



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:53 am GMT

PDB ID : 2PFF
Title : Structural Insights of Yeast Fatty Acid Synthase
Authors : Xiong, Y.; Lomakin, I.B.; Steitz, T.A.
Deposited on : 2007-04-04
Resolution : 4.00 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
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

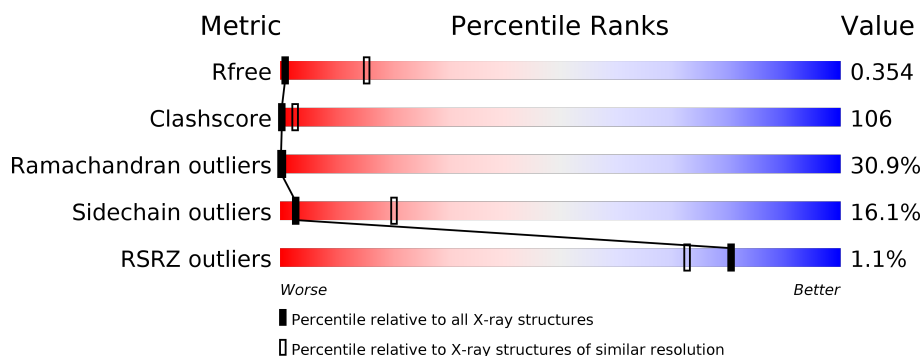
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.





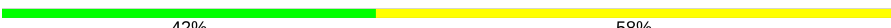
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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	1688	<div> <div>27%</div> <div>46%</div> <div>22%</div> <div>5%</div> </div>
1	D	1688	<div> <div>27%</div> <div>46%</div> <div>22%</div> <div>5%</div> </div>
1	G	1688	<div> <div>27%</div> <div>46%</div> <div>22%</div> <div>5%</div> </div>
2	B	2006	<div> <div>%</div> <div>34%</div> <div>54%</div> <div>11%</div> <div>•</div> </div>
2	E	2006	<div> <div>%</div> <div>34%</div> <div>54%</div> <div>11%</div> <div>•</div> </div>
2	H	2006	<div> <div>%</div> <div>34%</div> <div>54%</div> <div>11%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	65	 48% 52%
3	F	65	 45% 55%
3	I	65	 42% 58%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71862 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	D	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	G	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			
2	E	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			
2	H	2006	Total	C	N	O	S	0	0	0
			12310	7625	2253	2416	16			

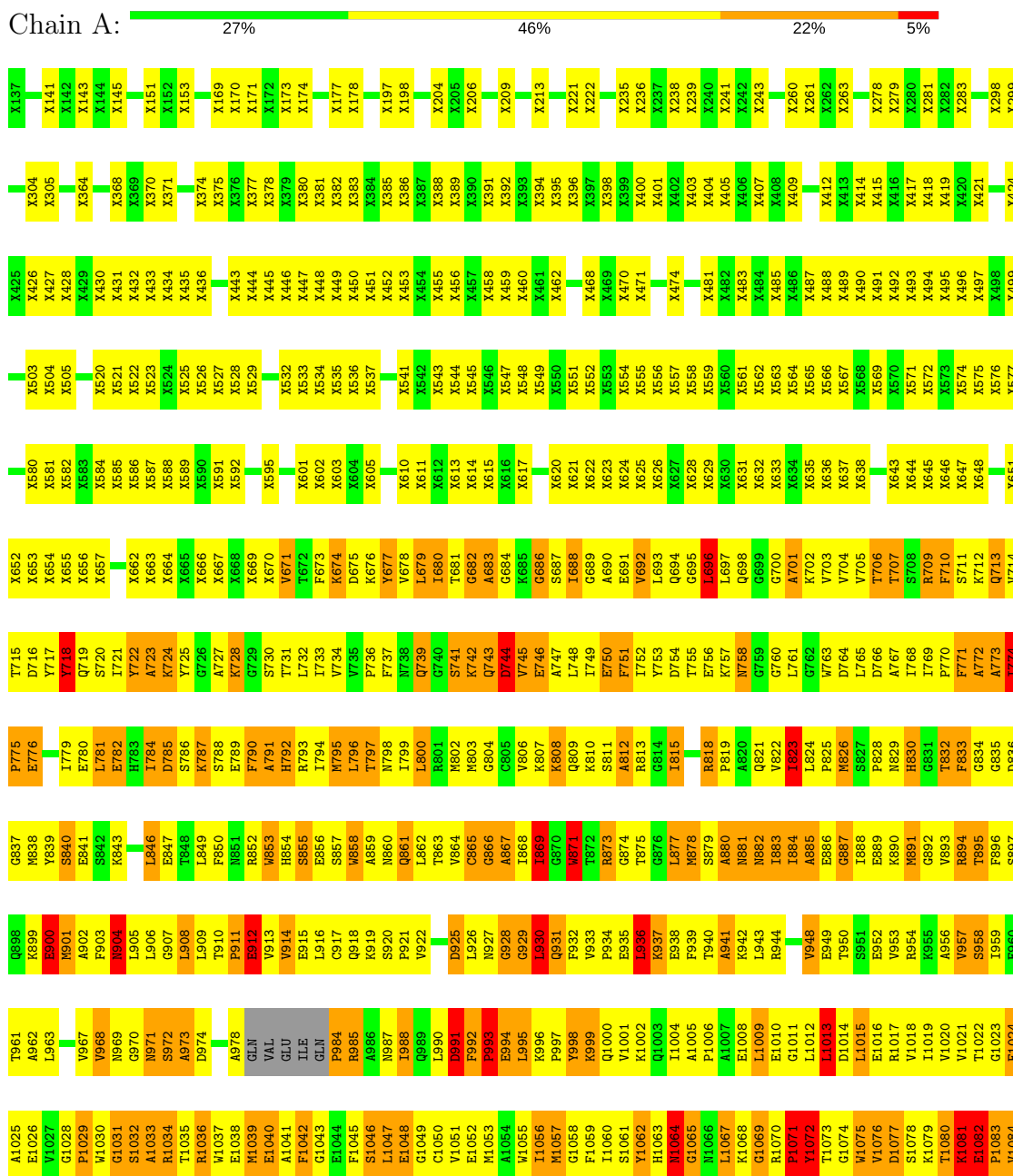
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	F	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	I	65	Total	C	N	O	0	0	0
			325	195	65	65			

