



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:36 PM UTC

PDB ID : 4V8W / pdb_00004v8w
EMDB ID : EMD-2357
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 : 17.50 Å(reported)
Based on initial model : 3ZEN

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

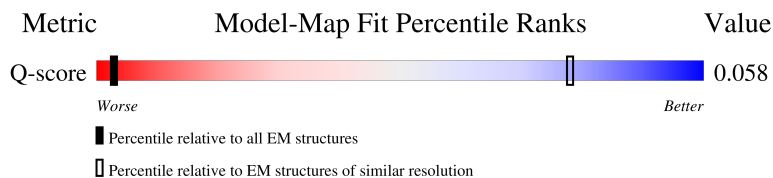
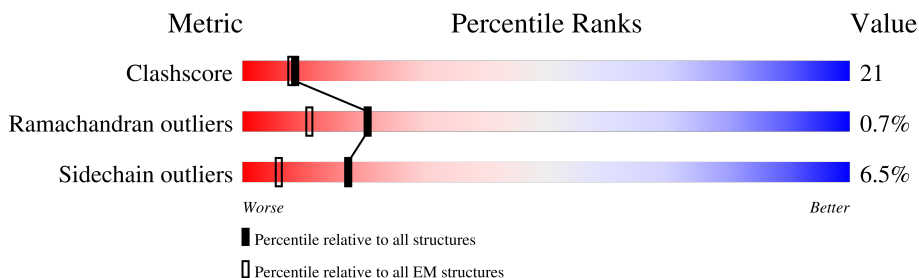
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.50 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	45 (17.00 - 18.00)

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	55% 32% 9%

2 Entry composition [i](#)

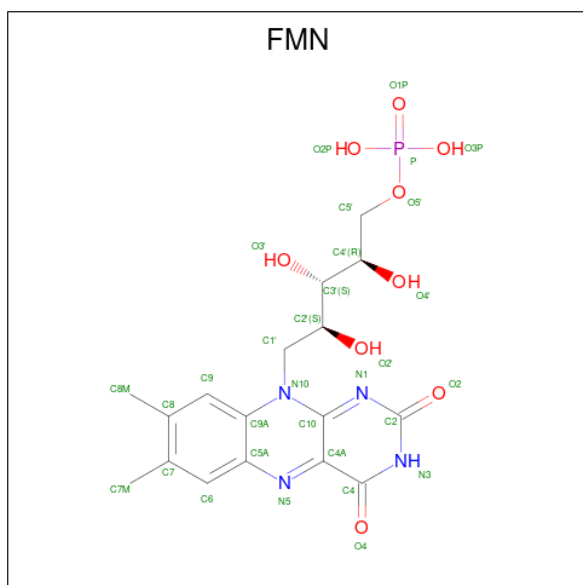
There are 2 unique types of molecules in this entry. The entry contains 123082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	D	2452	Total	C	N	O	S	0	0
			18171	11459	3176	3473	63		
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		
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		

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



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

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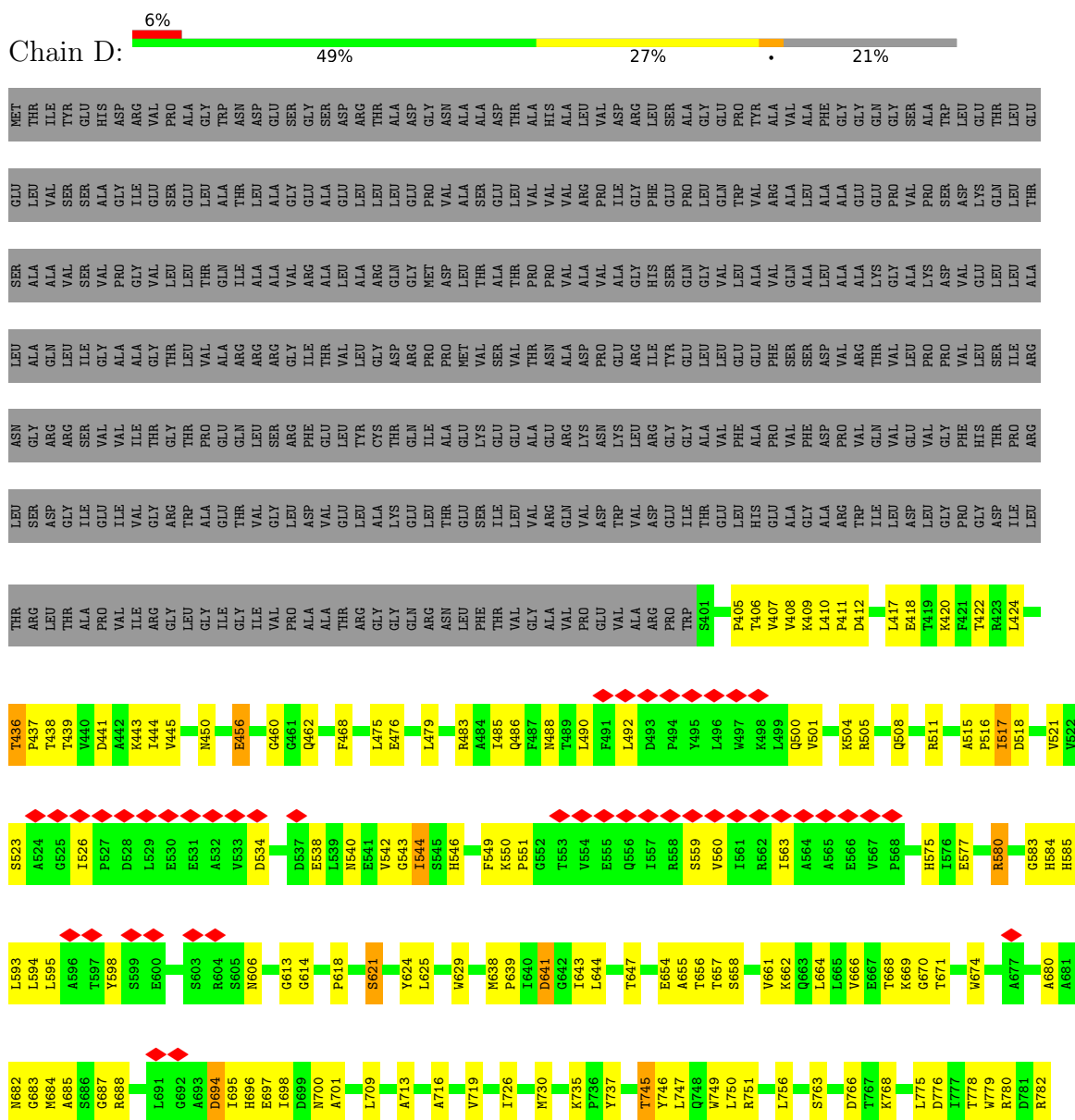
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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total 31	C 17	N 4	O 9	P 1	0
2	F	1	Total 31	C 17	N 4	O 9	P 1	0
2	A	1	Total 31	C 17	N 4	O 9	P 1	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0

