



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 11:24 am BST

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.; Mikolasek, 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

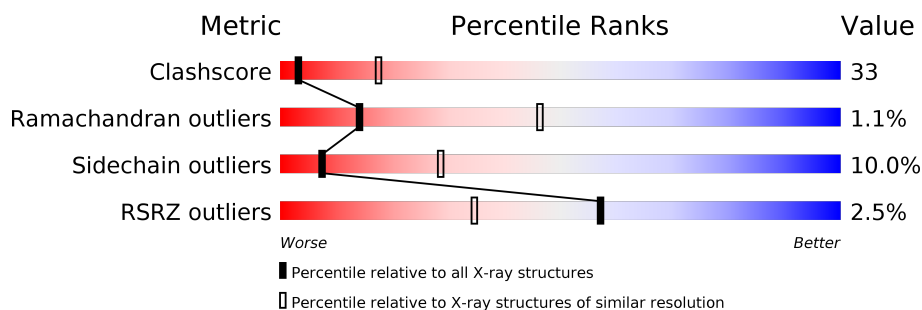
1 Overall quality at a glance

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.



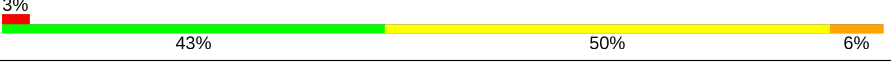
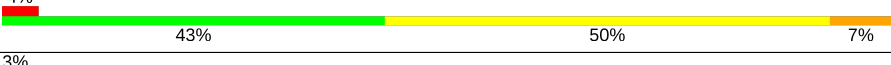
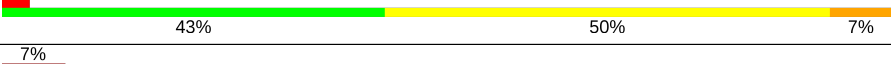
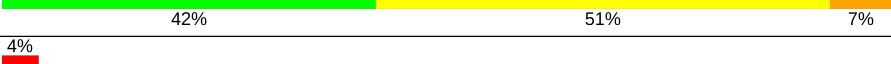
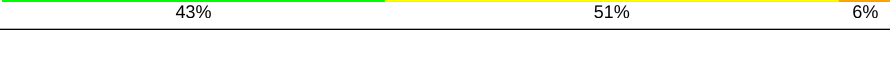
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 respectively. 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.

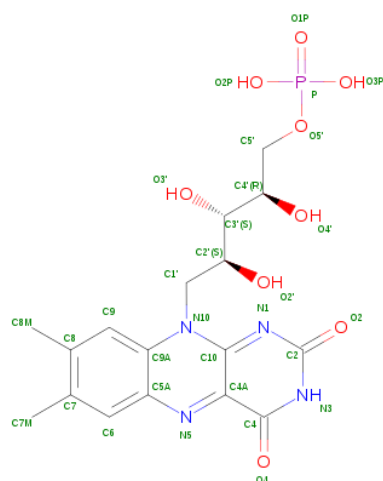
- Molecule 1 is a protein called FATTY ACID SYNTHASE ALPHA SUBUNITS.

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).

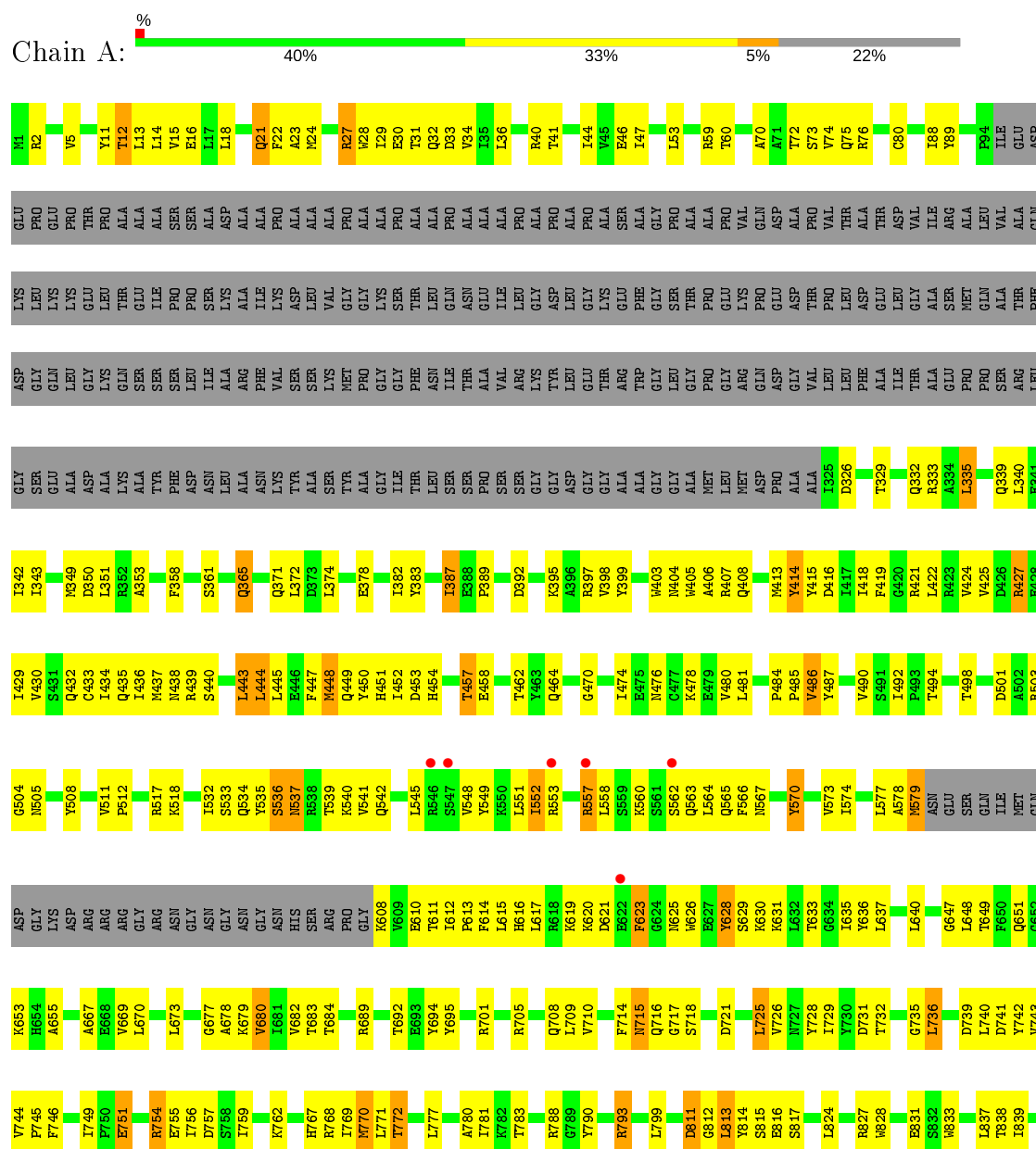


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	K	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	L	1	Total 31	C 17	N 4	O 9	P 1	0	0

