



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 04:37 PM EDT

PDB ID : 9ZN6 / pdb_00009zn6
EMDB ID : EMD-74436
Title : Structure of rabbit RyR1 complexed with FKBP12.6 and calmodulin in the presence of dantrolene, ADP, 4-chloro-m-cresol, caffeine, and Mg²⁺
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.58 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

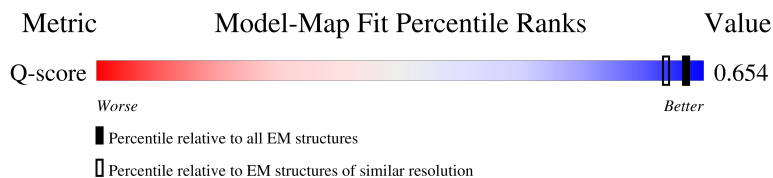
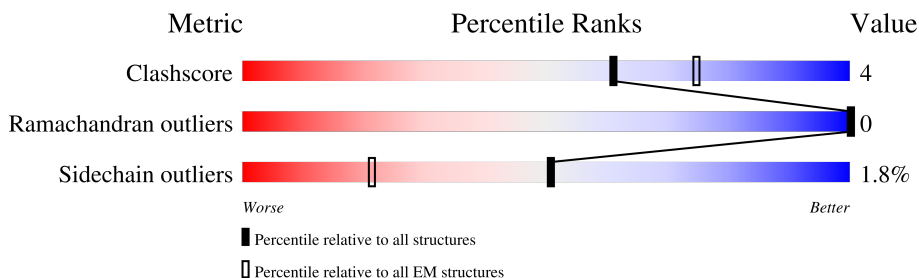
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7675 (2.08 - 3.08)

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	E	107	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	148	55% 92% 7%
2	J	148	55% 91% 7%
2	K	148	55% 89% 9%
2	L	148	55% 91% 9%
3	A	5037	9% 74% 10% 16%
3	B	5037	9% 74% 10% 16%
3	C	5037	9% 74% 10% 16%
3	D	5037	9% 74% 10% 16%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 144280 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 FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	148	Total	C	N	O	S	0	0
			990	606	169	211	4		
2	J	148	Total	C	N	O	S	0	0
			990	606	169	211	4		
2	K	148	Total	C	N	O	S	0	0
			990	606	169	211	4		
2	L	148	Total	C	N	O	S	0	0
			990	606	169	211	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23
L	-1	HIS	-	expression tag	UNP P0DP23

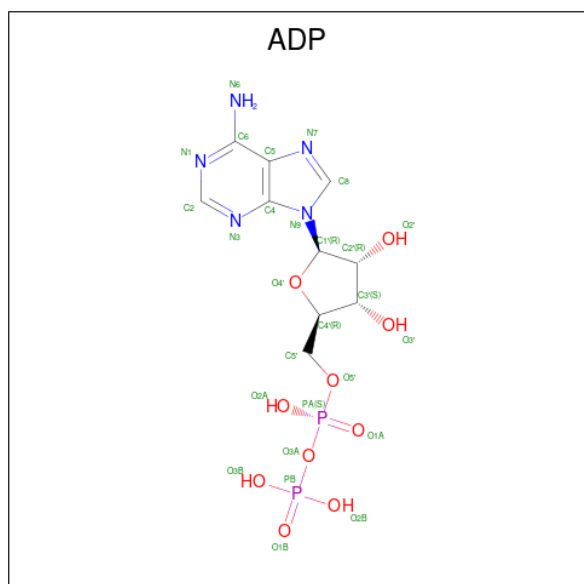
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4240	Total	C	N	O	S	2	0
			33207	21124	5739	6114	230		
3	D	4240	Total	C	N	O	S	2	0
			33207	21124	5739	6114	230		
3	B	4240	Total	C	N	O	S	2	0
			33207	21124	5739	6114	230		
3	C	4240	Total	C	N	O	S	2	0
			33207	21124	5739	6114	230		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



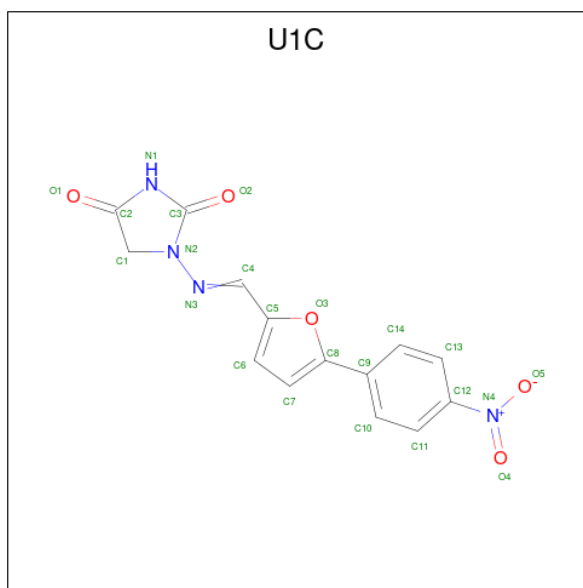
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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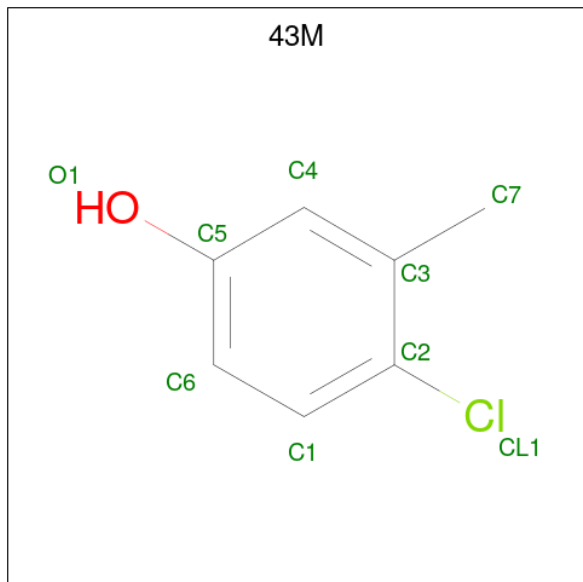
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is Dantrolene (CCD ID: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			23	14	4	5	
6	D	1	Total	C	N	O	0
			23	14	4	5	
6	B	1	Total	C	N	O	0
			23	14	4	5	
6	C	1	Total	C	N	O	0
			23	14	4	5	

- Molecule 7 is 4-CHLORO-3-METHYLPHENOL (CCD ID: 43M) (formula: C_7H_7ClO) (labeled as "Ligand of Interest" by depositor).

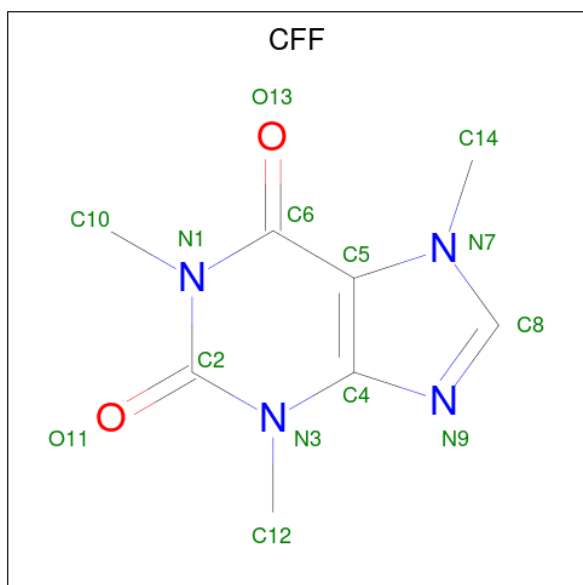


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



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

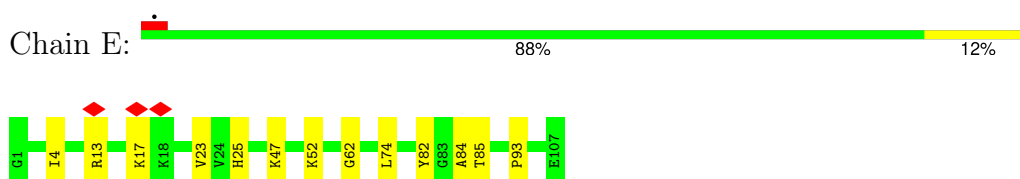
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	E	13	Total 13	O 13	0
10	F	13	Total 13	O 13	0
10	G	14	Total 14	O 14	0
10	H	12	Total 12	O 12	0
10	I	56	Total 56	O 56	0
10	J	61	Total 61	O 61	0
10	K	63	Total 63	O 63	0
10	L	61	Total 61	O 61	0
10	A	870	Total 870	O 870	0
10	D	855	Total 855	O 855	0
10	B	864	Total 864	O 864	0
10	C	858	Total 858	O 858	0

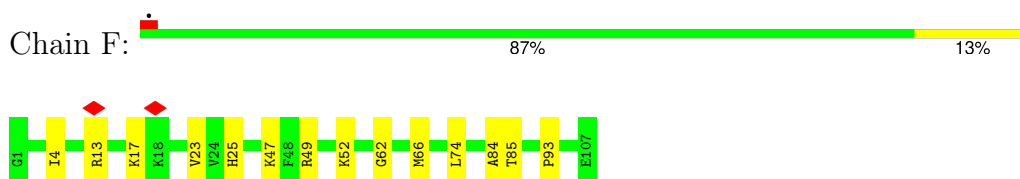
3 Residue-property plots

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.

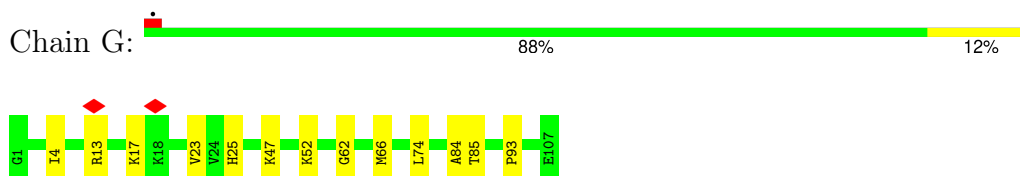
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



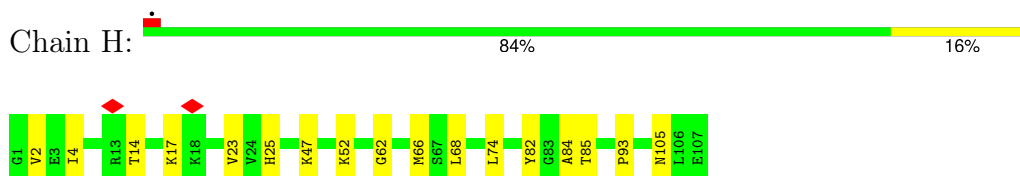
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



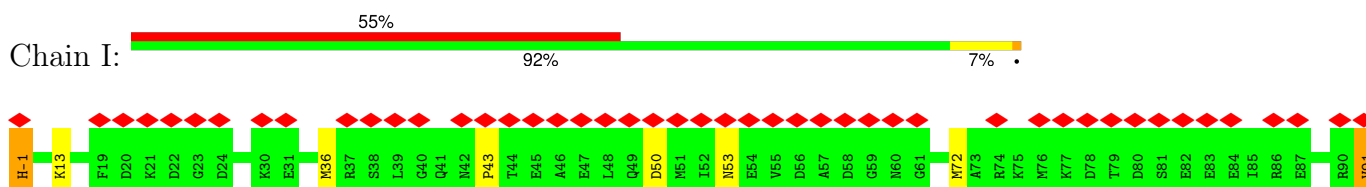
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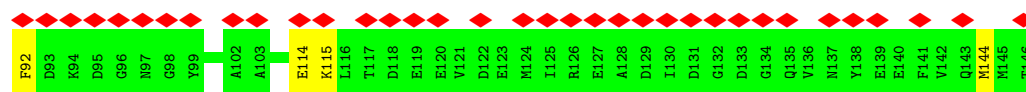


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

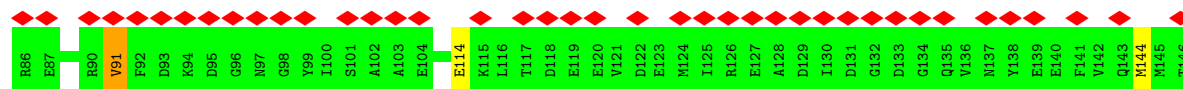
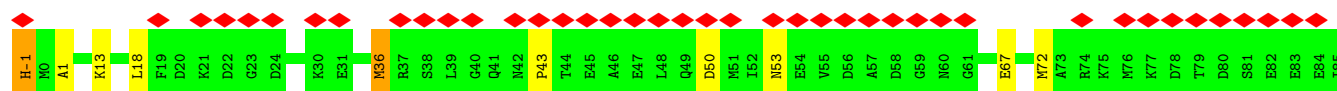
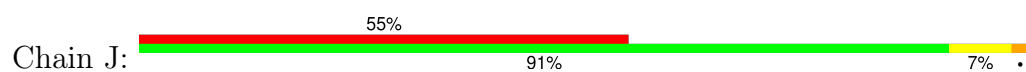


- Molecule 2: Calmodulin-1

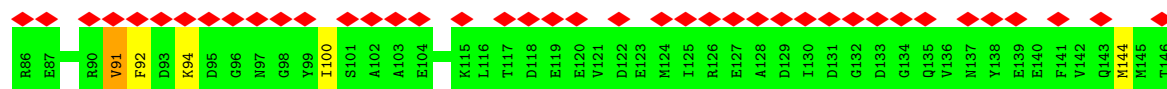
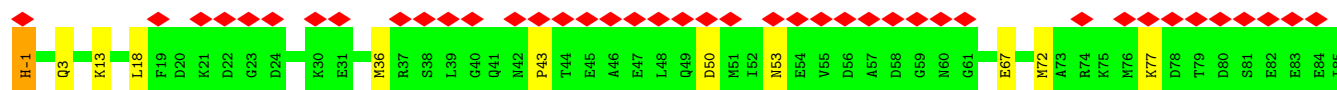
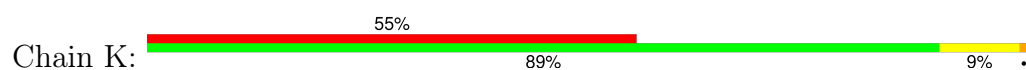




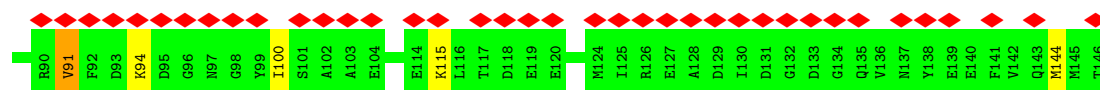
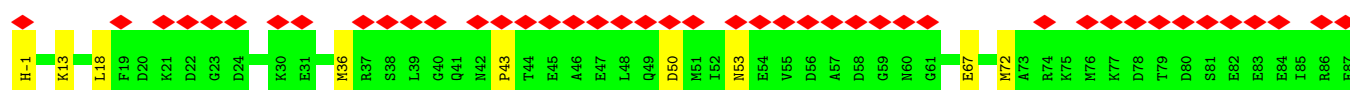
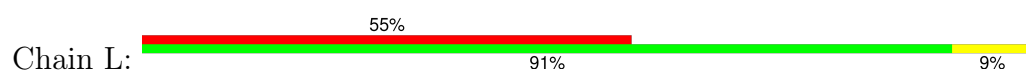
• Molecule 2: Calmodulin-1



