



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 03:11 PM UTC

PDB ID : 9UTW / pdb_00009utw
EMDB ID : EMD-64502
Title : Structure of dimeric FKS1 in complex with tRNA
Authors : Li, J.L.; Zhu, A.Q.; Liu, J.X.; Dai, X.L.; Wang, X.; Yan, C.Y.; Deng, D.
Deposited on : 2025-05-05
Resolution : 2.96 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

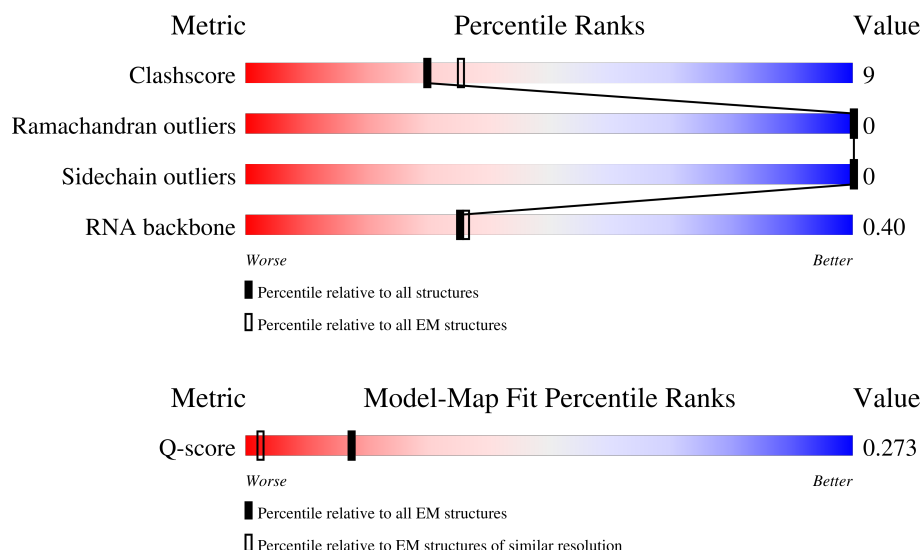
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	C	197	
1	G	197	
2	B	1876	

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Mol	Chain	Length	Quality of chain
2	H	1876	55% 20% 25%
3	A	76	61% 22% 39% 18% 18%
4	J	3	67% 67% 33%
5	D	2	100% 100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25408 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 Uncharacterized protein YMR295C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	25	Total	C	N	O	0	0
			203	124	38	41		
1	G	25	Total	C	N	O	0	0
			203	124	38	41		

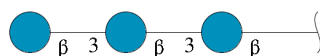
- Molecule 2 is a protein called 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1409	Total	C	N	O	S	0	0
			11499	7526	1918	1981	74		
2	B	1409	Total	C	N	O	S	0	0
			11499	7526	1918	1981	74		

- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	62	Total	C	N	O	P	0	0
			1319	587	228	442	62		

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
4	J	3	Total	C	O	0	0
			34	18	16		

- Molecule 5 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.

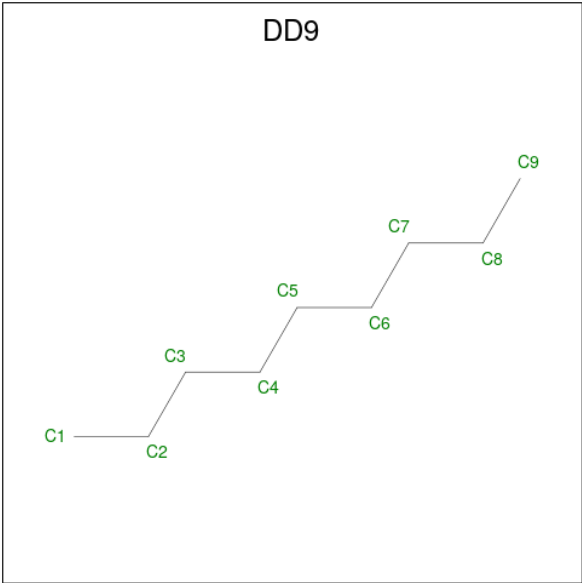


Mol	Chain	Residues	Atoms			AltConf	Trace
5	D	2	Total	C	O	0	0
			23	12	11		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	H	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	

- Molecule 7 is nonane (CCD ID: DD9) (formula: C₉H₂₀) (labeled as "Ligand of Interest" by depositor).



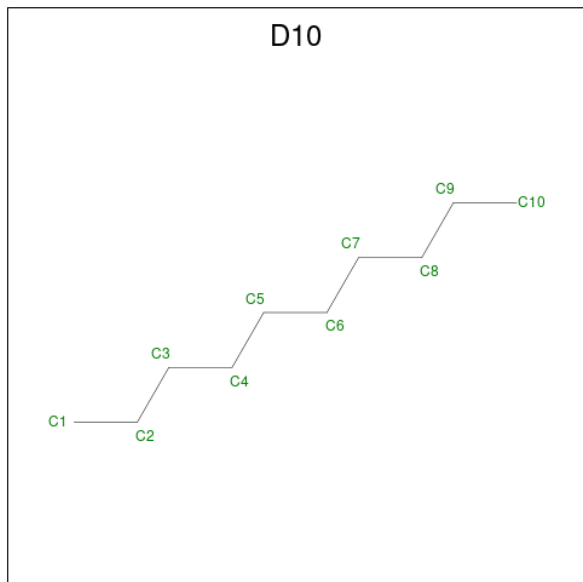
Mol	Chain	Residues	Atoms		AltConf
7	H	1	Total	C	0
			9	9	
7	H	1	Total	C	0
			9	9	
7	H	1	Total	C	0
			9	9	

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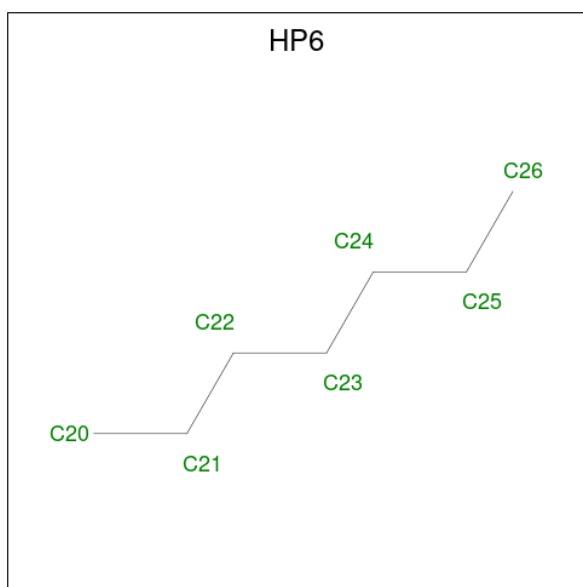
Mol	Chain	Residues	Atoms	AltConf
7	H	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0

- Molecule 8 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



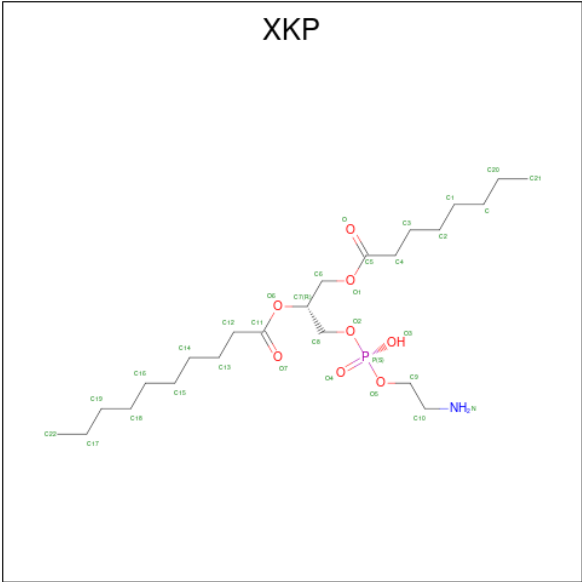
Mol	Chain	Residues	Atoms	AltConf
8	H	1	Total C 10 10	0
8	B	1	Total C 10 10	0

- Molecule 9 is HEPTANE (CCD ID: HP6) (formula: C_7H_{16}) (labeled as "Ligand of Interest" by depositor).



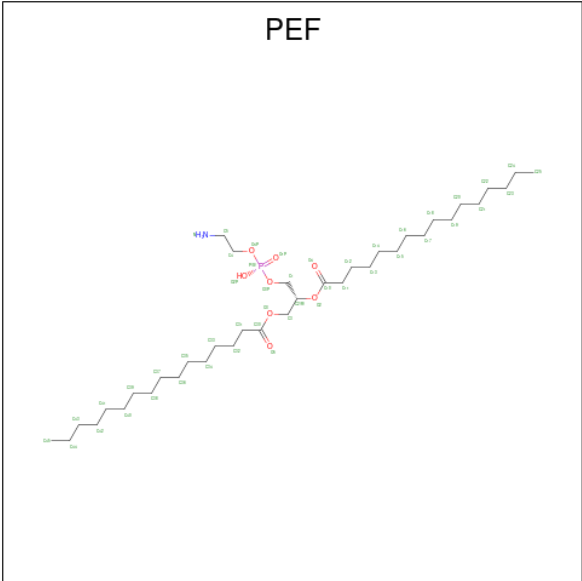
Mol	Chain	Residues	Atoms	AltConf
9	H	1	Total C 7 7	0
9	H	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0

- Molecule 10 is (11R,14S)-17-amino-14-hydroxy-8,14-dioxo-9,13,15-trioxa-14lambda 5 -phosphahaheptadecan-11-yl decanoate (CCD ID: XKP) (formula: $C_{23}H_{46}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	H	1	Total	C	N	O	P	0
			33	23	1	8	1	
10	B	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 11 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).



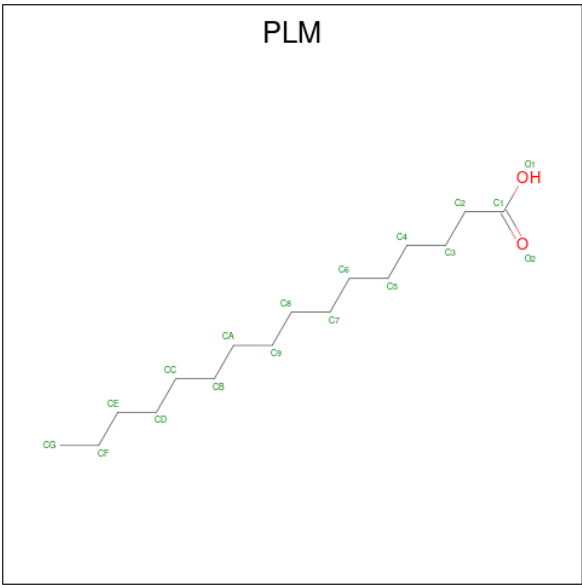
Mol	Chain	Residues	Atoms					AltConf
11	H	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 12 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



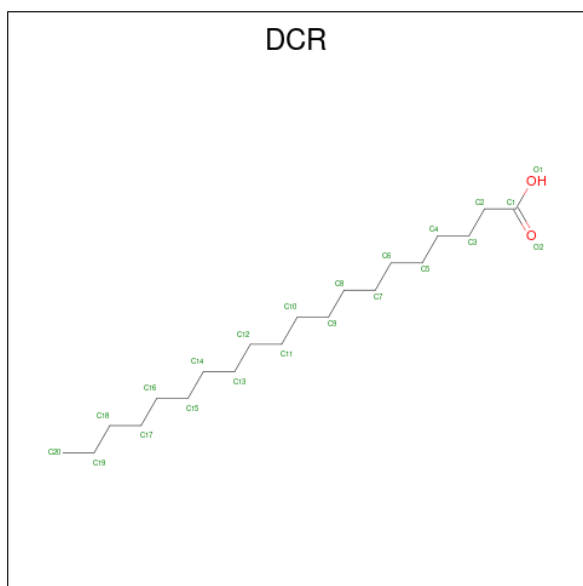
Mol	Chain	Residues	Atoms			AltConf
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	

- Molecule 13 is icosanoic acid (CCD ID: DCR) (formula: $C_{20}H_{40}O_2$) (labeled as "Ligand of Interest" by depositor).



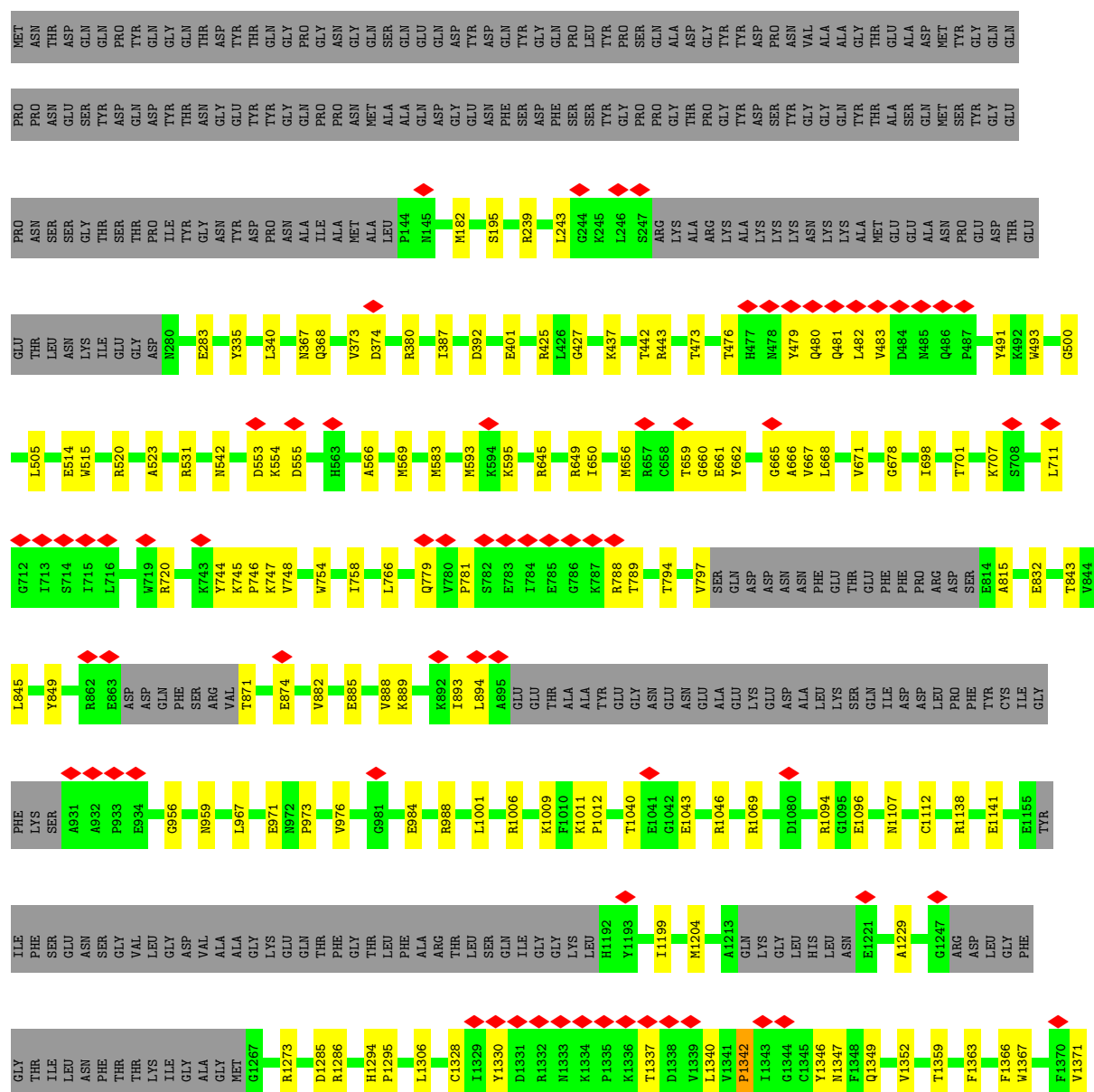
Mol	Chain	Residues	Atoms			AltConf
13	H	1	Total	C	O	0
			22	20	2	
13	B	1	Total	C	O	0
			22	20	2	

