



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 03:15 PM EDT

PDB ID : 8EAQ  
EMDB ID : EMD-27982  
Title : Structure of the full-length IP3R1 channel determined at high Ca<sup>2+</sup>  
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 : 3.26 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](mailto: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>.

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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

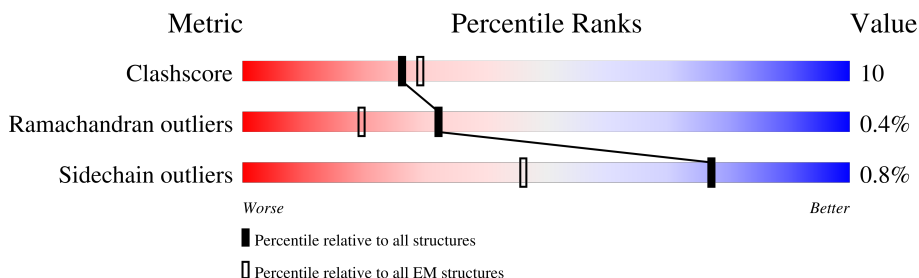
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.26 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  $\geq 3$ , 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	
1	B	2750	
1	C	2750	
1	D	2750	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 77928 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	2374	Total	C	N	O	S	1	0
			19195	12189	3321	3567	118		
1	B	2374	Total	C	N	O	S	1	0
			19195	12189	3321	3567	118		
1	C	2374	Total	C	N	O	S	1	0
			19195	12189	3321	3567	118		
1	D	2374	Total	C	N	O	S	1	0
			19195	12189	3321	3567	118		

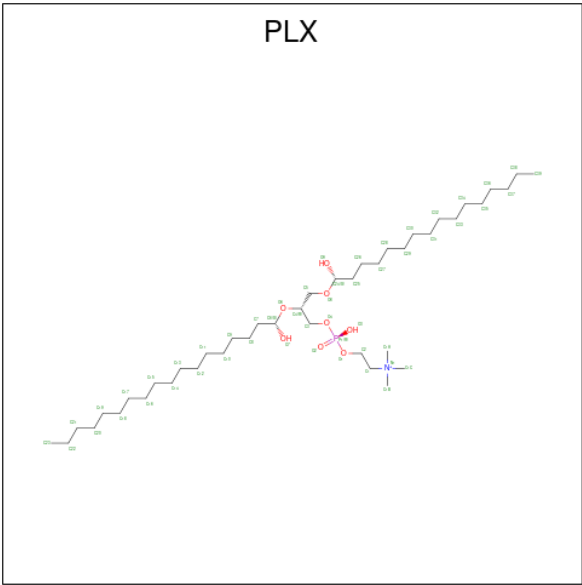
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	6	Total	Ca	0
			6	6	
3	B	5	Total	Ca	0
			5	5	
3	C	5	Total	Ca	0
			5	5	
3	D	4	Total	Ca	0
			4	4	

- Molecule 4 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: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	B	1	Total	C	N	O	P	0
			39	29	1	8	1	

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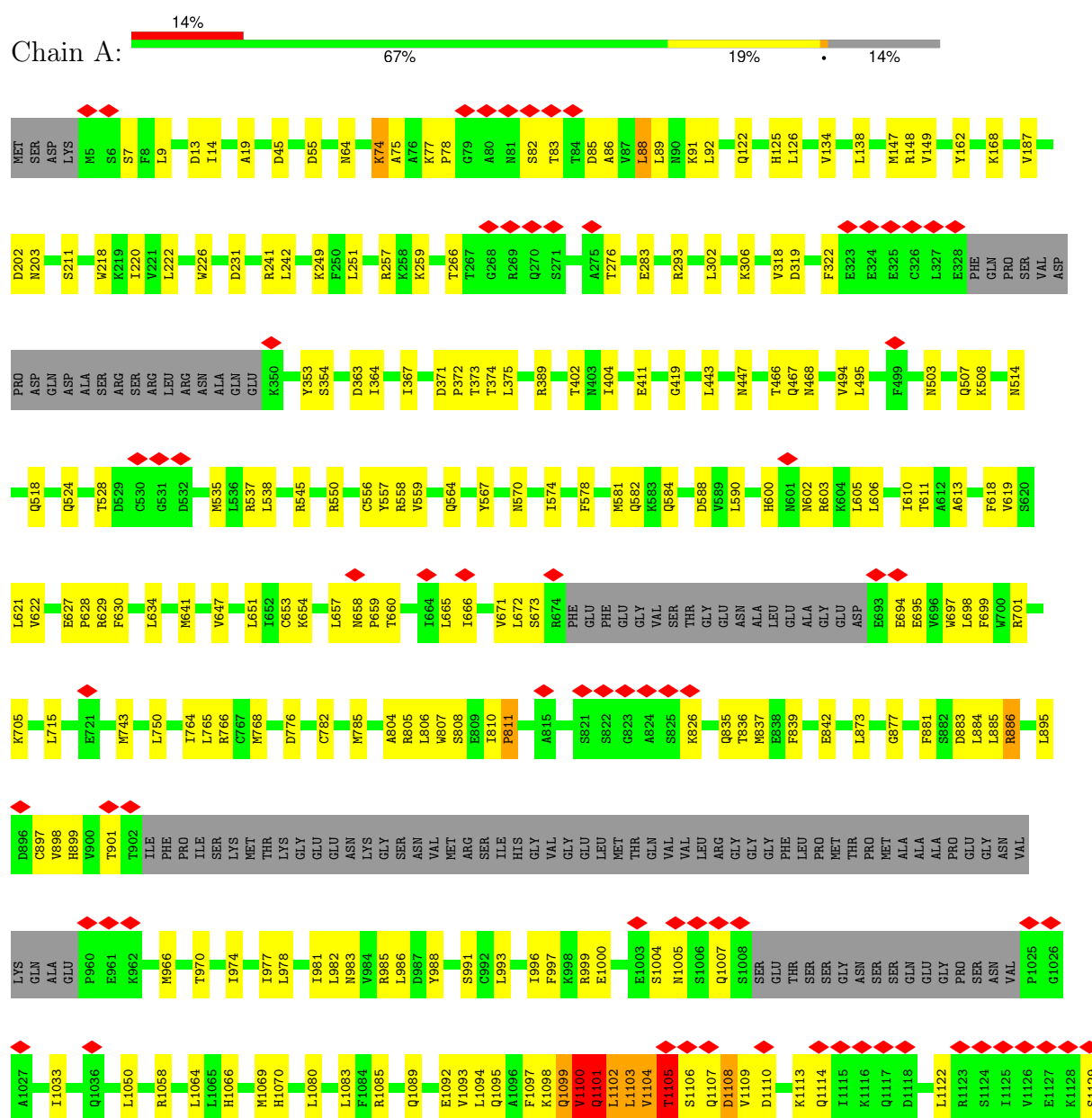
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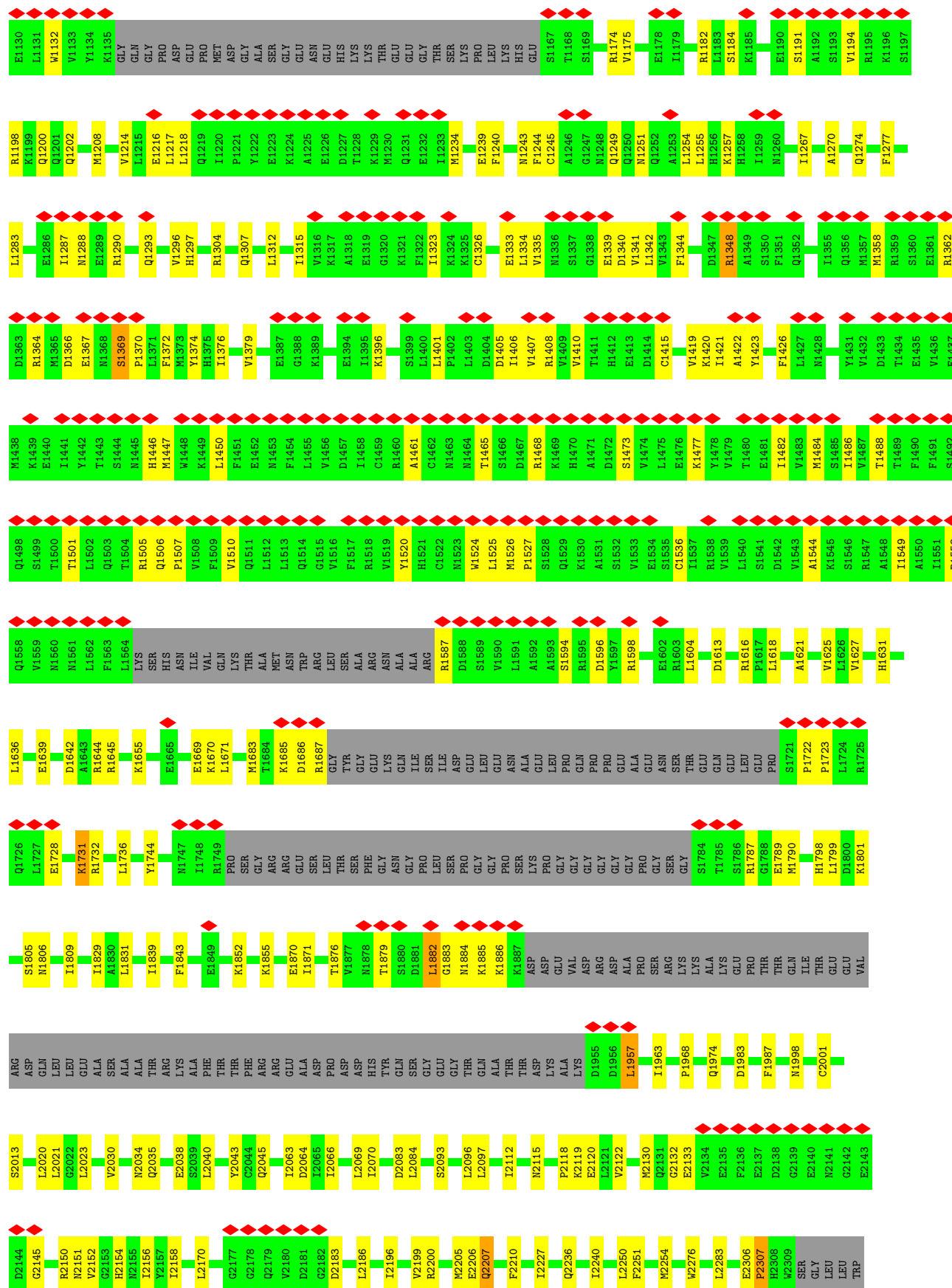
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	D	1	Total	C	N	O	P	0
			46	36	1	8	1	

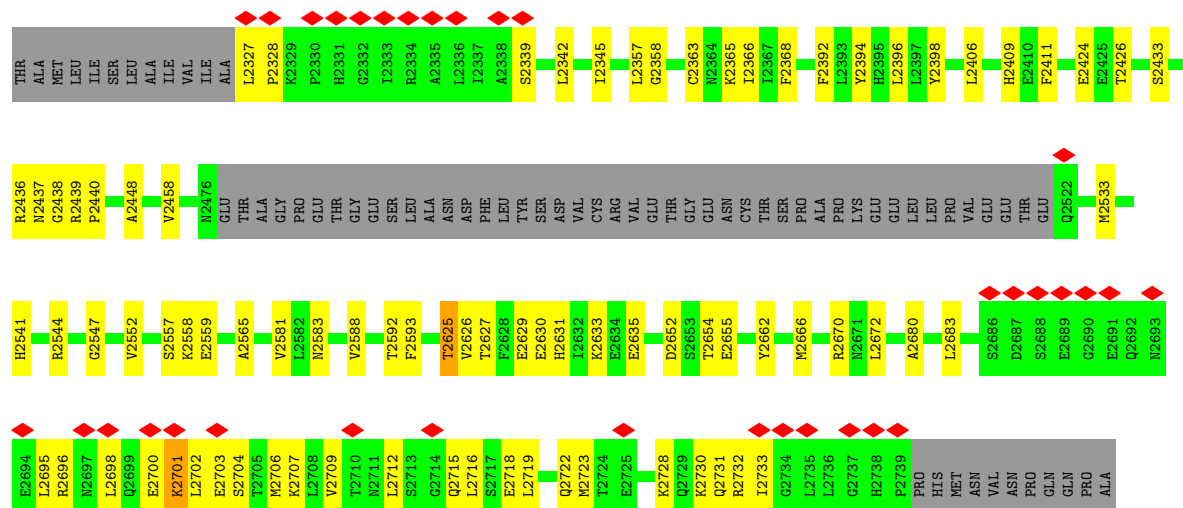
### 3 Residue-property plots

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.

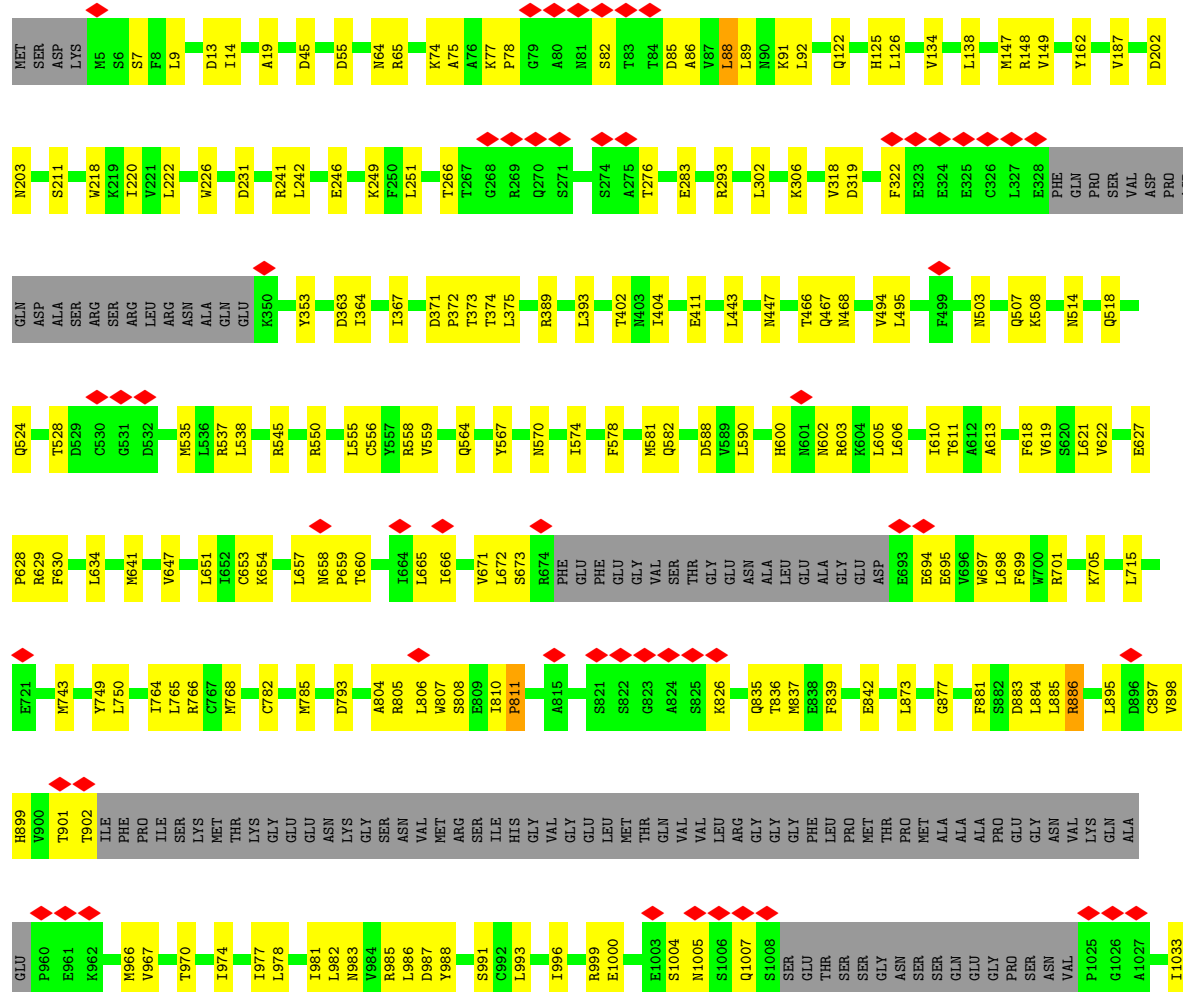
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





