



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:30 PM BST

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 : 2013-04-18  
Resolution : 17.50 Å(reported)  
Based on PDB ID : 3ZEN

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

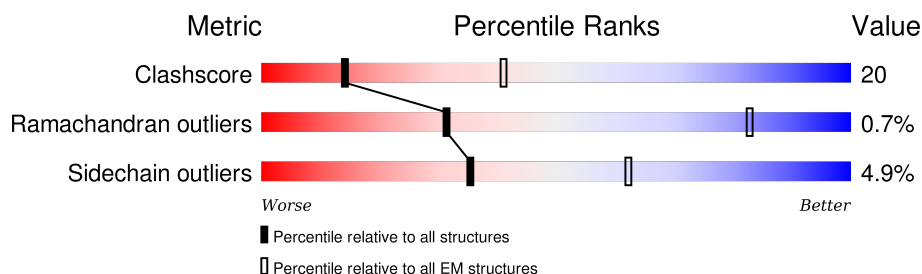
# 1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	57% 31% • 9%
1	B	3089	57% 31% • 9%
1	C	3089	57% 32% • 9%
1	D	3089	50% 27% • 21%
1	E	3089	57% 31% • 9%
1	F	3089	56% 32% • 9%

## 2 Entry composition [i](#)

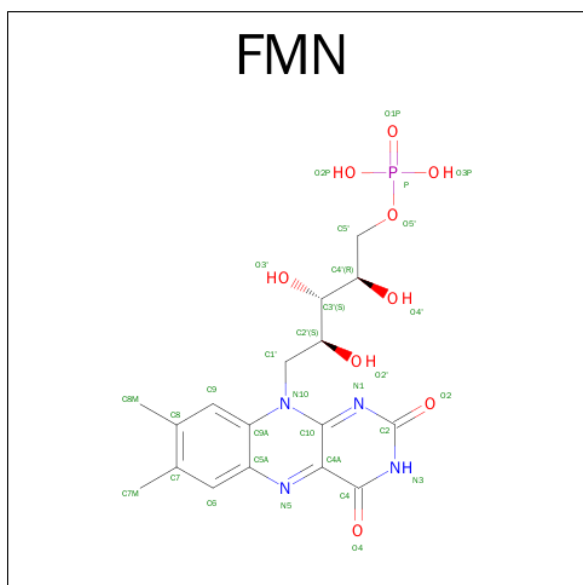
There are 2 unique types of molecules in this entry. The entry contains 123082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	

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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	