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 subunit alpha

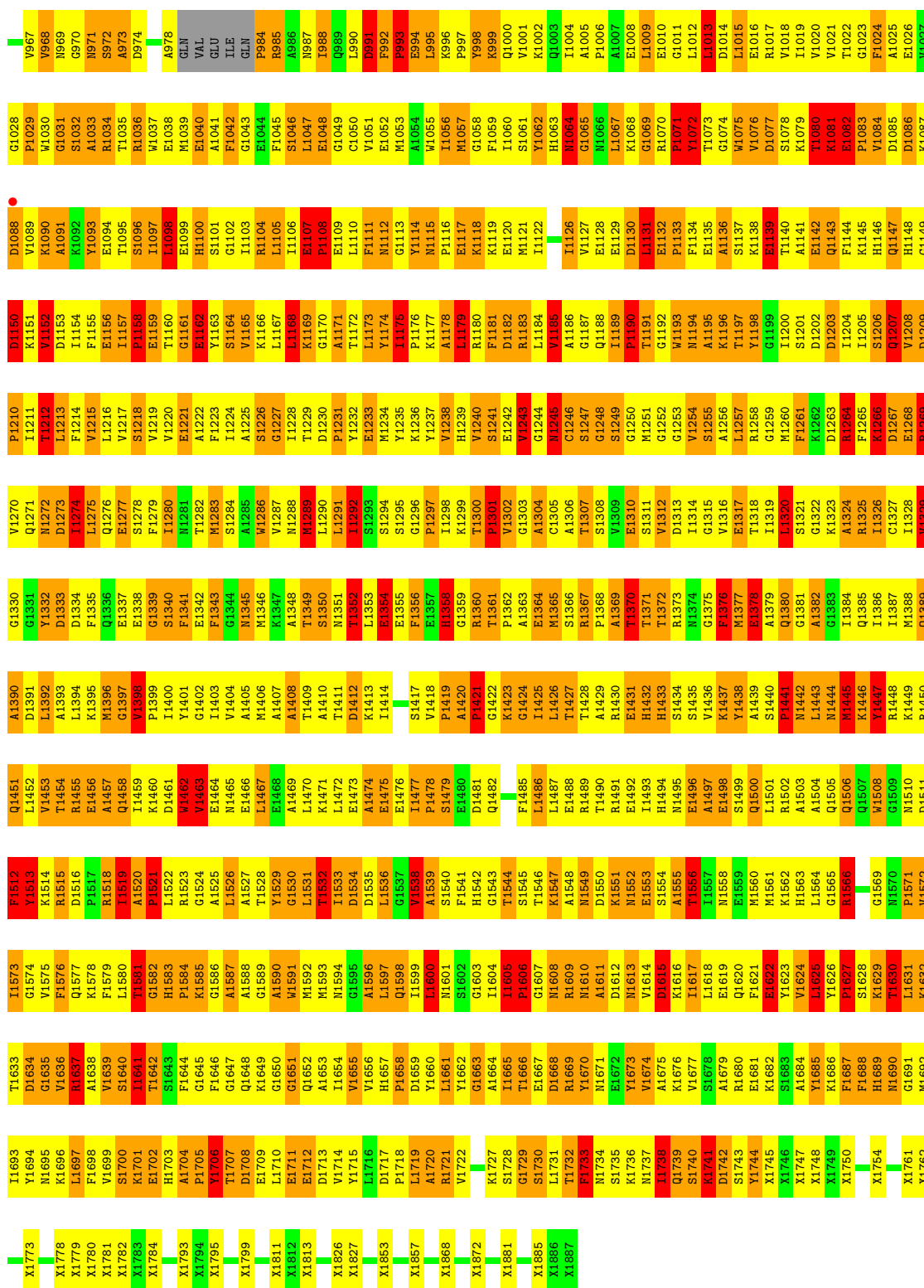


- Molecule 1: Fatty acid synthase subunit alpha

Frequency	Percentage
Daily	27%
Often	46%
Sometimes	22%
Never	5%



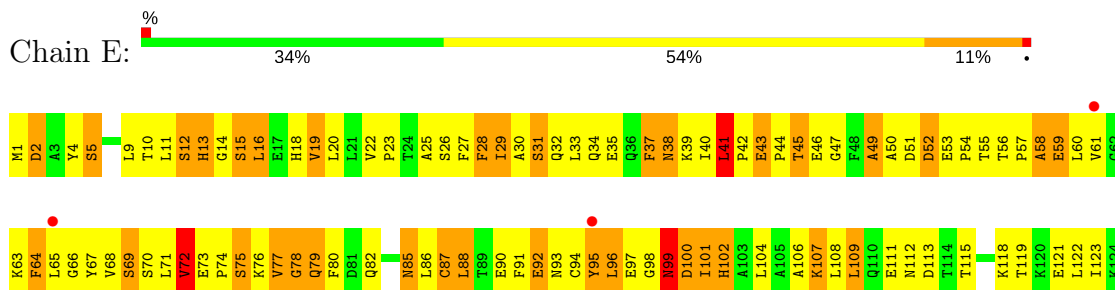
T1454	R1455	E1456	A1457	T1458	L1459	K1460	D1461	V1462	E1463	E1464	M1465	E1466	L1467	E1468	A1469	T1470	L1471	K1472	E1473	A1474	E1475	E1476	L1477	V1478	P1479	E1480	D1481	Q1482		F1485	L1486	L1487	E1488	R1489	T1490	R1491	E1492	I1493	H1494	N1495	E1496	A1497	E1498	S1499	Q1500	L1501	R1502	M1503	F1504	L1505	M1506	K1507	Y1508	R1509	L1510	F1511	L1512	L1513																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L1394	K1395	M1396	Q1397	P1398	E1399	L1400	Y1401	G1402	E1403	V1404	A1405	M1406	A1407	A1408	T1409	L1410	T1411	D1412	K1413	L1414	G1415	E1416	E1417	V1418	P1419	A1420	P1421	G1422	K1423	G1424	L1425	L1426	T1427	T1428	A1429	R1430	E1431	H1432	H1433	H1434	A1435	E1436	K1437	M1438	L1439	Q1440	P1441	N1442	L1443	N1444	M1445	K1446	Y1447	R1448	K1449	R1450	Q1451	L1452	R1453																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
D1333	D1334	F1335	Q1336	E1337	E1338	G1339	F1340	F1341	E1342	F1343	G1344	M1345	M1346	K1347	V1348	T1349	L1350	M1351	L1352	L1353	E1354	E1355	F1356	E1357	H1358	L1359	P1360	P1361	P1362	A1363	E1364	M1365	L1366	R1367	T1368	S1369	E1370	E1371	L1372	L1373	E1374	F1375	M1376	L1377	L1378	L1379	G1380	G1381	A1382	G1383	K1384	Q1385	L1386	L1387	M1388	Q1389	A1390	D1391	L1392	A1393																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
D1273	L1274	L1275	Q1276	E1277	S1278	V1279	L1280	M1281	T1282	M1283	S1284	A1285	M1286	V1287	L1288	M1289	L1290	L1291	L1292	S1293	S1294	S1295	G1296	P1297	L1298	K1299	T1300	P1301	V1302	G1303	A1304	L1305	L1306	T1307	S1308	E1309	E1310	S1311	D1312	V1313	G1314	G1315	L1316	E1317	L1318	L1319	L1320	S1321	G1322	K1323	A1324	R1325	L1326	C1327	M1328	L1329	V1330	G1331	Y1332																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L1213	F1214	V1215	L1216	V1217	S1218	V1219	L1220	E1221	A1222	F1223	L1224	A1225	S1226	G1227	L1228	T1229	D1230	P1231	Y1232	E1233	M1234	Y1235	K1236	V1237	L1238	H1239	L1240	S1241	E1242	V1243	G1244	R1245	G1246	S1247	G1248	S1249	G1250	M1251	G1252	G1253	V1254	S1255	A1256	L1257	L1258	L1259	G1260	F1261	K1262	D1263	R1264	F1265	K1266	D1267	M1268	F1269	L1270	Q1271	N1272																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
D1153	L1154	F1155	E1156	L1157	P1158	E1159	T1160	G1161	E1162	L1163	S1164	L1165	K1166	L1167	L1168	K1169	G1170	A1171	T1172	L1173	Y1174	L1175	P1176	K1177	A1178	L1179	R1180	F1181	D1182	R1183	L1184	V1185	G1186	G1187	Q1188	L1189	P1190	T1191	G1192	M1193	V1194	A1195	L1196	T1197	L1198	G1199	L1200	S1201	D1202	D1203	L1204	L1205	S1206	Q1207	V1208	L1209	P1210	L1211	T1212																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
A1091	K1092	Y1093	E1094	L1095	S1096	L1097	L1098	E1099	H1100	S1101	G1102	L1103	R1104	F1045	L1106	E1107	P1108	E1109	L1110	F1111	M1112	G1113	Y1114	L1115	P1116	E1117	L1118	F1181	D1182	R1183	L1184	V1185	G1186	G1187	Q1188	L1189	P1190	T1191	G1192	M1193	V1194	A1195	L1196	T1197	L1198	G1199	L1200	S1201	D1202	D1203	L1204	L1205	S1206	Q1207	V1208	L1209	P1210	L1211	T1212																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1031	S1032	A1033	R1034	T1035	R1036	V1037	E1038	M1039	E1040	A1041	F1042	G1043	E1044	F1045	L1106	E1107	P1108	E1109	L1110	F1111	M1112	G1113	Y1114	L1115	P1116	E1117	L1118	F1181	D1182	R1183	L1184	V1185	G1186	G1187	Q1188	L1189	P1190	T1191	G1192	M1193	V1194	A1195	L1196	T1197	L1198	G1199	L1200	S1201	D1202	D1203	L1204	L1205	S1206	Q1207	V1208	L1209	P1210	L1211	T1212																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
N971	S972	A973	E974	A975	A976	Y977	A978	GLN	VAL	GLU	ILE	GLN	P984	R985	S986	E987	I988	Q989	L990	D991	E992	F993	E994	L995	K996	P997	Y998	R999	F1000	Q1001	S1002	L1003	A1004	G1005	N1006	E1007	P1008	D1009	L1010	G1011	N1012	L1013	D1014	L1015	E1016	R1017	V1018	I1019	V1020	V1021	T1022	G1023	F1024	A1025	E1026	V1027	G1028	N1029	L1030																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L906	G907	L908	L909	T910	P911	E912	V913	V914	L915	L916	G917	Q918	K919	S920	P921	V922		D925	L926	N927	G928	R929	G930	Q931	P932	V933	P934	E935	L936	K937	E938	F939	T940	A941	K942	L943	R944		V948	E949	T950	S951	E952	V953	R954	K955	A956	V957	R958	L959	E960	T961	A962	L963		V967	V968	N969	K970	G971																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L846	E847	T848	L849	F850	N851	R852	W853	H854	S855	E856	S857	W858	A859	N860	Q861	L862	T863	V864	C865	G866	A867	L868	I869	G870	K871	T872	R873	G874	T875	G876	L877	M878	S879	A880	N881	N882	V883	L884	E885	E886	G887	L888	E889	K890	M891	G892	V893	R894	T895	F896	S897	Q898	K899	M900	M901	A902	P903	N904	L905																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
