



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 08:40 AM EDT

PDB ID : 8EAR
EMDB ID : EMD-27983
Title : Structure of the full-length IP3R1 channel determined in the presence of Calcium/IP3/ATP
Authors : Fan, G.; Baker, M.R.; Terry, L.E.; Arige, V.; Chen, M.; Seryshev, A.B.; Baker, M.L.; Ludtke, S.J.; Yule, D.I.; Serysheva, I.I.
Deposited on : 2022-08-29
Resolution : 3.50 Å (reported)
Based on initial model : 7LHE

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

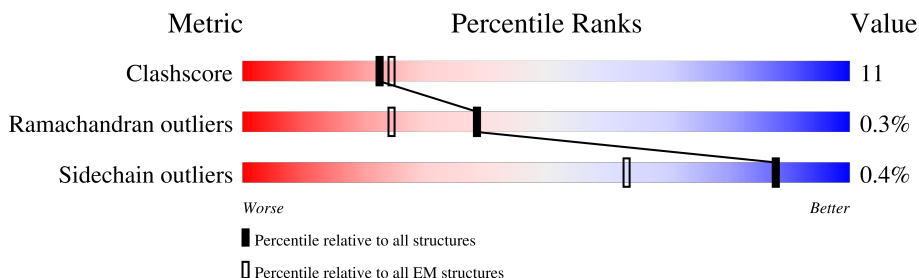
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2750	<div> <div>20%</div> <div>64%</div> <div>22%</div> <div>13%</div> </div>
1	B	2750	<div> <div>20%</div> <div>64%</div> <div>22%</div> <div>13%</div> </div>
1	C	2750	<div> <div>20%</div> <div>64%</div> <div>22%</div> <div>13%</div> </div>
1	D	2750	<div> <div>20%</div> <div>64%</div> <div>22%</div> <div>13%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 78512 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.

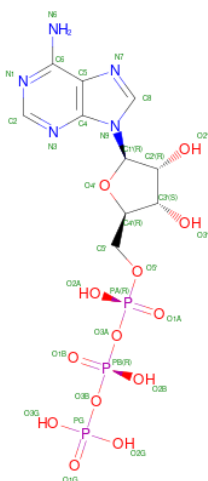
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	B	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	C	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	D	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0

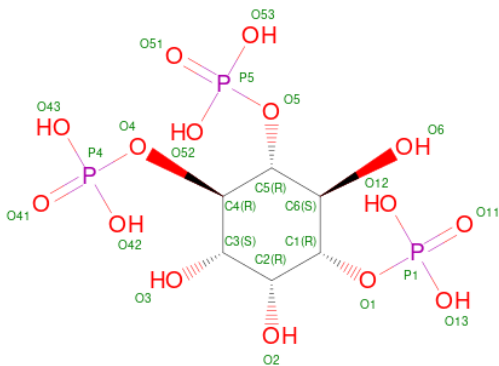
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



- Molecule 4 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $\text{C}_6\text{H}_{15}\text{O}_{15}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

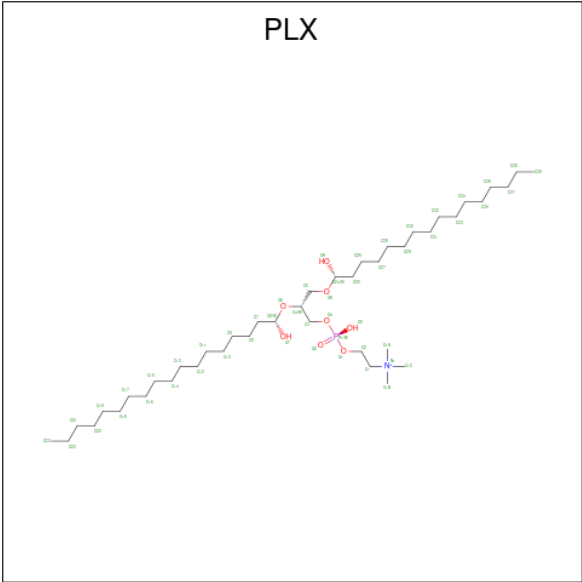


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			24	6	15	3	
4	B	1	Total	C	O	P	0
			24	6	15	3	
4	C	1	Total	C	O	P	0
			24	6	15	3	
4	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Ca	0
			4	4	
5	B	4	Total	Ca	0
			4	4	
5	C	4	Total	Ca	0
			4	4	
5	D	4	Total	Ca	0
			4	4	

- Molecule 6 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
6	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
6	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
6	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	D	1	Total	C	N	O	P	0
			40	30	1	8	1	

Continued on next page...

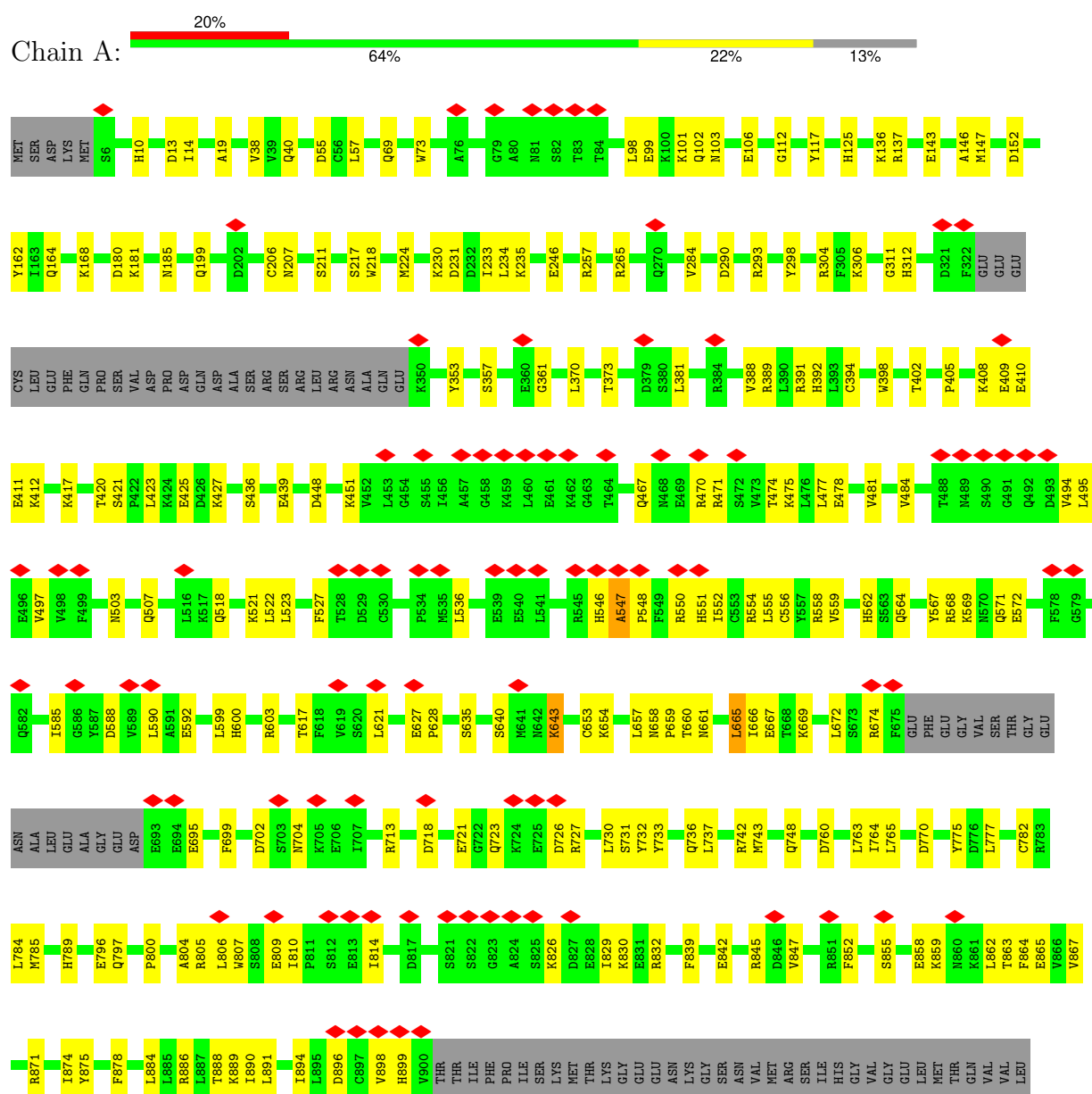
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
6	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	D	1	Total	C	N	O	P	0
			37	27	1	8	1	

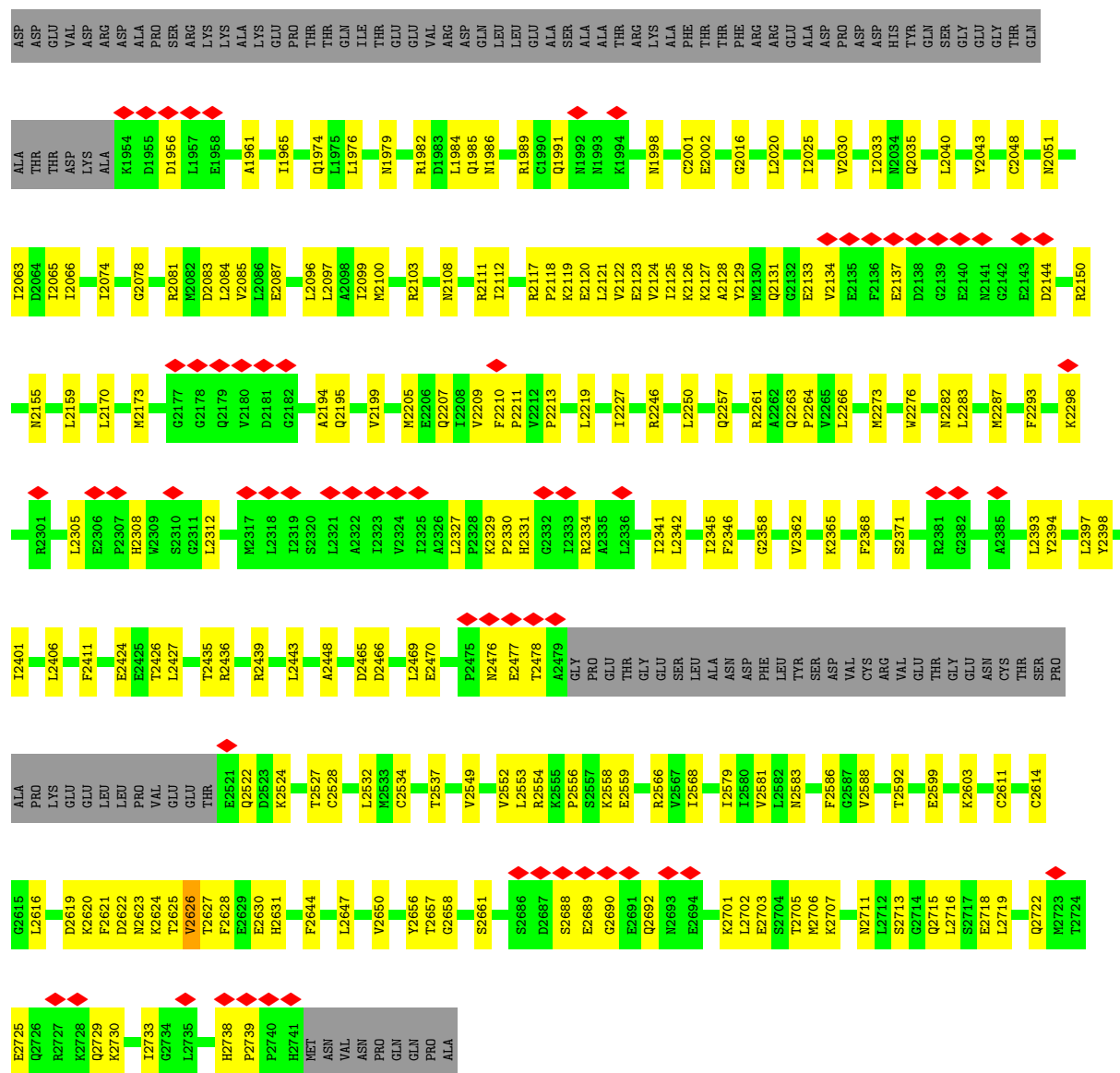
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

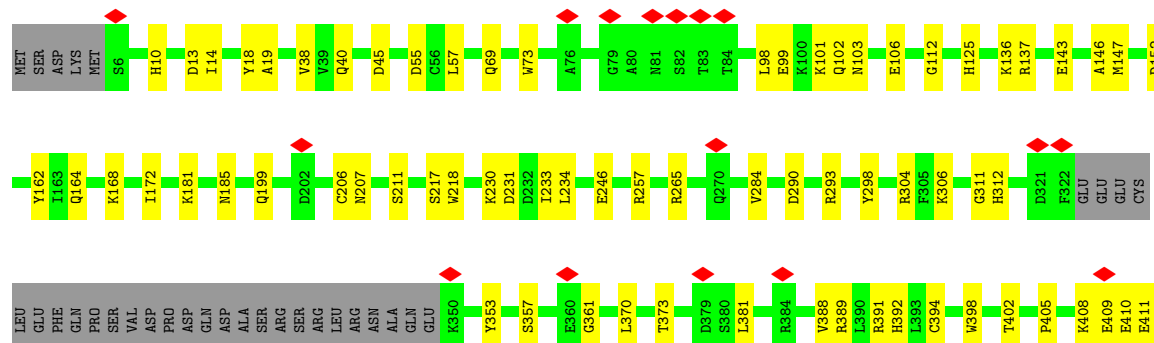
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





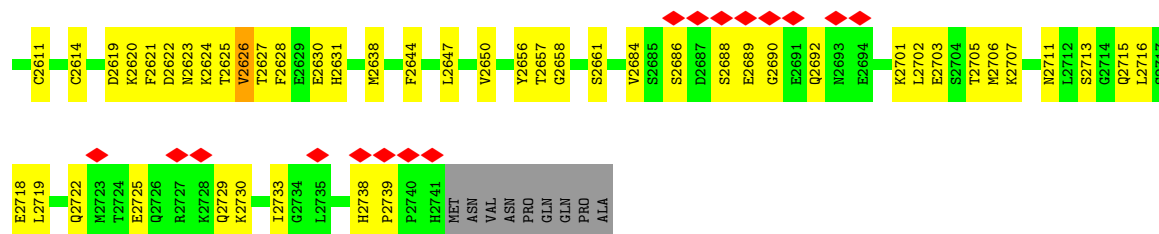


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

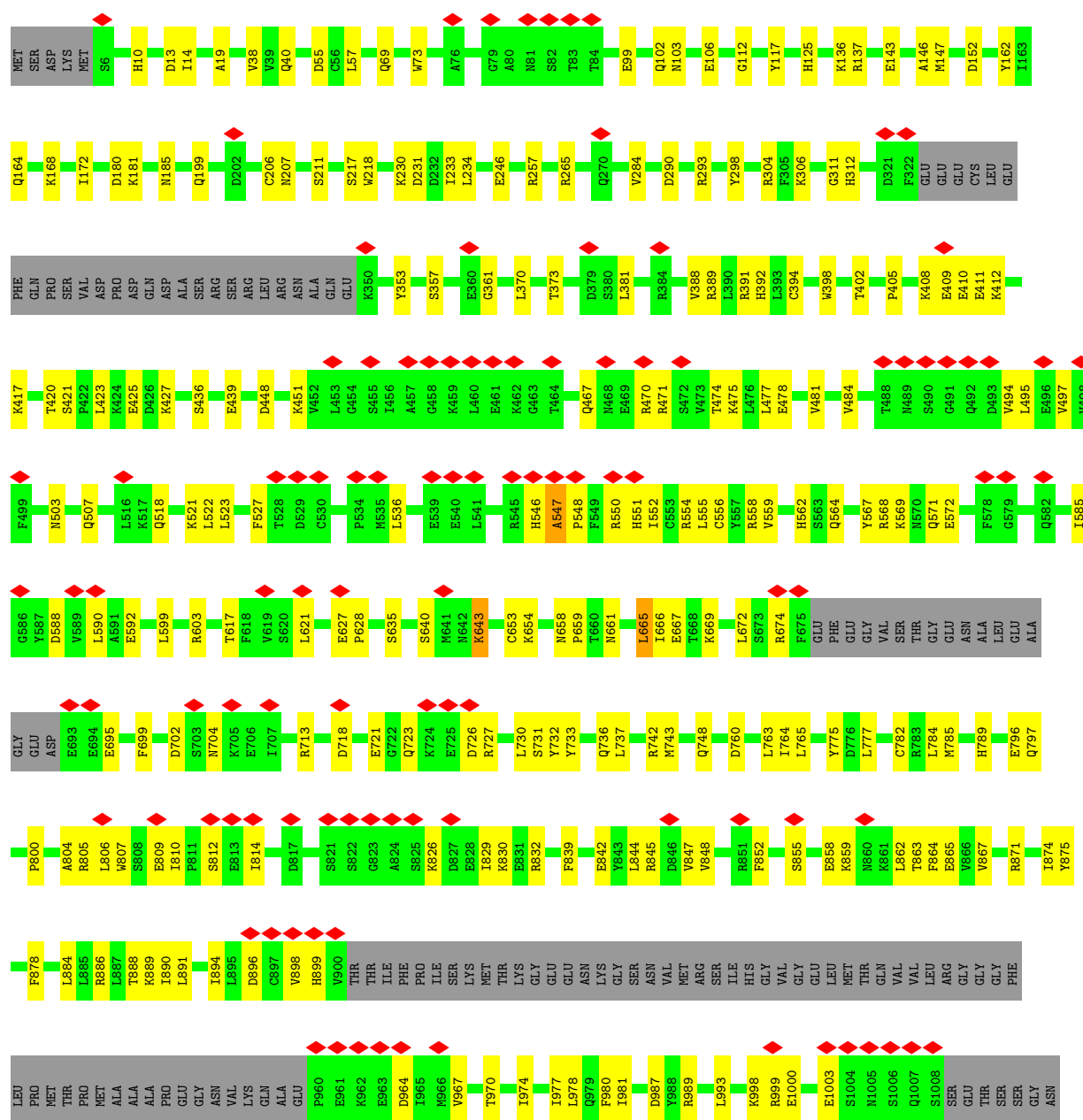




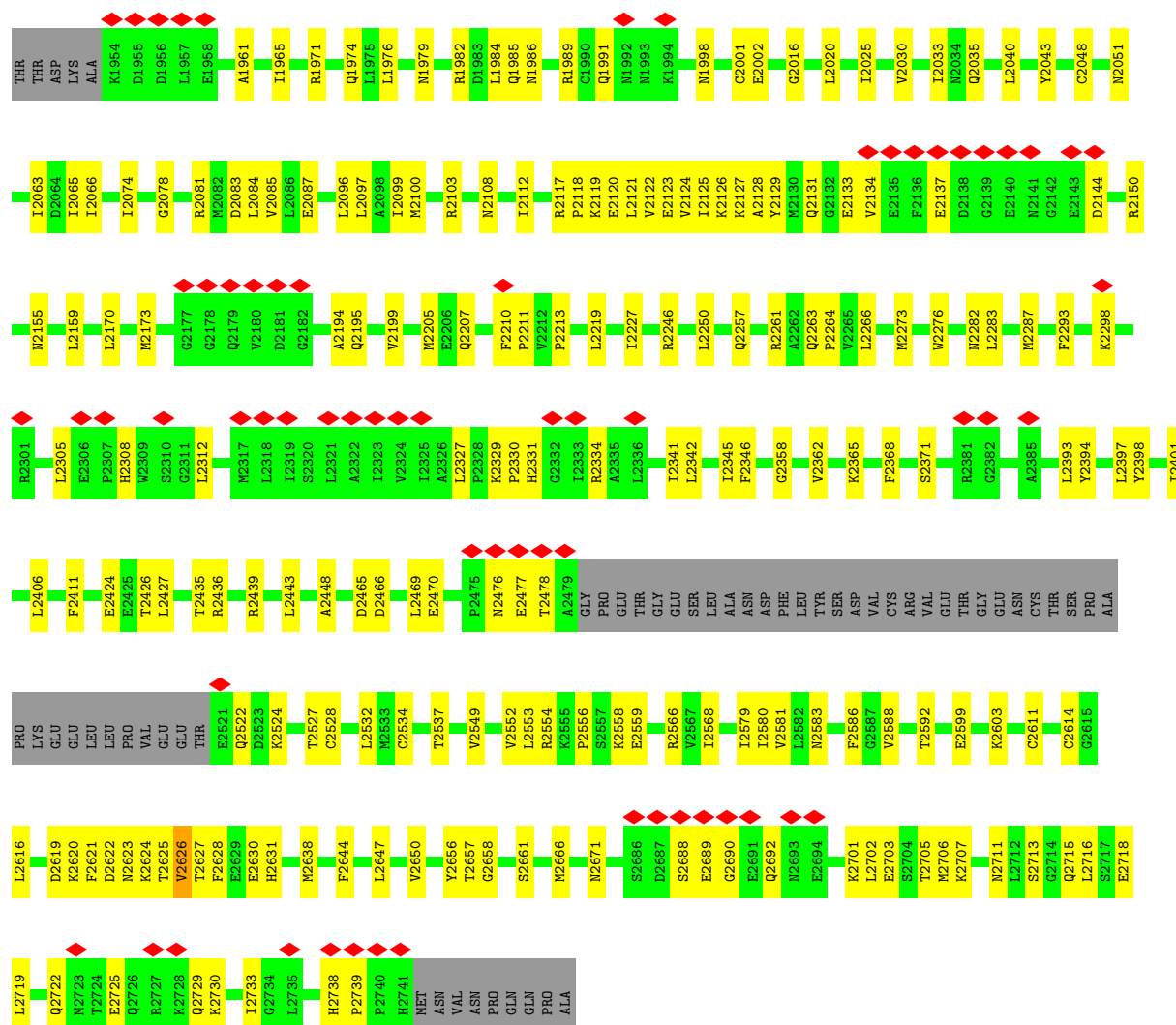




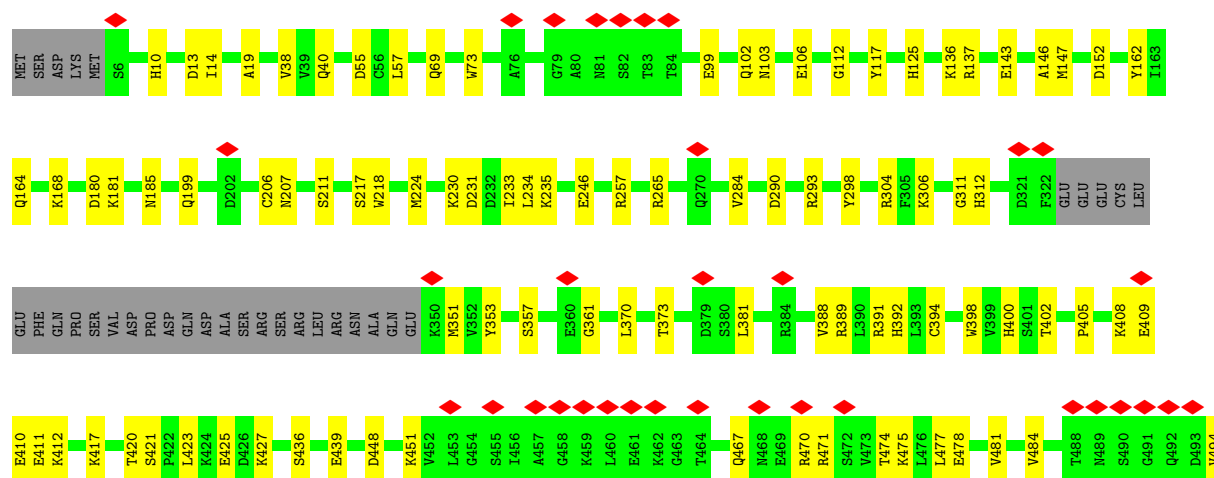
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