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

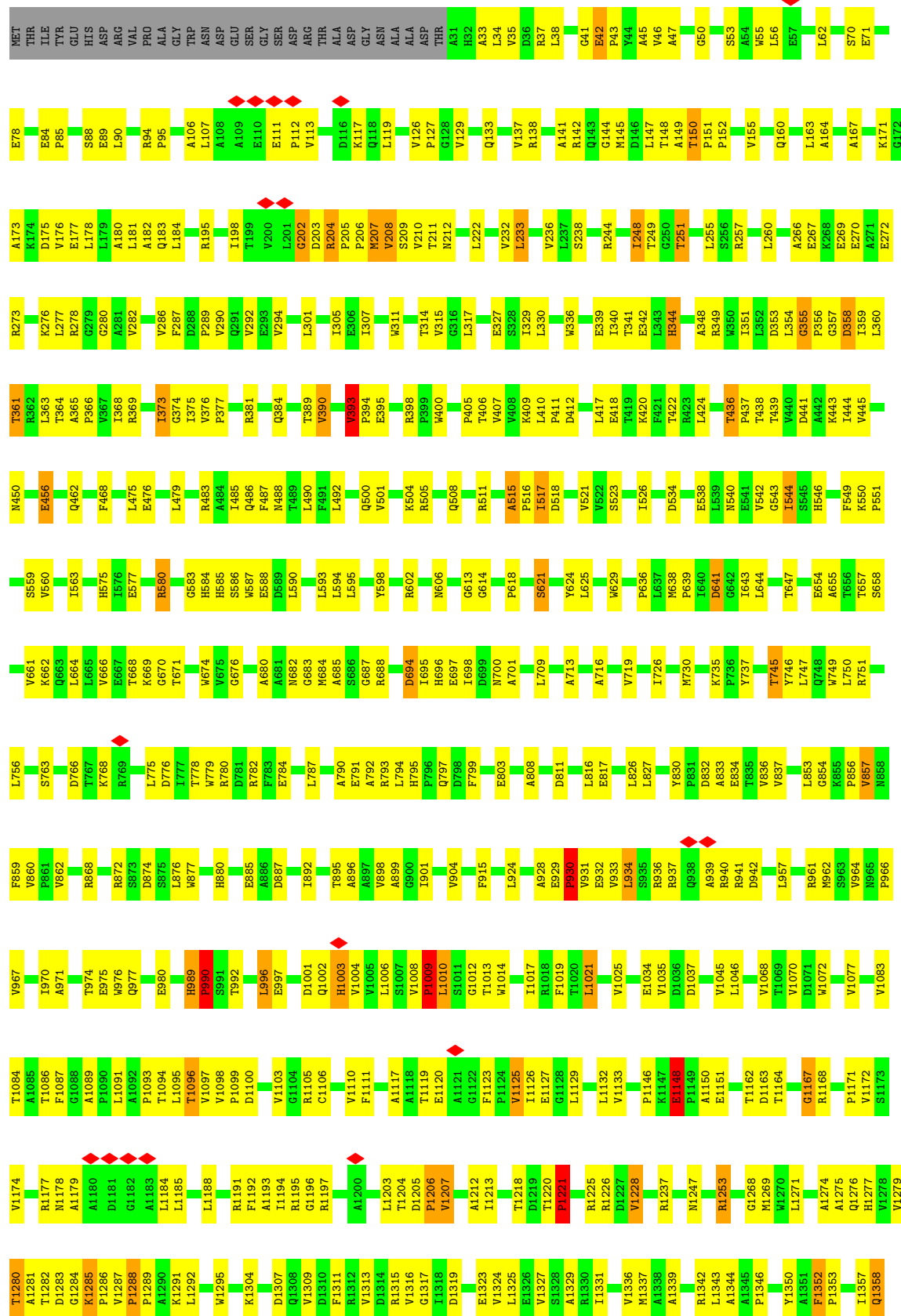




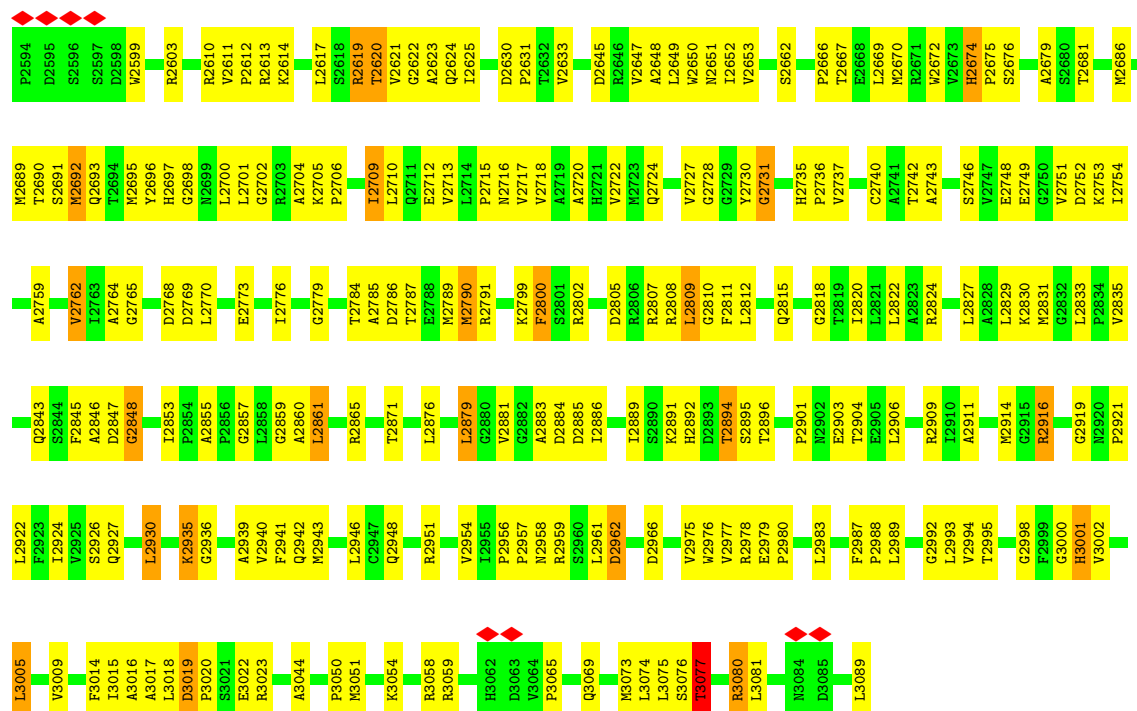
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G2882	A2883	D2884	D2885	L2886	L2889	S2890	K2891	L2892	D2893	L2894	L2895	T2896	P2901	L2902	E2903	T2904	F2905	L2906	R2909	T2910	A2911	M2914	G2915	R2916	G2919	N2920	P2921	L2922	F2923	T2924	V2925	S2926	Q2927	L2930	K2935	P2936	A2939	V2940	F2941	Q2942	M2943	L2946	C2947	Q2948	R2951	V2954	L2955	P2956			
K2799	F2800	S2801	R2802	D2805	R2806	R2807	L2808	L2809	G2810	F2811	L2812	Q2815	G2818	T2819	L2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	G2830	M2831	G2832	L2833	P2834	V2835	Q2843	S2844	F2845	A2846	D2847	G2848	L2853	P2854	A2855	G2856	L2857	V2858	F2859	A2860	L2861	R2865	T2871	L2876	L2879	G2880	V2881		
V2717	V2718	A2719	A2720	H2721	V2722	H2723	Q2724	V2727	G2728	G2729	V2730	G2731	H2735	P2736	V2737	C2740	A2741	T2742	A2743	S2746	V2747	E2748	E2749	G2750	V2751	D2752	K2753	L2754	A2759	V2762	L2763	A2764	G2765	D2768	D2769	L2770	E2773	L2776	G2779	T2784	A2785	D2786	T2787	F2788	M2789	M2790	R2791				
P2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	D2650	N2651	L2652	V2653	S2662	P2666	T2667	E2668	L2669	K2670	W2672	V2673	D2674	P2675	S2676	G2677	V2678	P2679	S2680	T2681	E2686	R2591	P2592	L2593	P2594	D2595	V2599	R2603	R2610	V2611	P2612	R2613	K2614	L2617	S2618	R2619	T2620	V2621	G2622	A2623	Q2624	L2625	D2630	
F2436	S2437	P2438	P2439	R2444	K2445	F2446	F2447	R2448	D2449	W2450	D2451	D2452	L2453	D2454	A2458	V2461	V2462	E2468	L2469	G2470	V2471	V2472	R2478	W2481	E2482	V2483	L2487	V2492	L2495	M2501	V2502	K2503	V2504	E2505	W2512	V2513	E2516	L2520	V2521	F2522	E2523	C2524	E2525	T2526	V2527	E2528					
Q2348	I2352	V2353	S2354	E2358	A2359	G2360	V2361	M2369	M2372	L2376	V2379	E2380	K2391	V2392	D2393	T2394	T2395	L2398	G2399	D2400	L2401	K2402	L2403	M2405	L2408	A2409	A2412	M2416	S2417	G2418	A2419	A2420	D2421	E2422	S2423	D2424	D2425	E2426	A2427	P2428	T2431	R2432	A2434	L2435							
P2234	T2235	L2236	F2238	R2244	V2245	A2246	V2252	R2255	K2261	W2265	Q2268	R2269	L2270	L2274	L2277	D2282	R2286	L2287	H2288	L2291	S2294	N2295	N2296	G2298	M2299	F2300	D2303	K2310	S2311	R2319	K2324	S2331	L2332	A2333	H2334	L2337	G2338	W2339													
H2115	L2118	I2122	A2123	A2124	G2125	A2126	E2127	N2128	F2129	G2130	K2131	E2137	V2140	V2141	V2164	A2165	A2166	T2167	R2170	D2173	D2174	R2175	L2176	K2180	R2188	F2189	T2192	L2193	W2194	V2195	P2197	A2198	N2199	M2200	D2205	L2209	V2210	E2211	W2212	V2213	G2214	T2215	E2216	K2229							
T2019	P2020	E2021	A2022	A2023	T2024	D2025	V2032	T2047	A2053	V2054	F2055	F2056	D2057	D2058	W2060	L2067	L2070	E2074	L2078	D2079	A2080	Q2081	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094	V2095	A2097	T2098	Q2099	A2100	N2101	W2102	W2103	Q2104	G2105	L2108	R2112	W2113	V2114				
ASP	LYS	VAL	ILE	ASP	GLY	ALA	VAL	ALA	ALA	ALA	ARG	ARG	GLY	ILE	SER	VAL	SER	LEU	PRO	SER	ALA	GLY	GLY	ALA	SER	GLY	VAL	VAL	ASP	S1983	A1984	L1985	L1986	F1989	K1992	P1996	L2000	R2005	L2006	V2007	L2008	W2009	Q2010	L2011	G2012	L2013	S2014	D2015	V2016	W2017	T2018

• Molecule 1: TYPE-I FATTY ACID SYNTHASE

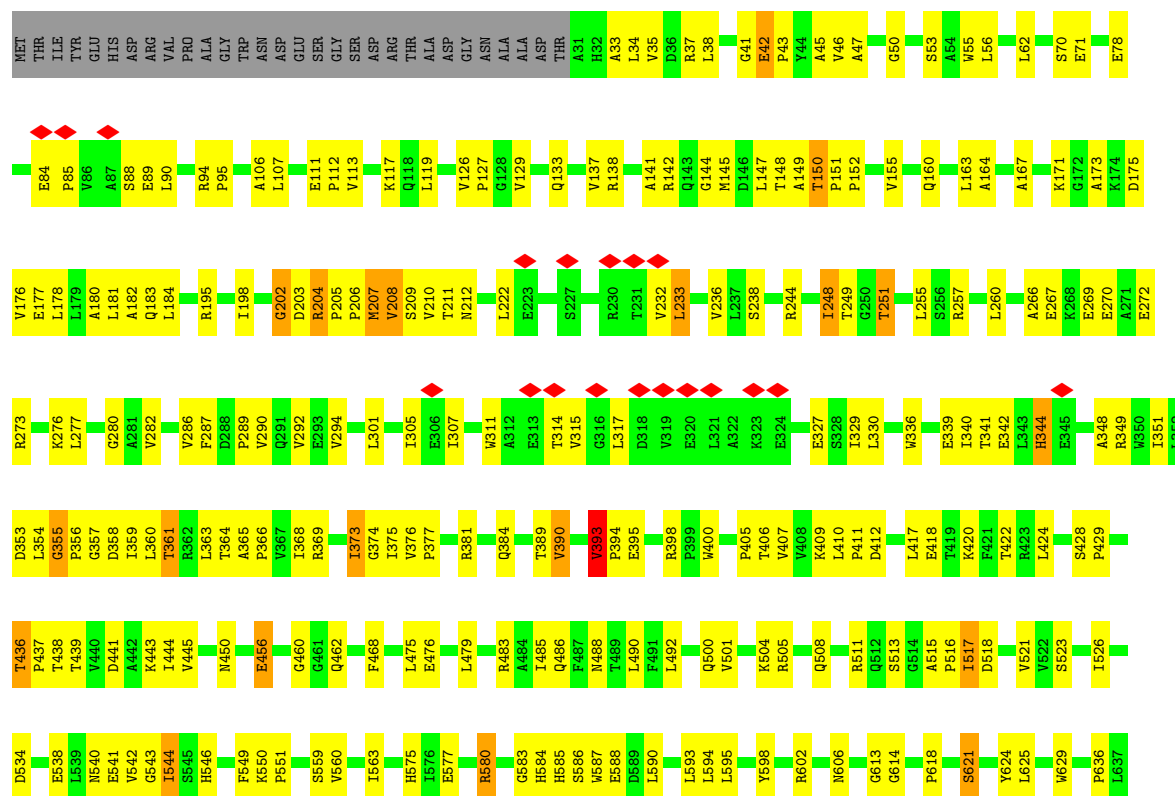
Chain E:  56% 32% 9%







• Molecule 1: TYPE-I FATTY ACID SYNTHASE





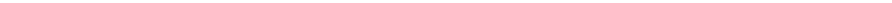
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GLY	SER	SER	VAL	ARG	GLY	GLY	ASP	LEU	GLY	GLY	ASP	LEU	HIS	ALA	ALA	LEU	ALA	ALA	ALA	ASP	VAL	ASP	LYS	VAL	ILE	ASP	GLY	ALA	VAL	SER	VAL	THR	ALA	SER	GLY	GLY	VAL	GLY	VAL	ASP	ASP	GLY	THR	ARG	GLU							
F1989	K1992	F1996	L2000	V2007	L2008	W2009	Q2010	G2012	L2013	S2014	D2015	V2016	V2017	T2018	T2019	P2020	E2021	A2022	A2023	T2024	D2025	V2032	T2047	A2053	V2054	V2055	F2056	W2060	V2164	L2067	L2070	E2074	T2078	Q2081	Q2084	L2085	S2086	Q2087	R2088	F2089	E2090	G2091	T2092	G2093	H2094							
V2095	A2097	T2098	Q2099	A2100	W2101	W2102	W2103	Q2105	L2108	R2112	N2113	L2114	H2115	L2118	I2122	A2123	G2125	A2126	E2127	N2128	P2129	Y2134	E2137	V2140	V2141	S2145	S2148	T2163	V2164	I2165	A2166	T2167	R2170	D2173	D2174	R2175	L2176	K2180	R2188	F2189	T2192											
L2193	W2194	V2195	W2196	F2197	A2198	W2199	W2200	D2205	L2209	W2210	E2211	W2212	W2213	T2215	E2216	K2229	P2234	T2235	L2236	L2237	F2238	R2244	V2245	A2246	G2247	D2248	V2252	R2255	K2261	W2265	Q2268	R2269	L2270	L2274	I2277	D2282	R2286	L2287	H2288	L2291	S2294	P2295										
N2296	R2297	G2298	M2299	F2300	D2303	K2310	S2311	R2319	S2331	L2332	A2333	H2334	L2337	G2338	W2339	M2346	G2347	Q2348	N2349	I2352	V2353	S2354	E2358	A2361	M2369	M2372	L2376	K2391	V2392	D2393	L2394	T2395	L2398	T2401	K2402	I2403	D2404	M2405	A2406	A2407	L2408	A2409	A2410	K2411								
A2412	M2416	S2417	Q2418	D2421	E2422	S2423	D2424	D2425	E2426	A2427	D2428	A2429	T2431	L2432	R2433	A2434	L2435	P2436	D2437	P2438	P2439	P2444	A2445	A2447	D2448	E2449	W2450	D2451	D2452	L2453	D2454	A2458	V2461	V2462	L2469	G2470	P2471	Y2472	R2478	M2481	D2482	V2483	L2487	V2492	L2495							
W2501	V2502	K2503	S2504	E2505	W2512	W2513	D2514	T2515	L2520	W2521	P2522	E2523	C2524	V2527	D2528	R2541	E2542	F2543	T2549	D2550	P2551	V2552	W2553	A2554	L2557	L2558	L2563	F2567	F2580	W2581	Q2582	F2583	D2584	P2585	E2586	R2591	P2592	L2593	P2594	D2595	S2596	D2597	D2598	W2599	R2603							
R2610	V2611	P2612	R2613	K2614	L2617	S2618	R2619	T2620	W2621	Q2622	A2623	Q2624	L2625	D2630	T2632	W2645	V2647	A2648	L2649	W2650	N2651	L2652	V2653	S2662	P2666	T2667	E2668	L2669	M2670	R2671	W2672	H2673	H2674	P2675	S2676	A2679	S2680	T2681	M2686	T2690	S2691	M2692	Q2693	T2694	M2695	H2696	D2697	G2698				
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L2770	E2773	I2776	G2779	T2784	A2785	D2786	T2787	E2788	M2789	M2790	R2791	K2799	F2800	S2801	R2802	D2805	R2806	R2807	R2808	L2809	G2810	F2811	L2812	Q2815	G2818	T2819	L2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	K2830	M2831	G2832	L2833	P2834	V2835	Q2843	S2844	F2845	A2846	D2847	G2848	I2853	P2854				
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G2936	A2939	V2940	F2941	Q2942	M2943	L2946	G2947	Q2948	R2951	V2954	I2955	P2956	P2957	N2958	R2959	S2960	L2961	D2962	D2965	V2975	W2976	V2977	R2978	E2979	P2980	L2983	F2987	P2988	L2989	G2992	L2993	V2994	T2995	G2998	F2999	G3000	H3001	V3002	L3005	V3009	F3014	I3015	A3016	A3017	L3018	D3019						
P3020	S3021	R3022	R3023	A3044	P3050	M3051	K3054	D3057	R3058	R3059	H3062	D3063	V3064	P3065	S2960	L2961	D2962	K3067	R3068	Q3069	A3072	K3073	L3074	L3075	S3076	T3077	R3080	L3081	N3084	D3085	L3089																					

