



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:13 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB 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/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

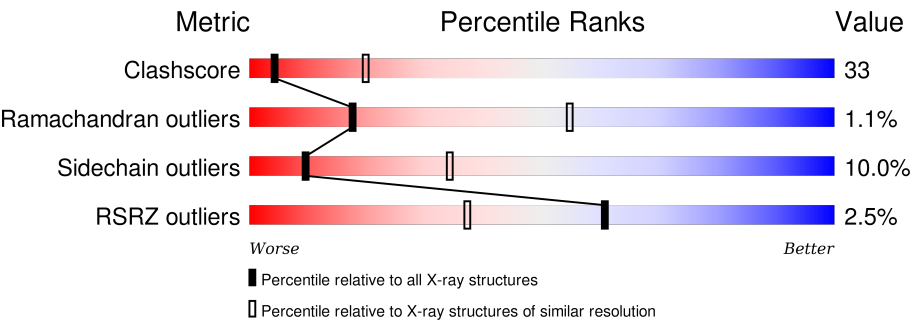
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



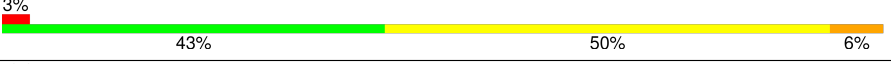
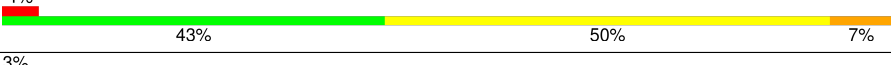
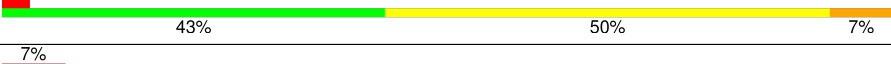
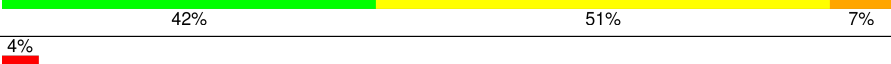
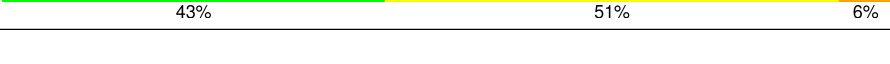
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1878	<div><div>40%33%5%22%</div></div>
1	B	1878	<div><div>42%32%.22%</div></div>
1	C	1878	<div><div>41%32%.22%</div></div>
1	D	1878	<div><div>41%33%5%22%</div></div>
1	E	1878	<div><div>40%33%.22%</div></div>
1	F	1878	<div><div>41%32%.22%</div></div>
2	G	2060	<div><div>2%44%49%6%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	2060	
2	I	2060	
2	J	2060	
2	K	2060	
2	L	2060	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-
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.

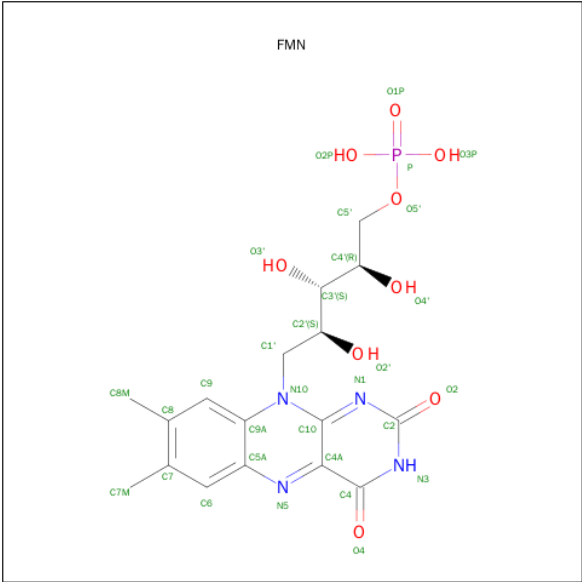
- Molecule 1 is a protein called FATTY ACID SYNTHASE ALPHA SUBUNITS.

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 (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					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		





WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





LEU  
GLN  
ALA  
VAL  
ALA  
VAL  
ALA  
VAL  
SER  
ARG  
THR

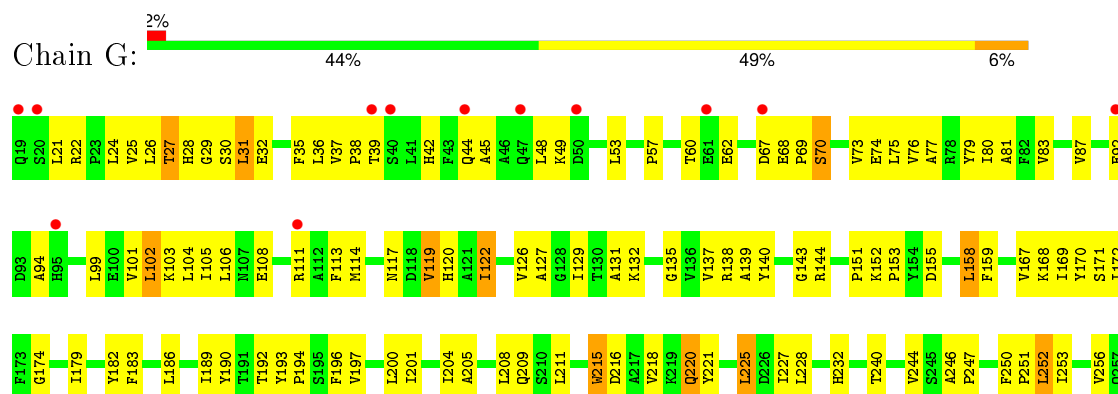
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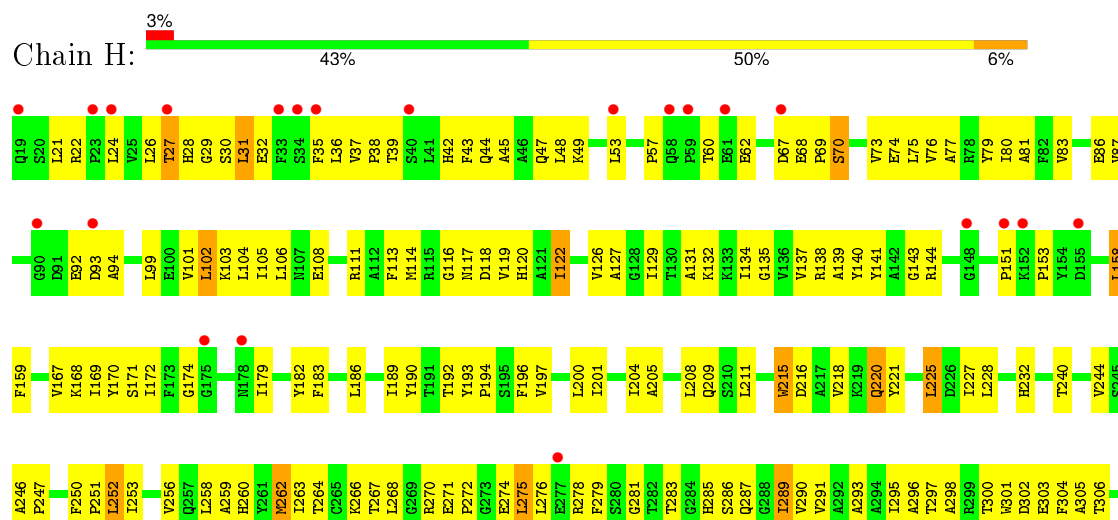
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK







