



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:00 am 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28972

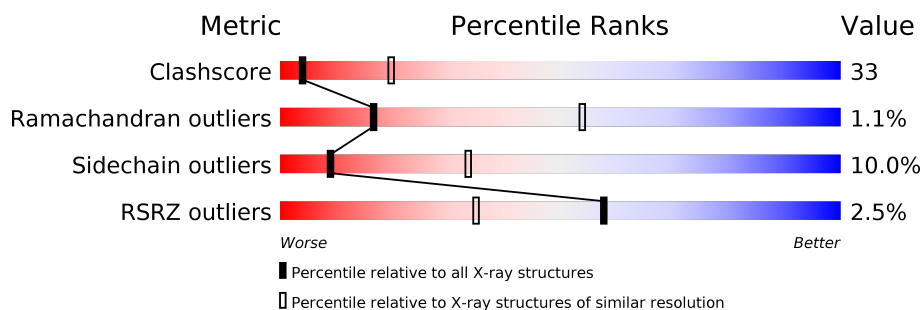
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



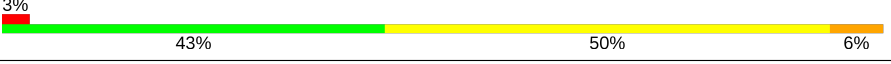
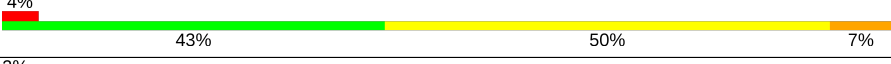
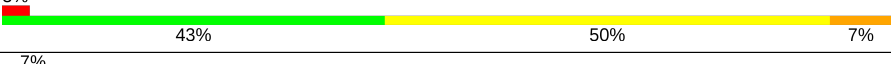
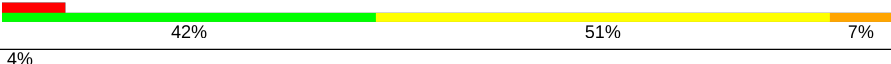
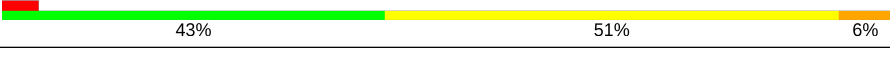
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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%</div> <div>33%</div> <div>5%</div> <div>22%</div> </div>
1	B	1878	<div> <div>42%</div> <div>32%</div> <div>•</div> <div>22%</div> </div>
1	C	1878	<div> <div>41%</div> <div>32%</div> <div>•</div> <div>22%</div> </div>
1	D	1878	<div> <div>41%</div> <div>33%</div> <div>5%</div> <div>22%</div> </div>
1	E	1878	<div> <div>40%</div> <div>33%</div> <div>•</div> <div>22%</div> </div>
1	F	1878	<div> <div>41%</div> <div>32%</div> <div>•</div> <div>22%</div> </div>
2	G	2060	<div> <div>2%</div> <div>44%</div> <div>49%</div> <div>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: C₁₇H₂₁N₄O₉P).

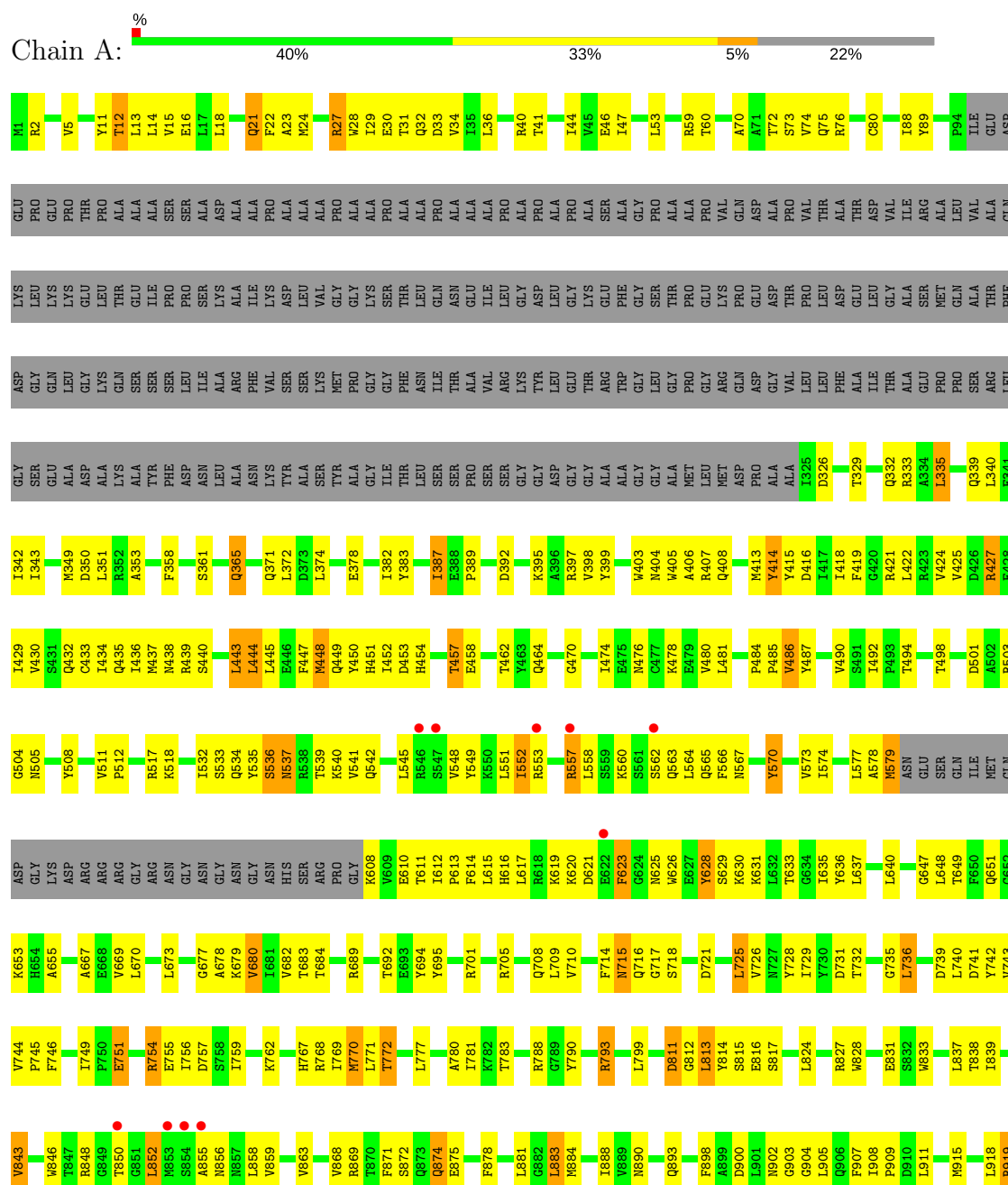


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	K	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	L	1	Total 31	C 17	N 4	O 9	P 1	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