D785	S786	E787	S788	E789	F790	A791	H792	R793	L794	W795	L796	T797	N798	I799	L800	R801	N802	N803	G804	C805	F806	K807	X808	Q809	K810	S811	A812	R813	G814	L815	R816	P817	A818	P819	Q821	V822	L823	L824	P825	G826	H827	T828	F829	G830	H831	T832	N833	G834	D835	G836	H837	N838	Y839	S840	E841	S842	K843	L844	S845																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
K724	Y725	G726	A727	K728	G729	S730	T731	L732	F733	G734	W735	F736	F737	N738	Q739	G740	S741	K742	Q743	D744	V745	E746	A747	L748	I749	E750	F751	I752	Y753	L754	T755	E756	N757	M758	G759	G760	L761	G762	W763	D764	L765	T766	A767	I768	R769	F770	S771	K772	A773	I774	P775	E776		I779	L780	E781	H782	H783	I784																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
X564	X565	X566	X567	X568	X569	X570	X571	X572	X573	X574	X575	X576	X577		X580	X581	X582	X583	X584	X585	X586	X587	X588	X589	X590	X591	X592	X593	X594	X595		X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X608	X609	X610	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X624	X625	X626	X627	X628																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
X629	X630	X631	X632	X633	X634	X635	X636	X637	X638	X639	X640	X641	X642	X643	X644	X645	X646	X647	X648	X649	X650	X651	X652	X653	X654	X655	X656	X657	X658	X659	X660	X661	X662	X663	X664	X665	X666	X667	X668	X669	X670	X671	X672	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X687	X688	X689	X690	X691	X692	X693	X694	X695	X696	X697	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X708	X709	X710	X711	X712	X713	X714	X715	X716	X717	X718	X719	X720	X721	X722	X723	X724	X725	X726	X727	X728	X729	X730	X731	X732	X733	X734	X735	X736	X737	X738	X739	X740	X741	X742	X743	X744	X745	X746	X747	X748	X749	X750	X751	X752	X753	X754	X755	X756	X757	X758	X759	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X773	X774	X775	X776	X777	X778	X779	X780	X781	X782	X783	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803	X804	X805	X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886	X887	X888	X889	X890	X891	X892	X893	X894	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X937	X938	X939	X940	X941	X942	X943	X944	X945	X946	X947	X948	X949	X950	X951	X952	X953	X954	X955	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X967	X968	X969	X970	X971	X972	X973	X974	X975	X976	X977	X978	X979	X980	X981	X982	X983	X984	X985	X986	X987	X988	X989	X990	X991	X992	X993	X994	X995	X996	X997	X998	X999	X1000	X1001	X1002	X1003	X1004	X1005	X1006	X1007	X1008	X1009	X1010	X1011	X1012	X1013	X1014	X1015	X1016	X1017	X1018	X1019	X1020	X1021	X1022	X1023	X1024	X1025	X1026	X1027	X1028	X1029	X1030	X1031	X1032	X1033	X1034	X1035	X1036	X1037	X1038	X1039	X1040	X1041	X1042	X1043	X1044	X1045	X1046	X1047	X1048	X1049	X1050	X1051	X1052	X1053	X1054	X1055	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1064	X1065	X1066	X1067	X1068	X1069	X1070	X1071	X1072	X1073	X1074	X1075	X1076	X1077	X1078	X1079	X1080	X1081	X1082	X1083	X1084	X1085	X1086	X1087	X1088	X1089	X1090	X1091	X1092	X1093	X1094	X1095	X1096	X1097	X1098	X1099	X1100	X1101	X1102	X1103	X1104	X1105	X1106	X1107	X1108	X1109	X1110	X1111	X1112	X1113	X1114	X1115	X1116	X1117	X1118	X1119	X1120	X1121	X1122	X1123	X1124	X1125	X1126	X1127	X1128	X1129	X1130	X1131	X1132	X1133	X1134	X1135	X1136	X1137	X1138	X1139	X1140	X1141	X1142	X1143	X1144	X1145	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1154	X1155	X1156	X1157	X1158	X1159	X1160	X1161	X1162	X1163	X1164	X1165	X1166	X1167	X1168	X1169	X1170	X1171	X1172	X1173	X1174	X1175	X1176	X1177	X1178	X1179	X1180	X1181	X1182	X1183	X1184	X1185	X1186	X1187	X1188	X1189	X1190	X1191	X1192	X1193	X1194	X1195	X1196	X1197	X1198	X1199	X1200	X1201	X1202	X1203	X1204	X1205	X1206	X1207	X1208	X1209	X1210	X1211	X1212	X1213	X1214	X1215	X1216	X1217	X1218	X1219	X1220	X1221	X1222	X1223	X1224	X1225	X1226	X1227	X1228	X1229	X1230	X12