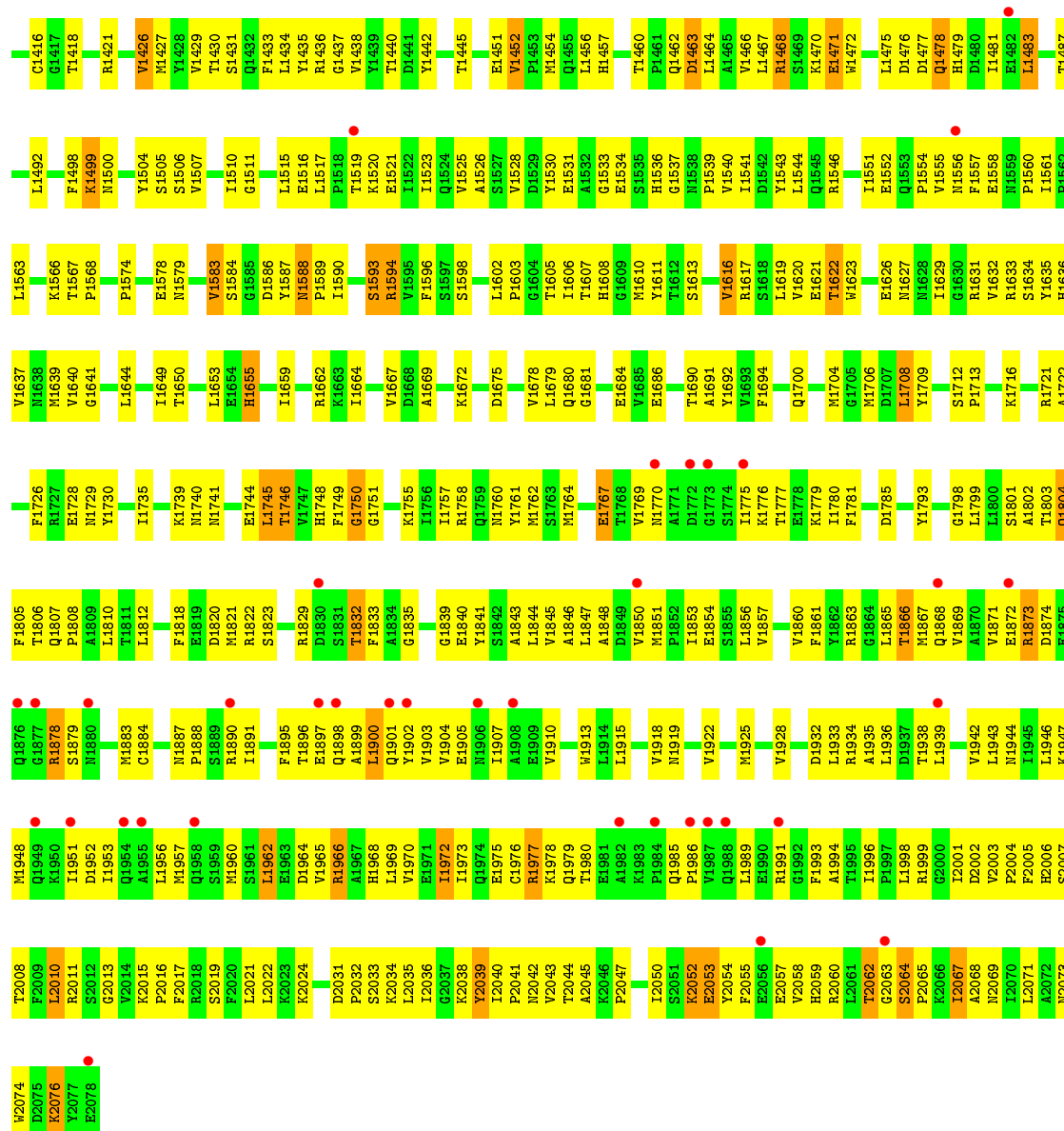




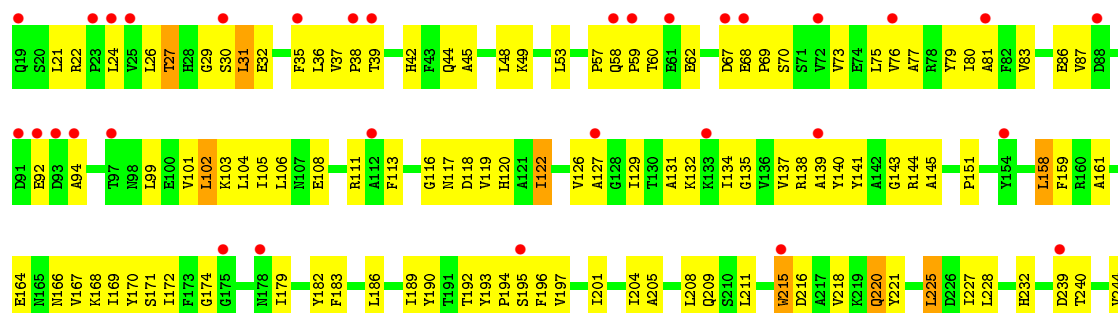


[illegible]

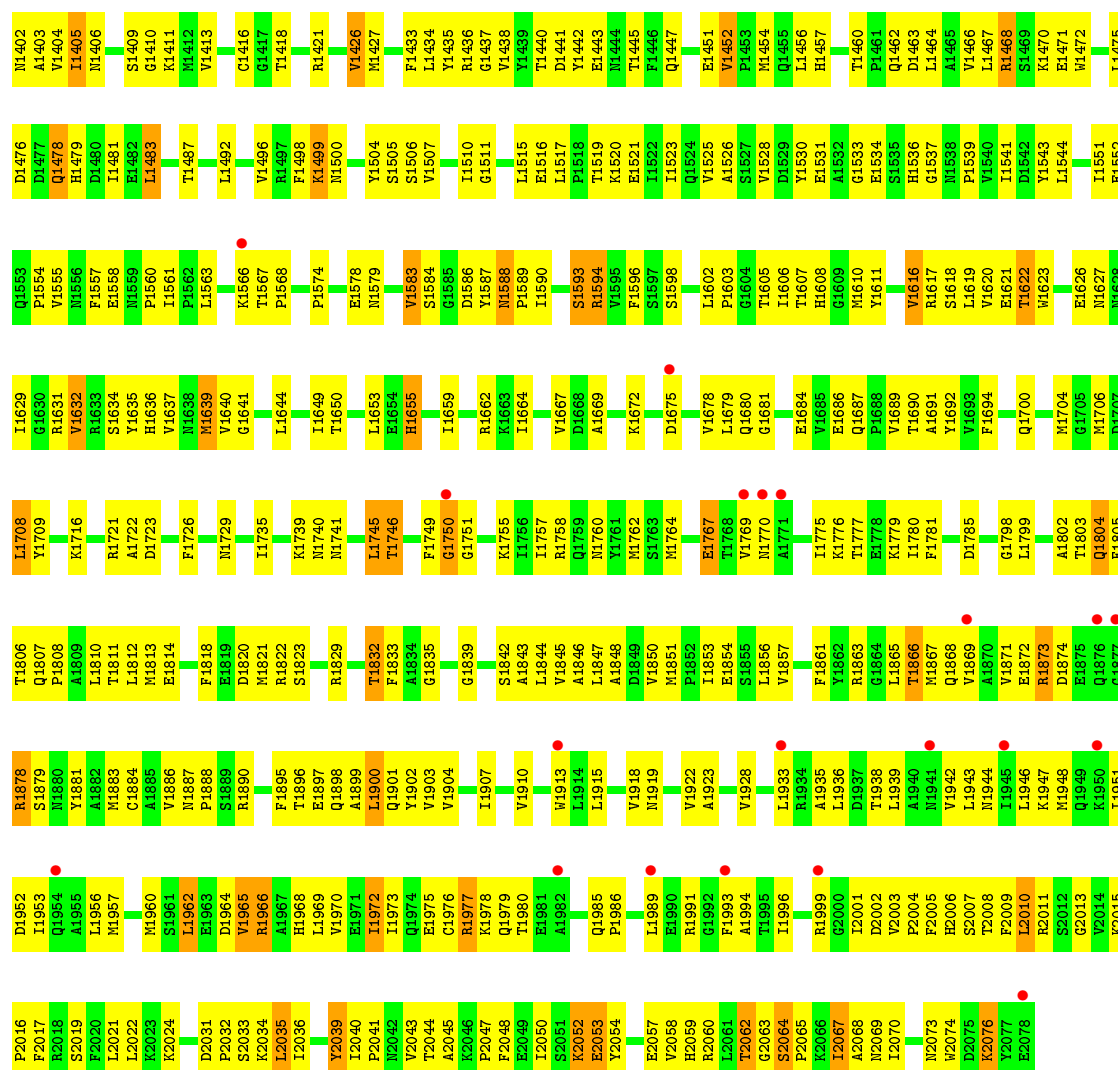