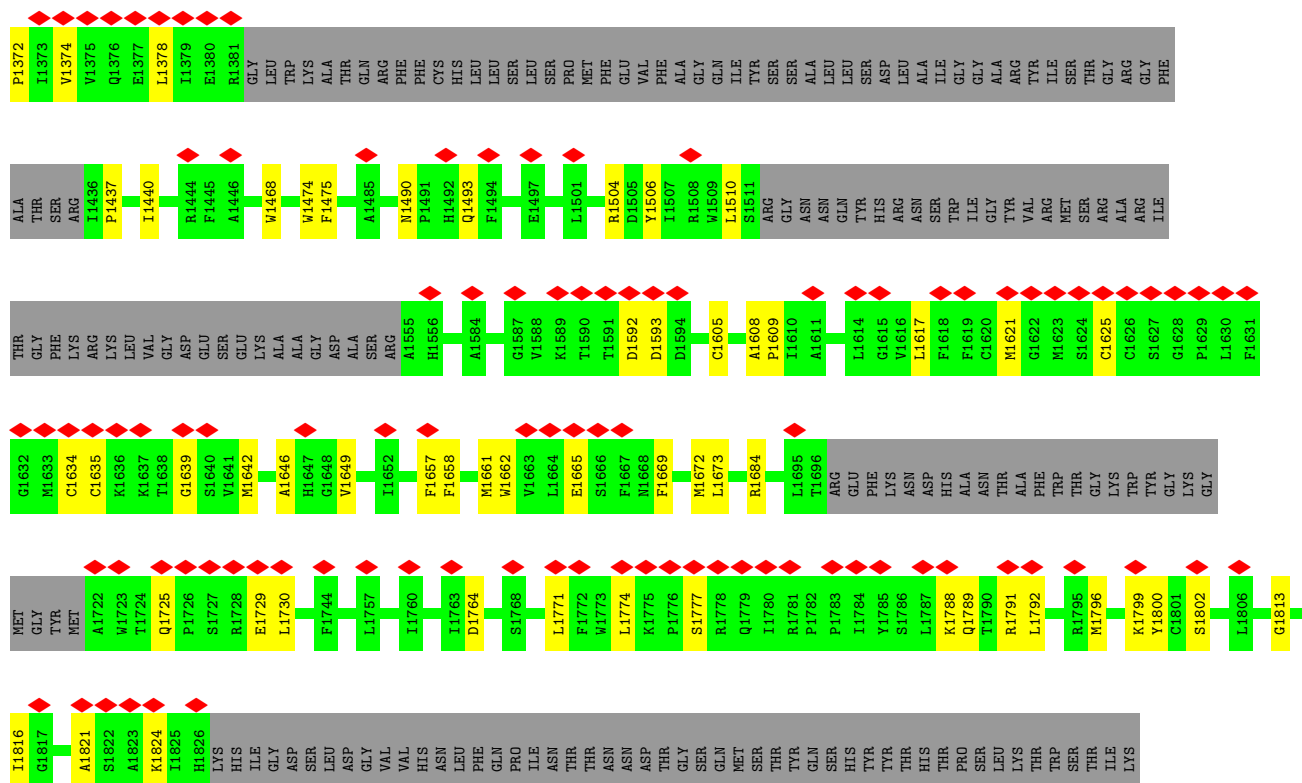


PHE	LYS	SER	A931	A932	P933	P934	Y935	T936	L937	R938	T939	R940	Y941	W942	A943	S944	L945	R946	S947	Q948	T949	L950	Y951	R952	S955	G956	F957	M958	N959	Y960	S961	R962	A963	I964	K965	L966	L967	Y968	P973	E974	I975	V976	Q977	M978	F979	G980	G981	N982	A983	E984	G985	L986	E987	R988	E989	L990	E991		
K992	M993	A994	K997	F998	K999	F1000	L1001	V1002	S1003	M1004	Q1005	R1006	L1007	A1008	K1009	F1010	K1011	P1012	H1013	E1014	L1015	E1016	M1017	A1018	E1019	F1020	G1021	L1022	R1023	A1024	Y1025	P1026	D1027	L1028	Q1029	I1030	A1031	Y1032	L1033	D1034	E1035	E1036	P1037	P1038	L1039	T1040	E1041	G1042	E1043	E1044	P1045	R1046	I1047	Y1048	S1049	A1050	L1051	T1052	
D1053	G1054	H1055	C1056	E1057	I1058	L1059	D1060	N1061	R1062	R1063	R1064	P1065	P1066	K1067	F1068	R1069	Q1070	Q1071	L1072	P1076	I1077	L1078	G1079	D1080	G1081	K1082	N1085	Q1086	L1090	I1091	F1092	Y1093	R1094	I1098	Q1099	L1100	I1101	D1102	E1036	A1103	ASP	N1104	P1105	D1106	N1107	Y1108	L1109	E1110	E1111	C1112	L1113	K1114	I1115	R1116	S1117	V1118	L1119		
A1120	E1121	F1122	E1123	E1124	L1125	M1126	V1127	E1128	Q1129	V1130	M1131	P1132	Y1133	A1134	P1135	G1136	L1137	R1138	Y1139	E1140	E1141	Q1142	T1143	T1144	M1145	H1146	P1147	V1148	G1152	A1153	R1154	E1155	TYR	ILE	PHE	SER	GLU	ASN	SER	GLY	VAL	LEU	GLY	ASP	VAL	ALA	ALA	LYS	GLU	GLN	THR	PHE	GLY	THR	LEU	ALA			
ARG	THR	LEU	SER	GLN	ILE	GLY	GLY	LYS	LEU	H1192	Y1193	G1194	H1195	P1196	D1197	F1198	I1199	N1200	A1201	T1202	F1203	M1204	T1205	R1206	G1208	G1209	V1210	S1211	K1212	A1213	GLN	LYS	GLY	LEU	HIS	LEU	ASN	E1221	D1222	I1223	Y1224	A1225	G1226	M1227	N1228	A1229	M1230	L1231	R1232	G1233	G1234	R1235	I1236	K1237	H1238	C1239	E1240	Y1241	
Y1242	Q1243	C1244	G1245	K1246	G1247	ARG	ASP	LEU	GLY	PHE	THR	GLY	ILE	ASN	PHE	THR	THR	LYS	I1326	GLY	ALA	GLY	MET	G1267	E1268	Q1269	M1270	L1271	S1272	R1273	E1274	Y1275	L1278	G1279	P1283	V1284	D1285	R1286	F1287	L1288	T1289	A1293	H1294	P1295	G1296	F1297	H1298	L1299	N1300	N1301	L1302	F1303	I1304	Q1305	L1306				
S1307	L1308	Q1309	M1310	F1311	M1312	L1313	T1314	L1315	V1316	S1320	L1321	A1322	H1323	E1324	S1325	T1326	M1327	C1328	I1329	Y1330	D1331	R1332	N1333	K1334	P1335	K1336	T1337	D1338	V1339	V1340	V1341	P1342	I1343	G1344	C1345	Y1346	N1347	F1348	Q1349	P1350	V1351	V1352	D1353	V1354	V1355	R1356	T1359	L1360	S1361	I1362	F1363	I1364	V1365	F1366	W1367	T1368	A1369		
F1370	V1371	P1372	I1373	V1374	V1375	Q1376	E1377	L1378	E1380	R1381	GLY	TRP	LYS	ALA	THR	GLN	ARG	PHE	PHE	CYS	HIS	LEU	LEU	ASN	SER	LEU	PRO	MET	PHE	GLU	VAL	PHE	ALA	GLY	GLN	ILE	TYR	SER	SER	ALA	LEU	ASP	LEU	ALA	LYS	ILE	GLY	ALA	ARG	TYR	ILE	SER	THR	GLY	ARG				
GLY	PHE	ALA	THR	SER	ARG	I1436	P1437	F1438	S1439	I1440	L1441	Y1442	S1443	R1444	F1445	A1446	G1447	S1448	A1449	I1450	Y1451	M1452	G1453	A1454	R1455	S1456	M1457	L1458	M1459	L1460	L1461	F1462	G1463	T1464	V1465	A1466	H1467	V1468	Q1469	A1470	P1471	L1472	L1473	V1474	F1475	W1476	A1477	S1478	L1479	S1480	L1481	L1482	T1483	F1484	A1485	P1486	F1487	V1488	F1489
N1490	P1491	H1492	Q1493	F1494	A1495	W1496	E1497	D1498	F1499	F1500	L1501	D1502	Y1503	D1505	Y1506	I1507	R1508	W1509	L1510	S1511	ARG	GLY	ASN	GLN	ASN	THR	TYS	HIS	ARG	ASN	SER	TRP	ILE	GLY	ALA	VAL	ARG	MET	SER	ARG	ARG	ALA	ARG	ILE	GLY	PHE	GLY	LYS	ARG	VAL	GLY	ASP	GLU	SER	GLU	LYS	ALA	ALA	
GLY	ASP	ALA	SER	ARG	A1555	H1556	R1557	T1558	N1559	L1560	I1561	M1562	A1563	E1564	I1565	I1566	P1567	C1568	A1569	I1570	Y1571	A1572	A1573	G1574	C1575	F1576	I1577	A1578	T1579	F1580	F1581	N1582	N1583	A1584	Q1585	T1586	G1587	V1588	K1589	T1590	T1591	D1592	D1593	D1594	R1595	V1596	N1597	S1598	V1599	L1600	R1601	I1602	Y1603	I1604	C1605	P1606	T1607	A1608	P1609
I1610	A1611	V1612	N1613	L1614	G1615	V1616	L1617	F1618	F1619	C1620	M1621	G1622	M1623	S1624	C1625	C1626	S1627	G1628	P1629	L1630	F1631	G1632	M1633	C1634	C1635	K1636	L1637	T1638	S1639	S1640	V1641	M1642	A1643	G1644	I1645	A1646	H1647	G1648	V1649	V1650	V1651	I1652	V1653	H1654	T1655	T1656	A1657	F1658	I1659	V1660	M1661	W1662	V1663	L1664	E1665	S1666	F1667	N1668	F1669
V1670	R1671	M1672	L1673	I1674	G1675	V1676	V1677	T1678	C1679	I1680	Q1681	C1682	Q1683	R1684	F1687	H1688	C1689	M1690	T1691	A1692	L1693	M1694	L1695	T1696	ARG	GLU	PHE	LYS	ASN	ASP	ALA	ASN	THR	ALA	PHE	TRP	THR	GLY	LYS	TRP	GLY	LYS	GLY	MET	TYR	GLY	MET	A1722	W1723	T1724	Q1725	P1726	S1727	R1728	E1729	L1730			

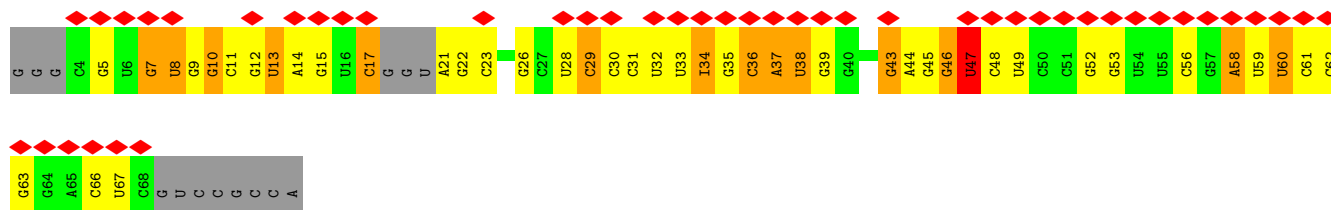
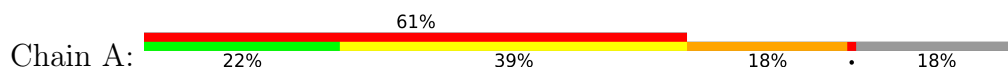
SER GLN MET SER THR TYR GLN SER HIS TYR TYR THR HIS THR PRO SER SER LEU LYS THR TRP SER THR ILE LYS

- Molecule 2: 1,3-beta-glucan synthase component FKS1





• Molecule 3: tRNA



• Molecule 4: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



• Molecule 5: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	243849	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.750	Depositor
Minimum map value	-1.782	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: BGC, DCR, XKP, MG, PEF, HP6, D10, DD9, PLM

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	C	0.16	0/206	0.33	0/279
1	G	0.15	0/206	0.37	0/279
2	B	0.27	0/11813	0.48	1/16028 (0.0%)
2	H	0.18	0/11813	0.43	0/16028
3	A	0.40	2/1469 (0.1%)	0.37	1/2283 (0.0%)
All	All	0.24	2/25507 (0.0%)	0.45	2/34897 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	34	I	C5-C6	7.31	1.54	1.39
3	A	34	I	N3-C4	6.78	1.49	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1342	PRO	CA-N-CD	-14.28	92.01	112.00
3	A	47	U	P-O3'-C3'	-7.27	109.29	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	203	0	194	4	0
1	G	203	0	194	3	0
2	B	11499	0	11514	132	0
2	H	11499	0	11513	274	0
3	A	1319	0	668	35	0
4	J	34	0	28	1	0
5	D	23	0	21	0	0
6	B	1	0	0	0	0
6	H	1	0	0	0	0
7	B	36	0	80	0	0
7	H	36	0	80	1	0
8	B	10	0	22	0	0
8	H	10	0	22	0	0
9	B	28	0	64	1	0
9	H	14	0	32	0	0
10	B	33	0	0	0	0
10	H	33	0	0	0	0
11	B	47	0	73	6	0
11	H	47	0	73	7	0
12	B	162	0	279	9	0
12	H	126	0	217	18	0
13	B	22	0	39	0	0
13	H	22	0	39	0	0
All	All	25408	0	25152	461	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 9.

The worst 5 of 461 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)
2:B:660:GLY:HA3	2:B:666:ALA:HA	1.44	0.97
2:H:514:GLU:OE1	2:H:531:ARG:NH2	2.02	0.93
2:H:1579:PHE:HA	2:H:1674:ILE:HD12	1.53	0.90
2:H:671:VAL:HG13	2:H:674:LYS:HE2	1.55	0.86
2:B:1107:ASN:ND2	2:B:1112:CYS:SG	2.53	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	23/197 (12%)	23 (100%)	0	0	100	100
1	G	23/197 (12%)	23 (100%)	0	0	100	100
2	B	1387/1876 (74%)	1339 (96%)	48 (4%)	0	100	100
2	H	1387/1876 (74%)	1342 (97%)	45 (3%)	0	100	100
All	All	2820/4146 (68%)	2727 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	22/167 (13%)	22 (100%)	0	100	100
1	G	22/167 (13%)	22 (100%)	0	100	100
2	B	1238/1620 (76%)	1238 (100%)	0	100	100
2	H	1238/1620 (76%)	1238 (100%)	0	100	100
All	All	2520/3574 (70%)	2520 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	1349	GLN
2	B	1281	GLN
2	H	1683	GLN
2	B	1469	GLN
2	B	614	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	58/76 (76%)	21 (36%)	2 (3%)

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	8	U
3	A	10	G
3	A	13	U
3	A	17	C
3	A	23	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	7	G
3	A	37	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BGC	D	1	5	12,12,12	0.18	0	17,17,17	0.15	0
5	BGC	D	2	5	11,11,12	0.21	0	15,15,17	0.51	0
4	BGC	J	1	4	12,12,12	0.34	0	17,17,17	0.57	0
4	BGC	J	2	4	11,11,12	0.35	0	15,15,17	0.70	0
4	BGC	J	3	4	11,11,12	0.21	0	15,15,17	0.55	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
5	BGC	D	1	5	-	2/2/22/22	0/1/1/1
5	BGC	D	2	5	-	2/2/19/22	0/1/1/1
4	BGC	J	1	4	-	2/2/22/22	0/1/1/1
4	BGC	J	2	4	-	2/2/19/22	0/1/1/1
4	BGC	J	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

