



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:30 PM UTC

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:

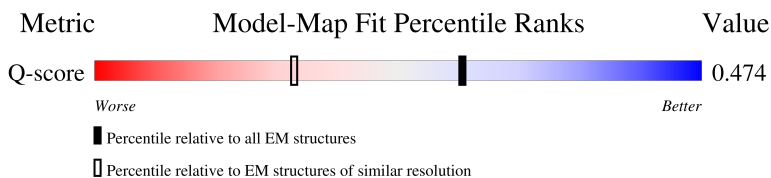
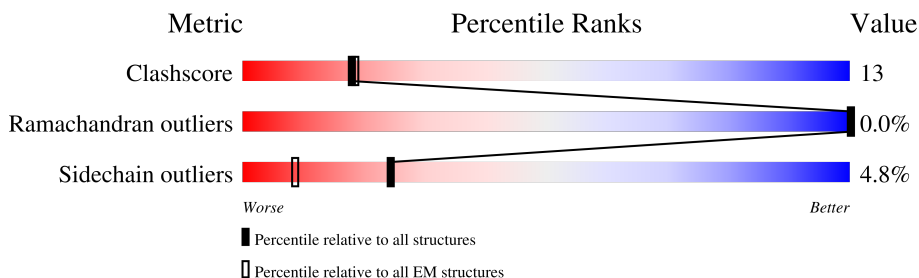
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
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	 5% 63% 25% • 10%
1	B	3069	 5% 63% 26% • 10%
1	C	3069	 5% 61% 27% • 10%
1	D	3069	 5% 63% 26% • 10%

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

2 Entry composition [i](#)

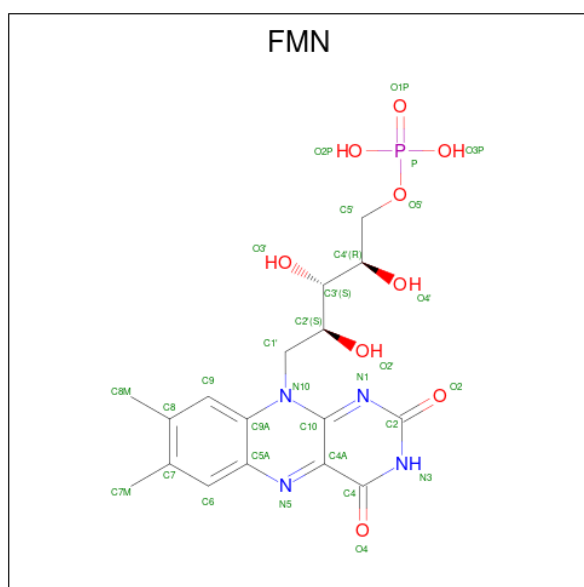
There are 2 unique types of molecules in this entry. The entry contains 124914 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

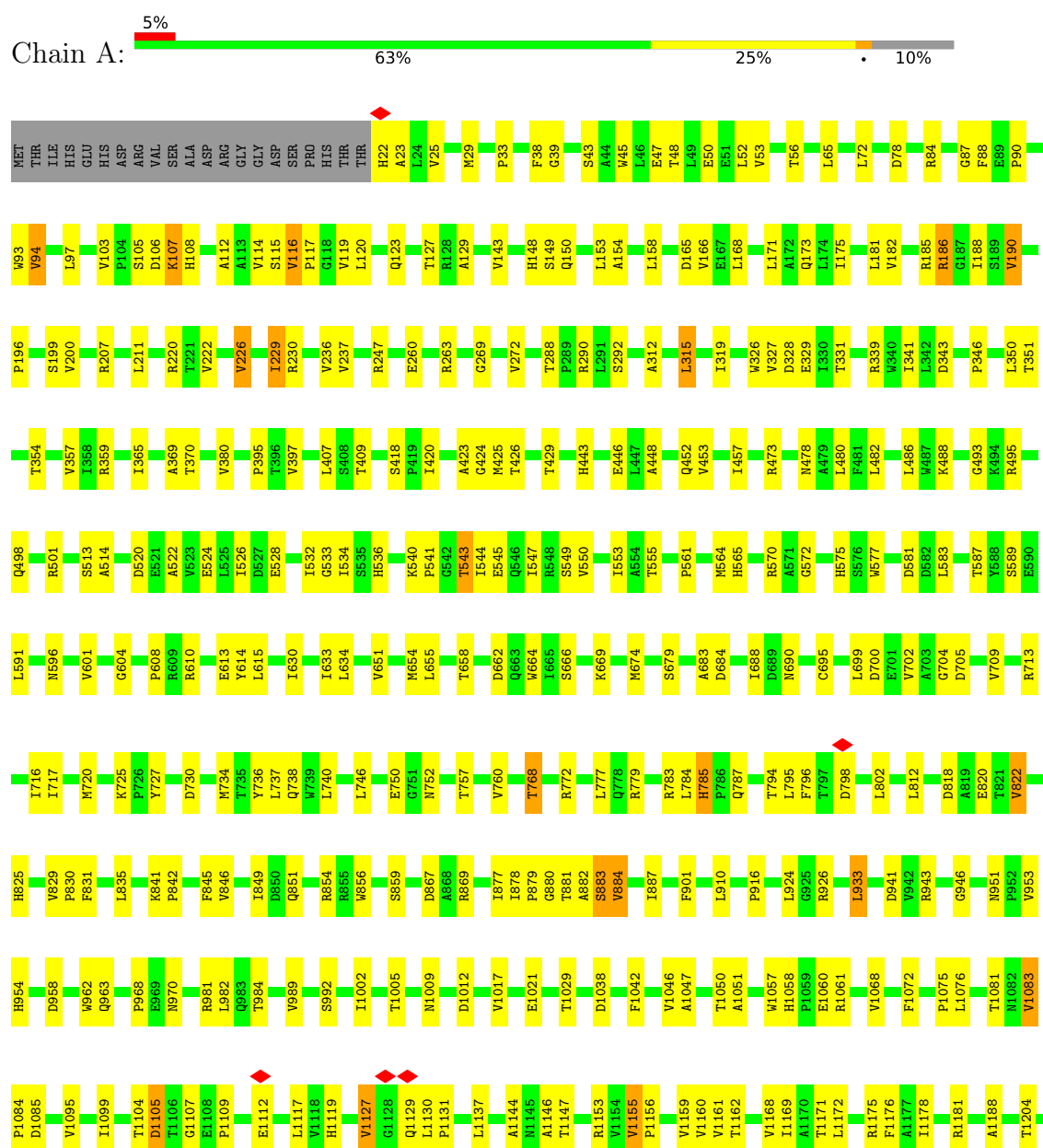


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0
2	D	1	Total 31	C 17	N 4	O 9	P 1	0
2	E	1	Total 31	C 17	N 4	O 9	P 1	0
2	F	1	Total 31	C 17	N 4	O 9	P 1	0

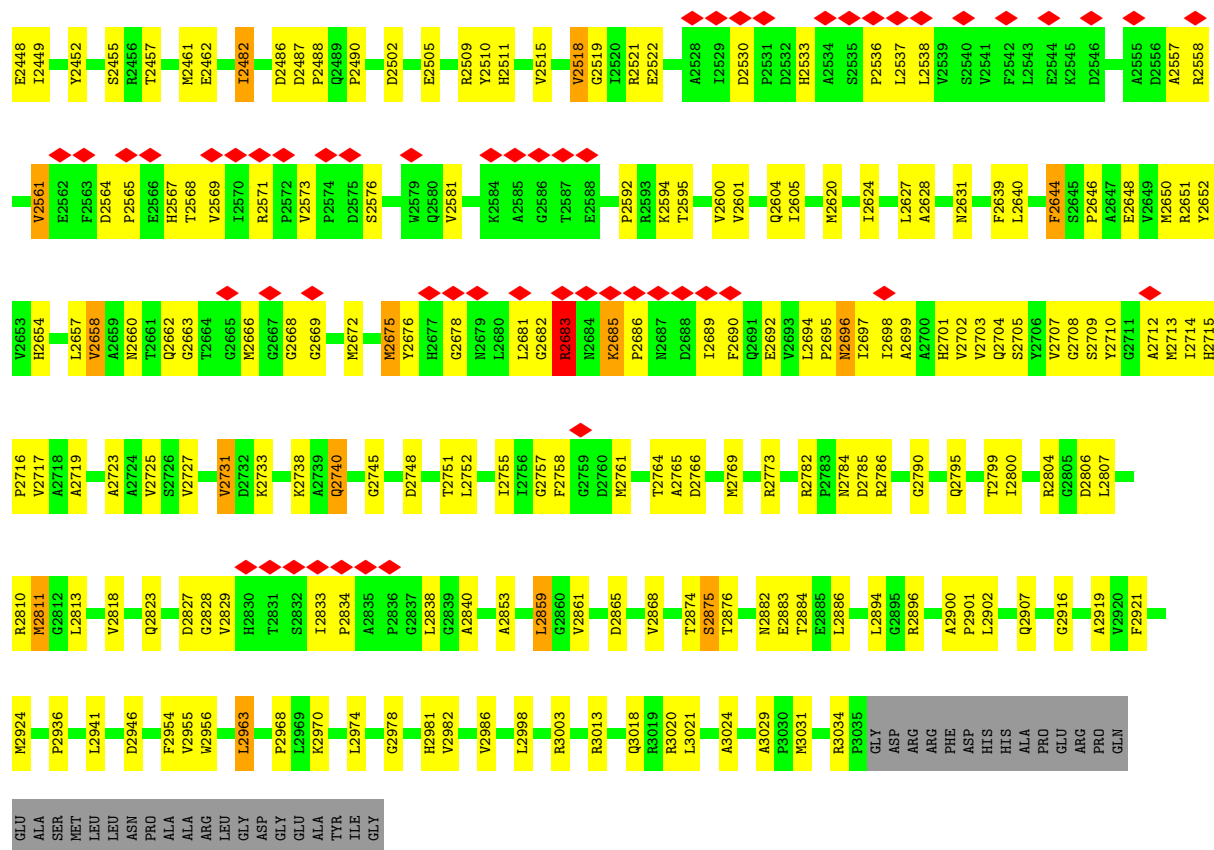
3 Residue-property plots

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.

