



## wwPDB EM Validation Summary Report ⓘ

Nov 12, 2025 – 01:33 PM EST

PDB ID : 9NMP / pdb\_00009nmp  
EMDB ID : EMD-49536  
Title : Structure of mouse RyR1 with simvastatin (Ca<sup>2+</sup>/CFF/ATP dataset; open pore)  
Authors : Weninger, G.; Marks, A.R.  
Deposited on : 2025-03-04  
Resolution : 3.09 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](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.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

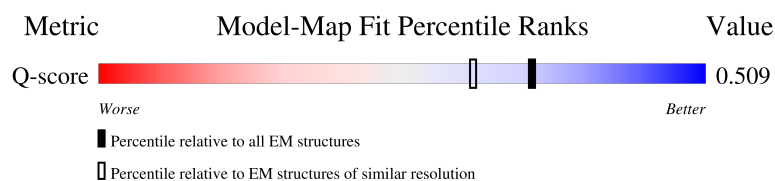
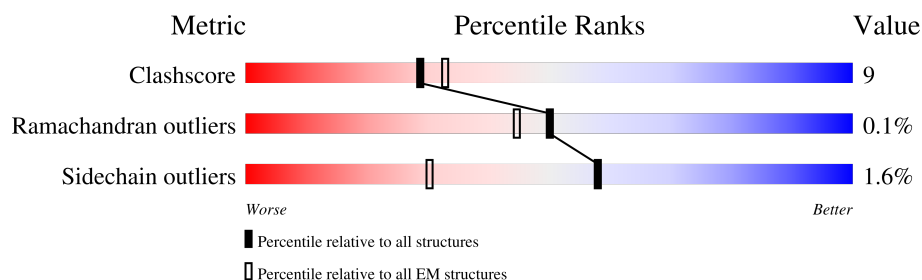
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.09 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14003 ( 2.59 - 3.59 )

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	E	108	
1	F	108	
1	G	108	
1	H	108	

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Mol	Chain	Length	Quality of chain
2	A	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	B	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	C	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	D	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 143492 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 Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	F	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	G	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	H	107	Total	C	N	O	S	0	0
			830	526	146	155	3		

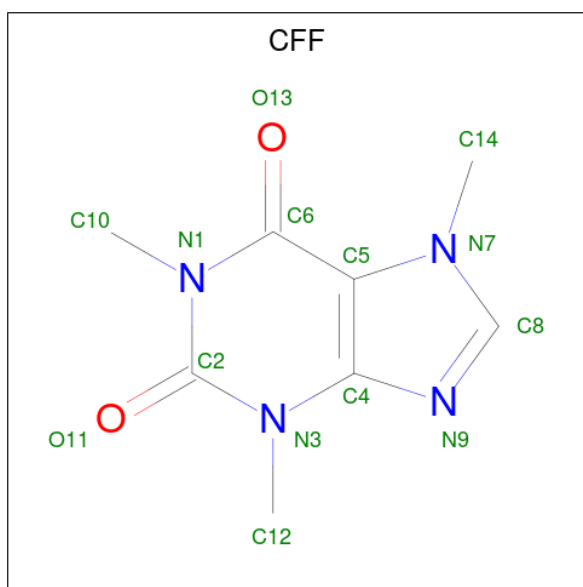
- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

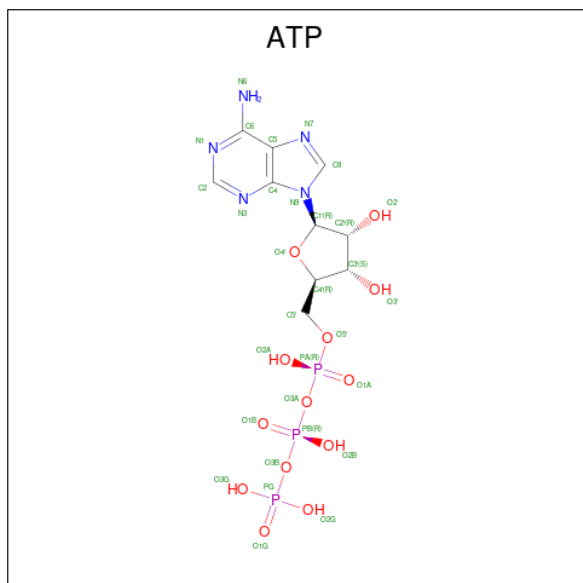
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

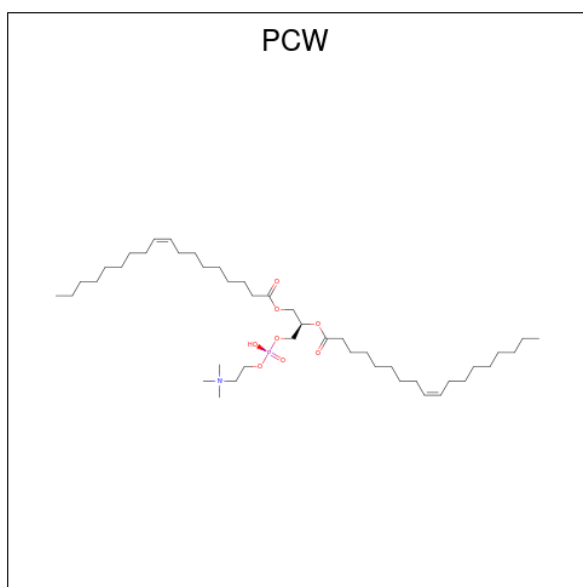


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

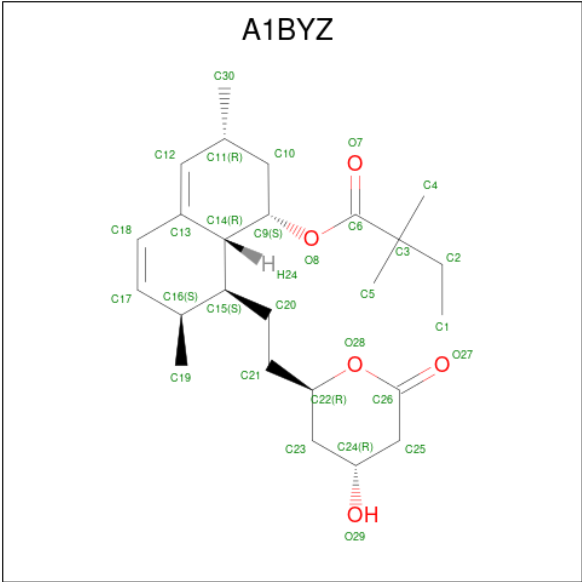
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is Simvastatin (CCD ID: A1BYZ) (formula:  $C_{25}H_{38}O_5$ ) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	

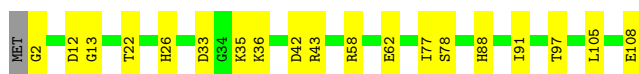


### 3 Residue-property plots [i](#)


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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 




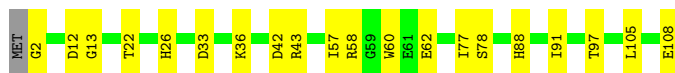
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 



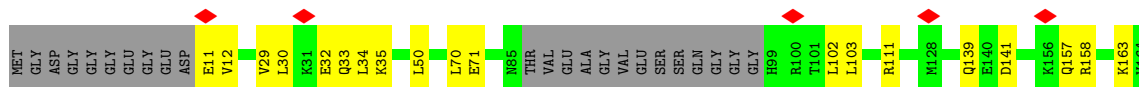
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 



- Molecule 2: Ryanodine receptor 1

Chain D: 



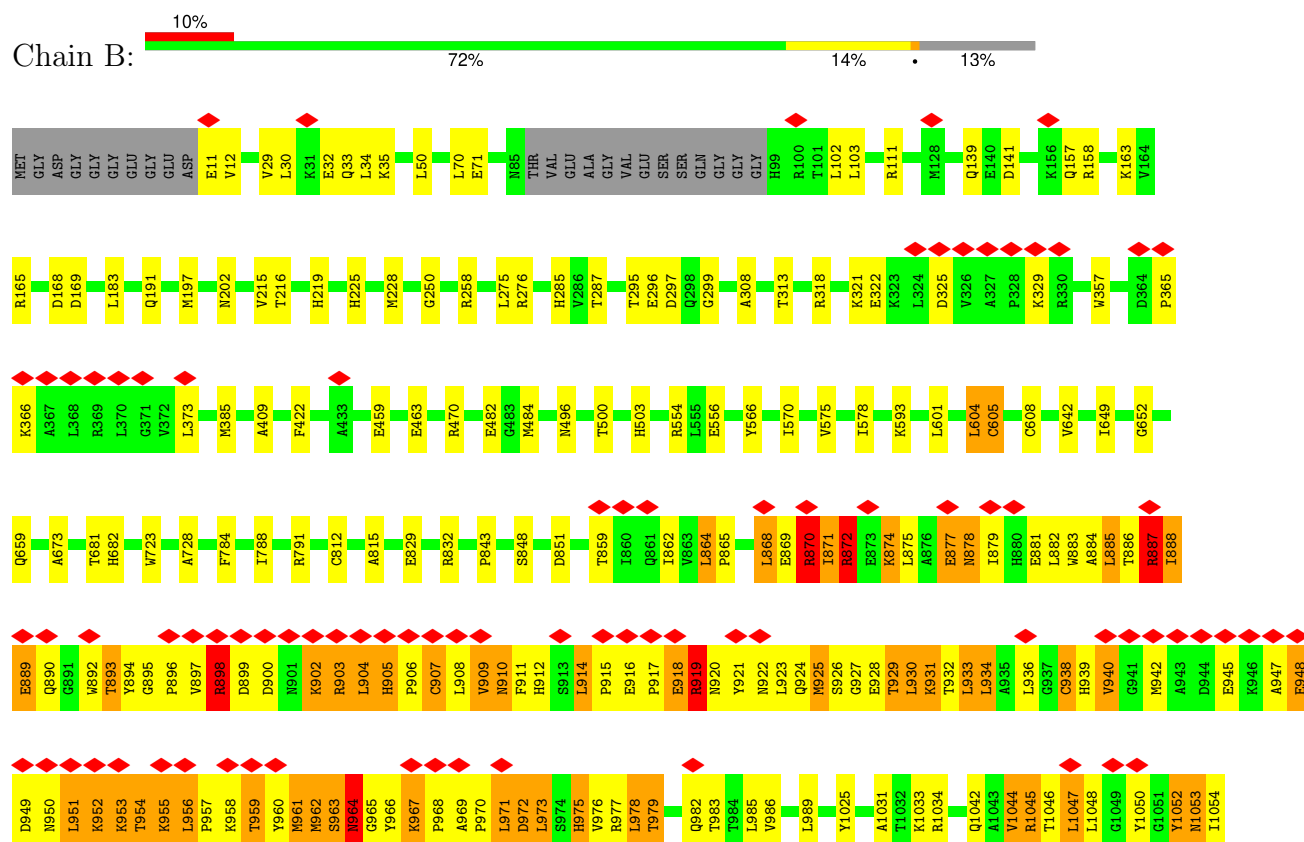








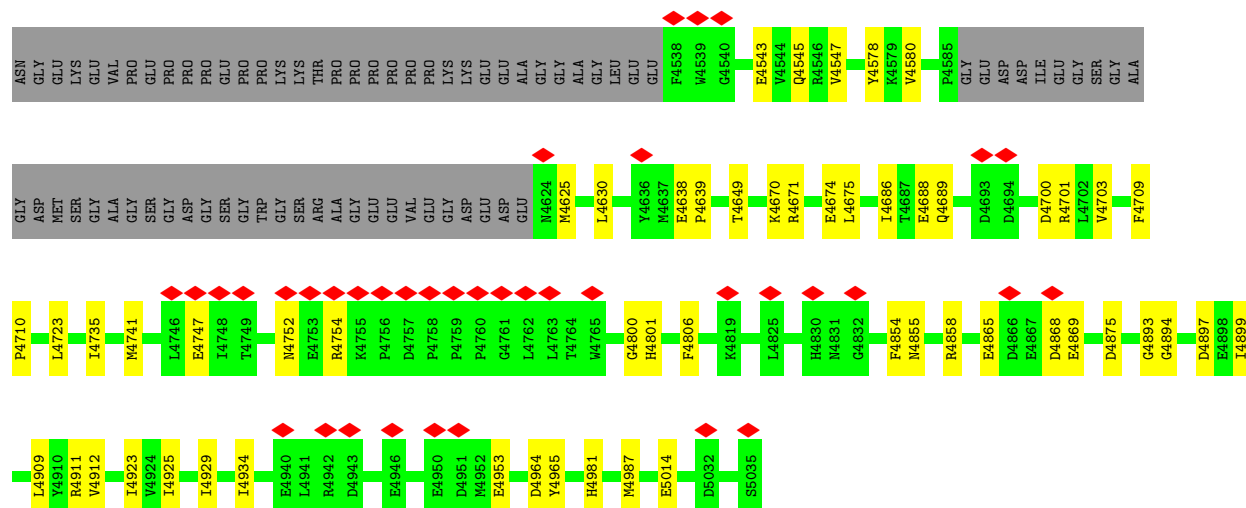




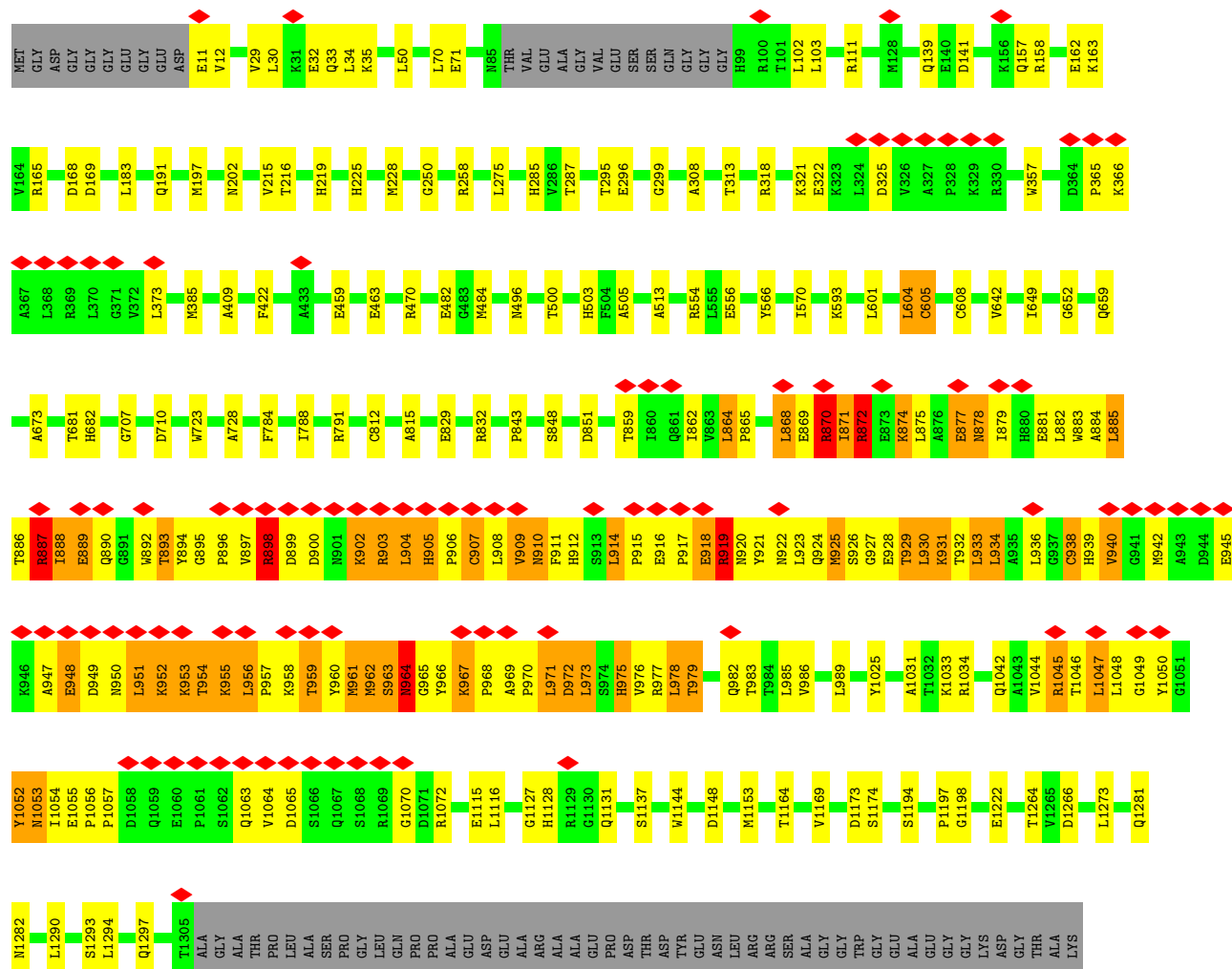
D2862	D2863	S2864	V2865	V2866	T2867	L2868	S2869	R2870	E2871	L2872	Q2873	A2874	M2875	A2876	E2877	Q2878	L2879	A2880	E2881	N2882	T2883	H2884	N2885	T2886	Q2887	Q2888	R2889	K2890	K2891	K2892	Q2893	E2894	L2895	E2896	A2897	K2898	K2899	G2900	G2901	S2902	H2903	P2904	L2905	L2906	V2907	P2908	Y2909	D2910	T2911	L2912	T2913	A2914	E2916	K2915	K2917	A2918	R2919	D2920	R2921	
D2802	K2803	E2804	I2805	Y2806	R2807	L2808	P2809	I2810	K2811	E2812	S2813	L2814	K2815	A2816	M2817	L2818	A2819	W2820	E2821	W2822	T2823	V2824	E2825	K2826	K2827	A2828	E2829	G2830	E2831	GLY	GLY	LYS	THR	GLY	LYS	LYS	LYS	THR	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	THR	TYR	ASP	PRO	ARG	GLY	Y2856	N2857	P2858	Q2859	P2860	P2861
E2742	T2743	L2744	N2745	V2746	L2747	I2748	P2749	E2750	K2751	L2752	D2753	S2754	F2755	I2756	N2757	K2758	F2759	A2760	E2761	Y2762	T2763	H2764	E2765	K2766	W2767	A2768	F2769	D2770	K2771	I2772	Q2773	N2774	K2775	W2776	S2777	Y2778	G2779	E2780	N2781	I2782	D2783	E2784	E2785	L2786	K2787	T2788	H2789	P2790	M2791	L2792	R2793	P2794	Y2795	K2796	T2797	F2798	E2800	K2801		
L2604	C2607	L2611	M2619	L2623	L2624	L2627	V2628	L2634	N2635	A2638	L2645	T2668	L2673	H2674	L2675	L2679	S2686	E2695	R2698	D2717	A2718	S2719	Y2720	S2721	K2723	T2724	E2725	K2726	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2735	F2736	D2737	P2738	R2739	P2740	V2741																		
R2370	G2371	G2372	E2382	E2383	R2386	D2394	V2398	ARG	ASP	ARG	ARG	GLY	HIS	PHE	GLY	GLY	P2411	P2412	E2413	E2414	N2415	R2416	V2417	H2418	L2419	Q2445	D2483	G2484	L2519	L2523	D2524	G2526	L2560	I2563	T2564	T2573	E2574	H2575	M2583	Q2600																				
K2228	M2229	C2233	C2234	R2235	F2236	L2237	C2238	F2239	F2240	C2241	R2245	Q2246	R2249	S2250	M2251	H2254	L2255	S2256	Y2257	L2258	L2259	E2260	N2261	S2262	G2263	T2264	L2266	Q2267	M2268	Q2269	S2270	S2271	T2272	D2282	D2283	N2284	V2285	E2286	K2298	L2314	Y2319	C2327	D2334	V2337	V2342															
LYS	VAL	LEU	VAL	LYS	LYS	THR	GLY	GLY	LYS	PRO	GLY	GLY	GLY	PRO	ALA	PRO	E2089	H2090	K2091	R2119	L2156	L2166	Q2174	L2178	M2179	M2186	M2187	M2199	M2204	M2209	E2210	V2211	M2212	V2213	V2215	L2216	G2217	Q2218	G2219	E2220	S2221	K2222	E2223	R2225	F2226	P2227														
GLY	GLY	ALA	ASP	ALA	ALA	GLY	GLY	LYS	GLY	GLY	L1923	L1927	F1985	T1986	M1987	S1988	A1989	A1990	E1991	R1995	T1996	R1997	E2005	Q2006	I2007	R2029	V2033	L2047	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLY	GLY	SER	THR	LEU	GLY	SER	LEU	MET	SER	LEU	GLY													
ASP	VAL	VAL	PRO	ALA	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
LYS	GLY	THR	PRO	GLY	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661	L1670	S1673																		
GLY	THR	PRO	GLY	THR	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	H1646	R1647	L1654	Q1661																				





