



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 10:17 AM UTC

PDB ID : 4V8V / pdb_00004v8v
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 initial model : 4B3Y

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

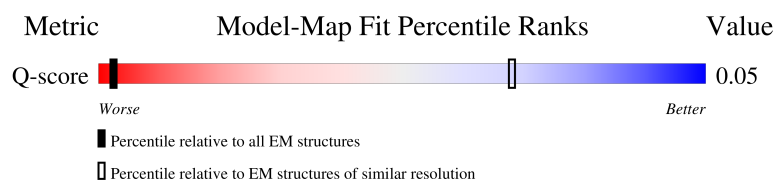
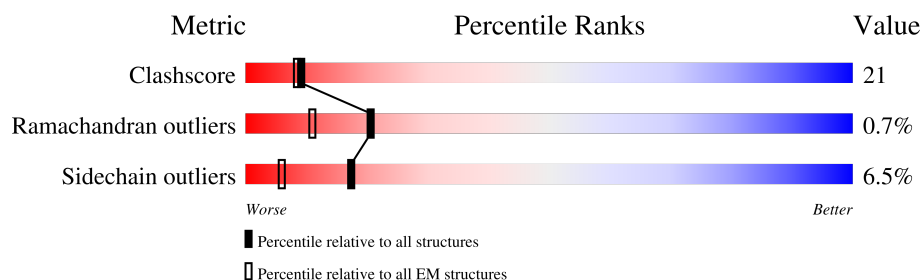
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	28 (19.50 - 20.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3089	
1	B	3089	
1	C	3089	
1	D	3089	

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Mol	Chain	Length	Quality of chain
1	E	3089	56% 32% • 9%
1	F	3089	5% 56% 32% • 9%

2 Entry composition [i](#)

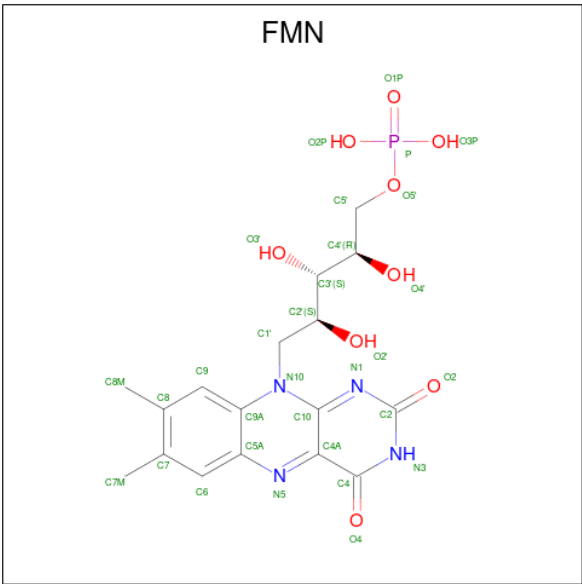
There are 2 unique types of molecules in this entry. The entry contains 125856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

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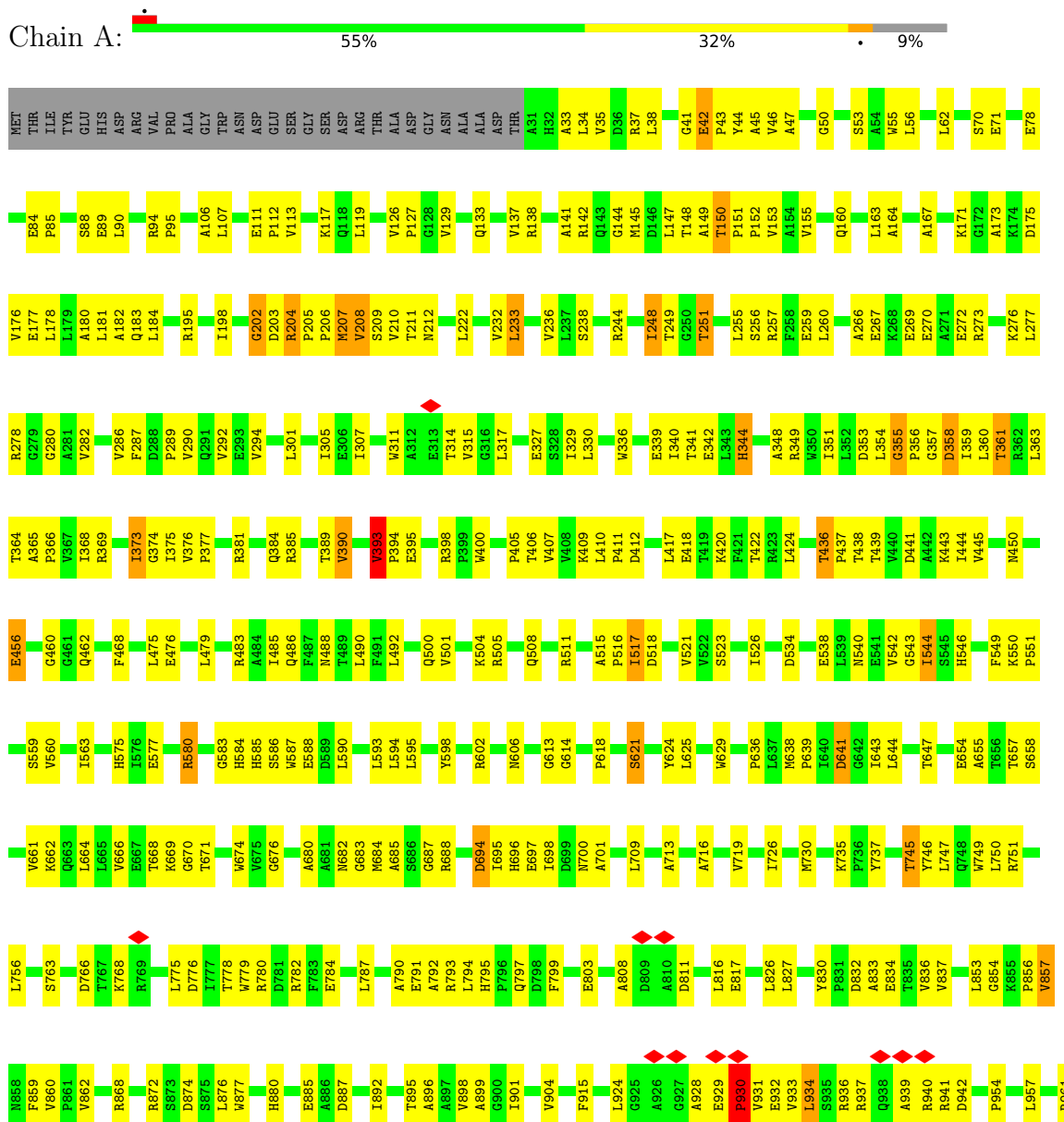
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

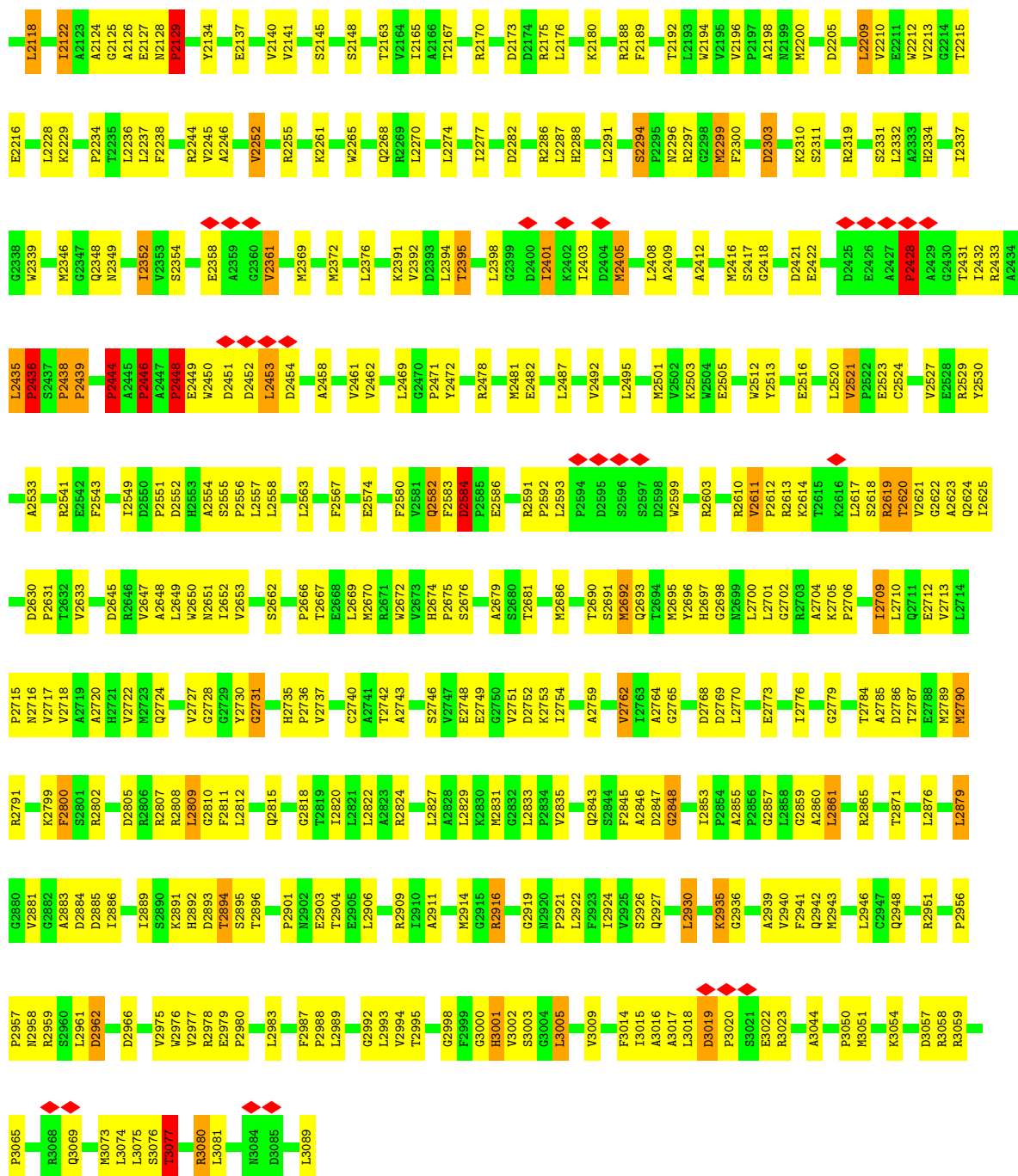
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

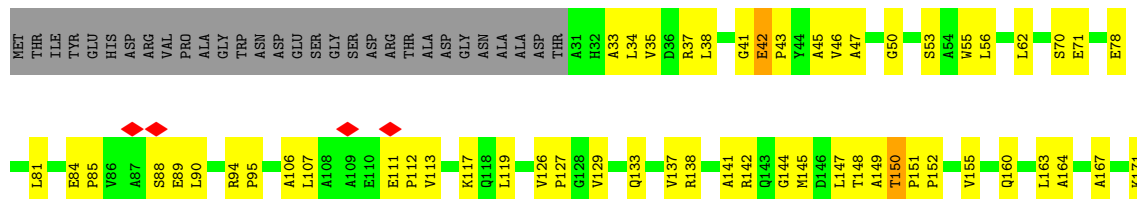
• Molecule 1: TYPE-I FATTY ACID SYNTHASE