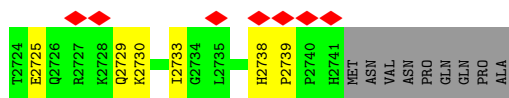


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



L495	E496	V497	V498	F499	N503	Q507	L516	K517	Q518	K521	L522	L523	F527	T528	D529	C530	P534	M535	L536	E539	E540	L541	R545	H546	A547	P548	F549	R550	H551	I552	R554	L555	C556	Y557	R558	V559	H562	S563	Q564	Y567	R568	K569	N570	Q571	E572	F578	G579											
+	Q582		I585	G586	Y587	D588	V589	L590	A591	E592	L599	H600		R603	T617	F618	V619	S620	L621	E627		S635	S640	M641	N642	K643	C653	K654	L657	N658	P659	T660	N661	L665	I666	E667	T668	K669	L672	S673	F675	GLU	PHE	GLU	GLY	VAL	T863	F864	E865	V866								
ASN	ALA	LEU	ALA	GLY	GLU	ASP	E693	E694	E695	F699	D702	S703	N704	K705	E706	I707	R713		D718	E721	G722	Q723	K724	E725	D726	R727	L730	S731	Y732	Y733	Q736	L737	R742	M743	Q748	D760	L763	I764	L765	D770	Y775	D776	L777	C782	R783													
L784	M785		H789	E796	Q797	P800	R805	L806	W807	S808	E809	I810	P811	S812	E813	I814	D817	S821	S822	G823	A824	S825	K826	D827	E828	I829	K830	E831	R832	F839	E842	R845	D846	V847	R851	F852	S855	E858	K859	N860	K861	L862	T863	F864	E865	V866												
R871	I874	Y875	F878	L884	L885	R886	L887	T888	K889	I890	L891	I894	L895	D896	C897	V898	H899	V900	THR	THR	ILE	PHE	PRO	ILE	LYS	THR	LYS	GLY	GLU	ASN	LYS	GLY	ASN	VAL	MET	VAL	GLY	LEU	MET	THR	GLN	VAL	LEU	ARG														
GLY	GLY	GLY	PHE	LEU	PRO	MET	THR	PRO	MET	ALA	ALA	PRO	GLU	ASN	VAL	LYS	GLN	ALA	GLU	P960	E961	K962	E963	D964	I965	M966	V967	T970	I974	I977	E979	F980	I981	D987	Y988	R989	K998	R999	E1000	E1003	S1004	N1005	S1006	Q1007	S1008	SER	GLU	THR	SER									
GLY	ASN	SER	GLN	GLU	GLY	PRO	ASN	SER	VAL	P1025	G1026	A1027	L1028	E1031	E1035	Q1036	G1039	I1040	F1041	G1042	G1043	S1044	E1045	E1046	N1047	D1051	L1052	G1057	F1060	V1063	L1064	L1065	H1066	L1067	T1068	M1069	L1075	V1076	F1084	R1085	H1086	Q1089	R1090	Q1091	L1094	Q1095	A1096											
F1097	K1098	Q1099	V1100	Q1101	L1102	L1103	V1104	T1105	S1106	Q1107	D1108	V1109	D1110	N1111	Y1112	K1113	Q1114	I1115	K1116	Q1117	D1118	L1119	D1120	Q1121	L1122	R1123	S1124	I1125	E1127	K1128	S1129	Y1132	V1133	Y1134	K1135	G1136	GLN	PRO	ASP	GLU	PRO	MET	ASP	GLY	ALA	SER	GLY	ASN	HIS	LYS	THR	GLU						
GLY	THR	SER	LYS	PRO	LEU	LYS	HIS	E1166	S1167	T1168	S1169	S1170	Y1171	N1172	Y1173	R1174	V1175	K1176	E1177	I1179	L1180	I1181	N1182	L1183	S1184	K1185	V1188	Q1189	E1190	S1191	A1192	S1193	V1194	R1195	K1196	S1197	R1198	Q1200	Q1201	R1206	M1207	M1208	G1209	A1210	H1211	A1212	V1213	L1215	E1216	L1218	Q1219	I1220	P1221					
Y1222	E1223	K1224	A1225	E1226	D1227	T1228	K1229	M1230	Q1231	E1232	L1233	M1234	R1235	H1238	E1239	F1240	L1241	Q1242	G1247	N1248	Q1249	Q1250	L1254	K1257	H1258	I1259	N1260	L1263	I1267	L1268	M1273	F1277	N1280	F1281	Q1282	L1283	C1284	S1285	E1286	I1287	N1288	E1289	R1290	V1291	V1292	Q1293	H1294	F1295	V1296	H1297								
C1298	I1299	E1300	T1301	H1302	G1303	R1304	I1309	K1310	F1311	L1312	K1317	G1320	K1321	F1322	I1323	K1324	K1325	C1326	Q1327	D1328	M1329	V1330	M1331	A1332	E1333	L1334	V1335	N1336	S1337	G1338	E1339	D1340	V1341	L1342	V1343	F1344	N1346	D1347	R1348	A1349	S1350	F1351	Q1352	T1353	L1354	I1355	Q1356	M1357	M1358	R1359	S1360	R1362	R1363	R1364				
M1365	D1366	E1367	N1368	S1369	P1370	L1371	F1372	M1373	I1376	H1377	L1378	V1379	E1380	C1385	T1386	E1387	G1388	K1389	N1390	V1391	Y1392	T1393	E1394	I1395	K1396	C1397	N1398	S1399	L1400	L1401	P1402	L1403	D1404	D1405	I1406	V1410	T1411	H1412	E1413	D1414	C1415	L1416	P1417	E1418	V1419	K1420	I1421	A1422	Y1423	Y1424	N1428	H1429	C1430	Y1431	V1432			
D1433	T1434	E1435	V1436	E1437	M1438	K1439	I1440	I1441	Y1442	T1443	S1444	N1446	H1446	M1447	N1448	K1449	L1450	F1451	E1452	N1453	F1454	L1455	V1456	D1457	I1458	C1459	R1460	A1461	C1462	N1463	N1464	T1465	S1466	D1467	R1468	K1469	H1470	A1471	D1472	S1473	V1474	L1475	E1476	K1477	Y1478	V1479	T1480	E1481	I1482	V1483	M1484	S1485	I1486	V1487	T1488	F1489	F1491	A1492

L2816	D2819	K2820	F2821	D2822	N2823	K2824	T2825	V2826	T2827	F2828	E2829	E2830	H2831	M2838	F2844	L2847	V2850	Y2856	T2857	G2858	S2861	S2886	D2887	S2888	E2889	G2890	E2891	Q2892	N2893	E2894	K2701	L2702	E2703	S2704	T2705	N2706	K2707	N2711	L2712	S2713	G2714	Q2715	L2716	S2717	E2718	L2719	Q2722	N2723															
PRO	LYS	GLU	GLU	LEU	LEU	PRO	VAL	GLU	GLU	THR	E2521	Q2522	D2523	K2524	T2527	C2528	L2532	M2533	C2534	T2537	V2549	V2552	L2553	R2554	K2555	P2556	K2558	S2557	L2559	R2566	V2567	I2568	L2579	T2580	V2581	L2582	N2583	F2586	G2587	V2588	T2592	E2599	K2603	C2611	C2614	G2615	L2616	N2617															
L2406	F2411	E2424	E2425	T2426	L2427	T2435	R2436	R2439	L2443	A2448	D2465	D2466	L2469	E2470	P2475	N2476	E2477	T2478	A2479	GLY	PRO	GLU	THR	GLY	GLU	SER	LEU	ALA	ASN	ASP	PHE	LEU	TYR	SER	ASP	VAL	ARG	GLU	THR	GLY	ASN	THR	PRO	ALA																			
K2301	L2305	E2306	P2307	H2308	W2309	S2310	G2311	L2312	M2317	L2318	L2319	S2320	L2321	A2322	L2323	V2324	L2325	A2326	L2327	P2328	K2329	P2330	H2331	G2332	L2333	K2334	A2335	L2336	I2341	L2342	I2345	F2346	G2358	V2362	K2365	F2368	S2371	R2381	G2382	A2385	L2393	Y2394	L2397	Y2398	I2401																		
N2155	L2159	L2170	M2173	G2177	Q2178	V2180	D2181	G2182	A2194	Q2195	V2199	M2205	E2206	Q2207	F2210	P2211	V2212	P2213	L2219	I2227	R2246	L2250	Q2257	R2261	Q2263	P2264	V2265	L2266	M2273	W2276	N2282	L2283	M2287	F2293	K2298																												
T2063	D2064	L2065	L2066	L2074	G2078	R2081	W2082	D2083	L2084	V2085	E2087	L2096	L2097	L2098	M2100	R2103	N2108	I2112	R2117	P2118	K2119	E2120	L2121	V2122	E2123	V2124	I2125	K2126	K2127	A2128	Y2129	Q2131	E2133	V2134	E2135	F2136	E2137	D2138	Q2139	E2140	N2141	G2142	E2143	D2144	R2150																		
THR	THR	ASP	LYS	ALA	K1954	D1955	D1956	L1957	E1958	A1961	L1965	R1971	Q1974	L1975	L1976	N1979	R1982	D1983	L1984	Q1985	N1986	R1989	C1990	Q1991	N1992	N1993	K1994	N1998	F1856	F1857	F1860	M1864	Q1868	Q1869	E1870	I1871	T1874	S1880	D1881	L1882	G1883	N1884	K1885	LYS	ASP																		
ASP	GLU	VAL	ASP	LYS	ARG	ALA	PRO	SER	ARG	LYS	LYS	GLU	THR	GLN	ILE	THR	GLU	VAL	ARG	ASP	GLN	LEU	LEU	SER	GLY	ALA	SER	THR	PHE	THR	THR	ARG	ARG	GLU	ALA	ASP	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP																	
GLU	ALA	GLU	ASN	SER	THR	GLN	GLN	GLN	GLN	SER	P1722	P1723	L1724	R1725	Q1726	D1729	L1736	I1748	ARG	PRO	SER	GLY	ARG	GLU	SER	THR	PHE	GLY	ASN	GLY	PRO	LEU	TYR	GLY	LYS	ILE	ILE	ASP	GLN	LEU	GLY	ASN	ALA	GLU	PRO	PRO																	
L1618	V1619	Q1620	A1621	E1622	L1623	S1624	V1625	L1626	E1639	A1643	R1644	R1645	C1646	E1648	S1649	Q1650	C1654	K1655	L1656	I1657	K1658	H1659	L1663	L1664	E1665	E1666	E1669	K1674	D1686	R1687	G1688	TYR	GLY	LYS	GLN	ILE	SER	ILE	ASP	GLN	LEU	GLY	ASN	ALA	GLU	PRO	PRO																
D1554	L1555	D1556	S1557	Q1558	Q1498	S1499	N1560	N1561	N1562	F1563	L1564	K1565	S1566	HIS	ASN	ILE	VAL	GLN	THR	ALA	MET	ASN	TRP	ARG	LEU	SER	ALA	ARG	ASN	Y1519	Y1520	H1521	C1522	N1523	W1524	L1525	M1526	P1527	S1528	Q1529	K1530	A1531	S1532	V1533	E1534	S1535	C1536	I1537	R1538	V1539	L1540	S1541	D1542	V1543	A1544	K1545	S1546	R1547	A1548	I1549	I1551	P1552	V1553



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	133740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P, PLX, CA, ATP, ZN

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	0.27	0/19653	0.50	0/26530
1	B	0.27	0/19653	0.50	0/26530
1	C	0.27	0/19653	0.50	0/26530
1	D	0.27	0/19653	0.50	0/26530
All	All	0.27	0/78612	0.50	0/106120

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1099	GLN	Mainchain
1	B	1099	GLN	Mainchain
1	C	1099	GLN	Mainchain
1	D	1099	GLN	Mainchain

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	19296	0	19387	435	0
1	B	19296	0	19387	437	0
1	C	19296	0	19387	436	0
1	D	19296	0	19387	432	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	24	0	9	1	0
4	B	24	0	9	1	0
4	C	24	0	9	1	0
4	D	24	0	9	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	272	0	387	18	0
6	B	272	0	387	13	0
6	C	272	0	387	13	0
6	D	272	0	387	16	0
All	All	78512	0	79180	1752	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 11.

The worst 5 of 1752 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:D:2213:PRO:HG3	1:D:2647:LEU:HB3	1.54	0.89
1:B:2213:PRO:HG3	1:B:2647:LEU:HB3	1.54	0.88
1:A:2213:PRO:HG3	1:A:2647:LEU:HB3	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2213:PRO:HG3	1:C:2647:LEU:HB3	1.54	0.86
1:D:806:LEU:HG	1:D:1103:LEU:HD22	1.58	0.85

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	2369/2750 (86%)	2264 (96%)	98 (4%)	7 (0%)	37	68
1	B	2369/2750 (86%)	2264 (96%)	98 (4%)	7 (0%)	37	68
1	C	2369/2750 (86%)	2265 (96%)	97 (4%)	7 (0%)	37	68
1	D	2369/2750 (86%)	2265 (96%)	97 (4%)	7 (0%)	37	68
All	All	9476/11000 (86%)	9058 (96%)	390 (4%)	28 (0%)	38	68

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	ALA
1	B	547	ALA
1	C	547	ALA
1	D	547	ALA
1	A	665	LEU

5.3.2 Protein sidechains [i](#)

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	2163/2459 (88%)	2153 (100%)	10 (0%)	86	93
1	B	2163/2459 (88%)	2153 (100%)	10 (0%)	86	93
1	C	2163/2459 (88%)	2153 (100%)	10 (0%)	86	93
1	D	2163/2459 (88%)	2153 (100%)	10 (0%)	86	93
All	All	8652/9836 (88%)	8612 (100%)	40 (0%)	88	93

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2583[B]	ASN
1	D	1603	ARG
1	C	2626	VAL
1	D	871	ARG
1	D	2583[A]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2715	GLN
1	D	2207	GLN
1	D	40	GLN
1	D	1238	HIS
1	D	2623	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 20 are monoatomic - leaving 36 for Mogul analysis.

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
3	ATP	A	2802	-	28,33,33	0.69	0	34,52,52	0.60	1 (2%)
6	PLX	D	2812	-	38,38,51	1.22	5 (13%)	40,46,59	0.77	0
6	PLX	A	2813	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	A	2810	-	36,36,51	1.24	5 (13%)	38,44,59	0.77	1 (2%)
6	PLX	A	2808	-	39,39,51	1.22	4 (10%)	41,47,59	0.77	0
4	I3P	D	2804	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)
3	ATP	D	2803	-	28,33,33	0.70	0	34,52,52	0.59	1 (2%)
6	PLX	B	2812	-	35,35,51	1.26	5 (14%)	37,43,59	0.73	0
6	PLX	C	2814	-	39,39,51	1.22	4 (10%)	41,47,59	0.77	0
6	PLX	D	2809	-	44,44,51	1.19	5 (11%)	46,52,59	0.79	0
6	PLX	C	2803	-	36,36,51	1.25	5 (13%)	38,44,59	0.77	1 (2%)
3	ATP	B	2803	-	28,33,33	0.70	0	34,52,52	0.59	1 (2%)
6	PLX	B	2811	-	36,36,51	1.24	5 (13%)	38,44,59	0.77	1 (2%)
6	PLX	C	2804	-	35,35,51	1.27	5 (14%)	37,43,59	0.74	0
6	PLX	C	2805	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
6	PLX	D	2813	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	B	2814	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	D	2814	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	1 (2%)
6	PLX	B	2813	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
4	I3P	C	2808	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)
6	PLX	A	2814	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	1 (2%)
6	PLX	A	2812	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
6	PLX	D	2810	-	36,36,51	1.25	5 (13%)	38,44,59	0.77	1 (2%)
4	I3P	B	2804	-	24,24,24	1.33	3 (12%)	39,39,39	0.83	1 (2%)
3	ATP	C	2807	-	28,33,33	0.70	0	34,52,52	0.60	1 (2%)
6	PLX	B	2810	-	44,44,51	1.18	5 (11%)	46,52,59	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	I3P	A	2803	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)
6	PLX	A	2809	-	44,44,51	1.19	5 (11%)	46,52,59	0.78	0
6	PLX	C	2802	-	44,44,51	1.19	5 (11%)	46,52,59	0.79	0
6	PLX	B	2809	-	39,39,51	1.22	5 (12%)	41,47,59	0.77	0
6	PLX	C	2813	-	36,36,51	1.21	5 (13%)	38,44,59	0.75	1 (2%)
6	PLX	C	2806	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	D	2811	-	35,35,51	1.26	4 (11%)	37,43,59	0.74	0
6	PLX	D	2802	-	39,39,51	1.22	5 (12%)	41,47,59	0.77	0
6	PLX	A	2811	-	35,35,51	1.26	4 (11%)	37,43,59	0.74	0
6	PLX	B	2802	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	0

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
3	ATP	A	2802	-	-	8/18/38/38	0/3/3/3
6	PLX	D	2812	-	-	23/42/42/55	-
6	PLX	A	2813	-	-	21/41/41/55	-
6	PLX	A	2810	-	-	14/40/40/55	-
6	PLX	A	2808	-	-	19/43/43/55	-
4	I3P	D	2804	-	-	1/15/39/39	0/1/1/1
3	ATP	D	2803	-	-	8/18/38/38	0/3/3/3
6	PLX	B	2812	-	-	24/39/39/55	-
6	PLX	C	2814	-	-	19/43/43/55	-
6	PLX	D	2809	-	-	28/48/48/55	-
6	PLX	C	2803	-	-	14/40/40/55	-
3	ATP	B	2803	-	-	8/18/38/38	0/3/3/3
6	PLX	B	2811	-	-	14/40/40/55	-
6	PLX	C	2804	-	-	24/39/39/55	-
6	PLX	C	2805	-	-	23/42/42/55	-
6	PLX	D	2813	-	-	21/41/41/55	-
6	PLX	B	2814	-	-	21/41/41/55	-
6	PLX	D	2814	-	-	22/40/40/55	-
6	PLX	B	2813	-	-	23/42/42/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	I3P	C	2808	-	-	1/15/39/39	0/1/1/1
6	PLX	A	2814	-	-	22/40/40/55	-
6	PLX	A	2812	-	-	23/42/42/55	-
6	PLX	D	2810	-	-	14/40/40/55	-
4	I3P	B	2804	-	-	1/15/39/39	0/1/1/1
3	ATP	C	2807	-	-	8/18/38/38	0/3/3/3
6	PLX	B	2810	-	-	28/48/48/55	-
4	I3P	A	2803	-	-	1/15/39/39	0/1/1/1
6	PLX	A	2809	-	-	28/48/48/55	-
6	PLX	C	2802	-	-	28/48/48/55	-
6	PLX	B	2809	-	-	19/43/43/55	-
6	PLX	C	2813	-	-	22/40/40/55	-
6	PLX	C	2806	-	-	21/41/41/55	-
6	PLX	D	2811	-	-	24/39/39/55	-
6	PLX	D	2802	-	-	19/43/43/55	-
6	PLX	A	2811	-	-	24/39/39/55	-
6	PLX	B	2802	-	-	22/40/40/55	-

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2804	PLX	O6-C4	-3.77	1.39	1.44
6	B	2809	PLX	O6-C4	-3.71	1.39	1.44
6	C	2814	PLX	O6-C4	-3.71	1.39	1.44
6	B	2812	PLX	O6-C4	-3.69	1.39	1.44
6	D	2809	PLX	O6-C4	-3.69	1.39	1.44

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2802	ATP	C5-C6-N6	2.36	123.91	120.31
3	C	2807	ATP	C5-C6-N6	2.35	123.88	120.31
3	D	2803	ATP	C5-C6-N6	2.31	123.83	120.31
3	B	2803	ATP	C5-C6-N6	2.31	123.83	120.31
6	B	2811	PLX	C8-C7-C6	-2.18	108.30	113.38

There are no chirality outliers.