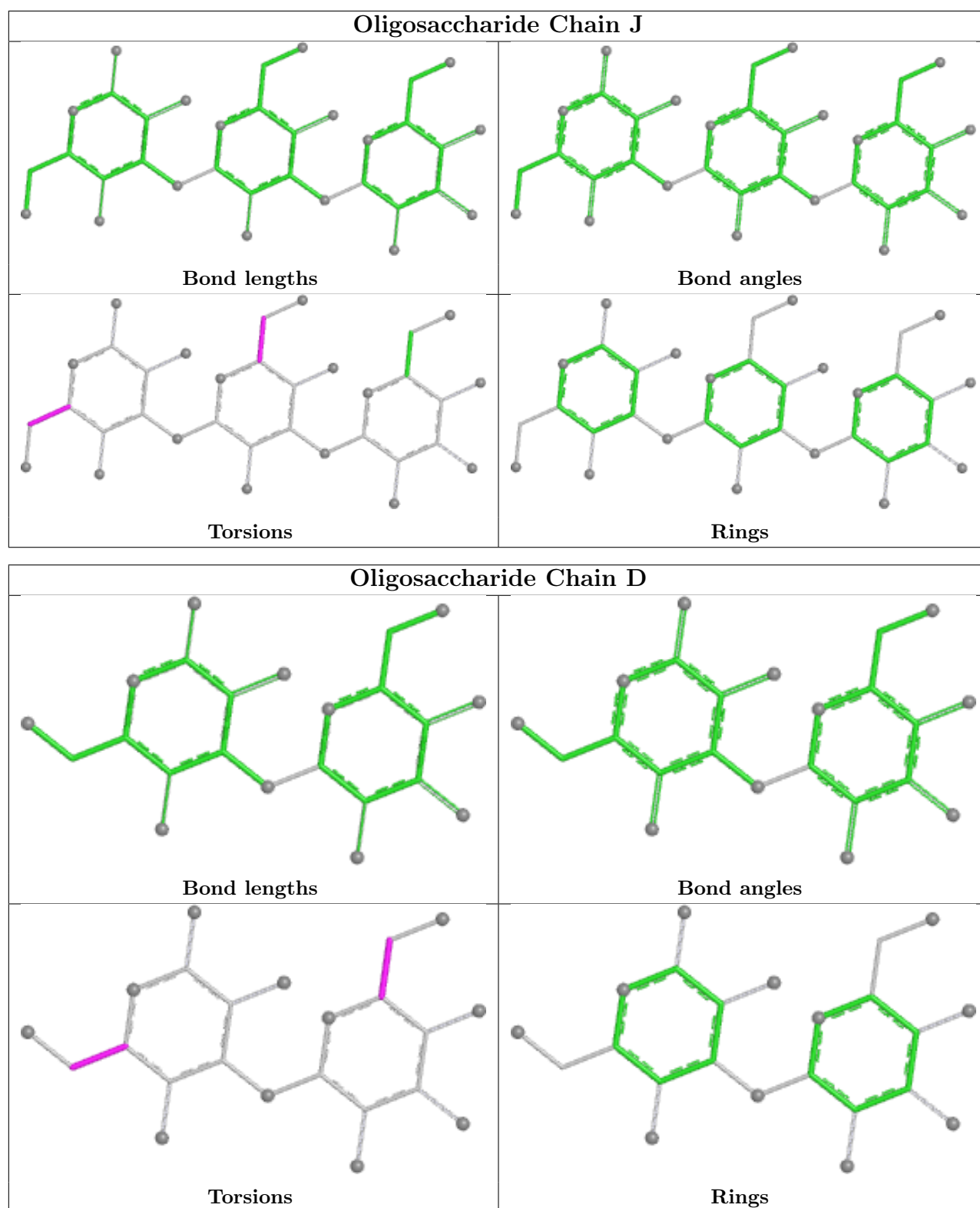
Mol	Chain	Res	Type	Atoms
5	D	2	BGC	O5-C5-C6-O6
5	D	2	BGC	C4-C5-C6-O6
4	J	2	BGC	C4-C5-C6-O6
4	J	1	BGC	C4-C5-C6-O6
4	J	1	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	BGC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	$\# Z > 2$
9	HP6	H	1908	-	6,6,6	0.32	0	5,5,5	0.66	0
12	PLM	B	1913	-	17,17,17	0.57	0	17,17,17	1.10	0
13	DCR	B	1917	-	21,21,21	0.52	0	21,21,21	1.07	0
7	DD9	B	1902	-	8,8,8	0.26	0	7,7,7	0.86	0
12	PLM	H	1914	-	17,17,17	0.60	0	17,17,17	1.05	0
9	HP6	B	1908	-	6,6,6	0.29	0	5,5,5	0.72	0
12	PLM	H	1912	-	17,17,17	0.59	0	17,17,17	1.08	0
12	PLM	H	1916	-	17,17,17	0.61	0	17,17,17	1.06	0
7	DD9	H	1903	-	8,8,8	0.30	0	7,7,7	0.79	0
10	XKP	H	1909	-	32,32,32	1.07	4 (12%)	35,37,37	1.05	2 (5%)
9	HP6	B	1907	-	6,6,6	0.31	0	5,5,5	0.65	0
12	PLM	B	1920	-	17,17,17	0.57	0	17,17,17	1.11	1 (5%)
12	PLM	B	1922	-	17,17,17	0.59	0	17,17,17	1.10	0
12	PLM	H	1913	-	17,17,17	0.56	0	17,17,17	1.09	1 (5%)
13	DCR	H	1915	-	21,21,21	0.55	0	21,21,21	1.02	0
8	D10	H	1906	-	9,9,9	0.32	0	8,8,8	0.78	0
12	PLM	B	1915	-	17,17,17	0.57	0	17,17,17	1.14	0
9	HP6	H	1907	-	6,6,6	0.35	0	5,5,5	0.60	0
12	PLM	H	1917	-	17,17,17	0.59	0	17,17,17	1.11	0
12	PLM	B	1916	-	17,17,17	0.57	0	17,17,17	1.08	0
11	PEF	B	1912	-	46,46,46	1.32	6 (13%)	49,51,51	1.19	2 (4%)
10	XKP	B	1911	-	32,32,32	1.08	4 (12%)	35,37,37	1.01	2 (5%)
12	PLM	B	1918	-	17,17,17	0.58	0	17,17,17	1.11	1 (5%)
7	DD9	B	1905	-	8,8,8	0.30	0	7,7,7	0.80	0
8	D10	B	1906	-	9,9,9	0.27	0	8,8,8	0.84	0
7	DD9	H	1902	-	8,8,8	0.29	0	7,7,7	0.78	0
7	DD9	B	1904	-	8,8,8	0.31	0	7,7,7	0.73	0
12	PLM	B	1921	-	17,17,17	0.54	0	17,17,17	1.17	1 (5%)
9	HP6	B	1909	-	6,6,6	0.32	0	5,5,5	0.65	0
7	DD9	H	1905	-	8,8,8	0.31	0	7,7,7	0.85	0
12	PLM	B	1914	-	17,17,17	0.56	0	17,17,17	1.09	0
7	DD9	B	1903	-	8,8,8	0.29	0	7,7,7	0.81	0
12	PLM	H	1911	-	17,17,17	0.59	0	17,17,17	1.06	0
12	PLM	B	1919	-	17,17,17	0.57	0	17,17,17	1.09	0
12	PLM	H	1918	-	17,17,17	0.62	0	17,17,17	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PEF	H	1910	-	46,46,46	1.37	6 (13%)	49,51,51	1.01	2 (4%)
7	DD9	H	1904	-	8,8,8	0.31	0	7,7,7	0.79	0
9	HP6	B	1910	-	6,6,6	0.31	0	5,5,5	0.69	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
9	HP6	H	1908	-	-	0/4/4/4	-
12	PLM	B	1913	-	-	6/15/15/15	-
13	DCR	B	1917	-	-	7/19/19/19	-
7	DD9	B	1902	-	-	2/6/6/6	-
12	PLM	H	1914	-	-	4/15/15/15	-
9	HP6	B	1908	-	-	0/4/4/4	-
12	PLM	H	1912	-	-	7/15/15/15	-
12	PLM	H	1916	-	-	6/15/15/15	-
7	DD9	H	1903	-	-	1/6/6/6	-
10	XKP	H	1909	-	-	21/36/36/36	-
9	HP6	B	1907	-	-	0/4/4/4	-
12	PLM	B	1920	-	-	9/15/15/15	-
12	PLM	B	1922	-	-	11/15/15/15	-
12	PLM	H	1913	-	-	10/15/15/15	-
13	DCR	H	1915	-	-	7/19/19/19	-
8	D10	H	1906	-	-	3/7/7/7	-
12	PLM	B	1915	-	-	10/15/15/15	-
9	HP6	H	1907	-	-	0/4/4/4	-
12	PLM	H	1917	-	-	5/15/15/15	-
12	PLM	B	1916	-	-	7/15/15/15	-
11	PEF	B	1912	-	-	18/50/50/50	-
10	XKP	B	1911	-	-	13/36/36/36	-
12	PLM	B	1918	-	-	6/15/15/15	-
7	DD9	B	1905	-	-	0/6/6/6	-
8	D10	B	1906	-	-	2/7/7/7	-
7	DD9	H	1902	-	-	2/6/6/6	-
7	DD9	B	1904	-	-	2/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PLM	B	1921	-	-	10/15/15/15	-
9	HP6	B	1909	-	-	1/4/4/4	-
7	DD9	H	1905	-	-	0/6/6/6	-
12	PLM	B	1914	-	-	5/15/15/15	-
7	DD9	B	1903	-	-	1/6/6/6	-
12	PLM	H	1911	-	-	8/15/15/15	-
12	PLM	B	1919	-	-	4/15/15/15	-
12	PLM	H	1918	-	-	7/15/15/15	-
11	PEF	H	1910	-	-	20/50/50/50	-
7	DD9	H	1904	-	-	3/6/6/6	-
9	HP6	B	1910	-	-	0/4/4/4	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1910	PEF	O2-C10	3.83	1.45	1.34
11	B	1912	PEF	O3-C30	3.81	1.44	1.33
11	H	1910	PEF	O3-C30	3.79	1.44	1.33
11	B	1912	PEF	O2-C10	3.63	1.44	1.34
11	B	1912	PEF	O2-C2	-2.74	1.40	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1912	PEF	O2-C10-C11	4.18	120.52	111.48
10	H	1909	XKP	O6-C11-C12	4.05	120.24	111.48
10	B	1911	XKP	O6-C11-C12	4.00	120.14	111.48
11	H	1910	PEF	O2-C10-C11	3.66	119.39	111.48
10	B	1911	XKP	O1-C5-C4	2.90	120.69	111.83

There are no chirality outliers.

5 of 218 torsion outliers are listed below:

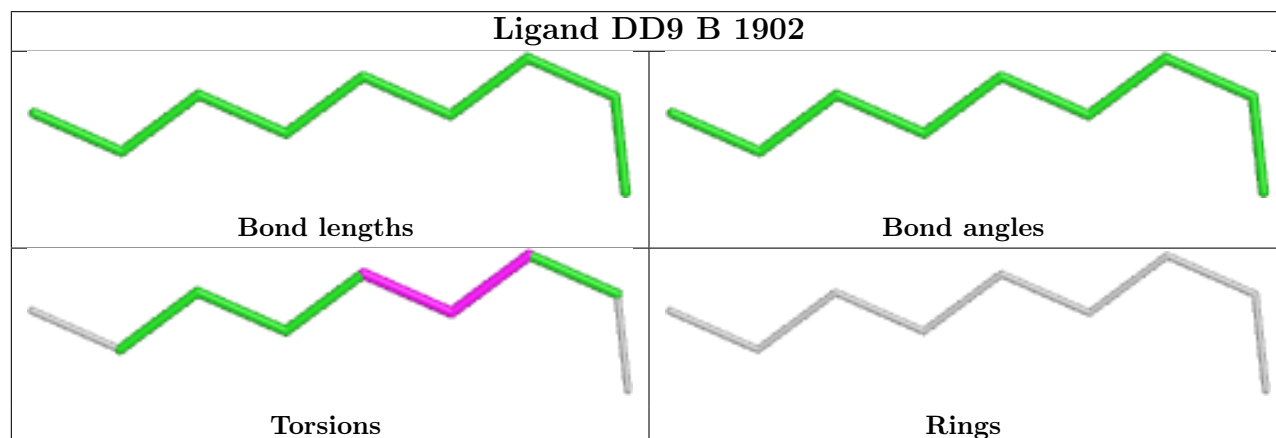
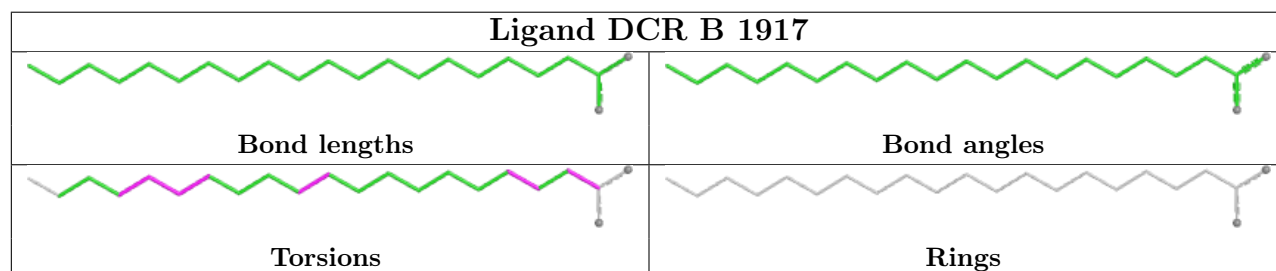
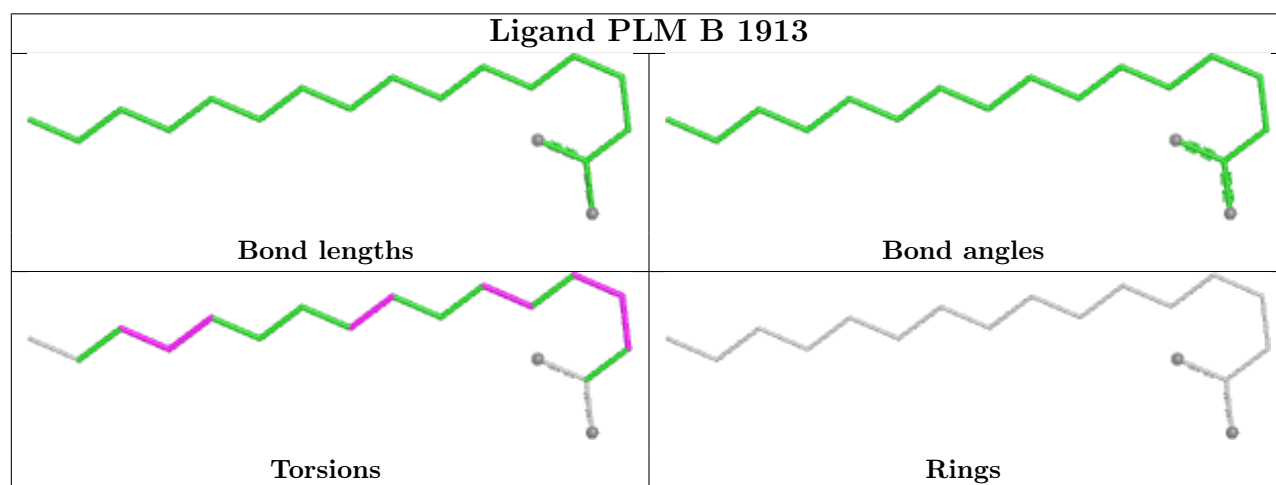
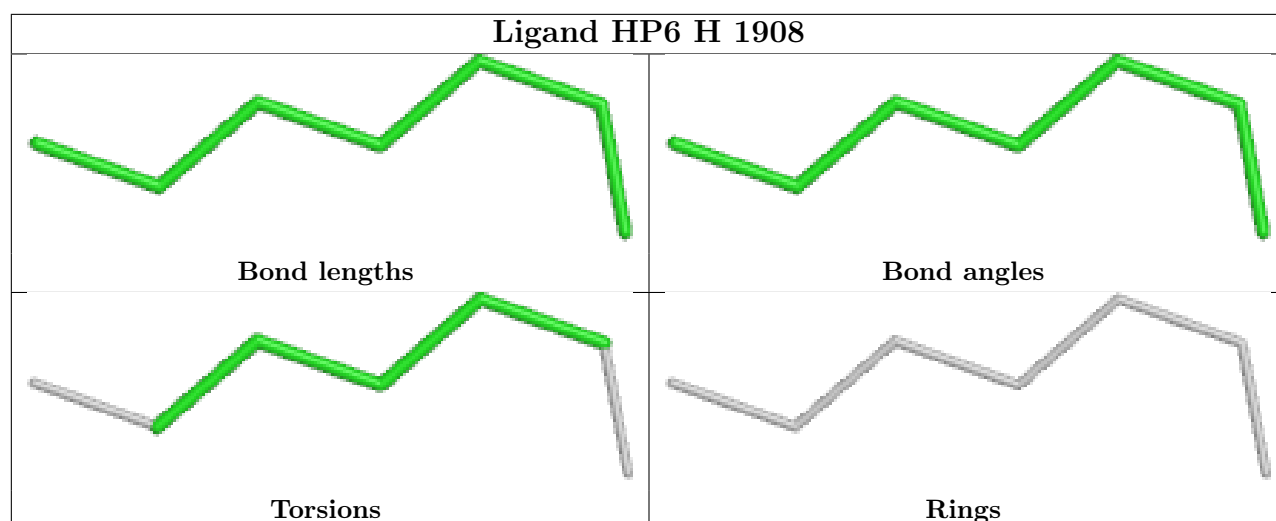
Mol	Chain	Res	Type	Atoms
10	H	1909	XKP	C12-C11-O6-C7
10	H	1909	XKP	C7-C8-O2-P
10	H	1909	XKP	C8-O2-P-O3
10	H	1909	XKP	C8-O2-P-O4
10	H	1909	XKP	C8-O2-P-O5

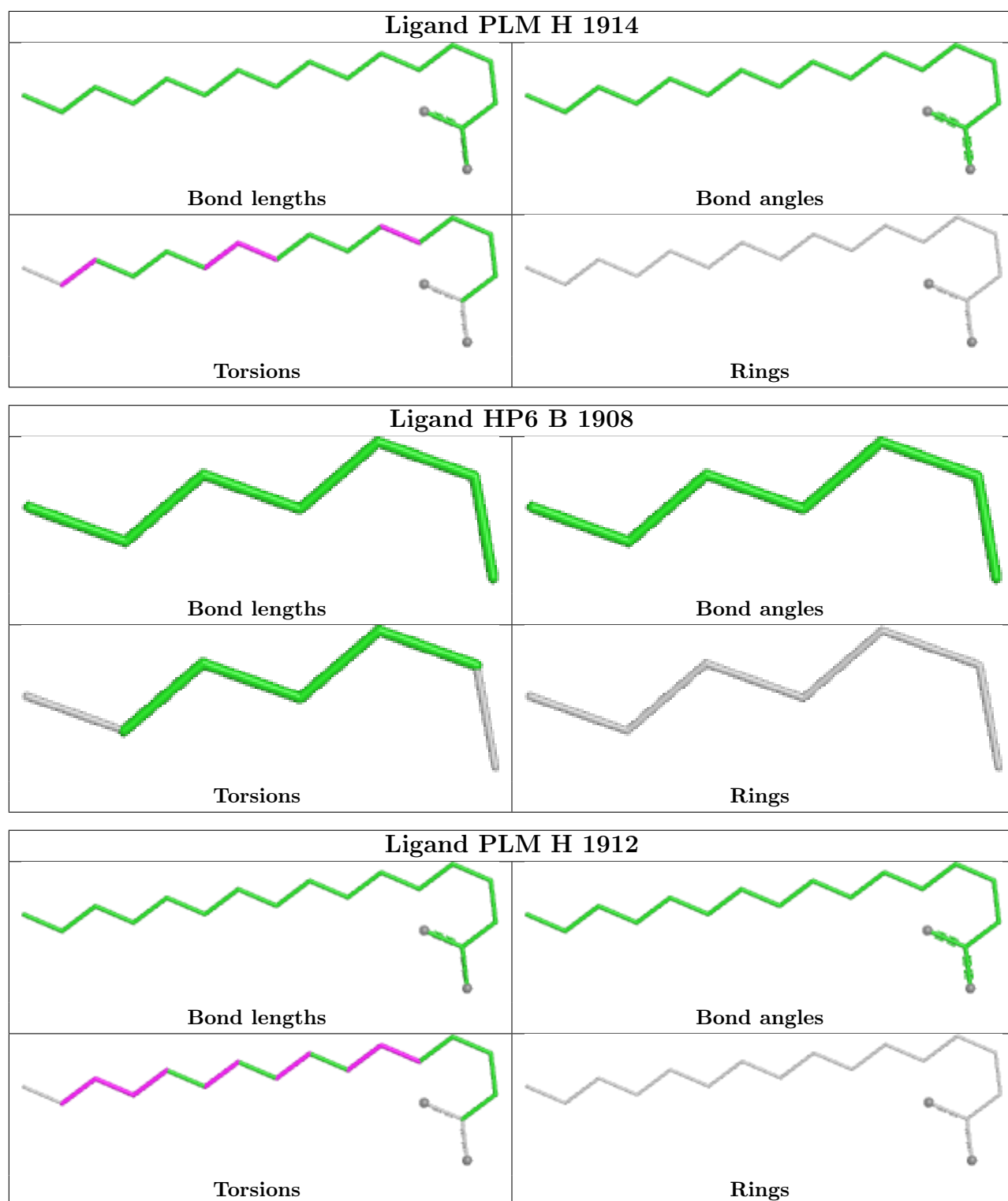
There are no ring outliers.

