



wwPDB EM Validation Summary Report ⓘ

Dec 4, 2025 – 10:37 AM EST

PDB ID : 9PQX / pdb_00009pqx
EMDB ID : EMD-71792
Title : Structure of M. tuberculosis type-I FAS in the apo state
Authors : Mazhab-Jafari, M.T.; Samani, E.K.
Deposited on : 2025-07-23
Resolution : 2.83 Å (reported)
Based on initial model : 6GJC

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:

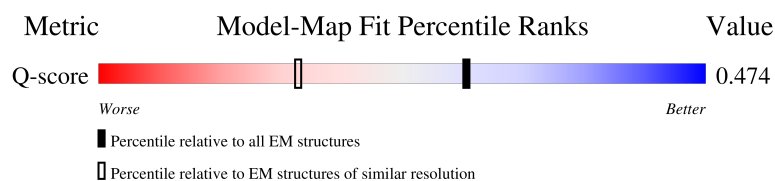
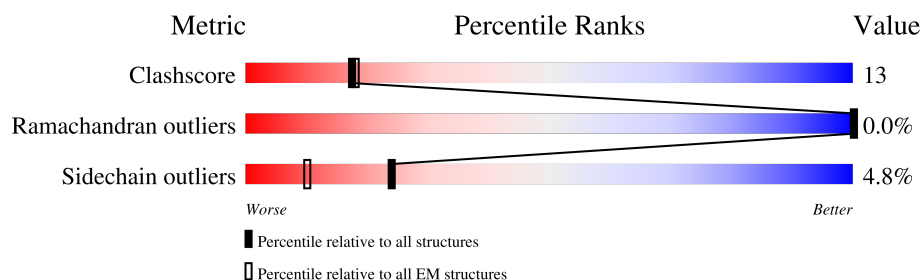
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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 2.83 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	3069	<div> <div>5%</div> <div>63%</div> <div>25%</div> <div>10%</div> </div>
1	B	3069	<div> <div>5%</div> <div>63%</div> <div>26%</div> <div>10%</div> </div>
1	C	3069	<div> <div>5%</div> <div>61%</div> <div>27%</div> <div>10%</div> </div>
1	D	3069	<div> <div>5%</div> <div>63%</div> <div>26%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	3069	<div><div>5%</div><div><div></div><div>63%</div><div>26%</div><div>• 10%</div></div></div>
1	F	3069	<div><div>5%</div><div><div></div><div>62%</div><div>26%</div><div>• 10%</div></div></div>

2 Entry composition [i](#)

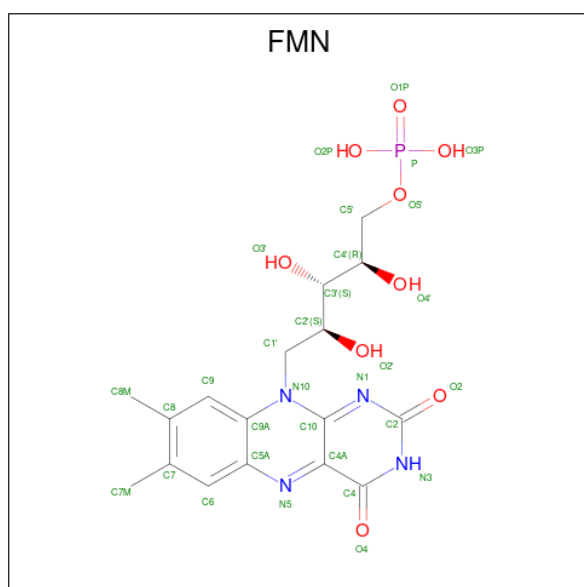
There are 2 unique types of molecules in this entry. The entry contains 124914 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-ACP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2770	Total	C	N	O	S	0	0
			20787	13071	3700	3951	65		
1	B	2770	Total	C	N	O	S	0	0
			20788	13072	3700	3951	65		
1	C	2770	Total	C	N	O	S	0	0
			20779	13067	3700	3947	65		
1	D	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	E	2770	Total	C	N	O	S	0	0
			20782	13068	3699	3950	65		
1	F	2770	Total	C	N	O	S	0	0
			20791	13073	3700	3953	65		

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

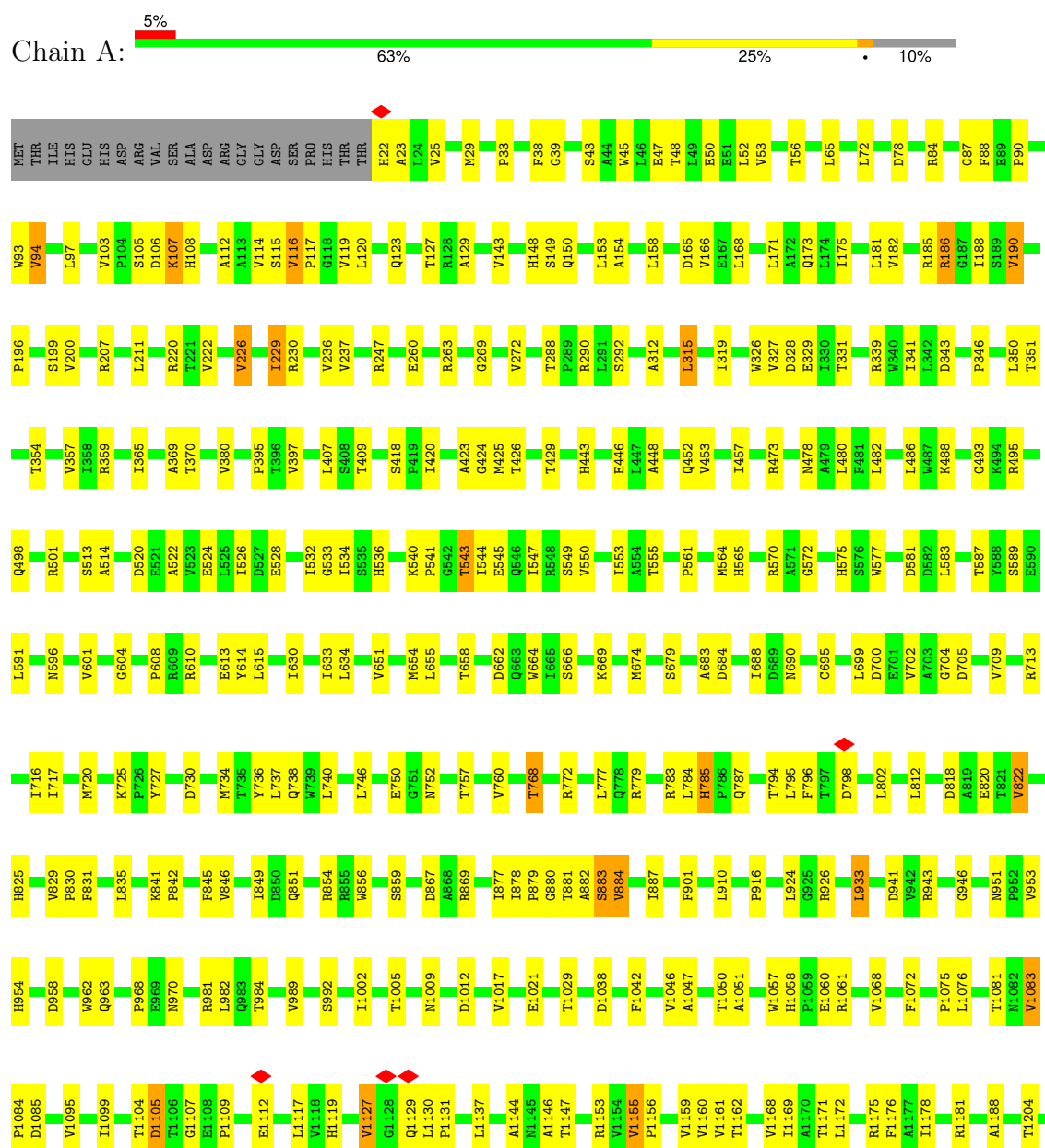


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0
2	D	1	Total 31	C 17	N 4	O 9	P 1	0
2	E	1	Total 31	C 17	N 4	O 9	P 1	0
2	F	1	Total 31	C 17	N 4	O 9	P 1	0

3 Residue-property plots [i](#)

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: 3-oxoacyl-ACP synthase



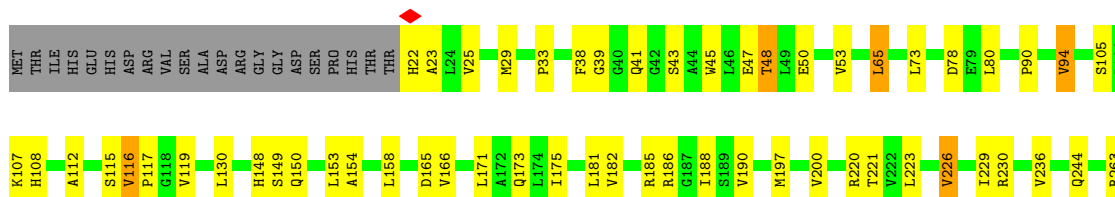
S2345	L2271	V2186	R2044	THR	GLY	THR	ASP	A1709	I1617	G1530	S1524	C1447	A1323	R1207
E2360	S2274	D2187	L2050	VAL	GLY	VAL	ALA	H1710	R1618	E1624	Y1525		S1324	R1208
R2367	ASN	L2189	W2051	VAL	THR	VAL	SER	S1711	D1619	P1625	Y1526	A1456	A1325	R1209
S2368	ARG	S2200	L2052	ALA	ILE	ALA	GLN	V1713	L1620	L1626	A1527	L1457	R1326	R1210
P2369	GLY		L2053	LEU	ASP	LEU	VAL						F1223	
I2370	GLY	S2205	D2054	GLY		GLY	THR	N1717	E1624	G1530			V1226	
D2373	GLY	S2206	L2058	THR	THR	THR	LYS	A1718	P1625	R1533			S1227	
L2378	GLY	H2207	E2067	ARG	GLY	ARG	ALA	E1719	L1626	F1462			V1286	
A2379	D2210		G2071	SER	GLY	THR	LYS	L1725	D1627	G1534			E1246	
L2383	A2211		R2074	THR	THR	THR	LYS	D1729	A1631	M1468			S1247	
L2388	Q2212		R2078	VAL	VAL	VAL	ARG	T1750	D1632	H1469			V1280	
K2391	T2213		T2078	GLY	THR	THR	PRO	D1731	R1640	D1470			I1341	
A2392	T2214		R1975	GLY	PRO	PRO	ILE	PR0	P1641	I1471			Q1342	
R2393	T2215		R1976	GLY	GLY	GLY	GLN	PR0	A1642	V1472			M1253	
E2394	L2216		E1977	MET	VAL	VAL	ILE	PR0	E1643	P1473			L1254	
Q2395	L2217		L1980	GLY	GLY	GLY	GLU	PR0	E1651	D1474			S1256	
M2396	F2218		R1985	HIS	HIS	HIS	SER	PR0	L1652	D1475			Q1260	
S2397	F2220		Q2093	LEU	LEU	LEU	ASP	GLU	L1653	E1476			H1261	
A2398	A2221		L2094	GLY	GLY	GLY	ILE	GLU	Q1656	L1548			V1263	
A2399	A2222		L2098	ALA	ASP	ASP	SER	PR0	F1657	T1549			S1375	
A2400	R2223		R2101	LEU	LEU	LEU	ILE	ALA	V1661	G1550			V1376	
A2401	R2224		E2107	ASP	ASP	ASP	THR	GLU	R1662	G1551			P1273	
V2402	Q2227		R2113	THR	THR	THR	GLY	PR0	W1663	R1482			A1274	
D2403	D2228		R2114	ALA	VAL	VAL	ALA	ALA	I1664	R1483			R1275	
E2404	L2229		Q1992	SER	LEU	LEU	SER	PR0	E1665	A1485			L1276	
D2405	S2230		L1993	VAL	VAL	VAL	GLY	ASP	T1666	I1556			V1277	
A2406	E2231		D1994	ASP	PRO	PRO	ARG	VAL	L1670	L1557			T1280	
E2407	A2232		D1995	LYS	SER	SER	ARG	VAL	F1671	G1560			F1283	
L2412	R2235		P1996	VAL	VAL	VAL	ASN	SER	I1672	I1561			L1284	
L2415			V1997	ILE	ASP	ASP	GLN	GLU	A1675	D1493			M1411	
P2418			A1998	ARG	PRO	PRO	LEU	ALA	E1682	D1495			R1288	
P2419			A1999	ALA	GLY	GLY	VAL	VAL	E1686	D1496			V1289	
R2420			L2000	VAL	ALA	ALA	ASP	VAL	I1687	S1567			V1293	
P2428			P2001	SER	SER	SER	GLY	PR0	G1688	R1568			E1298	
Q2429			D2005	ALA	VAL	VAL	GLU	ALA	V1689	A1497			V1297	
W2430			E2007	ARG	VAL	VAL	LEU	ALA	K1690	D1498			E1299	
L2433			L2008	GLN	LYS	LYS	ASN	SER	P1693	A1501			V1300	
D2434			L2009	THR	THR	THR	LEU	ALA	G1694	F1502			G1301	
V2435			L2010	VAL	GLY	GLY	GLY	GLY	T1694	G1505			I1302	
A2438			L2011	SER	VAL	VAL	ILE	PR0	V1695	I1506			E1307	
D2439			W2020	VAL	VAL	VAL	ASP	ARG	A1696	A1507			I1308	
L2440			L2023	LEU	GLY	GLY	GLY	PR0	G1697	A1434			V1309	
V2441			W2024	GLY	GLY	GLY	ASP	ASP	L1698	D1310			V1311	
V2442			V2027	PRO	TRP	TRP	ALA	LEU	M1701	S1438			V1315	
G2446			W2035	ALA	ALA	ALA	SER	VAL	T1702	G1511			E1441	
			P2036	GLY	LYS	LYS	ASP	PHE	L1703	G1512			L1319	
			D2037	SER	HIS	HIS	LEU	ALA	P1706	F1513			A1444	
			R2039	GLY	VAL	VAL	ALA	ALA	E1707	L1514				
									Y1708	E1515				
										N1518				
										F1519				
										N1520				
										L1521				



