



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 12:52 PM EST

PDB ID : 4V8V
EMDB ID: : EMD-2358
Title : Structure and conformational variability of the Mycobacterium tuberculosis fatty acid synthase multienzyme complex
Authors : Ciccarelli, L.; Connell, S.R.; Enderle, M.; Mills, D.J.; Vonck, J.; Grininger, M.
Deposited on : 2013-04-18
Resolution : 20.00 Å (reported)
Based on PDB ID : 4B3Y

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

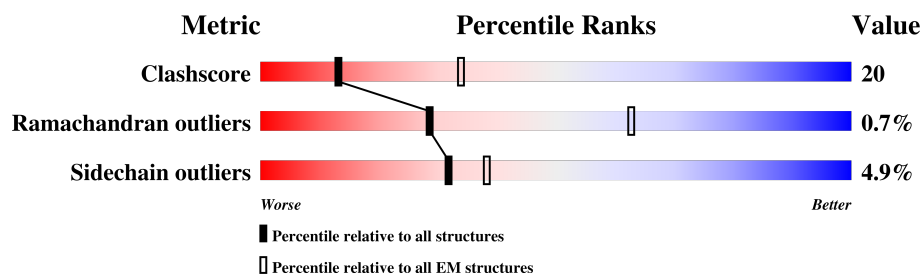
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	3089	57% 31% • 9%
1	B	3089	57% 31% • 9%
1	C	3089	57% 31% • 9%
1	D	3089	57% 31% • 9%
1	E	3089	57% 31% • 9%
1	F	3089	57% 31% • 9%

2 Entry composition [i](#)

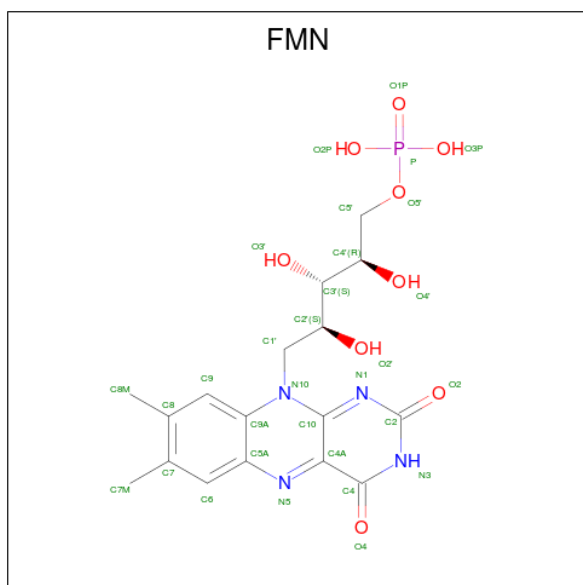
There are 2 unique types of molecules in this entry. The entry contains 125856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TYPE-I FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	B	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	C	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	D	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	E	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		
1	F	2822	Total	C	N	O	S	0	0
			20945	13219	3662	3998	66		

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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

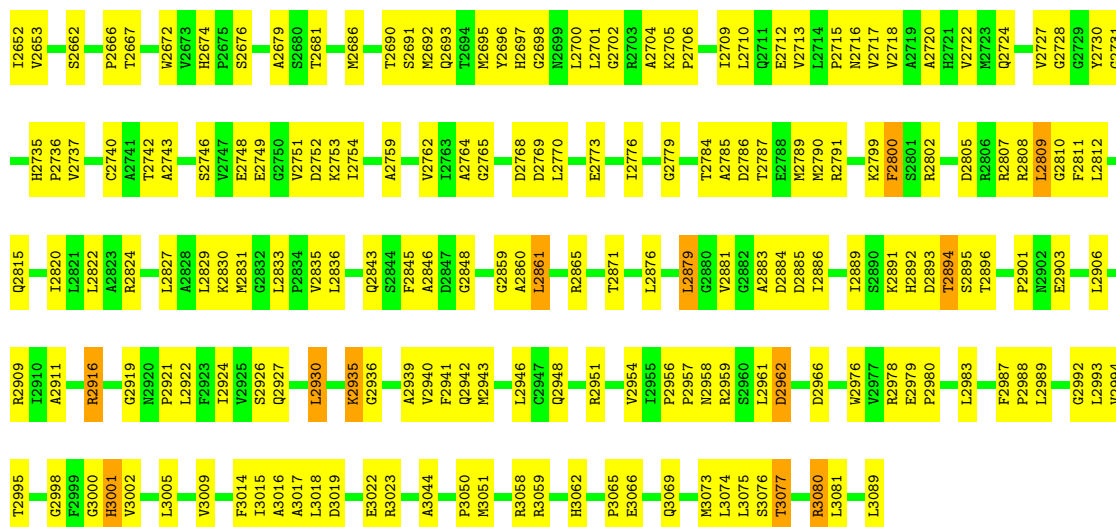
- Molecule 1: TYPE-I FATTY ACID SYNTHASE