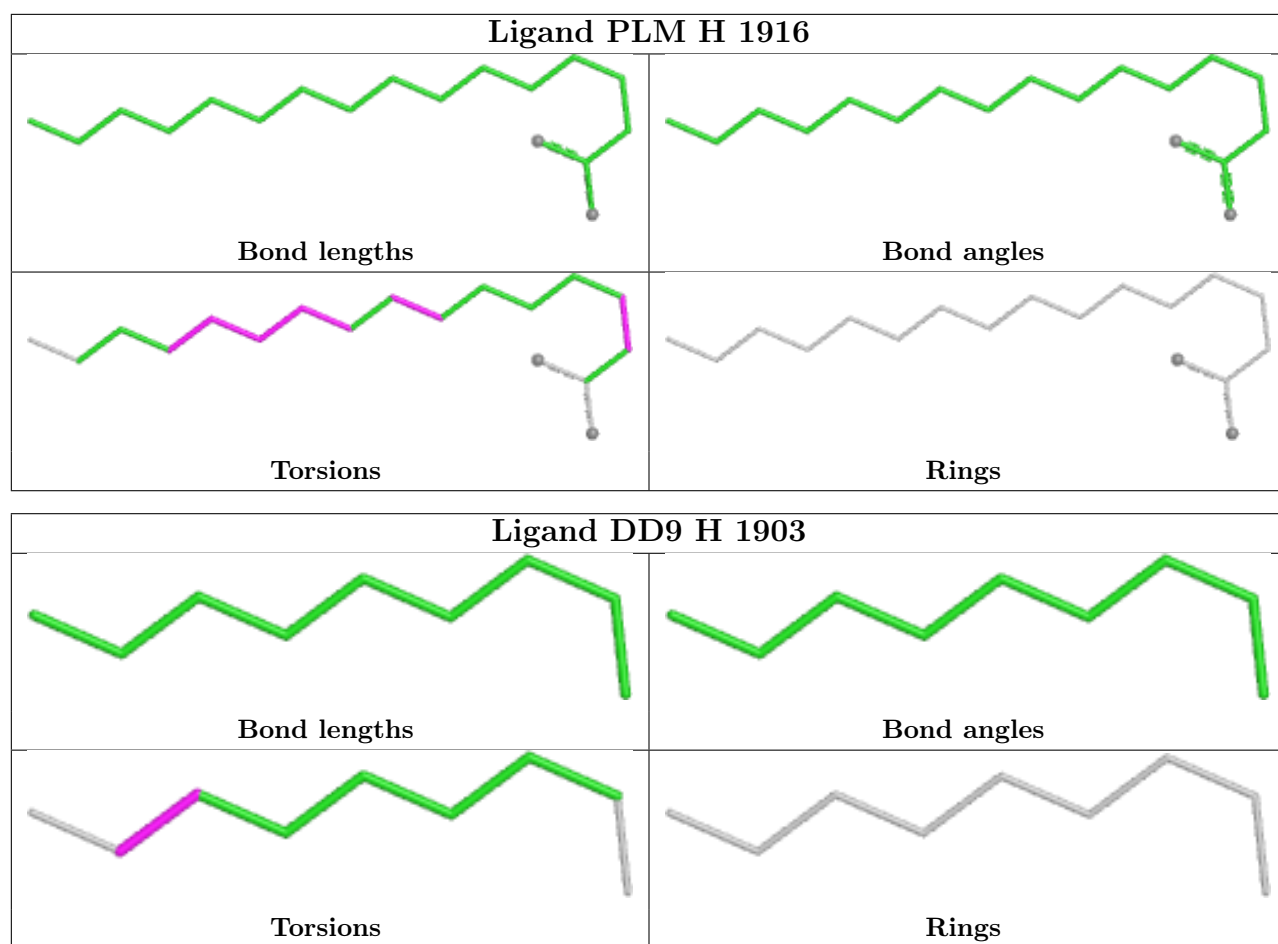
17 monomers are involved in 42 short contacts:

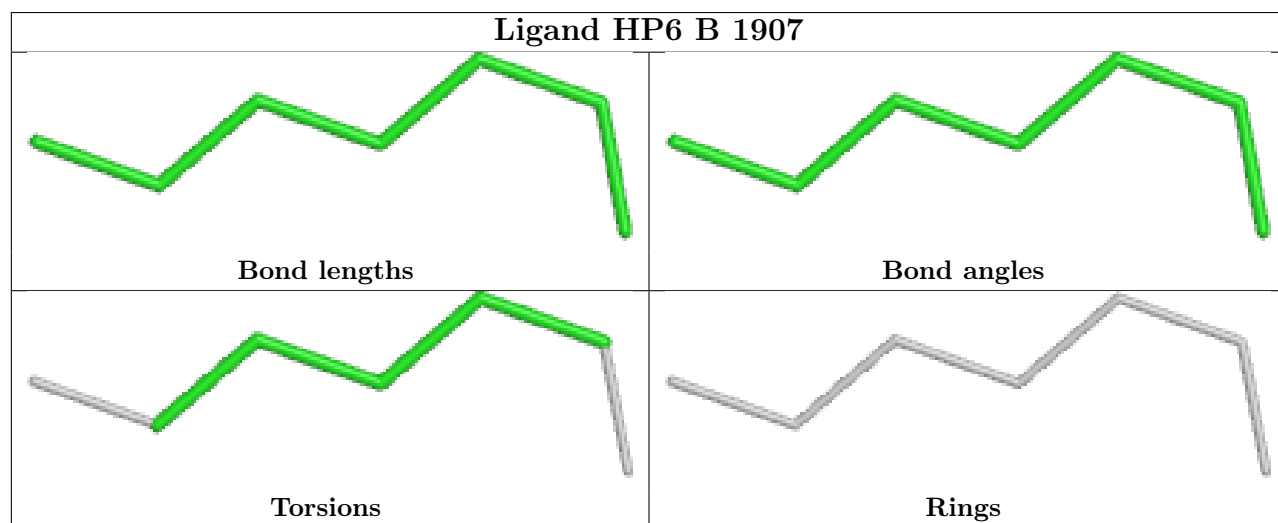
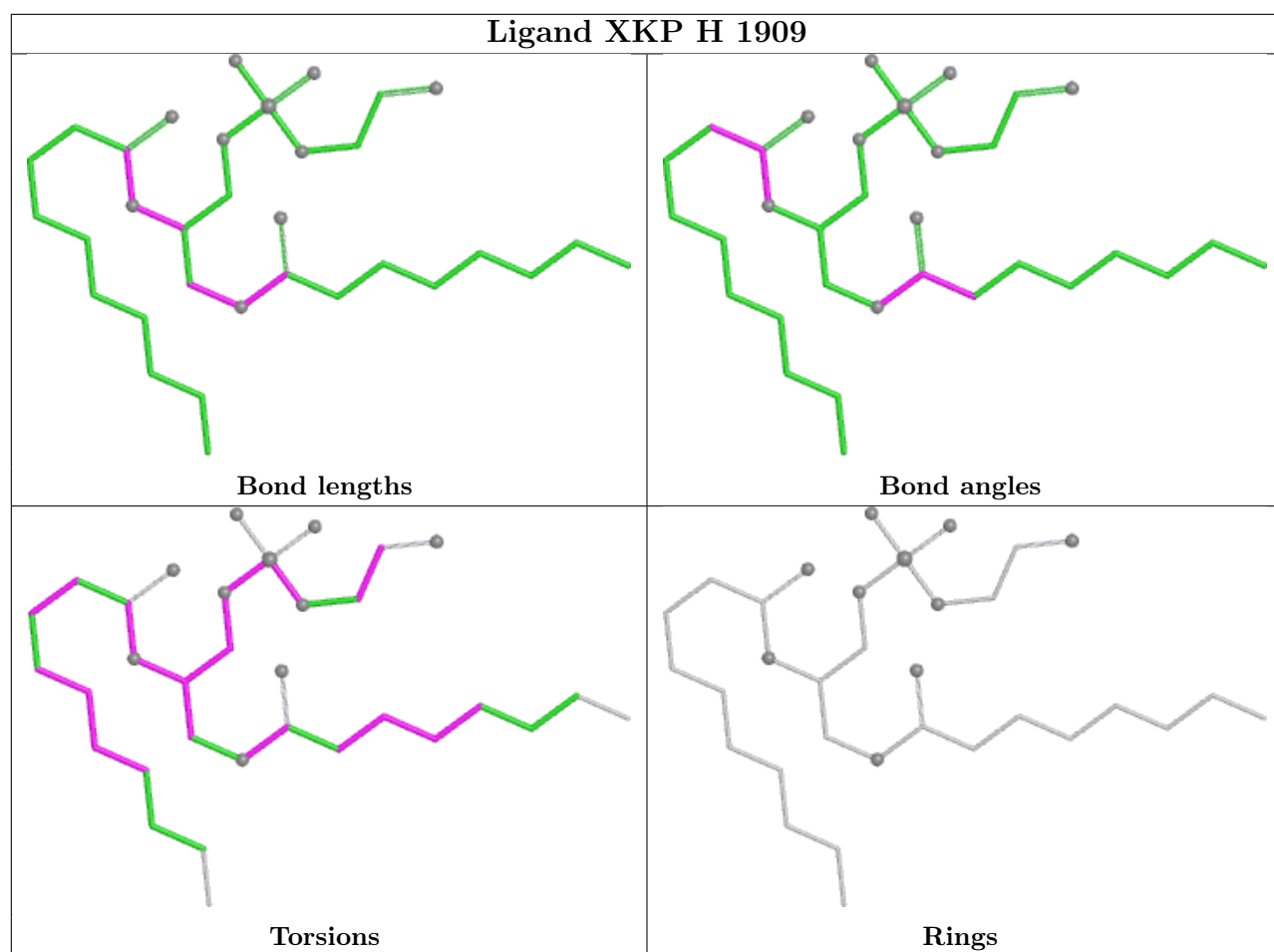
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1913	PLM	1	0
12	H	1914	PLM	3	0
9	B	1908	HP6	1	0
12	H	1912	PLM	2	0
12	H	1916	PLM	2	0
12	B	1920	PLM	1	0
12	H	1913	PLM	7	0
12	B	1915	PLM	3	0
12	H	1917	PLM	1	0
11	B	1912	PEF	6	0
7	H	1902	DD9	1	0
12	B	1921	PLM	2	0
12	B	1914	PLM	1	0
12	H	1911	PLM	2	0
12	B	1919	PLM	1	0
12	H	1918	PLM	2	0
11	H	1910	PEF	7	0

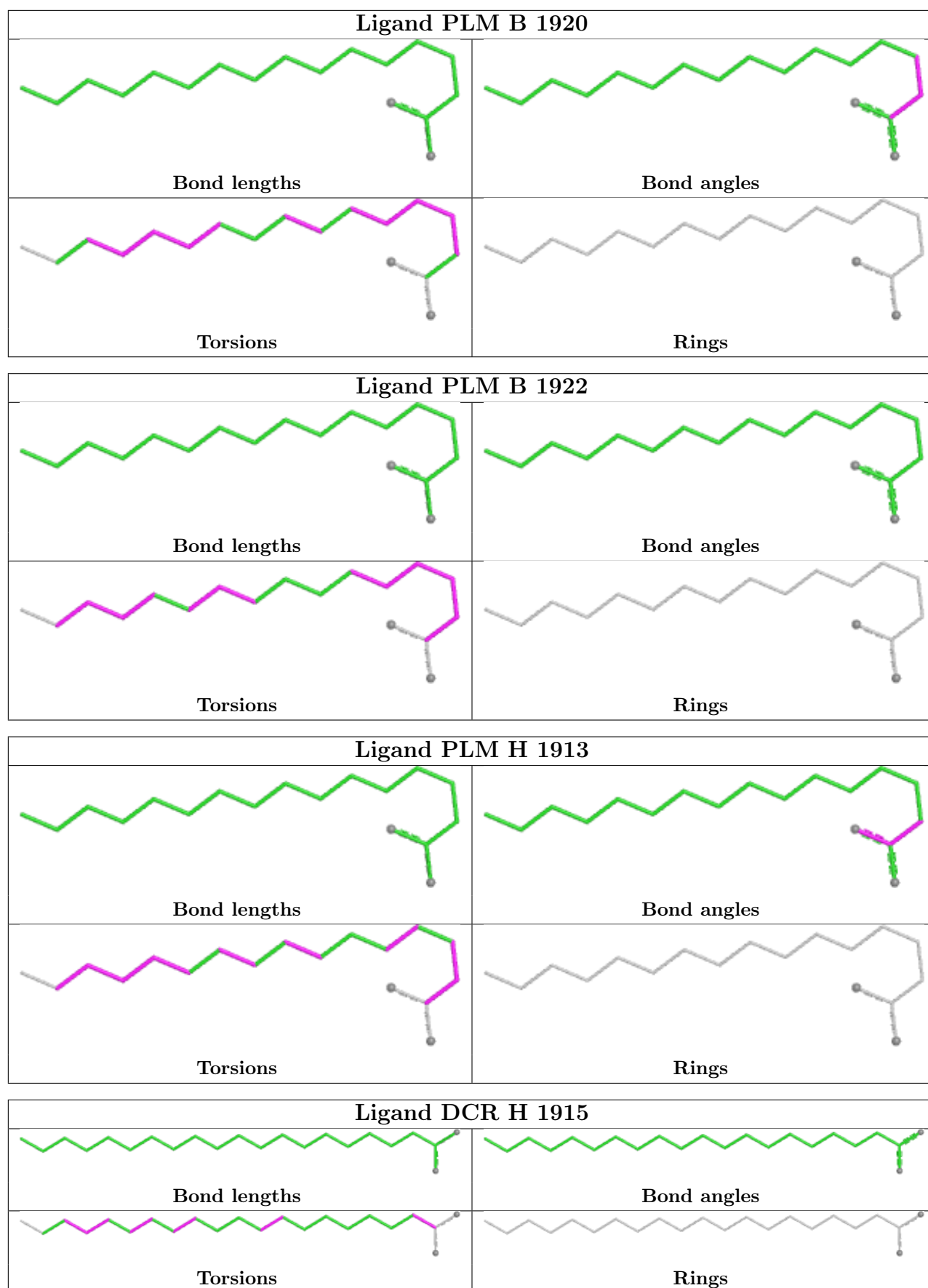
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

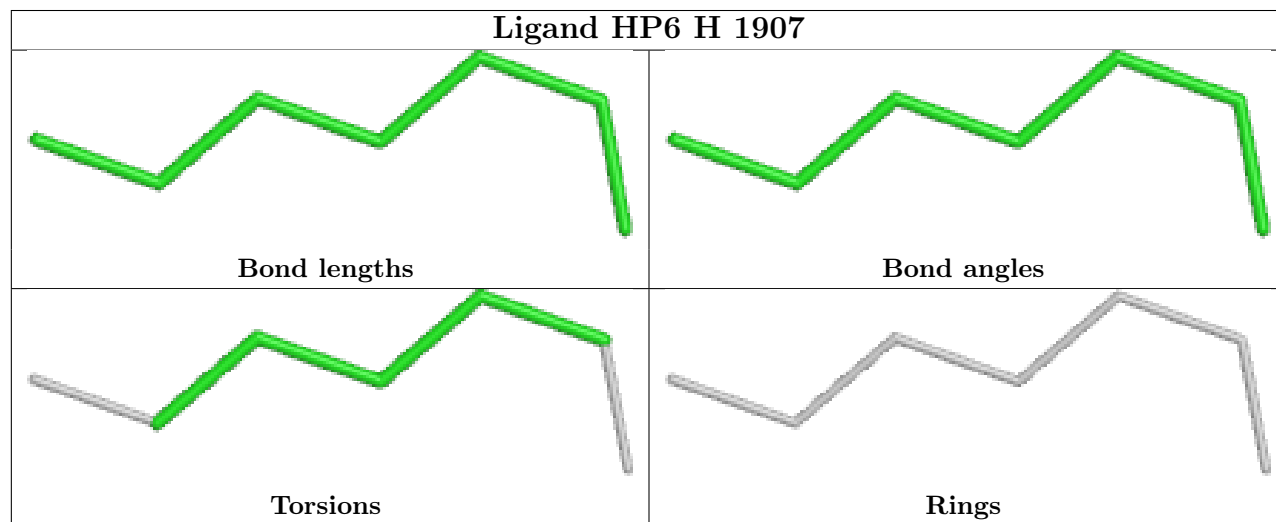
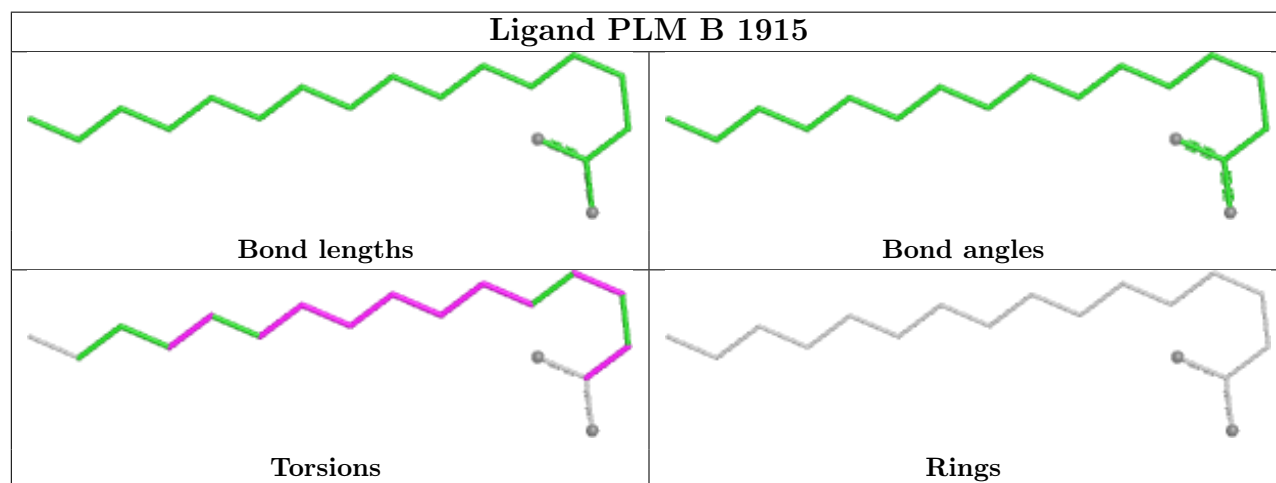
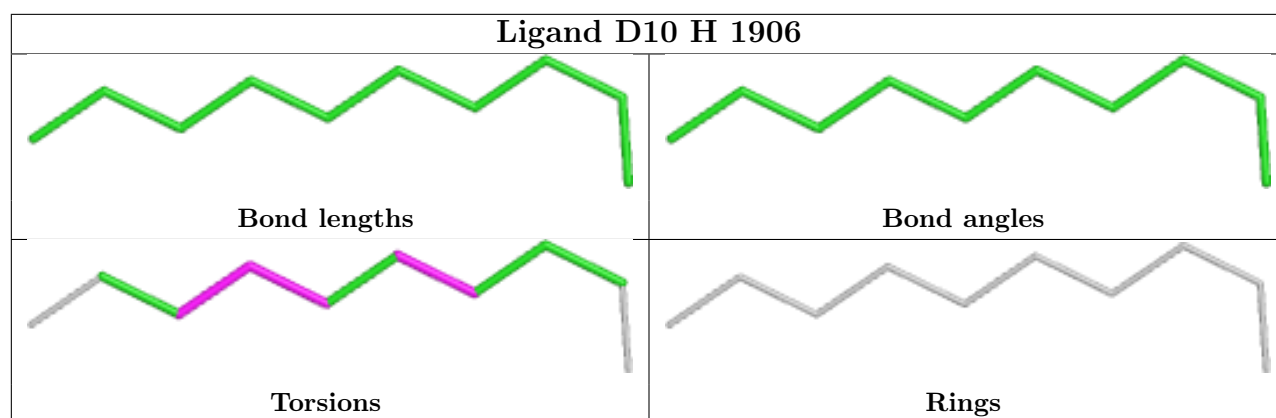