L1362	M1363	D1288	F1209	K1113	S1091	V943	V943	V843	E751	R653	ASP	T494	L422	E341	LEU	PHE	GLN
T1364	A1365	Y1291	K1211	E1117	L1022	E946	E946	R848	R754	R654	GLY	T498	R423	I342	GLY	ASP	LYS
L1367	Q1366	I1294	Y1212	F1129	M1028	D947	D947	G849	E755	A655	LYS	T499	V424	I343	SER	GLN	LEU
A1368	L1367	I1294	V1213	F1130	A1029	H948	H948	T850	I756	G663	ARG	F500	V425	L347	ALA	LEU	LYS
	A1368	A1299	H1214	E1131	M1031	E949	E949	G851	D757	V669	ARG	D501	R427	K348	ASP	GLY	GLU
M1371	S1301	R1300	L1216	T1135	M1032	A950	A950	R852	S758	L673	GLY	N505	E428	M349	ALA	LYS	LEU
G1372	C1302	C1302	S1217	G1136	N1037	L951	L951	M853	I759	L673	ASN	Y508	V430	D350	LYS	THR	THR
L1373	L1303	V1304	Q1218	Y1137	H1038	Y952	Y952	S854	K762	G677	GLY	P512	Q432	L351	ALA	GLN	ILE
P1374	P1374	V1304	G1219	Y1138	N1039	R953	R953	A855	R767	A678	ASN	V511	S431	A353	ASP	PRO	PRO
I1375	I1375		M1220	T1139	G1040	I956	I956	N856	H767	K679	GLY	P512	Q433	K356	ILE	SER	SER
				V1140	P1041			N857	R768	V680	ASN		T434	A357	LEU	LYS	LYS
I1378				R1141	L1042	P959	P959	V868	R768	I681	GLY		Q435	F358	ALA	ALA	ALA
M1381				L1142	L1042	R960	R960	R869	M770	V682	ASN		M437		ALA	PHE	ILE
T1382				R1143	Y1047	A961	A961	T870	L771	T683	ASN		R438	S361	LYS	VAL	LYS
						N962	N962	T870	T772		SER		R439		TYR	SER	ASP
						L963	L963	F871	R776	S688	ARG		S440	Q365	ALA	SER	LEU
						K964	K964		L777	R689	PRO				SER	LYS	VAL
T1386	D1387	E1313	G1226	L1148	V1080	Y965	Y965	Q874	R776	T692	GLY		L443	Q371	TYR	MET	GLY
D1387	K1388	S1315	T1229	I1150	V1081	P966	P966	L881	A780	V695	GLY		L444	L372	ALA	PRO	GLY
I1389	Y1316	E1317	A1231	P1151	D1052	P967	P967	G882	I781		GLY		L445	D373	ILE	GLY	LYS
G1390	G1390	E1317	L1232	A1153	T1055	P968	P968	L883	K782	T611	THR		E446	L374	THR	PHE	THR
				L1154	G1056	E969	E969	M884	T733	I612	LEU		M443	E378	LEU	ASN	LEU
				Q1155	L970	L970	L970	M884	T733	P613	SER		Q449		GLN	ILE	GLN
P1394				F1156	P1058			I888	R788	R705	PRO				SER	THR	ASN
				D1157	D1061	W973	W973	P896	Y790	L615	GLY		H451	Y383	PRO	ALA	GLU
				R1158	D1061	Q983	Q983	P896	Y790	H616	ILE		I452		SER	VAL	ILE
				L1159	K1087	Q983	Q983	V897	L709	L617	LEU		D453	I387	SER	ARG	LEU
				V1160	Y1088	M987	M987	F898	R703	R618	GLY		H454		GLY	LYS	GLY
				A1161	Y1088	V988	V988	A999	L799	K619	ASP			P389	GLY	TYR	ASP
				G1162	Y1071	N989	N989	A999	L799	K620	LEU				GLY	LEU	LEU
				Q1163	I1072	L990	L990	L901	D811	E621	GLY		E458	A390	ASP	GLY	LEU
				P1165	I1072	D991	D991	N902	G812	E622	GLY			D392	THR	LYS	LYS
						K992	K992	G903	L813	F623	GLY		T462		ALA	ARG	GLU
						V993	V993	G904	L813	G624	ALA		Y463	K395	ALA	TRP	PHE
						V994	V994	L905	Y814	N625	GLY		Q464	A395	GLY	GLY	GLY
						V995	V995	F907	S816	W626	GLY				GLY	SER	SER
						T997	T997	P908	K818	E627	THR			V398	ALA	GLY	THR
						P1083	P1083	P909	L819	S561	LEU				MET	PRO	PRO
						G998	G998	D910	L824	S562	GLY			D400	LEU	GLY	GLU
						F1086	F1086	D911	L824	S563	LYS				MET	ARG	LYS
						E1001	E1001	L911	R827	K630	PRO			W405	ASP	GLN	PRO
						I1002	I1002	M915	W828	L632	GLY			A406	PHO	GLY	GLU
						G1003	G1003	L918	R827	L632	GLY			R407	ALA	ASP	GLY
						P1004	P1004	R919	W828	G634	THR			Q408	ALA	VAL	THR
						Q1095	Q1095	K920	W828	I635	PRO			D409	LEU	LEU	PRO
						L1096	L1096	E921	W828	A568	LEU				LEU	LEU	LEU
						L1097	L1097	E921	W828	L569	ASP					PHE	ASP
						Q1098	Q1098	I922	W828	Y570	GLU			S412	ALA	ALA	GLU
						E1099	E1099	I922	W828	V573	ILE			M413	ILE	ILE	GLU
						V1100	V1100	S926	S830	P485	THR			Y415	Q332	THR	GLY
						L1106	L1106	S926	S830	V486	ALA			D416	R333	ALA	ALA
						E1107	E1107	S926	S830	Y487	GLU			Y417	A334	GLU	SER
						P1108	P1108	S926	S830	V490	PRO			I418	L335	PRO	MET
						S1201	S1201	S926	S830	S491	GLN			P419	Q339	GLN	GLN
								S926	S830	T492	ALA			R421	L340	SER	ALA
								S926	S830	F746	THR					ARG	THR