<div><div></div><div>P2522</div><div>D2630</div><div>E2523</div><div>C2524</div><div>T2632</div><div>V2633</div></div>	<div><div></div><div>E2422</div><div>E2426</div><div>E2427</div><div>P2428</div><div>T2431</div><div>L2432</div><div>R2433</div><div>A2434</div><div>L2435</div><div>P2436</div><div>P2437</div><div>P2438</div><div>P2439</div></div>	<div><div></div><div>G2298</div><div>M2299</div><div>F2300</div><div>L2193</div><div>D2303</div><div>Y2306</div><div>Y2196</div><div>K2310</div><div>A2434</div><div>R2319</div><div>S2331</div><div>L2332</div><div>A2333</div><div>H2334</div><div>W2339</div><div>M2346</div><div>G2347</div><div>Q2348</div><div>N2349</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>F2089</div><div>E2090</div><div>G2091</div><div>T2092</div><div>L2093</div><div>H2094</div><div>Y2095</div><div>V2096</div><div>A2097</div><div>T2098</div><div>Q2099</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192</div><div>L2193</div><div>Y2194</div><div>Y2195</div><div>Y2196</div><div>A2197</div><div>G2198</div><div>D2205</div><div>L2209</div><div>W2210</div><div>E2211</div><div>W2212</div><div>Q2213</div><div>G2214</div><div>T2215</div><div>E2216</div><div>R2217</div><div>L2218</div><div>Q2219</div><div>K2220</div><div>P2234</div><div>L2235</div><div>L2236</div><div>L2237</div><div>F2238</div><div>I2352</div><div>V2353</div><div>S2354</div><div>L2453</div><div>D2454</div></div>	<div><div></div><div>P2089</div><div>T2192<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Q1002	T895	L787	V675	G583	E476	G374	V286	L178	E84	THR	THR	A2720
H1003	A896	A790	G676	H584	L479	L375	F287	L179	P85	ILE	ILE	H2721
V1004	A899	A791	A680	H585	A483	V376	P289	A180	S88	TYR	TYR	V2722
V1008	G900	A792	A681	S586	R484	R381	V292	L181	L90	GLU	GLU	Q2724
P1009	P1009	R793	G683	E588	I485	Q384	E293	Q183	R94	HIS	HIS	V2727
L1010	L1011	L794	M684	D589	Q486	Q384	V294	L184	P95	ASP	ASP	G2728
G1012	G1012	H795	G686	L590	Q487	Q384	V294	R195	R95	ARG	ARG	G2729
T1013	F915	H796	G687	L593	I488	T389	L301	R196	P96	PRO	PRO	F2811
V1014	L924	D798	R688	L594	T489	V390	L301	R197	A106	VAL	VAL	Y2730
I1017	L924	F799	R688	L595	L490	V390	L301	R198	L107	ALA	ALA	G2731
R1018	A928	E803	D684	R602	Q500	V393	I305	I198	A107	GLY	GLY	Q2815
F1019	E929	H696	I695	R602	V501	P394	I307	D203	E111	TRP	TRP	H2735
P1020	P930	A808	E697	N606	K504	E395	W311	R204	P112	ASN	ASN	P2736
L1021	V931	D811	I698	N606	K504	W400	W311	P205	P113	ASP	ASP	V2737
V1025	E932	D811	G613	G614	Q505	P405	T314	P206	K117	GLU	GLU	C2740
E1034	L934	L816	G614	G614	Q505	P405	G316	N207	Q118	SER	SER	A2741
V1035	S935	E817	P618	P618	R511	V408	G316	V208	L119	GLY	GLY	T2742
D1036	R936	L826	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	A2743
D1037	R937	L827	P618	P618	R511	V408	G316	V208	Q118	ALA	ALA	S2746
V1045	A939	D832	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	V2747
L1046	R940	A833	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	E2748
V1068	L957	E834	P618	P618	R511	V408	G316	V208	Q118	GLY	GLY	G2749
H1072	R961	V836	P618	P618	R511	V408	G316	V208	Q118	ASN	ASN	G2750
V1077	R962	V837	P618	P618	R511	V408	G316	V208	Q118	ALA	ALA	V2751
T1084	R963	L853	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	T2752
F1087	R964	G854	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	I2754
G1088	R965	G855	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	A2759
P1089	R966	P856	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	F2762
V1092	R967	V857	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	I2763
P1093	R970	L858	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	A2764
T1094	R971	F859	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	G2765
L1095	R972	V860	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	D2768
V1098	R973	V861	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	D2769
P1099	R974	V862	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	L2770
D1100	R975	V863	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	E2773
V1103	R976	R868	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	I2776
G1104	R977	R872	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	G2779
L1105	R978	D873	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	L2879
C1106	R979	D874	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	G2880
V1110	R980	S875	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	L2881
F1111	R981	S876	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	G2882
	R982	L876	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	A2883
	R983	L877	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	D2884
	R984	L878	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	D2885
	R985	L879	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	E2788
	R986	L880	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	M2789
	R987	L881	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	M2790
	R988	L882	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	R2791
	R989	L883	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	S2890
	R990	L884	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	K2891
	R991	L885	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	H2892
	R992	L886	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	F2899
	R993	L887	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	S2801
	R994	L888	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R995	L889	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R996	L890	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R997	L891	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R998	L892	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R999	L893	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1000	L894	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1001	L895	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1002	L896	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1003	L897	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1004	L898	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1005	L899	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1006	L900	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1007	L901	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1008	L902	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1009	L903	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1010	L904	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1011	L905	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1012	L906	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1013	L907	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1014	L908	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1015	L909	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1016	L910	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1017	L911	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1018	L912	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1019	L913	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1020	L914	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1021	L915	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1022	L916	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1023	L917	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1024	L918	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1025	L919	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1026	L920	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1027	L921	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1028	L922	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1029	L923	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1030	L924	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1031	L925	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1032	L926	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1033	L927	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1034	L928	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1035	L929	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1036	L930	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1037	L931	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1038	L932	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1039	L933	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1040	L934	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1041	L935	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1042	L936	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1043	L937	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1044	L938	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1045	L939	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1046	L940	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1047	L941	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1048	L942	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1049	L943	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1050	L944	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1051	L945	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1052	L946	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1053	L947	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1054	L948	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1055	L949	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1056	L950	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1057	L951	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1058	L952	P618	P618	R511	V408	G316	V208	Q118	ASP	ASP	
	R1059	L953	P									