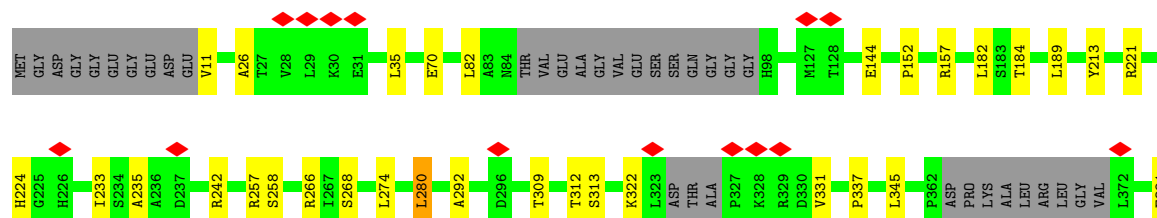
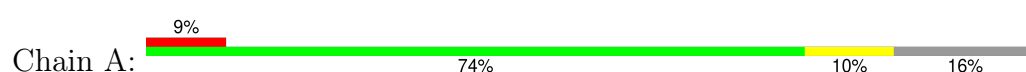
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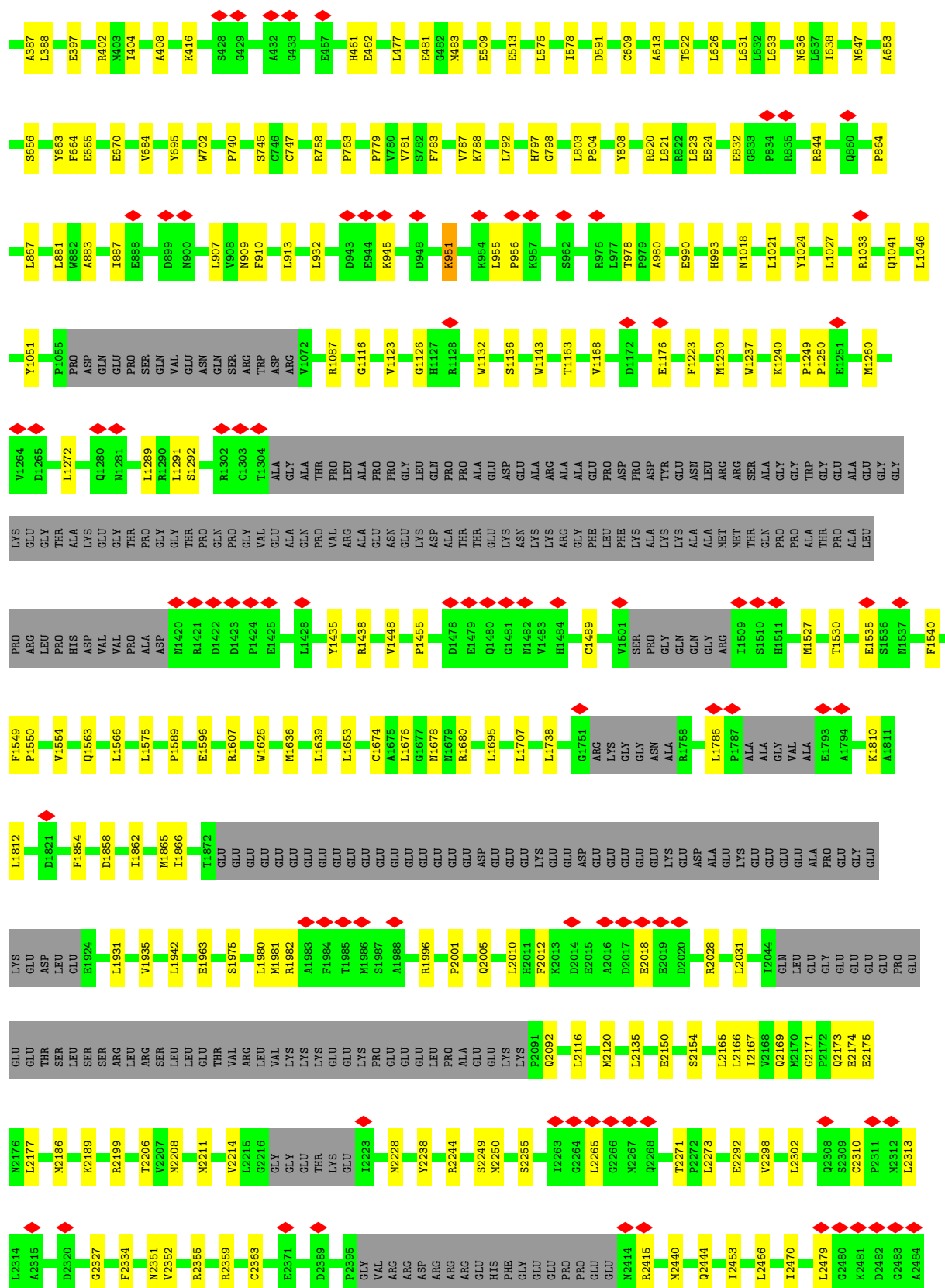


• Molecule 2: Calmodulin-1

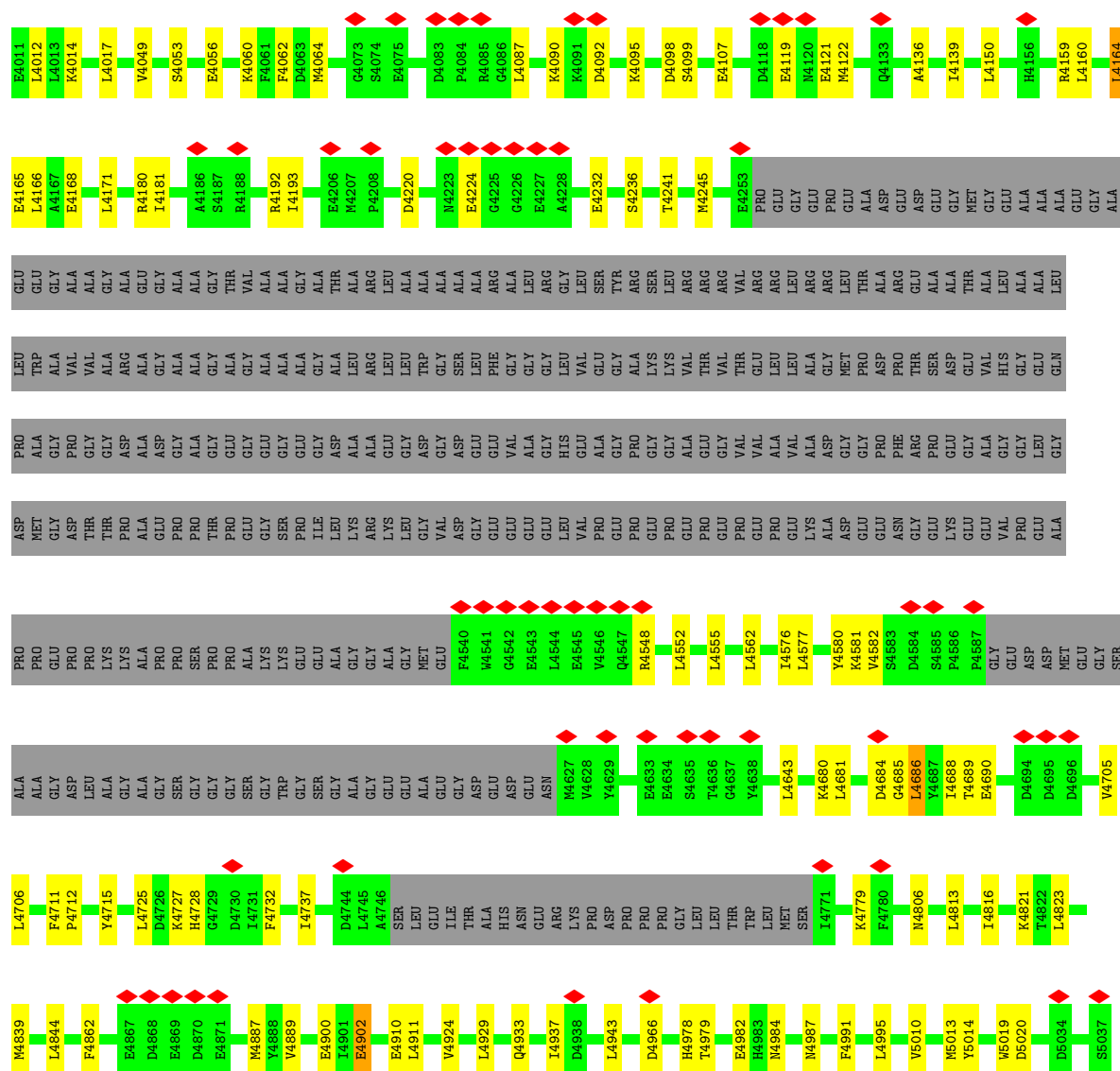


• Molecule 3: Ryanodine receptor 1

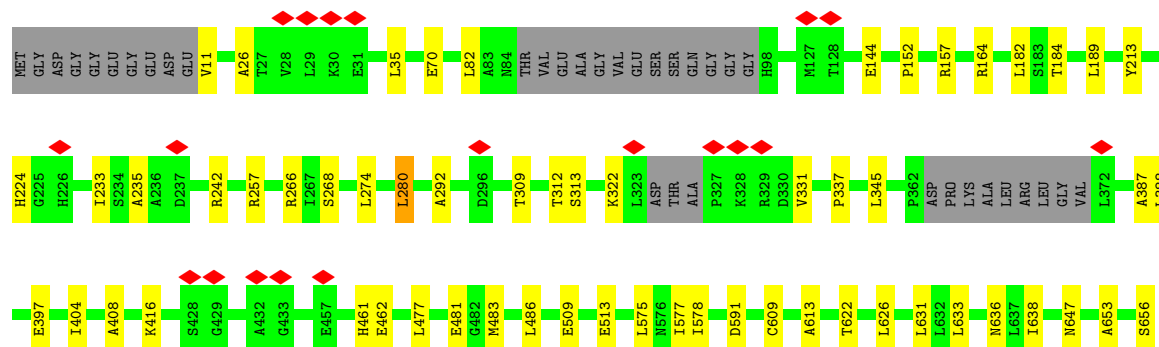
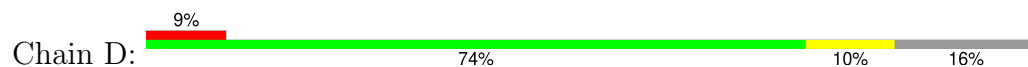


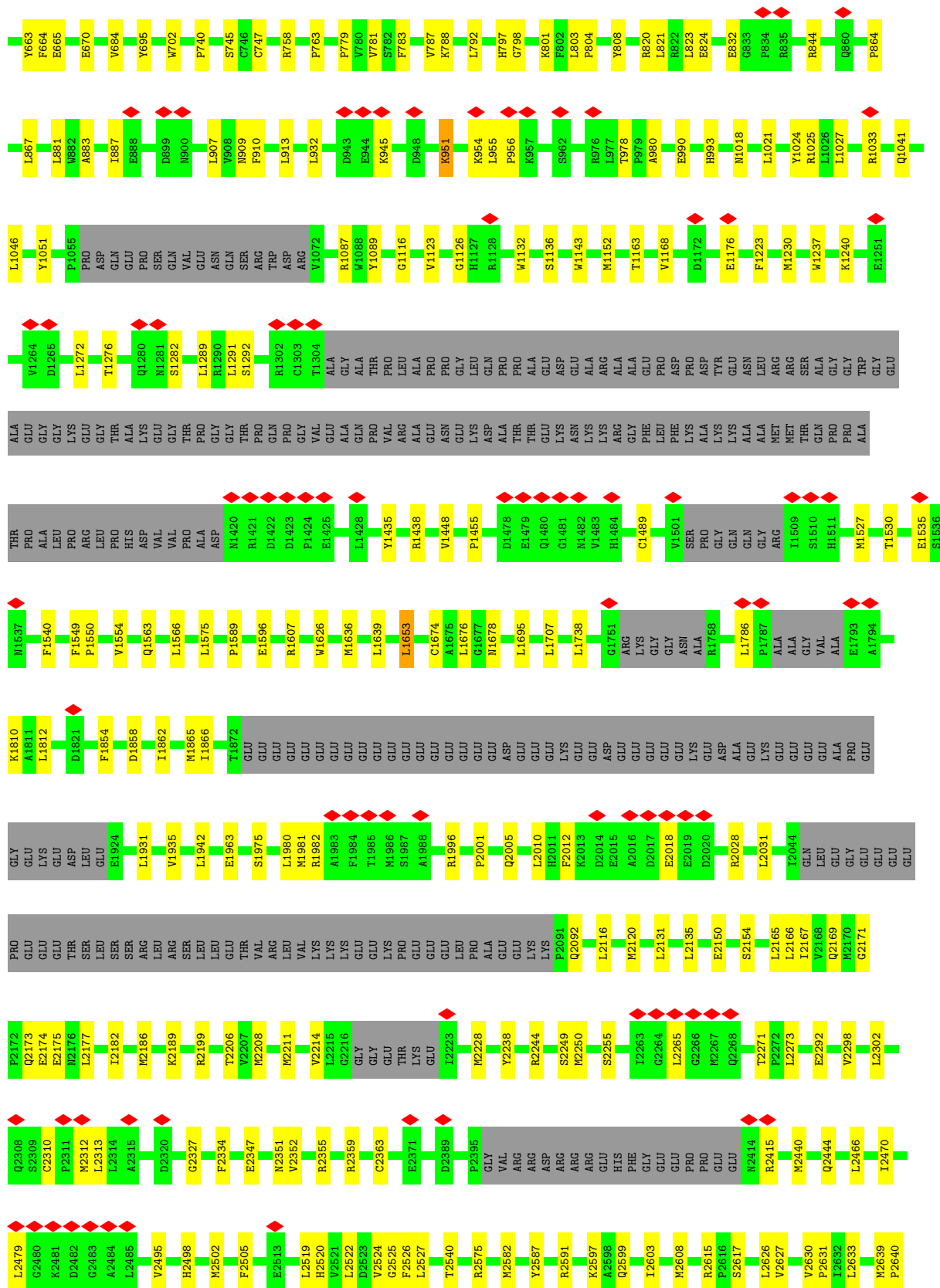




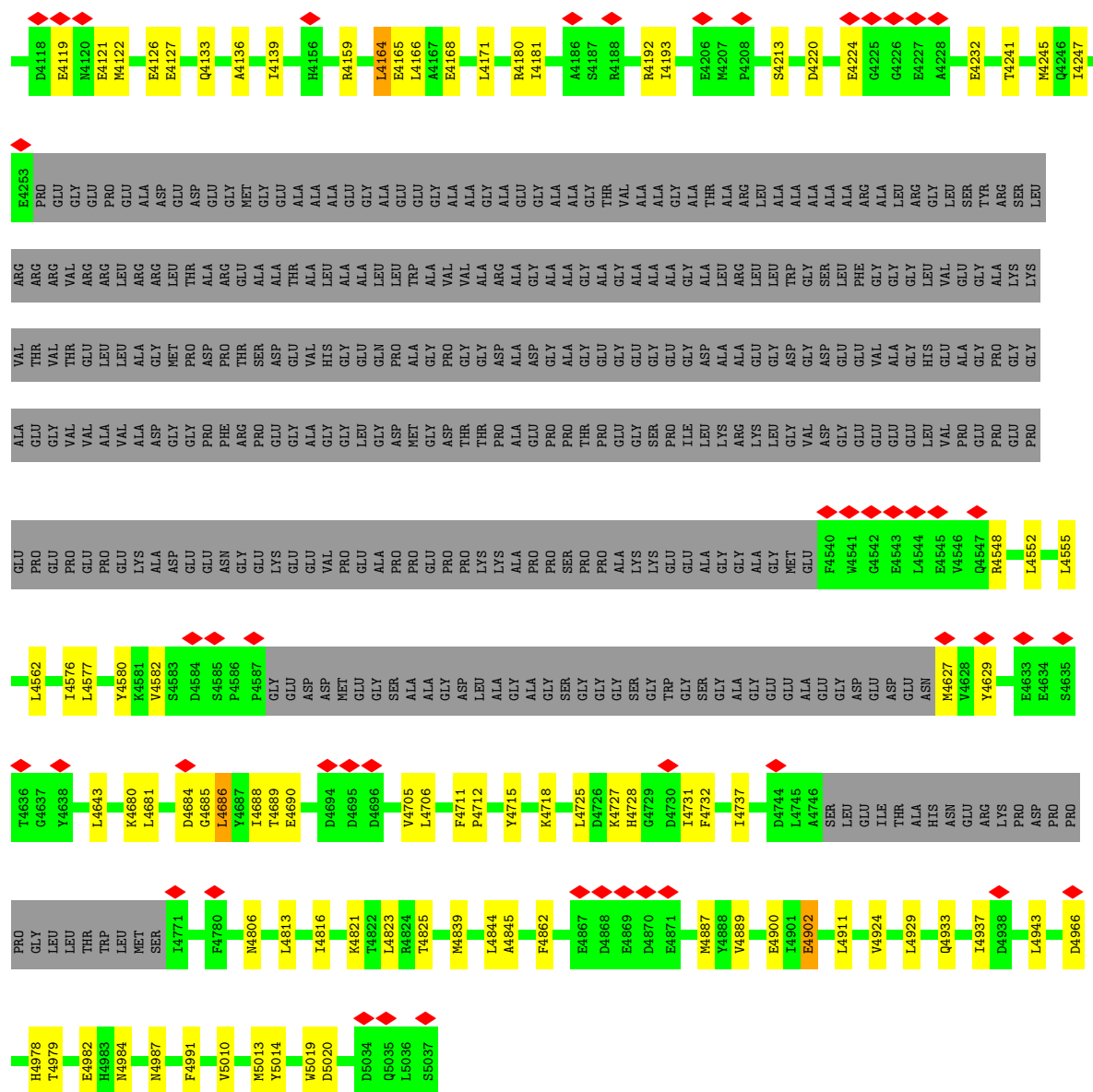


• Molecule 3: Ryanodine receptor 1

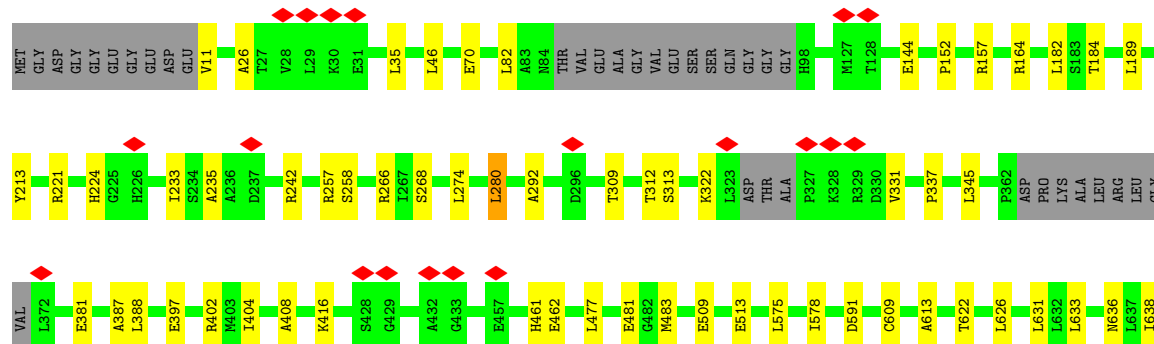
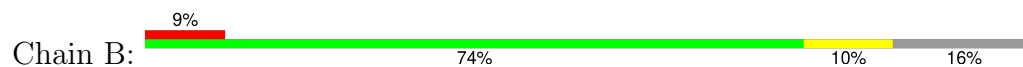