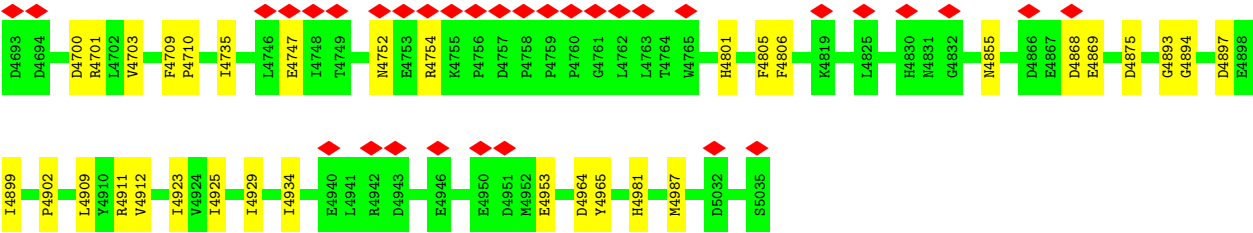


• Molecule 2: Ryanodine receptor 1









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25791	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PCW, CFF, ATP, A1BYZ, 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	E	0.24	0/848	0.40	0/1143
1	F	0.25	0/848	0.40	0/1143
1	G	0.25	0/848	0.41	0/1143
1	H	0.24	0/848	0.40	0/1143
2	A	0.29	0/35586	0.47	13/48203 (0.0%)
2	B	0.29	0/35586	0.47	14/48203 (0.0%)
2	C	0.29	0/35586	0.47	13/48203 (0.0%)
2	D	0.29	0/35586	0.47	13/48203 (0.0%)
All	All	0.29	0/145736	0.47	53/197384 (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
2	A	0	10
2	B	0	10
2	C	0	10
2	D	0	10
All	All	0	40

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	B	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	C	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	A	2238	CYS	CA-CB-SG	9.55	136.37	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3241	CYS	CA-CB-SG	7.71	132.13	114.40

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	605	CYS	Peptide
2	D	870	ARG	Sidechain
2	D	872	ARG	Sidechain
2	D	887	ARG	Sidechain
2	D	898	ARG	Sidechain

## 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	E	830	0	828	16	0
1	F	830	0	828	15	0
1	G	830	0	828	16	0
1	H	830	0	828	16	0
2	A	34797	0	34382	638	0
2	B	34797	0	34382	643	0
2	C	34797	0	34382	644	0
2	D	34797	0	34382	642	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	108	0	168	5	0
7	B	108	0	168	5	0
7	C	108	0	168	5	0
7	D	108	0	168	5	0
8	A	60	0	0	2	0
8	B	60	0	0	3	0
8	C	60	0	0	3	0
8	D	60	0	0	2	0
All	All	143492	0	141648	2626	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 2626 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:899:ASP:HB3	2:B:902:LYS:HB2	1.30	1.10
2:A:899:ASP:HB3	2:A:902:LYS:HB2	1.30	1.09
2:D:899:ASP:HB3	2:D:902:LYS:HB2	1.30	1.08
2:C:899:ASP:HB3	2:C:902:LYS:HB2	1.30	1.08
1:H:2:GLY:N	1:H:78:SER:HG	1.55	1.03

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	E	105/108 (97%)	102 (97%)	3 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	79
2	B	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	79
2	C	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	79
2	D	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	79
All	All	17800/20572 (86%)	17318 (97%)	470 (3%)	12 (0%)	50	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2574	GLU
2	D	4055	SER
2	A	2574	GLU
2	A	4055	SER
2	B	2574	GLU

### 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	E	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	A	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
2	B	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
2	C	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
2	D	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
All	All	15580/17544 (89%)	15324 (98%)	256 (2%)	58	79

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	952	LYS
2	C	962	MET
2	A	939	HIS
2	A	933	LEU
2	C	971	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2037	GLN
2	C	2992	HIS
2	A	1762	HIS
2	A	1641	HIS
2	C	3423	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 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	CFF	C	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
8	A1BYZ	C	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
5	ATP	B	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
5	ATP	D	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
8	A1BYZ	C	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	B	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
4	CFF	A	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
8	A1BYZ	B	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
8	A1BYZ	D	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
8	A1BYZ	A	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
5	ATP	A	8007	-	28,33,33	0.60	0	34,52,52	0.88	1 (2%)
4	CFF	D	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
5	ATP	C	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	B	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
5	ATP	C	8003	-	28,33,33	0.66	0	34,52,52	0.90	2 (5%)
8	A1BYZ	A	8008	-	32,32,32	0.67	1 (3%)	40,47,47	0.85	1 (2%)
8	A1BYZ	B	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	D	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
8	A1BYZ	D	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
5	ATP	A	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
7	PCW	C	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
4	CFF	B	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)

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	CFF	C	8002	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1BYZ	C	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	B	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	D	8007	-	-	8/18/38/38	0/3/3/3
8	A1BYZ	C	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	B	8005	-	-	25/57/57/57	-
8	A1BYZ	B	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
8	A1BYZ	D	8009	-	-	4/18/59/59	0/3/3/3
7	PCW	B	8006	-	-	29/57/57/57	-
8	A1BYZ	A	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	A	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	C	8007	-	-	8/18/38/38	0/3/3/3
4	CFF	D	8002	-	-	-	0/2/2/2
7	PCW	D	8006	-	-	29/57/57/57	-
7	PCW	A	8005	-	-	25/57/57/57	-
5	ATP	B	8003	-	-	9/18/38/38	0/3/3/3
5	ATP	C	8003	-	-	9/18/38/38	0/3/3/3
8	A1BYZ	A	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	B	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	C	8006	-	-	29/57/57/57	-
5	ATP	D	8003	-	-	9/18/38/38	0/3/3/3
7	PCW	D	8005	-	-	25/57/57/57	-
8	A1BYZ	D	8008	-	-	3/18/59/59	0/3/3/3
5	ATP	A	8003	-	-	9/18/38/38	0/3/3/3
7	PCW	C	8005	-	-	25/57/57/57	-
4	CFF	B	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	29/57/57/57	-

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8002	CFF	C5-C4	-3.52	1.33	1.39
4	A	8002	CFF	C5-C4	-3.49	1.33	1.39
4	D	8002	CFF	C5-C4	-3.49	1.33	1.39
4	C	8002	CFF	C5-C4	-3.49	1.33	1.39
4	D	8002	CFF	C6-N1	-3.34	1.32	1.38

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	B	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	C	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	A	8006	PCW	O2-C31-C32	4.13	120.41	111.48
7	C	8005	PCW	O2-C31-C32	3.98	120.09	111.48

There are no chirality outliers.

5 of 312 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O3A
5	D	8007	ATP	PB-O3B-PG-O3G
5	D	8007	ATP	C5'-O5'-PA-O2A

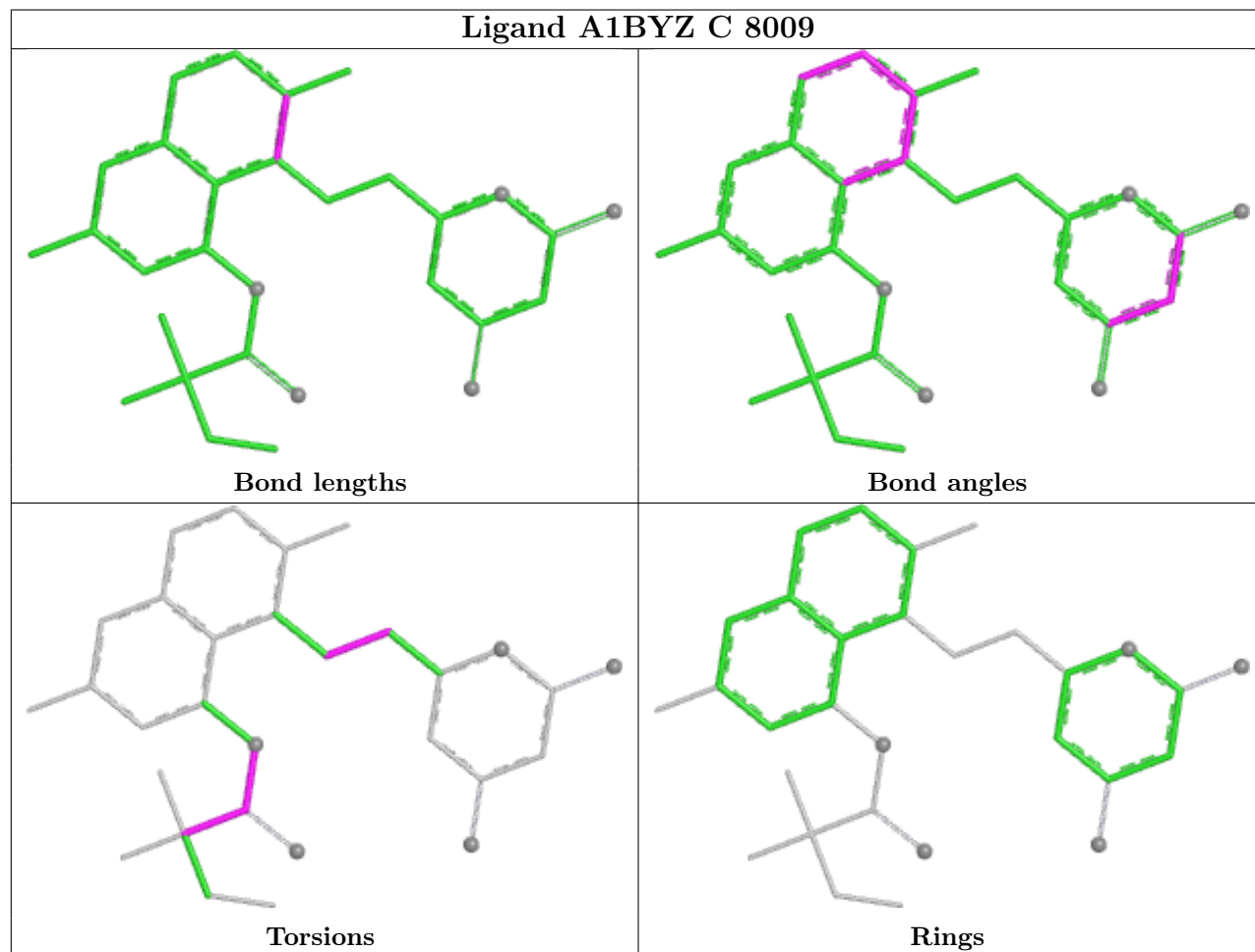
There are no ring outliers.

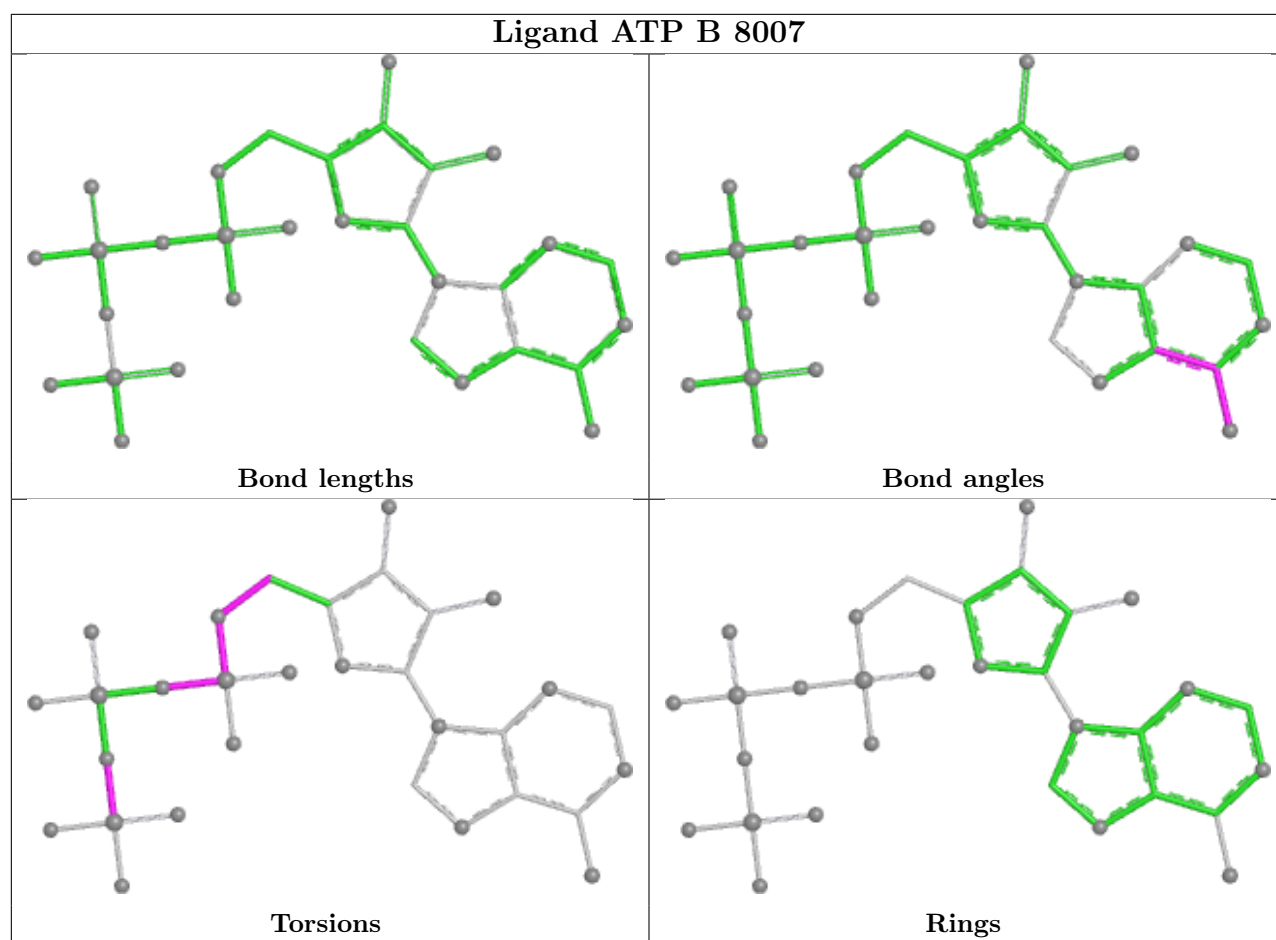
18 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	8009	A1BYZ	2	0
8	C	8008	A1BYZ	1	0
7	B	8005	PCW	2	0
8	B	8009	A1BYZ	2	0
8	D	8009	A1BYZ	2	0
7	B	8006	PCW	3	0
8	A	8009	A1BYZ	2	0
7	D	8006	PCW	3	0
7	A	8005	PCW	2	0
5	B	8003	ATP	1	0
5	C	8003	ATP	1	0
8	B	8008	A1BYZ	1	0
7	C	8006	PCW	3	0
5	D	8003	ATP	1	0
7	D	8005	PCW	2	0
5	A	8003	ATP	1	0
7	C	8005	PCW	2	0
7	A	8006	PCW	3	0

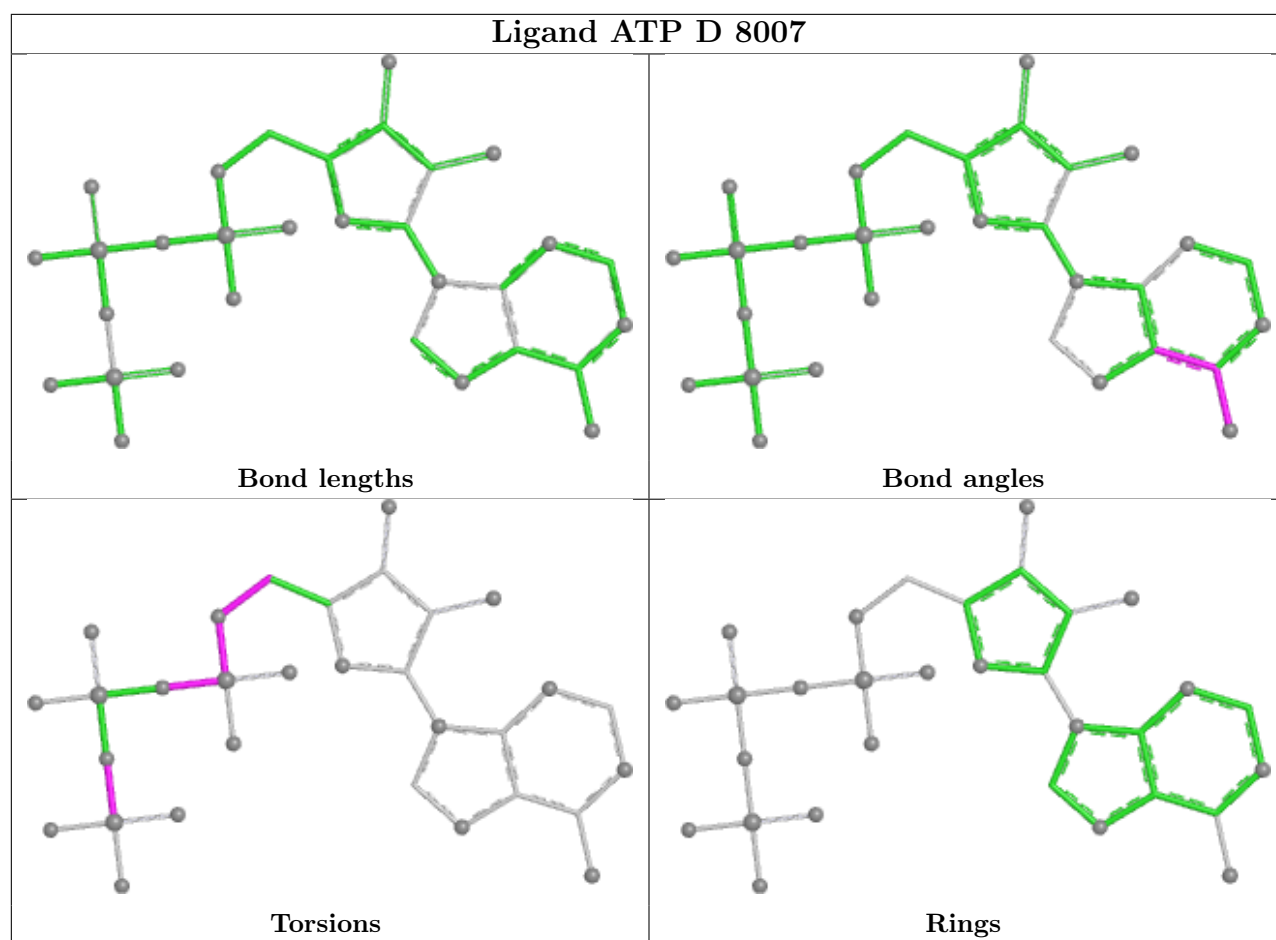
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