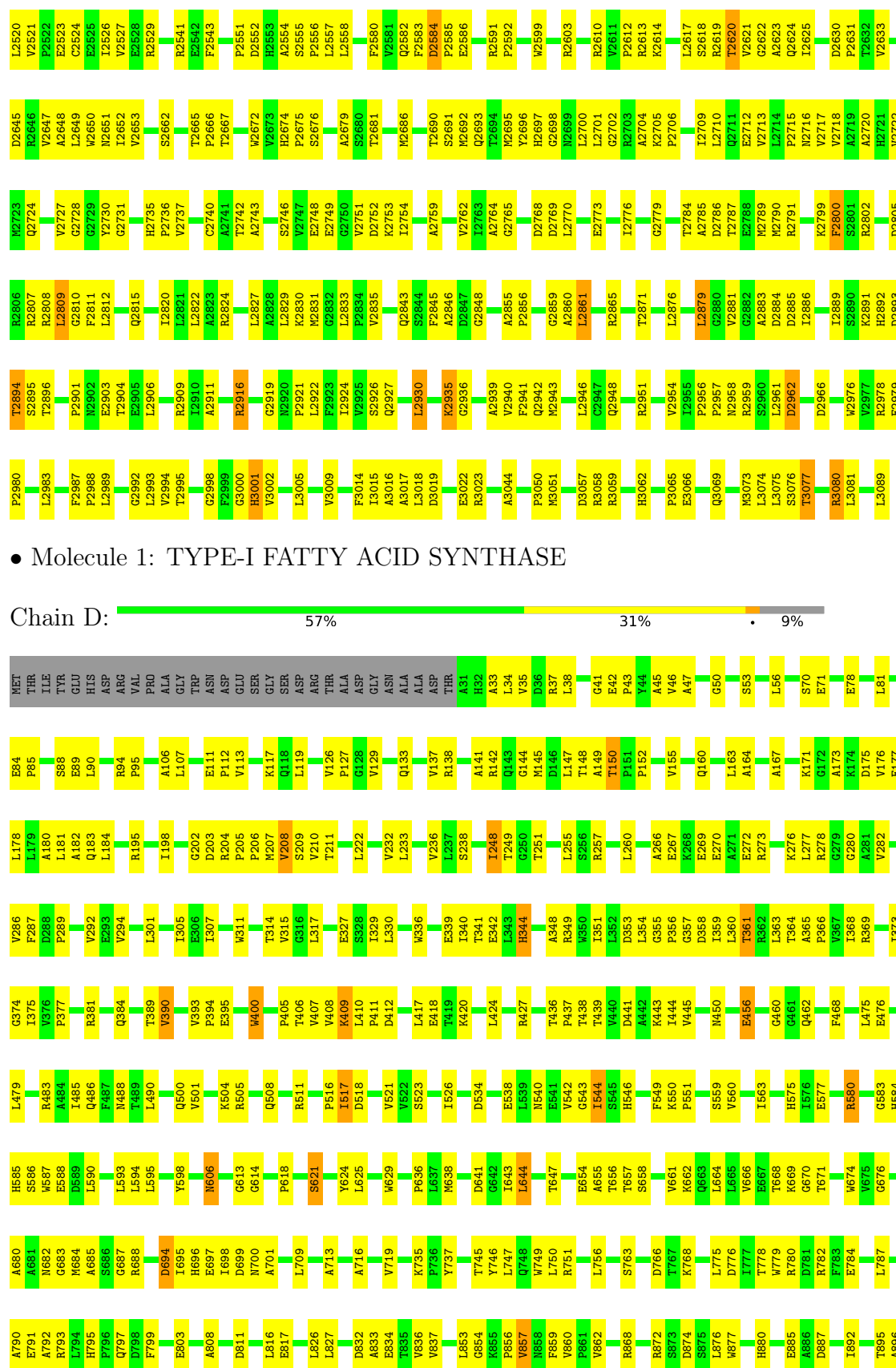


• Molecule 1: TYPE-I FATTY ACID SYNTHASE

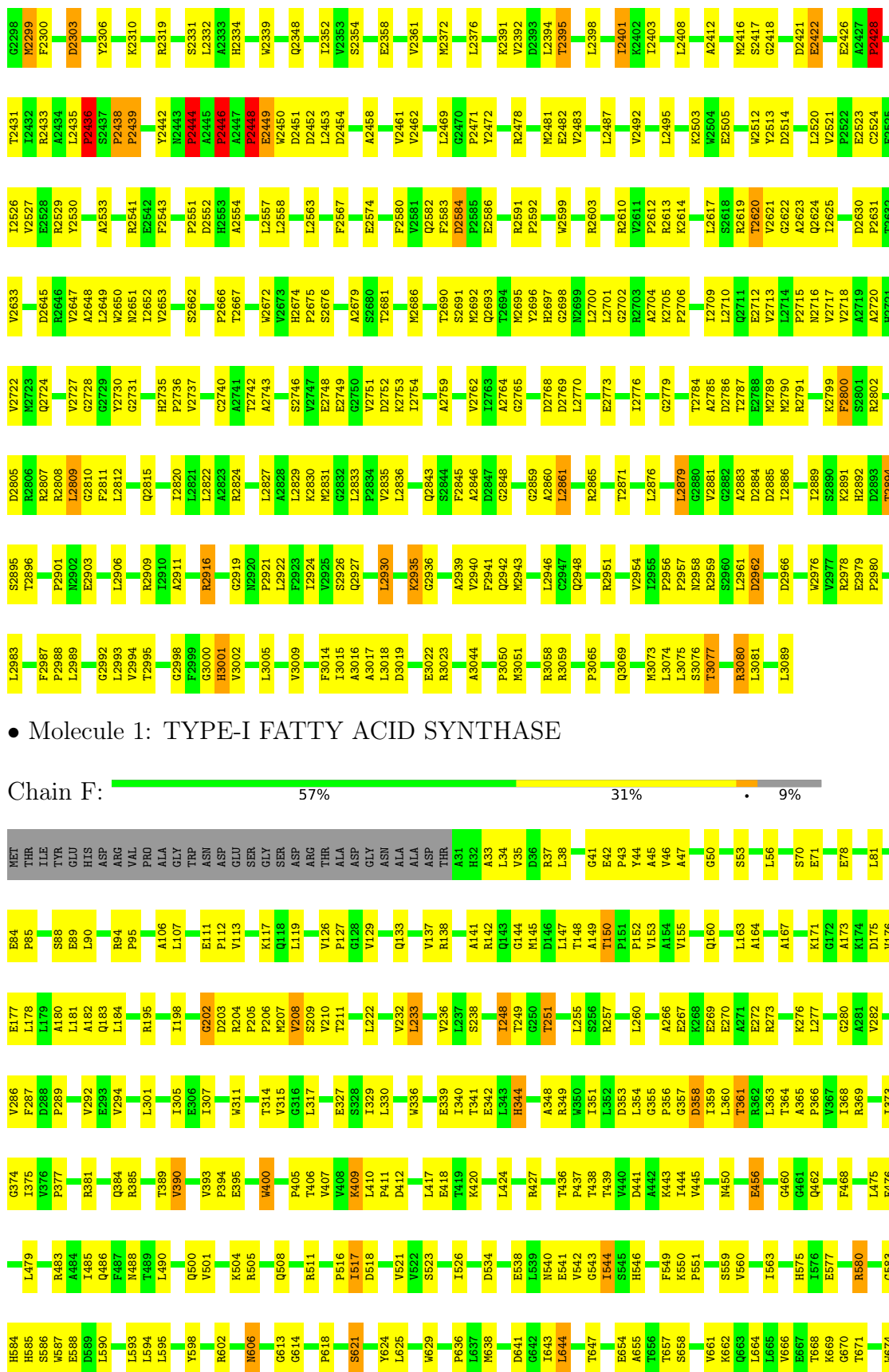


[illegible]



D2303	L2193	T2092	GLY	HIS	LEU	ALA	V1731	P1638	V1533	V1430	EL323	T1218	A1118	V1005	A899
Y2306	W2194	G2093	ALA	VAL	GLY	ALA	L1732	A1639	M1534	A1431	EL324	D1219	T1119	V1008	G900
K2310	V2195	W2094	SER	THR	ALA	ASP	S1733	V1535	M1536	V1435	L1325	T1220	E1120	P1009	I901
R2319	V2196	W2095	GLY	GLY	LYS	THR	S1734	V1436	M1537	V1436	EL326	P1221	F1123	L1010	V904
S2331	A2198	A2097	VAL	PHE	GLN	ALA	R1736	K1656	R1538	Q1441	S1327	R1225	P1124	S1011	V904
L2332	D2205	T2098	VAL	ALA	VAL	LEU	D1737	P1657	S1540	V1445	S1328	R1226	V1125	G1012	F915
H2334	Q2099	Q2099	THR	GLY	THR	ILE	L1741	K1658	Q1542	A1448	A1329	R1227	I1126	T1013	L924
W2339	W2210	W2101	THR	THR	LYS	ALA	D1745	L1660	Y1542	I1449	R1330	V1228	G1128	W1014	
Q2348	G2214	W2102	GLY	GLY	ALA	SER	THR	C1661	I1544	A1450	I1331	R1237	L1129	T1017	
I2352	T2215	L2108	SER	SER	THR	LYS	ASP	R1662	L1551	V1455	M1337	R1249	L1132	R1018	A928
V2353	E2216	R2112	VAL	VAL	LYS	THR	PRO	K1663	E1552	V1455	A1336	P1249	V1133	F1019	E929
S2354	K1992	W2113	ARG	ARG	PRO	ILE	GLU	I1666	A1553	T1459	A1339	R1253	P1146	T1020	P830
E2358	P1996	H2114	GLY	GLY	PHE	ASP	GLU	E1667	L1554	A1460	R1342	R1253	K1147	V1025	V931
V2361	L2000	W2115	GLY	GLY	GLY	GLN	ALA	L1668	E1555	A1461	L1343	G1268	P1148	L934	V932
W2372	Q2010	H2116	ASP	ASP	PRO	ILE	ALA	W1671	E1556	A1462	A1344	M1269	A1150	E1034	S935
L2376	G2012	L2118	LEU	LEU	VAL	GLU	GLU	P1672	E1557	C1463	P1346	W1270	E1151	V1035	R336
K2391	L2011	F2119	GLY	GLY	SER	LEU	GLU	A1674	R1560	V1467	Y1350	A1274	F1152	D1037	R937
V2392	G2012	F2119	GLY	GLY	SER	LEU	GLU	A1674	R1562	V1467	A1351	A1274	T1162	V1045	A939
L2394	L2013	F2119	GLY	GLY	SER	LEU	GLU	A1674	Q1563	E1468	F1352	A1275	D1163	L1046	R940
T2395	S2014	F2119	HIS	HIS	ALA	SER	THR	W1679	I1564	E1471	P1353	Q1276	T1164	R941	
L2398	E2015	L2122	ALA	ALA	ILE	ILE	ASP								L957
I2401	V2016	A2123	GLY	GLY	ASN	GLU	ALA	D1684	D1578	T1474	I1357	W1278	G1167	V1068	
K2402	W2054	E2137	ALA	ALA	ASP	SER	PRO	L1685	P1579	T1279	Q1358	T1280	R1168	T1069	R961
L2403	F2056	W2140	LEU	LEU	GLN	ILE	ALA	F1687	P1580	T1280	Q1358	T1280	P1171	V1070	M962
M2405	D2057	V2141	ALA	ALA	LEU	THR	GLU		F1687	T1281	M1362	T1282	P1172	W1072	S963
L2408	R2059	T2163	SER	SER	ARG	ASP	ALA	E1690	F1581	R1480	V1376	T1283	S1173	V1077	V964
A2409	W2060	W2164	ALA	ALA	THR	GLY	ALA		S1583	K1483	V1376	G1284	V1174		R965
A2412	L2067	I2165	ASP	ASP	VAL	SER	ALA	G1694	L1586	H1484	A1380	K1285	T1084	P966	P967
M2416	L2070	T2167	VAL	VAL	GLY	PRO	ALA	L1695	L1586	D1486	D1381	P1286			
S2417	E2074	R2170	LYS	LYS	SER	SER	ALA	R1699	V1590	I1487	F1390	V1287	R1177	T1087	I970
G2418	Q2081	D2173	VAL	VAL	GLY	ASN	ALA	F1700	E1598	V1488	S1391	P1288	A1179	G1088	A971
D2421	W2082	R2175	ILE	ILE	THR	GLN	PRO	V1701	E1598	P1489	S1391	P1288			T974
E2422	Q2084	L2176	ARG	ARG	THR	LEU	ALA	E1702	K1605	R1490	P1400	A1290	L1184	P1090	E975
E2426	S2086	K2180	ARG	ARG	THR	LEU	VAL	I1703	G1605	D1491	P1400	L1292	L1185	A1092	W976
K2427	Q2087	W2164	THR	THR	LYS	LEU	GLY	G1713	I1611	R1495	A1405	W1295	L1188	P1093	Q977
P2428	R2088	R2188	GLY	GLY	THR	LEU	ALA	L1714	R1621	S1496	V1408			T1094	V978
T2431	F2089	F2189	ILE	ILE	THR	GLY	PRO	L1719	P1622	I1503	V1408	K1304	R1191	L1095	R979
	E2090	T2192	ALA	ALA	THR	GLY	ALA	S1707	R1613	R1504	H1412		F1192	T1096	E980
	G2091		ASP	ASP	LYS	ASP	ASP		R1613	I1504	P1412		A1193	V1097	H989
									L1617	R1504	P1413		I1194	V1098	P990
									L1618	Q1507	D1414		R1195	P1099	S991
									L1619	I1508	G1415		G1196	D1100	T992
									P1620		V1416		R1197		
									R1621	D1511	L1417			V1103	
									L1622	T1514	R1312		E1202	G1104	L996
									L1623	D1514	R1313		L1203	R1105	E997
									L1624	Q1421	D1314		C1106	V998	
									L1625	F1422	D1315		T1204	D1205	
									R1634	V1519	F1423		P1206	V1110	D1001
										S1725	T1423		W1207	F1111	Q1002
											Q1424			I1318	H1003
											V1425			A1117	V1004