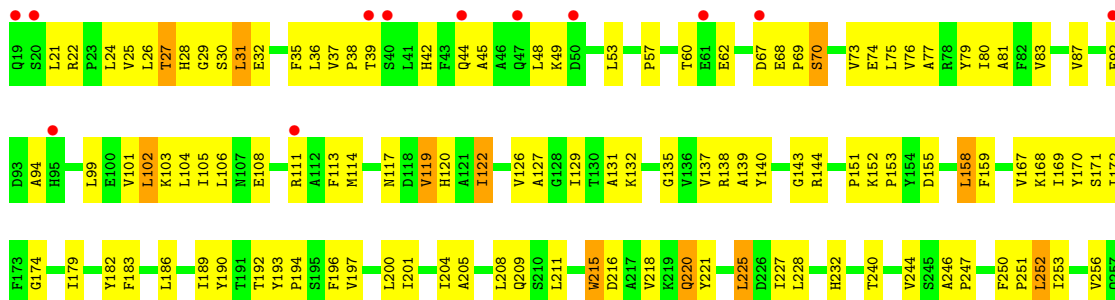


- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



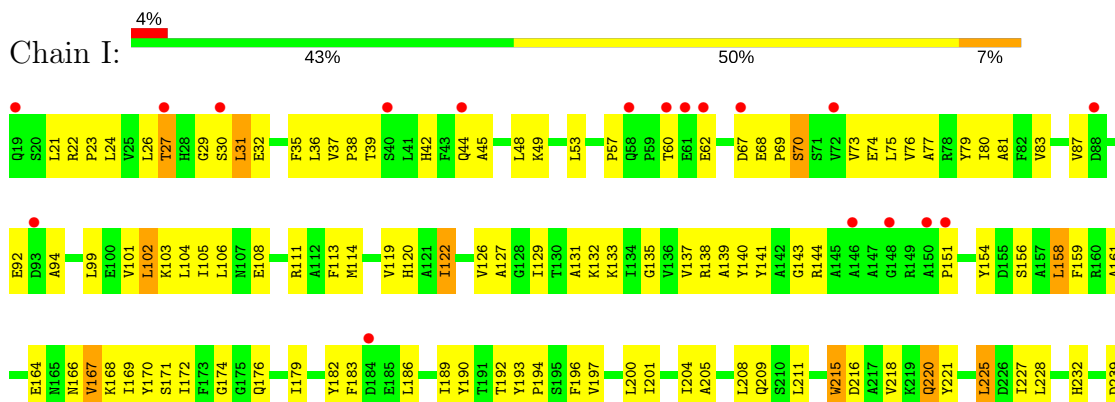
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V1661	Q1579	F1489	T1418	E1336	S1253	W1168	R1079	V994	P909	S830	L736	L640	A578	I500	D426
Q1662	V1580	G1490	K1419	P1337	F1254	D1169	L1080	V995	D910	E831	L736	G647	ASN	D501	R427
K1663	L1581	E1492	V1420	G1338	T1257	A1170	E1082	V996	L911	S832	L740	L648	GLU	A502	E428
		F1493	R1421	E1339	M1258		P1083	T997	M915	W833	D741	T649	SER	G504	V430
		W1494	R1422	M1340	Y1173	Y1173	F1086	G998	L918	L837	Y742	F650	GLN	N505	S431
		R1495	R1423	S1341	G1174	G1174	F1086	L999	R919	T838	V743	Q651	ILE	Q432	Q432
		R1496	Q1424	R1342	L1267	P1176	Y1089	A1000	R919	T839	V744	G652	MET	C433	C433
		R1499	L1425	T1344	S1268	E1177	D1090	E1001	K920	T839	P745	H653	GLN	L434	L434
			E1426	T1344	S1269	D1178	D1090	E1001	E921	W843	F746	H654	ASP	R517	Q435
					T1270	D1178	W1092	P1004	I922			A655	GLY	K518	L436
						I1180	R1093	W1005		R848	E751		LYS	L437	L437
							R1093	G1006	S926	G849		A687	ASP	K534	W436
							Q1094	A1007		T850	R754	E688	ARG	R439	W436
							Q1094	A1007	R929	G851	E755	V669	ARG	A527	S440
							L1096	Q930	Q930	L852	I756	L670	ARG		
							L1097			L853		L673	GLY	G530	L443
							Q1098	R1011	I933	W853	I759		ARG	P531	L444
							Q1099	M1014	K934	S854			ASN	I532	L445
							V1100	E1015	E935	A855			GLY	S533	E446
									I938	W857	K762	G677	ASN	S536	F447
							L1106	G1018		L858	H767	K679	GLY	S536	N448
							E1107	K1019		W859	R768	V680	ASN	N537	Q449
							P1108	F1020	V943		I769	I681	GLY	R538	Y450
								S1021	N944	W863	M770	V632	ASN	T539	H451
							K1113	L1022	G945	L866	L771	T633	HIS	K540	L452
							E1117	M1028	E946	G867	T772		SER	V541	D453
							E1118		H948	W868	R776	S688	ARG	Q542	H454
									H948	R869	L777	R639	PRO	N643	
										T870			GLY	P544	T457
							I1129	M1032	A850		T692			L545	E458
							F1130		L951	F871	A780	E693		V548	T462
							E1131	M1037	Y952	S872	I781			V549	L463
								N1038	R953		K782			K650	Q464
							Q1137	N1039	R954	Q874	T783			L551	
							Y1138	G1046	V955	E875		R701		L551	
							T1139	P1041	I956		R788			L552	
							V1140	L1042	P957	F876		R705		L553	
							L1141		E958	L881	Y790			R557	L474
							R1143	Y1046	P959		R793			L558	N476
								P1046	R960	L883				S559	C477
							L1148	W1050	N962	W884	L799			K560	K478
							L1149	V1051	L963					S561	E479
							I1150	D1052	K964	T888	D811			S562	E479
							P1151		Y965	W889	G812			S562	L481
							K1152	T1055	P966	N890	L813			L564	
							A1153	G1056	P967		Y814			Q565	P484
							L1154	E1057	P968	P896	S915			P566	
							Q1155	P1058	E969	W897	E916			E527	P485
							F1156		L970	F898	D721			N567	V486
							D1157	D1061		A899	S817			A588	Y487
							R1158		W973	D900	L725			L569	V490
							L1159	K1067			V726			K630	
							V1160	Y1068	Q983		W727			Y570	
							A1161			G903	L821			K571	S491
							Q1162	Y1072	V988	G904	L824			D572	L492
							L1250	I1071	N989	L905	Y730			V573	P493
							I1164	I1072	N989	Q906	R627			I574	T494
									L990	F907	W828			A576	T498