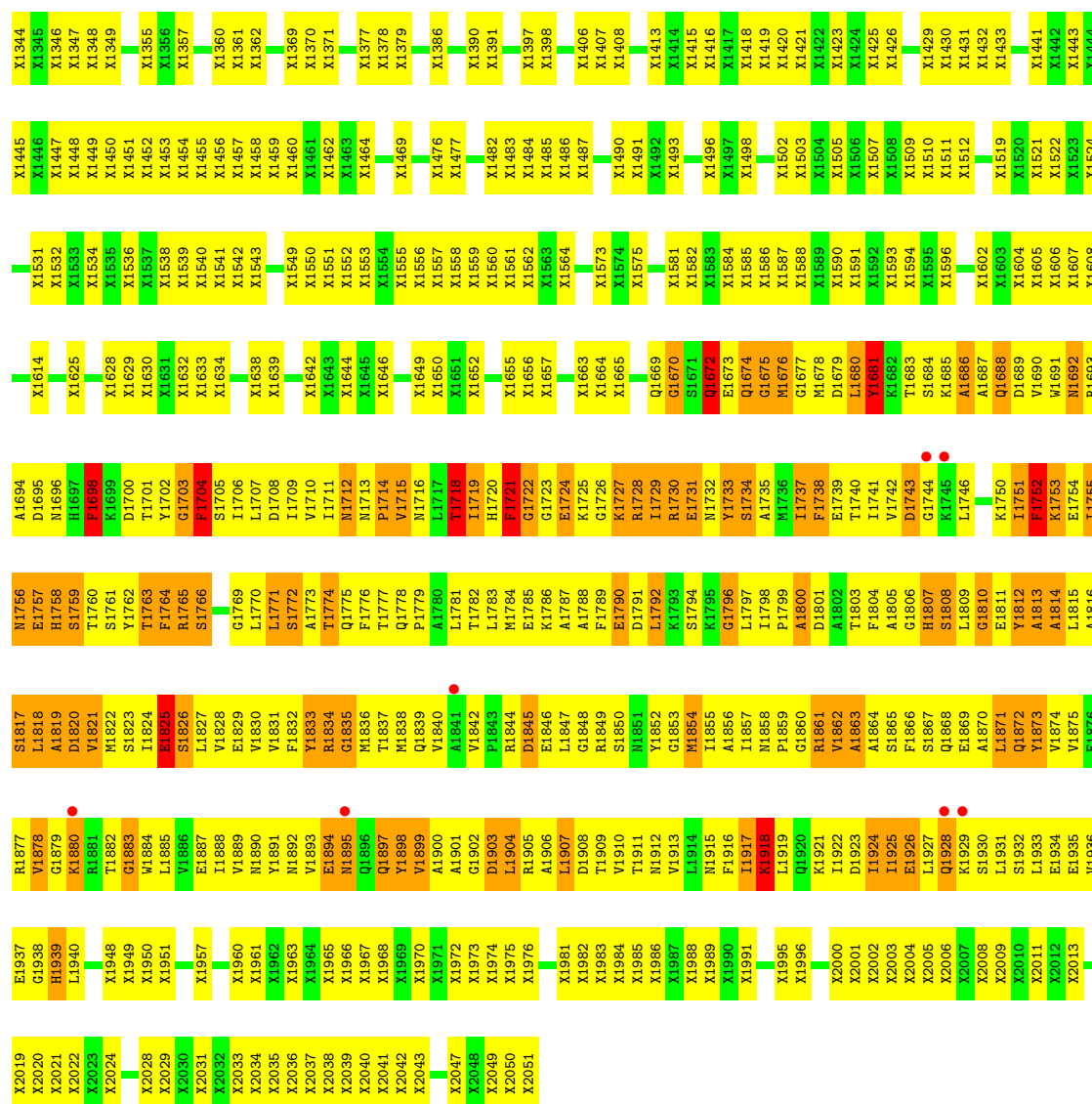
- Molecule 2: Fatty acid synthase subunit beta



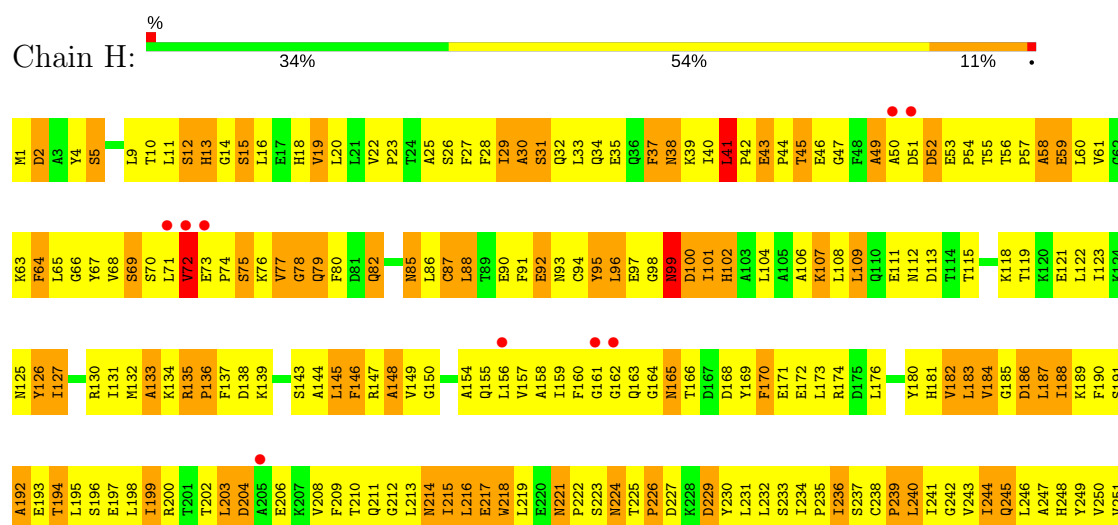
X1049	X1050	X1051	X1052	X1053	X1054	X1055	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1066	X1067	X1068	X1069	X1074	X1075	X1076	X1137	X1138	X1139	X1140	X1141	X1142	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1157	X1162	X1163	X1164	X1165	X1166	X1167	X1168	X1169	X1170	X1171	X1172	X1173	X1177	X1178	X1179	X1180																																																																				
X974	X975	X976	X977	X978	X979	X980	X981	X982	X983	X989	X985	X986	X987	X988	X996	X997	X998	X999	X1002	X1008	X1009	X1010	X1011	X1012	X1013	X1014	X1015	X1016	X1017	X1018	X1019	X1020	X1021	X1022	X1023	X1024	X1025	X1028	X1029	X1030	X1031	X1034	X1035	X1036	X1037	X1038	X1039	X1040	X1041	X1042	X1043	X1044	X1045	X1047	X1048																																																																	
X887	X888	X895	X896	X897	X898	X899	X900	X905	X906	X907	X911	X912	X915	X916	X917	X918	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X948	X949	X950	X951	X956	X957	X958	X959	X961	X962	X963	X964	X969	X970	X971	X972	X973																																																																								
X806	X807	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X836	X837	X838	X841	X842	X843	X844	X845	X846	X847	X848	X849	X851	X852	X853	X862	X863	X864	X865	X866	X867	X868	X870	X871	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886																																																																			
X725	X726	X727	X728	X729	X730	X731	X732	X735	X736	X737	X738	X739	X742	X743	X744	X745	X746	X752	X753	X754	X755	X756	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X775	X776	X777	X784	X785	X786	X796	X797	X798	X799	X800	X801	X802	X803																																																																							
X648	X649	X650	X651	X652	X653	X654	X655	X660	X661	X662	X667	X668	X669	X670	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X689	X690	X691	X692	X693	X694	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X710	X711	X712	X716	X719	X720	X721	X722	X723	X724																																																																				
X568	X569	X570	X571	X572	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X627	X628	X629	X633	X634	X635	X646	X647																																																																			
X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565	X566	X567																																																					
X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500																																																												
X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	
T252	A253	K254	L255	T317	L256	G257	F258	T259	P260	G261	T262	L263	G264	S265	Y266	K267	L268	G269	F270	T271	G272	L273	H274	G275	L276	L277	V278	L279	E280	L281	G282	L283	T284	E285	T286	D287	K288	L289	F292	G293	L294	E295	L296	T297	G298	L299	I300	E301	V302	L303	G304	F305	L306	G307	V308	L309	C310	X311	L312	F313	X314	E315																																																										
P315	N316	L317	S318	L319	P320	G321	S322	L323	L324	E325	L328	E329	N330	L331	K332	G333	V334	P335	S336	P337	N338	L339	S340	L341	S342	L343	N344	L345	T346	G347	E348	L349	V349	Q350	D351	V352	V353	N354	K355	T356	N357	P358	H359	L360	P361	Q365	V366	E367	L368	S369	L370	V371	N372	G373	A374	N376																																																																