[illegible]



A2097	T2098	Q2099	A2100	R2101	W2102	W2103	T2104	G2105	L2108	R2112	W2113	H2114	H2115	L2118	F2119	T2122	A2123	A2124	G2125	A2126	E2127	R2128	R2129	Y2134	E2137	V2140	V2141	T2163	W2164	I2166	A2166	T2167	R2170	D2173	R2174	R2175	L2176	K2180	R2188	F2189	T2192	T2193	R2194	V2195	F2197			
GLY	GLY	VAL	VAL	ASP	ASP	L1983	L1986	F1989	K1992	P1996	L2000	G2012	L2013	S2014	V2015	V2016	P2020	V2032	T2047	A2053	V2054	V2055	F2056	D2057	R2058	R2059	W2060	L2067	L2070	E2074	Q2081	W2082	E2083	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	T2091	T2092	G2093	H2094	V2095	V2096		
ALA	THR	VAL	GLN	LEU	ILE	LYS	LEU	ARG	LYS	THR	THR	MET	ARG	LYS	THR	ILE	GLN	ASP	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
ALA	THR	VAL	GLN	LEU	ILE	LYS	LEU	ARG	LYS	THR	THR	MET	ARG	LYS	THR	ILE	GLN	ASP	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
P1638	A1639	T1651	W1652	K1656	P1657	E1659	L1660	C1661	R1662	K1663	I1666	E1667	L1668	W1671	Q1672	F1673	A1674	W1679	D1684	L1685	L1686	F1687	E1690	G1694	L1695	R1699	F1700	V1701	E1702	L1703	G1704	V1705	K1706	T1710	V1711	A1712	G1713	L1714	P1722	E1723	Y1724	S1725	E1730	V1731	L1733	L1734	W1735	
F1535	N1536	R1537	G1538	S1540	Q1541	Y1542	I1544	L1551	E1552	A1553	L1554	E1555	A1556	E1557	R1560	R1561	Q1562	I1564	D1578	V1579	P1580	F1581	H1582	L1586	V1590	E1598	K1605	I1611	G1612	R1613	P1616	L1617	V1619	P1620	R1621	P1622	F1623	T1624	L1625	F1629	L1633	R1634	V1637	W1638	W1639			
E1323	V1324	L1325	E1326	S1328	A1329	R1330	I1331	V1336	M1337	A1338	A1339	R1342	L1343	C1463	V1464	V1467	A1468	E1469	E1470	E1471	L1474	V1479	Q1480	K1483	M1484	L1485	D1486	L1487	V1488	F1489	P1490	D1491	R1495	S1496	I1503	Q1507	D1511	D1514	P1515	D1516	P1517	P1518	P1519	P1520	P1521	P1522	P1523	
A1212	T1218	D1219	F1221	R1225	R1226	D1227	V1228	R1237	R1253	G1268	M1269	L1271	A1274	A1275	Q1276	H1277	V1278	T1280	A1281	T1282	D1283	G1284	K1285	P1286	V1287	P1288	P1289	A1290	K1291	L1292	I1293	G1294	W1295	K1304	D1307	Q1308	V1309	D1310	F1311	R1312	V1313	D1315	V1316	G1317	L1318	D1319		
A1117	A1118	T1119	E1120	F1123	P1124	V1125	I1126	E1127	G1128	W1129	L1132	V1133	L1141	P1146	K1147	E1148	P1149	A1150	E1151	T1162	D1163	T1164	G1167	R1168	P1171	V1172	S1173	V1174	R1177	N1178	A1179	L1184	L1185	L1188	R1191	F1192	A1193	I1194	R1195	G1196	R1197	E1202	L1203	T1204	D1205	P1206	V1207	
Q1002	H1003	V1004	V1005	V1008	P1009	L1010	S1011	G1012	T1013	W1014	I1017	R1018	F1019	T1020	L1021	V1025	E1034	V1035	D1036	D1037	V1045	L1046	V1068	W1072	V1077	P1084	F1087	G1088	A1089	P1090	L1091	A1092	P1093	T1094	T1096	V1097	V1098	P1099	D1100	V1103	G1104	R1105	C1106	V1110	F1111	D1112		
T895	A896	A899	G899	I901	V904	F915	G797	D798	F799	A928	E929	P930	V931	E932	V933	L934	S935	R936	R937	Q938	A939	R940	R941	L957	R961	M962	S963	V964	P965	P966	V967	I970	A971	T974	E975	W976	Q977	V978	S979	E980	H989	P990	S991	T992	L996	E997	V998	D1001
L787	A790	E791	A792	R793	L794	H795	T796	G797	D798	E803	A808	D811	L816	E817	L826	L827	D832	A833	E834	T835	V836	V837	L853	G854	K855	P856	L857	N858	F859	V860	P861	V862	R868	R872	S873	D874	S875	L876	W877	H880	E885	A886	D887	I892				
G675	G676	A680	N682	G683	M684	A685	S686	G687	R688	D694	L695	H696	E697	T698	D699	W700	A701	L709	A713	A716	V719	K735	P736	Y737	T745	Y746	L747	G748	W749	L750	R751	L756	S763	D766	T767	K768	L775	D776	I777	T778	W779	R780	D781	R782	F783	E784		