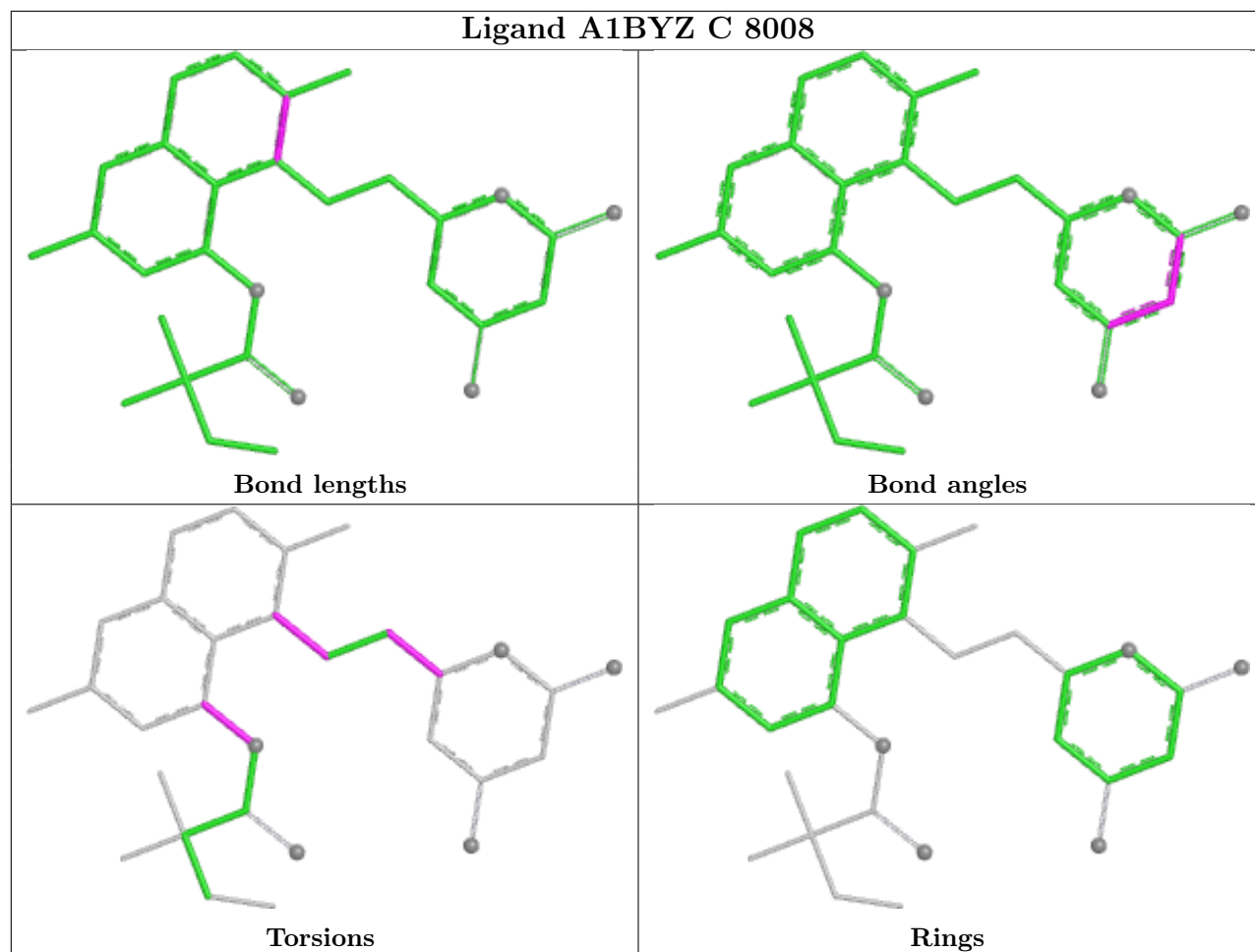


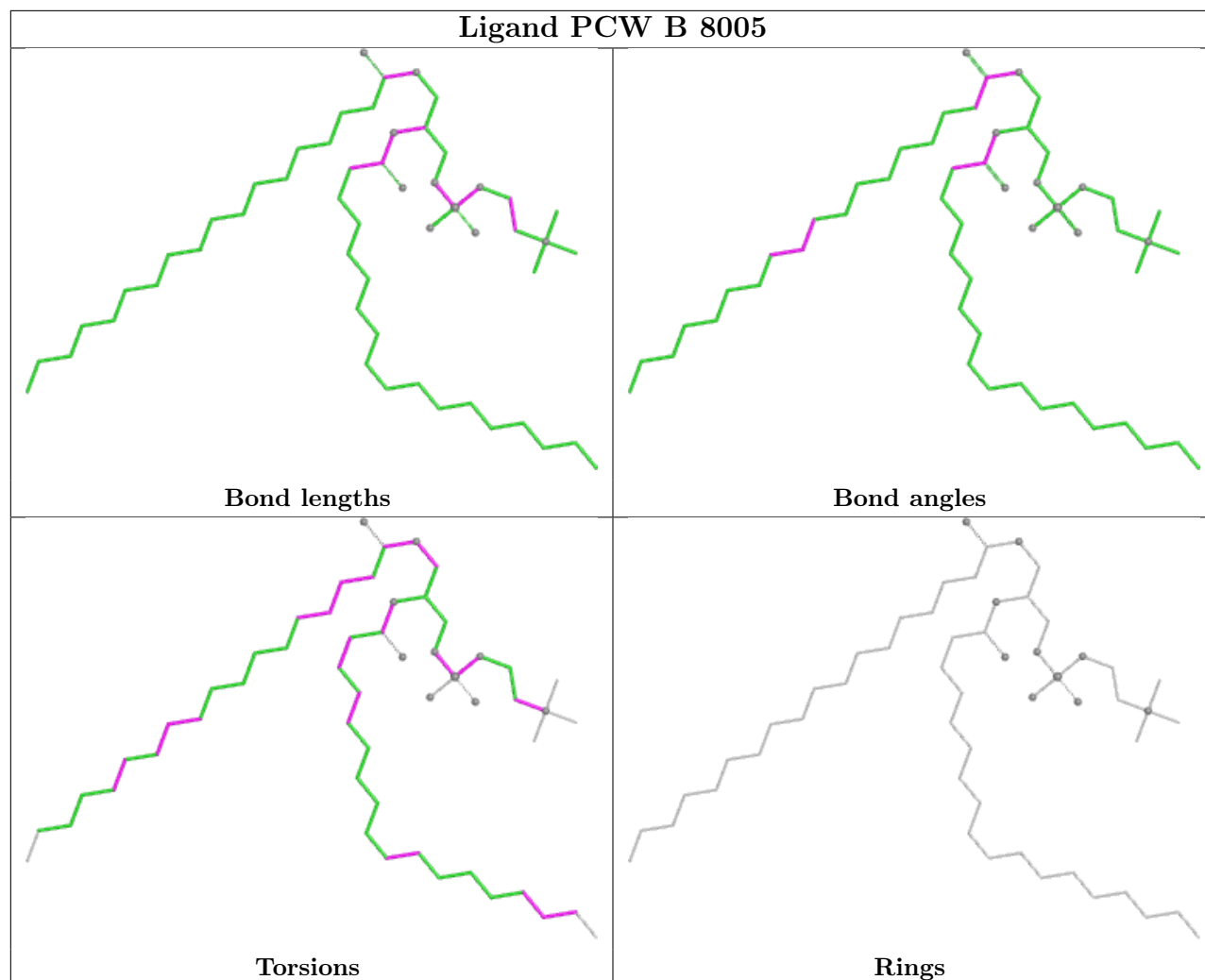




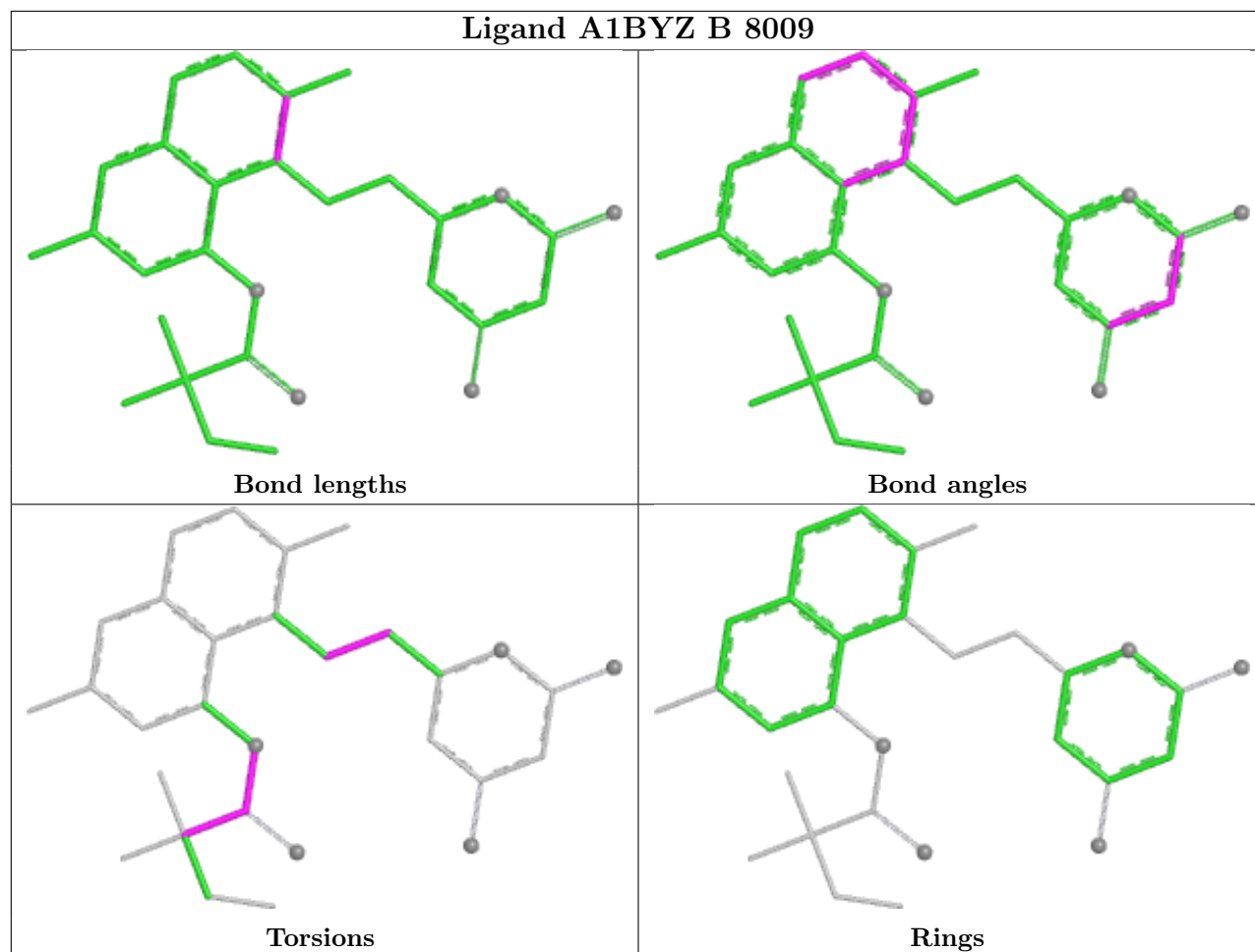


## Ligand A1BYZ C 8008

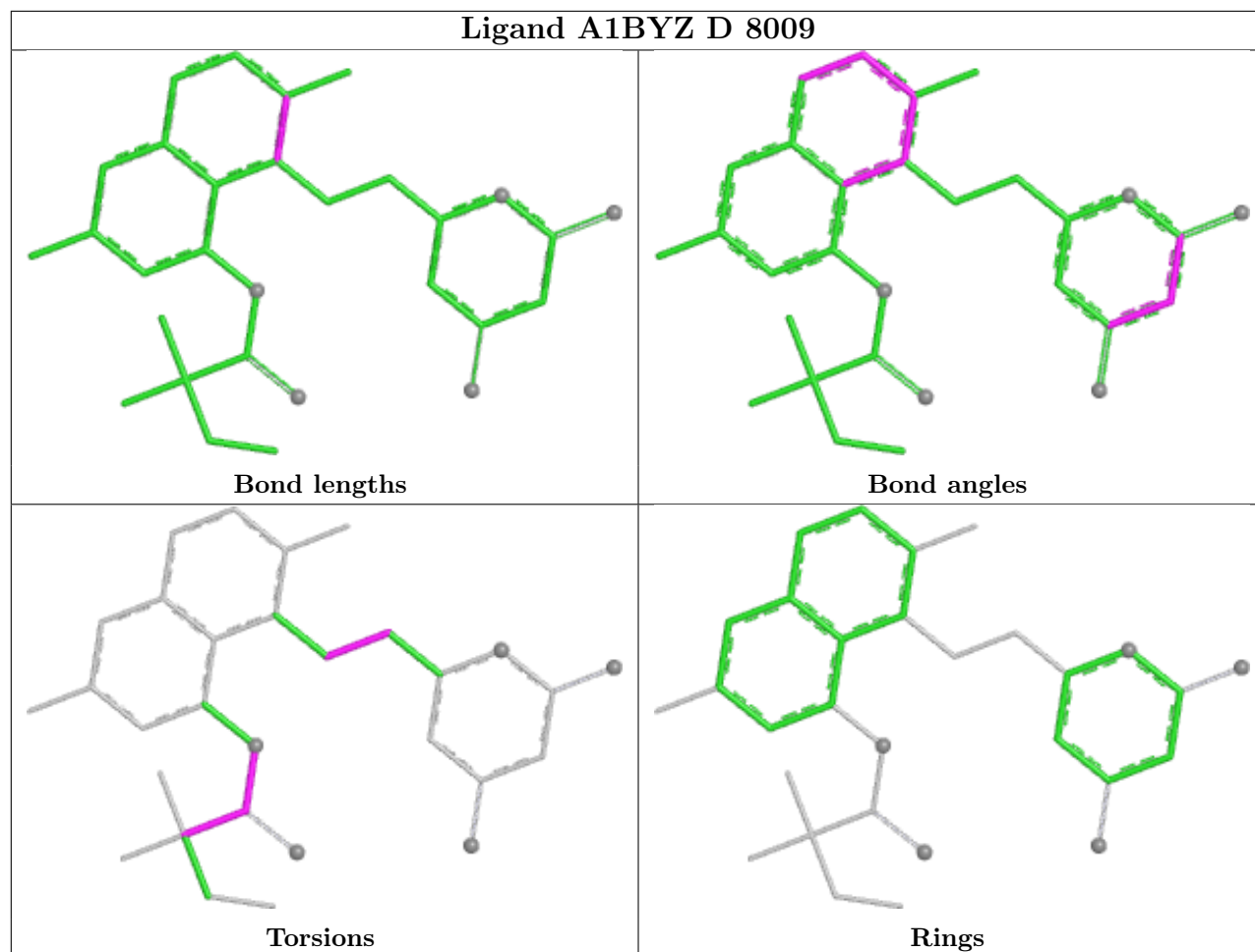


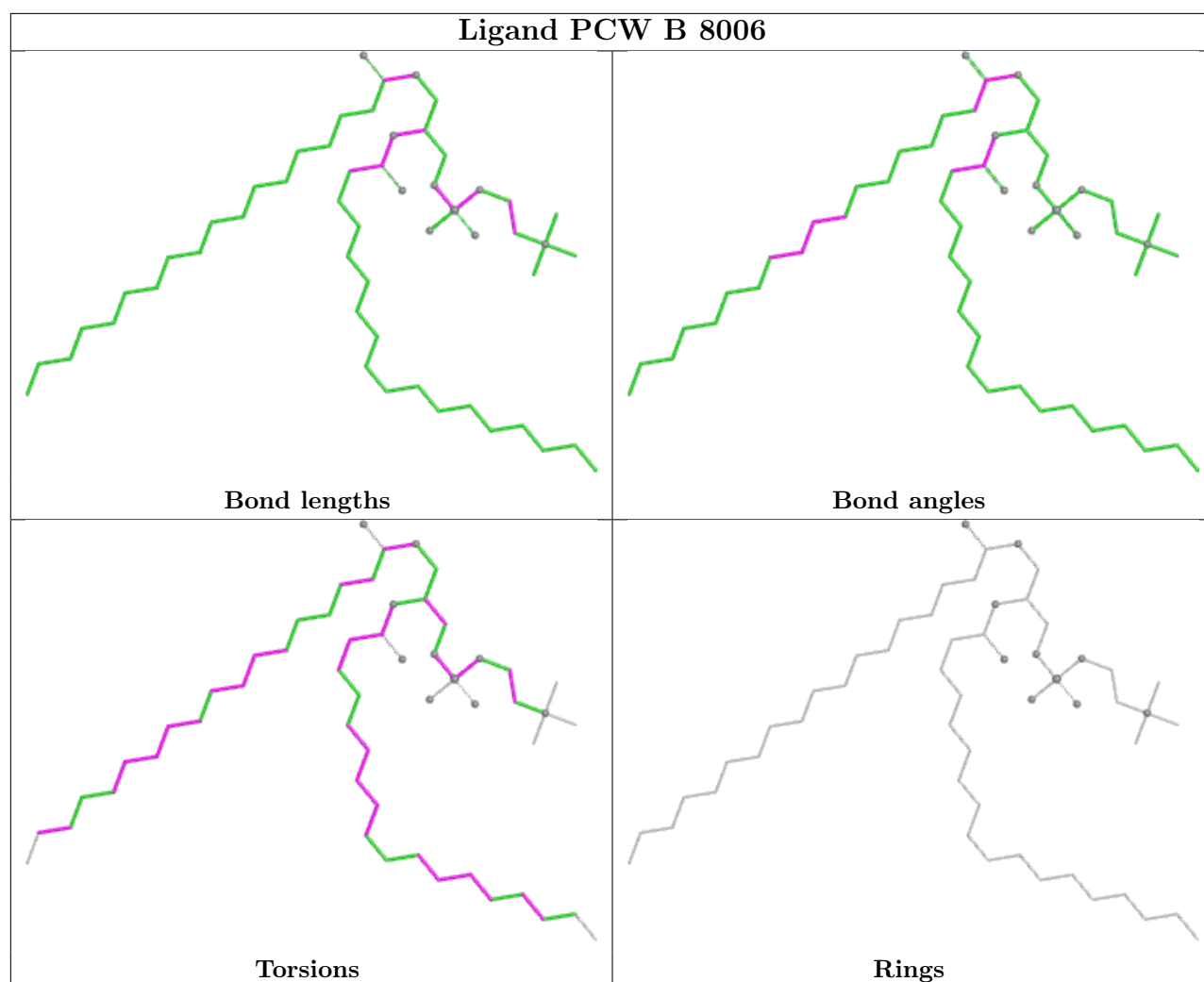


## Ligand A1BYZ B 8009

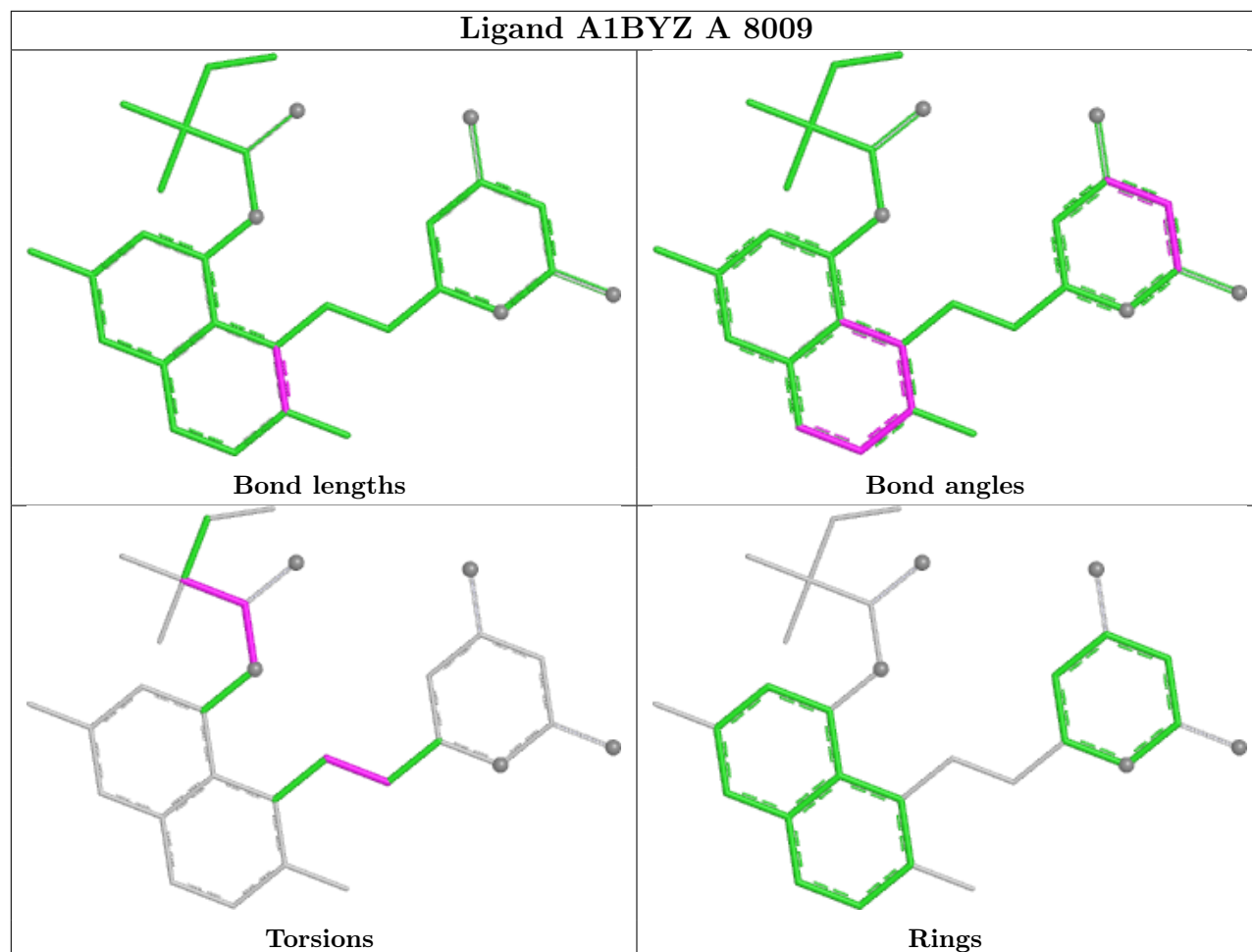


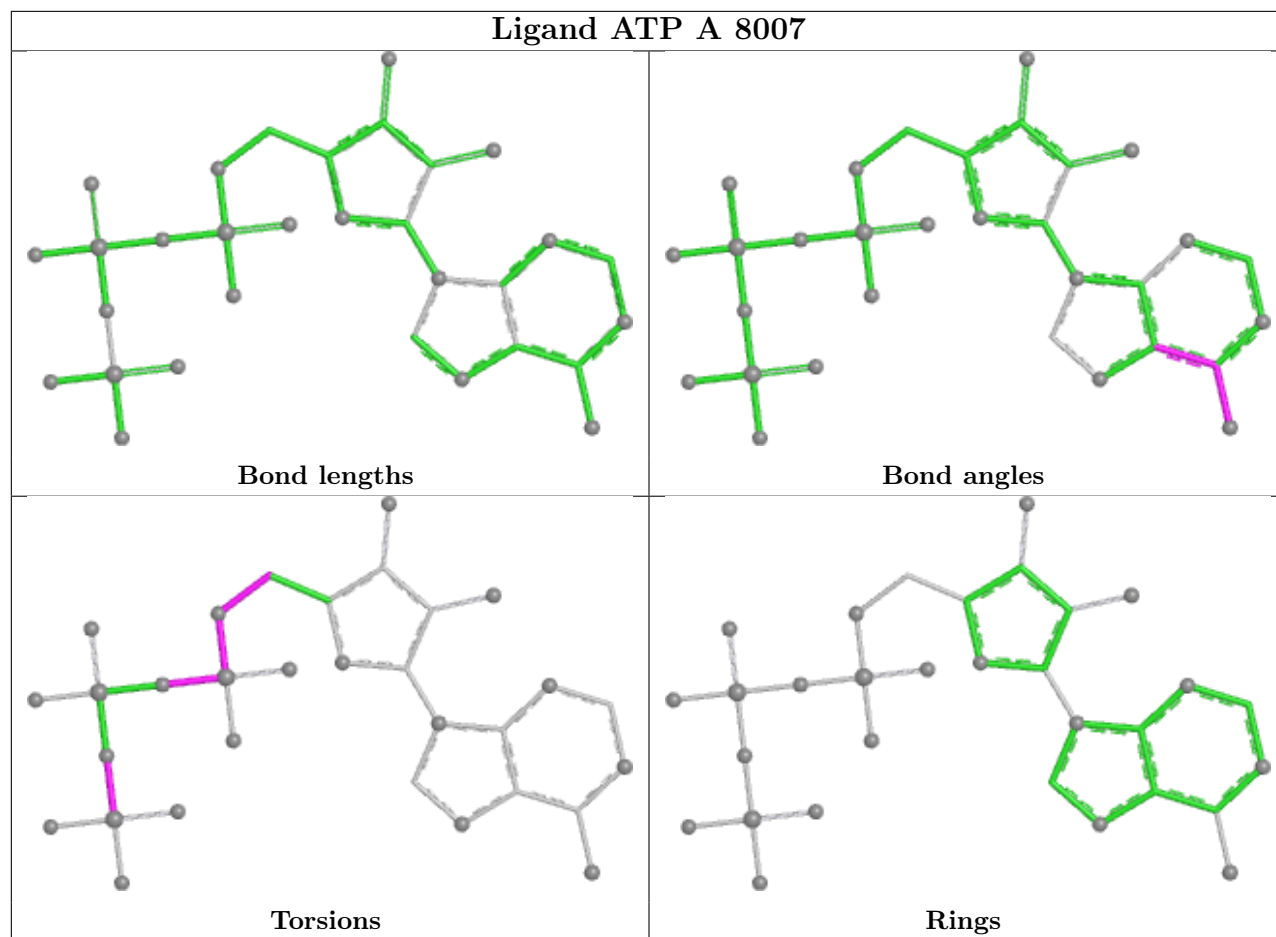
