



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2025 – 12:14 PM EDT

PDB ID : 9NMN / pdb_00009nmn
EMDB ID : EMD-49534
Title : Structure of mouse RyR1 (Ca²⁺/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

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.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

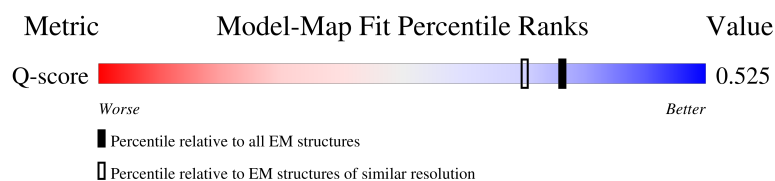
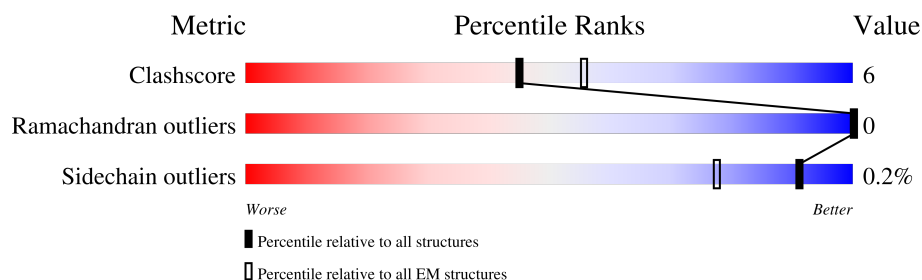
1 Overall quality at a glance

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5035	
1	B	5035	
1	C	5035	
1	D	5035	

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Mol	Chain	Length	Quality of chain
2	E	108	 87% 12% •
2	F	108	 88% 11% •
2	G	108	 89% 10% •
2	H	108	 89% 10% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143248 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 Ryanodine receptor 1.

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

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

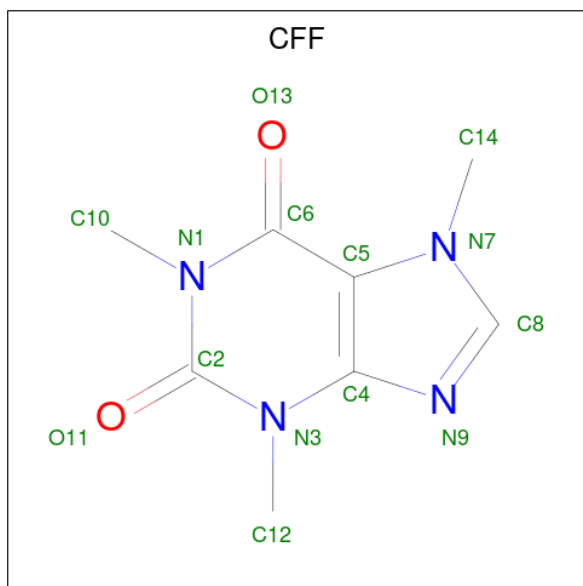
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

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

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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂) (labeled as "Ligand of

Interest" by depositor).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

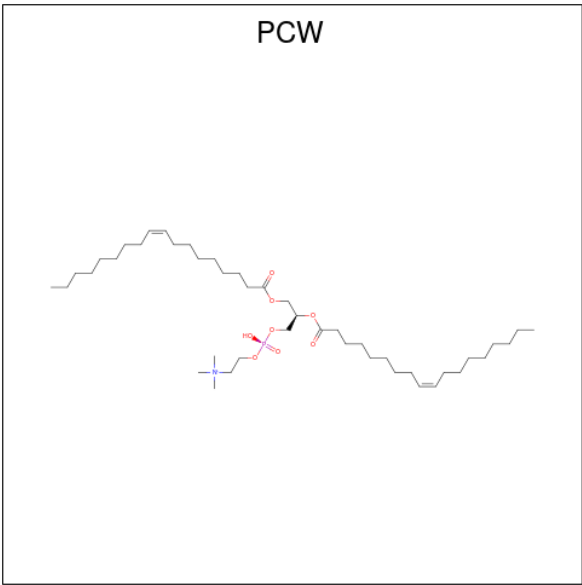
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	1	Total Ca 1 1	0
6	C	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).

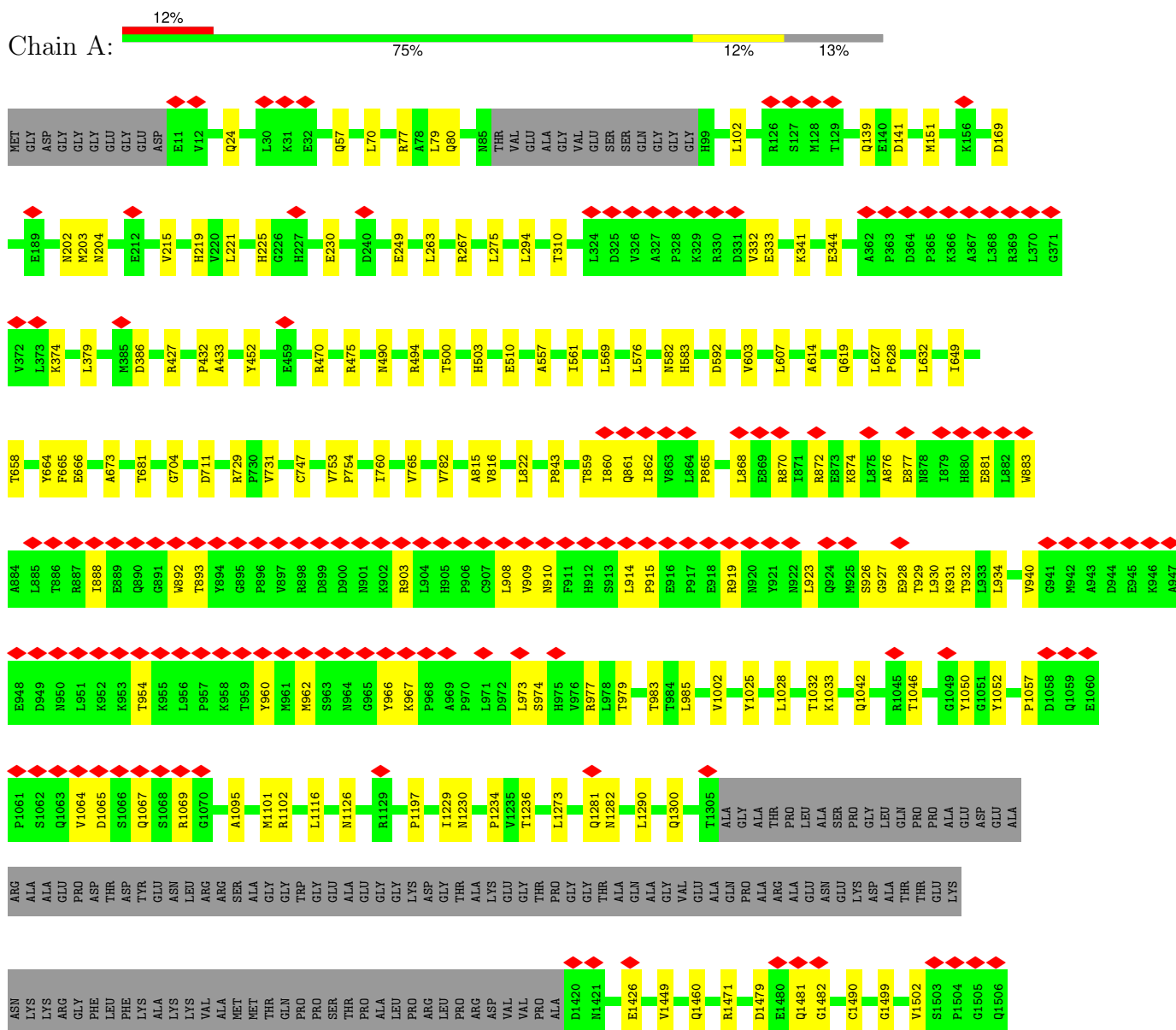


Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	A	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	B	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	B	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	C	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	C	1	Total	C	N	O	P	0	
			54	44	1	8	1		
7	D	1	Total	C	N	O	P	0	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

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1

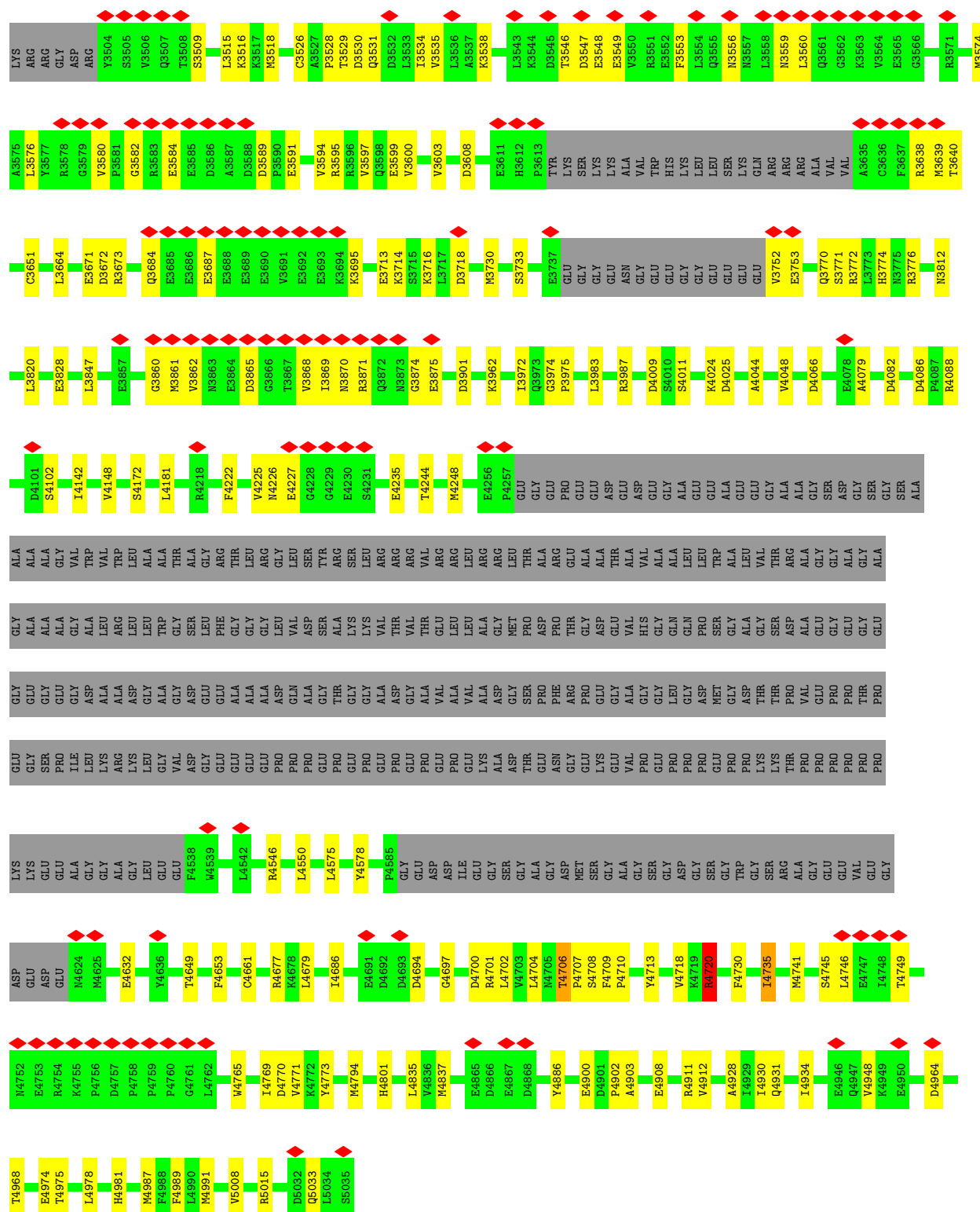




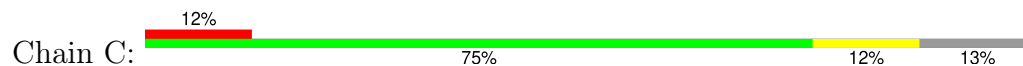




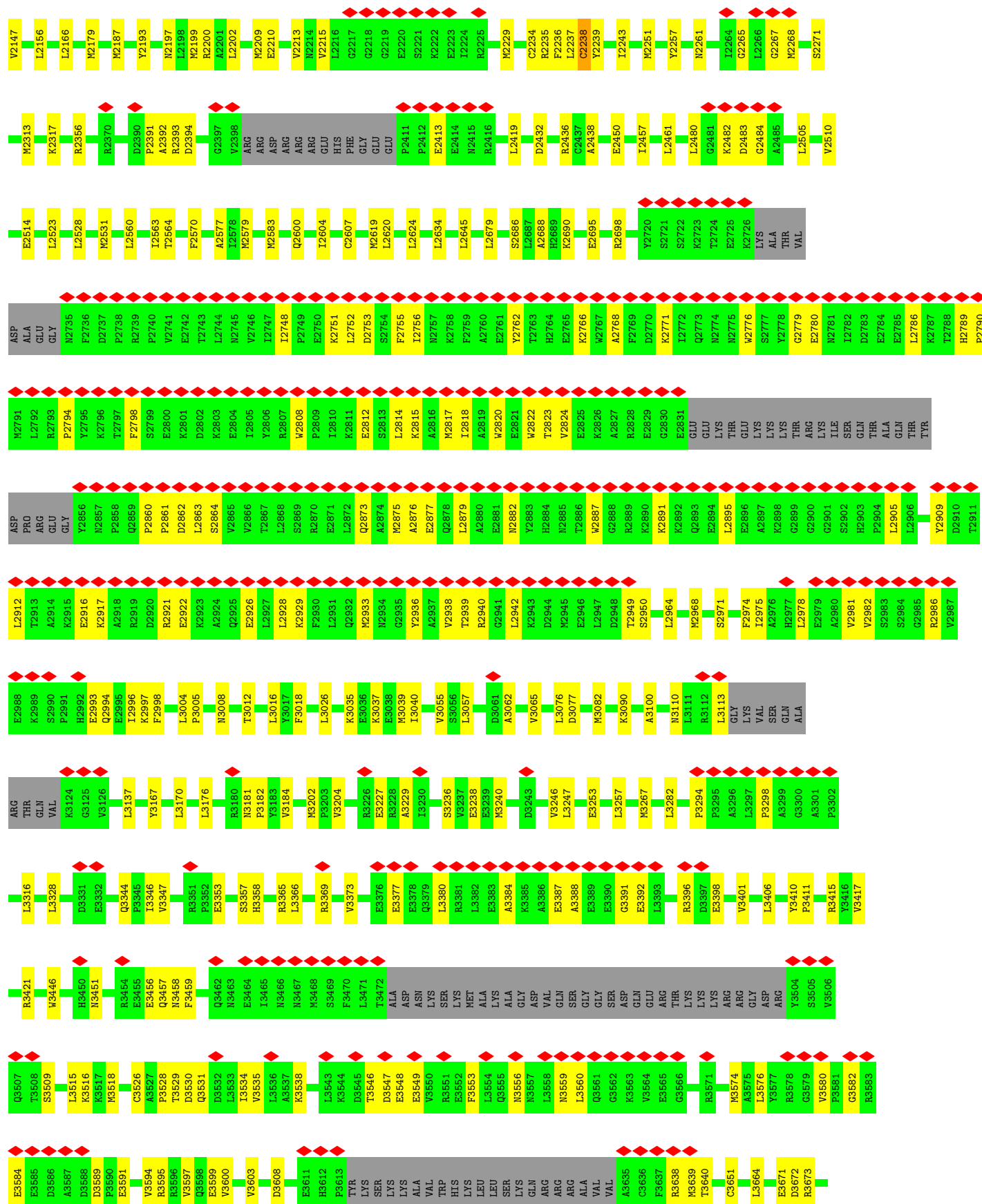
Y3410	P3298	L3113	V2981	F2904	E2784	T2724	A2485	N2261	Q2128	D2018	GLU
P3411	A3299	LYS	V2982	L2905	E2785	E2725	K2490	G2264	L2132	C2022	ALA
R3415	G3300	VAL	S2983	L2906	L2786	K2726	L2605	L2265	L2136	P2025	LYS
Y3416	A3301	SER	S2984	Y2909	K2787	ALA	V2610	L2266	L2139	R2029	ASP
Y3417	P3302	GLN	G2985	D2910	H2788	THR	E2514	G2267	P2140	I2045	GLU
R3421	L3316	ALA	R2986	T2911	H2789	VAL	E2523	M2268	V2147	Q2046	LYS
Y3424	L3328	ARG	V2987	L2912	P2790	ASP	L2623	S2271	L2156	L2047	GLU
K3446	L3328	GLN	E2988	T2913	M2791	ALA	L2628	M2313	L2166	GLU	ALA
H3450	D3331	VAL	K2989	A2914	R2793	GLY	L2631	K2317	L2166	GLY	GLU
H3451	E3332		S2990	K2915	P2794		M2531	R2356	L2179	GLU	ASP
R3454	Q3344		E2916	E2916	Y2795	D2737	L2660	R2370	M2187	GLU	ALA
I3455	P3345		H2992	K2917	K2796	P2738	I2663	D2391	Y2193	GLU	GLU
I3456	I3346		Q2994	A2918	P2797	R2739	T2664	P2392	L2198	PRO	GLU
I3457	V3347		Q2995	R2919	F2798	R2740	F2670	A2393	GLU	GLU	LYS
I3458	R3351		I2996	D2920	S2799	V2741	E2577	R2393	L2199	GLU	GLU
F3459	P3352		K2997	R2921	E2800	E2742	M2579	D2394	R2200	THR	GLU
	E3353		F2998	E2922	K2801	T2743	M2583	L2202	L2202	SER	GLU
	L3354			K2923	D2802	L2744	Q2600	G2397	ARG	ARG	
	R3355			A2924	K2803	L2745	I2604	V2398	E2210	LEU	
	I3356			Q2925	E2804	V2746	L2620	ARG	E1964	MET	
	H3358			E2926	R2805	I2747	L2624	ASP	C1965	SER	
	R3365			L2927	Y2806	L2748	L2634	LEU	K1969	LEU	
	L3366			K2928	R2807	P2749	L2645	ARG	N1973	GLU	
	R3369			L2929	W2808	E2750	L2679	ARG	Q1974	LYS	
	V3373			F2930	I2810	K2751	M2619	GLU	Y1978	LYS	
	E3376			L2931	K2811	L2752	L2624	GLU	L1981	LYS	
	E3377			K2932	E2812	D2753	L2634	P2411	A1984	THR	
	E3378			M2933	S2813	S2754	L2645	P2412	F1985	GLU	
	Q3379			N2934	L2814	F2755	L2679	E2413	T1986	LYS	
	L3380			Q2935	K2815	L2756	S2686	E2414	M1987	PRO	
	R3381			G2936	A2816	N2757	L2687	N2415	S1988	GLU	
	L3382			V2938	M2817	K2758	A2688	R2416	A1989	GLU	
	E3383			T2939	L2818	F2759	H2689	L2419	A1990	PRO	
	A3384			R2940	I2819	A2760	K2690	A2438	E1991	PRO	
	K3385			G2941	A2819	E2761	E2695	E2450	T1992	GLU	
	K3386			L2942	W2820	K2762	R2698	I2457	A1993	GLU	
	A3387			K2943	E2821	Y2763	L2687	L2461	R1995	GLU	
	E3388			D2944	W2822	H2764	A2688	L2480	F1999	GLU	
	E3389			M2945	T2823	E2765	K2690	M2251	R2000	GLU	
	E3390			E2946	V2824	K2766	E2695	Y2257	S2001	GLU	
	G3391			L2947	E2825	N2767	R2698	L2124	P2002	GLU	
	E3392			D2948	K2826	A2768	Y2720		Q2006	GLU	
	L3393			T2949	A2827	F2769	S2721				
	P3294			S2950	R2828	D2770	S2722				
	P3295			L2964	E2829	K2771	K2723				
	A3296			M2968	G2830	L2772					
	R3397				E2831	Q2773					
	E3398				GLU	N2774					
	V3401				GLU	W2775					
	L3406				THR	W2776					
					LYS	S2777					
					GLU	G2778					
					LYS	Q2779					
					LYS	E2780					
					THR	N2781					
					ARG	L2782					
					LYS	D2783					