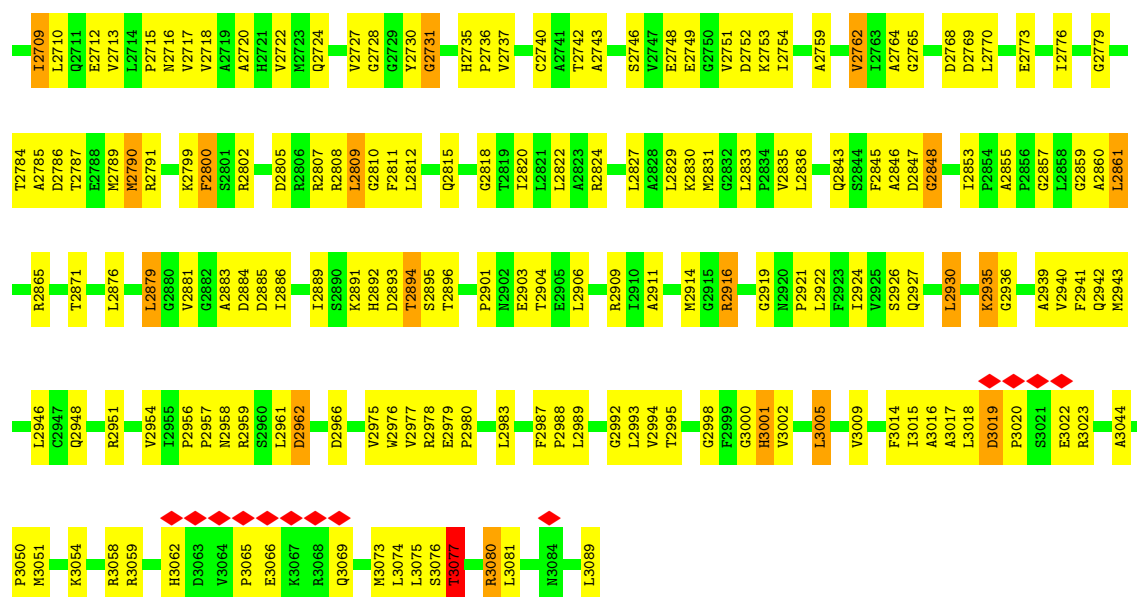


• Molecule 1: TYPE-I FATTY ACID SYNTHASE

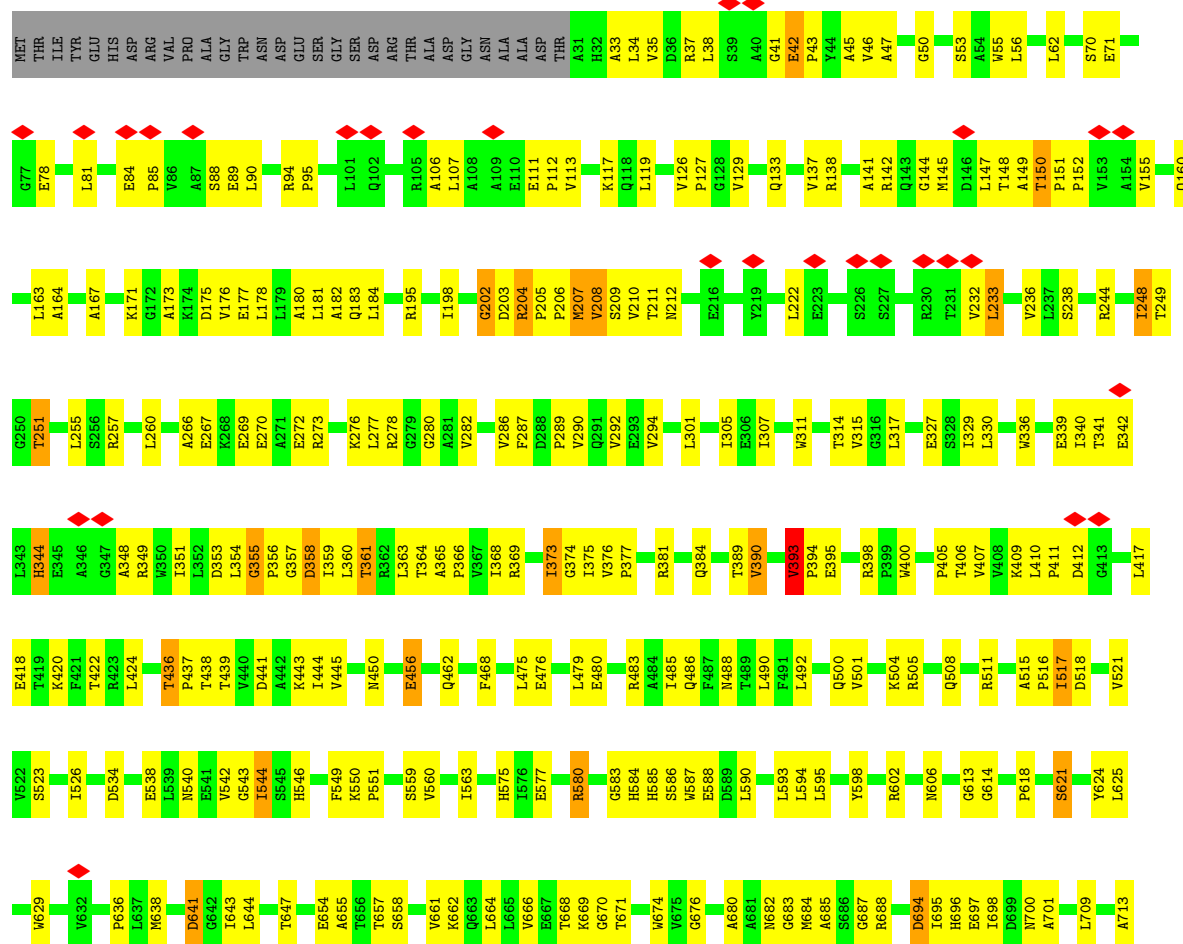


G172	A173	K174	D175	V176	E177	L178	L179	A180	L181	A182	Q183	L184	R195	I198	G202	D203	R204	P205	P206	M207	V208	S209	V210	T211	N212	L222	T231	V232	L233	V236	L237	S238	R244	I248	T249	G250	T251	L255	S256	R257	L260	A266	E267	K268	E269	E270	A271	E272		
R273	K276	L277	G355	P356	G357	G280	V282	V286	F287	D288	P289	V290	Q291	V292	E293	V294	L301	I305	E306	I307	R310	W311	A312	E313	T314	V315	G316	V232	L317	D318	V319	E320	L321	K323	E324	E327	S328	I329	L330	W336	E339	I340	T341	E342	L343	H344	A348	R349	W350	I351
L352	D353	P437	G355	P356	G357	D358	A281	L359	R362	L363	T364	A365	P366	V367	Q291	R369	I373	G374	I375	V376	P377	R381	Q384	T389	V390	V393	P394	L490	E395	R398	P399	W400	P405	T406	V407	V408	K409	L410	P411	D412	L417	E418	T419	K420	F421	T422	L423	L424	S428	P429
T436	P437	T438	E541	V440	D441	A442	K443	L444	V445	N450	E456	G460	Q461	Q462	F468	L475	E476	L479	R483	A484	S486	W487	Q487	N488	T489	L490	F491	L492	Q500	V501	K504	R505	Q508	R511	A515	P516	I517	D518	V521	V522	S523	I526	D534							
E538	L539	N540	E541	V542	G543	I544	S545	H546	F549	K550	P551	S559	V560	I563	H575	I576	E577	R580	G583	H584	S586	W587	E588	D589	L590	L593	L594	L595	R602	N606	G613	G614	P618	S621	Y624	L625	W629	P636	L637	M638	D641									
G642	I643	L644	T647	E654	A655	T656	S658	V661	K662	Q663	L664	V665	F667	T668	K669	G670	T671	W674	V675	G676	A680	N682	Q683	M684	A685	S686	R687	D688	D694	L695	H696	E697	I698	D699	N700	A701	L709	A713	A716	V719	I726	W730	K735							
P736	Y737	T745	Y746	L747	Q748	W749	R751	L756	D760	G761	N762	S763	D766	T767	K768	P770	D771	L775	A680	I777	T778	W779	R780	D781	R782	F783	E784	L787	A790	E791	A792	R793	L794	H795	P796	Q797	F799	E803	A808	D811	L816	E817	L826	L827						
D832	A833	E834	T835	V836	V837	L853	K855	P856	V857	H858	F859	V860	P861	V862	R868	R872	S873	D874	S875	L876	W877	H880	E885	A886	D887	I892	T895	A896	A897	V898	A899	G900	I901	V904	F915	L924	G925	A926	G927	A928	E929	P930	V931	G932	V933	L934	S935			
R936	R937	Q938	A939	R940	R941	D942	L957	R961	N962	S963	V964	N965	P966	V967	T970	T971	T974	E975	W976	Q977	E980	D983	N984	R985	S986	A987	S988	H989	P990	S991	T992	L996	E997	D1001	Q1002	H1003	V1004	V1005	L1006	S1007	P1009	L1010	G1011	G1012	T1013	W1014	I1017	F1019		
T1020	L1021	V1025	E1034	V1035	D1036	D1037	V1045	L1046	E1056	N1057	L1058	P1059	K1060	D1063	N1064	V1068	T1069	V1070	D1071	W1072	V1077	V1083	T1084	A1085	T1086	F1087	G1088	A1089	P1090	L1091	A1092	P1093	T1094	L1095	T1096	V1097	V1098	P1099	V1103	G1104	R1105	C1106	V1110	F1111	A1117	A1118	T1119			
E1120	A1121	G1122	F1123	T1124	V1125	I1126	E1127	G1128	L1129	L1132	V1133	P1146	K1147	E1148	P1149	A1150	E1151	T1162	D1163	T1164	G1167	R1168	P1171	V1172	S1173	V1174	R1177	N1178	A1179	A1180	D1181	G1182	L1184	L1185	L1188	R1191	F1192	I1193	R1195	G1196	R1197	A1200	A1201	E1202	L1203	T1204	D1205	P1206		
V1207	A1212	I1213	T1218	D1219	V1220	P1221	R1225	R1226	D1227	V1228	R1237	N1247	R1253	G1268	M1269	W1270	L1271	A1274	A1275	Q1276	H1277	V1278	V1279	L1280	A1281	T1282	D1283	G1284	K1285	P1286	V1287	P1288	P1289	A1290	K1291	L1292	W1295	K1304	D1307	Q1308	V1309	D1310	F1311	R1312	V1313	D1314	R1315	V1316		
G1317	I1318	D1319	E1323	V1324	L1325	E1326	S1327	S1328	A1329	R1330	I1331	V1336	M1337	A1338	A1339	R1342	L1343	A1344	A1345	P1346	Y1350	A1351	F1352	P1353	I1357	Q1358	L1470	E1471	L1474	A1380	F1390	S1391	K1483	H1484	H1485	D1486	I1487	V1488	P1489	D1490	D1491	E1492	L1493	G1494	R1495	S1496	T1503	R1504	Q1507	