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

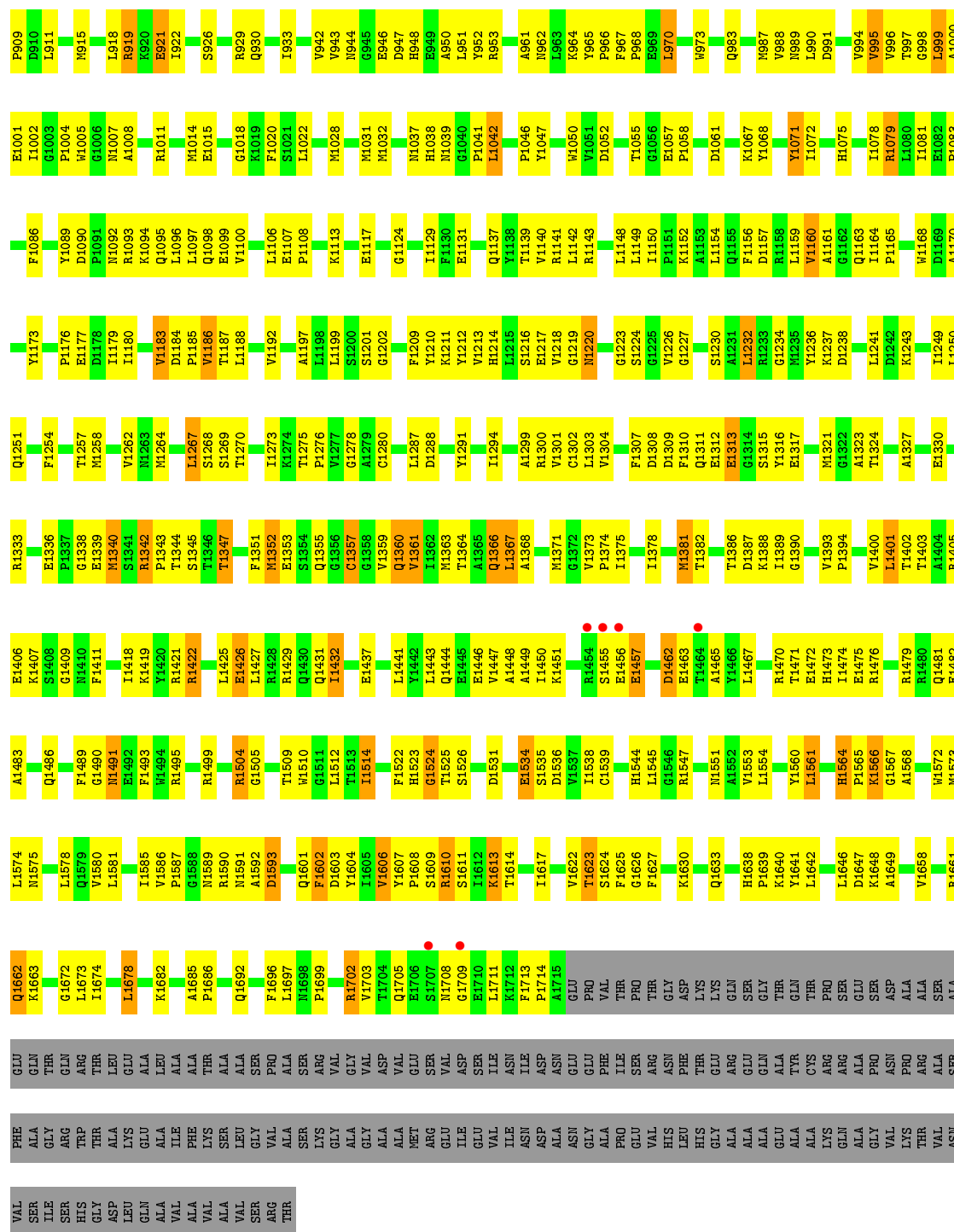


F1209	K1113	S1021	V943	V643	E751	K653	K654	A655	R648	R754	R755	R756	D757	S758	R759	K762	R767	R768	I769	W770	L771	I772	R776	L777	T692	W695	R701	R705	Q708	L709	V710	R793	L799	D811	G812	L813	S814	S815	R816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839
K1211	E1117	M1028	E946	R648	R754	R654	R655	R656	R754	R755	R756	D757	S758	R759	K762	R767	R768	I769	W770	L771	I772	R776	L777	T692	W695	R701	R705	Q708	L709	V710	R793	L799	D811	G812	L813	S814	S815	R816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839	
Y1212	I1129	M1028	E946	R648	R754	R654	R655	R656	R754	R755	R756	D757	S758	R759	K762	R767	R768	I769	W770	L771	I772	R776	L777	T692	W695	R701	R705	Q708	L709	V710	R793	L799	D811	G812	L813	S814	S815	R816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839	
Y1213	I1129	M1028	E946	R648	R754	R654	R655	R656	R754	R755	R756	D757	S758	R759	K762	R767	R768	I769	W770	L771	I772	R776	L777	T692	W695	R701	R705	Q708	L709	V710	R793	L799	D811	G812	L813	S814	S815	R816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839	
Y1214	E1131	M1030	E949	R649	R755	R655	R656	R657	R755	R756	R757	D758	S759	R760	K763	R768	I769	W770	L771	I772	R776	L777	T692	W695	R701	R705	Q708	L709	V710	R793	L799	D811	G812	L813	S814	S815	R816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839		
L1216	T1135	N1037	A950	R653	R758	R654	R655	R656	R758	R759	R760	D761	S762	R763	K764	R769	I770	W771	L772	I773	R777	L778	T693	W696	R702	R706	R710	R714	Q717	L718	V719	R794	L799	D812	G813	L814	S815	S816	R817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839	
S1217	E1137	H1038	Y952	R654	R759	R655	R656	R657	R759	R760	R761	D762	S763	R764	K765	R770	I771	W772	L773	I774	R778	L779	T694	W697	R703	R707	R711	Q714	L715	V716	R795	L799	D813	G814	L815	S816	S817	R818	L819	A820	L821	L824	R827	R828	W829	S830	E831	S832	R833	L837	W838	R839			
E1218	R1143	P1047	N962	R655	R760	R656	R657	R658	R760	R761	R762	D763	S764	R765	K766	R771	I772	W773	L774	I775	R779	L780	T695	W698	R704	R708	R712	Q715	L716	V717	R796	L799	D814	G815	L816	S817	S818	R819	L820	A821	L822	L825	R828	R829	W830	S831	E832	R833	L838	W839	R840				
G1219	L1148	L1149	L963	R656	R761	R657	R658	R659	R761	R762	R763	D764	S765	R766	K767	R772	I773	W774	L775	I776	R780	L781	T696	W699	R705	R709	R713	Q716	L717	V718	R797	L799	D815	G816	L817	S818	S819	R820	L821	A822	L823	L826	R829	R830	W831	S832	R833	L839	W840	R841					
N1220	L1149	L1150	L964	R657	R762	R658	R659	R660	R762	R763	R764	D765	S766	R767	K768	R773	I774	W775	L776	I777	R781	L782	T697	W700	R706	R710	R714	Q717	L718	V719	R798	L799	D816	G817	L818	S819	S820	R821	L822	A823	L824	L827	R830	R831	W832	S833	L840	W841	R842						
G1223	L1150	L1151	L965	R658	R763	R659	R660	R661	R763	R764	R765	D766	S767	R768	K769	R774	I775	W776	L777	I778	R782	L783	T698	W701	R707	R711	R715	Q718	L719	V720	R799	L799	D817	G818	L819	S820	S821	R822	L823	A824	L825	L828	R831	R832	W833	S834	L841	W842	R843						
S1224	L1151	L1152	L966	R659	R764	R660	R661	R662	R764	R765	R766	D767	S768	R769	K770	R775	I776	W777	L778	I779	R783	L784	T699	W702	R708	R712	R716	Q719	L720	V721	R800	L799	D818	G819	L820	S821	S822	R823	L824	A825	L826	L829	R832	R833	W834	S835	L842	W843	R844						
V1226	L1152	L1153	L967	R660	R765	R661	R662	R663	R765	R766	R767	D768	S769	R770	K771	R776	I777	W778	L779	I780	R784	L785	T700	W703	R709	R713	R717	Q720	L721	V722	R801	L799	D819	G820	L821	S822	S823	R824	L825	A826	L827	L830	R833	R834	W835	S836	L843	W844	R845						
G1227	L1153	L1154	L968	R661	R766	R662	R663	R664	R766	R767	R768	D769	S770	R771	K772	R777	I778	W779	L780	I781	R785	L786	T701	W704	R710	R714	R718	Q721	L722	V723	R802	L799	D820	G821	L822	S823	S824	R825	L826	A827	L828	L831	R834	R835	W836	S837	L844	W845	R846						
G1228	L1154	L1155	L969	R662	R767	R663	R664	R665	R767	R768	R769	D770	S771	R772	K773	R778	I779	W780	L781	I782	R786	L787	T702	W705	R711	R715	R719	Q722	L723	V724	R803	L799	D821	G822	L823	S824	S825	R826	L827	A828	L829	L832	R835	R836	W837	S838	L845	W846	R847						
M1235	L1155	L1156	L970	R663	R768	R664	R665	R666	R768	R769	R770	D771	S772	R773	K774	R779	I780	W781	L782	I783	R788	L789	T703	W706	R712	R716	R720	Q723	L724	V725	R804	L799	D822	G823	L824	S825	S826	R827	L828	A829	L830	L833	R836	R837	W838	S839	L846	W847	R848						
G1236	L1156	L1157	L971	R664	R769	R665	R666	R667	R769	R770	R771	D772	S773	R774	K775	R780	I781	W782	L783	I784	R789	L790	T704	W707	R713	R717	R721	Q724	L725	V726	R805	L799	D823	G824	L825	S826	S827	R828	L829	A830	L831	L834	R837	R838	W839	S840	L847	W848	R849						
D1237	L1157	L1158	L972	R665	R770	R666	R667	R668	R770	R771	R772	D773	S774	R775	K776	R781	I782	W783	L784	I785	R790	L791	T705	W708	R714	R718	R722	Q725	L726	V727	R806	L799	D824	G825	L826	S827	S828	R829	L830	A831	L832	L835	R838	R839	W840	S841	L848	W849	R850						
D1238	L1158	L1159	L973	R666	R771	R667	R668	R669	R771	R772	R773	D774	S775	R776	K777	R782	I783	W784	L785	I786	R791	L792	T706	W709	R715	R719	R723	Q726	L727	V728	R807	L799	D825	G826	L827	S828	S829	R830	L831	A832	L833	L836	R840	R841	W841	S842	L849	W850	R851						
L1241	L1159	L1160	L974	R667	R772	R668	R669	R670	R772	R773	R774	D775	S776	R777	K778	R783	I784	W785	L786	I787	R792	L793	T707	W710	R716	R720	R724	Q727	L728	V729	R808	L799	D826	G827	L828	S829	S830	R831	L832	A833	L834	L837	R841	R842	W842	S843	L850	W851	R852						
D1242	L1160	L1161	L975	R668	R773	R669	R670	R671	R773	R774	R775	D776	S777	R778	K779	R784	I785	W786	L787	I788	R793	L794	T708	W711	R717	R721	R725	Q728	L729	V730	R809	L799	D827	G828	L829	S830	S831	R832	L833	A834	L835	L838	R842	R843	W843	S844	L851	W852	R853						
K1243	L1161	L1162	L976	R669	R774	R670	R671	R672	R774	R775	R776	D777	S778	R779	K780	R785	I786	W787	L788	I789	R794	L795	T709	W712	R718	R722	R726	Q729	L730	V731	R810	L799	D828	G829	L830	S831	S832	R833	L834	A835	L836	L839	R843	R844	W844	S845	L852	W853	R854						
L1250	L1162	L1163	L977	R670	R775	R671	R672	R673	R775	R776	R777	D778	S779	R780	K781	R786	I787	W788	L789	I790	R795	L796	T710	W713	R719	R723	R727	Q730	L731	V732	R811	L799	D829	G830	L831	S832	S833	R834	L835	A836	L837	L840	R844	R845	W845	S846	L853	W854	R855						
Q1251	L1163	L1164	L978	R671	R776	R672	R673	R674	R776	R777	R778	D779	S780	R781	K782	R787	I788	W789	L790	I791	R796	L797	T711	W714	R720	R724	R728	Q731	L732	V733	R812	L799	D830	G831	L832	S833	S834	R835	L836	A837	L838	L841	R845	R846	W846	S847	L854	W855	R856						
F1254	L1164	L1165	L979	R672	R777	R673	R674	R675	R777	R778	R779	D780	S781	R782	K783	R788	I789	W790	L791	I792	R797	L798	T712	W715	R721	R725	R729	Q732	L733	V734	R813	L799	D831	G832	L833	S834	S835	R836	L837	A838	L839	L842	R846	R847	W847	S848	L855	W856	R857						
T1257	L1165	L1166	L980	R673	R778	R674	R675	R676	R778	R779	R780	D781	S782	R783	K784	R789	I790	W791	L792	I793	R798	L799	T713	W716	R722	R726	R730	Q733	L734	V735	R814	L799	D832	G833	L834	S835	S836	R837	L838	A839	L840	L843	R847	R848	W848	S849	L856	W857	R858						
M1264	L1166	L1167	L981	R674	R779	R675	R676	R677	R779	R780	R781	D782	S783	R784	K785	R790	I791	W792	L793	I794	R799	L800	T714	W717	R723	R727	R731	Q734	L735	V736	R815	L799	D833	G834	L835	S836	S837	R838	L839	A840	L841	L844	R848	R849	W849	S850	L857	W858	R859						
M1267	L1167	L1168	L982	R675	R780	R676	R677	R678	R780	R781	R782	D783	S784	R785	K786	R791	I792	W793	L794	I795	R800	L801	T715	W718	R724	R728	R732	Q735	L736	V737	R816	L799	D834	G835	L836	S837	S838	R839	L840	A841	L842	L845	R849	R850	W850	S851	L858	W859	R860						
S1268	L1168	L1169	L983	R676	R781	R677	R678	R679	R781	R782	R783	D784	S785	R786	K787	R792	I793	W794	L795	I796	R801	L802	T716	W719	R725	R729	R733	Q736	L737	V738	R817	L799	D835	G836	L837	S838	S839	R840	L841	A842	L843	L846	R850	R851	W851	S852	L859	W860	R861						
S1269	L11																																																						



L1678	N1589	T1509	I1432	F1351	S1269	V1183	R1093	M1007	I922	T838	P750	E668	ARG
A1592	N1591	G1511	E1437	M1352	T1270	D1184	K1094	A1008	S926	I839	E751	P669	ARG
D1593	G1512	G1513	L1441	L1354	T1273	P1185	Q1095	R1011	R929	V843	R754	Q671	GLY
Q1601	T1512	T1513	L1442	Q1355	T1275	T1187	L1096	M1014	R930	R848	I756	L672	ARG
P1602	L1614	L1614	L1443	G1356	P1276	L1188	Q1098	E1015	I933	R848	D757	G673	ASN
D1603	F1522	F1522	E1445	G1358	G1278	A1197	V1100	G1018	V942	G851	S758	G677	GLY
H1604	H1523	H1523	E1446	L1198	C1280	L1198	L1106	K1019	V942	L852	I759	A678	GLY
V1606	G1524	G1524	V1447	Q1360	C1280	L1199	L1107	F1020	A855	A855	K762	K679	ASN
S1526	T1525	T1525	A1448	V1361	L1287	S1200	P1108	S1021	E946	N856	I681	V680	ASN
P1608	S1526	S1526	L1449	I1361	D1288	S1201	P1108	L1022	E948	N857	V682	R683	HIS
S1609	T1627	T1627	M1363	M1363	D1288	F1209	K1113	M1028	E949	V859	I769	G529	SER
R1610	D1531	D1531	K1451	A1364	Y1291	F1209	E1117	M1031	A950	V863	L771	S688	ARG
S1611	E1534	E1534	R1453	A1366	I1294	K1211	E1117	M1031	L951	V863	T772	R689	PRO
K1613	S1535	S1535	R1454	L1367	I1294	V1212	G1124	M1032	Y952	V868	R776	Q534	LYS
T1614	D1536	D1536	A1455	A1368	A1299	H1213	E1131	M1037	R953	R688	I781	S536	VAL
I1617	V1537	V1537	E1457	M1371	R1300	H1215	E1131	H1038	R954	R689	L777	N537	GLY
V1622	C1538	C1538	D1458	G1372	V1301	L1216	E1134	M1039	V955	T870	R788	S536	LYS
T1623	C1539	C1539	G1459	G1373	C1302	E1217	E1134	G1040	V956	F871	Y790	N537	VAL
S1624	L1542	L1542	P1460	P1374	L1303	V1218	Q1137	P1041	P959	Q873	I781	Q542	GLY
F1625	K1543	K1543	F1461	L1375	V1304	G1219	V1140	L1042	A961	Q874	I783	N543	VAL
G1626	H1544	H1544	T1463	I1378	D1307	G1223	L1142	K1045	N962	L881	R788	R546	GLY
F1627	L1545	L1545	T1464	M1381	D1308	G1223	L1142	P1046	L963	G882	L777	S547	GLY
K1630	G1546	G1546	A1465	T1382	D1309	S1224	G1224	Y1047	K964	L883	Y790	V548	GLY
Q1633	R1547	R1547	L1466	L1386	F1311	V1226	T1147	M1050	Y965	M884	I793	L551	VAL
Q1633	G1550	G1550	R1470	D1387	E1312	G1227	L1148	Y1051	P967	L888	R793	L552	VAL
H1638	M1551	M1551	T1471	K1388	E1313	G1227	L1149	Y1052	P968	V889	L799	R553	GLY
P1639	A1552	A1552	E1472	L1389	G1314	S1230	P1155	G1056	E969	N890	S802	Q624	GLY
K1640	L1554	L1554	H1473	G1390	S1315	L1232	L1152	E1057	L970	Q893	S802	Q624	GLY
Y1641	Y1560	Y1560	I1474	P1394	E1317	R1234	L1154	E1057	W973	Q893	P803	H556	LYS
L1642	L1561	L1561	R1476	V1400	M1321	G1234	Q1155	P1058	Q983	P896	N804	R557	LYS
L1646	H1564	H1564	R1479	L1401	G1322	H1235	F1156	D1061	Q983	V897	D721	S562	GLY
D1647	P1565	P1565	R1480	T1402	A1323	V1236	D1157	L1081	N987	P898	L725	S629	GLY
K1648	K1566	K1566	Q1481	T1402	T1324	R1237	L1158	K1067	N987	A899	V726	K630	GLY
A1649	G1567	G1567	E1482	K1407	A1327	L1241	V1160	Y1068	N989	D900	L632	K631	GLY
Q1650	A1568	A1568	A1483	S1406	E1330	D1242	G1162	Y1071	L990	L901	T633	F566	GLY
Y1651	Y1572	Y1572	Q1486	G1409	E1330	K1243	Q1163	I1072	D991	G903	Y729	N567	GLY
C1655	M1573	M1573	Q1486	G1409	E1330	K1243	Q1163	I1072	K992	L905	T732	A568	GLY
Y1658	L1574	L1574	F1489	K1418	R1333	I1249	P1165	I1078	V994	Q906	L821	V573	GLY
Y1658	M1575	M1575	Q1490	Y1420	E1336	L1250	W1168	L1080	V995	F907	L735	I574	GLY
Q1662	L1578	L1578	N1491	R1421	F1337	Q1251	D1169	I1081	V996	I908	L824	R575	GLY
K1663	Q1579	Q1579	E1492	R1422	E1338	F1254	A1170	E1082	T997	P909	D739	A576	GLY
L1670	L1581	L1581	F1493	Q1423	E1339	F1254	A1170	P1083	G998	L911	L740	L577	GLY
F1669	H1581	H1581	W1494	Q1424	M1340	T1257	Y1173	F1086	A1000	N915	D741	Q651	GLY
H1670	L1581	L1581	R1495	L1425	S1341	M1258	P1176	E1086	I1002	E831	V743	M585	GLY
H1671	L1585	L1585	R1499	E1426	P1343	W1284	E1177	Y1089	G1003	L918	V744	Q586	GLY
G1672	V1586	V1586	G1672	R1429	T1344	W1284	D1178	D1090	P1004	R919	P745	R654	GLY
L1673	P1587	P1587	R1504	Q1430	T1344	L1267	L1179	P1091	W1005	K920	F746	A655	GLY
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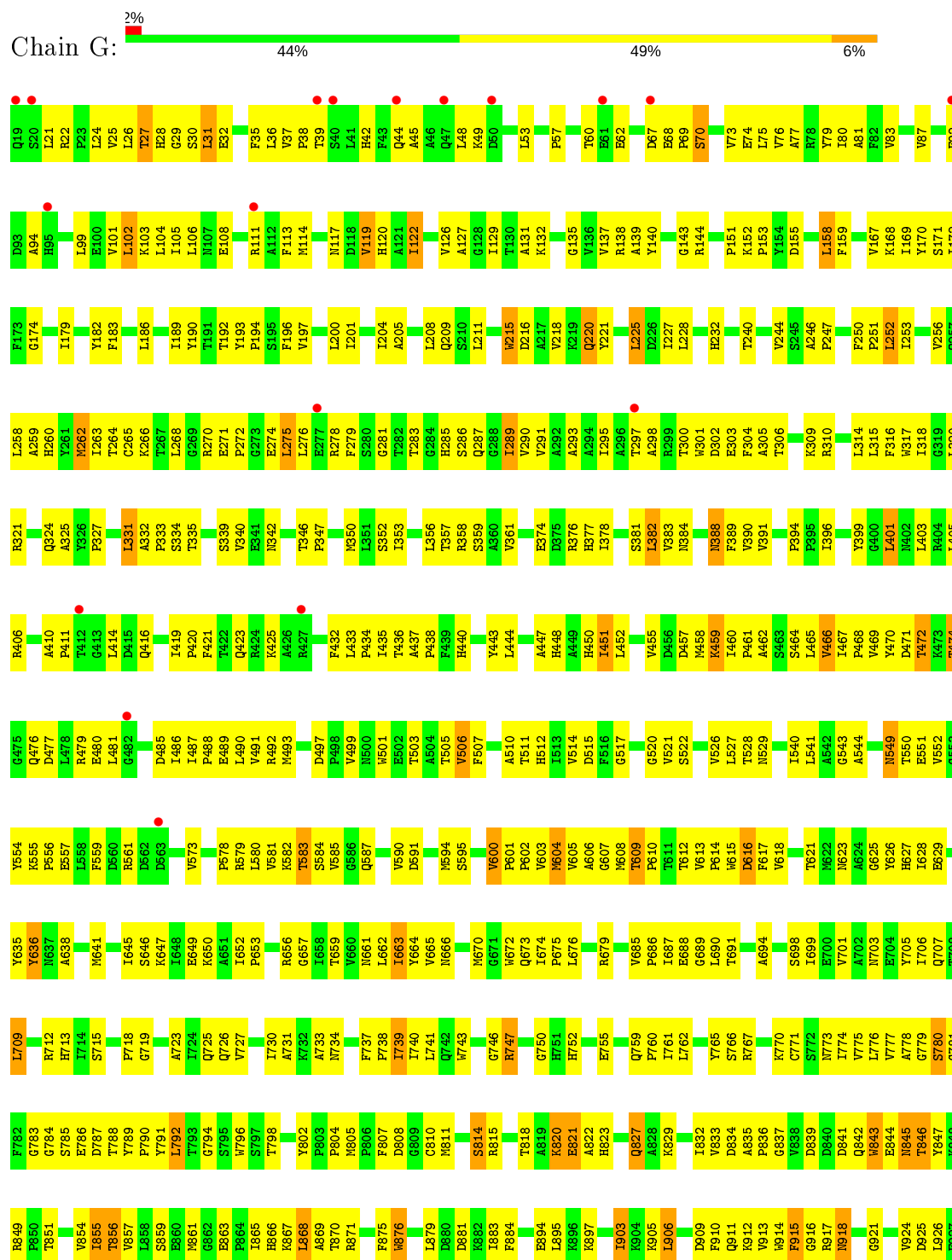
• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS