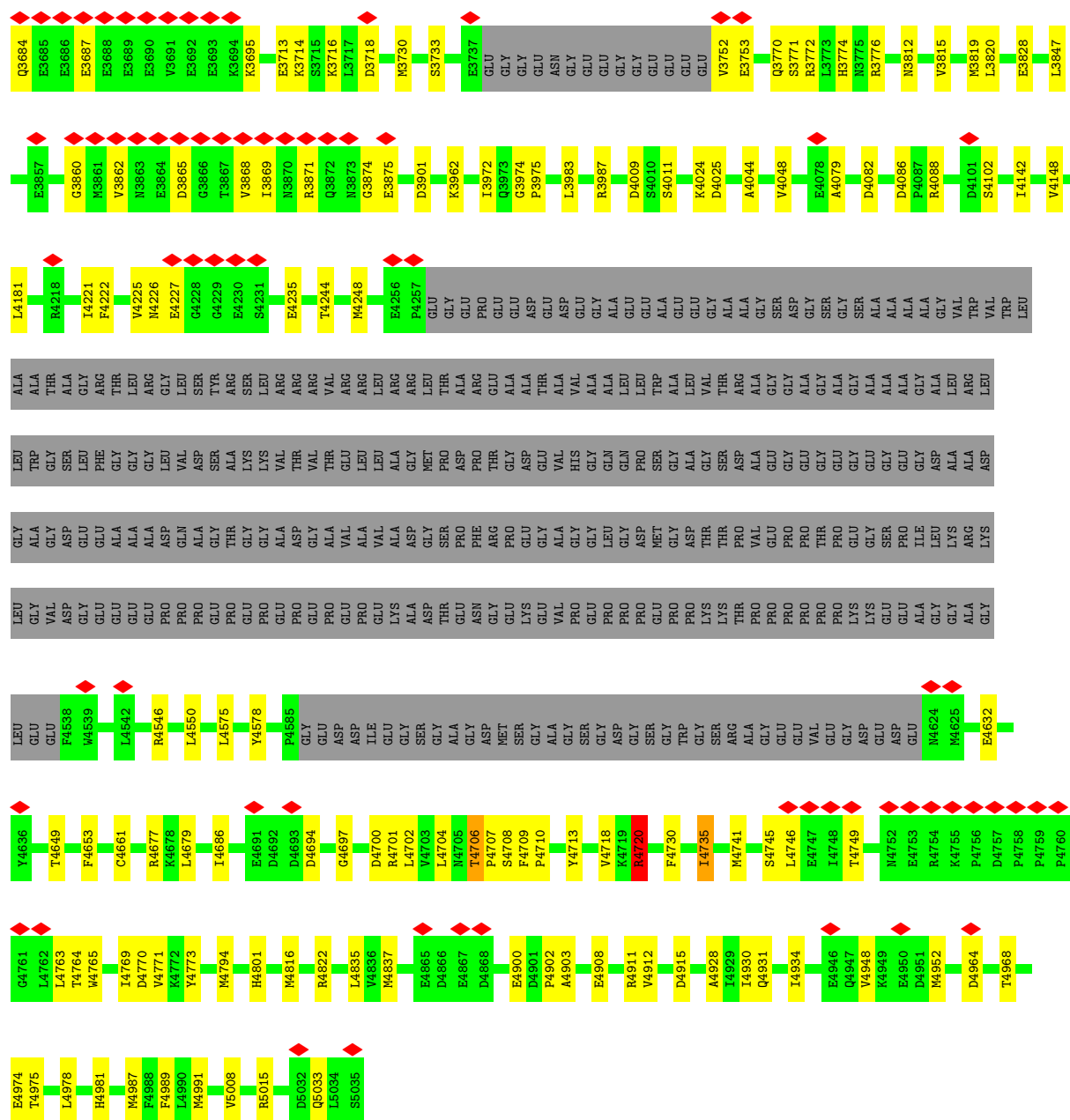


• Molecule 1: Ryanodine receptor 1

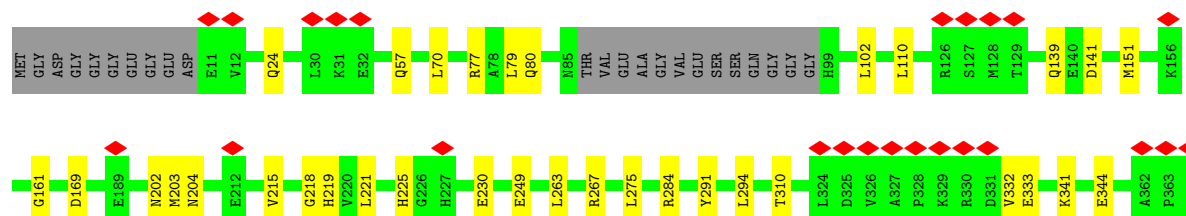
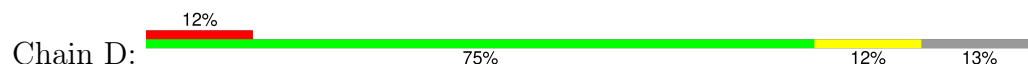






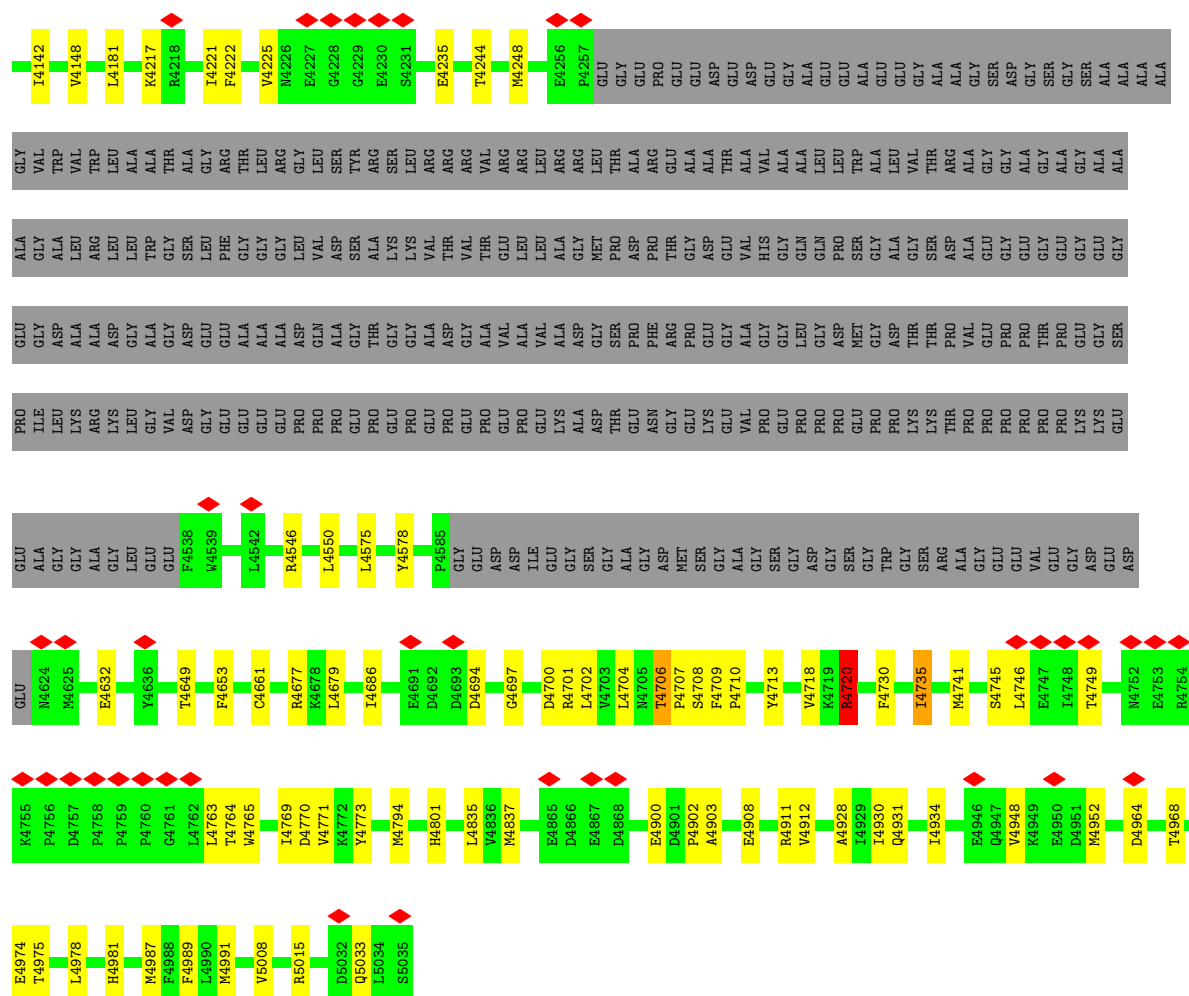


● Molecule 1: Ryanodine receptor 1



M2268	L2139	R2029	E1756	G1N	Q1042	L934	K874	L607	P365
S2271	P2140	T2045	D1757	PRO	Q1045	H939	L875	A614	K366
V2281	V2147	G2046	G1758	ALA	T1046	V940	A877	L627	A367
M2313	L2156	L2047	G1481	ALA	G1049	G941	N878	P628	L368
K2317	L2166	GLY	G1482	ASN	G1051	M942	I879	L632	R369
R2356	M2179	GLU	G1499	GLU	G1052	A943	H880	I649	L370
R2370	M2187	ALA	V1502	ASP	P1057	E945	L882	T658	G371
D2390	Y2193	GLU	S1503	THR	D1058	K946	W883	K374	V372
P2391	N2197	GLU	P1504	GLU	E1059	A947	A884	L379	L373
A2392	L2198	GLU	G1505	GLU	E1060	E948	L885	L379	L373
R2393	M2199	GLU	Q1506	ASN	P1061	D949	T886	M385	D386
D2394	R2200	GLU	Q1507	GLY	S1062	N950	R887	R427	R427
G2397	A2201	THR	Q1508	ALA	Q1063	L951	I888	P432	P432
V2398	L2202	LEU	R1509	ARG	V1064	K952	G891	A433	A433
ARG	M2209	ARG	I1510	PHE	D1065	T954	W892	Y452	Y452
ASP	E2210	LEU	S1511	LEU	S1066	L956	T993	E459	E459
ARG	V2213	SER	H1512	THR	Q1067	P957	D711	R470	R470
ASP	M2214	GLU	N1546	ALA	S1068	K958	Y894	R475	R475
ARG	V2215	VAL	V1555	LYS	R1069	T959	G895	M490	M490
ARG	L2216	VAL	T1558	VAL	G1070	Y960	P730	R494	R494
GLU	G2217	LYS	V1562	MET	A1095	M961	R898	T500	T500
HIS	G2218	LEU	I1642	MET	M1101	M962	D899	H503	H503
PHE	G2219	LYS	E1645	THR	R1102	N964	D900	E510	E510
GLY	E2220	LYS	N1646	GLN	L1116	G965	N901	C538	C538
GLU	S2221	THR	R1647	PRO	N1126	K967	N902	R554	R554
GLU	K2222	GLU	M1649	SER	P1129	A969	K902	L555	L555
P2411	L2223	VAL	D1659	GLU	P1197	L971	R903	V816	V816
P2412	E2224	GLU	L1677	PRO	I1229	D972	R904	L822	L822
E2413	L2225	GLU	A1685	ARG	T1235	S974	N910	P843	P843
E2414	M2229	GLU	L1695	VAL	T1236	H975	F911	T859	T859
N2415	C2234	GLU	R1703	ALA	L1273	V976	H912	I860	I860
R2416	F2235	GLU	L1716	ARG	Q1281	T979	L914	Q861	Q861
L2419	R2236	ALA	E1734	THR	N1282	P980	P915	I862	I862
A2438	F2237	PRO	T1740	VAL	L1290	T983	P917	V863	V863
E2450	C2238	ASP	R1744	VAL	Q1300	L985	P918	L864	L864
I2457	Y2239	GLU	G1752	ALA	T1305	T988	P919	P865	P865
L2461	L2096	GLU	R1753	D1420	ALA	T984	R918	L868	L868
L2480	L2124	GLU	S1754	N1421	GLY	L985	R919	E869	E869
G2481	Q2128	GLU	A1755	E1426	THR	L985	N920	H582	H582
K2482	L2132	ALA		V1449	ALA	T985	Y921	R370	R370
D2483	L2136	HIS		Q1460	GLN	L985	R922	I871	I871
G2484	L2136	LYS		R1471	VAL	L985	N922	R872	R872
A2485		GLU			GLU	L985	E873	V603	V603
L2505		GLU			ALA	L985			
					THR	L985			





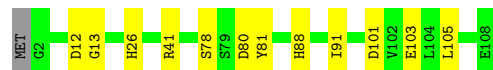
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 87% 12%



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 88% 11%




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 89% 10%



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:  89% 10% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26588	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	0.463	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.776, 427.776, 427.776	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8355, 0.8355, 0.8355	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/35586	0.36	4/48203 (0.0%)
1	B	0.20	0/35586	0.36	4/48203 (0.0%)
1	C	0.20	0/35586	0.36	4/48203 (0.0%)
1	D	0.20	0/35586	0.36	4/48203 (0.0%)
2	E	0.17	0/847	0.34	0/1142
2	F	0.17	0/847	0.32	0/1142
2	G	0.18	0/847	0.33	0/1142
2	H	0.18	0/847	0.33	0/1142
All	All	0.20	0/145732	0.36	16/197380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2237	LEU	CA-C-N	8.49	134.18	120.60
1	C	2237	LEU	C-N-CA	8.49	134.18	120.60
1	A	2237	LEU	CA-C-N	8.48	134.16	120.60
1	A	2237	LEU	C-N-CA	8.48	134.16	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2237	LEU	CA-C-N	8.48	134.16	120.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4701	ARG	Sidechain
1	A	4720	ARG	Sidechain
1	B	4701	ARG	Sidechain
1	B	4720	ARG	Sidechain
1	C	4701	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	A	34797	0	34384	428	0
1	B	34797	0	34384	432	0
1	C	34797	0	34384	425	0
1	D	34797	0	34384	427	0
2	E	829	0	826	11	0
2	F	829	0	826	11	0
2	G	829	0	826	10	0
2	H	829	0	826	9	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	2	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	0	0
7	B	108	0	168	0	0
7	C	108	0	168	1	0
7	D	108	0	168	1	0
All	All	143248	0	141648	1734	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 6.

The worst 5 of 1734 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2234:CYS:SG	1:D:2271:SER:OG	2.24	0.94
1:A:2234:CYS:SG	1:A:2271:SER:OG	2.24	0.94
1:B:2234:CYS:SG	1:B:2271:SER:OG	2.24	0.94
1:C:2234:CYS:SG	1:C:2271:SER:OG	2.24	0.94
1:C:2879:LEU:HD12	1:C:2928:LEU:HD21	1.55	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4345/5035 (86%)	4201 (97%)	144 (3%)	0	100	100
1	B	4345/5035 (86%)	4200 (97%)	145 (3%)	0	100	100
1	C	4345/5035 (86%)	4203 (97%)	142 (3%)	0	100	100
1	D	4345/5035 (86%)	4201 (97%)	144 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17800/20572 (86%)	17210 (97%)	590 (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	A	3806/4296 (89%)	3799 (100%)	7 (0%)	92	96
1	B	3806/4296 (89%)	3799 (100%)	7 (0%)	92	96
1	C	3806/4296 (89%)	3799 (100%)	7 (0%)	92	96
1	D	3806/4296 (89%)	3799 (100%)	7 (0%)	92	96
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15580/17544 (89%)	15552 (100%)	28 (0%)	91	96

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	219	HIS
1	D	4771	VAL
1	C	4718	VAL
1	D	4718	VAL
1	C	4706	THR

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

Mol	Chain	Res	Type
1	D	2963	GLN
1	D	3557	ASN
1	B	1632	GLN
1	B	1591	GLN
1	D	3892	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	B	8002	-	8,15,15	2.08	3 (37%)	8,23,23	1.40	1 (12%)
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	D	8002	-	8,15,15	2.08	3 (37%)	8,23,23	1.40	1 (12%)
4	CFF	C	8002	-	8,15,15	2.08	3 (37%)	8,23,23	1.39	1 (12%)
5	ATP	B	8007	-	28,33,33	0.65	0	34,52,52	0.92	1 (2%)
4	CFF	A	8002	-	8,15,15	2.08	3 (37%)	8,23,23	1.39	1 (12%)
5	ATP	C	8007	-	28,33,33	0.65	0	34,52,52	0.92	1 (2%)
5	ATP	A	8007	-	28,33,33	0.65	0	34,52,52	0.92	1 (2%)
5	ATP	B	8003	-	28,33,33	0.64	0	34,52,52	0.88	1 (2%)
5	ATP	C	8003	-	28,33,33	0.63	0	34,52,52	0.89	1 (2%)
7	PCW	B	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
5	ATP	A	8003	-	28,33,33	0.64	0	34,52,52	0.89	1 (2%)
5	ATP	D	8007	-	28,33,33	0.65	0	34,52,52	0.92	1 (2%)
7	PCW	C	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
5	ATP	D	8003	-	28,33,33	0.63	0	34,52,52	0.89	1 (2%)

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	B	8002	-	-	-	0/2/2/2
7	PCW	B	8006	-	-	22/57/57/57	-
7	PCW	D	8006	-	-	22/57/57/57	-
7	PCW	C	8006	-	-	22/57/57/57	-
7	PCW	A	8005	-	-	26/57/57/57	-
7	PCW	A	8006	-	-	22/57/57/57	-
4	CFF	C	8002	-	-	-	0/2/2/2
4	CFF	D	8002	-	-	-	0/2/2/2
5	ATP	B	8007	-	-	6/18/38/38	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
5	ATP	C	8007	-	-	6/18/38/38	0/3/3/3
5	ATP	A	8007	-	-	6/18/38/38	0/3/3/3
5	ATP	B	8003	-	-	4/18/38/38	0/3/3/3
5	ATP	C	8003	-	-	4/18/38/38	0/3/3/3
7	PCW	B	8005	-	-	26/57/57/57	-
5	ATP	A	8003	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	D	8007	-	-	6/18/38/38	0/3/3/3
7	PCW	C	8005	-	-	26/57/57/57	-
7	PCW	D	8005	-	-	26/57/57/57	-
5	ATP	D	8003	-	-	4/18/38/38	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8002	CFF	C5-C4	-3.44	1.33	1.39
4	D	8002	CFF	C5-C4	-3.44	1.33	1.39
4	A	8002	CFF	C5-C4	-3.42	1.33	1.39
4	C	8002	CFF	C5-C4	-3.42	1.33	1.39
4	A	8002	CFF	C6-N1	-3.26	1.32	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	8005	PCW	O2-C31-C32	4.11	120.38	111.48
7	A	8005	PCW	O2-C31-C32	4.10	120.36	111.48
7	D	8005	PCW	O2-C31-C32	4.09	120.34	111.48
7	B	8005	PCW	O2-C31-C32	4.08	120.32	111.48
7	B	8005	PCW	C21-C20-C19	4.08	155.39	124.83

There are no chirality outliers.