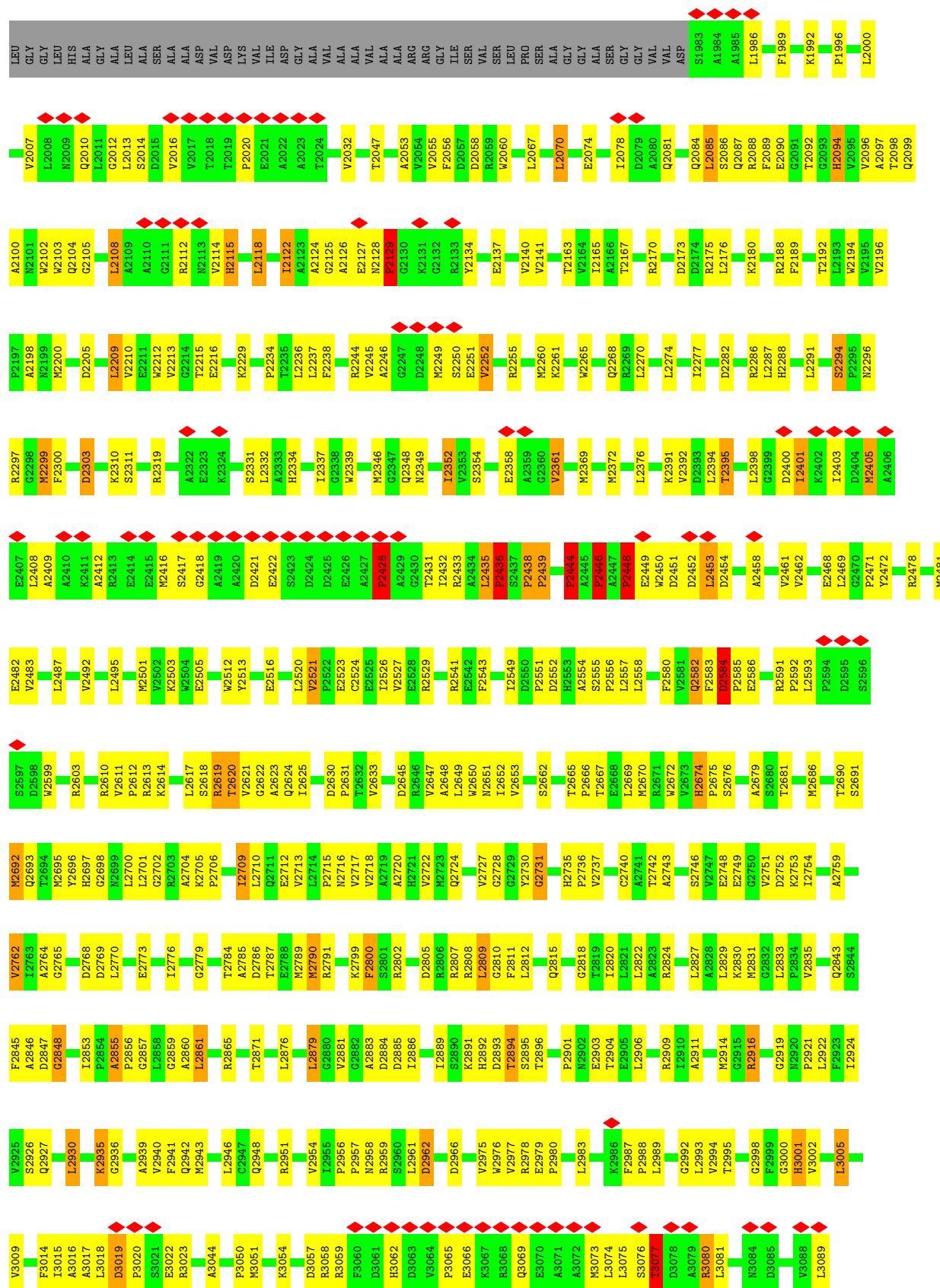




• Molecule 1: TYPE-I FATTY ACID SYNTHASE

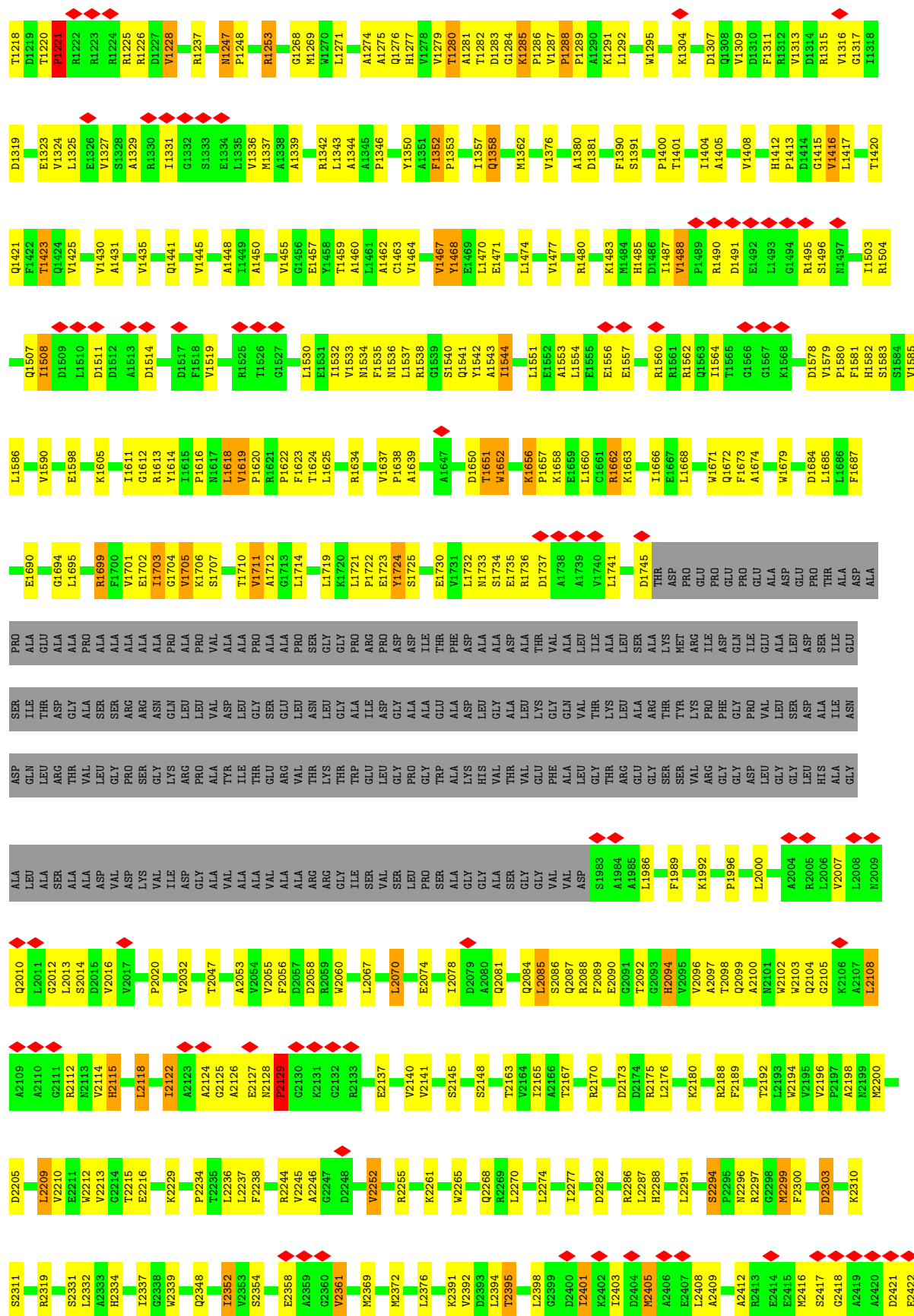






• Molecule 1: TYPE-I FATTY ACID SYNTHASE



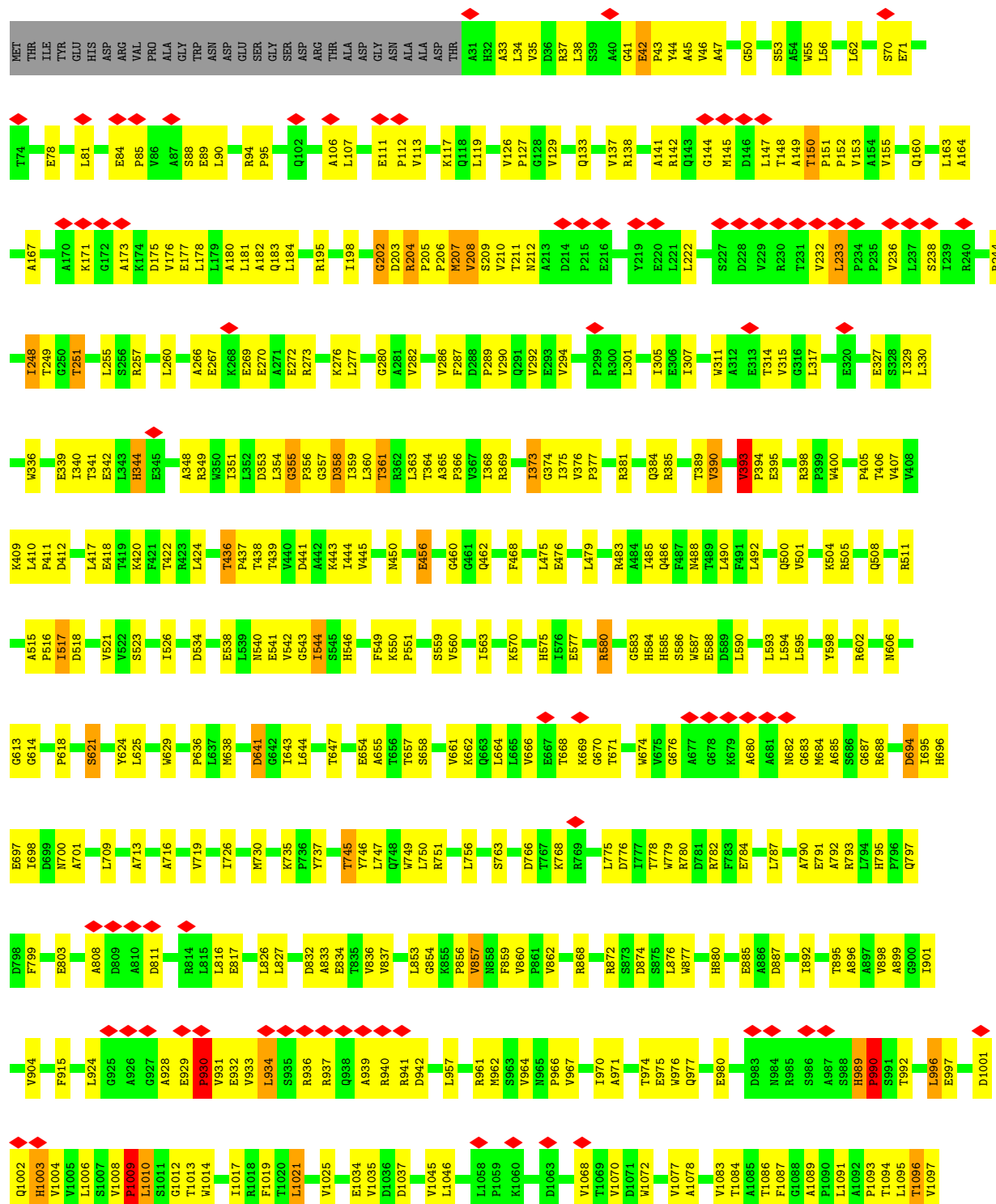


L1714	P1620	F1529	G1456	R1253	P1149	V1045	R961	F859	S763	K662	I563	Q462
L1721	R1621	L1530	E1457	G1288	A1150	L1046	M962	V860	D766	Q663	I563	F468
P1722	F1622	E1531	Y1458	G1269	E1151	L1058	S963	P861	T767	L664	H576	L476
E1723	F1623	T1459	T1459	T1269	N964	L1058	N964	N962	K768	L665	E577	E476
L1625	P1346	P1346	L1461	L1270	D1162	V1068	N965	B868	R769	E667	R580	L479
S1725	L1625	M1534	A1462	L1271	T1164	V1069	P966	H880	P770	T668	L479	L483
E1730	R1634	F1535	A1463	A1274	G1167	T1089	T970	R872	L775	G670	G583	R483
V1731	P1637	R1536	V1464	A1275	R1168	D1071	A971	S873	D776	T671	H584	L485
N1733	P1638	R1538	V1467	V1278	P1171	V1070	T974	S875	T777	W674	H585	L486
S1734	A1639	G1539	E1468	V1279	V1172	T1071	W976	L876	T778	W675	Q486	F487
E1735	D1650	Q1358	L1470	T1280	S1173	D1072	W977	W877	W779	G676	E588	N488
R1736	T1651	E1471	E1471	T1281	V1174	V1072	Q977	H880	R781	A680	D589	L489
D1737	W1652	L1474	L1474	T1282	A1281	V1077	E980	E885	F782	A681	L590	L490
L1741	K1656	L1551	V1477	G1283	N1177	T1085	D983	E886	F783	N682	L593	L491
D1745	P1657	E1552	V1477	K1285	A1179	F1087	N984	D887	E784	G683	L594	L492
THR	K1658	A1553	P1286	G1284	D1180	G1088	R985	I892	L787	M684	L595	Q500
ASP	E1659	L1554	P1287	G1285	D1181	A1089	A987	A896	A790	S686	Y598	V501
GLU	C1660	E1555	P1288	A1089	G1182	P1090	R989	A999	A791	G687	R602	K504
GLU	C1661	K1483	P1289	A1092	G1183	L1094	R990	I901	A792	R688	R505	R505
PRO	R1662	M1484	A1290	A1093	A1183	T1095	S988	V904	R793	D684	N606	Q508
GLU	K1663	H1485	L1291	P1093	A1183	L1096	H989	V904	R794	I695	G613	R511
PRO	I1666	H1487	L1292	T1095	L1185	T1097	P990	V904	R795	H696	G614	R511
GLU	E1667	V1488	L1295	P1097	L1188	A1097	S991	V904	R796	G697	P618	A515
GLU	L1668	P1489	K1304	P1098	L1188	T1098	T992	V904	R797	I698	S621	P516
ALA	W1671	D1491	V1408	P1099	R1191	D1100	L996	V904	R798	D699	D629	D518
ALA	Q1672	F1673	D1307	P1103	F1192	V1103	E997	F915	R808	N700	L625	V521
ALA	A1674	S1496	Q1308	G1104	A1194	R1105	Q1002	F915	R809	A701	Y624	V521
ALA	W1679	D1578	P1309	R1105	R1195	C1106	H1003	D921	D809	L709	L625	V521
ALA	D1684	F1581	D1310	R1106	G1196	V1110	H1004	L924	A810	A713	W629	V523
GLU	L1685	H1582	G1311	L1107	R1197	F1111	V1005	G925	D811	A716	A630	S523
ALA	L1686	S1583	V1312	A1117	G1197	F1111	L1006	A926	R814	V719	E631	I526
ALA	F1687	S1584	R1313	A1118	P1206	A1118	L1007	G927	R815	I726	P636	D634
ALA	E1690	L1586	D1318	E1120	V1207	E1120	P1008	A928	L816	P637	L637	E538
ALA	G1694	V1590	D1319	E1121	A1212	E1121	P1009	E929	L817	M638	P638	L539
ALA	L1695	E1598	E1323	E1122	A1121	G1122	L1010	E930	L826	P639	N540	E541
ALA	R1699	K1605	L1324	F1123	G1122	G1122	G1012	V931	L827	K735	I640	V542
ALA	F1700	D1606	L1325	F1124	D1219	F1124	T1013	E932	L832	P736	D641	G543
VAL	E1702	P1607	V1327	P1125	T1220	P1125	W1014	V933	D833	Y737	I643	I544
ALA	E1703	T1611	S1328	V1126	R1225	V1126	I1017	L934	A833	T745	L644	H546
ALA	G1704	A1520	A1329	E1127	R1226	E1127	R1018	S935	E834	Y746	T647	F549
ALA	K1706	I1522	R1330	G1128	D1227	G1128	F1019	R936	T835	Q748	E654	K550
ALA	T1710	S1523	L1331	L1129	V1228	L1129	T1020	R937	V836	Q748	A655	P551
PRO	L1615	E1524	M1337	L1132	V1228	L1132	L1021	Q938	V837	L750	T657	L750
SER	P1616	R1525	M1337	L1133	R1237	V1133	V1025	A939	L853	R751	S658	S559
GLY	L1617	T1526	A1448	L1134	R1247	V1134	E1034	R940	K855	L756	V661	V560
GLY	L1618	G1527	A1450	P1146	P1248	K1146	V1035	R941	K856	L756	V661	V560
GLY	V1619	E1528	V1455	E1148	P1248	K1148	D1037	D942	V857	L756	V661	V560