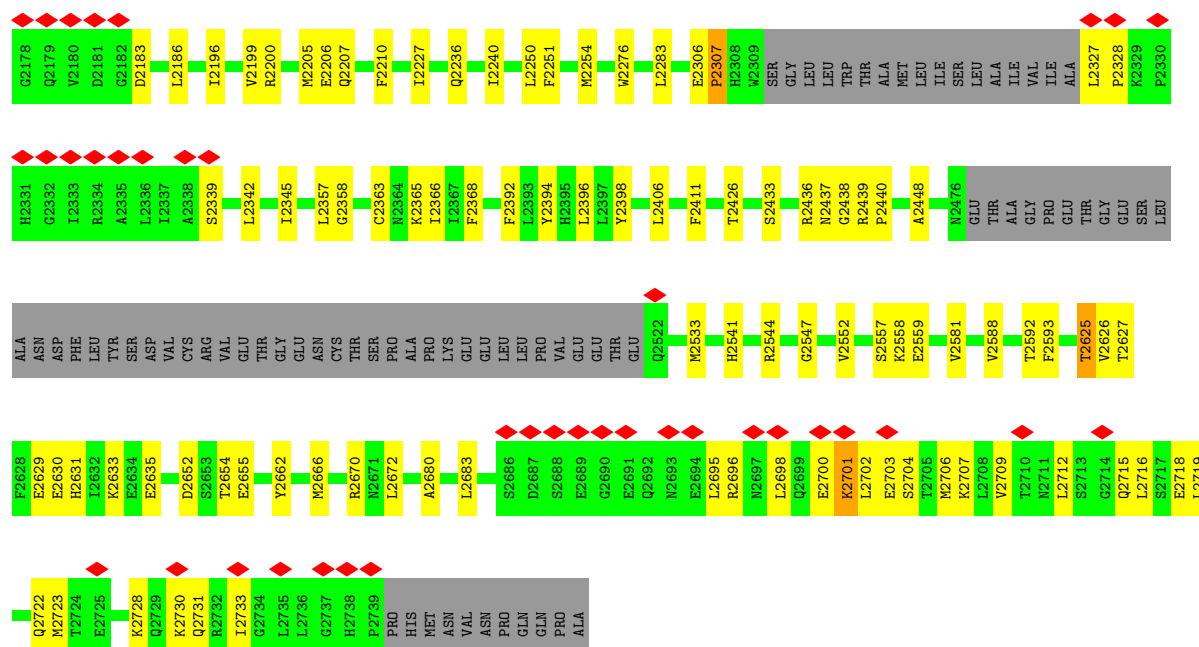


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

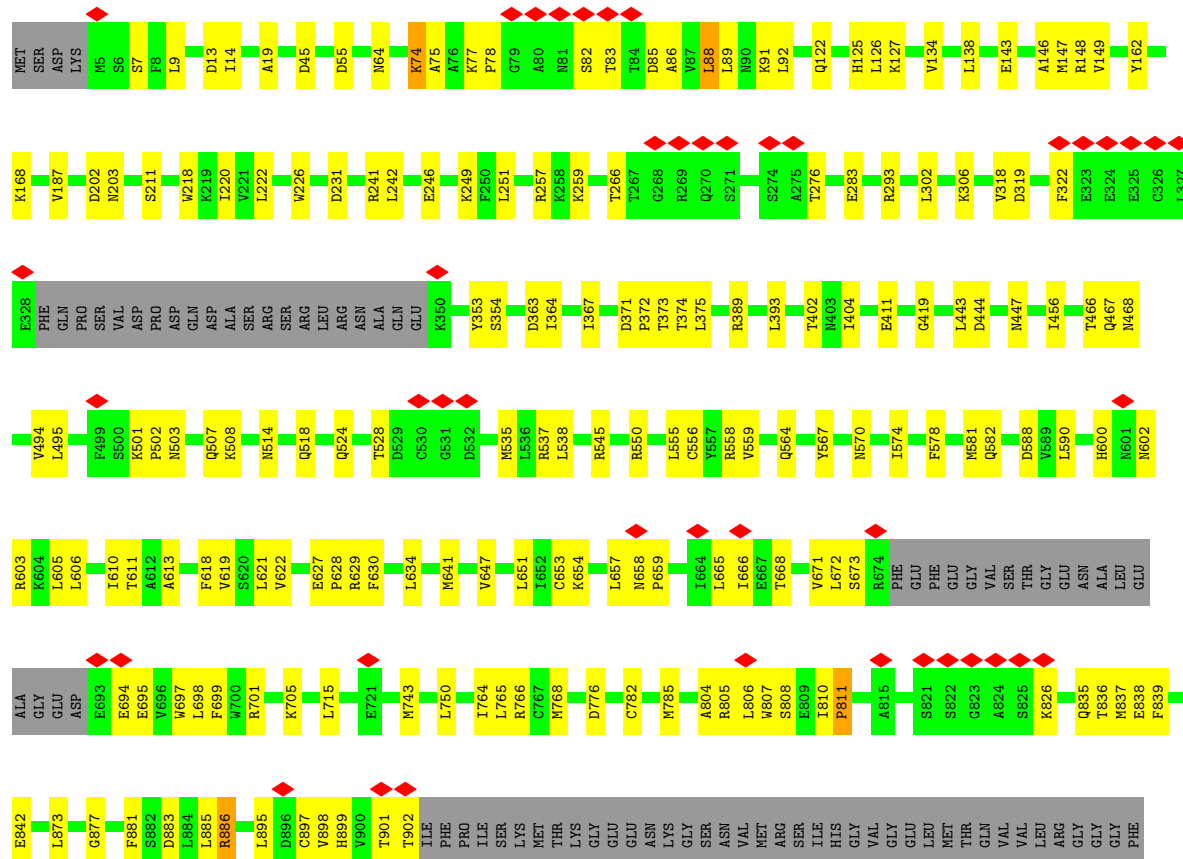




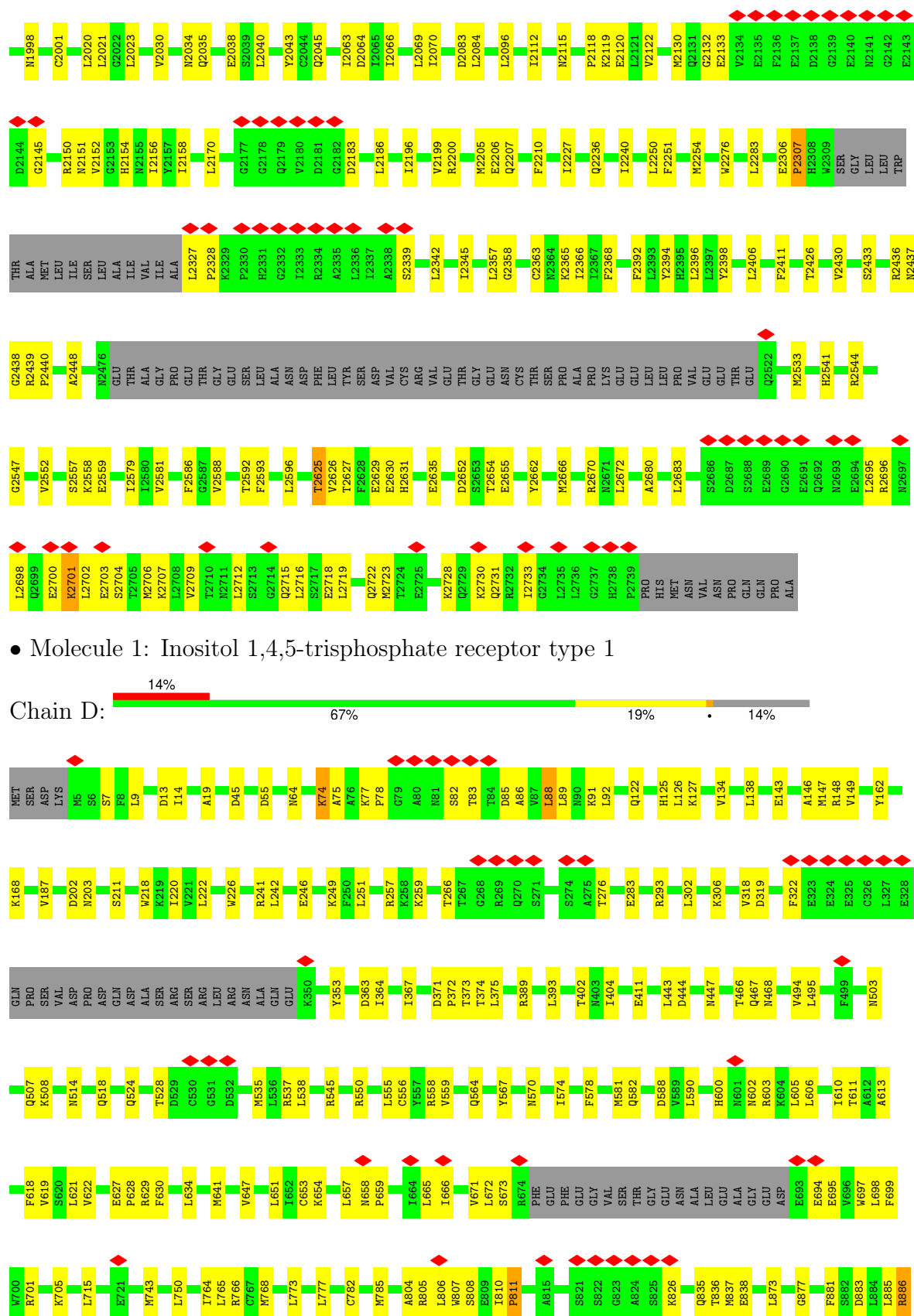
52039	L2040	Y2043	C2044	Q2045	L2063	D2064	L2065	L2066	L2069	L2070	D2083	L2084	L2096	L2112	N2115	P2118	K2119	E2120	L2121	V2122	N2130	Q2131	E2133	V2134	E2135	F2136	E2137	D2138	G2139	E2140	N2141	G2142	F1987	L2020	L2021	G2022	L2023	N2026	V2030	N2034	Q2035	E2038	L2170	G2177																				
ALA	THR	ARG	LYS	PHE	THR	PHE	ARG	ARG	GLU	ALA	ASP	PRO	ASP	ASP	HIS	TYR	GLN	SER	GLY	GLY	GLY	THR	THR	THR	THR	ASP	LYS	ASP	LYS	ALA	LYS	GLU	THR	THR	THR	THR	THR	THR	GLN	ILE	THR	GLU	GLU	VAL	ARG	ASP	GLN	LEU	GLU	ALA	SER	ALA												
L1831	I1839	F1843	E1849	K1852	K1855	E1870	T1876	V1877	N1878	T1879	S1880	D1881	L1882	G1883	N1884	K1885	K1886	K1887	ASP	ASP	GLU	VAL	ASP	ARG	ARG	ALA	PRO	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY													
R1737	Y1744	N1747	I1748	R1749	PRO	SER	GLY	ARG	ARG	GLU	SER	LEU	THR	THR	PHE	GLY	ASN	GLY	GLY	PRO	SER	LEU	ILE	ASP	GLU	GLY	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY												
R1644	R1645	K1655	E1655	E1669	K1670	L1671	K1685	D1686	R1687	GLY	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY													
V1559	N1560	N1561	L1562	F1563	L1564	LYS	SER	HIS	ASN	ILE	VAL	GLN	LYS	THR	THR	ALA	MET	GLY	N1453	F1454	V1455	G1456	F1457	S1458	C1459	R1460	A1461	C1462	N1463	N1464	L1465	S1466	D1467	R1468	K1469	H1470	A1471	D1472	S1473	V1474	E1475	E1476	K1477	V1478	V1479	L1480	E1481	L1482	V1483	M1484	S1485	L1486	V1487	T1488	T1489	F1490	F1491	S1492	S1493	P1494	S1495	L1496	D1497	Q1498
S1499	T1500	T1501	L1502	Q1503	T1504	R1505	Q1506	V1507	V1508	K1509	V1510	F1511	E1512	N1513	Q1514	G1515	V1516	F1517	R1518	C1459	R1460	A1461	C1462	N1463	N1464	L1465	S1466	D1467	R1468	K1469	H1470	A1471	D1472	S1473	V1474	E1475	E1476	K1477	V1478	V1479	L1480	E1481	L1482	V1483	M1484	S1485	L1486	V1487	T1488	T1489	F1490	F1491	S1492	S1493	P1494	S1495	L1496	D1497	Q1498					
K1439	E1440	I1441	T1442	T1443	S1444	N1445	H1446	M1447	N1448	K1449	L1450	F1451	E1452	N1453	F1454	L1455	V1456	D1457	I1458	C1459	R1460	A1461	C1462	N1463	N1464	L1465	S1466	D1467	R1468	K1469	H1470	A1471	D1472	S1473	V1474	E1475	E1476	K1477	V1478	V1479	L1480	E1481	L1482	V1483	M1484	S1485	L1486	V1487	T1488	T1489	F1490	F1491	S1492	S1493	P1494	S1495	L1496	D1497	Q1498					
N1368	S1369	P1370	F1372	M1373	Y1374	H1375	I1376	V1379	E1380	L1381	L1382	E1387	G1388	K1389	N1390	E1394	I1395	K1396	S1399	L1400	L1401	F1402	L1403	D1404	I1405	V1406	V1407	R1408	V1409	V1410	T1411	H1412	E1413	D1414	C1415	V1419	K1420	I1421	A1422	Y1423	F1426	L1427	N1428	Y1431	V1432	D1433	T1434	E1435	V1436	E1437	M1438													
I1287	N1288	E1289	R1290	Q1293	V1296	H1297	R1304	Q1307	L1312	I1315	A1318	E1319	G1320	K1321	F1322	I1323	K1324	K1325	C1326	E1333	L1334	V1335	N1336	S1337	G1338	E1339	D1340	V1341	L1342	V1343	F1344	D1347	R1348	A1349	Q1352	I1355	Q1356	M1357	M1358	R1359	S1360	F1361	E1362	D1363	R1364	M1365	E1367																	
Q1201	Q1202	M1208	V1214	L1215	E1216	L1217	L1218	Q1219	I1220	P1221	Y1222	E1223	K1224	A1225	E1226	D1227	L1228	K1229	M1230	Q1231	E1232	I1233	M1234	E1239	F1240	N1243	F1244	C1245	A1246	G1247	N1248	Q1249	N1251	Q1252	A1253	L1254	H1256	K1257	H1258	I1259	N1260	I1267	A1270	Q1274	F1277	L1283	E1286																	
V1133	Y1134	K1135	GLY	GLY	PRO	ASP	GLU	PRO	MET	ASP	GLY	ALA	SER	GLY	GLY	ASN	GLY	HIS	LYS	LYS	THR	GLU	GLY	THR	SER	LYS	PRO	V1100	Q1101	L1102	L1103	V1104	T1105	S1106	D1107	V1109	D1110	K1113	Q1114	I1115	K1116	Q1117	D1118	L1122	R1123	S1124	I1125	V1126	E1127	K1128	S1129	E1130	L1131	W1132										



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









S2704	T2705	K2706	K2707	L2708	V2709	T2710	N2711	L2712	S2713	G2714	Q2715	L2716	S2717	E2718	L2719		Q2722	M2723	T2724	E2725	K2728	Q2729	K2730	Q2731	R2732	L2733	G2734	L2735	L2736	G2737	H2738	P2739	PRO	HIS	MET	ASN	VAL	ASN	ASN	PRO	GLN	PRO	ALA								
S2557	K2558	E2559	V2581	V2588	T2592	F2593	L2596	T2625	V2626	T2627	F2628	E2629	E2630	H2631	T2632	K2633	E2634	E2635	D2652	S2653	T2654	E2655	V2662	M2666	R2670	N2671	L2672	A2680	L2683	S2686	D2687	S2688	E2689	G2690	E2691	Q2692	N2693	E2694	L2695	R2696	N2697	L2698	Q2699	E2700	K2701	L2702	E2703				
A2448	N2476	GLU	THR	ALA	GLY	PRO	GLU	GLU	THR	GLY	GLU	SER	LEU	ALA	ASN	ASP	PHE	LEU	TYR	SER	ASP	VAL	CYS	ARG	VAL	THR	GLU	ASN	CYS	THR	SER	PRO	ALA	PRO	LYS	GLU	GLU	LEU	PRO	VAL	GLU	THR	GLU	Q2522	M2533	H2541	R2544	G2547	V2552		
ILE	SER	LEU	ALA	ILE	VAL	ILE	ALA	L2327	P2328	K2329	P2330	H2331	G2332	I2333	R2334	A2335	L2336	I2337	A2338	S2339	L2342	I2345	L2357	G2358	C2363	N2364	K2365	I2366	T2367	F2368	F2392	L2393	Y2394	H2395	L2396	L2397	Y2398	L2406	H2409	E2410	F2411	T2426	S2433	R2436	N2437	G2438	R2439	P2440			
GLU	VAL	ASP	GLN	LEU	LEU	GLU	ALA	SER	ALA	ALA	THR	ARG	ARG	LYS	PHE	THR	THR	PHE	ARG	ARG	GLU	ALA	ASP	PRO	ASP	ASP	HIS	TYR	GLN	SER	GLY	GLU	THR	GLN	ALA	THR	THR	ASP	LYS	ALA	LYS	D1955	D1956	L1957	I1963	P1968	Q1974	D1983	F1987	L2020	L2021
G2092	L2023	V2030	N2034	Q2035	E2038	S2039	L2040	Y2043	C2044	Q2045	I2063	D2064	I2065	I2066	L2069	I2070	D2083	L2084	S2093	L2096	L2097	I2112	N2115	P2118	K2119	E2120	V2122	M2130	Q2131	G2132	E2133	V2134	E2135	F2136	E2137	D2138	G2139	E2140	N2141	G2142	E2143	D2144	G2145	R2150							

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	346731	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	0.116	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0118	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.07, 1.07, 1.07	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: ZN, PLX, CA

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	0/19547	0.50	4/26382 (0.0%)
1	B	0.27	0/19547	0.50	4/26382 (0.0%)
1	C	0.27	0/19547	0.51	4/26382 (0.0%)
1	D	0.27	0/19547	0.50	4/26382 (0.0%)
All	All	0.27	0/78188	0.50	16/105528 (0.0%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	C	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	1882	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1882	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	1957	LEU	CA-CB-CG	5.47	127.88	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	1098	LYS	Mainchain
1	A	665	LEU	Peptide
1	B	1098	LYS	Mainchain
1	B	665	LEU	Peptide
1	C	665	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19195	0	19276	410	0
1	B	19195	0	19276	400	0
1	C	19195	0	19276	409	0
1	D	19195	0	19276	398	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	6	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	281	0	412	21	0
4	B	281	0	412	20	0
4	C	281	0	412	19	0
4	D	281	0	412	23	0
All	All	77928	0	78752	1551	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 10.