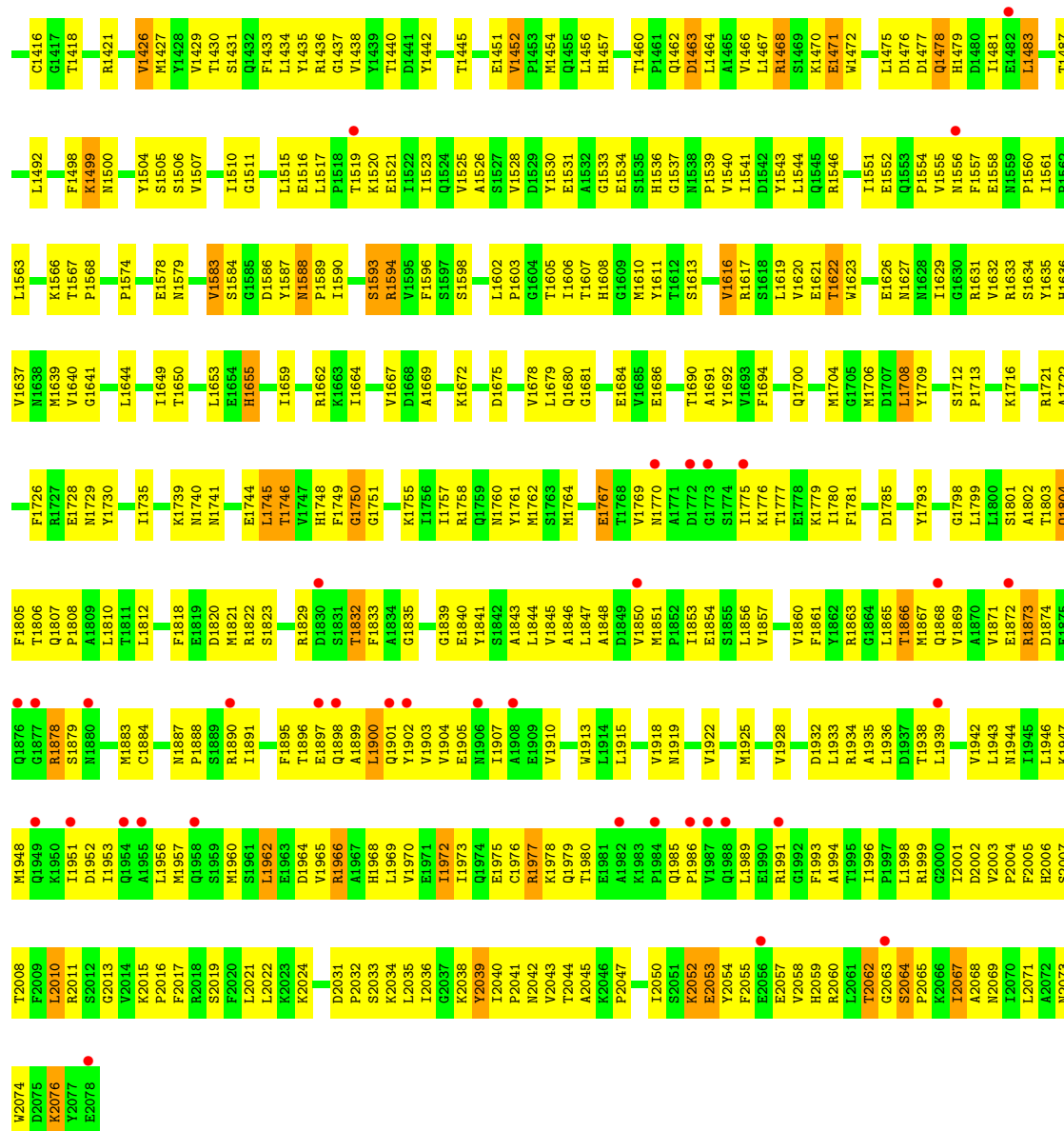


R1281	N1208	R1137	L1067	A999	D928	R849	F782	L709	Y635	Y554	G475	R406	R321	L258
P1209	P1209	D138	Q1068	Y1000	M929	P859	G783	R712	Y636	K555	Q476		Q324	A259
D1210	D1210	A139	G1069	P1001	Y931	T851	G784	H713	M637	P556	D477	A410	P324	H260
D1211	D1211	N140	P1070	E1002	T930		S785	H713	A638	E557	L478	P411	Y261	Y261
P1212	P1212	K141	A1071	A1003	A932	H854	E786	I714	M641	L558	R479	T412	Y326	M262
		I142	A1072	S1004	E933	T855	D787	S715		F559	E480	G413	P327	L263
F1288	T1215	S143	A1073	T1005	V934	T856	T788			D560	L481	L414		T264
Y1289	V1216		K1074	Q1006	V935	H857	T789	P718	T645	R561	G482	D415	L331	C265
Y1290	I1217	L146	Y1075	L1007	H936	L858	P790	G719	S646	D562		Q416	A332	K266
R1291	S1218		Y1076	M1008	R937	S859	Y791		S646	D563			A332	K266
V1292	S1219	N153	K1077	M1009	M938	E860	L792	A723	I648		D485	I419	P333	L268
V1293	R1220	L154		A1010	V939	H861	G794	G725	E650	V573	L486	P420	T335	G269
F1294		P155	D1080	Q1011	E940	G862	G795	G726	K651		L487	F421		R270
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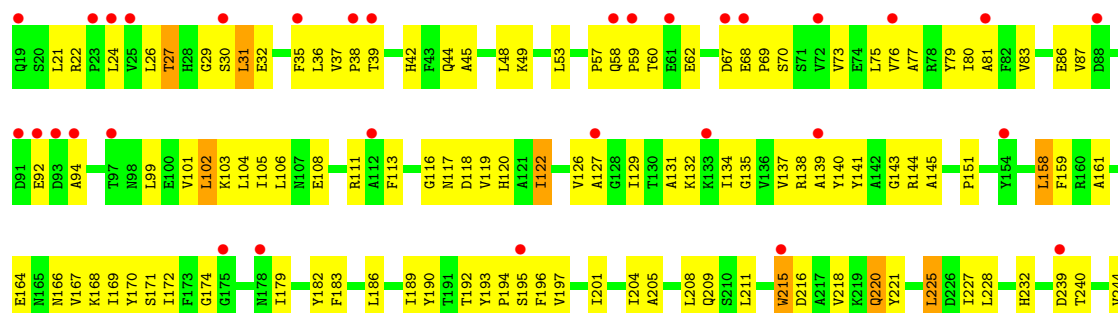
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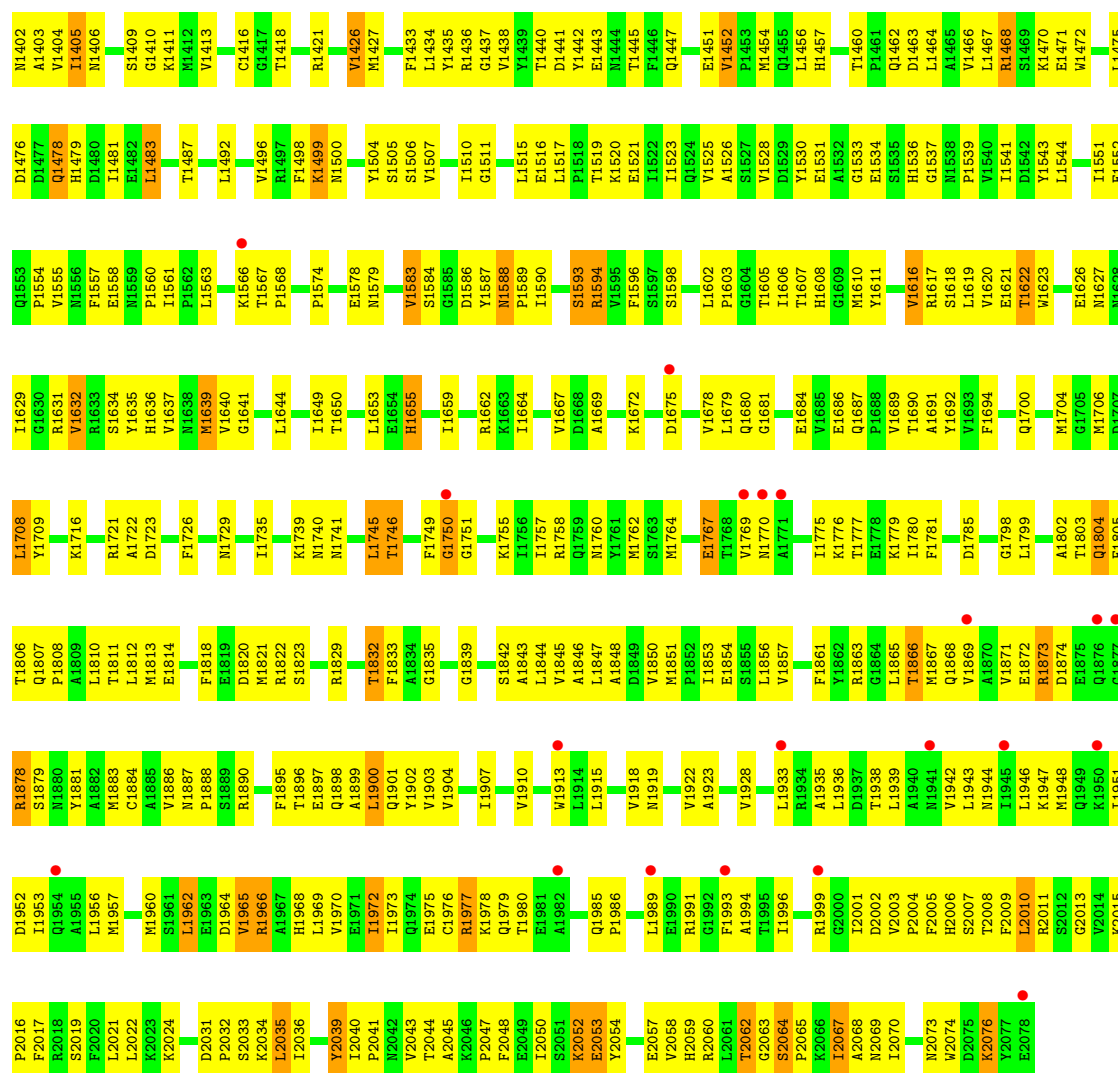