• Molecule 1: TYPE-I FATTY ACID SYNTHASE





L3005	V3009	F3014	I3015	A3016	A3017	L3018	D3019	P3020	S3021	E3022	R3023	A3044	P3050	M3051	K3054	D3057	R3058	R3059	H3062	P3065	E3066	Q3069	M3073	L3074	L3075	S3076	T3077	R3080	L3081	L3089																						
P2921	L2922	F2923	I2924	V2925	S2926	Q2927	L2930	K2935	G2936	A2939	V2940	F2941	Q2942	M2943	L2946	C2947	Q2948	R2951	V2954	I2955	P2956	P2957	N2958	R2959	S2960	L2961	D2962	D2966	V2975	W2976	V2977	R2978	E2979	P2980	L2983	F2987	P2988	L2989	G2992	L2993	V2994	T2995	G2998	F2999	G3000	H3001	V3002					
V2835	Q2843	S2844	F2845	A2846	D2847	G2848	T2853	P2854	A2855	P2856	G2857	L2858	G2859	A2860	L2861	R2865	T2871	L2876	L2879	G2880	V2881	G2882	A2883	D2884	D2885	L2886	T2889	S2890	K2891	H2892	D2893	T2894	S2895	T2896	P2901	R2902	E2903	T2904	E2905	L2906	R2909	I2910	A2911	M2914	G2915	R2916	G2919	L2920	N2920			
I2754	A2759	V2762	I2763	A2764	G2765	D2768	D2769	L2770	E2773	I2776	G2779	T2784	A2785	D2786	T2787	E2788	M2789	R2790	R2791	K2799	V2717	F2800	S2801	R2802	D2805	R2806	R2807	L2808	L2809	G2810	F2811	L2812	Q2815	G2818	T2819	I2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	K2830	M2831	G2832	P2834					
M2686	T2690	S2691	M2692	Q2693	T2694	M2695	H2697	G2698	N2699	L2700	L2701	G2702	R2703	A2704	K2705	P2706	I2709	L2710	Q2711	E2712	V2713	L2714	P2715	N2716	V2717	V2718	A2719	A2720	H2721	V2722	M2723	Q2724	V2727	G2728	G2729	Y2730	G2731	H2735	P2736	V2737	C2740	A2741	T2742	A2743	S2746	V2747	E2748	E2749	G2750	V2751	D2752	K2753
P2592	L2593	P2594	D2595	S2596	S2597	D2598	W2599	R2603	R2610	V2611	P2612	R2613	K2614	L2617	S2618	R2619	T2620	V2621	G2622	A2623	Q2624	I2625	D2630	P2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	W2650	N2651	I2652	V2653	S2662	P2666	E2668	L2669	M2670	R2671	W2672	V2673	H2674	P2675	S2676	A2679	T2681				
M2501	V2502	K2503	M2504	E2505	W2512	Y2513	D2514	T2515	E2516	L2520	V2521	P2522	E2523	C2524	V2527	E2528	R2529	R2541	G2542	F2543	I2549	D2550	P2551	D2552	H2553	A2554	S2555	P2556	L2557	L2558	L2563	D2564	K2565	D2566	F2567	S2573	E2574	A2575	D2576	A2577	R2578	A2579	P2580	V2581	Q2582	F2583	D2584	P2585	S2586	R2591		
A2412	M2416	S2417	G2418	A2419	A2420	D2421	E2422	S2423	D2424	D2425	E2426	A2427	P2428	T2431	I2432	R2433	A2434	L2435	P2436	S2437	P2438	P2439	P2444	A2445	P2446	A2447	P2448	E2449	W2450	D2451	D2452	L2453	D2454	A2458	V2461	V2462	L2469	G2470	P2471	Y2472	R2478	M2481	E2482	V2483	L2487	V2492	L2495					
N2296	R2297	G2298	M2299	F2300	D2303	K2310	S2311	R2319	S2331	L2332	A2333	H2334	L2337	G2338	W2339	M2346	G2347	Q2348	W2349	I2352	V2353	S2354	E2358	A2359	G2360	V2361	N2369	W2372	L2376	K2391	V2392	D2393	T2395	L2398	G2399	D2400	I2401	K2402	L2403	D2404	N2405	A2406	F2407	L2408								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4337	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	10.361	Depositor
Minimum map value	-2.852	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.8	Depositor
Map size ($\text{\AA}$)	456.0, 456.0, 456.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.28, 2.28, 2.28	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	18/21335 (0.1%)	0.90	61/29037 (0.2%)
1	B	0.45	18/21335 (0.1%)	0.90	60/29037 (0.2%)
1	C	0.45	18/21335 (0.1%)	0.90	60/29037 (0.2%)
1	D	0.45	18/21335 (0.1%)	0.90	60/29037 (0.2%)
1	E	0.45	18/21335 (0.1%)	0.90	61/29037 (0.2%)
1	F	0.45	18/21335 (0.1%)	0.90	59/29037 (0.2%)
All	All	0.45	108/128010 (0.1%)	0.90	361/174222 (0.2%)

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 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2094	HIS	CB-CG	-5.85	1.42	1.50
1	A	996	LEU	CB-CG	-5.81	1.41	1.53
1	A	2094	HIS	CB-CG	-5.80	1.42	1.50
1	F	2115	HIS	CB-CG	-5.80	1.42	1.50
1	B	1003	HIS	CB-CG	-5.80	1.42	1.50

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2438	PRO	N-CA-CB	13.73	110.88	103.19
1	A	2438	PRO	N-CA-CB	13.58	110.79	103.19
1	F	2438	PRO	N-CA-CB	13.53	110.77	103.19
1	D	2438	PRO	N-CA-CB	13.51	110.76	103.19
1	E	2438	PRO	N-CA-CB	13.51	110.75	103.19

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 [i](#)

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	914	0
1	B	20945	0	20595	906	0
1	C	20945	0	20595	909	0
1	D	20945	0	20595	909	0
1	E	20945	0	20595	913	0
1	F	20945	0	20595	917	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	5	0
2	E	31	0	19	4	0
2	F	31	0	19	5	0
All	All	125856	0	123684	5122	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 21.

The worst 5 of 5122 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%)	21	59
1	B	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	18	56
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	18	56
1	D	2818/3089 (91%)	2641 (94%)	158 (6%)	19 (1%)	18	56
1	E	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	21	59
1	F	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	18	56
All	All	16908/18534 (91%)	15849 (94%)	947 (6%)	112 (1%)	20	56

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%)	1958 (94%)	136 (6%)	15	37
1	B	2097/2402 (87%)	1961 (94%)	136 (6%)	15	37
1	C	2094/2402 (87%)	1958 (94%)	136 (6%)	15	37
1	D	2093/2402 (87%)	1957 (94%)	136 (6%)	15	37
1	E	2095/2402 (87%)	1959 (94%)	136 (6%)	15	37
1	F	2094/2402 (87%)	1958 (94%)	136 (6%)	15	37
All	All	12567/14412 (87%)	11751 (94%)	816 (6%)	17	37

5 of 816 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1280	THR
1	E	621	SER
1	F	2827	LEU
1	D	1544	ILE
1	D	1253	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2288	HIS
1	F	2587	HIS
1	E	2651	ASN
1	F	633	HIS
1	C	386	ASN

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 oligosaccharides 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	-	33,33,33	1.03	2 (6%)	48,50,50	1.28	7 (14%)
2	FMN	F	4000	-	33,33,33	1.04	2 (6%)	48,50,50	1.28	7 (14%)
2	FMN	E	4000	-	33,33,33	1.04	2 (6%)	48,50,50	1.29	7 (14%)
2	FMN	D	4000	-	33,33,33	1.05	2 (6%)	48,50,50	1.29	9 (18%)
2	FMN	B	4000	-	33,33,33	1.04	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	C	4000	-	33,33,33	1.04	2 (6%)	48,50,50	1.29	9 (18%)

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	F	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	E	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	D	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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	3.72	1.38	1.30
2	F	4000	FMN	C4A-N5	3.71	1.38	1.30
2	E	4000	FMN	C4A-N5	3.69	1.38	1.30
2	A	4000	FMN	C4A-N5	3.68	1.38	1.30
2	D	4000	FMN	C4A-N5	3.67	1.38	1.30

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4000	FMN	C4-N3-C2	-3.14	120.06	125.64
2	C	4000	FMN	C4-N3-C2	-3.11	120.12	125.64
2	E	4000	FMN	C4-N3-C2	-3.10	120.13	125.64
2	D	4000	FMN	C4-N3-C2	-3.10	120.13	125.64
2	B	4000	FMN	C4-N3-C2	-3.09	120.15	125.64

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'

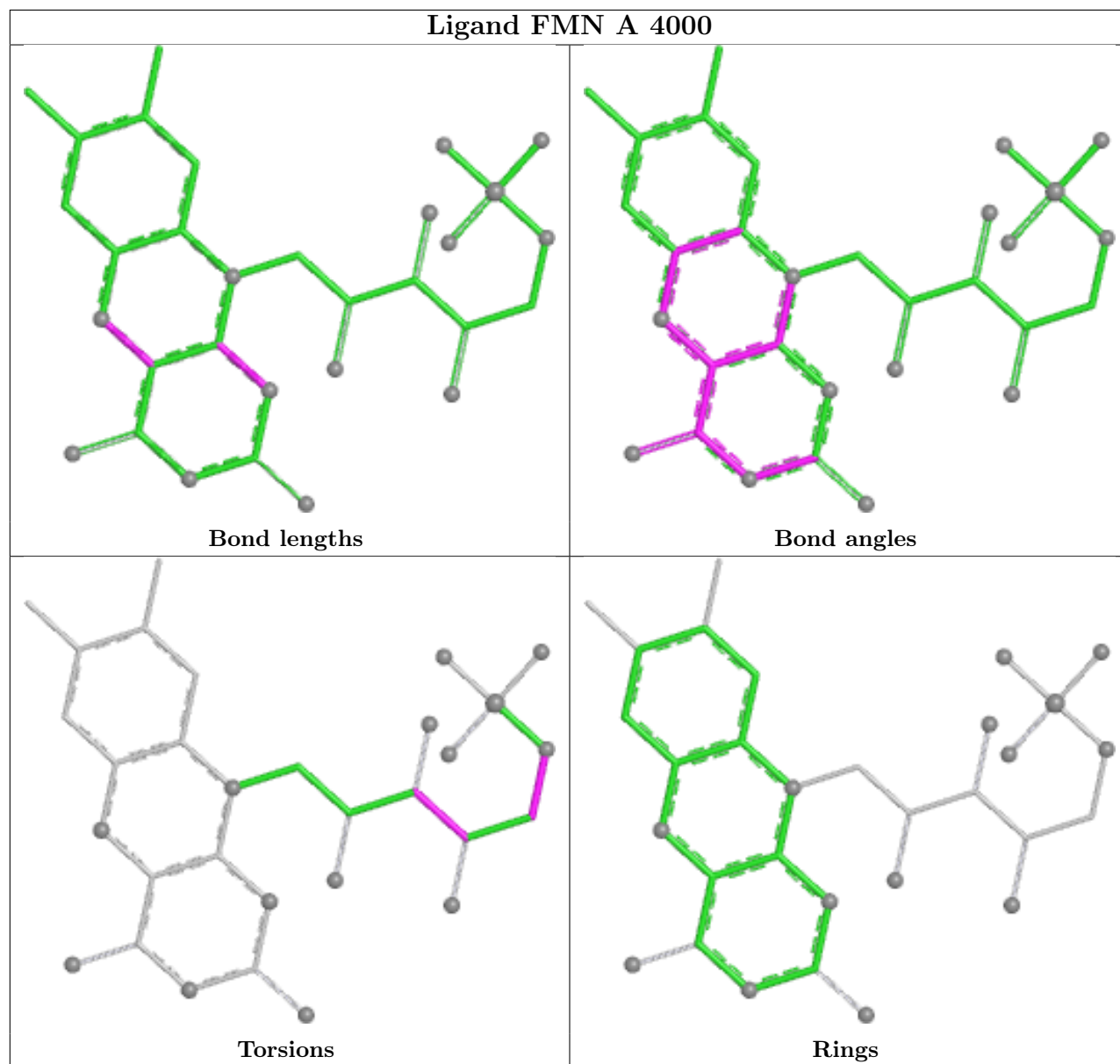
There are no ring outliers.