The worst 5 of 1551 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:806:LEU:HD11	1:D:1104:VAL:N	1.84	0.93
1:A:806:LEU:HD11	1:A:1104:VAL:N	1.84	0.92
1:B:806:LEU:HD11	1:B:1104:VAL:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:LEU:HD11	1:C:1104:VAL:N	1.84	0.92
1:A:1101:GLN:O	1:A:1102:LEU:HB2	1.75	0.86

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	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	30	60
1	B	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	30	60
1	C	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	30	60
1	D	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	30	60
All	All	9404/11000 (86%)	8978 (96%)	390 (4%)	36 (0%)	32	60

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	PRO
1	A	1101	GLN
1	A	1102	LEU
1	A	1108	ASP
1	A	2307	PRO

### 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	2154/2459 (88%)	2137 (99%)	17 (1%)	79	86
1	B	2154/2459 (88%)	2137 (99%)	17 (1%)	79	86
1	C	2154/2459 (88%)	2137 (99%)	17 (1%)	79	86
1	D	2154/2459 (88%)	2137 (99%)	17 (1%)	79	86
All	All	8616/9836 (88%)	8548 (99%)	68 (1%)	77	86

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1101	GLN
1	D	1104	VAL
1	D	2045	GLN
1	B	1103	LEU
1	B	1101	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1558	GLN
1	C	2699	GLN
1	C	1998	ASN
1	D	1005	ASN
1	B	1005	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 52 ligands modelled in this entry, 24 are monoatomic - leaving 28 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
4	PLX	D	5111	-	37,37,51	1.24	5 (13%)	39,45,59	0.77	0
4	PLX	D	5108	-	36,36,51	1.17	5 (13%)	38,44,59	1.17	1 (2%)
4	PLX	B	5110	-	35,35,51	1.24	4 (11%)	37,43,59	0.77	1 (2%)
4	PLX	A	5109	-	44,44,51	1.19	2 (4%)	46,52,59	0.78	0
4	PLX	B	5108	-	39,39,51	1.22	5 (12%)	41,47,59	0.76	0
4	PLX	D	5112	-	45,45,51	1.17	5 (11%)	47,53,59	0.78	0
4	PLX	C	5108	-	44,44,51	1.19	3 (6%)	46,52,59	0.78	0
4	PLX	D	5110	-	38,38,51	1.20	5 (13%)	40,46,59	0.80	0
4	PLX	B	5111	-	38,38,51	1.20	5 (13%)	40,46,59	0.80	0
4	PLX	C	5109	-	39,39,51	1.22	5 (12%)	41,47,59	0.76	0
4	PLX	D	5106	-	44,44,51	1.19	3 (6%)	46,52,59	0.78	0
4	PLX	C	5110	-	36,36,51	1.17	5 (13%)	38,44,59	1.17	1 (2%)
4	PLX	A	5108	-	45,45,51	1.17	5 (11%)	47,53,59	0.78	0
4	PLX	B	5113	-	45,45,51	1.17	5 (11%)	47,53,59	0.78	0
4	PLX	A	5112	-	35,35,51	1.23	4 (11%)	37,43,59	0.77	1 (2%)
4	PLX	A	5114	-	37,37,51	1.23	5 (13%)	39,45,59	0.77	0
4	PLX	B	5109	-	36,36,51	1.18	5 (13%)	38,44,59	1.17	1 (2%)
4	PLX	D	5109	-	35,35,51	1.23	4 (11%)	37,43,59	0.77	1 (2%)
4	PLX	A	5110	-	39,39,51	1.22	5 (12%)	41,47,59	0.76	0
4	PLX	A	5111	-	36,36,51	1.18	5 (13%)	38,44,59	1.17	1 (2%)
4	PLX	B	5112	-	37,37,51	1.24	5 (13%)	39,45,59	0.77	0
4	PLX	D	5107	-	39,39,51	1.22	5 (12%)	41,47,59	0.76	0
4	PLX	C	5111	-	35,35,51	1.23	4 (11%)	37,43,59	0.77	1 (2%)
4	PLX	C	5113	-	37,37,51	1.23	5 (13%)	39,45,59	0.76	0
4	PLX	C	5107	-	45,45,51	1.18	5 (11%)	47,53,59	0.78	0
4	PLX	A	5113	-	38,38,51	1.20	5 (13%)	40,46,59	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PLX	C	5112	-	38,38,51	1.19	5 (13%)	40,46,59	0.80	0
4	PLX	B	5107	-	44,44,51	1.19	2 (4%)	46,52,59	0.78	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
4	PLX	D	5111	-	-	15/41/41/55	-
4	PLX	D	5108	-	-	18/40/40/55	-
4	PLX	B	5110	-	-	25/39/39/55	-
4	PLX	A	5109	-	-	24/48/48/55	-
4	PLX	B	5108	-	-	20/43/43/55	-
4	PLX	D	5112	-	-	30/49/49/55	-
4	PLX	C	5108	-	-	24/48/48/55	-
4	PLX	D	5110	-	-	19/42/42/55	-
4	PLX	B	5111	-	-	19/42/42/55	-
4	PLX	C	5109	-	-	20/43/43/55	-
4	PLX	D	5106	-	-	24/48/48/55	-
4	PLX	C	5110	-	-	18/40/40/55	-
4	PLX	A	5108	-	-	30/49/49/55	-
4	PLX	B	5113	-	-	30/49/49/55	-
4	PLX	A	5112	-	-	25/39/39/55	-
4	PLX	A	5114	-	-	15/41/41/55	-
4	PLX	B	5109	-	-	18/40/40/55	-
4	PLX	D	5109	-	-	25/39/39/55	-
4	PLX	A	5110	-	-	20/43/43/55	-
4	PLX	A	5111	-	-	18/40/40/55	-
4	PLX	B	5112	-	-	14/41/41/55	-
4	PLX	D	5107	-	-	20/43/43/55	-
4	PLX	C	5111	-	-	25/39/39/55	-
4	PLX	C	5113	-	-	15/41/41/55	-
4	PLX	C	5107	-	-	30/49/49/55	-
4	PLX	A	5113	-	-	20/42/42/55	-
4	PLX	C	5112	-	-	19/42/42/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLX	B	5107	-	-	24/48/48/55	-

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5106	PLX	O6-C4	-3.75	1.39	1.44
4	D	5111	PLX	O6-C4	-3.68	1.39	1.44
4	A	5109	PLX	O6-C4	-3.68	1.39	1.44
4	B	5107	PLX	O6-C4	-3.68	1.39	1.44
4	C	5108	PLX	O6-C4	-3.68	1.39	1.44

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5111	PLX	C6-O6-C4	5.24	125.67	115.20
4	B	5109	PLX	C6-O6-C4	5.24	125.66	115.20
4	D	5108	PLX	C6-O6-C4	5.21	125.59	115.20
4	C	5110	PLX	C6-O6-C4	5.21	125.59	115.20
4	B	5110	PLX	C8-C7-C6	-2.06	108.59	113.38

There are no chirality outliers.

5 of 604 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5108	PLX	O7-C6-O6-C4
4	A	5108	PLX	C3-O4-P1-O1
4	A	5108	PLX	C3-O4-P1-O2
4	A	5108	PLX	C3-O4-P1-O3
4	A	5108	PLX	C2-O1-P1-O4

There are no ring outliers.

28 monomers are involved in 83 short contacts:

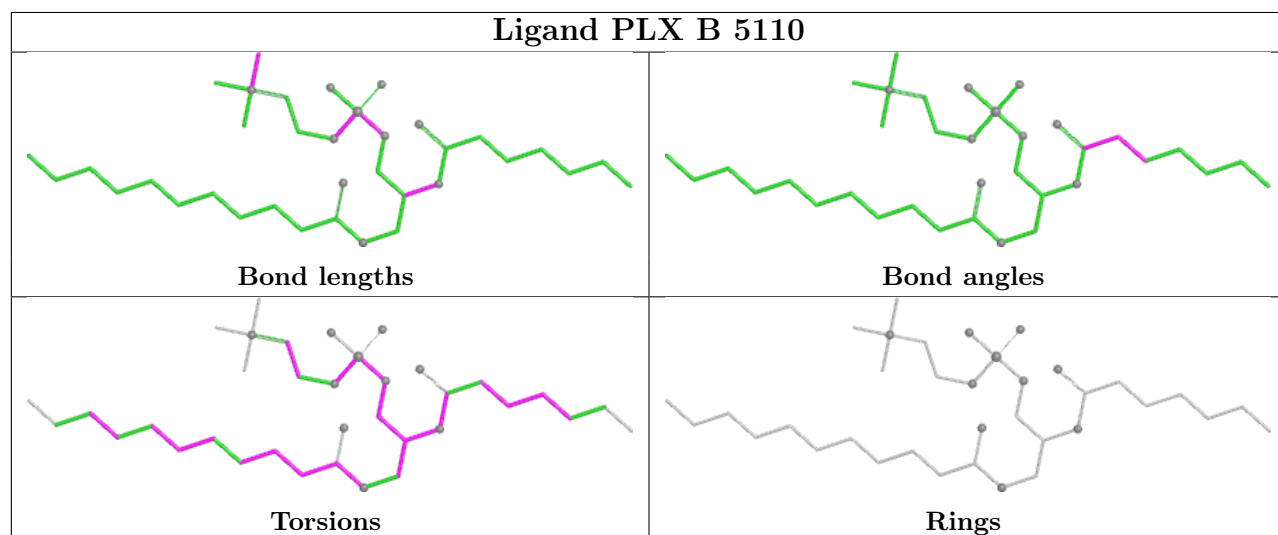
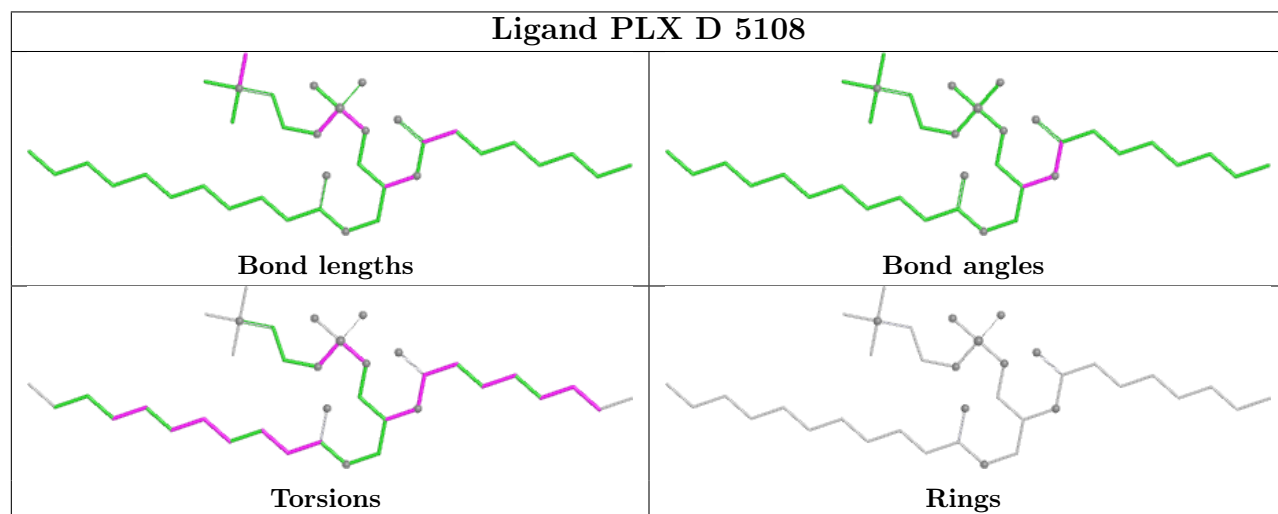
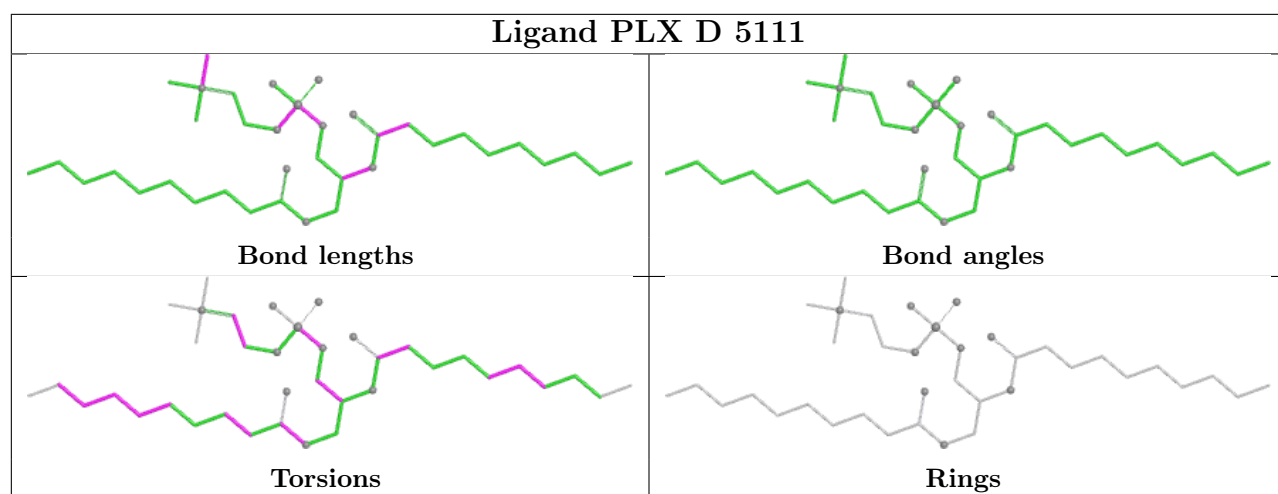
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5111	PLX	4	0
4	D	5108	PLX	5	0
4	B	5110	PLX	2	0
4	A	5109	PLX	4	0
4	B	5108	PLX	3	0
4	D	5112	PLX	2	0
4	C	5108	PLX	3	0