L377	V378	V379	G381	P382	P383	Q384	S385	L386	G387	E388	N389	N390	L391	T392	L393	R394	K395	A396	G401	L402	H403	D404	S405	R406	L407	S408	L409	F409	L410	S411	E411	R412	K413	L414	K415	L416	S417	N418	F419	V420	L421	L422	V423	A424	S425	P426	F427	H428	S429	L430	L431	S432	L433	T434	G435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500
M1	D2	A3	Y4	S5	L9	L10	L11	S12	H13	E73	P74	G14	S15	L16	E17	G78	F79	L80	S26	L21	V22	P23	T24	A25	S26	L87	L88	F28	L29	A30	E92	N93	Q32	L33	Q34	E35	Q36	G97	G98	N99	D100	L101	H102	A103	L104	A105	T45	A106	K107	L108	L109	Q110	A149	A50	D51	D52	E53	T55	T56	P57	A58	E59	L60	V61	K124																																																							
K63	F64	L65	G66	Y67	V68	S69	S70	L71	S12	E73	P74	G14	S15	L16	E17	G78	F79	L80	S26	L21	V22	P23	T24	A25	S26	L87	L88	F28	L29	A30	E92	N93	Q32	L33	Q34	E35	Q36	G97	G98	N99	D100	L101	H102	A103	L104	A105	T45	A106	K107	L108	L109	Q110	A149	A50	D51	D52	E53	T55	T56	P57	A58	E59	L60	V61	K124																																																							
N125	Y126	L127	R130	L131	M132	A133	L134	L135	P136	F137	R138	D139	K139	S143	E207	V208	F209	T210	Q211	G212	L213	N214	L215	G216	Q155	L156	V157	A158	E159	Q160	G161	G162	Q163	G164	N165	T166	D167	D168	Y169	F170	E171	E172	L173	R174	D175	L176	Y180	H181	L182	L183	V184	G185	L186	D187	A188	L189	F190	S191																																																														
A192	E193	L194	T195	S196	E197	L198	L199	R200	P201	G202	L203	R204	A205	E206	K207	V208	F209	T210	Q211	G212	L213	N214	L215	G216	Q155	L156	V157	A158	E159	Q160	G161	G162	Q163	G164	N165	T166	D167	D168	Y169	F170	E171	E172	L173	R174	D175	L176	Y180	H181	L182	L183	V184	G185	L186	D187	A188	L189	F190	S191																																																														
P315	N316	L317	S318	L319	P320	G321	S322	L323	L324	E325	L328	E329	N330	L331	K332	G333	V334	P335	S336	P337	N338	L339	S340	L341	S342	L343	N344	L345	T346	G347	E348	L349	V349	Q350	D351	V352	V353	N354	K355	T356	N357	P358	H359	L360	P361	Q365	V366	E367	L368	S369	L370	V371	N372	G373	A374	N376																																																																
L377	V378	V379	G381	P382	P383	Q384	S385	L386	G387	E388	N389	N390	L391	T392	L393	R394	K395	A396	G401	L402	H403	D404	S405	R406	L407	S408	L409	F409	L410	S411	E411	R412	K413	L414	K415	L416	S417	N418	F419	V420	L421	L422	V423	A424	S425	P426	F427	H428	S429	L430	L431	S432	L433	T434	G435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500
K441	K442	L443	L444	K445	K446	N447	N448	N449	N450	N451	N452	K453	D454	L455	L456	L457	P458	V459	Y460	D461	T462	F463	G464	G465	S466	L467	L468	L469	L470	L471	L472	L473	G474	S475	I476	S476	E477	R478	L479	V480	D481	C482	I483	I484	L485	L486	L487	L488	K489	L490	E491	L492	T493	L494	Q495	F496	K497	L498	L499	T499																																																												
H500	L501	L502	D503	F504	G505	P506	G507	G508	A509	S510	G511	L512	A513	G514	D515	L516	N517	N518	N519	D520	D521	G522	T523	G524	V525	R526	V527	L528	L529	L530	L531	L532	L533	L534	L535	N536	P537	D538	D539	L540	G541	G542	F543	K544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567																																																					
X568	X569	X570	X571	X572	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X627	X628	X629	X633	X634	X635	X646	X647																																																																			
X648	X649	X650	X651	X652	X653	X654	X655	X660	X661	X662	X667	X668	X669	X670	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X689	X690	X691	X692	X693	X694	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X710	X711	X712	X716	X719	X720	X72																																																																							