E1252	P1165	I1078	D991	Y008	R829	G735	L640	L577	T499	V425	E341	LEU	PHE	GLN	ASP
S1253	W1168	R1079	V994	P909	S830	G736	L640	A578	I500	D426	I342	GLY	ASP	LYS	GLU
F1254	D1169	L1080	V995	E331	E832	L736	L640	MET	D501	E427	I343	SER	GLY	LEU	PRO
T1257	A1170	I1081	V996	L911	S833	L740	G647	ASN	A502	E428	E428	ALA	GLY	LYS	GLU
M1258	P1083	E1082	T997	N915	R833	D741	T649	SER	R503	I429	K347	LYS	GLY	THR	PRO
M1284	P1086	F1086	G998	N915	L837	Y742	R650	GLN	N505	S431	K348	ALA	LYS	PRO	ALA
G1174	L999	L918	L999	L918	R838	Y743	R651	ILE	N505	Q432	K349	LYS	GLN	THR	ALA
G1174	A1000	R919	A1000	R919	R839	Y744	R652	MET	Y508	C433	D360	ALA	SER	GLU	ALA
P1176	E1001	R920	E1001	R920	R839	Y745	R653	GLN	R517	I434	L351	ALA	SER	ILE	ALA
E1177	P1091	D1090	P1091	E321	R843	F745	R654	ASP	R517	Q435	R352	THR	SER	PRO	SER
D1178	P1092	P1091	P1092	I922	R843	F746	R655	GLY	K518	I436	A353	ASP	SER	SER	SER
I1179	H1005	N1092	H1005	I922	R848	E751	A655	GLY	K518	M437	K356	ASN	ILE	PRO	ALA
I1180	G1006	R1093	G1006	S926	R848	E751	A655	ASP	K524	M438	K357	LEU	ALA	ASP	ASP
T1273	N1007	K1094	N1007	S926	R849	A667	A667	ARG	K524	M438	K357	LEU	ALA	ASP	ASP
K1274	A1008	Q1095	A1008	R929	R850	R754	R668	ARG	A527	R440	F358	ALA	ARG	ALA	ALA
T1275	L1096	L1096	L1096	Q930	R851	E755	R669	ARG	A527	R440	F358	ALA	ARG	ALA	ALA
P1185	L1097	L1097	L1097	R930	R852	L756	L670	ARG	A527	R440	F358	ALA	ARG	ALA	ALA
V1276	R1011	R1097	R1011	R933	R853	L759	L673	GLY	G530	L443	S361	TYR	VAL	ASP	ALA
V1277	M1014	Q1098	M1014	R933	R853	L759	L673	ARG	G530	L443	S361	TYR	VAL	ASP	ALA
G1278	E1015	E1098	E1015	R935	R856	K762	L673	ASN	I532	L444	Q865	SER	SER	LEU	ALA
A1279	G1018	V1100	G1018	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
C1280	K1019	V1100	K1019	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	F1020	P1108	F1020	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	S1021	P1108	S1021	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	L1022	P1108	L1022	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	G1018	P1108	G1018	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	K1019	P1108	K1019	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	F1020	P1108	F1020	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	S1021	P1108	S1021	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	L1022	P1108	L1022	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	G1018	P1108	G1018	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	K1019	P1108	K1019	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	F1020	P1108	F1020	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	S1021	P1108	S1021	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	L1022	P1108	L1022	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	G1018	P1108	G1018	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	K1019	P1108	K1019	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
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L1188	K1019	P1108	K1019	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	F1020	P1108	F1020	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
L1188	S1021	P1108	S1021	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
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L1188	F1020	P1108	F1020	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
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L1188	G1018	P1108	G1018	R935	R856	K762	L673	GLY	I532	L444	Q865	SER	SER	LEU	ALA
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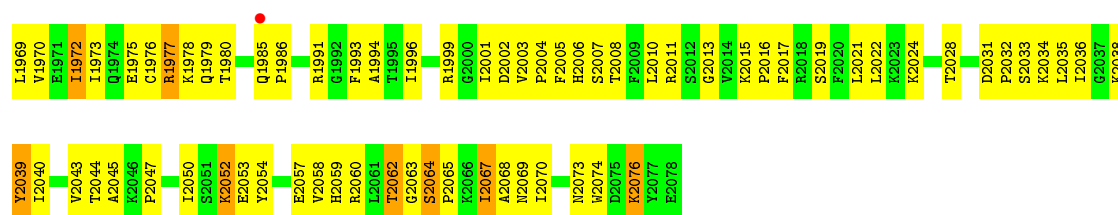


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LEU	ALA	ASP
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ALA	GLU	LEU
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ALA	VAL	ALA
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THR	LYS	VAL
THR	LEU	THR
ALA	GLY	GLY
SER	SER	SER
PRO	VAL	ARG
ALA	ALA	THR
SER	SER	
ARG	LYS	
VAL	GLY	
GLY	ALA	
VAL	GLY	
ASP	ALA	
VAL	ALA	
GLU	MET	
SER	ARG	
VAL	GLU	
ILE	ILE	
ASP	GLY	
SER	ILE	
ILE	ASN	
ASN	ASN	
ASP	ASP	
ASN	ALA	
GLU	ASN	
GLU	GLY	
PHE	ALA	
ILE	PRO	
SER	GLU	
ARG	VAL	
ASN	HIS	
PHE	LEU	
THR	HIS	
GLY	GLY	
ARG	ALA	
GLU	ALA	
GLN	ALA	
ALA	ALA	
TYR	ALA	
CYS	ALA	
ARG	LYS	
ARG	GLN	
ALA	ALA	
PRO	GLY	
ASN	VAL	
ASN	LYS	
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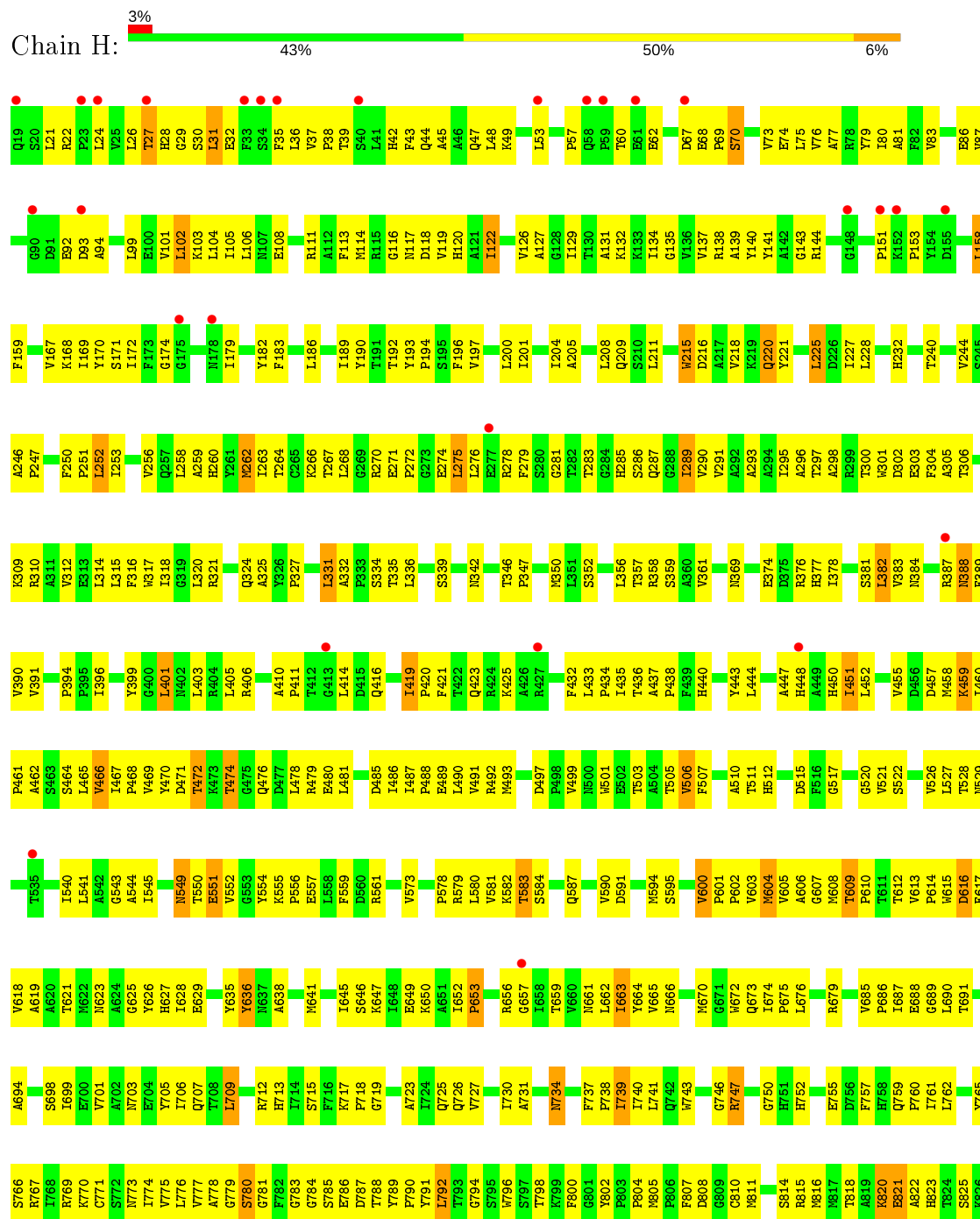
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