V2027	ALA	GLY	GLY	V1689	A1589	L1514	V1439	P1337	N1231	A1124	D1012	V853	R741
F2028	LEU	ASP	ALA	K1690	I1594	E1515	G1440	G1338	H1234	R1125	A1012	R854	V744
V2035	PRO	ASP	GLU	P1693	I1594	E1515	E1441	G1339	H1234	V1126	V1017	V745	L746
R2039	GLY	PHE	VAL	R1597	R1597	N1518	A1444	G1340	S1247	V1127	T1020	S859	L746
R2044	GLY	ASP	ASP	V1695	T1694	F1519	L1445	G1342	V1250	G1128	T1020	D867	E750
R2044	GLY	ALA	LEU	A1696	I1599	N1520	A1446	H1343	V1250	Q1129	T1024	L1130	T757
D2054	GLY	ALA	ALA	P1600	P1600	L1521	C1447	M1346	M1253	P1131	T1024	L1130	T757
I2058	GLY	GLY	GLY	T1702	M1601	S1524	I1451	G1347	S1256	M1027	M1027	G880	V760
D2059	GLY	GLY	GLY	K1703	L1602	M1525	I1451	G1348	S1256	R1028	R1028	T881	V760
I2068	GLY	GLY	GLY	L1705	L1611	Y1526	A1456	E1349	H1261	T1137	T1029	A882	T768
D2069	GLY	GLY	GLY	P1706	R1611	A1527	L1457	E1349	H1261	T1138	T1029	S883	T768
A2066	ASP	LEU	VAL	E1707	I1614	G1530	M1460	R1558	A1282	V1139	D1038	S883	T768
A2066	GLY	ILE	THR	Y1708	I1614	G1530	M1460	R1558	A1282	V1139	D1038	S883	T768
G2071	GLY	THR	LYS	V1715	R1618	R1533	V1461	R1359	V1263	A1144	S1039	V884	L777
L1966	GLY	LEU	LEU	D1619	D1619	G1534	V1461	V1360	T1286	H1145	P1040	V884	L777
S2087	GLY	ALA	ALA	P1622	P1622	L1535	G1465	D1362	T1286	A1146	E1041	T887	R779
R2092	GLY	THR	THR	A1623	A1623	E1536	H1469	D1365	R1271	T1147	V1046	P901	R783
Q2093	GLY	THR	THR	E1624	E1624	A1537	D1470	K1366	R1275	T1149	A1047	T906	H784
I2094	GLY	THR	THR	P1625	P1625	L1538	I1471	F1367	L1277	R1153	T1050	T906	H784
T1970	GLY	THR	THR	L1626	L1626	E1539	V1472	T1368	G1278	V1154	T1050	T906	H784
G1975	GLY	THR	THR	D1627	D1627	E1542	F1473	F1374	M1279	V1155	A1051	L910	D788
R1976	GLY	THR	THR	A1631	A1631	E1543	D1474	S1375	M1279	P1156	H1058	P916	T794
E1977	GLY	THR	THR	E1632	E1632	R1544	D1475	V1376	L1284	V1157	P1059	T916	L795
V1979	GLY	THR	THR	Y1633	Y1633	R1545	E1476	V1376	L1284	S1158	P1059	L924	L795
L1980	GLY	THR	THR	P1636	P1636	R1546	L1477	D1381	V1287	V1159	R1061	L924	L795
R1985	GLY	THR	THR	L1637	L1637	E1547	G1478	D1382	R1288	V1160	R1061	L924	L795
L1986	GLY	THR	THR	R1640	R1640	E1548	R1479	I1387	V1293	T1162	V1068	L926	D798
V1987	GLY	THR	THR	P1641	P1641	L1549	S1480	I1388	V1297	V1168	F1072	L933	P805
L1988	GLY	THR	THR	E1642	E1642	G1550	N1481	H1393	I1302	A1170	F1072	L937	P805
Q1990	GLY	THR	THR	M1644	M1644	G1551	Y1482	H1396	G1301	T1171	T1081	L937	L812
L1991	GLY	THR	THR	A1645	A1645	R1552	L1483	P1397	I1302	L1172	N1082	R943	D818
G1992	GLY	THR	THR	R1646	R1646	S1554	A1485	D1398	E1307	E1173	V1083	G946	V822
L1993	GLY	THR	THR	L1652	L1652	F1556	R1488	G1399	T1308	R1175	P1084	R947	Q823
D1994	GLY	THR	THR	F1657	F1657	I1556	Q1491	V1400	D1310	F1176	P1084	P952	L824
D1995	GLY	THR	THR	V1661	V1661	L1557	T1492	L1401	V1311	A1177	L1087	V953	H825
P1996	GLY	THR	THR	R1662	R1662	G1560	D1493	L1402	V1311	I1178	V1088	H954	V829
V1997	GLY	THR	THR	E1663	E1663	I1561	L1494	T1404	V1315	R1181	V1099	P958	P830
H1998	GLY	THR	THR	I1664	I1664	D1562	L1494	Q1405	L1319	T1182	I1099	F931	F831
L1999	GLY	THR	THR	T1666	T1666	D1562	L1494	F1406	L1319	A1188	T1104	T834	T834
L2000	GLY	THR	THR	L1670	L1670	H1566	D1496	T1407	M1321	A1188	T1104	L835	L835
P2001	GLY	THR	THR	F1671	F1671	S1567	A1497	Q1408	V1320	T1204	T1106	C836	C836
A2003	GLY	THR	THR	L1672	L1672	R1568	D1498	V1409	M1322	T1204	T1106	P968	L839
P2004	GLY	THR	THR	F1673	F1673	E1571	A1501	M1411	S1324	R1207	G1107	P969	G840
D2005	GLY	THR	THR	L1674	L1674	R1571	F1502	A1418	L1327	R1207	E1108	N970	L839
S2006	GLY	THR	THR	F1684	F1684	E1576	G1505	Q1418	L1327	R1207	E1108	N970	L839
E2007	GLY	THR	THR	V1685	V1685	R1579	L1506	V1419	L1327	R1207	E1108	N970	L839
L2008	GLY	THR	THR	I1687	I1687	D1582	G1507	T1433	L1327	R1207	E1108	N970	L839
I2009	GLY	THR	THR	G1688	G1688	D1582	E1508	S1438	L1327	R1207	E1108	N970	L839
D2010	GLY	THR	THR	L1688	L1688	M1585	S1509	S1438	L1327	R1207	E1108	N970	L839
L2011	GLY	THR	THR	P1688	P1688	R1587	G1511	T1433	L1327	R1207	E1108	N970	L839
E2015	GLY	THR	THR	G1688	G1688	D1588	E1512	S1438	L1327	R1207	E1108	N970	L839