T2995	R2909	G2731	Q2815	R2909	A2198
G2998	I2910	H2735	I2820	E2542	D2205
F2999	A2911	P2736	L2821	S2437	S2331
G3000	R2916	V2737	L2822	P2438	L2332
H3001	G2919	C2740	A2823	A2438	V2210
V3002	R2920	A2741	R2824	P2439	E2211
L3005	P2921	T2742	L2827	Y2442	W2212
V3009	L2922	A2743	L2828	N2443	W2213
F2923	F2923	A2828	K2829	P2444	G2214
I2924	I2924	S2746	L2830	A2445	T2215
V2925	V2925	V2747	M2831	G2446	E2216
S2926	Q2927	E2748	G2832	L2447	K2229
Q2927	L2930	E2749	L2833	P2448	N2349
L2930	V2835	D2751	V2835	E2449	P2234
K2935	G2936	D2752	P2836	D2450	T2235
G2936	A2939	K2753	Q2843	D2451	L2236
F2845	F2845	I2754	S2844	L2453	L2237
V2940	F2941	A2759	A2846	D2454	F2238
D2847	D2847	V2762	G2848	A2458	R2244
G2848	M2943	I2763	G2849	V2461	V2245
M2943	L2946	A2764	G2859	V2462	A2246
L2946	C2947	G2765	A2860	L2469	V2252
Q2948	Q2948	D2768	L2861	G2470	R2255
R2951	R2951	L2770	R2865	P2471	K2261
V2954	V2954	E2773	T2871	Y2472	L2394
I2955	P2956	I2776	L2876	R2478	T2395
P2957	N2958	G2779	L2879	M2481	L2398
N2958	R2959	V2881	G2880	E2482	T2401
S2960	L2961	D2883	V2881	V2483	K2402
D2962	D2962	D2884	D2885	L2487	L2403
D2966	D2966	D2886	I2886	V2492	D2282
W2976	W2976	I2889	I2889	L2495	R2286
V2977	R2978	S2890	K2891	L2495	L2287
R2979	E2979	D2892	D2893	K2503	H2288
P2980	P2980	T2894	T2894	W2504	L2291
L2983	L2983	S2895	S2895	E2505	S2294
F2987	F2987	T2896	T2896	M2416	S2417
P2988	P2988	R2901	R2901	W2512	N2296
L2989	L2989	R2808	R2808	Y2513	R2297
G2992	G2992	W2902	W2902	D2514	M2299
L2993	L2993	E2903	E2903	D2421	G2299
V2994	V2994	L2906	L2906	E2422	F2300
				A2427	D2303
				P2428	Y2306
				T2431	K2310
				I2432	
				R2433	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4337	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	B	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	C	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	D	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	E	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
1	F	0.39	27/21335 (0.1%)	0.51	13/29037 (0.0%)
All	All	0.39	162/128010 (0.1%)	0.51	78/174222 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2442	TYR	CB-CG	-6.38	1.42	1.51
1	A	2442	TYR	CB-CG	-6.36	1.42	1.51
1	B	2442	TYR	CB-CG	-6.35	1.42	1.51
1	F	2442	TYR	CB-CG	-6.33	1.42	1.51
1	D	2442	TYR	CB-CG	-6.31	1.42	1.51

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	930	PRO	N-CA-CB	7.04	111.75	103.30
1	B	930	PRO	N-CA-CB	7.01	111.71	103.30
1	D	930	PRO	N-CA-CB	6.99	111.69	103.30
1	E	930	PRO	N-CA-CB	6.98	111.68	103.30
1	A	930	PRO	N-CA-CB	6.97	111.66	103.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1148	GLU	Peptide
1	A	150	THR	Peptide
1	A	202	GLY	Peptide
1	A	2584	ASP	Peptide
1	A	357	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20945	0	20595	881	0
1	B	20945	0	20595	872	0
1	C	20945	0	20595	872	0
1	D	20945	0	20595	873	0
1	E	20945	0	20595	878	0
1	F	20945	0	20595	878	0
2	A	31	0	19	4	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	4	0
2	E	31	0	19	4	0
2	F	31	0	19	5	0
All	All	125856	0	123684	4910	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 4910 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:A:1013:THR:HG23	1:A:1014:TRP:H	1.15	1.10
1:E:1013:THR:HG23	1:E:1014:TRP:H	1.15	1.09
1:A:2112:ARG:H	1:A:2115:HIS:CG	1.73	1.07
1:C:2094:HIS:CG	1:C:2096:VAL:HG22	1.90	1.06
1:D:1013:THR:HG23	1:D:1014:TRP:H	1.15	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	27	70
1	B	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	24	67
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	24	67
1	D	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	24	67
1	E	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	27	70
1	F	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	24	67
All	All	16908/18534 (91%)	15849 (94%)	947 (6%)	112 (1%)	28	67

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	930	PRO
1	A	1148	GLU
1	A	2428	PRO
1	A	2436	PRO
1	A	2446	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2094/2402 (87%)	1992 (95%)	102 (5%)	27	58
1	B	2097/2402 (87%)	1994 (95%)	103 (5%)	27	58
1	C	2094/2402 (87%)	1992 (95%)	102 (5%)	27	58
1	D	2093/2402 (87%)	1991 (95%)	102 (5%)	27	58
1	E	2095/2402 (87%)	1993 (95%)	102 (5%)	27	58
1	F	2094/2402 (87%)	1992 (95%)	102 (5%)	27	58
All	All	12567/14412 (87%)	11954 (95%)	613 (5%)	32	58

5 of 613 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2395	THR
1	D	1009	PRO
1	F	1651	THR
1	C	2448	PRO
1	D	233	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2349	ASN
1	D	1277	HIS
1	F	1617	ASN
1	C	2815	GLN
1	D	486	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	A	4000	-	31,33,33	1.34	4 (12%)	40,50,50	1.57	7 (17%)
2	FMN	B	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.57	7 (17%)
2	FMN	C	4000	-	31,33,33	1.37	4 (12%)	40,50,50	1.58	7 (17%)
2	FMN	D	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.58	7 (17%)
2	FMN	E	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.58	7 (17%)
2	FMN	F	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.55	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
2	FMN	A	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	D	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	E	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	F	4000	-	-	5/18/18/18	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	3.76	1.38	1.33
2	F	4000	FMN	C4A-N5	3.74	1.38	1.33
2	E	4000	FMN	C4A-N5	3.71	1.38	1.33
2	A	4000	FMN	C4A-N5	3.71	1.38	1.33
2	D	4000	FMN	C4A-N5	3.69	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	FMN	C4-N3-C2	5.94	120.16	115.14
2	B	4000	FMN	C4-N3-C2	5.93	120.15	115.14
2	D	4000	FMN	C4-N3-C2	5.91	120.13	115.14
2	E	4000	FMN	C4-N3-C2	5.91	120.13	115.14
2	C	4000	FMN	C4-N3-C2	5.90	120.12	115.14

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4000	FMN	O3'-C3'-C4'-C5'
2	B	4000	FMN	O3'-C3'-C4'-C5'
2	C	4000	FMN	O3'-C3'-C4'-C5'
2	D	4000	FMN	O3'-C3'-C4'-C5'
2	E	4000	FMN	O3'-C3'-C4'-C5'