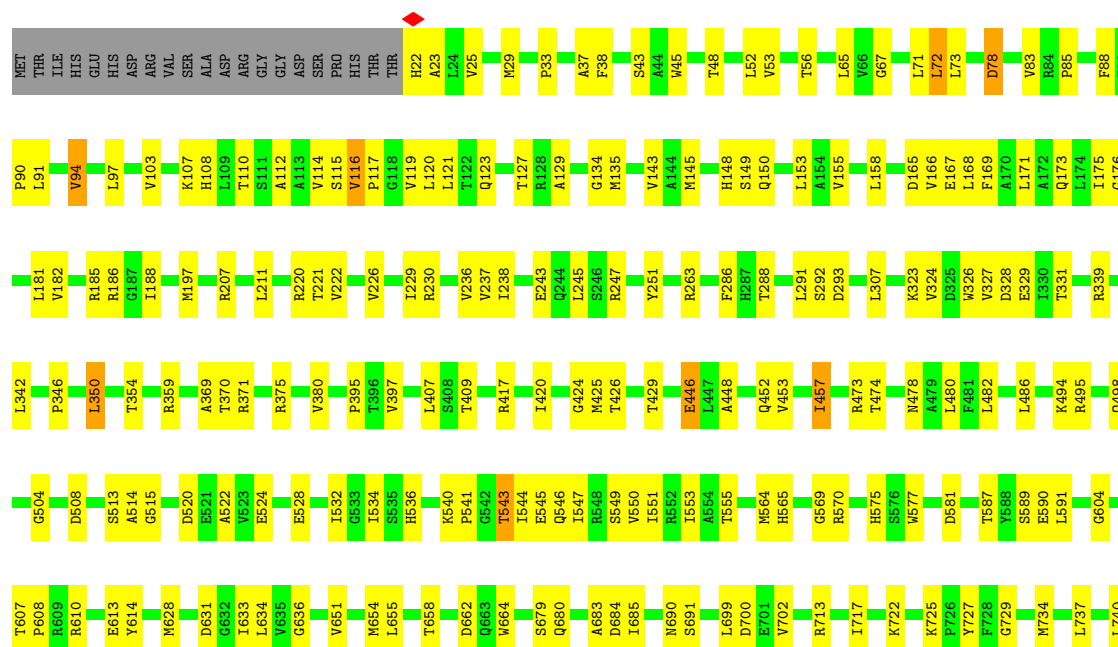
• Molecule 1: 3-oxoacyl-ACP synthase



S2345	L2271	V2186	R2044	GLY	THR	ALA	ASP	A1709	I1617	G1530	S1524	C1447	A1323	R1207
E2360	S2274	D2187	L2050	GLY	VAL	ALA	ALA	H1710	R1618	G1530	Y1525		S1324	R1208
R2367	ASN	L2189	W2051	THR	VAL	THR	THR	S1711	D1619	Y1526	Y1526	A1456	R1325	R1209
S2368	ARG	S2200	L2052	ILE	ALA	ALA	ALA	V1713	L1620	A1527	A1527	L1457	R1326	R1210
P2369	GLY	S2205	L2053	ASP	LEU	THR	THR	N1717	E1624	G1530	G1530	R1460	F1223	
I2370	MET	L2206	D2054		GLY	THR	THR	A1718	P1625			V1461	V1226	
D2373	GLY	H2207	L2058		THR	THR	THR	E1719	L1626	R1533	R1533	F1462	S1227	
L2378	GLY	D2210	E2067		GLY	THR	THR	L1725	D1627	G1534	G1534	H1463	E1246	
A2379	S2283	A2211	E2071		THR	THR	THR	D1729	A1631	E1536	E1536	M1468	S1247	
L2383	A2289	Q2212	Q2074		VAL	THR	THR	T1750	D1632			H1469	V1260	
L2388	A2290	T2213	R2078		GLY	THR	THR	D1731	R1640	E1539	E1539	D1470		
K2391	L2293	T2215	R1976		GLY	GLY	GLY	PR0	R1641	V1542	V1542	V1471	M1253	
A2392	D2294	L2216	E1977		ALA	ALA	PRO	PR0	A1642	E1543	E1543	I1472	W1254	
R2393	A2295	L2217	E1977		MET	VAL	VAL	GLU	E1643	R1544	R1544	P1473	L1255	
E2394	A2296	L2218	L1980		GLY	LEU	LEU	PRO	E1651	R1545	R1545	D1474	S1256	
Q2395	Q2093	L2094	L1980		HIS	THR	THR	GLU	L1652	E1547	E1547	D1475	Q1260	
M2396	F2220	L2098	L1980		HIS	LEU	ASP	ASP	L1653	L1548	L1548	E1476	H1261	
S2397	A2221	L2098	L1980		GLY	ASP	ASP	VAL	Q1656	T1549	T1549	G1477	A1262	
A2398	R2224	R2101	R2101		ALA	ASP	ASP	ALA	F1657	G1550	G1550	R1478	V1263	
A2399	V2225	E2107	E2107		LEU	THR	THR	GLU	V1661	G1551	G1551	S1481	Q1269	
A2400	Q2227	R2113	R2113		ASP	GLY	GLY	GLU	R1662	R1482	R1482	I1388	P1273	
A2401	D2228	R2114	R2114		ALA	THR	THR	PRO	W1663	R1552	R1552	A1274	A1274	
V2402	L2229	W2114	W2114		ALA	VAL	VAL	ALA	I1664	R1553	R1553	H1393	R1275	
D2403	S2230	V2121	V2121		VAL	LEU	LEU	PRO	E1665	S1554	S1554	L1401	L1276	
E2404	E2231	T2122	T2122		ASP	GLY	GLY	ASP	T1666	I1556	I1556	R1488	V1277	
D2405	A2232	G2123	G2123		VAL	THR	THR	VAL	L1670	L1557	L1557	T1404	T1280	
A2406	L2235	A2124	A2124		ALA	ASP	ASP	ALA	F1671	G1560	G1560	T1407	F1283	
E2407	R2235	T2129	T2129		ALA	ASP	ASP	ALA	I1672	I1561	I1561	Q1408	L1284	
L2412	W2240	L2137	L2137		VAL	ALA	ALA	VAL	A1675	D1562	D1562	M1411	V1287	
L2415	K2241	Q2141	Q2141		VAL	ALA	ALA	VAL	E1682	H1566	H1566	A1415	R1288	
P2418	L2242	A2142	A2142		SER	ILE	ILE	VAL	E1686	S1567	S1567	A1416	V1293	
P2419	L2243	L2151	L2151		VAL	GLY	GLY	PRO	I1687	R1568	R1568	Q1417	V1297	
R2420	W2244	D2152	D2152		ALA	GLU	GLU	ALA	G1688			Q1418	E1298	
P2428	A2246	E2153	E2153		ARG	VAL	VAL	ALA	V1689	R1571	R1571	V1419	E1299	
Q2429	Q2247	Y2159	Y2159		GLN	THR	THR	SER	K1690	V1572	V1572	A1420	V1300	
W2430	Q2248	A2167	A2167		VAL	TRP	TRP	ALA	P1693	G1573	G1573	M1422	G1301	
L2433	R2249	R2168	R2168		SER	GLU	GLU	GLY	T1694	V1574	V1574	F1428	I1302	
D2434	L2250	W2020	W2020		VAL	LEU	LEU	PRO	V1695	R1578	R1578	A1507	E1307	
V2435	I2251	L2023	L2023		VAL	GLY	GLY	ARG	A1696	A1589	A1589	I1506	I1308	
A2438	R2261	Q2170	Q2170		LEU	GLY	GLY	ASP	G1697	R1597	R1597	A1434	V1309	
D2439	S2265	W2179	W2179		PRO	TRP	TRP	ALA	L1698	Y1598	Y1598	S1438	D1310	
L2440	R2266	W2180	W2180		ALA	ALA	ALA	VAL	M1701	T1510	T1510	V1439	V1311	
V2441	L2267	A2171	A2171		GLY	THR	THR	PHE	T1702	G1511	G1511	G1440	V1315	
V2442	H2268	N2179	N2179		SER	ALA	ALA	ASP	L1703	P1600	P1600	E1441	V1319	
G2446	V2269	R2036	R2036		HIS	LEU	LEU	ALA	P1706	N1601	N1601	F1512		
	V2270	D2037	D2037		GLY	VAL	VAL	ALA	E1707	L1602	L1602	L1514	L1319	
		R2039	R2039						Y1708	T1608	T1608	E1515		
										F1613	F1613	N1518		
												F1519		
												N1520		
												L1521		



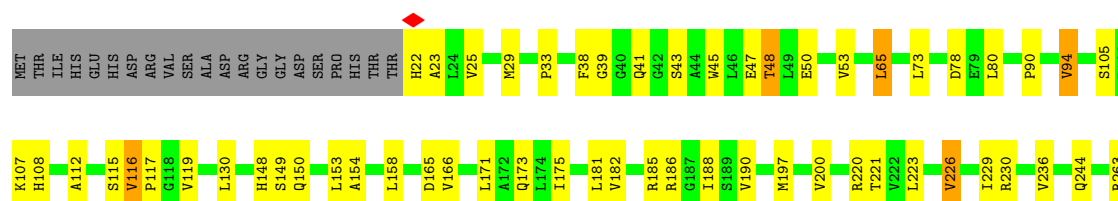
• Molecule 1: 3-oxoacyl-ACP synthase



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	D1012	R854	V744
V2035	PRO	GLY	GLU	P1693	I1594	E1515	E1441	G1339	H1234	V1126	V1017	V745	L746
R2039	GLY	PHE	ASP	R1597	R1597	N1518	A1444	G1340	S1247	V1127	T1020	S859	L746
R2044	GLY	ASP	LEU	V1695	T1694	F1519	L1445	G1342	V1250	G1128	T1020	D867	E750
R2044	GLY	ALA	ALA	A1696	P1600	N1520	A1446	H1343	V1250	Q1129	T1024	L1130	T757
D2054	GLY	ASP	GLY	T1702	M1601	S1524	I1451	M1346	M1253	P1131	T1024	L1130	T757
I2058	GLY	LEU	ALA	K1703	L1602	G1525	I1451	G1347	S1256	M1027	M1027	G880	V760
D2059	ALA	THR	ARG	L1705	L1611	Y1526	A1456	M1348	S1256	R1028	R1028	T881	V760
A2066	THR	LEU	LEU	P1706	R1611	A1527	L1457	E1349	H1261	T1138	T1029	A882	T768
A2066	ASP	LEU	LEU	E1707	I1614	G1530	M1460	R1558	H1261	V1139	D1038	S883	T768
G2071	GLY	ILE	ILE	Y1708	R1618	R1533	V1461	R1359	A1282	A1144	S1039	V884	L777
L1966	LEU	LEU	LEU	V1715	D1619	G1534	V1461	V1360	V1263	H1145	P1040	L778	L777
S2087	ALA	LEU	ALA	E1719	P1622	L1535	G1465	D1362	T1286	A1146	E1041	R887	R779
R2092	LYS	THR	THR	A1723	P1622	E1536	H1469	D1365	R1271	T1147	F1042	T888	R783
Q2093	MET	TYR	TYR	D1729	A1623	A1537	D1470	K1366	R1275	T1149	V1046	P901	L784
I2094	ARG	PRO	PRO	T1730	E1624	L1538	I1471	F1367	L1277	R1153	A1047	T906	H785
T1970	ILE	ILE	ILE	D1731	P1625	E1539	V1472	T1368	V1276	V1154	T1050	T906	P786
G1975	ASP	TYR	GLY	PRO	L1626	E1539	F1473	D1382	G1278	V1155	A1051	L910	Q787
R1976	GLY	GLY	GLN	GLU	D1627	V1542	R1474	F1374	M1279	F1156	V1068	L910	D788
E1977	ALA	ILE	ILE	PRO	L1637	E1543	D1475	S1375	H1279	V1157	H1058	P916	T794
G1978	VAL	PRO	PRO	GLU	A1631	R1544	E1476	V1376	L1284	F1157	P1059	P916	L795
V1979	LEU	GLY	GLY	PRO	P1632	R1545	E1476	V1376	L1284	S1158	P1059	L924	F796
L1980	ASP	LEU	LEU	GLU	Y1633	R1546	L1477	D1381	V1287	V1159	R1061	L924	F796
V2121	ASP	ASP	ASP	ASP	V1636	R1547	G1478	R1382	R1288	V1160	R1061	R926	T797
T2122	ILE	ILE	ILE	GLU	L1637	E1547	R1479	D1382	R1288	V1161	V1068	R926	D798
G2123	ASN	ILE	ASN	GLU	L1637	V1548	S1480	I1387	V1293	T1162	V1068	L933	P805
A2124	ALA	ASP	ASP	PRO	R1640	T1549	N1481	I1388	V1297	V1168	F1072	L937	L812
I2129	ALA	ILE	ILE	ALA	P1641	G1550	Y1482	H1393	G1301	A1170	T1081	L937	L812
V2133	ASP	THR	THR	GLY	P1642	G1551	R1483	H1396	I1302	T1171	N1082	R943	D818
R2136	GLY	ARG	ARG	PRO	E1643	R1552	L1484	P1397	E1307	L1172	V1083	G946	V822
L2137	ALA	THR	THR	ALA	M1644	R1553	A1485	D1398	E1307	E1173	P1084	R947	Q823
R2137	ALA	VAL	VAL	ALA	A1645	S1554	A1485	G1399	T1308	R1175	D1085	P952	L824
L2142	VAL	LEU	LEU	PRO	R1646	F1555	R1488	V1400	V1309	F1176	L1087	P952	H825
T2143	ASP	GLY	GLY	ASP	L1652	I1556	Q1491	L1401	D1310	A1177	V1088	V953	V829
V2144	ASP	ARG	ARG	VAL	F1657	L1557	T1492	L1402	V1311	I1178	V1088	H954	P830
I2145	ASN	ASN	ASN	VAL	F1657	L1557	D1493	T1404	V1315	R1181	V1099	P958	F831
L2151	LYS	LYS	LYS	GLU	V1661	G1560	L1494	Q1405	V1319	T1182	I1099	P958	F831
D2152	ILE	LYS	LYS	ALA	R1662	I1561	L1494	F1406	L1319	A1188	T1104	P963	T834
E2153	ALA	PRO	PRO	ALA	W1663	D1562	D1495	T1407	M1321	A1188	D1105	P963	L835
R2155	ALA	VAL	VAL	PRO	I1664	H1566	D1496	Q1408	V1320	T1204	T1106	P968	C836
E2154	ALA	ILE	ILE	ALA	E1665	S1567	A1497	V1409	M1322	T1204	T1106	P968	C836
A2003	ALA	ALA	ALA	PRO	T1666	R1568	D1498	A1410	A1323	R1207	G1107	P969	L839
P2004	ALA	GLY	GLY	ALA	L1670	R1571	A1501	M1411	S1324	R1207	G1107	P969	G840
D2005	ALA	LEU	LEU	ALA	F1671	R1571	F1502	A1417	A1325	R1208	E1108	P970	K841
S2006	ASN	VAL	VAL	SER	I1672	E1576	G1505	Q1418	R1326	R1209	V1110	P974	P842
E2007	LYS	LYS	LYS	GLY	F1684	E1576	I1506	V1419	L1327	F1223	V1111	L982	V843
L2008	THR	THR	THR	GLY	V1685	R1579	G1506	T1433	V1333	V1226	G1113	L982	V843
I2009	ALA	ILE	ILE	ARG	E1686	D1582	A1507	T1433	V1334	V1226	G1113	L982	V843
D2010	ASP	LEU	LEU	PRO	I1687	D1582	E1508	S1438	F1336	V1226	G1113	L982	V843
L2011	ASP	ASP	ASP	PRO	G1688	M1585	S1509	S1438	F1336	V1226	G1113	L982	V843
E2015	ASP	ASP	ASP	PRO	G1688	M1585	S1509	S1438	F1336	V1226	G1113	L982	V843