## Ligand A1BYZ D 8009



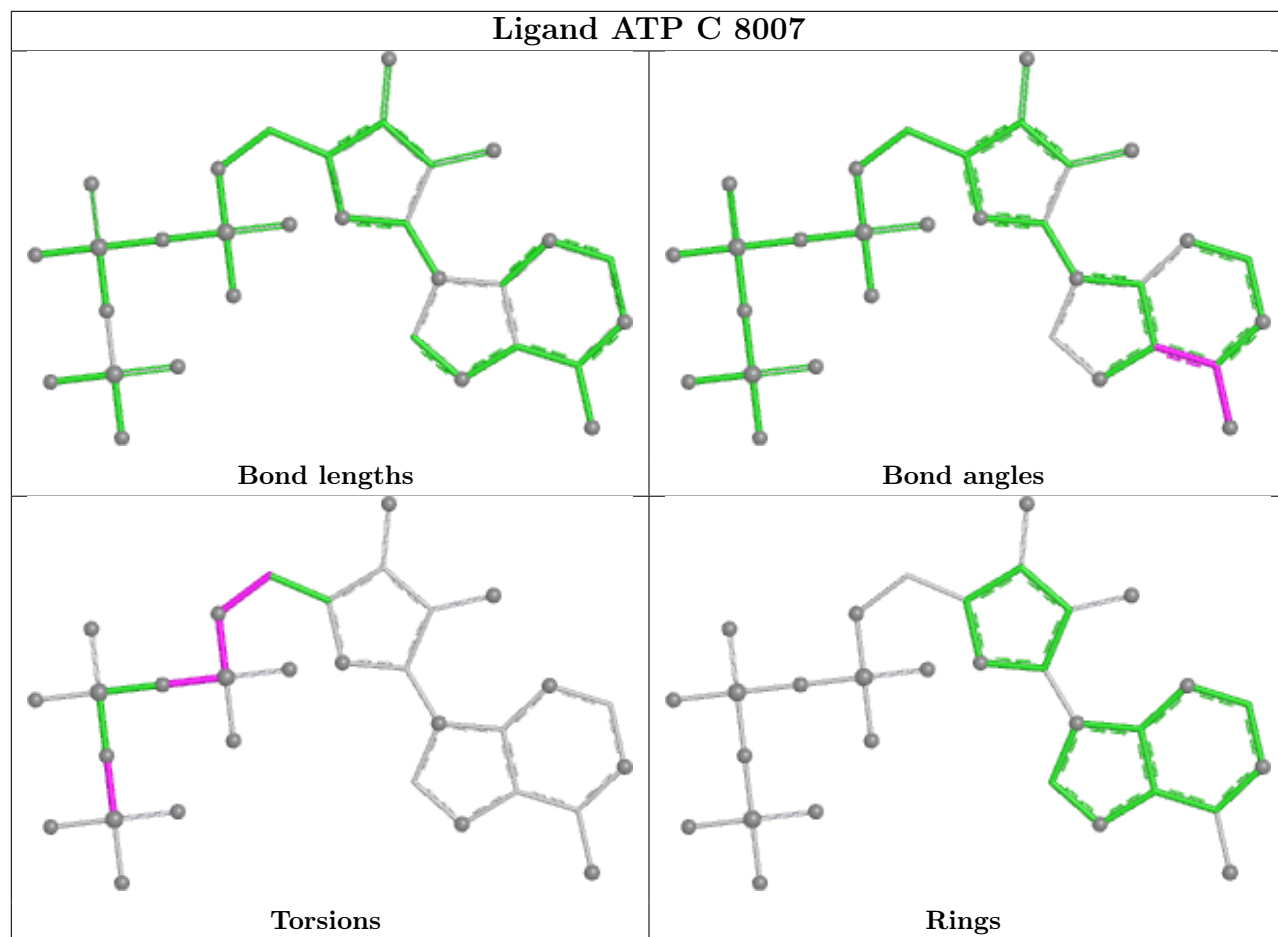


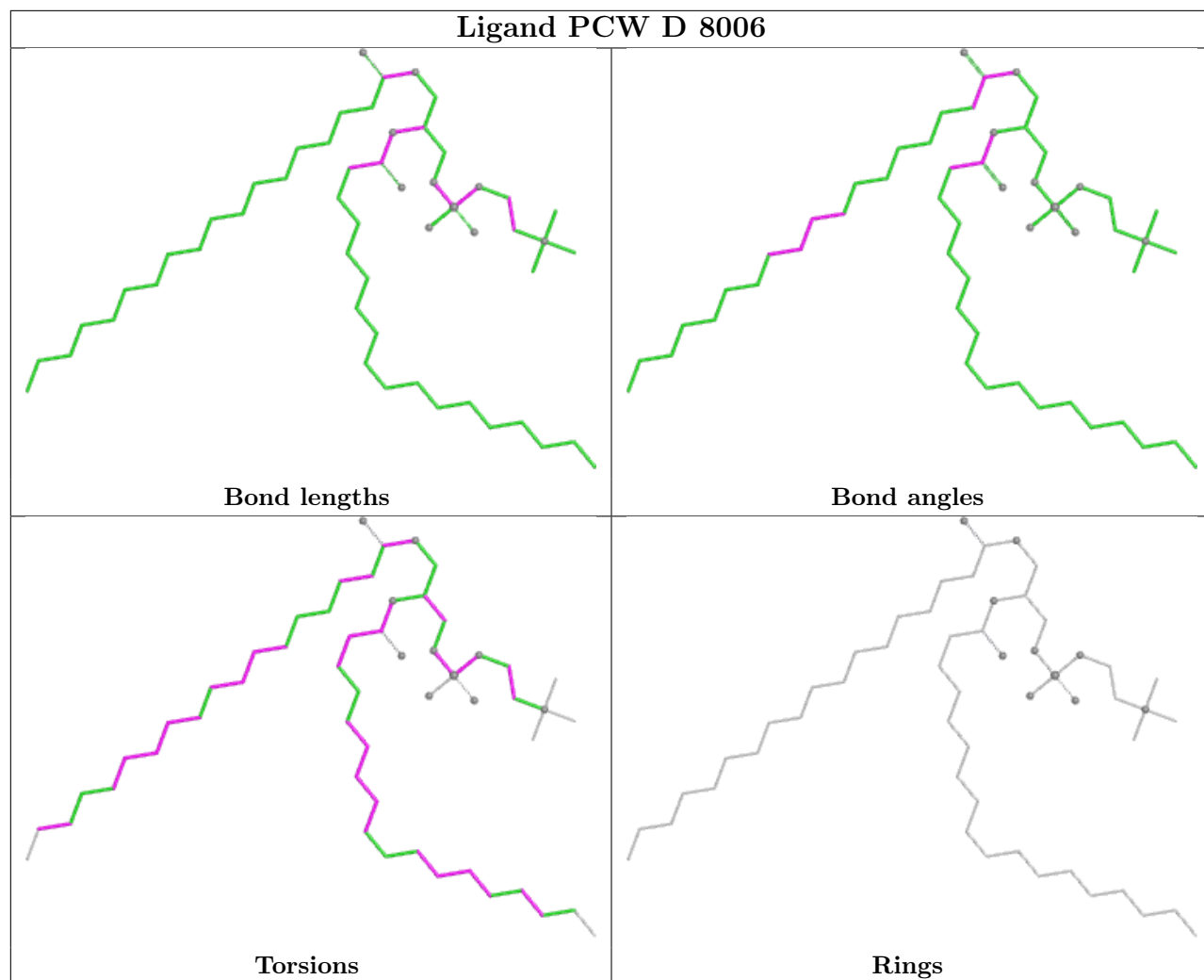
## Ligand A1BYZ A 8009

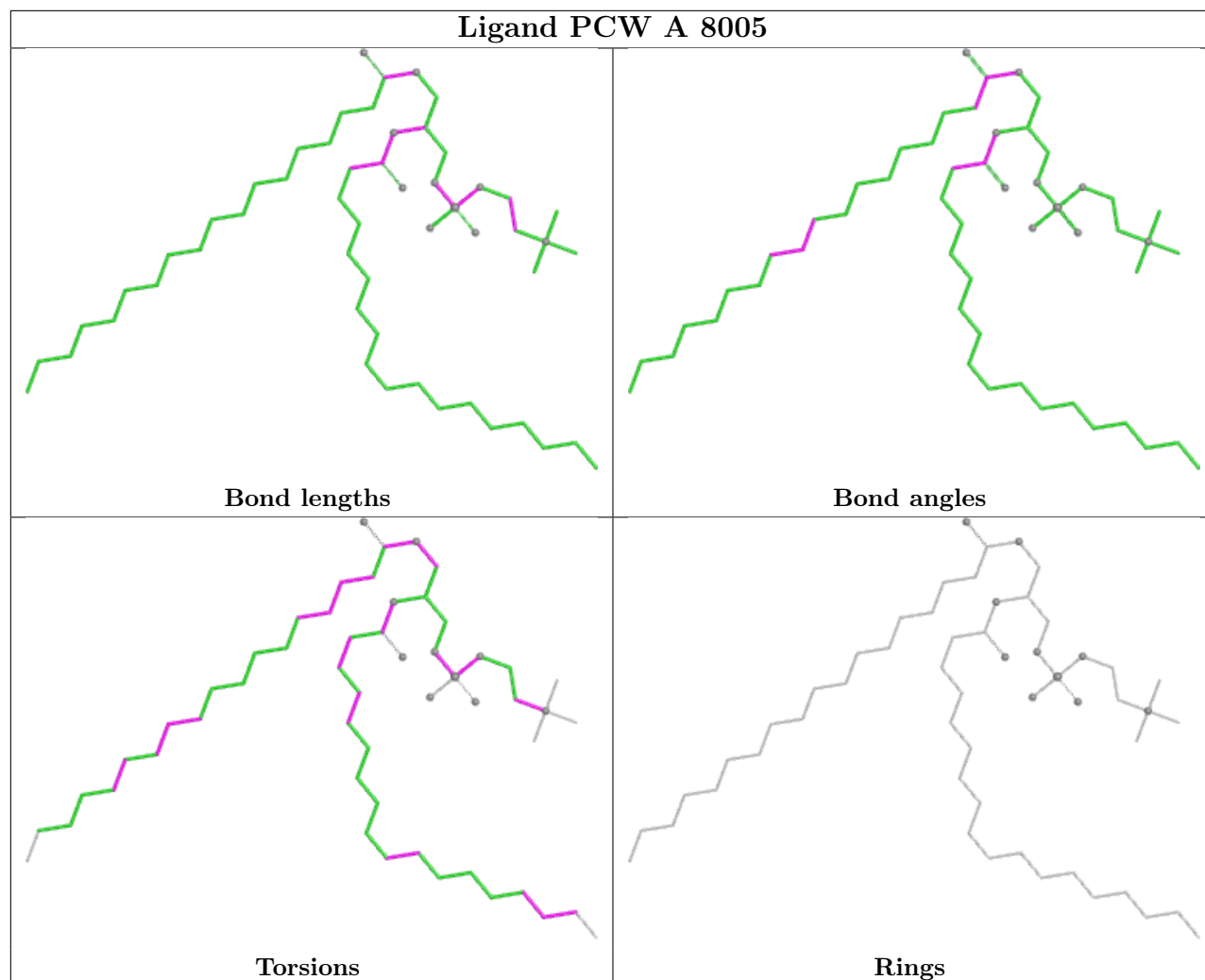


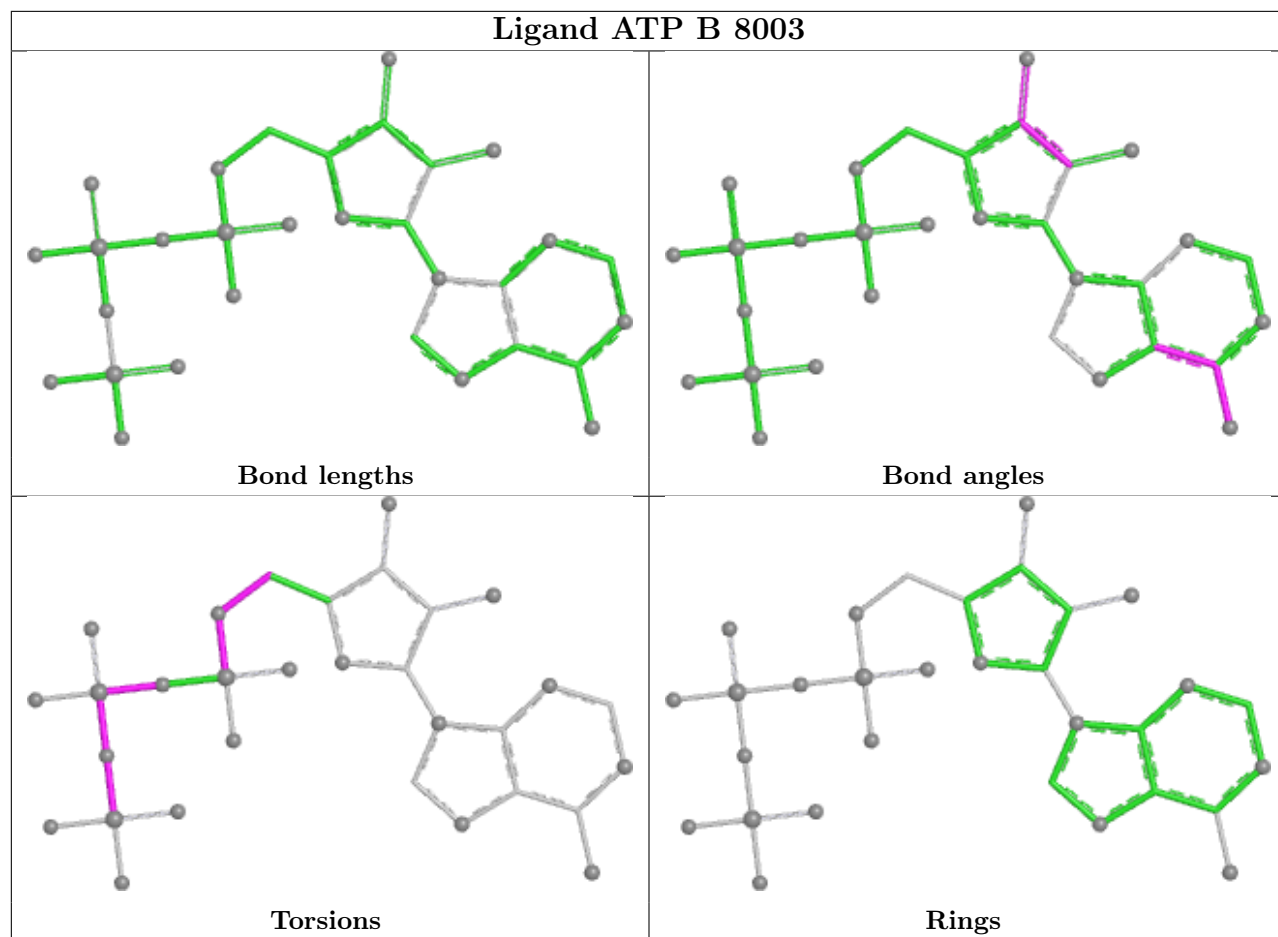


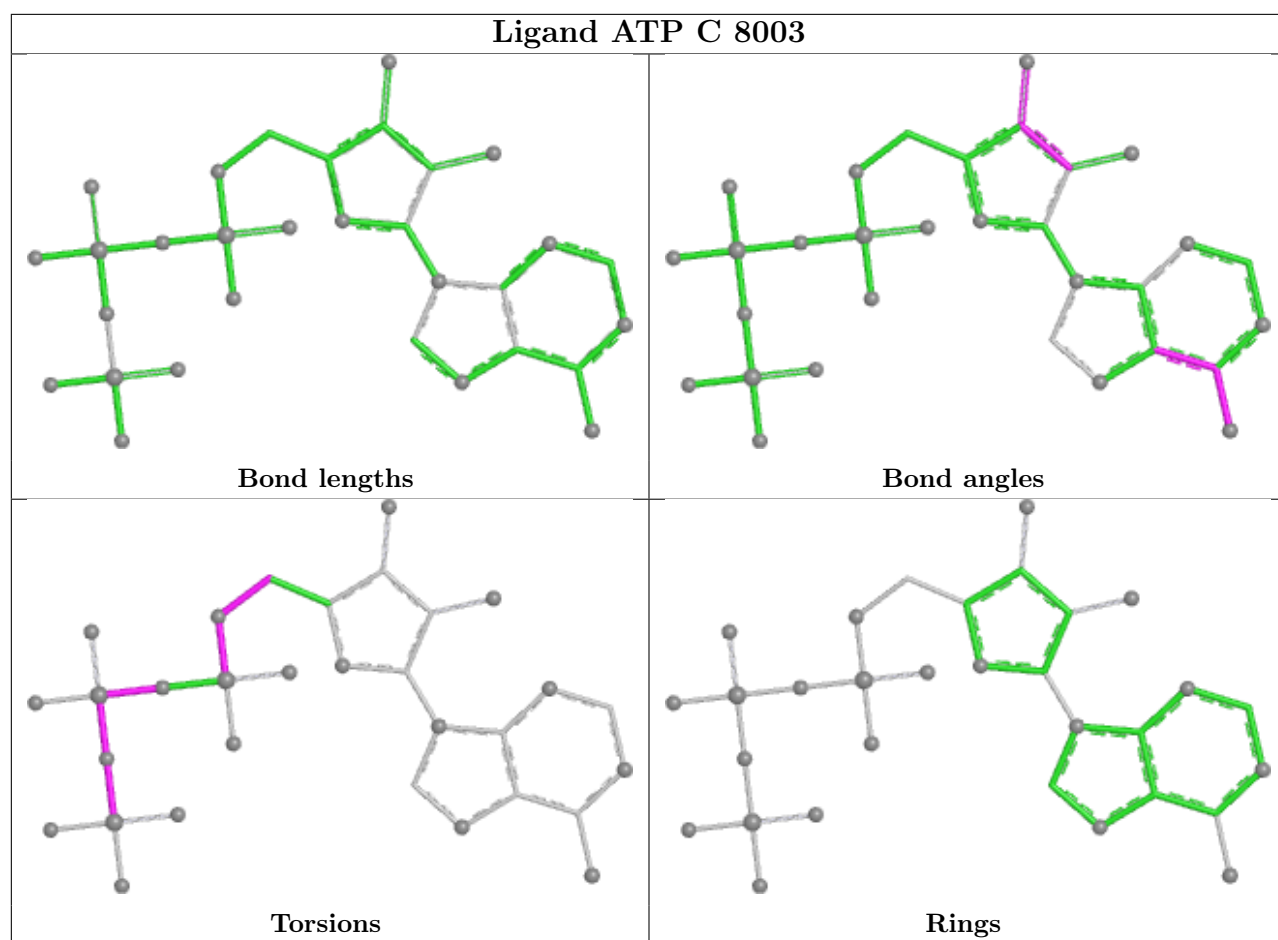




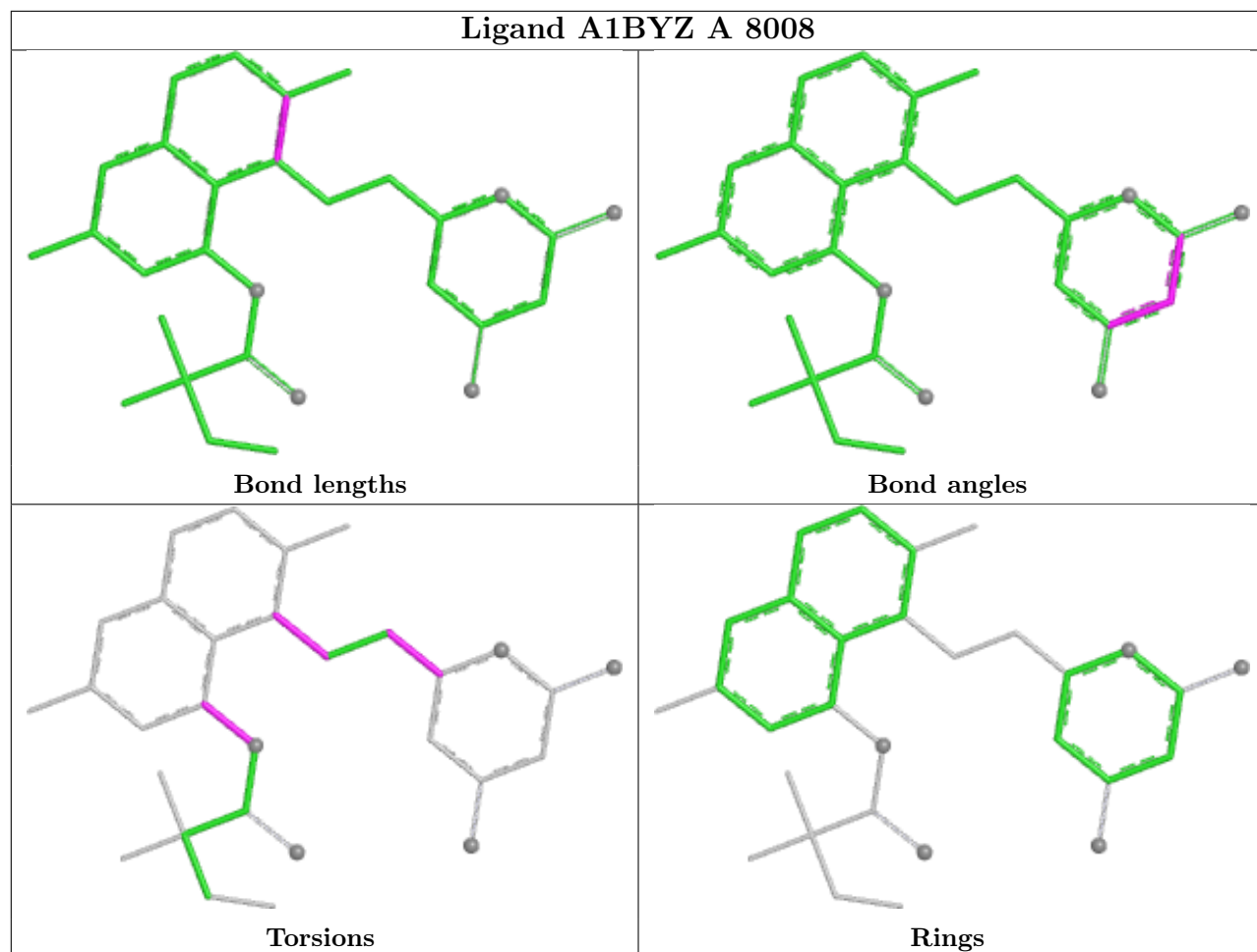