Response	Percentage
Yes	57%
No	31%
Don't know	9%



R2319	D2205	T2098	VAL	PHE	GLY	VAL	R1736	W1652	G1539	A1448	A1329	P1221	F1123	V1008	A899
S2331	L2209	Q2099	VAL	ALA	GLN	LEU	D1737	K1656	S1540	I1449	R1330	R1225	P1124	P1009	G900
L2332	V2210	A2100	GLY	LEU	THR	ILE	L1741	P1657	Y1542	A1450	I1331	Q1541	R1125	L1010	I901
A2333	E2211	W2102	THR	ARG	LYS	ALA	L1745	K1658	A1543	V1455	M1336	D1227	E1126	G1011	V904
E2334	W2212	Q2104	GLY	ARG	LEU	SER	D1745	E1659	I1544	G1456	M1337	V1228	E1127	G1012	F915
W2339	G2214	G2105	ALA	GLY	ALA	THR	ASP	L1660	L1551	E1457	A1338	R1237	G1128	T1013	
Q2348	K1992	L2108	THR	THR	THR	LYS	PRO	C1661	E1552	T1458	A1339		L1129	W1014	L924
L2352	P1996	R2112	VAL	VAL	ARG	PRO	GLU	K1663	A1553	T1459	R1342	R1253	V1132	I1017	I928
W2353	L2228	W2113	GLY	GLY	PRO	GLU	GLU	E1666	L1554	L1461	L1343	G1268	V1133	R1018	A928
S2354	K2229	E2114	GLY	GLY	PHE	ASP	PRO	E1667	E1556	A1462	A1344	M1269	T1020	F1019	E929
E2358	P2200	L2000	ASP	ASP	THR	GLU	GLU	L1668	E1557	G1463	P1346	W1270	K1147	T1021	E930
V2361	Q2010	H2115	ALA	ALA	ILE	ALA	ALA	W1671	R1560	V1464	Y1350	L1271	E1148	L1021	V931
W2372	L2011	L2118	LEU	LEU	VAL	GLU	ASP	G1672	R1561	Y1467	A1351	P1149	V1025	V933	
L2376	G2012	F2119	GLY	GLY	LEU	ALA	GLU	F1673	R1562	Y1468	A1350	A1274	P1150	R1018	R934
K2391	L2013	L2013	SER	SER	THR	LEU	PRO	A1674	Q1563	E1469	F1352	A1275	E1151	E1034	S935
W2392	S2014	S2014	HIS	ASP	ASP	ASP	ALA	W1679	I1564	E1471	P1353	Q1276	E1151	V1035	R936
D2393	L2015	I2122	ALA	ALA	ILE	ALA	ALA	F1687	S1583	G1484	G1284	H1277	T1162	D1036	R937
T2395	W2016	A2123	ALA	GLY	THR	GLY	PRO	E1690	L1586	H1485	A1380	P1286	V1172	T1037	Q938
L2401	P2020	G2125	LEU	ALA	ASP	ALA	ALA	D1684	P1580	R1480	Q1358	T1279	T1164	V1045	A939
W2402	W2082	E2127	LEU	LEU	GLN	ILE	ALA	L1685	F1581	R1480	H1362	T1280	G1167	L1046	R940
R2403	L2032	N2128	SER	SER	THR	ALA	ALA	F1687	H1582	K1483	V1376	T1282	R1168	L1046	R941
L2408	T2047	Y2134	ALA	ASP	THR	ALA	ALA	E1690	L1586	H1486	A1380	P1286	V1172	V1068	L957
A2412	A2053	E2137	VAL	VAL	GLY	SER	ALA	G1694	V1590	I1487	F1390	T1287	S1173	W1072	R961
M2416	W2054	W2140	ASP	ASP	PRO	ARG	ALA	L1695		V1488	P1400	P1288	V1174	W1072	R962
G2418	F2056	V2141	VAL	VAL	LYS	ARG	ALA	R1699	E1598	R1490	A1405	A1290	N1178	T1084	N965
D2421	R2059	T2163	ASP	ILE	GLN	ARG	ALA	V1701	K1605	D1491	A1405	L1292	A1179	F1087	P966
E2422	W2060	V2164	GLY	GLY	PRO	LEU	PRO	E1702	P1606	R1495	V1408	W1295	L1184	G1088	V967
P2427	L2067	I2165	ALA	VAL	THR	VAL	VAL	G1704	D1607	S1496	H1412	W1295	L1185	A1089	I970
R2428	L2070	A2166	ALA	VAL	ILE	ASP	ALA	V1705	G1612	I1503	P1413	K1304	L1188	P1090	A971
G2418	E2074	T2167	ALA	VAL	THR	ALA	ALA	K1706	R1613	R1504	D1414	D1307	R1191	A1092	T974
S2417	R2170	R2170	ALA	ALA	GLY	SER	ALA	T1710	Y1614	P1505	G1415	Q1307	R1191	P1093	E975
D2418	D2173	D2174	ARG	ARG	VAL	LEU	PRO	V1711	I1615	S1506	V1416	V1309	F1192	T1094	E976
E2422	Q2081	D2175	THR	THR	LYS	LEU	GLY	A1712	I1616	Q1507	L1417	D1310	F1192	L1095	Q977
L2291	Q2084	L2176	GLY	GLY	THR	GLY	GLY	G1713	H1617	I1508	T1420	F1311	R1195	T1096	Q978
S2294	L2085	L2176	ILE	ILE	THR	ALA	PRO	L1714	V1618	D1511	Q1421	R1312	G1196	V1098	E980
P2295	S2086	K2180	SER	SER	GLY	ILE	ARG	L1719	V1619	D1514	T1422	D1314	R1197	D1100	H989
W2296	Q2087	R2188	VAL	VAL	LEU	ASP	PRO	P1722	P1622	V1519	Q1424	R1315	E1202	V1103	P990
R2297	R2088	F2189	SER	SER	GLY	GLY	ASP	E1723	F1623	V1531	V1425	W1316	L1203	G1104	S991
G2298	Q2089	R2189	PRO	PRO	PRO	ALA	ILE	Y1724	L1624	E1531	V1430	G1317	T1204	R1105	T992
R2299	E2090	L2192	SER	THR	THR	GLU	THR	S1725	L1625	I1530	V1430	D1319	D1205	C1106	I996
F2300	G2091	T2192	ALA	ALA	ALA	ALA	PHE	E1730	R1634	V1532	A1431	D1319	P1206	V1207	V998
E2426	L2092	L2193	GLY	GLY	LYS	ASP	ASP	V1731	V1637	M1533	V1435	E1323	V1207	F1111	
A2427	H2094	W2194	VAL	GLY	HIS	LEU	ALA	E1731	P1637	N1534		V1324	A1212	D1001	D1001
P2428	W2095	V2195	THR	THR	GLY	LEU	ALA	L1732	P1638	F1535	Q1441	L1325	T1218	A1117	Q1002
T2431	V2306	D2197	SER	SER	THR	ALA	ASP	N1733	A1639	M1536	V1445	E1326	T1218	H1003	V1004
R2433	F2300	P2197	GLY	GLY	VAL	LEU	ALA	S1734	T1651	L1537		V1327	D1219	T1119	V1005
E2426	W2310	A2198	GLY	GLY	THR	THR	THR	E1735	T1651	R1537		V1327	T1220	F1420	