5 of 640 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	C5'-O5'-PA-O1A
3	A	2802	ATP	C5'-O5'-PA-O2A
3	A	2802	ATP	C5'-O5'-PA-O3A
3	A	2802	ATP	O4'-C4'-C5'-O5'
3	B	2803	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

35 monomers are involved in 67 short contacts:

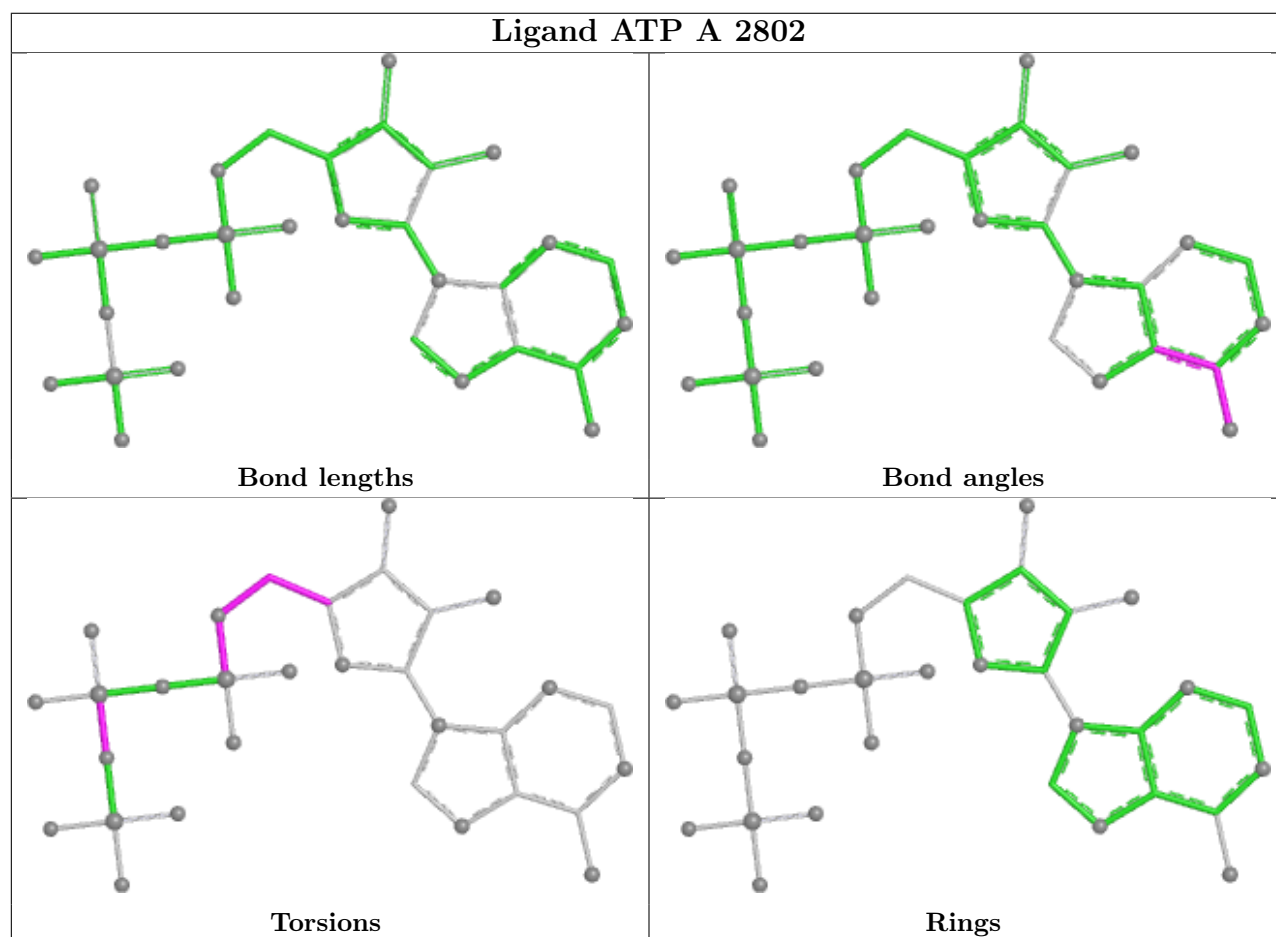
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2812	PLX	1	0
6	A	2813	PLX	6	0
6	A	2810	PLX	2	0
6	A	2808	PLX	1	0
4	D	2804	I3P	1	0
3	D	2803	ATP	1	0
6	B	2812	PLX	1	0
6	C	2814	PLX	1	0
6	D	2809	PLX	3	0
6	C	2803	PLX	1	0
3	B	2803	ATP	1	0
6	B	2811	PLX	2	0
6	C	2804	PLX	1	0
6	C	2805	PLX	1	0
6	D	2813	PLX	6	0
6	B	2814	PLX	4	0
6	D	2814	PLX	2	0
6	B	2813	PLX	1	0
4	C	2808	I3P	1	0
6	A	2814	PLX	1	0
6	A	2812	PLX	2	0
6	D	2810	PLX	2	0
4	B	2804	I3P	1	0
3	C	2807	ATP	1	0
6	B	2810	PLX	4	0
4	A	2803	I3P	1	0
6	A	2809	PLX	5	0
6	C	2802	PLX	4	0
6	B	2809	PLX	1	0
6	C	2813	PLX	1	0
6	C	2806	PLX	5	0
6	D	2811	PLX	1	0
6	D	2802	PLX	2	0

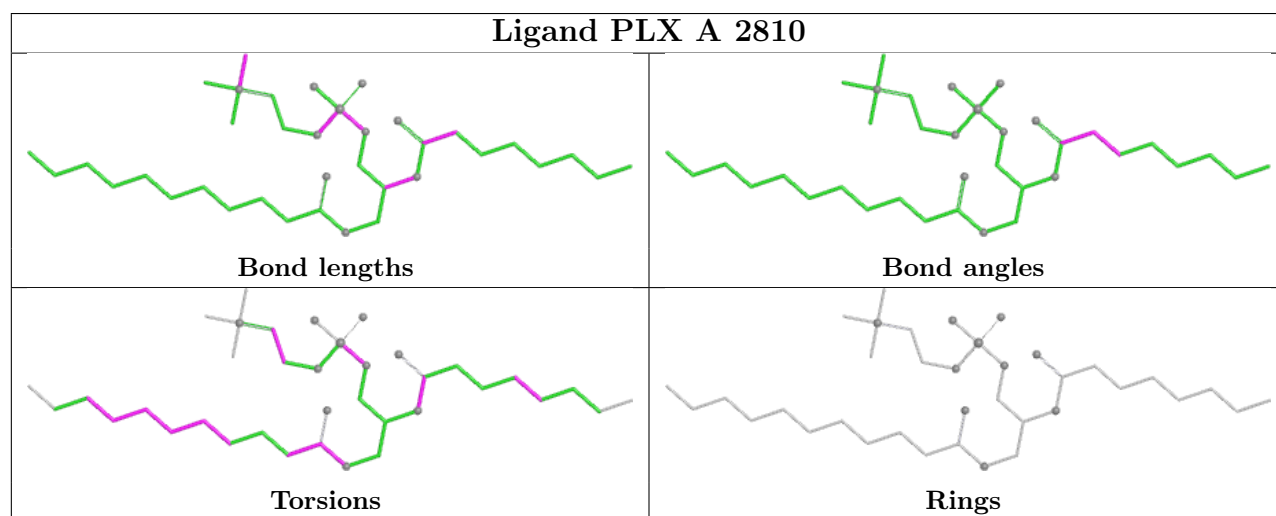
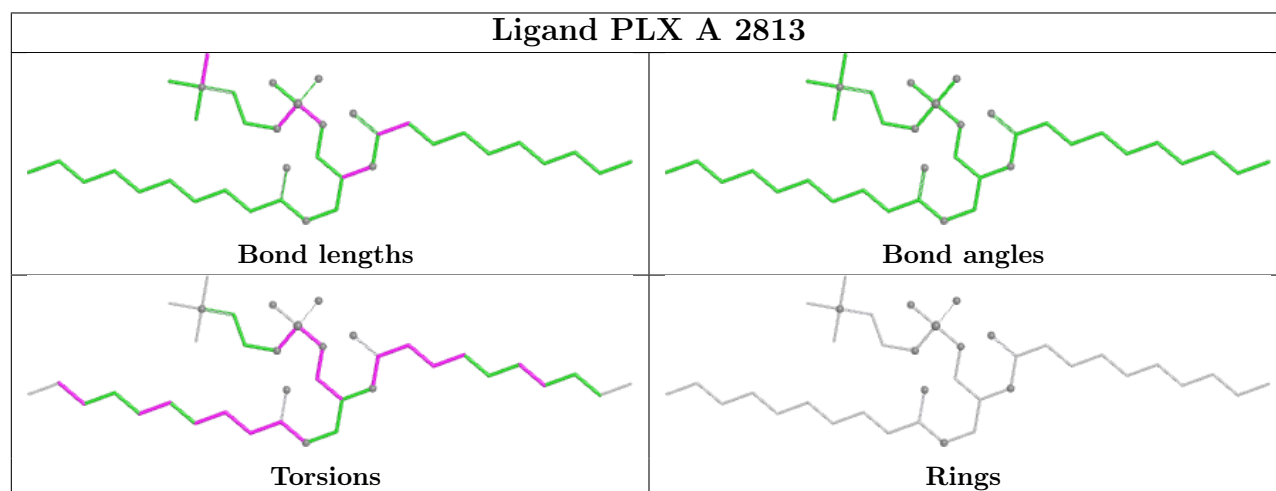
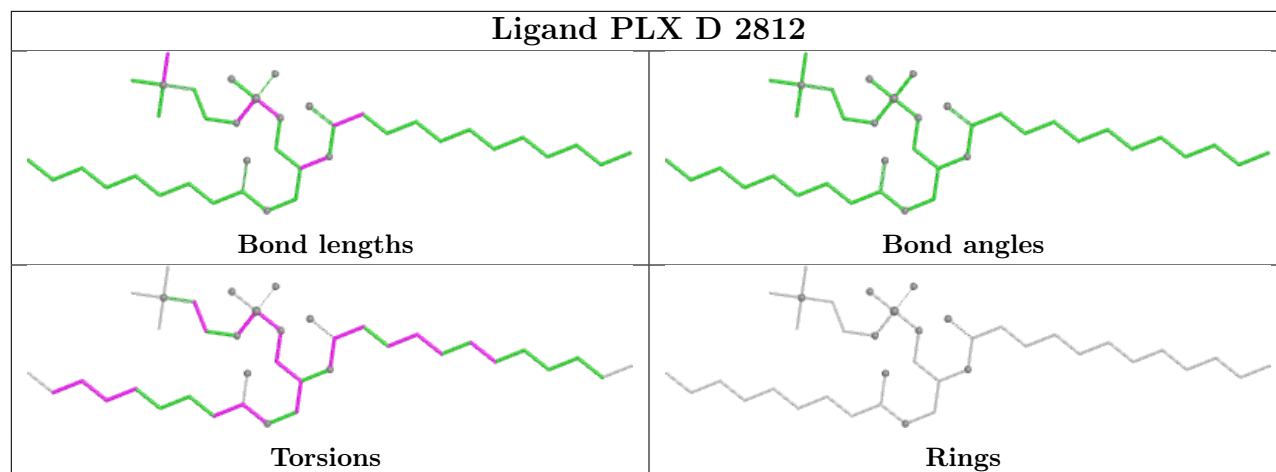
Continued on next page...

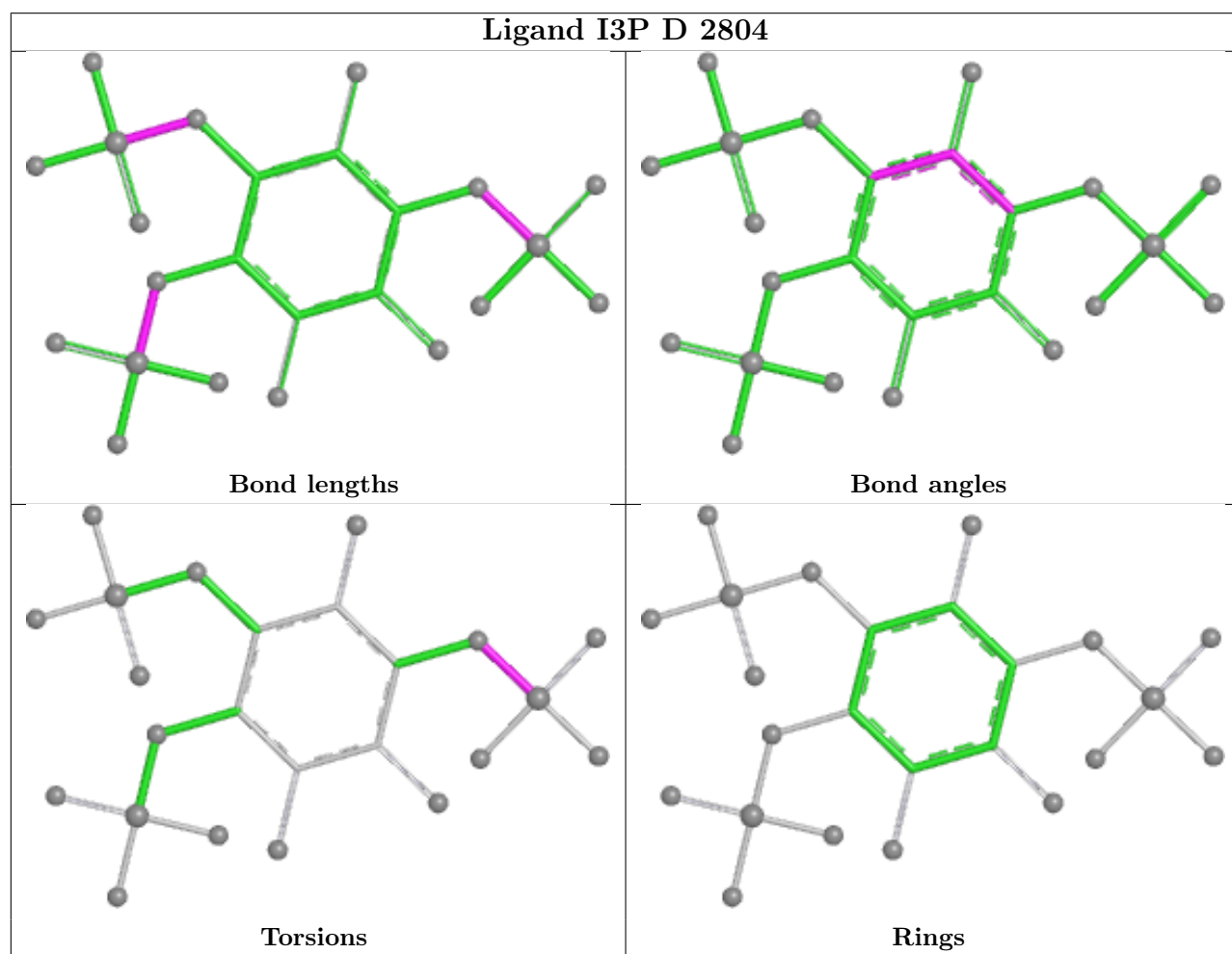
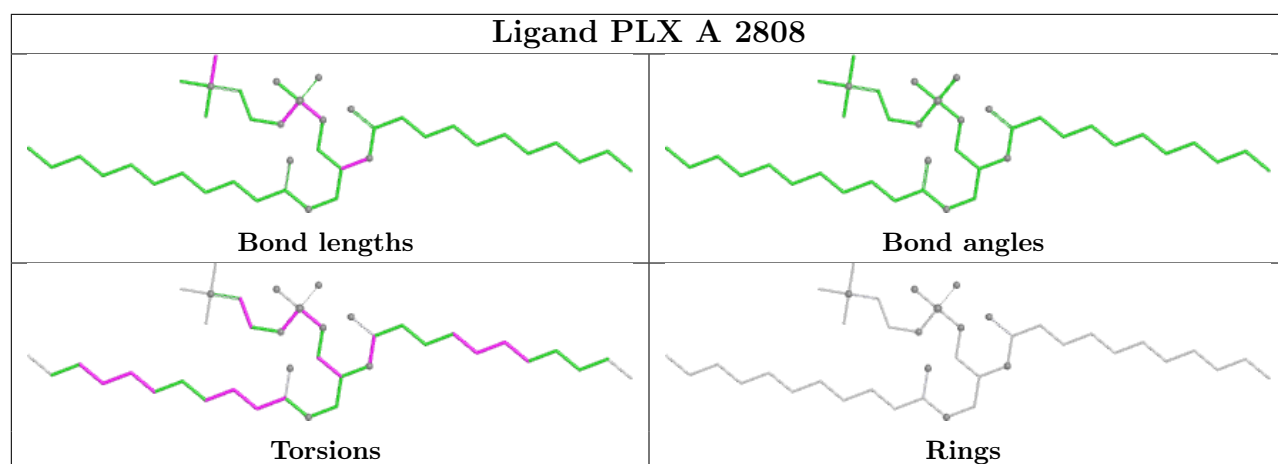
Continued from previous page...