• Molecule 1: 3-oxoacyl-ACP synthase



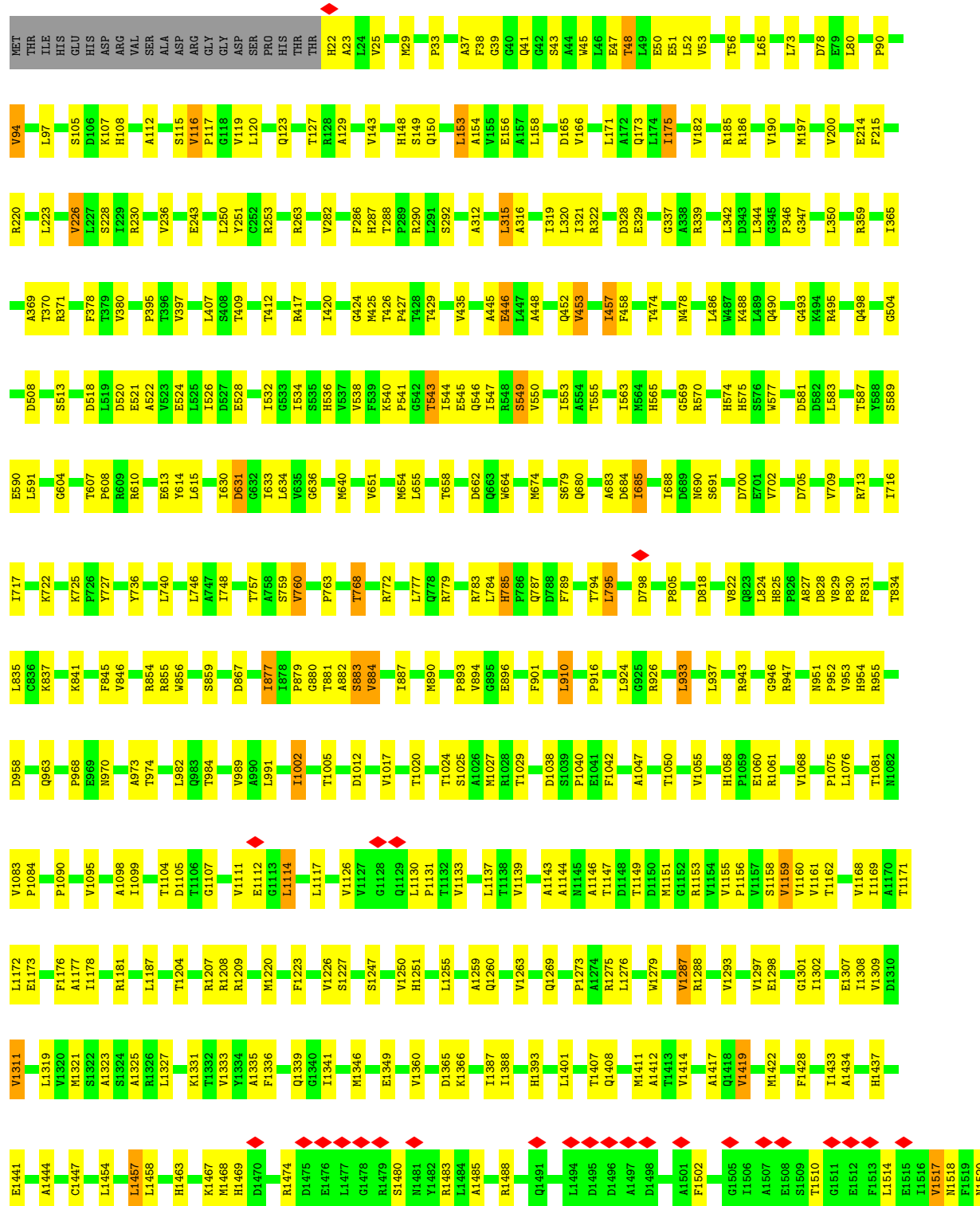




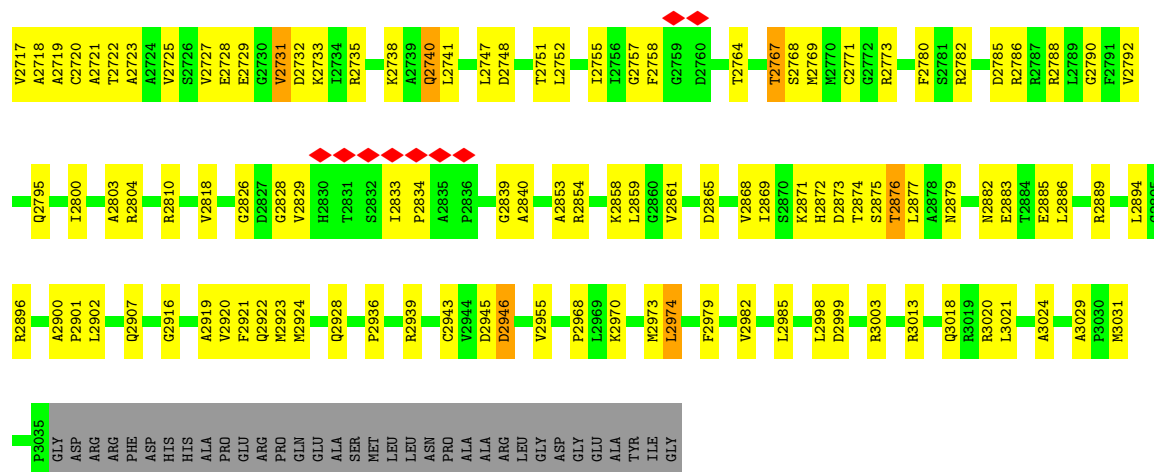
MET
LEU
LEU
ASN
PRO
ALA
ALA
ARG
LEU
GLY
ASP
GLY
GLU
ALA
TYR
ILE
GLY

● Molecule 1: 3-oxoacyl-ACP synthase

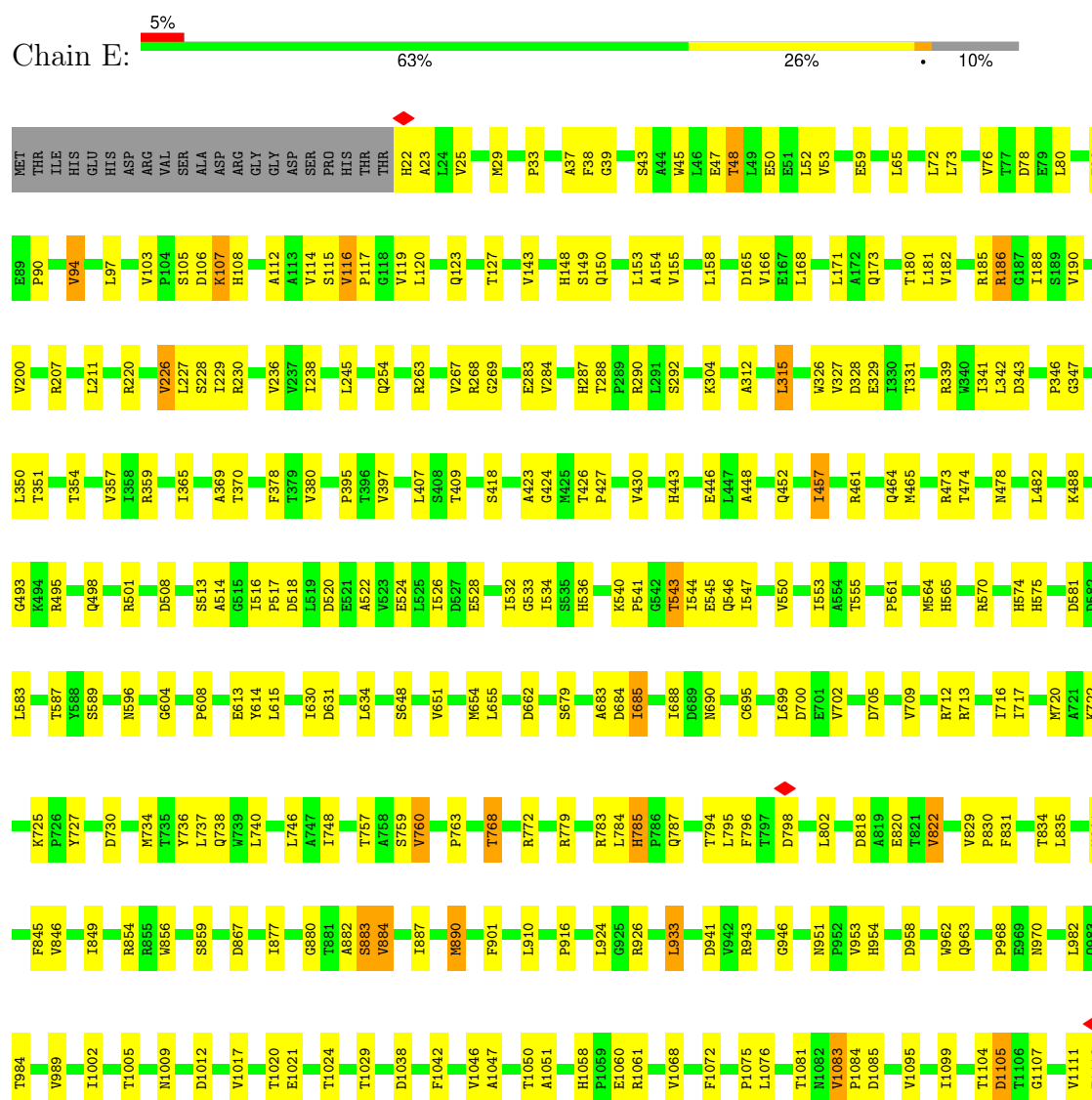
Chain D: 5% 63% 26% 10%







• Molecule 1: 3-oxoacyl-ACP synthase







Q3018	S2875	T2764	F2690	K2594	V2518	E2407	GLY	I2251	Y2159	T2009
R3019	T2876	T2767	Q2691	T2695	G2519	A2408	HIS	I2259	D2165	D2010
R3020	S2768	S2768	E2692	K2696	I2520	I2412	D2329	A2259	D2166	L2011
A3029	N2881	M2769	V2693	Q2604	R2521	P2416	D2331	D2262	A2167	V2027
P3030	E2883	M2770	L2694	P2606	A2528	S2417	I2332	S2265	R2168	A2033
M3031	T2884	C2771	P2695	W2614	I2529	P2418	V2333	R2266	W2174	A2034
R3034	L2885	C2771	I2697	W2614	D2530	P2419	A2334	L2267	L2176	V2035
P3035	L2886	R2782	T2698	L2627	D2532	R2420	V2336	H2268	N2179	R2039
GLY	R2889	D2785	A2699	A2628	H2533	W2430	E2337	V2269	M2180	R2044
ASP	L2894	R2787	V2702	N2631	A2534	L2433	G2340	G2273	A2188	R2052
ARG	G2895	R2788	Q2703	D2637	S2535	D2434	V2341	S2274	E2191	T2053
ARG	R2896	L2789	Q2704	D2637	P2536	V2435	S2345	PRO	W2192	D2054
PHE	G2790	G2790	S2705	A2638	L2537	A2438	M2349	ARG	Q2197	T2058
ASP	Q2795	Q2795	V2706	F2639	L2537	L2439	A2350	GLY	L2201	A2066
HIS	G2796	G2796	S2707	L2640	V2539	L2440	A2351	MET	G2202	E2067
HIS	Q2796	S2641	S2709	S2641	S2540	V2441	C2357	PHE	R2068	R2068
ALA	W2710	F2644	V2710	E2648	L2541	V2442	E2360	GLY	S2087	S2087
ALA	G2711	A2712	G2711	E2648	L2543	V2443	S2361	GLY	H2207	H2207
PRO	A2803	M2713	I2714	Y2652	E2544	V2444	K2362	GLY	I2208	I2208
GLU	R2804	D2806	P2715	H2654	E2545	G2445	V2363	GLY	K2209	K2209
ARG	G2805	L2807	P2716	H2654	D2546	G2446	E2366	GLY	Q2093	Q2093
GLU	L2807	L2807	V2717	H2654	D2546	G2446	V2363	GLY	T2094	T2094
ALA	R2810	A2718	A2718	L2657	A2555	Y2452	A2366	GLY	R2101	R2101
MET	M2811	A2719	C2720	V2658	D2556	T2457	R2367	GLY	E2107	E2107
LEU	V2818	A2658	A2723	A2658	A2557	M2461	S2368	GLY	R2113	R2113
ASN	D2827	N2660	A2724	N2661	R2558	V2462	P2369	GLY	Y2114	Y2114
PRO	G2828	Q2662	V2725	Q2662	E2561	E2463	I2370	GLY	V2118	V2118
ALA	V2829	G2663	S2726	G2663	E2562	E2464	D2373	GLY	V2121	V2121
ARG	H2830	T2664	V2727	T2664	F2563	L2467	L2374	GLY	G2227	G2227
LEU	T2831	G2665	E2728	G2665	P2564	L2467	L2374	GLY	R2223	R2223
GLY	T2831	M2666	E2729	M2666	D2564	L2475	L2375	GLY	V2225	V2225
ASP	S2832	Q2667	D2730	Q2667	P2565	L2475	E2303	GLY	A2124	A2124
GLY	I2833	G2668	D2732	G2668	P2566	L2482	S2304	GLY	T2129	T2129
GLU	P2834	G2668	V2733	G2668	H2567	R2483	S2305	GLY	V2134	V2134
TYR	A2835	M2672	L2734	M2672	T2568	D2486	A2308	GLY	R2136	R2136
ILE	P2836	Q2673	K2735	Q2673	V2569	D2487	R2309	GLY	L2137	L2137
GLY	A2840	T2674	R2735	T2674	I2570	P2488	V2310	GLY	V2144	V2144
GLY	A2853	M2675	Q2740	M2675	P2571	Q2489	S2311	GLY	I2145	I2145
GLY	A2853	Y2676	L2741	Y2676	P2572	G2491	L2312	GLY	A2146	A2146
GLY	A2853	H2677	D2748	H2677	V2573	G2491	L2312	GLY	M2238	M2238
GLY	A2853	G2678	D2749	G2678	P2574	T2495	L2312	GLY	K2241	K2241
GLY	A2853	L2680	L2750	L2680	D2575	E2499	L2316	GLY	V2242	V2242
GLY	A2853	L2681	T2751	L2681	S2576	M2500	L2317	GLY	L2243	L2243
GLY	A2853	G2682	T2755	G2682	W2579	H2511	G2318	GLY	V2245	V2245
GLY	A2853	R2683	L2756	R2683	Q2580	H2511	G2318	GLY	A2246	A2246
GLY	A2853	N2684	G2757	N2684	V2581	H2511	G2318	GLY	V2247	V2247
GLY	A2853	K2685	F2758	K2685	T2582	H2511	G2318	GLY		
GLY	A2853	P2686	Q2759	P2686	R2583	H2511	G2318	GLY		
GLY	A2853	N2687	D2873	N2687	K2584	H2511	G2318	GLY		
GLY	A2853	D2688	T2874	D2688	A2585	H2511	G2318	GLY		
GLY	A2853	L2689		L2689	T2587	H2511	G2318	GLY		
GLY	A2853				E2588	H2511	G2318	GLY		
GLY	A2853				P2592	H2511	G2318	GLY		
GLY	A2853				R2593	H2511	G2318	GLY		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.517	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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	0.13	0/21209	0.36	3/28918 (0.0%)
1	B	0.13	0/21210	0.38	4/28919 (0.0%)
1	C	0.14	0/21200	0.49	9/28905 (0.0%)
1	D	0.13	0/21223	0.36	5/28935 (0.0%)
1	E	0.21	3/21203 (0.0%)	0.46	13/28909 (0.0%)
1	F	0.13	0/21213	0.36	4/28923 (0.0%)
All	All	0.15	3/127258 (0.0%)	0.41	38/173509 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2223	PRO	CG-CD	-20.42	0.81	1.50
1	E	2223	PRO	CB-CG	10.05	1.99	1.49
1	E	2223	PRO	N-CD	5.72	1.55	1.47

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1707	GLU	CA-C-N	33.23	170.59	122.40
1	C	1707	GLU	C-N-CA	33.23	170.59	122.40
1	C	1707	GLU	N-CA-C	-27.44	68.80	109.96
1	E	2223	PRO	N-CD-CG	-24.95	65.78	103.20
1	E	1708	TYR	N-CA-C	19.89	135.88	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20787	0	20642	542	0
1	B	20788	0	20644	569	0
1	C	20779	0	20631	600	0
1	D	20801	0	20661	570	0
1	E	20782	0	20632	569	0
1	F	20791	0	20646	571	0
2	A	31	0	19	4	0
2	B	31	0	19	4	0
2	C	31	0	19	5	0
2	D	31	0	19	4	0
2	E	31	0	19	4	0
2	F	31	0	19	4	0
All	All	124914	0	123970	3306	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 13.

The worst 5 of 3306 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:C:2677:HIS:HB3	1:C:2683:ARG:NH1	1.62	1.13
1:C:2677:HIS:CB	1:C:2683:ARG:HH12	1.62	1.10
1:C:1705:LEU:O	1:C:1707:GLU:O	1.69	1.09
1:F:2678:GLY:HA2	1:F:2683:ARG:HD3	1.40	1.03
1:F:2681:LEU:HB2	1:F:2683:ARG:HD2	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	2762/3069 (90%)	2629 (95%)	133 (5%)	0	100	100
1	B	2762/3069 (90%)	2643 (96%)	119 (4%)	0	100	100
1	C	2762/3069 (90%)	2630 (95%)	132 (5%)	0	100	100
1	D	2762/3069 (90%)	2633 (95%)	129 (5%)	0	100	100
1	E	2762/3069 (90%)	2630 (95%)	132 (5%)	0	100	100
1	F	2762/3069 (90%)	2636 (95%)	125 (4%)	1 (0%)	100	100
All	All	16572/18414 (90%)	15801 (95%)	770 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	2203	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	2132/2359 (90%)	2038 (96%)	94 (4%)	24	47
1	B	2132/2359 (90%)	2038 (96%)	94 (4%)	24	47
1	C	2129/2359 (90%)	2010 (94%)	119 (6%)	17	35
1	D	2135/2359 (90%)	2025 (95%)	110 (5%)	19	39
1	E	2130/2359 (90%)	2022 (95%)	108 (5%)	20	40
1	F	2133/2359 (90%)	2038 (96%)	95 (4%)	23	46
All	All	12791/14154 (90%)	12171 (95%)	620 (5%)	24	43

5 of 620 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1083	VAL
1	F	1137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1319	LEU
1	E	1068	VAL
1	E	2859	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2580	GLN
1	E	2696	ASN
1	D	2704	GLN
1	E	1145	ASN
1	F	92	GLN

5.3.3 RNA [i](#)

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	3101	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	E	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	D	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	8 (16%)
2	FMN	B	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	F	3101	-	33,33,33	1.06	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	C	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.24	8 (16%)