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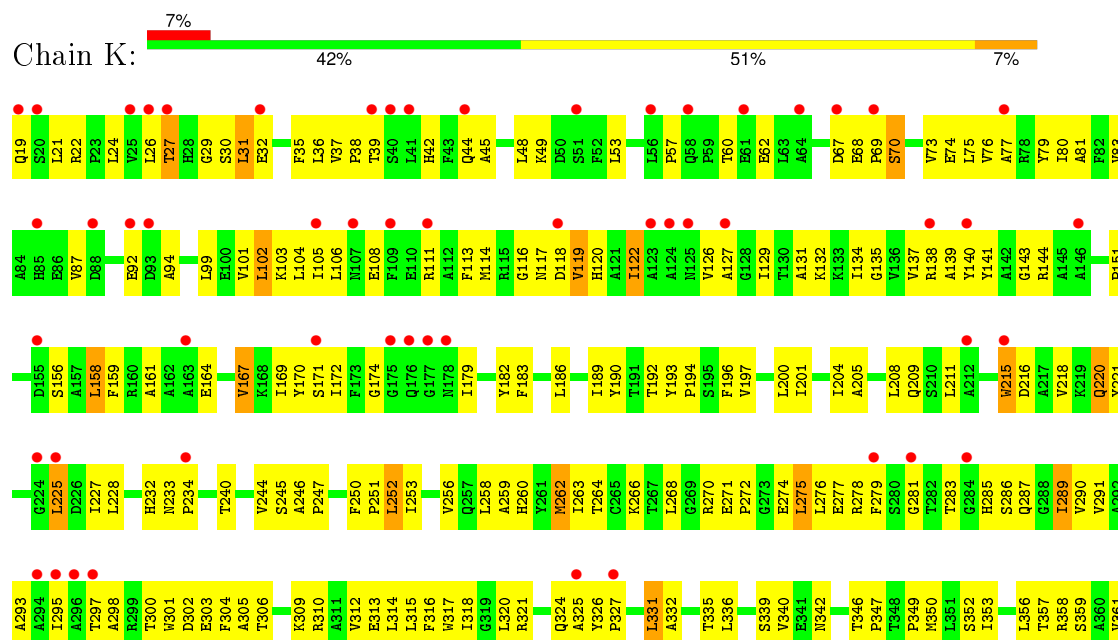
## ● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