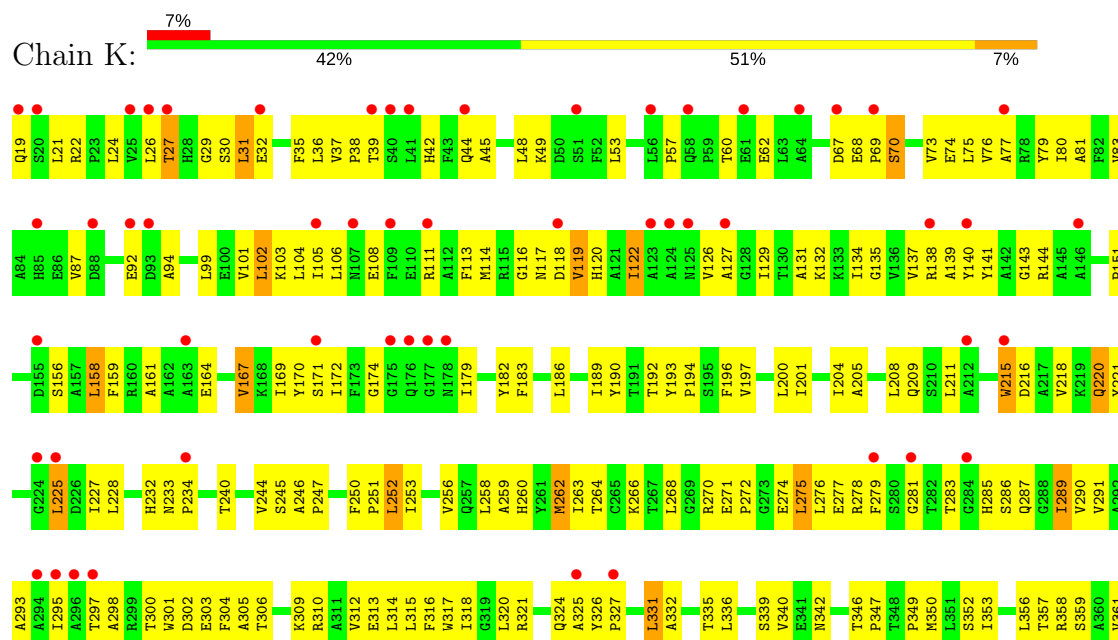
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



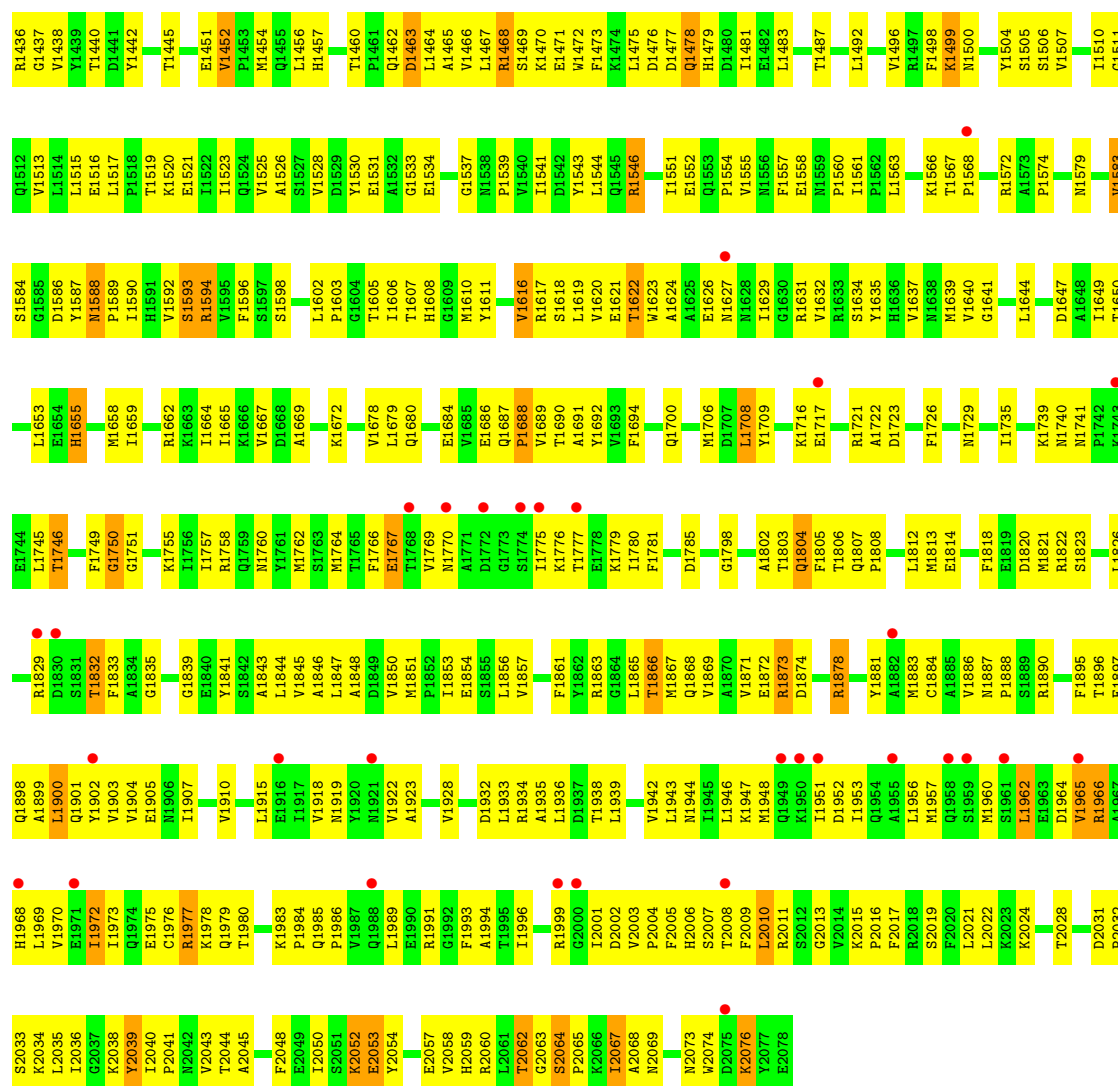
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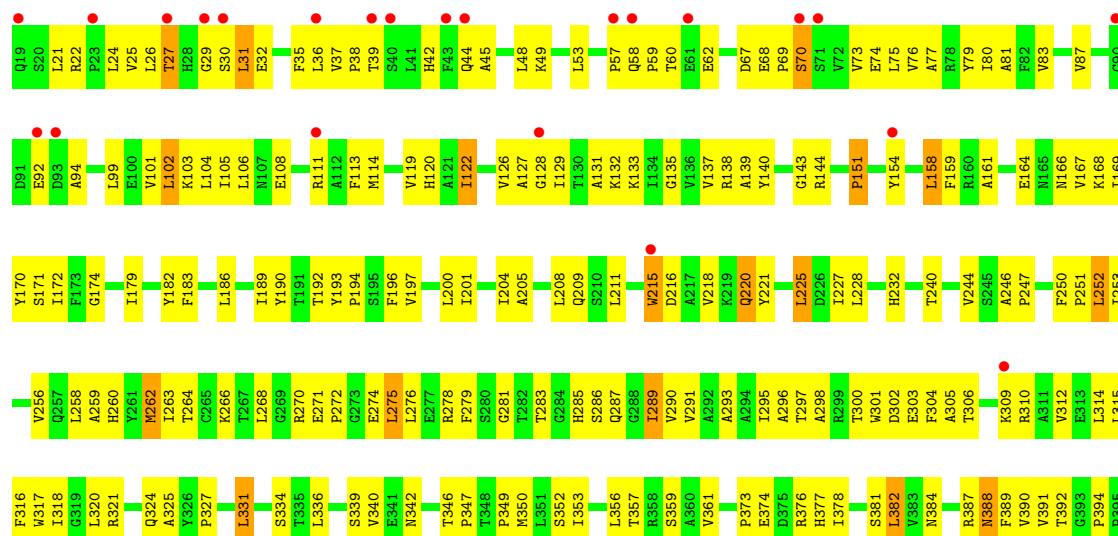
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