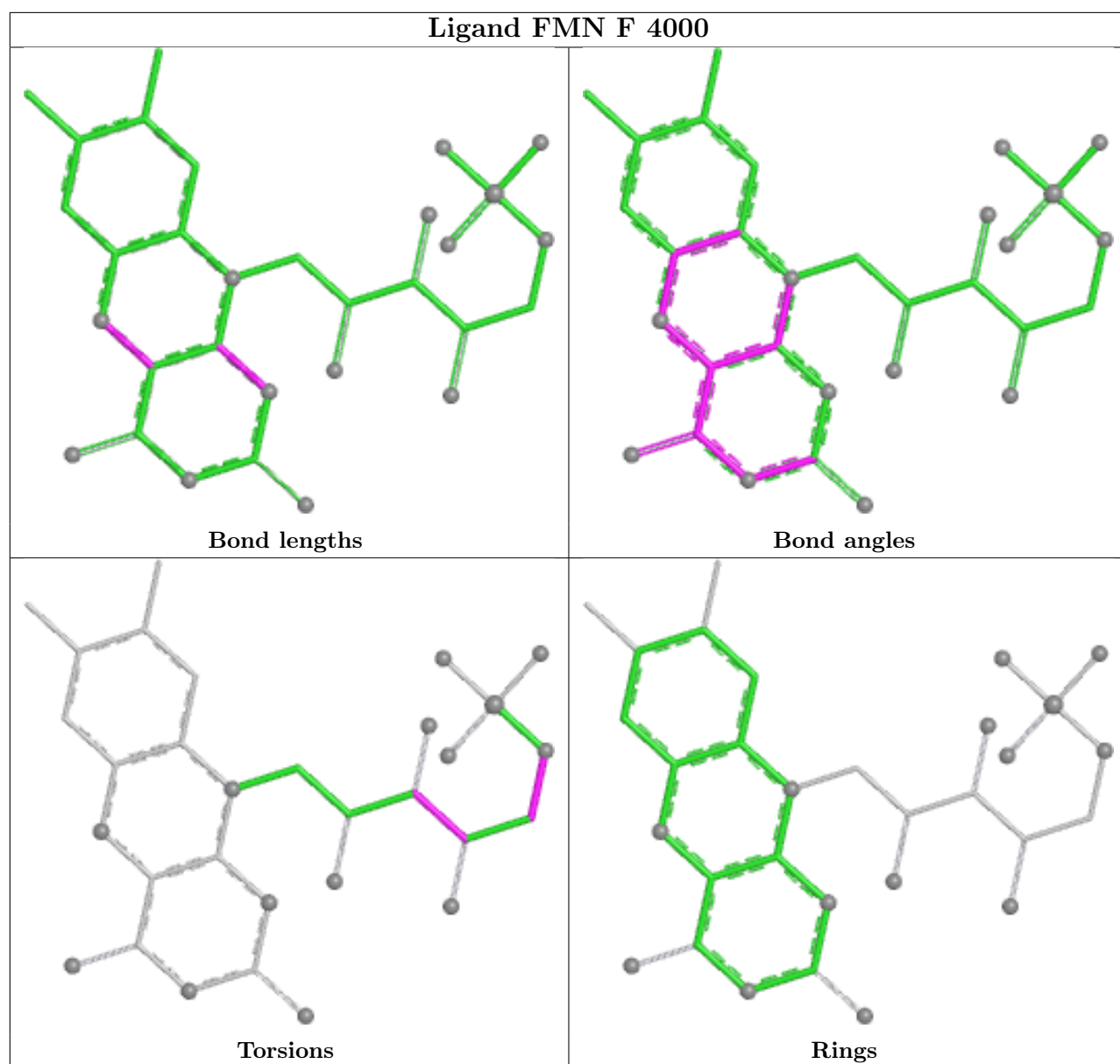
6 monomers are involved in 27 short contacts:

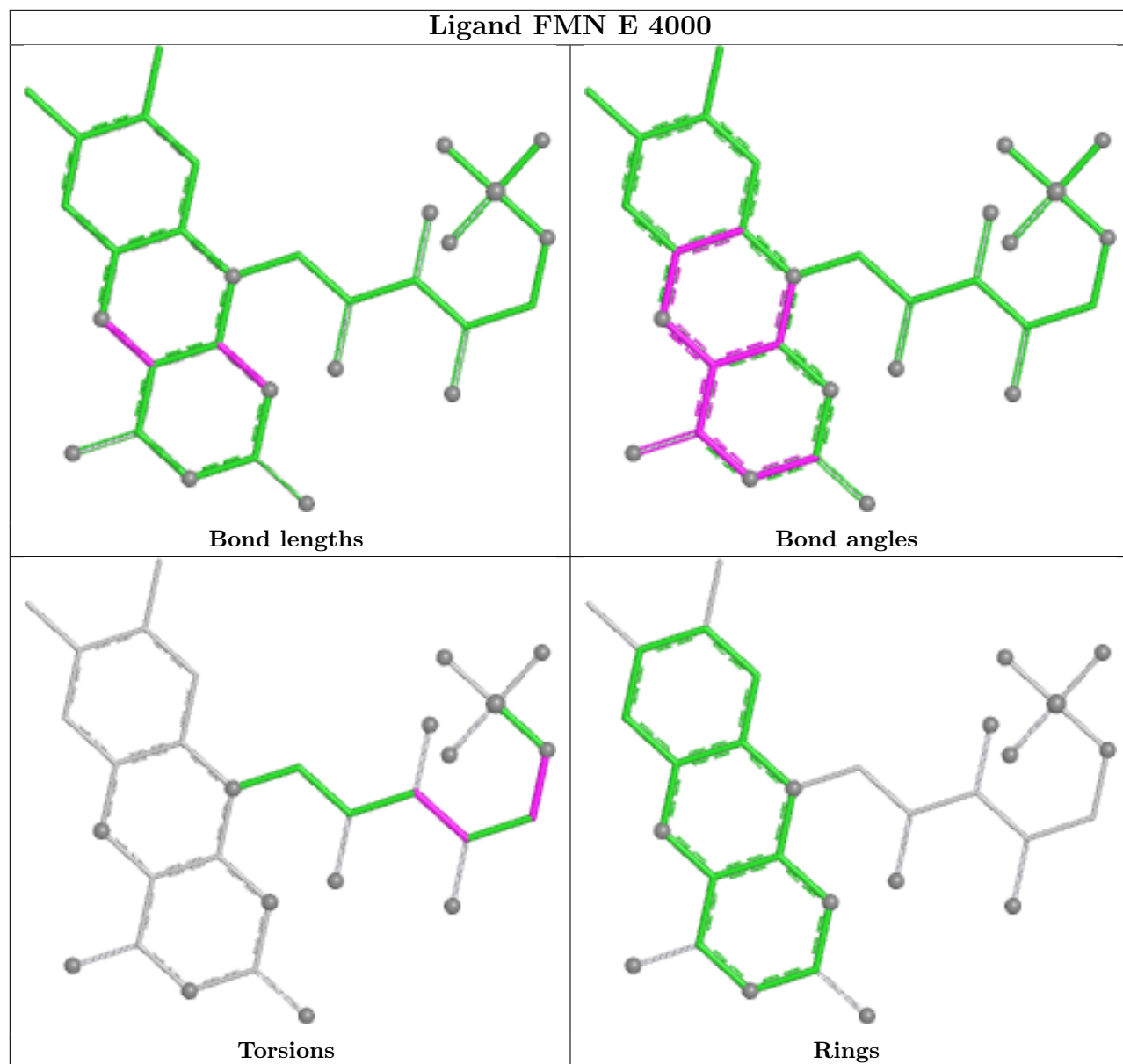
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	FMN	4	0
2	F	4000	FMN	5	0
2	E	4000	FMN	4	0
2	D	4000	FMN	5	0
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0

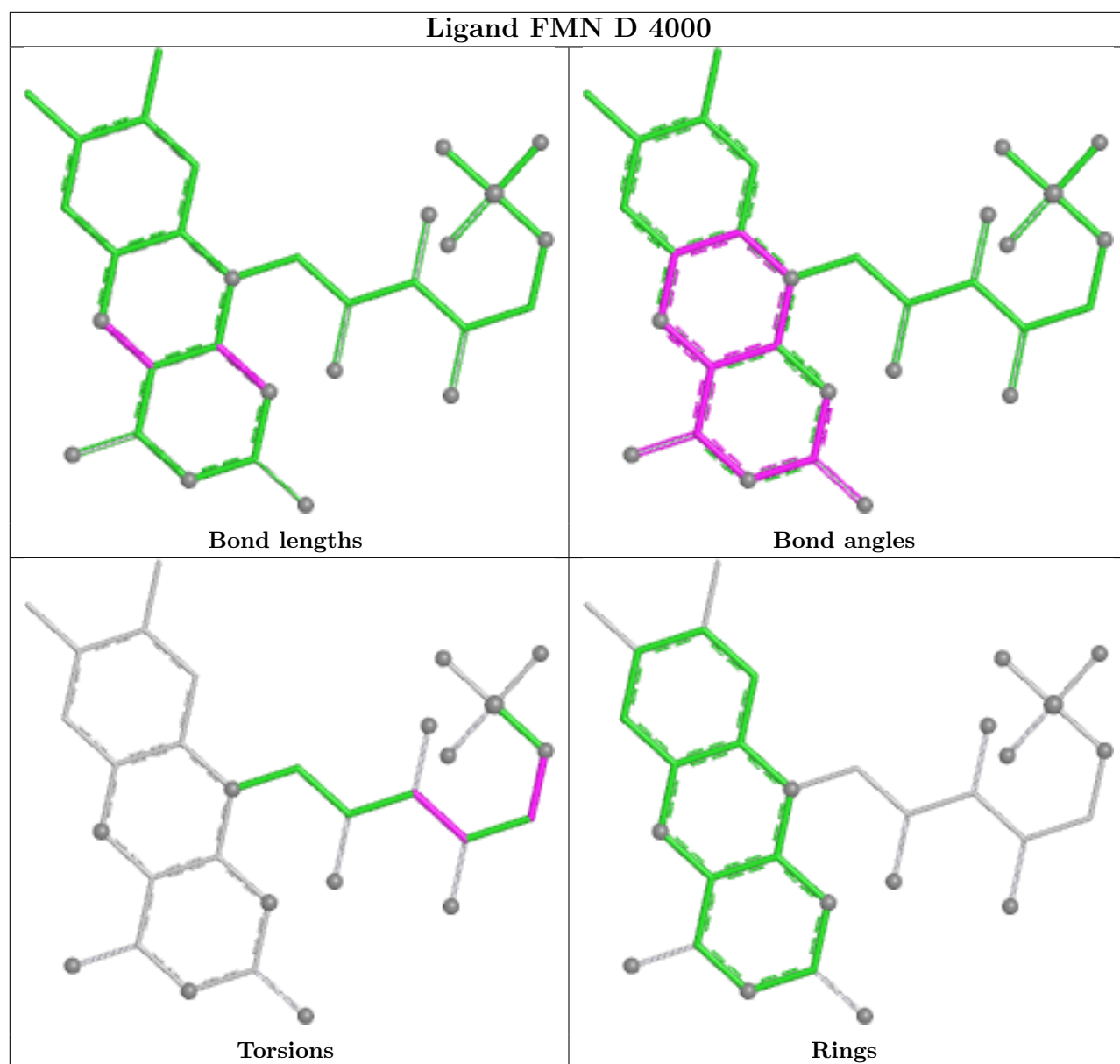
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