• Molecule 3: Ryanodine receptor 1





F3996	I3802	GLU	G3581	LYS	Y3409	K3123	Q2971	K2890	GLU	S2685
M4000	M3816	GLU	R3582	ARG	P3410	G3124	E2972	K2891	GLU	K2770
I4010	E4011	GLU	GLU	ARG	L3411	V3125	F2973	Q2892	ARG	K2689
L4012	E3825	GLU	ASP	ASP	L3412	G3126	H2976	E2893	THR	N2773
L4013	A3834	VAL	ASP	ALA	I3413	G3127	L2977	L2894	GLU	N2774
K4014	T3838	GLU	D3587	ARG	Y3415	T3132	E2978	E2895	LYS	W2775
L4017	F3847	GLU	D3588	Y3503	V3416	T3133	A2979	A2896	LYS	S2776
D4018	E3861	GLU	F3589	S3504	R3420	L3136	V2980	K2897	THR	Y2777
V4049	D3862	GLU	E3590	Q3506	L3434	Q3145	V2981	G2898	ARG	G2778
E4056	R3865	GLU	E3591	T3507	F3435	Q3149	S2982	G2899	LYS	E2779
K4060	I3866	GLU	R3595	L3509	R3436	G3160	S2983	G2900	SER	N2780
F4061	ASN	GLU	V3596	M3524	T3443	T3177	E2979	H2901	GLN	V2781
F4062	ARG	GLU	Y3604	D3531	Y3444	T3178	V2986	P2902	ALA	A2782
M4064	GLN	GLU	E3607	L3535	V3445	K3179	S2987	P2903	THR	E2784
G4073	ASN	GLU	E3610	L3536	S3446	T3182	K2988	L2904	VAL	E2785
S4074	GLY	GLU	H3611	R3538	R3452	Y3186	S2989	L2905	ASP	K2786
A4075	E3872	GLU	P3612	R3539	R3453	L3186	H2991	D2909	ARG	T2787
D4083	D3877	LYS	TYR	Y3540	V3460	L3190	E2992	T2912	GLU	H2788
P4084	D3883	SER	LYS	A3541	M3334	L3194	I2995	A2913	GLY	P2789
R4085	L3884	LYS	L3542	R3542	M3335	Y3213	I2995	A2914	N2856	M2790
G4086	F3885	ALA	K3543	K3543	V3346	S3223	L3003	K2915	N2857	L2791
L4087	F3889	VAL	D3544	D3544	T3361	P3224	P3004	E2916	Q2858	M2792
K4090	F3899	TRP	T3545	N3465	R3364	R3225	L3005	K2917	P2859	R2793
T3907	T3907	HIS	D3546	N3466	L3365	R3225	S3027	R2918	P2860	Y2794
T3919	T3919	LYS	E3547	M3467	L3365	R3225	K3036	D2919	D2861	K2795
D4091	T3919	LEU	E3548	L3470	E3375	R3225	I3039	R2920	L2862	V2740
D4092	T3919	GLY	V3548	T3471	E3376	R3225	V3050	E2921	L2863	E2741
K4095	T3931	GLU	R3550	ALA	E3377	R3225	K3056	K2922	Q2864	L2742
S4099	D3941	GLU	F3551	ASP	Q3378	R3225	E3086	A2923	V2865	L2743
E4107	V3942	GLU	E3552	SER	L3379	R3225	K3053	Q2924	T2866	N2744
F4110	Q3946	GLU	Q3554	LYS	R3381	R3225	L3056	E2925	L2867	V2745
D4118	K3948	GLU	N3555	ALA	A3383	R3225	E3086	L2926	S2868	L2746
E4119	F3951	GLU	N3556	GLY	K3384	R3225	K3105	L2927	R2869	L2747
M4120	F3951	VAL	N3556	ASP	E3385	R3225	M3106	F2929	L2871	P2748
M4122	M3955	GLU	N3556	GLY	E3387	R3225	V3107	K2928	L2872	E2749
A4136	T3969	GLU	E3557	GLY	E3388	R3225	E3108	L2930	Q2872	K2750
I4139	Q3970	GLU	L3557	SER	E3388	R3225	E3109	Q2931	A2873	L2751
L4159	G3971	GLU	P3557	GLN	E3389	R3225	L3110	M2932	A2875	D2752
E4165	P3972	GLU	L3663	ASP	G3390	R3225	R3111	N2933	E2876	S2753
L4166	L3980	GLU	D3666	GLU	E3391	R3225	L3112	Q2934	E2877	K2754
	L3985	GLU	E3670	THR	E3392	R3225	LYS	Y2935	Q2877	L2755
		GLN	E3682	LYS	L3392	R3225	VAL	A2936	L2878	N2756
		GLN	E3682	LYS	L3392	R3225	SER	V2937	A2879	K2757
		GLN	E3682	LYS	L3392	R3225	GLN	E2880	E2881	F2758
		GLN	E3682	LYS	L3392	R3225	GLN	N2881	A2815	F2759
		GLN	E3682	LYS	L3392	R3225	GLN	Y2882	E2760	E2761
		GLN	E3682	LYS	L3392	R3225	GLN	H2883	L2817	V2761
		GLN	E3682	LYS	L3392	R3225	GLN	N2884	A2818	T2762
		GLN	E3682	LYS	L3392	R3225	GLN	T2885	W2819	H2763
		GLN	E3682	LYS	L3392	R3225	GLN	W2886	E2764	E2764
		GLN	E3682	LYS	L3392	R3225	GLN	G2887	K2765	K2765
		GLN	E3682	LYS	L3392	R3225	GLN	R2888	W2766	W2766
		GLN	E3682	LYS	L3392	R3225	GLN	R2888	A2767	A2767
		GLN	E3682	LYS	L3392	R3225	GLN	R2888	F2768	F2768
		GLN	E3682	LYS	L3392	R3225	GLN	R2888	D2769	D2769







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	66232	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)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, U1C, CA, 43M, ZN, CFF

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	0.12	0/834	0.29	0/1123
1	F	0.12	0/834	0.31	0/1123
1	G	0.12	0/834	0.30	0/1123
1	H	0.13	0/834	0.32	0/1123
2	I	0.10	0/999	0.27	0/1355
2	J	0.10	0/999	0.27	0/1355
2	K	0.10	0/999	0.27	0/1355
2	L	0.11	0/999	0.30	0/1355
3	A	0.13	0/33927	0.28	0/45977
3	B	0.13	0/33927	0.29	0/45977
3	C	0.13	0/33927	0.28	0/45977
3	D	0.13	0/33927	0.28	0/45977
All	All	0.13	0/143040	0.28	0/193820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	824	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	818	0	824	8	0
1	G	818	0	824	8	0
1	H	818	0	824	11	0
2	I	990	0	775	11	0
2	J	990	0	775	10	0
2	K	990	0	775	11	0
2	L	990	0	775	11	0
3	A	33207	0	32374	284	0
3	B	33207	0	32374	294	0
3	C	33207	0	32374	281	0
3	D	33207	0	32374	300	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	54	0	24	1	0
5	B	54	0	24	1	0
5	C	54	0	24	1	0
5	D	54	0	24	1	0
6	A	23	0	0	0	0
6	B	23	0	0	0	0
6	C	23	0	0	0	0
6	D	23	0	0	0	0
7	A	27	0	18	0	0
7	B	27	0	18	0	0
7	C	27	0	18	0	0
7	D	27	0	18	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	14	0	10	2	0
9	B	14	0	10	2	0
9	C	14	0	10	2	0
9	D	14	0	10	2	0
10	A	870	0	0	1	0
10	B	864	0	0	1	0
10	C	858	0	0	1	0
10	D	855	0	0	1	0
10	E	13	0	0	0	0
10	F	13	0	0	0	0
10	G	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	12	0	0	0	0
10	I	56	0	0	0	0
10	J	61	0	0	0	0
10	K	63	0	0	0	0
10	L	61	0	0	0	0
All	All	144280	0	136100	1206	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 4.

The worst 5 of 1206 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)
3:A:4232:GLU:HG2	3:A:5019:TRP:HE1	1.50	0.77
3:B:4232:GLU:HG2	3:B:5019:TRP:HE1	1.50	0.76
3:B:3996:PHE:O	3:B:4000:MET:HG3	1.86	0.76
3:A:3996:PHE:O	3:A:4000:MET:HG3	1.86	0.76
3:C:3996:PHE:O	3:C:4000:MET:HG3	1.86	0.75

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	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	G	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	I	146/148 (99%)	142 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	K	146/148 (99%)	143 (98%)	3 (2%)	0	100	100
2	L	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
3	A	4188/5037 (83%)	4121 (98%)	67 (2%)	0	100	100
3	B	4188/5037 (83%)	4119 (98%)	69 (2%)	0	100	100
3	C	4188/5037 (83%)	4121 (98%)	67 (2%)	0	100	100
3	D	4188/5037 (83%)	4122 (98%)	66 (2%)	0	100	100
All	All	17756/21168 (84%)	17454 (98%)	302 (2%)	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	E	88/88 (100%)	85 (97%)	3 (3%)	32	58
1	F	88/88 (100%)	85 (97%)	3 (3%)	32	58
1	G	88/88 (100%)	85 (97%)	3 (3%)	32	58
1	H	88/88 (100%)	85 (97%)	3 (3%)	32	58
2	I	74/127 (58%)	71 (96%)	3 (4%)	27	51
2	J	74/127 (58%)	68 (92%)	6 (8%)	11	23
2	K	74/127 (58%)	70 (95%)	4 (5%)	20	40
2	L	74/127 (58%)	71 (96%)	3 (4%)	27	51
3	A	3528/4276 (82%)	3465 (98%)	63 (2%)	51	74
3	B	3528/4276 (82%)	3471 (98%)	57 (2%)	55	77
3	C	3528/4276 (82%)	3471 (98%)	57 (2%)	55	77
3	D	3528/4276 (82%)	3465 (98%)	63 (2%)	51	74
All	All	14760/17964 (82%)	14492 (98%)	268 (2%)	51	74

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	2173	GLN
3	C	2971	GLN
3	C	4580	TYR
3	D	578	ILE
3	D	184	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	4216	GLN
3	C	4005	GLN
3	C	181	HIS
3	C	1938	GLN
3	C	4805	ASN

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
5	ADP	C	5607	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
7	43M	C	5606	-	9,9,9	0.39	0	12,12,12	0.50	0
5	ADP	B	5607	-	28,29,29	1.42	5 (17%)	43,45,45	1.85	8 (18%)
7	43M	B	5604	-	9,9,9	0.39	0	12,12,12	0.53	0
6	U1C	D	5603	-	25,25,25	0.61	0	33,35,35	0.51	0
7	43M	B	5605	-	9,9,9	0.40	0	12,12,12	0.53	0
5	ADP	A	5602	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
5	ADP	B	5602	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
9	CFF	B	5609	-	15,15,15	0.59	0	23,23,23	0.76	1 (4%)
9	CFF	A	5609	-	15,15,15	0.59	0	23,23,23	0.75	1 (4%)
7	43M	D	5604	-	9,9,9	0.40	0	12,12,12	0.52	0
6	U1C	C	5603	-	25,25,25	0.61	0	33,35,35	0.50	0
7	43M	A	5605	-	9,9,9	0.40	0	12,12,12	0.52	0
5	ADP	D	5607	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	8 (18%)
5	ADP	C	5602	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
9	CFF	C	5609	-	15,15,15	0.59	0	23,23,23	0.75	1 (4%)
7	43M	D	5605	-	9,9,9	0.39	0	12,12,12	0.53	0
7	43M	C	5605	-	9,9,9	0.39	0	12,12,12	0.51	0
7	43M	B	5606	-	9,9,9	0.38	0	12,12,12	0.50	0
9	CFF	D	5609	-	15,15,15	0.59	0	23,23,23	0.75	1 (4%)
7	43M	C	5604	-	9,9,9	0.38	0	12,12,12	0.52	0
7	43M	A	5606	-	9,9,9	0.40	0	12,12,12	0.50	0
5	ADP	A	5607	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	8 (18%)
5	ADP	D	5602	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
7	43M	A	5604	-	9,9,9	0.38	0	12,12,12	0.52	0
7	43M	D	5606	-	9,9,9	0.39	0	12,12,12	0.51	0
6	U1C	B	5603	-	25,25,25	0.62	0	33,35,35	0.50	0
6	U1C	A	5603	-	25,25,25	0.61	0	33,35,35	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	C	5607	-	-	2/16/32/32	0/3/3/3
7	43M	C	5606	-	-	-	0/1/1/1
5	ADP	B	5607	-	-	2/16/32/32	0/3/3/3
7	43M	B	5604	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U1C	D	5603	-	-	0/11/25/25	0/3/3/3
7	43M	B	5605	-	-	-	0/1/1/1
5	ADP	A	5602	-	-	2/16/32/32	0/3/3/3
5	ADP	B	5602	-	-	2/16/32/32	0/3/3/3
9	CFF	B	5609	-	-	-	0/2/2/2
9	CFF	A	5609	-	-	-	0/2/2/2
7	43M	D	5604	-	-	-	0/1/1/1
6	U1C	C	5603	-	-	0/11/25/25	0/3/3/3
7	43M	A	5605	-	-	-	0/1/1/1
5	ADP	D	5607	-	-	2/16/32/32	0/3/3/3
5	ADP	C	5602	-	-	2/16/32/32	0/3/3/3
9	CFF	C	5609	-	-	-	0/2/2/2
7	43M	D	5605	-	-	-	0/1/1/1
7	43M	C	5605	-	-	-	0/1/1/1
7	43M	B	5606	-	-	-	0/1/1/1
9	CFF	D	5609	-	-	-	0/2/2/2
7	43M	C	5604	-	-	-	0/1/1/1
7	43M	A	5606	-	-	-	0/1/1/1
5	ADP	A	5607	-	-	2/16/32/32	0/3/3/3
5	ADP	D	5602	-	-	2/16/32/32	0/3/3/3
7	43M	A	5604	-	-	-	0/1/1/1
7	43M	D	5606	-	-	-	0/1/1/1
6	U1C	B	5603	-	-	0/11/25/25	0/3/3/3
6	U1C	A	5603	-	-	0/11/25/25	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5607	ADP	C5-C4	4.72	1.47	1.39
5	C	5602	ADP	C5-C4	4.70	1.47	1.39
5	A	5602	ADP	C5-C4	4.70	1.47	1.39
5	B	5607	ADP	C5-C4	4.69	1.47	1.39
5	C	5607	ADP	C5-C4	4.68	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5607	ADP	C5-C4-N3	-6.02	118.42	126.72
5	B	5607	ADP	C5-C4-N3	-6.00	118.46	126.72
5	D	5602	ADP	C5-C4-N3	-5.99	118.47	126.72
5	A	5607	ADP	C5-C4-N3	-5.98	118.48	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5607	ADP	C5-C4-N3	-5.98	118.48	126.72