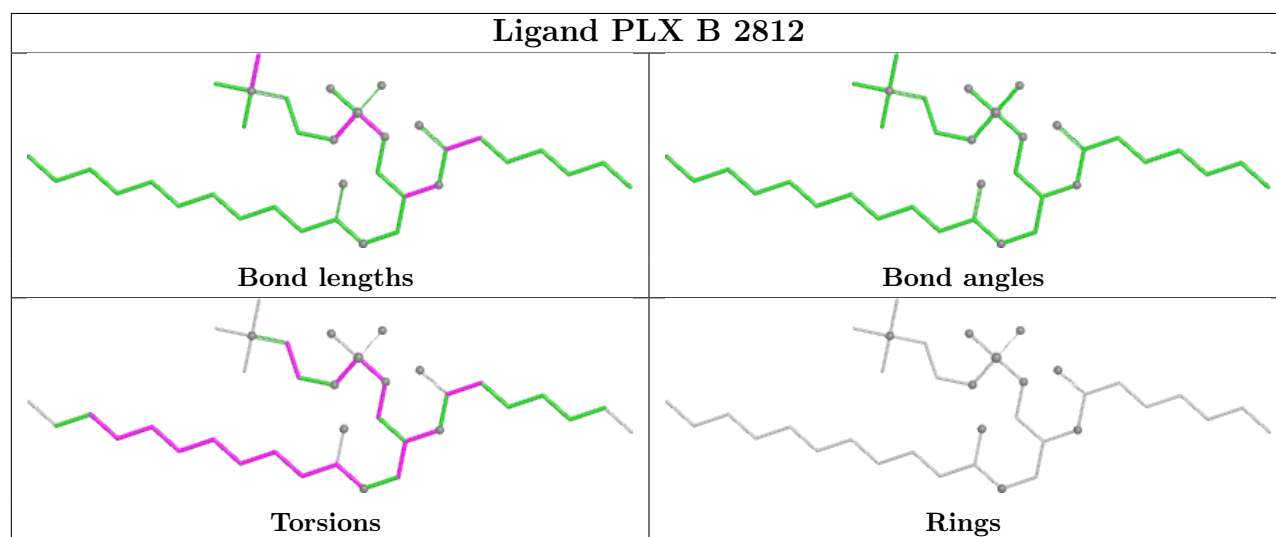
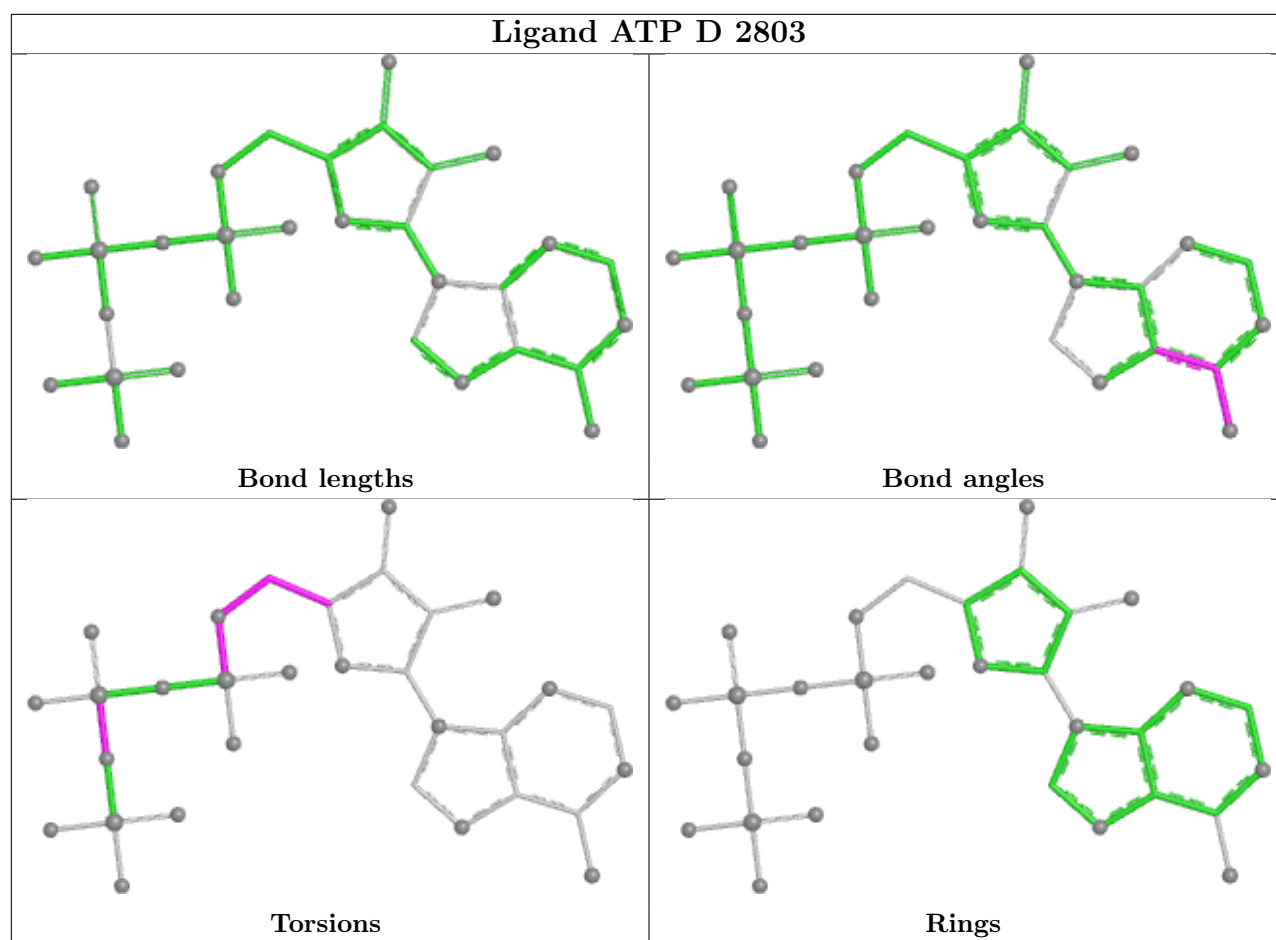
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2811	PLX	2	0
6	B	2802	PLX	1	0

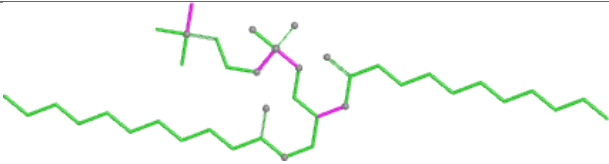
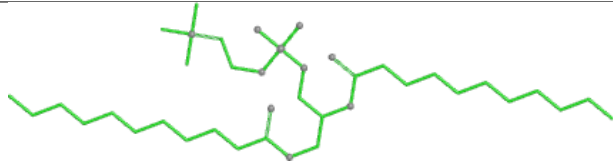
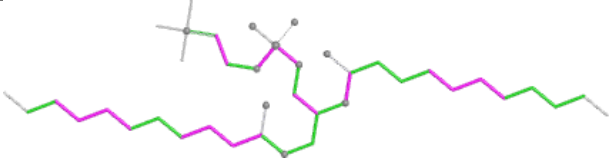
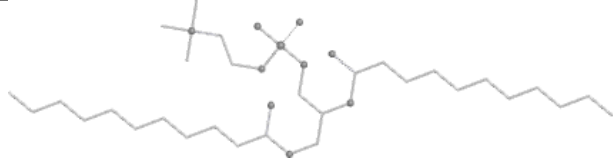
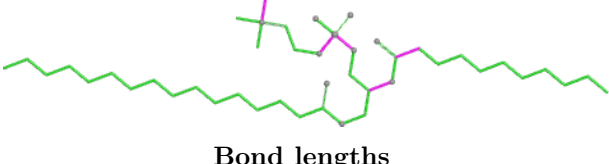
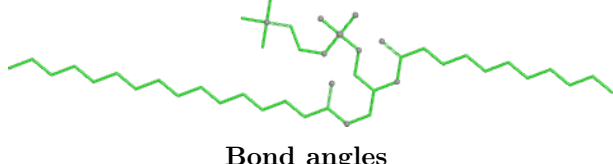
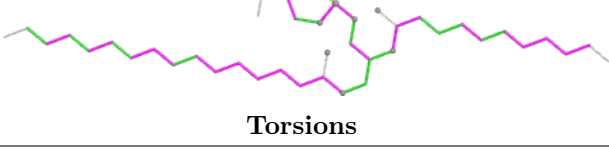
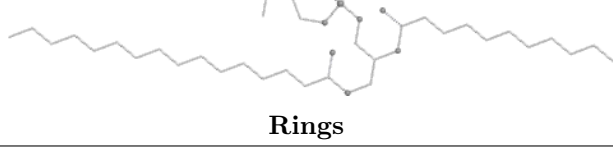
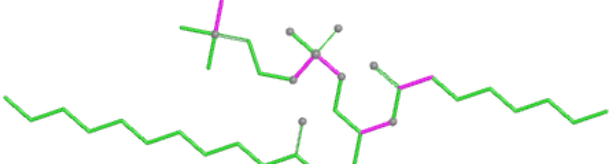
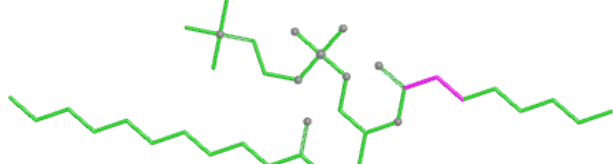
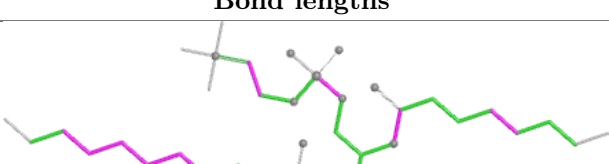
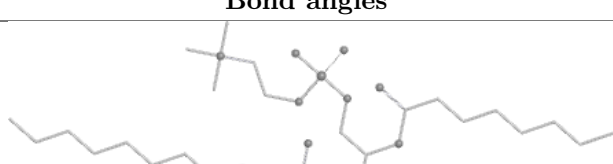
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

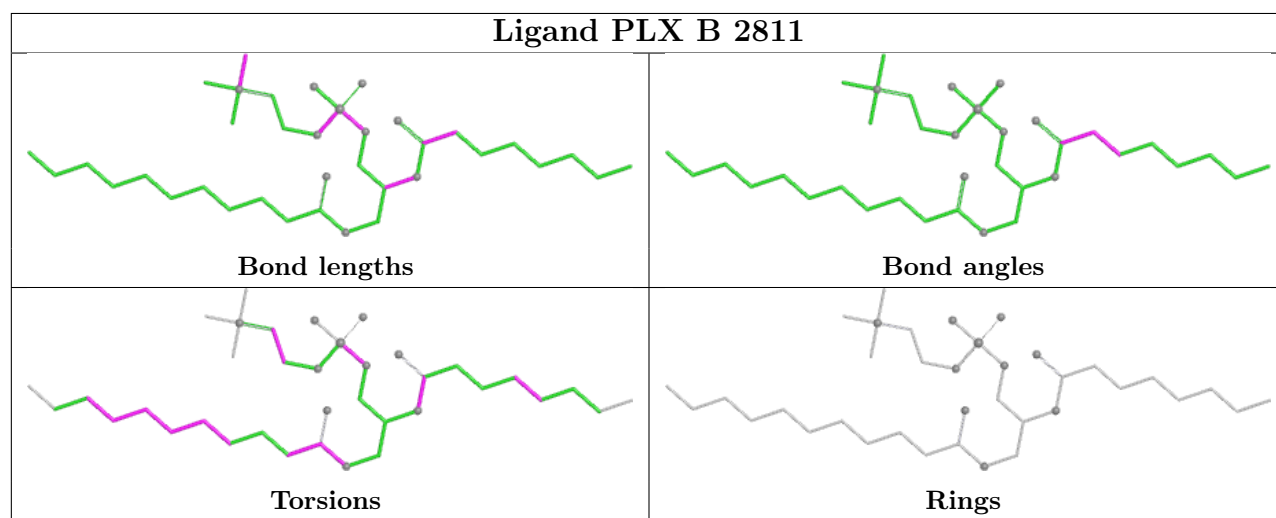
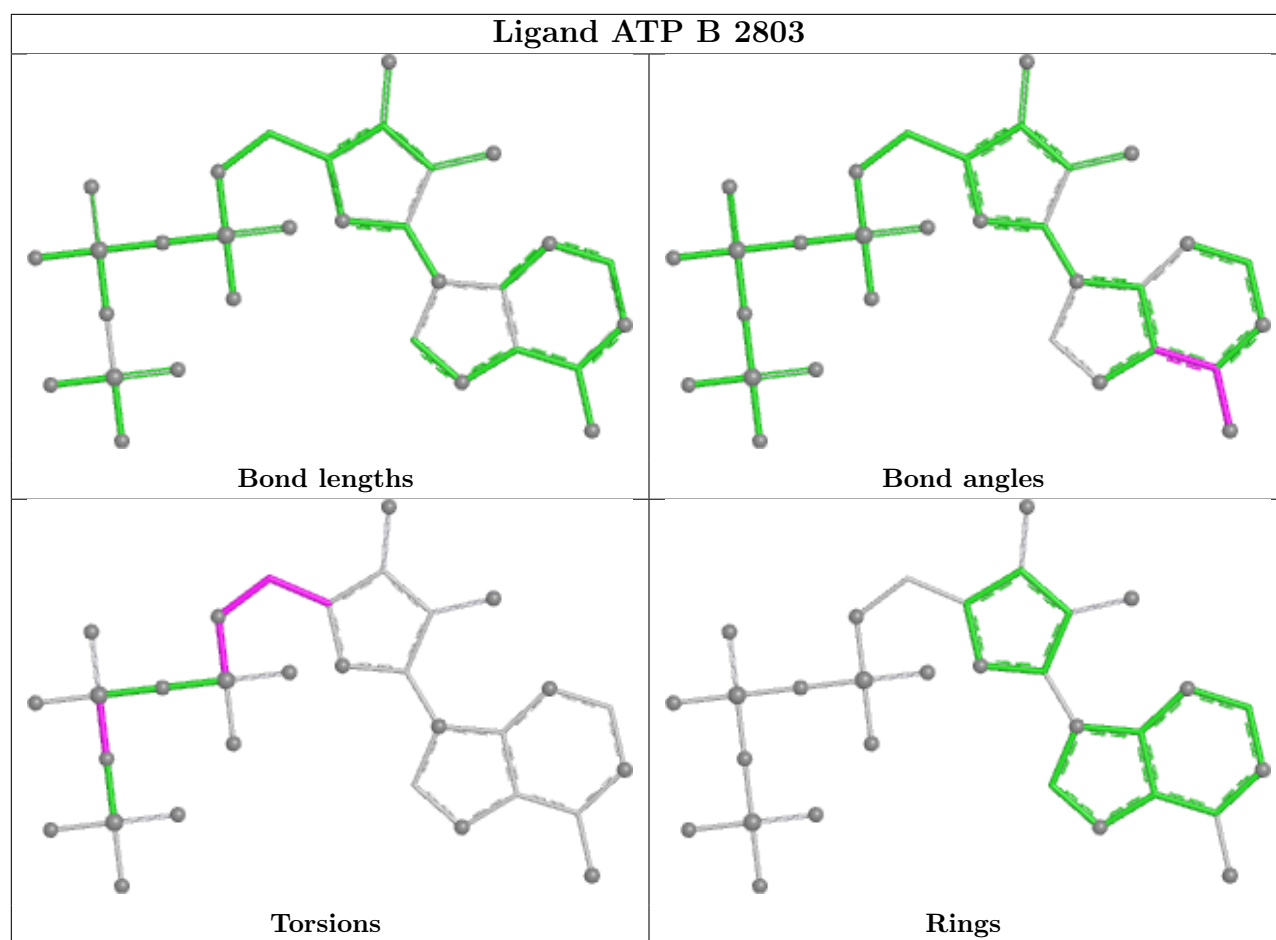


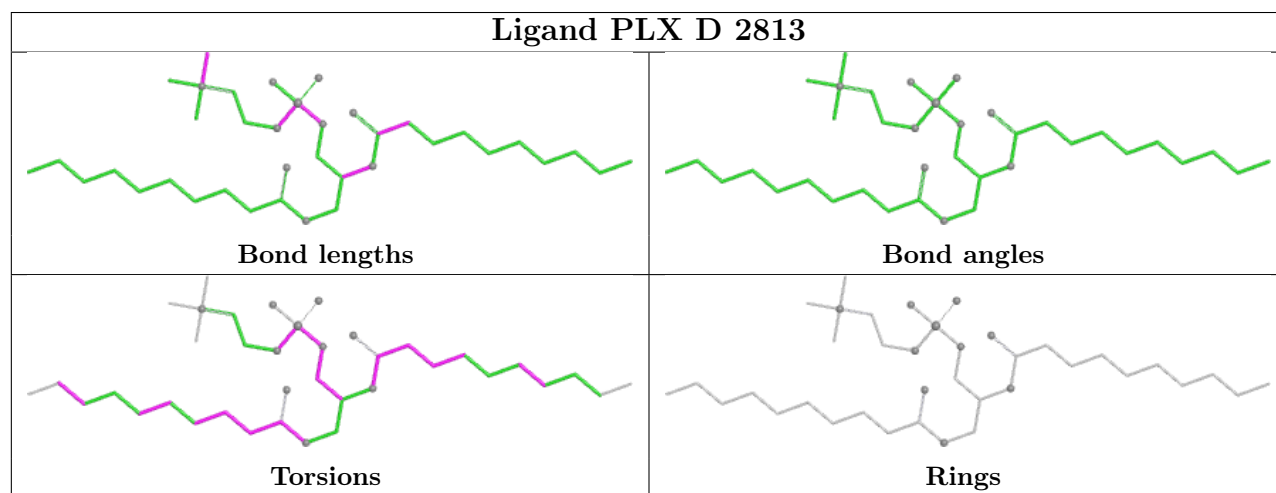
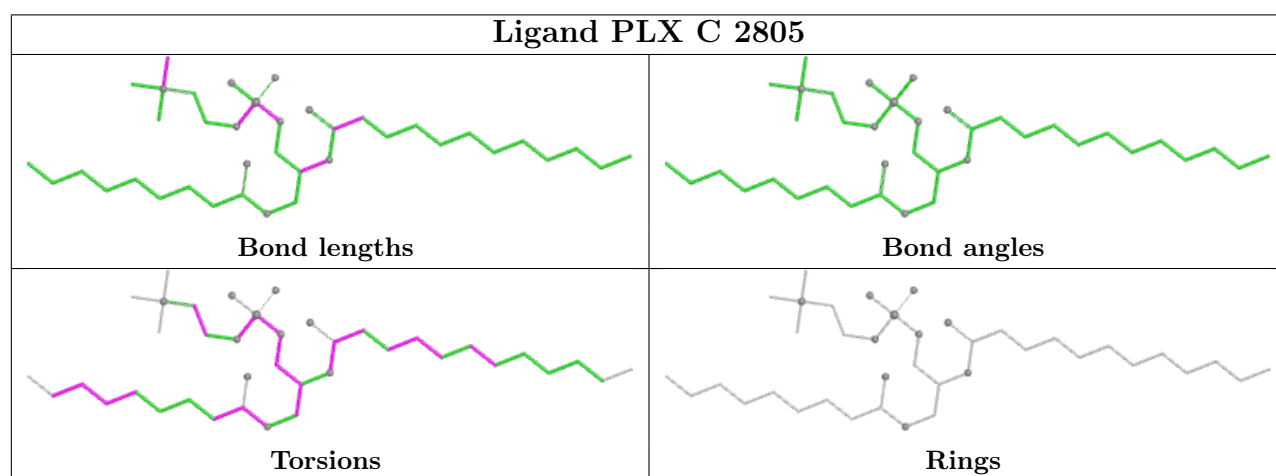
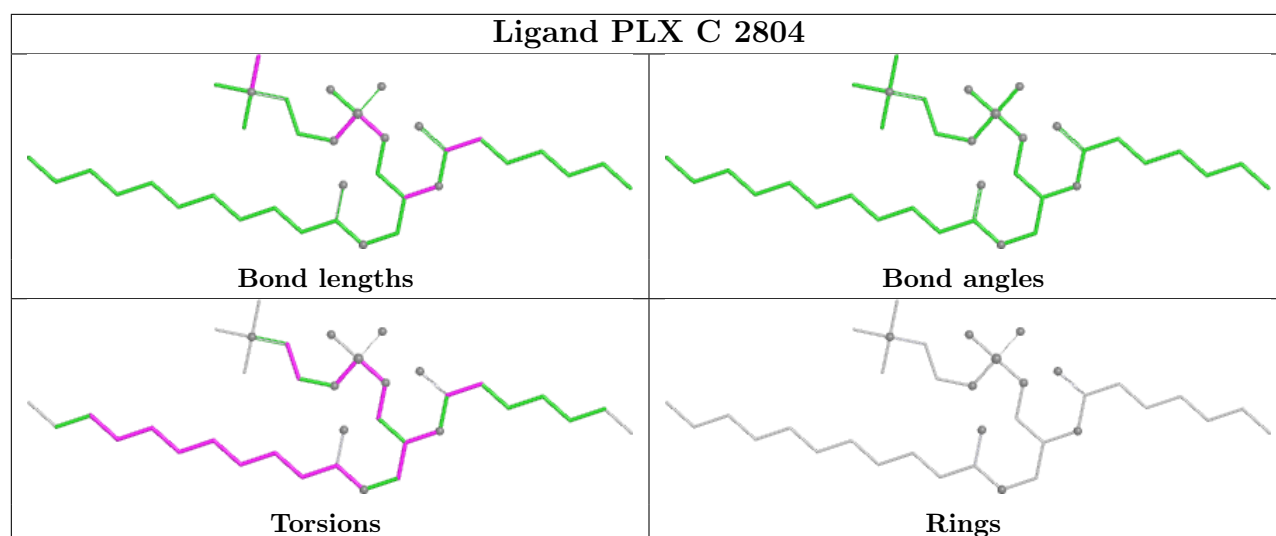


