	Q2711	E2712	V2713	L2714	P2715	N2716	V2717	V2718	A2719	A2720	H2721	V2722	M2723	Q2724	V2727	G2728	G2729	L2730	G2731	H2735	P2736	V2737	C2740	A2741	T2742	A2743	S2746	V2747	E2748	E2749	G2750	V2751	D2752	K2753	I2754	K2758	A2759	M2692	Q2693	T2694	M2695	E2697	G2698	M2699	L2700	L2701	G2702	R2703	A2704	K2705	P2706	I2709	L2710	S2618	R2619	T2620	V2621	G2622	A2623	Q2624	L2625	D2630	A2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	M2650	N2651	I2652	V2653	S2662	T2665	P2666	T2667	M2672	S2676	A2679	S2680	T2681	M2686	T2690	S2691	M2692	Q2693	T2694	M2695	E2697	G2698	M2699	L2700	L2701	G2702	R2703	A2704	K2705	P2706	I2709	L2710	E2505	M2512	Y2513	L2520	V2521	F2522	E2523	C2524	E2525	L2526	V2527	E2528	R2529	Y2530	A2533	R2541	E2542	F2543	P2551	D2552	H2553	A2554	S2555	P2556	L2557	L2558	L2563	F2567	E2574	F2580	V2581	Q2582	F2583	D2584	P2585	E2586	R2591	P2592	M2481	E2482	V2483	L2487	D2492	L2495	K2503	M2504	M2416	S2417	G2418	D2421	E2422	E2426	A2427	P2428	T2431	L2432	R2433	L2435	P2436	S2437	L2438	P2439	Y2442	N2443	P2444	A2445	P2446	A2447	P2448	E2449	V2450	D2451	D2452	L2453	D2454	A2458	V2461	V2462	L2469	G2470	P2471	Y2472	R2478	M2481	E2482	V2483	L2487	D2492	L2495	K2503	M2504	N2296	R2297	G2298	M2299	F2300	D2303	Y2306	K2310	R2319	K2324	E2328	S2331	L2332	H2334	M2339	M2346	G2347	Q2348	N2349	T2352	L2352	V2353	S2354	R2244	V2245	A2246	V2252	R2255	K2261	M2265	Q2268	L2274	T2277	R2286	L2287	H2288	L2291	S2294	P2295	L2176	K2180	R2188	F2189	T2192	L2193	M2194	V2195	P2197	A2198	D2205	L2209	V2210	E2211	M2212	V2213	G2214	E2215	E2216	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	V2096	A2097	Q2098	Q2099	A2100	N2101	H2102	M2103	Q2104	G2105	L2108	R2112	N2113	V2114	H2115	L2118	F2119	I2122	A2123	A2124	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	T2163	V2164	I2165	A2166	L2167	R2170	D2173	D2174	R2175	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9136	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	B	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	C	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	D	0.41	26/18511 (0.1%)	0.50	13/25179 (0.1%)
1	E	0.39	26/21335 (0.1%)	0.51	13/29037 (0.0%)
1	F	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
All	All	0.40	160/125186 (0.1%)	0.51	78/170364 (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	5
1	B	0	5
1	C	0	5
1	D	0	2
1	E	0	5
1	F	0	5
All	All	0	27

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2442	TYR	CB-CG	-6.39	1.42	1.51
1	A	2442	TYR	CB-CG	-6.35	1.42	1.51
1	B	2442	TYR	CB-CG	-6.35	1.42	1.51
1	D	2442	TYR	CB-CG	-6.33	1.42	1.51
1	F	2442	TYR	CB-CG	-6.33	1.42	1.51