• Molecule 1: 3-oxoacyl-ACP synthase



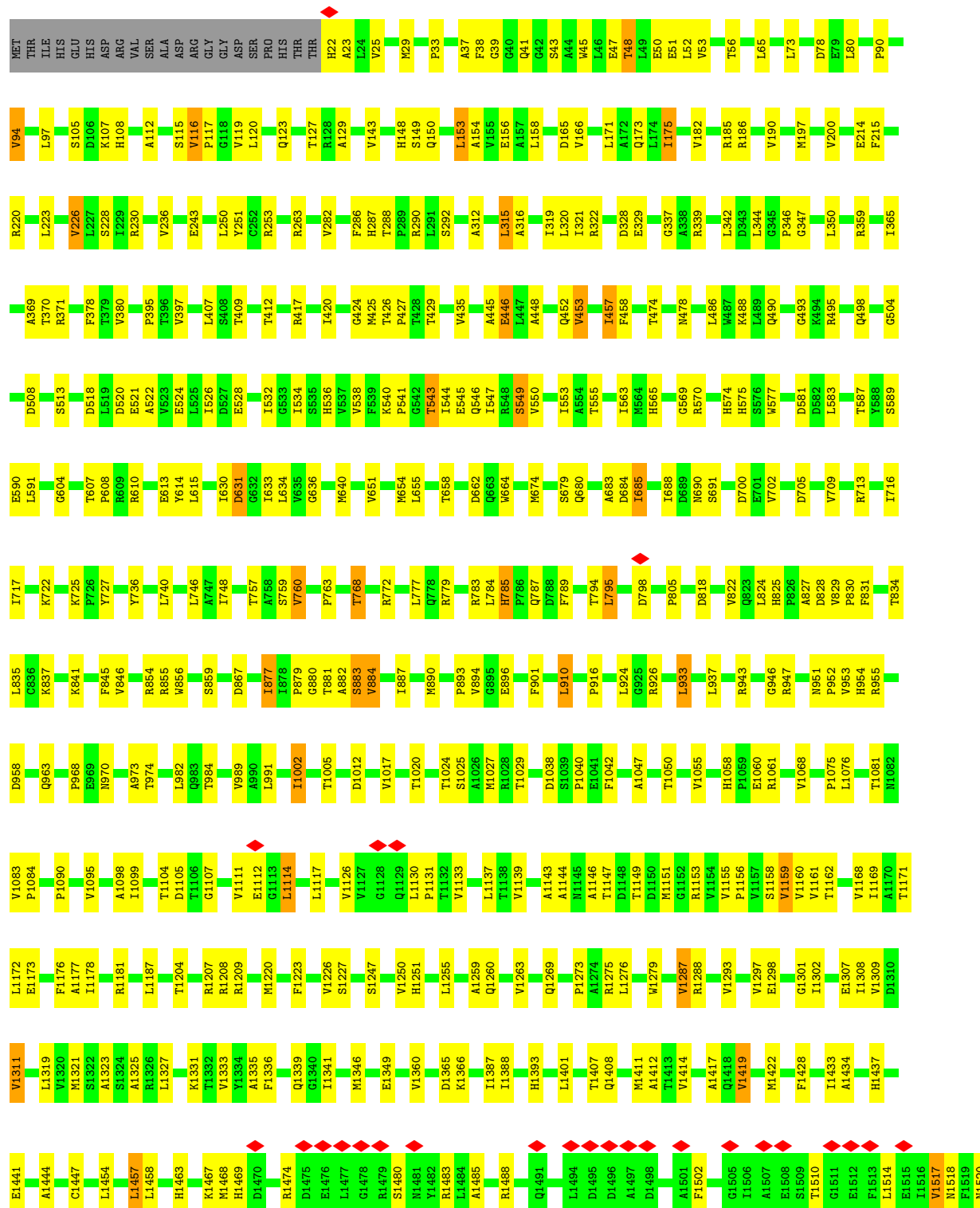
PRO	R1662	F1565	D1498	M1411	V1287	I1169	L1087	N970	K841	P726	G604	L519	T412
GLU	W1663	H1666	A1501	A1412	R1288	A1170	G1088	T974	P842	Y727	T607	D520	R417
GLU	E1665	ASP	F1502	V1414	V1293	E1171	P1090	L982	H845	T735	P608	A522	F286
GLU	P1666	R1568	F1502	V1414	V1293	E1173	P1090	L982	H845	T735	P608	A522	F286
PRO	Q1667	R1571	G1505	A1418	V1297	E1174	V1095	T984	H855	Q738	R610	E524	I420
VAL	D1668	R1571	G1505	A1418	V1297	E1174	V1095	T984	H855	Q738	R610	E524	I420
ALA	L1669	E1576	I1506	V1419	G1301	R1175	A1098	V989	B613	W739	E823	I526	A423
ALA	L1669	E1576	I1506	V1419	G1301	R1175	A1098	V989	B613	W739	E823	I526	A423
GLU	L1670	E1576	I1506	V1419	G1301	R1175	A1098	V989	B613	W739	E823	I526	A423
SER	F1671	PRO	E1508	M1422	I1302	A1177	I1099	A990	Y614	L740	L615	E528	M425
PRO	L1672	PRO	S1509	F1428	E1307	I1178	I1099	L991	H866	L746	L615	L529	P427
ALA	A1675	ALA	T1510	F1428	E1307	I1178	V1103	I1002	H866	L746	L615	L529	P427
PRO	A1675	ALA	T1510	F1428	E1307	I1178	V1103	I1002	H866	L746	L615	L529	P427
ASP	G1678	I1594	E1511	I1433	D1310	L1187	T1016	T1005	I877	I748	I630	I532	T429
VAL	G1678	I1594	E1511	I1433	D1310	L1187	T1016	T1005	I877	I748	I630	I532	T429
SER	E1682	Y1598	F1513	A1434	V1311	D1188	E1108	T1005	I877	I748	I630	I532	T429
GLU	R1683	I1599	F1513	A1434	V1311	D1188	E1108	T1005	I877	I748	I630	I532	T429
ALA	I1599	ALA	E1515	E1441	L1319	P1190	P1109	D1012	P879	A758	I534	I534	I434
ALA	E1686	M1601	I1516	E1441	L1319	P1190	P1109	D1012	P879	A758	I534	I534	I434
PRO	I1687	P1602	V1517	A1444	V1320	G1194	V1111	V1017	T881	V760	L634	H536	W444
PRO	I1687	P1602	V1517	A1444	V1320	G1194	V1111	V1017	T881	V760	L634	H536	W444
VAL	G1688	V1603	F1518	I1445	V1320	G1194	V1111	V1017	T881	V760	L634	H536	W444
VAL	G1688	V1603	F1518	I1445	V1320	G1194	V1111	V1017	T881	V760	L634	H536	W444
ALA	V1689	P1604	N1520	C1446	A1323	S1322	E1112	G636	A882	V538	L447	F539	E446
ALA	V1689	P1604	N1520	C1446	A1323	S1322	E1112	G636	A882	V538	L447	F539	E446
PRO	P1693	T1608	L1521	V1448	R1326	T1204	G1113	T1020	V894	P763	G636	K540	A448
ALA	L1694	ALA	L1521	V1448	R1326	T1204	G1113	T1020	V894	P763	G636	K540	A448
ALA	L1694	ALA	L1521	V1448	R1326	T1204	G1113	T1020	V894	P763	G636	K540	A448
SER	V1695	R1618	Q1525	L1454	T1332	M1220	V1126	T1024	I887	R772	V651	G542	Q452
SER	V1695	R1618	Q1525	L1454	T1332	M1220	V1126	T1024	I887	R772	V651	G542	Q452
SER	V1695	R1618	Q1525	L1454	T1332	M1220	V1126	T1024	I887	R772	V651	G542	Q452
GLY	G1697	D1619	A1527	L1454	Y1334	Y1334	Y1127	A1026	M776	M776	M654	E545	I457
GLY	G1697	D1619	A1527	L1454	Y1334	Y1334	Y1127	A1026	M776	M776	M654	E545	I457
GLY	G1697	D1619	A1527	L1454	Y1334	Y1334	Y1127	A1026	M776	M776	M654	E545	I457
PRO	L1698	L1620	I1528	L1457	F1337	F1223	G1128	T1029	R779	R779	L655	Q546	F458
PRO	L1698	L1620	I1528	L1457	F1337	F1223	G1128	T1029	R779	R779	L655	Q546	F458
ARG	E1624	ARG	G1530	L1458	P1337	V1226	L1130	D1038	F901	L784	D622	I544	Q464
ARG	E1624	ARG	G1530	L1458	P1337	V1226	L1130	D1038	F901	L784	D622	I544	Q464
ARG	E1624	ARG	G1530	L1458	P1337	V1226	L1130	D1038	F901	L784	D622	I544	Q464
PRO	T1700	PRO	L1630	L1458	P1337	V1226	L1130	D1038	F901	L784	D622	I544	Q464
PRO	T1700	PRO	L1630	L1458	P1337	V1226	L1130	D1038	F901	L784	D622	I544	Q464
ASP	L1702	ASP	F1537	H1463	Q1339	T1132	P1133	S1039	M674	P786	M674	A554	T474
ASP	L1702	ASP	F1537	H1463	Q1339	T1132	P1133	S1039	M674	P786	M674	A554	T474
LEU	L1703	LEU	L1538	L1467	F1366	S1247	V1133	F1042	L910	Q787	Q680	E556	Q476
LEU	L1703	LEU	L1538	L1467	F1366	S1247	V1133	F1042	L910	Q787	Q680	E556	Q476
LEU	L1703	LEU	L1538	L1467	F1366	S1247	V1133	F1042	L910	Q787	Q680	E556	Q476
LEU	L1704	LEU	L1538	L1467	F1366	S1247	V1133	F1042	L910	Q787	Q680	E556	Q476
LEU	L1704	LEU	L1538	L1467	F1366	S1247	V1133	F1042	L910	Q787	Q680	E556	Q476
VAL	L1705	VAL	E1536	H1469	M1346	H1251	A1143	N1048	L924	T794	A683	K560	T351
VAL	L1705	VAL	E1536	H1469	M1346	H1251	A1143	N1048	L924	T794	A683	K560	T351
PHE	P1706	PHE	L1537	H1469	M1346	H1251	A1143	N1048	L924	T794	A683	K560	T351
ASP	E1707	ASP	L1538	L1474	F1374	Q1260	V1149	T1055	L937	D818	S691	R570	T354
ALA	Y1708	ALA	L1538	L1474	F1374	Q1260	V1149	T1055	L937	D818	S691	R570	T354
ALA	Y1708	ALA	L1538	L1474	F1374	Q1260	V1149	T1055	L937	D818	S691	R570	T354
ASP	A1709	ASP	E1541	D1475	D1365	G1252	A1143	N1048	L924	T794	A683	K560	T354
ASP	A1709	ASP	E1541	D1475	D1365	G1252	A1143	N1048	L924	T794	A683	K560	T354
ALA	S1711	ALA	E1543	E1476	D1366	L1255	A1146	T1154	G925	L795	D684	H574	N376
ALA	S1711	ALA	E1543	E1476	D1366	L1255	A1146	T1154	G925	L795	D684	H574	N376
THR	S1711	THR	E1543	E1476	D1366	L1255	A1146	T1154	G925	L795	D684	H574	N376
LEU	L1713	LEU	R1544	L1477	R1544	Q1263	V1150	T1058	L943	W822	C695	H574	N376
ALA	L1713	ALA	R1544	L1477	R1544	Q1263	V1150	T1058	L943	W822	C695	H574	N376
LEU	L1713	LEU	R1544	L1477	R1544	Q1263	V1150	T1058	L943	W822	C695	H574	N376
LEU	L1713	LEU	R1544	L1477	R1544	Q1263	V1150	T1058	L943	W822	C695	H574	N376
ILE	A1718	ILE	E1547	N1480	H1388	T1264	M1151	P1059	G946	Q823	L824	H575	L377
ALA	A1718	ALA	E1547	N1480	H1388	T1264	M1151	P1059	G946	Q823	L824	H575	L377
LEU	E1719	LEU	L1548	R1482	H1393	R1271	V1155	R1061	R947	H825	L699	W577	T379
LEU	E1719	LEU	L1548	R1482	H1393	R1271	V1155	R1061	R947	H825	L699	W577	T379
SER	R1720	SER	L1549	L1484	D1398	A1274	P1156	R1061	R947	H825	L699	W577	T379
SER	R1720	SER	L1549	L1484	D1398	A1274	P1156	R1061	R947	H825	L699	W577	T379
ALA	M1644	ALA	Q1550	A1485	D1398	A1274	P1156	R1061	R947	H825	L699	W577	T379
ALA	M1644	ALA	Q1550	A1485	D1398	A1274	P1156	R1061	R947	H825	L699	W577	T379
LYS	L1725	LYS	G1551	R1488	T1404	R1276	S1158	V1068	N951	W829	V702	D511	G504
LYS	L1725	LYS	G1551	R1488	T1404	R1276	S1158	V1068	N951	W829	V702	D511	G504
MET	D1729	MET	R1552	A1514	Q1405	R1276	V1159	P1075	P952	P830	A703	D582	D608
MET	D1729	MET	R1552	A1514	Q1405	R1276	V1159	P1075	P952	P830	A703	D582	D608
ARG	L1730	ARG	L1653	L1653	F1406	L1276	V1159	L1076	R954	F831	R713	L583	T396
ARG	L1730	ARG	L1653	L1653	F1406	L1276	V1159	L1076	R954	F831	R713	L583	T396
ILE	D1731	ILE	E1554	T1407	A1280	W1279	V1160	P1075	P953	T834	T717	T587	S513
ASP	PRD	ASP	S1554	Q1408	A1280	W1279	V1160	P1075	P953	T834	T717	T587	S513
GLN	GLU	GLN	F1655	Q1408	A1280	W1279	V1160	P1075	P953	T834	T717	T587	S513
GLN	GLU	GLN	F1655	Q1408	A1280	W1279	V1160	P1075	P953	T834	T717	T587	S513
ILE	PRD	ILE	L1556	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
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GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1165	P1084	P968	L839	K722	L591	I516
GLU	GLU	GLU	L1557	L1494	V1409	R1282	D1						



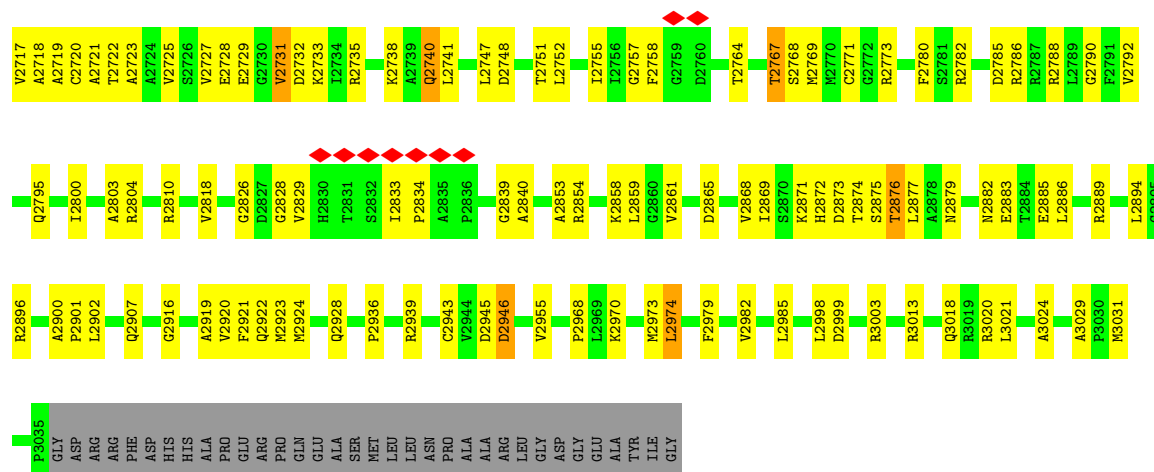
MET
LEU
LEU
ASN
PRO
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GLY
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GLY
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ALA
TYR
ILE
GLY