E2128	V2032	SER	ARG	ASP	ALA	P1580	H4484	P1288	L1185	L1091	S991	D887	L787
E2129	T2047	ALA	THR	GLY	ALA	F1581	H1485	A1290	L1188	A1092	T992	I892	A790
Y2134		ASP	VAL	ALA	PRO	H582	D1486	K1291		P1093	I996	T895	E791
	A2053	VAL	GLY	SER	ALA	L1586	V1488	L1292	R1191	T1094	L996	T895	A792
E2137	A2054	ASP	PRO	ARG	ALA	L1586	P1488	K1304	F1192	T1096	V998	A896	R793
V2140	V2055	LYS	SER	ARG	ALA	V1590	P1489	D1307	A1193	V1097	D1001	A899	L794
V2141	F2056	VAL	GLY	ASN	ALA	E1598	D1491	Q1308	I1194	V1098	Q1002	G900	H795
T2163	T2059	ILE	LYS	GLN	PRO	E1702	V1496	V1309	R1195	P1099	H1003	G900	P796
V2164	W2060	GLY	ARG	LEU	ALA	I1703	S1496	D1310	G1196	D1100	H1004	I901	T797
T2165	ALA	ALA	VAL	LEU	VAL	G1704	H1412	F1311	R1197	V1103	V1004	V904	D798
A2166	L2067	VAL	ILE	ASP	ALA	V1705	L1500	R1312	E1202	G1104	V1005	F915	F799
T2167	L2070	ALA	THR	LEU	ALA	K1706	D1414	V1313	L1203	R1105	V1008	F915	E803
R2170	E2074	VAL	THR	GLY	PRO	S1707	G1415	D1314	T1204	P1009	P1009	L924	A808
D2173	Q2081	ALA	THR	GLY	ALA	T1710	R1504	R1315	D1205	V1110	G1012	A928	D811
E2175	E2082	ALA	THR	GLY	ALA	A1711	R1504	V1316	P1206	F1111	T1013	E929	L816
T2176	Q2084	ILE	TRP	ALA	ALA	A1712	R1508	G1317	V1207	V1110	W1014	P830	E817
L2176	L2085	SER	GLY	ILE	ARG	L1714	D1511	D1319	A1212	A1117	W1014	P830	L826
K2180	S2086	VAL	GLY	ASP	PRO	P1722	D1514	E1323	T1218	A1118	I1017	V931	L827
R2188	Q2087	SER	GLY	GLY	ASP	E1723	V1519	V1326	D1221	A1118	I1018	E932	D832
F2189	R2088	LEU	PRO	ALA	ASP	Y1724	L1530	S1327	R1225	A1119	I1019	R937	A833
T2192	F2089	PRO	GLY	ALA	ILE	S1725	E1531	S1328	R1226	T1119	T1020	Q938	E834
L2193	E2090	SER	TRP	GLY	THR	S1725	I1532	A1329	R1227	E1126	T1021	A939	T835
W2194	G2091	ALA	ALA	ALA	ALA	A1730	I1533	R1330	V1228	A1127	I1022	R940	V836
E2195	G2093	GLY	LYS	ASP	ALA	W1731	N1534	I1331	V1228	G1128	L1021	R941	V837
T2196	H2094	ALA	VAL	LEU	ALA	L1732	F1535	V1336	P1233	L1129	G1028		L838
V2197	V2095	SER	THR	ALA	ASP	N1733	N1536	M1337	M1236	S1131	G1029	A953	H839
A2198	V2096	GLY	VAL	LEU	ALA	E1734	R1537	A1338	R1237	P1031	P1031	V956	P840
T2199	A2097	GLY	GLY	LYS	THR	S1735	R1538	A1339	M1237	I1032	V1033	L957	L853
K2200	T2098	VAL	PHE	GLY	VAL	D1736	G1539	P1346	G1268	A1150	V1033	W958	G854
D2205	A2100	ASP	ALA	VAL	ALA	L1737	S1540	R1342	M1269	E1151	A1039	W964	R855
L2209	R2101	S1983	GLY	THR	ILE	Q1541	Y1542	L1343	L1268	P1146	V1035	G960	P856
W2210	W2103	L1986	THR	LYS	ALA	P1657	A1543	A1344		P1147	D1036	R961	W857
E2211	Q2104	F1989	GLY	LEU	ALA	E1659	I1544	P1346	G1268	P1149	D1037	M962	V857
W2212	G2105	ASP	ALA	LEU	SER	C1661	L1551	Y1350	M1269	E1151	A1039	S963	N858
G2214	L2108	THR	THR	ARG	ALA	R1662	E1552	A1351	W1270	T1162	T1040	W964	F859
T2215	R2112	LYS	TYR	THR	LYS	K1663	A1553	F1352	L1271	D1163	A1041	W965	V860
E2216	T2113	VAL	VAL	ARG	ARG	L1666	L1554	P1363	A1274	T1164	M1042	P866	P861
W2217	W2114	GLY	GLY	PHE	ILE	E1667	E1555	A1463	A1275	D1163	A1044	P866	V862
K2229	E2115	ASP	GLY	GLY	GLN	L1668	E1556	T1357	Q1276	G1167	V1045	I970	R868
P2234	L2118	LEU	ASP	PRO	ILE	W1671	E1557	Q1358	W1278	R1168	L1046	A971	R872
T2235	F2119	GLY	GLY	VAL	GLU	Q1672	R1560	M1362	V1279	P1171	V1068	T974	S873
L2236	L2012	LEU	GLY	LEU	ALA	F1673	R1561	W1376	T1280	V1172	W1072	E975	D874
L2237	L2013	ASP	LEU	LEU	LEU	A1674	L1470	V1376	A1281	S1173	W1072	W976	S875
F2238	L2122	ALA	ALA	ASP	ASP	W1679	Q1563	E1471	T1282	V1174	V1077	Q977	L876
R2244	A2124	ILE	ALA	ALA	ALA	W1679	I1564	A1380	D1283	R1177	V1077	W978	W877
V2245	G2125	GLY	GLY	ASP	GLY	D1684	V1574	D1381	K1285	N1178	T1084	E980	H880
A2246	E2127	LEU	ALA	LEU	ALA	L1685	D1578	R1385	P1286	A1179	T1089	H989	E885
		LEU	THR	THR	THR	F1687	V1579	K1483	P1288	L1184	P1090	P990	A886