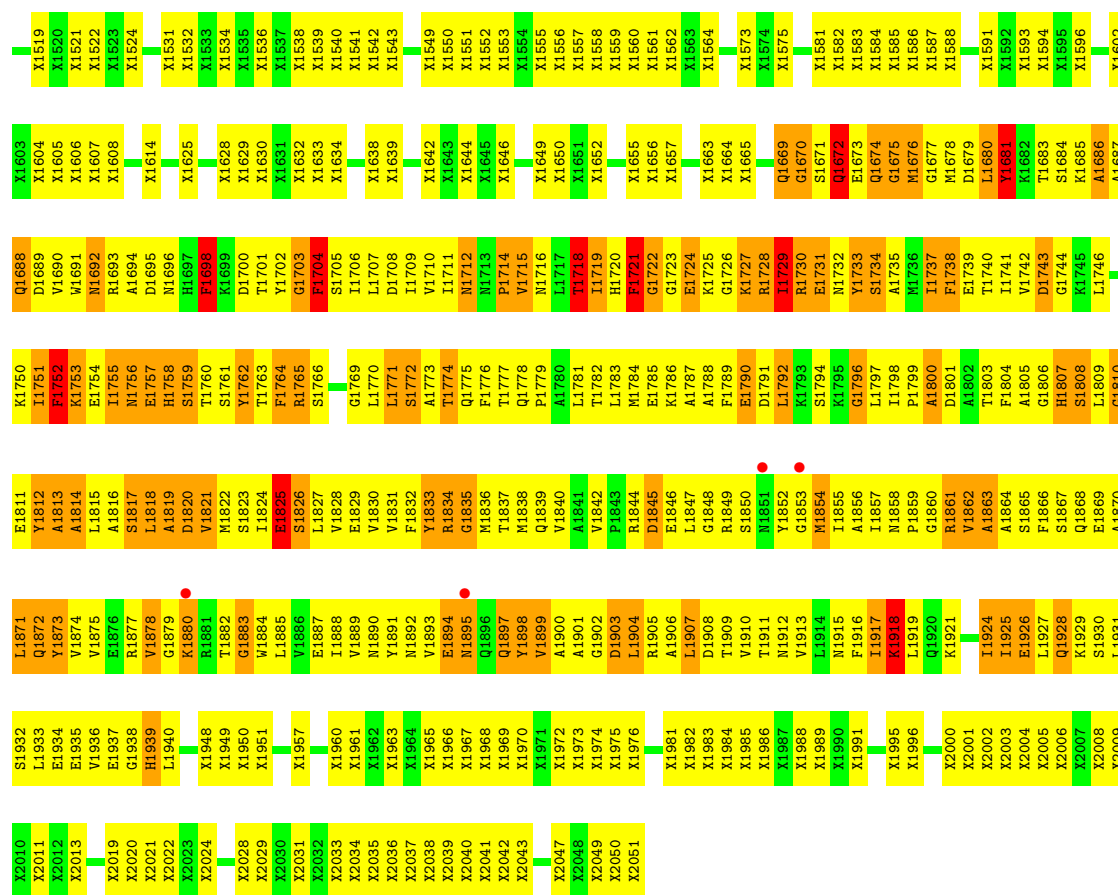
X1265	X1180	X1051	X973	X897	X809	X726	X650	X570	I501	K441	L377	P315	V251	S191	N125
X1266	X1181	X1052	X974	X898	X810	X727	X651	X571	I502	D442	V378	P316	T252	A192	Y126
X1267	X1182	X1053	X975	X899	X811	X728	X652	X572	D503	L443	V379	N316	T253	A193	I127
X1268	X1183	X1054	X976	X900	X812	X729	X653	X730	F504	V444	S380	T317	K254	T194	
X1269	X1192	X1055	X977	X905	X813	X730	X654	X577	G505	K445	G381	S318	L255	L195	R130
X1270	X1193	X1056	X978	X906	X814	X731	X655	X578	P506	L446	P382	L319	L256	S196	I131
X1271	X1194	X1057	X979	X907	X815	X732	X656	X579	G507	N447	P383	P320	G257	E197	M132
X1272	X1195	X1058	X982	X908	X816	X733	X657	X580	G508	V448	Q384	P321	F258	E198	M133
X1275	X1196	X1059	X983	X911	X817	X735	X660	X581	A509	S349	S322	S322	T259	I199	A134
X1276	X1197	X1060	X989	X912	X818	X736	X661	X582	S510	L386	P260	L323	G261	T201	R135
X1280	X1198	X1062	X995	X915	X820	X738	X662	X584	L512	A452	E262	L324	E262	F137	F138
X1281	X1199	X1063	X996	X916	X821	X739	X667	X585	G513	K388	L263	E325	L263	L203	L138
X1282	X1200	X1066	X997	X918	X822	X742	X668	X586	V514	D454	R264	L328	R264	D204	K139
X1283	X1201	X1067	X998	X917	X823	X743	X669	X587	L515	I455	S265	E206	S265	A205	
X1284	X1202	X1068	X999	X919	X824	X744	X670	X591	T516	K267	L267	E207	L267	E207	S143
X1205	X1205	X1069	X1002	X920	X825	X745	X671	X592	H517	L457	K268	L393	K268	L145	A144
X1206	X1206	X1071	X1003	X921	X826	X746	X674	X593	R518	P458	E332	E332	G269	F209	F146
X1207	X1207	X1074	X1008	X922	X836	X747	X675	X594	N519	V459	V334	A270	A270	T210	R147
X1208	X1208	X1075	X1009	X923	X841	X748	X676	X595	D521	D461	P335	A271	A271	Q211	A148
X1209	X1209	X1076	X1010	X924	X842	X749	X677	X596	G522	F463	S336	G272	G272	G212	V149
X1210	X1210	X1077	X1011	X925	X843	X750	X678	X597	T523	K464	L402	P337	H273	L213	G150
X1211	X1211	X1078	X1012	X926	X844	X751	X679	X598	G524	D465	Q403	K338	Q275	N214	
X1212	X1212	X1079	X1013	X927	X845	X752	X680	X599	V525	G466	Q404	L339	Q275	T215	A154
X1215	X1215	X1136	X1014	X928	X846	X754	X681	X600	K526	S466	S405	S340	G276	L216	Q155
X1301	X1301	X1137	X1015	X929	X847	X755	X682	X601	V527	D467	R406	L341	G277	E217	L156
X1304	X1304	X1138	X1016	X930	X848	X756	X683	X602	T528	L468	L278	L342	V278	L218	V157
X1305	X1305	X1139	X1017	X931	X851	X760	X685	X603	V529	R469	N343	N343	T279	L219	A158
X1306	X1306	X1140	X1018	X932	X852	X761	X686	X604	A530	V470	L444	L344	A280	I159	I159
X1307	X1307	X1141	X1019	X933	X853	X762	X687	X605	G531	L471	T345	V281	D227	N221	F160
X1308	X1308	X1142	X1020	X934	X854	X763	X688	X606	T532	S472	Q346	A282	D228	P222	G161
X1309	X1309	X1143	X1021	X935	X855	X764	X689	X607	L533	K473	E347	L283	D229	S223	G162
X1314	X1314	X1144	X1022	X936	X856	X765	X692	X611	D534	S474	Q348	A284	Y230	Q224	L231
X1315	X1315	X1145	X1023	X939	X857	X766	X694	X612	L535	I475	Q349	E285	L232	E171	F170
X1320	X1320	X1150	X1024	X946	X858	X767	X698	X613	N536	S477	Q350	T286	L233	G163	
X1321	X1321	X1151	X1025	X947	X859	X768	X699	X614	P537	E477	D351	D287	L234	N165	T166
X1322	X1322	X1152	X1026	X948	X860	X769	X700	X615	D538	R478	V352	S288	E236	D227	T166
X1323	X1323	X1153	X1027	X949	X861	X770	X701	X616	D539	I479	V353	W289	L235	K238	D167
X1324	X1324	X1154	X1028	X950	X862	X771	X702	X617	D540	V480	P420	D168	L236	D229	D168
X1325	X1325	X1155	X1029	X951	X863	X772	X703	X618	Y541	D481	L421	Y169	L237	Y230	Y169
X1246	X1246	X1157	X1030	X952	X864	X773	X704	X619	G542	C482	P422	F293	L238	L231	F170
X1247	X1247	X1158	X1031	X953	X865	X774	X705	X620	F543	I483	V423	F294	L239	E171	E171
X1248	X1248	X1159	X1032	X954	X866	X775	X706	X621	K544	I484	A424	S295	L240	G172	L173
X1249	X1249	X1160	X1033	X955	X867	X776	X707	X622	Q545	R485	S425	V296	L241	L234	L173
X1250	X1250	X1161	X1034	X956	X868	X777	X708	X623	X551	L486	P426	V297	L242	P235	R174
X1251	X1251	X1162	X1035	X957	X869	X778	X709	X624	X552	L487	K298	K298	L243	L236	D175
X1252	X1252	X1163	X1036	X958	X870	X779	X710	X625	X553	V488	P427	A299	L244	S237	L176
X1253	X1253	X1164	X1037	X959	X871	X780	X711	X626	X554	K489	H428	C238	L245	C238	Y177
X1254	X1254	X1165	X1038	X960	X872	X781	X712	X627	X555	V490	H429	A299	L246	P239	Y180
X1255	X1255	X1166	X1039	X961	X873	X782	X713	X628	X556	I491	L431	V366	L247	T241	Y180
X1256	X1256	X1167	X1040	X962	X874	X783	X714	X629	X557	T492	L432	E367	L248	G242	H181
X1257	X1257	X1168	X1041	X963	X875	X784	X715	X630	X558	V491	L433	S368	L249	G243	L182
X1258	X1258	X1169	X1042	X964	X876	X785	X716	X631	X559	T493	V433	S369	L250	V243	L183
X1259	X1259	X1170	X1043	X965	X877	X786	X717	X632	X560	I494	P434	S370	L251	L244	V184
X1260	X1260	X1171	X1044	X966	X878	X787	X718	X633	X561	K495	A435	V371	L252	Q245	G185
X1261	X1261	X1172	X1045	X967	X879	X788	X719	X634	X562	Q496	S436	N372	L253	L246	D186
X1262	X1262	X1173	X1046	X968	X880	X789	X720	X635	X563	K497	D437	G373	L254	A247	L187
X1340	X1340	X1174	X1047	X969	X881	X790	X721	X646	X564	A498	L438	A374	L255	H248	I388
X1341	X1341	X1175	X1048	X970	X882	X791	X722	X647	X565	T499	L439	K375	L256	C310	L189
X1342	X1342	X1176	X1049	X971	X883	X792	X723	X648	X566	K499	L440	N376	L257	V249	
X1343	X1343	X1177	X1050	X972	X884	X793	X724	X649	X567	H500	N440		L258	V250	F190