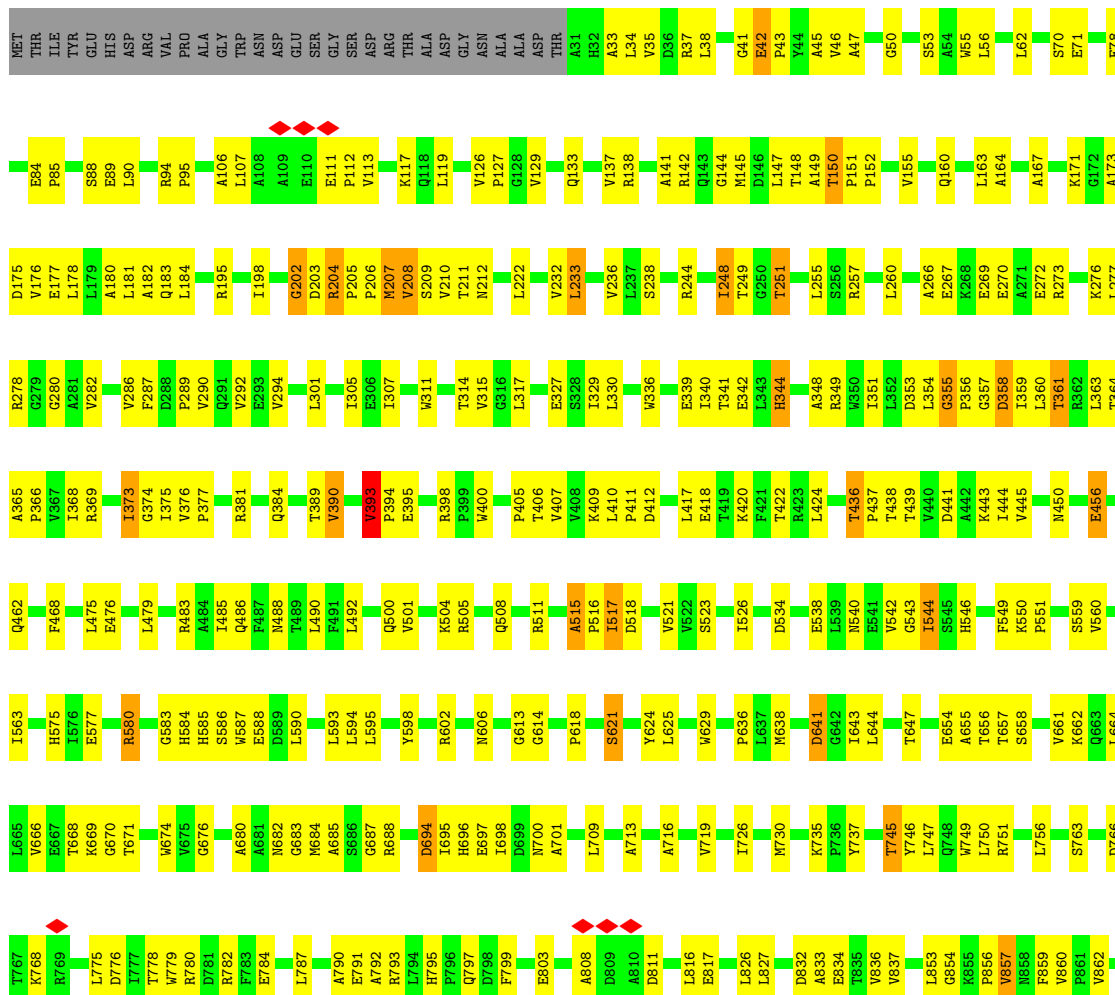
Chain A: 56% 32% 9%





- Molecule 1: TYPE-I FATTY ACID SYNTHASE

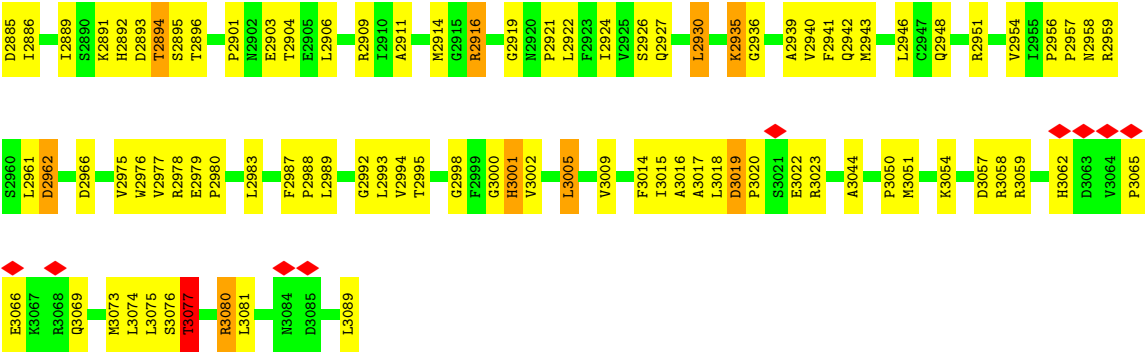
Chain B:  56% 31% 9%





V1445	L1530	A1448	A1339	R1342	L1343	A1344	A1345	P1346	V1350	A1351	A1460	F1352	P1353	V1455	G1456	E1457	F1458	T1459	A1460	L1461	A1462	C1463	V1464	V1467	Y1468	E1469	L1470	E1471	L1474	V1477	R1480	F1581	K1483	M1484	H1485	D1486	I1487	V1488	P1489	R1490	D1491	E1492	R1495	S1496	I1503	R1504	P1505	S1506	Q1507	I1508	D1511	D1514	V1519	E1524	L1525	T1526	G1527	M1337	A1338	A1339	R1342	L1343	A1344	A1345	M1247	P1248	R1253	G1268	M1269	I1270	L1271	A1274	A1275	Q1276	H1277	P1171	V1172	S1173	V1174	R1177	N1178	A1179	A1180	D1181	G1182	A1183	L1184	L1185	L1188	R1191	F1192	A1193	I1194	R1195	G1196	R1197	L1203	T1204	D1205	P1206	V1207	A1212	I1213	T1218	D1219	I1220	P1221	R1225	R1226	D1227	V1228	R1237	A939	R940	R941	D942	P954	L957	R961	N962	S963	V964	N965	P966	V967	I970	A971	T974	E975	N976	Q977	E980	D983	H984	H989	P990	S991	T992	L996	E997	D1001	Q1002	H1003	V1004	V1005	L1006	S1007	P1009	L1010	S1011	G1012	T1013	W1014	V931	E932	V933	L934	S935	R936	R937	Q938	V836	V837	L853	G854	K855	P856	V857	N858	F859	V860	P861	V862	R868	R872	S873	D874	S875	L876	W877	H880	E885	A886	D887	T895	A896	V898	A899	G900	I901	V904	F915	D921	L924	G925	A926	G927	A928	E929	P930	V931	E932	V933	T1020	L1021	S935	R936	R937	Q938	T745	Y746	L747	Q748	W749	L750	R751	L756	S763	D766	T767	K768	R769	P770	L775	D776	T777	W778	V779	R780	D781	R782	F783	G784	L787	A790	E791	A792	R793	L794	H795	P796	Q797	F799	E803	A808	D809	A810	D811	L816	E817	L826	L827	D832	A833	E834	T835	L644	T647	E654	K655	L656	T657	S658	V661	K662	G663	L664	L665	V666	E667	T668	K669	G670	T671	W674	V675	G676	A680	A681	N682	G683	M684	A685	S686	R688	D684	I695	H696	I698	N700	A701	L709	A713	A716	V719	T726	M730	K735	G642	A833	P736	Y737	E541	V542	I544	H546	F549	K550	P551	S559	V560	I563	H575	I576	E577	R580	G583	H584	H585	S586	W587	E588	N488	L590	L593	L594	L595	Y598	R602	N606	G613	G614	P618	S621	Y624	L625	W629	P636	L637	M638	D641	G642	I643	D383	L384	G385	P386	D387	L389	V390	R398	W399	W400	P405	T406	V407	V408	K409	L410	P411	D412	L417	E418	T419	K420	F421	E342	T422	L343	H344	A348	R349	V350	I351	L352	E270	A271	R272	R273	K276	L277	R278	G279	G280	A281	V282	V286	D287	D288	P289	V290	Q291	E292	E293	V294	L301	I305	E306	I307	W311	A312	E313	T314	V315	G316	L317	D318	V319	E320	L321	E327	S328	I329	L330	W336	E339	I340	T341	E342	L343	H344	A348	R349	V350	I351	L352
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R2802	H2721	H2846	I2549	V2353	W2249	Y2134	D2067	ALA	ARG	GLU	ALA	A1712	P1622
D2550	V2722	V2847	D2550	S2354	S2250	Y2134	D2068	ALA	VAL	LEU	VAL	G1713	F1623
P2551	M2723	A2848	P2551	E2358	E2251	E2137	W2060	ARG	THR	ASN	THR	L1714	T1624
H2553	Q2724	L2849	H2553	E2358	E2252	E2137	W2060	ARG	GLY	LEU	GLY	L1719	L1625
A2554	V2727	W2850	A2554	V2361	R2255	V2140	L2067	ILE	THR	ALA	PRO	K1726	F1629
S2555	R2807	N2851	S2555	W2369	W2260	V2141	L2070	SER	ARG	ILE	ARG	L1721	I1633
L2557	C2728	I2852	L2557	M2372	K2261	T2163	E2074	SER	PRO	ASP	PRO	P1722	R1634
L2558	G2729	V2853	L2558	M2372	K2261	V2164	E2074	PRO	ALA	ALA	ILE	Y1724	V1637
L2563	G2731	S2862	L2563	A2458	W2265	I2165	L2078	SER	THR	GLU	THR	H1726	P1638
F2567	H2735	T2665	F2567	V2461	Q2268	T2167	D2079	ALA	ALA	ASP	PHE	A1639	A1639
E2574	P2736	P2666	E2574	V2462	R2269	A2080	D2079	GLY	LYS	ASP	ALA	E1730	D1650
A2575	V2737	T2667	A2575	K2391	L2270	R2170	Q2081	GLY	HIS	LEU	ALA	V1731	T1651
F2580	C2740	E2668	F2580	D2392	L2274	D2173	Q2081	ALA	VAL	GLY	ALA	L1732	D1652
V2581	L2741	L2669	V2581	D2393	L2277	L2175	Q2081	SER	THR	ALA	ASP	N1733	N1733
Q2582	T2742	M2670	Q2582	T2395	L2277	R2176	Q2081	GLY	VAL	LEU	THR	S1734	S1734
F2583	A2743	R2672	F2583	L2398	R2286	K2180	Q2081	VAL	GLY	GLN	VAL	E1735	E1735
P2585	K2744	G2673	P2585	I2401	H2288	F2188	Q2081	ASP	THR	LEU	ALA	D1737	K1656
E2586	A2745	S2680	E2586	K2402	H2288	F2188	Q2081	ASP	THR	LEU	ALA	L1741	P1657
P2592	S2746	T2681	P2592	I2403	L2291	R2189	Q2081	ASP	THR	LEU	ALA	L1741	K1658
L2593	E2747	P2675	L2593	D2404	L2291	R2189	Q2081	ASP	THR	LEU	ALA	L1741	E1659
P2594	P2748	S2676	P2594	M2405	S2294	T2192	Q2081	ASP	THR	LEU	ALA	D1745	K1661
S2596	V2749	S2676	S2596	L2408	P2295	L2193	Q2081	ASP	THR	LEU	ALA	D1745	R1662
S2597	E2750	F2583	S2597	A2409	N2296	V2194	Q2081	ASP	THR	LEU	ALA	THR	I1666
D2598	A2751	D2584	D2598	A2412	R2297	V2195	Q2081	ASP	THR	LEU	ALA	GLU	E1667
W2599	G2752	P2685	W2599	A2412	W2298	V2196	Q2081	ASP	THR	LEU	ALA	GLU	L1668
R2603	K2753	T2686	R2603	M2416	F2300	P2197	Q2081	ASP	THR	LEU	ALA	GLU	W1671
R2610	A2754	G2687	R2610	S2417	D2303	M2200	Q2081	ASP	THR	LEU	ALA	GLU	Q1672
V2611	P2755	L2689	V2611	G2418	K2310	W2200	Q2081	ASP	THR	LEU	ALA	GLU	F1673
P2612	E2756	P2522	P2612	A2419	S2311	D2205	Q2081	ASP	THR	LEU	ALA	GLU	A1674
R2613	G2757	E2523	R2613	A2420	R2319	L2209	Q2081	ASP	THR	LEU	ALA	GLU	W1679
K2614	E2758	C2524	K2614	D2421	R2319	V2210	Q2081	ASP	THR	LEU	ALA	GLU	D1684
L2617	A2759	E2525	L2617	E2422	K2324	E2211	Q2081	ASP	THR	LEU	ALA	GLU	L1685
S2618	P2760	E2525	S2618	S2423	E2328	V2212	Q2081	ASP	THR	LEU	ALA	GLU	L1686
R2619	L2709	T2526	R2619	D2424	E2328	G2214	Q2081	ASP	THR	LEU	ALA	GLU	F1687
V2621	G2761	V2527	V2621	D2425	S2331	T2215	Q2081	ASP	THR	LEU	ALA	GLU	E1690
A2622	E2762	V2527	A2622	E2426	L2332	E2216	Q2081	ASP	THR	LEU	ALA	GLU	G1694
Q2624	V2713	R2528	Q2624	E2427	H2333	E2216	Q2081	ASP	THR	LEU	ALA	GLU	L1695
L2625	L2714	W2530	L2625	A2427	H2334	K2229	Q2081	ASP	THR	LEU	ALA	GLU	L1695
P2630	P2715	A2533	P2630	P2428	E2334	P2234	Q2081	ASP	THR	LEU	ALA	GLU	R1699
D2631	N2716	T2631	D2631	T2431	T2337	T2235	Q2081	ASP	THR	LEU	ALA	GLU	F1700
P2632	V2717	S2632	P2632	I2432	G2338	L2236	Q2081	ASP	THR	LEU	ALA	GLU	V1701
V2633	W2718	R2541	V2633	R2433	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	E1702
D2645	A2719	F2543	D2645	A2434	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	I1703
				P2436	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	G1704
				S2437	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	V1705
				P2438	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	K1706
				P2439	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	S1707
				P2440	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1710
				P2441	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711
				P2442	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711
				P2443	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711
				P2444	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711
				P2445	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711
				P2446	W2339	L2237	Q2081	ASP	THR	LEU	ALA	GLU	T1711