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	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	E	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	D	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	B	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	F	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	C	3101	-	-	2/18/18/18	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	3101	FMN	C4A-N5	3.49	1.38	1.30
2	D	3101	FMN	C4A-N5	3.49	1.38	1.30
2	E	3101	FMN	C4A-N5	3.47	1.38	1.30
2	C	3101	FMN	C4A-N5	3.45	1.38	1.30
2	F	3101	FMN	C4A-N5	3.43	1.38	1.30

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3101	FMN	C4-N3-C2	-3.27	119.83	125.64
2	A	3101	FMN	C4-N3-C2	-3.25	119.86	125.64
2	E	3101	FMN	C4-N3-C2	-3.23	119.91	125.64
2	B	3101	FMN	C4-N3-C2	-3.21	119.95	125.64
2	D	3101	FMN	C4-N3-C2	-3.18	119.99	125.64

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

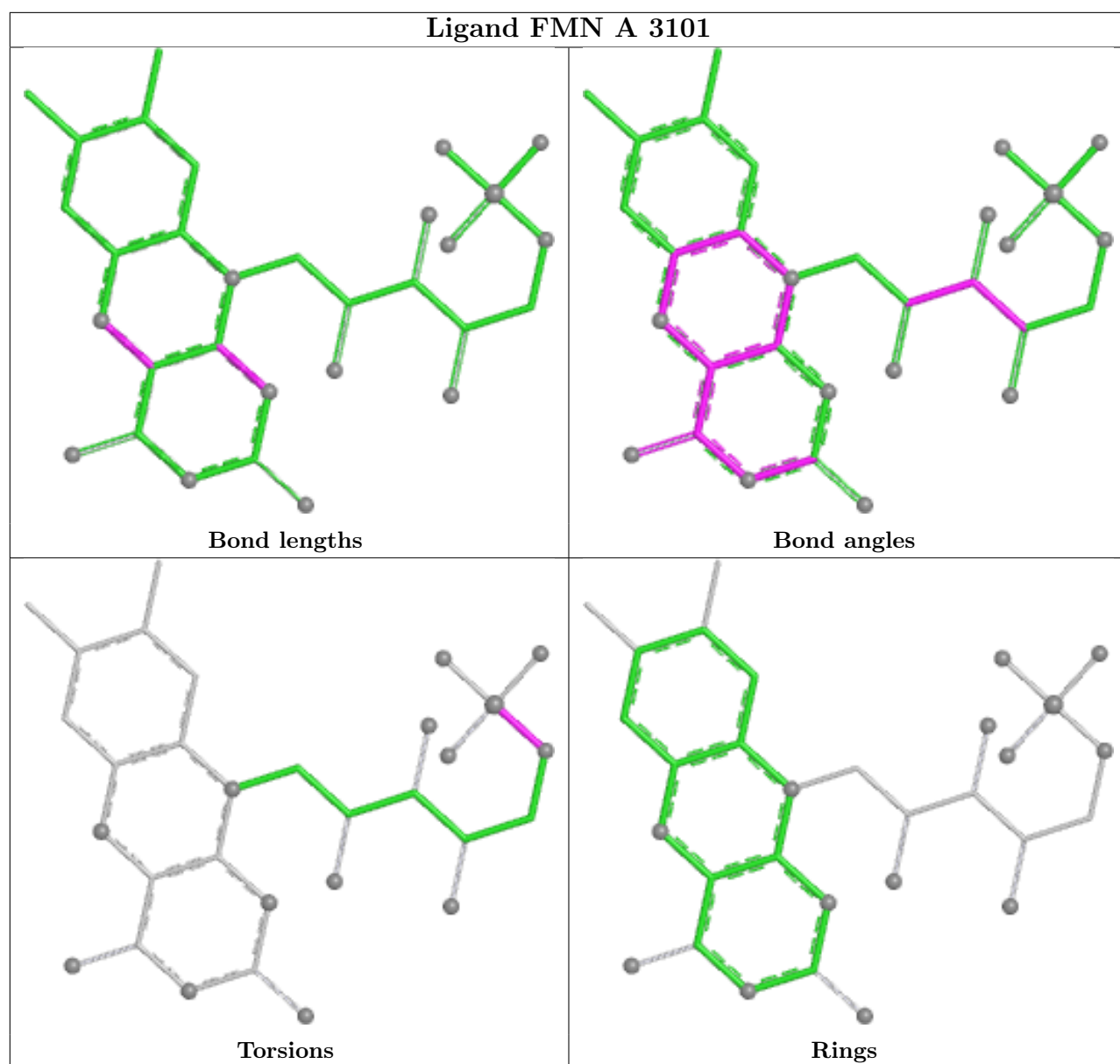
Mol	Chain	Res	Type	Atoms
2	A	3101	FMN	C5'-O5'-P-O1P
2	B	3101	FMN	C5'-O5'-P-O1P
2	E	3101	FMN	C5'-O5'-P-O1P
2	F	3101	FMN	C5'-O5'-P-O1P
2	C	3101	FMN	C5'-O5'-P-O1P

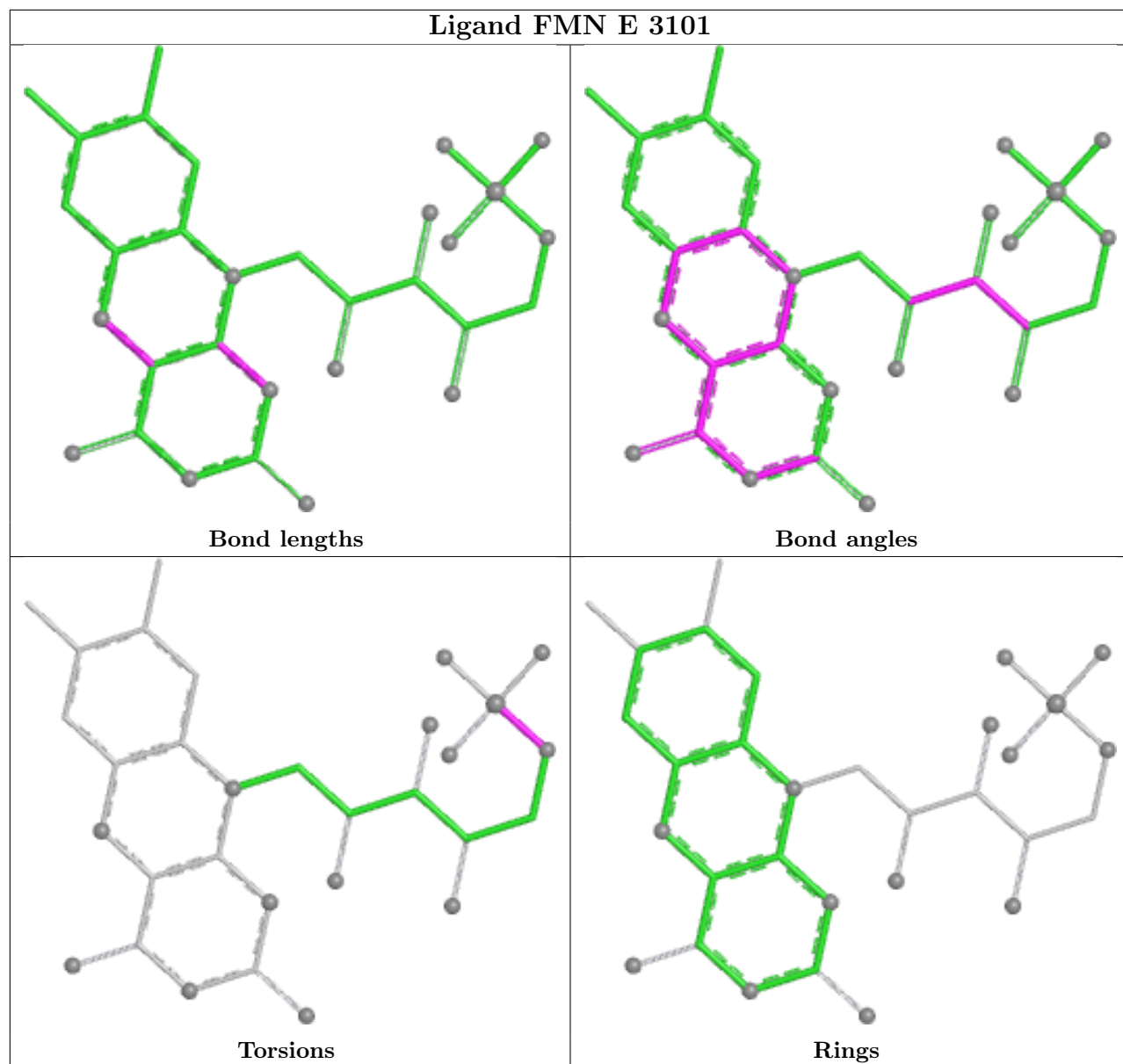
There are no ring outliers.

6 monomers are involved in 25 short contacts:

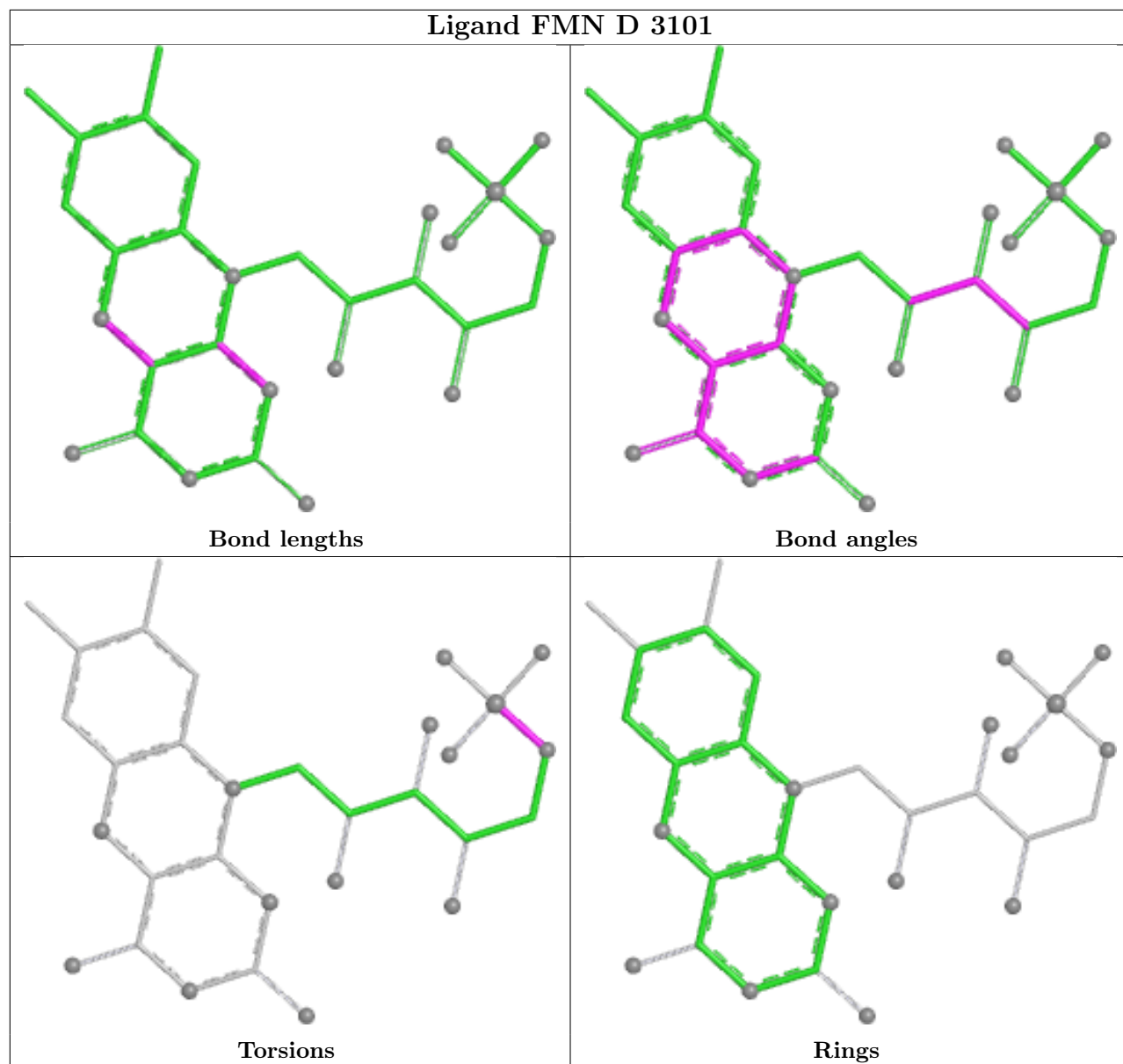
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3101	FMN	4	0
2	E	3101	FMN	4	0
2	D	3101	FMN	4	0
2	B	3101	FMN	4	0
2	F	3101	FMN	4	0
2	C	3101	FMN	5	0

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.