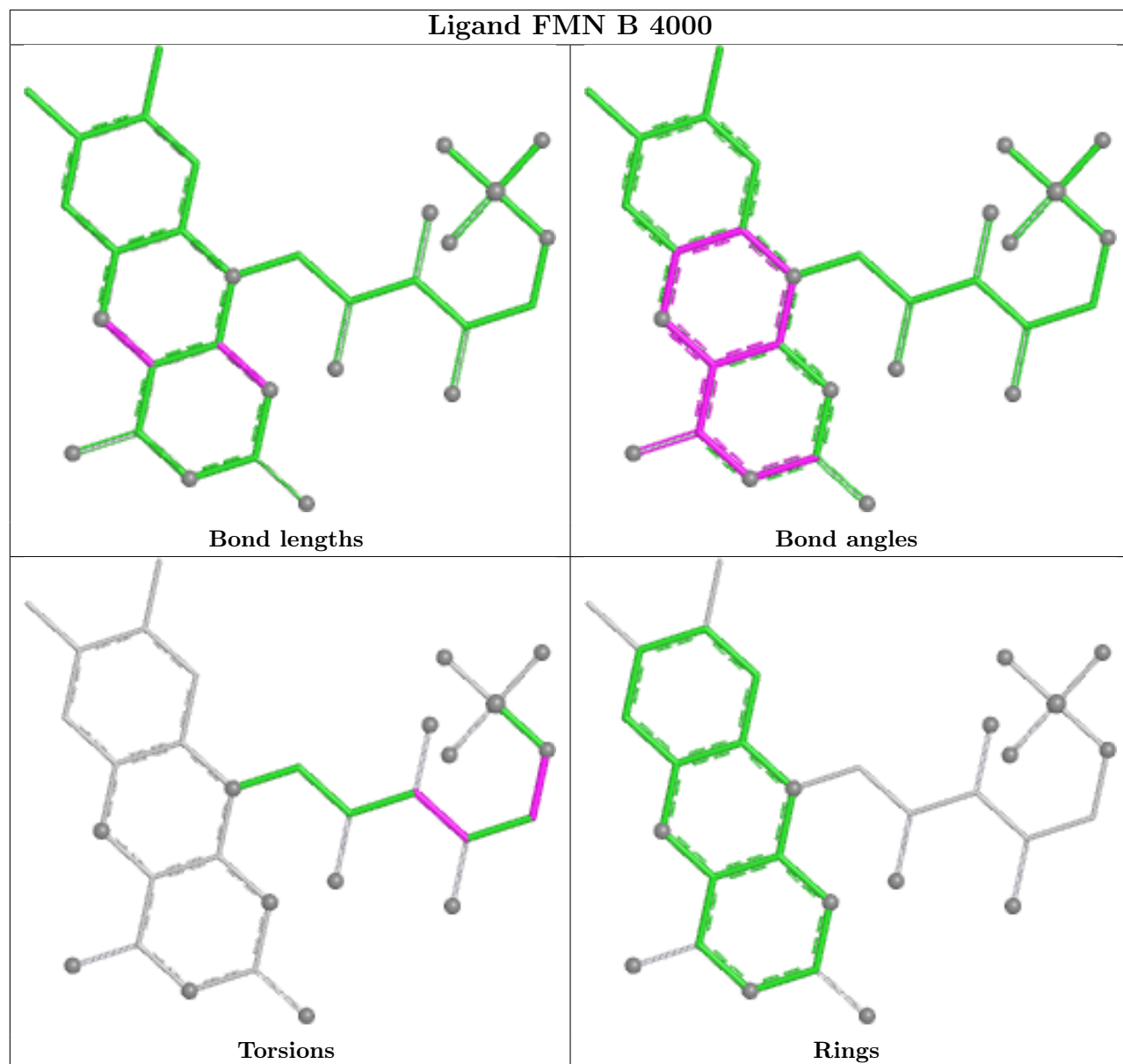
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

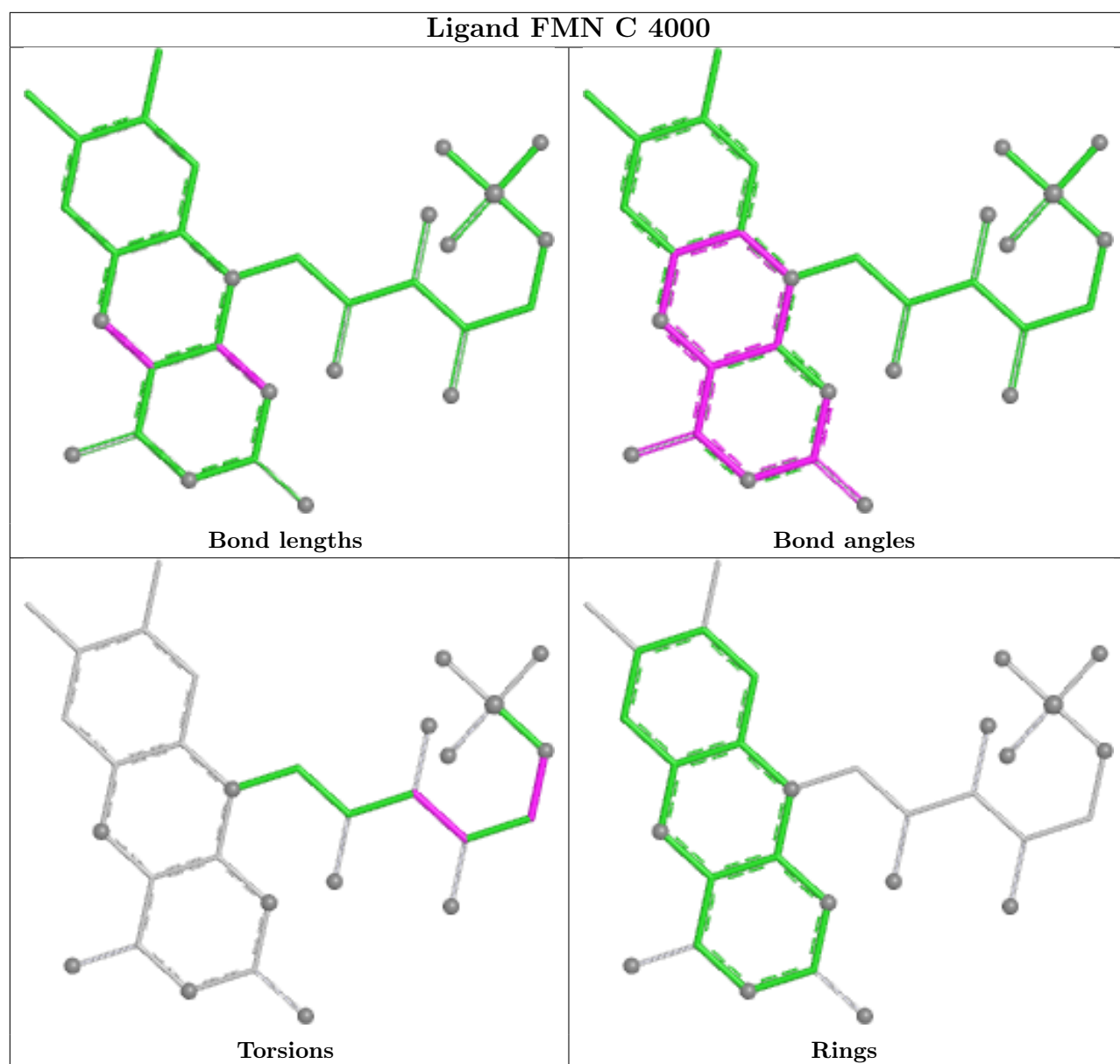












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

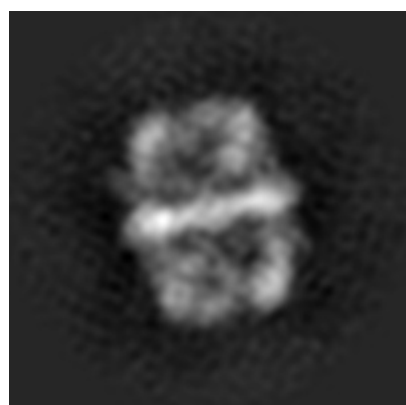
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2358. These allow visual inspection of the internal detail of the map and identification of artifacts.

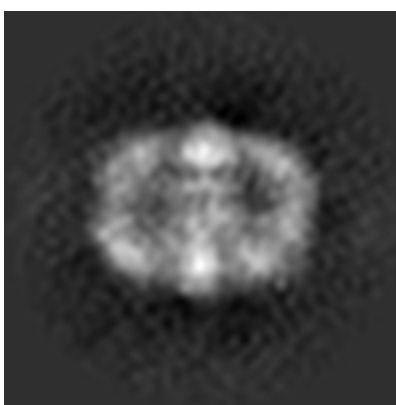
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

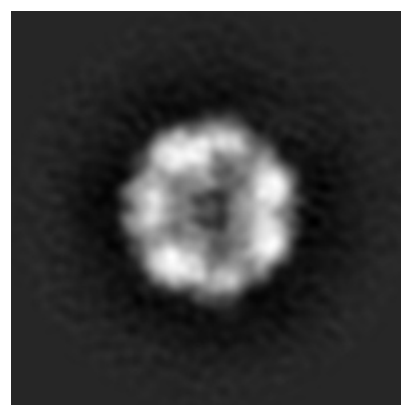
6.1.1 Primary map



X



Y

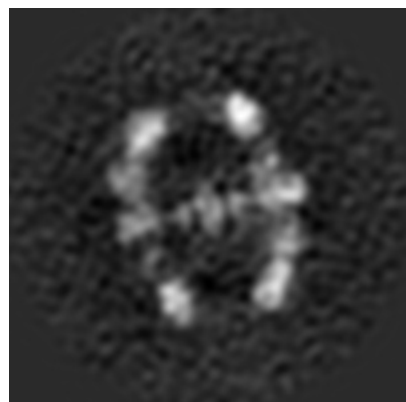


Z

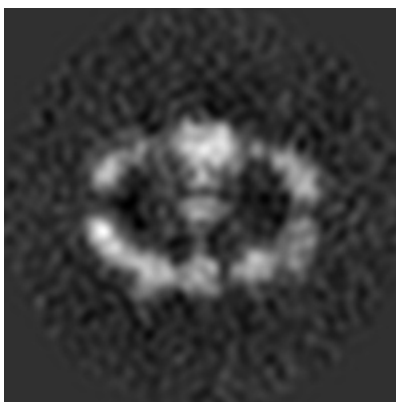
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

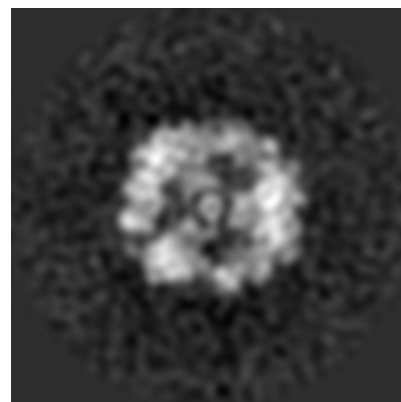
6.2.1 Primary map



X Index: 100



Y Index: 100

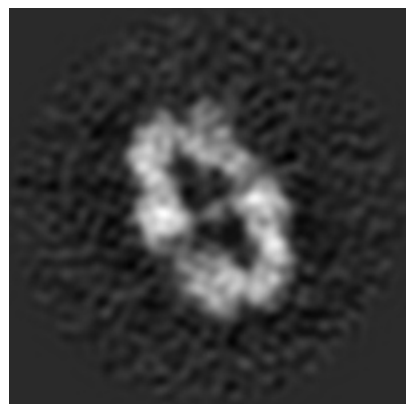


Z Index: 100

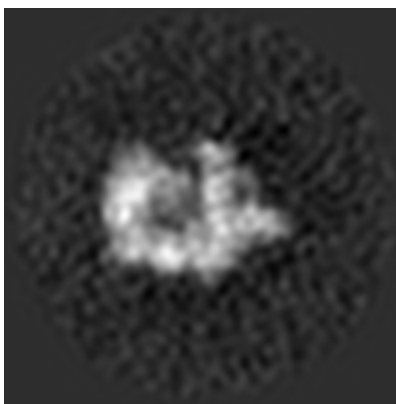
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