P2089	LEU	ALA	ASP	E1723	P1622	D1514	F1422	D1314	E1202	V1103	L986	A886	F783	W674	G583
E2090	PRO	ALA	ILE	Y1724	F1623	D1514	T1423	R1315	L1203	G1104	L987	D837	E784	W675	H584
G2091	SER	ALA	THR	S1725	T1624	V1519	Q1424	V1316	L1203	R1105	E997	I892	L787	G676	H585
T2092	ALA	ALA	PHE		L1625		V1425	G1317	T1204	C1106	V998				S586
G2093	GLY	ASP	ASP	E1730	R1634	L1530	V1430	D1319	P1206	V1110	D1001	T895	A790	A650	W587
H2094	GLY	LEU	ALA	V1731		E1531	A1431	I1318	V1207	F1111	D1002	A896	E791	A681	E588
V2095	ALA	GLY	ALA	L1732	V1637	I1532		E1323	A1212	A1117	H1003	M882	A792	M882	D589
V2096	SER	THR	ASP	N1733	P1638	V1533	V1435	V1324	A1212	A1118	H1004	A899	R793	M884	L590
A2097	GLY	VAL	ALA	S1734	A1639	N1534		L1325	T1218	T1119	V1005	G900	L794	M884	L593
Q2098	GLY	GLY	THR	E1735		F1535	Q1441	E1326	T1218	A1119		I901	H795	A685	L594
Q2099	VAL	PHE	VAL	R1736	T1651	N1536	Q1441	S1327	T1220	E1120	V1008	P796	T796	S686	L594
A2100	VAL	ALA	ALA	D1737	M1652	L1537	V1445	V1328	P1221		P1003	W904	Q797	G687	L595
N2101	ASP	VAL	LEU			L1537		S1328	T1220		F1008				
W2102	ASP	THR	ILE	L1741		R1538	V1445	A1329	P1221	F1123	L1010	F799	D799	R688	
W2103	THR	LYS	ALA		K1656	G1539	A1448	A1330	R1225	P1124	S1011	F915	F799		Y698
Q2104	ARG	LEU	LEU	D1745	P1657	S1540	I1449	I1331	R1225	P1124	S1011	F915	F799	D694	
G2105	GLY	GLY	ALA	THR	K1658	Q1541	A1450	I1331	R1226	V1125	G1012	I924	E803	I695	R602
	GLY	ARG	ALA	ASP	E1659	Y1542		V1336	D1227	L1127	T1013	L924	E803	H696	
L2108	SER	THR	LYS	PRO	L1660	A1543	V1455	M1337	V1228	G1128	A928	A928	A808	E697	B606
	SER	TYR	MET	GLU	K1661	I1544	G1456	A1338		L1129	I1017	E929	A808	I698	
	VAL	LYS	ILE	PRO	R1662	L1551	Y1458	A1339	R1237		R1018	P930	D811	D899	
R2112	ARG	PRO	ILE	GLU	K1663	E1552	T1459	I1343	R1253	L1132	F1019	V931	L816	N700	6613
N2113	GLY	PHE	ASP	PRO		A1553	A1460	L1343		L1133	T1020	E932	L816	A701	6614
V2114	GLY	GLY	GLY	GLU	E1665	L1554	A1461	A1344	G1268	P1146	L1021	V933	E817	P618	
H2115	ASP	PRO	ILE	ALA	L1666	E1555	I1463	A1344	M1269			L934		L709	
L2118	LEU	VAL	GLY	ASP	L1667	A1555	A1462	A1345	M1270	K1147	V1025	S985	L826	S621	
F2119	GLY	LEU	ALA	ASP	L1668	E1556	C1463	A1346	M1270	E1149	E1034	R936	L827	A713	
	GLY	SER	LEU	PRO	W1671	E1557	V1464	P1346	L1271	P1149	T1035	R937	Y830	A716	Y624
T2122	LEU	ASP	ASP	THR	F1672	E1564	E1471	Y1350	V1279	A1150	D1036	R940	D832	V719	L625
A2123	HIS	ALA	SER	ALA	Q1673	L1564	E1471		V1279	E1151	T1037	R941	D833	K735	P636
G2124	ALA	ILE	ILE	ASP	A1674	R1560	V1467	M1362	A1274	F1152	D1037		D832	P736	L637
A2125	ASN	ASN	GLY	ALA		R1561	Y1468	V1376	A1275				D833	Y737	M638
G2126	ASP	LEU	SER	ALA	W1679	R1562	E1469		Q1276	T1162	V1045	P954	A834	K735	P636
E2127	VAL	GLY	THR	PRO	D1684	Q1663	E1471	I1357	H1277	D1163	L1046		D835	P736	L637
N2128	ALA	LEU	ILE	ALA	L1685	E1564	E1471	Q1358	V1279	T1164	L1046		D835	Y737	M638
P2129	SER	SER	THR	GLU	L1686	D1578	L1474	M1362	T1280	G1167	T1068	I957	D837	T745	D641
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G2125	ALA	VAL	ALA	PRO		P1580	R1480		T1282			M962	L853	L747	1643
E2137	VAL	ASP	SER	ALA	E1690	H1582	K1483	A1380	D1283	P1171	W1072	S963	R855	Q748	L644
V2140	ASP	VAL	ARG	ALA		F1581	M1484	D1381	K1285	S1172	P856	V964	R855	W749	
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T2163	VAL	ILE	ASN	ALA	L1695	V1590	D1487	S1391	V1287	V1174		P966	R858	R751	
V2164	ASP	ASP	GLN	ALA			I1487		P1288		T1084	V967	F859		E654
A2166	ASP	GLY	LEU	ALA	R1699	E1598	P1489	P1400	A1290	R1177	F1087	I970	V860	L756	A655
T2167	VAL	ALA	VAL	VAL	F1700	E1598	P1489	P1400	K1291	N1178	G1088	A971	V861	T656	T656
	VAL	VAL	TYR	ALA	E1702	K1605	R1490	A1405	L1292	A1179	V862		V862	S763	T657
R2170	ALA	ALA	ILE	PRO	G1704	K1605	D1491	A1405				T974	R868	D766	S658
E2074	VAL	THR	GLY	ALA	V1705	L1611	R1495	V1408	W1295	L1184	P1090	E975	R868	T767	V661
Q2081	ALA	ARG	SER	ALA	K1706	R1612	S1496		K1304		A1092	I976	R872	K768	K662
D2173	ALA	VAL	GLU	ALA		Y1613		H1412		L1188	P1093	Q977	S873	S873	K663