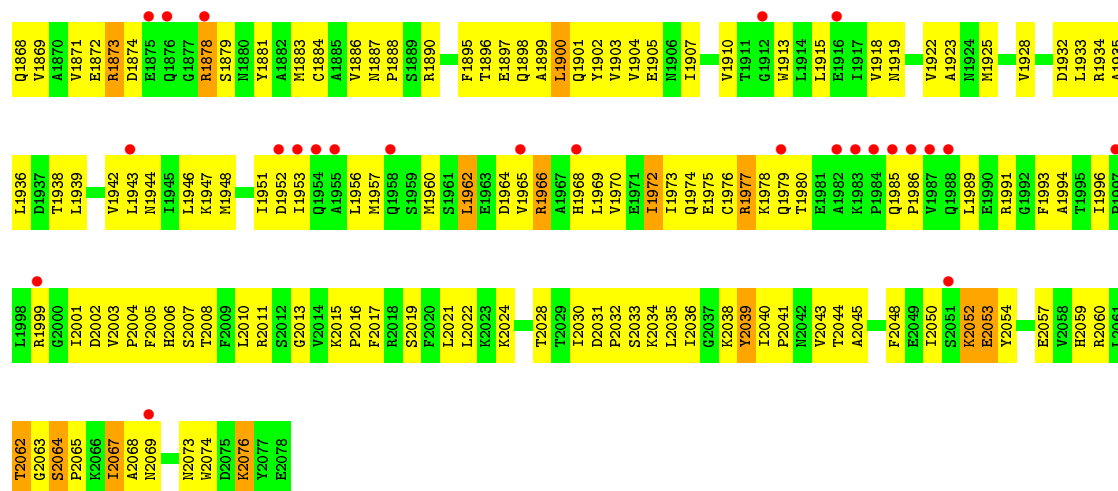
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	T1803			V1619	I1541	E1472	L1401	V1325	E1248	E1179	Y1103	A1033	R964
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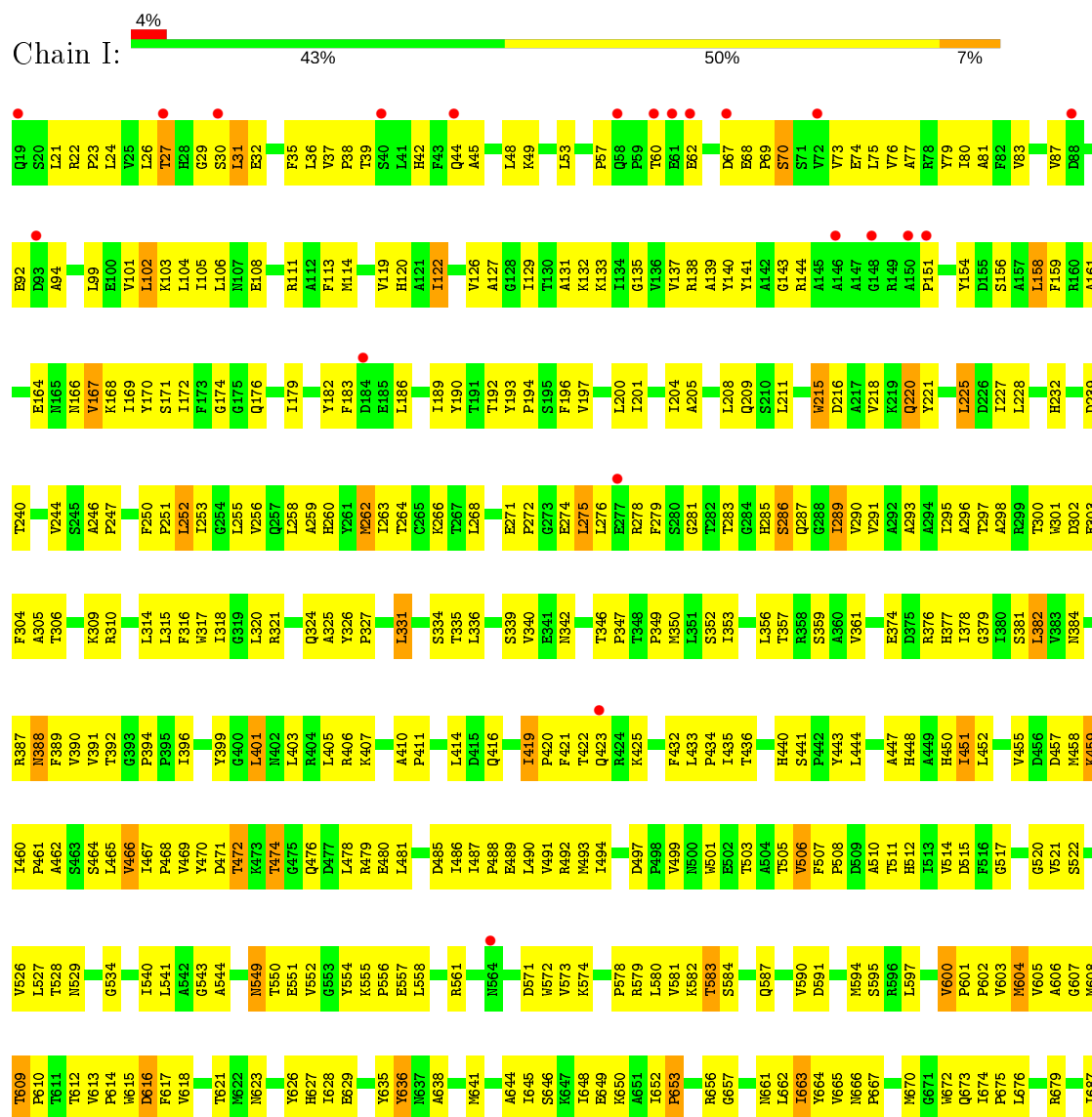
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



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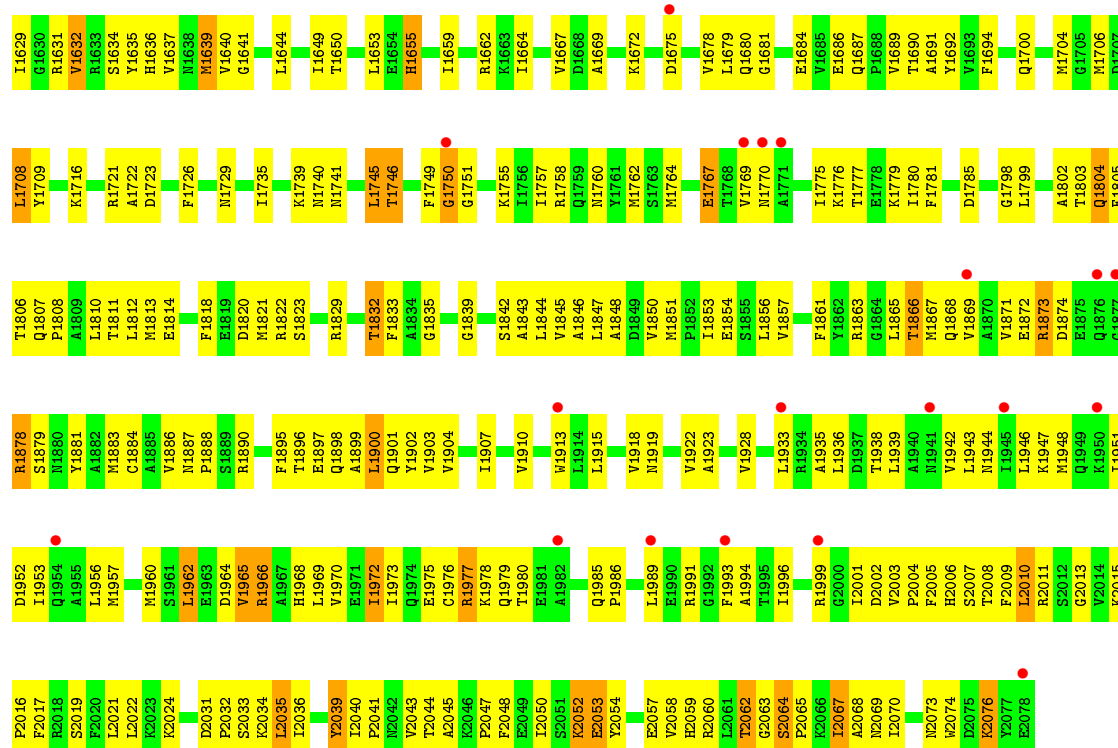


• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

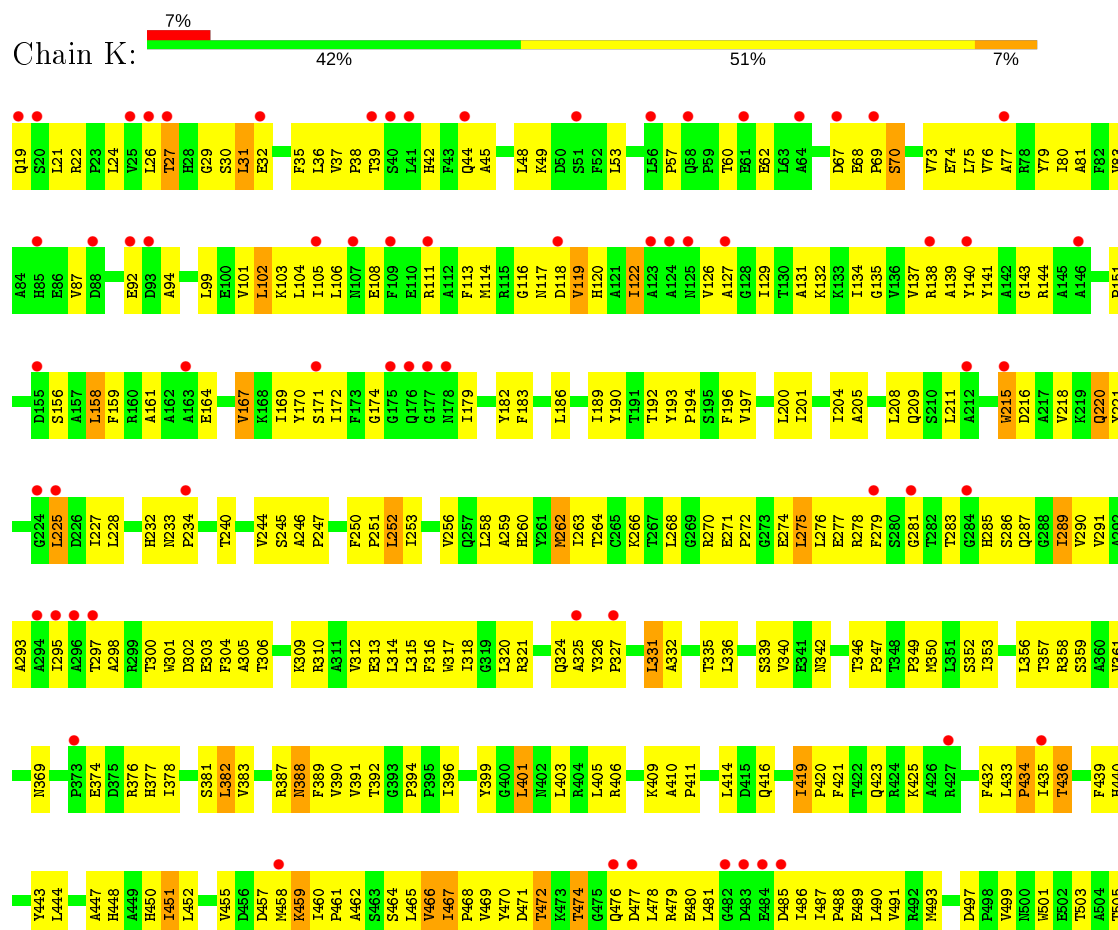


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L1344	P1345	M1346	D1347	F1348	A1349	H1350	V1351	V1352	G1353	A1354	K1355	A1356	K1359	P1360	I1361	F1362	P1363	A1364	K1365	I1366	D1367	G1368	L1369	L1370	L1371	K1372	L1373	V1374	H1375	M1382	V1383	P1384	P1388	V1391	G1392	D1393	V1394	L1395	D1396	L1397	T1398	A1399	Q1400	I1401	N1402	A1403	V1404	I1405	N1406	S1409	G1410	K1411	V1413					
T1259	T1260	R1262	Y1265	H1266	P1267	E1268	A1269	G1270	Y1271	I1274	R1275	E1276	V1277	R1284	L1285	K1286	F1288	Y1289	Y1290	R1291	V1292	L1293	F1294	L1295	A1296	K1297	E1298	V1299	P1300	F1301	L1305	V1308	F1309	R1313	E1314	L1315	V1316	M1317	A1318	F1324	V1325	L1326	A1334	E1335	F1335	R1338	G1339	F1342	F1343									
F1187	Q1188	T1189	M1190	P1191	L1192	K1193	R1194	L1195	A1197	P1198	T1199	G1200	E1201	M1202	Y1203	V1204	E1205	T1207	N1208	P1209	T1215	L1216	D1217	S1218	L1219	A1295	K1296	L1297	E1298	V1299	P1300	F1301	L1305	V1308	F1309	R1313	E1314	L1315	V1316	M1317	A1318	F1324	V1325	L1326	A1334	E1335	F1335	R1338	G1339	F1342	F1343							
D1104	G1105	K1106	E1107	E1108	M1109	Y1110	F1111	V1112	I1113	E1114	Y1115	K1122	A1123	T1124	I1125	E1126	F1127	P1128	D1129	I1130	L1133	R1137	D1138	A1139	L1140	K1141	I1142	S1143	L1146	A1149	M1153	L1154	P1155	D1156	V1157	D1158	S1159	F1160	I1164	Y1169	S1170	M1171	R1172	H1173	A1174	M1175	T1178	E1179	V1180	F1181								
E968	R969	F970	T971	E974	Q975	Q976	P977	D985	S986	L987	Q981	D985	L986	D987	E988	P989	Y990	P991	R995	I996	L997	A998	A999	Y1000	P1001	E1002	A1003	S1004	T1005	Q1006	R937	I1008	M938	V939	A1010	Q1011	D1012	N942	Y943	Q1014	H1015	F1016	L1017	L1018	L1019	G1020	R1022	K1026	P1027	V1028	F962	P1029	F1030	V1031	P1032	A1033	L1034	
B1035	E1036	E1039	Y1040	Y1041	F1042	K1043	K1044	M1048	L1049	S1050	E1051	I1052	T1053	Y1057	V1061	G1062	R1063	T1064	G1065	L1066	L1067	Q1068	G1069	P1070	V1071	A1072	A1073	K1074	Y1075	S1076	K1077	D1080	E1081	T1082	K1083	Y943	D1085	I1086	L1087	D1088	G1089	I1090	H1091	N1092	D1093	H1094	I1095	F1097	L1098	L1099	R1100	Y1103						
B821	A822	H823	Q827	K828	K829	T832	R833	D834	A835	P836	D839	E840	T841	D841	Q842	H843	E844	M845	T846	K848	L926	E927	D928	M929	P1001	E1002	A1003	S1004	T1005	Q1006	R937	I1008	M938	V939	A1010	Q1011	D1012	N942	Y943	Q1014	H1015	F1016	L1017	L1018	L1019	G1020	R1022	K1026	P1027	V1028	F962	P1029	F1030	V1031	P1032	A1033	L1034	
B88	G689	L1690	T891	I692	G693	A694	P697	S698	I699	K700	E701	A702	M703	E704	Y705	L706	V707	T708	L709	R712	H713	I714	S715	P718	G719	A723	I724	Q725	W726	V727	I730	A731	R732	A733	N734	F737	P738	I739	L740	L741	P800	Q801	Y802	P803	P804	M805	P806	F807	W742	W743	G746	R747	G750	H751	H752	S753	F754	E755