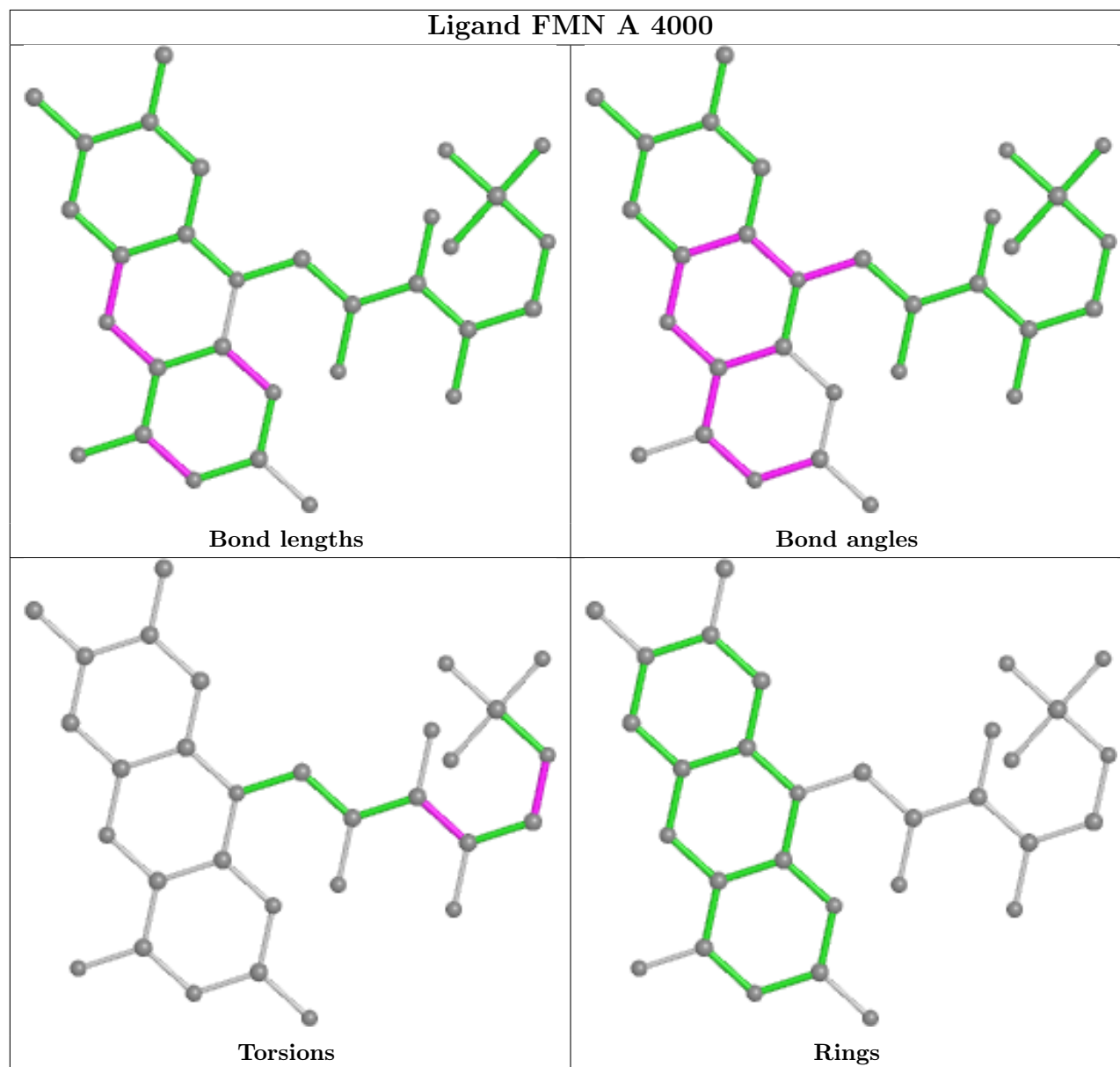
There are no ring outliers.

6 monomers are involved in 26 short contacts:

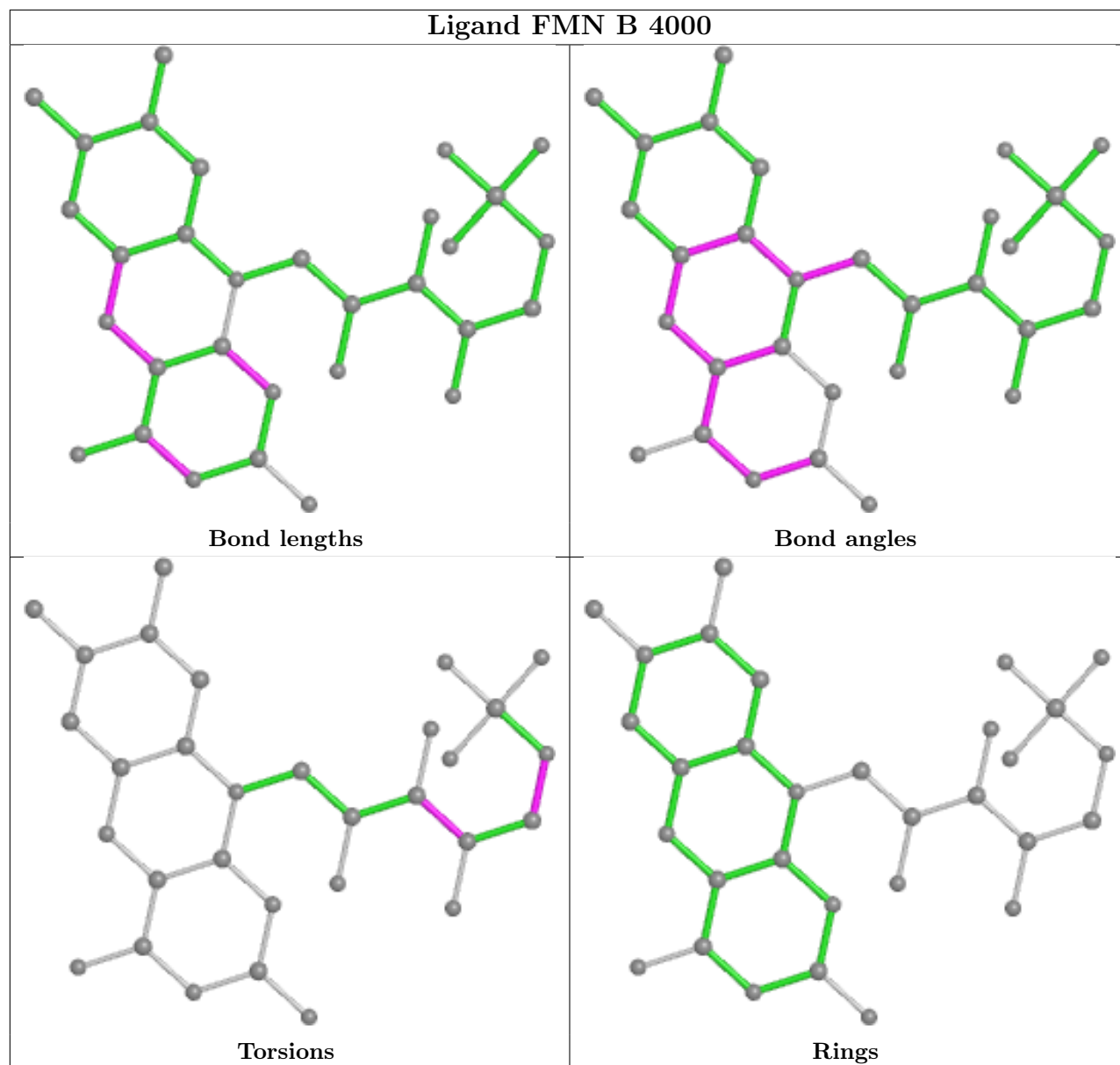
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	FMN	4	0
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0
2	D	4000	FMN	4	0
2	E	4000	FMN	4	0
2	F	4000	FMN	5	0

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.