E2083	ARG	THR	ASN	PRO	T1710	L1615	R1503	P1413			T1094	Q977	D874	L775	L664
Q2084	ARG	LYS	GLY	SER	V1711	P1616	R1504	D1414	D1307	R1191	L1095	V978	S875	D776	L665
L2176	GLY	THR	GLY	GLY	A1712	P1617	P1505	Q1308	F1192	F1192	T1096	E980	L876	I777	V666
L2085	ILE	TRP	ALA	PRO	G1713	L1618	Q1507	V1416	V1309	A1193	V1097	H989	R877	T778	V667
K2180	SER	GLU	ILE	ARG	L1714	V1619	I1508	D1417	D1310	I1194	V1098	P990	H880	W779	T668
Q2087	VAL	LEU	ASP	PRO		P1620	T1508	T1420	F1311	R1195	P1099	P990	H880	R780	R669
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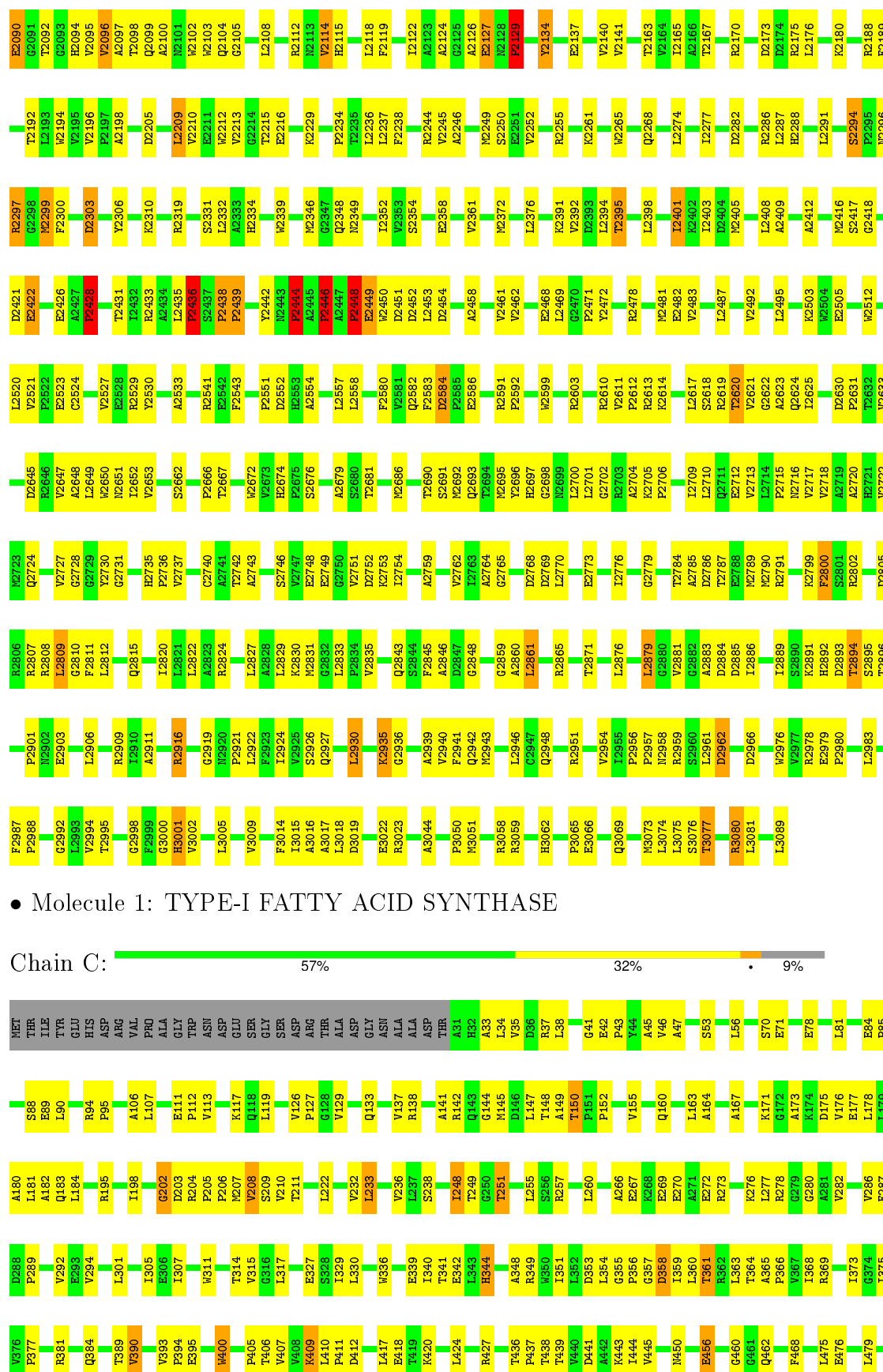
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L2193	D2303	P2428	E2523	P2632	E2721	D2805	T2894	L2983
V2194	C2524	P2428	C2525	V2633	V2722	R2806	S2895	L2983
V2195	Y2306	T2431	L2526	D2645	M2723	R2807	T2896	F2987
V2196	K2310	L2432	V2527	E2646	Q2724	R2808	P2901	P2988
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A2198	R2319	L2435	R2529	A2648	G2728	G2810	R2903	L2993
D2205	S2331	P2436	Y2530	L2649	G2729	F2811	V2994	V2994
L2209	S2331	S2437	A2533	M2650	G2731	L2812	T2995	T2995
V2210	L2332	P2438	P2533	L2652	Q2731	Q2815	R2909	G2998
E2211	A2333	P2439	R2541	V2653	H2735	I2820	I2910	F2999
V2212	H2334	Y2442	E2542	S2662	P2736	L2821	A2911	G3000
V2213	V2339	R2443	F2543	P2666	V2737	L2822	R2916	H3001
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K2229	M2349	P2448	A2554	V2673	A2743	A2828	L2922	L3005
P2234	I2352	E2449	L2557	H2674	S2746	L2829	F2923	V3009
T2235	V2353	D2450	L2558	S2675	V2747	K2830	L2924	F3014
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L2237	E2358	D2452	F2567	A2679	G2750	G2832	S2926	A3016
F2238	E2358	D2454	T2567	S2680	V2751	L2833	Q2927	A3017
R2244	V2361	A2458	F2580	T2681	D2752	V2835	L2930	L3018
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A2246	L2376	V2462	Q2582	T2690	A2759	Q2843	G2936	E3022
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R2255	K2391	L2469	D2584	M2692	I2763	F2845	V2940	A3044
K2261	V2392	P2470	E2586	Q2693	A2764	D2847	F2941	P3050
V2265	D2393	P2471	R2591	M2695	G2765	G2848	Q2942	M3051
Q2268	L2394	Y2472	P2592	L2696	D2768	G2859	L2946	R3058
L2274	T2395	R2478	M2599	H2697	D2769	A2860	C2947	R3059
I2277	L2401	M2481	R2603	G2698	L2770	L2861	Q2948	P3065
D2282	L2402	E2482	R2610	I2699	E2773	R2865	R2951	Q3069
L2286	L2403	V2483	V2611	L2700	I2776	T2871	V2954	M3073
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R2297	M2417	G2512	S2618	E2712	E2788	L2961	D2962	L3081
G2298	G2418	G2512	G2622	V2713	M2789	D2885	D2966	L3089
	D2421	Y2513	A2623	P2715	R2791	I2886	D2976	
	E2422	D2514	Q2624	N2716	K2799	I2889	V2977	
		L2520	I2625	I2717	F2800	S2890	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
TYR	L90	A182	V292	R381	F487
GLU	R94	Q183	E293	Q384	N488
ASP	P95	L194	V294	T389	T489
ARG	A106	R195	L301	V390	L490
VAL	L107	I198	I305	V393	Q500
PRO	E111	G202	D203	P394	K504
GLY	P112	R204	R204	E395	R505
TRP	V113	P205	P205	W400	Q508
ASN	K117	P206	W311	P400	R511
ASP	Q118	M207	T314	P405	R511
SER	L119	V208	V315	T406	A515
SER	V126	S209	G316	V407	P516
ASP	P127	V210	L317	V408	I517
ARG	V129	T211	E327	L410	D518
THR	Q133	L222	I329	P411	V521
ALA	V137	V232	L330	D412	V522
ASP	R138	L233	W336	L417	S523
ASN	A141	V236	E339	E418	I526
ALA	Q143	L237	T341	T419	D534
ASP	G144	S238	T342	K420	
THR	M145	L248	E342	L424	
A31	D146	T249	I343	R427	
H32	L147	G250	H344	T436	
A33	T148	T251	A348	P437	
V35	A149	L255	R349	T438	
D36	T150	S256	I351	T439	
R37	P151	R257	L352	V440	
L38	P152	L260	D353	D441	
G41	V155	A266	L354	K442	
E42	Q160	E267	G355	K443	
P43	L163	K268	P356	T444	
Y44	A164	E269	G357	V445	
A45	A167	L363	D358	N450	
V46	K171	L277	L364	E456	
A47	G172	R278	A365	Q462	
G50	A175	P366	P366	F468	
S53	K174	G279	V367	L475	
L56	E171	G280	I368	E476	
S70	D175	A281	R369	L479	
E78	V176	V282	I373	H584	
E84	E177	V286	G374	H585	
P85	L178	F287	I375	S586	
	L479	A484		W587	