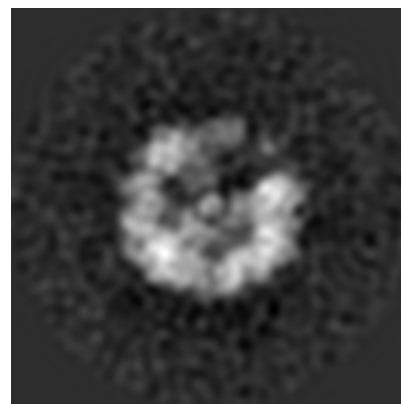
6.3.1 Primary map



X Index: 76



Y Index: 131

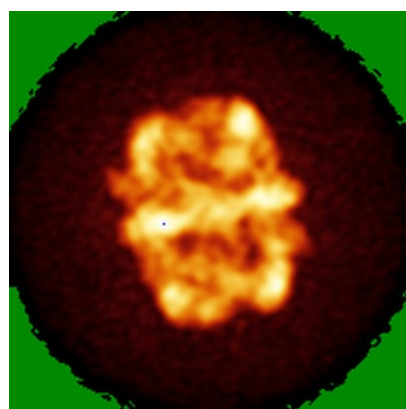


Z Index: 96

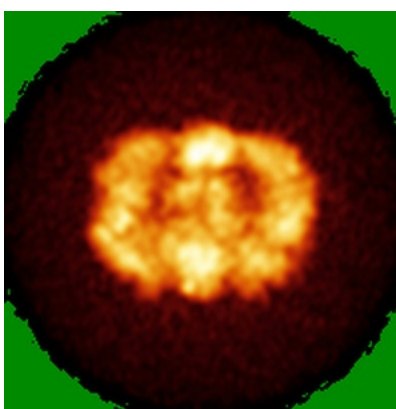
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

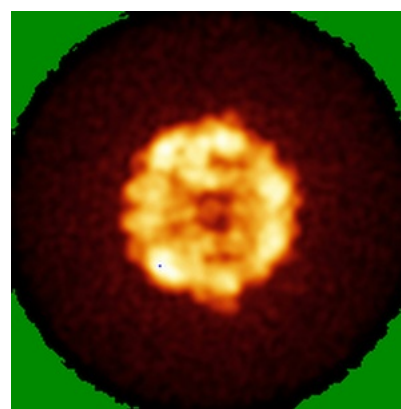
6.4.1 Primary map



X



Y

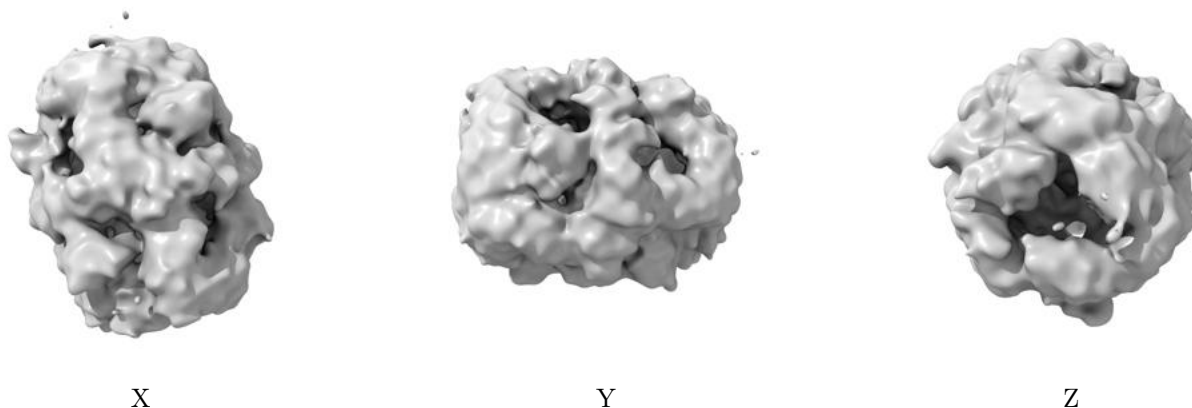


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

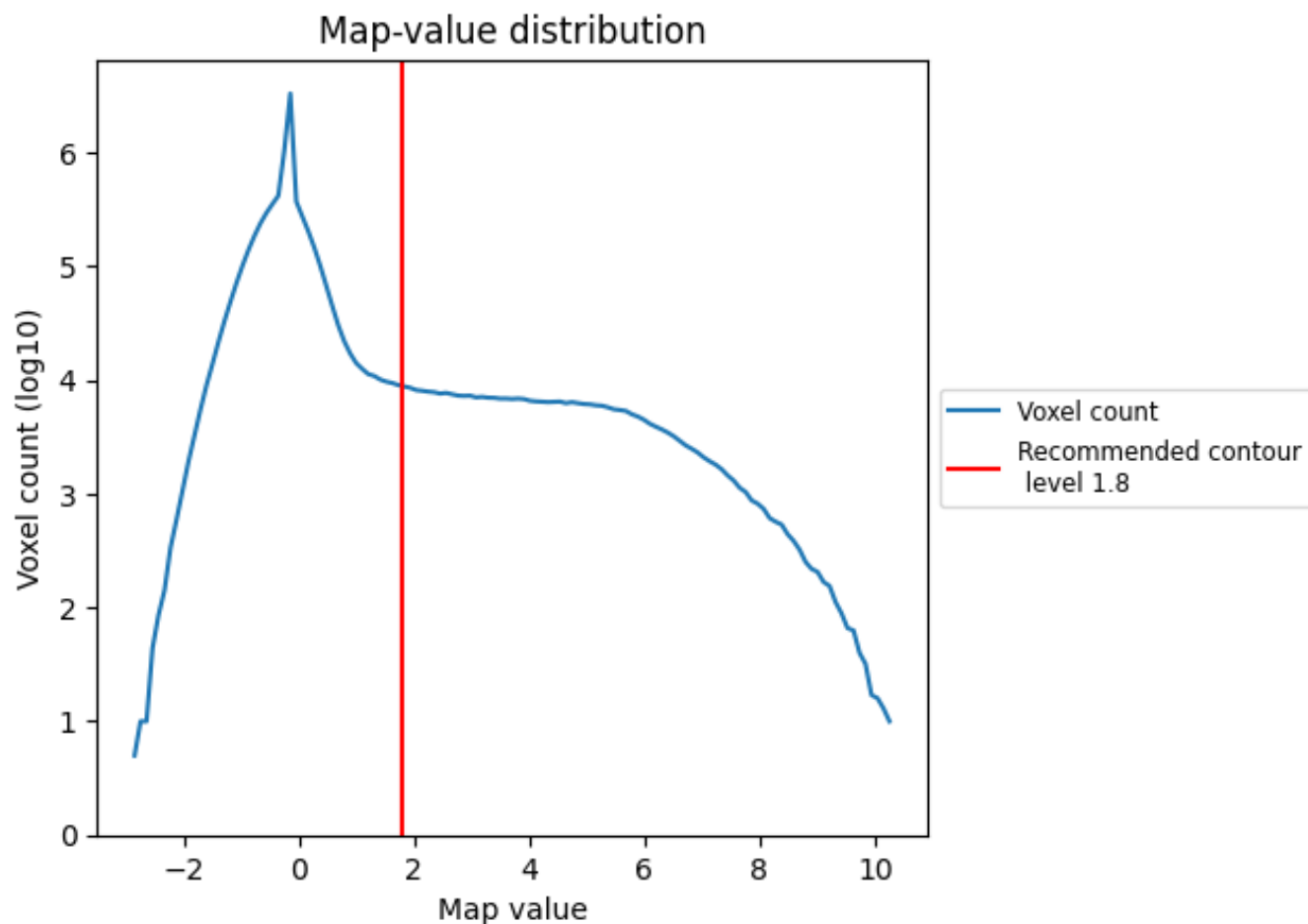
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

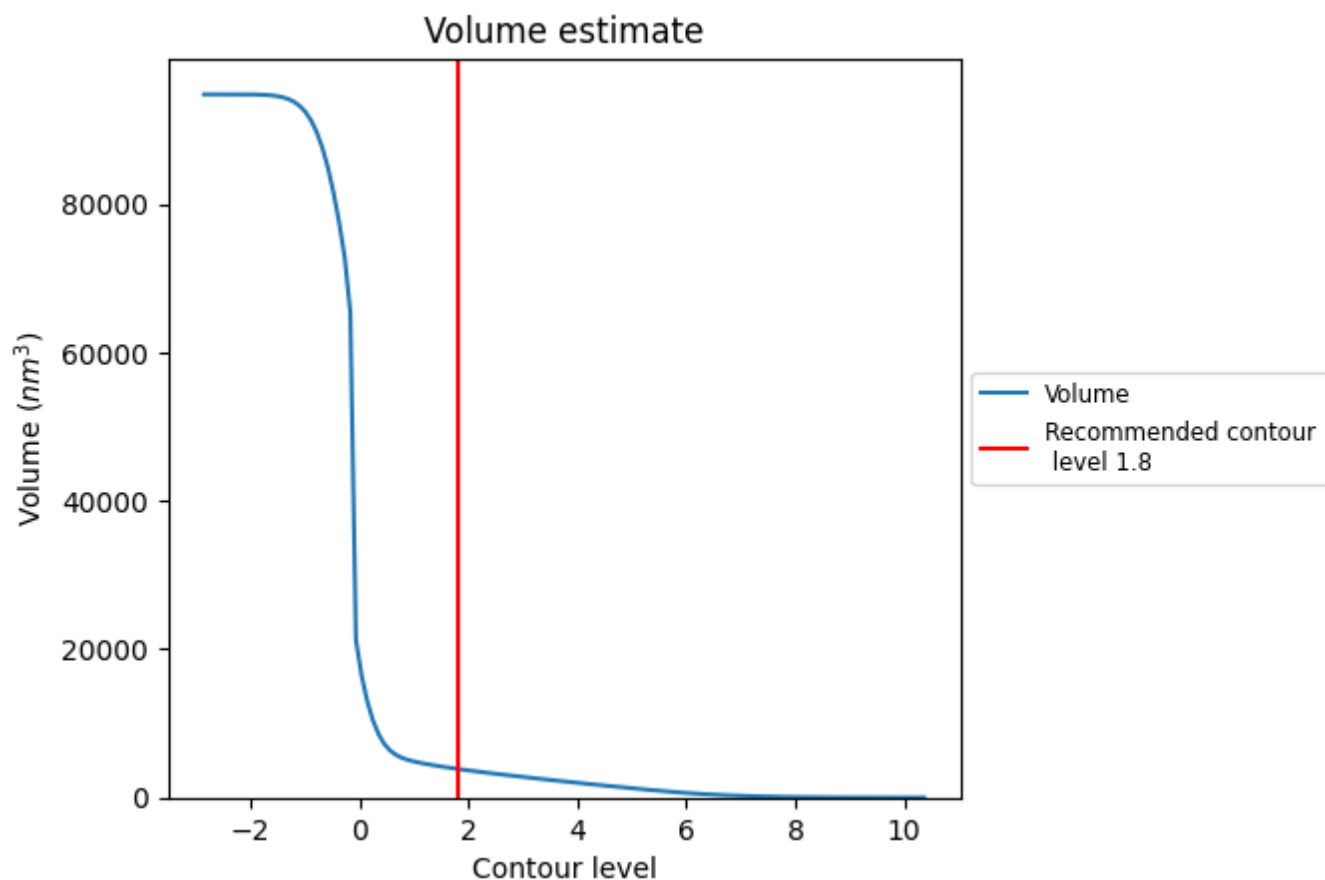
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