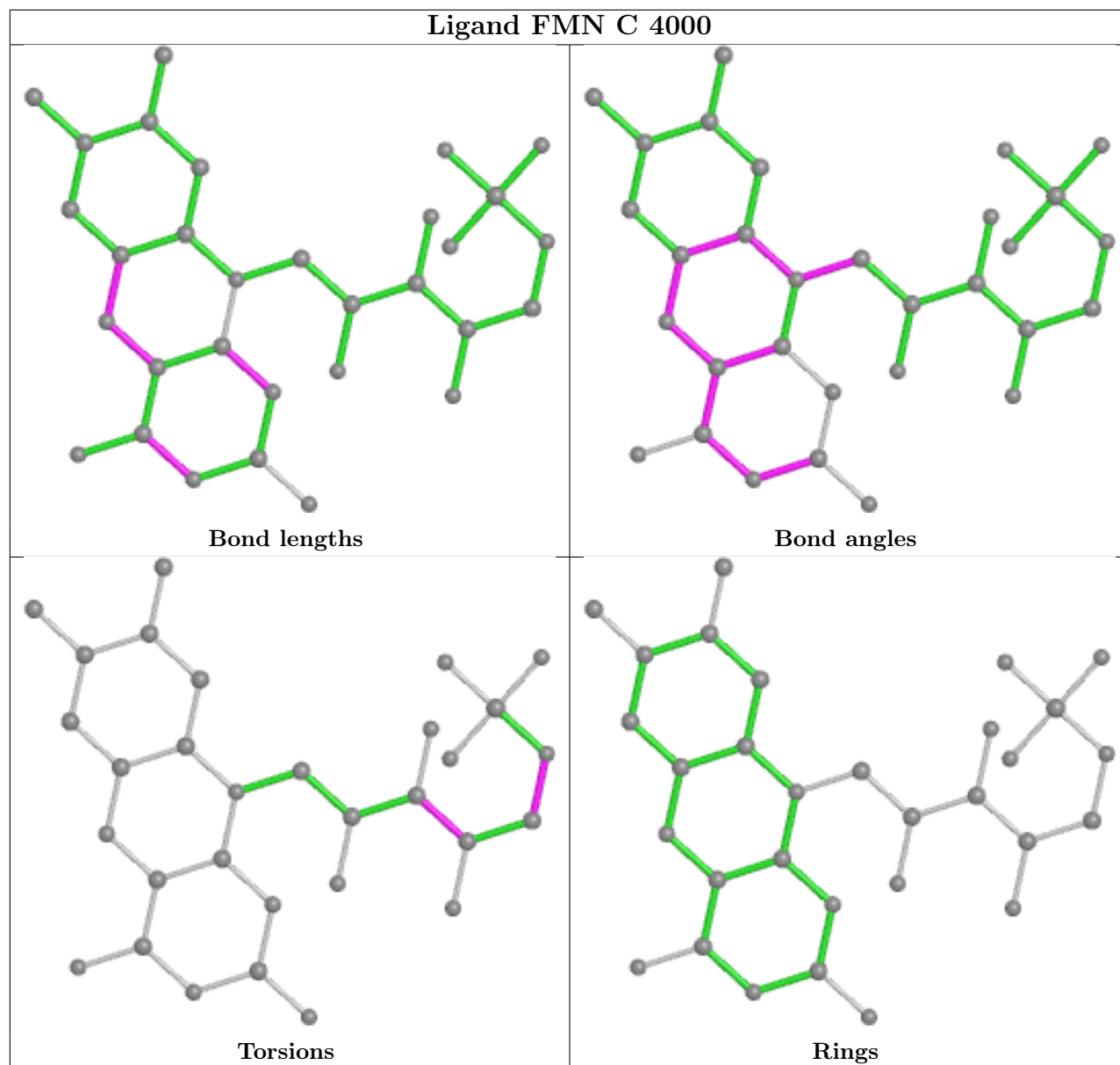
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