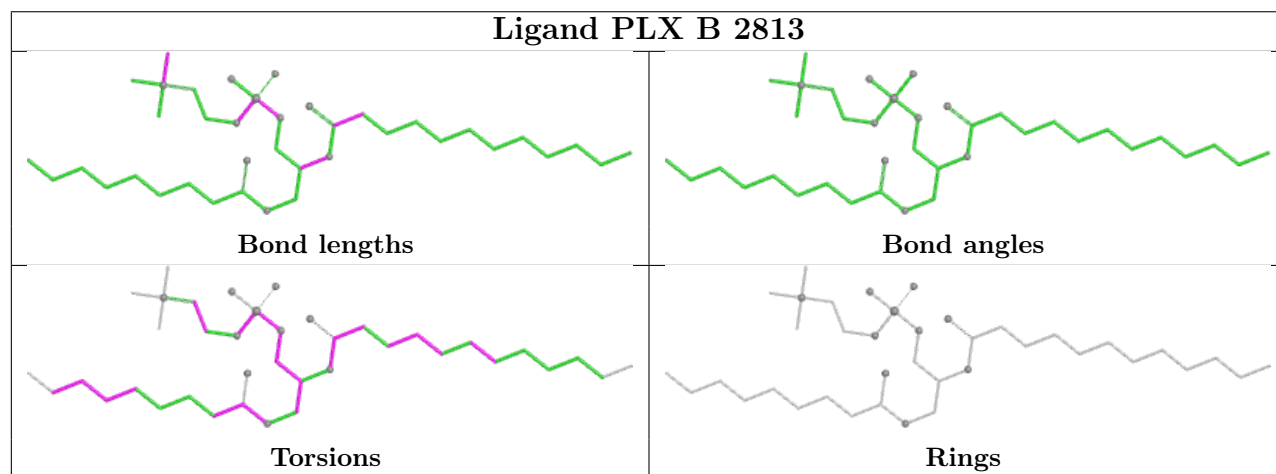
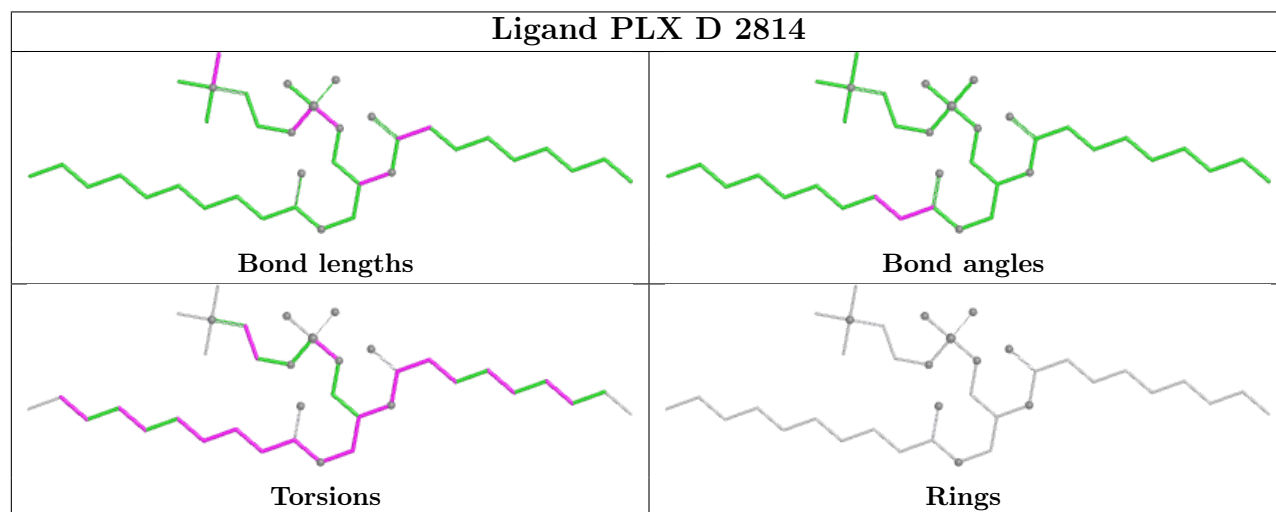
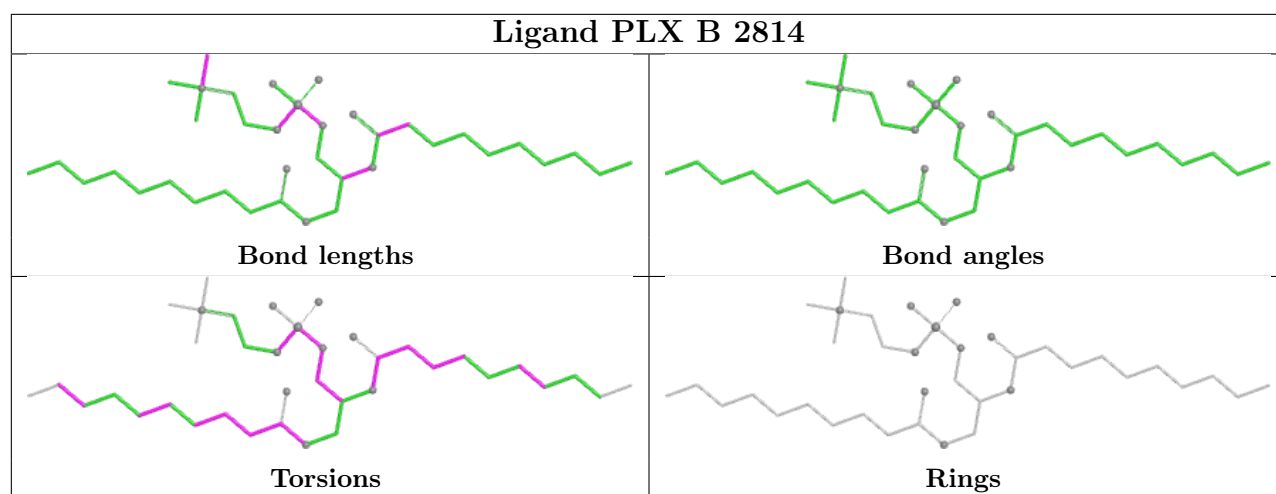


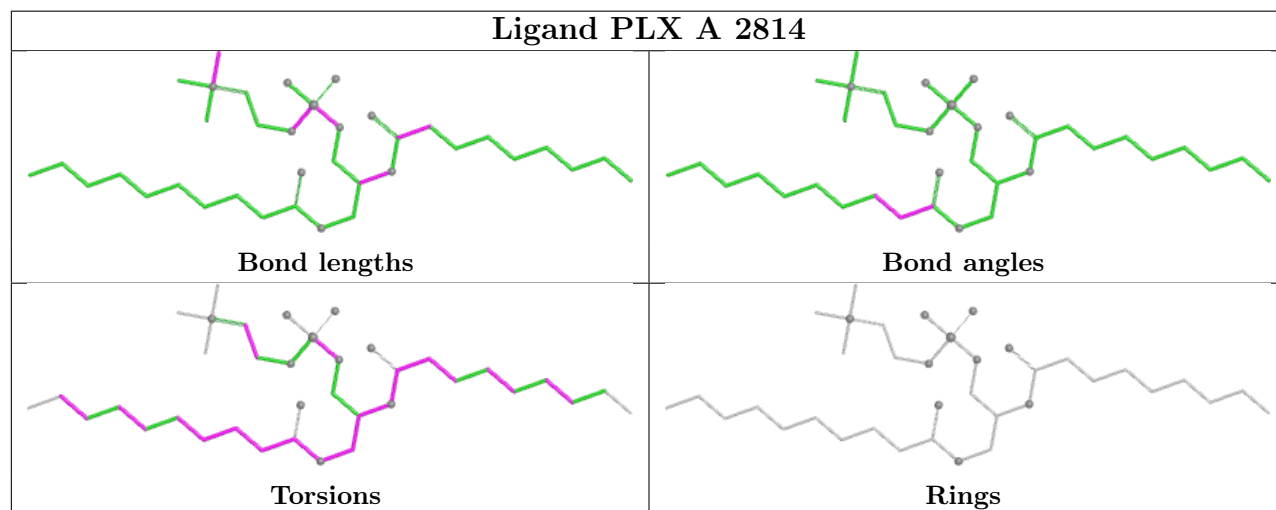
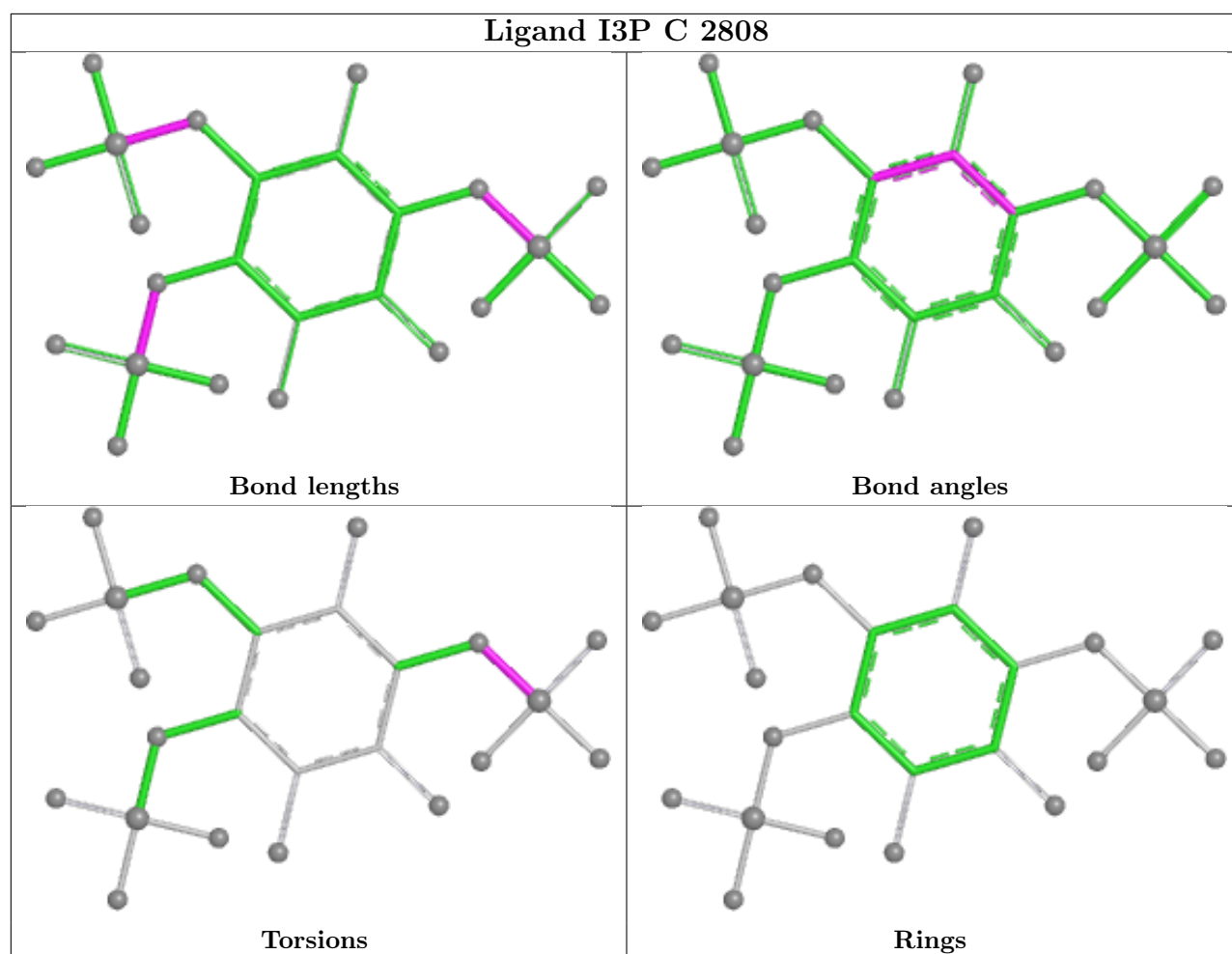


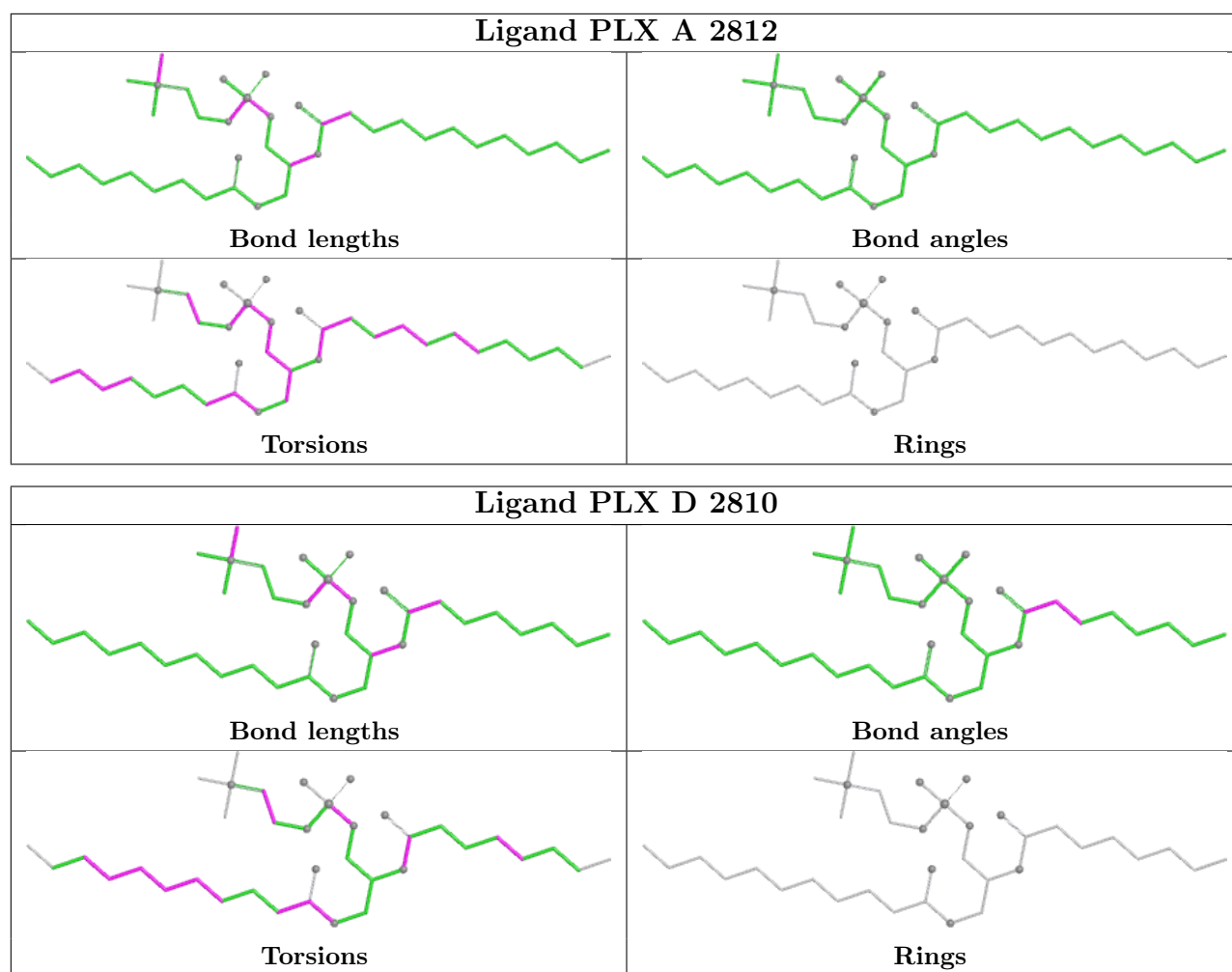
Ligand PLX C 2814	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX D 2809	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX C 2803	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