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9136	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	9.063	Depositor
Minimum map value	-2.149	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	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 i

5.1 Standard geometry i

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	56/29037 (0.2%)
1	B	0.45	18/21335 (0.1%)	0.90	62/29037 (0.2%)
1	C	0.45	18/21335 (0.1%)	0.90	60/29037 (0.2%)
1	D	0.46	18/18511 (0.1%)	0.88	47/25179 (0.2%)
1	E	0.45	18/21335 (0.1%)	0.90	61/29037 (0.2%)
1	F	0.45	18/21335 (0.1%)	0.89	59/29037 (0.2%)
All	All	0.45	108/125186 (0.1%)	0.89	345/170364 (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	2
1	E	0	5
1	F	0	5
All	All	0	27

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1003	HIS	CB-CG	-5.84	1.42	1.50
1	D	2094	HIS	CB-CG	-5.82	1.42	1.50
1	B	989	HIS	CB-CG	-5.78	1.42	1.50
1	A	2094	HIS	CB-CG	-5.78	1.42	1.50
1	A	996	LEU	CB-CG	-5.77	1.42	1.53

The worst 5 of 345 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2438	PRO	N-CA-CB	13.70	110.86	103.19
1	B	2438	PRO	N-CA-CB	13.62	110.82	103.19
1	D	2438	PRO	N-CA-CB	13.55	110.78	103.19
1	E	2438	PRO	N-CA-CB	13.53	110.77	103.19
1	F	2438	PRO	N-CA-CB	13.50	110.75	103.19

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1148	GLU	Peptide
1	D	2584	ASP	Peptide
1	E	150	THR	Peptide
1	E	202	GLY	Peptide
1	E	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	915	0
1	B	20945	0	20595	907	0
1	C	20945	0	20595	938	0
1	D	18171	0	17756	796	0
1	E	20945	0	20595	917	0
1	F	20945	0	20594	1059	0
2	A	31	0	19	5	0
2	B	31	0	19	4	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	4	0
All	All	123082	0	120844	5181	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 5181 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:F:1039:ALA:HB2	1:F:1125:VAL:CG1	1.35	1.53
1:F:958:TRP:CH2	1:F:1131:SER:OG	1.76	1.38
1:F:1385:ARG:NH1	1:F:2411:LYS:NZ	1.74	1.36
1:F:953:ALA:CB	1:F:1032:ILE:HD11	1.58	1.33
1:F:1385:ARG:CD	1:F:2411:LYS:HZ3	1.44	1.30

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%)	2642 (94%)	157 (6%)	19 (1%)	18	56
1	B	2818/3089 (91%)	2642 (94%)	158 (6%)	18 (1%)	21	59
1	C	2818/3089 (91%)	2642 (94%)	157 (6%)	19 (1%)	18	56
1	D	2448/3089 (79%)	2293 (94%)	138 (6%)	17 (1%)	18	56
1	E	2818/3089 (91%)	2641 (94%)	159 (6%)	18 (1%)	21	59
1	F	2818/3089 (91%)	2630 (93%)	163 (6%)	25 (1%)	14	51
All	All	16538/18534 (89%)	15490 (94%)	932 (6%)	116 (1%)	20	56

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	930	PRO
1	D	1148	GLU
1	D	2428	PRO
1	D	2436	PRO
1	D	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	2096/2402 (87%)	1960 (94%)	136 (6%)	15	37
1	B	2096/2402 (87%)	1960 (94%)	136 (6%)	15	37
1	C	2095/2402 (87%)	1959 (94%)	136 (6%)	15	37
1	D	1808/2402 (75%)	1691 (94%)	117 (6%)	15	37
1	E	2097/2402 (87%)	1961 (94%)	136 (6%)	15	37
1	F	2097/2402 (87%)	1957 (93%)	140 (7%)	15	36
All	All	12289/14412 (85%)	11488 (94%)	801 (6%)	17	37

5 of 801 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1564	ILE
1	B	1083	VAL
1	C	3077	THR
1	A	2070	LEU
1	A	1551	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2296	ASN
1	C	2651	ASN
1	B	2815	GLN
1	C	1057	ASN
1	E	2973	HIS

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

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	D	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	F	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	A	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	E	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	3.74	1.38	1.30
2	A	4000	FMN	C4A-N5	3.70	1.38	1.30
2	E	4000	FMN	C4A-N5	3.69	1.38	1.30
2	D	4000	FMN	C4A-N5	3.67	1.38	1.30
2	F	4000	FMN	C4A-N5	3.66	1.38	1.30

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4000	FMN	C4-N3-C2	-3.14	120.06	125.64
2	E	4000	FMN	C4-N3-C2	-3.11	120.11	125.64
2	F	4000	FMN	C4-N3-C2	-3.10	120.13	125.64
2	D	4000	FMN	C4-N3-C2	-3.08	120.17	125.64
2	B	4000	FMN	C4-N3-C2	-3.08	120.17	125.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

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

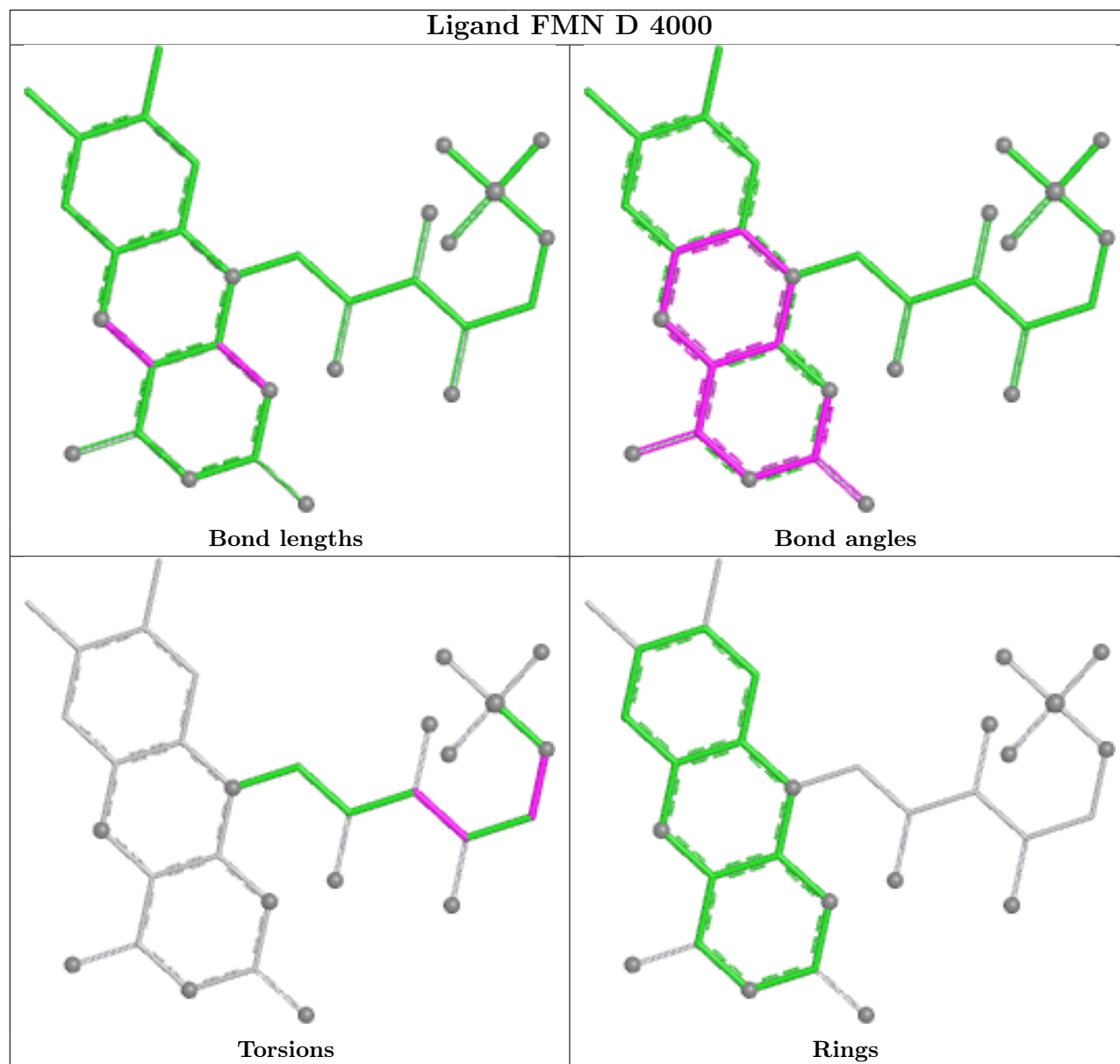
There are no ring outliers.