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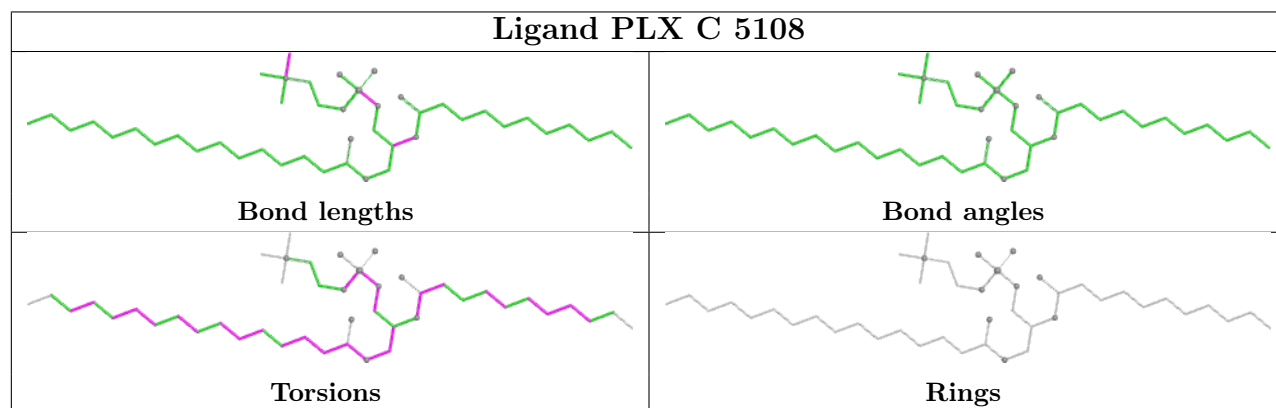
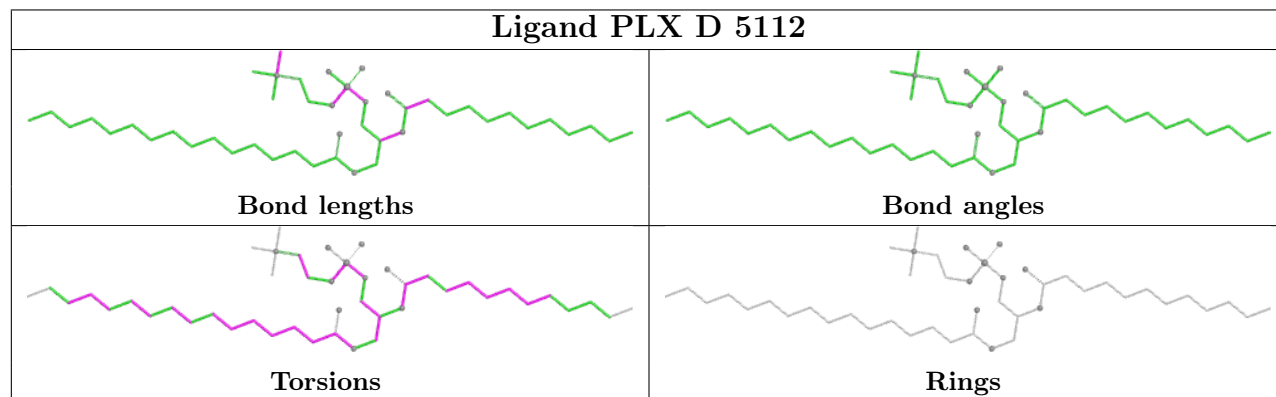
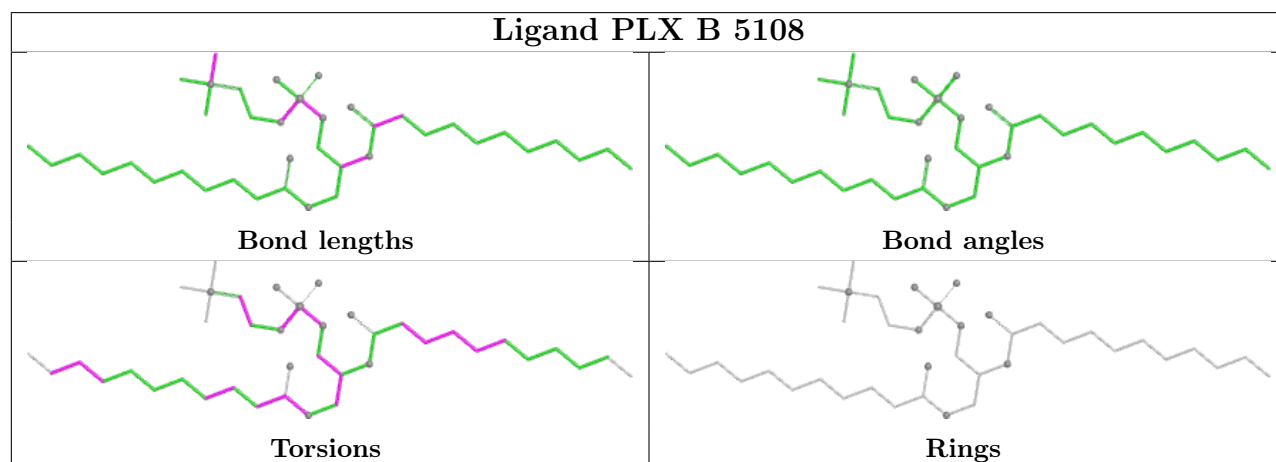
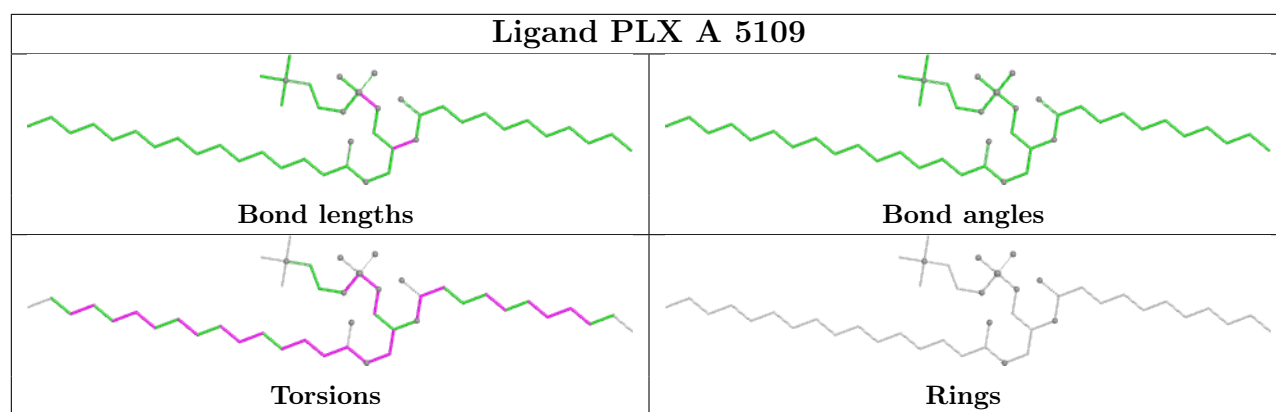
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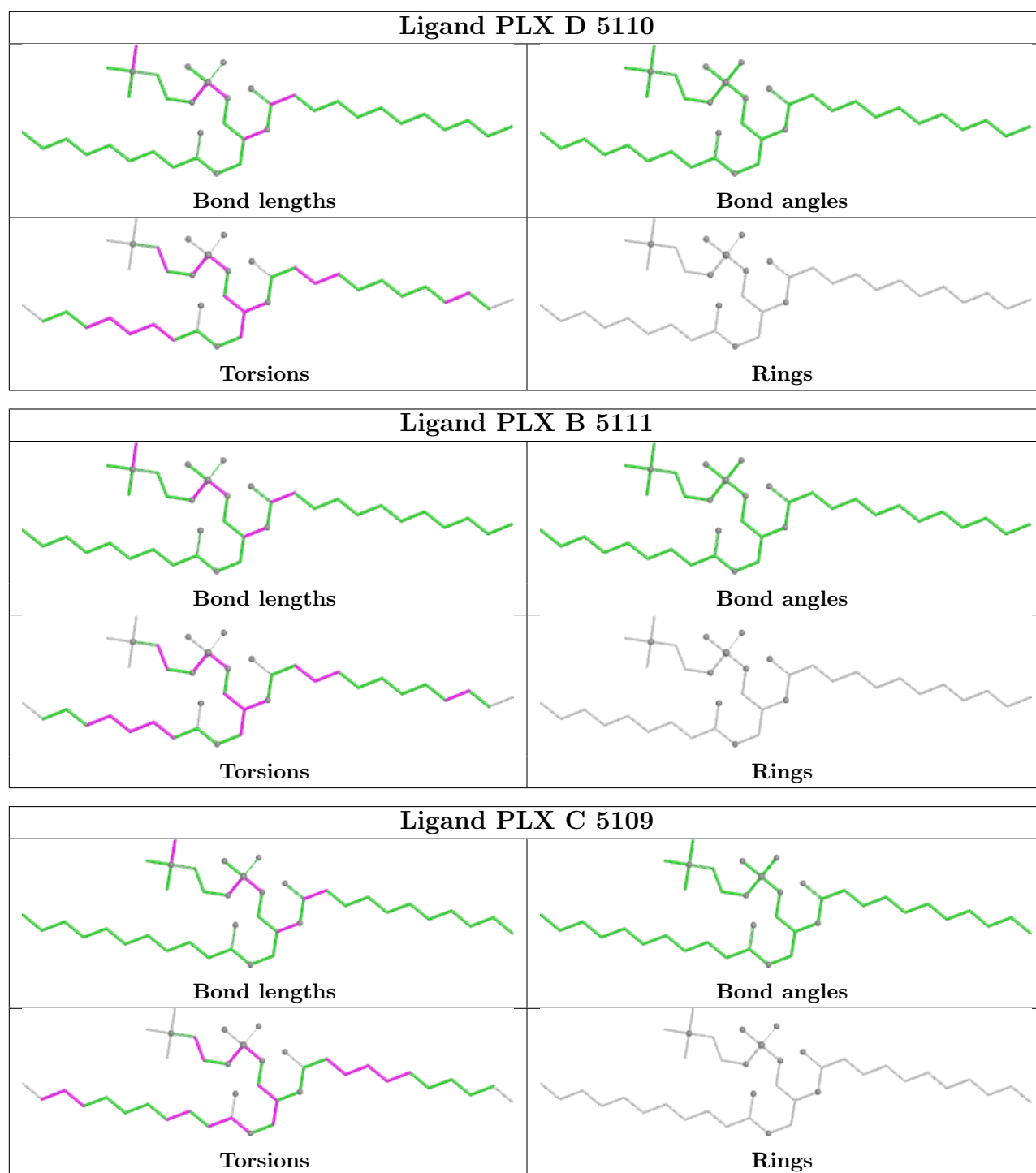
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5110	PLX	3	0
4	B	5111	PLX	3	0
4	C	5109	PLX	3	0
4	D	5106	PLX	3	0
4	C	5110	PLX	4	0
4	A	5108	PLX	4	0
4	B	5113	PLX	2	0
4	A	5112	PLX	1	0
4	A	5114	PLX	3	0
4	B	5109	PLX	3	0
4	D	5109	PLX	3	0
4	A	5110	PLX	3	0
4	A	5111	PLX	4	0
4	B	5112	PLX	3	0
4	D	5107	PLX	3	0
4	C	5111	PLX	3	0
4	C	5113	PLX	3	0
4	C	5107	PLX	1	0
4	A	5113	PLX	2	0
4	C	5112	PLX	2	0
4	B	5107	PLX	4	0

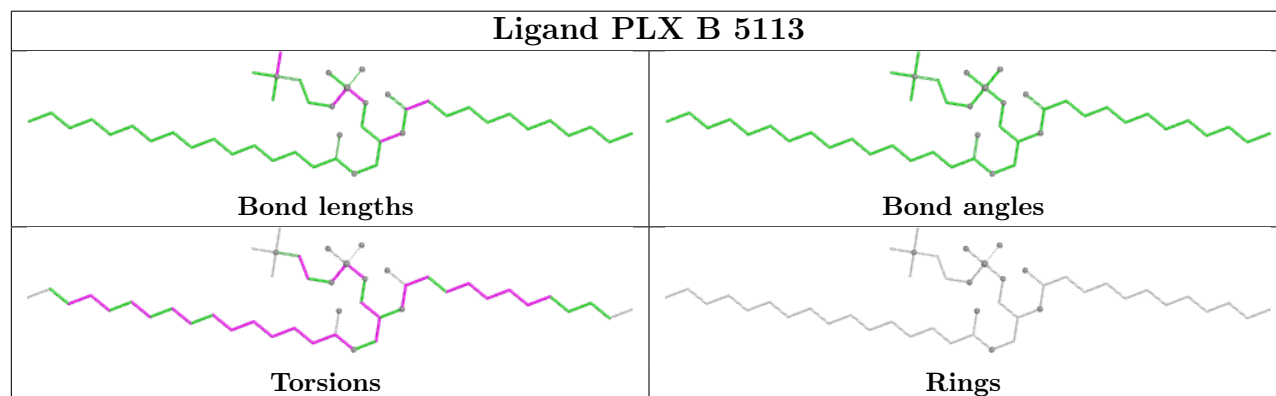
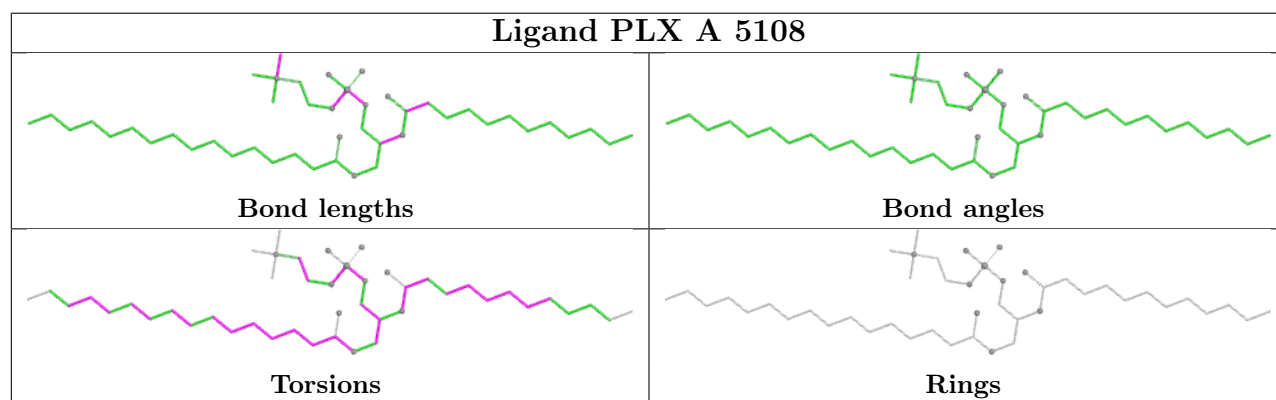
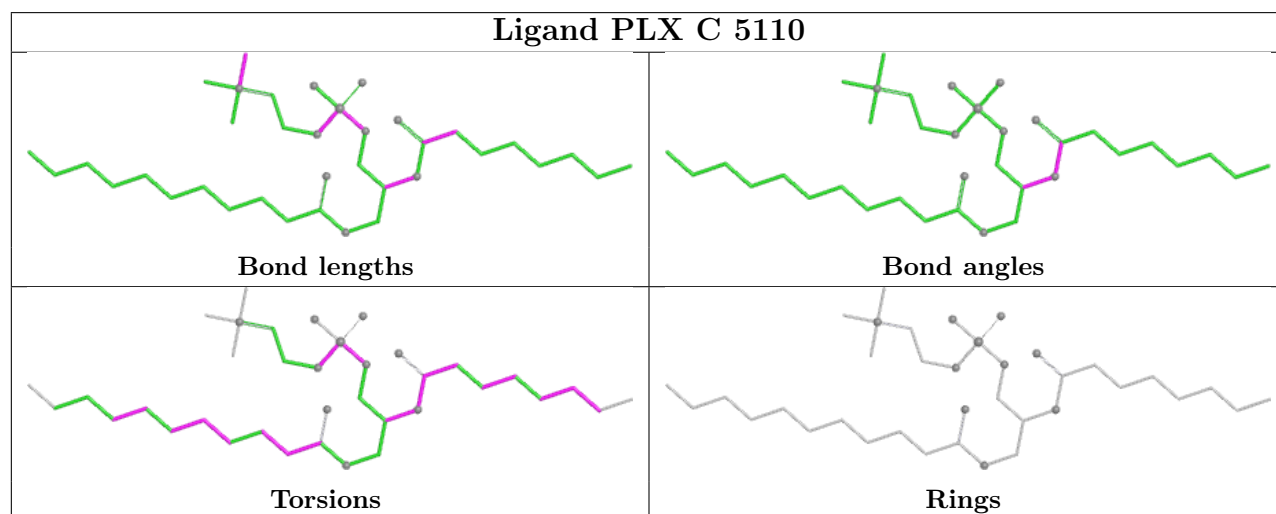
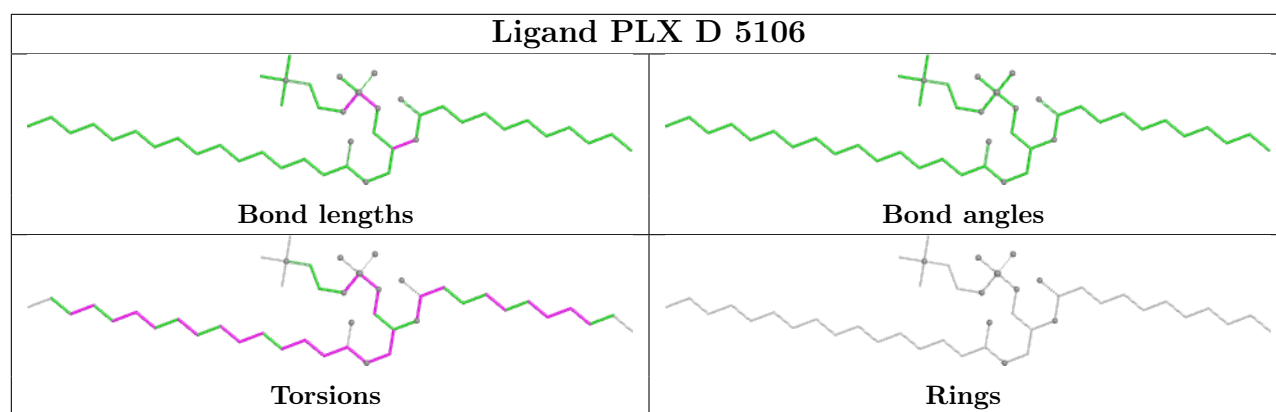
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