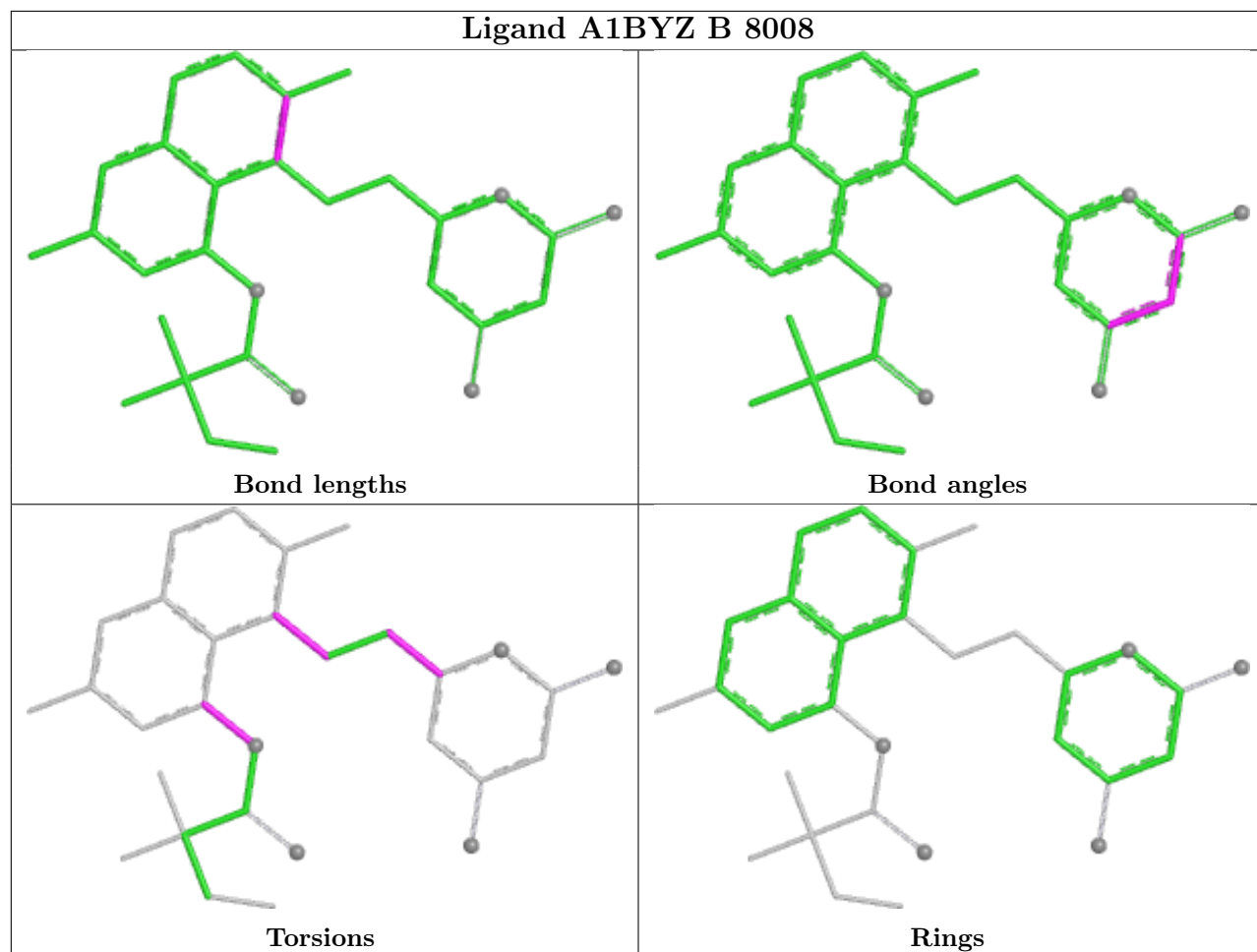


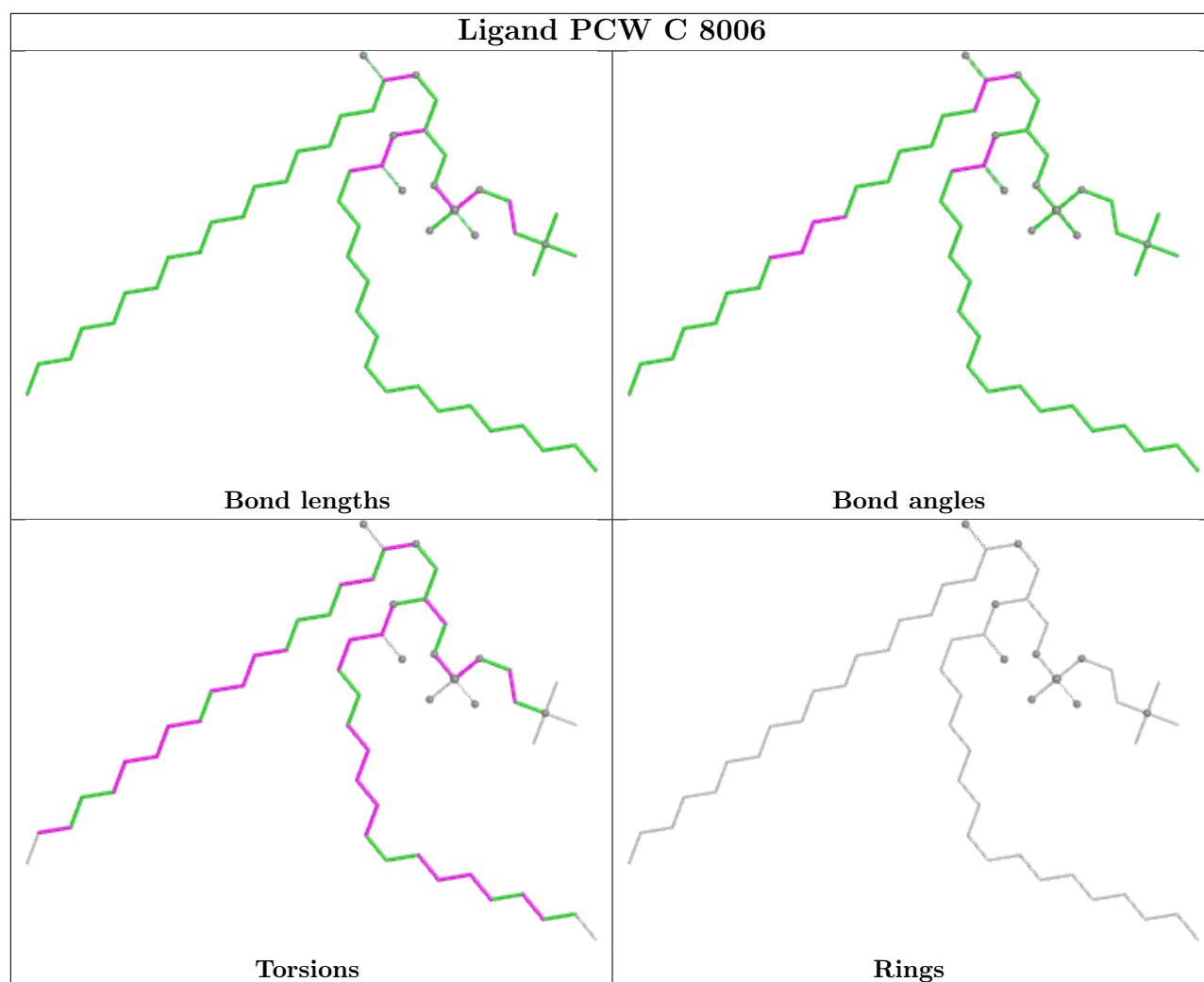




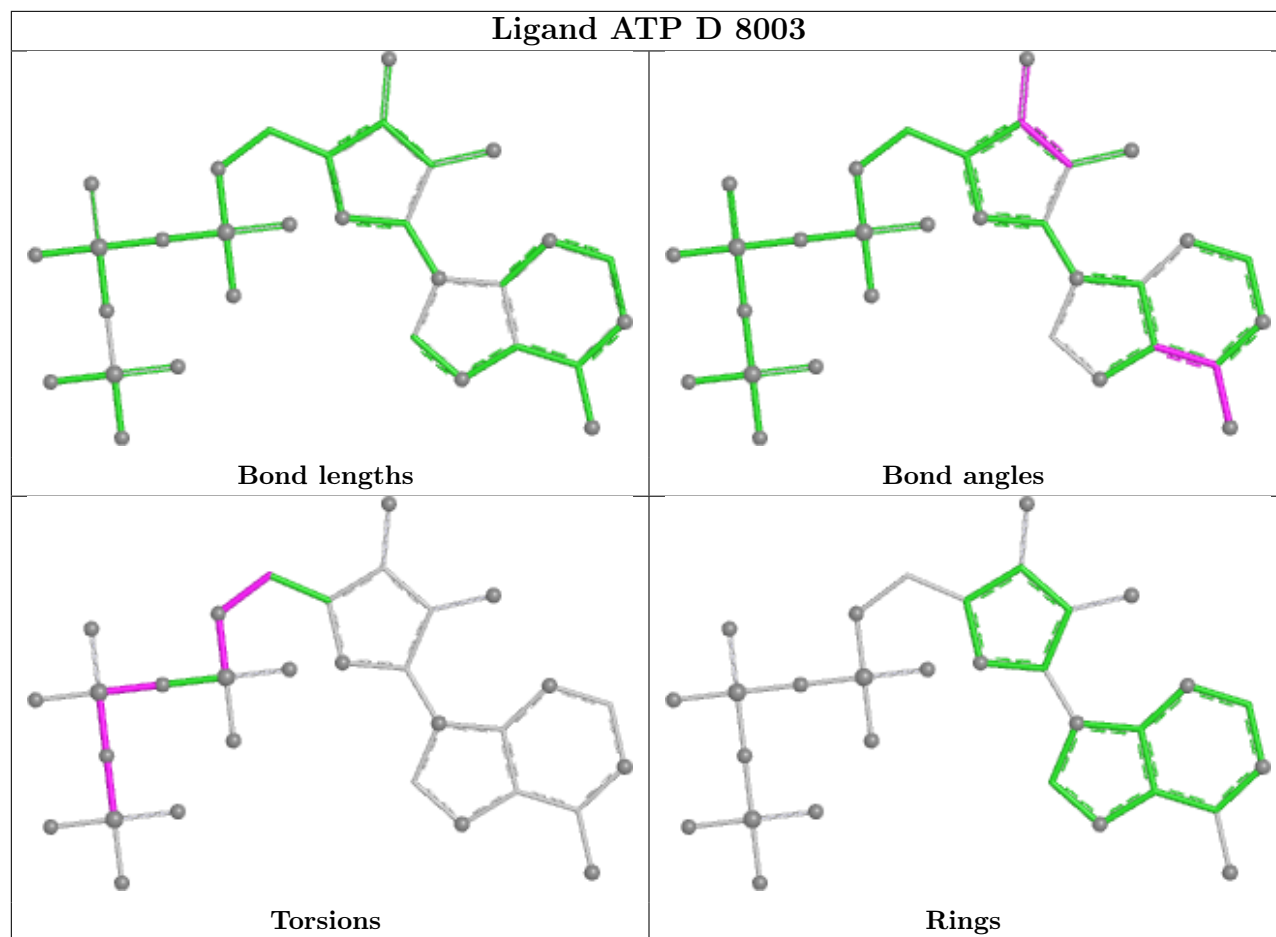
## Ligand A1BYZ A 8008

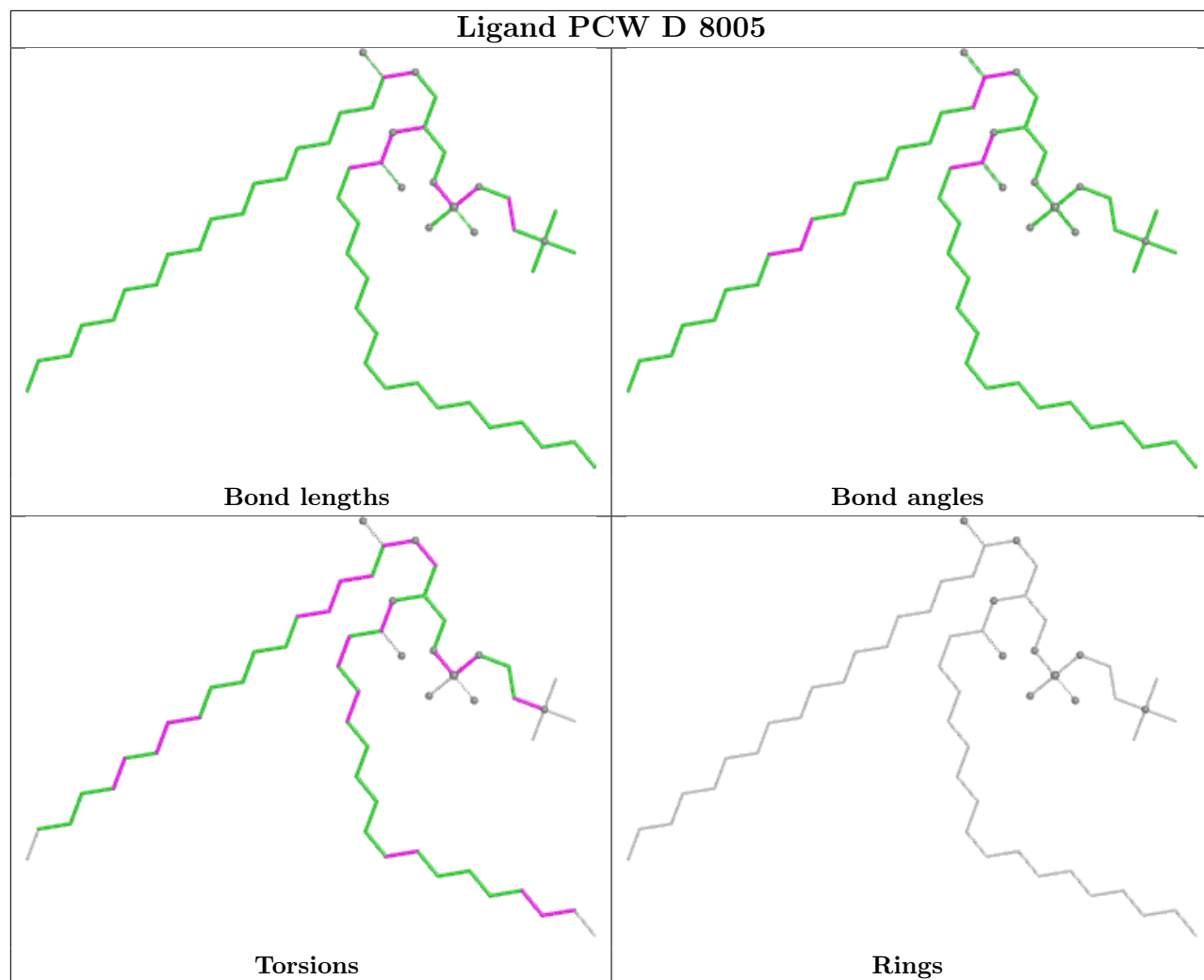




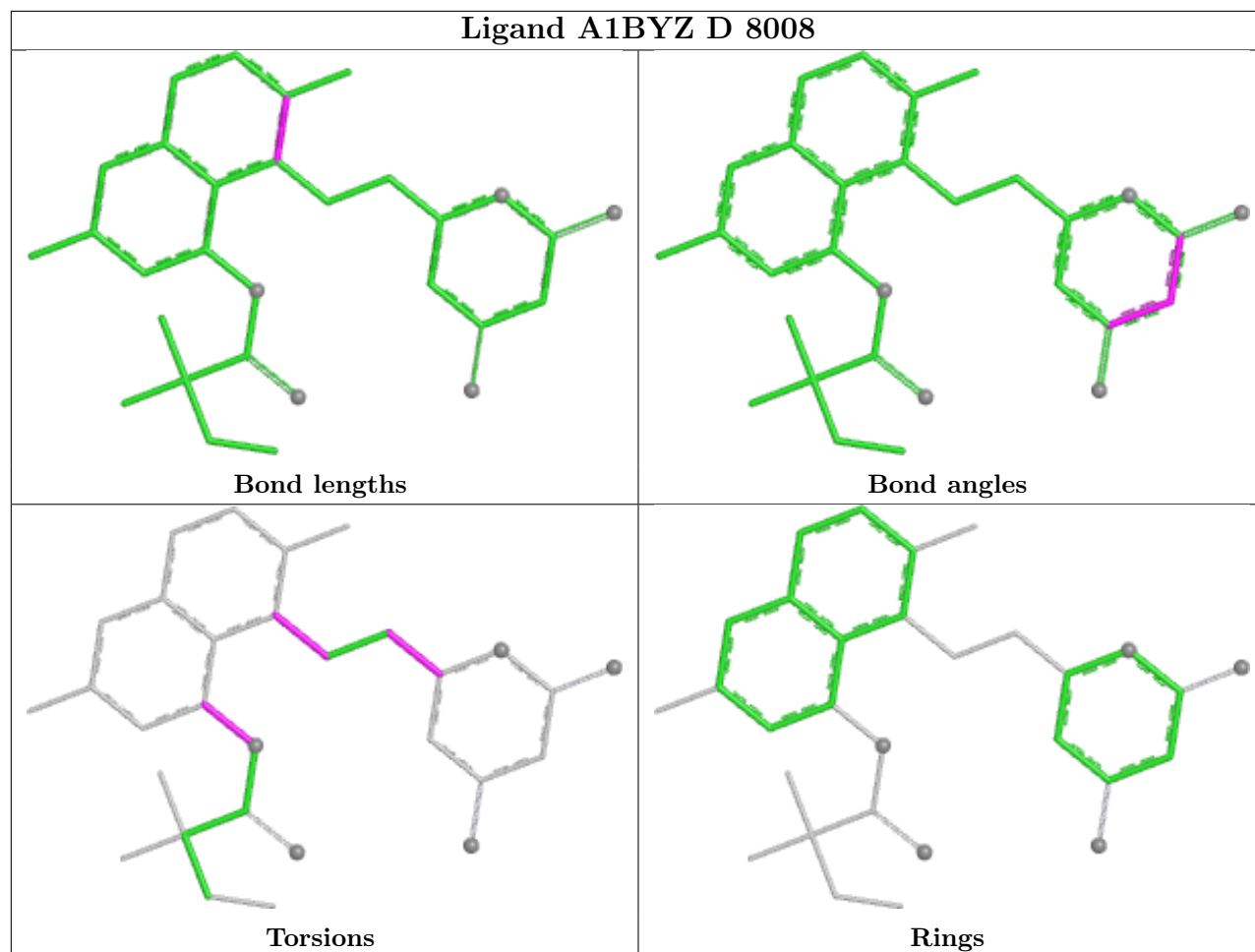


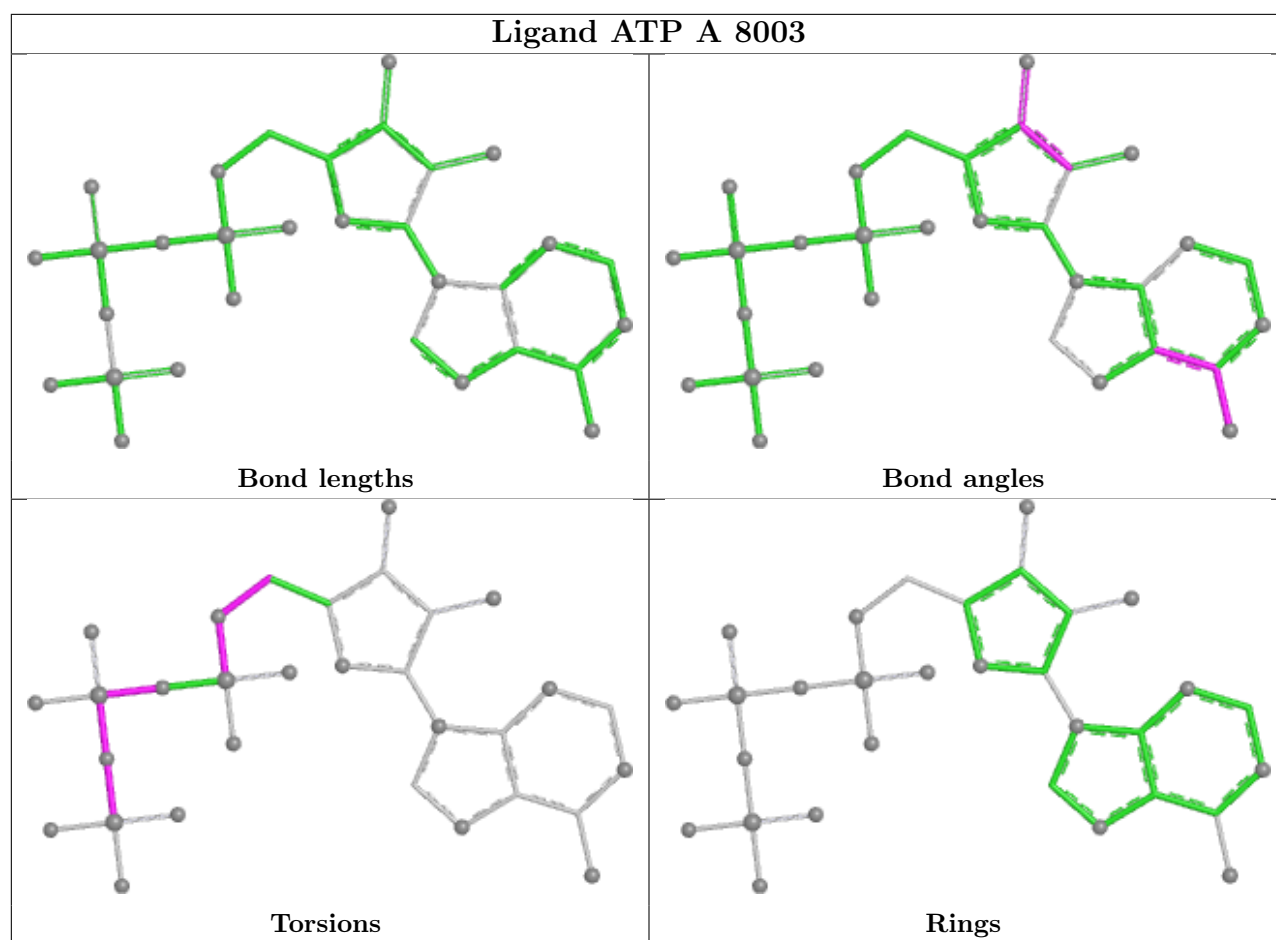


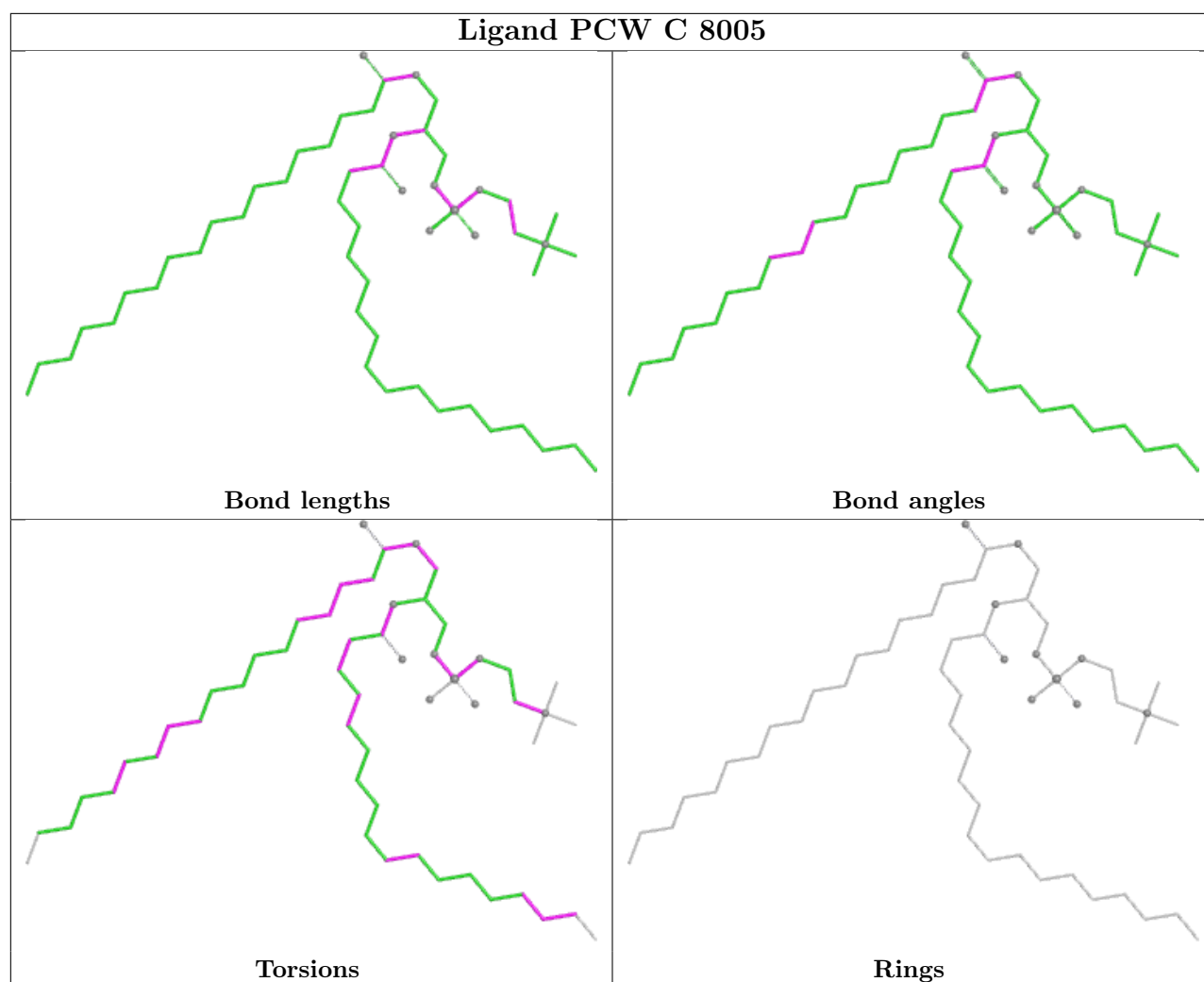