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

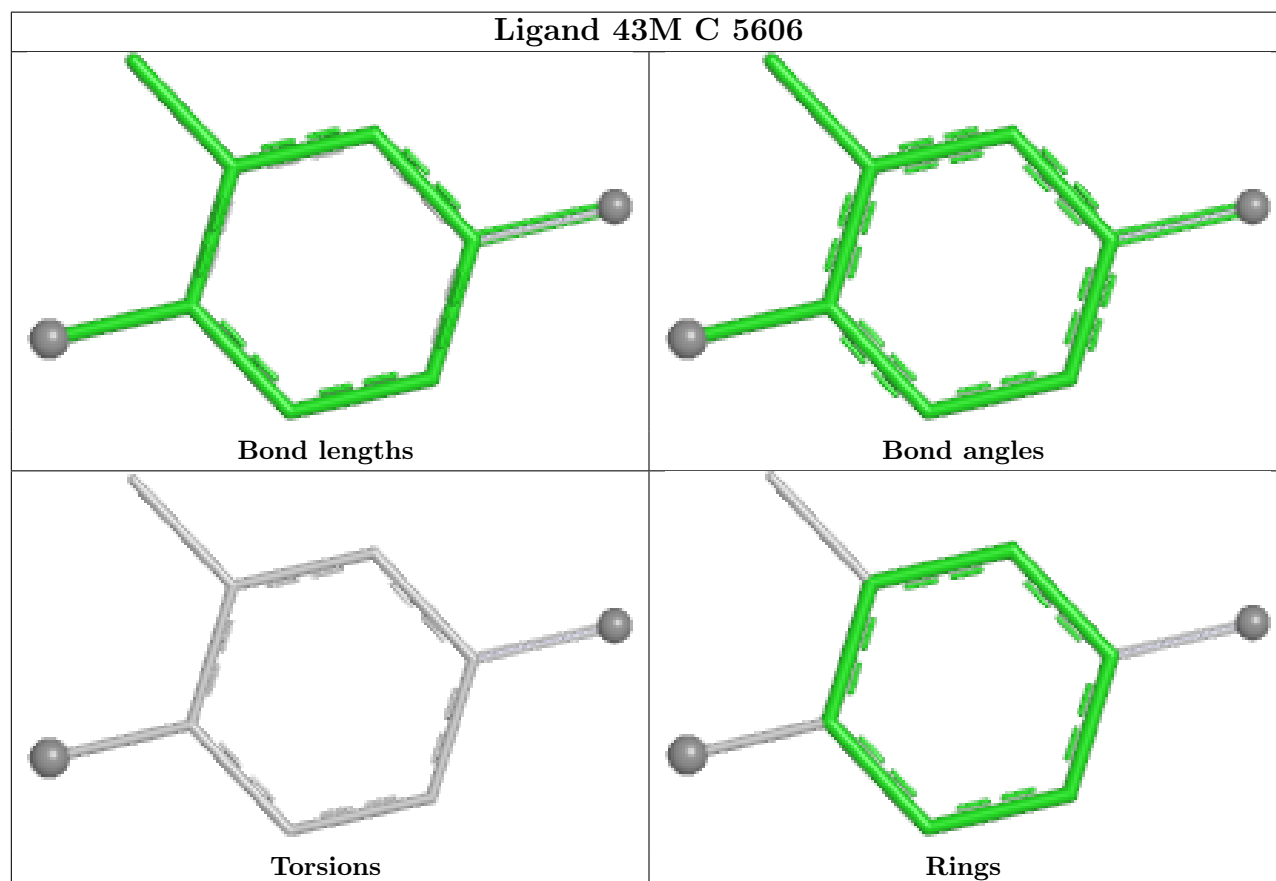
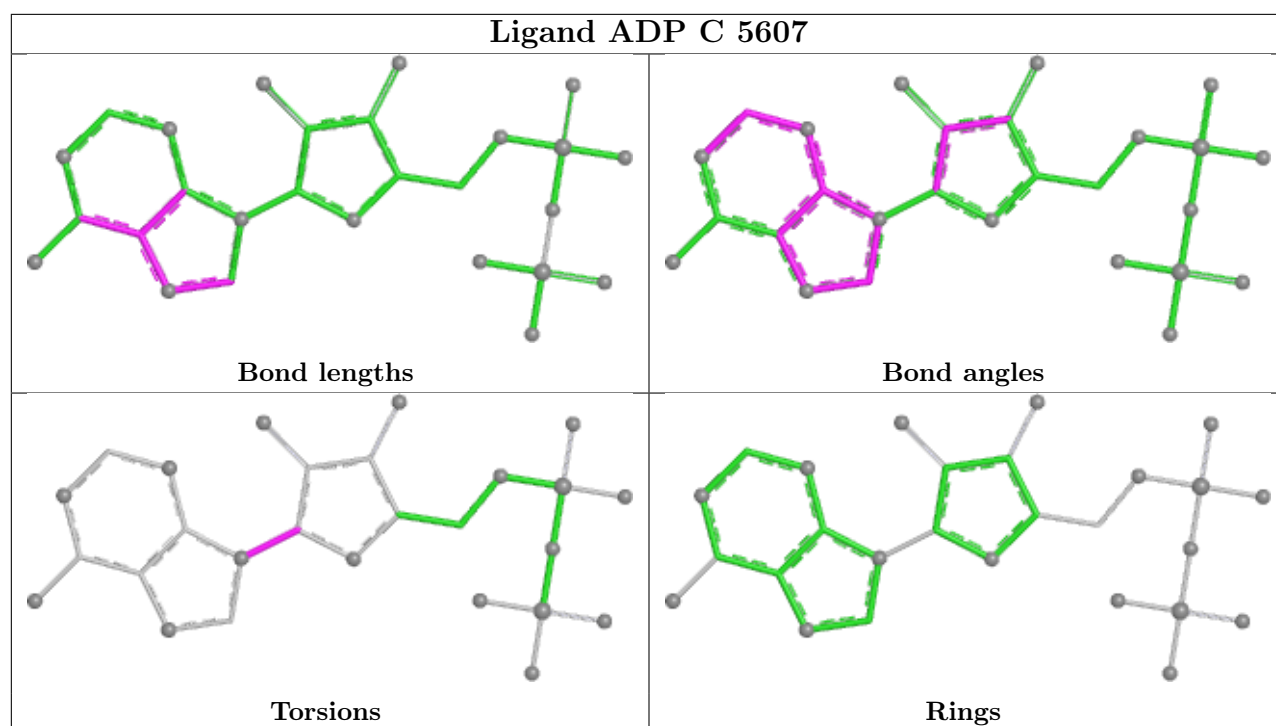
Mol	Chain	Res	Type	Atoms
5	A	5602	ADP	O4'-C4'-C5'-O5'
5	D	5602	ADP	O4'-C4'-C5'-O5'
5	B	5602	ADP	O4'-C4'-C5'-O5'
5	C	5602	ADP	O4'-C4'-C5'-O5'
5	A	5607	ADP	O4'-C1'-N9-C8

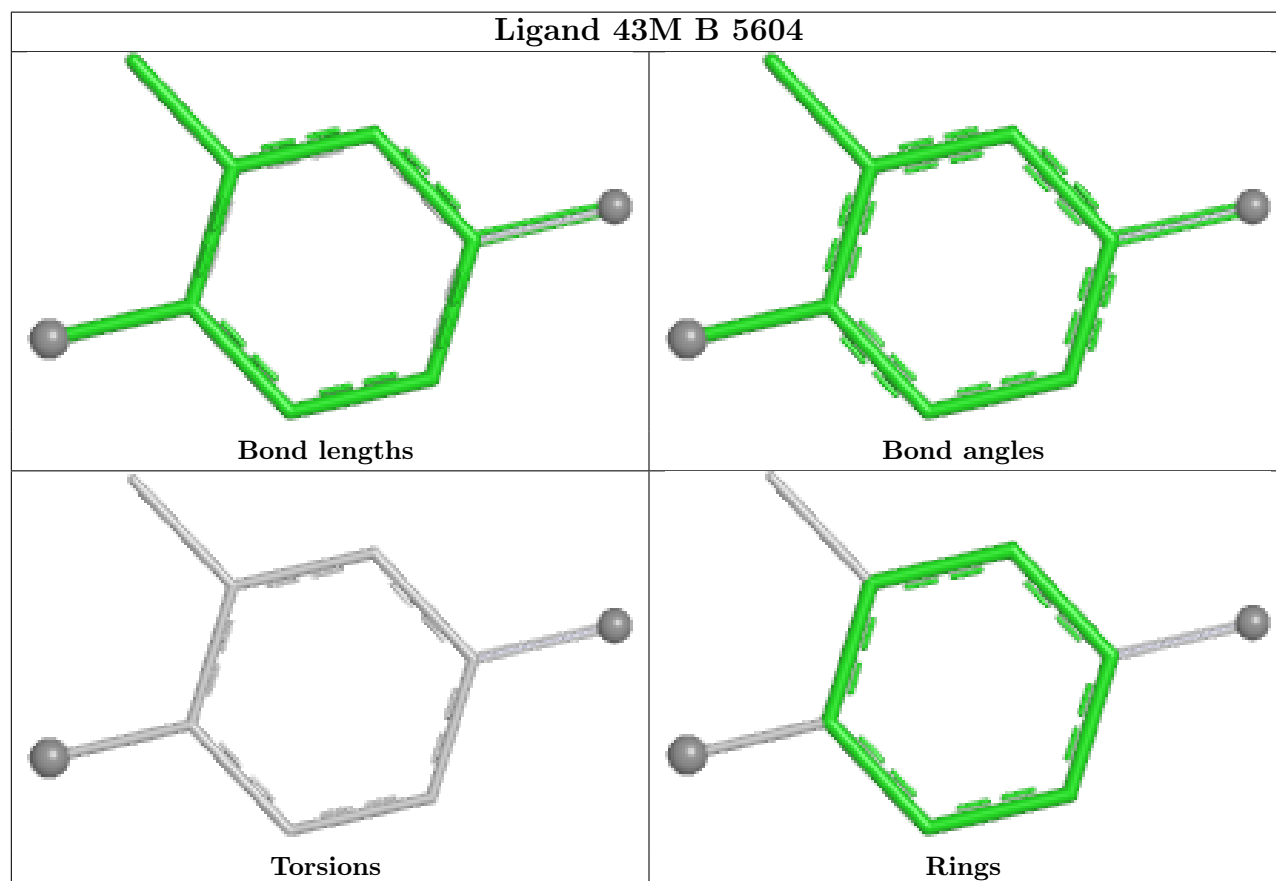
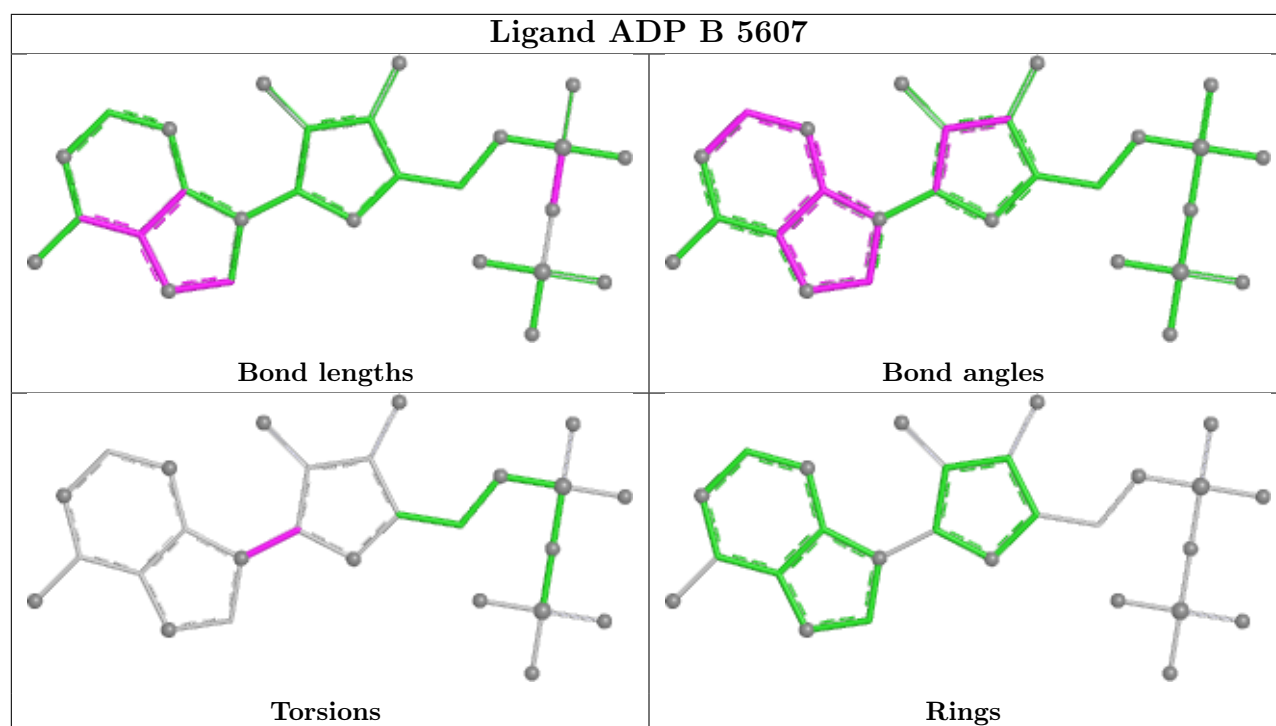
There are no ring outliers.

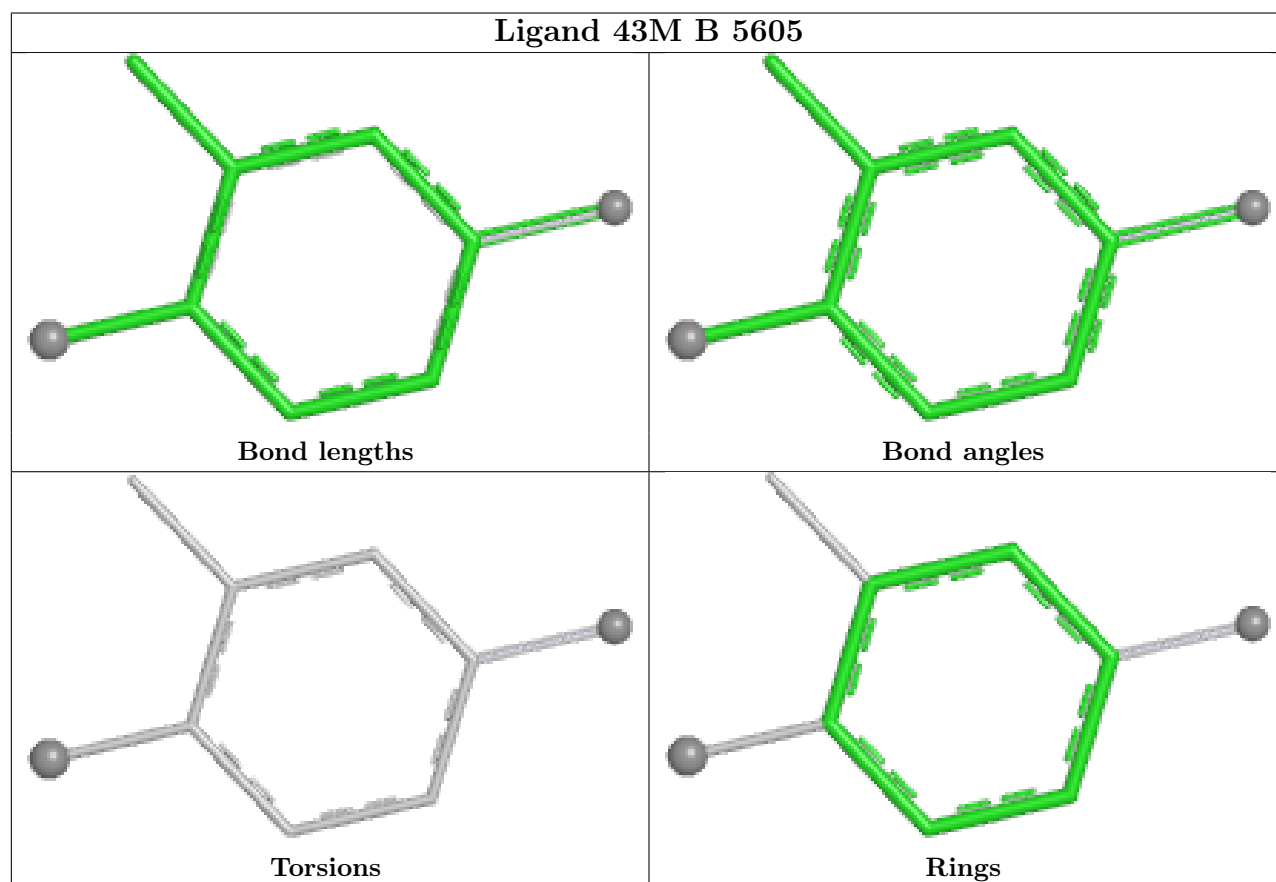
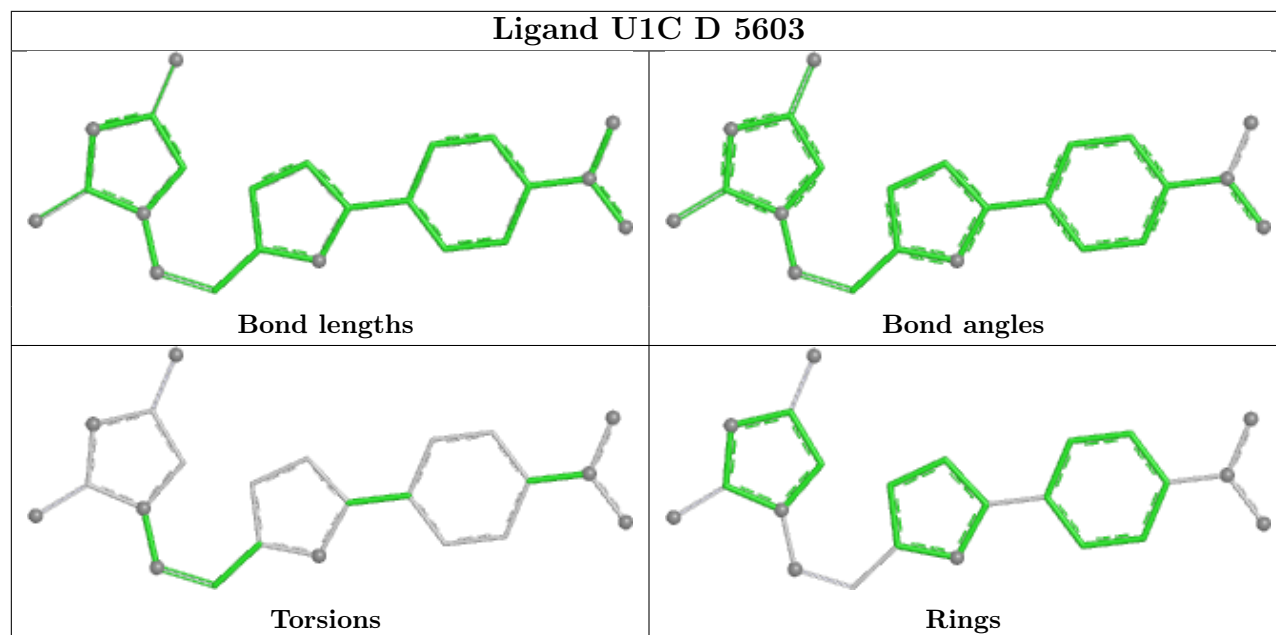
8 monomers are involved in 12 short contacts:

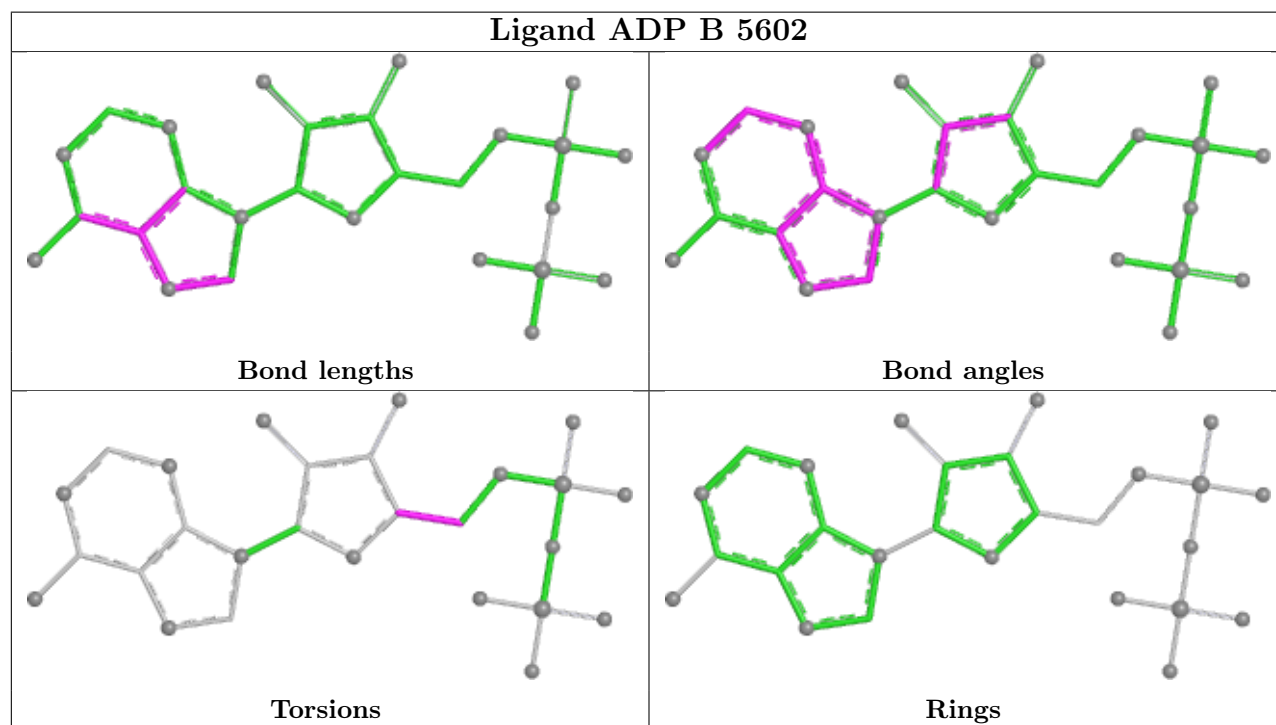
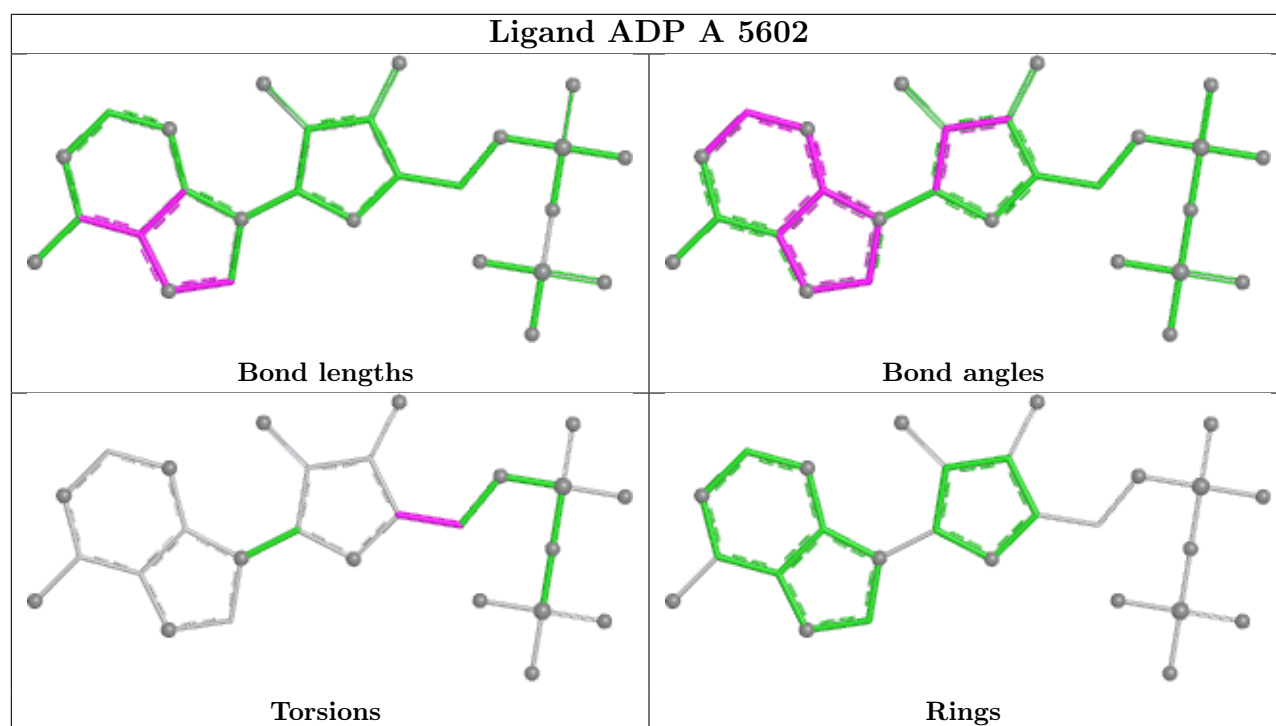
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5607	ADP	1	0
5	B	5607	ADP	1	0
9	B	5609	CFF	2	0
9	A	5609	CFF	2	0
5	D	5607	ADP	1	0
9	C	5609	CFF	2	0
9	D	5609	CFF	2	0
5	A	5607	ADP	1	0

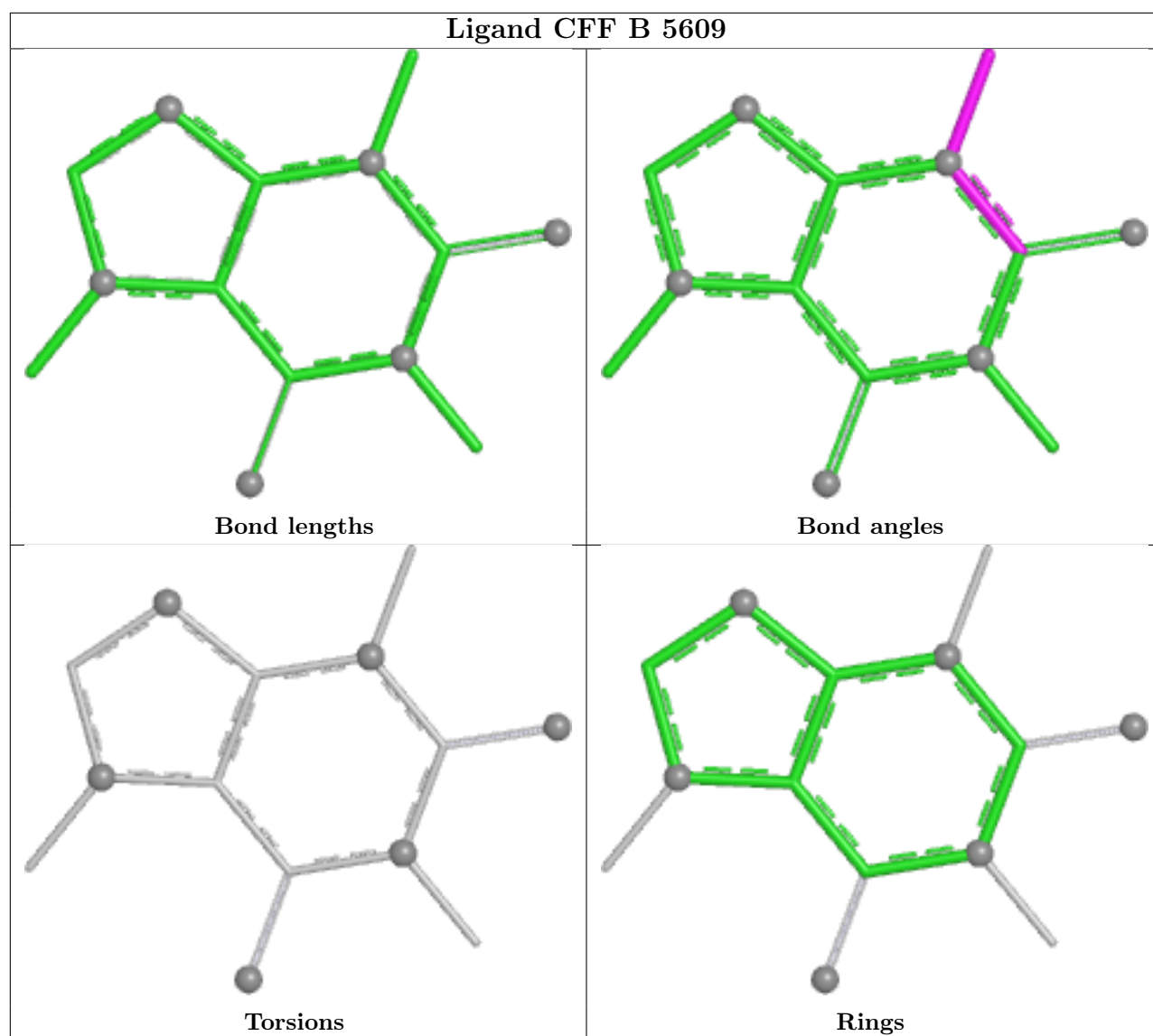
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