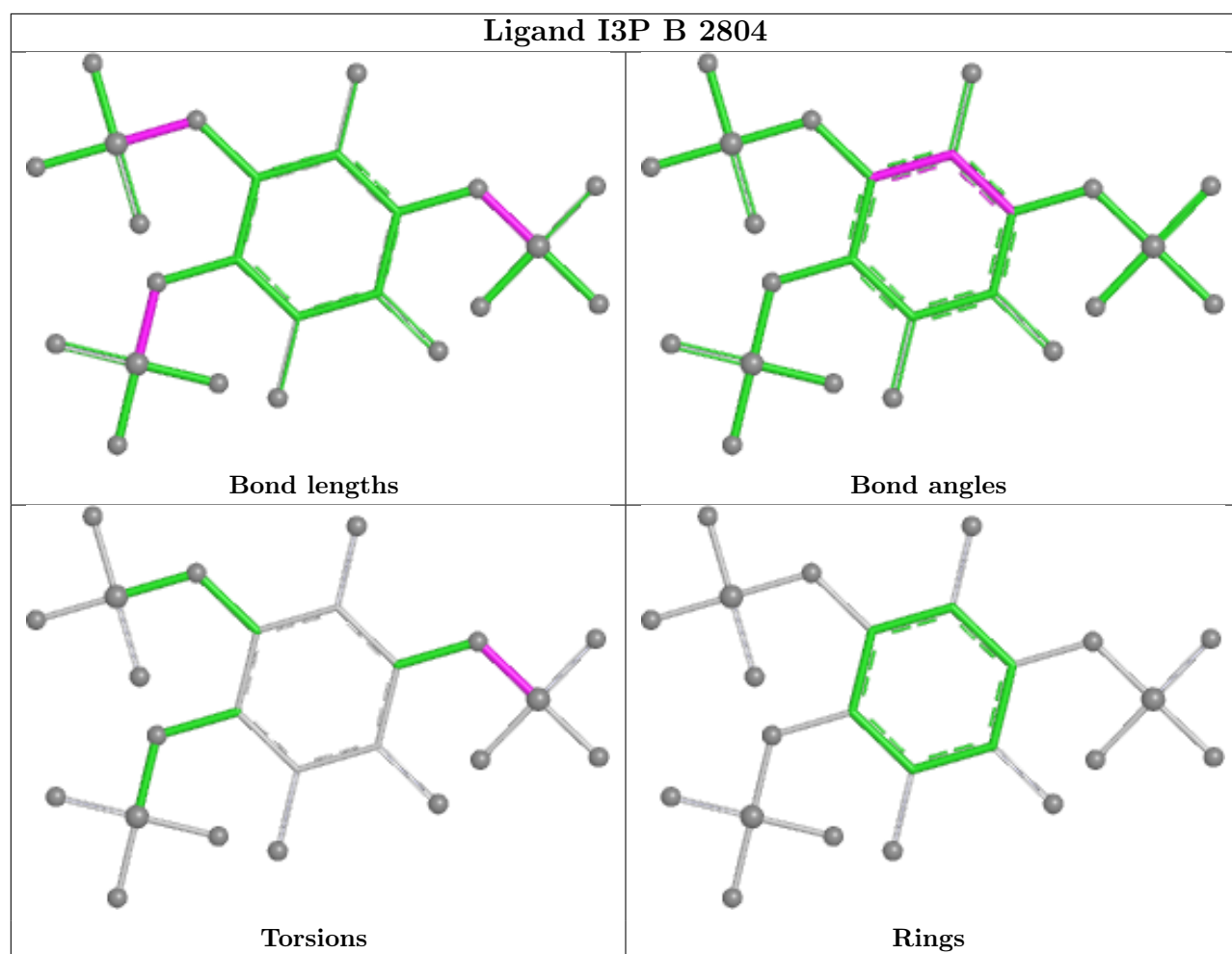


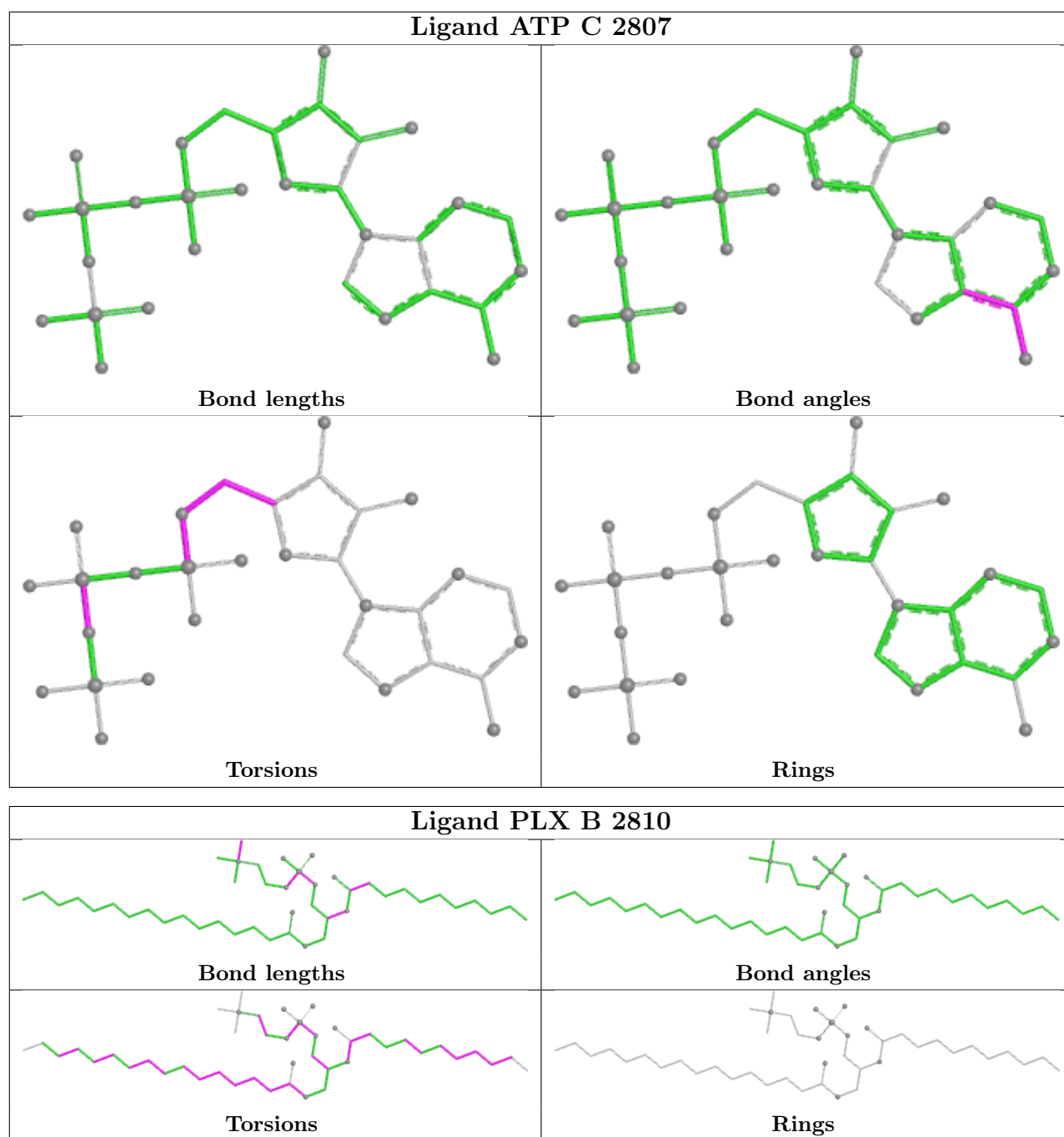


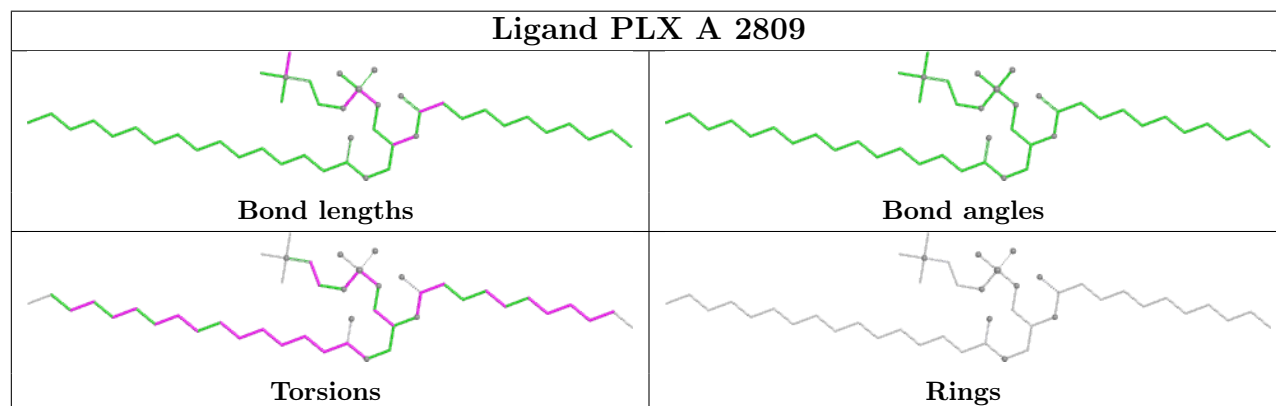
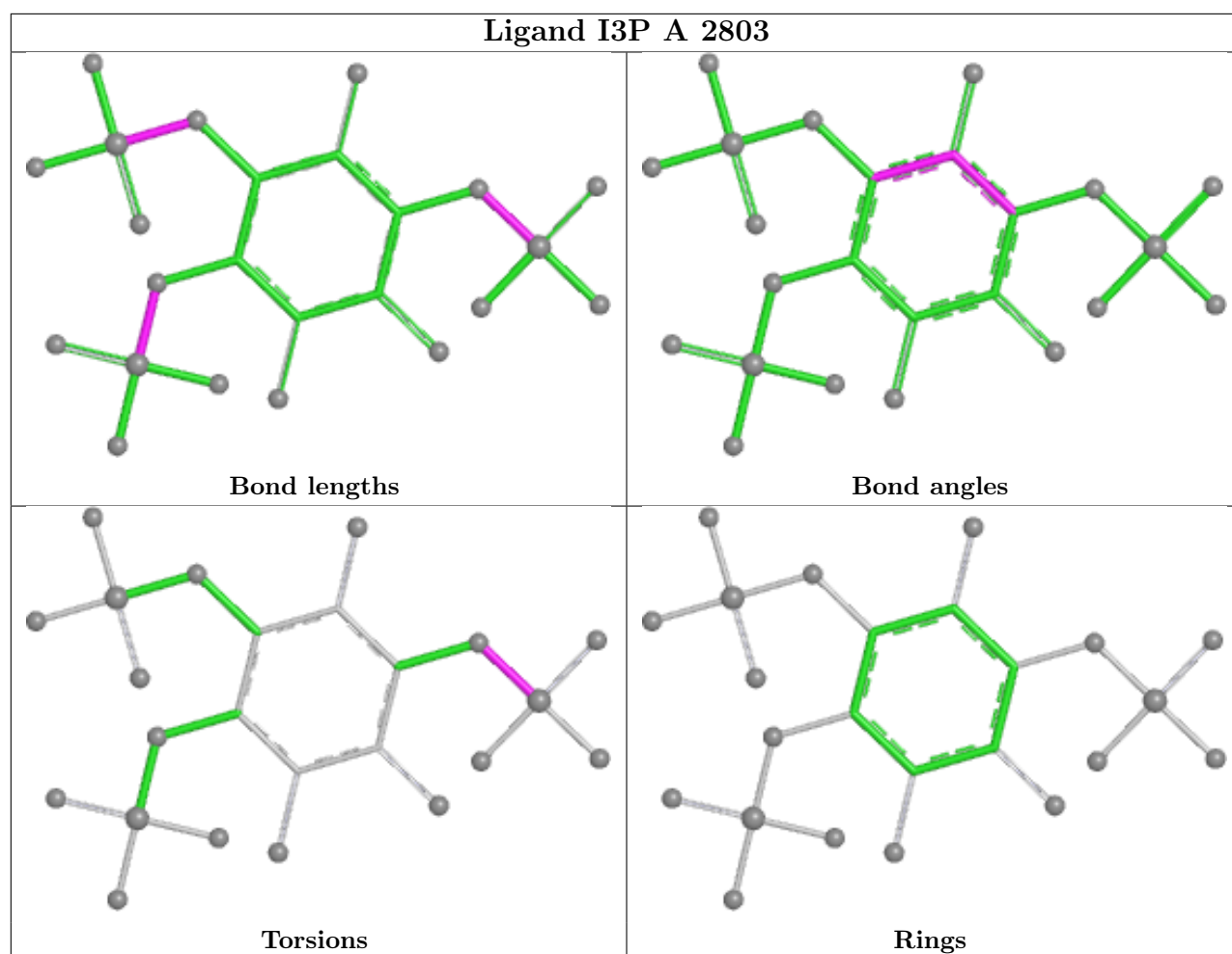


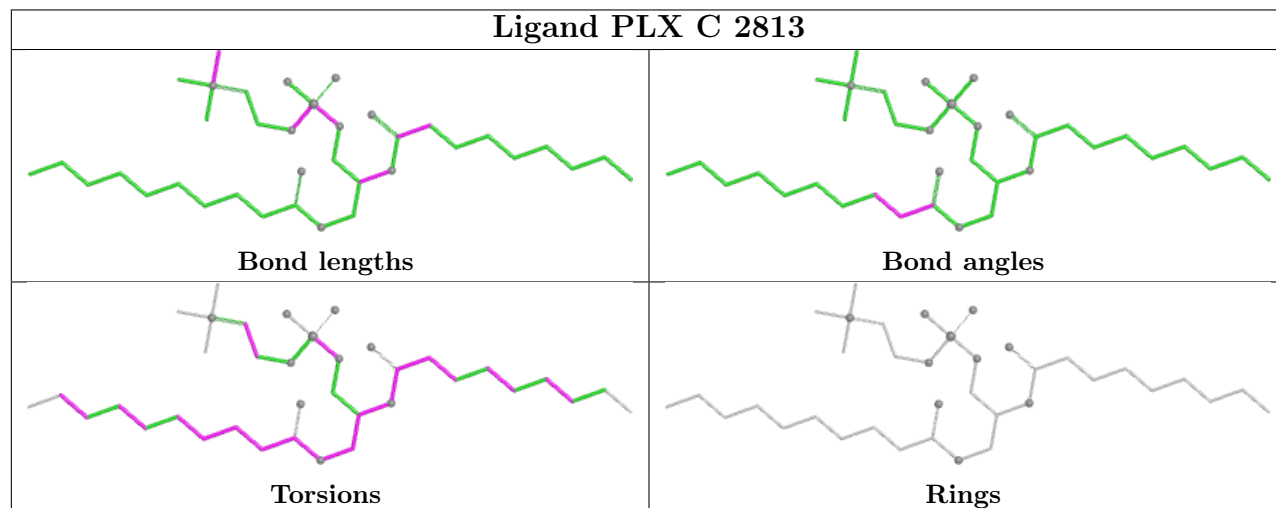
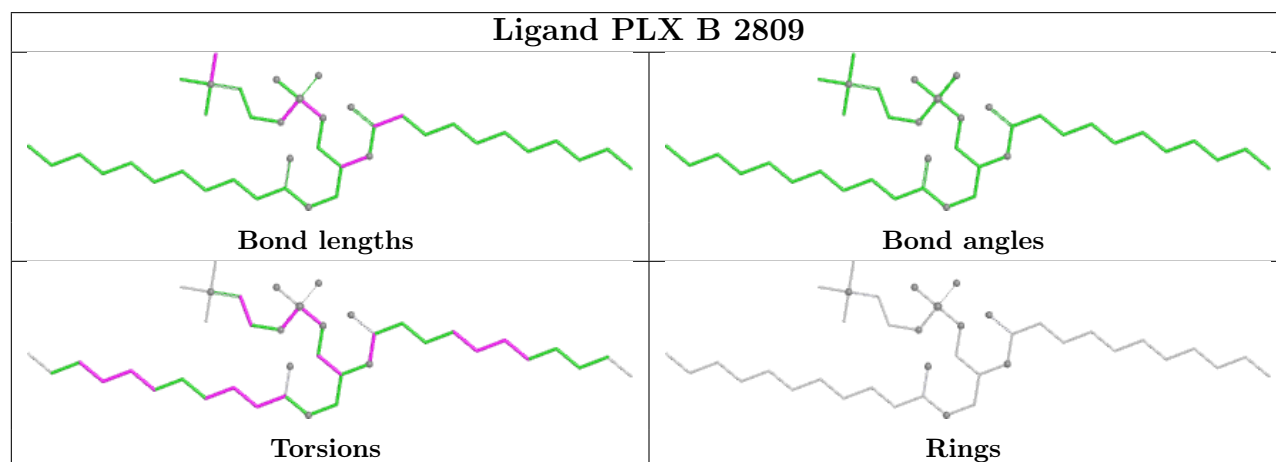
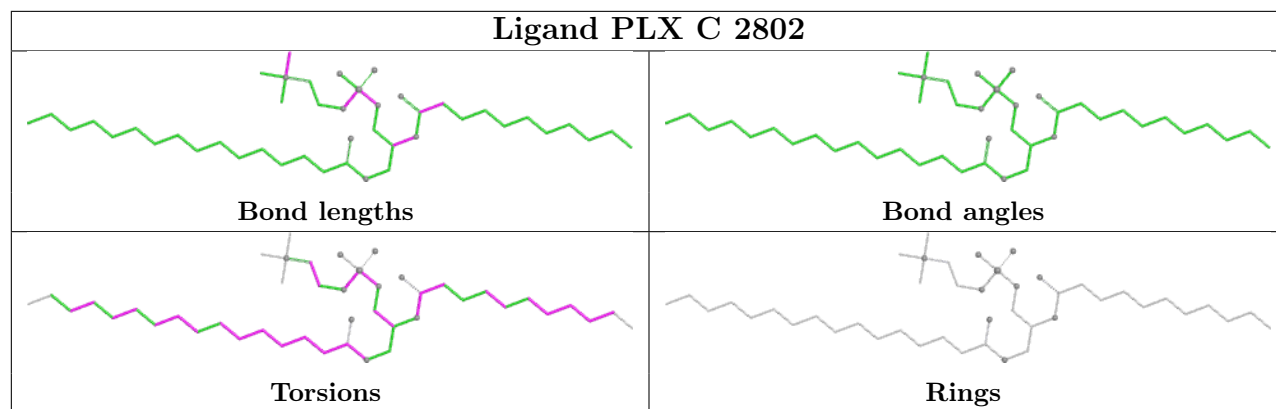


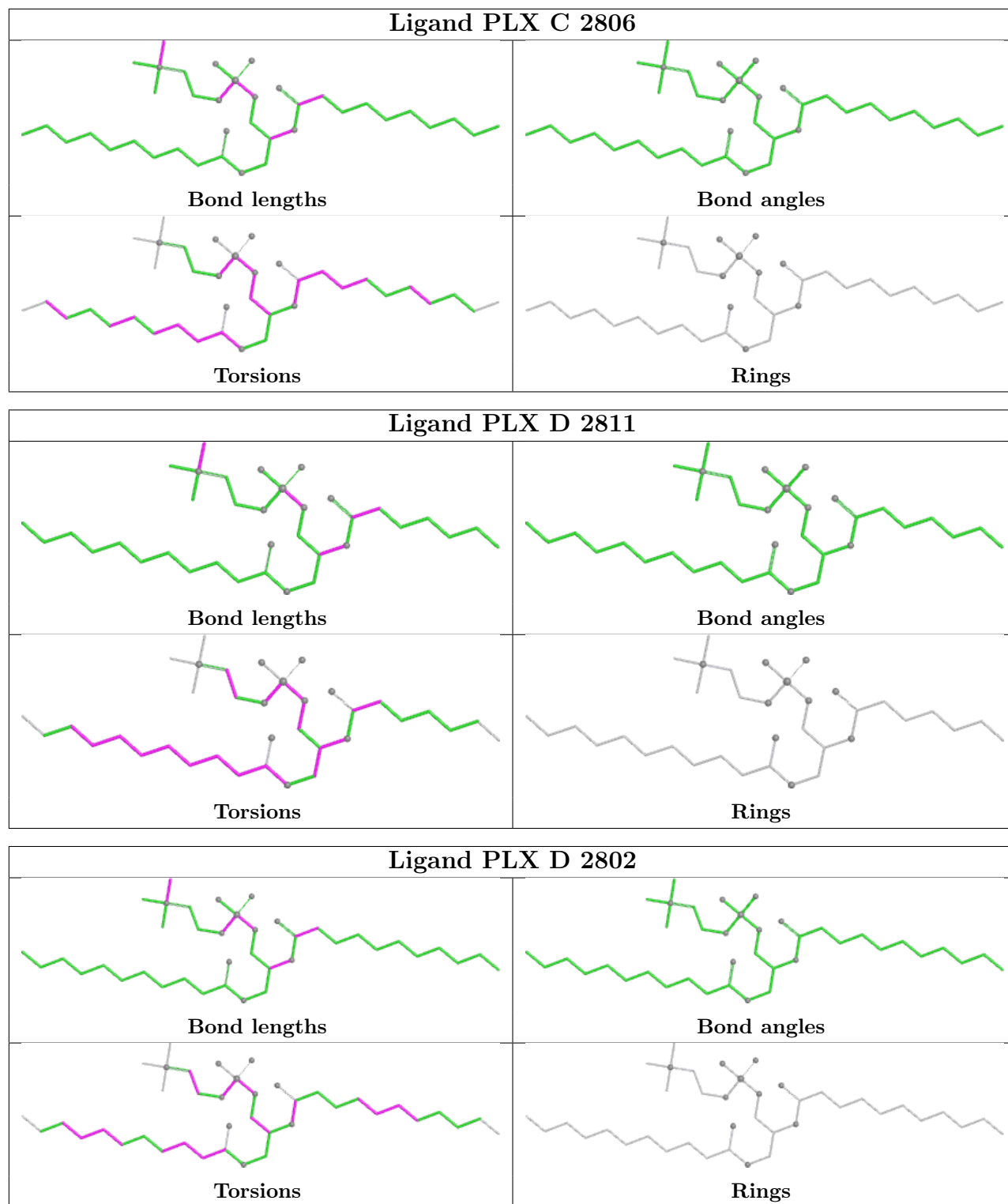


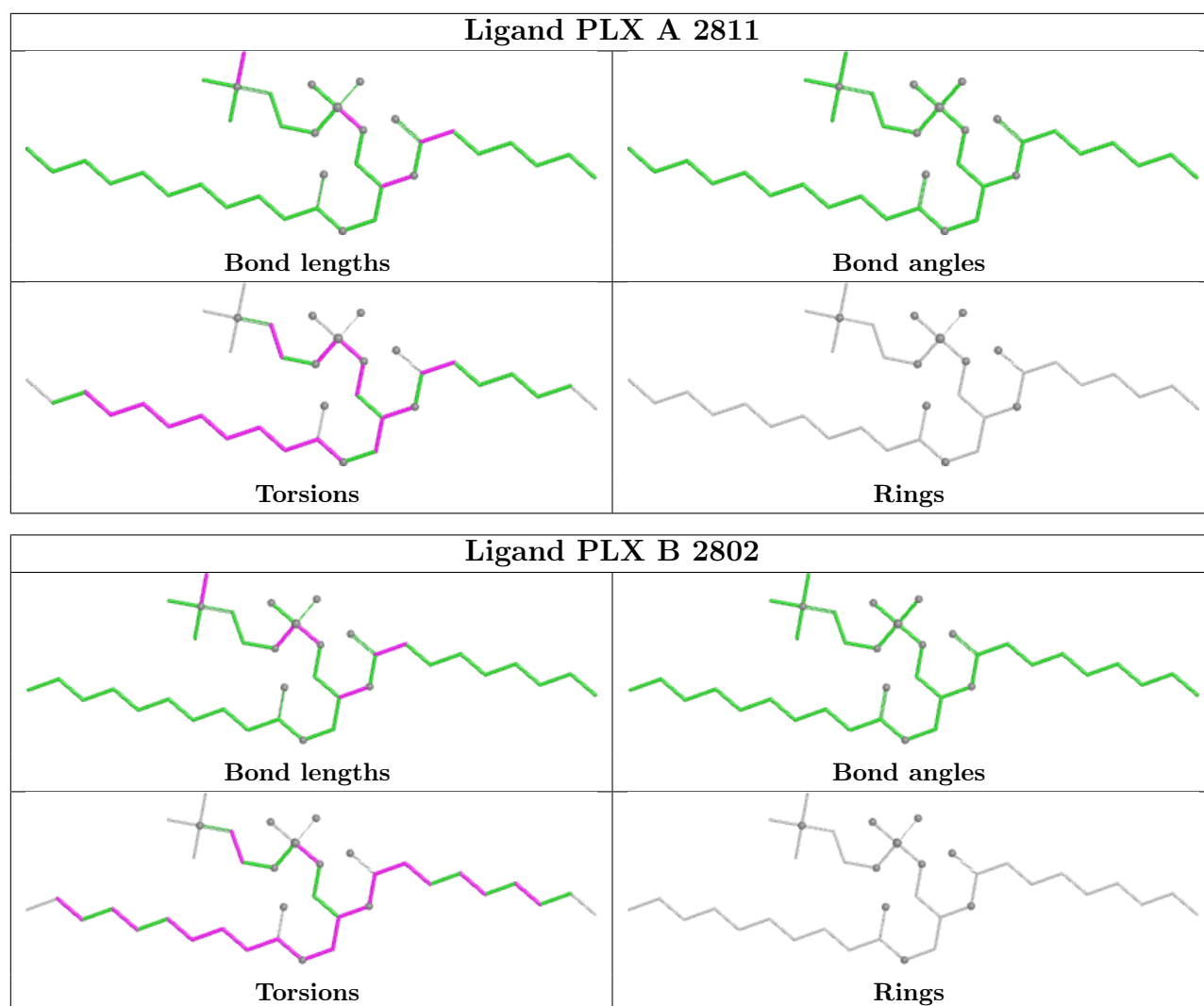












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

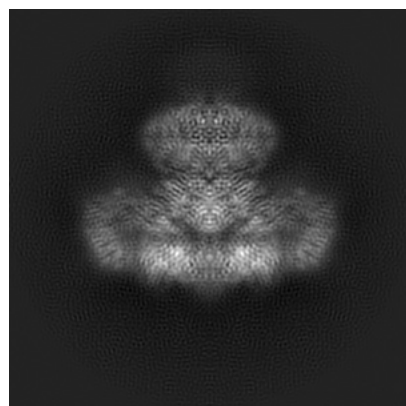
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27983. These allow visual inspection of the internal detail of the map and identification of artifacts.