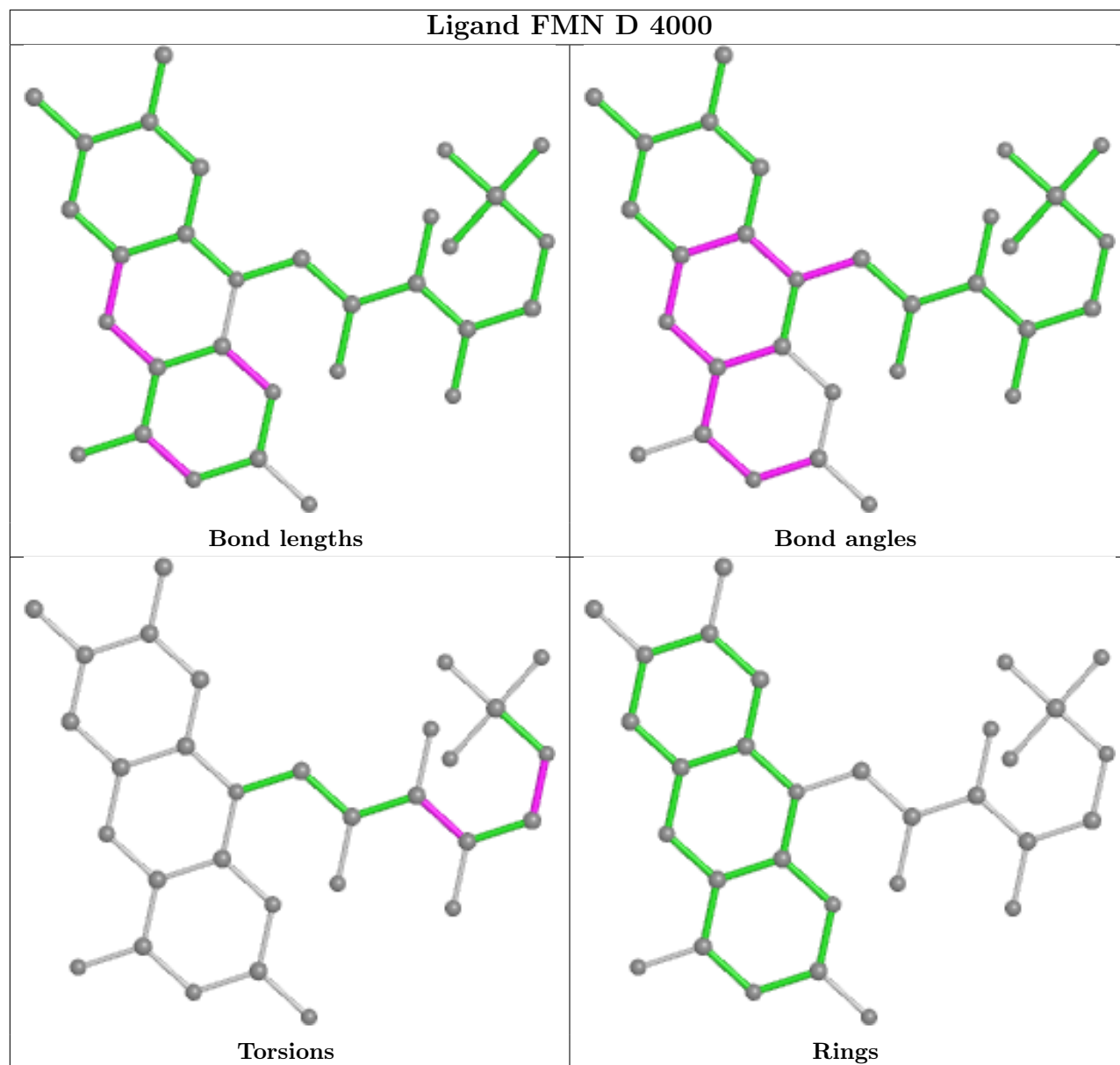
Ligand FMN B 4000



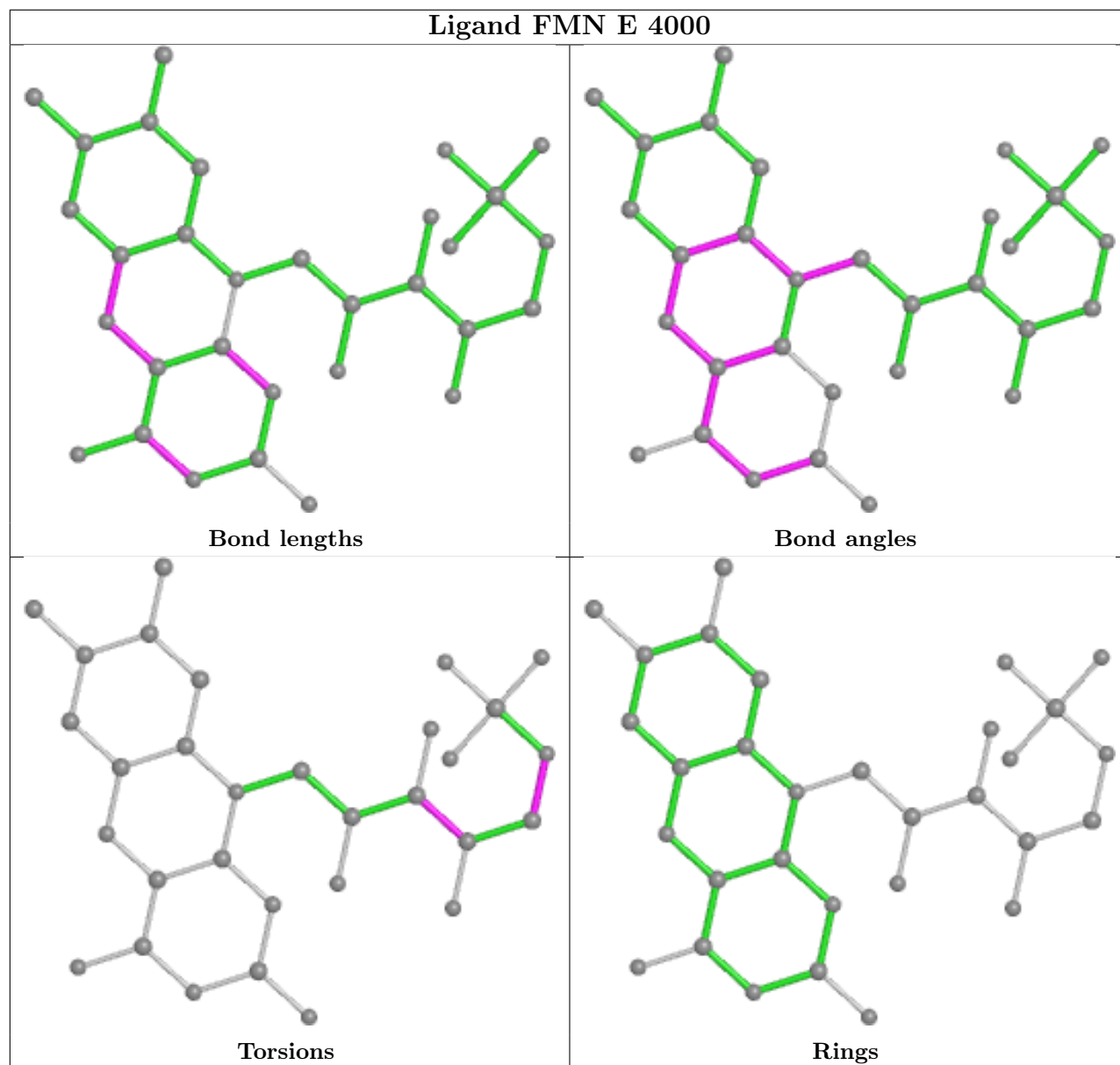
Ligand FMN C 4000

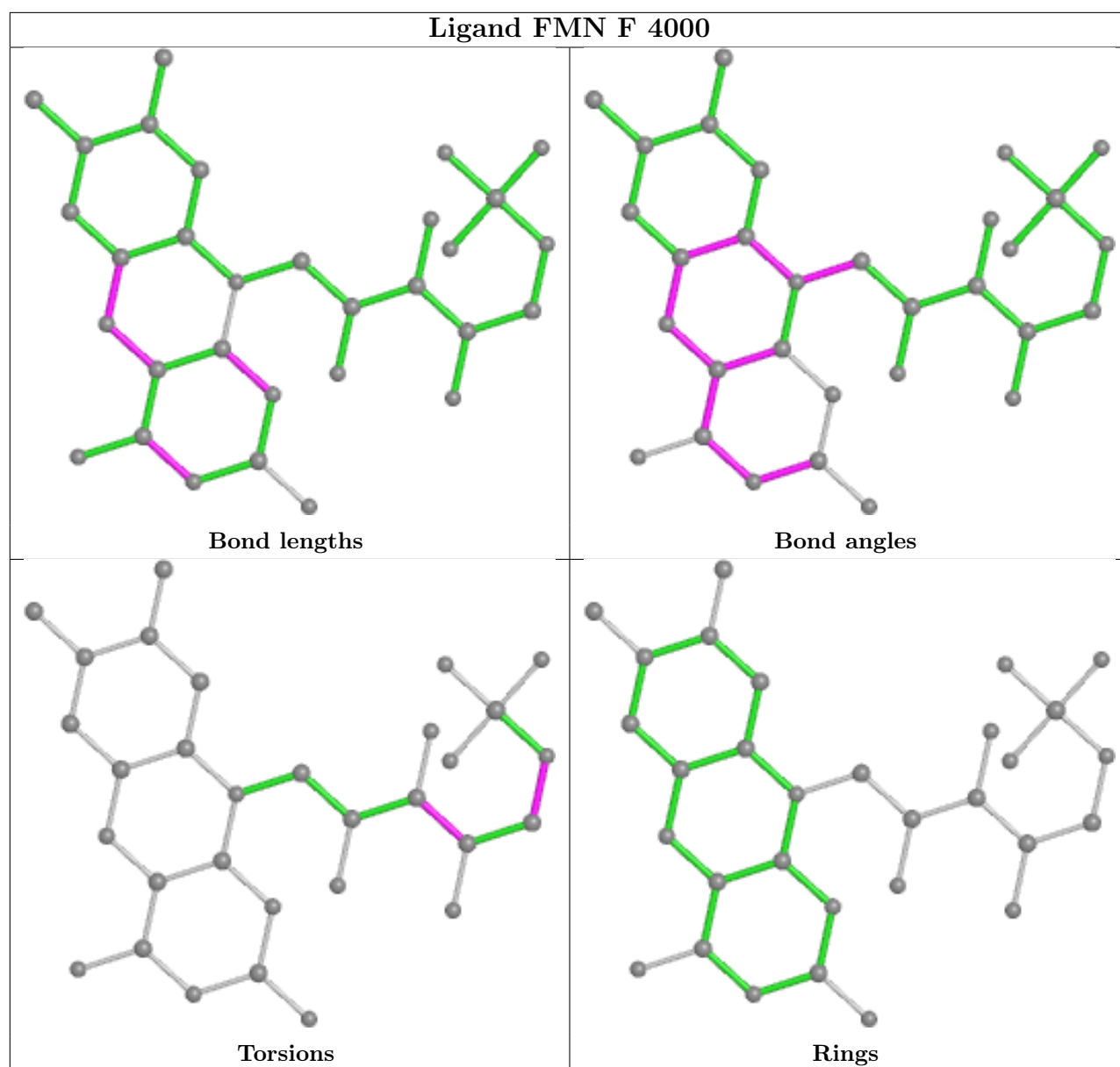


Ligand FMN D 4000



Ligand FMN E 4000





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.