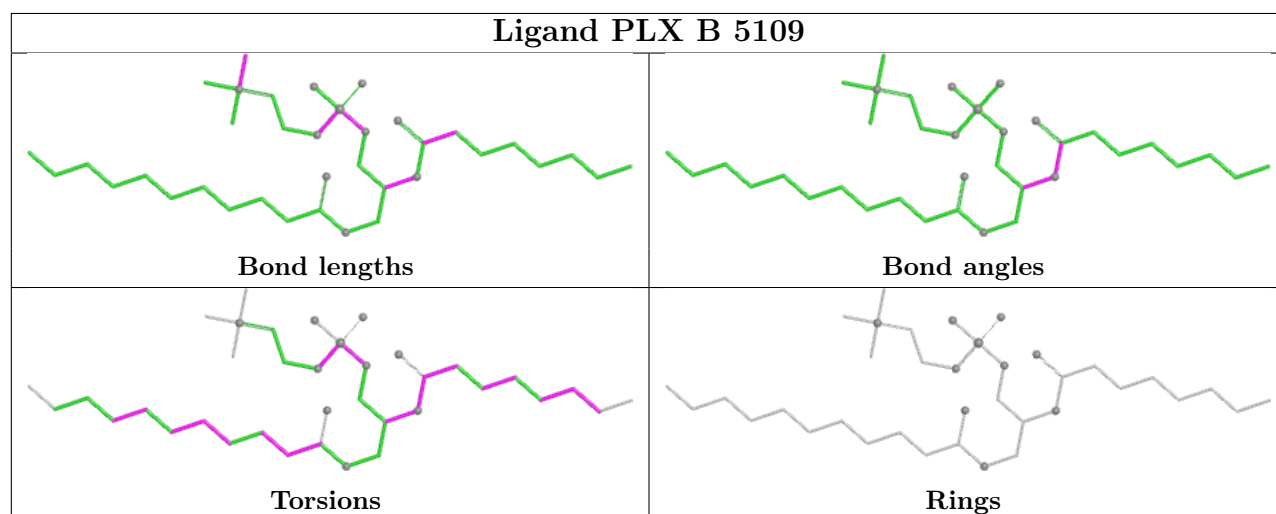
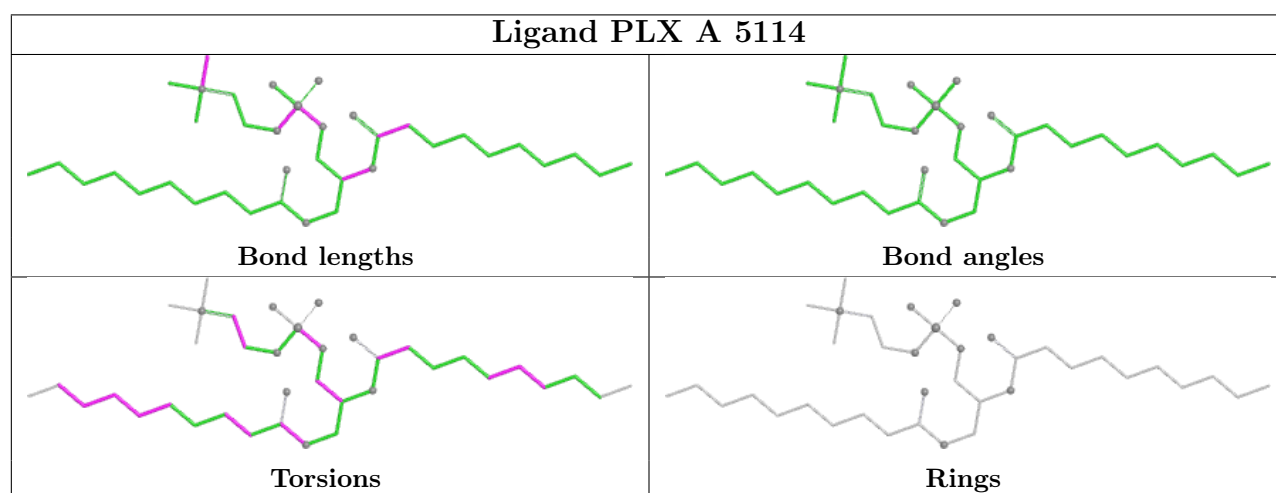
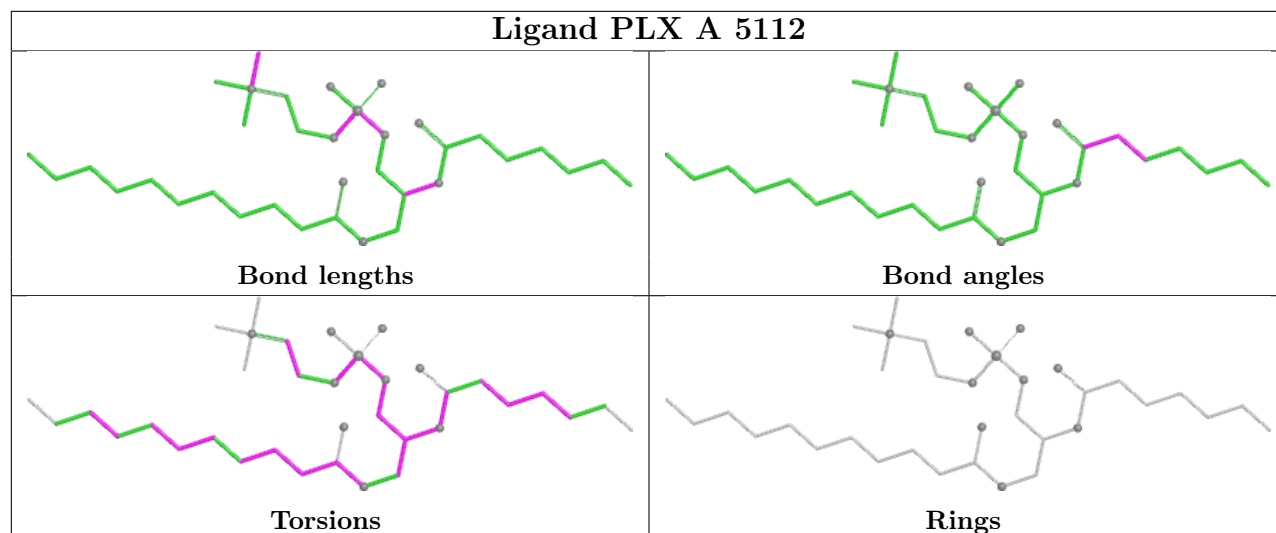


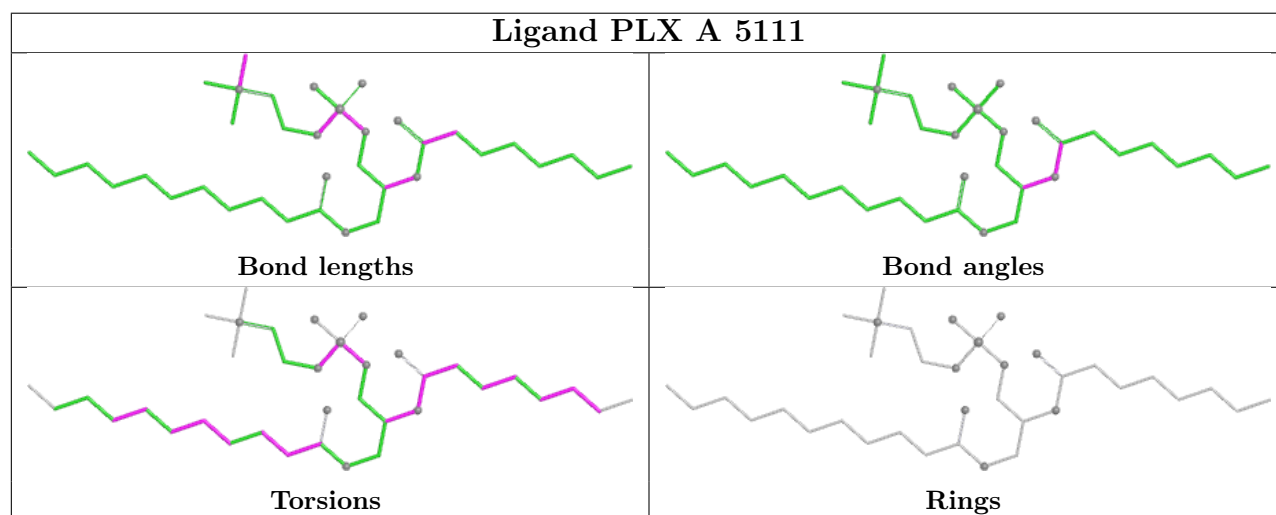
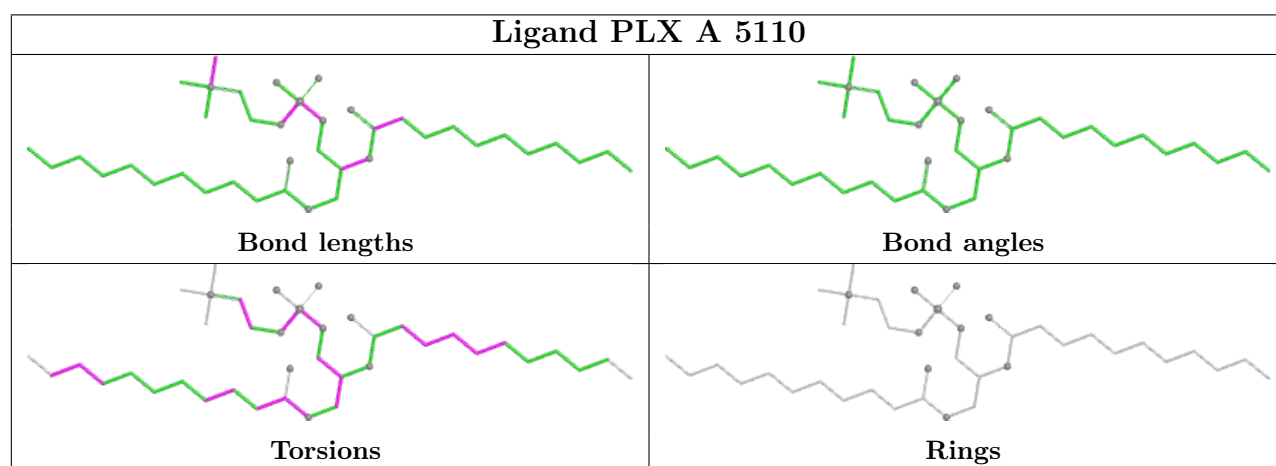
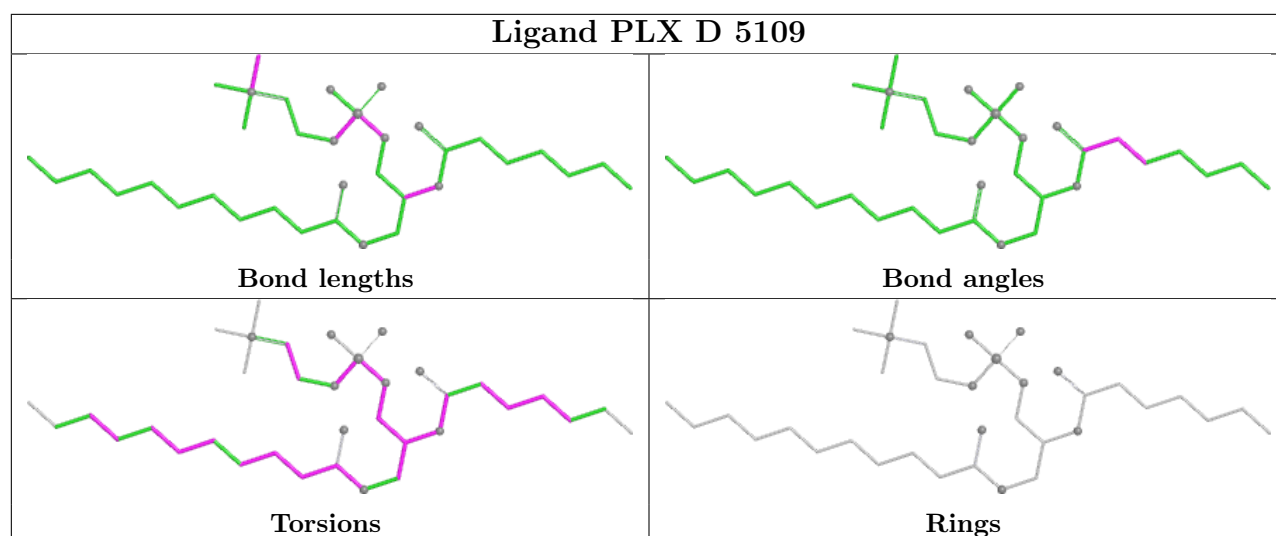