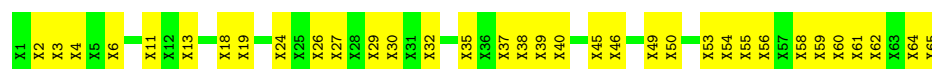
• Molecule 2: Fatty acid synthase subunit beta



X1433	X1345	X1268	X1180	X1051	X971	X887	X803	X722	X651	X570	X502	D442	V378	P315	T252
X1441	X1346	X1269	X1181	X1052	X972	X888	X803	X723	X652	X571	D503	L443	V379	N316	A253
X1442	X1347	X1270	X1182	X1053	X973	X888	X806	X724	X653	X572	F504	V444	G381	N318	K254
X1443	X1348	X1271	X1183	X1054	X974	X888	X806	X725	X654	X573	G505	V445	G382	N318	L255
X1444	X1349	X1272	X1192	X1055	X975	X895	X807	X726	X655	X577	P506	N446	P382	N319	L256
X1445	X1355	X1275	X1193	X1056	X976	X896	X808	X727	X656	X578	G507	N447	P383	P320	G257
X1446	X1356	X1276	X1194	X1057	X977	X897	X809	X728	X657	X579	G508	V448	Q384	P321	F258
X1447	X1357	X1277	X1195	X1058	X978	X898	X810	X729	X658	X580	A509	S449	S385	S322	T289
X1448	X1360	X1280	X1196	X1059	X979	X899	X811	X730	X659	X581	S510	F450	L386	L323	P260
X1449	X1361	X1281	X1197	X1060	X980	X899	X812	X731	X660	X582	G511	N451	V387	L324	G261
X1450	X1362	X1282	X1198	X1061	X981	X899	X813	X732	X661	X583	L512	A452	G388	L325	E262
X1451	X1363	X1283	X1199	X1062	X982	X899	X814	X733	X662	X584	G513	A453	L389	L263	L263
X1452	X1364	X1284	X1200	X1063	X983	X899	X815	X734	X663	X585	V514	D454	N390	R264	R264
X1453	X1365	X1285	X1201	X1064	X984	X899	X816	X735	X664	X586	L515	A455	L391	S265	S265
X1454	X1366	X1286	X1202	X1065	X985	X899	X817	X736	X665	X587	T516	Q456	L392	L266	L266
X1455	X1367	X1287	X1203	X1066	X986	X899	X818	X737	X666	X588	H517	L457	L393	N331	L267
X1456	X1368	X1288	X1204	X1067	X987	X899	X819	X738	X667	X589	P458	V459	R518	E332	K268
X1457	X1369	X1289	X1205	X1068	X988	X899	X820	X739	X668	X590	N519	V459	K395	G333	G269
X1458	X1370	X1290	X1206	X1069	X989	X899	X821	X740	X669	X591	K520	Y460	A396	V334	A270
X1459	X1371	X1291	X1207	X1070	X990	X899	X822	X741	X670	X592	D521	D461	G401	P335	T271
X1460	X1372	X1292	X1208	X1071	X991	X899	X823	X742	X671	X593	G522	L462	L402	S336	G272
X1461	X1373	X1293	X1209	X1072	X992	X899	X824	X743	X672	X594	T523	F463	L403	N337	H273
X1462	X1374	X1294	X1210	X1073	X993	X899	X825	X744	X673	X595	G524	D464	D403	N338	S274
X1463	X1375	X1295	X1211	X1074	X994	X899	X826	X745	X674	X596	V525	G465	Q404	L339	Q275
X1464	X1376	X1296	X1212	X1075	X995	X899	X827	X746	X675	X597	R526	S466	S405	S340	G276
X1465	X1377	X1297	X1213	X1076	X996	X899	X828	X747	X676	X598	V527	D467	R406	I341	L277
X1466	X1378	X1298	X1214	X1077	X997	X899	X829	X748	X677	X599	V528	L468	R407	S342	V278
X1467	X1379	X1299	X1215	X1078	X998	X899	X830	X749	X678	X600	V529	L469	S343	N343	V278
X1468	X1380	X1300	X1216	X1079	X999	X899	X831	X750	X679	X601	A530	V470	F408	L344	A280
X1469	X1381	X1301	X1217	X1080	X1000	X899	X832	X751	X680	X602	G531	L471	F409	T345	V281
X1470	X1382	X1302	X1218	X1081	X1001	X899	X833	X752	X681	X603	T532	S472	S410	Q346	A282
X1471	X1383	X1303	X1219	X1082	X1002	X899	X834	X753	X682	X604	L533	G473	E411	E347	T283
X1472	X1384	X1304	X1220	X1083	X1003	X899	X835	X754	X683	X605	D534	S474	R412	K348	A284
X1473	X1385	X1305	X1221	X1084	X1004	X899	X836	X755	X684	X606	T535	L475	F416	V349	E285
X1474	X1386	X1306	X1222	X1085	X1005	X899	X837	X756	X685	X607	N536	S476	S417	Q350	T286
X1475	X1387	X1307	X1223	X1086	X1006	X899	X838	X757	X686	X608	P537	E477	E418	D351	D287
X1476	X1388	X1308	X1224	X1087	X1007	X899	X839	X758	X687	X609	D538	R478	N418	Y352	S288
X1477	X1389	X1309	X1225	X1088	X1008	X899	X840	X759	X688	X610	D539	L479	E419	V353	W289
X1478	X1390	X1310	X1226	X1089	X1009	X899	X841	X760	X689	X611	D540	V480	F420	N354	F292
X1479	X1391	X1311	X1227	X1090	X1010	X899	X842	X761	X690	X612	Y541	D481	L421	K355	F293
X1480	X1392	X1312	X1228	X1091	X1011	X899	X843	X762	X691	X613	G542	C482	P422	T356	V294
X1481	X1393	X1313	X1229	X1092	X1012	X899	X844	X763	X692	X614	F543	L483	V423	N357	S295
X1482	X1394	X1314	X1230	X1093	X1013	X899	X845	X764	X693	X615	G544	L484	A424	S358	S295
X1483	X1395	X1315	X1231	X1094	X1014	X899	X846	X765	X694	X616	Q545	P485	S425	H359	V296
X1484	X1396	X1316	X1232	X1095	X1015	X899	X847	X766	X695	X617	X546	L486	P426	L360	R297
X1485	X1397	X1317	X1233	X1096	X1016	X899	X848	X767	X696	X618	X550	P487	F427	P361	K298
X1486	X1398	X1318	X1234	X1097	X1017	X899	X849	X768	X697	X619	X551	V488	H428	A299	A299
X1487	X1406	X1320	X1235	X1098	X1018	X899	X850	X769	X698	X620	X552	K489	S429	T301	I300
X1488	X1407	X1321	X1236	X1099	X1019	X899	X851	X770	X699	X621	X553	E491	H430	V366	I301
X1489	X1408	X1322	X1246	X1100	X1020	X899	X852	X771	X700	X622	X554	L492	L431	E367	V302
X1490	X1409	X1323	X1247	X1101	X1021	X899	X853	X772	X701	X623	X555	T493	L432	I368	L303
X1491	X1410	X1324	X1248	X1102	X1022	X899	X854	X773	X702	X624	X556	L494	V433	F304	F304
X1492	X1411	X1325	X1249	X1103	X1023	X899	X855	X774	X703	X625	X557	Q495	P434	L370	F305
X1493	X1412	X1326	X1250	X1104	X1024	X899	X856	X775	X704	X626	X558	A435	A435	V371	I306
X1494	X1413	X1327	X1251	X1105	X1025	X899	X857	X776	X705	X627	X559	F496	S436	N372	G307
X1495	X1414	X1328	X1252	X1106	X1026	X899	X858	X777	X706	X628	X560	L497	D437	G373	V308
X1496	X1415	X1329	X1253	X1107	X1027	X899	X859	X778	X707	X629	X561	A498	L438	A374	R309
X1497	X1416	X1330	X1254	X1108	X1028	X899	X860	X779	X708	X630	X562	L499	I439	K375	C310
X1498	X1417	X1331	X1255	X1109	X1029	X899	X861	X780	X709	X631	X563	H500	M440	N376	X311
X1499	X1418	X1332	X1256	X1110	X1030	X899	X862	X781	X710	X632	X564	L501	K441	L377	L377
X1500	X1419	X1333	X1257	X1111	X1031	X899	X863	X782	X711	X633	X565	T499	L439	A374	A374
X1501	X1420	X1334	X1258	X1112	X1032	X899	X864	X783	X712	X634	X566	L501	L439	K375	C310
X1502	X1421	X1335	X1259	X1113	X1033	X899	X865	X784	X713	X635	X567	L501	L439	K375	C310
X1503	X1422	X1336	X1260	X1114	X1034	X899	X866	X785	X714	X636	X568	L501	L439	K375	C310
X1504	X1423	X1337	X1261	X1115	X1035	X899	X867	X786	X715	X637	X569	L501	L439	K375	C310
X1505	X1424	X1338	X1262	X1116	X1036	X899	X868	X787	X716	X638	X570	L501	L439	K375	C310
X1506	X1425	X1339	X1263	X1117	X1037	X899	X869	X788	X717	X639	X571	L501	L439	K375	C310
X1507	X1426	X1340	X1264	X1118	X1038	X899	X870	X789	X718	X640	X572	L501	L439	K375	C310
X1508	X1427	X1341	X1265	X1119	X1039	X899	X871	X790	X719	X641	X573	L501	L439	K375	C310
X1509	X1428	X1342	X1266	X1120	X1040	X899	X872	X791	X720	X642	X574	L501	L439	K375	C310
X1510	X1429	X1343	X1267	X1121	X1041	X899	X873	X792	X721	X643	X575	L501	L439	K375	C310
X1511	X1430	X1344	X1268	X1122	X1042	X899	X874	X793	X722	X644	X576	L501	L439	K375	C310
X1512	X1431	X1345	X1269	X1123	X1043	X899	X875	X794	X723	X645	X577	L501	L439	K375	C310
X1513	X1432	X1346	X1270	X1124	X1044	X899	X876	X795	X724	X646	X578	L501	L439	K375	C310
X1514	X1433	X1347	X1271	X1125	X1045	X899	X877	X796	X725	X647	X579	L501	L439	K375	C310
X1515	X1434	X1348	X1272	X1126	X1046	X899	X878	X797	X726	X648	X580	L501	L439	K375	C310
X1516	X1435	X1349	X1273	X1127	X1047	X899	X879	X798	X727	X649	X581	L501	L439	K375	C310
X1517	X1436	X1350	X1274	X1128	X1048	X899	X880	X799	X728	X650	X582	L501	L439	K375	C310
X1518	X1437	X1351	X1275	X1129	X1049	X899	X881	X800	X729	X651	X583	L501	L439	K375	C310
X1519	X1438	X1352	X1276	X1130	X1050	X899	X882	X801	X730	X652	X584	L501	L439	K375	C310
X1520	X1439	X1353	X1277	X1131	X1051	X899	X883	X802	X731	X653	X585	L501	L439	K375	C310
X1521	X1440	X1354	X1278	X1132	X1052	X899	X884	X803	X732	X654	X586	L501	L439	K375	C310
X1522	X1441	X1355	X1279	X1133	X1053	X899	X885	X804	X733	X655	X587	L501	L439	K375	C310
X1523	X1442	X1356	X1280	X1134	X1054	X899	X886	X805	X734	X656	X588	L501	L439	K375	C310
X1524	X1443	X1357	X1281	X1135	X1055	X899	X887	X806	X735	X657	X589	L501	L439	K375	C310
X1525	X1444	X1358	X1282	X1136	X1056	X899	X888	X807	X736	X658	X590	L501	L439	K375	C310
X1526	X1445	X1359	X1283	X1137	X1057	X899	X889	X808	X737	X659	X591	L501	L439	K375	C310
X1527	X1446	X1360	X1284	X1138	X1058	X899	X890	X809	X738	X660	X592	L501	L439	K375	C310
X1528	X1447	X1361	X1285	X1139	X1059	X899	X891	X810	X739	X661	X593	L501	L439	K375	