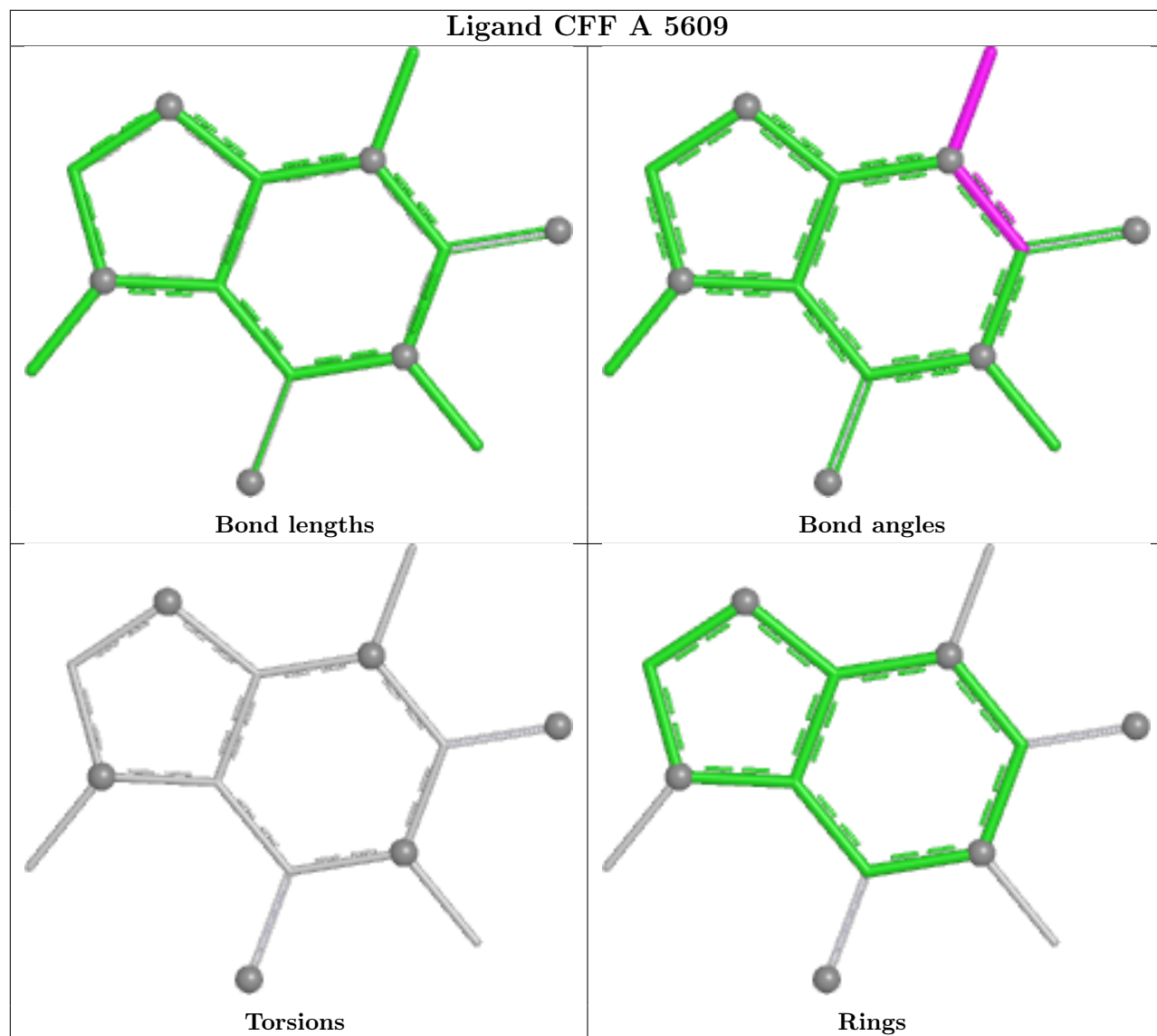




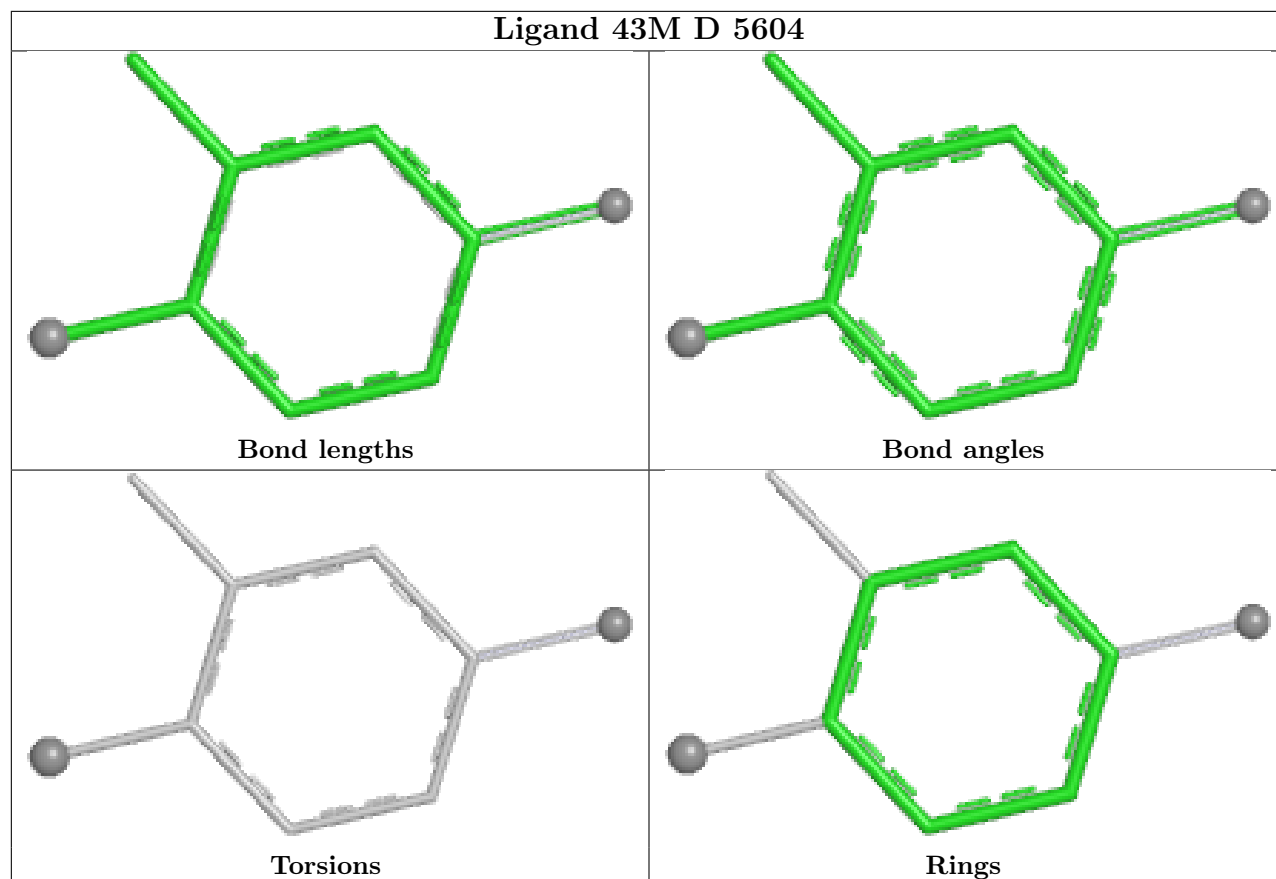




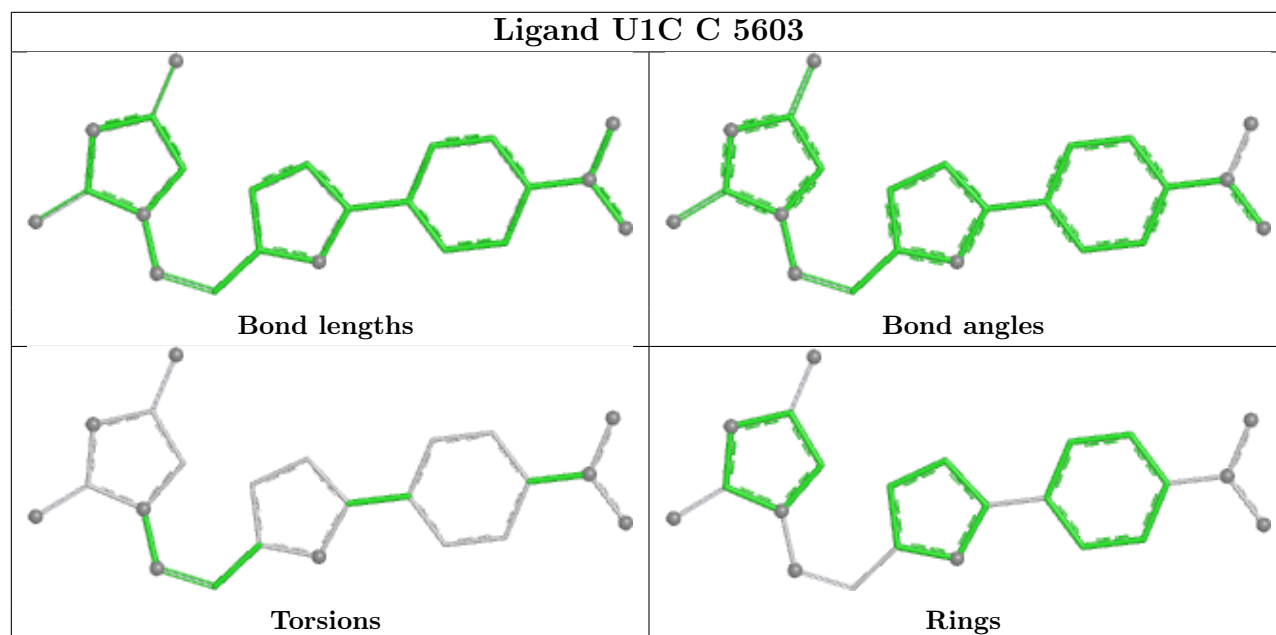




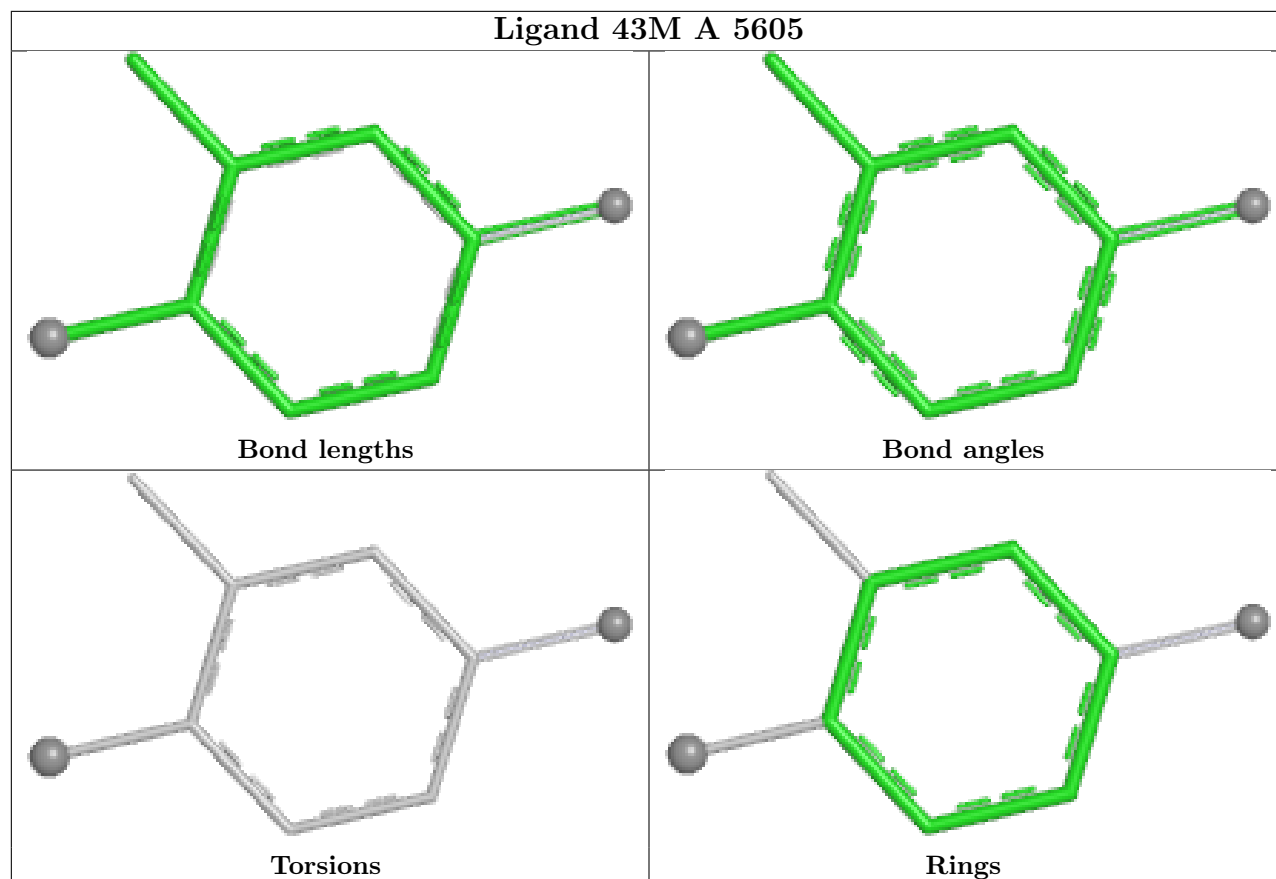
Ligand 43M D 5604



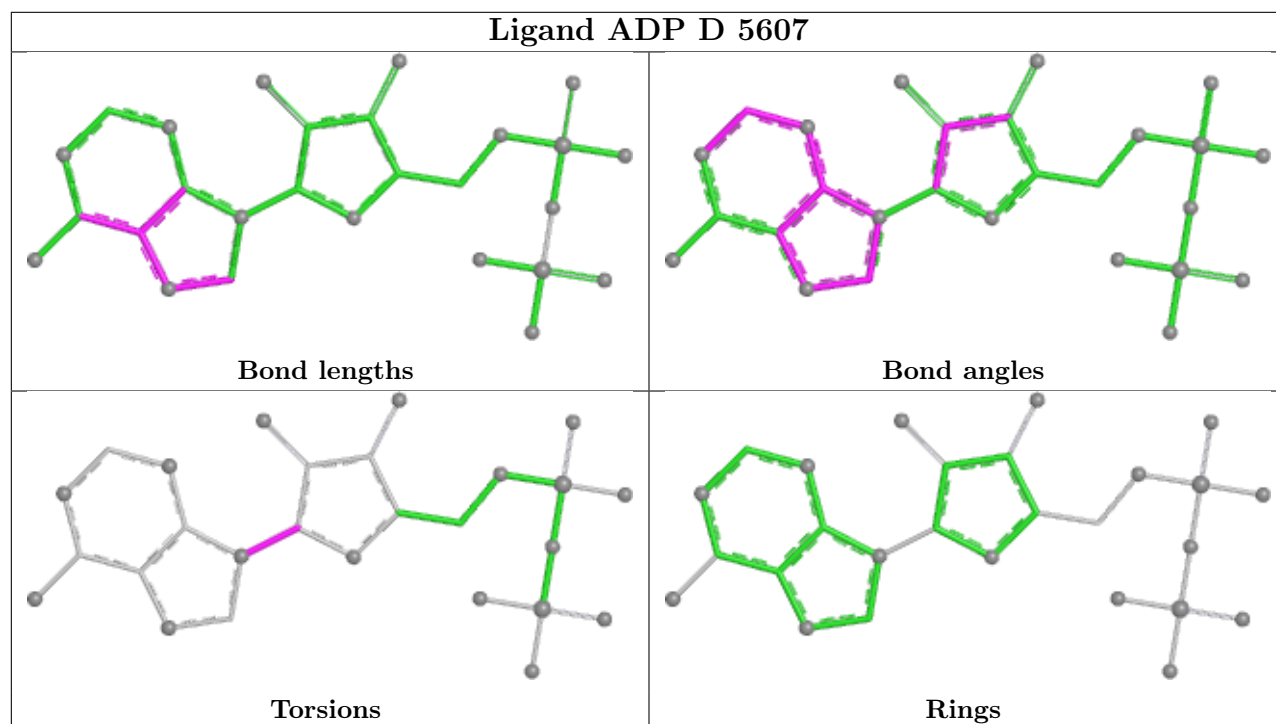
Ligand U1C C 5603

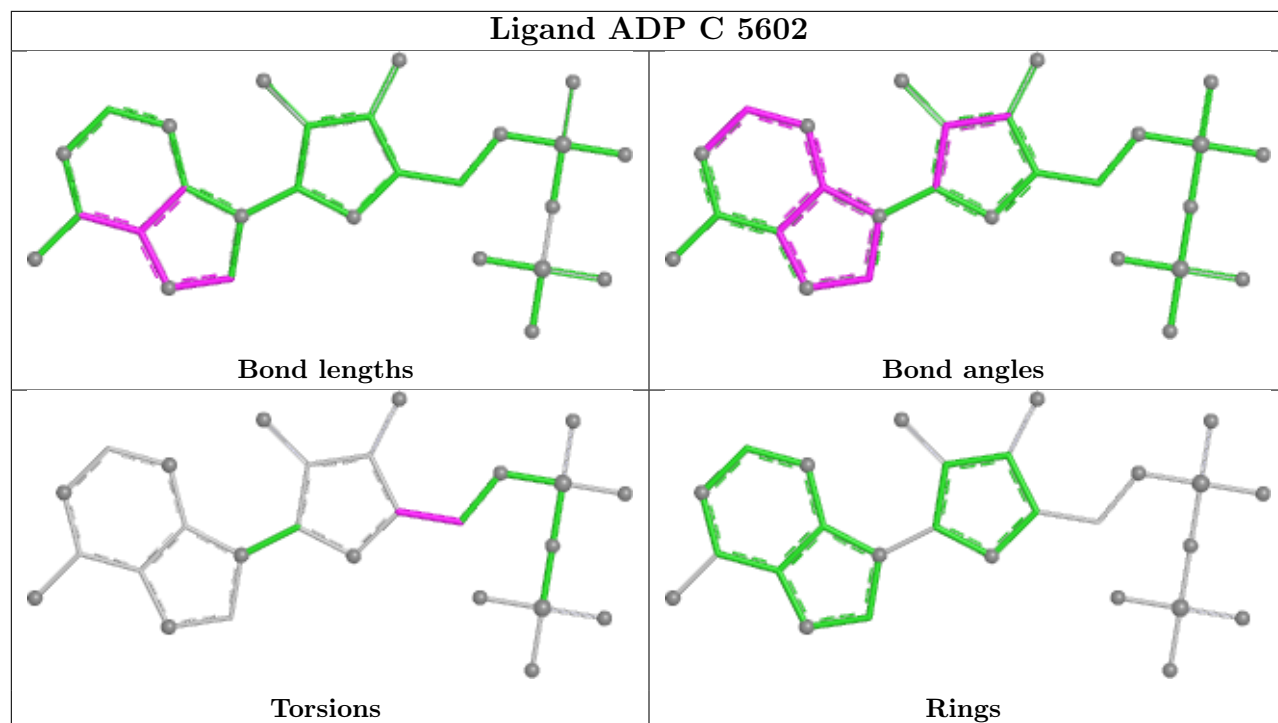