● Molecule 1: 3-oxoacyl-ACP synthase

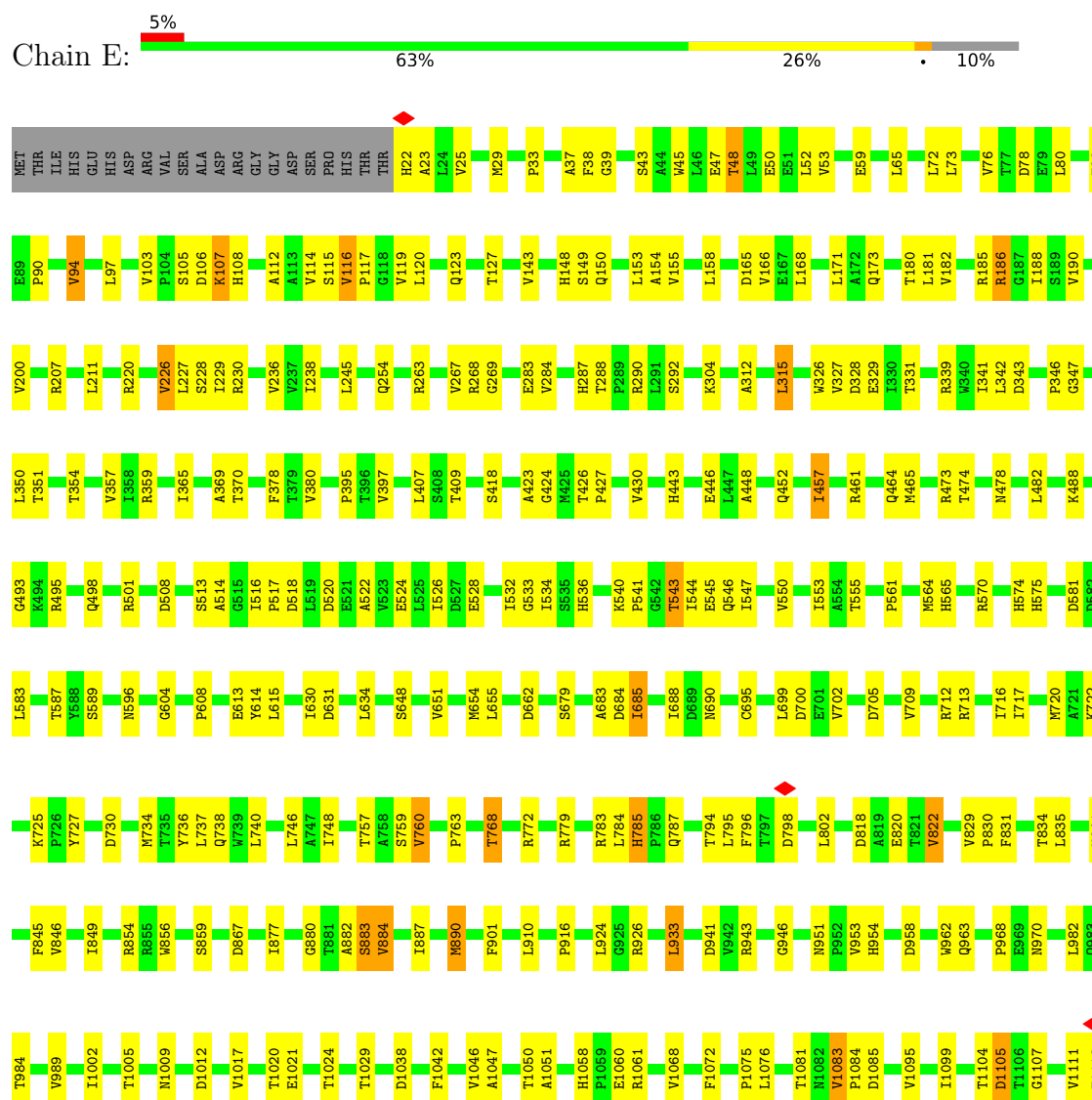
Chain D: 5% 63% 26% 10%





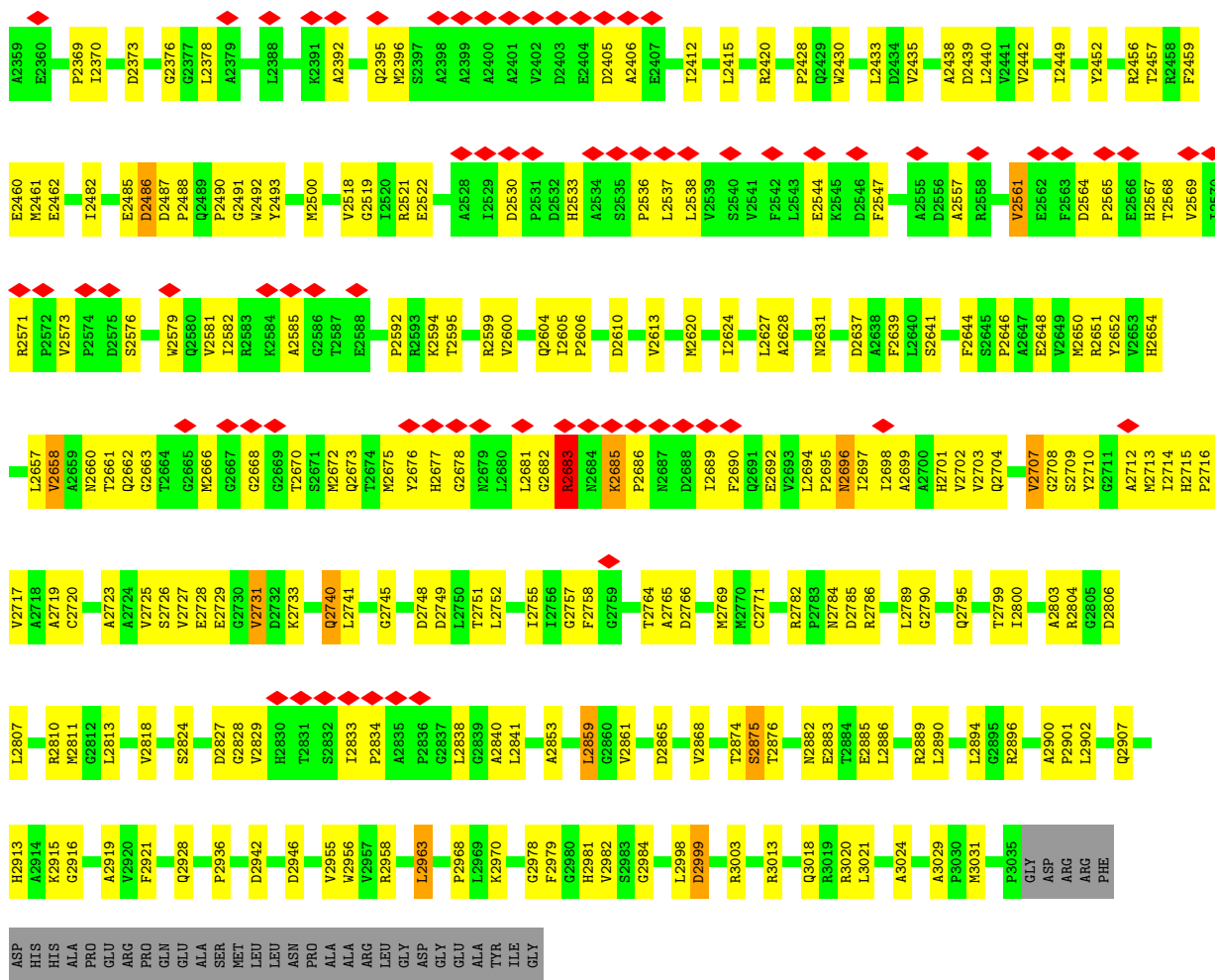


• Molecule 1: 3-oxoacyl-ACP synthase

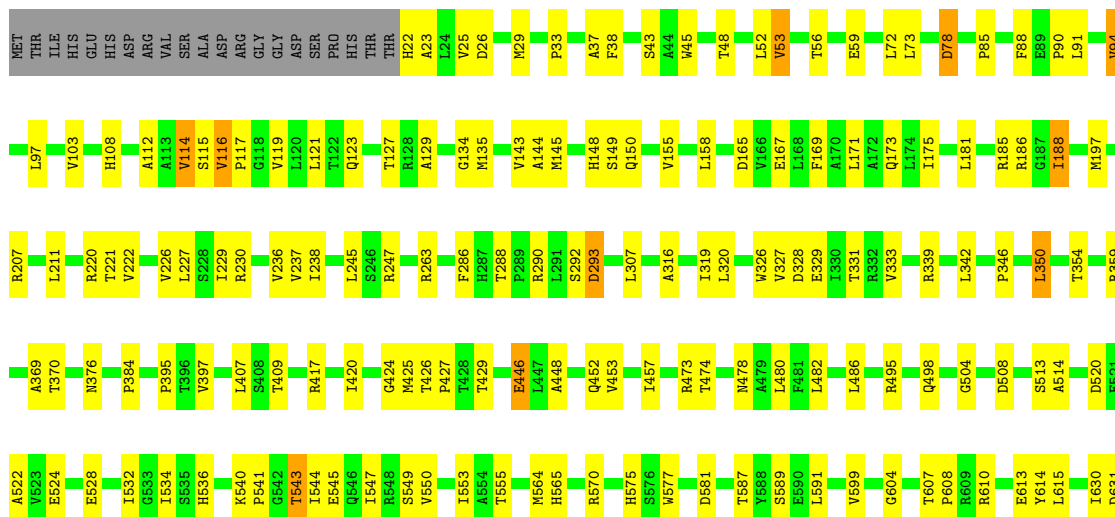




WORLDWIDE
PDB
PROTEIN DATA BANK



• 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	P2881	S2768	E2692	K2696	I2520	I2412	D2329	A2259	D2166	L2011
A3029	N2882	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	E2885	R2782	I2697	W2614	D2530	P2419	A2334	L2267	L2175	V2035
P3035	L2886	D2785	T2698	L2627	P2531	R2420	V2336	H2268	N2179	R2039
GLY	R2889	D2786	A2699	A2628	H2533	W2430	E2337	V2269	M2180	R2044
ASP	L2894	R2787	V2702	N2631	A2534	L2433	G2340	G2273	A2188	L2052
ARG	G2895	Q2704	V2703	D2637	S2535	D2434	V2341	S2274	E2191	T2053
ARG	R2896	S2705	Q2704	D2637	P2536	V2435	S2345	PRO	W2192	D2054
ASP	A2900	T2706	A2638	L2537	L2537	A2438	M2349	ARG	Q2197	T2058
HIS	Q2795	Q2708	F2639	L2537	V2539	L2439	A2350	GLY	L2201	A2066
HIS	G2796	L2640	L2640	L2539	S2540	L2440	A2351	GLY	E2202	E2067
ALA	Q2796	S2641	S2641	S2540	V2541	V2441	C2357	GLY	R2068	R2068
ALA	W2710	F2644	F2644	V2541	P2542	V2442	E2360	GLY	S2087	S2087
PRO	G2711	E2648	E2648	L2543	L2543	V2443	S2361	GLY	H2207	H2207
GLU	A2712	Y2652	Y2652	E2544	E2544	V2444	K2362	GLY	I2208	I2208
ARG	M2713	H2654	H2654	E2545	E2545	G2445	V2363	GLY	K2209	K2209
PRO	D2800	R2654	R2654	D2546	D2546	G2446	E2366	GLY	Q2093	Q2093
ARG	A2803	L2657	L2657	A2555	A2555	Y2452	A2366	GLY	T2094	T2094
GLN	R2804	V2658	V2658	D2556	D2556	T2457	R2367	GLY	R2101	R2101
GLU	G2805	A2658	A2658	A2557	A2557	M2461	S2368	GLY	E2107	E2107
GLU	D2806	M2660	M2660	R2558	R2558	V2463	P2369	GLY	R2113	R2113
ALA	L2807	Q2662	Q2662	V2561	V2561	E2464	I2370	GLY	Y2114	Y2114
ALA	L2807	G2663	G2663	E2562	E2562	L2467	D2373	GLY	V2118	V2118
LEU	H2830	T2664	T2664	F2563	F2563	L2475	L2374	GLY	A2221	A2221
GLY	T2831	G2665	G2665	P2564	P2564	L2475	L2375	GLY	V2121	V2121
ASP	S2832	M2666	M2666	P2565	P2565	L2475	L2375	GLY	G2223	G2223
GLY	I2833	Q2667	Q2667	P2566	P2566	L2482	L2378	GLY	R2224	R2224
GLU	P2834	G2668	G2668	E2566	E2566	R2483	A2379	GLY	V2225	V2225
TYR	A2835	M2672	M2672	H2567	H2567	D2486	L2388	GLY	V2226	V2226
ILE	P2836	Q2673	Q2673	T2568	T2568	D2487	R2309	GLY	G2227	G2227
GLY	A2840	T2674	T2674	V2569	V2569	P2488	V2310	GLY	D2228	D2228
GLY	A2853	M2675	M2675	L2570	L2570	Q2489	S2311	GLY	V2134	V2134
GLY	A2853	Y2676	Y2676	V2573	V2573	G2491	L2312	GLY	A2135	A2135
GLY	A2853	H2677	H2677	P2574	P2574	T2495	L2313	GLY	R2136	R2136
GLY	A2853	N2679	N2679	D2575	D2575	E2499	A2314	GLY	L2137	L2137
GLY	A2853	L2680	L2680	S2576	S2576	M2500	A2315	GLY	E2231	E2231
GLY	A2853	G2682	G2682	W2579	W2579	E2499	L2317	GLY	A2232	A2232
GLY	A2853	R2683	R2683	Q2580	Q2580	M2500	G2318	GLY	R2235	R2235
GLY	A2853	N2684	N2684	V2581	V2581	H2511	W2319	GLY	A2146	A2146
GLY	A2853	K2685	K2685	T2582	T2582	Q2515	T2320	GLY	M2238	M2238
GLY	A2853	P2686	P2686	R2583	R2583	Q2516	R2321	GLY	D2152	D2152
GLY	A2853	N2687	N2687	K2584	K2584	R2517	G2302	GLY	E2153	E2153
GLY	A2853	D2688	D2688	A2585	A2585	Q2517	T2323	GLY	R2154	R2154
GLY	A2853	L2689	L2689	T2587	T2587	E2517	GLY	GLY	E2155	E2155
GLY	A2853	L2689	L2689	E2588	E2588	R2517	MET	GLY	V2242	V2242
GLY	A2853	L2689	L2689	E2588	E2588	R2517	GLY	GLY	L2243	L2243
GLY	A2853	L2689	L2689	E2588	E2588	R2517	GLY	GLY	V2245	V2245
GLY	A2853	L2689	L2689	E2588	E2588	R2517	GLY	GLY	A2246	A2246
GLY	A2853	L2689	L2689	E2588	E2588	R2517	GLY	GLY	V2247	V2247

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%)	25	49
1	B	2132/2359 (90%)	2038 (96%)	94 (4%)	25	49
1	C	2129/2359 (90%)	2010 (94%)	119 (6%)	19	40
1	D	2135/2359 (90%)	2025 (95%)	110 (5%)	21	43
1	E	2130/2359 (90%)	2022 (95%)	108 (5%)	21	44
1	F	2133/2359 (90%)	2038 (96%)	95 (4%)	24	48
All	All	12791/14154 (90%)	12171 (95%)	620 (5%)	24	46

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	D	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	3101	-	33,33,33	1.07	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	A	3101	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	E	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	D	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	B	3101	-	-	2/18/18/18	0/3/3/3
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	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

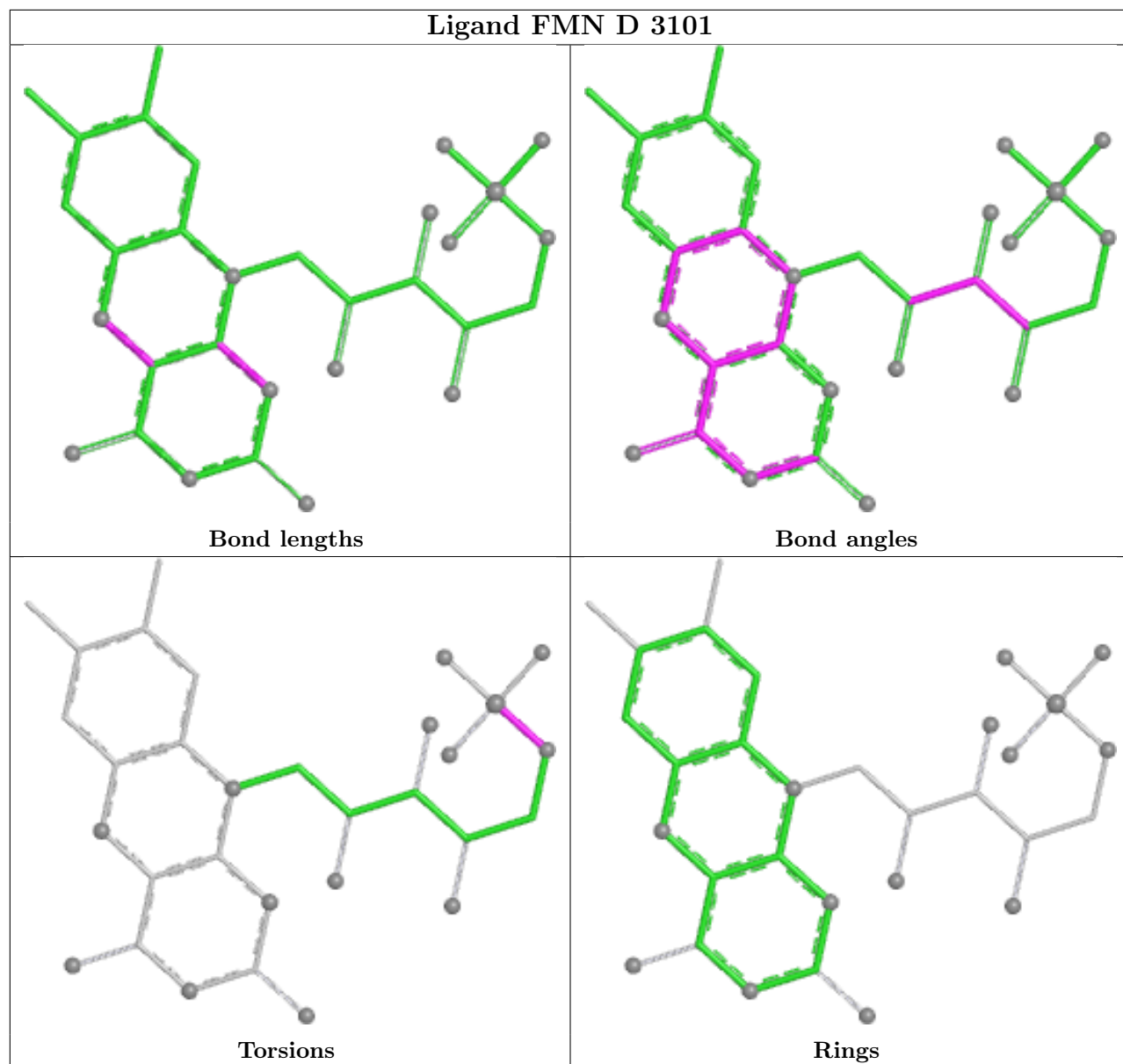
There are no ring outliers.