5 of 232 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O3A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	C	8003	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 7 short contacts:

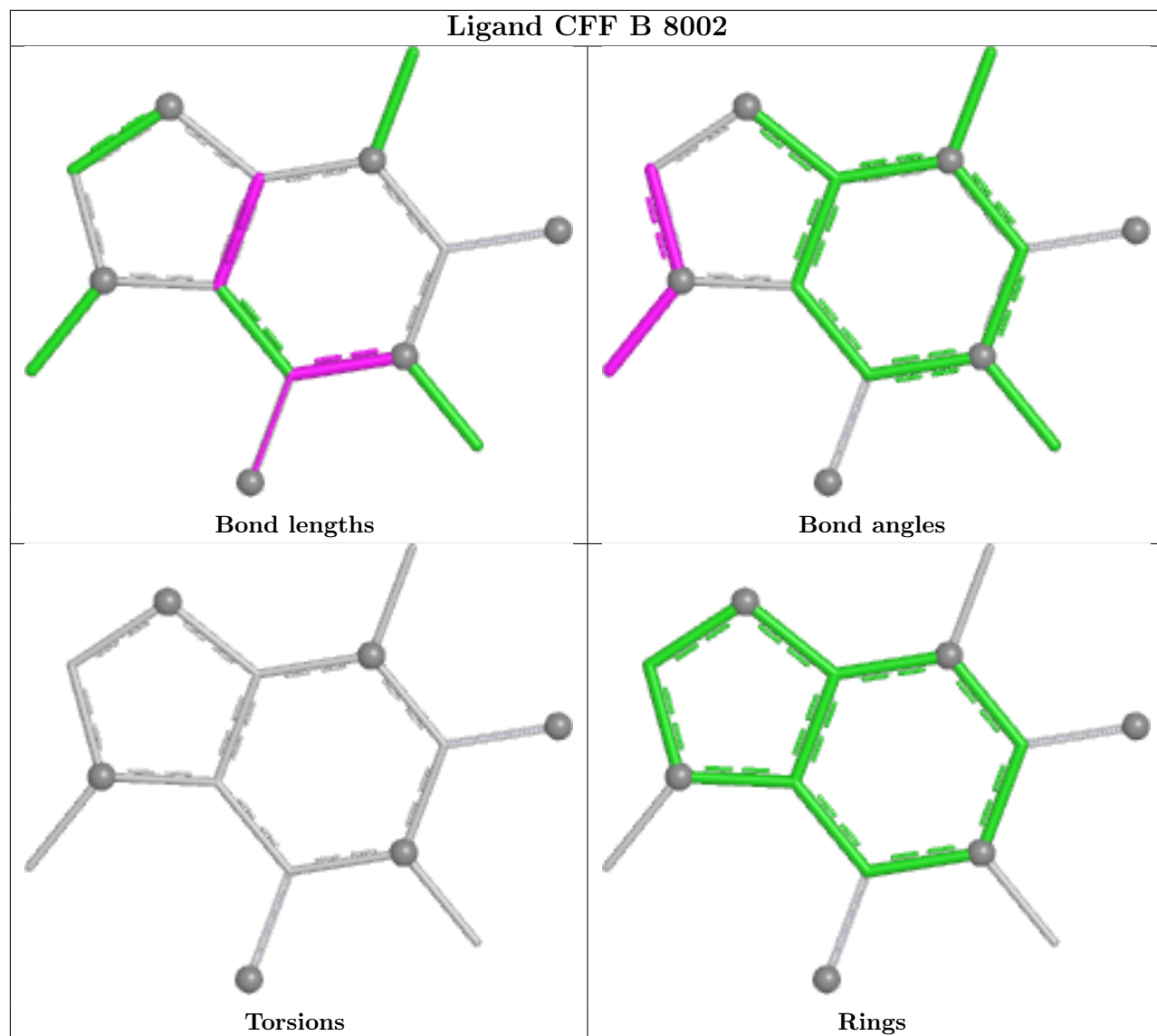
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	8006	PCW	1	0
7	C	8006	PCW	1	0
5	B	8003	ATP	1	0

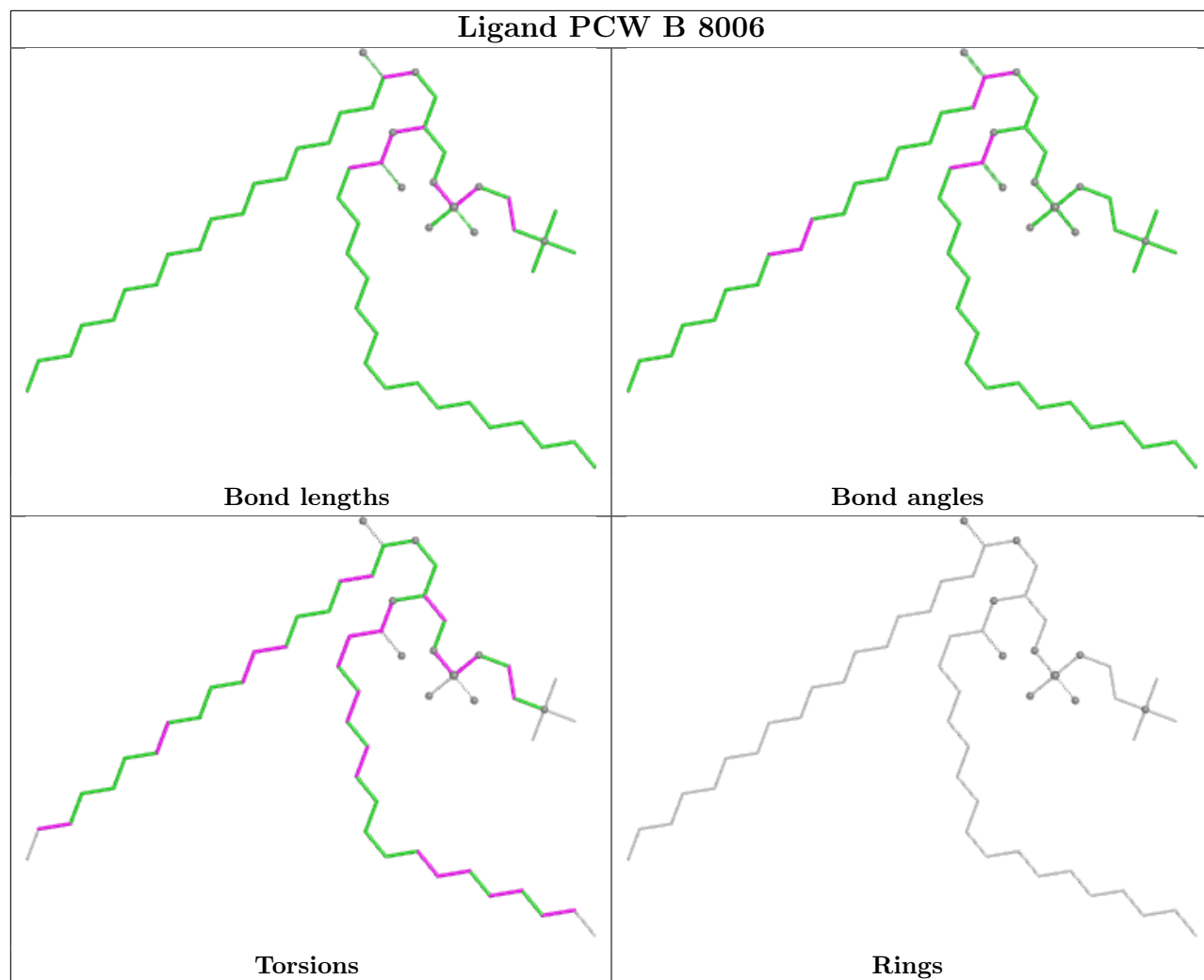
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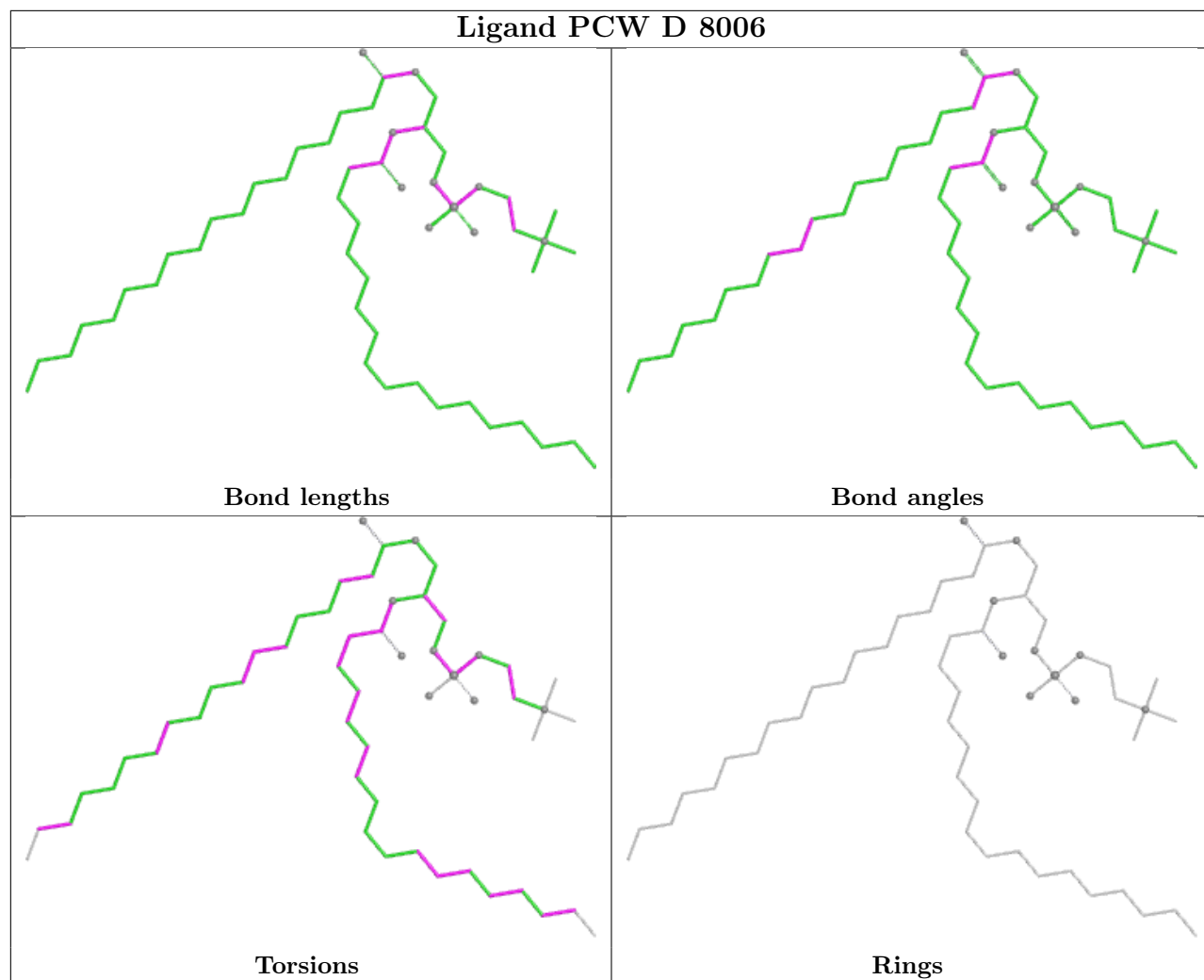
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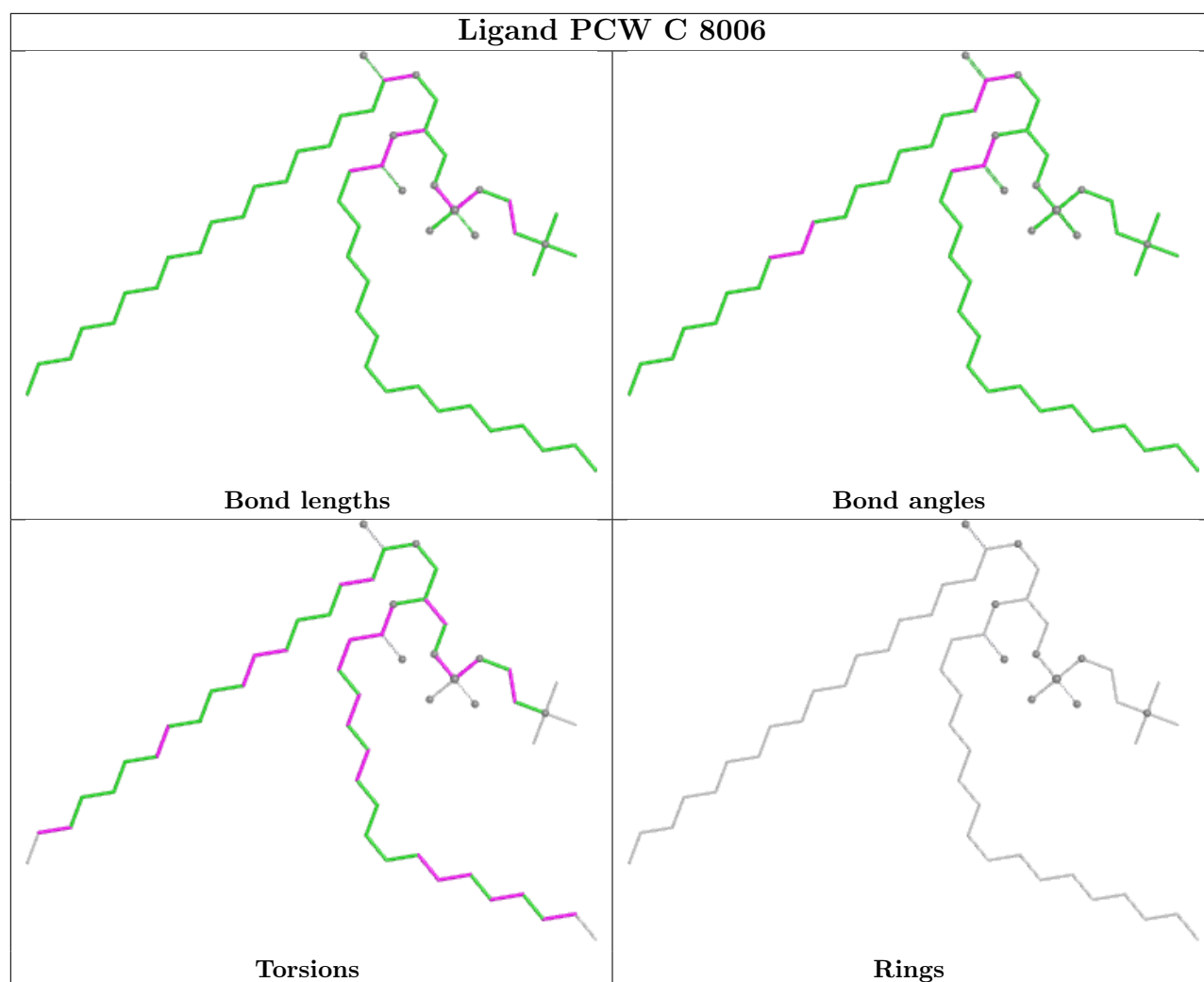
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8003	ATP	1	0
5	A	8003	ATP	1	0
5	D	8003	ATP	2	0

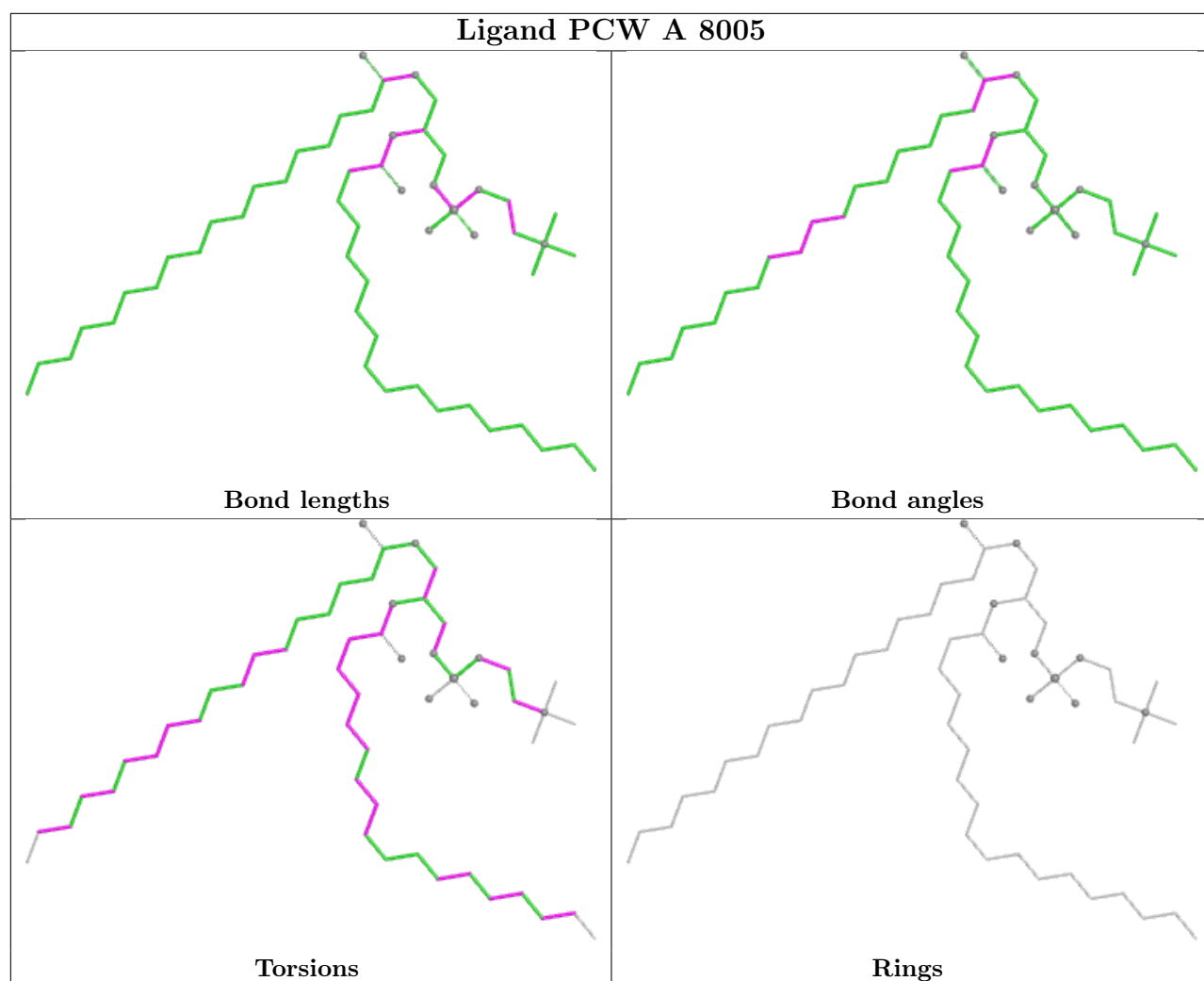
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