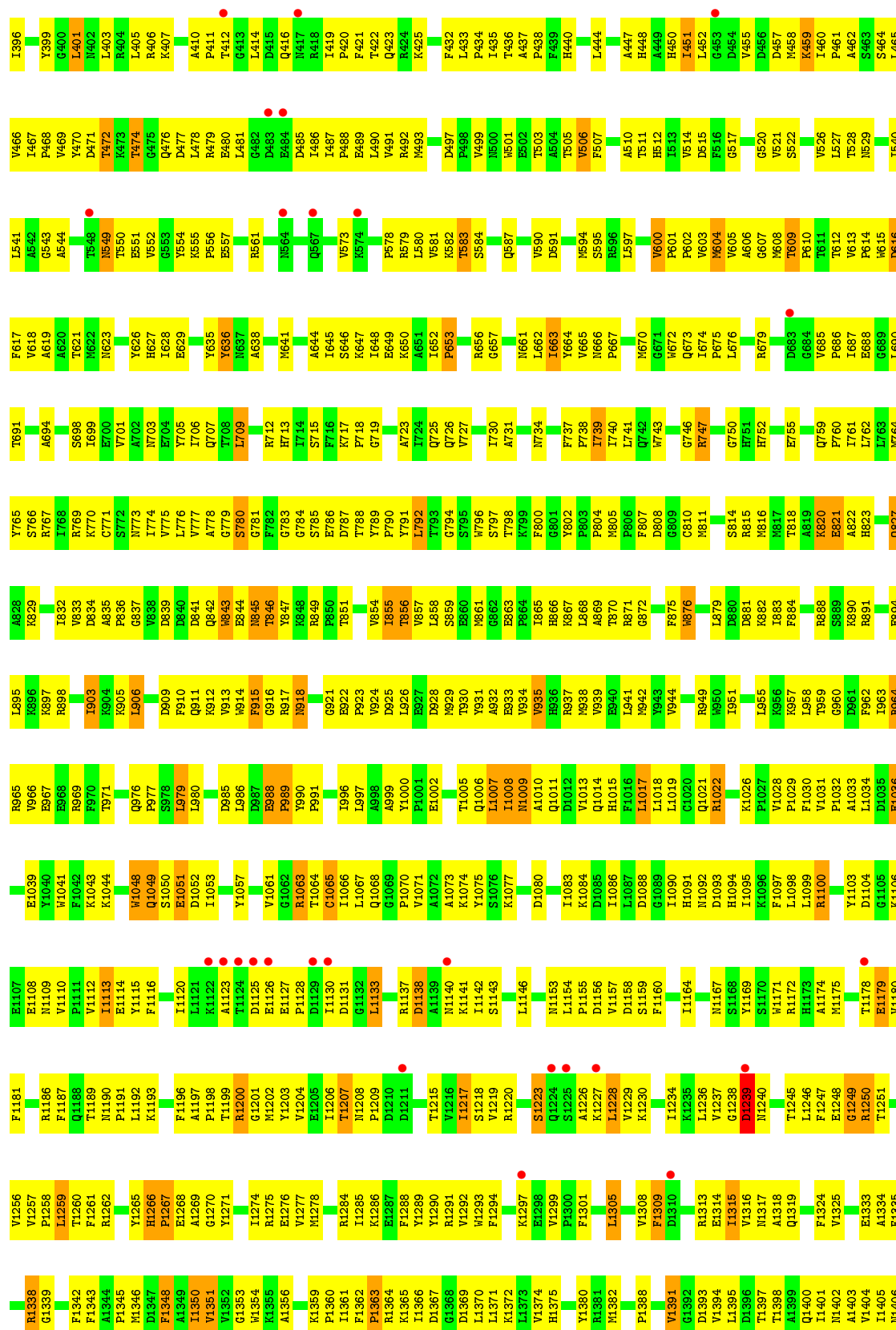


• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



R1436	T1358	Y1289	A1213	S1143	A1073	Q1006	H836	I865	Y802	I740	V664	F589	V506
G1437	K1359	Y1290	A1214	L1146	K1074	L1007	R937	H866	P803	L741	V665	V690	F507
V1438	P1360	R1291	V1215	L1147	Y1075	I1008	N938	K867	M804	W742	V666	D591	D509
V1439	V1292	V1293	V1216	A1152	K1076	M1009	V939	L868	M005	Q743	M670	M594	A510
F1362	W1293	W1293	I1217	N1153	V1078	Q1011	E940	A869	P806	G746	N670	S595	T511
D1441	P1363	D1441	I1218	L1154	L1079	Q1012	N942	T870	F807	R747	N672	V600	H512
R1364	R1364	F1294	V1219	P1155	D1080	V1013	Y943	R871	D808	G748	Q673	P601	F516
K1365	K1365	K1297	A1220	F1156	D1080	Q1014	Y944	G872	G809	G749	P675	P602	G517
E1298	E1298	E1298	S1223	V1157	K1083	H1015	K948	F875	S814	H752	L676	V604	G520
P1300	P1300	P1300	Q1224	V1157	K1083	F1016	R949	R876	K877	R679	A606	V521	V521
D1302	D1302	D1302	S1225	S1159	F1160	L1017	N950	P878	R815	E755	A606	S522	S522
F1303	F1303	F1303	A1226	F1160	D1088	L1019	I951	L879	M816	D756	N607	N608	V526
P1304	P1304	P1304	K1227	F1160	G1089	Q1020	N952	D880	M817	P686	T609	P610	L527
L1305	L1305	L1305	V1228	T1164	H1091	G1021	P953	D881	T818	P686	P610	P610	T528
T1306	T1306	T1306	K1230	Y1169	N1092	R1022	S954	K882	A819	Q759	N611	N611	N529
A1307	A1307	A1307	S1170	S1170	D1093	Q1025	L955	I883	K820	P760	T611	T612	T528
V1308	V1308	V1308	H1171	H1171	H1094	F1030	K956	P884	R821	I761	L690	L690	N529
F1309	F1309	F1309	R1172	R1172	I1095	P1027	K957	F884	A822	L762	L690	L690	D533
R1313	R1313	R1313	K1235	A1173	K1096	K1026	L958	R888	H823	L762	L690	L690	I540
E1314	E1314	E1314	V1237	A1174	F1097	P1028	T959	P888	S824	L762	L690	L690	L541
I1315	I1315	I1315	G1238	M1175	L1098	P1029	F962	R891	S825	L762	L690	L690	A542
V1316	V1316	V1316	D1239	F1177	L1099	F1031	T963	E894	K826	Y765	A694	A694	G543
N1317	N1317	N1317	N1240	T1178	R1100	P1032	R864	L895	A828	R767	T616	T616	A544
A1318	A1318	A1318	T1245	E1179	Y1103	A1033	R965	K897	K829	I768	P697	P697	A544
Q1319	Q1319	Q1319	L1246	H1180	D1104	L1034	V966	K897	I832	W700	T621	T621	I545
F1324	F1324	F1324	F1247	F1181	K1105	E1035	E967	K897	I903	K771	N623	N623	D546
D1323	D1323	D1323	I1248	F1182	K1106	E1036	E968	K905	K834	W772	A624	A624	G547
V1328	V1328	V1328	V1256	Q1188	E1108	E1039	P970	K905	D839	N773	G625	G625	T548
N1330	N1330	N1330	P1257	H1188	E1109	Y1040	S972	L906	P836	W775	L626	L626	N549
A1334	A1334	A1334	P1258	T1189	P1111	F1042	L980	N918	G837	L776	L627	L627	T550
F1335	F1335	F1335	L1259	N1190	V1112	K1043	S978	Q911	D841	A778	E629	E629	G553
V1336	V1336	V1336	T1260	P1191	E1114	L1047	L979	Q912	Q842	S780	V635	V635	Y554
D1337	D1337	D1337	F1261	L1192	F1115	W1048	N980	V913	W843	G781	V636	V636	K555
R1338	R1338	R1338	R1262	K1193	F1116	Q1049	Q981	W914	E844	H713	P556	P556	P556
G1339	G1339	G1339	Y1265	L1195	L1121	S1050	D985	G916	N845	F782	E557	E557	L558
K1340	K1340	K1340	H1265	F1196	K1122	E1051	D987	R917	T846	G783	D560	D560	F559
D1341	D1341	D1341	P1267	A1197	A1123	D1052	E987	N918	X847	S785	A561	A561	D560
F1342	F1342	F1342	E1268	P1198	E1126	I1053	E988	G921	K848	G719	I645	I645	R561
A1343	A1343	A1343	A1269	T1199	E1127	Y1057	P989	E922	R849	A723	S646	S646	P566
V1345	V1345	V1345	G1270	R1200	P1128	Q1062	Y990	P923	P850	I724	K647	K647	E557
M1346	M1346	M1346	Y1271	G1201	D1129	V1061	P991	V924	T851	Q725	I648	I648	L558
D1347	D1347	D1347	I1274	Y1202	I1130	G1063	D925	D925	V854	Y791	K650	K650	D560
F1348	F1348	F1348	R1275	Y1203	D1131	R1063	R995	L926	I855	L792	A651	A651	F578
A1349	A1349	A1349	E1276	V1204	L1132	T1064	L996	E927	T856	T793	I652	I652	R579
I1350	I1350	I1350	E1276	E1205	L1133	C1065	L997	D928	V857	G794	P653	P653	L580
P1345	P1345	P1345	V1277	I1206	L1133	I1066	A998	M929	L858	K732	V581	V581	V581
V1352	V1352	V1352	M1278	T1207	R1137	L1067	A999	T930	L858	K732	K656	K656	K582
G1353	G1353	G1353	R1284	N1208	D1138	Q1068	Y1000	X931	P860	N734	G657	G657	T583
V1354	V1354	V1354	I1285	P1209	A1139	G1069	P1001	A932	M861	T798	N661	N661	S584
K1355	K1355	K1355	D1210	D1211	N1140	P1070	E1002	E933	G862	K799	F737	F737	Q587
A1356	A1356	A1356	F1212	P1212	I1142	A1072	T1005	V934	E863	F738	L662	L662	T588
I1357	I1357	I1357	F1288	F1212	I1142	A1072	T1005	V934	E863	F738	L662	L662	T588





K2015	Q1954	M1813	K1716	R1631	M1556	E1482	S1409
P2016	A1955	E1814	R1721	V1632	F1557	L1483	G1410
F2017	L1956	F1818	A1722	R1633	M1558	T1487	K1411
R2018	M1957	D1819	F1726	S1634	M1559	V1488	M1412
S2019	M1960	D1820	F1726	H1635	P1560	L1489	V1413
F2020	S1961	M1821	K1739	H1636	P1562	C1416	C1416
L2021	L1962	S1822	M1740	V1637	L1563	G1417	G1417
L2022	E1963	S1823	M1741	M1638	T1567	T1418	T1418
K2023	D1964	Q1828	P1742	M1639	K1566	F1498	F1498
K2024	V1965	R1829	M1745	G1641	T1567	K1499	K1499
T2028	R1966	D1830	T1746	L1644	P1568	M1500	R1421
T2029	A1967	S1831	T1746	P1645	R1572	Y1504	K1424
I2030	H1968	T1832	F1749	M1646	A1573	S1505	P1426
D2031	L1969	F1833	G1751	D1647	P1574	S1506	V1426
P2032	V1970	G1835	K1755	T1650	A1575	V1507	M1427
S2033	E1971	G1839	K1755	L1653	M1579	I1510	L1434
K2034	I1972	E1840	R1758	E1654	V1583	G1511	Y1435
L2035	I1973	Y1841	Q1759	H1655	S1584	L1514	R1436
L2036	Q1974	S1842	N1760	R1659	G1585	L1515	G1437
G2037	E1975	L1844	M1761	I1659	D1586	E1516	V1438
T2038	C1976	V1845	M1762	R1662	Y1587	L1517	Y1439
D2039	R1977	A1846	S1763	K1663	M1588	F1518	Y1440
P2040	K1978	L1847	M1763	R1664	P1589	T1519	D1441
P2041	Q1979	A1848	F1766	I1664	I1590	K1520	Y1442
H2042	T1980	D1849	F1766	V1667	V1592	E1521	T1445
V2043	E1981	L1849	E1767	R1668	S1593	I1522	T1445
T2044	A1982	M1850	T1768	R1668	R1594	I1523	E1451
A2045	K1983	M1851	V1769	A1669	V1595	Q1524	V1452
K2046	P1984	E1852	M1770	K1672	F1596	V1525	P1453
K2047	Q1985	S1855	I1775	D1675	L1602	S1527	M1454
P2047	P1986	L1856	K1776	D1675	P1603	L1456	L1456
I2050	V1987	V1857	T1777	V1678	G1604	H1457	H1457
S2051	Q1988	F1861	E1778	L1679	T1605	T1460	T1460
K2052	L1989	Y1862	K1779	Q1680	I1606	P1461	P1461
E2053	A1990	R1863	F1781	G1681	T1607	S1469	S1469
Y2054	R1991	G1864	D1785	E1684	H1608	K1470	K1470
E2057	G1992	L1865	S1788	V1685	G1609	E1471	E1471
V2058	F1993	T1866	S1788	E1686	M1610	D1542	D1542
H2059	A1994	M1867	K1793	Q1687	Y1611	Y1543	Y1543
R2060	I1996	Q1868	L1799	P1688	V1616	Y1544	Y1544
L2061	P1997	V1869	A1802	V1689	R1617	F1472	F1472
T2062	L1998	D1870	T1803	T1690	S1618	K1475	K1475
G2063	A1999	E1871	Q1804	A1691	L1619	D1476	D1476
S2064	G2000	R1872	F1805	V1692	V1620	E1551	E1551
K2066	I2001	D1874	T1806	F1694	E1621	E1552	E1552
P2065	D2002	S1875	Q1807	M1706	T1622	Q1553	Q1553
I2067	V2003	D1874	P1808	E1707	V1623	P1554	P1554
A2068	P2004	R1878	L1812	Y1709	E1626	D1477	D1477
N2069	F2005	S1879			M1627	Q1478	Q1478
N2073	H2006	M1880			M1628	H1479	H1479
W2074	S2007	Y1881			G1630	D1480	D1480
K2076	T2008	A1882				V1555	V1555
Y2077	L2010	E1882					
E2078	R2011	S2012					
	G2013	V2014					