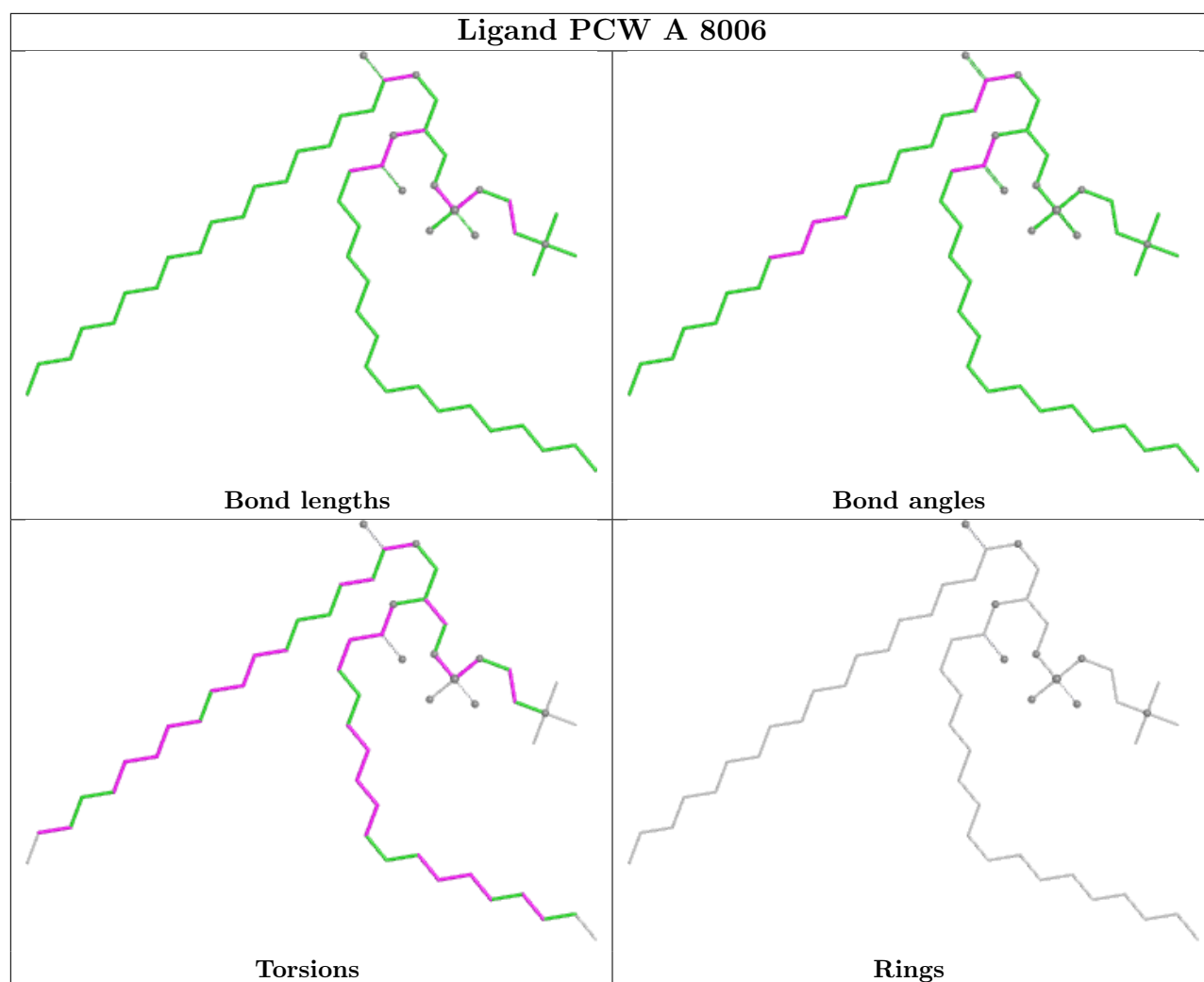


## Ligand A1BYZ D 8008









## 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.

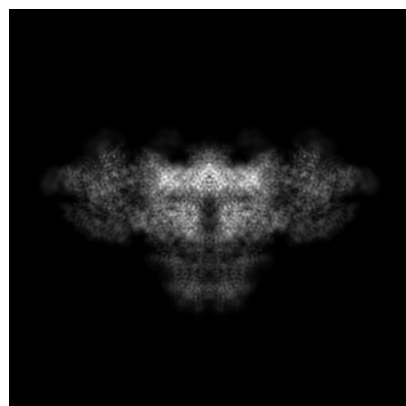
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49536. These allow visual inspection of the internal detail of the map and identification of artifacts.