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	930	PRO	N-CA-CB	6.99	111.69	103.30
1	C	930	PRO	N-CA-CB	6.98	111.68	103.30
1	F	930	PRO	N-CA-CB	6.97	111.66	103.30
1	A	930	PRO	N-CA-CB	6.96	111.66	103.30
1	D	930	PRO	N-CA-CB	6.96	111.65	103.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1148	GLU	Peptide
1	D	2584	ASP	Peptide
1	E	150	THR	Peptide
1	E	202	GLY	Peptide
1	E	357	GLY	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	20945	0	20595	882	0
1	B	20945	0	20595	872	0
1	C	20945	0	20595	896	0
1	D	18171	0	17756	765	0
1	E	20945	0	20595	882	0
1	F	20945	0	20594	1028	0
2	A	31	0	19	4	0
2	B	31	0	19	4	0
2	C	31	0	19	4	0
2	D	31	0	19	4	0
2	E	31	0	19	4	0
2	F	31	0	19	4	0
All	All	123082	0	120844	4979	0

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 20.

The worst 5 of 4979 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1039:ALA:HB2	1:F:1125:VAL:CG1	1.35	1.53
1:F:958:TRP:CH2	1:F:1131:SER:OG	1.76	1.38
1:F:1385:ARG:NH1	1:F:2411:LYS:NZ	1.74	1.36
1:F:953:ALA:CB	1:F:1032:ILE:HD11	1.58	1.33
1:F:2407:GLU:O	1:F:2411:LYS:HG3	1.26	1.29

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	25	68
1	B	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	28	71
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	25	68
1	D	2448/3089 (79%)	2293 (94%)	138 (6%)	17 (1%)	25	68
1	E	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	28	71
1	F	2818/3089 (91%)	2630 (93%)	163 (6%)	25 (1%)	20	63
All	All	16538/18534 (89%)	15490 (94%)	932 (6%)	116 (1%)	30	68

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	930	PRO
1	D	1148	GLU
1	D	2428	PRO
1	D	2436	PRO
1	D	2446	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	2096 / 2402 (87%)	1994 (95%)	102 (5%)	29	61
1	B	2096 / 2402 (87%)	1993 (95%)	103 (5%)	29	61
1	C	2095 / 2402 (87%)	1993 (95%)	102 (5%)	29	61
1	D	1808 / 2402 (75%)	1720 (95%)	88 (5%)	29	61
1	E	2097 / 2402 (87%)	1995 (95%)	102 (5%)	29	61
1	F	2097 / 2402 (87%)	1992 (95%)	105 (5%)	28	60
All	All	12289 / 14412 (85%)	11687 (95%)	602 (5%)	33	61

5 of 602 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	2446	PRO
1	A	1162	THR
1	C	1662	ARG
1	F	2809	LEU
1	A	361	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	2334	HIS
1	A	1276	GLN
1	C	1617	ASN
1	F	2651	ASN
1	A	386	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
2	FMN	A	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.51	6 (15%)
2	FMN	B	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	C	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.49	6 (15%)
2	FMN	D	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.52	6 (15%)
2	FMN	E	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	F	4000	-	31,33,33	1.34	4 (12%)	38,50,50	1.50	6 (15%)

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
2	FMN	A	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	B	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	C	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	D	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	E	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	F	4000	-	-	0/16/18/18	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C5A-N5	2.27	1.38	1.35
2	E	4000	FMN	C5A-N5	2.31	1.38	1.35
2	A	4000	FMN	C5A-N5	2.31	1.38	1.35
2	F	4000	FMN	C5A-N5	2.32	1.38	1.35
2	C	4000	FMN	C5A-N5	2.35	1.38	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4000	FMN	C4A-C4-N3	-2.60	119.78	123.48
2	A	4000	FMN	C4A-C4-N3	-2.60	119.78	123.48
2	F	4000	FMN	C4A-C4-N3	-2.60	119.78	123.48
2	E	4000	FMN	C4A-C4-N3	-2.57	119.82	123.48
2	B	4000	FMN	C4A-C4-N3	-2.57	119.83	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	FMN	4	0
2	B	4000	FMN	4	0
2	C	4000	FMN	4	0
2	D	4000	FMN	4	0
2	E	4000	FMN	4	0
2	F	4000	FMN	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.