A1334	P1258	T1189	P1111	W048	F970	I903	V833	R769	P697	V622	L541	S463	F389	R310	S245
F1335	L1289	M1190	V1112	Q1049	T971	K904	D834	K770	S698	M623	A542	S464	V390	A311	A246
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G1339	F1261	L1192	E1114	E1051	L980	L906	P836	T772	I699	G625	A544	I467	G393	E313	F250
K1340	R1262	K1193	F1115	E1052	L985	L906	G837	T773	E700	H627	I545	P468	P394	L314	P251
D1341	Y1265	L1195	G1116	L1053	D885	D909	D839	V775	A702	I628	M549	V469	P395	L315	L252
F1342	R1266	F1196	R1119	E1054	L986	F910	D840	V776	E704	E629	T550	Y470	I396	R317	L253
F1343	T1267	L1197	G1120	A1055	D987	Q911	D841	T777	E705	E551	E551	D471	G254	I318	G254
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P1345	A1269	T1199	V1057	A1133	P989	V913	M843	G779	T706	G473	G553	T473	L320	G319	V256
M1346	G1270	R1200	T1124	Y1061	Y990	G914	E344	S780	Q707	M637	Y554	T474	L401	R321	Q257
D1347	Y1271	G1201	T1125	V1061	P991	G915	M845	G781	T708	A638	K555	G475	M402	K21	L258
F1348	M1202	M1202	E1126	G1082	G916	G916	T846	F782	L709	Q641	P556	Q476	L403	Q324	K258
A1349	T1274	Y1203	E1127	R1083	R917	N918	Y847	G783	R712	M641	E557	Q476	R404	A325	A259
T1350	R1275	T1204	E1128	T1064	L997	N918	K848	G784	H713	A644	L558	R479	R405	A325	H260
V1351	E1276	E1205	D1129	C1085	A998	A998	R849	S785	H713	A644	F559	E480	R406	Y261	M262
V1352	V1277	E1206	I1130	I1066	A999	A999	R849	S786	H713	A644	D560	L481	R406	R328	L263
G1353	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
K1354	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
K1355	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
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K1364	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
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K1424	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
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K1427	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
K1428	M1278	T1207	D1131	L1067	Y1000	T930	T851	D787	P718	S646	R561	D485	A410	T329	T264
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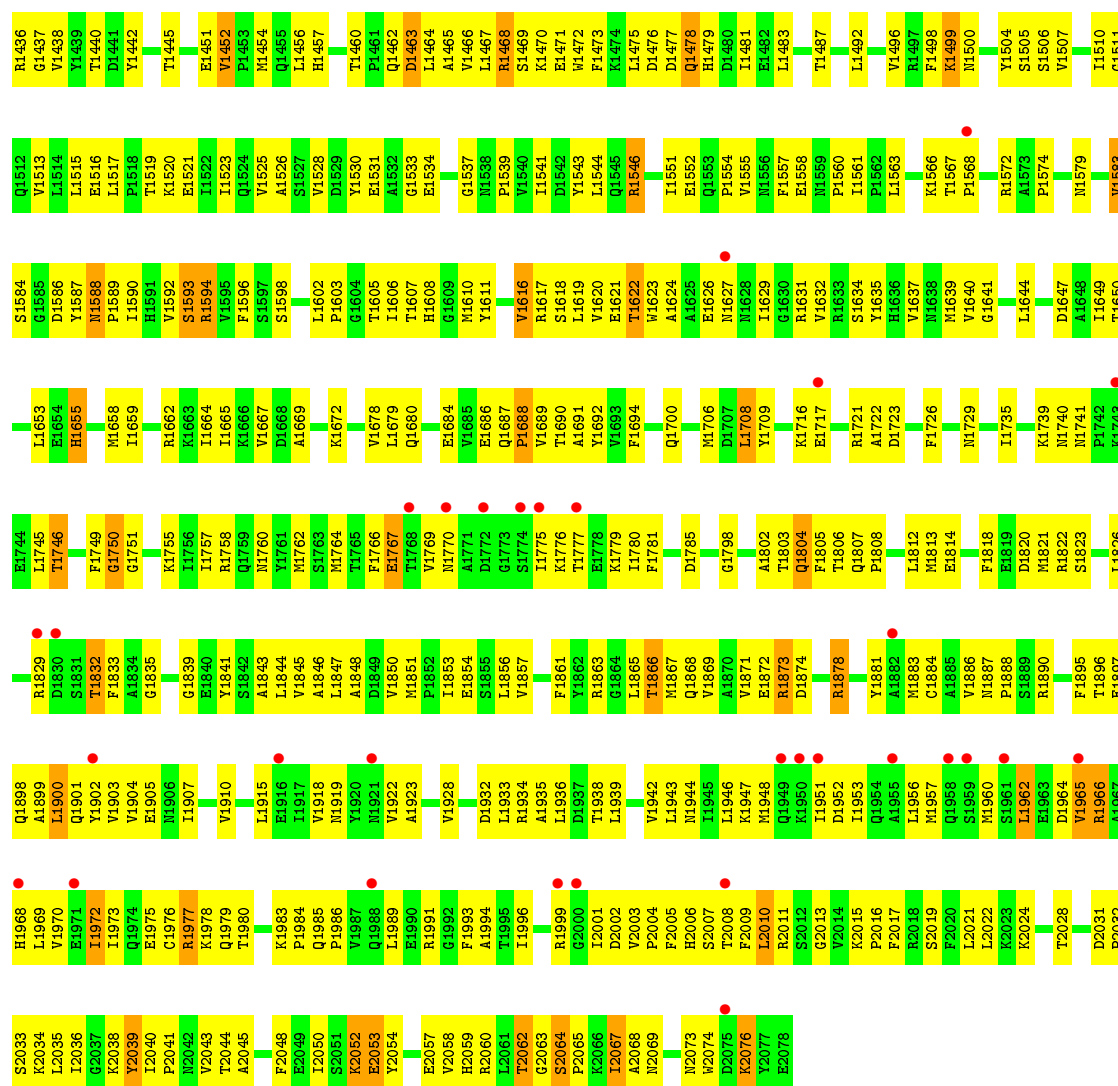


## ● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

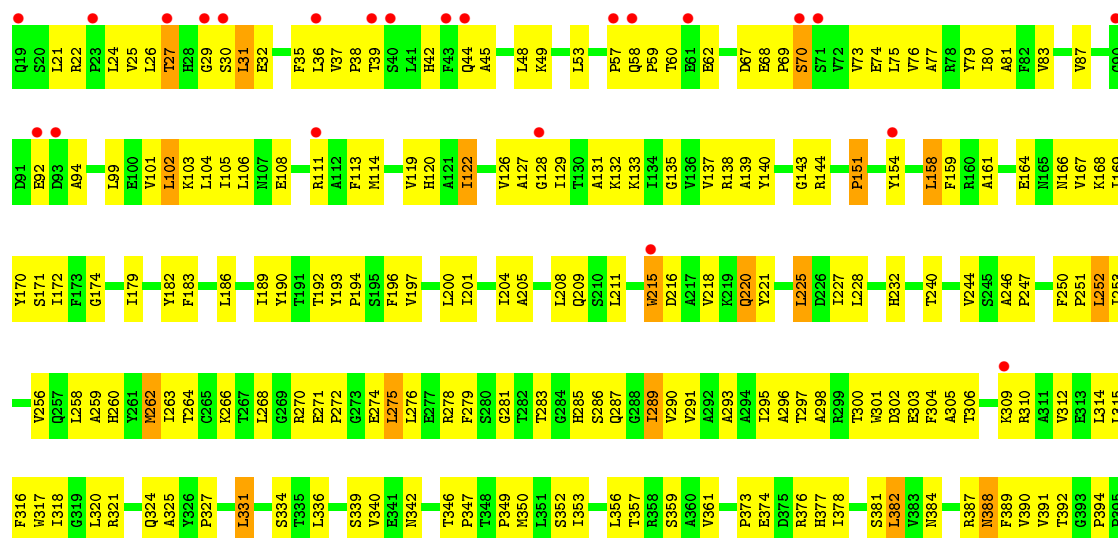








● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



S1409	R1338	V1256	F1181	E1107	E1039	R965	L895	A828	Y765	T691	F617	L541	Y486	I396
G1410	G1339	V1257	R1186	E1108	Y1040	V966	R996	R829	S766	A694	V618	A542	I467	
G1411		P1258	F1187	V1110	M1109	E967	R898		E768		A619	A544	P468	Y399
M1412	F1342	L1259	G1188	P1111	E968	E969	R899	T832	R770	S698	T621	T548	G420	G401
V1413	F1343	T1260	T1189	V1112	K1042	R969	I903	R834	K770	T699	G622	N549	D471	N402
	A1344	R1261	M1190	E1113	K1043	T971	K904	A835	C771	E700	N623	T550	T972	L403
C1416	F1345	R1262	P1191	E1114	K1044		K905	R836	S772	V701		T550	K473	R404
G1417	M1346	Y1265	L1192	F1116	W1048	Q976	L906	G837	N773	A702	Y626	E551	K474	L405
T1418	F1347	H1266	Y1115		Q1049	P977		R838	N774	E703	H627	G552	R406	K407
	P1348	E1268	F1116		S1050	S978	D909	W839	V775	E704	G628	G553	D477	
R1421	A1349	E1269	I1120		E1051	L979	F910	D840	L776	Y705	E629	Y554	L478	A410
K1424	L1350	A1269	L1121		L980	L980	Q911	D841	V777	L706		K555	L478	P411
P1425	V1351	G1270	I1052		I1053		K912	Q842	A778	Q707	Y635	P556	A479	P411
V1426	G1352	Y1271	Y1057			D985	V913	R843	G779	T708	Y636	E557	E480	T412
M1427	K1353	I1274				L986	W914	E844	S780	L709	N637		L481	G413
	K1354	R1275	V1061		V1061	E987	F915	T846	G781	R712	A638	R561	G482	L414
L1434	A1355	E1276	G1062		G1062	P989	R917	Y847	G783	H713		N564	D483	D415
Y1435	K1356	V1277	R1064		R1064	Y990	R918	R848	G784	T714	M641		P484	Q416
G1437	P1360	M1278	C1065		C1065		G921	R849	S785	S715	A644	Q667	D485	R417
V1438	I1361	I1206	I1130		I1130		E922	R850	E786	F716	I645	V573	I487	I419
Y1439	F1362	T1207	L1067		L1067	I996	P923	T851	D787	K717	S646	K574	P488	P420
T1440	K1286	N1208	G1132		G1132	L997	V924		T788	F718	K647		E489	F421
D1441	P1209	L1133	Q1068		Q1068	A998	R925	W854	Y789	G719	I648		I480	T422
Y1442	E1210		G1069		G1069	A999	D925	I855	P790		E649	P578	V491	Q423
T1445	D1211		P1070		P1070	Y1000	L926	T856	Y791	A723	K850	R579	R492	R424
	T1215		V1071		V1071	E1002	E927	R857	L792	T724	A651	L580	M493	K425
E1451	V1216		A1073		A1073		N929	S859	G794	Q726	I652	K882	D497	F432
Y1452	I1217		K1074		K1074	Q1006	T930	E960	S795	V727	P653	T583	P498	L433
F1453	S1076		S1076		S1076	L1007	A932	R861	Y796		R656	S584	V499	P434
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Q1455	L1146		D1080		D1080	N1009	V934	P864	T799		N661	Q587	E502	A437
L1456	N1153		N1153		N1153	Q1011	V935	I865	R800	N734	L662	V590	T503	P438
H1457	L1154		L1154		L1154	D1012	H936	R866	G801		I663	D591	A504	F439
	P1301		P1301		P1301	V1013	R937	K867	X802	F737	Y664	M594	T505	R440
T1460	R1381	A1226	K1084		K1084	Q1014	N938	L868	P903	F738	P665	S995	V506	L444
Q1462	M1382	K1227	D1085		D1085	H1015	V939	A869	P804	I739	N666	R596	F507	
D1463	L1305	L1228	L1086		L1086	F1016	E940	T870	M805	L740	P675		A510	A447
L1464	V1308	V1229	L1087		L1087	L1017	L941	R871	P906	L741	L676	V605		H448
A1465	F1309	K1230	G1088		G1088	L1018	M942	G872	R807	Q742	G671	A606	A510	T511
V1466	D1310		I1089		I1089	L1019	Y943	F875	D808	W743		G607	H512	L449
L1467	R1391	I1234	H1091		H1091	Q1020	V944	W876	G809		W672	P601	I613	H450
R1468	G1392	L1236	N1092		N1092	Q1021	R949		C810	R747	Q673	P602	I614	I451
S1469	V1394	V1237	D1093		D1093	R1022	W950	L879	M811		I674	V603	D515	L452
K1470	I1315	G1238	H1094		H1094	K1026	I951	D880	S814	G750	P675	M604	F516	G453
E1471	V1316	D1238	I1095		I1095	P1027	L955	D881	R815	H751	L676	V605	G517	D454
F1472	N1317	N1240	K1096		K1096	V1028	L956	K882	M816	H752	R679	A606	G520	V455
T1397	A1318		F1087		F1087	P1029	K956	I883	N917	E755	D683	G607	G520	D456
F1473	Q1319		L1098		L1098	F1030	K957	F884	T818		P610	M608	V521	D457
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D1476	N1402	E1248	M1175		M1175	V1031	G969	R889	E821	P760	P686	T612	V526	I460
T1477	V1325	F1248	Y1103		Y1103	A1033	D861	K890	A822	I761	I687	V613	T528	P461
Q1478	A1403	G1249	G1104		G1104	L1034	F962	R891	H823	L762	G688	P614	N529	A462
L1479	V1404	R1250	G1105		G1105	D1035	I963			L763	G689	W615		S463
D1480	N1406	T1251	N1106		N1106	E1036	R964	E894	Q827	M764	L690	D616	I540	L465
I1481														