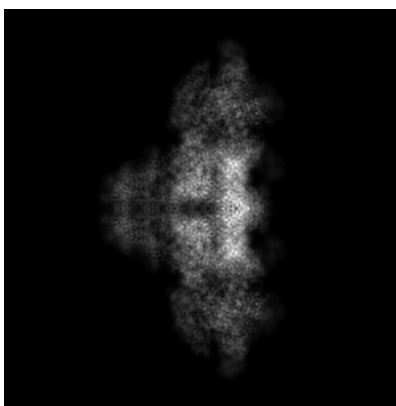
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

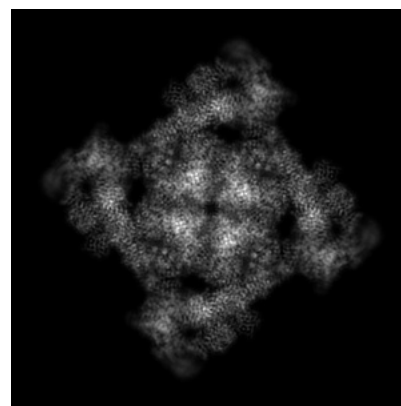
#### 6.1.1 Primary map



X

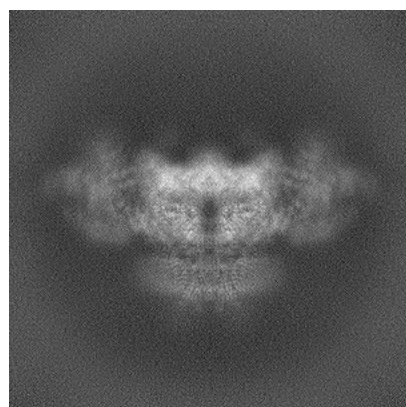


Y

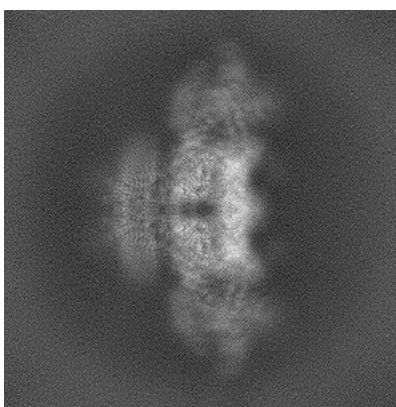


Z

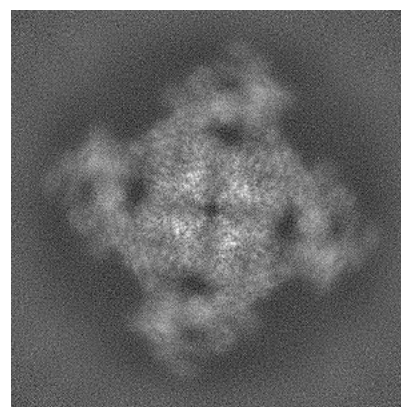
#### 6.1.2 Raw map



X



Y



Z

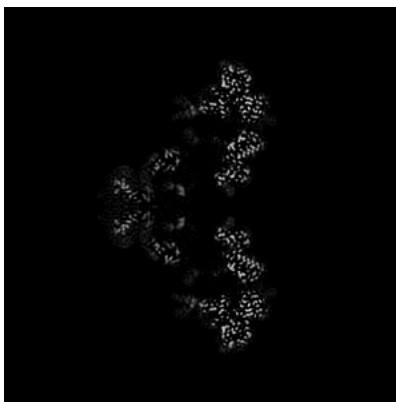
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

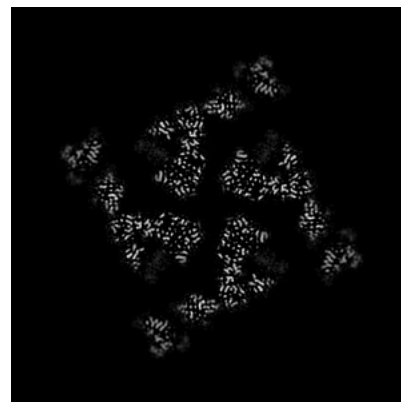
### 6.2.1 Primary map



X Index: 256



Y Index: 256

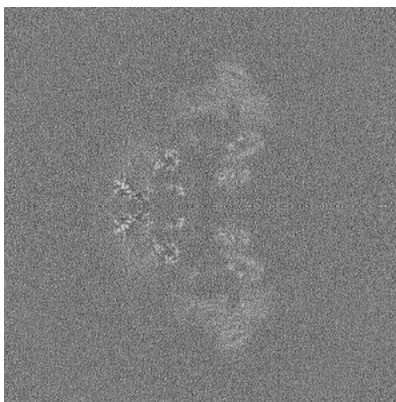


Z Index: 256

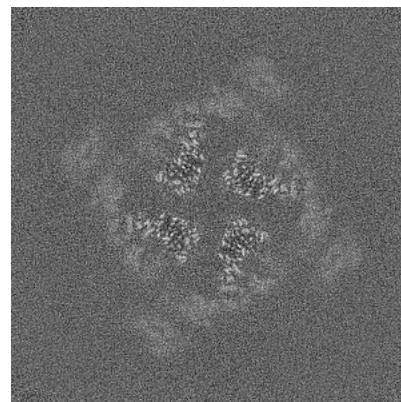
### 6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

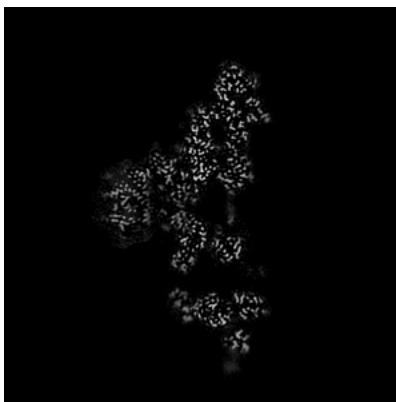


## 6.3 Largest variance slices [i](#)

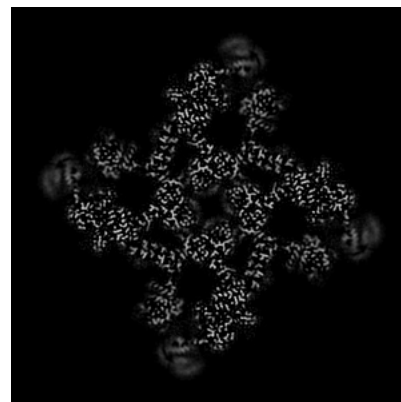
### 6.3.1 Primary map



X Index: 238

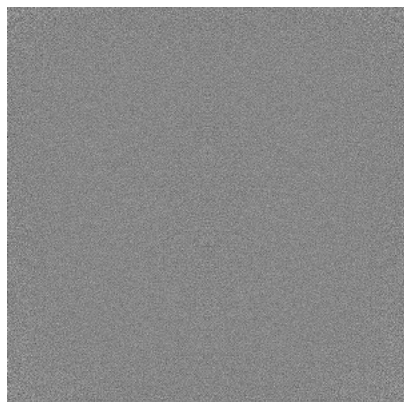


Y Index: 274

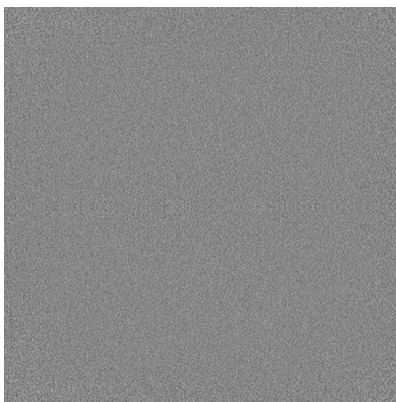


Z Index: 287

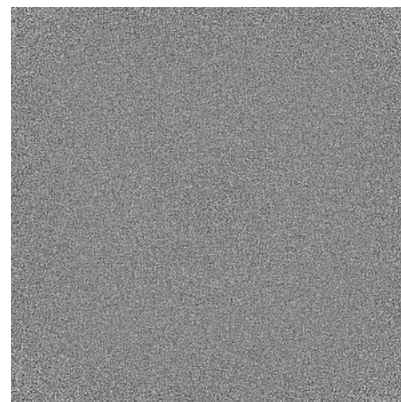
### 6.3.2 Raw map



X Index: 0



Y Index: 0

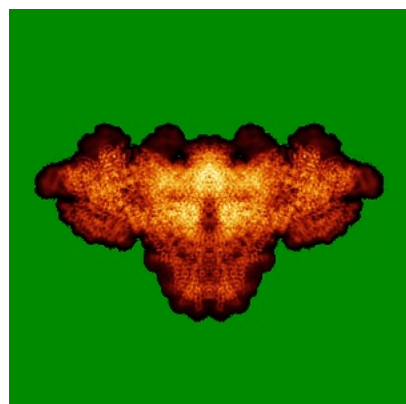


Z Index: 0

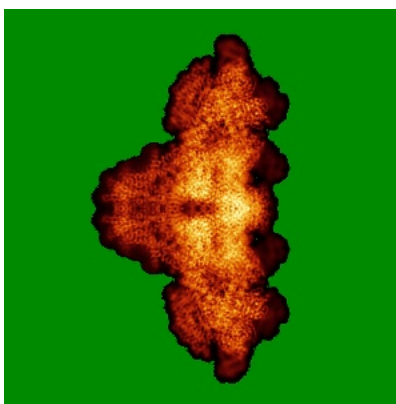
The images above show the largest variance slices of the map in three orthogonal directions.

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

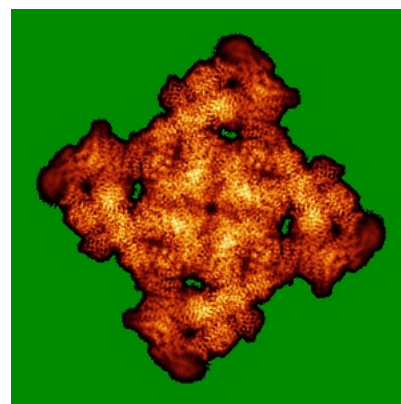
### 6.4.1 Primary map



X

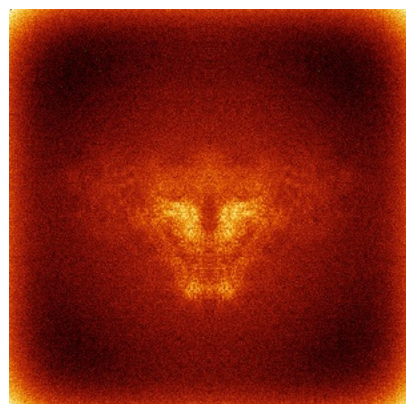


Y

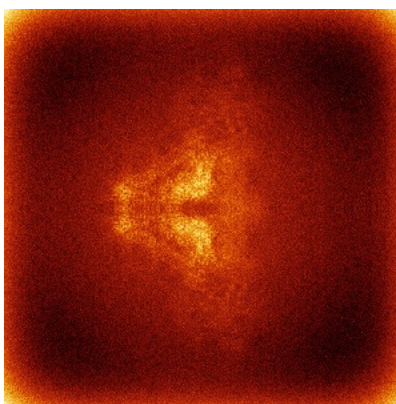


Z

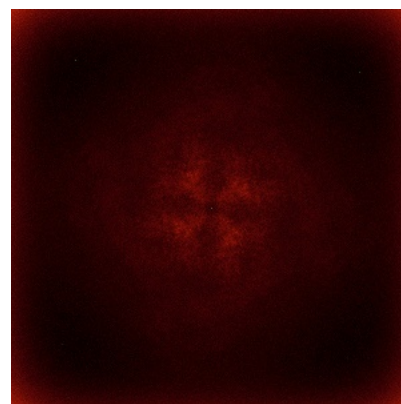
### 6.4.2 Raw map



X



Y

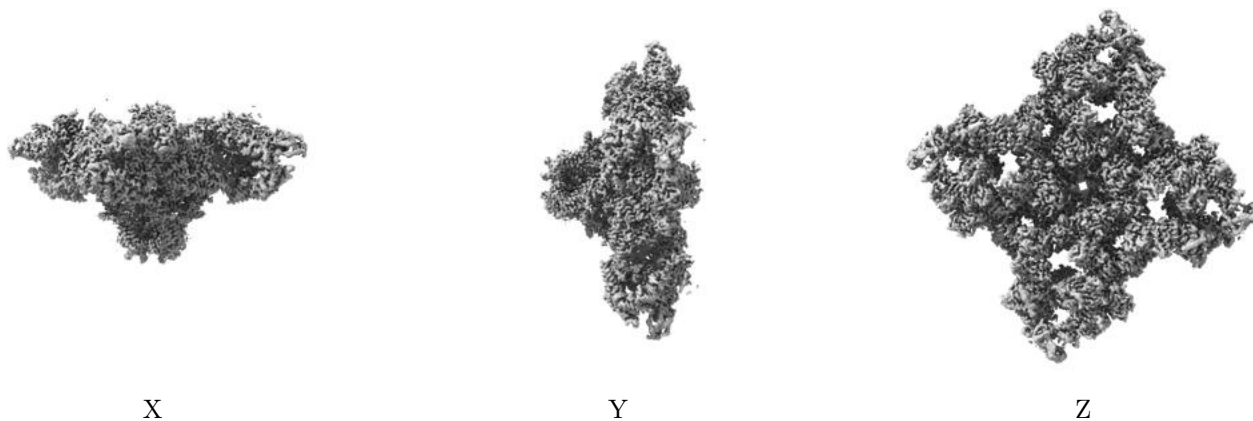


Z

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.

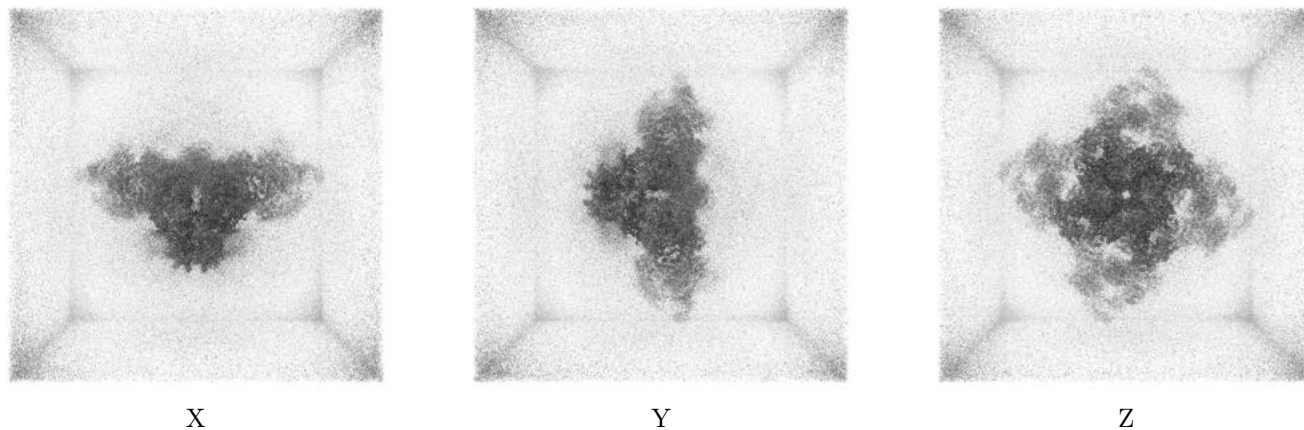
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

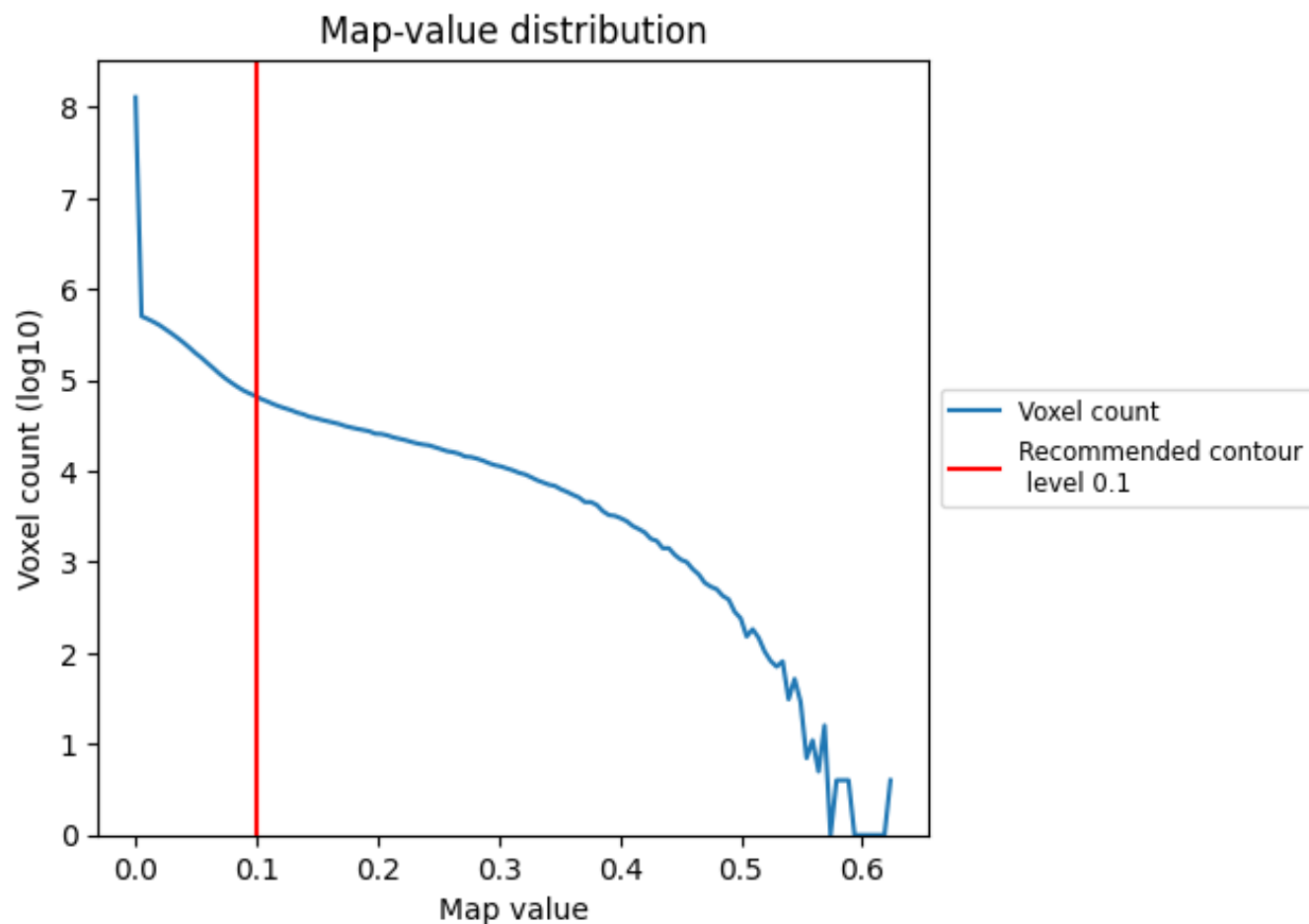
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

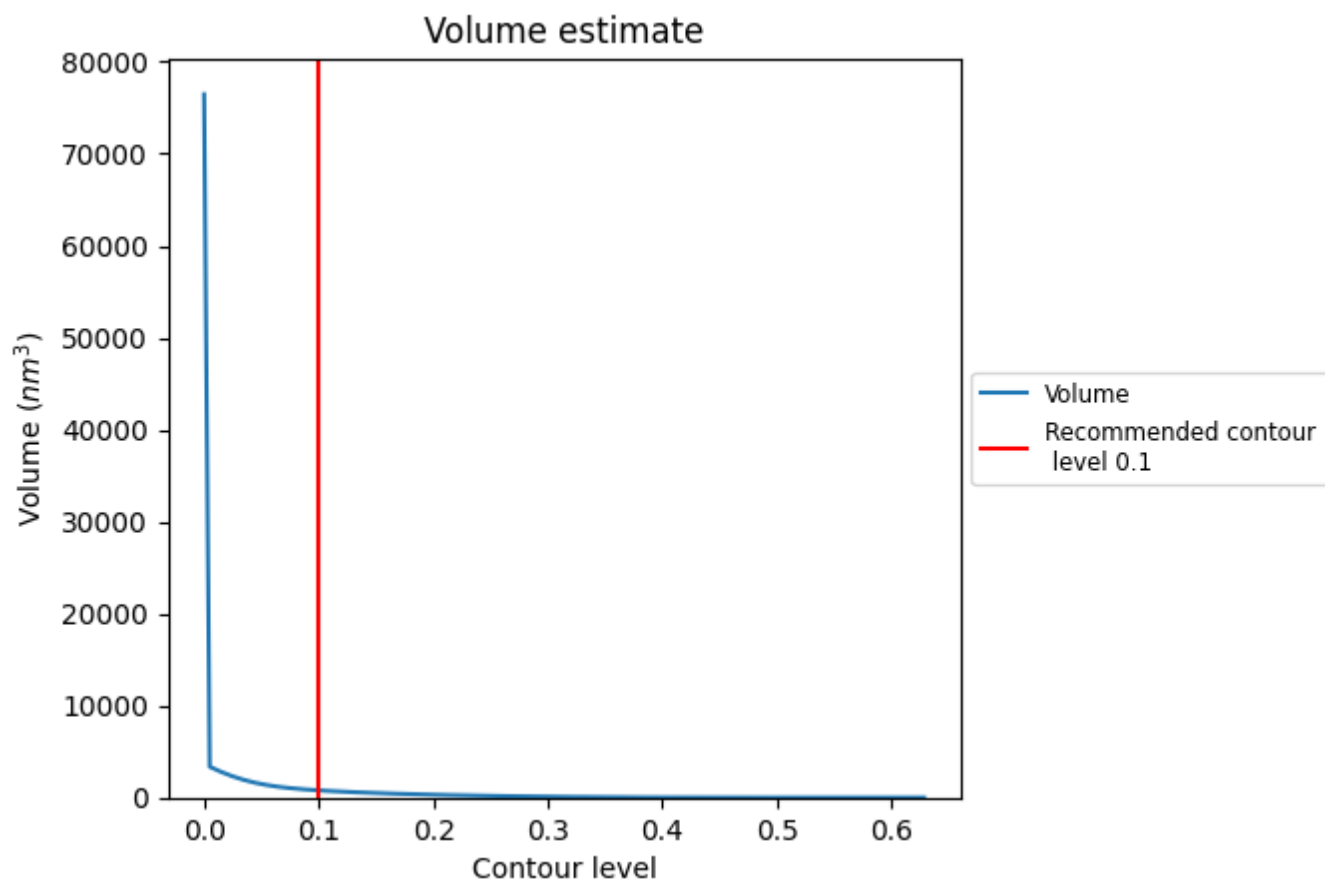
This section contains the results of statistical analysis of the map.