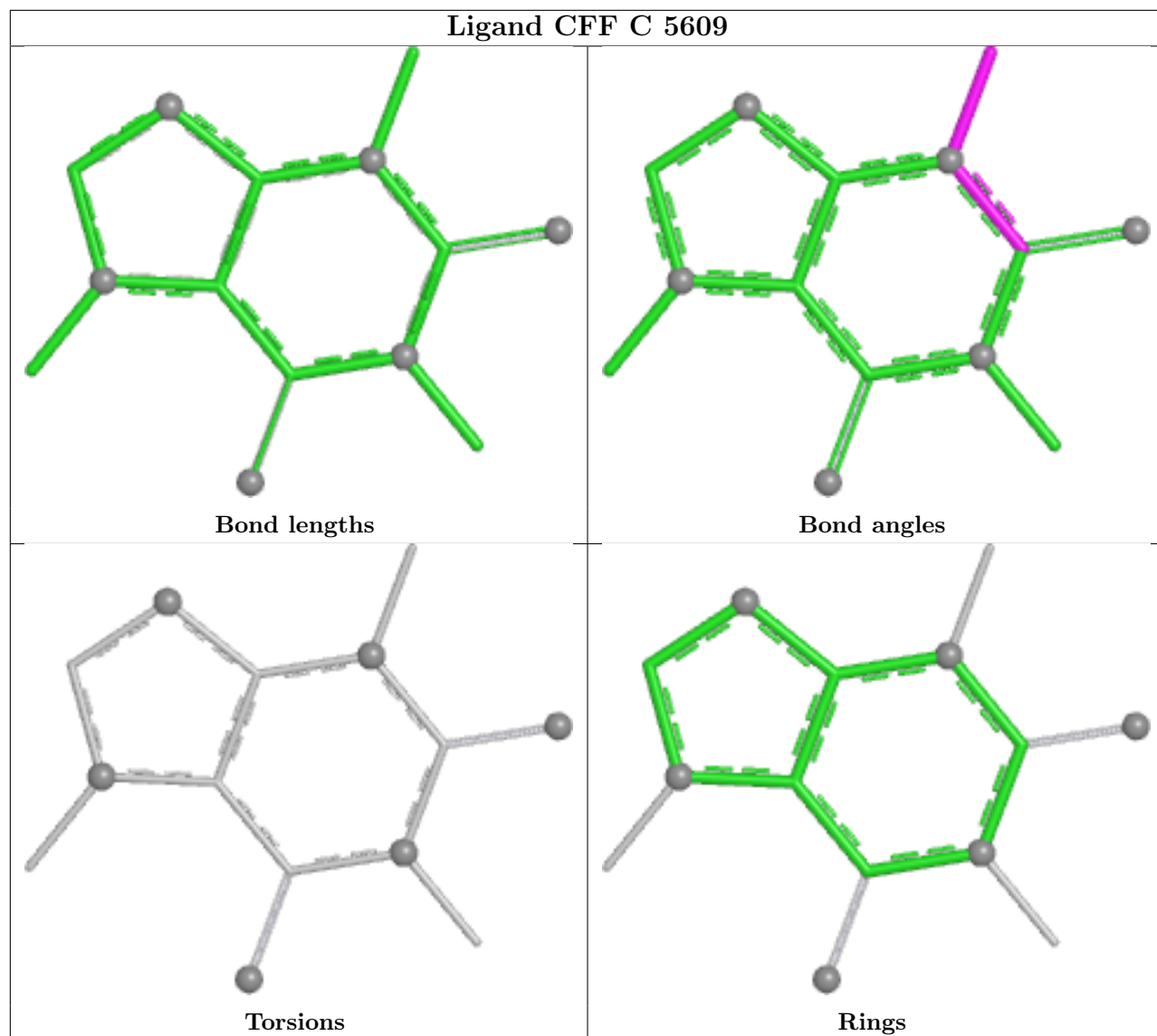
Ligand 43M A 5605



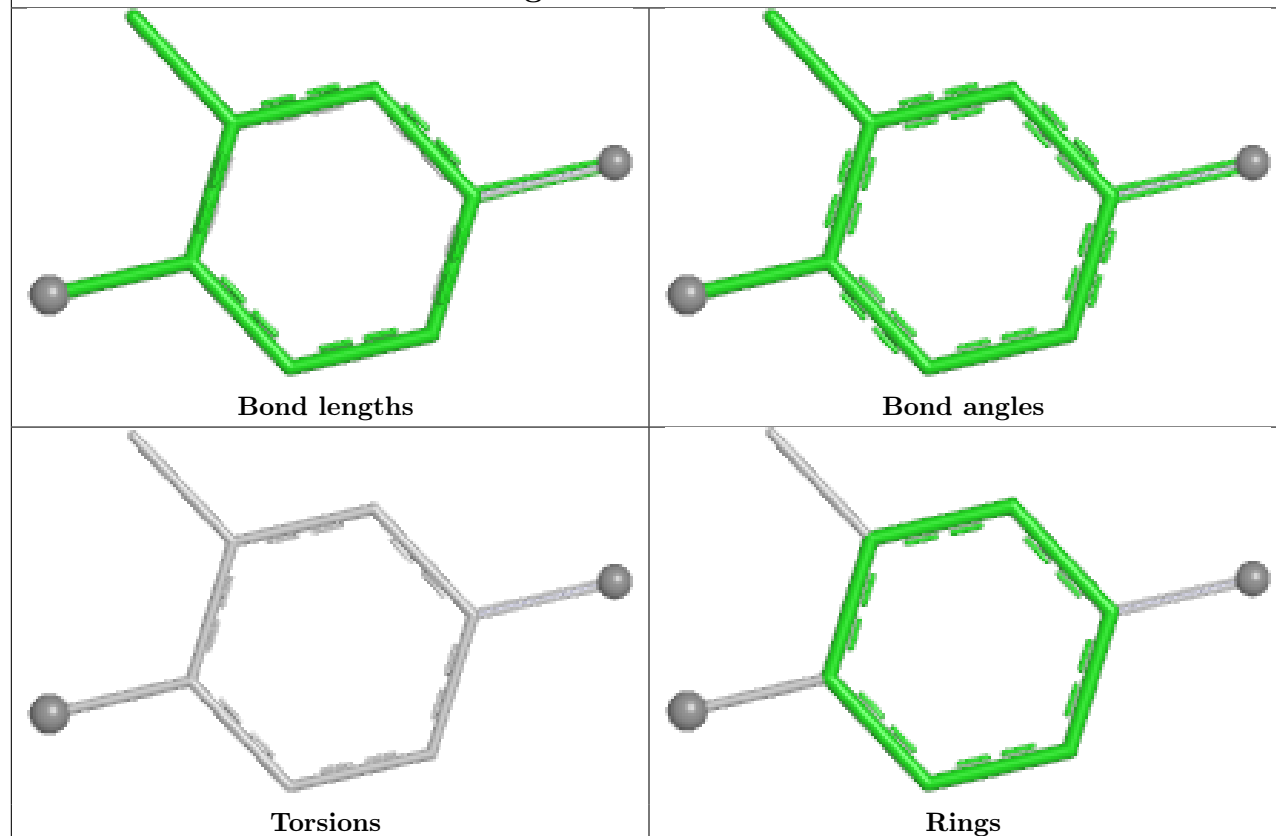
Ligand ADP D 5607



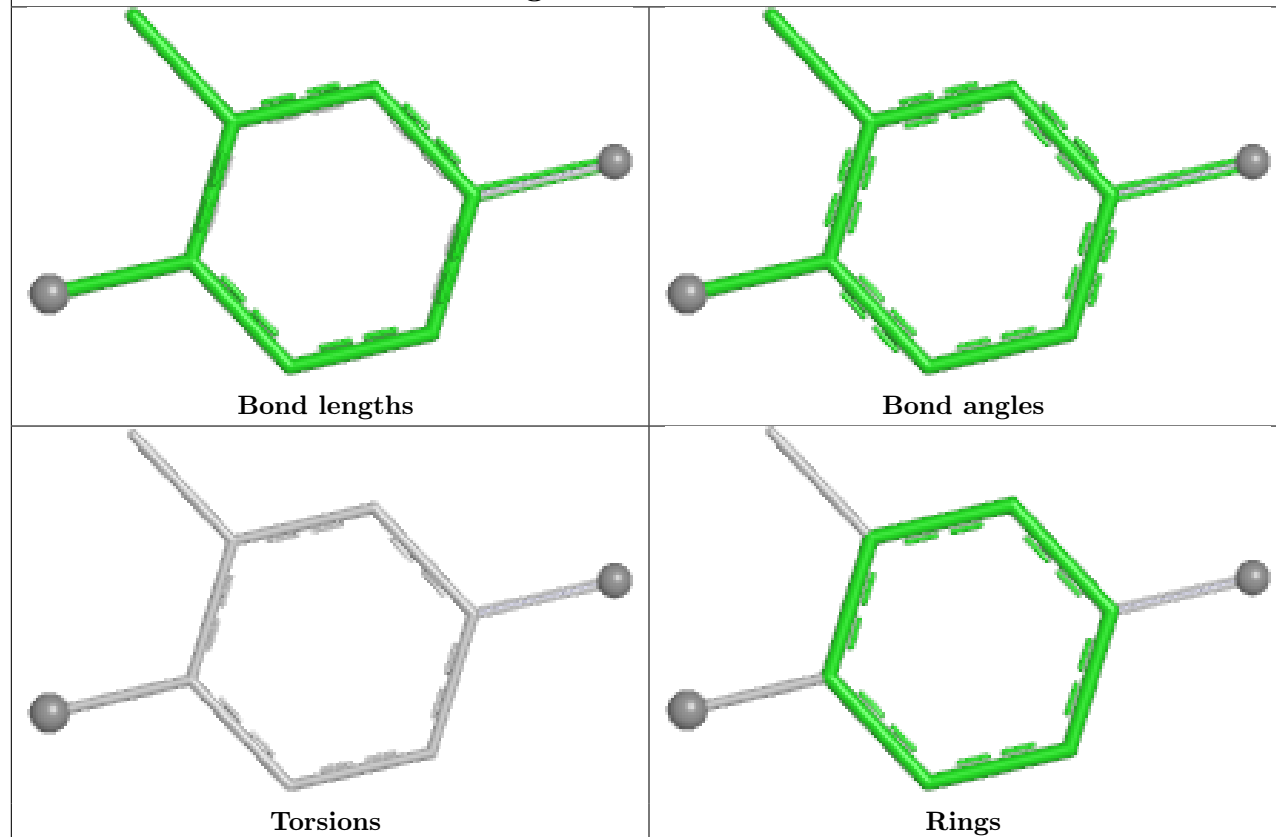


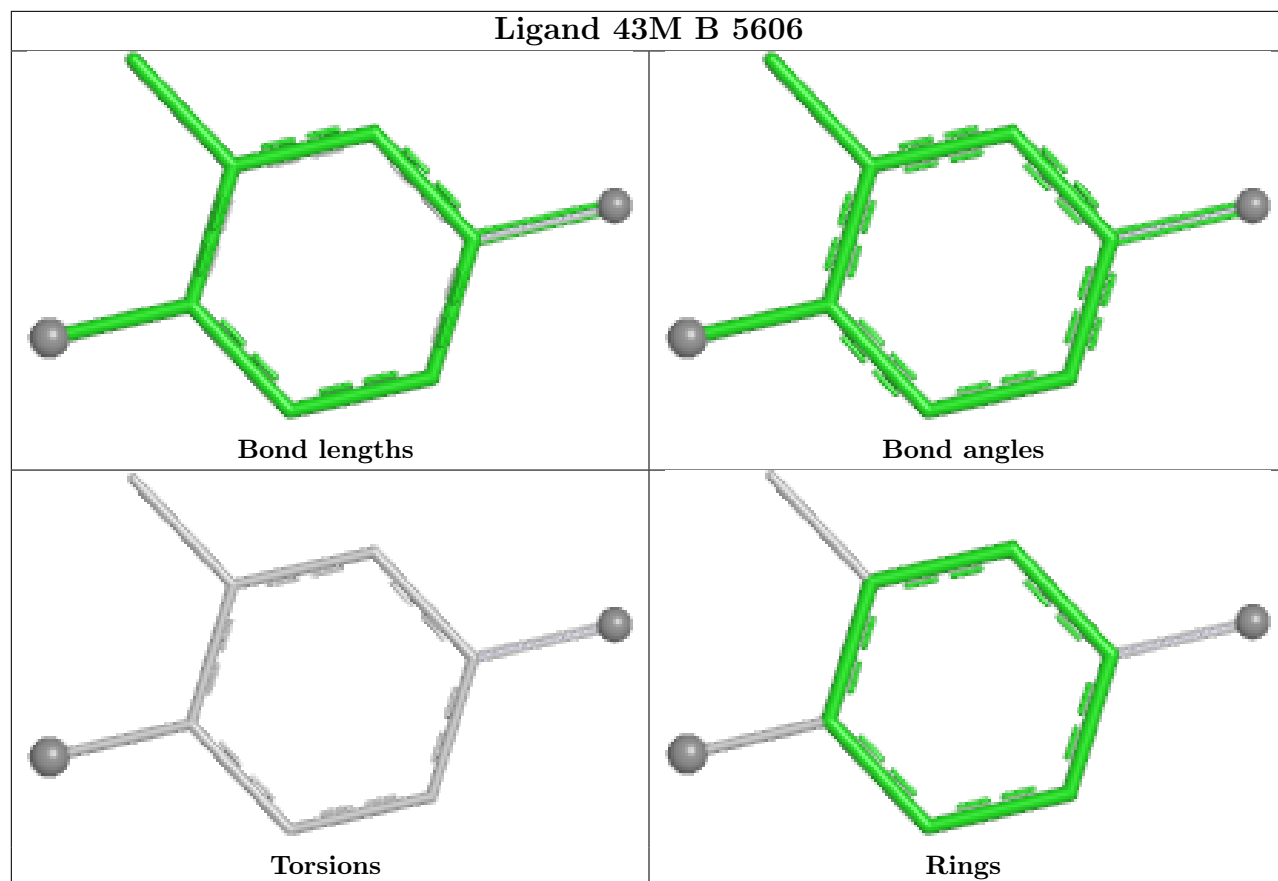


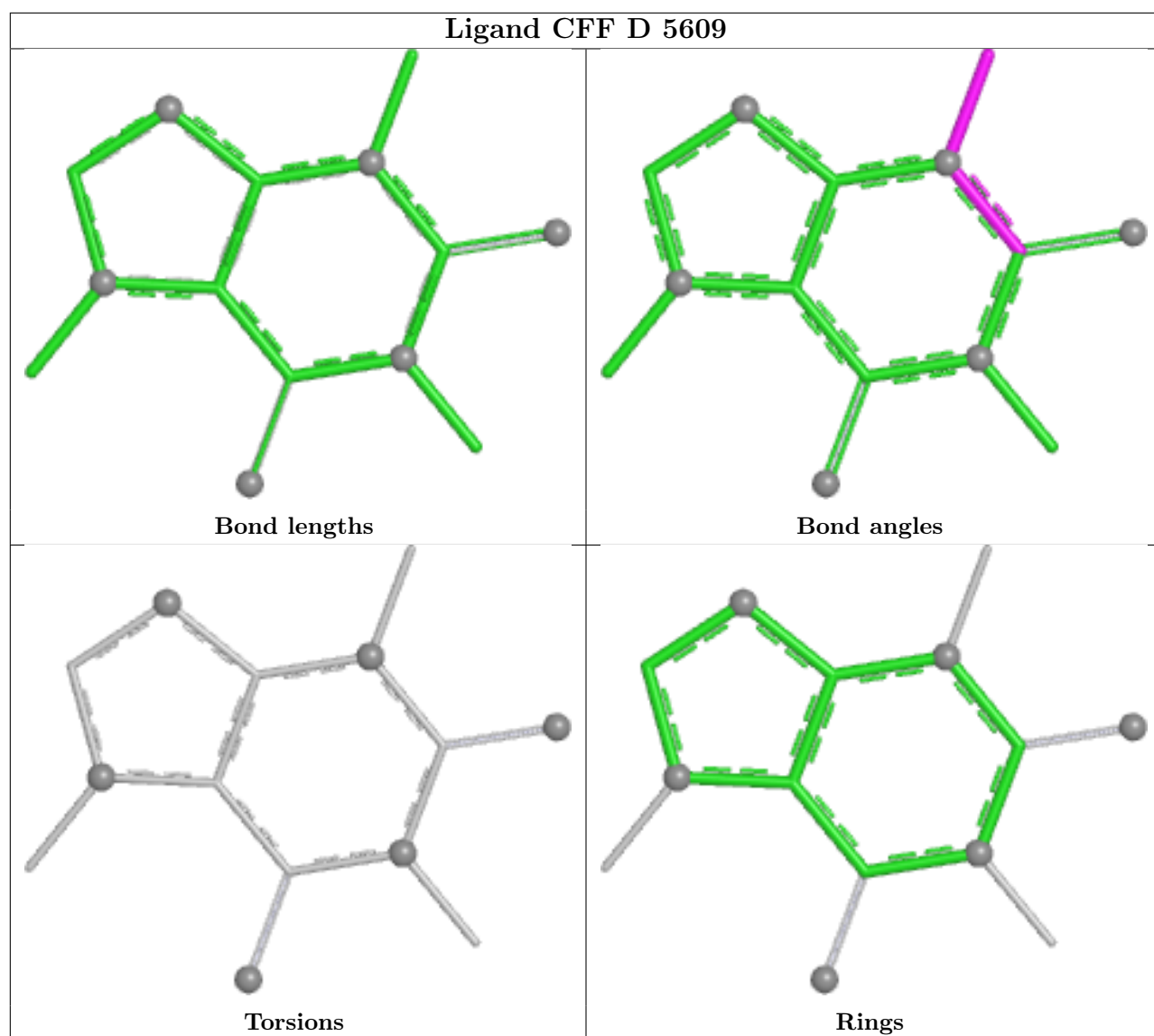
Ligand 43M D 5605