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	3.34 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.290 , 0.320 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.123	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	0.276 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1451/1878 (77%)	1291 (89%)	148 (10%)	12 (1%)	19	54
1	B	1458/1878 (78%)	1295 (89%)	151 (10%)	12 (1%)	19	54
1	C	1456/1878 (78%)	1293 (89%)	151 (10%)	12 (1%)	19	54
1	D	1461/1878 (78%)	1290 (88%)	155 (11%)	16 (1%)	14	46
1	E	1450/1878 (77%)	1292 (89%)	146 (10%)	12 (1%)	19	54
1	F	1455/1878 (78%)	1300 (89%)	140 (10%)	15 (1%)	15	49
2	G	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	12	42
2	H	2058/2060 (100%)	1786 (87%)	244 (12%)	28 (1%)	11	40
2	I	2058/2060 (100%)	1799 (87%)	233 (11%)	26 (1%)	12	42
2	J	2058/2060 (100%)	1792 (87%)	240 (12%)	26 (1%)	12	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	2058/2060 (100%)	1772 (86%)	258 (12%)	28 (1%)	11	40
2	L	2058/2060 (100%)	1777 (86%)	253 (12%)	28 (1%)	11	40
All	All	21079/23628 (89%)	18479 (88%)	2359 (11%)	241 (1%)	14	46

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%)	8	29
1	B	1227/1527 (80%)	1111 (90%)	116 (10%)	8	31
1	C	1225/1527 (80%)	1102 (90%)	123 (10%)	7	28
1	D	1229/1527 (80%)	1110 (90%)	119 (10%)	8	30
1	E	1219/1527 (80%)	1101 (90%)	118 (10%)	8	30
1	F	1224/1527 (80%)	1109 (91%)	115 (9%)	8	32
2	G	1752/1752 (100%)	1571 (90%)	181 (10%)	7	27
2	H	1752/1752 (100%)	1579 (90%)	173 (10%)	8	29
2	I	1752/1752 (100%)	1571 (90%)	181 (10%)	7	27
2	J	1752/1752 (100%)	1573 (90%)	179 (10%)	7	27
2	K	1752/1752 (100%)	1575 (90%)	177 (10%)	7	28
2	L	1752/1752 (100%)	1576 (90%)	176 (10%)	7	28
All	All	17856/19674 (91%)	16079 (90%)	1777 (10%)	7	28

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	6.81	21 (67%)	40,50,50	1.75	4 (10%)
3	FMN	K	2101	-	31,33,33	7.03	21 (67%)	40,50,50	1.85	9 (22%)
3	FMN	J	2101	-	31,33,33	7.03	21 (67%)	40,50,50	1.99	8 (20%)
3	FMN	I	2101	-	31,33,33	6.80	20 (64%)	40,50,50	1.91	7 (17%)
3	FMN	H	2101	-	31,33,33	6.77	20 (64%)	40,50,50	1.84	8 (20%)
3	FMN	L	2101	-	31,33,33	6.76	19 (61%)	40,50,50	1.83	7 (17%)

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	-	-	5/18/18/18	0/3/3/3
3	FMN	K	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	I	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	H	2101	-	-	5/18/18/18	0/3/3/3
3	FMN	L	2101	-	-	5/18/18/18	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	J	2101	FMN	C4A-C10	16.24	1.55	1.38
3	K	2101	FMN	C4A-C10	15.67	1.54	1.38
3	I	2101	FMN	C4A-C10	15.48	1.54	1.38
3	G	2101	FMN	C4A-C10	15.42	1.54	1.38
3	L	2101	FMN	C4A-C10	15.21	1.54	1.38

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2101	FMN	C4-N3-C2	6.51	120.64	115.14
3	H	2101	FMN	C4-N3-C2	6.25	120.42	115.14
3	I	2101	FMN	C4-N3-C2	6.04	120.25	115.14
3	L	2101	FMN	C4-N3-C2	6.01	120.22	115.14
3	J	2101	FMN	C1'-N10-C10	5.95	123.74	118.41

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2101	FMN	C2'-C3'-C4'-C5'
3	G	2101	FMN	O3'-C3'-C4'-C5'
3	I	2101	FMN	C2'-C3'-C4'-C5'
3	I	2101	FMN	O3'-C3'-C4'-C5'
3	H	2101	FMN	C2'-C3'-C4'-C5'

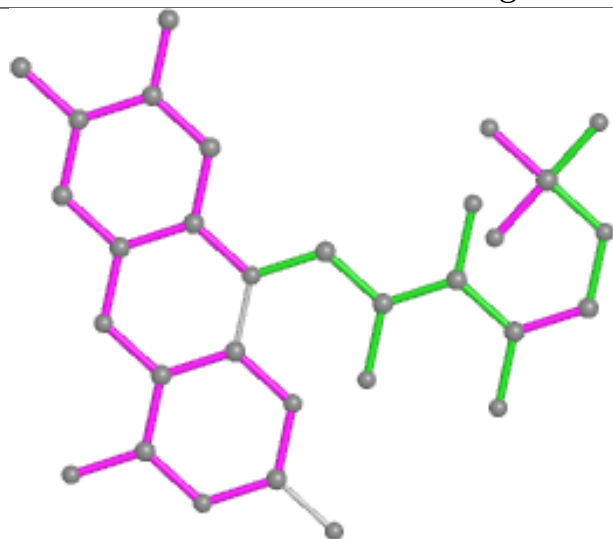
There are no ring outliers.

6 monomers are involved in 61 short contacts:

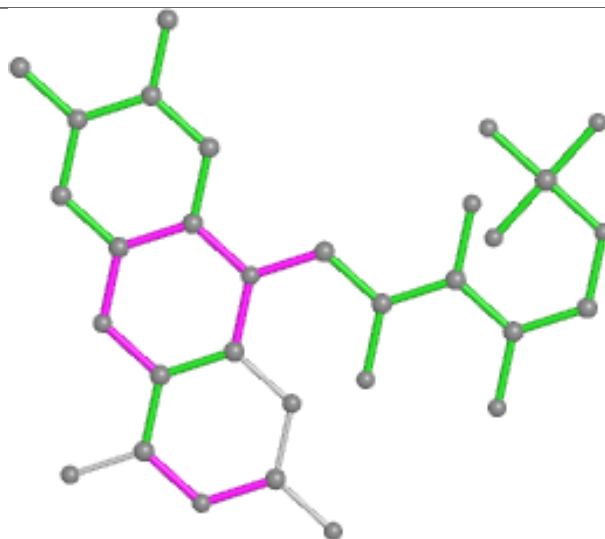
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2101	FMN	10	0
3	K	2101	FMN	12	0
3	J	2101	FMN	9	0
3	I	2101	FMN	9	0
3	H	2101	FMN	11	0
3	L	2101	FMN	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