6 monomers are involved in 25 short contacts:

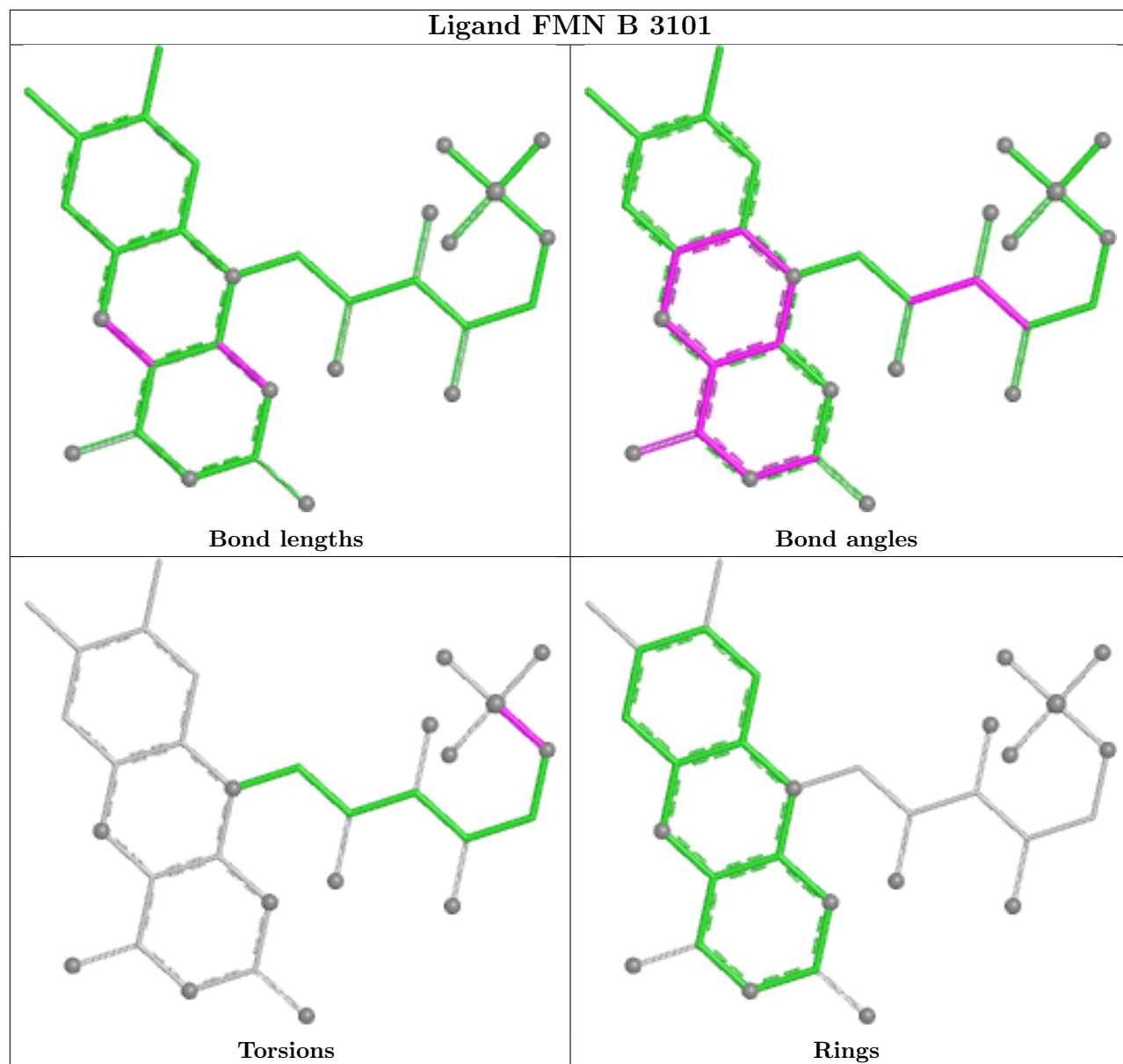
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3101	FMN	4	0
2	B	3101	FMN	4	0
2	A	3101	FMN	4	0
2	E	3101	FMN	4	0
2	F	3101	FMN	4	0
2	C	3101	FMN	5	0

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.