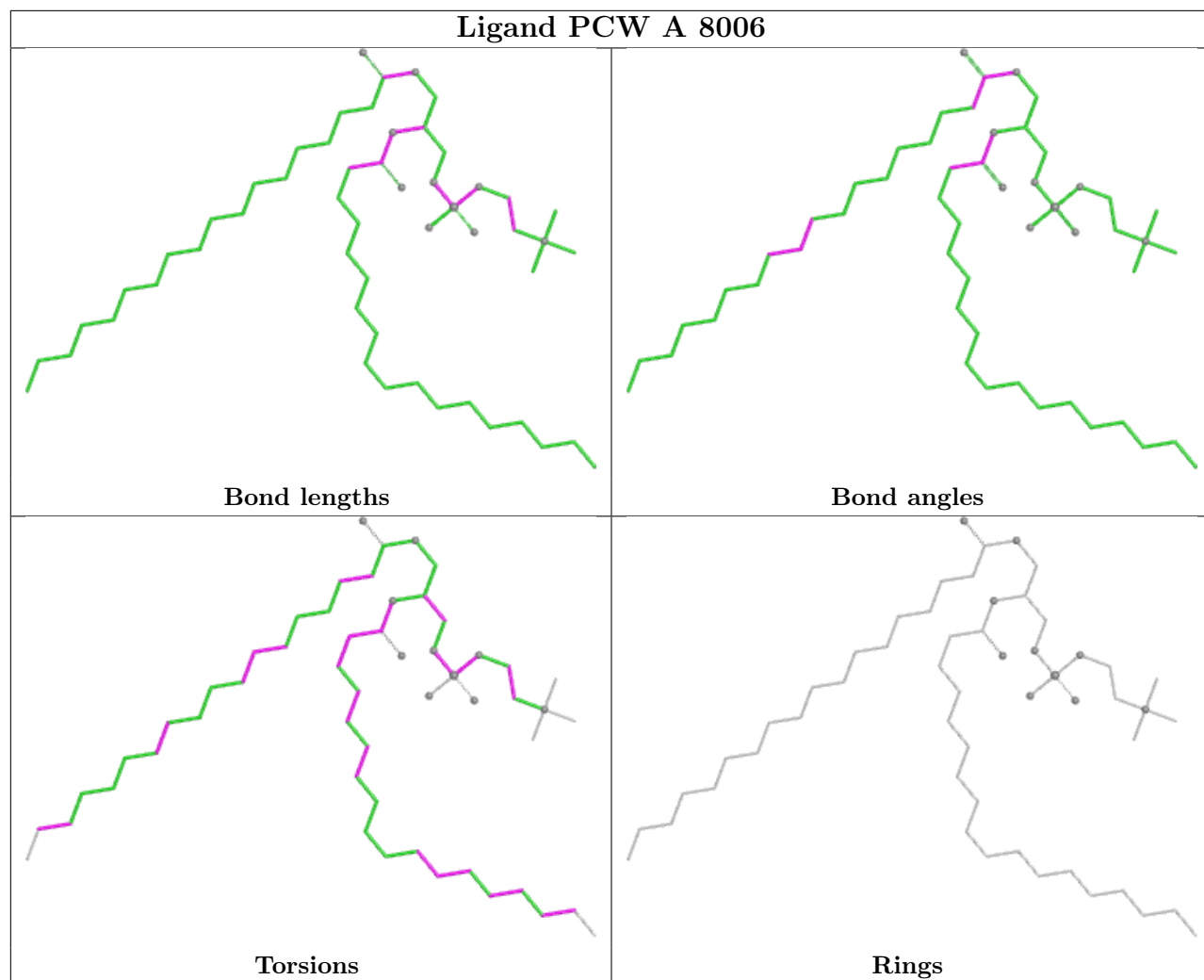


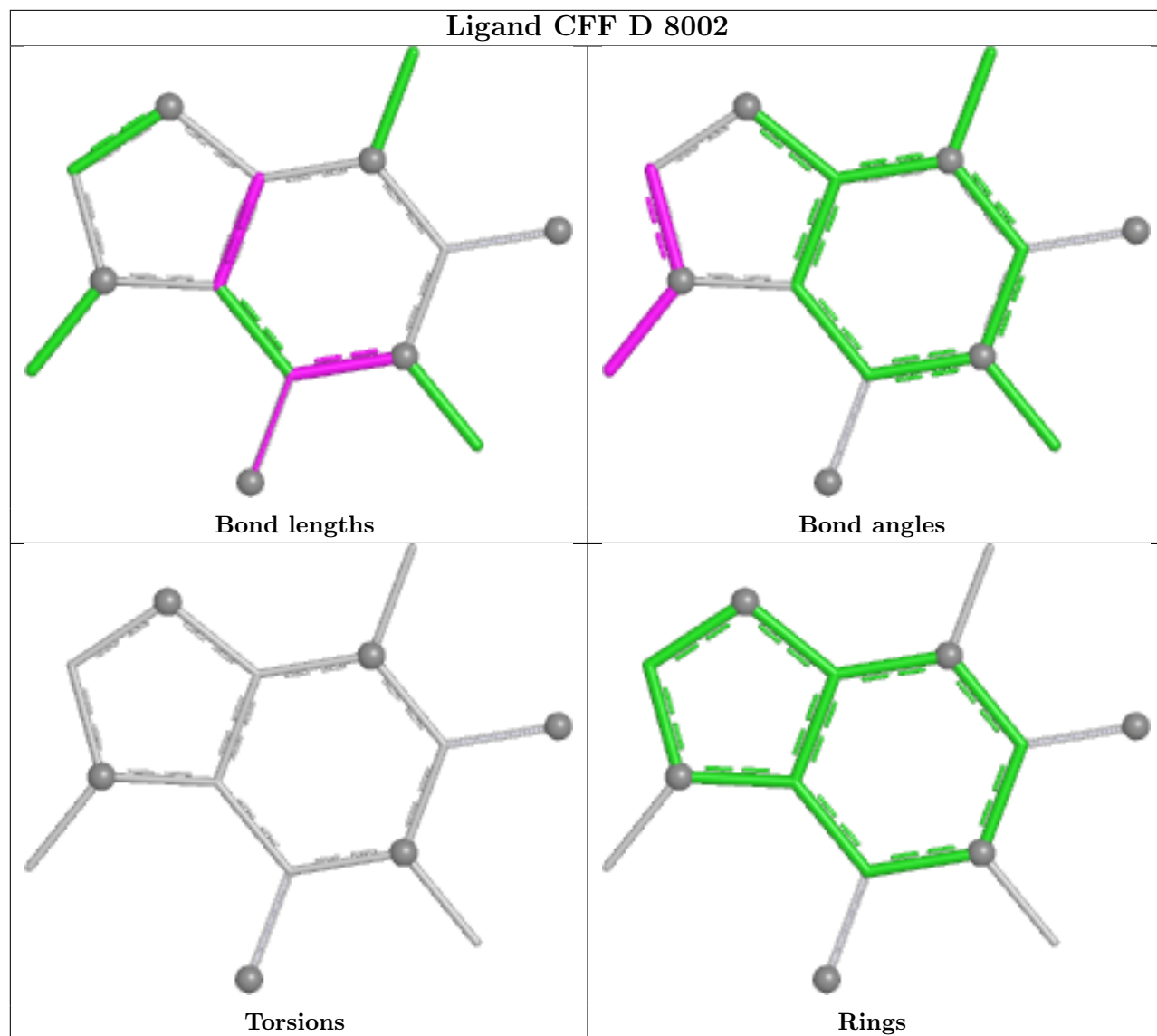


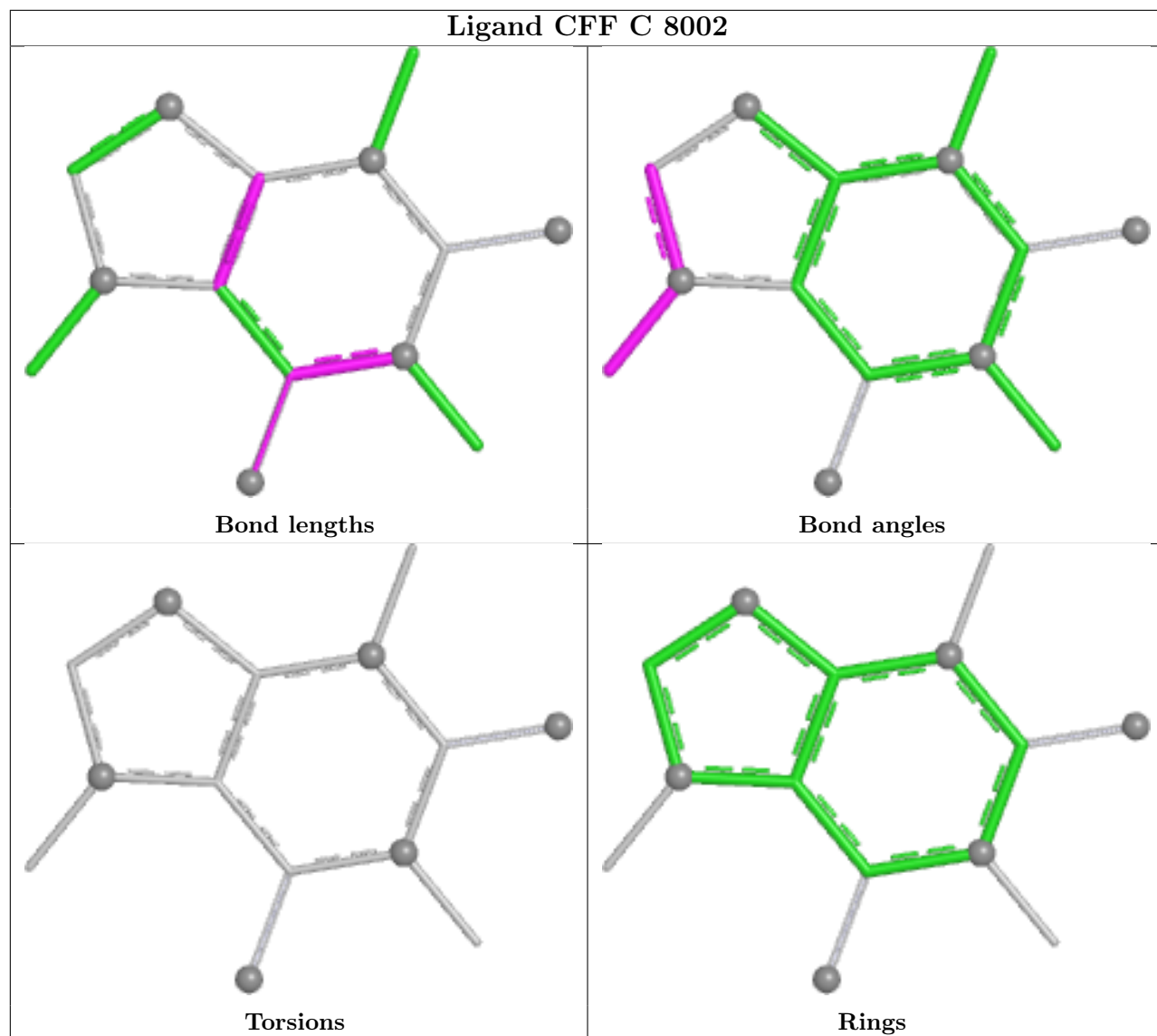


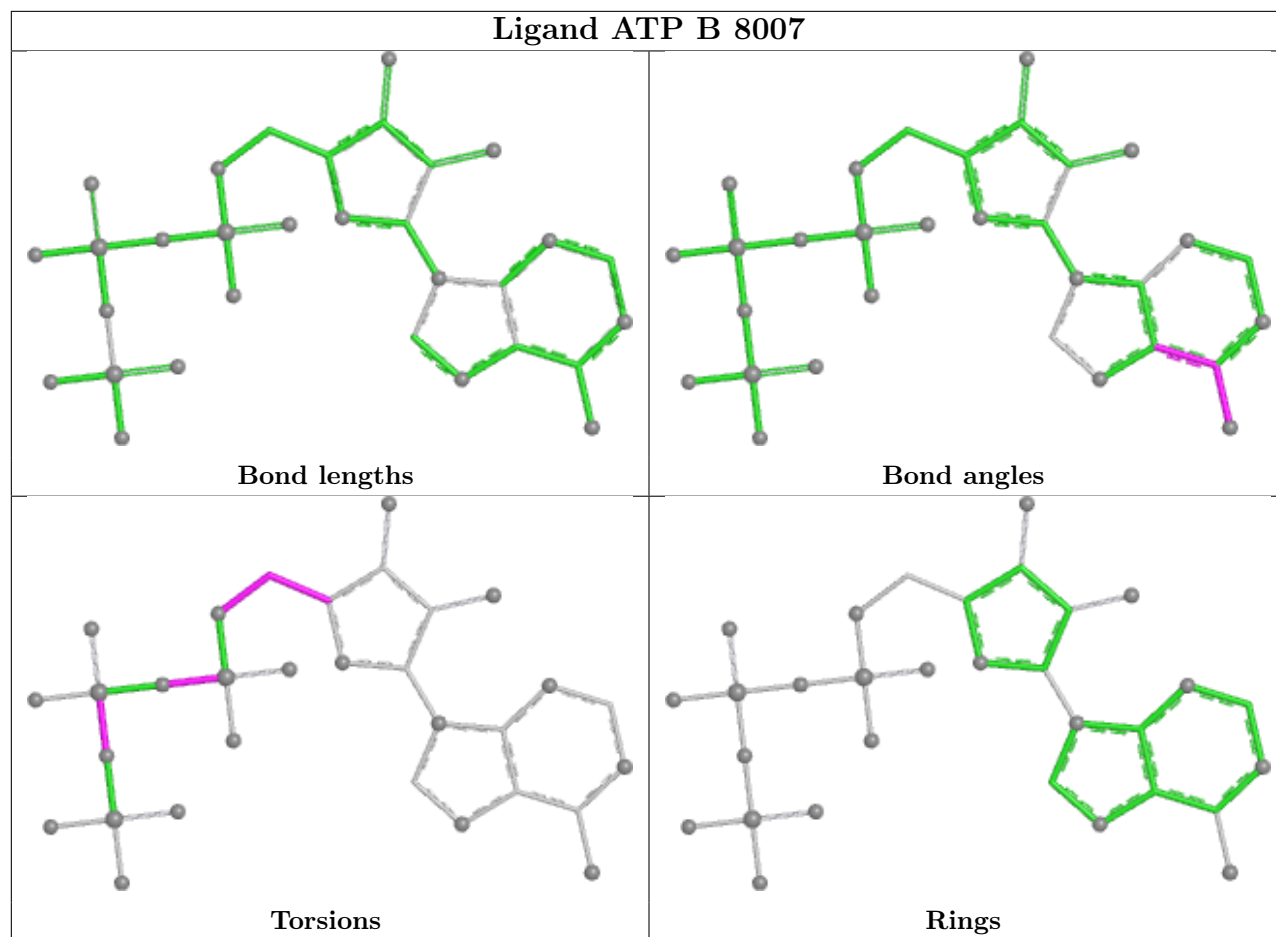


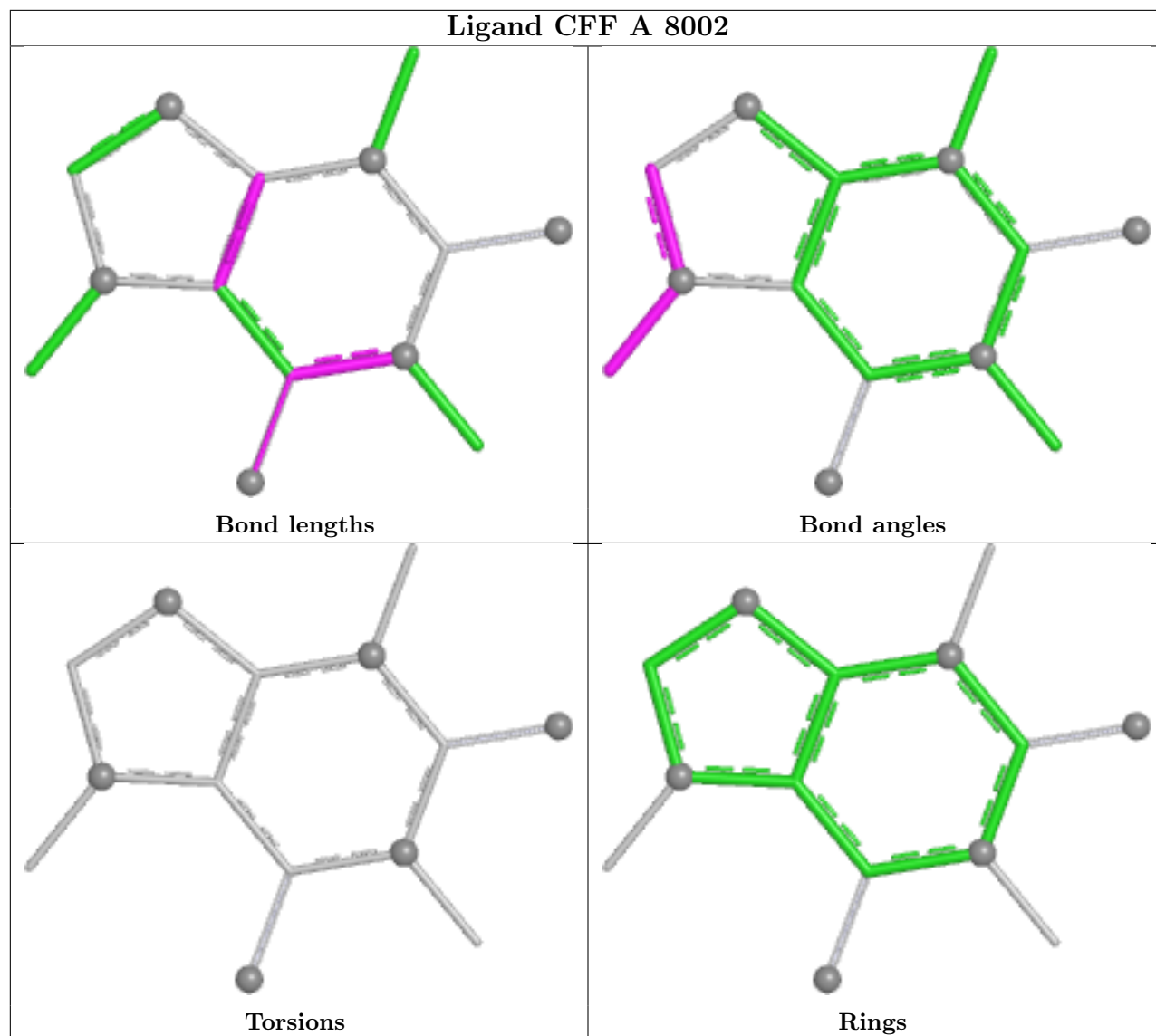


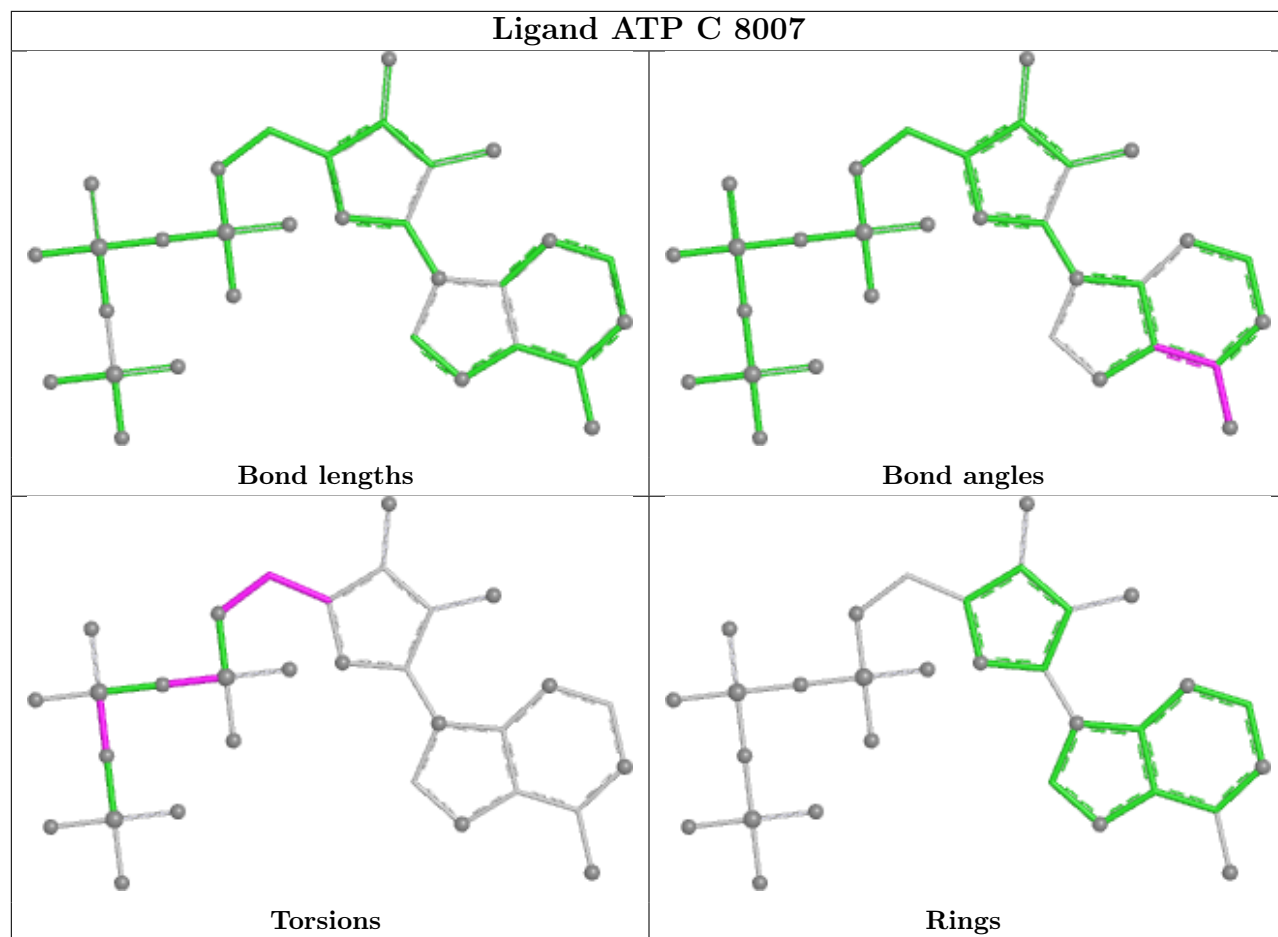


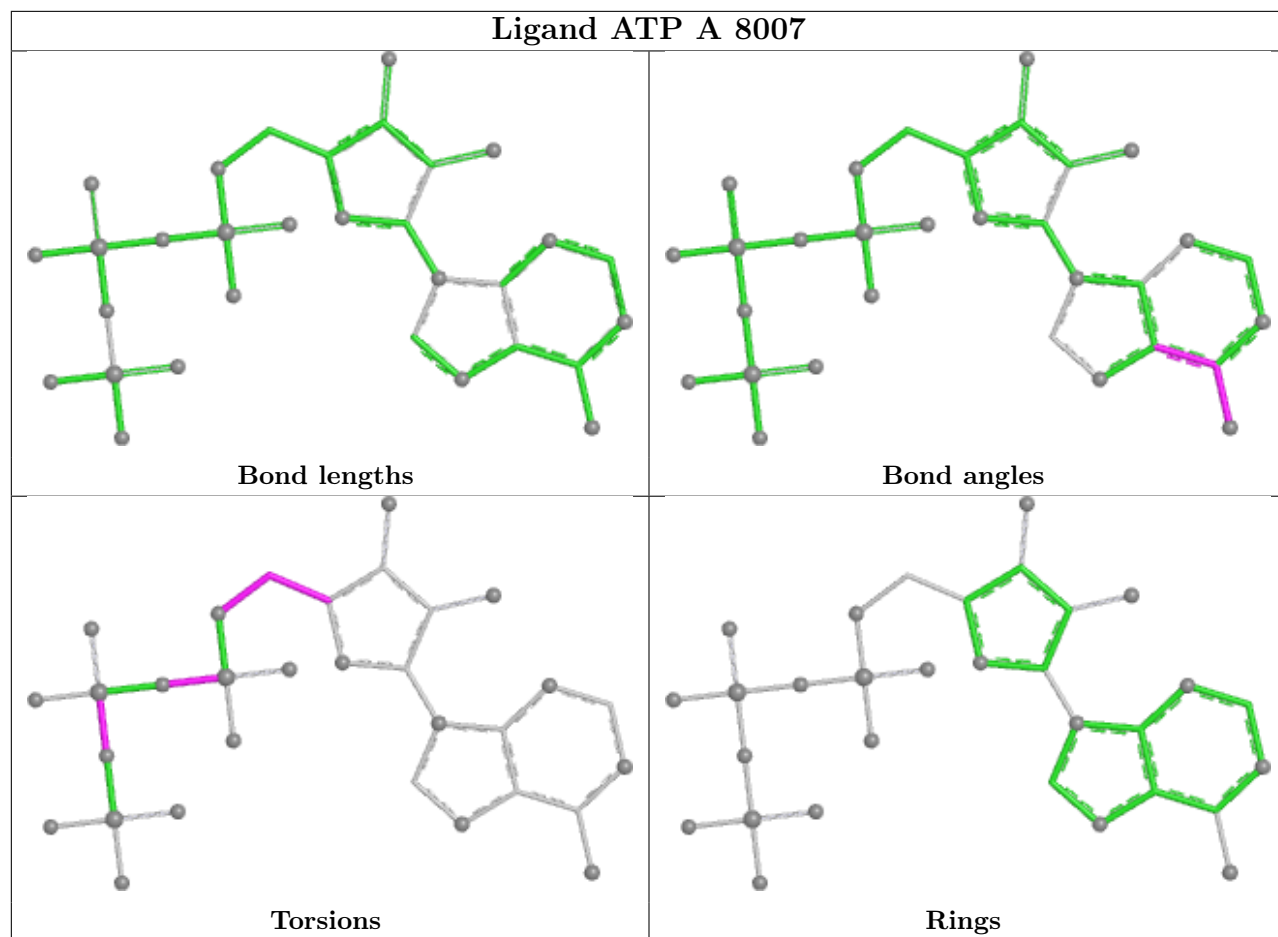