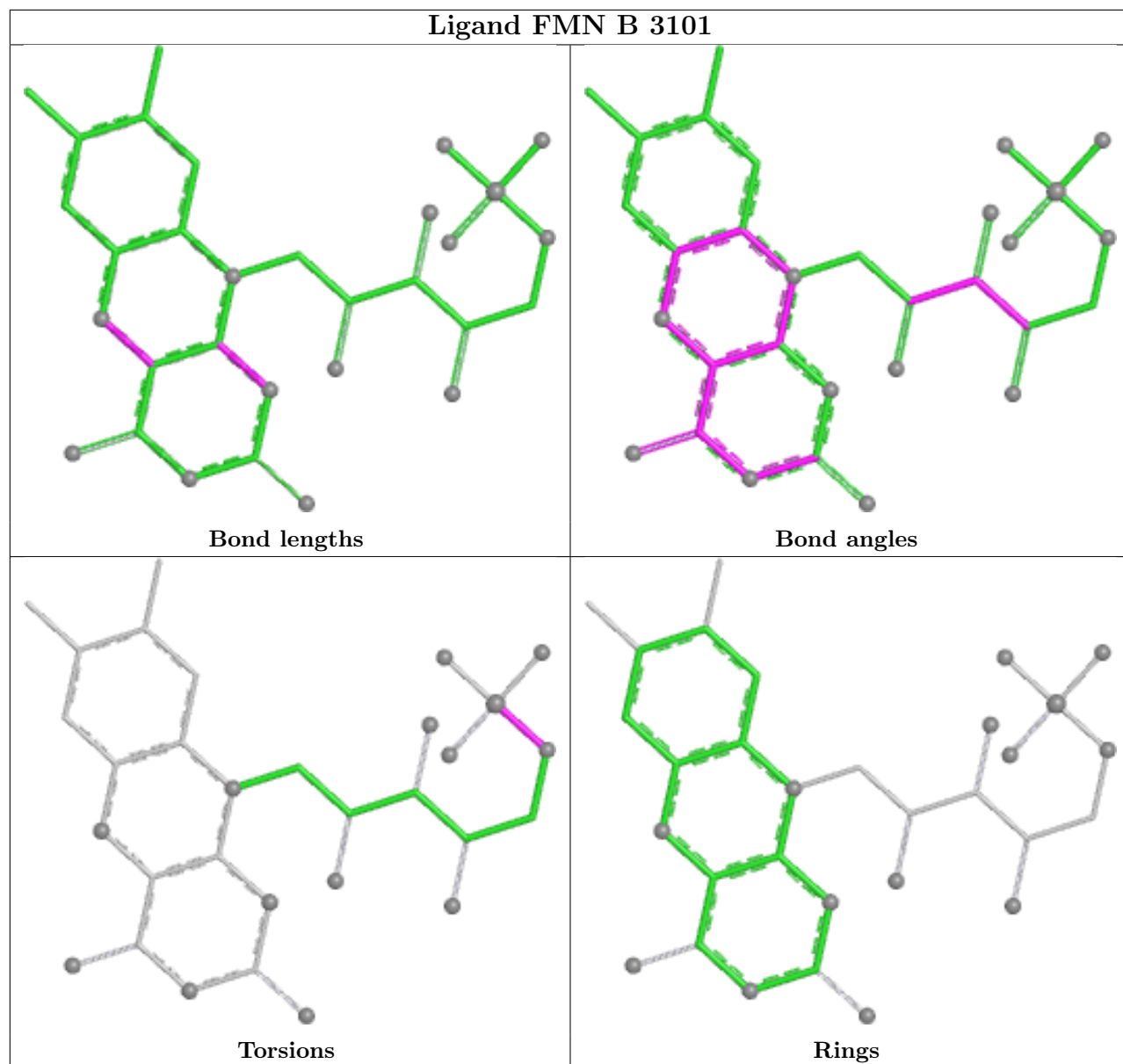


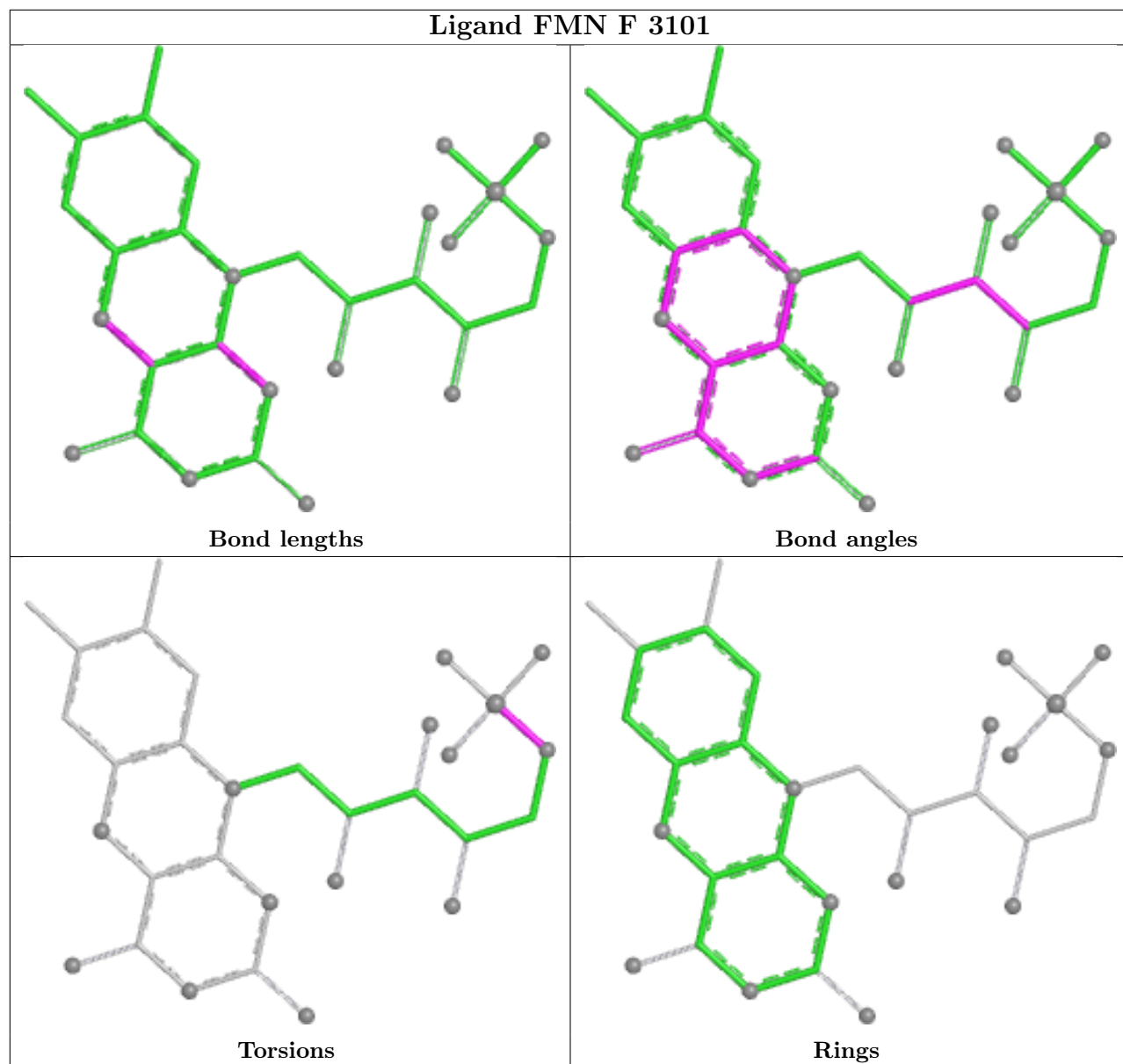


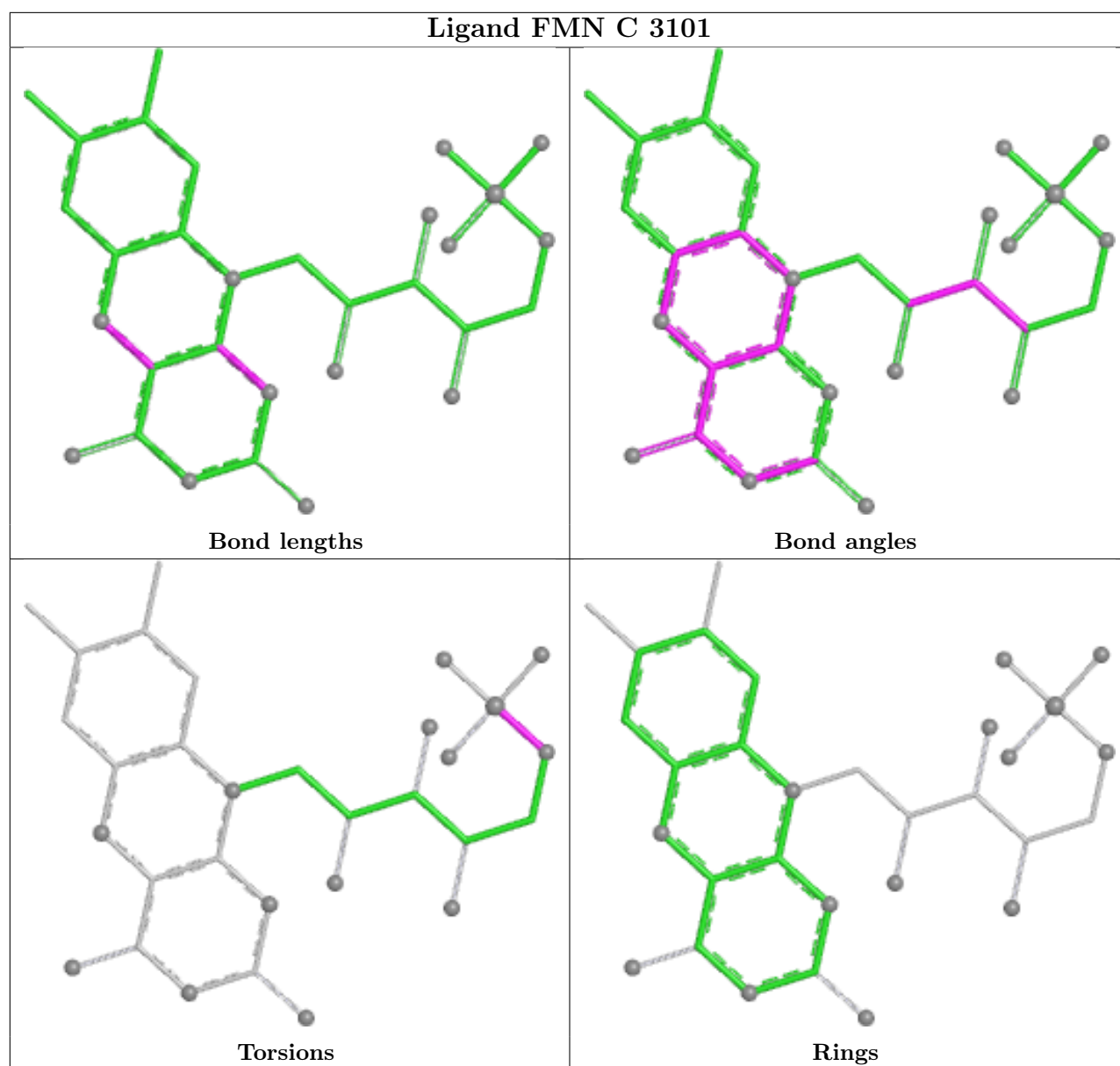
Ligand FMN D 3101



Ligand FMN B 3101







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.

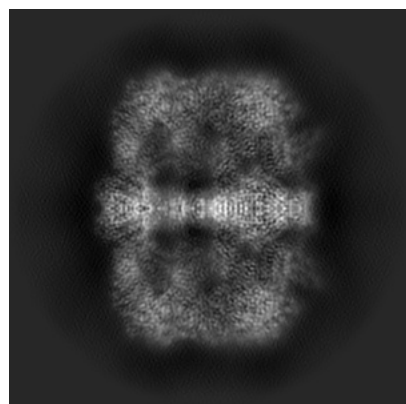
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71792. These allow visual inspection of the internal detail of the map and identification of artifacts.