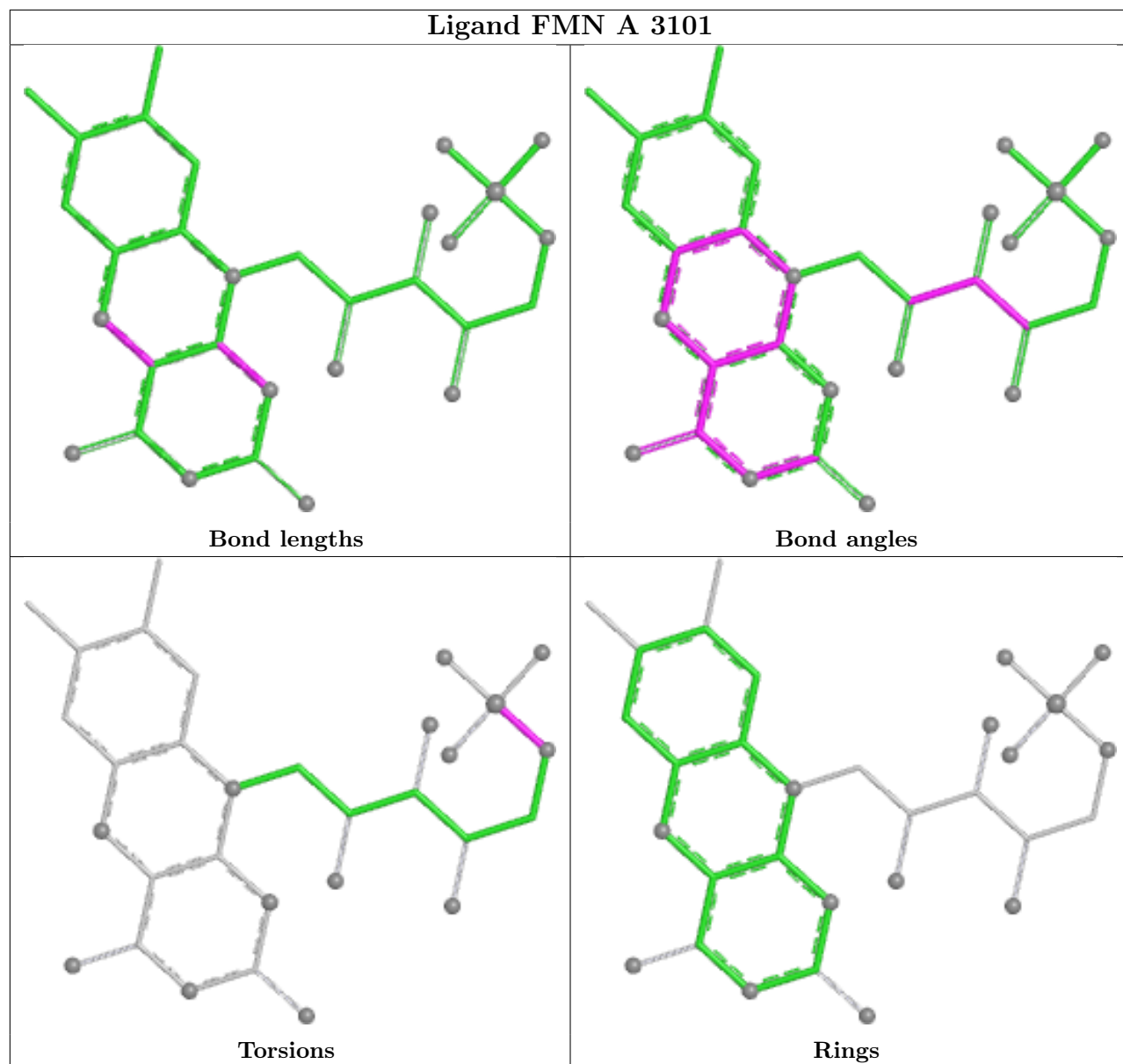
Ligand FMN D 3101

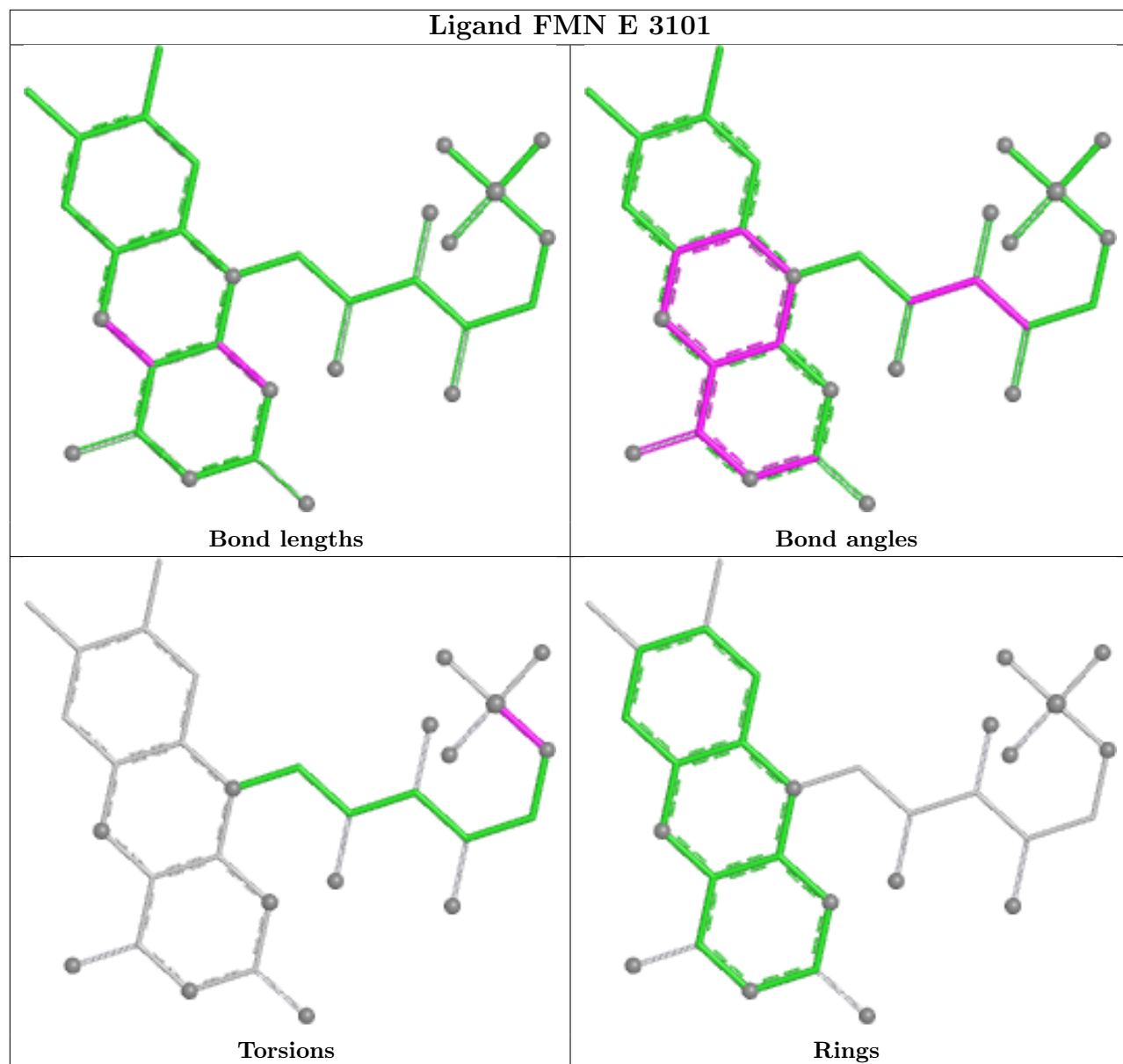


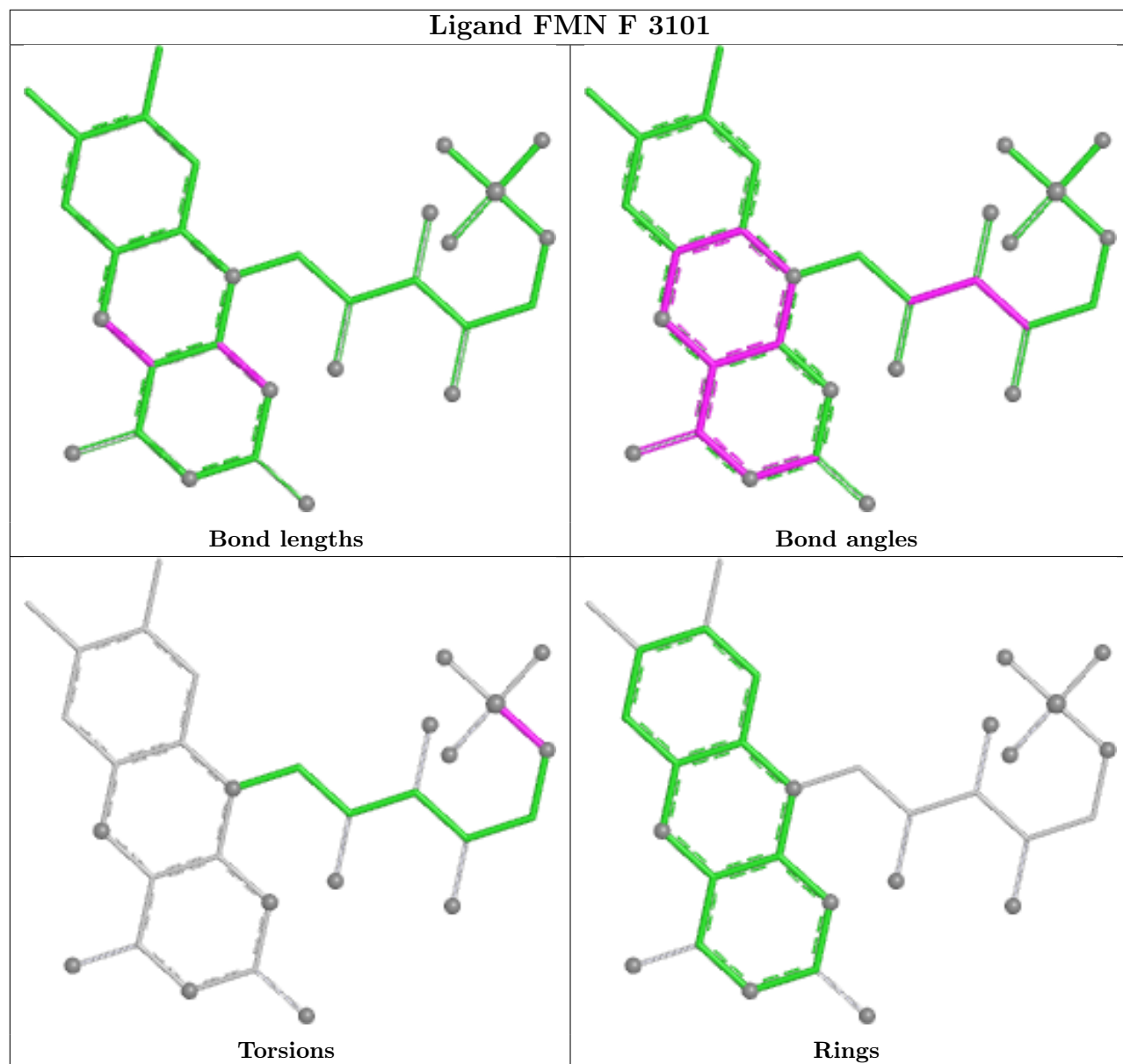
Ligand FMN B 3101

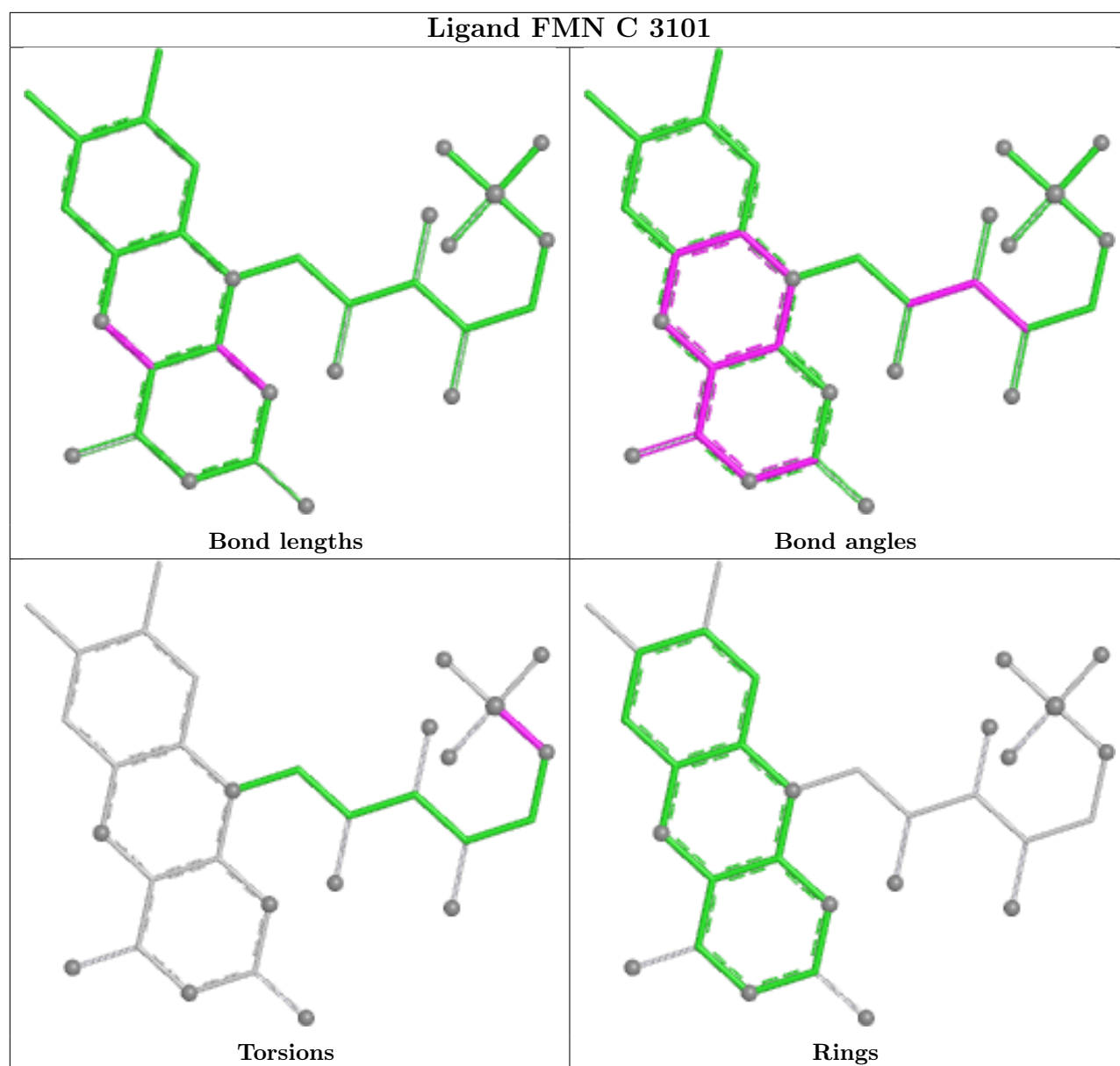


Ligand FMN A 3101









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.

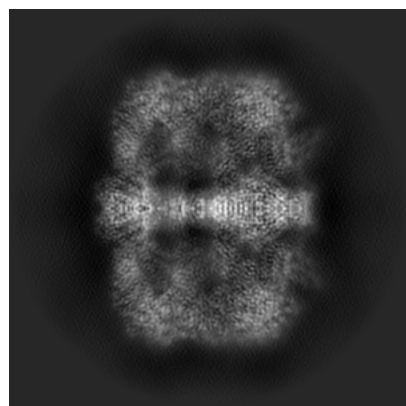
6 Map visualisation [i](#)

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.

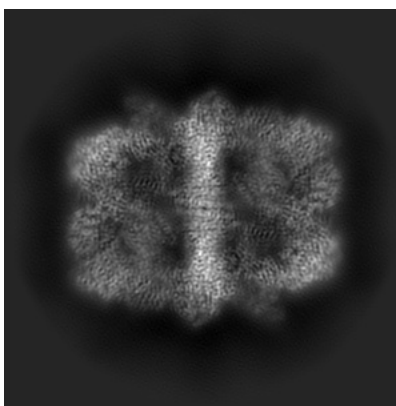
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

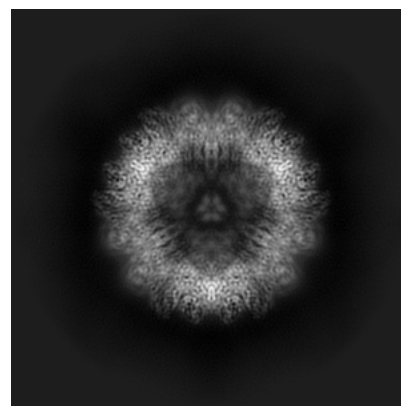
6.1.1 Primary map



X

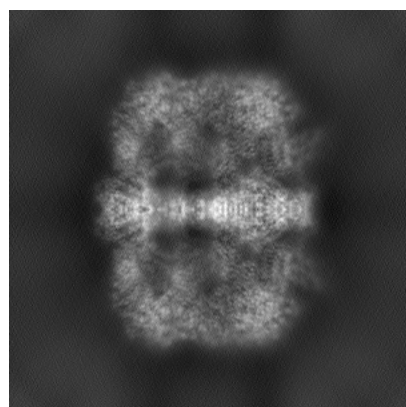


Y

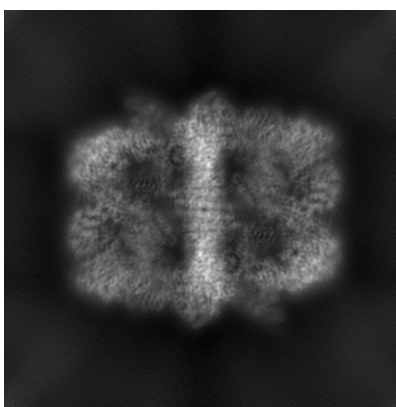


Z

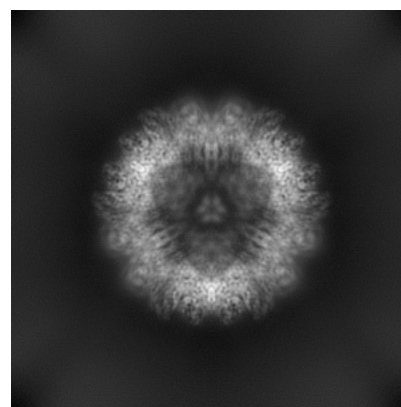
6.1.2 Raw map



X



Y

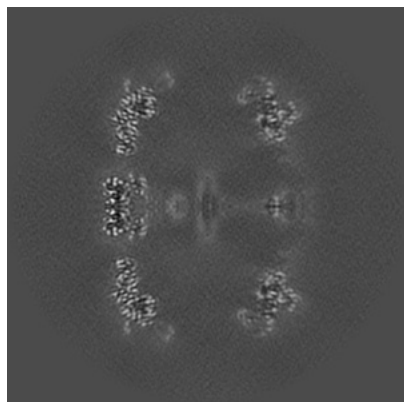


Z

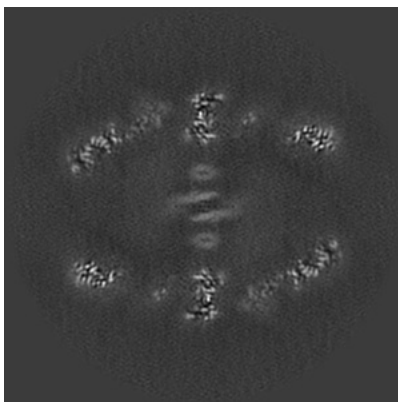
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

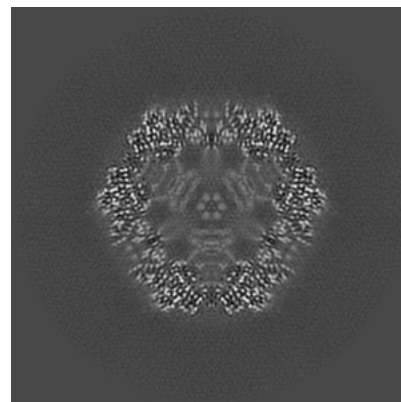
6.2.1 Primary map



X Index: 200

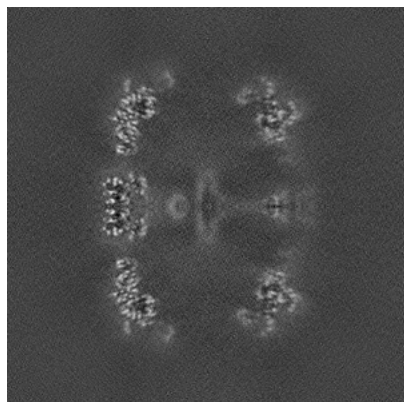


Y Index: 200

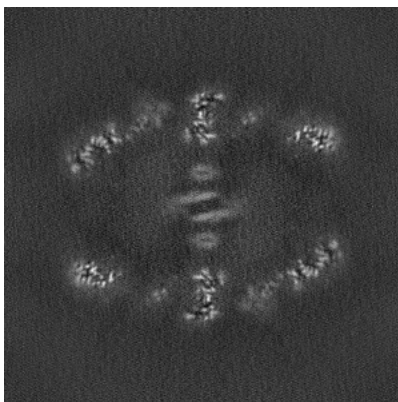


Z Index: 200

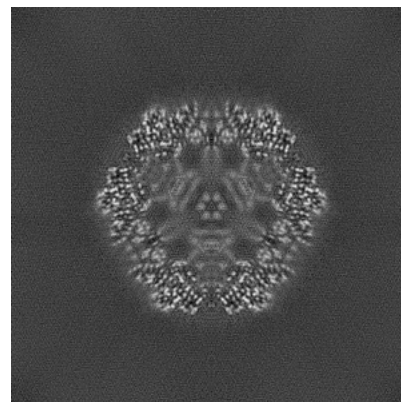
6.2.2 Raw map



X Index: 200



Y Index: 200

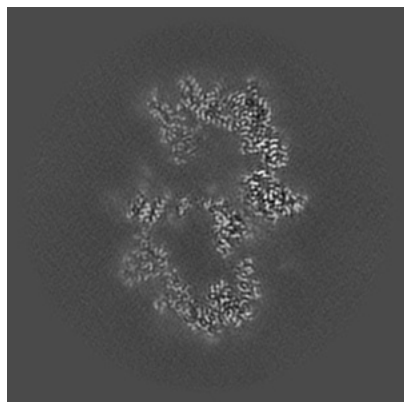


Z Index: 200

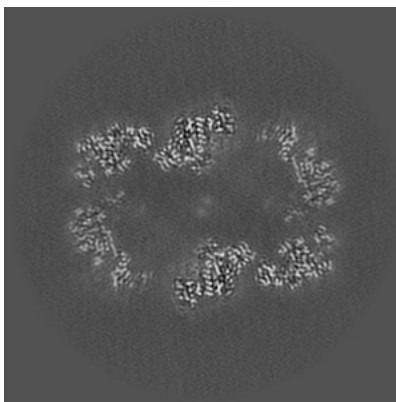
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

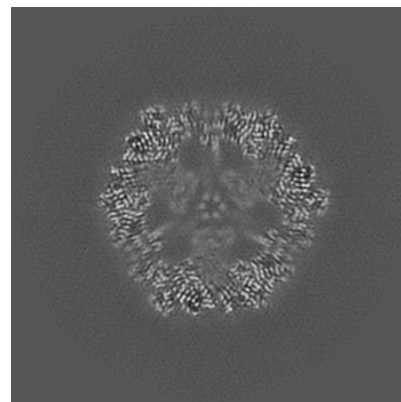
6.3.1 Primary map



X Index: 135

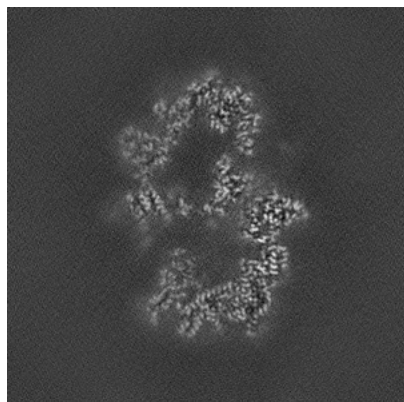


Y Index: 248

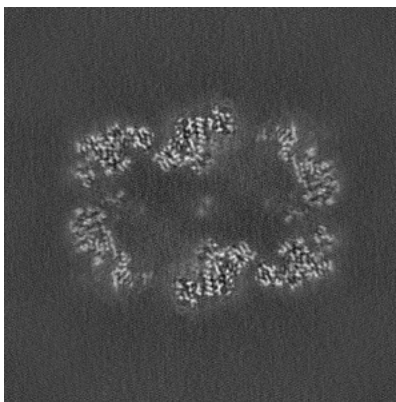


Z Index: 204

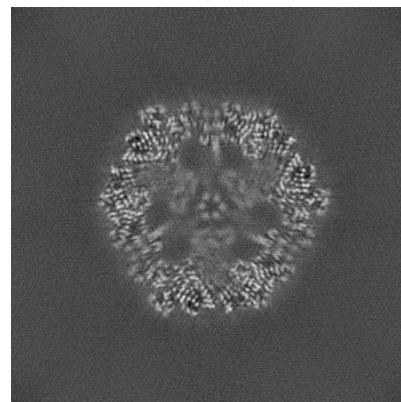
6.3.2 Raw map



X Index: 265



Y Index: 248

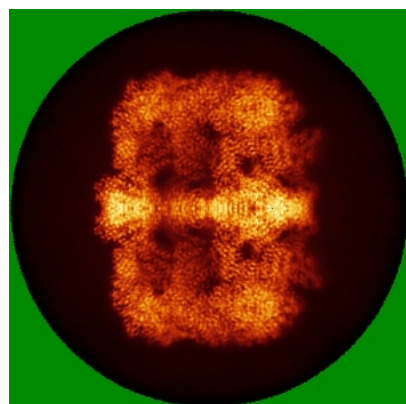


Z Index: 204

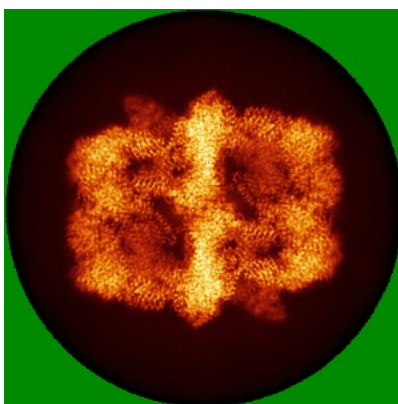
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