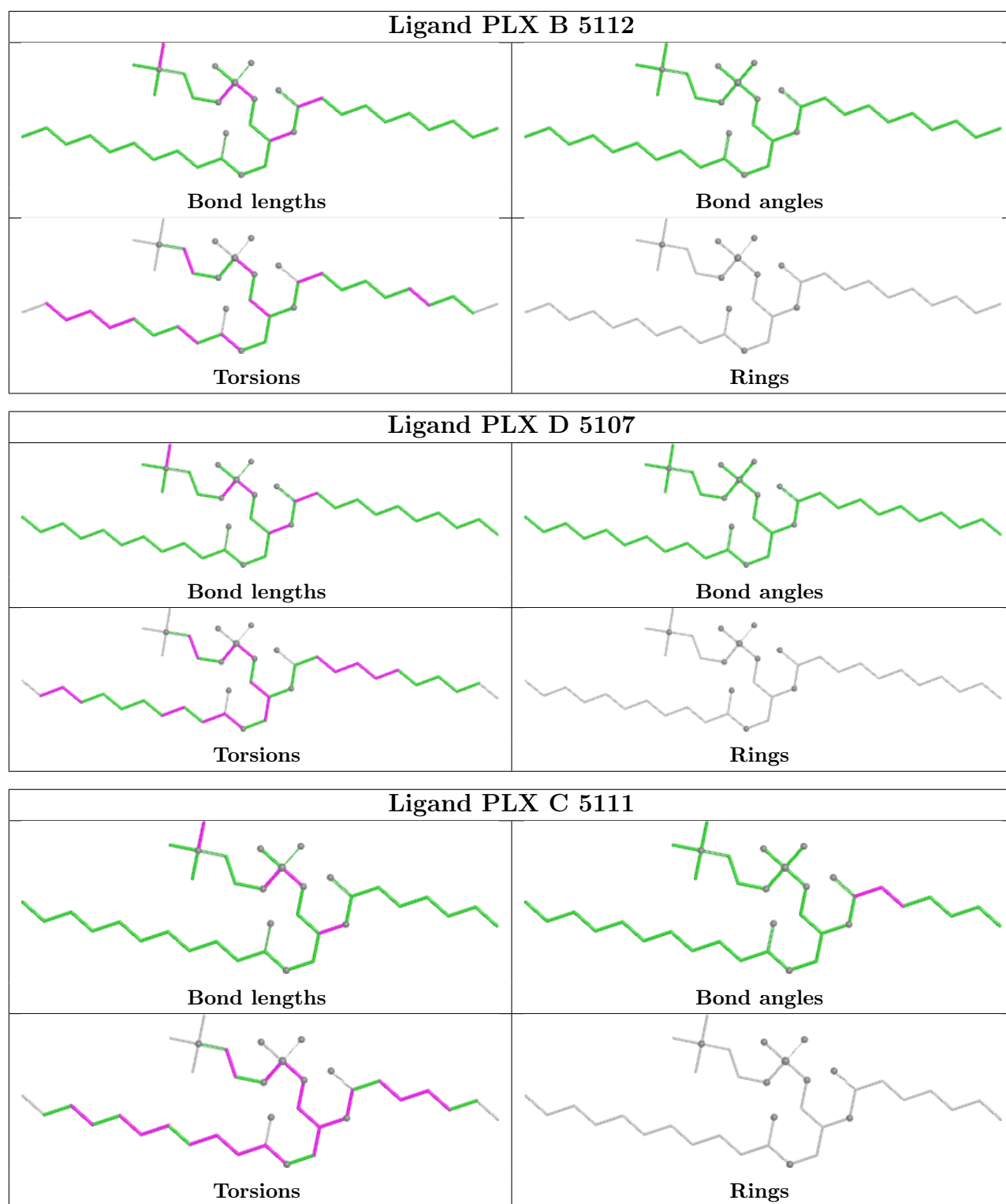


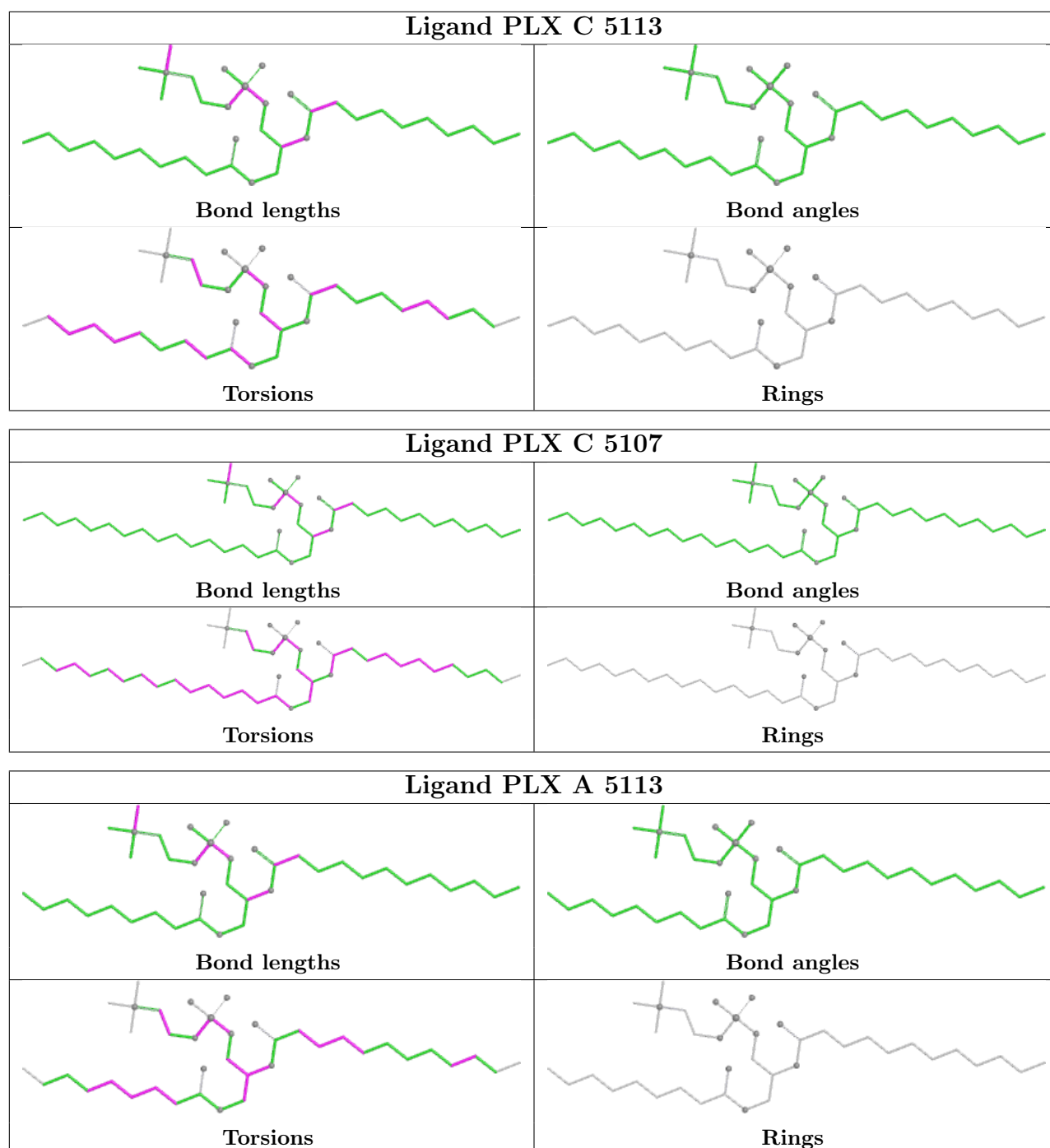


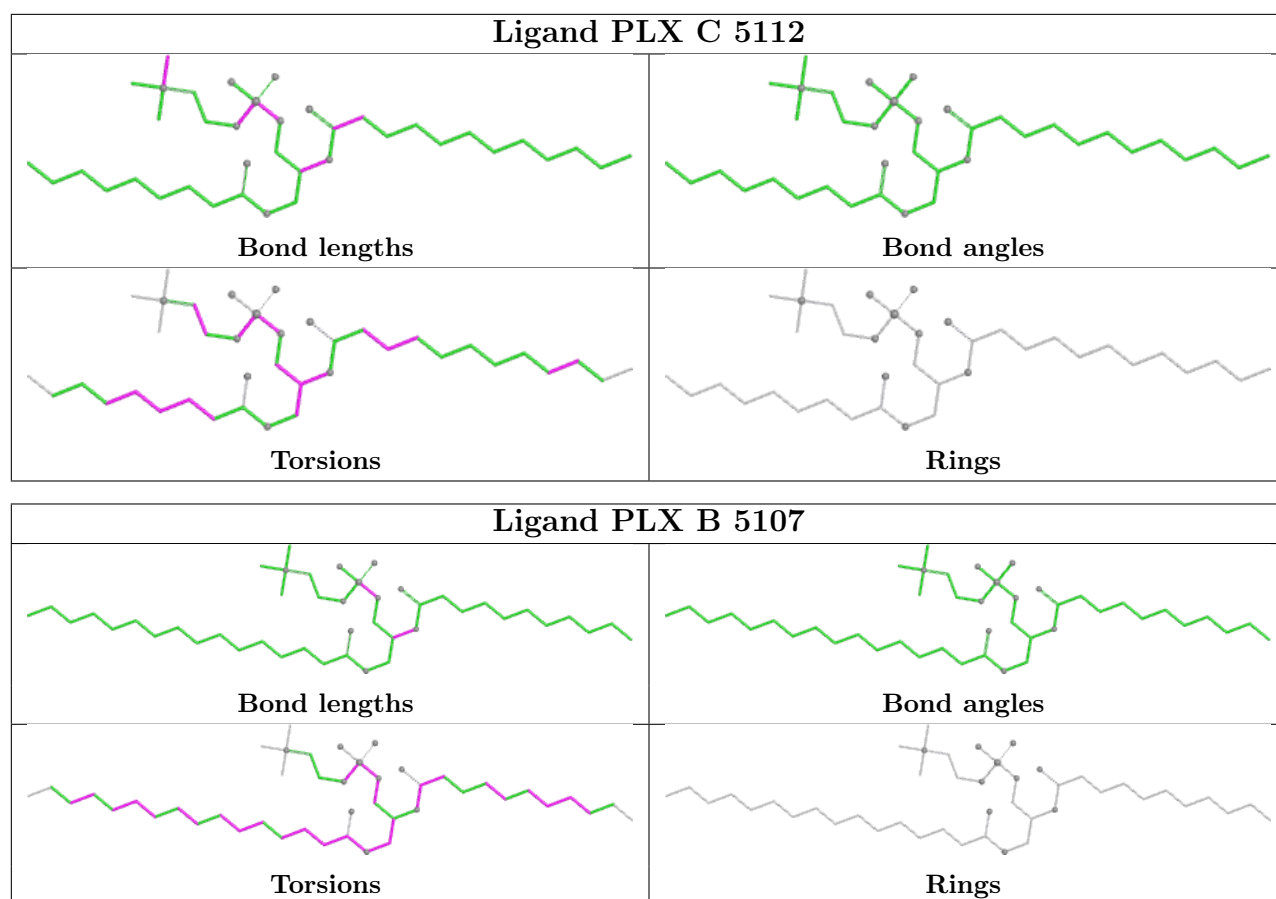












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



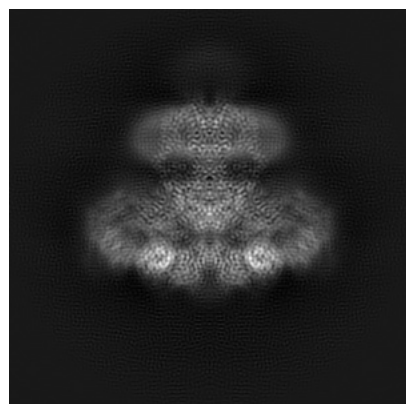
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27982. These allow visual inspection of the internal detail of the map and identification of artifacts.

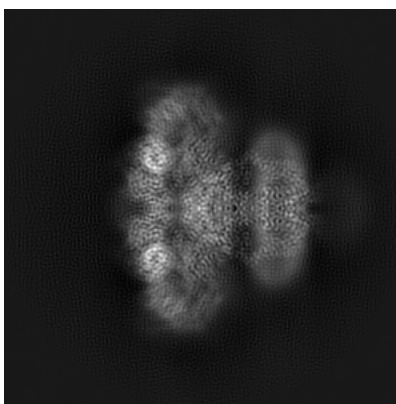
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

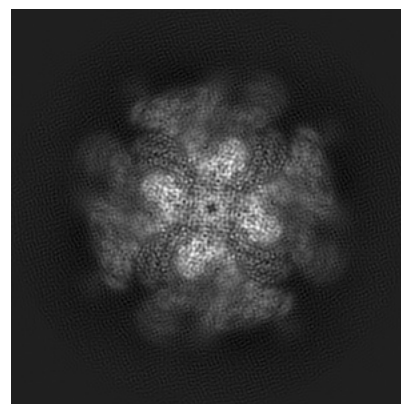
#### 6.1.1 Primary map



X

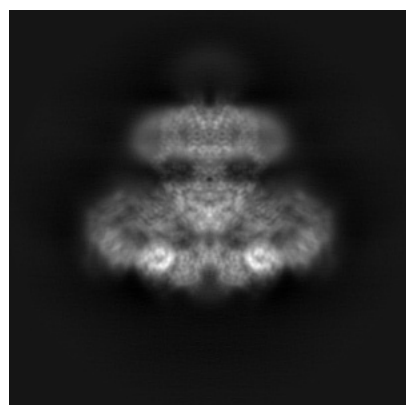


Y

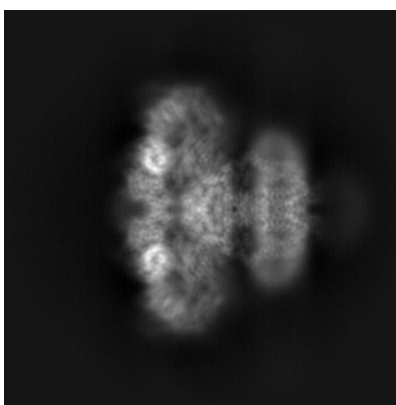


Z

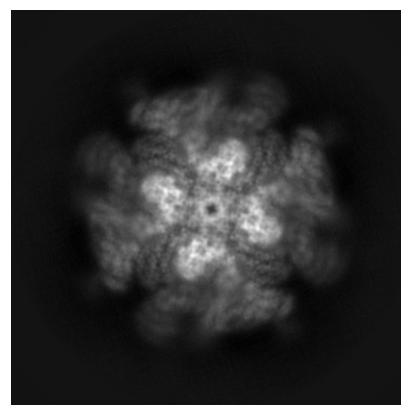
#### 6.1.2 Raw map



X



Y

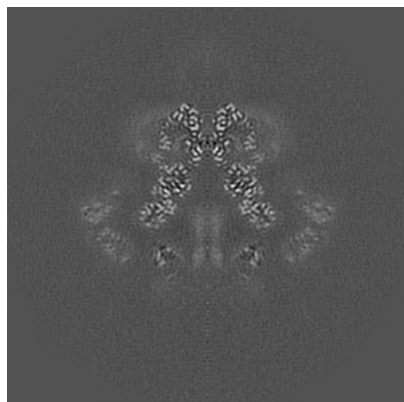


Z

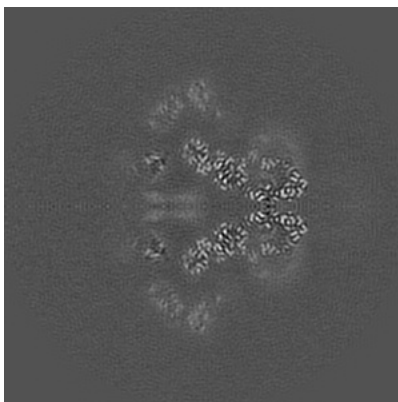
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

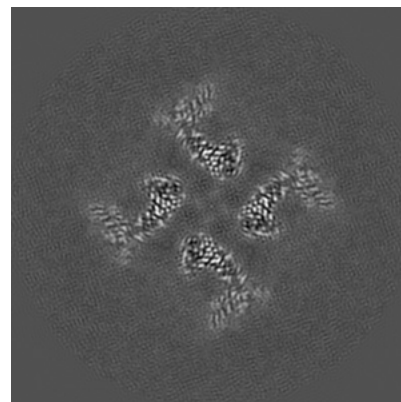
### 6.2.1 Primary map



X Index: 168

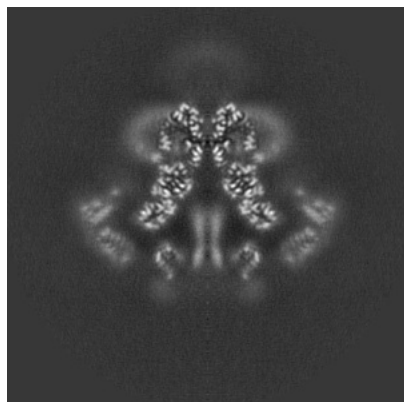


Y Index: 168

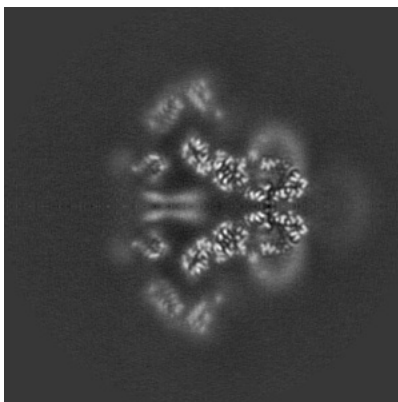


Z Index: 168

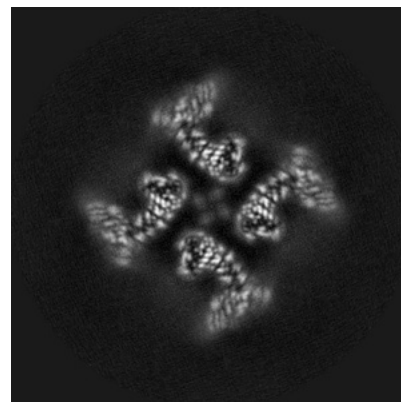
### 6.2.2 Raw map



X Index: 168



Y Index: 168

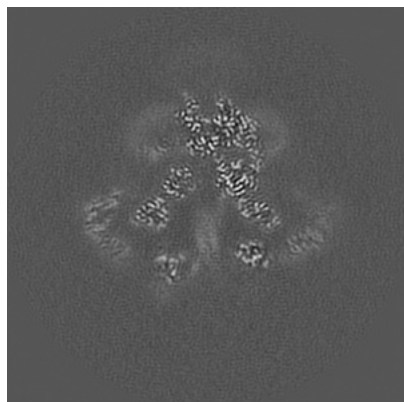


Z Index: 168

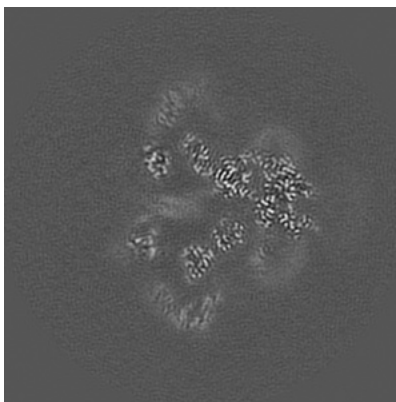
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