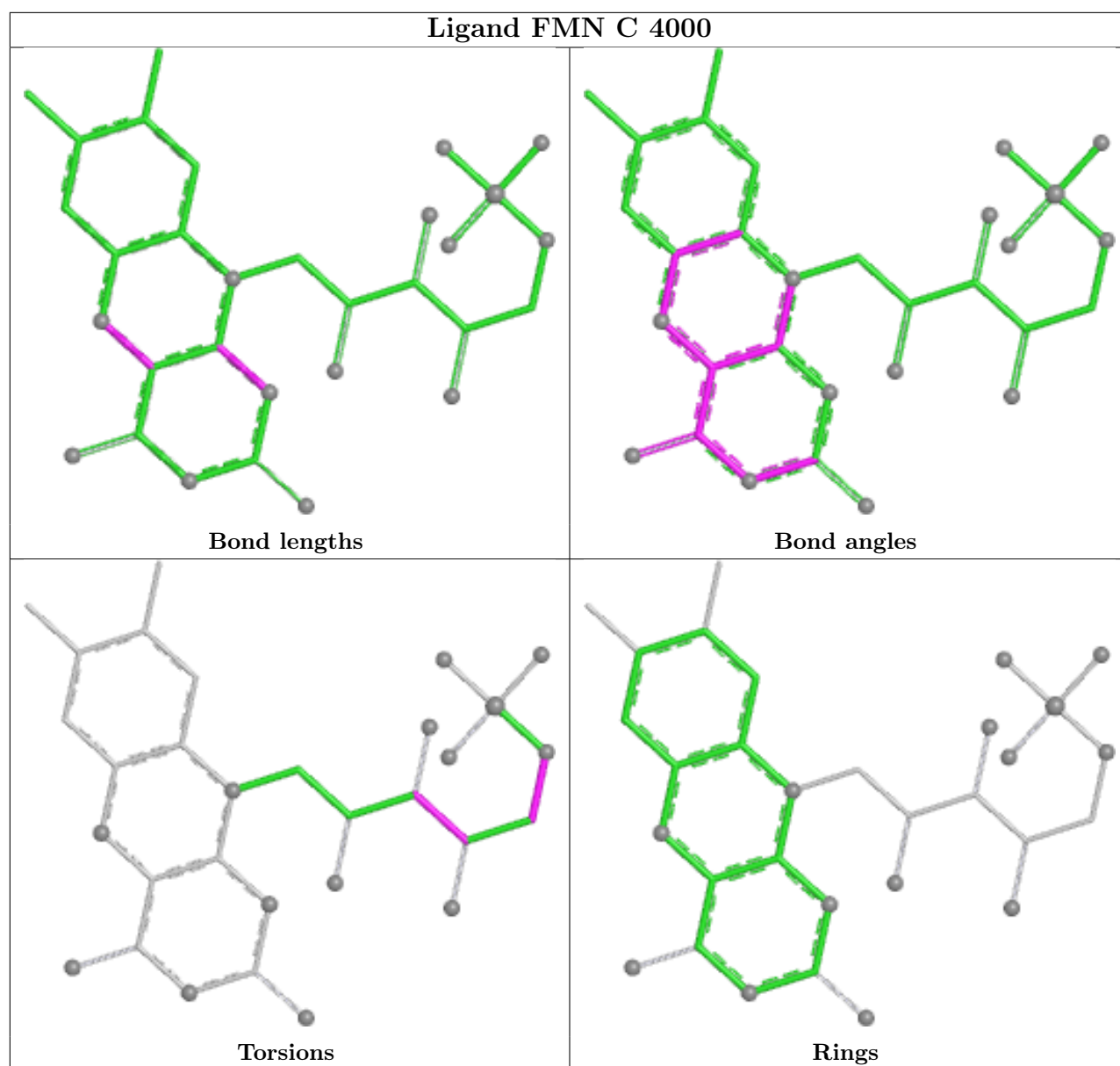
6 monomers are involved in 25 short contacts:

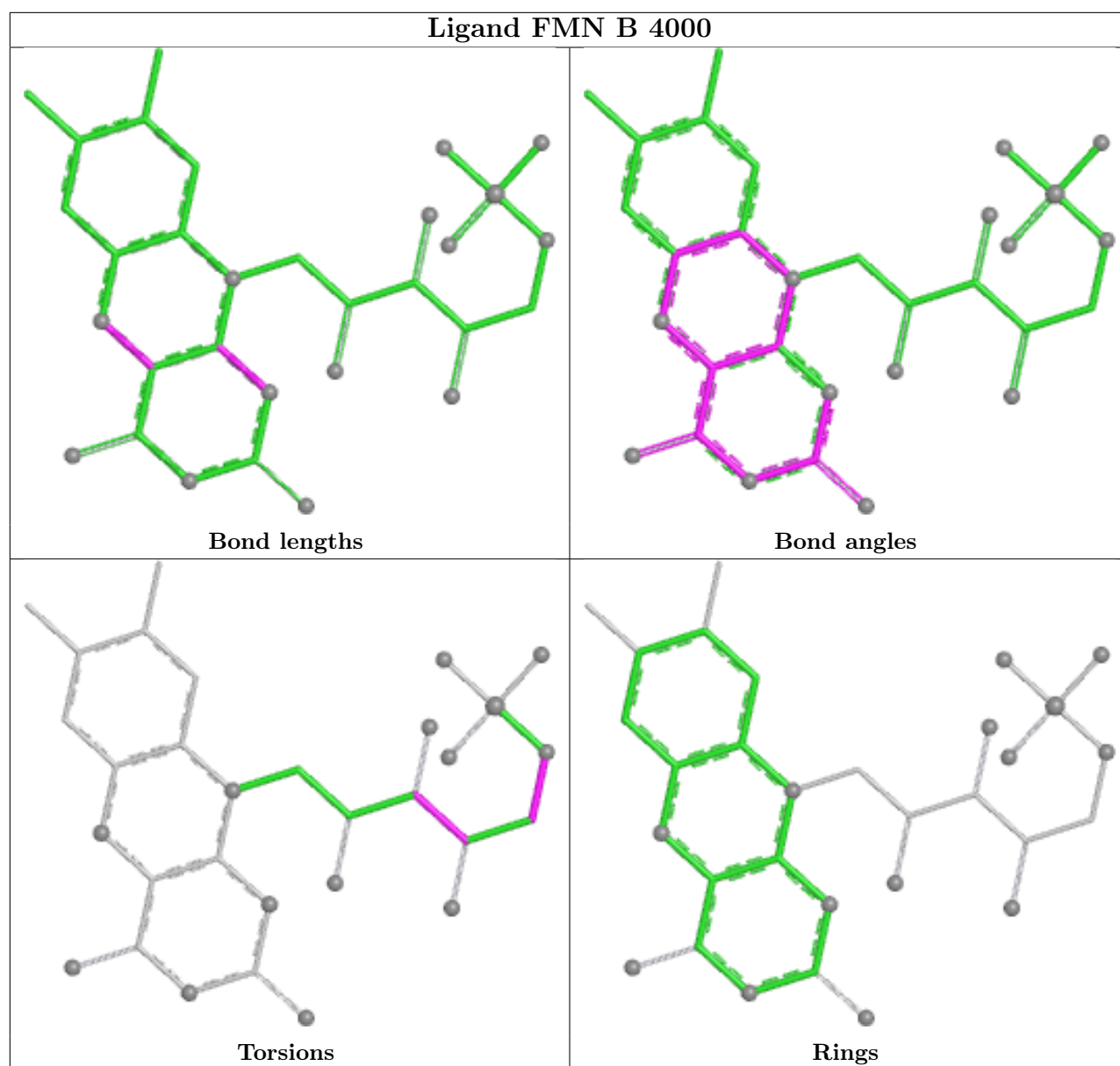
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4000	FMN	4	0
2	C	4000	FMN	4	0
2	B	4000	FMN	4	0
2	F	4000	FMN	4	0
2	A	4000	FMN	5	0
2	E	4000	FMN	4	0

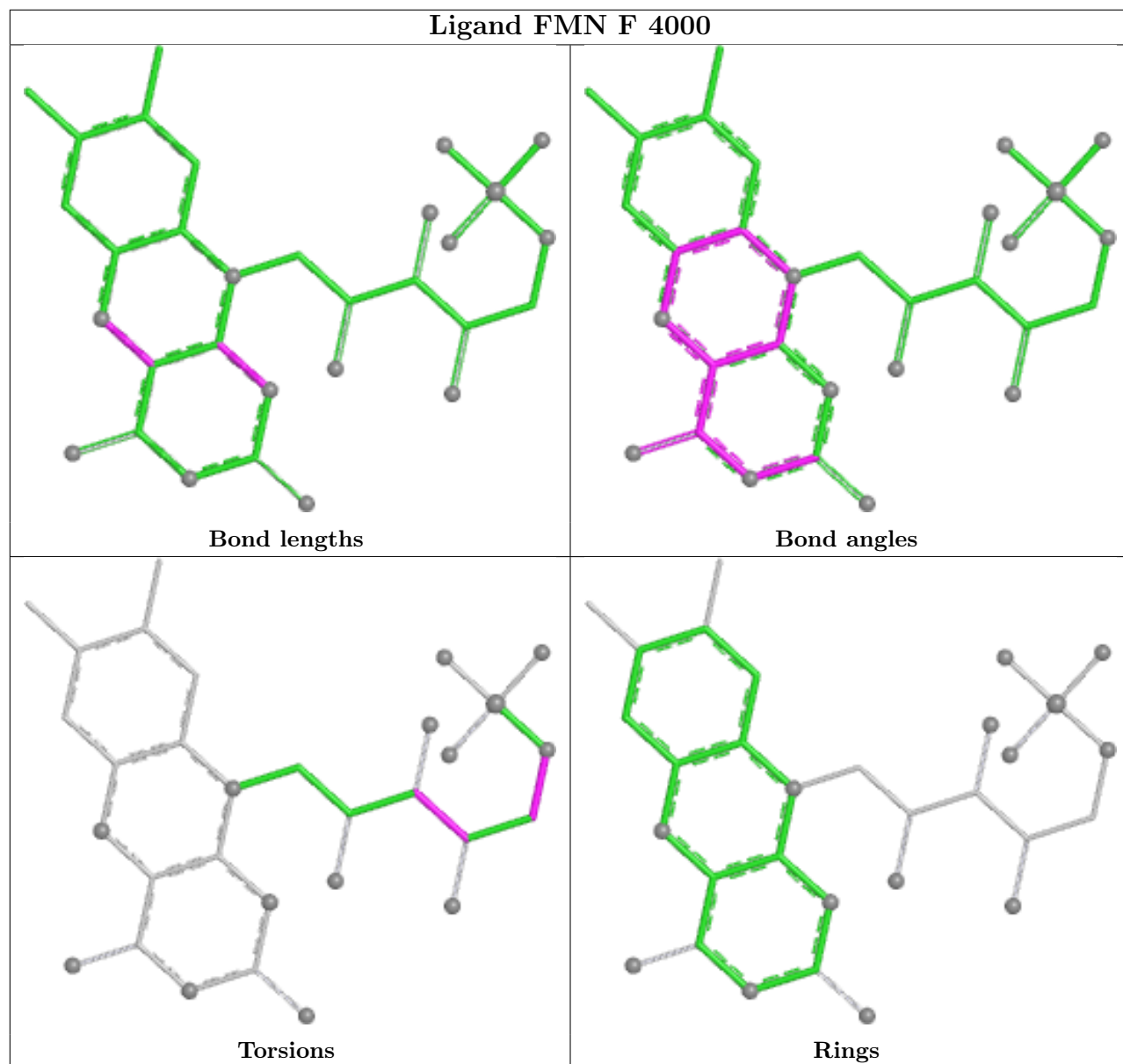
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