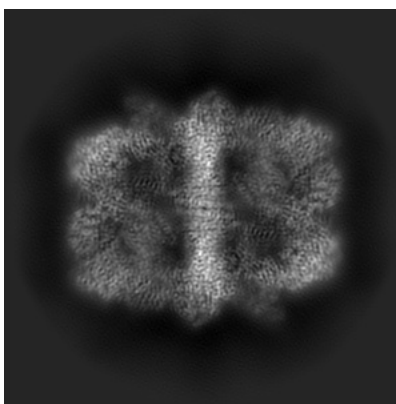
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

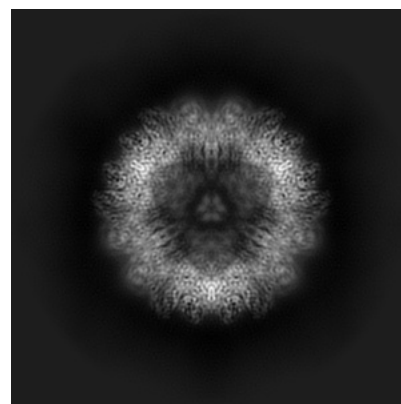
6.1.1 Primary map



X

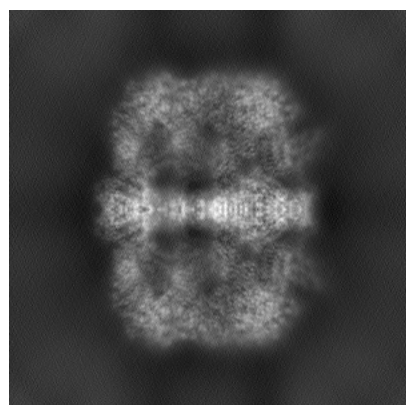


Y

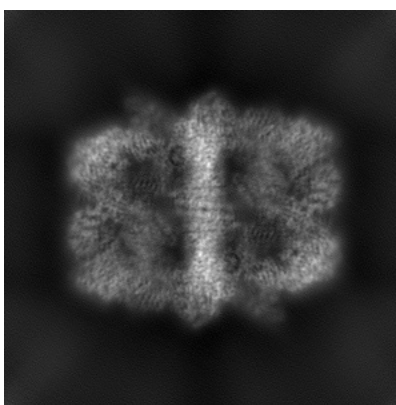


Z

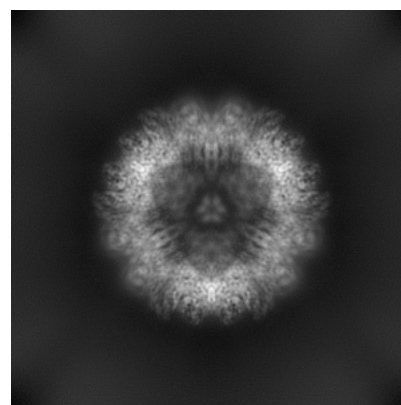
6.1.2 Raw map



X



Y

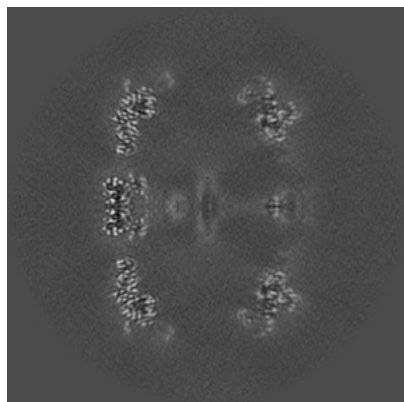


Z

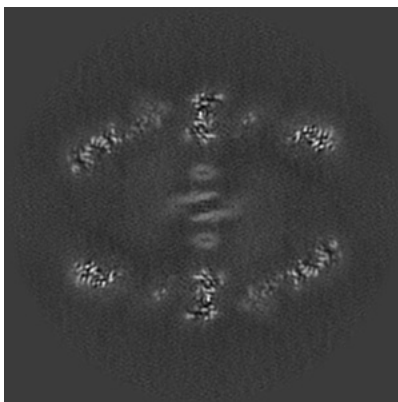
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

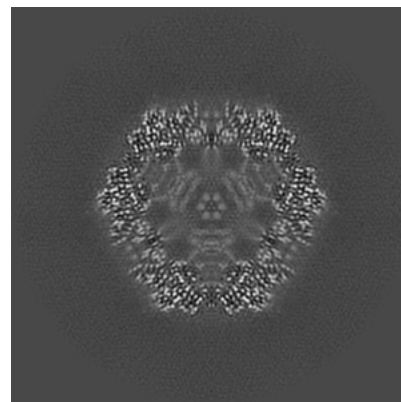
6.2.1 Primary map



X Index: 200

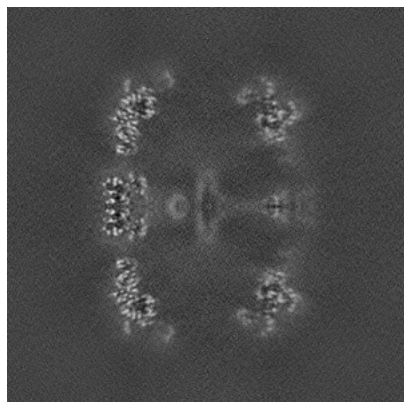


Y Index: 200

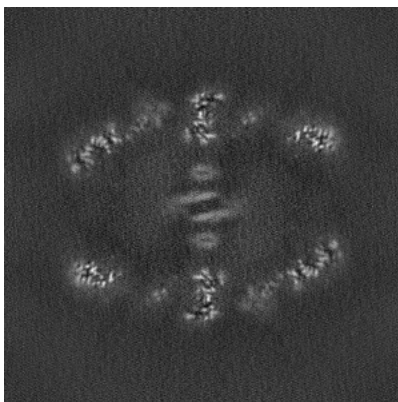


Z Index: 200

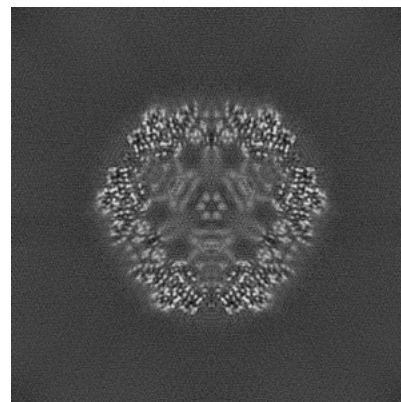
6.2.2 Raw map



X Index: 200



Y Index: 200

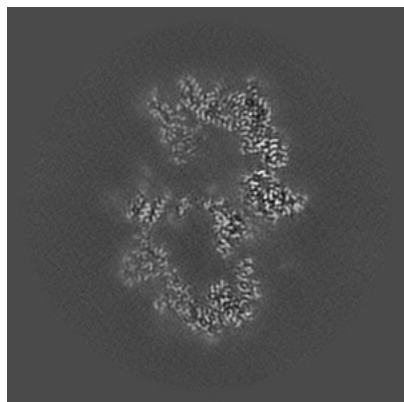


Z Index: 200

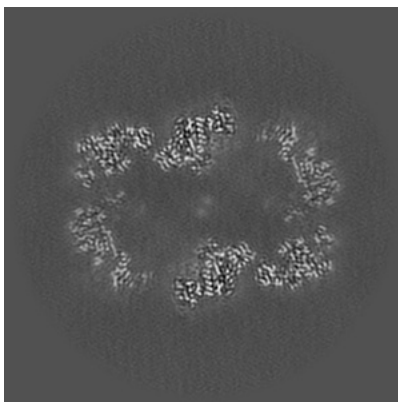
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

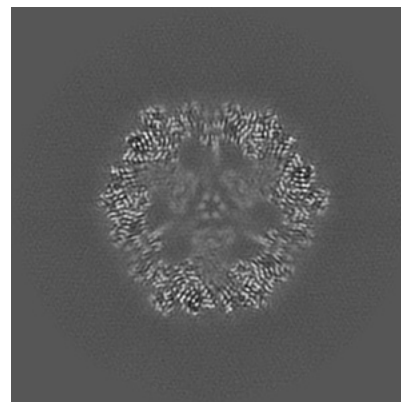
6.3.1 Primary map



X Index: 135

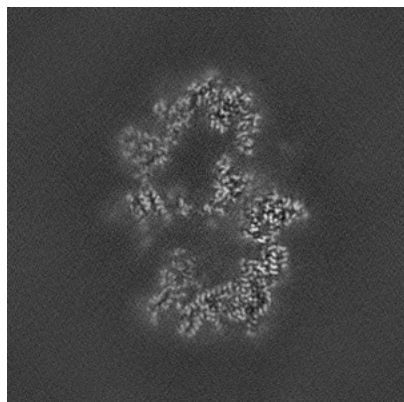


Y Index: 248

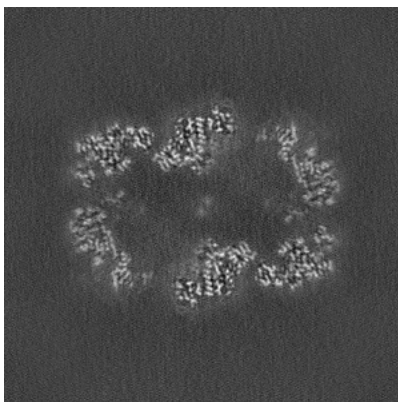


Z Index: 204

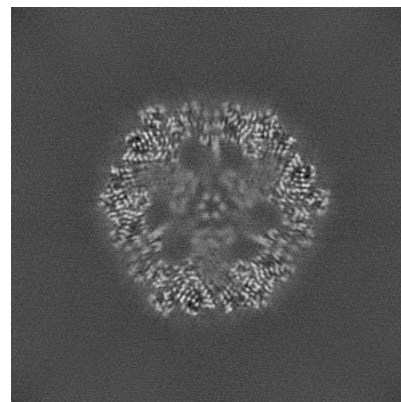
6.3.2 Raw map



X Index: 265



Y Index: 248

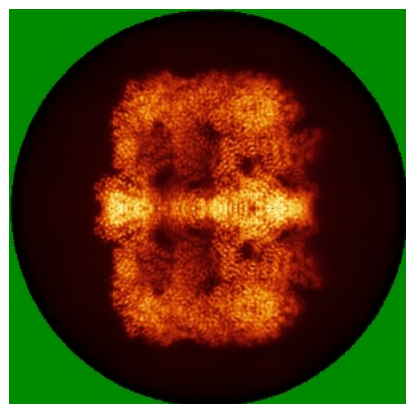


Z Index: 204

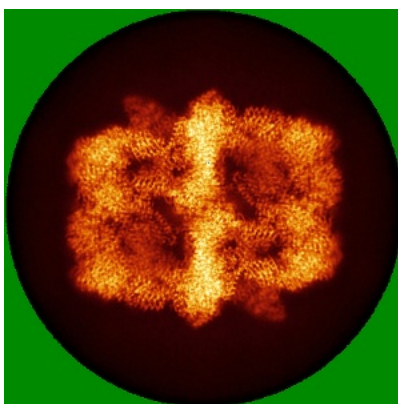
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

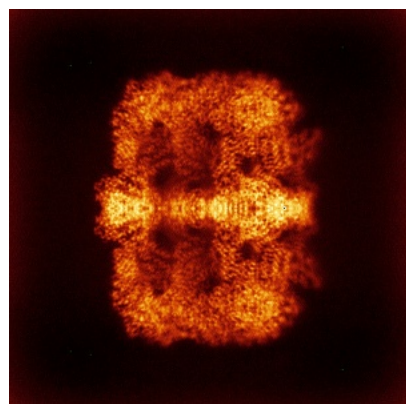


Y

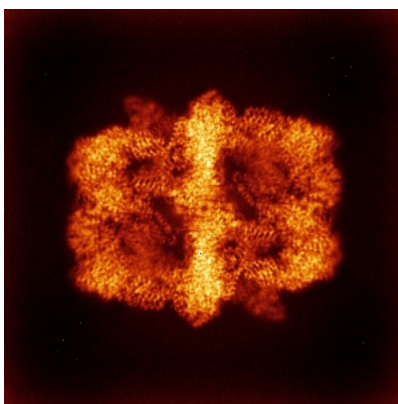


Z

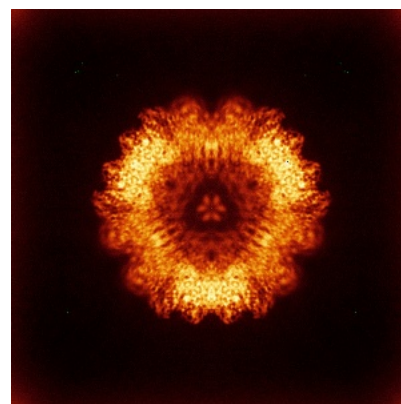
6.4.2 Raw map



X



Y

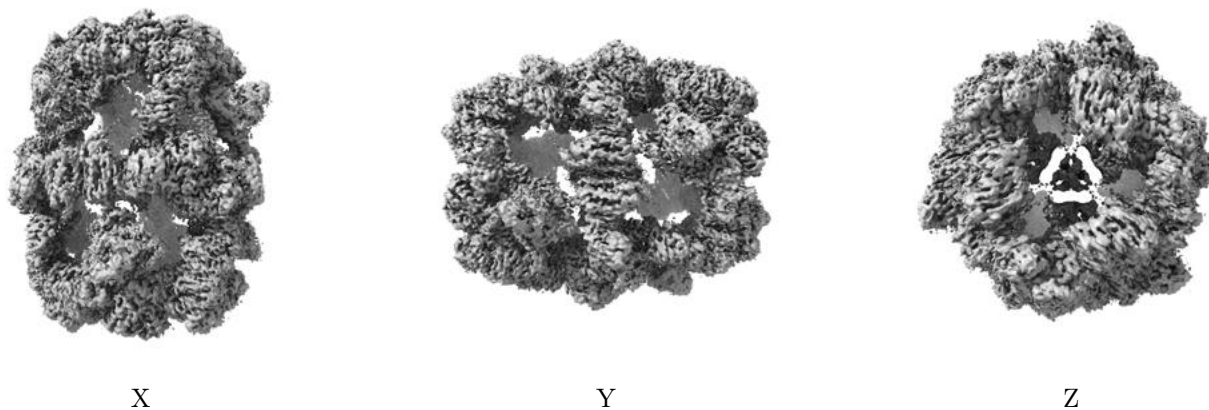


Z

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.