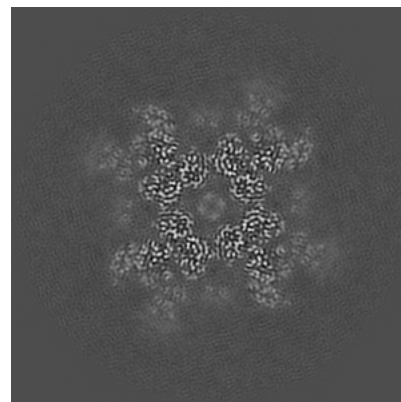
### 6.3.1 Primary map



X Index: 173

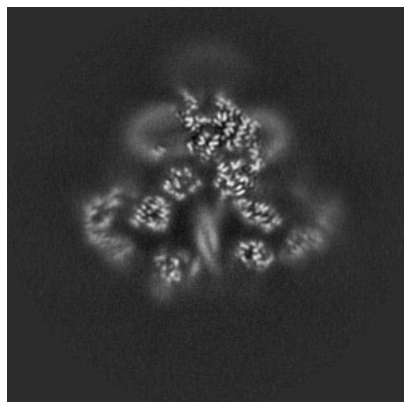


Y Index: 163

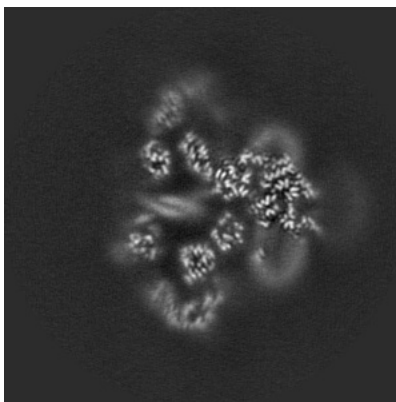


Z Index: 123

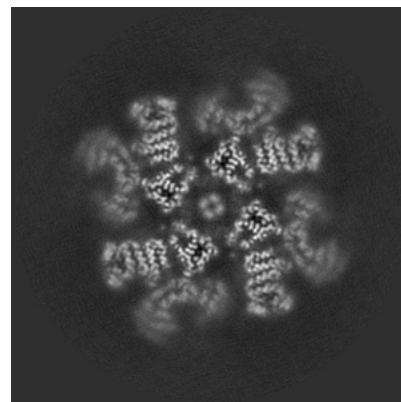
### 6.3.2 Raw map



X Index: 174



Y Index: 162

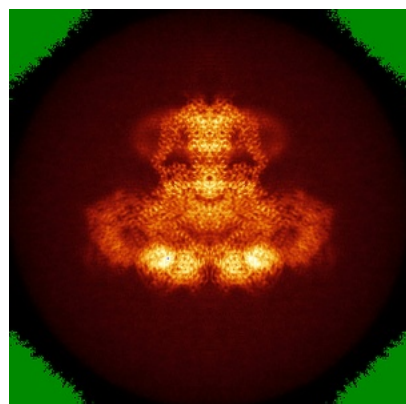


Z Index: 131

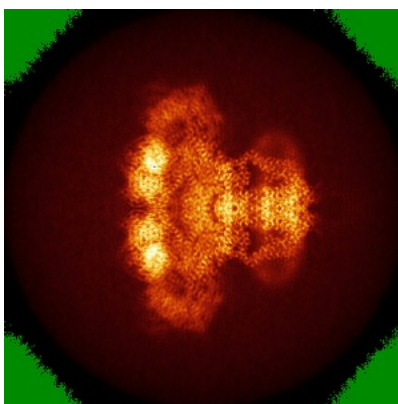
The images above show the largest variance slices of the map in three orthogonal directions.

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

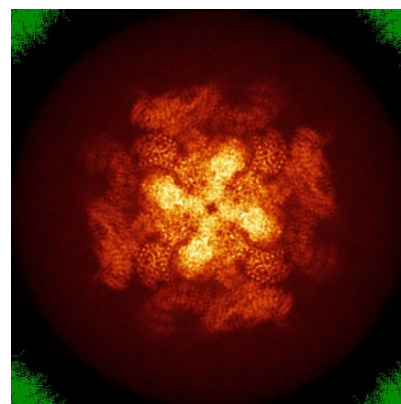
### 6.4.1 Primary map



X

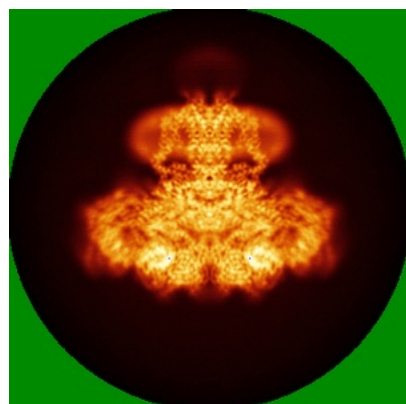


Y

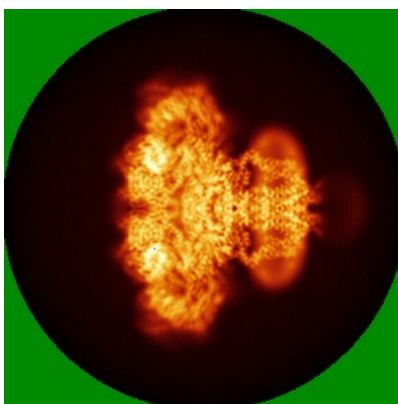


Z

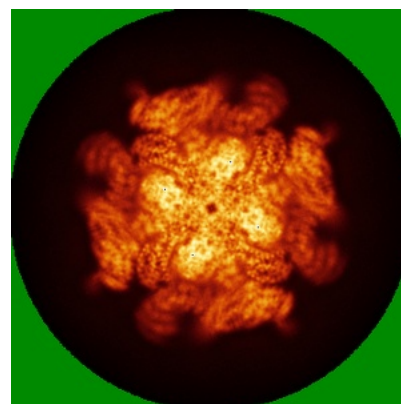
### 6.4.2 Raw map



X



Y



Z

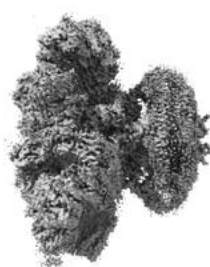
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

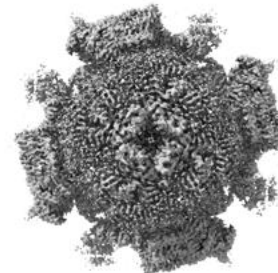
### 6.5.1 Primary map



X



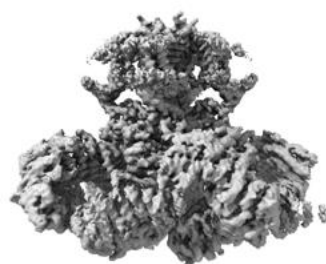
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

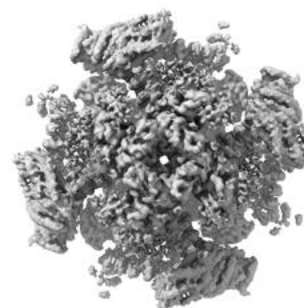
### 6.5.2 Raw map



X



Y



Z

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](#)

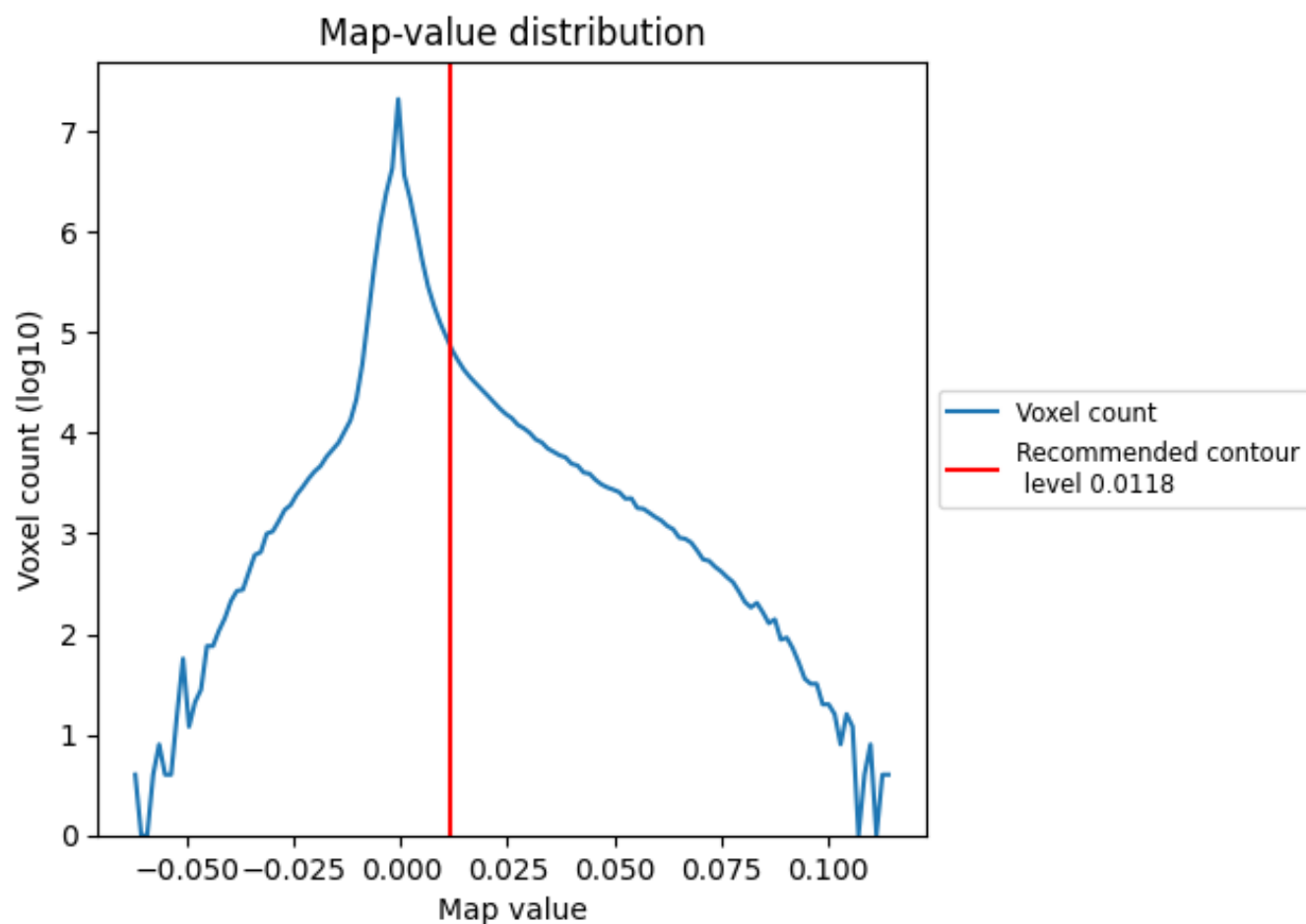
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

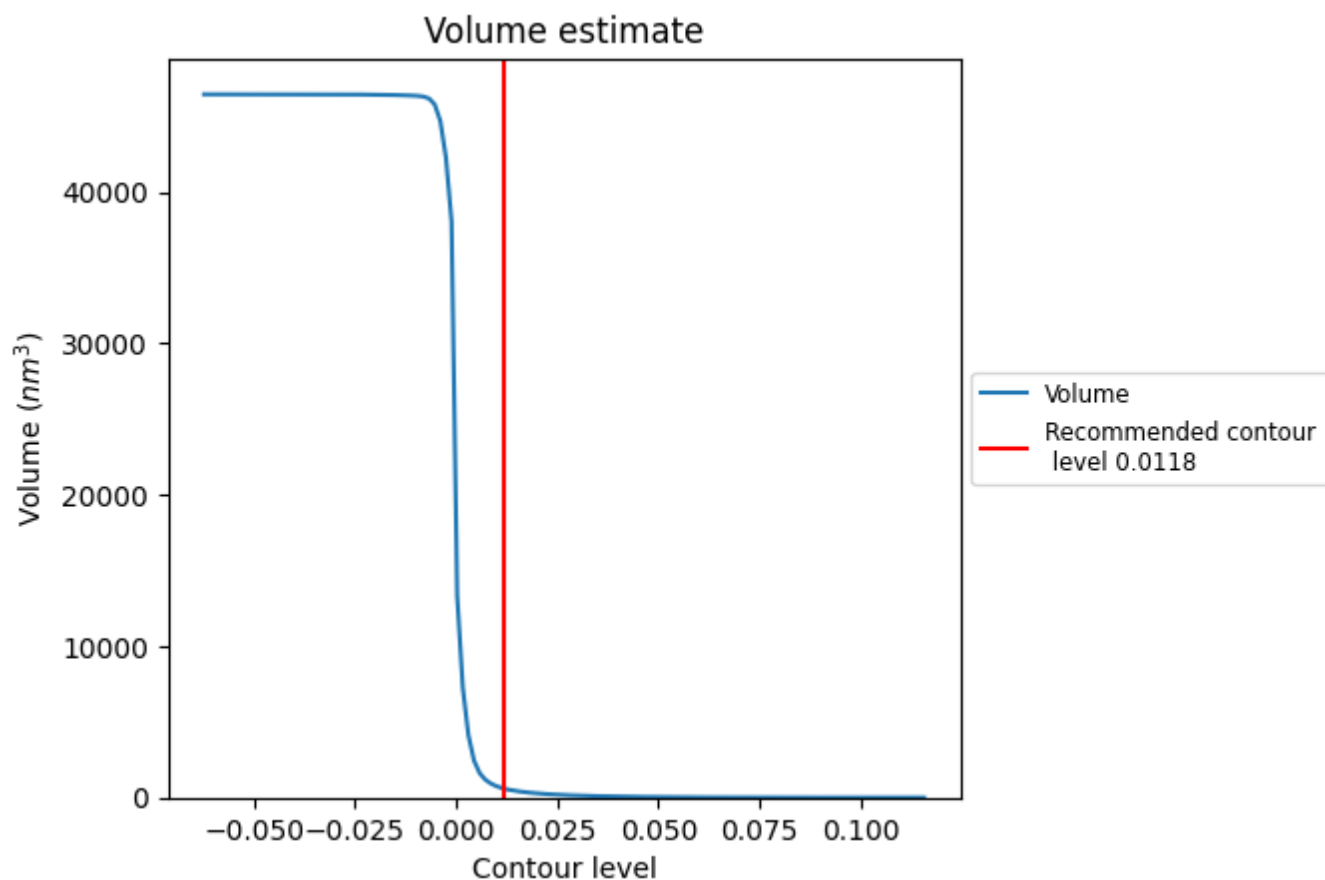
This section contains the results of statistical analysis of the map.