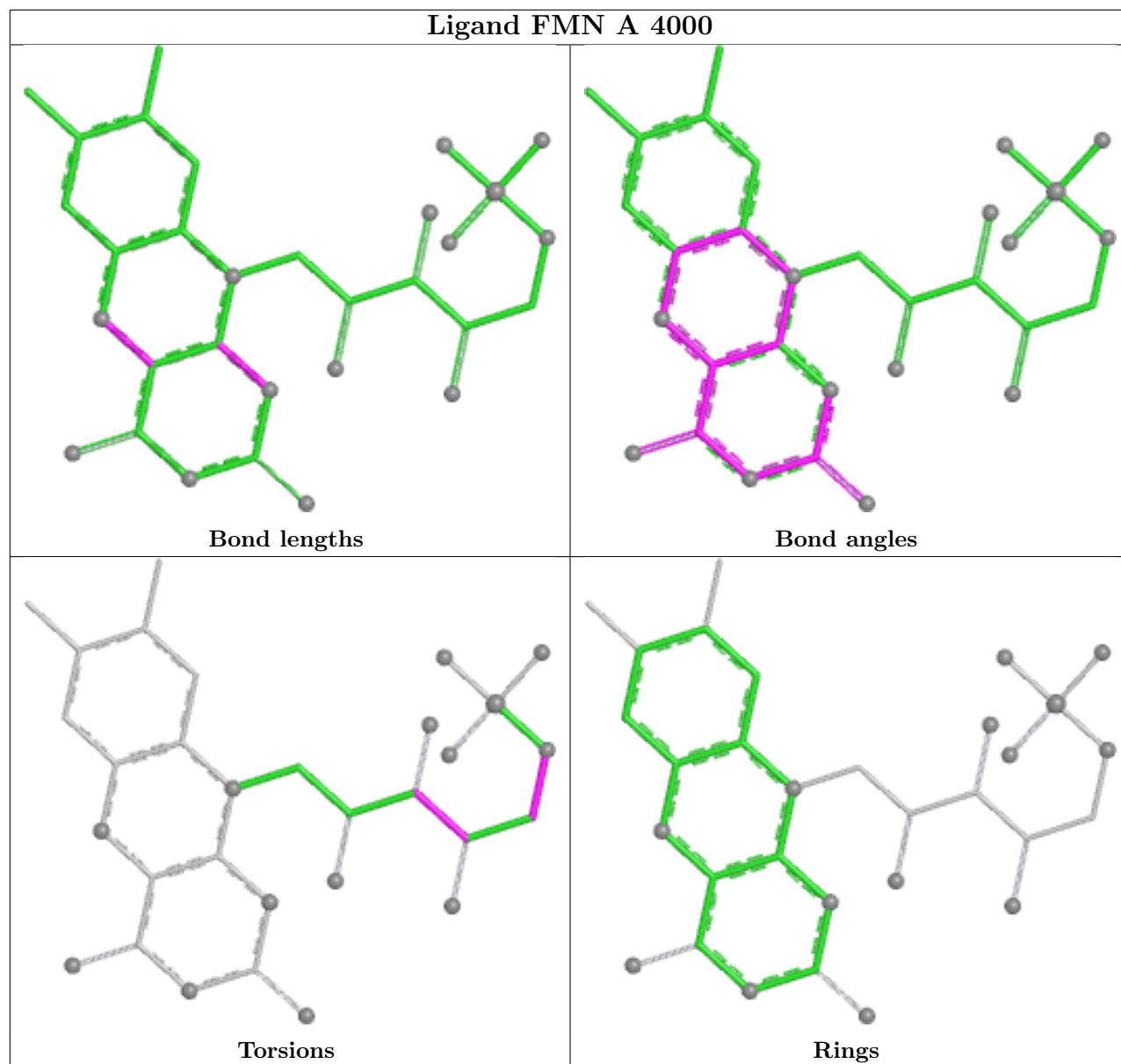
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

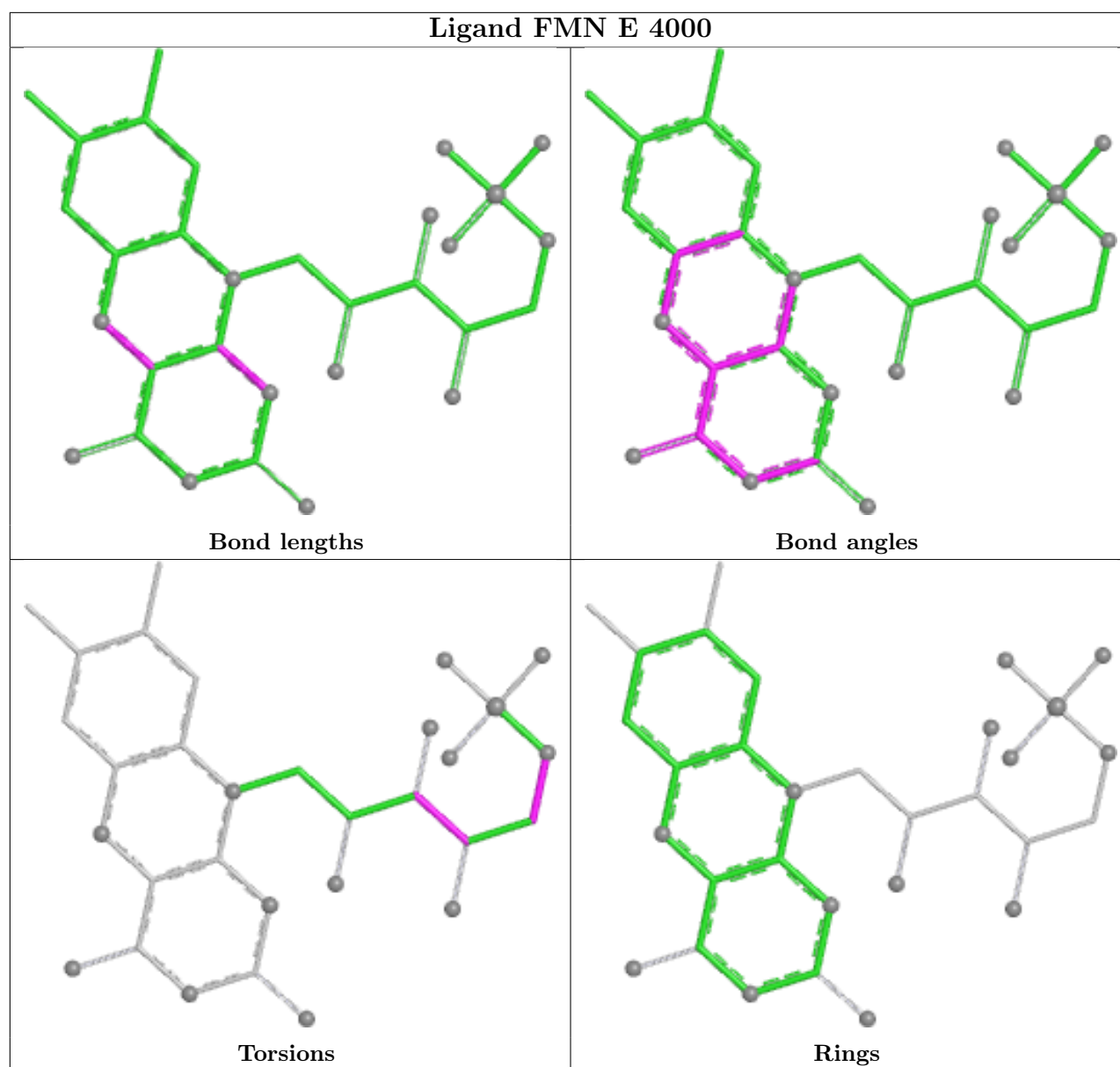












5.7 Other polymers [i](#)

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-2357. These allow visual inspection of the internal detail of the map and identification of artifacts.

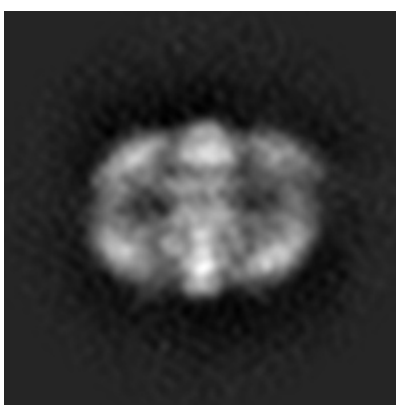
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

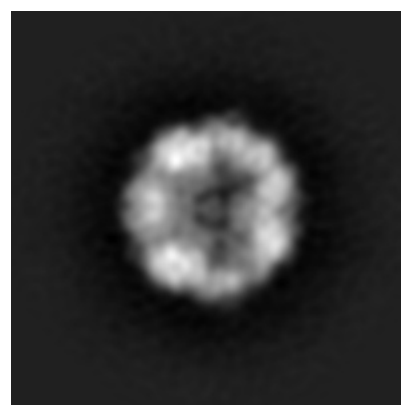
6.1.1 Primary map



X



Y

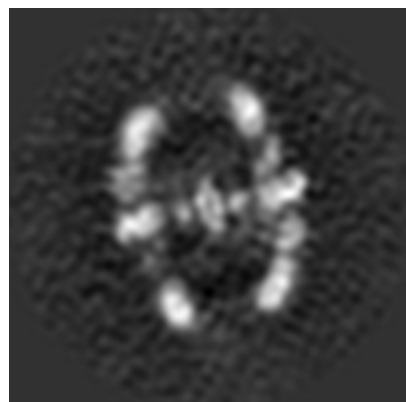


Z

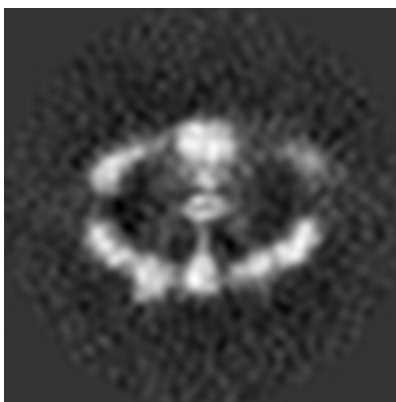
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

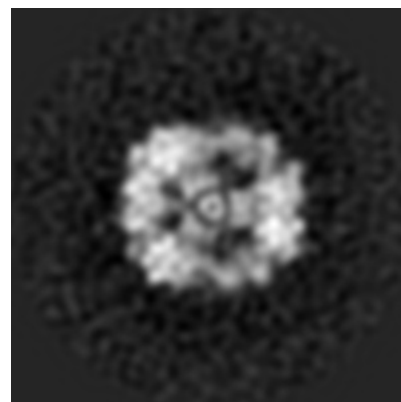
6.2.1 Primary map



X Index: 100



Y Index: 100

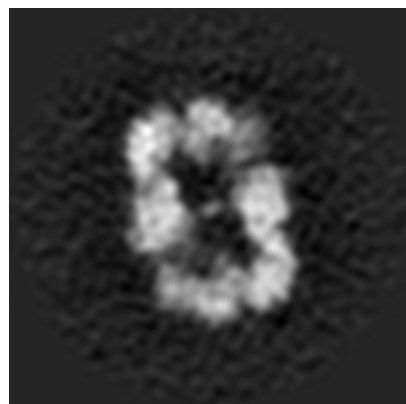


Z Index: 100

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

6.3 Largest variance slices [i](#)

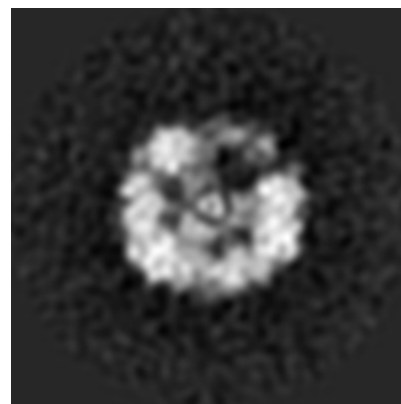
6.3.1 Primary map



X Index: 79



Y Index: 130

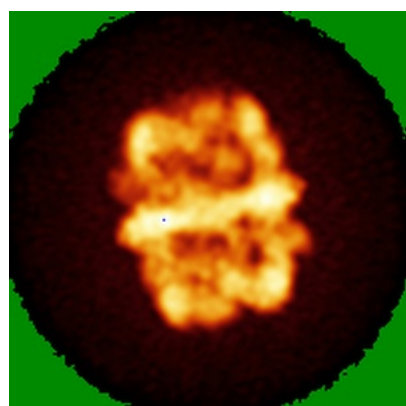


Z Index: 97

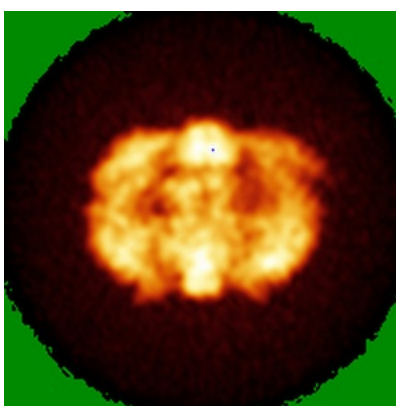
The images above show the largest variance slices of the map in three orthogonal directions.