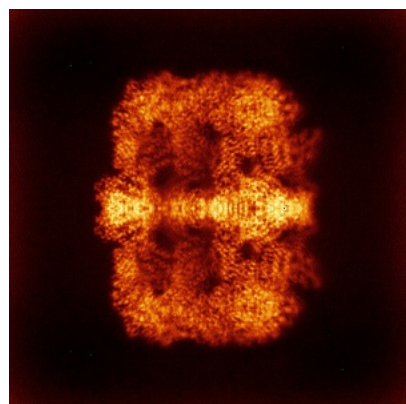


Y

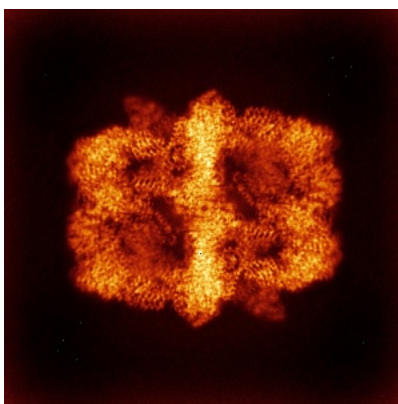


Z

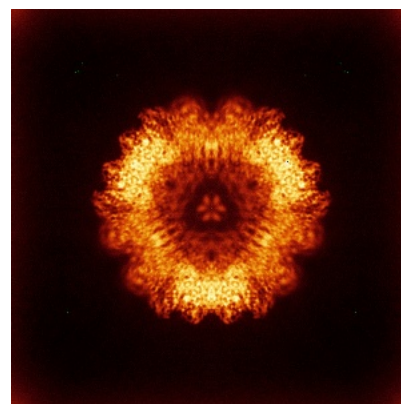
6.4.2 Raw map



X



Y

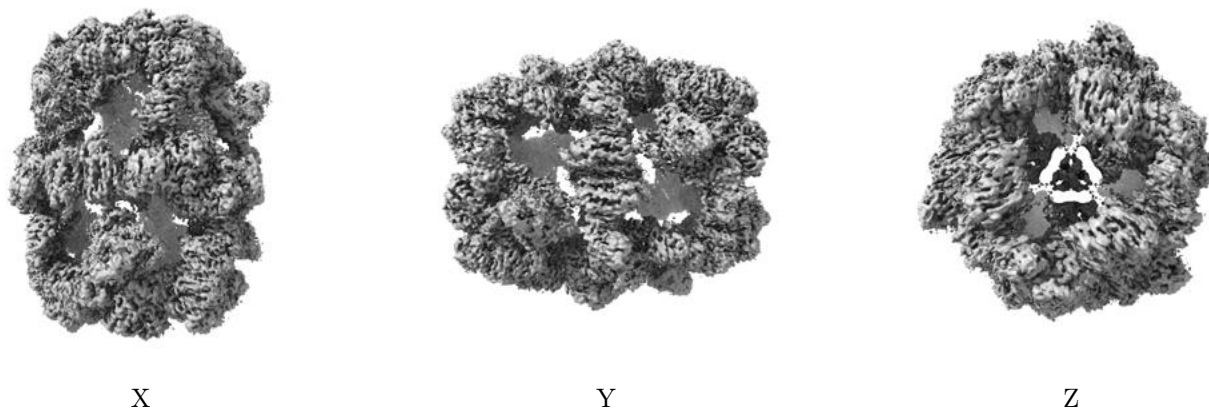


Z

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.

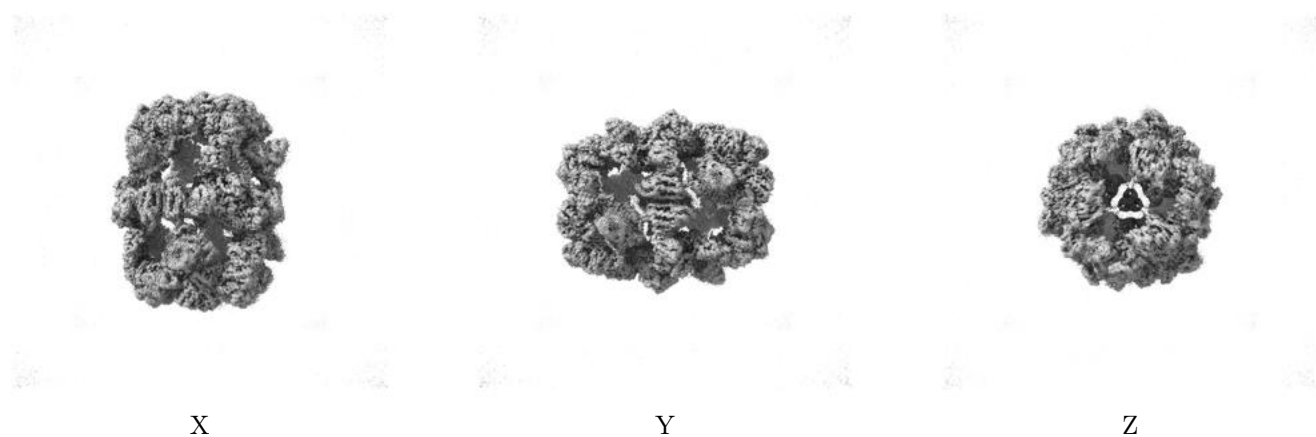
6.5 Orthogonal surface views [i](#)

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.

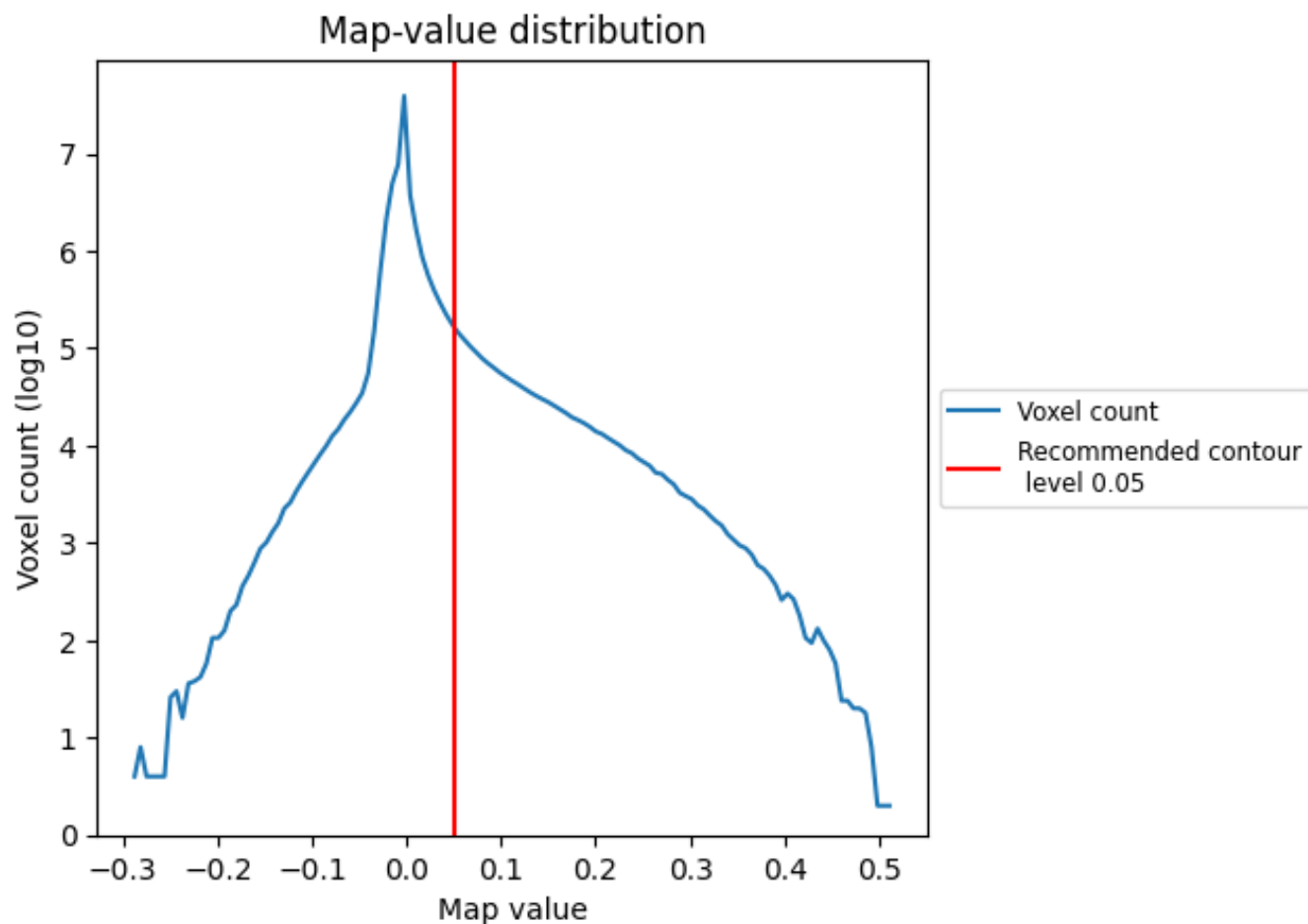
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

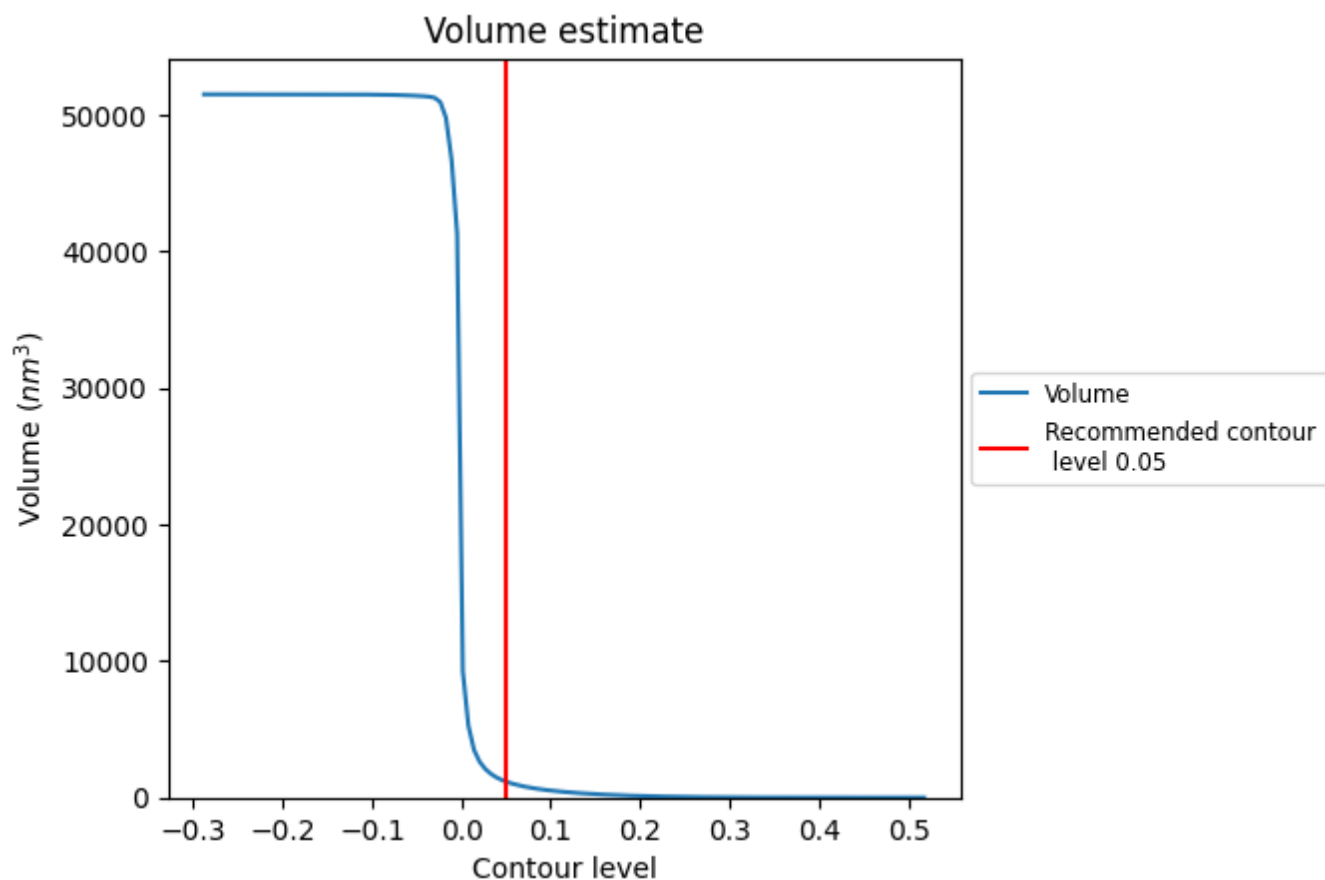
This section contains the results of statistical analysis of the map.

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.