### 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.

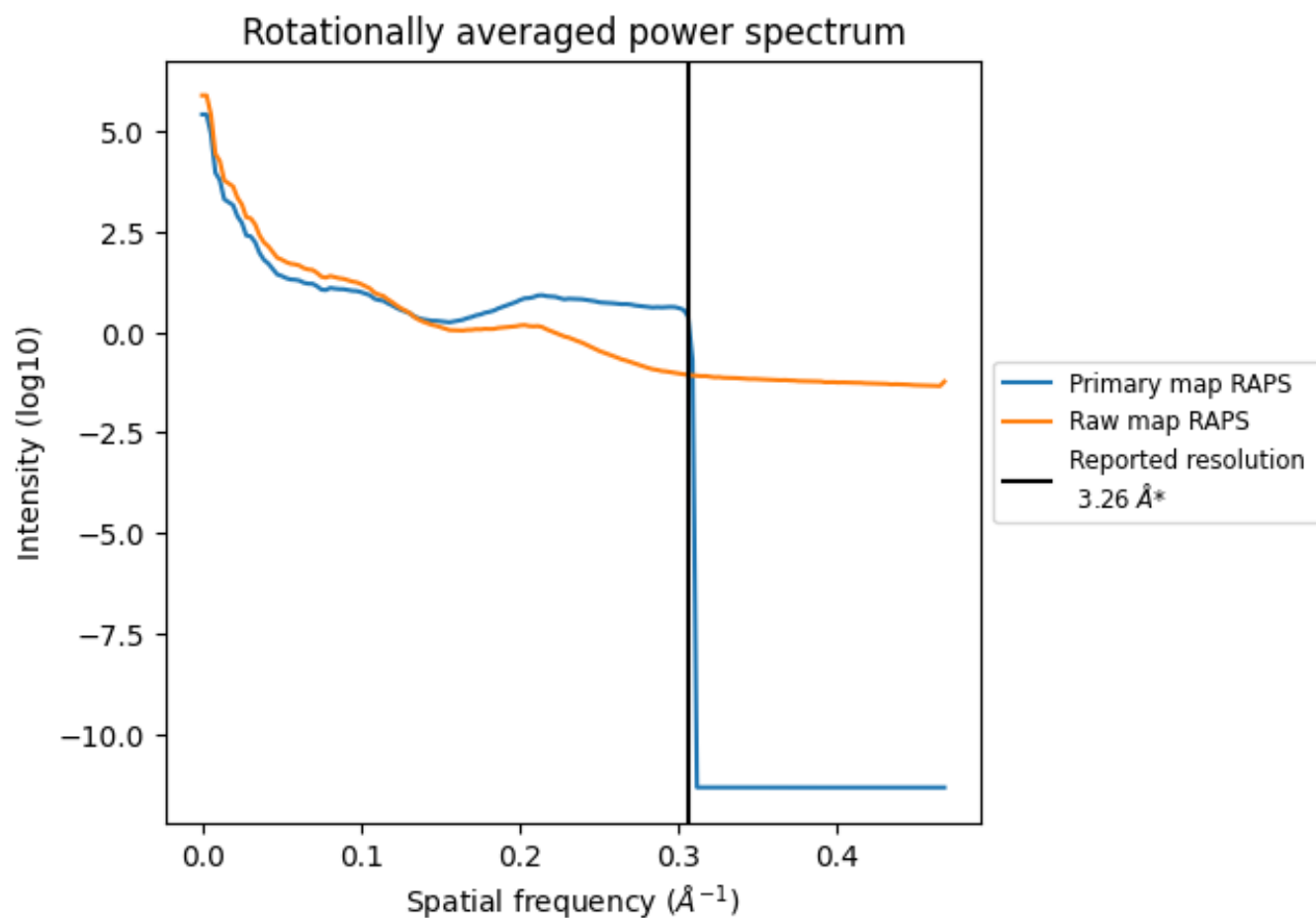
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 600 nm<sup>3</sup>; this corresponds to an approximate mass of 542 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 ⓘ



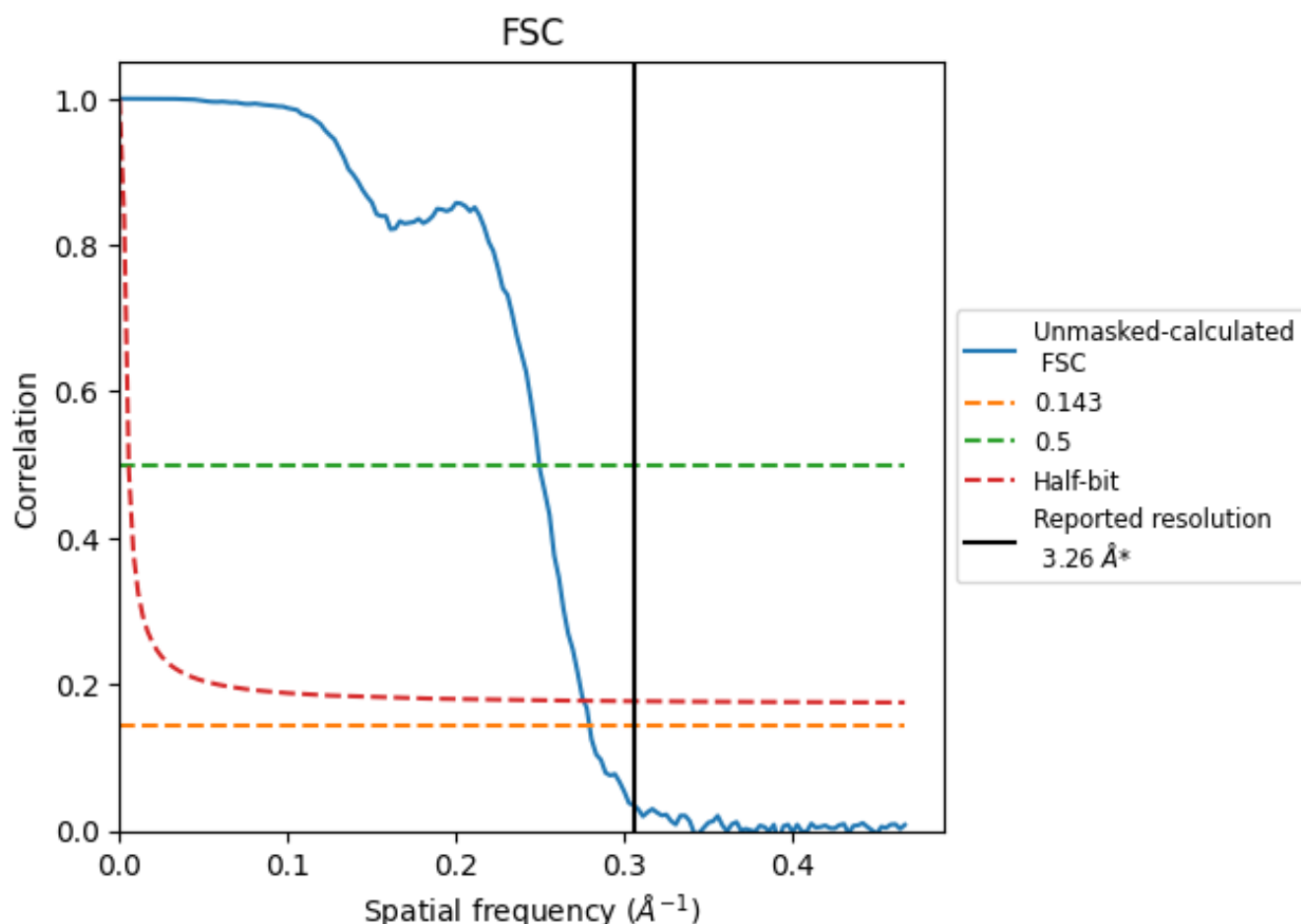
\*Reported resolution corresponds to spatial frequency of  $0.307 \text{ \AA}^{-1}$



## 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 0.307 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

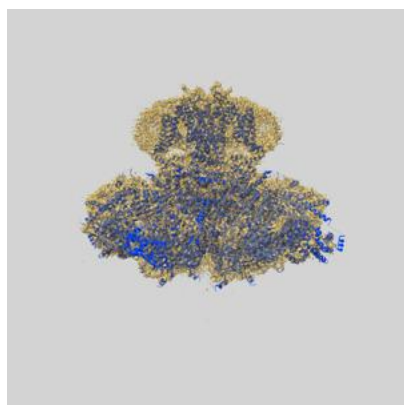
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.00	3.62

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

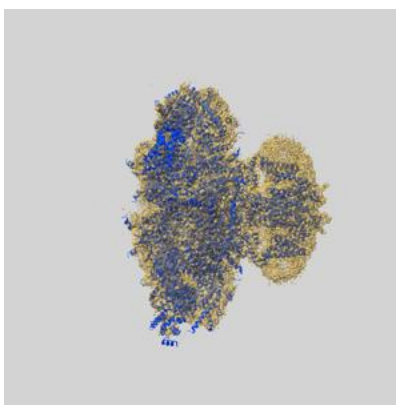
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27982 and PDB model 8EAQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

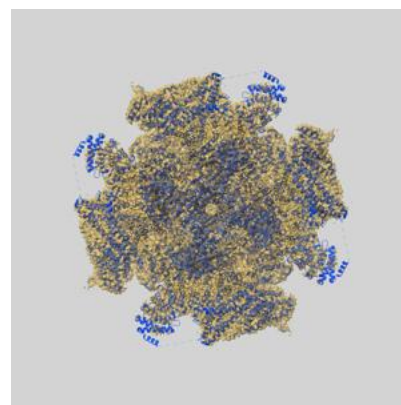
### 9.1 Map-model overlay [i](#)



X



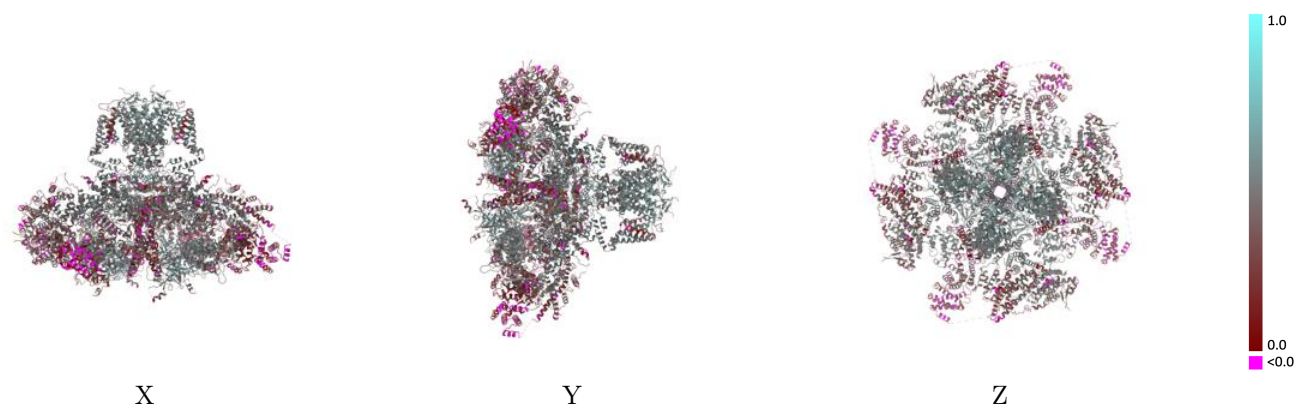
Y



Z

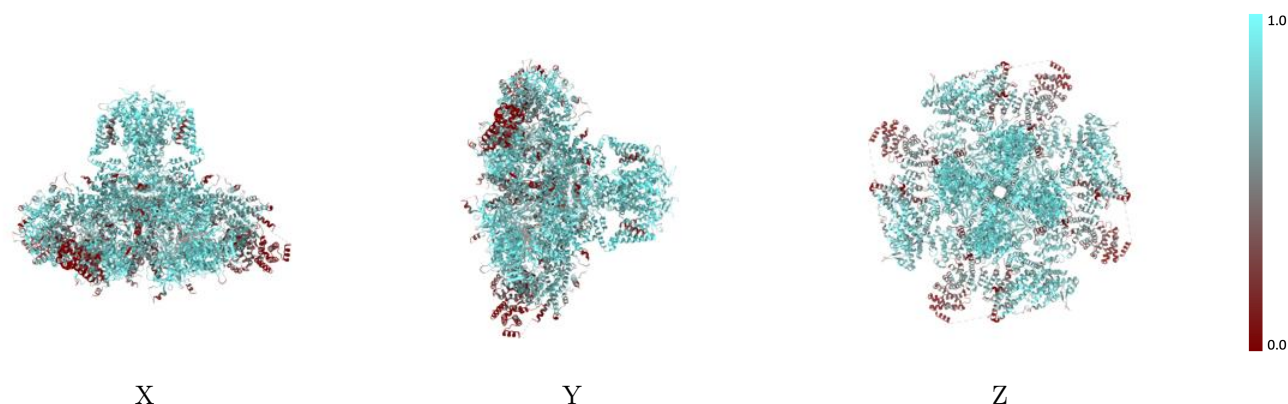
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



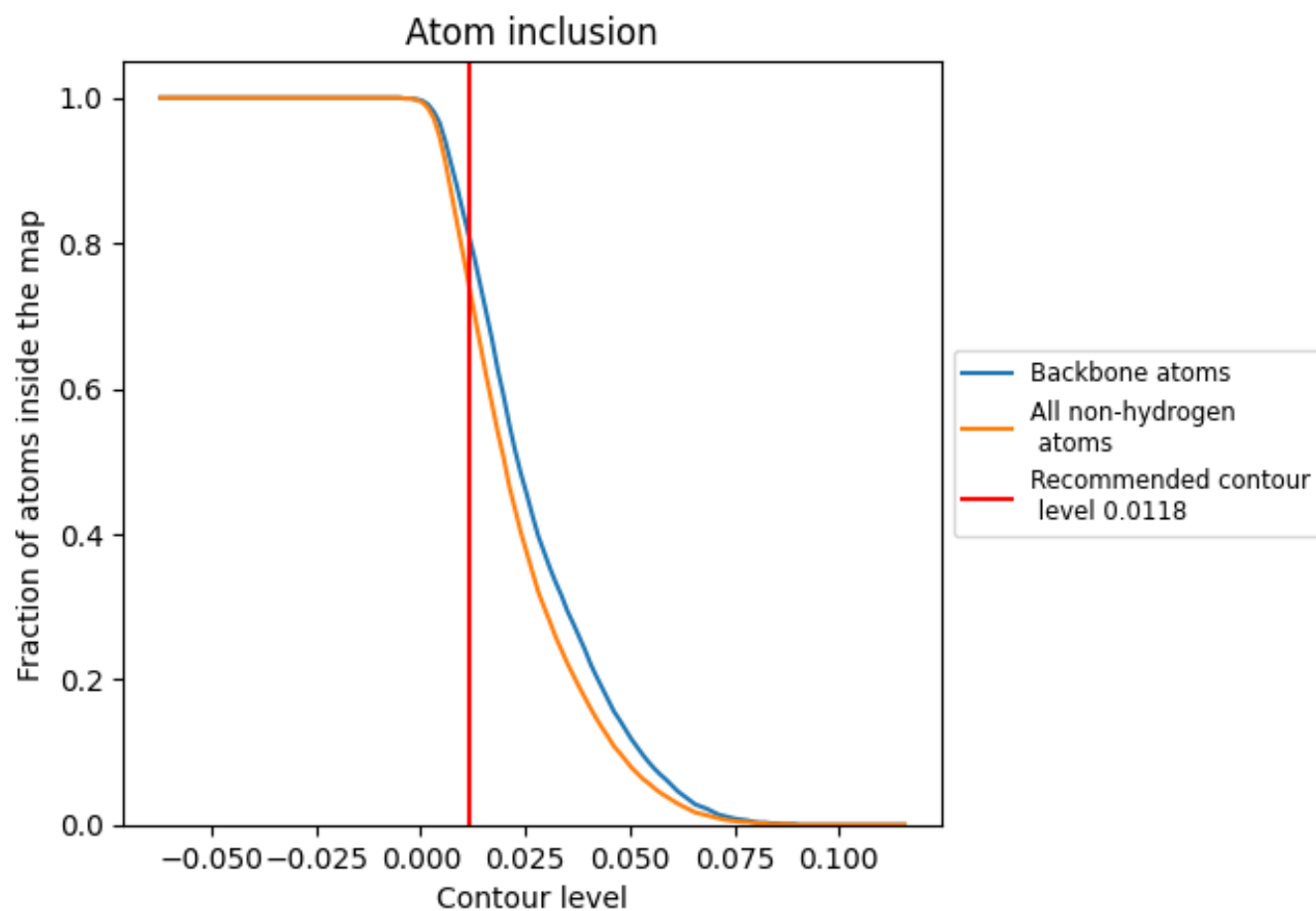
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0118).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7330	<div></div> 0.4030
A	<div></div> 0.7330	<div></div> 0.4030
B	<div></div> 0.7340	<div></div> 0.4030
C	<div></div> 0.7340	<div></div> 0.4030
D	<div></div> 0.7340	<div></div> 0.4030