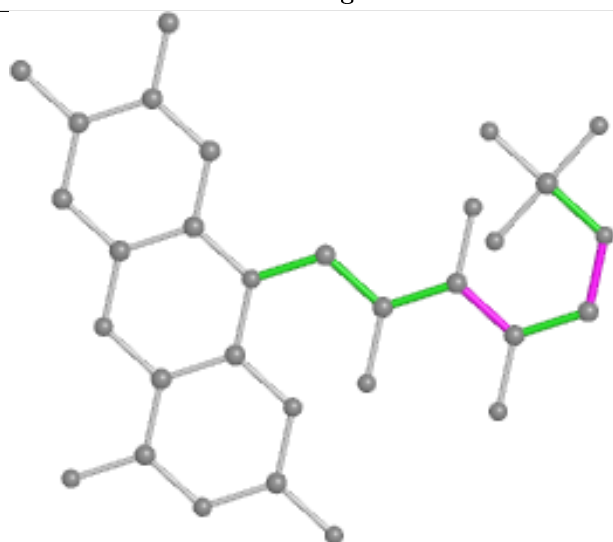
Ligand FMN G 2101



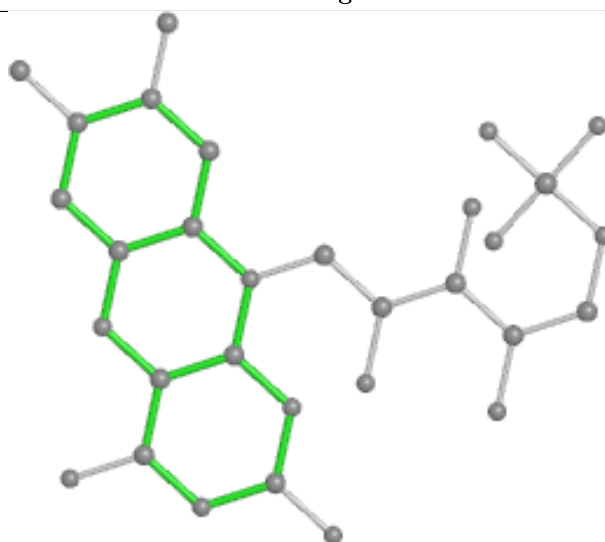
Bond lengths



Bond angles

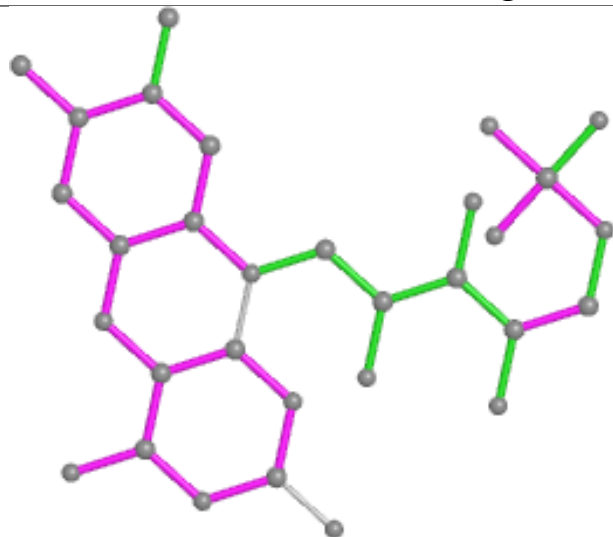


Torsions

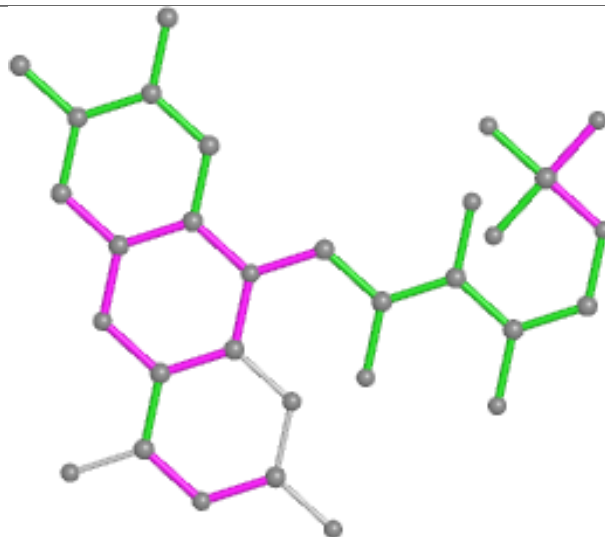


Rings

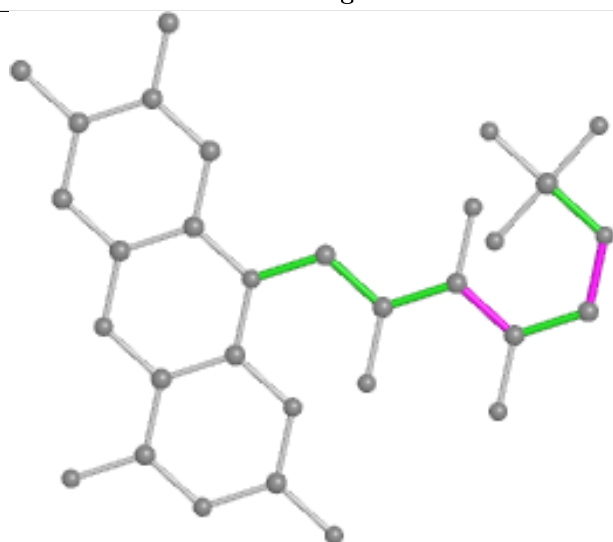
Ligand FMN K 2101



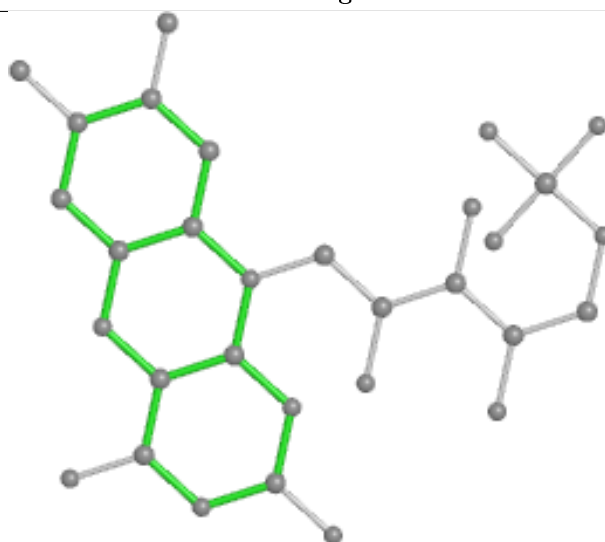
Bond lengths



Bond angles

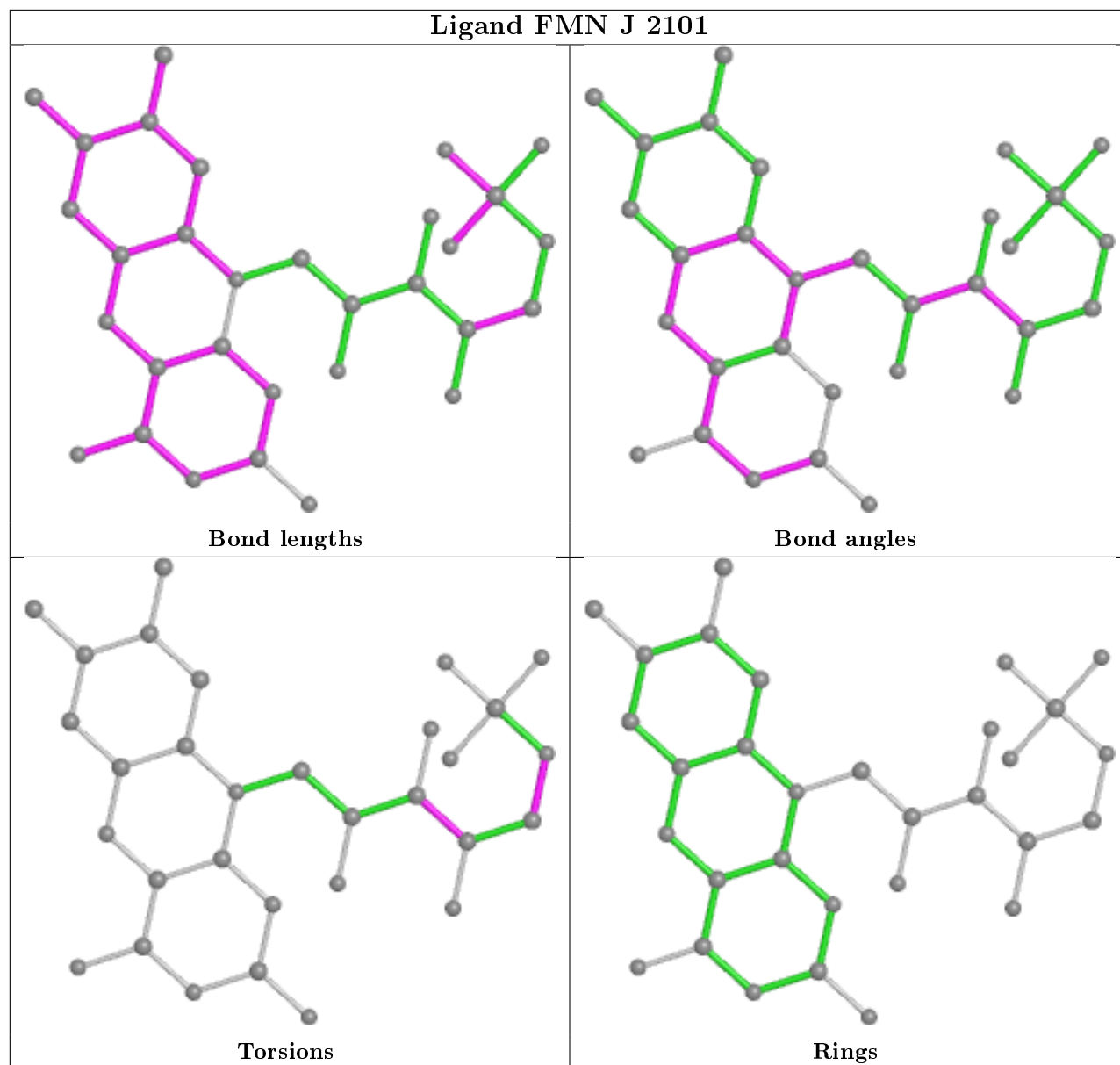


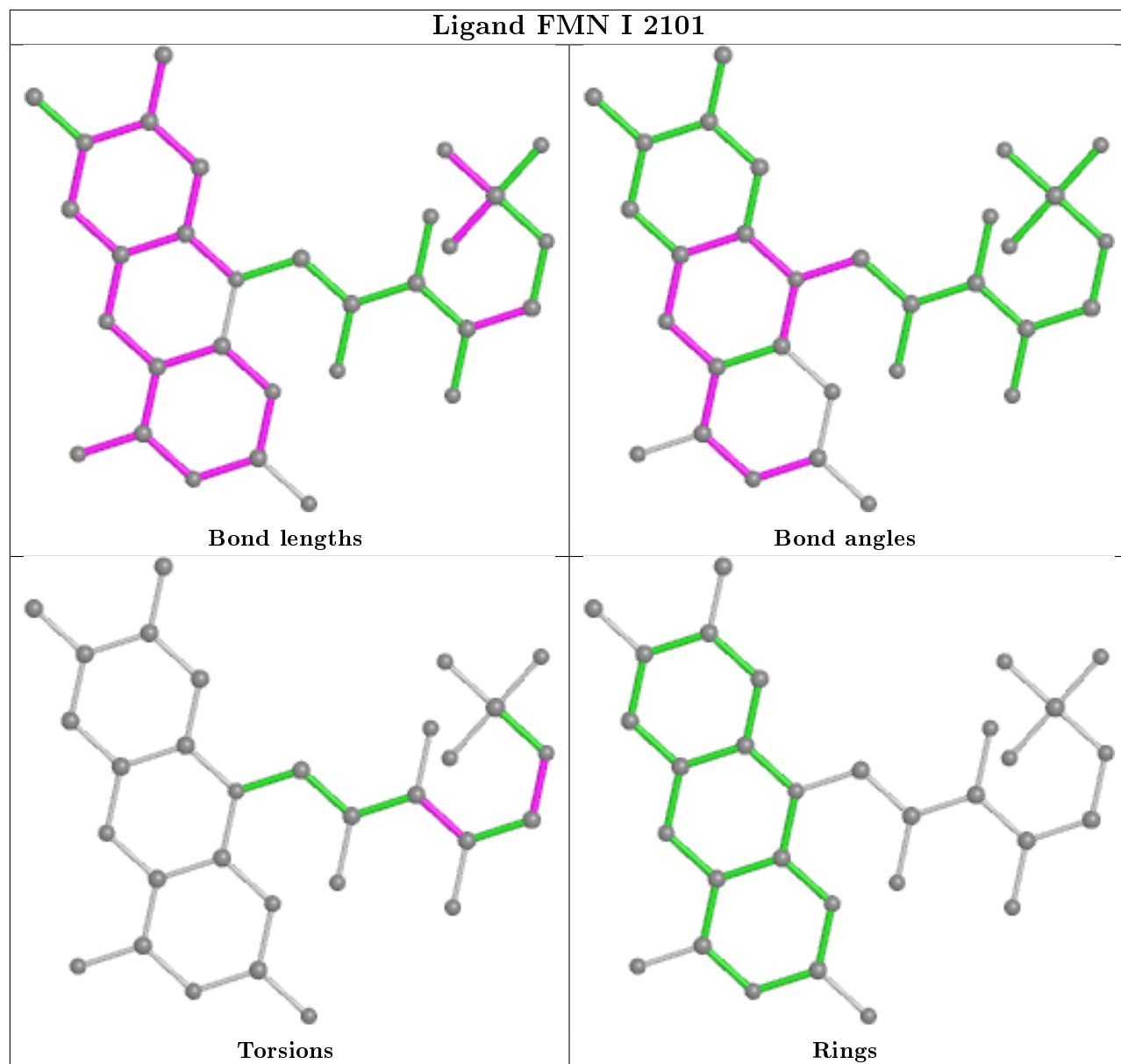
Torsions



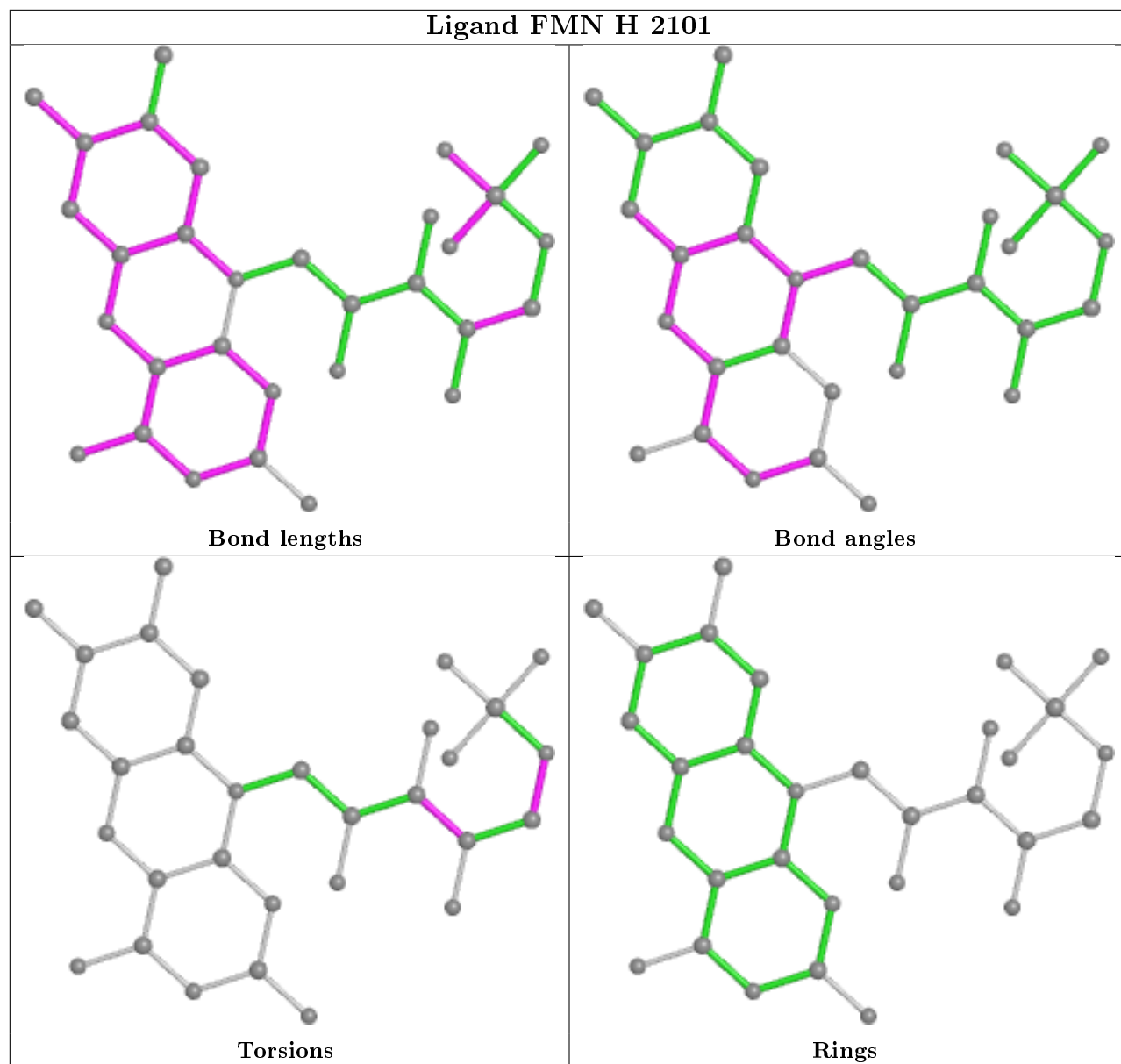
Rings

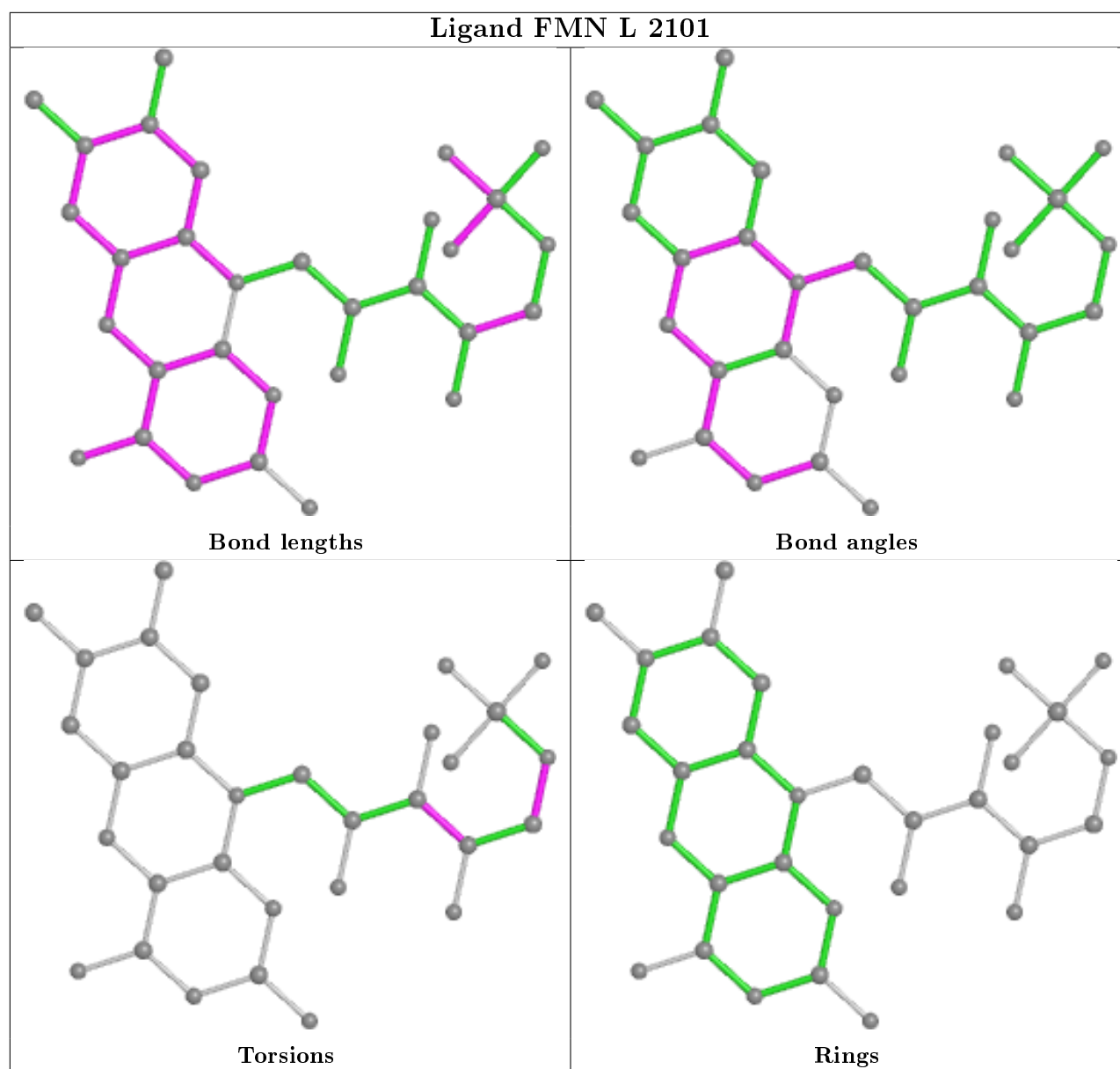
Ligand FMN J 2101





Ligand FMN H 2101





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(Å ²)	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 72	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 72	16, 51, 108, 159	0
2	G	2060/2060 (100%)	-0.12	38 (1%)	68 47	27, 83, 129, 169	0
2	H	2060/2060 (100%)	-0.05	69 (3%)	46 24	24, 86, 132, 167	0
2	I	2060/2060 (100%)	-0.02	73 (3%)	44 23	23, 86, 132, 167	0
2	J	2060/2060 (100%)	0.03	66 (3%)	47 25	28, 89, 133, 172	0
2	K	2060/2060 (100%)	0.25	134 (6%)	18 8	27, 91, 136, 172	0
2	L	2060/2060 (100%)	0.01	76 (3%)	41 21	23, 87, 133, 172	0
All	All	21127/23628 (89%)	-0.20	537 (2%)	57 34	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

There are no carbohydrates in this entry.