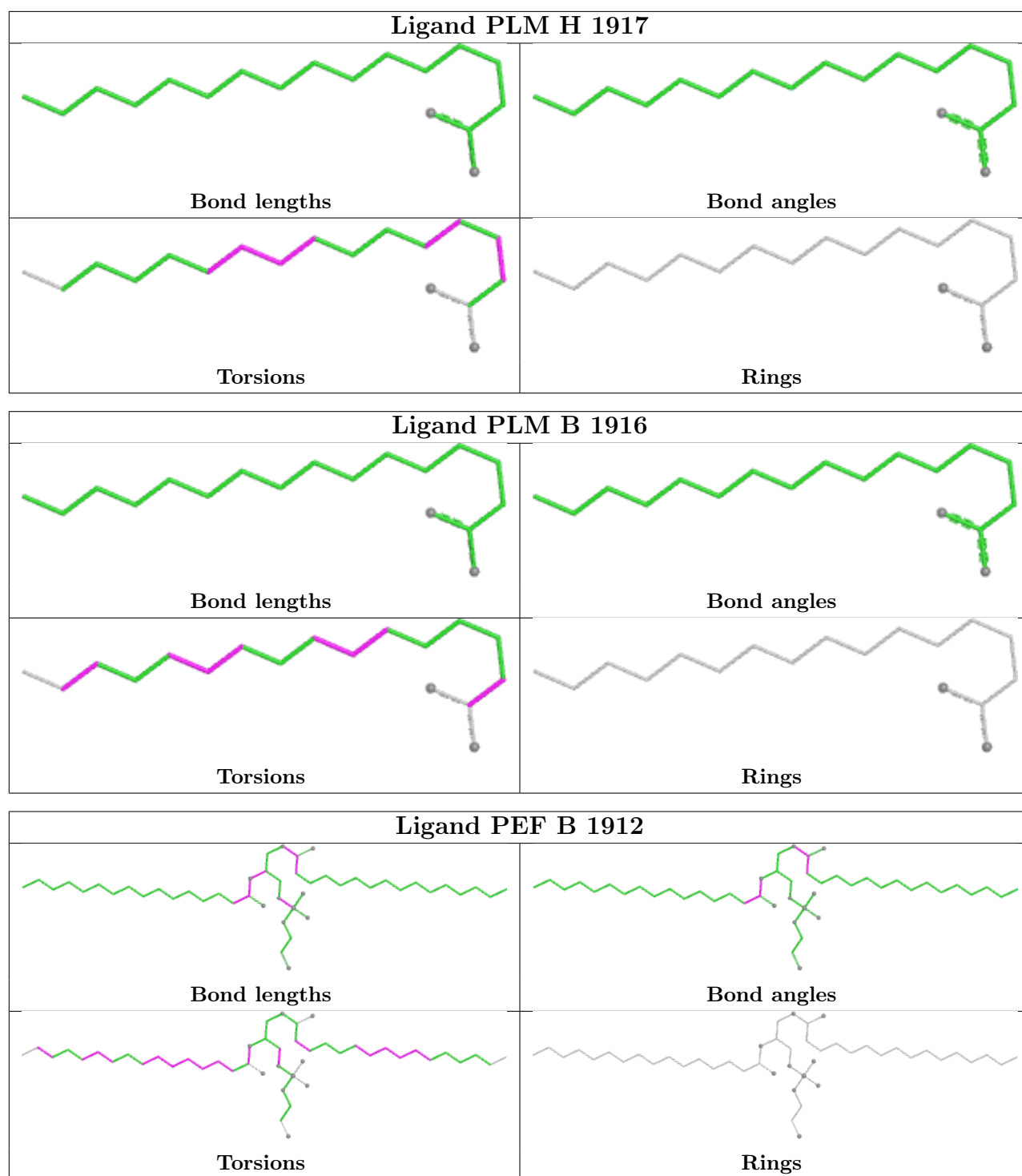


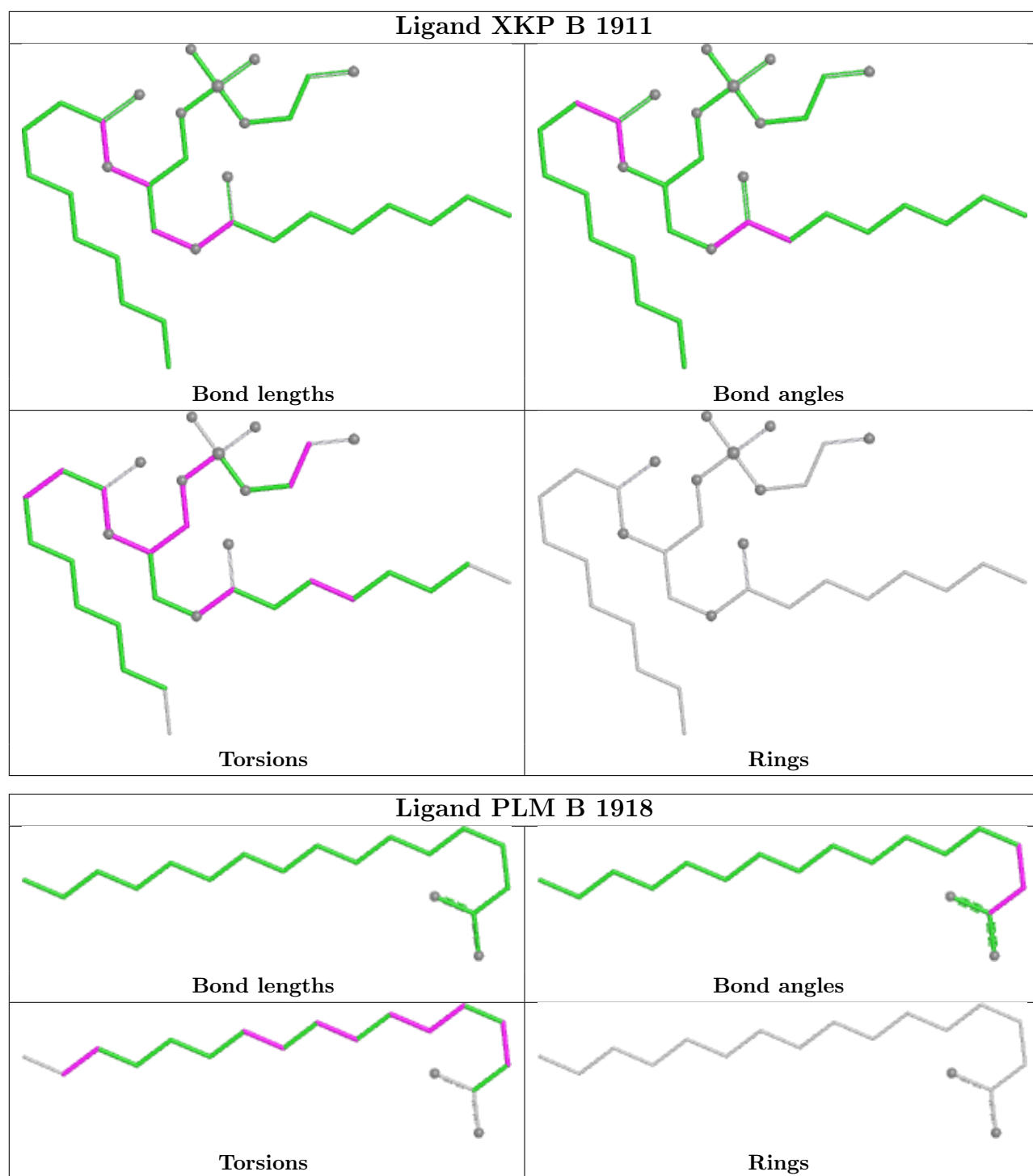


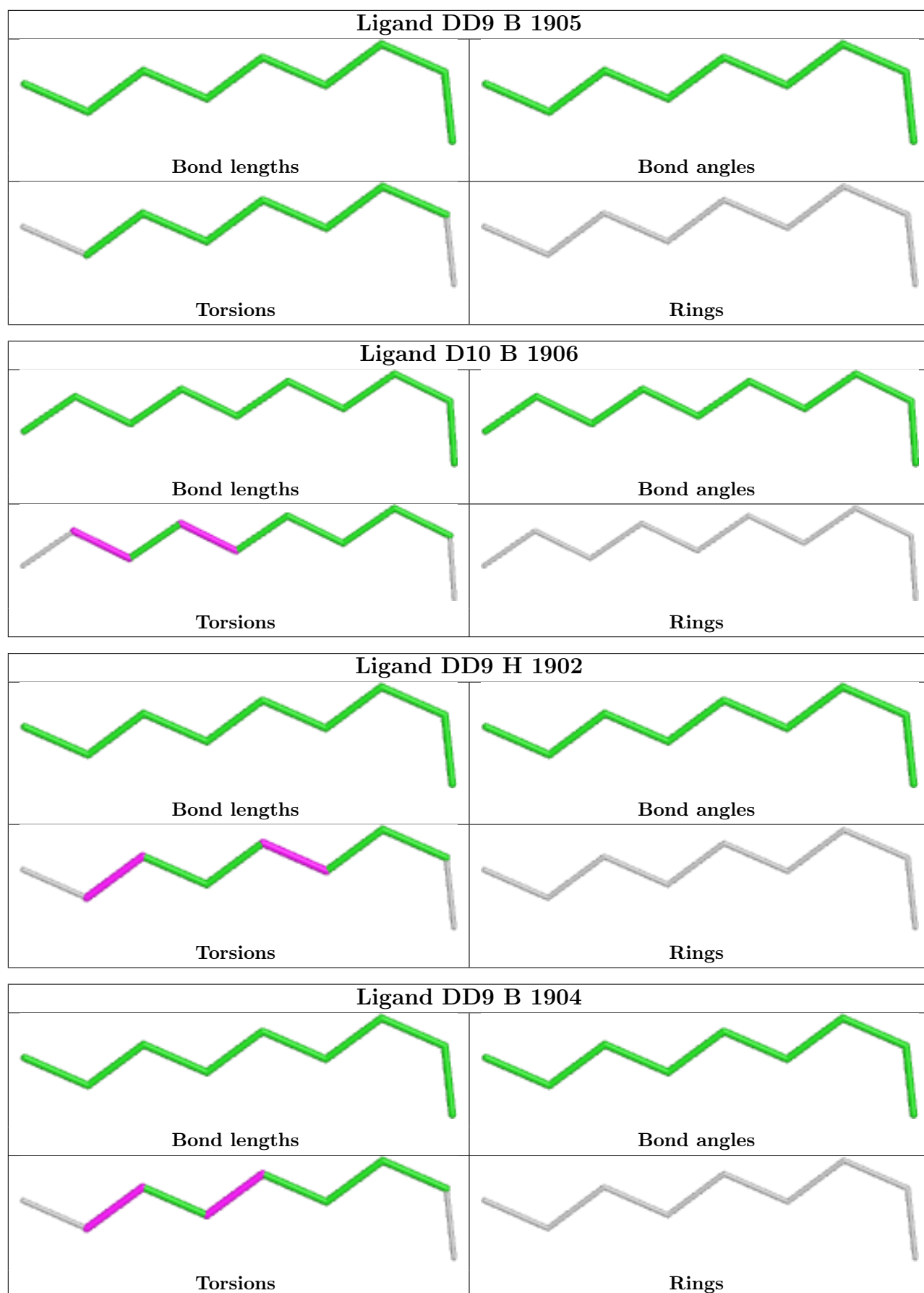


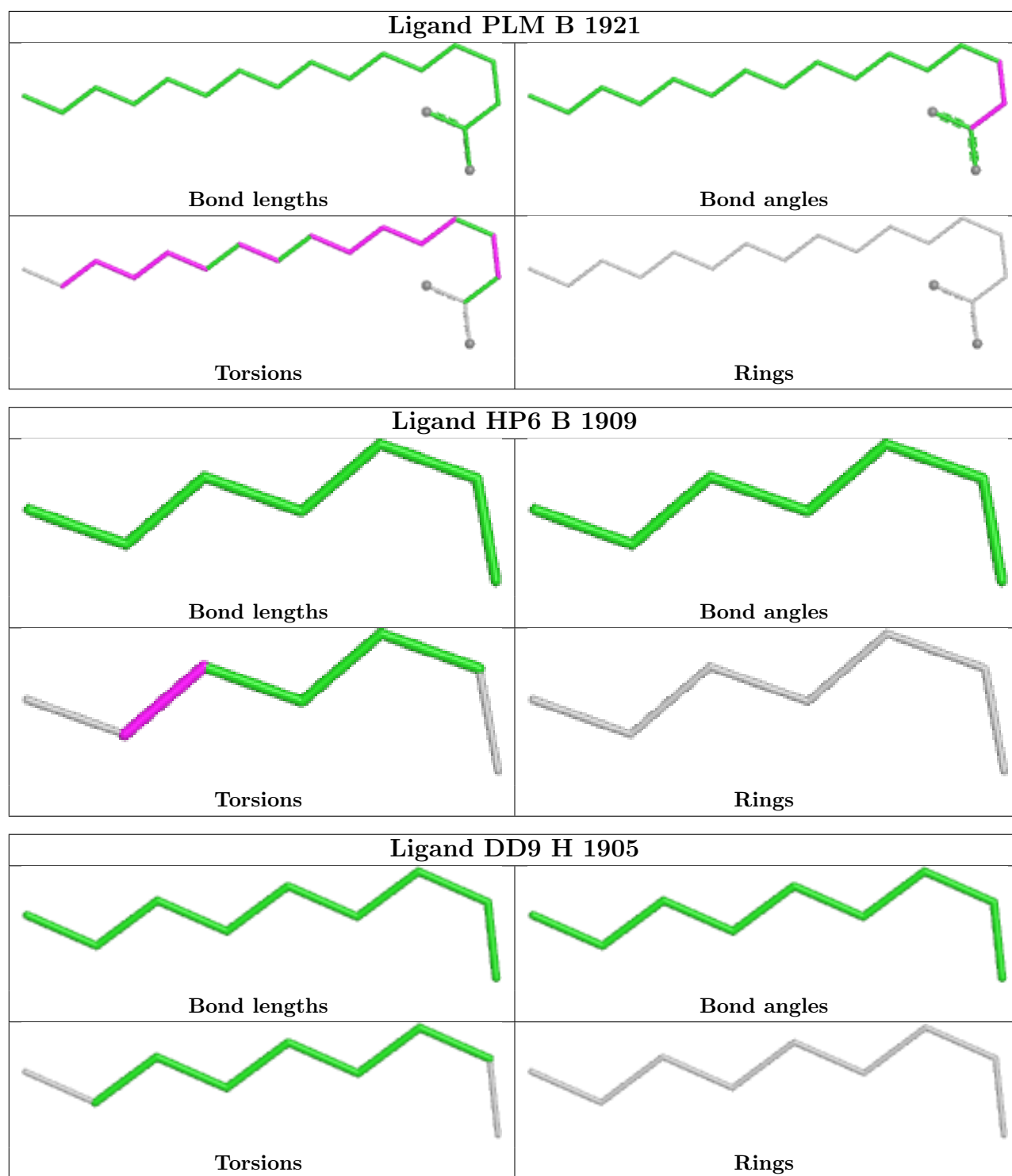


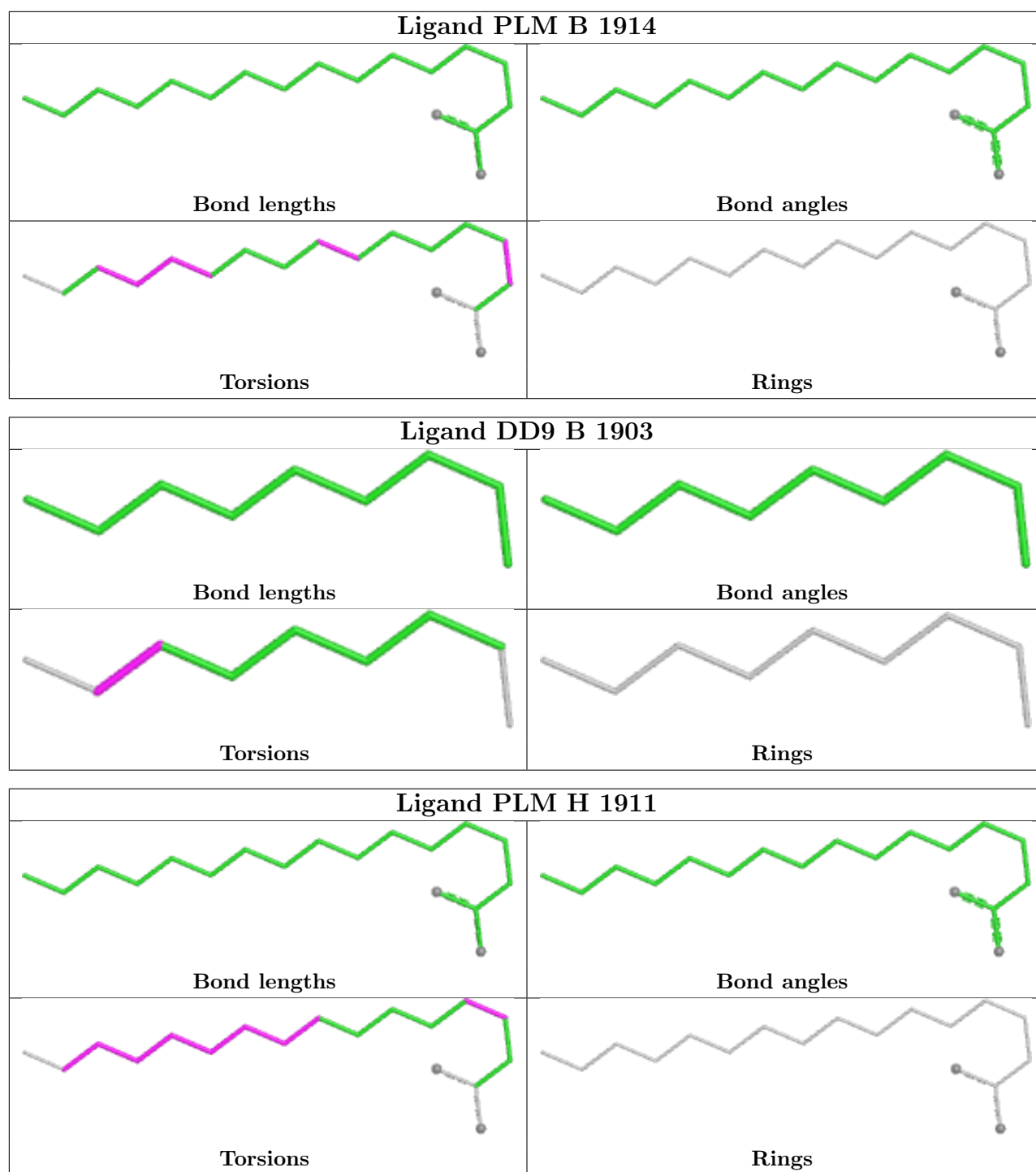


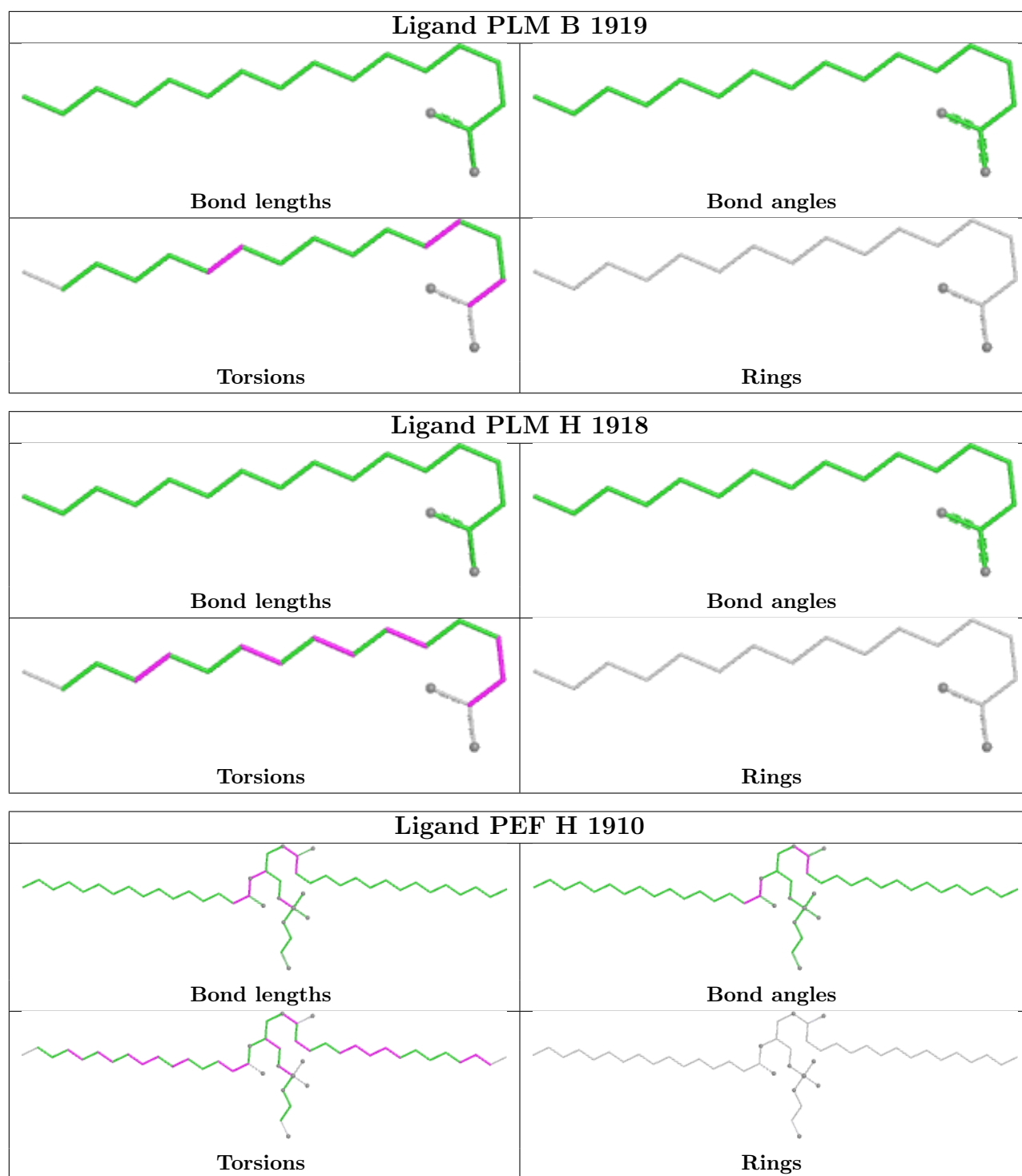


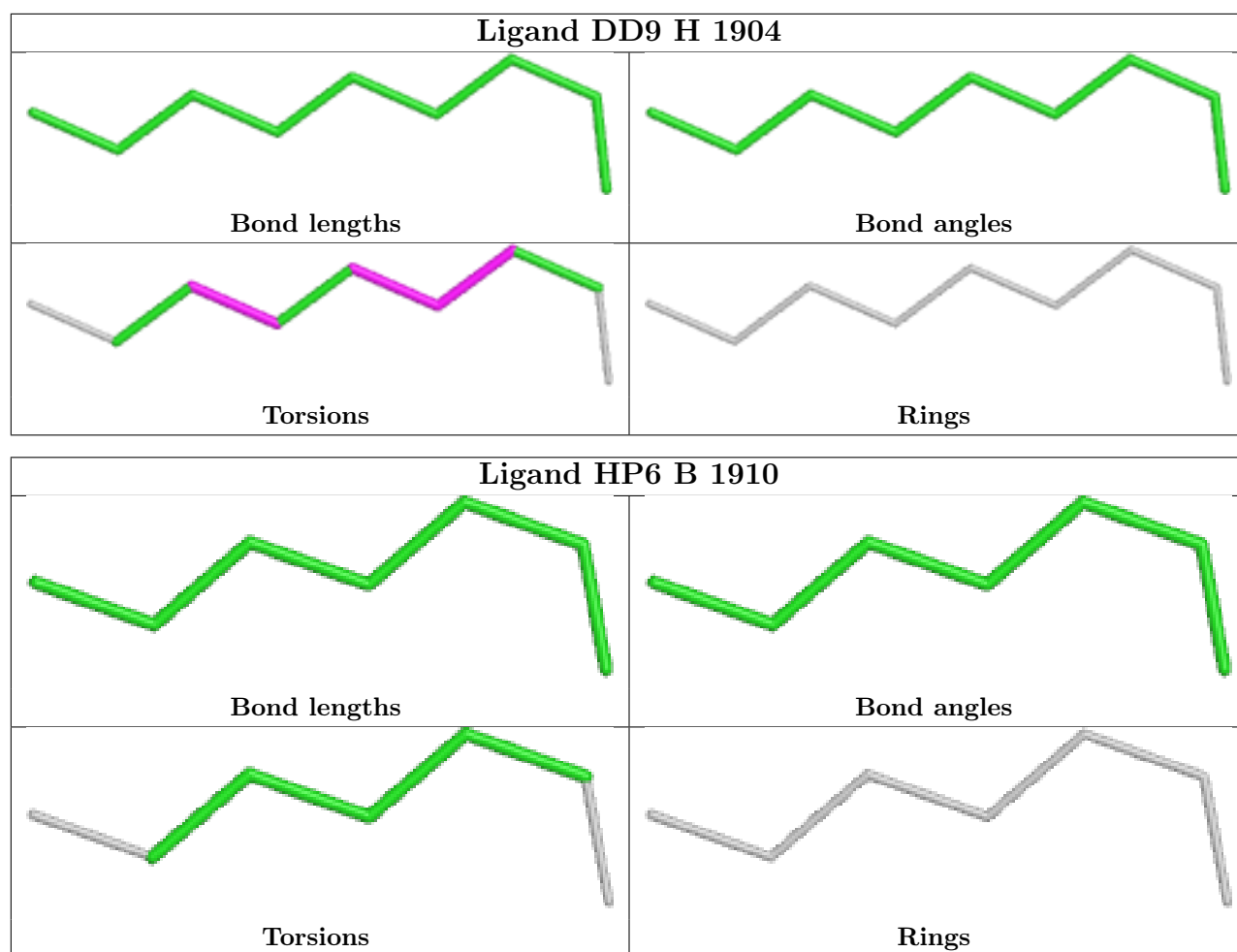












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

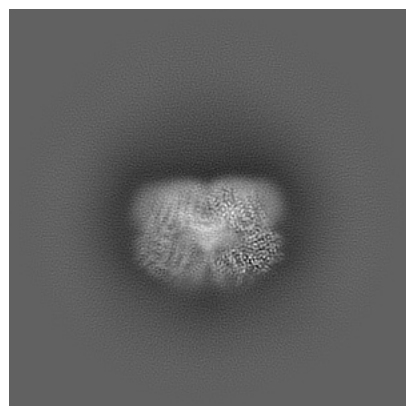
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64502. These allow visual inspection of the internal detail of the map and identification of artifacts.

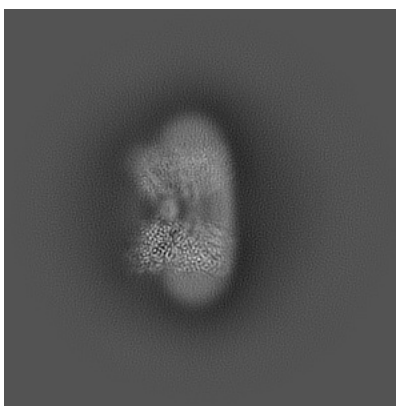
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

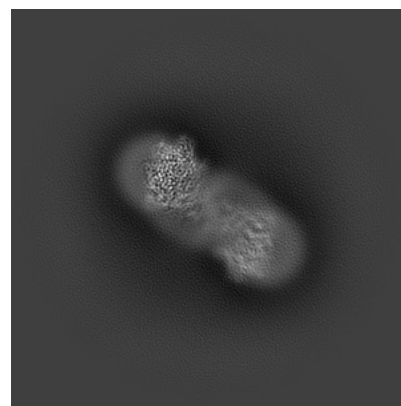
6.1.1 Primary map



X