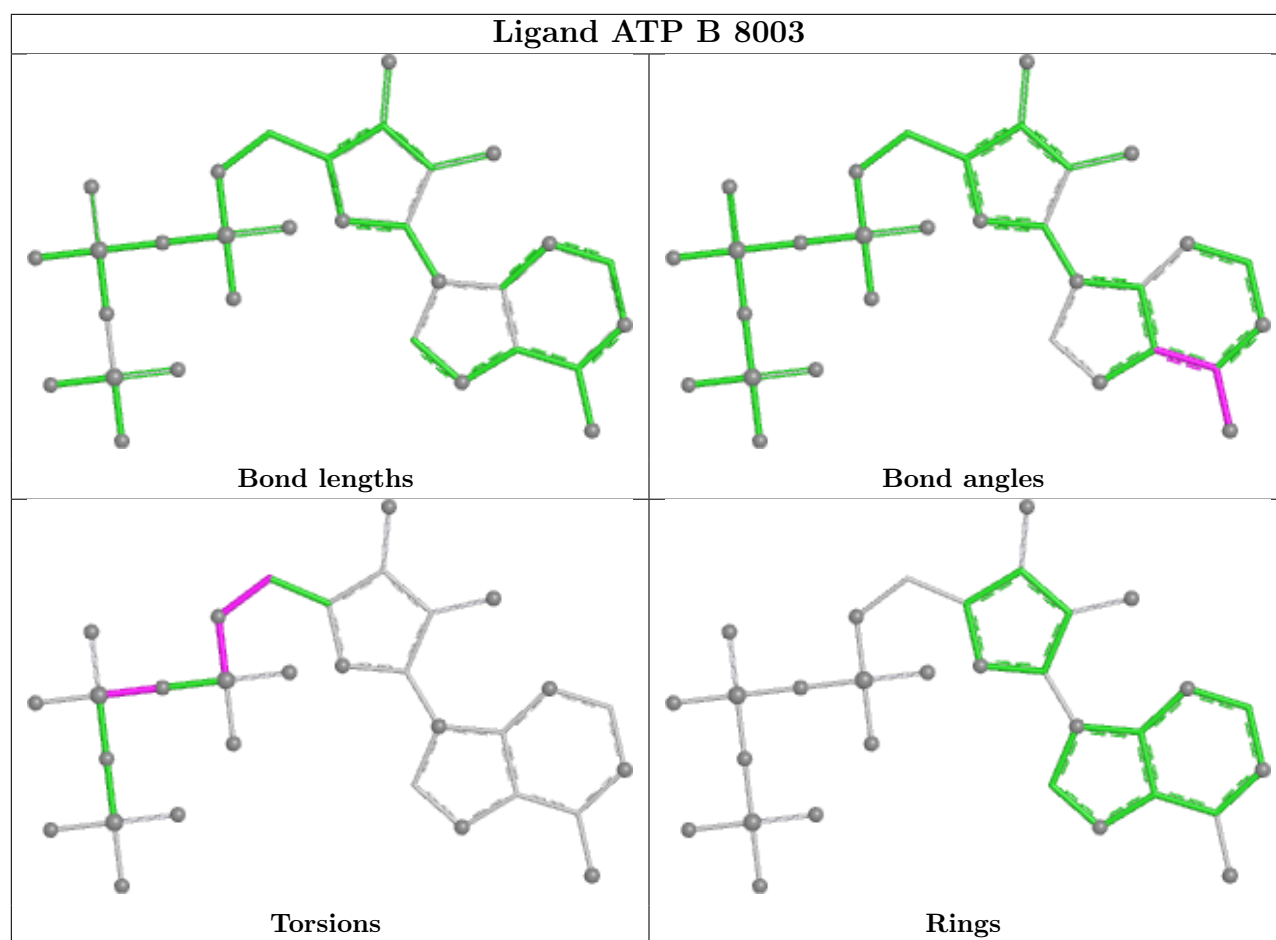


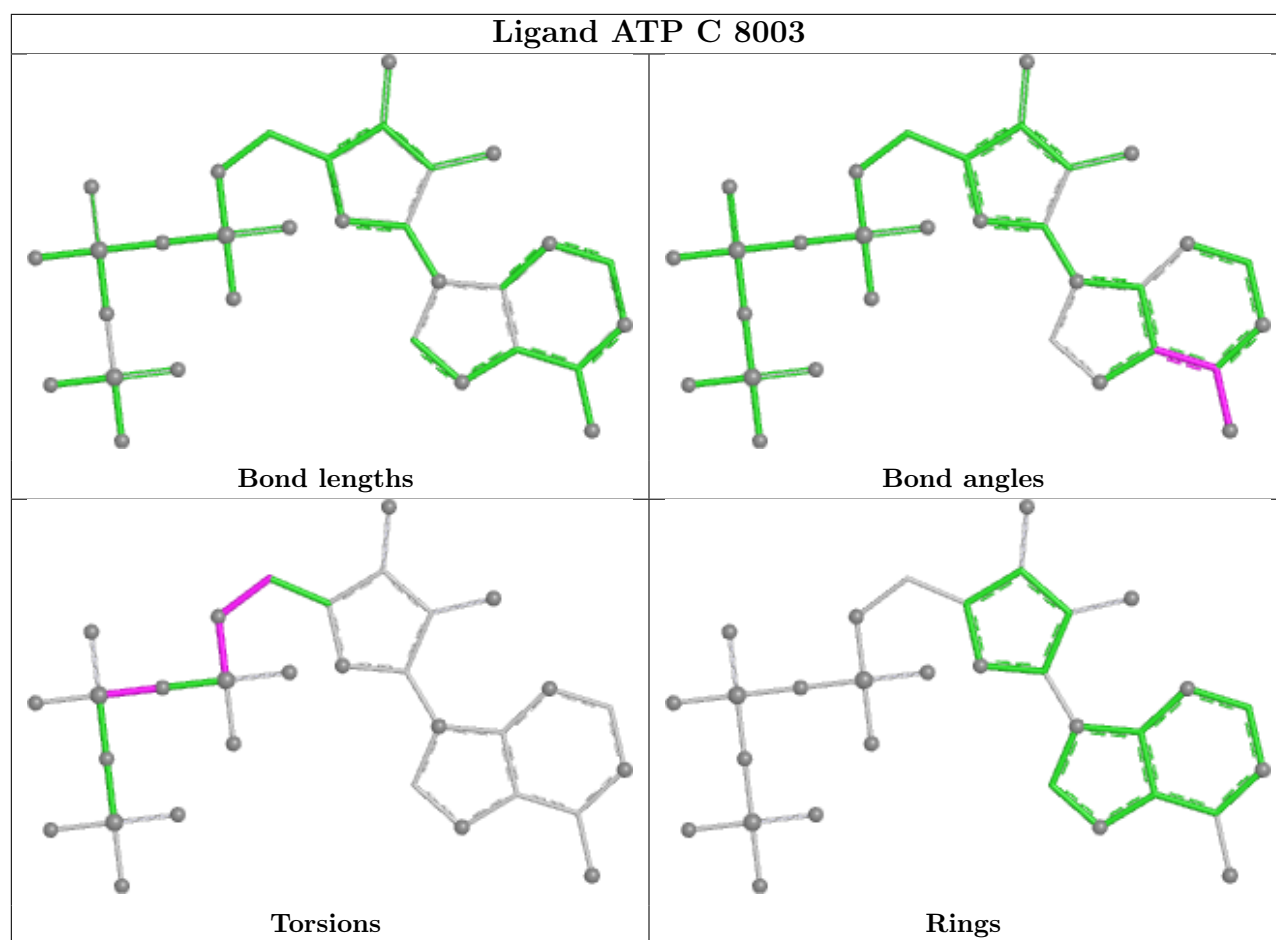


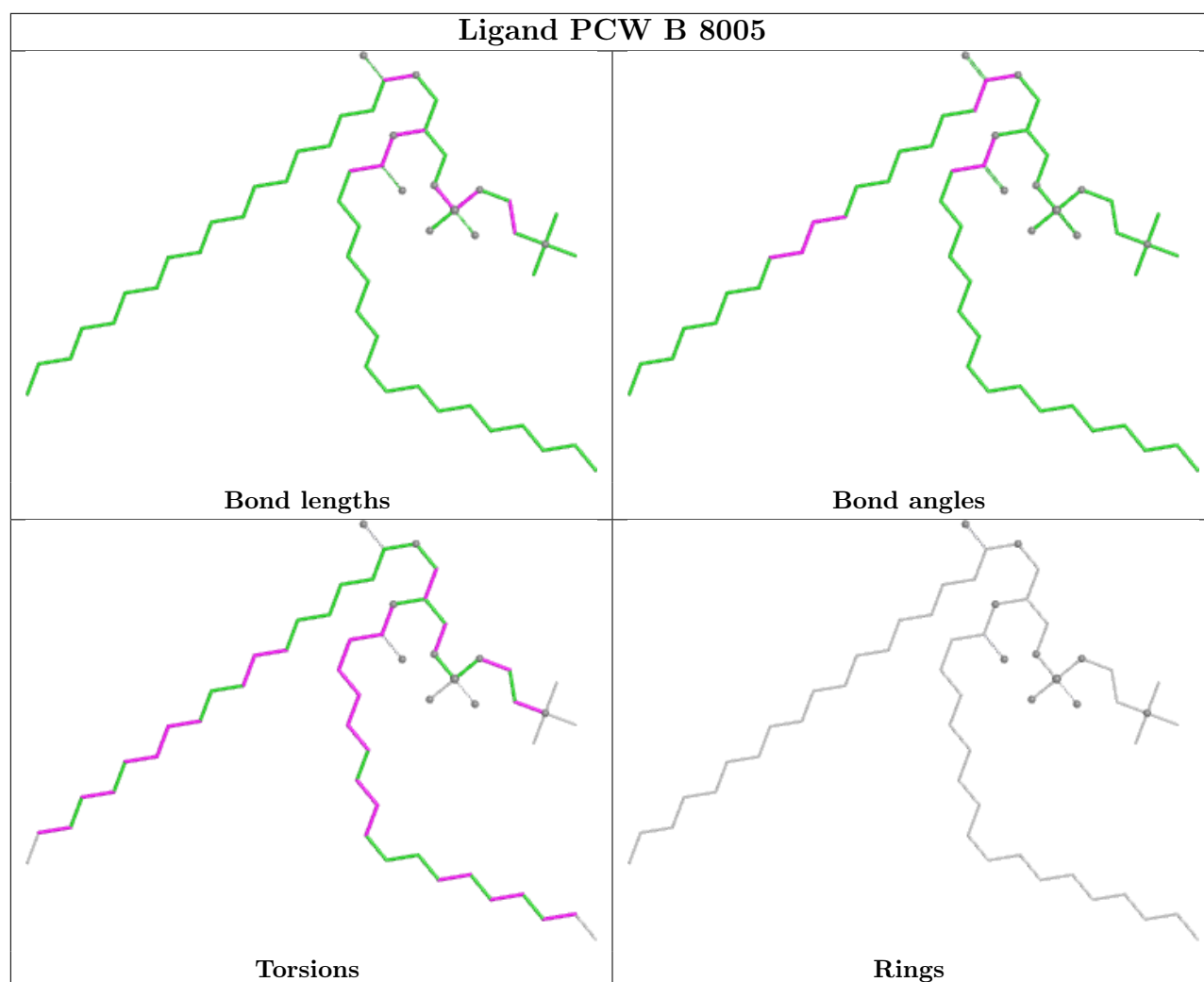


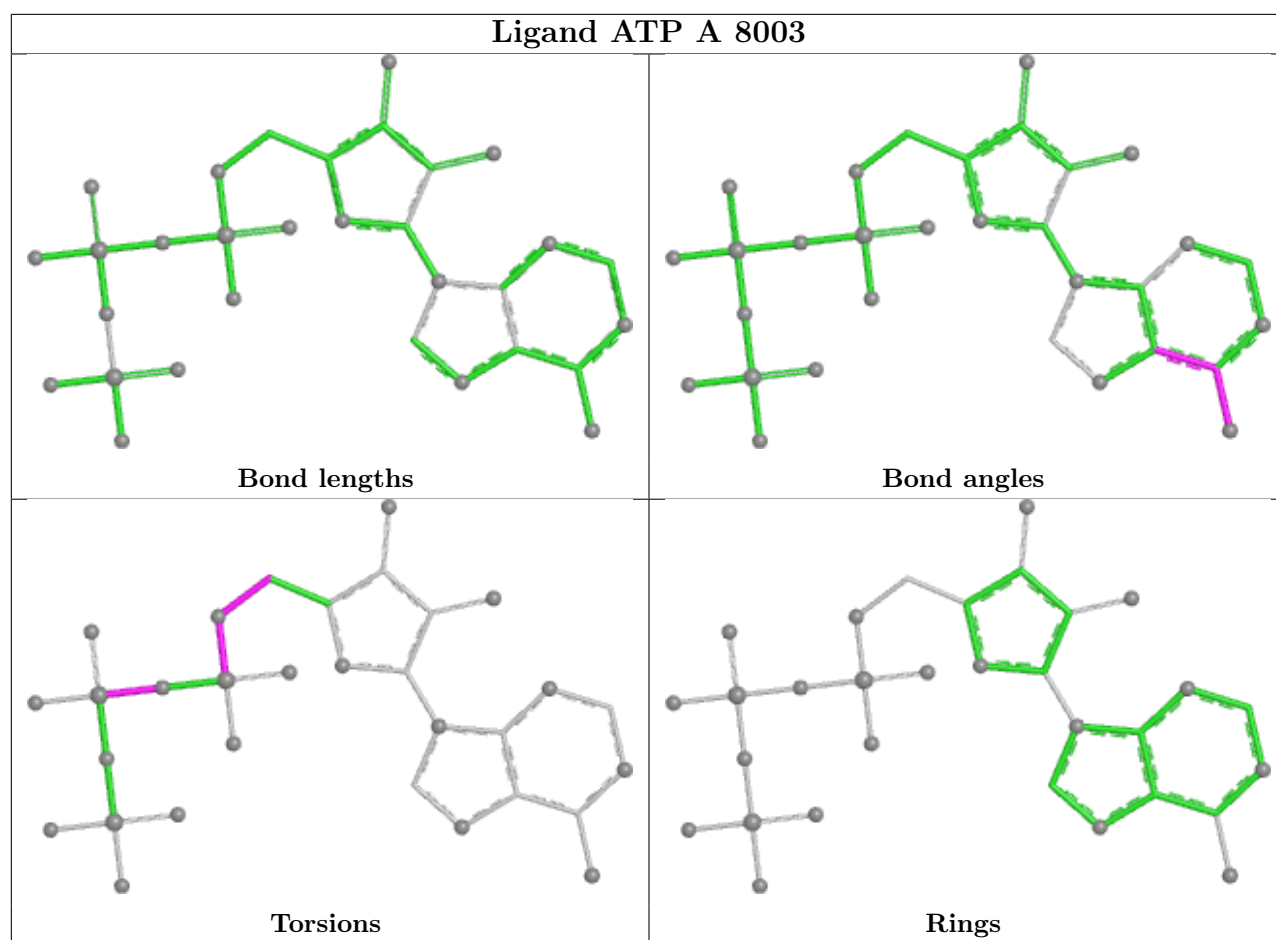


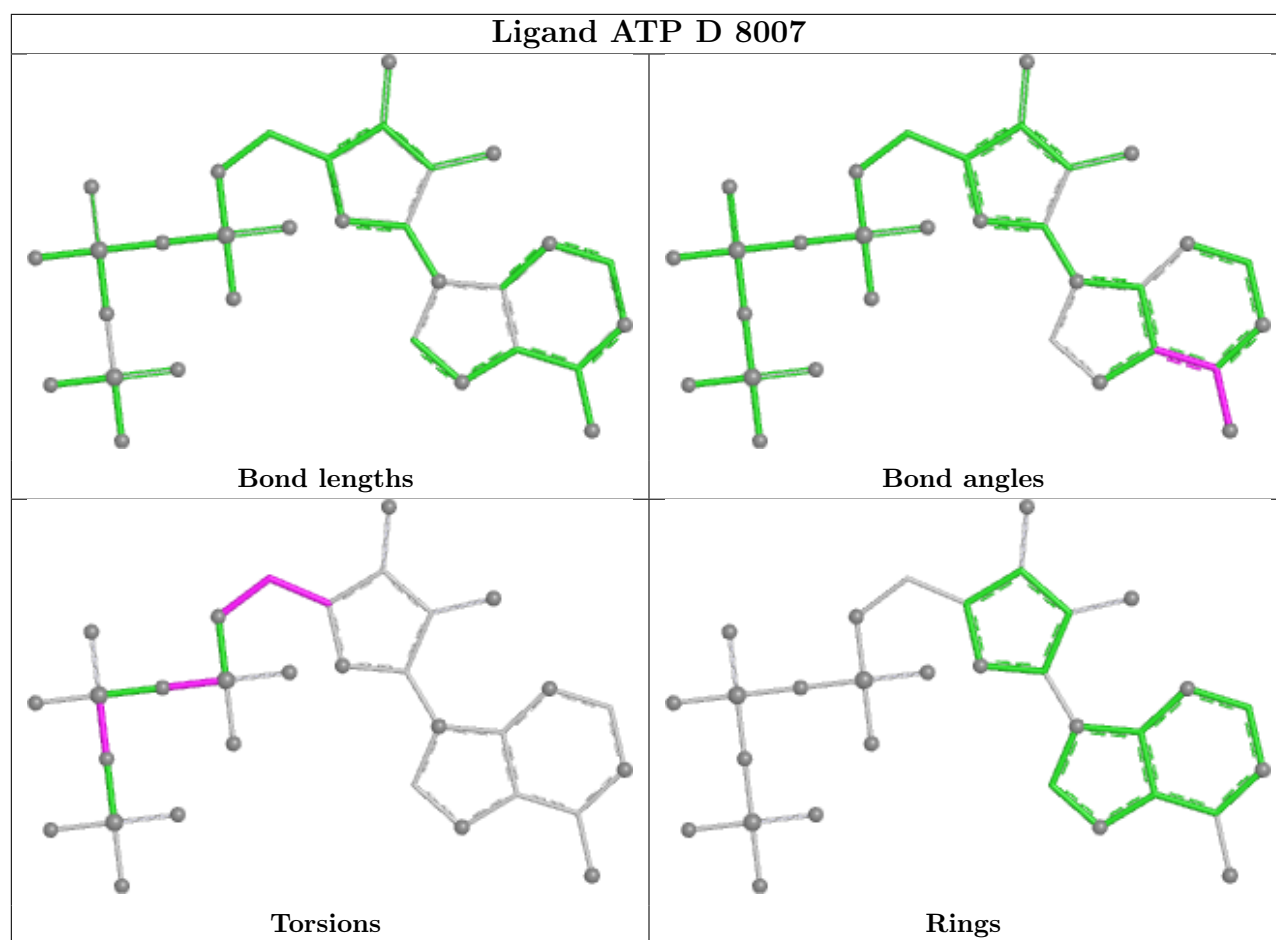


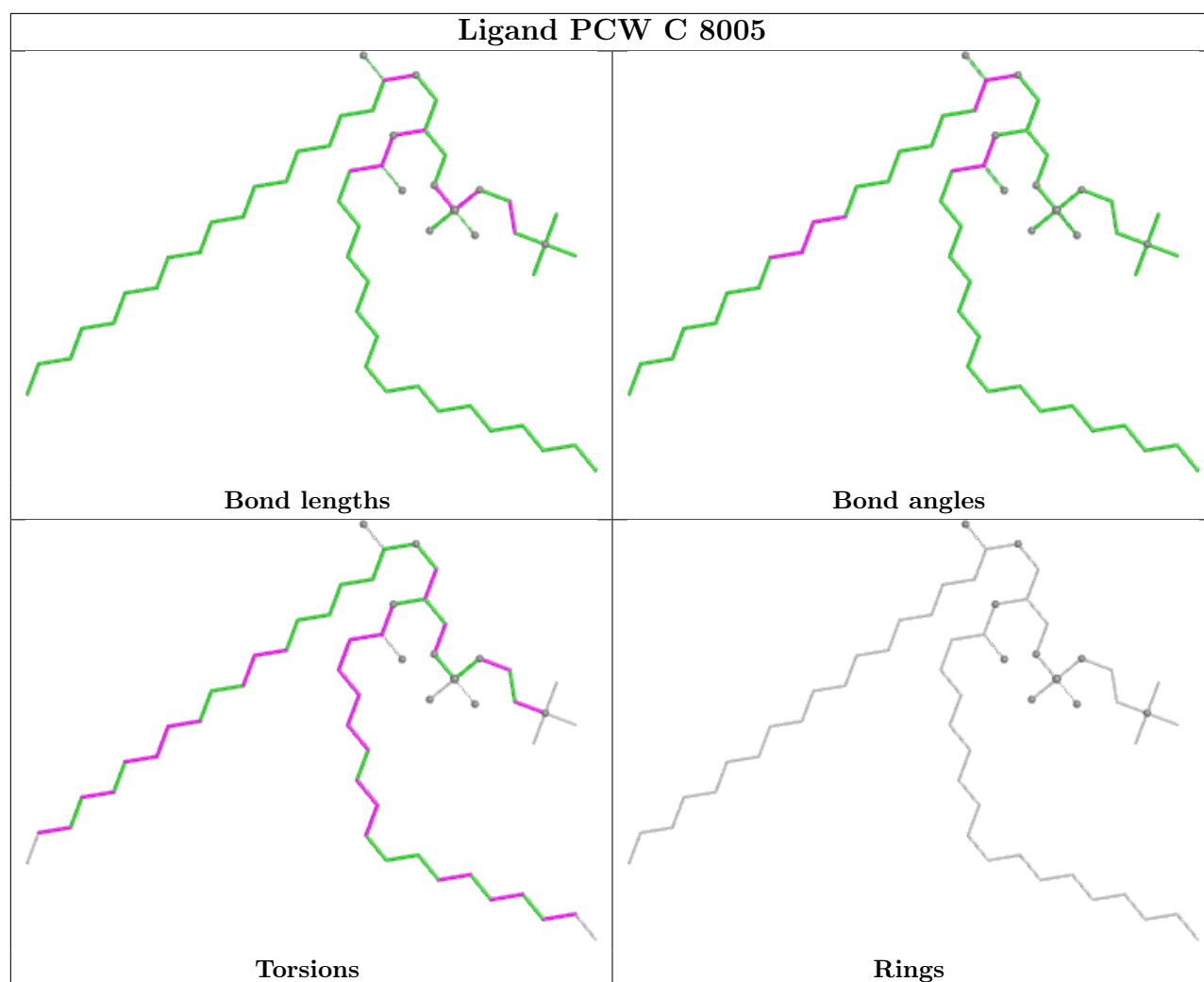


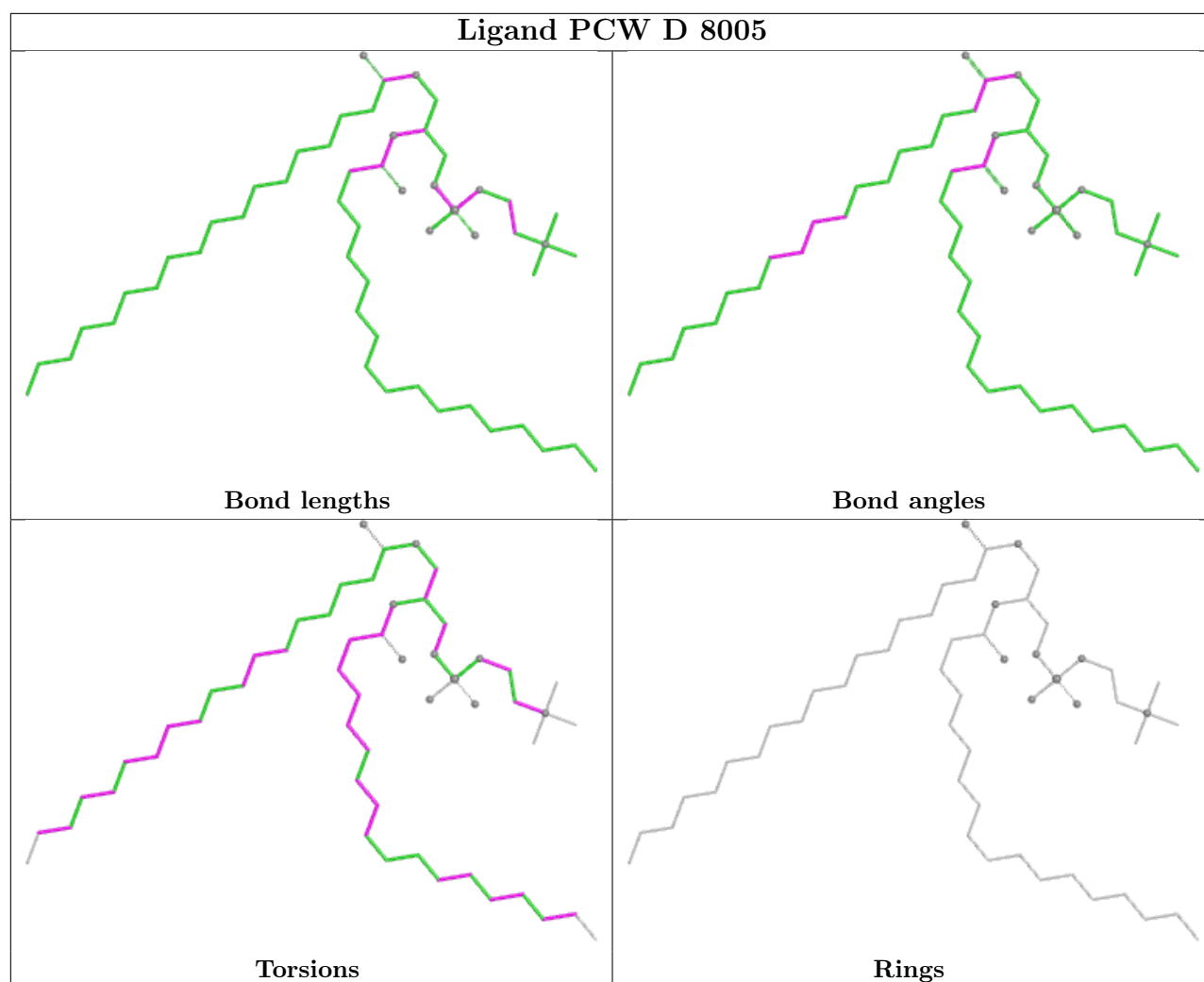