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P1363	W1294	K1218		V1078	D1012	R941	T870	D908	R747	W672	H512	H512	R376
I1364		V1219		I1079	V1013	K942	R871	G809	G748	Q673	P601	P601	H377
K1365	K1297	R1220		D1080	W944	G943	G872	M811	G750	P675	D515	D515	H378
I1366	E1298					Y944			H752	L676	G517	G517	S381
D1369	V1299	S1223		I1083	K948	K948	W875	S814	E785	B679	G520	V455	L382
L1370	F1300	K1224		T1084	R949	R949	K877	R815	D756	V605	V521	V456	V383
L1371	F1301	S1225		D1088	L1017	V950	E878	M816	F757	P685	S522	D457	R387
K1372	T1303	K1227		G1089	L1019	I951	L879	M818	D758	G607	R388	M458	N388
L1373	P1304	L1228		H1091	C1020	D952	D880	M817	F759	P686	M608	K459	V390
V1374	L1305	L1229		N1092	R1022	P953	D881	T818	H758	T609	V526	V526	P461
H1375	T1306	K1230		N1092	R1022	S954	K892	A819	Q759	E688	P610	P610	V391
	A1307			D1093	Q1025	L955	I883	K820	P760	G683	T528	T528	T392
	V1308			H1094	F1030	K956	F884	E821	I761	L690	N529	N529	G393
F1309	F1309			I1095	K1026	K957		A822	L762	V613	D533	D533	P394
R1313	R1313	L1236		F1097	P1027	L958	R888	H823	L763	P614	I540	I540	P395
E1314	E1314	V1237		L1098	V1028	T959		S825	W764	W615	V466	V466	I396
G1392	V1315	G1238		L1099	P1029	R891	R891	S825	W764	W615	V466	V466	I396
V1316	V1316	D1239		L1099	F1030	F962	E884	Q827	S766	D616	I540	I540	
A1317	A1317	N1240		R1100	V1031	I963	L895	K826	R767	V617	L541	L541	
A1318	A1318				P1032	R983		A828	P697	V618	A542	A542	
Q1319	Q1319	T1245		Y1103	A1033	R965	L896	K828	S698	G543	G543	G543	
D1323	D1323	L1246		D1104	L1034	V966	K897	K829	T621	L401	A544	A544	
F1324	F1324	F1247		G1105	D1035	E967			M622	T472	N402	N402	
		G1248		K1106	E1036	E968	I903	V833	C771	E700	I545	I545	
		R1250		E1107	D1036	R969	K904	D834	S773	A702	D546	D546	
		T1251		E1108	E1039	F970	K905	A835	N773	W703	T548	T548	
		V1256		N1109	V1040	I971	L906	P836	I774	E704	N549	N549	
		V1257		V1110	W1042	S972		G837	W775	Y705	T550	T550	
		L1258		Y1111	F1043	Q976	D909	V838	L776	I706	E551	E551	
		L1259		Y1112	K1044	P977		D839	W777	Q707	E629	E629	
		T1260		E1113	L1047	S978		D841	G779	L709	G553	G553	
		F1261		Y1115	W1048	L979		Q842	S780	K635	Y554	Y554	
		R1262		F1116	Q1049	L980		W843	G781	N637	K555	K555	
					S1050	Q981		E844	F782	A638	P556	P556	
					E1051	D985		N845	G783	E557	E557	E557	
					D1052	R986		T846	G784	L558	L558	L558	
					I1053	S987		Y847	S785	I419	F559	F559	
					Y1057	E988		K848	G794	I486	P420	P420	
					V1061	P989		R849	S786	T487	P421	P421	
					G1062	Y990		P850	D787	P488	T422	T422	
					R1063	P991		T851	Y789	E489	Q423	Q423	
					T1064	P991		V854	P790	V491	R424	R424	
					R1065	R995		T855	Y791	K492	K425	K425	
					T1066	R996		T856	L792	A851	A426	A426	
					I1067	L997		V857	G793	P578	R427	R427	
					L1068	A998		L858	S795	L580	F432	F432	
					G1069	A999		S859	G796	V581	L433	L433	
					P1070	Y1000		Y931	W796	N500	P434	P434	
					E1002	P1001		M861	S797	T583	I435	I435	
					T1005	E1002		G862	T798	S584	T436	T436	
								G862	F799	T503	F439	F439	
								G862	P738	T505	T505	T505	
								G862	T739	T505	T505	T505	



● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



S1409	R1338	V1256	F1181	E1107	E1039	R965	L895	K829	Y765	T691	F617	L541	V466	I396
G1410	G1339	V1257	R1186	E1108	Y1040	V966	K896	K829	S766	A694	V618	A542	I467	
K1411	L1259	P1258	F1187	N1109	Y1041	E967	R898	T832	R767	A694	A619	G543	P468	Y399
M1412	F1342	T1260	Q1188	P1111	E1042	E969	I903	R833	R769	S698	T621	N401	Y470	G400
V1413	F1261	R1261	T1189	V1112	K1043	E970	K904	D834	K770	L699	M622	N402	D471	N402
	R1262		N1190	I1113	K1044	T971	K905	A835	C771	E700	N623	L403	T472	L403
C1416	P1345	Y1265	P1191	E1114	W1048	Q976	L906	P836	S772	V701	Y626	T548	K473	R404
G1417	M1346	H1266	L1192	Y1115	Q1049	P977	L906	C837	N773	A702	H627	N549	T474	L405
T1418	F1347	P1267	K1193	F1116	S1050	S978		D839	E704	E703	Q475	E551	K475	R406
					E1061	L979		D840	Y705	Y706	Q476	G553	D477	K407
R1421	A1349	E1268	F1196	I1120	E1052	L980		D841	Y706	Y707	E629	Y554	L478	
K1424	I1350	A1269	A1197	D1121	I1062			D842	Y707	Y708	Y635	K555	R479	A410
P1425	V1352	G1270	P1199	I1083	I1083			Q842	Y708	Y709	Y636	P556	E480	P411
M1427	G1353	E1271	D1200	Y1057	Y1057	D985		W843	G779	L708	N637	E557	L481	T412
	K1354	I1274	G1201	V1061	V1061	L986		N845	S780	L709	R561			
L1434	K1355	R1275	M1202	E1126	G1082	D987		T846	F781	R712	A638	D483	D485	L414
Y1435	A1356	E1276	Y1203	E1127	R1083	P989		Y847	G783	H713	M641	F484		D415
G1437	K1359	M1278	V1204	P1128	R1083	Y990		K846	G784	T714	Q667	D485		Q416
V1438	P1360	R1284	I1206	C1085	C1085	P991		R849	S785		A644			N417
F1439	I1361	F1285	T1207	I1130	I1130			R850	E786	F716	I645	L486		L419
T1440	P1362	I1285	G1132	L1067	L1067	I996		T851	D787	K717	S646	P488		P420
D1441	F1363	K1286	Q1068	Q1068	Q1068	L997		V854	T788	P718	K647	E489		F421
Y1442	R1364	E1287	G1088	G1088	G1088	A999		I855	Y789	G719	I648	L490		T422
T1445	K1365	F1288	R1137	D1138	V1071	Y1000		T856	P790	A723	K650	P578		Q423
E1451	I1366	Y1289	T1215	N1140	A1073	E1002		W857	F791	T724	A651	L580		K425
P1452	D1367	R1290	I1216	K1141	A1073	I922		R858	T793	L792	I652	V581		F432
F1453	P1368	R1291	I1217	K1142	K1074	E922		S859	G794	Q726	P653	K574		L433
L1454	L1370	V1292	S1143	S1142	Y1075	T930		E860	Y796	V727	R656	S584		P434
Q1455	K1372	F1294	L1146	L1146	S1076	L1006		K861	S797	I730	G657	Q587		I435
V1456	V1374	K1297	S1223	N1153	D1080	L1007		E862	A932	A731	N661			H500
H1457	H1375	V1298	G1224	L1154	I1083	I1008		P864	K799	N734	L662	V590		T436
		P1300	S1225	P1155	K1084	A1010		R866	F800		I663	D591		P438
T1460	Y1380	F1301	A1226	D1156	D1085	D1012		K867	Y802	F737	Y664	M594		F439
P1461	R1381	L1305	K1227	D1157	D1086	Q1014		L868	P803	P738	V665	S595		H440
D1463	M1382	L1305	L1228	D1158	L1087	H1015		A869	P804	I739	N666	M594		L444
L1464	P1388	V1308	V1229	S1159	L1087	F1016		T870	M805	L741	P667	R595		L447
V1465	V1309	D1310	K1230	F1160	G1088	L1017		R871	P806	Q742	M670	L597		A447
V1466	V1391	I1234	I1234	I1164	I1090	L1018		G872	F807	W743	G671	V600		H448
L1467	G1392	K1235	L1236	L1154	H1091	L1019		F875	G809	W743	W672	P601		I449
R1468	D1393	L1236	L1237	P1155	N1092	C1020		W876	C810	G746	Q673	P602		H450
S1469	V1394	E1314	V1237	D1156	D1093	Q1021		L879	M811	R747	I674	V603		I451
K1470	L1395	I1315	G1238	D1157	H1094	R1022		P880	M815	G750	P675	M604		L452
E1471	P1396	V1316	D1239	Y1169	I1095	K1026		D881	R815	H751	L676	V605		G453
F1472	T1397	N1317	N1240	S1170	K1096	P1027		K882	R816	H752	R679	A606		D454
F1473	T1398	Q1319	T1245	W1171	F1097	V1028		I883	M817			G607		V455
K1474	A1399	Q1319	L1246	H1172	L1098	P1029		F884	T818	E755	D683	M608		D456
L1475	Q1400	R1173	R1173	L1099	F1030	L958		R888	A819		G684	T609		D457
I1401	F1324	H1174	F1247	R1100	I1031	T960		S889	K820	Q759	V685	P610		K459
D1477	N1402	M1175	E1248	Y1103	P1032	G960		R889	E821	T611	T612	T612		I460
Q1478	A1403	G1249	G1249	T1178	A1033	D861		K890	A822	I761	I687	V613		A462
H1479	V1404	R1250	R1250	G1104	I1034	F963		R891	E888	L762	P614	S463		S463
D1480	I1405	E1179	G1105	D1105	D1035	I963		E894	Q827	L763	W615	S464		S464
I1481	N1406	F1335	F1335	N1180	E1036	R964				M764	L690	D616		L465