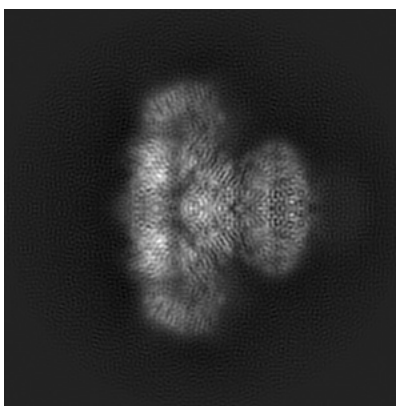
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

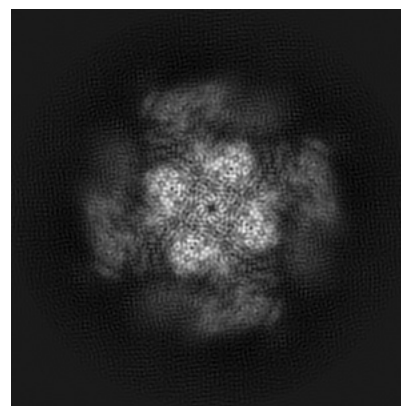
6.1.1 Primary map



X

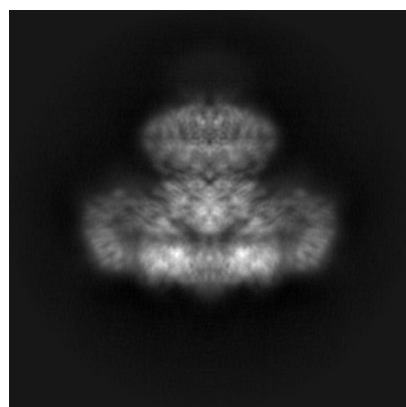


Y

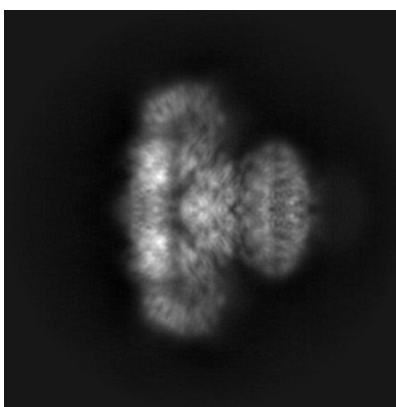


Z

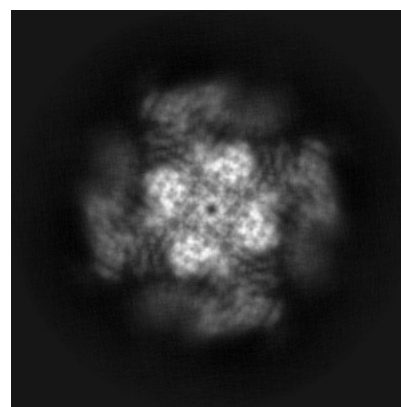
6.1.2 Raw map



X



Y

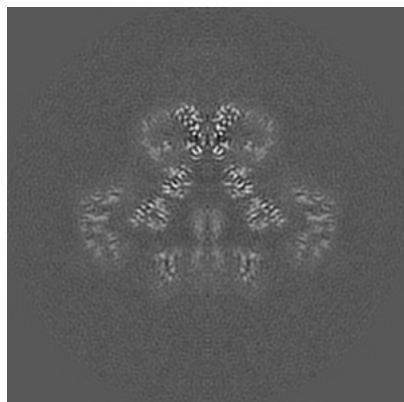


Z

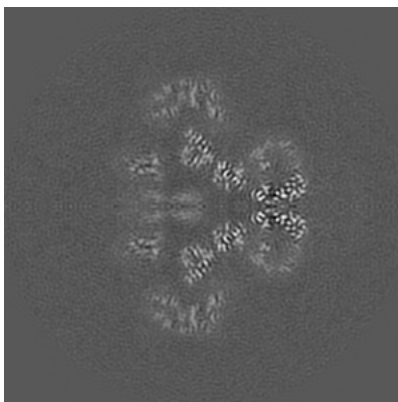
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

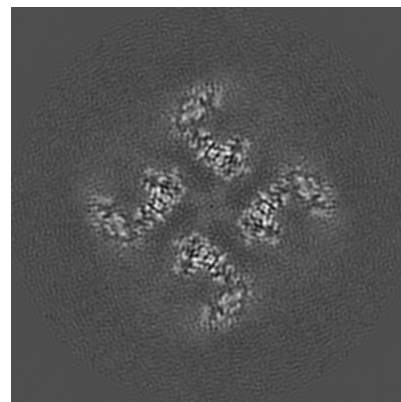
6.2.1 Primary map



X Index: 168

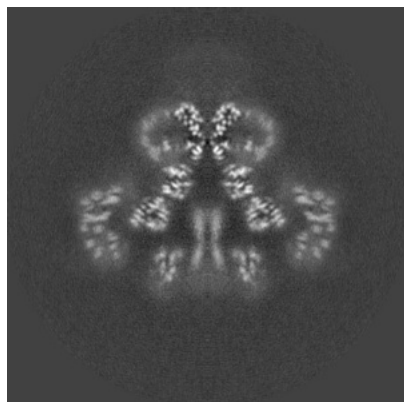


Y Index: 168

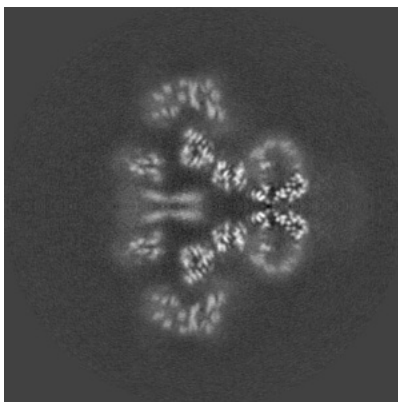


Z Index: 168

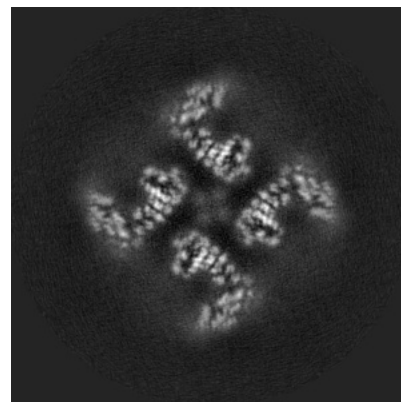
6.2.2 Raw map



X Index: 168



Y Index: 168

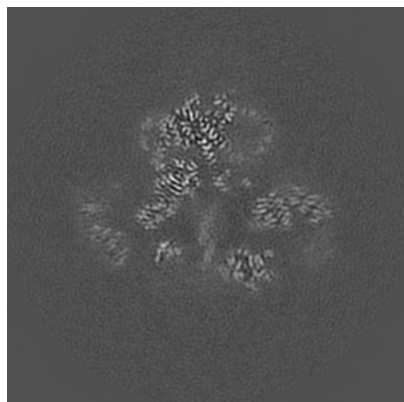


Z Index: 168

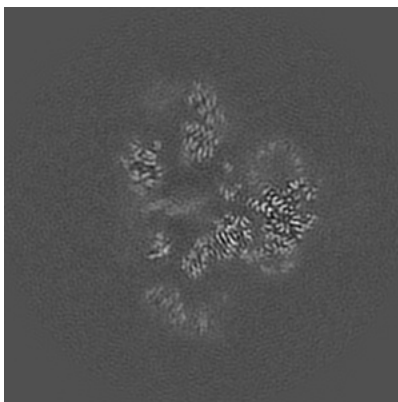
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

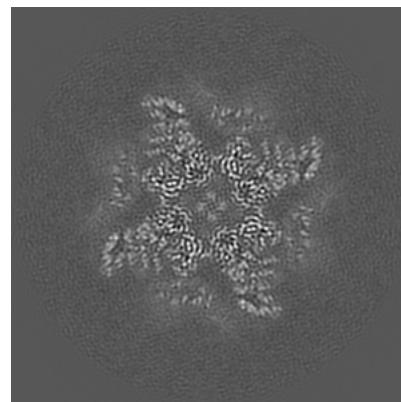
6.3.1 Primary map



X Index: 160

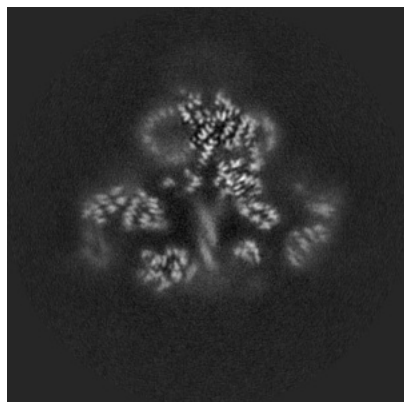


Y Index: 176

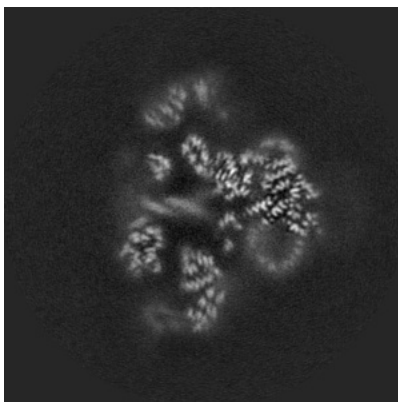


Z Index: 125

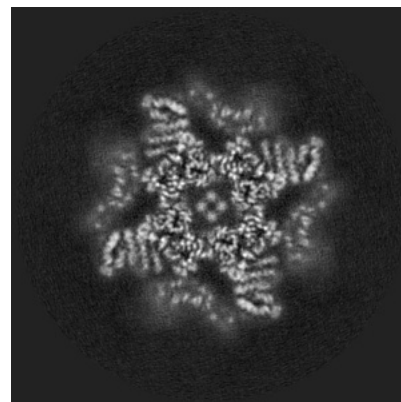
6.3.2 Raw map



X Index: 176



Y Index: 160

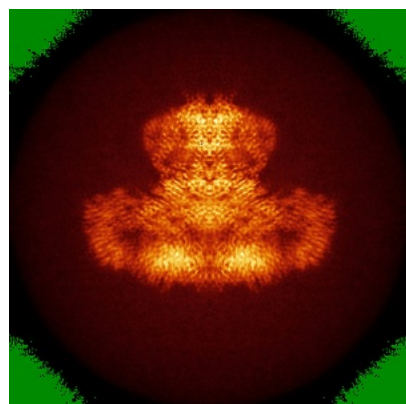


Z Index: 126

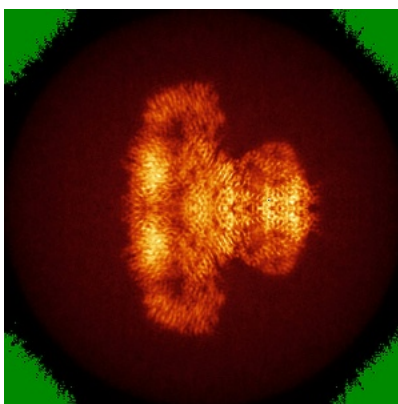
The images above show the largest variance slices of the map in three orthogonal directions.

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

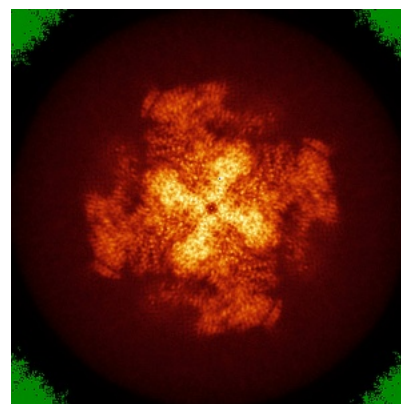
6.4.1 Primary map



X

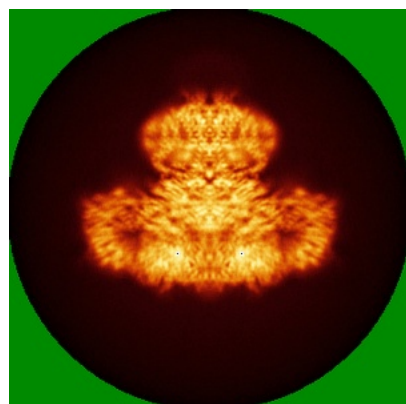


Y

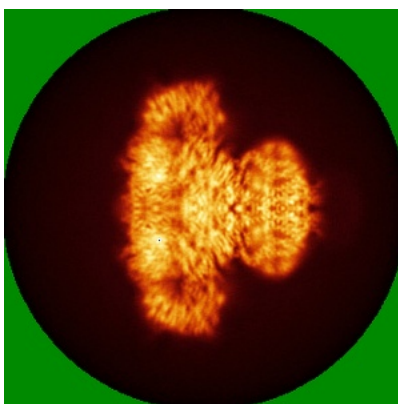


Z

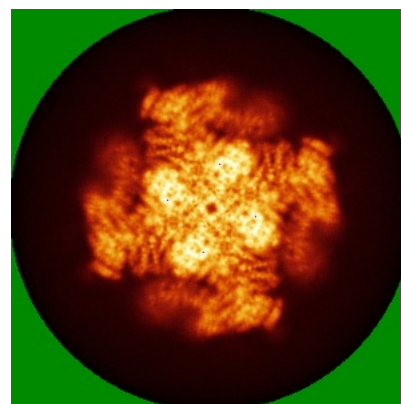
6.4.2 Raw map



X



Y

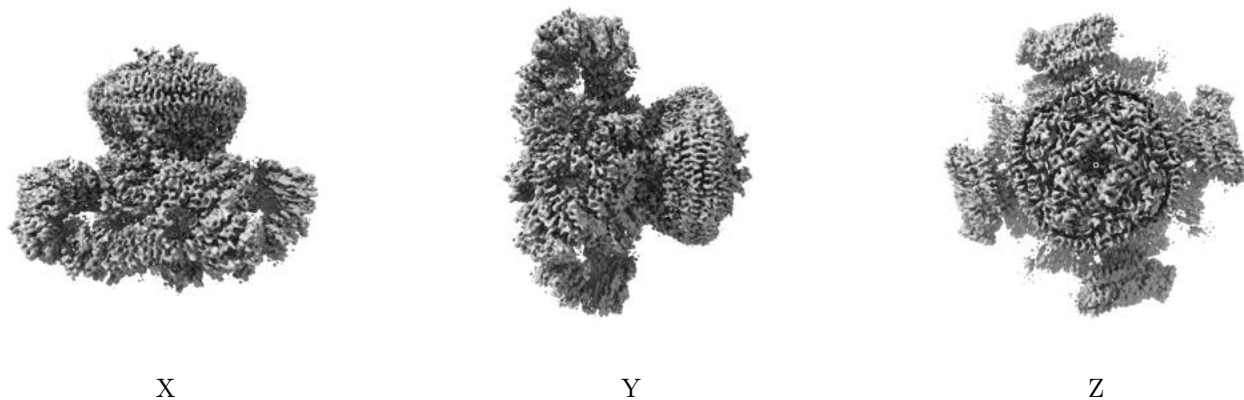


Z

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.

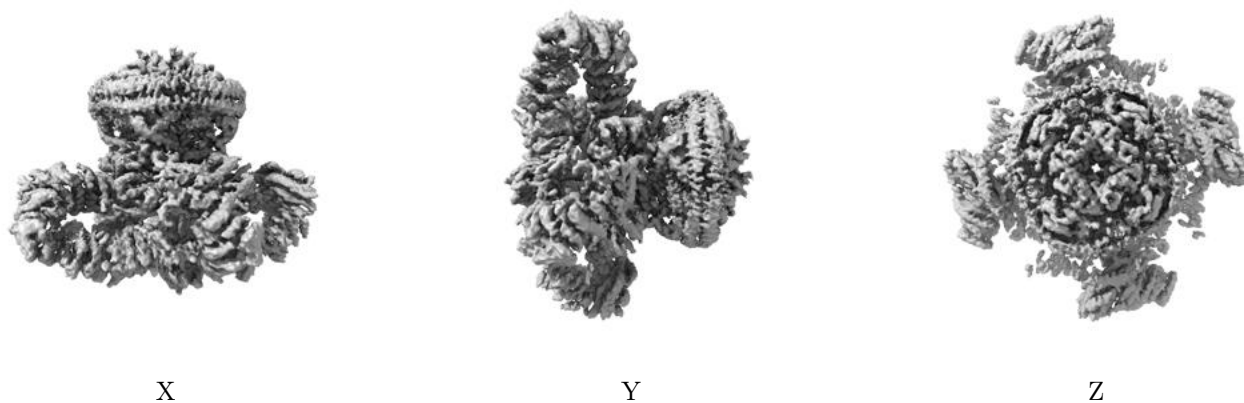
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

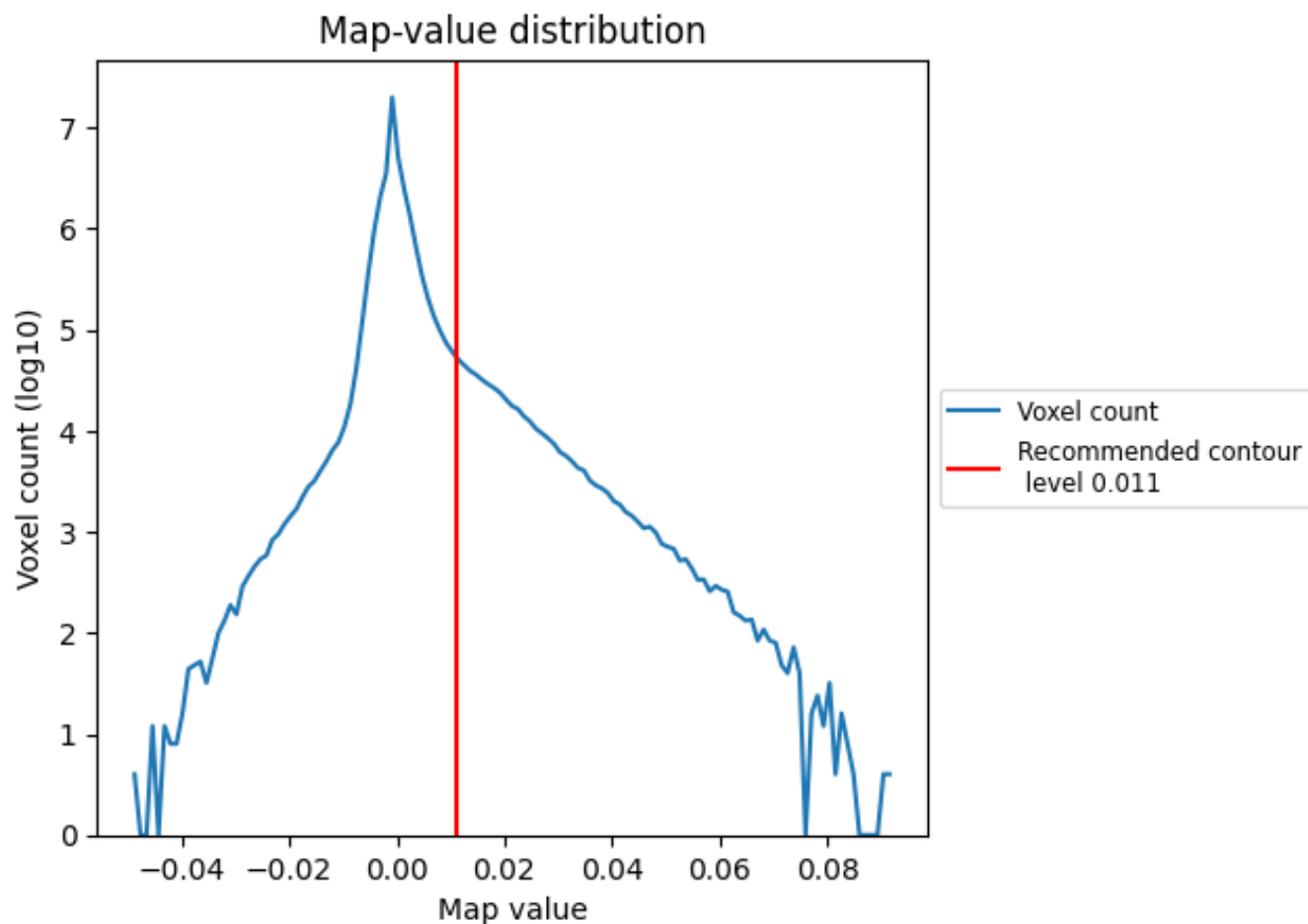
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