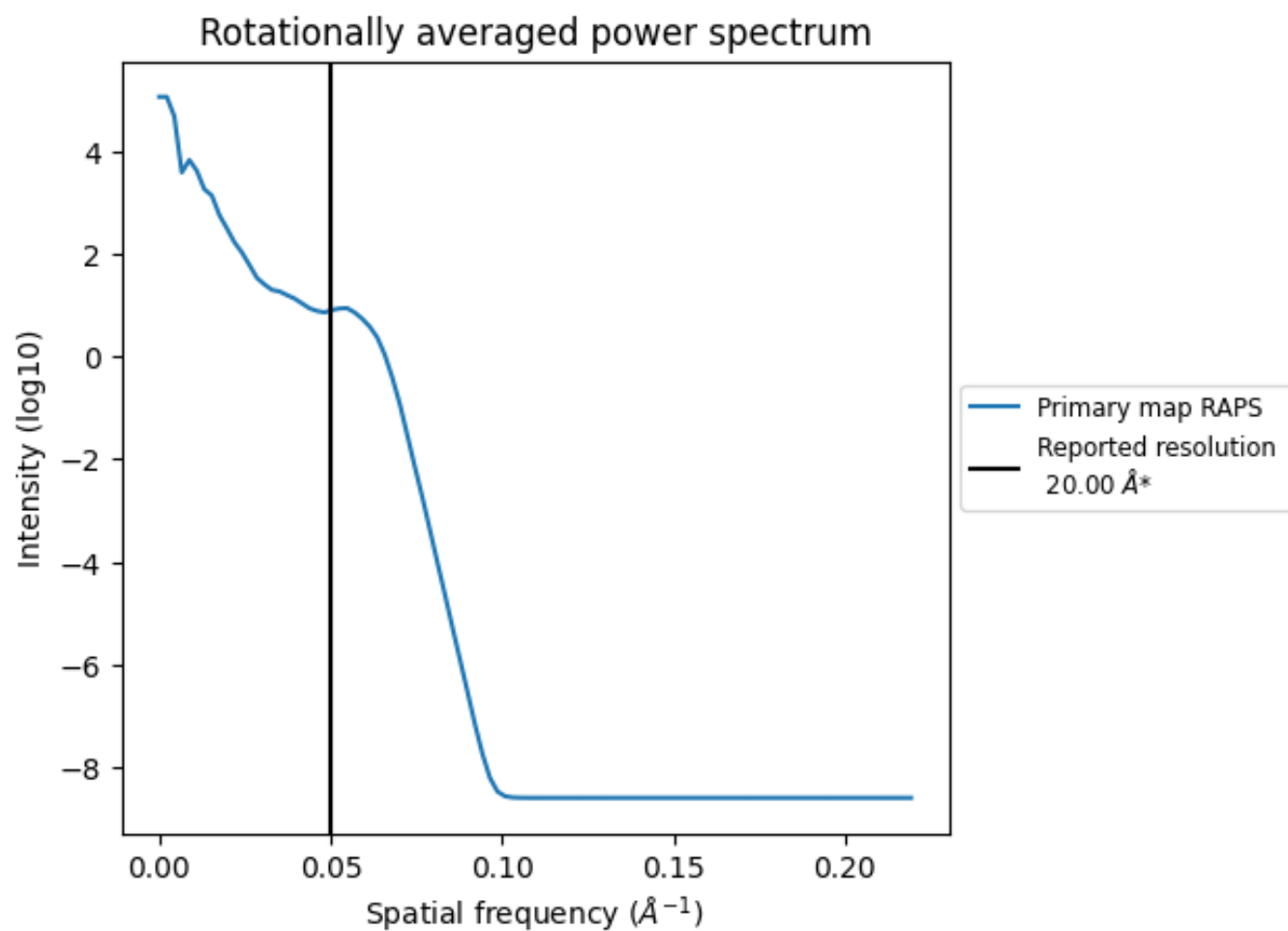
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3860 nm³; this corresponds to an approximate mass of 3487 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.050 Å⁻¹

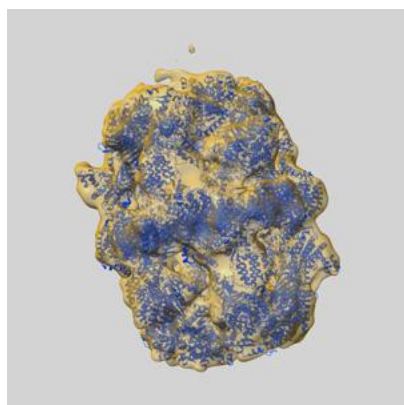
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

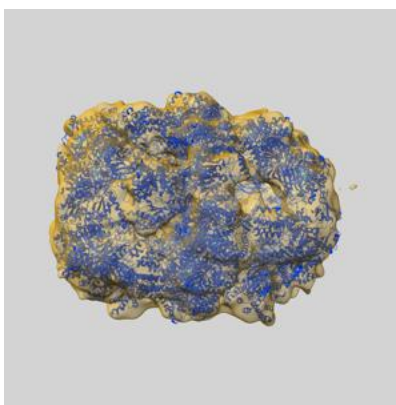
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2358 and PDB model 4V8V. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

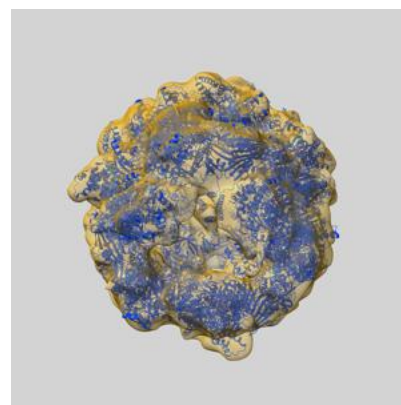
9.1 Map-model overlay [i](#)



X



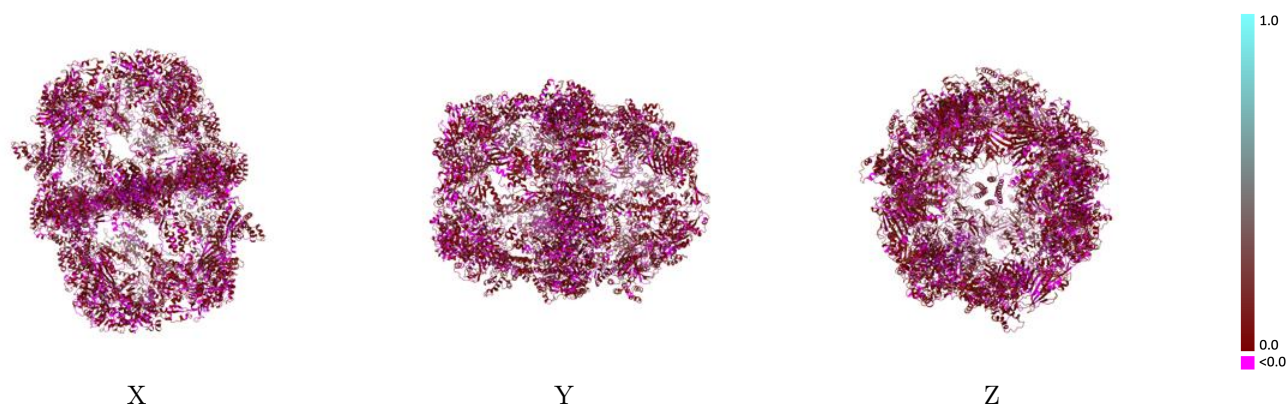
Y



Z

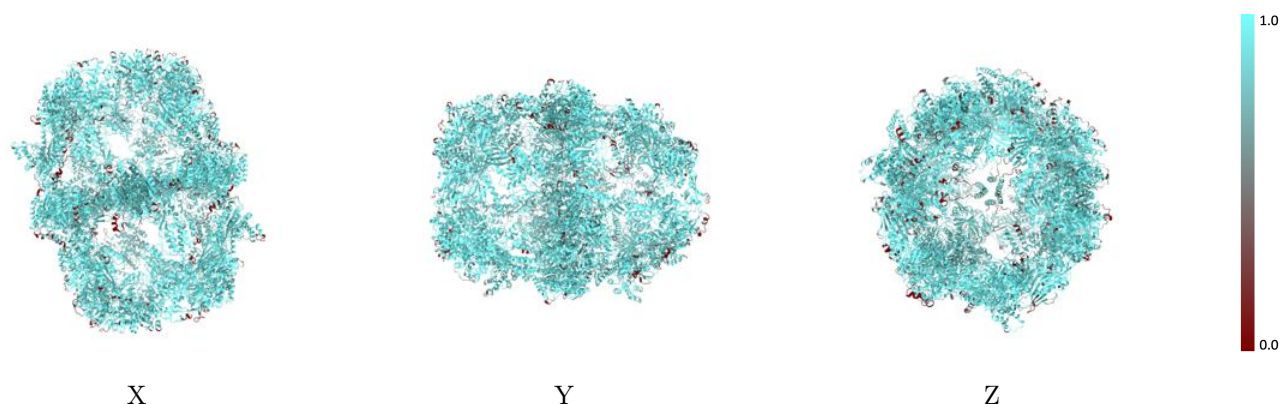
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



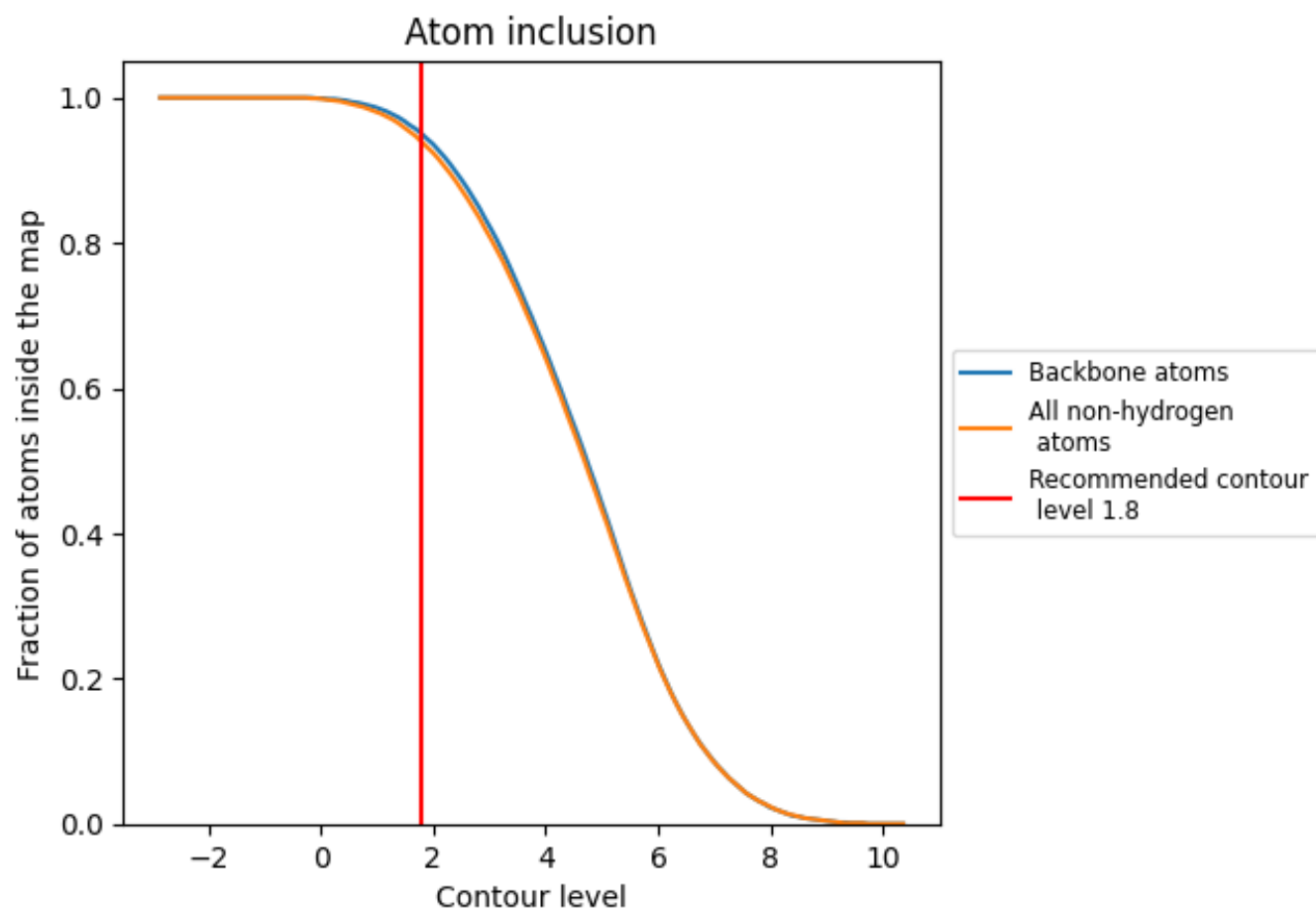
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.0500
A	0.9570	0.0520
B	0.9360	0.0450
C	0.9280	0.0440
D	0.9310	0.0490
E	0.9490	0.0560
F	0.9340	0.0520