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P2016	A1885	E1814		V1632	F1557	L1483
F2017	V1886		R1721	R1633	M1558	
R2018	M1887	F1818	A1722	S1634	M1559	T1487
S2019	P1888	E1819		H1635	I1561	L1488
P2020	S1889	D1820	F1726	H1636	P1562	V1489
L2021	R1890	M1821		V1637	L1563	
L2022	S1891	R1822	K1739	M1638		L1492
K2023	T1894	S1823	M1740	M1639	K1566	F1498
K2024		Q1828	P1742	G1641	T1567	K1499
		Q1829			P1568	M1500
T2028	E1897	D1830	L1745	L1644		
T2029	Q1898	S1831	T1746	P1645	R1572	Y1504
I2030	A1899	T1832		M1646	A1573	S1505
D2031	L1900	F1833	F1749	D1647	P1574	S1506
P2032	Y1901	G1834	G1750	A1648	A1575	V1507
S2033	Y1902	G1835	G1751	I1649		
K2034	V1903			T1650	M1579	I1510
K2035	V1904	G1839	K1755	L1653	V1583	G1511
I2036	E1905	E1840		E1654	S1584	L1514
G2037	M1906	Y1841	R1758	H1655	G1585	L1515
K2038	I1907	S1842	Q1759		D1586	E1516
Y2039		A1843	N1760		Y1587	L1517
I2040	V1910	L1844	Y1761	L1659	M1588	F1518
P2041	W1913	V1845	M1762		P1589	L1519
H2042	L1914	A1846	S1763	R1662	I1590	K1520
V2043	L1915	L1847	M1764	R1663	H1591	E1521
T2044	A1982	A1848	T1765	I1664	V1592	I1522
A2045	K1983	D1849	F1766	V1667	S1593	I1523
K2046	P1984	V1850	E1767	D1668	R1594	Q1524
P2047	Y1920	M1851	T1768	A1669	V1595	A1526
	Y1921	I1852	V1769		F1596	
I2050	V1922	E1853	M1770	K1672	L1602	V1528
K2051	A1923	S1854			P1603	D1529
E2053		L1855	I1775	D1675	G1604	Y1530
Y2054	Q1926	L1856	K1776		T1605	E1531
	Y1927	V1857	T1777	V1678	T1606	A1532
E2057	V1928		E1778	L1679	T1607	G1533
V2058		F1861		Q1680	H1608	E1534
H2059	D1932	Y1862	R1779	G1681	G1609	S1535
R2060	L1933	R1863	T1780		M1610	H1536
L2061	R1934	G1864	F1781	E1684	Y1611	G1537
T2062	A1935	L1865	D1785	V1685		M1538
G2063	L1936	T1866		Q1686	V1616	P1539
S2064	D1937	M1867	S1788	Q1687	R1617	V1540
P2065	L1938	V1868		P1688	S1618	E1541
K2066	T1938	V1869	Y1793	V1689	L1619	D1542
S2067	L1939	A1870		A1691	V1620	Y1543
I2067	V1942	V1871	L1799	E1621	T1622	Q1544
A2068	L1943	E1872		V1693	W1623	R1546
N2069	N1944	D1874	A1802	F1694		
	L1945	D1875	T1803		E1626	I1551
N2073	V1946	R1878	Q1804		M1627	E1552
V2074	K1947	F1805	T1806	M1706	M1628	Q1553
K2075	M1948	S1879	Q1807	D1707	I1629	P1554
E2076		H1880	P1808	Y1709		V1555
Y2077	I1951	Y1881				
E2078	S2012	A1882	L1812			
	V2014	M1883				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.37Å 414.43Å 221.51Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 88.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 89.5 (88.45-3.10)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 3.13Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, $R_{free}$	0.290 , 0.320 0.253 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.12 , -83.0	EDS
Estimated twinning fraction	0.280 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.21$ , $\langle L^2 \rangle = 0.07$	Xtriage
Outliers	0 of 629508 reflections	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	166671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

## 5.2 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	745	0
1	B	11571	0	11529	706	1
1	C	11555	0	11507	695	0
1	D	11593	0	11552	733	0
1	E	11506	0	11467	745	0
1	F	11546	0	11499	701	0
2	G	16200	0	16081	1178	1
2	H	16200	0	16081	1209	1
2	I	16200	0	16081	1238	0
2	J	16200	0	16081	1213	0
2	K	16200	0	16081	1262	1
2	L	16200	0	16081	1219	0
3	G	31	0	19	10	0
3	H	31	0	19	11	0
3	I	31	0	19	9	0
3	J	31	0	19	9	0
3	K	31	0	19	12	0
3	L	31	0	19	10	0
All	All	166671	0	165630	11004	2

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 33.

The worst 5 of 11004 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:HH11	2:H:1594:ARG:HG2	1.02	1.17
1:E:1610:ARG:HH11	1:E:1610:ARG:HG2	1.00	1.16
2:L:1594:ARG:HG2	2:L:1594:ARG:HH11	1.03	1.16

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	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%)	24	63
1	B	1458/1878 (78%)	1295 (89%)	151 (10%)	12 (1%)	24	63
1	C	1456/1878 (78%)	1293 (89%)	151 (10%)	12 (1%)	24	63
1	D	1461/1878 (78%)	1290 (88%)	155 (11%)	16 (1%)	17	55
1	E	1450/1878 (77%)	1292 (89%)	146 (10%)	12 (1%)	24	63
1	F	1455/1878 (78%)	1300 (89%)	140 (10%)	15 (1%)	19	58
2	G	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	15	50
2	H	2058/2060 (100%)	1786 (87%)	244 (12%)	28 (1%)	14	48
2	I	2058/2060 (100%)	1799 (87%)	233 (11%)	26 (1%)	15	50
2	J	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	2058/2060 (100%)	1772 (86%)	258 (12%)	28 (1%)	14	48
2	L	2058/2060 (100%)	1777 (86%)	253 (12%)	28 (1%)	14	48
All	All	21079/23628 (89%)	18479 (88%)	2359 (11%)	241 (1%)	17	55