Chain C:



• Molecule 3: Tail protein

Chain F:



• Molecule 3: Tail protein

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	231.34Å 231.34Å 754.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 4.00 59.69 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.00-4.00) 97.4 (59.69-3.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.346 0.320 , 0.354	Depositor DCC
R_{free} test set	8382 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 180.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	71862	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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 i

5.1 Standard geometry i

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	0.80	7/8414 (0.1%)	0.95	28/11377 (0.2%)
1	D	0.80	7/8414 (0.1%)	0.95	32/11377 (0.3%)
1	G	0.82	7/8414 (0.1%)	0.96	29/11377 (0.3%)
2	B	0.41	0/6495	0.72	2/8812 (0.0%)
2	E	0.40	0/6495	0.72	3/8812 (0.0%)
2	H	0.41	0/6495	0.72	2/8812 (0.0%)
All	All	0.66	21/44727 (0.0%)	0.86	96/60567 (0.2%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1150	ASP	CB-CG	33.05	2.21	1.51
1	D	1150	ASP	CB-CG	32.65	2.20	1.51
1	A	1150	ASP	CB-CG	32.54	2.20	1.51
1	D	1181	PHE	CD2-CE2	21.08	1.81	1.39
1	G	1181	PHE	CE2-CZ	20.68	1.76	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1150	ASP	CB-CG-OD1	12.15	129.24	118.30
1	D	1150	ASP	CB-CG-OD1	12.14	129.22	118.30
1	A	1150	ASP	CB-CG-OD1	11.62	128.76	118.30
1	D	992	PHE	C-N-CD	-11.23	95.89	120.60
1	G	992	PHE	C-N-CD	-10.81	96.82	120.60

There are no chirality outliers.

There are no planarity outliers.

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	11319	0	8817	2535	24
1	D	11319	0	8818	2518	14
1	G	11319	0	8817	2527	24
2	B	12310	0	7819	1753	0
2	E	12310	0	7817	1770	0
2	H	12310	0	7816	1770	0
3	C	325	0	76	25	0
3	F	325	0	76	28	0
3	I	325	0	76	35	0
All	All	71862	0	50132	12923	38

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 106.

The worst 5 of 12923 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:G:1181:PHE:CE2	1:G:1181:PHE:CZ	1.76	1.71
1:A:1181:PHE:CZ	1:A:1181:PHE:CE2	1.75	1.69
1:D:1181:PHE:CD2	1:D:1181:PHE:CE2	1.81	1.68
1:G:1181:PHE:CE1	1:G:1181:PHE:CZ	1.75	1.68
1:D:1181:PHE:CD1	1:D:1181:PHE:CE1	1.78	1.66

The worst 5 of 38 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)
1:D:1150:ASP:OD1	1:D:1181:PHE:CE2[7_555]	1.80	0.40
1:A:1150:ASP:OD1	1:G:1181:PHE:CE2[7_555]	1.85	0.35
1:A:1181:PHE:CE2	1:G:1150:ASP:OD1[7_555]	1.85	0.35
1:D:1150:ASP:CG	1:D:1181:PHE:CE2[7_555]	1.87	0.33
1:A:1150:ASP:CG	1:G:1181:PHE:CE2[7_555]	1.87	0.33

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	1069/1688 (63%)	401 (38%)	298 (28%)	370 (35%)	0	0
1	D	1069/1688 (63%)	396 (37%)	307 (29%)	366 (34%)	0	0
1	G	1069/1688 (63%)	398 (37%)	307 (29%)	364 (34%)	0	0
2	B	817/2006 (41%)	356 (44%)	245 (30%)	216 (26%)	0	1
2	E	817/2006 (41%)	357 (44%)	244 (30%)	216 (26%)	0	1
2	H	817/2006 (41%)	352 (43%)	247 (30%)	218 (27%)	0	1
All	All	5658/11082 (51%)	2260 (40%)	1648 (29%)	1750 (31%)	0	0

5 of 1750 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	723	ALA
1	A	724	LYS
1	A	741	SER
1	A	742	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	871/895 (97%)	700 (80%)	171 (20%)	1	12
1	D	871/895 (97%)	697 (80%)	174 (20%)	1	12
1	G	871/895 (97%)	696 (80%)	175 (20%)	1	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	703/703 (100%)	623 (89%)	80 (11%)	7	33
2	E	703/703 (100%)	623 (89%)	80 (11%)	7	33
2	H	703/703 (100%)	622 (88%)	81 (12%)	6	33
All	All	4722/4794 (98%)	3961 (84%)	761 (16%)	3	20

5 of 761 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1297	PRO
2	E	28	PHE
2	H	199	ILE
1	D	1354	GLU
1	D	1538	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1351	ASN
2	E	221	ASN
2	H	331	ASN
1	D	1389	GLN
1	D	1570	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 [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1069/1688 (63%)	-0.35	0 100 100	48, 122, 192, 203	0
1	D	1069/1688 (63%)	-0.32	2 (0%) 94 93	53, 123, 194, 203	0
1	G	1069/1688 (63%)	-0.37	1 (0%) 95 94	43, 112, 190, 203	0
2	B	818/2006 (40%)	-0.12	25 (3%) 49 39	107, 177, 202, 203	0
2	E	818/2006 (40%)	-0.10	15 (1%) 69 60	111, 190, 202, 203	0
2	H	818/2006 (40%)	-0.15	17 (2%) 64 54	94, 183, 202, 203	0
3	C	0/65	-	-	-	-
3	F	0/65	-	-	-	-
3	I	0/65	-	-	-	-
All	All	5661/11277 (50%)	-0.25	60 (1%) 80 72	43, 151, 201, 203	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1895	ASN	9.5
2	H	451	ASN	4.8
2	H	51	ASP	4.3
2	E	1928	GLN	4.2
2	B	1880	LYS	4.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.