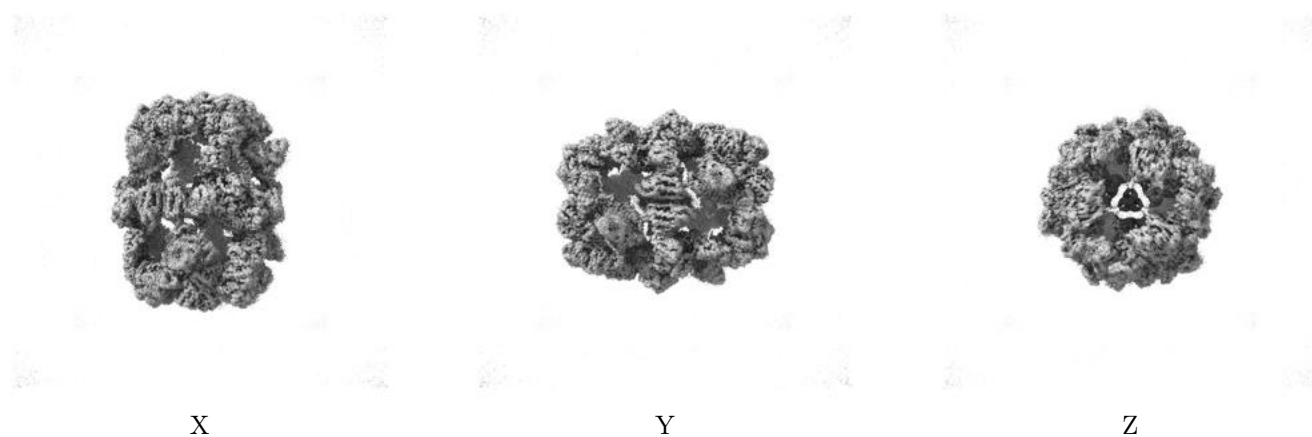
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

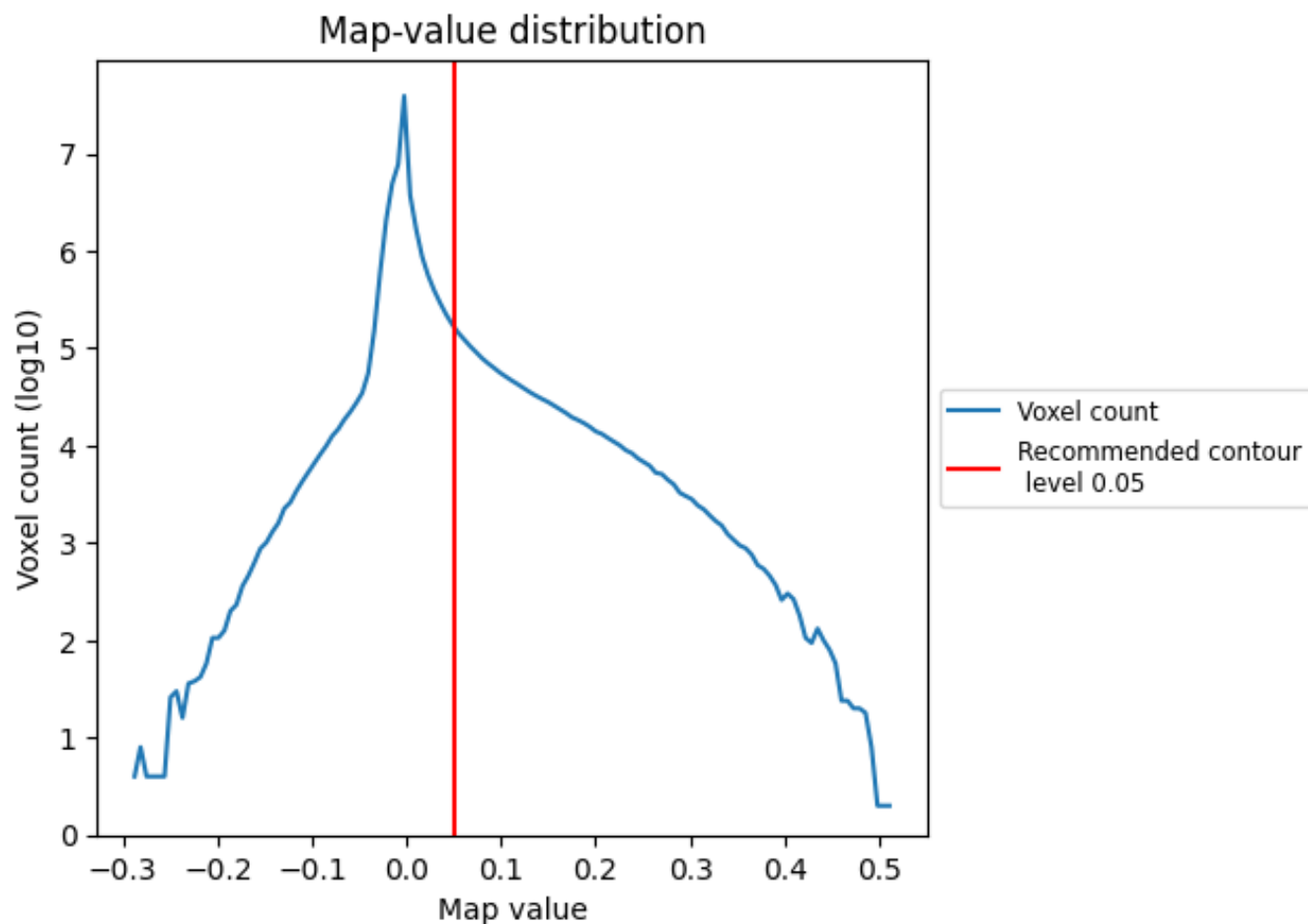
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

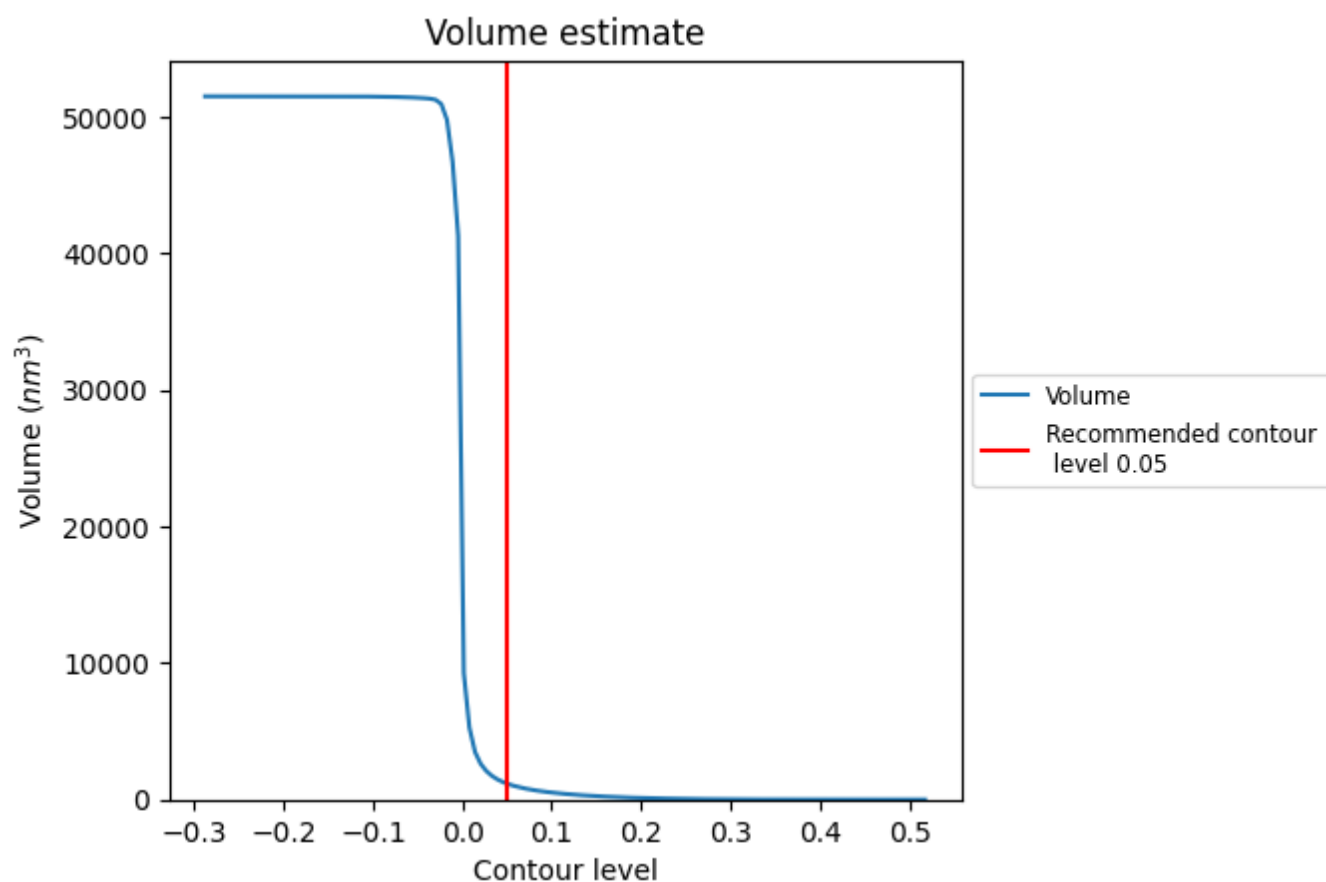
This section contains the results of statistical analysis of the map.

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.

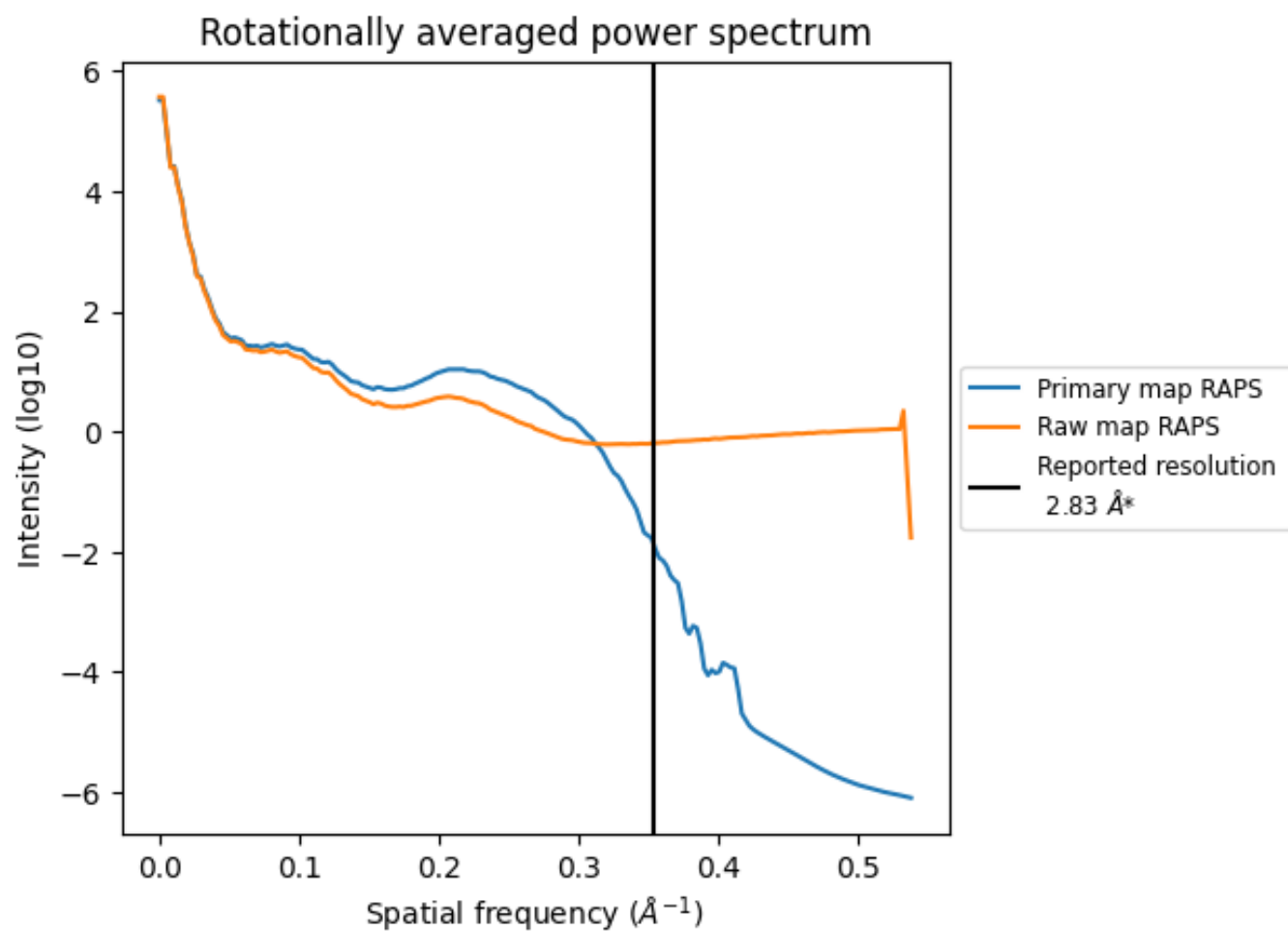
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm³; this corresponds to an approximate mass of 1055 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 [i](#)