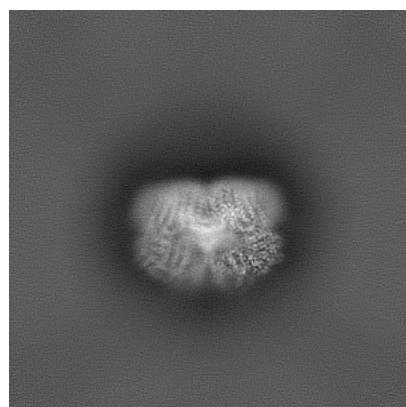


Y

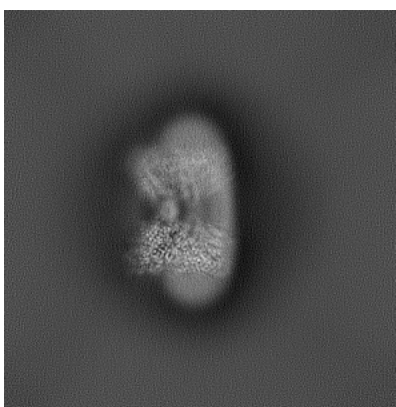


Z

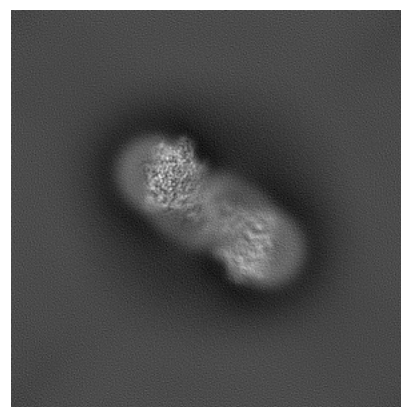
6.1.2 Raw map



X



Y

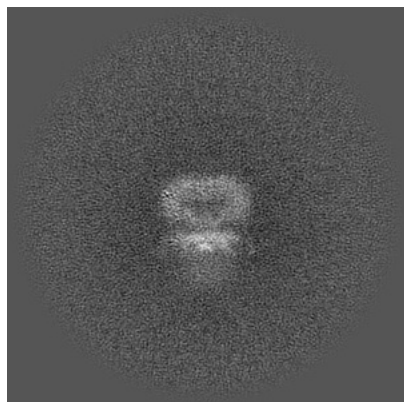


Z

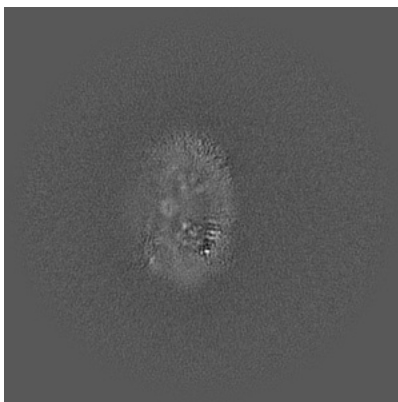
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

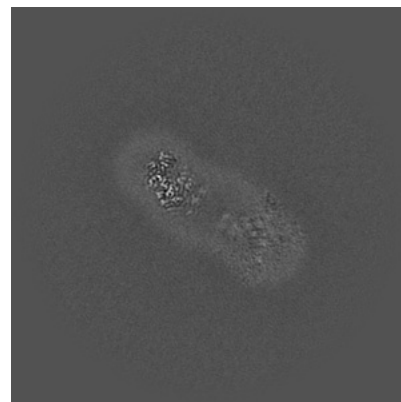
6.2.1 Primary map



X Index: 200

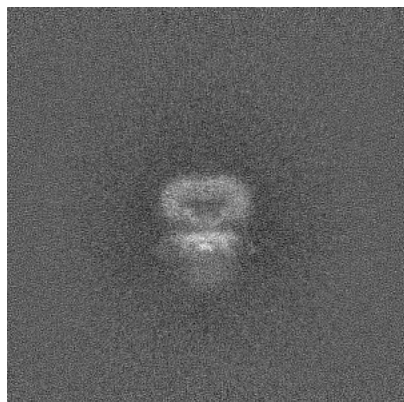


Y Index: 200

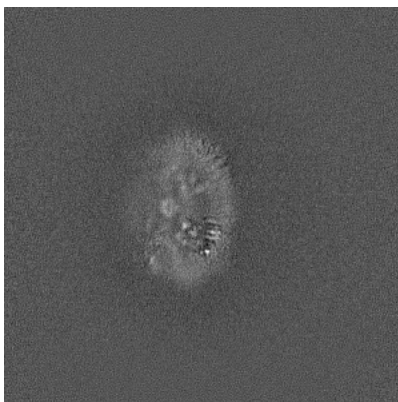


Z Index: 200

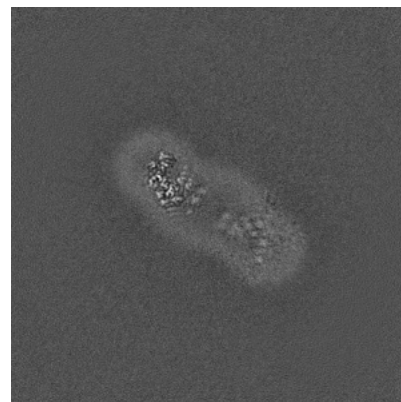
6.2.2 Raw map



X Index: 200



Y Index: 200

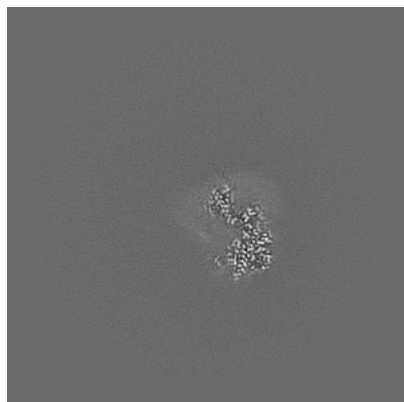


Z Index: 200

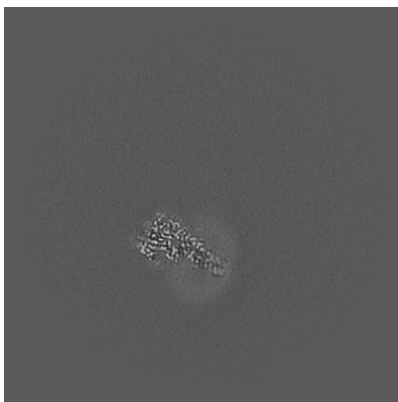
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