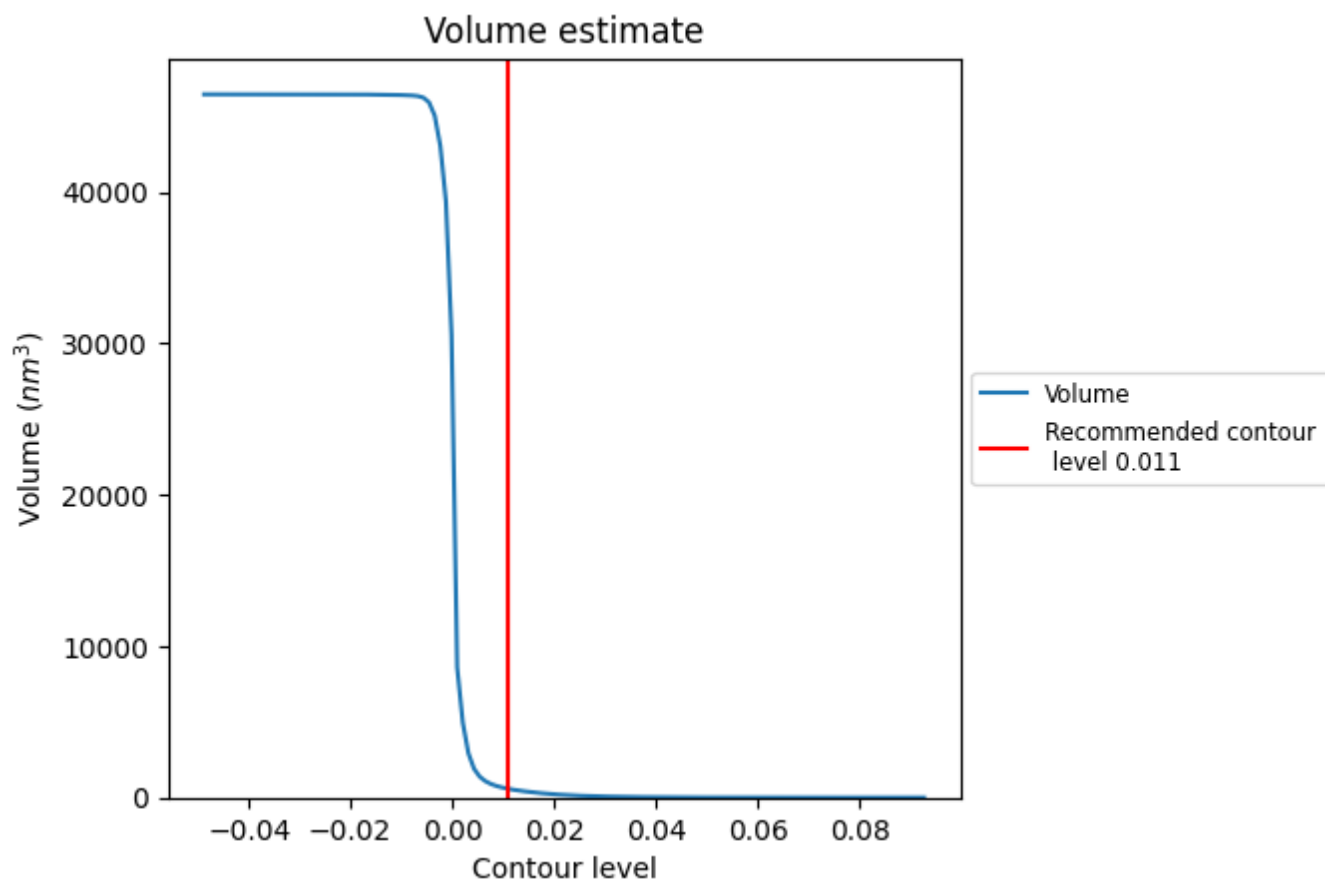
This section contains the results of statistical analysis of the map.

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.

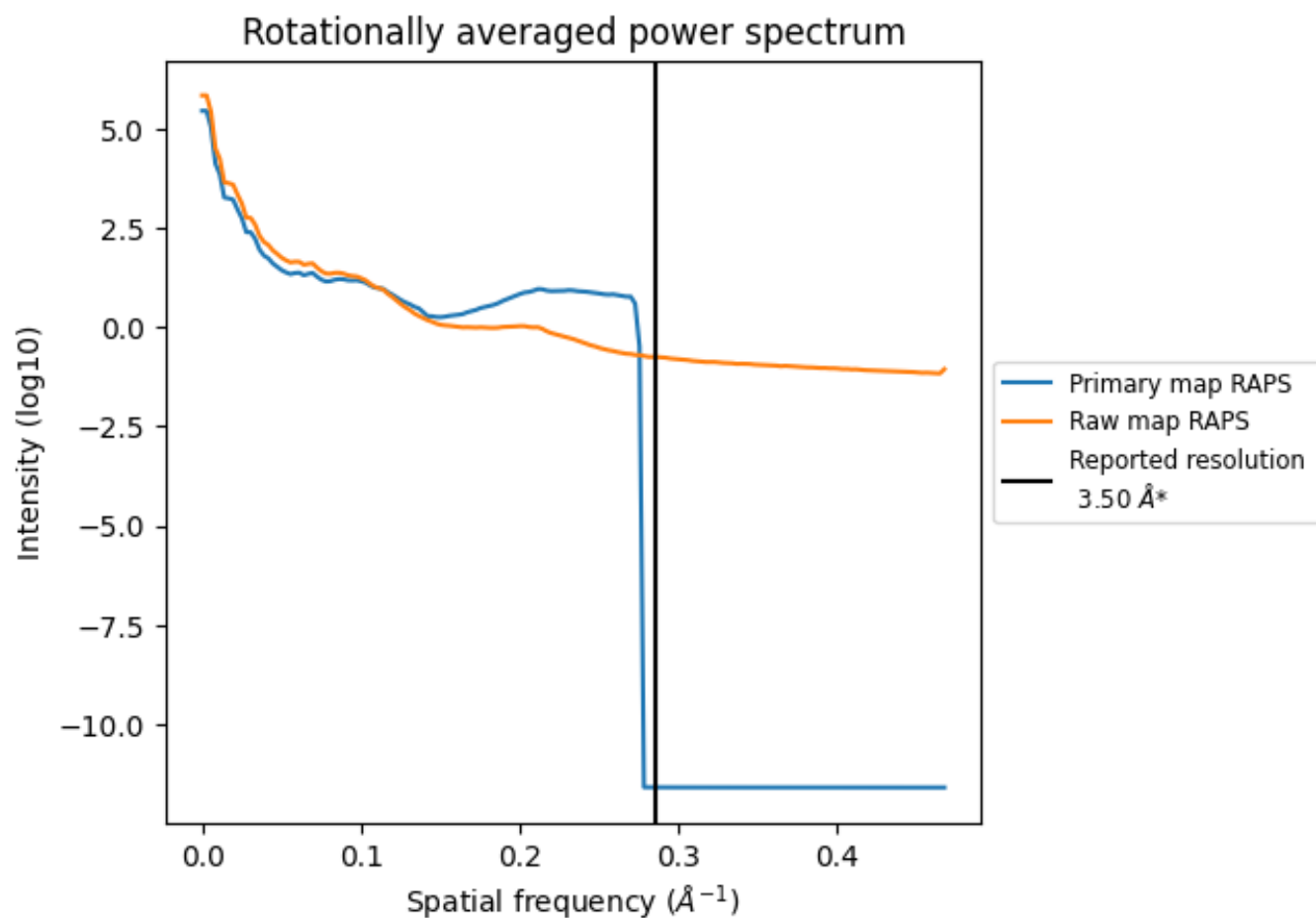
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 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 ⓘ

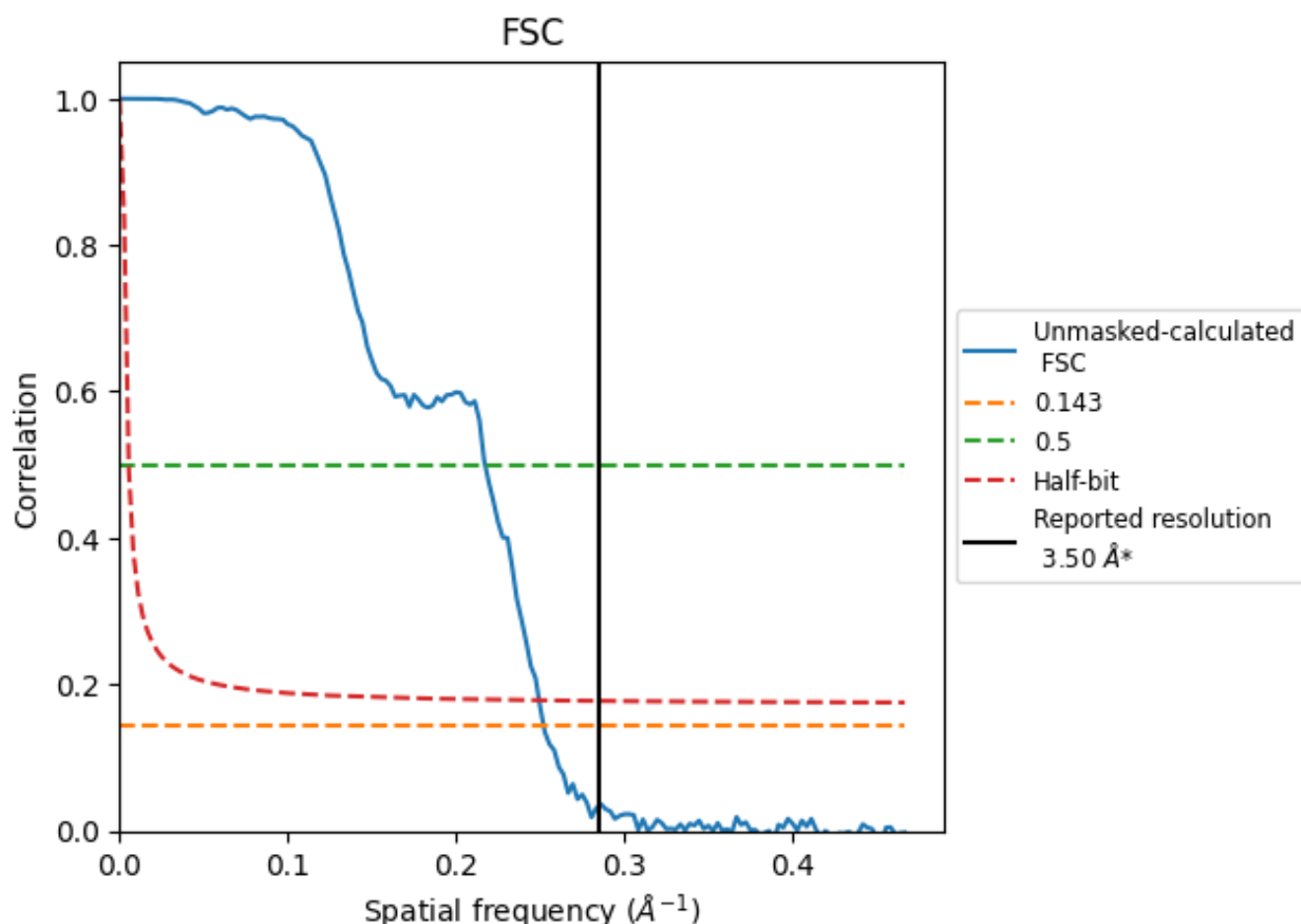


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

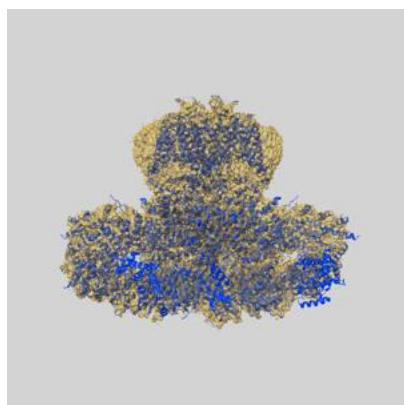
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	4.60	4.00

*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 3.96 differs from the reported value 3.5 by more than 10 %

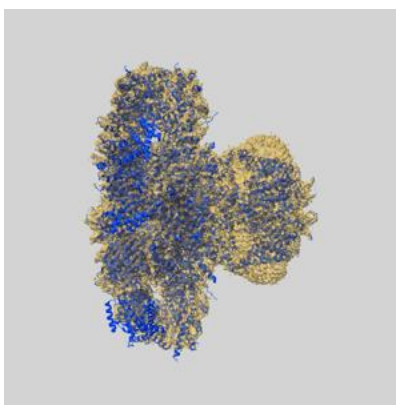
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27983 and PDB model 8EAR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

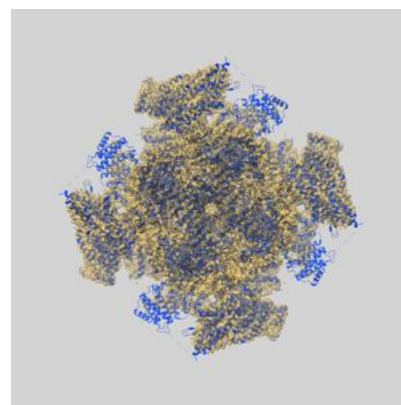
9.1 Map-model overlay [i](#)



X



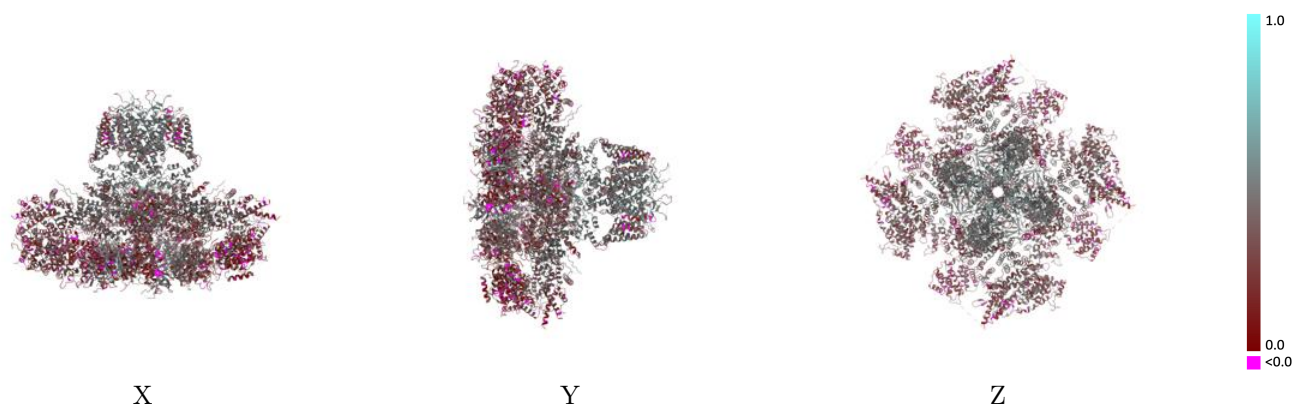
Y



Z

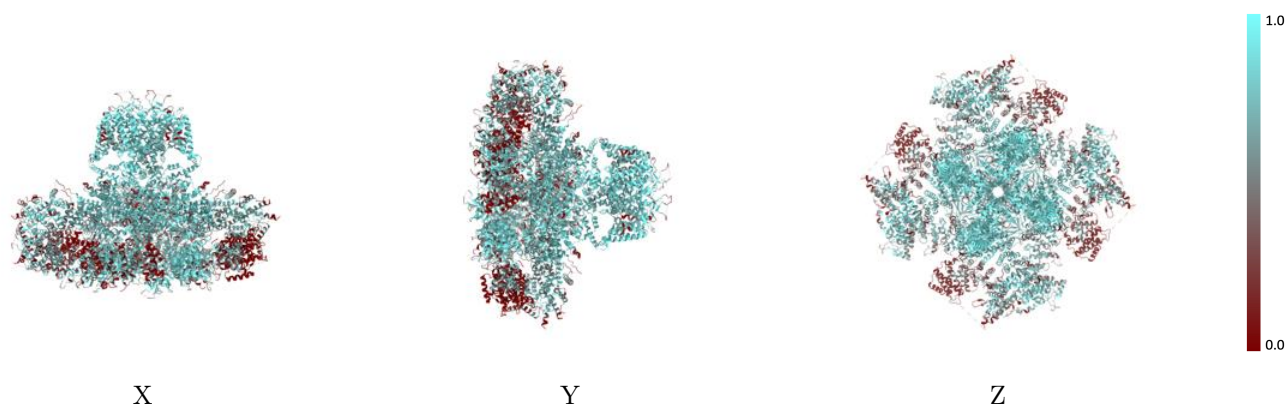
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



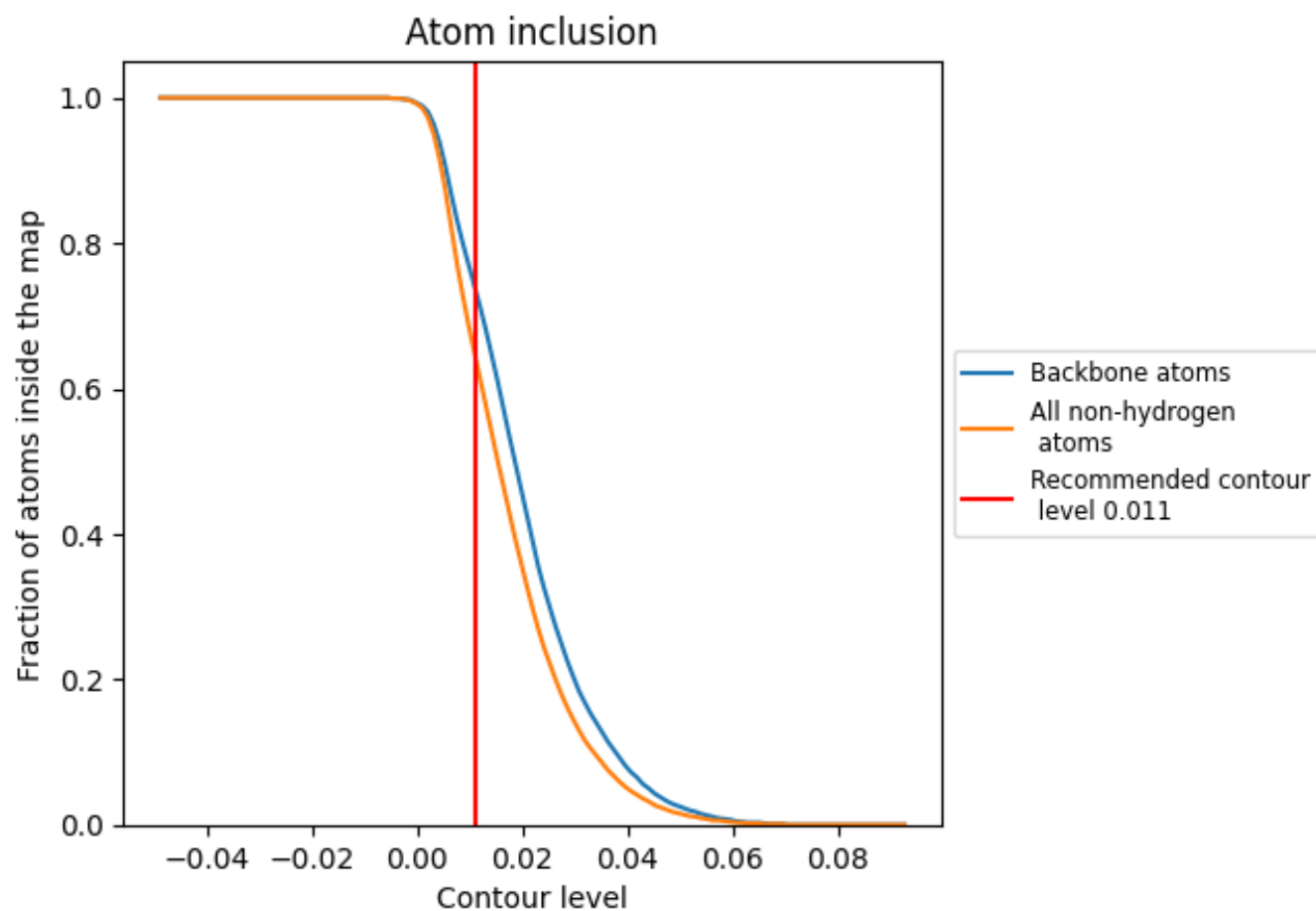
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6470	<div></div> 0.3500
A	<div></div> 0.6470	<div></div> 0.3500
B	<div></div> 0.6470	<div></div> 0.3500
C	<div></div> 0.6470	<div></div> 0.3500
D	<div></div> 0.6470	<div></div> 0.3500