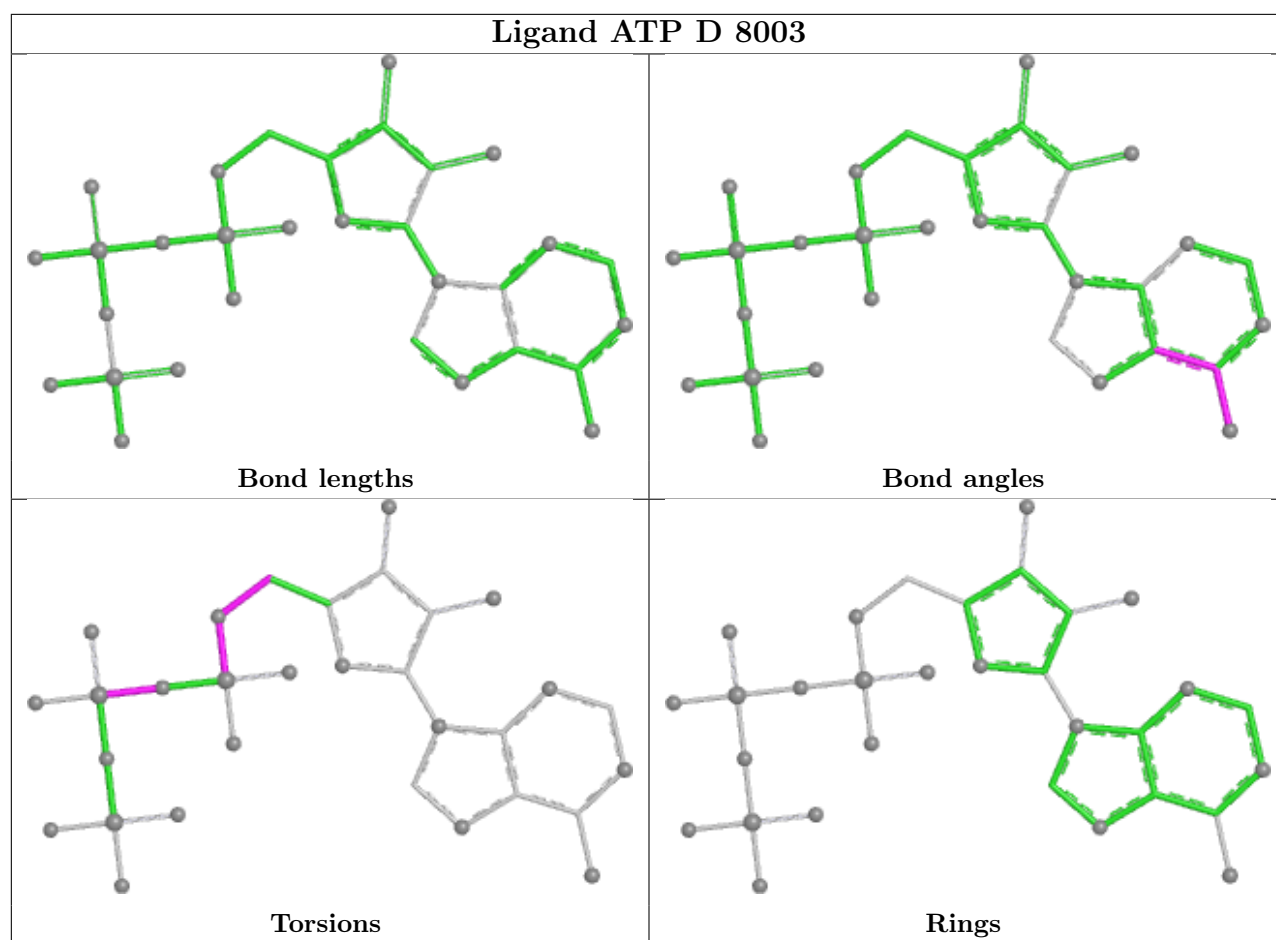












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

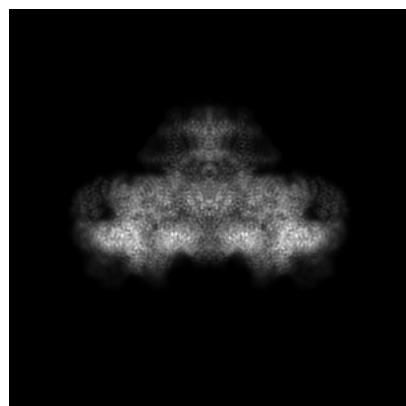
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49534. These allow visual inspection of the internal detail of the map and identification of artifacts.