### 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.

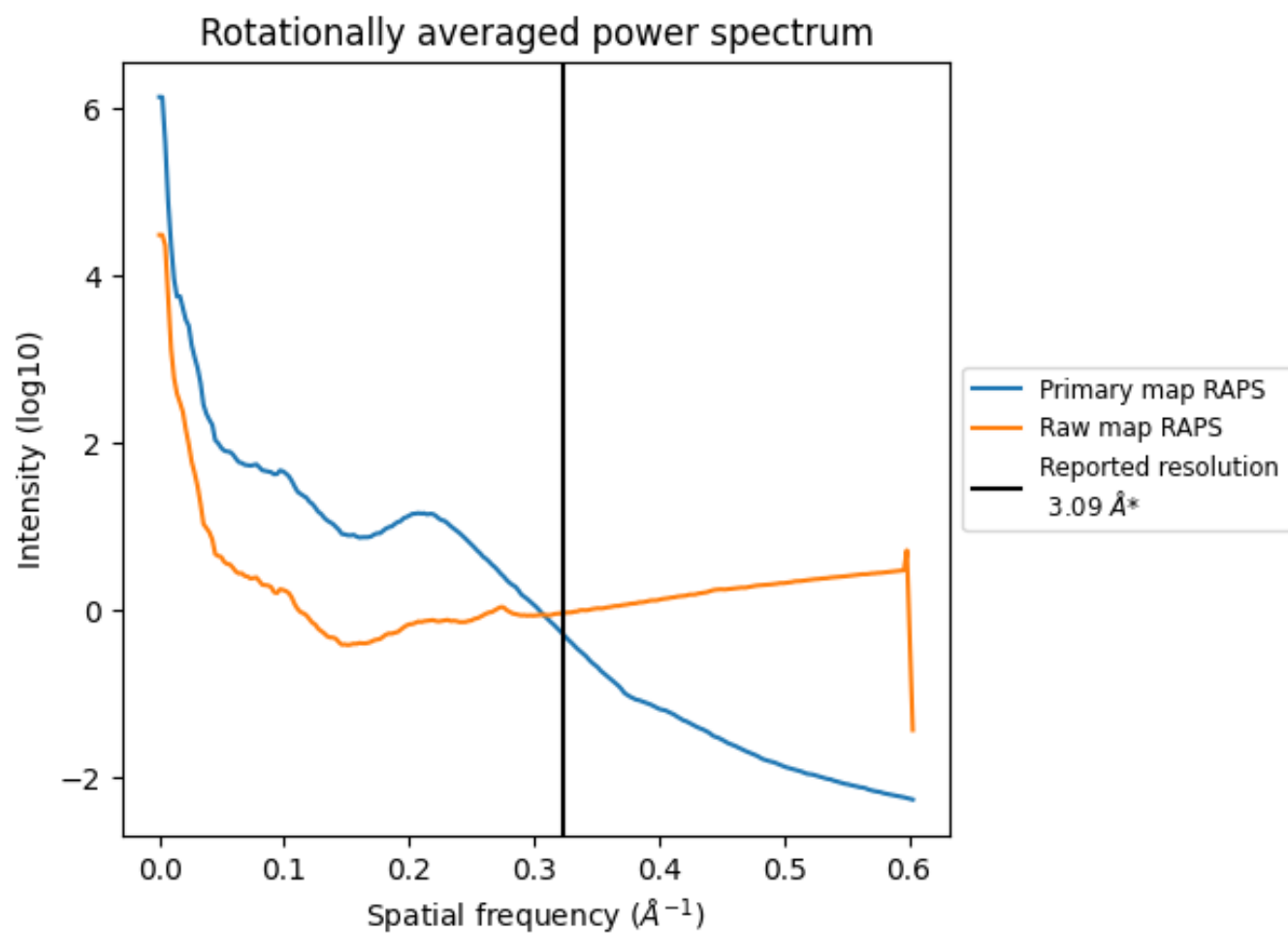
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm<sup>3</sup>; this corresponds to an approximate mass of 707 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 ⓘ

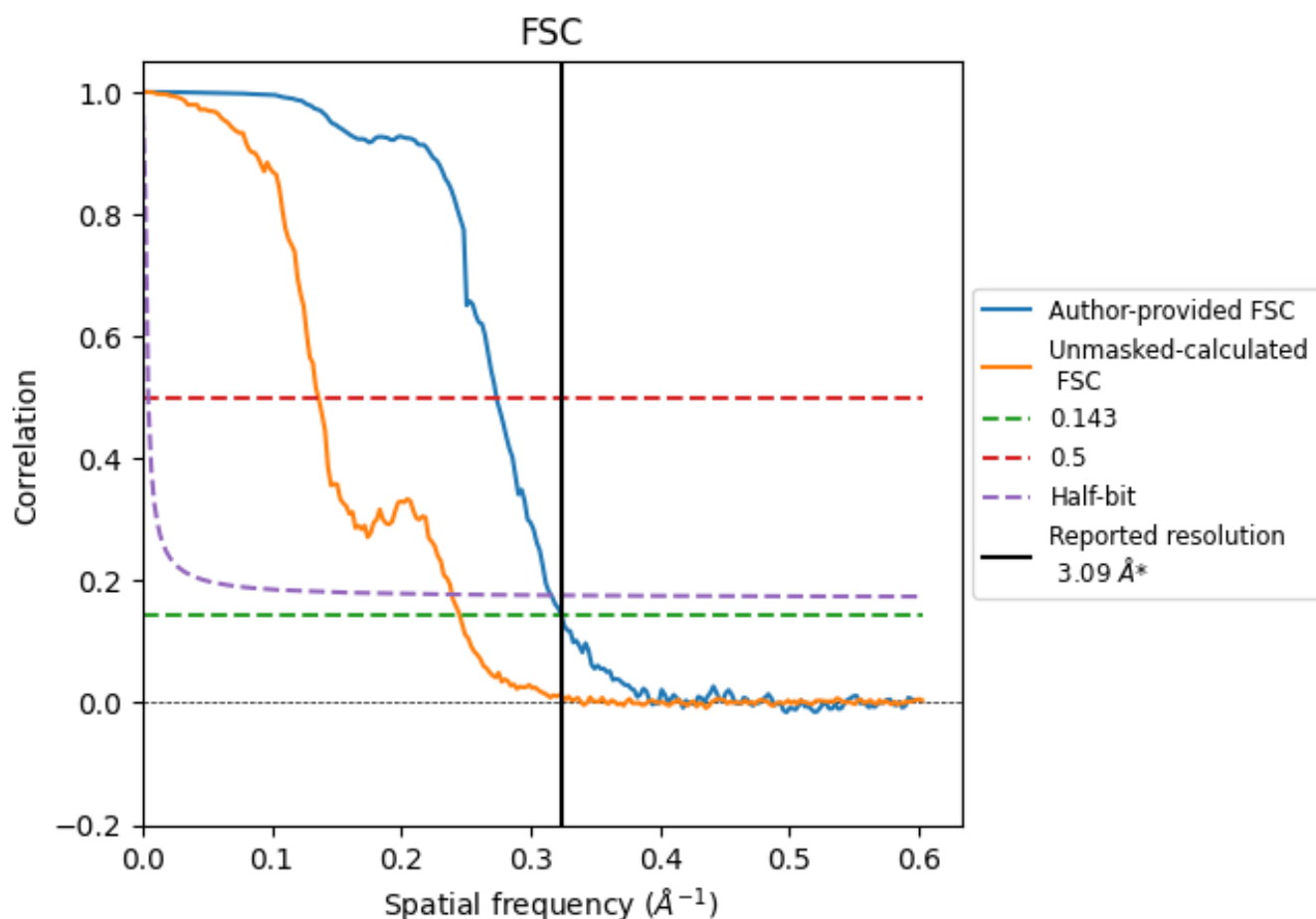


\*Reported resolution corresponds to spatial frequency of 0.324  $\text{\AA}^{-1}$

## 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  $0.324 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.16
Unmasked-calculated*	4.08	7.35	4.18

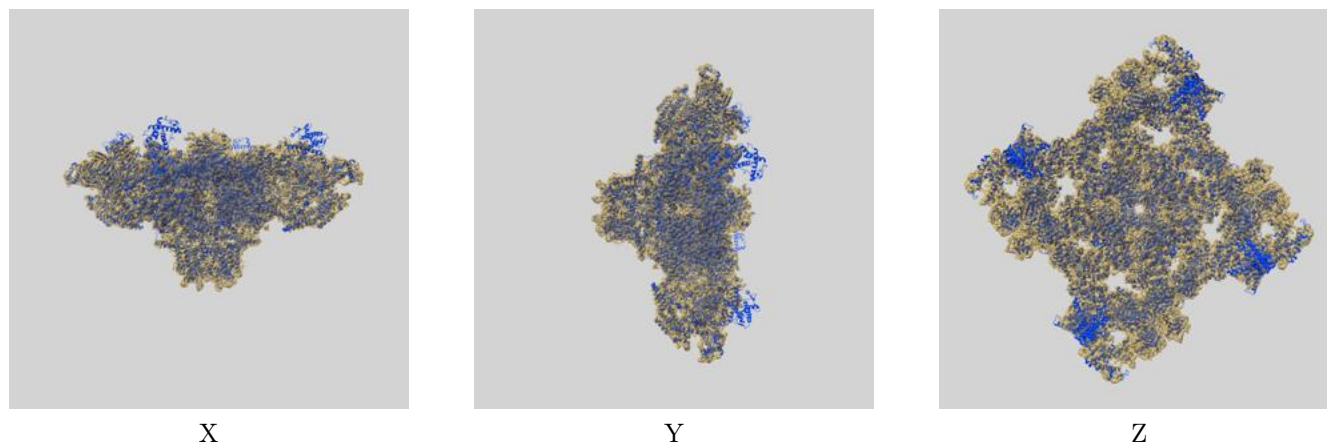
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.09 by more than 10 %



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

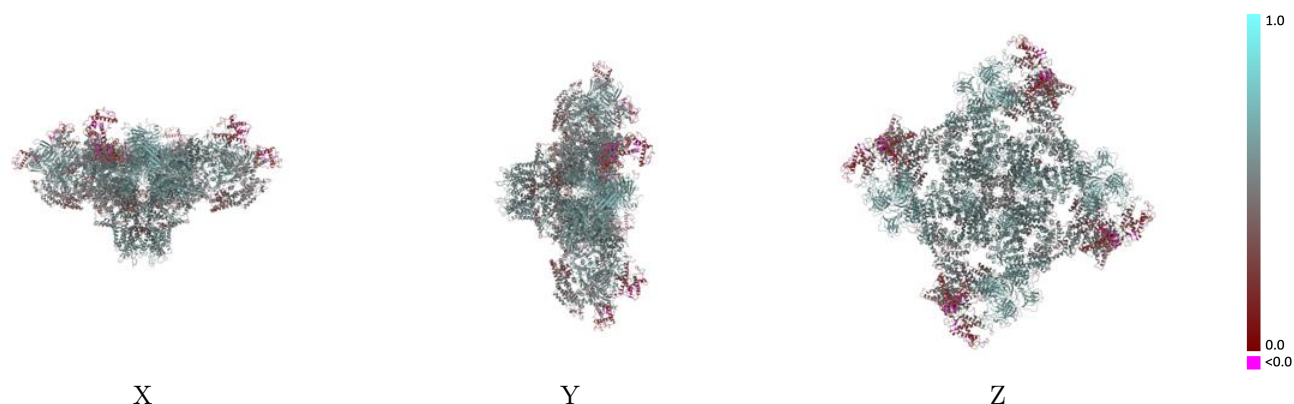
This section contains information regarding the fit between EMDB map EMD-49536 and PDB model 9NMP. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

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



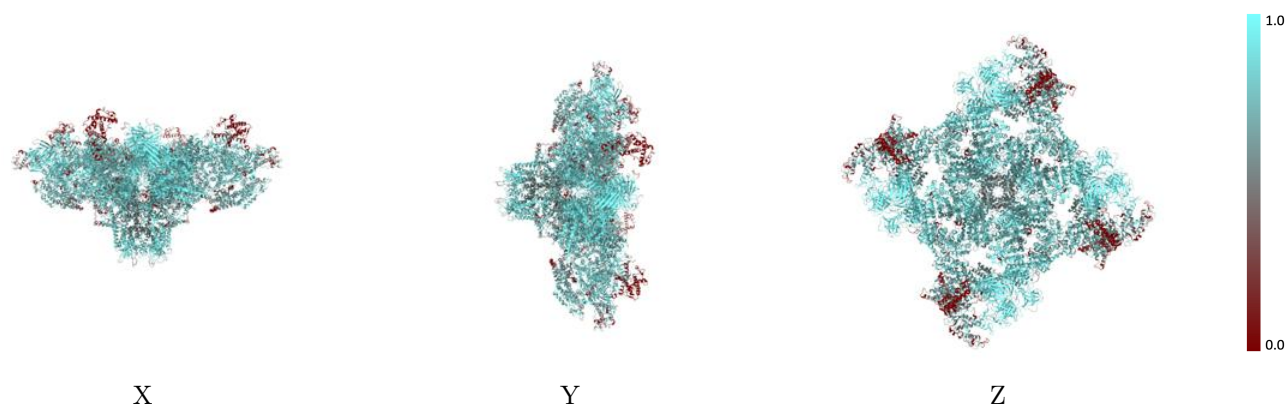
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



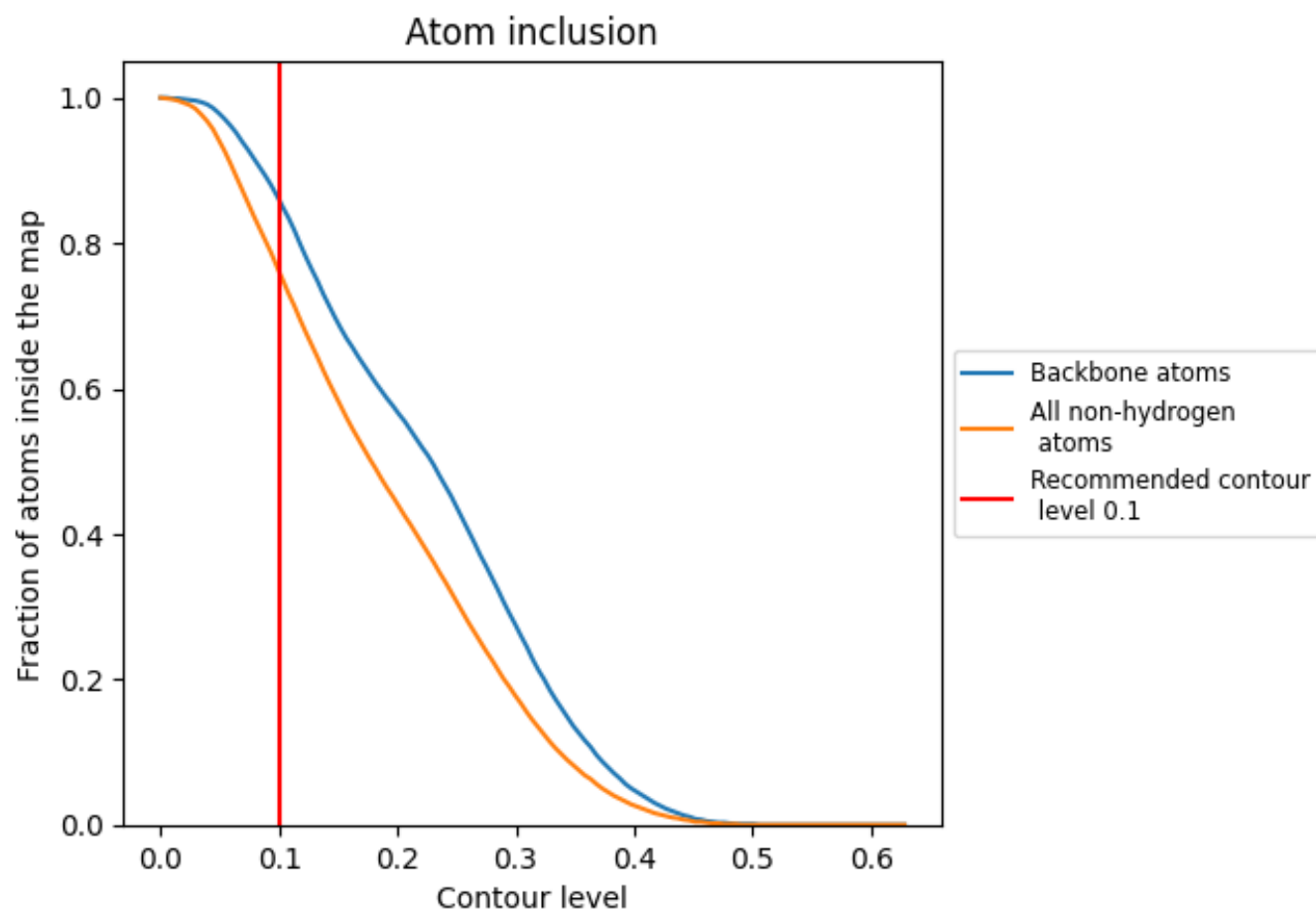
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7610	<div></div> 0.5090
A	<div></div> 0.7600	<div></div> 0.5080
B	<div></div> 0.7580	<div></div> 0.5070
C	<div></div> 0.7580	<div></div> 0.5070
D	<div></div> 0.7580	<div></div> 0.5070
E	<div></div> 0.8810	<div></div> 0.5870
F	<div></div> 0.8840	<div></div> 0.5890
G	<div></div> 0.8770	<div></div> 0.5850
H	<div></div> 0.8840	<div></div> 0.5910

1.0

0.0

<0.0