LEU	PRO	ALA	ASP	LEU723	TI624	LI530	YI430	DI319	AI212	AI117	VI004	A899	E791	A681	E588
PRO	GLY	ALA	ILE	YI724	LI625	LI531	AI431	YI323	TI218	AI118	VI005	G900	A792	M652	D699
SER	THR	GLU	THR	SI725	LI625	LI532	AI431	EI323	TI218	TI119	VI008	Y901	TI119	G683	L590
ALA	ALA	ALA	PHE	SI725	LI625	LI533	AI431	EI324	TI219	EI120	VI008	Y904	L794	M884	L593
LYS	ASP	ASP	ASP	EI730	LI634	LI534	VI435	LI325	TI220	F1123	P1009	Y915	H795	A685	L594
HIS	LEU	LEU	ALA	VI731	VI637	LI535	QI441	EI326	PI221	AI123	S1011	F915	P796	S686	L595
VAL	ALA	GLY	ALA	LI722	PI638	LI536	QI441	VI327	PI221	AI124	G1012	L924	Q797	G687	L598
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VAL	ALA	THR	ALA	LI723	PI639	LI538	VI445	LI329	PI221	AI126	G1013	L924	F799		
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LI1986		LYS	ALA	DI745	VI658	LI544	VI455	MI337	PI233	AI131	W1014	L924	D799		
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		ALA	THR	DI745	VI658	LI544	VI455	MI414	PI233	AI208	W1014	L924	D799		
		ALA	THR	DI745	VI658	LI544	VI455	MI415	PI233	AI209	W1014	L924	D799		
		ALA	THR	DI745	VI658	LI544	VI455	MI416	PI233	AI210	W1014	L924	D799		
		ALA	THR	DI745	VI658	LI544	VI455	MI417	PI233	AI211	W1014	L924	D799		
		ALA	THR	DI745	VI658	LI544	VI455	MI418	PI233	AI212	W1014	L924	D799		
		ALA	THR	DI745	VI658	LI544	VI455	MI419	PI233	AI213	W1014	L924	D799		
		ALA	THR	DI745	VI658</										