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

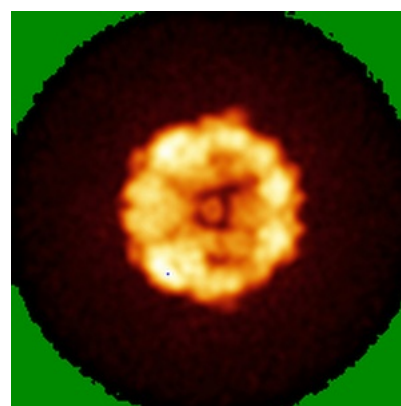
6.4.1 Primary map



X



Y

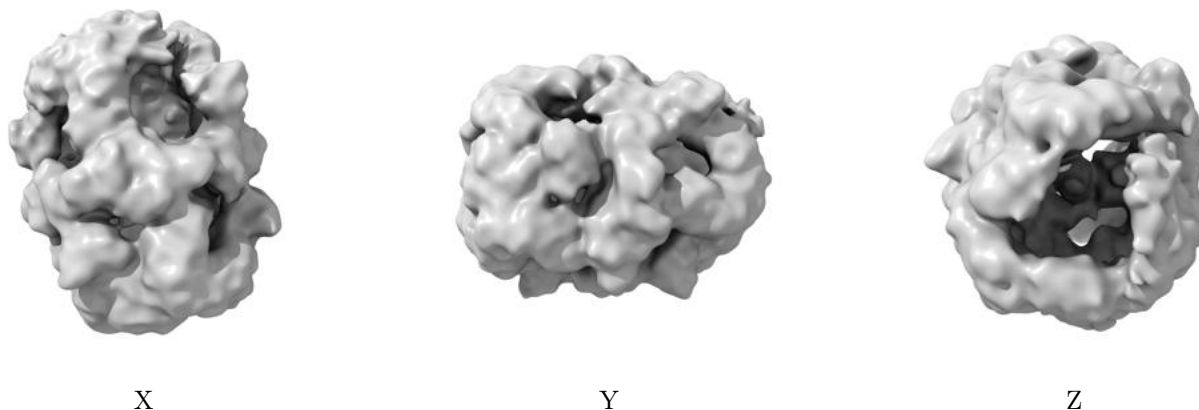


Z

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

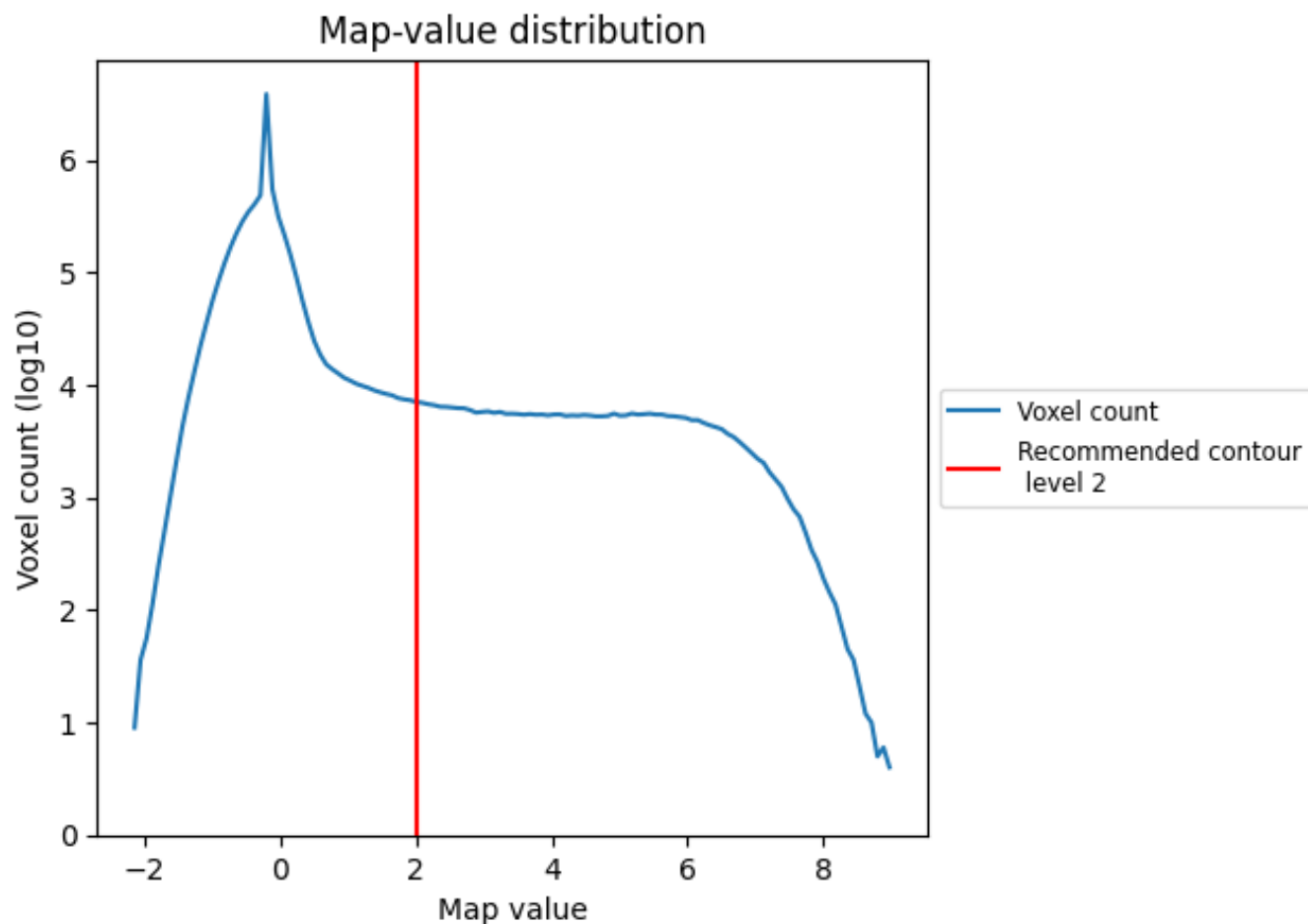
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

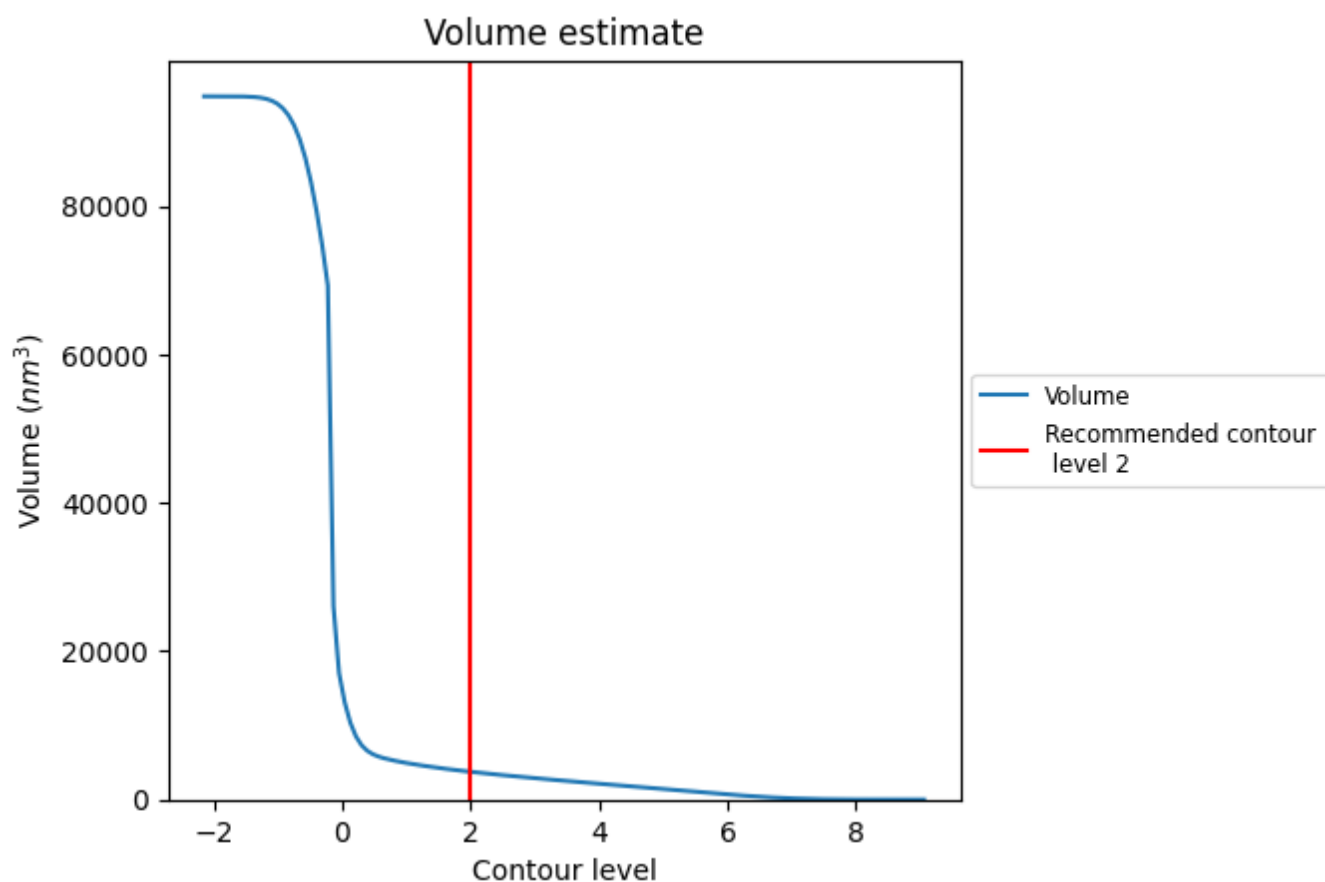
This section contains the results of statistical analysis of the map.

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.