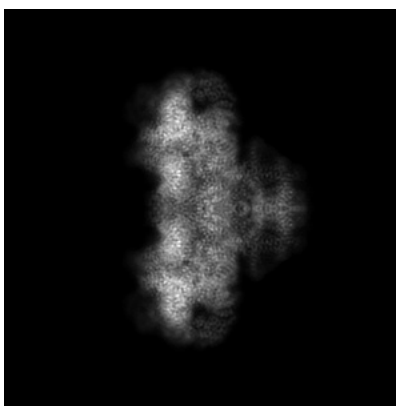
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

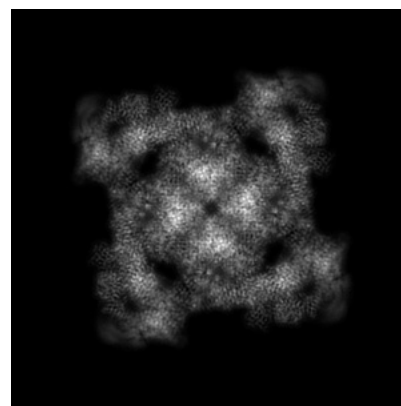
6.1.1 Primary map



X

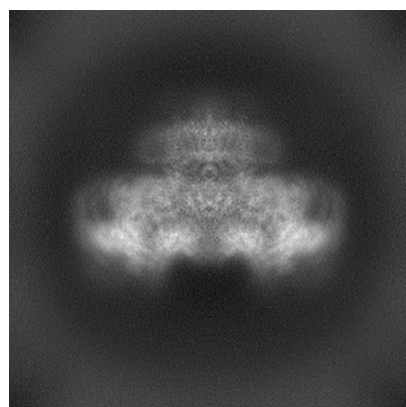


Y

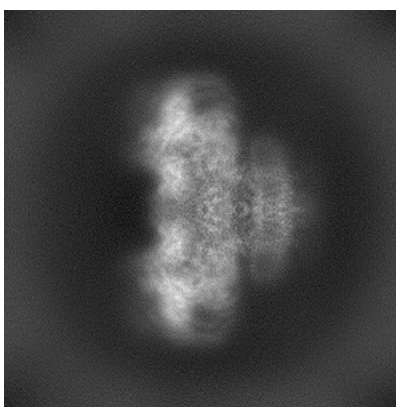


Z

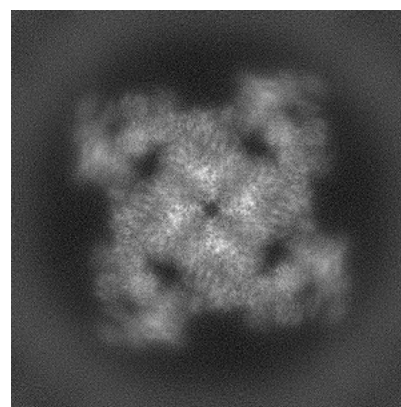
6.1.2 Raw map



X



Y

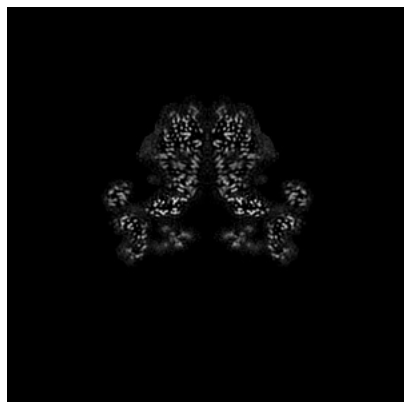


Z

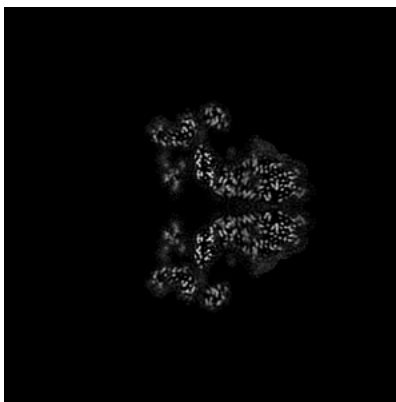
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

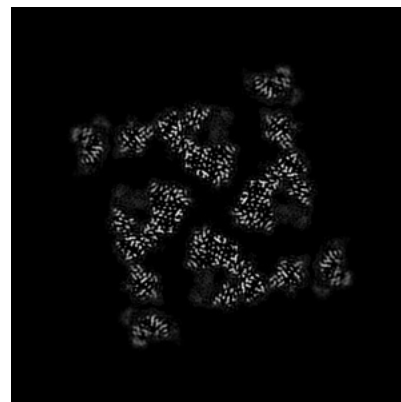
6.2.1 Primary map



X Index: 256

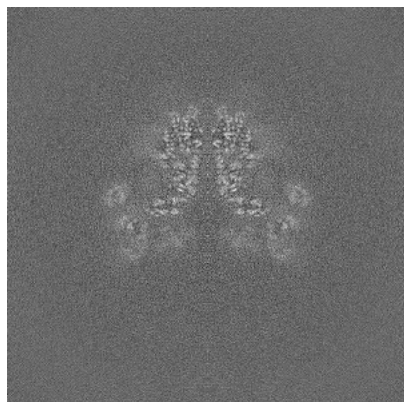


Y Index: 256

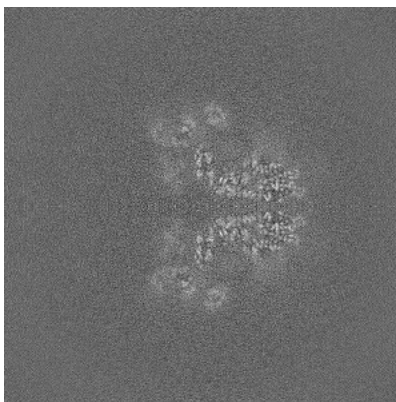


Z Index: 256

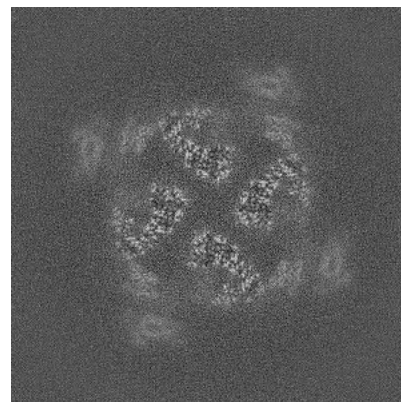
6.2.2 Raw map



X Index: 256



Y Index: 256

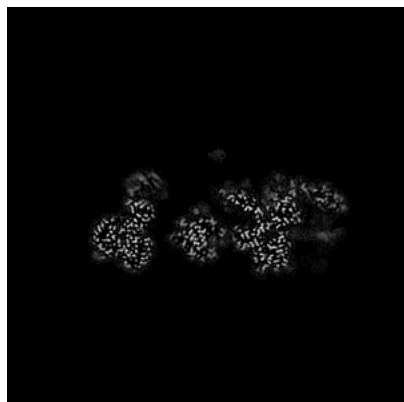


Z Index: 256

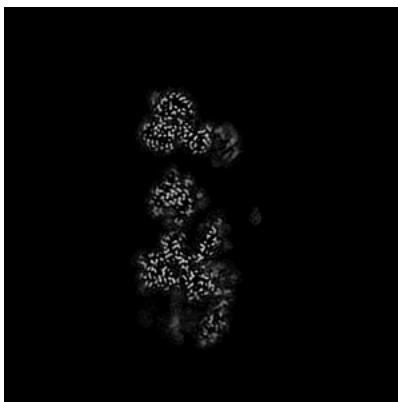
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

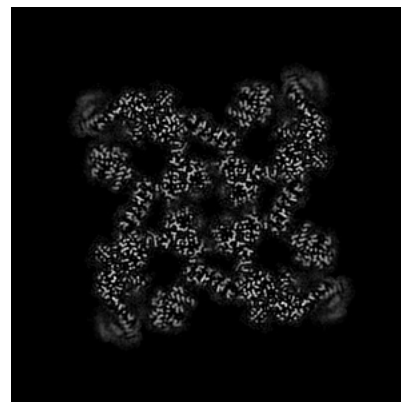
6.3.1 Primary map



X Index: 348

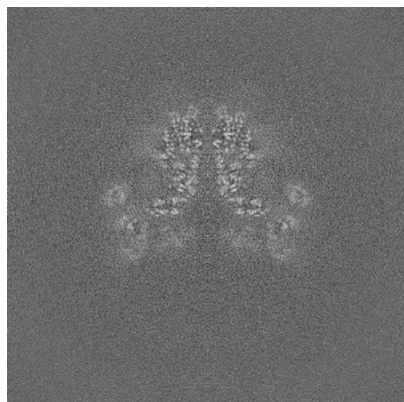


Y Index: 348

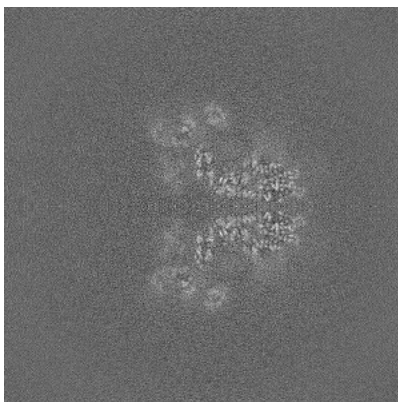


Z Index: 224

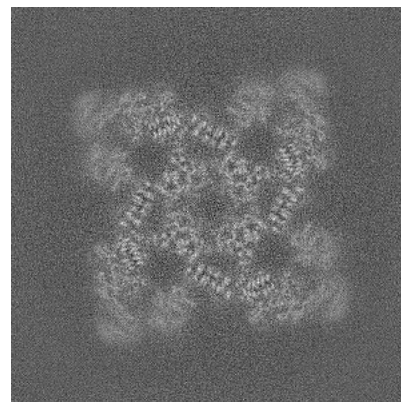
6.3.2 Raw map



X Index: 256



Y Index: 256

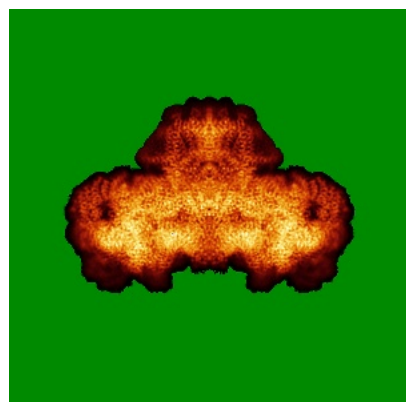


Z Index: 225

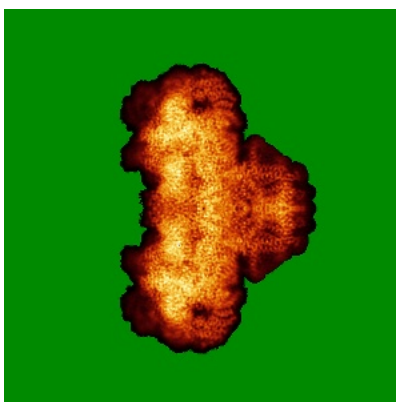
The images above show the largest variance slices of the map in three orthogonal directions.

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

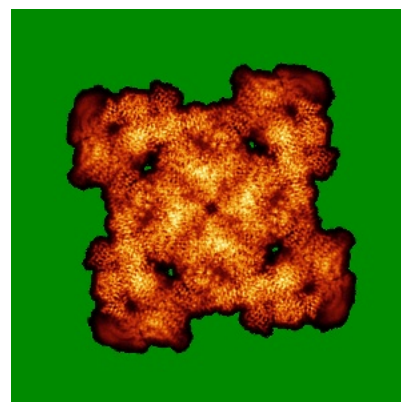
6.4.1 Primary map



X

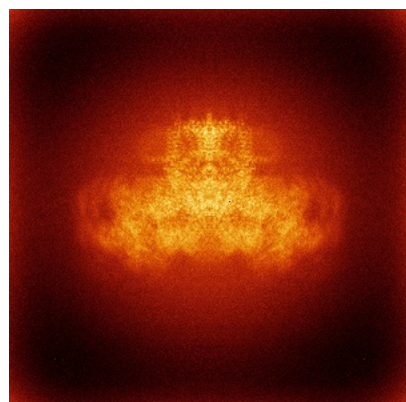


Y

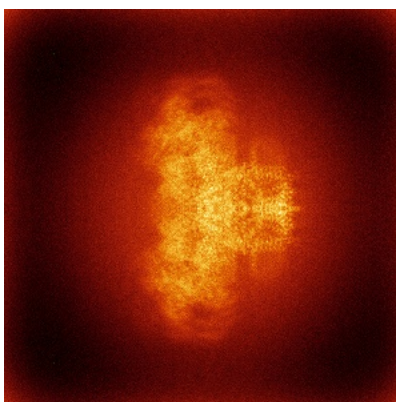


Z

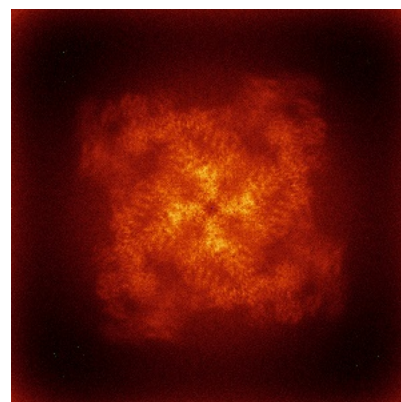
6.4.2 Raw map



X



Y

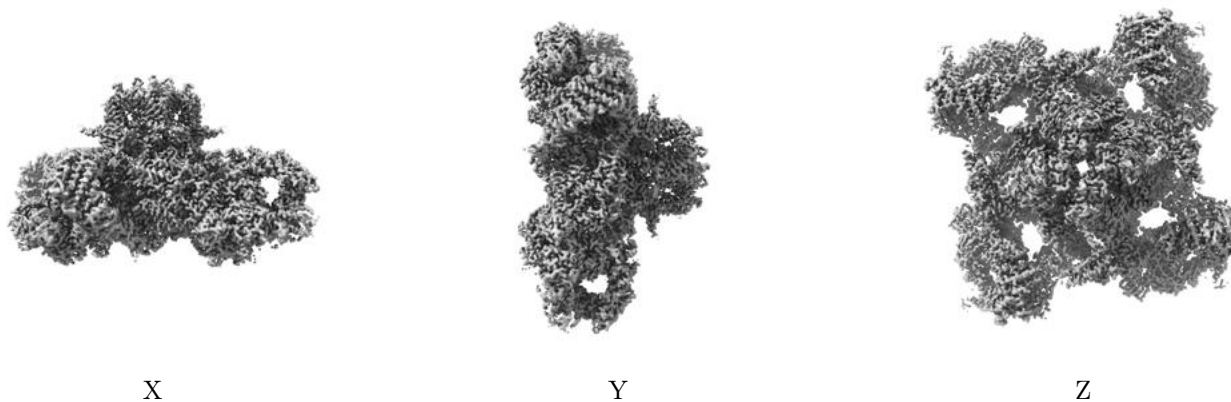


Z

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.

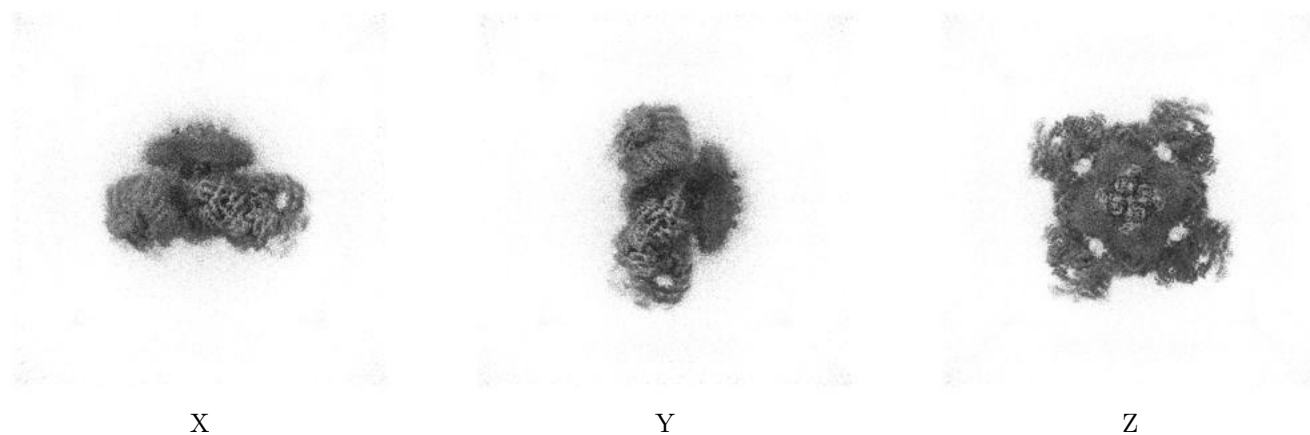
6.5 Orthogonal surface views [i](#)

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.

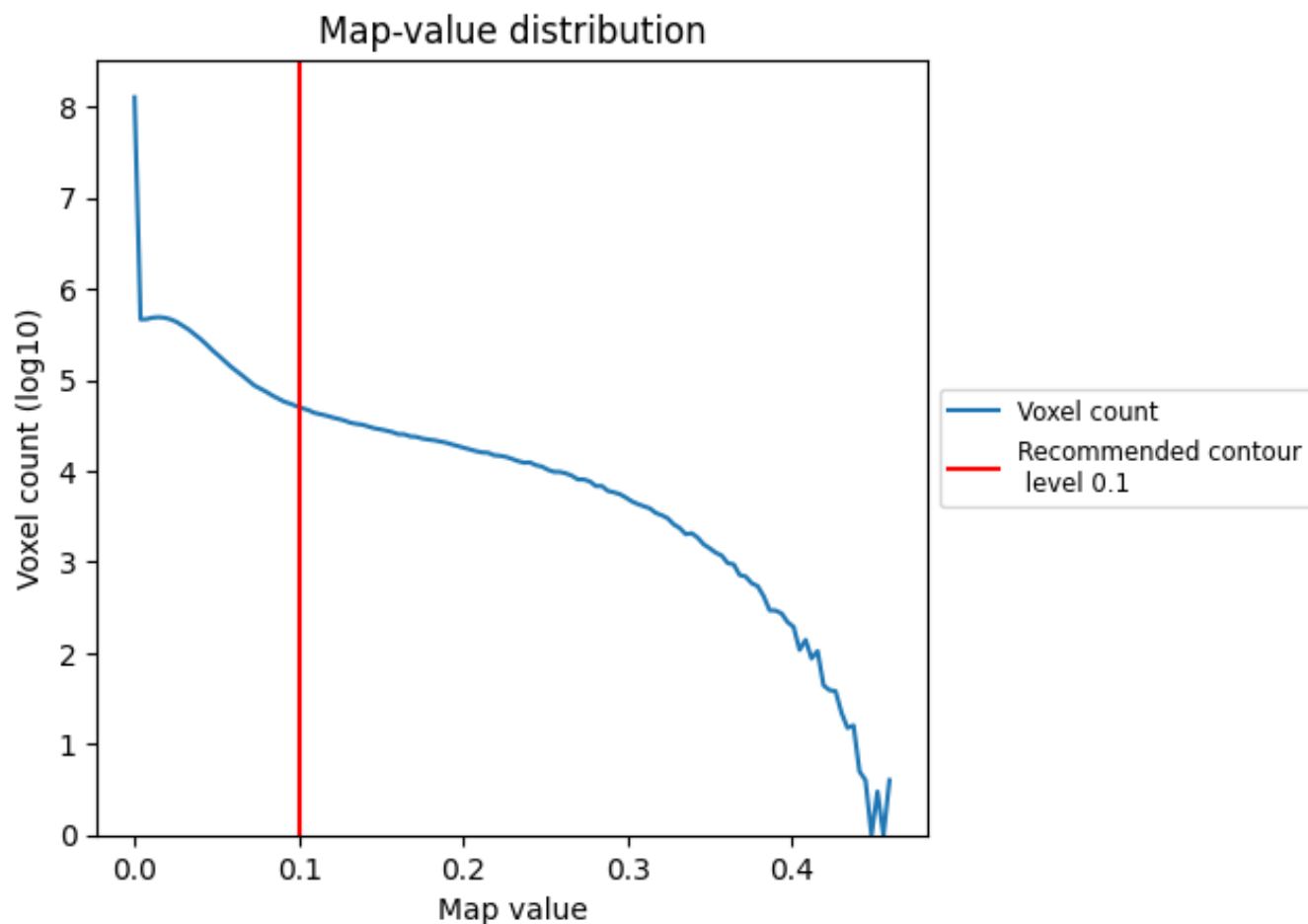
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

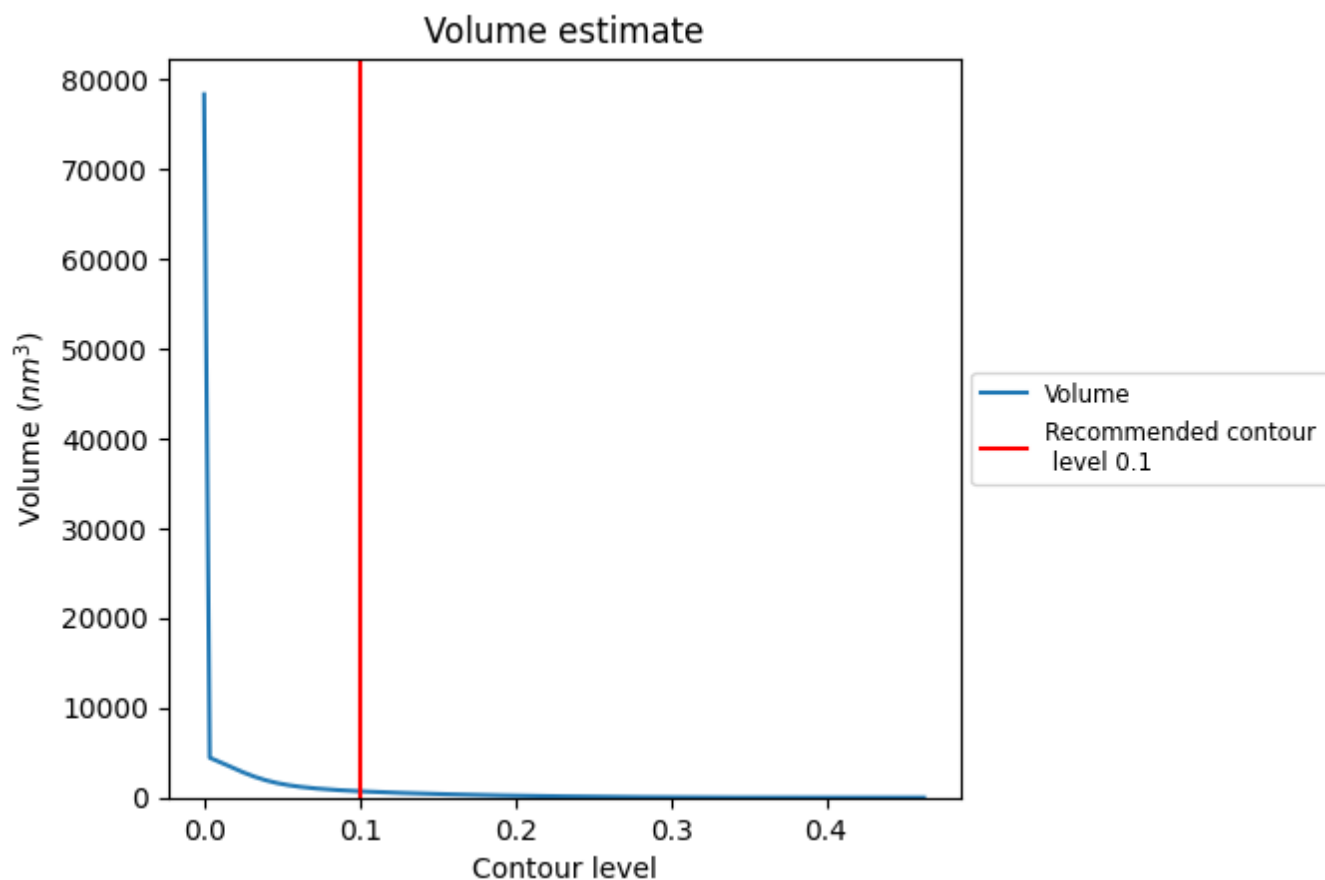
This section contains the results of statistical analysis of the map.