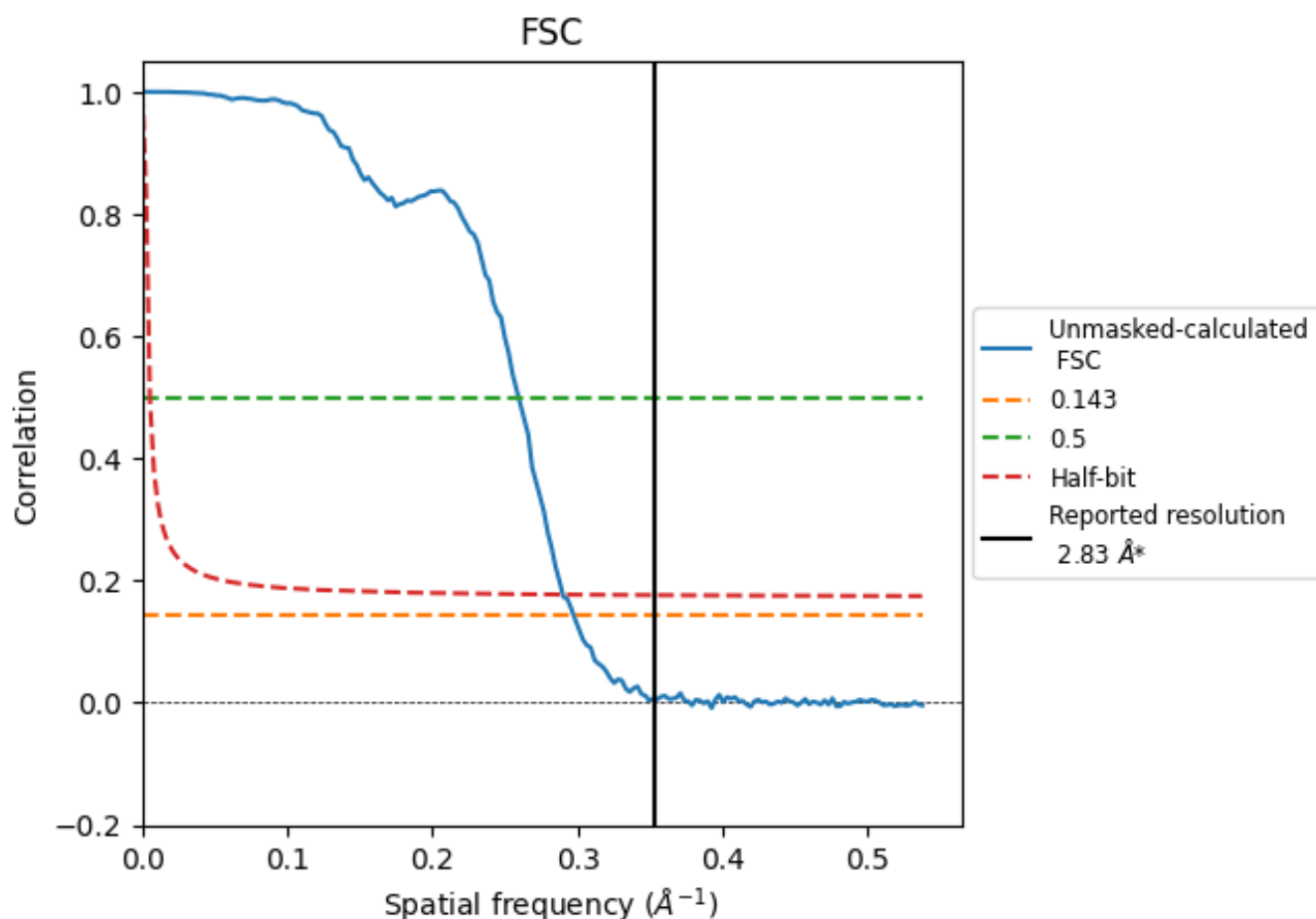


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

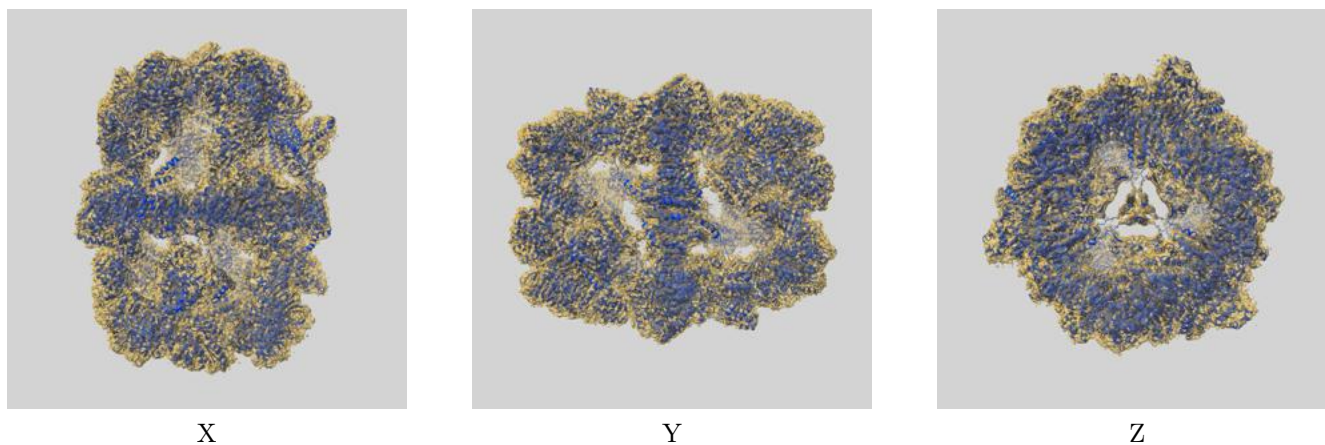
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.86	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

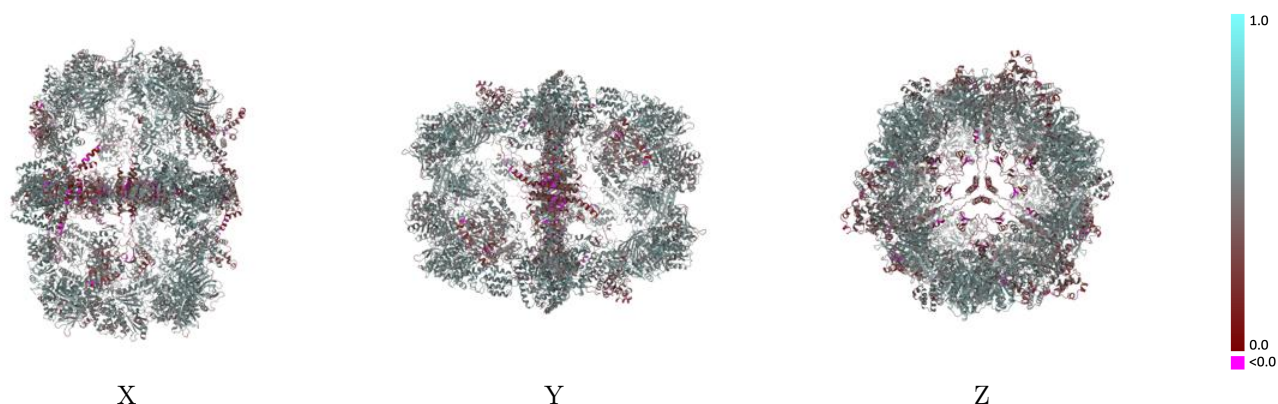
This section contains information regarding the fit between EMDB map EMD-71792 and PDB model 9PQX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



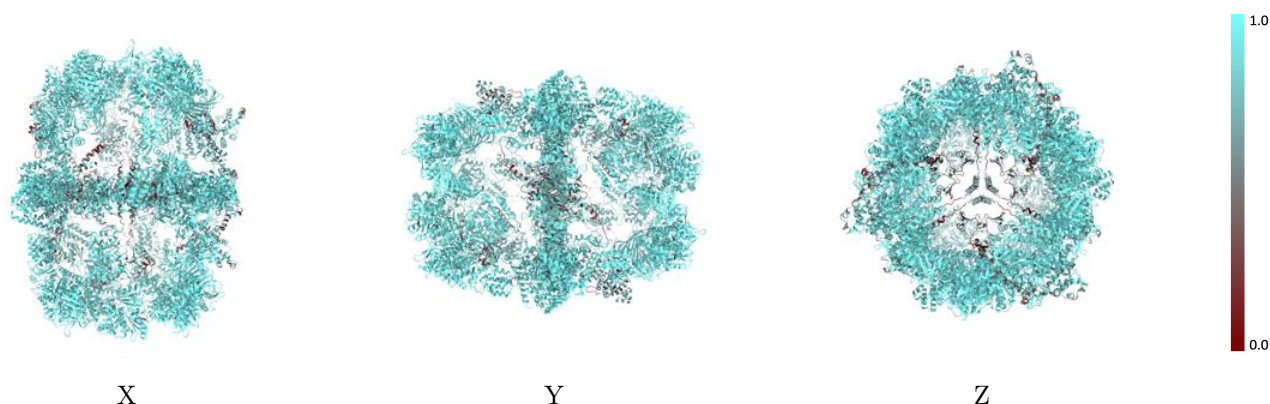
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



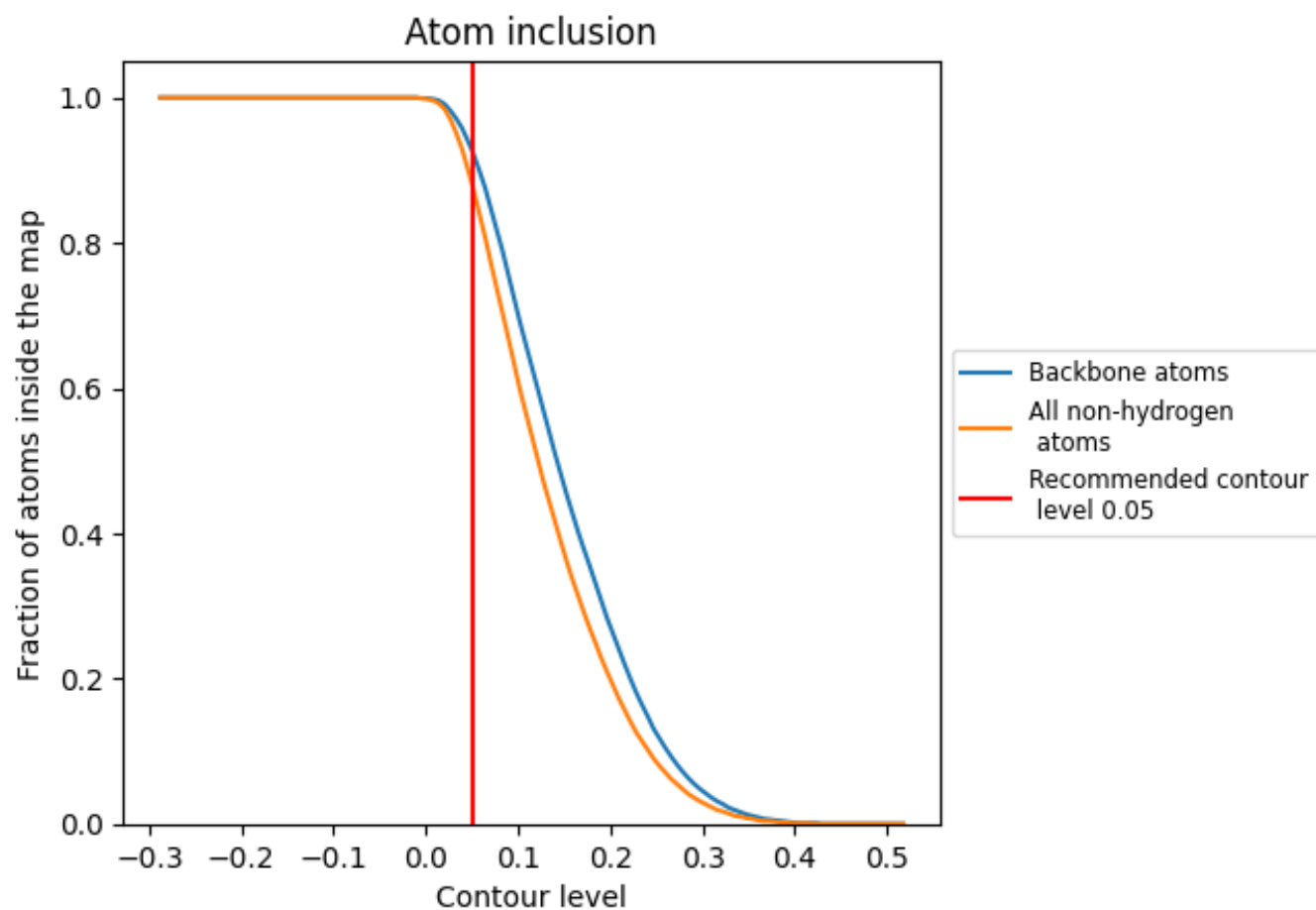
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8820	<div><div></div></div> 0.4740
A	<div><div></div></div> 0.8820	<div><div></div></div> 0.4750
B	<div><div></div></div> 0.8800	<div><div></div></div> 0.4730
C	<div><div></div></div> 0.8830	<div><div></div></div> 0.4740
D	<div><div></div></div> 0.8820	<div><div></div></div> 0.4730
E	<div><div></div></div> 0.8820	<div><div></div></div> 0.4730
F	<div><div></div></div> 0.8820	<div><div></div></div> 0.4740

1.0

0.0

<0.0