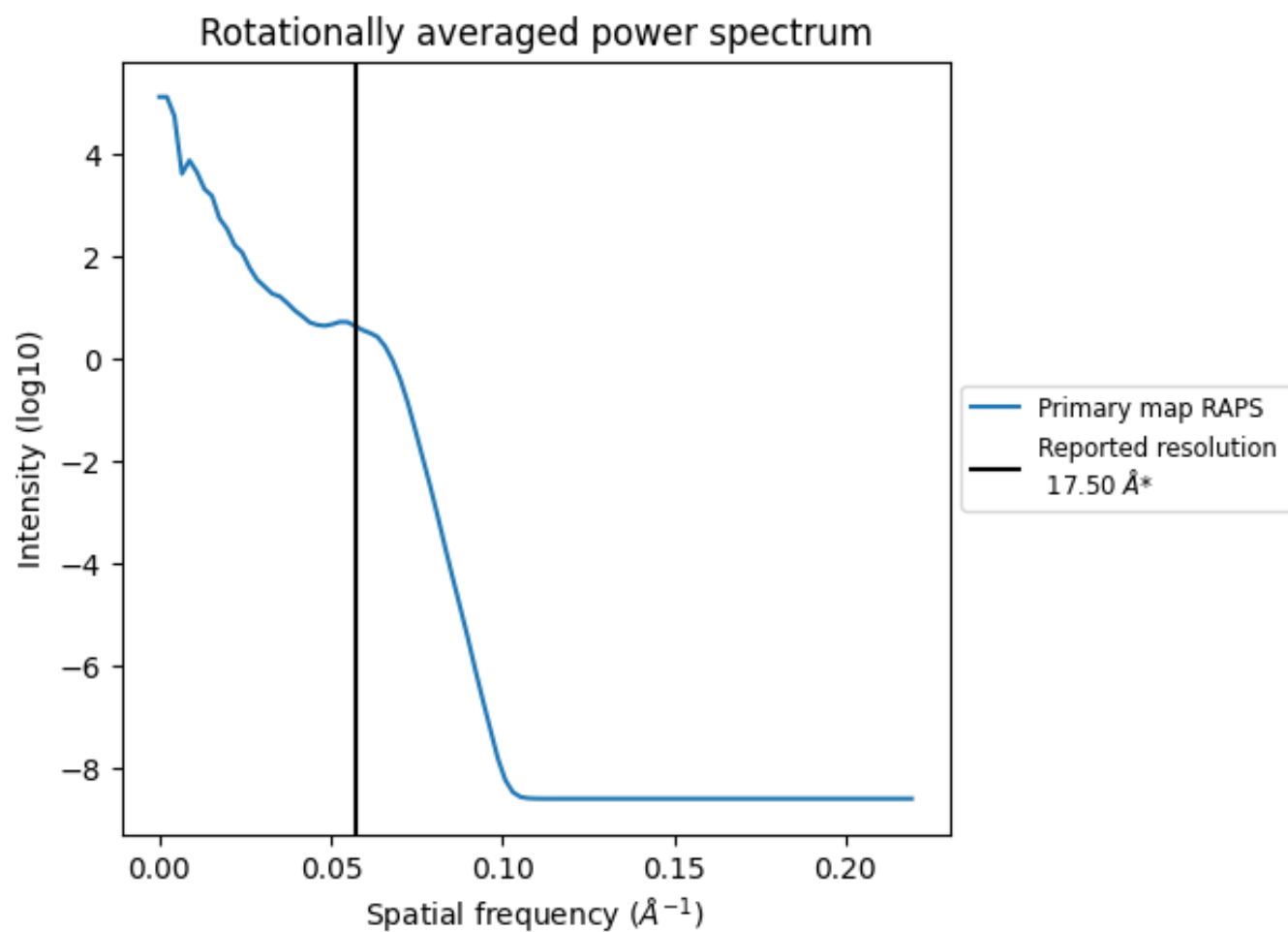
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3745 nm³; this corresponds to an approximate mass of 3383 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 0.057 Å⁻¹

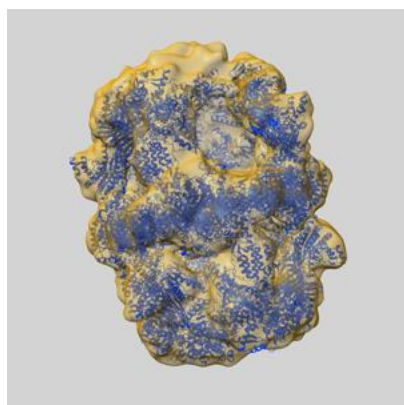
8 Fourier-Shell correlation

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

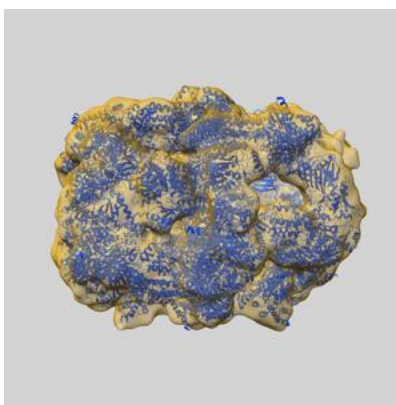
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2357 and PDB model 4V8W. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

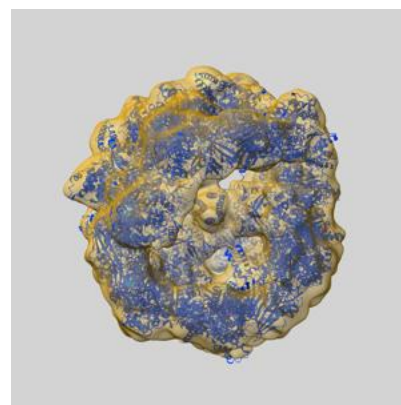
9.1 Map-model overlay [i](#)



X



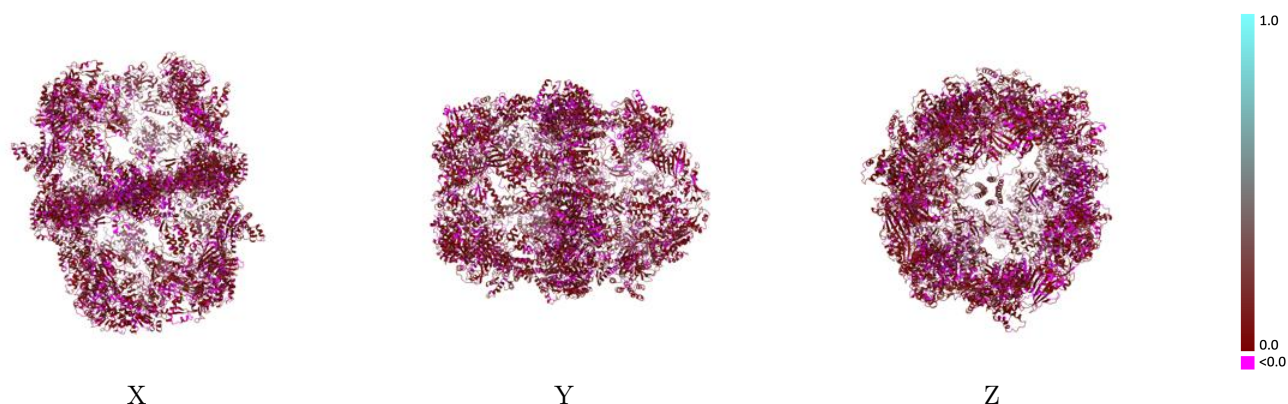
Y



Z

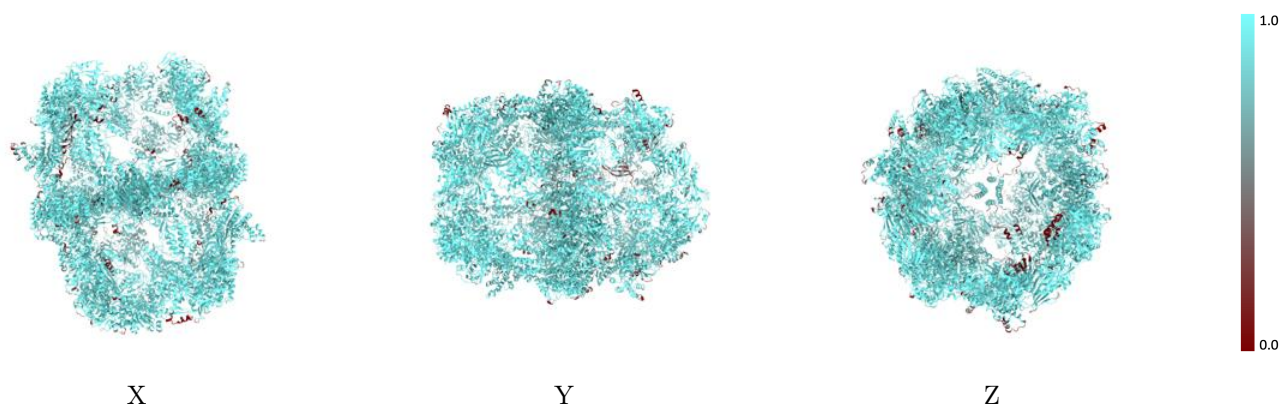
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



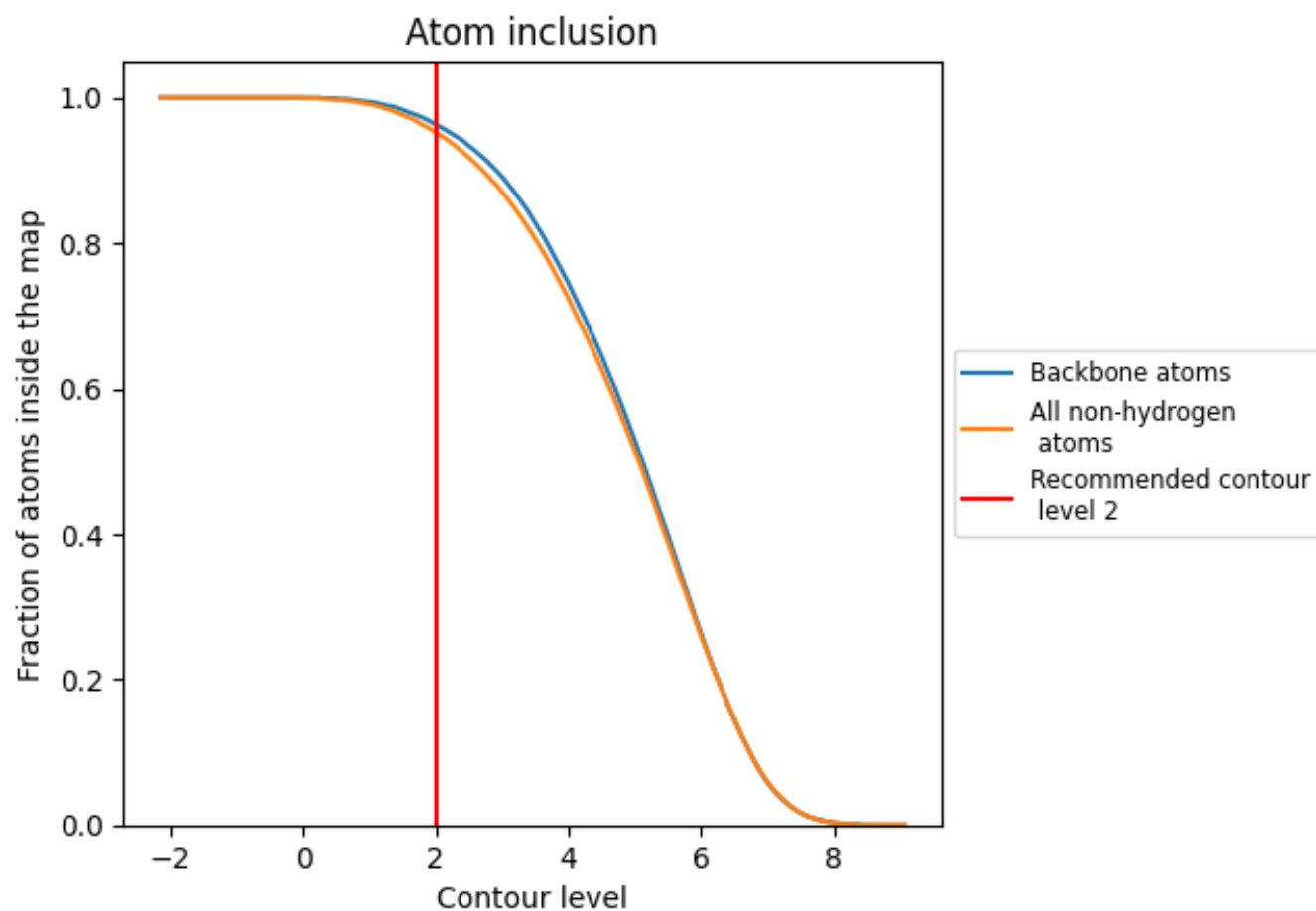
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.0580
A	0.9650	0.0610
B	0.9640	0.0600
C	0.9550	0.0590
D	0.9110	0.0500
E	0.9660	0.0610
F	0.9480	0.0570

1.0

0.0

<0.0