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.

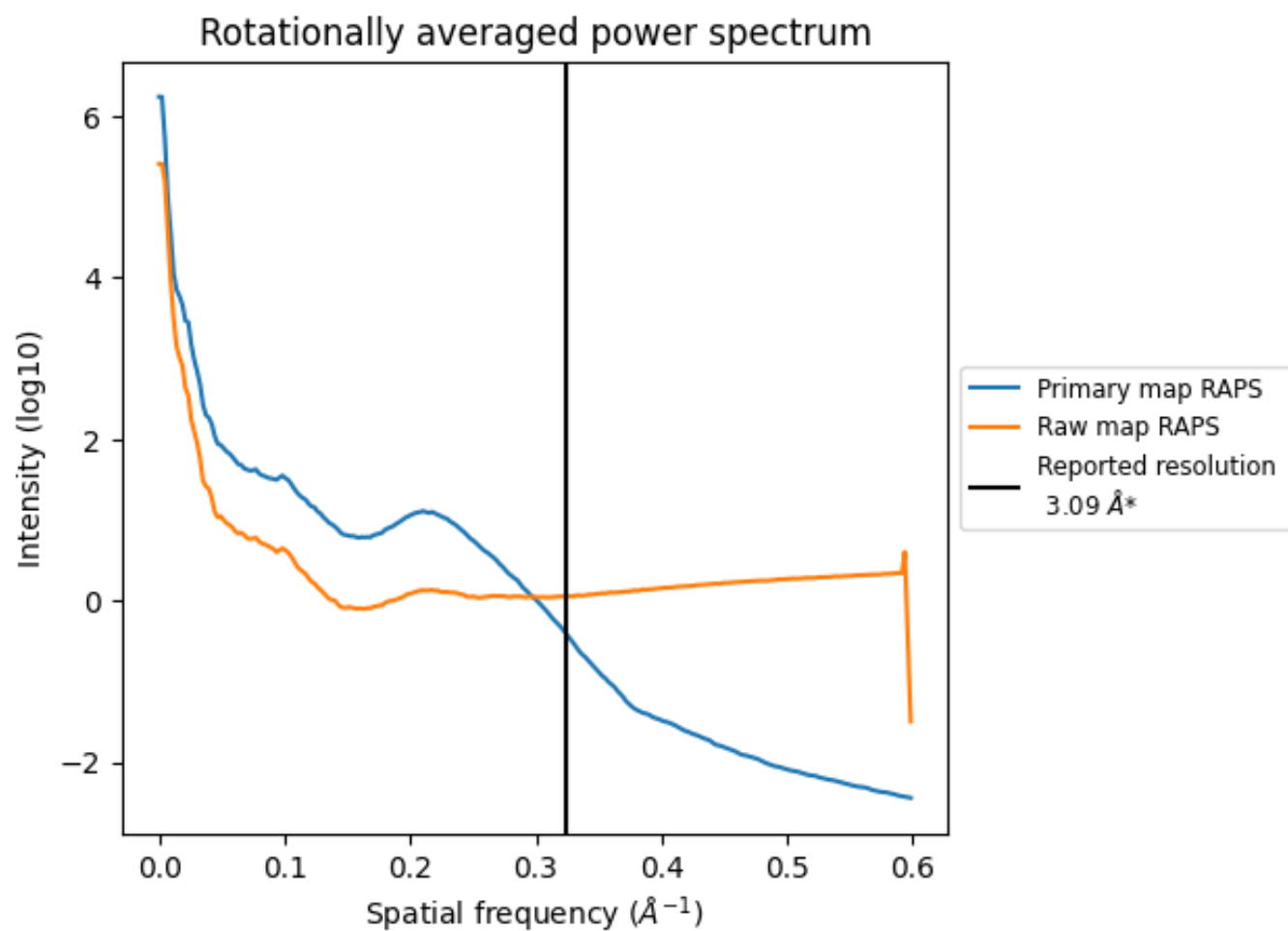
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 703 nm^3 ; this corresponds to an approximate mass of 635 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 ⓘ

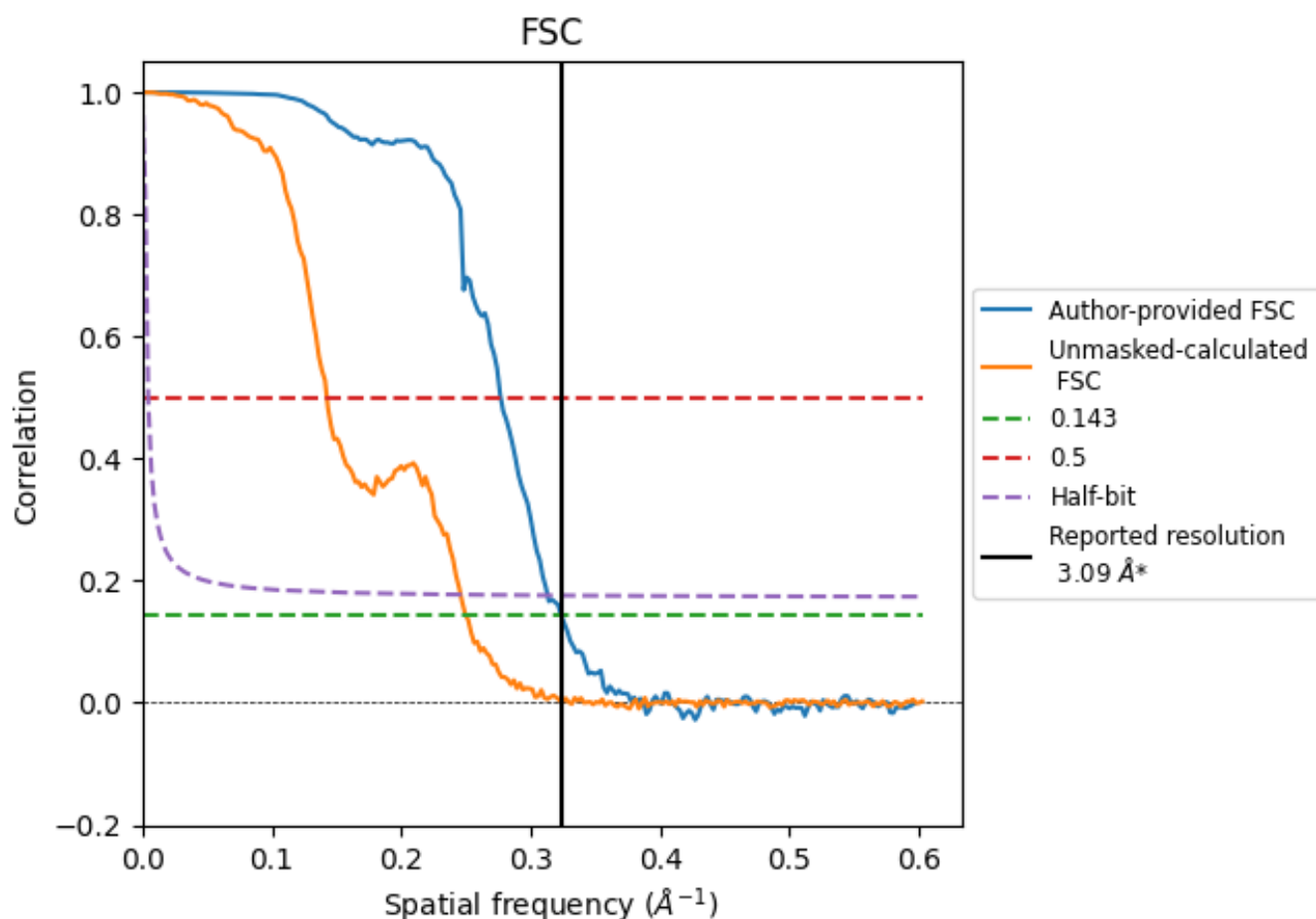


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

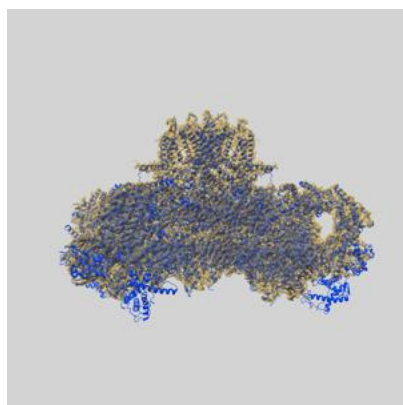
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.61	3.19
Unmasked-calculated*	4.00	7.01	4.07

*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 4.00 differs from the reported value 3.09 by more than 10 %

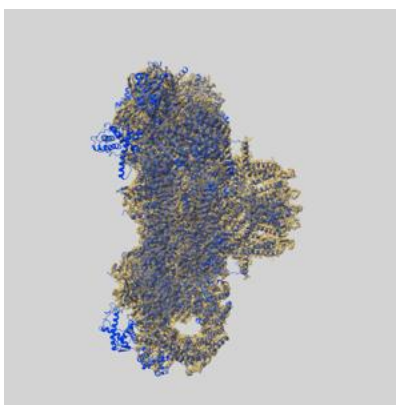
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49534 and PDB model 9NMN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

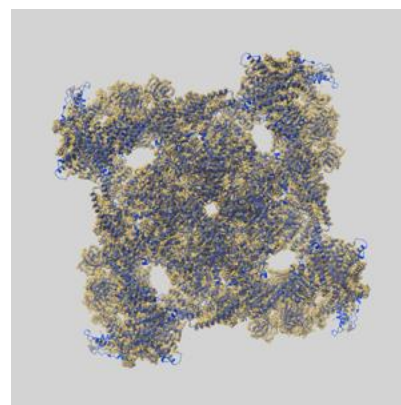
9.1 Map-model overlay [i](#)



X



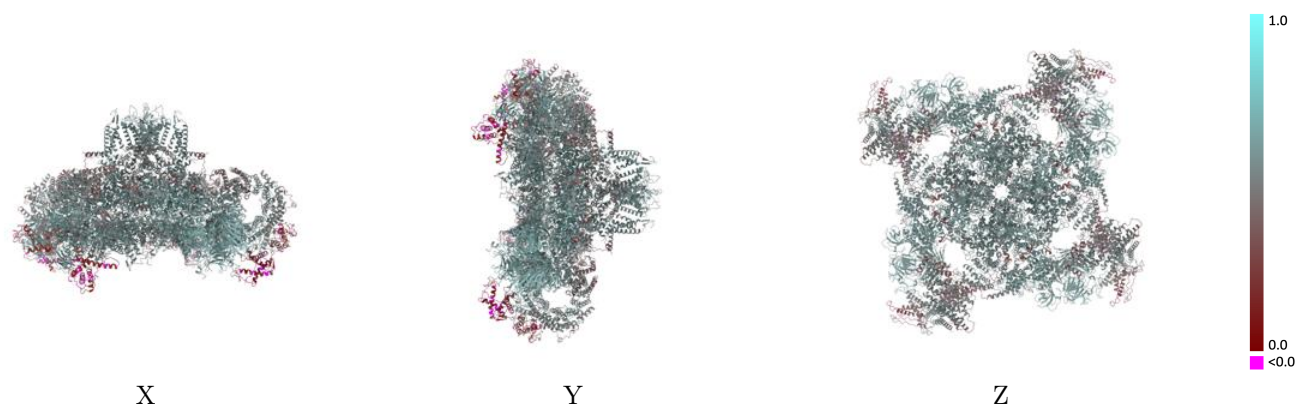
Y



Z

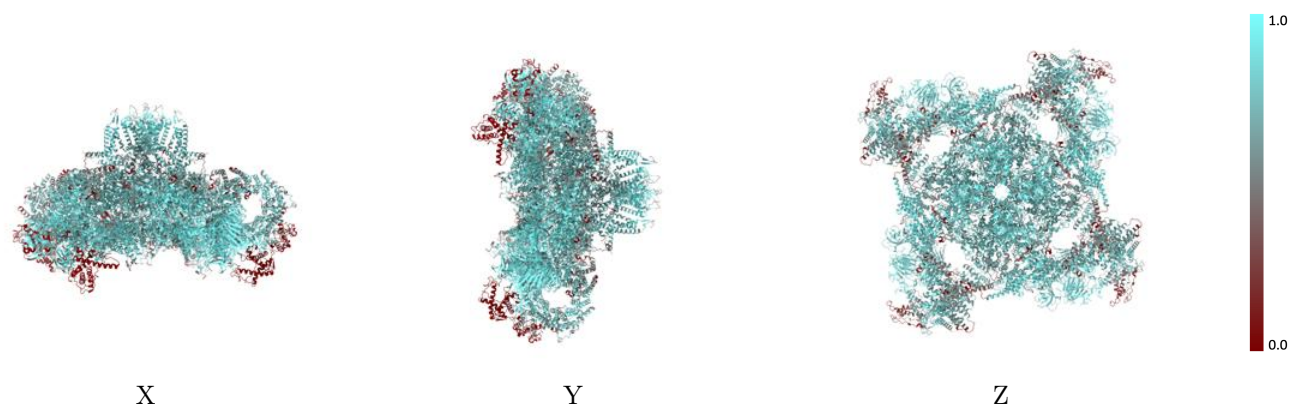
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



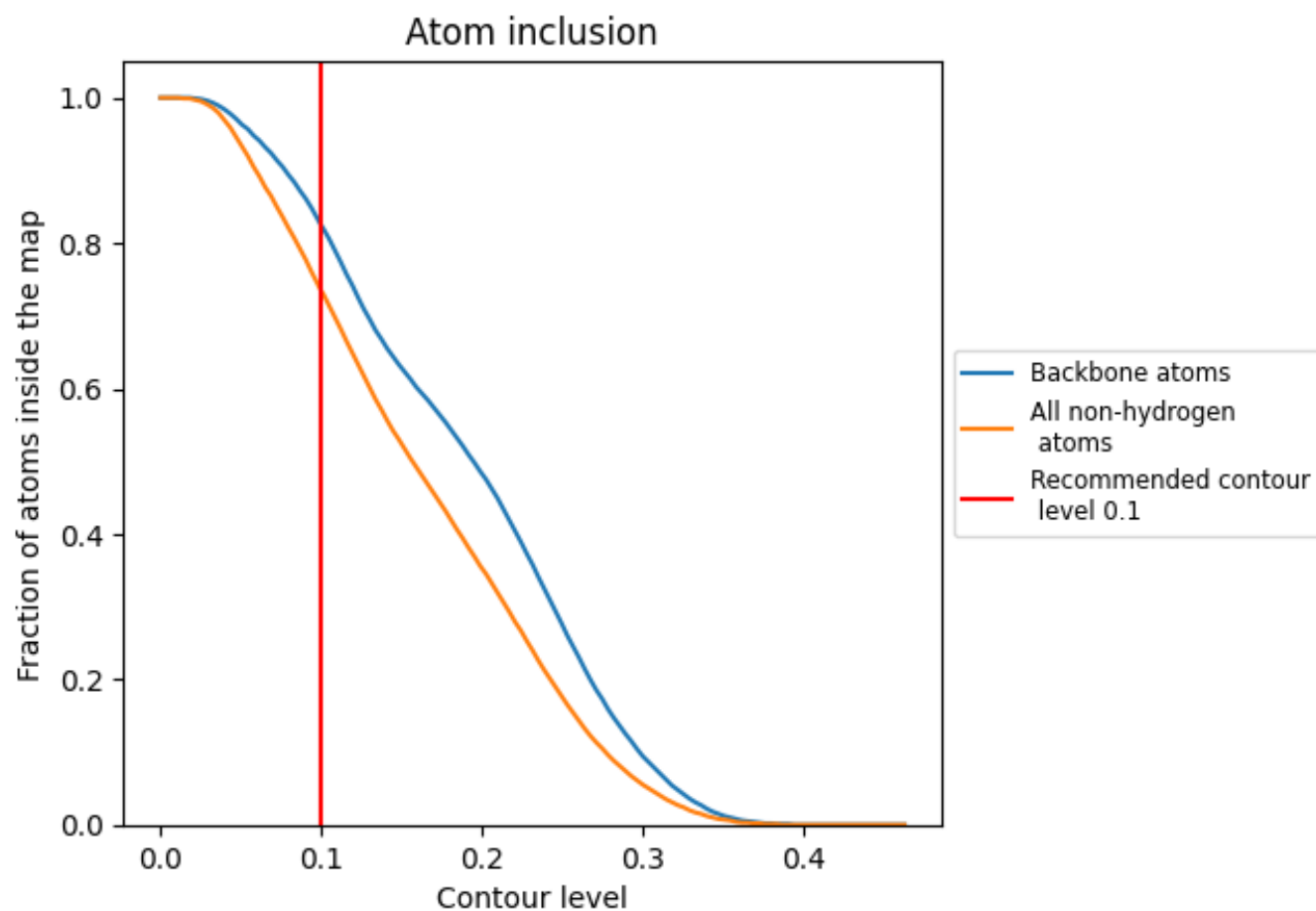
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 82% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7340	<div><div></div></div> 0.5250
A	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
B	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
C	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
E	<div><div></div></div> 0.8480	<div><div></div></div> 0.6050
F	<div><div></div></div> 0.8440	<div><div></div></div> 0.6060
G	<div><div></div></div> 0.8430	<div><div></div></div> 0.6070
H	<div><div></div></div> 0.8400	<div><div></div></div> 0.6050

1.0

0.0

<0.0