5 of 241 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1227	GLY
1	A	1566	LYS
1	A	1593	ASP
1	B	614	PHE
1	B	1566	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1220/1527 (80%)	1101 (90%)	119 (10%)	10	36
1	B	1227/1527 (80%)	1111 (90%)	116 (10%)	11	38
1	C	1225/1527 (80%)	1102 (90%)	123 (10%)	9	34
1	D	1229/1527 (80%)	1110 (90%)	119 (10%)	10	36
1	E	1219/1527 (80%)	1101 (90%)	118 (10%)	10	36
1	F	1224/1527 (80%)	1109 (91%)	115 (9%)	11	39
2	G	1752/1752 (100%)	1571 (90%)	181 (10%)	9	32
2	H	1752/1752 (100%)	1579 (90%)	173 (10%)	10	34
2	I	1752/1752 (100%)	1571 (90%)	181 (10%)	9	32
2	J	1752/1752 (100%)	1573 (90%)	179 (10%)	9	33
2	K	1752/1752 (100%)	1575 (90%)	177 (10%)	9	33
2	L	1752/1752 (100%)	1576 (90%)	176 (10%)	9	34
All	All	17856/19674 (91%)	16079 (90%)	1777 (10%)	9	34



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

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

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

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

### 5.3.3 RNA ⓘ

There are no RNA 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
3	FMN	G	2101	-	32,33,33	6.16	22 (68%)	34,50,50	1.84	5 (14%)
3	FMN	H	2101	-	32,33,33	6.14	22 (68%)	34,50,50	1.94	7 (20%)
3	FMN	I	2101	-	32,33,33	6.16	20 (62%)	34,50,50	1.93	6 (17%)
3	FMN	J	2101	-	32,33,33	6.36	23 (71%)	34,50,50	1.98	7 (20%)
3	FMN	K	2101	-	32,33,33	6.40	22 (68%)	34,50,50	1.88	8 (23%)
3	FMN	L	2101	-	32,33,33	6.13	20 (62%)	34,50,50	1.89	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
3	FMN	G	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	H	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	I	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	J	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	K	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	L	2101	-	-	0/18/18/18	0/3/3/3

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2101	FMN	C5'-C4'	2.02	1.54	1.51
3	G	2101	FMN	C7M-C7	2.06	1.55	1.51
3	G	2101	FMN	C8M-C8	2.10	1.55	1.51
3	H	2101	FMN	P-O5'	2.11	1.65	1.59
3	J	2101	FMN	C7M-C7	2.11	1.55	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2101	FMN	N3-C2-N1	-5.04	119.20	127.69
3	K	2101	FMN	N3-C2-N1	-4.96	119.33	127.69
3	H	2101	FMN	N3-C2-N1	-4.77	119.66	127.69
3	I	2101	FMN	N3-C2-N1	-4.65	119.86	127.69
3	L	2101	FMN	N3-C2-N1	-4.64	119.87	127.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 61 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	1457/1878 (77%)	-0.50	14 (0%)	84	69	17, 54, 105, 150	0
1	B	1464/1878 (77%)	-0.51	12 (0%)	87	75	16, 52, 111, 158	0
1	C	1462/1878 (77%)	-0.51	17 (1%)	81	64	15, 51, 111, 159	0
1	D	1467/1878 (78%)	-0.52	13 (0%)	85	72	17, 54, 108, 158	0
1	E	1456/1878 (77%)	-0.48	13 (0%)	85	72	15, 54, 110, 157	0
1	F	1461/1878 (77%)	-0.54	12 (0%)	87	75	16, 51, 108, 159	0
2	G	2060/2060 (100%)	-0.12	38 (1%)	71	50	27, 83, 129, 169	0
2	H	2060/2060 (100%)	-0.05	69 (3%)	50	26	24, 86, 132, 167	0
2	I	2060/2060 (100%)	-0.02	73 (3%)	48	23	23, 86, 132, 167	0
2	J	2060/2060 (100%)	0.03	66 (3%)	51	27	28, 89, 133, 172	0
2	K	2060/2060 (100%)	0.25	134 (6%)	22	8	27, 91, 136, 172	0
2	L	2060/2060 (100%)	0.01	76 (3%)	45	22	23, 87, 133, 172	0
All	All	21127/23628 (89%)	-0.20	537 (2%)	61	37	15, 75, 127, 172	0

The worst 5 of 537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	40	SER	13.0
2	J	93	ASP	11.0
2	K	27	THR	9.5
2	I	19	GLN	7.4
2	G	39	THR	6.7

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMN	G	2101	31/31	0.94	0.20	0.20	19,64,105,124	0
3	FMN	L	2101	31/31	0.94	0.18	-0.37	15,51,89,119	0
3	FMN	I	2101	31/31	0.93	0.18	-0.38	23,54,85,115	0
3	FMN	H	2101	31/31	0.94	0.18	-0.46	21,53,91,110	0
3	FMN	J	2101	31/31	0.94	0.15	-0.92	19,56,106,122	0
3	FMN	K	2101	31/31	0.90	0.19	-0.94	24,63,111,122	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.