M3073	Q2958	D2786	Q2711	S2618	E2505	M2416	N2296	L2176	Q2084
L3074	R2959	T2787	E2712	R2619	W2513	S2417	R2297	K2180	L2085
L3075	S2960	E2788	L2714	T2620	Y2513	G2418	G2298		S2086
S3076	L2961	M2789	L2713	V2621			M2299		Q2087
T3077	D2962	M2790	P2715	G2622	L2520	D2421	F2300	R2188	R2088
	D2966	R2791	N2716	A2623	W2521	E2422	D2303	F2189	E2090
		K2799	V2717	Q2624	P2522				G2091
	W2976	F2800	A2719	L2625	E2523	E2426	Y2306	T2192	T2092
	V2977	S2801	A2720	D2630	C2524	A2427	A2427	L2193	G2093
	R2978	K2891	H2721	V2630	E2525	P2428	K2310	W2194	H2094
	E2979	H2892	V2722	T2632	L2526			V2195	V2095
	P2980	D2893	M2723	V2633	V2527	T2431	R2319	P2197	V2096
		T2894	Q2724		E2526	L2432	A2198	A2198	A2097
	L2983	R2807	V2727	D2645	Y2529	R2433	K2324		Q2098
	F2987	R2808	G2728	V2646	Y2530	A2434	E2328	D2205	Q2099
	P2988	L2809	G2729	V2647	A2533	L2435			A2100
	L2989	G2810	A2730	A2648		P2436	S2331	L2209	N2101
		F2811	Q2731	L2649	R2541	S2437	L2332	V2210	W2102
		L2812		W2650	E2542	P2438	H2334	E2211	W2103
				N2651	F2543	P2439		W2212	Q2104
		Q2815	H2735	I2652		Y2442		G2214	G2105
		P2736	P2736	V2653	P2551	N2443	W2339	T2215	L2108
		V2737	V2737		D2552	P2444		E2216	
		L2820	L2821	S2662	H2553	A2445	W2346		R2112
		L2822	C2740		A2554	P2446	G2347	K2229	N2113
		A2823	A2741	T2665	S2555	A2447	Q2348	V2114	N2113
		R2824	T2742	P2666	P2556	P2448	N2349	P2234	H2115
			A2743	T2667	L2557	E2449		T2235	
		L2827	S2746	W2672	L2558	W2450	L2352	L2236	L2118
		A2828	W2747			D2451	W2353	L2237	F2119
		L2829	E2748	S2676	L2563	D2452	S2354		I2122
		K2830	E2749	A2679	F2567	L2453	E2358	R2244	A2123
		M2831	G2750	A2680		D2454		V2245	A2124
		L2833	V2751	T2681	E2574		V2361	A2246	G2125
		P2834	D2752						A2126
		V2835	K2753						E2127
			L2754	W2686	F2580	V2461	W2372	V2252	N2128
		Q2843			V2581	V2462		R2255	P2129
		S2844	K2758	T2690	Q2582		L2376		Y2134
		F2845	A2759	S2691	F2583	L2469		K2261	
		A2846		M2692	D2584	G2470	K2391	W2285	E2137
		D2847	V2762	Q2693	P2585	P2471	V2392	Q2268	V2140
		G2848	L2763	T2694	E2586	Y2472	L2394		V2141
			A2764	M2695					
		A2855	G2765	W2696	R2591	R2478	T2395		
		P2856		E2697	P2592				
				G2698					
		G2859	D2768	W2699	W2599	M2481	L2398	L2274	T2163
		A2860	D2769	L2700		E2482			V2164
		L2861	L2770	L2701	R2603	V2483	L2401	I2277	I2165
			E2773	G2702		L2487	K2402	R2286	A2166
		R2865	R2773	R2703	R2610		I2403	L2287	T2167
			I2776	A2704	V2611	V2492	M2405	H2288	
		T2871		K2705	R2612	L2495			R2170
		L2876	G2779	P2706	K2614		L2408	L2291	D2173
						K2503	A2409	S2294	D2174
		L2879	T2784	I2709	L2617	W2504		P2295	R2175
			A2785	L2710					