6.4 Ligands

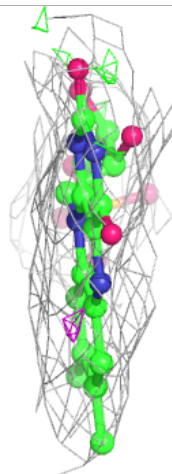
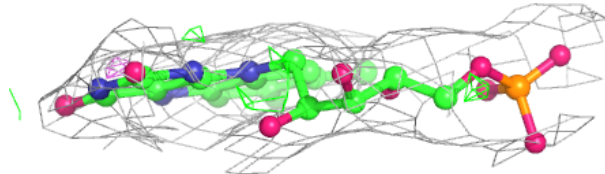
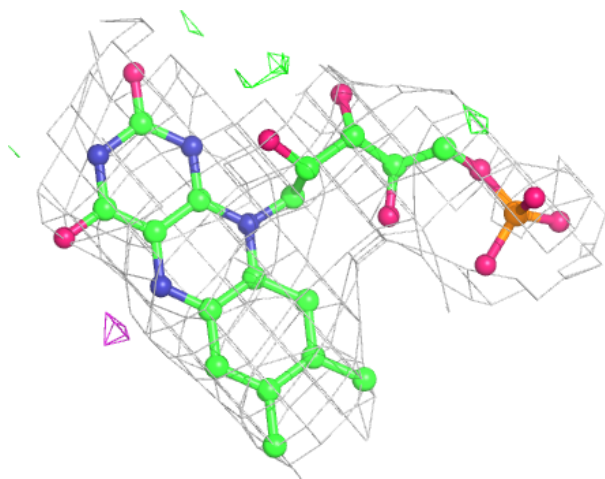
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

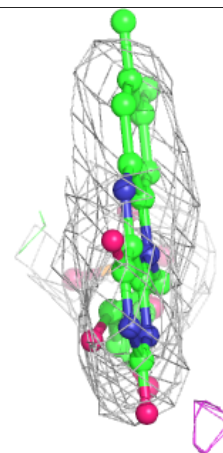
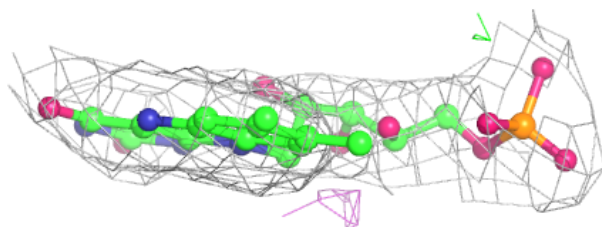
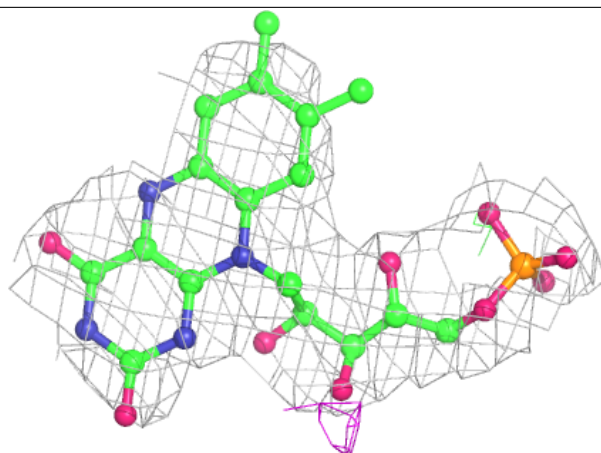
Electron density around FMN K 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

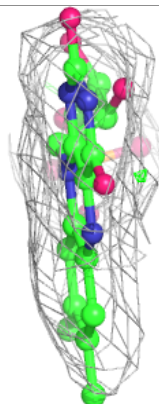
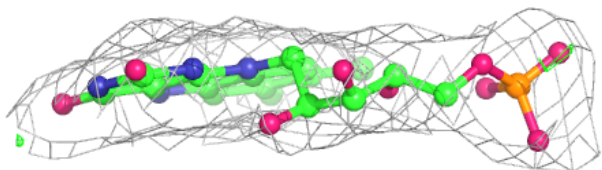
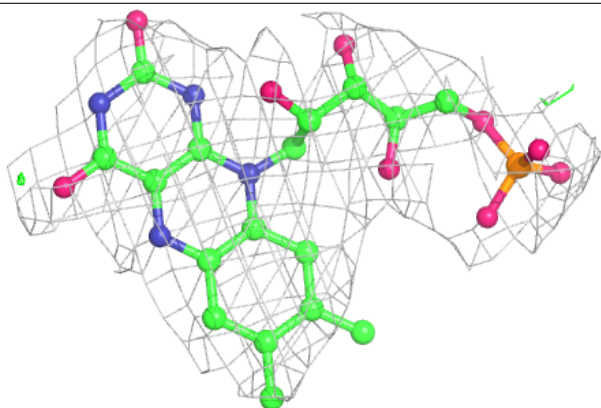


Electron density around FMN I 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

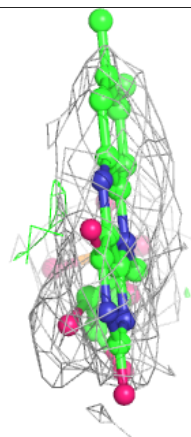
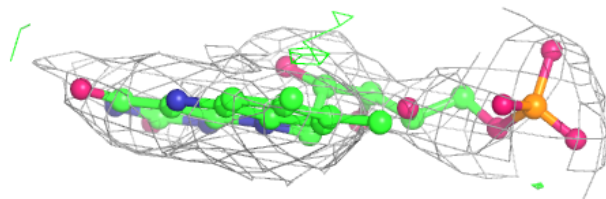
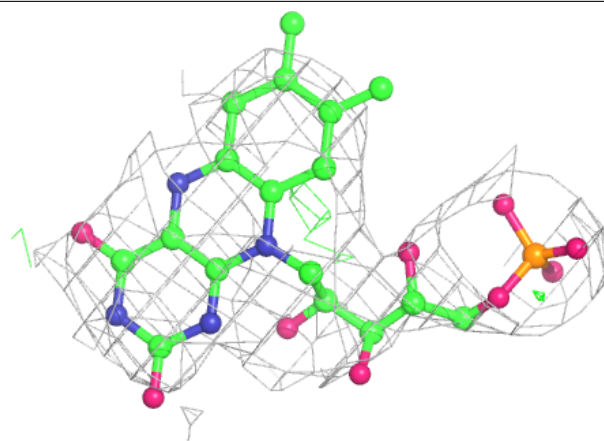
**Electron density around FMN J 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



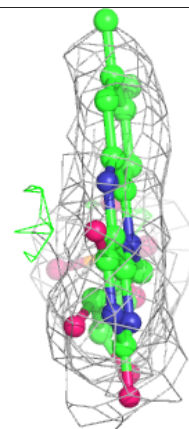
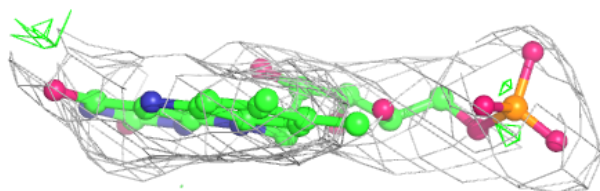
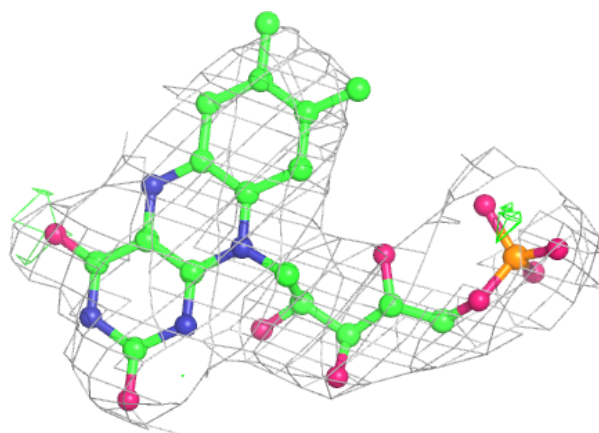
Electron density around FMN G 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



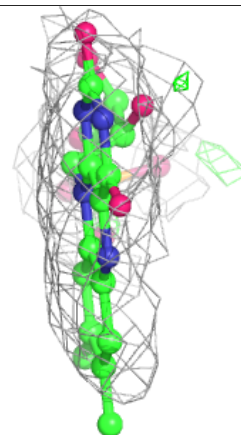
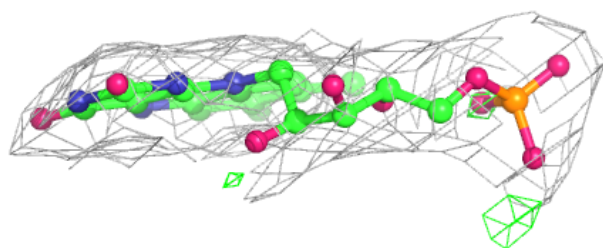
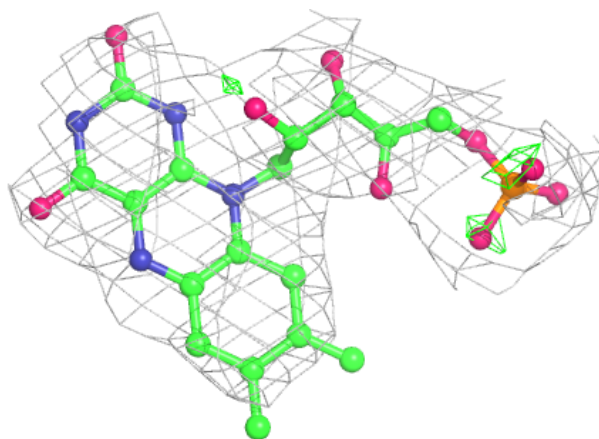
Electron density around FMN H 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN L 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.