K2015	Q1954	M1813	K1716	R1631	M1556	E1482
P2016	A1955	E1814		V1632	F1557	L1483
F2017	V1886		R1721	S1633	E1558	
R2018	M1887	F1818	A1722	S1634	M1559	T1487
S2019	P1888	E1819		V1635	P1560	L1488
P2020	S1889	D1820	F1726	H1636	I1561	V1489
L2021	R1890	M1821		V1637	P1562	
L2022	T1894	R1822	K1739	M1638	L1563	L1492
K2023	F1895	S1823	M1740	M1639	K1566	F1498
K2024	T1896		P1742	G1641	T1567	K1499
	E1897	Q1828			P1568	M1500
T2028	R1966	D1830	L1745	L1644	R1572	Y1504
T2029	A1967	S1831	T1746	P1645	A1573	S1505
I2030	H1968	T1832		M1646	P1574	S1506
D2031	L1969	F1833	F1749	D1647	A1575	V1507
P2032	V1970	G1834	G1750	A1648		
S2033	E1971	G1835	G1751	I1649		
K2034	I1972			T1650		
L2035	I1973	G1839	K1755	L1653	M1579	I1510
L2036	Q1974	E1840		E1654	V1583	G1511
G2037	E1975	Y1841	R1758	H1655	S1584	L1514
K2038	C1976	S1842	Q1759		G1585	L1515
Y2039	R1977	L1843	M1760		D1586	E1516
I2040	K1978	L1844	Y1761	I1659	Y1587	L1517
P2041	Q1979	V1845	M1762		M1588	F1518
N2042	T1980	A1846	S1763	R1662	P1589	L1519
V2043	E1981	L1847	M1764	K1663	I1590	K1520
T2044	A1982	A1848	T1765	I1664	H1591	E1521
A2045	K1983	D1849	F1766		V1592	I1522
K2046	P1984	V1850	E1767	V1667	S1593	I1523
P2047	Q1985	M1851	T1768	D1668	R1594	Q1524
	P1986	M1852	V1769	A1669	V1595	V1525
I2050	N1987	I1853	M1770		F1596	A1526
S2051	V1922	E1854		K1672		S1527
K2052	A1923	S1855	I1775		L1502	V1528
E2053		L1856	K1776		P1603	D1529
Y2054	Q1926	V1857	T1777	D1675	G1604	Y1530
	Y1927		E1778		T1605	E1531
E2057	V1928	F1861	K1779	V1678	T1606	A1532
V2058		Y1862	T1780	L1679	H1607	G1533
H2059	D1932	R1863	F1781	Q1680	H1608	E1534
R2060	L1933	G1864		G1681	G1609	S1535
L2061	R1934	L1865	D1785		M1610	H1536
T2062	A1935	T1866		E1684	Y1611	G1537
G2063	R1936	M1867	S1788	V1685		N1538
S2064	D1937	Q1868		Q1687	V1616	P1539
K2065	L1938	V1869	Y1793	P1688	R1617	V1540
P2066	I2001	A1870		T1690	S1618	I1541
K2067	D2002	V1871	L1799	A1691	L1619	D1542
A2068	V2003	E1872	A1802	V1692	V1620	Y1543
N2069	F2005	R1873	T1803	G1693	E1621	L1544
	H2006	D1874	Q1804	F1694	T1622	Q1545
N2073	S2007		F1805		W1623	R1546
W2074	L1946	R1878	T1806	M1706		
	T2008	S1879	Q1807	D1707	E1626	I1551
D2075	K1947	N1880	P1808	Y1709	M1627	E1552
K2076	M1948	Y1881			N1628	Q1553
		A1882			I1629	P1554
Y2077	I1951	M1883	L1812		G1630	V1555
E2078	D1952					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	216.37Å 414.43Å 221.51Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 88.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 89.5 (88.45-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.13Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, R_{free}	0.290 , 0.320 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , -83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.280 for l,-k,h	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	166671	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1451/1878 (77%)	1291 (89%)	148 (10%)	12 (1%)	22	62
1	B	1458/1878 (78%)	1295 (89%)	151 (10%)	12 (1%)	22	62
1	C	1456/1878 (78%)	1293 (89%)	151 (10%)	12 (1%)	22	62
1	D	1461/1878 (78%)	1290 (88%)	155 (11%)	16 (1%)	17	54
1	E	1450/1878 (77%)	1292 (89%)	146 (10%)	12 (1%)	22	62
1	F	1455/1878 (78%)	1300 (89%)	140 (10%)	15 (1%)	18	57
2	G	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	14	48
2	H	2058/2060 (100%)	1786 (87%)	244 (12%)	28 (1%)	13	47
2	I	2058/2060 (100%)	1799 (87%)	233 (11%)	26 (1%)	14	48
2	J	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	2058/2060 (100%)	1772 (86%)	258 (12%)	28 (1%)	13	47
2	L	2058/2060 (100%)	1777 (86%)	253 (12%)	28 (1%)	13	47
All	All	21079/23628 (89%)	18479 (88%)	2359 (11%)	241 (1%)	17	54

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%)	9	35
1	B	1227/1527 (80%)	1111 (90%)	116 (10%)	10	37
1	C	1225/1527 (80%)	1102 (90%)	123 (10%)	9	33
1	D	1229/1527 (80%)	1110 (90%)	119 (10%)	9	35
1	E	1219/1527 (80%)	1101 (90%)	118 (10%)	9	35
1	F	1224/1527 (80%)	1109 (91%)	115 (9%)	10	38
2	G	1752/1752 (100%)	1571 (90%)	181 (10%)	8	32
2	H	1752/1752 (100%)	1579 (90%)	173 (10%)	9	34
2	I	1752/1752 (100%)	1571 (90%)	181 (10%)	8	32
2	J	1752/1752 (100%)	1573 (90%)	179 (10%)	8	32
2	K	1752/1752 (100%)	1575 (90%)	177 (10%)	9	33
2	L	1752/1752 (100%)	1576 (90%)	176 (10%)	9	33
All	All	17856/19674 (91%)	16079 (90%)	1777 (10%)	9	33

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	-	31,33,33	6.25	21 (67%)	38,50,50	1.70	4 (10%)
3	FMN	H	2101	-	31,33,33	6.24	20 (64%)	38,50,50	1.82	8 (21%)
3	FMN	I	2101	-	31,33,33	6.25	19 (61%)	38,50,50	1.85	7 (18%)
3	FMN	J	2101	-	31,33,33	6.45	21 (67%)	38,50,50	1.93	8 (21%)
3	FMN	K	2101	-	31,33,33	6.47	22 (70%)	38,50,50	1.79	9 (23%)
3	FMN	L	2101	-	31,33,33	6.22	19 (61%)	38,50,50	1.78	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	G	2101	-	-	0/16/18/18	0/3/3/3
3	FMN	H	2101	-	-	0/16/18/18	0/3/3/3
3	FMN	I	2101	-	-	0/16/18/18	0/3/3/3
3	FMN	J	2101	-	-	0/16/18/18	0/3/3/3
3	FMN	K	2101	-	-	0/16/18/18	0/3/3/3
3	FMN	L	2101	-	-	0/16/18/18	0/3/3/3

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2101	FMN	C8M-C8	2.01	1.55	1.51
3	L	2101	FMN	C5'-C4'	2.04	1.54	1.51
3	G	2101	FMN	C7M-C7	2.08	1.55	1.51
3	G	2101	FMN	C8M-C8	2.11	1.55	1.51
3	J	2101	FMN	C7M-C7	2.13	1.55	1.51

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2101	FMN	C4A-C4-N3	-3.10	119.07	123.48
3	H	2101	FMN	C4A-C10-N10	-2.91	118.50	120.52
3	J	2101	FMN	C1'-N10-C9A	-2.82	115.76	118.35
3	L	2101	FMN	C4A-C4-N3	-2.60	119.78	123.48
3	K	2101	FMN	C1'-N10-C9A	-2.55	116.01	118.35

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	1457/1878 (77%)	-0.50	14 (0%)	82	67	17, 54, 105, 150	0
1	B	1464/1878 (77%)	-0.51	12 (0%)	86	71	16, 52, 111, 158	0
1	C	1462/1878 (77%)	-0.51	17 (1%)	79	61	15, 51, 111, 159	0
1	D	1467/1878 (78%)	-0.52	13 (0%)	84	69	17, 54, 108, 158	0
1	E	1456/1878 (77%)	-0.48	13 (0%)	84	69	15, 54, 110, 157	0
1	F	1461/1878 (77%)	-0.54	12 (0%)	86	71	16, 51, 108, 159	0
2	G	2060/2060 (100%)	-0.12	38 (1%)	69	47	27, 83, 129, 169	0
2	H	2060/2060 (100%)	-0.05	69 (3%)	47	24	24, 86, 132, 167	0
2	I	2060/2060 (100%)	-0.02	73 (3%)	44	22	23, 86, 132, 167	0
2	J	2060/2060 (100%)	0.03	66 (3%)	48	25	28, 89, 133, 172	0
2	K	2060/2060 (100%)	0.25	134 (6%)	20	7	27, 91, 136, 172	0
2	L	2060/2060 (100%)	0.01	76 (3%)	42	21	23, 87, 133, 172	0
All	All	21127/23628 (89%)	-0.20	537 (2%)	58	35	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 ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FMN	G	2101	31/31	0.94	0.20	0.20	19,64,105,124	0
3	FMN	I	2101	31/31	0.93	0.18	-0.38	23,54,85,115	0
3	FMN	L	2101	31/31	0.94	0.18	-0.38	15,51,89,119	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.