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	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	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 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	$\# Z  > 2$	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%)	26	71
1	B	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	30	74
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	26	71
1	D	2448/3089 (79%)	2293 (94%)	138 (6%)	17 (1%)	26	71
1	E	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	30	74
1	F	2818/3089 (91%)	2630 (93%)	163 (6%)	25 (1%)	21	67
All	All	16538/18534 (89%)	15490 (94%)	932 (6%)	116 (1%)	31	71

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	2100 / 2402 (87%)	1998 (95%)	102 (5%)	31	67
1	B	2100 / 2402 (87%)	1997 (95%)	103 (5%)	31	67
1	C	2100 / 2402 (87%)	1998 (95%)	102 (5%)	31	67
1	D	1810 / 2402 (75%)	1722 (95%)	88 (5%)	31	67
1	E	2100 / 2402 (87%)	1998 (95%)	102 (5%)	31	67
1	F	2100 / 2402 (87%)	1995 (95%)	105 (5%)	30	66
All	All	12310 / 14412 (85%)	11708 (95%)	602 (5%)	35	67

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	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	B	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	C	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.70	7 (20%)
2	FMN	D	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	E	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	F	4000	-	32,33,33	1.20	3 (9%)	34,50,50	1.71	7 (20%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C5A-N5	2.22	1.38	1.35
2	E	4000	FMN	C5A-N5	2.25	1.38	1.35
2	A	4000	FMN	C5A-N5	2.25	1.38	1.35
2	F	4000	FMN	C5A-N5	2.26	1.38	1.35
2	C	4000	FMN	C5A-N5	2.29	1.38	1.35

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	FMN	N3-C2-N1	-4.49	120.14	127.69
2	B	4000	FMN	N3-C2-N1	-4.48	120.14	127.69
2	E	4000	FMN	N3-C2-N1	-4.46	120.17	127.69
2	C	4000	FMN	N3-C2-N1	-4.45	120.19	127.69
2	F	4000	FMN	N3-C2-N1	-4.44	120.21	127.69

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.