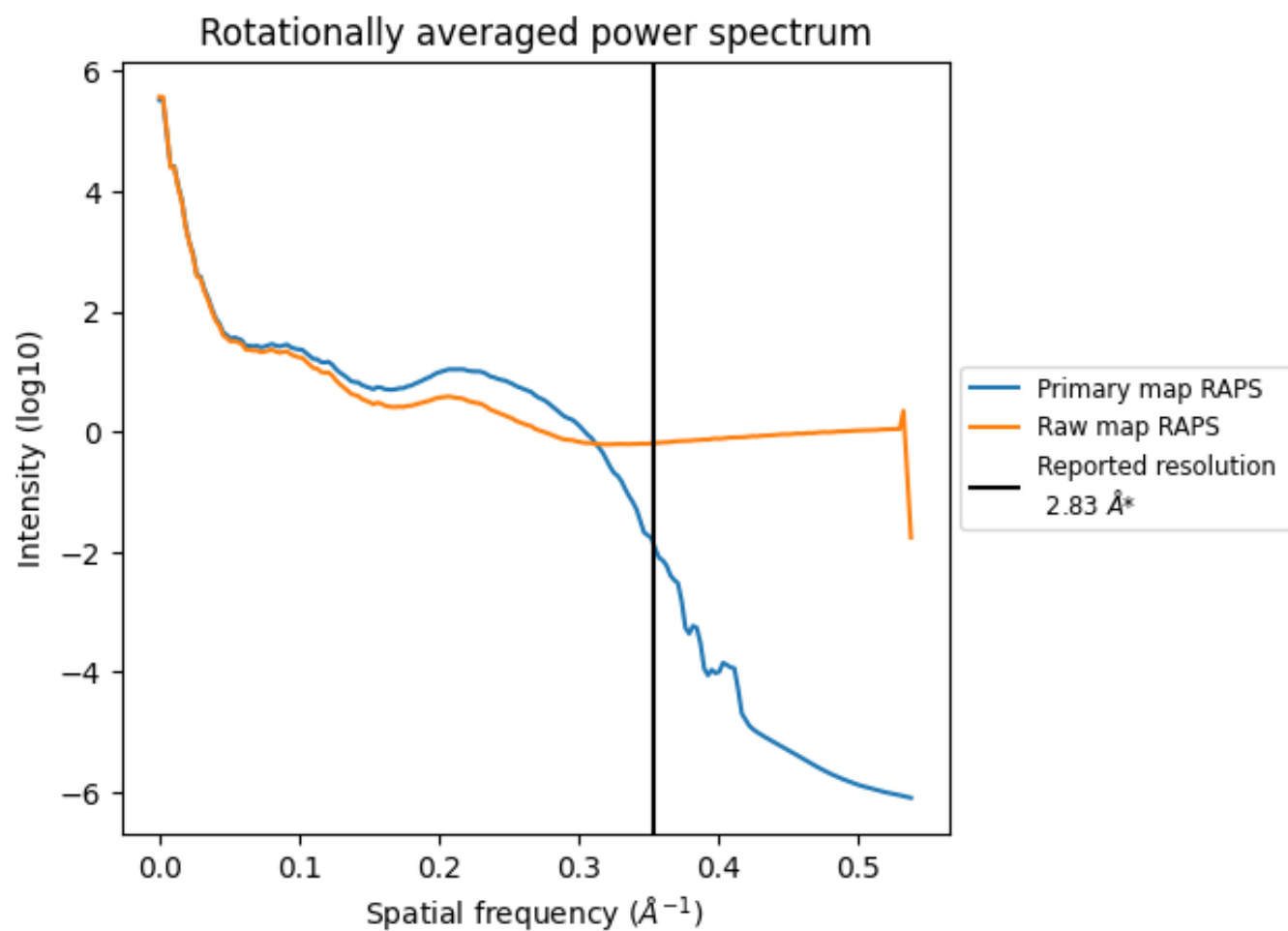
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm^3 ; 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](#)

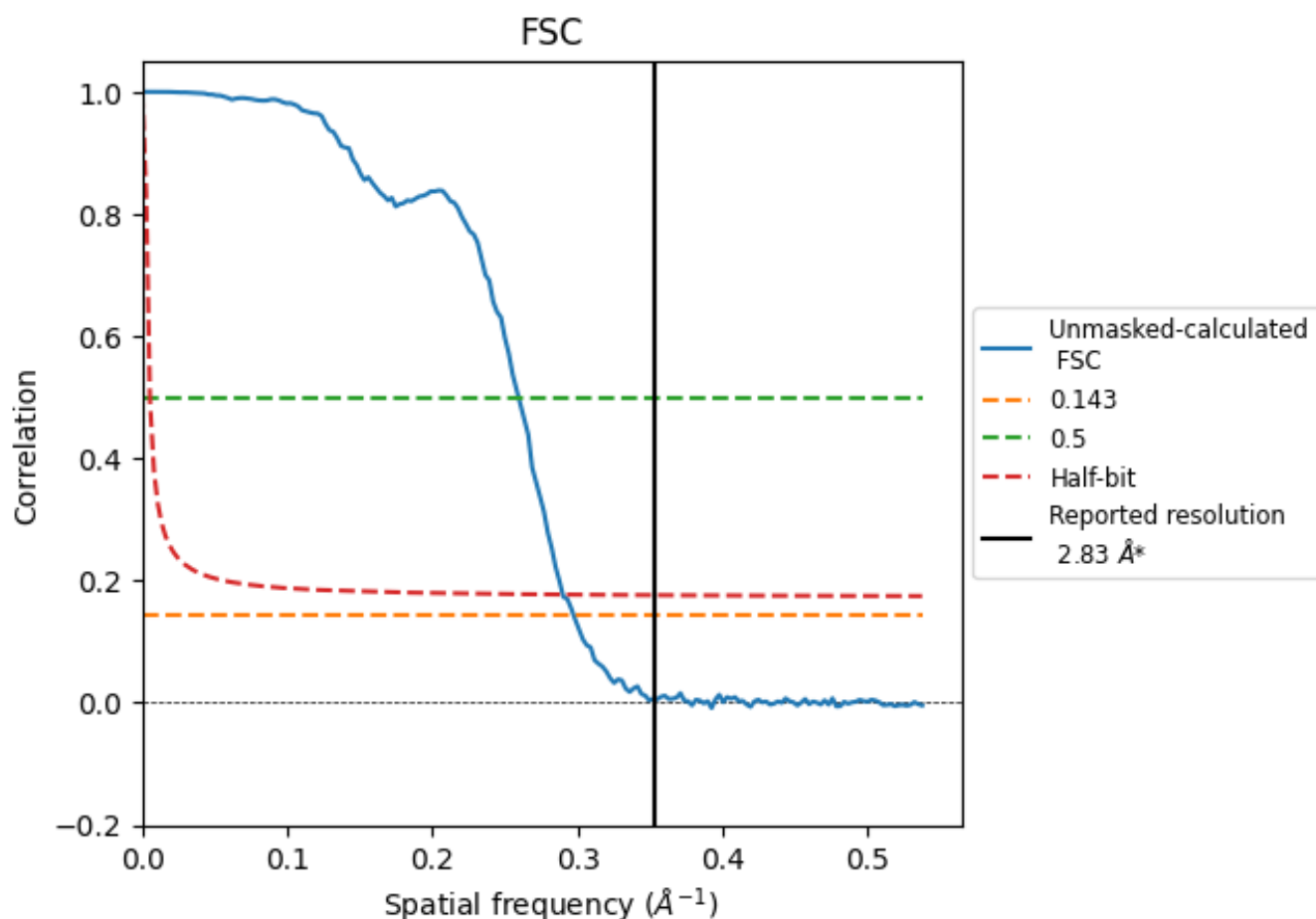


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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](#)

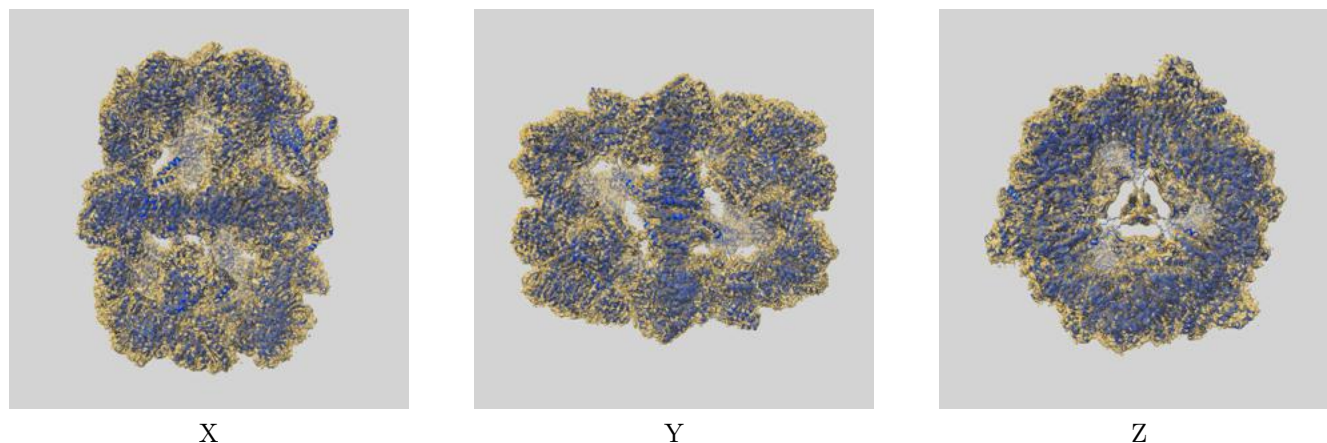
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.86	3.45

*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](#)

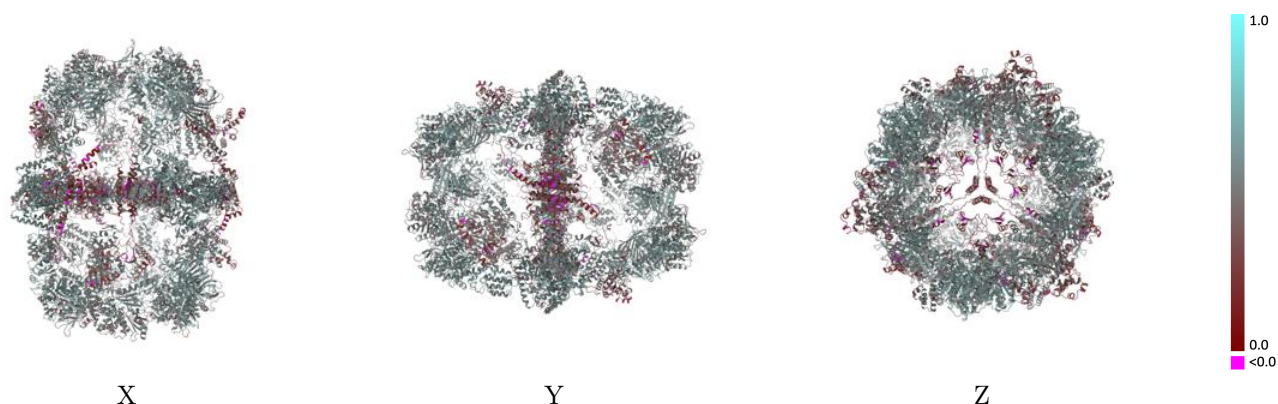
This section contains information regarding the fit between EMDB map EMD-71792 and PDB model 9PQX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



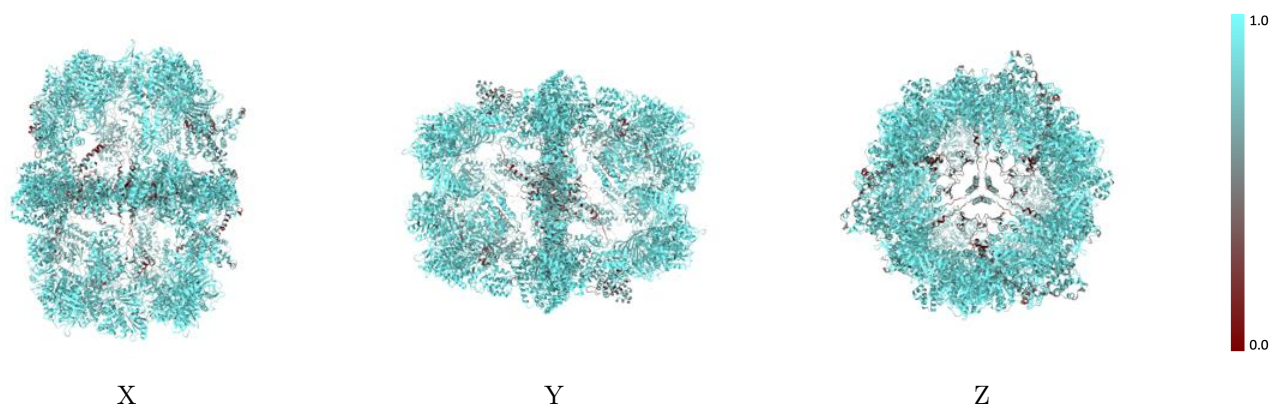
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



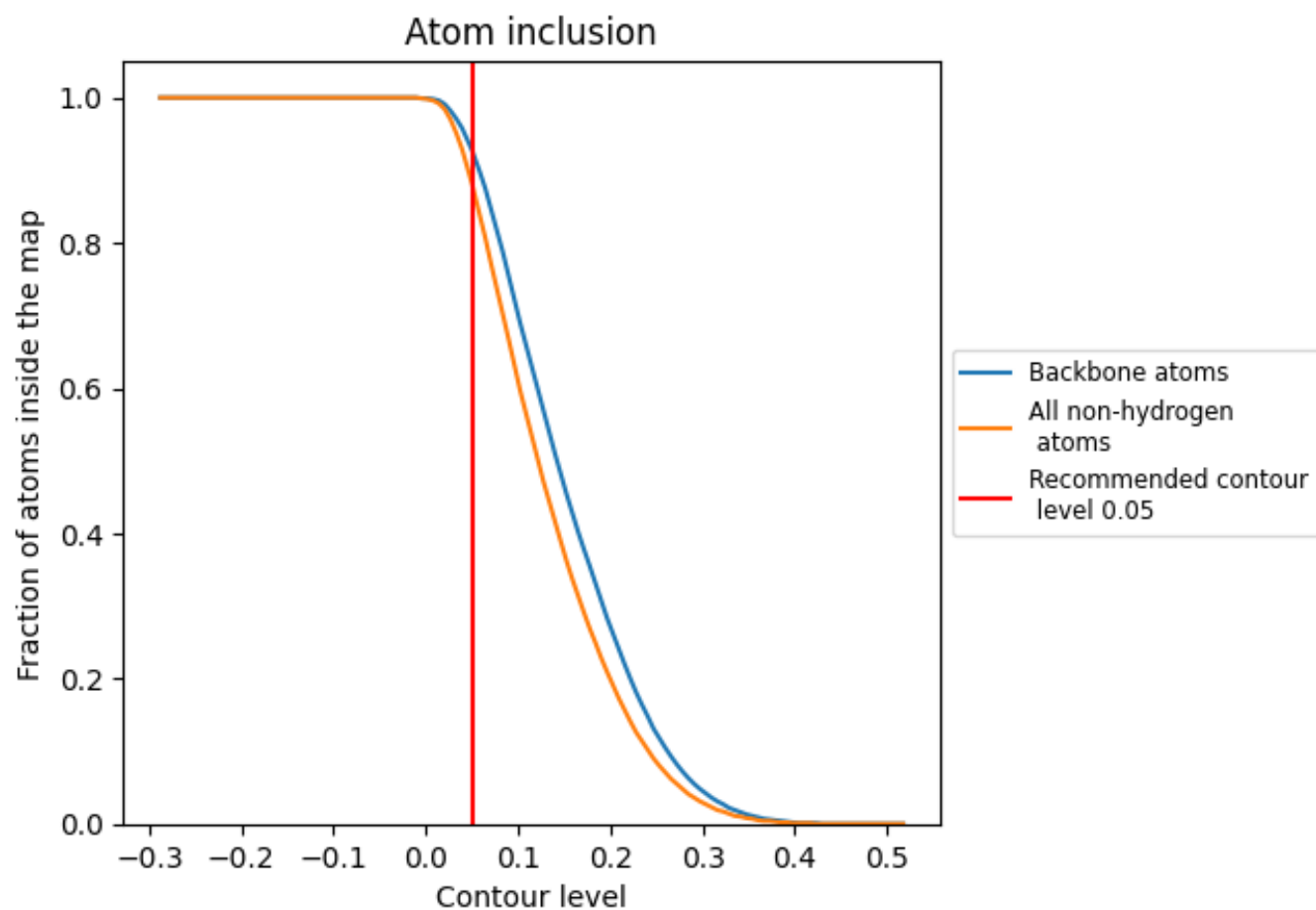
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8820	0.4740
A	0.8820	0.4750
B	0.8800	0.4730
C	0.8830	0.4740
D	0.8820	0.4730
E	0.8820	0.4730
F	0.8820	0.4740

1.0

0.0

<0.0