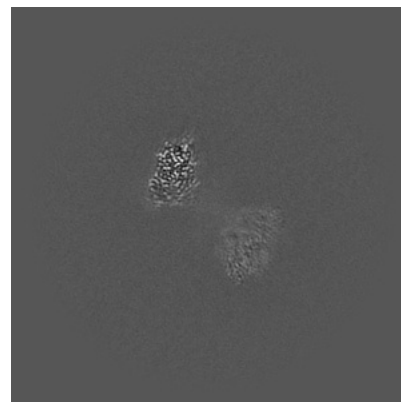
6.3.1 Primary map



X Index: 159

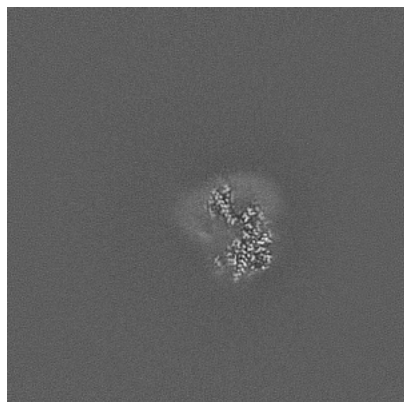


Y Index: 245

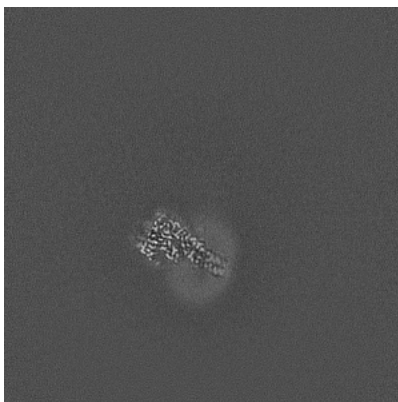


Z Index: 148

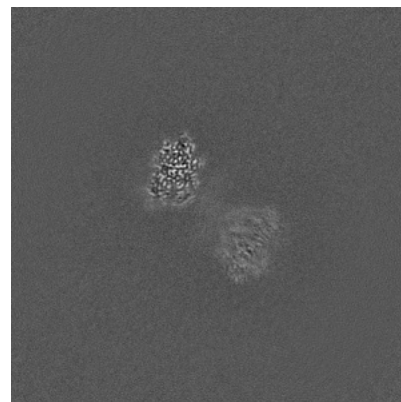
6.3.2 Raw map



X Index: 159



Y Index: 245

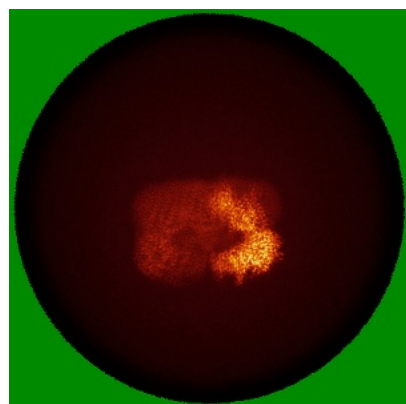


Z Index: 151

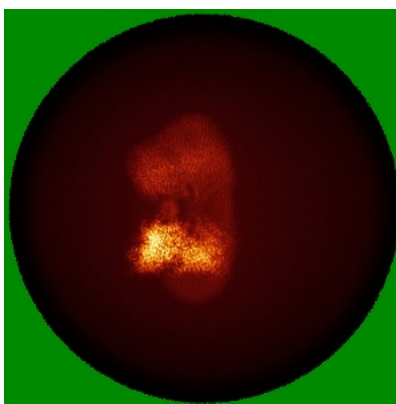
The images above show the largest variance slices of the map in three orthogonal directions.

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

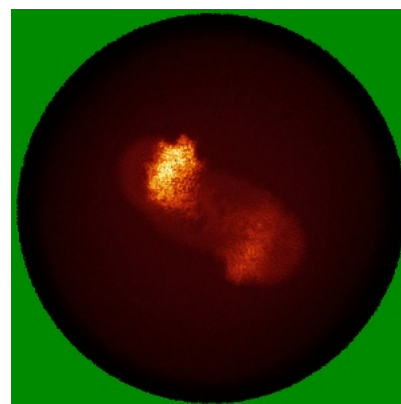
6.4.1 Primary map



X

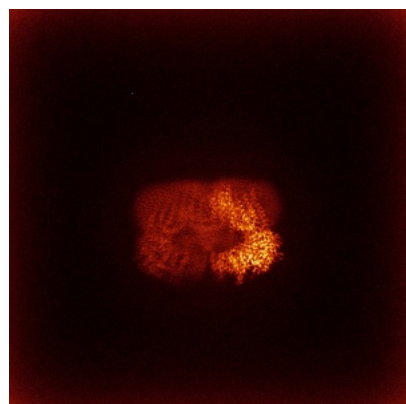


Y

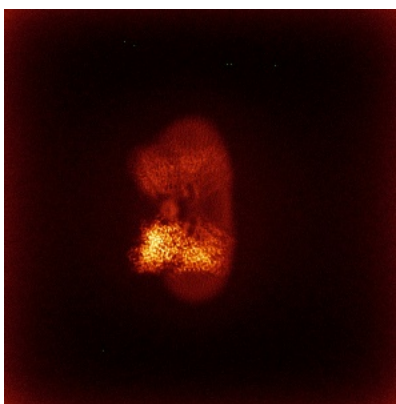


Z

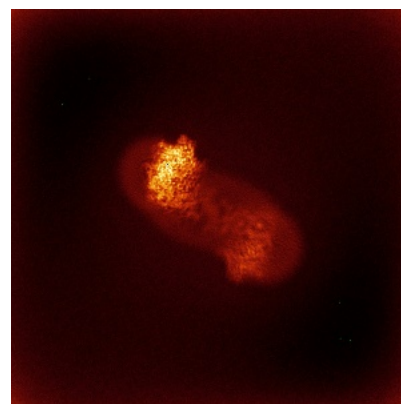
6.4.2 Raw map



X



Y

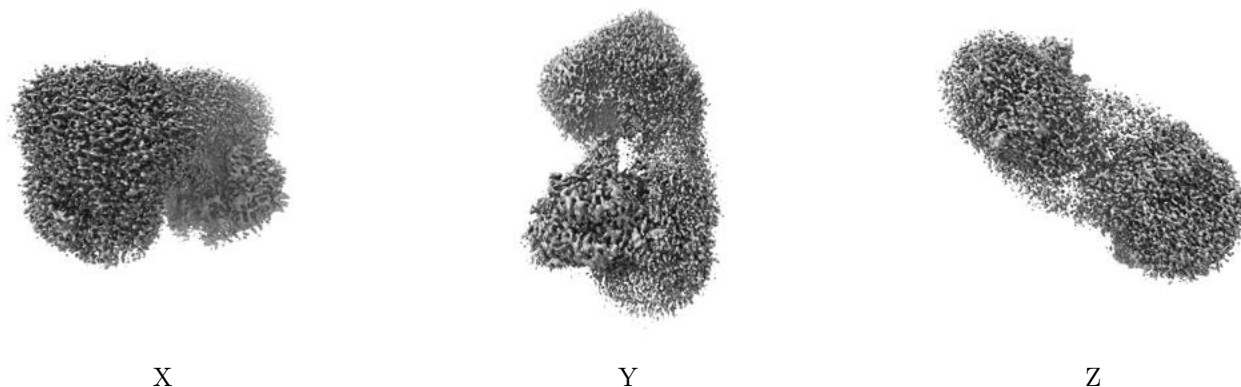


Z

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.

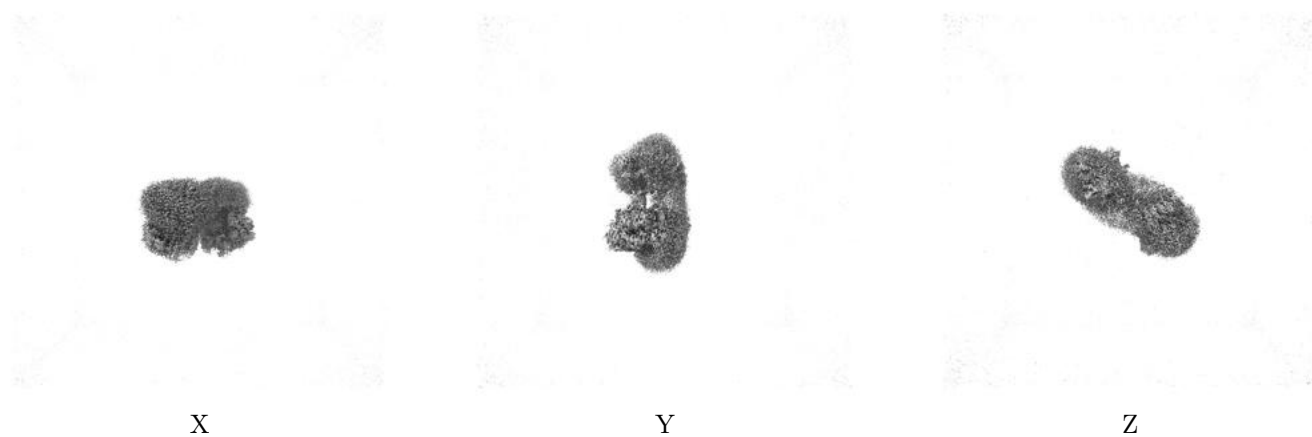
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

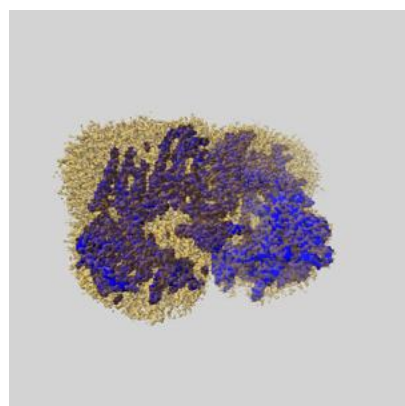
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

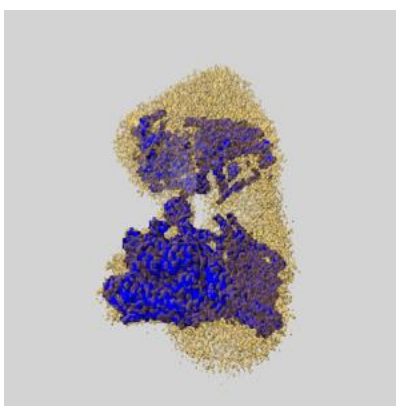
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

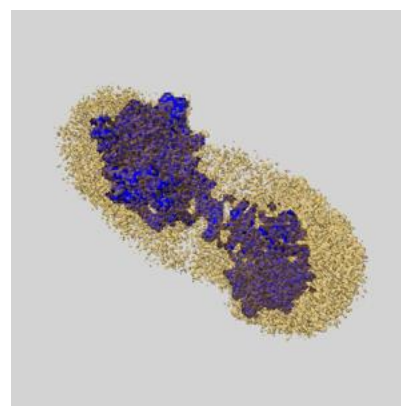
6.6.1 emd_64502_msk_1.map [i](#)



X



Y

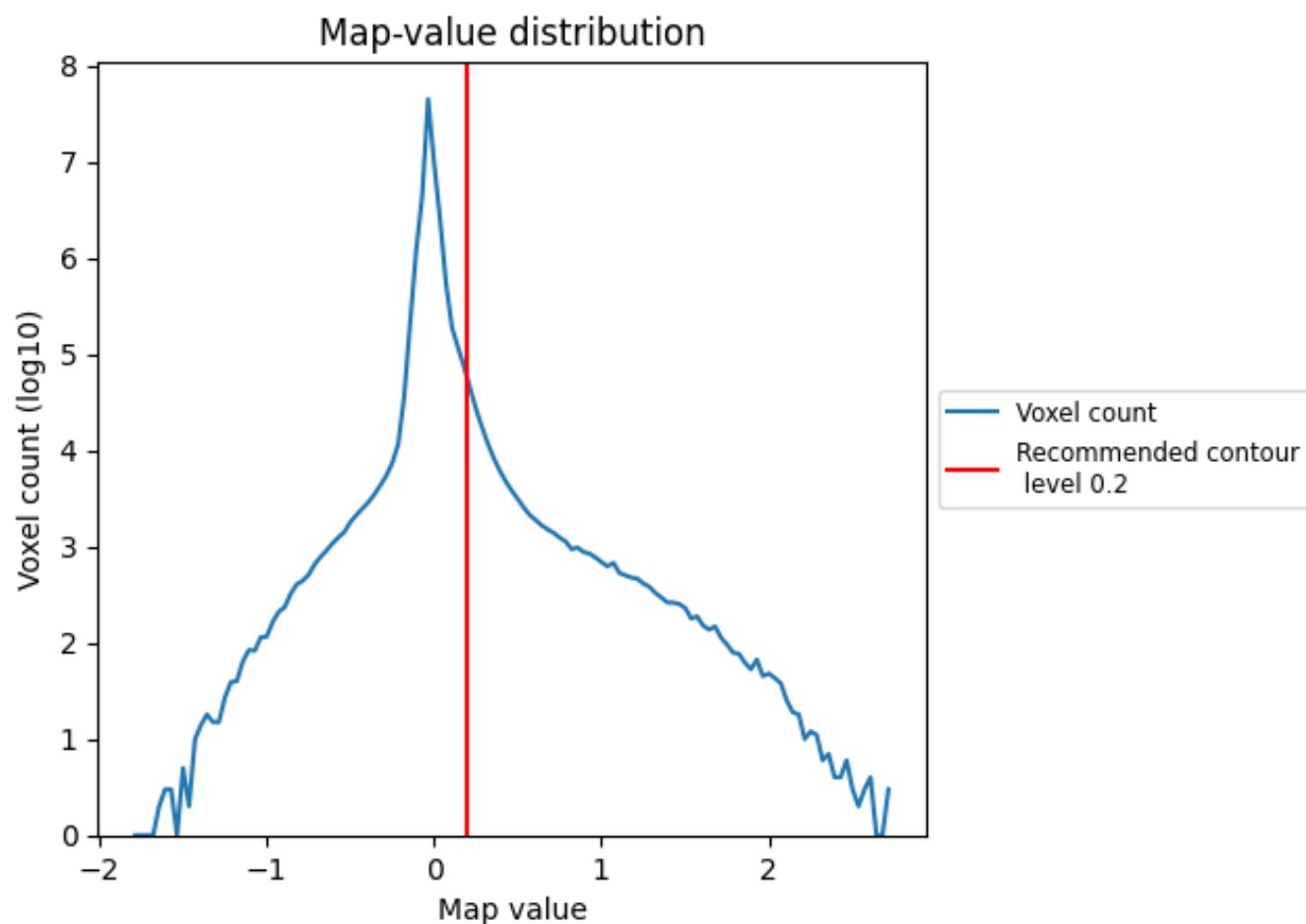


Z

7 Map analysis [i](#)

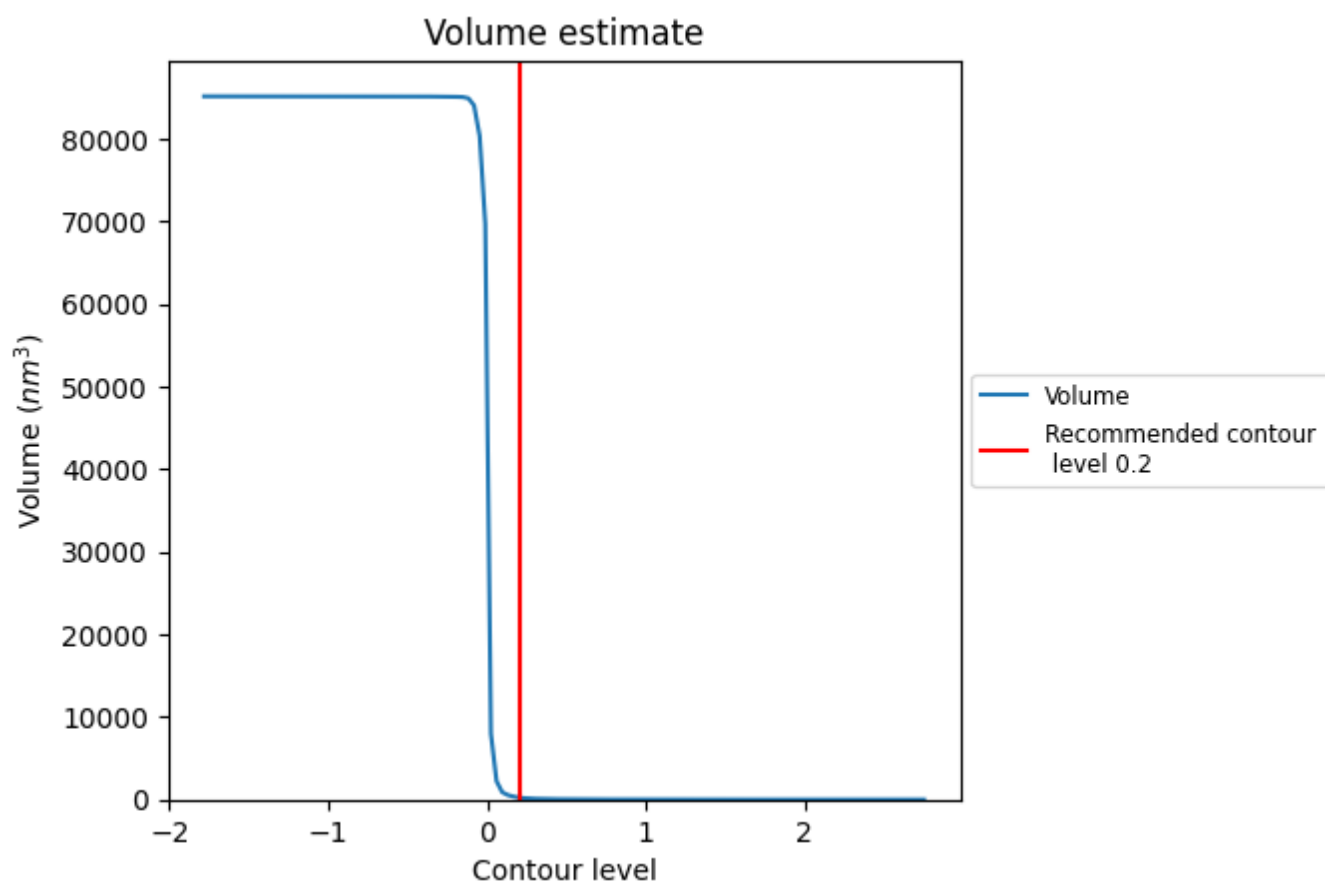
This section contains the results of statistical analysis of the map.

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.

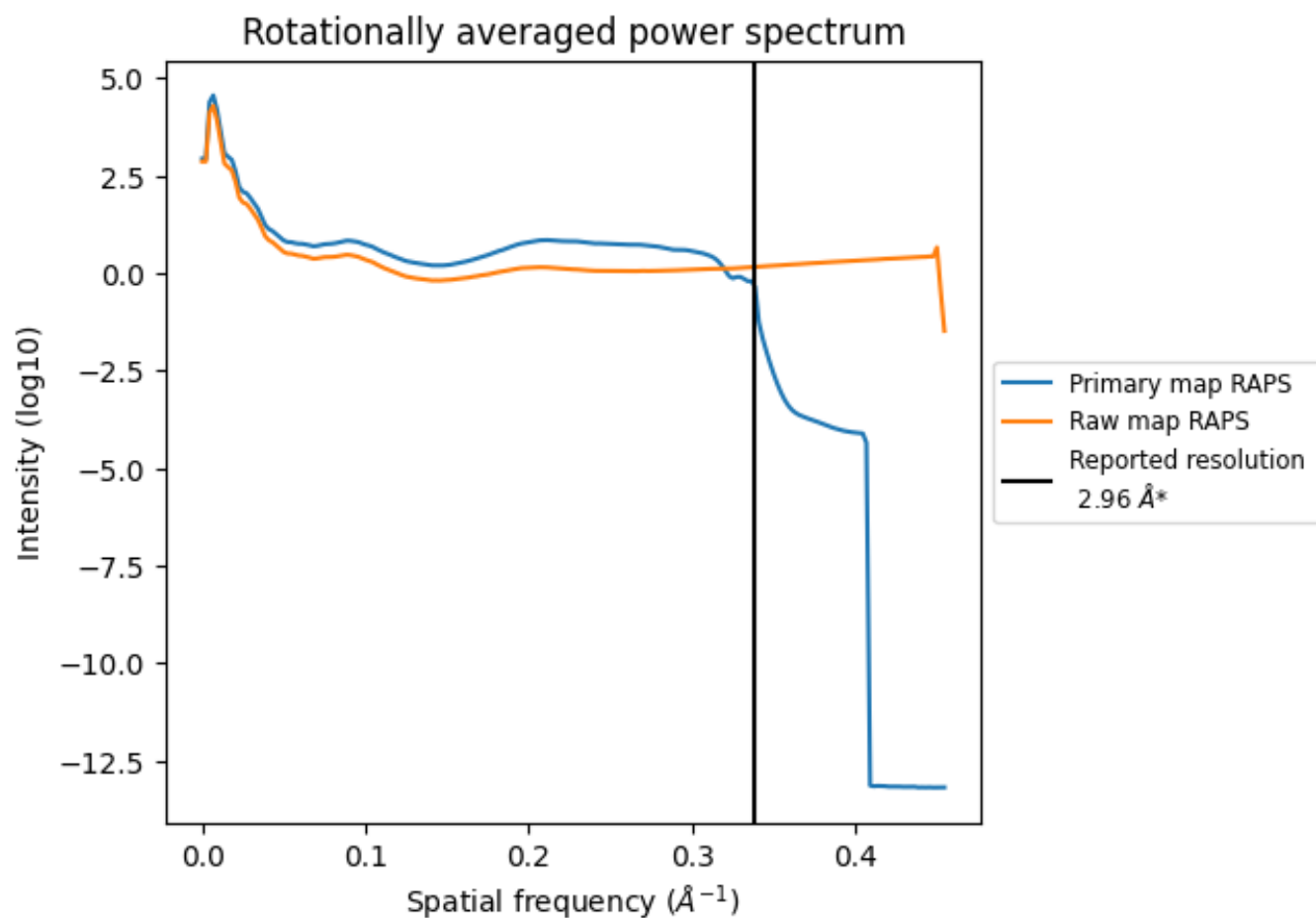
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm³; this corresponds to an approximate mass of 220 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 ⓘ

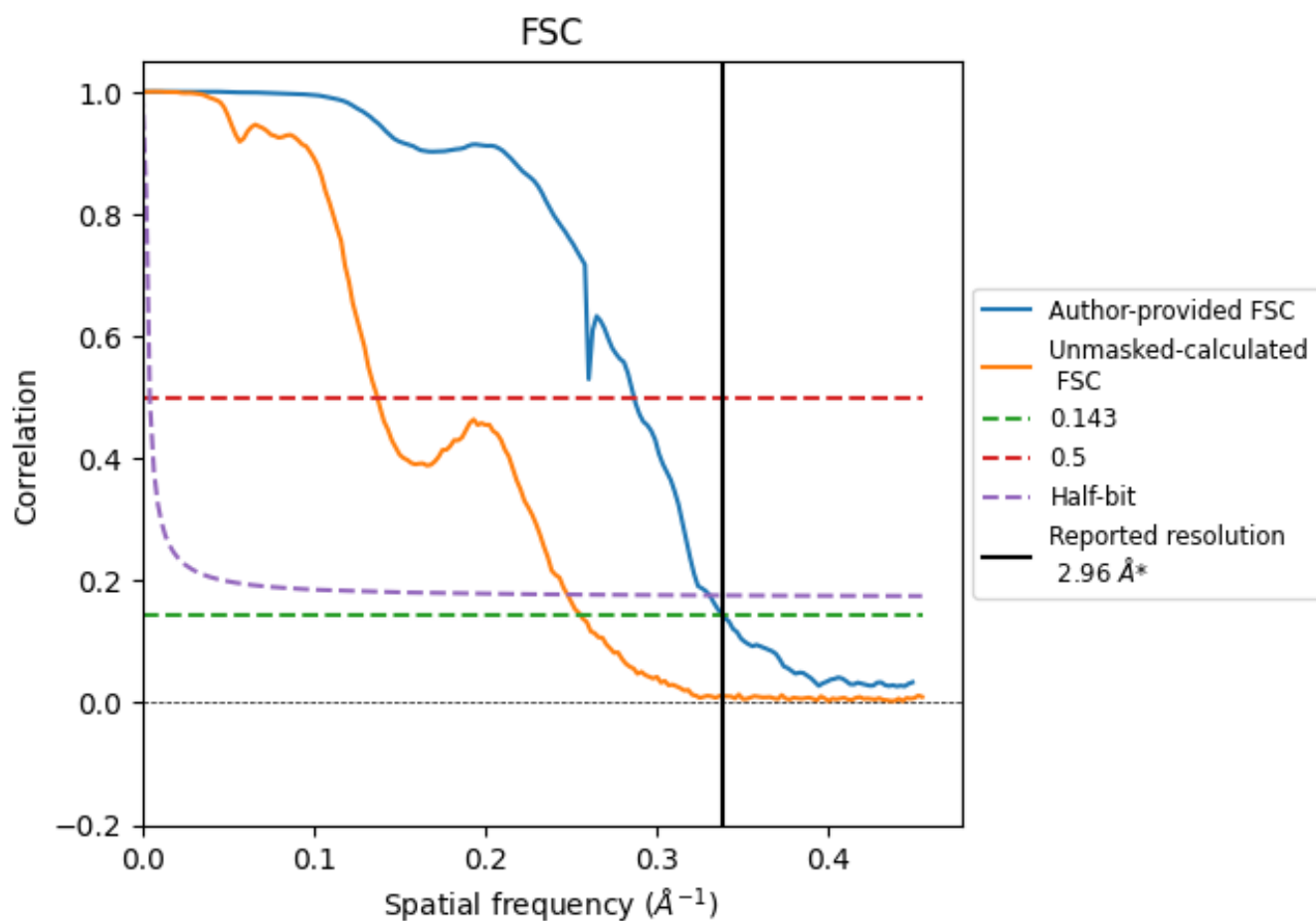


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

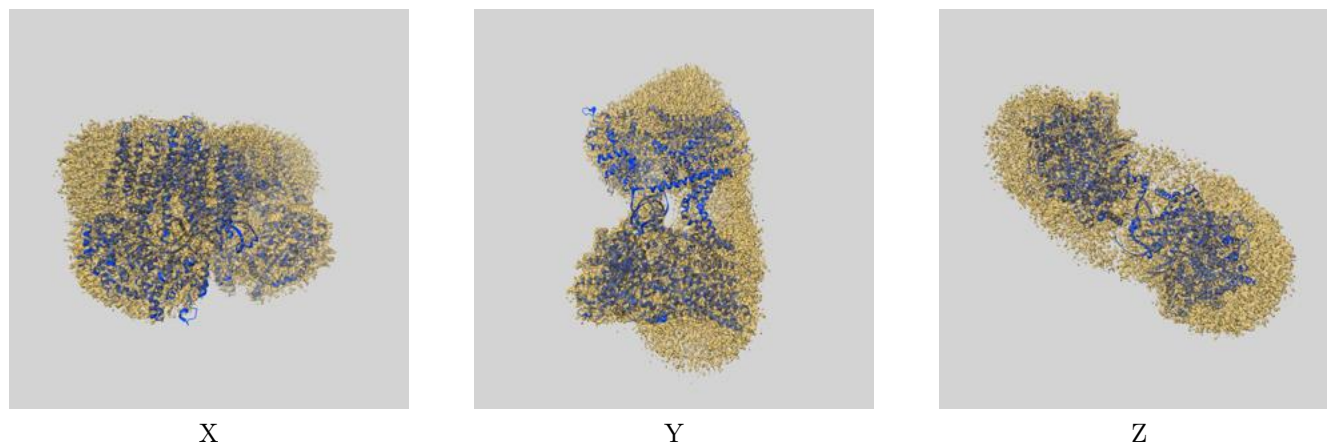
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.49	3.02
Unmasked-calculated*	3.91	7.30	4.04

*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 3.91 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

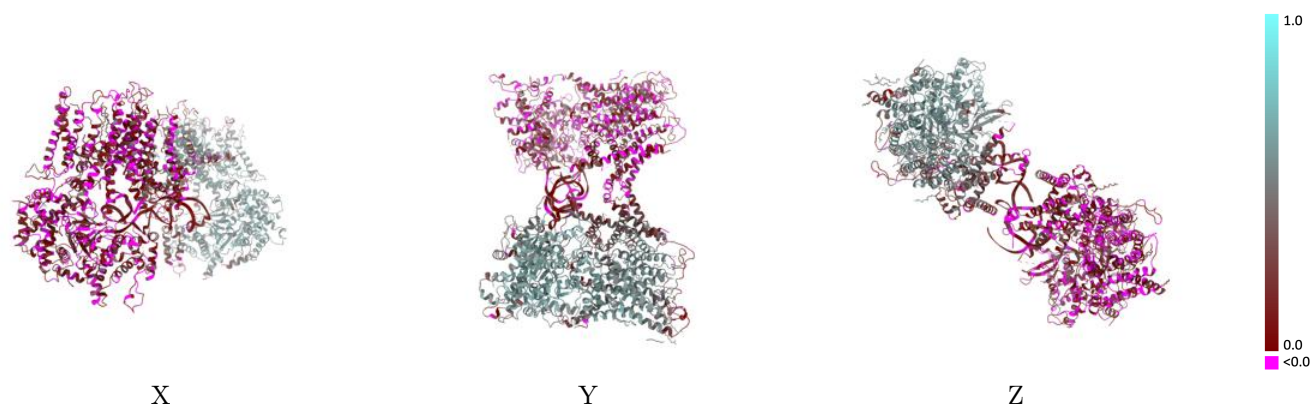
This section contains information regarding the fit between EMDB map EMD-64502 and PDB model 9UTW. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



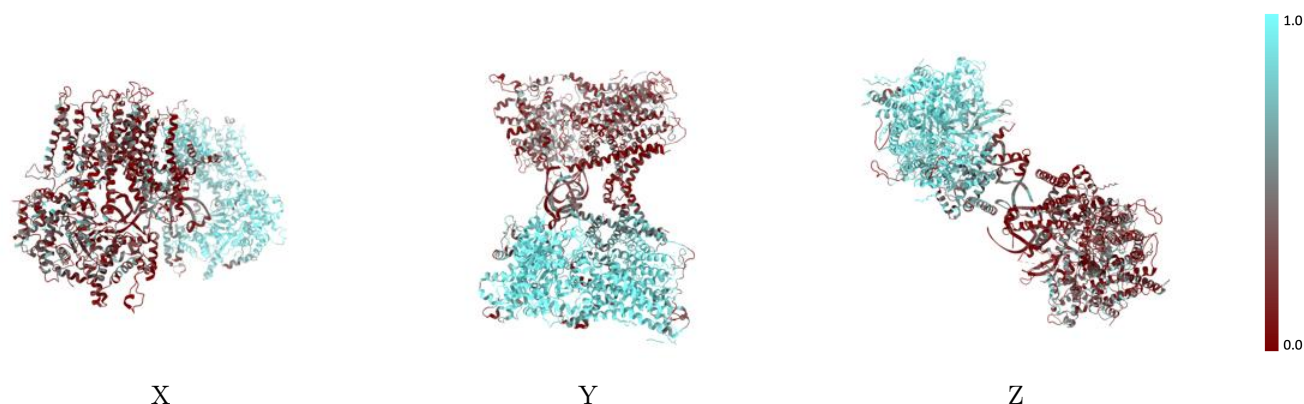
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



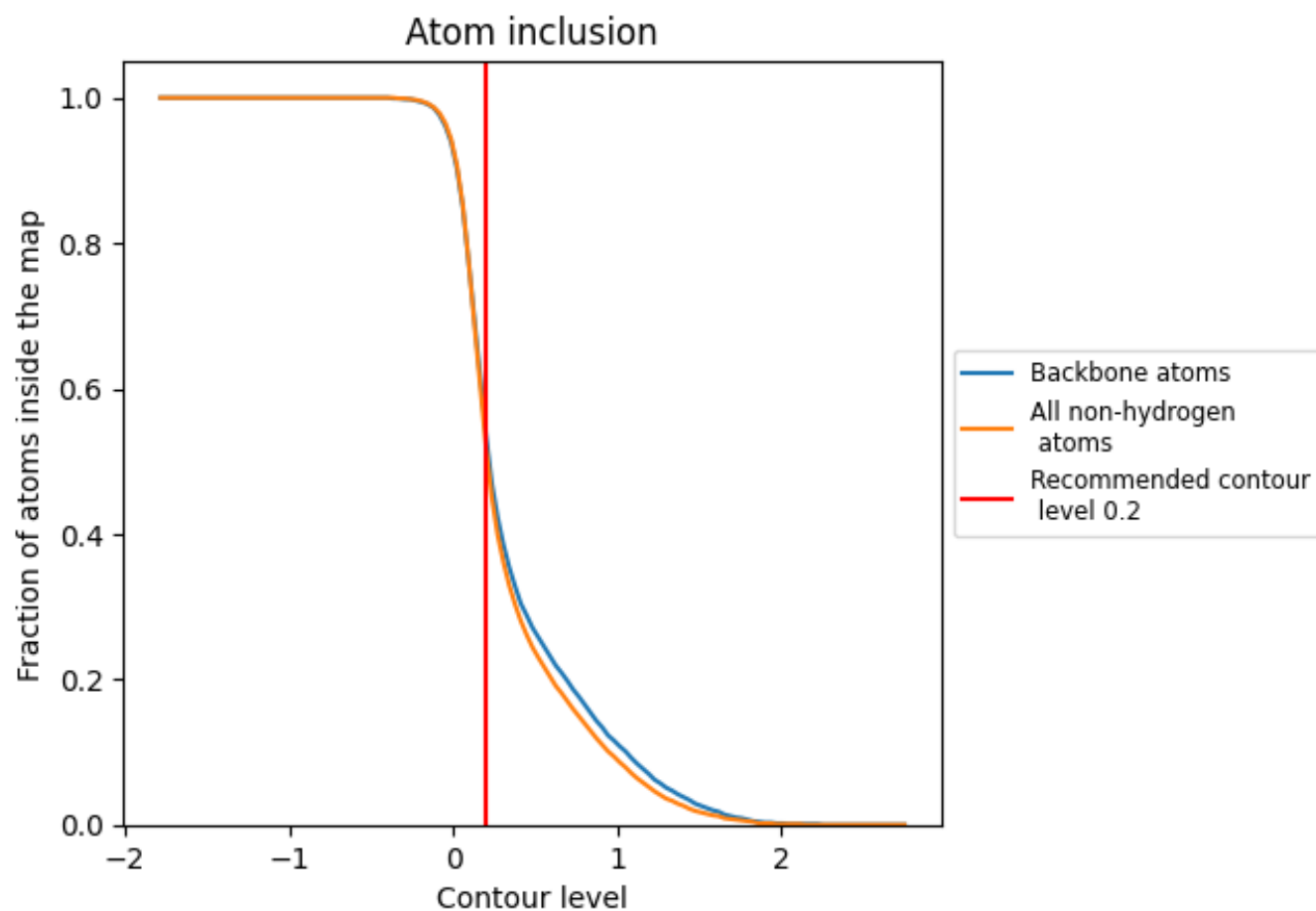
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 52% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.2730
A	0.2460	0.0720
B	0.8090	0.4790
C	0.5510	0.4170
D	0.1300	0.0170
G	0.2470	0.1020
H	0.2700	0.0900
J	0.2650	0.1750

1.0

0.0

<0.0