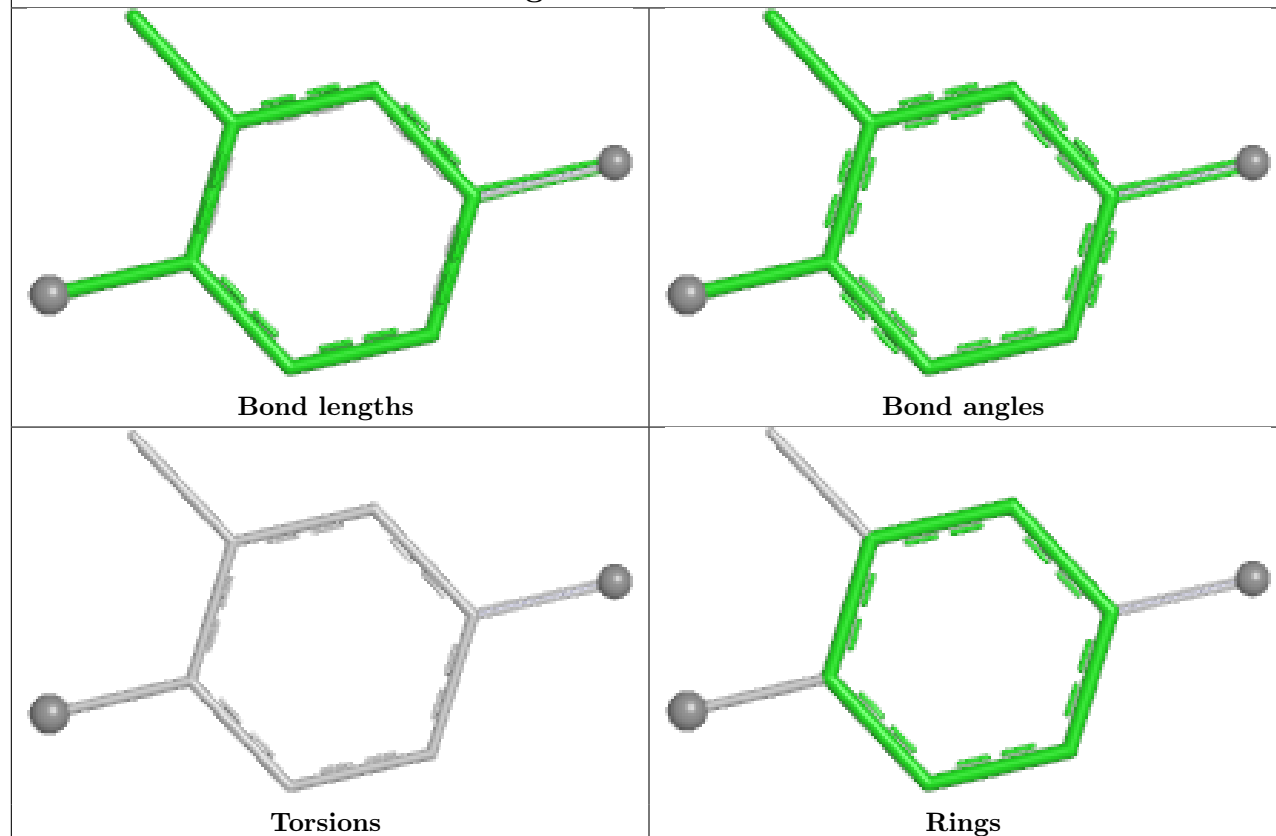
Ligand 43M C 5605



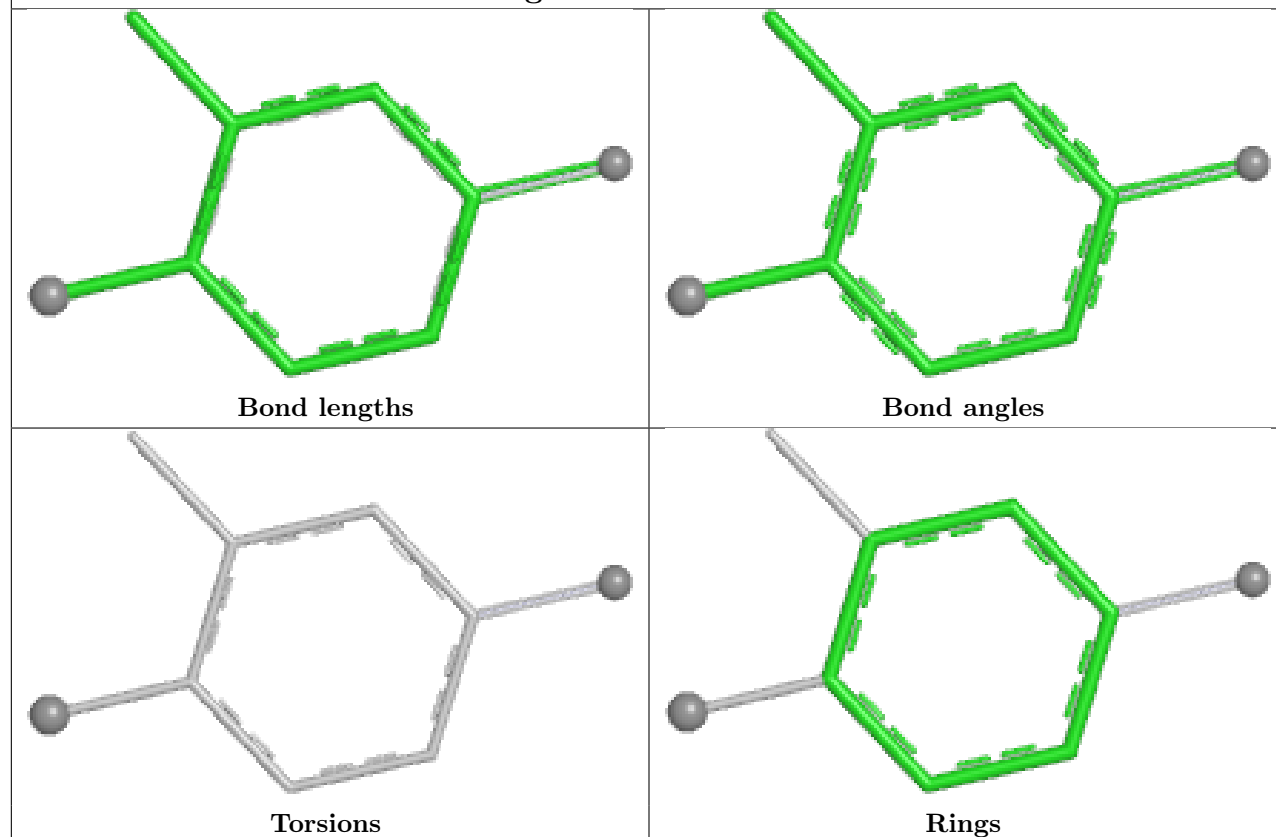


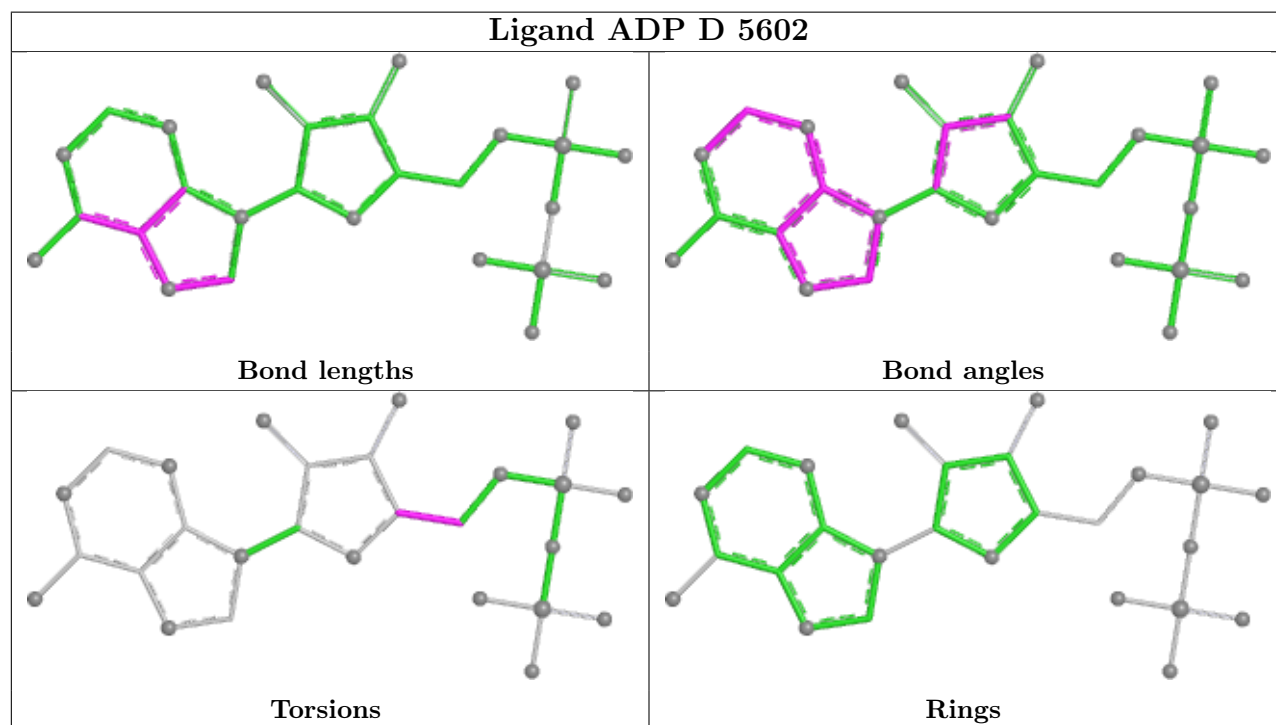
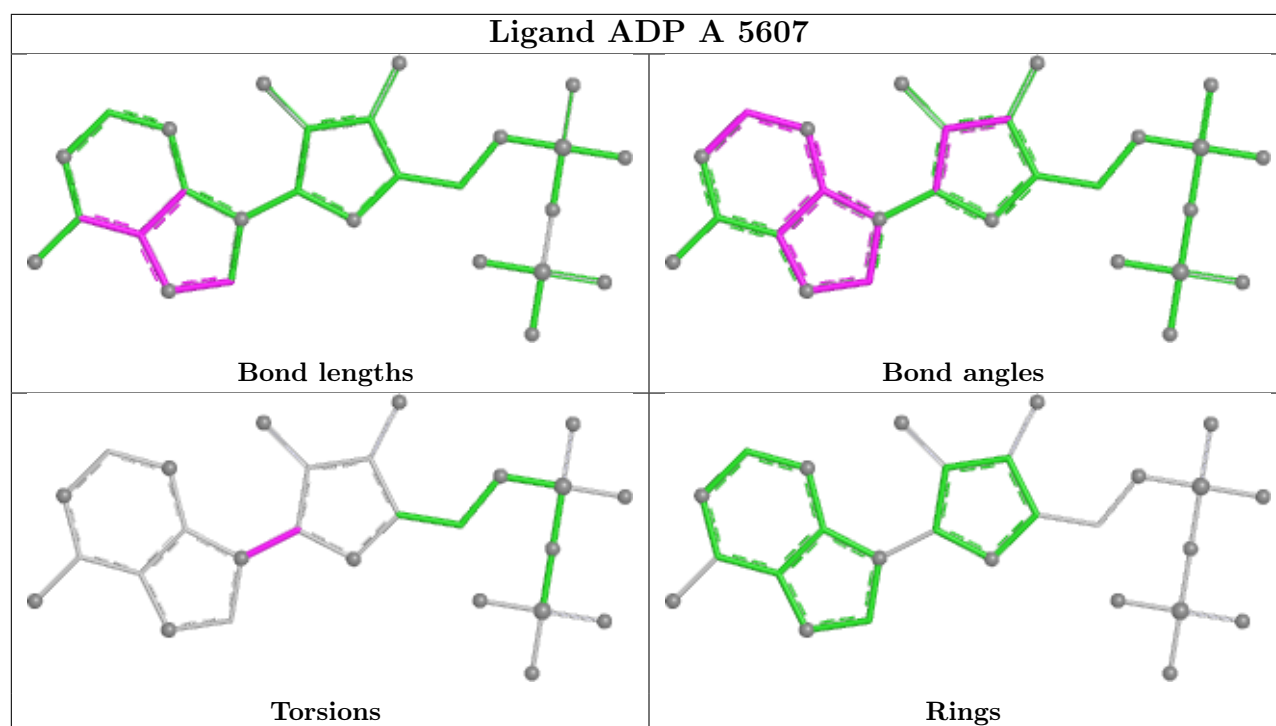


Ligand 43M C 5604

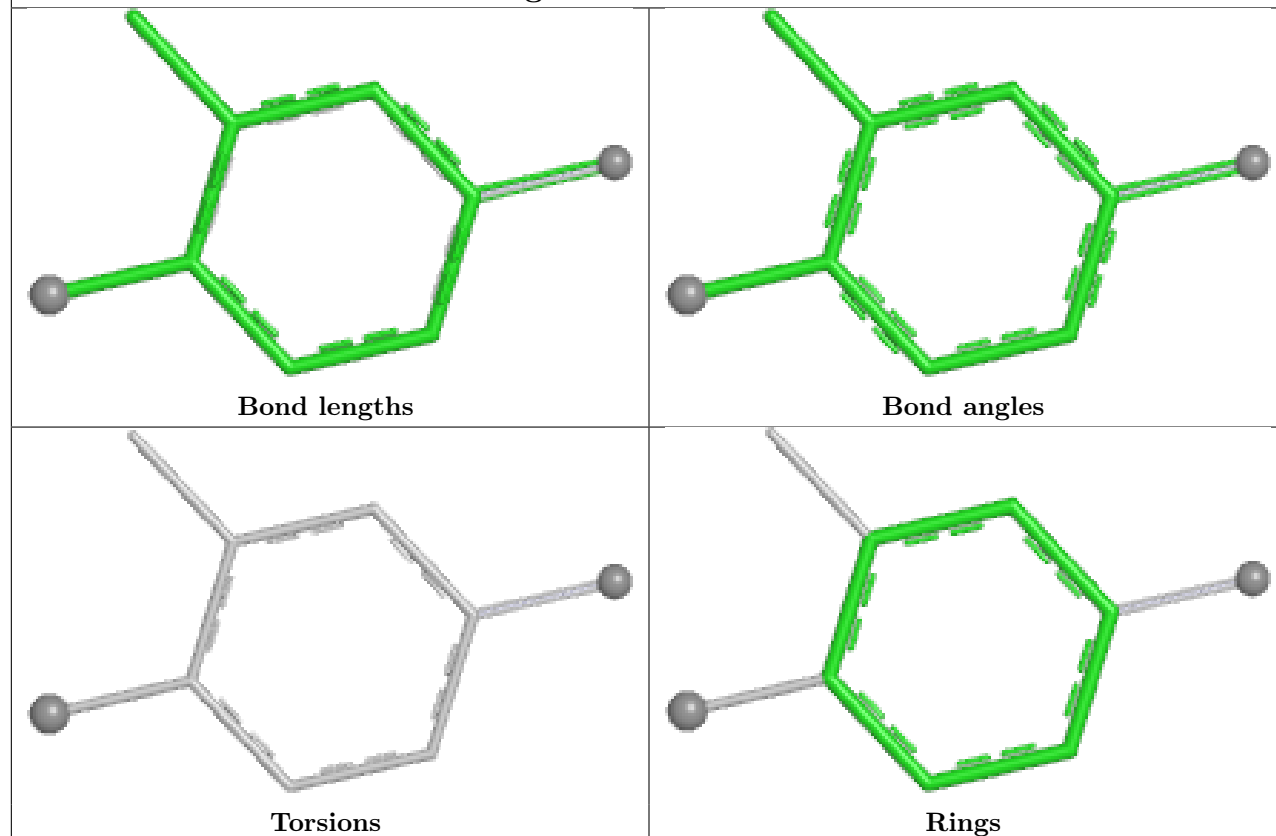


Ligand 43M A 5606

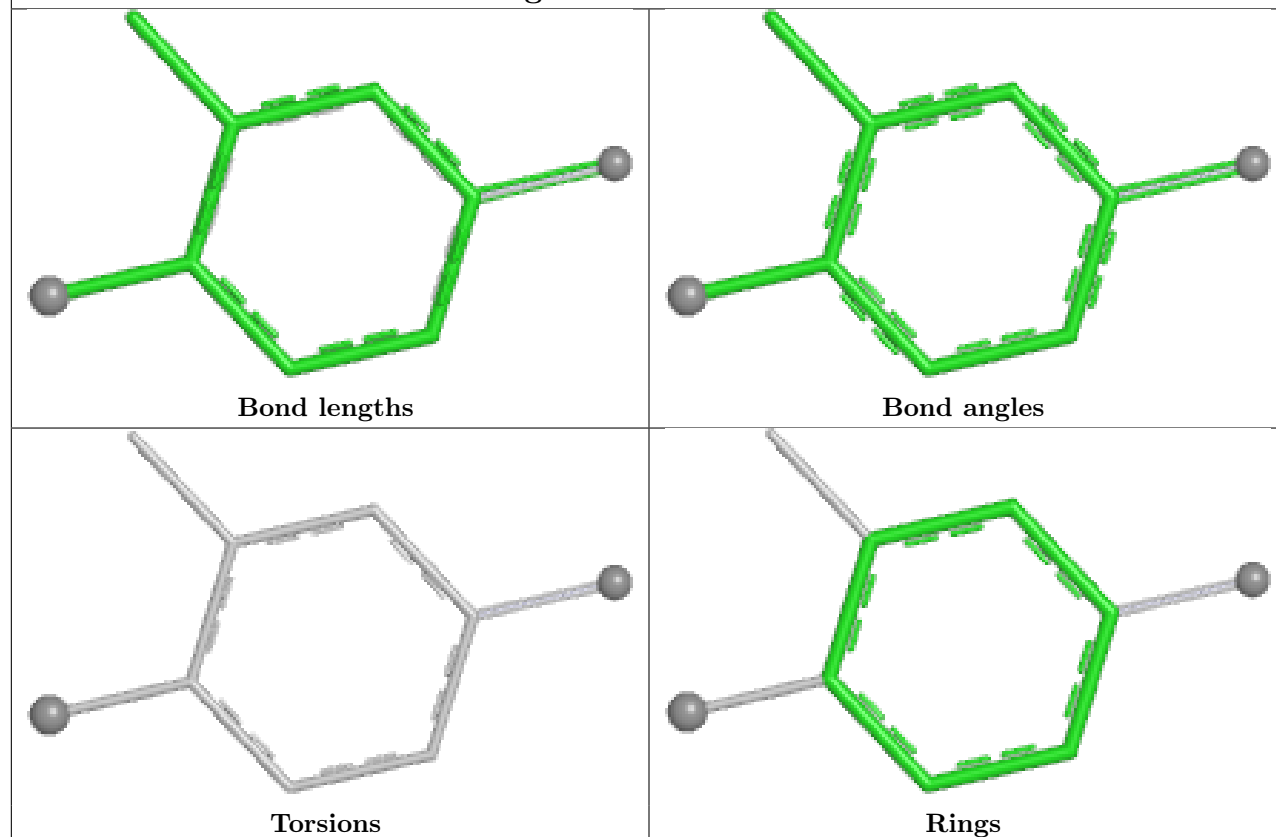


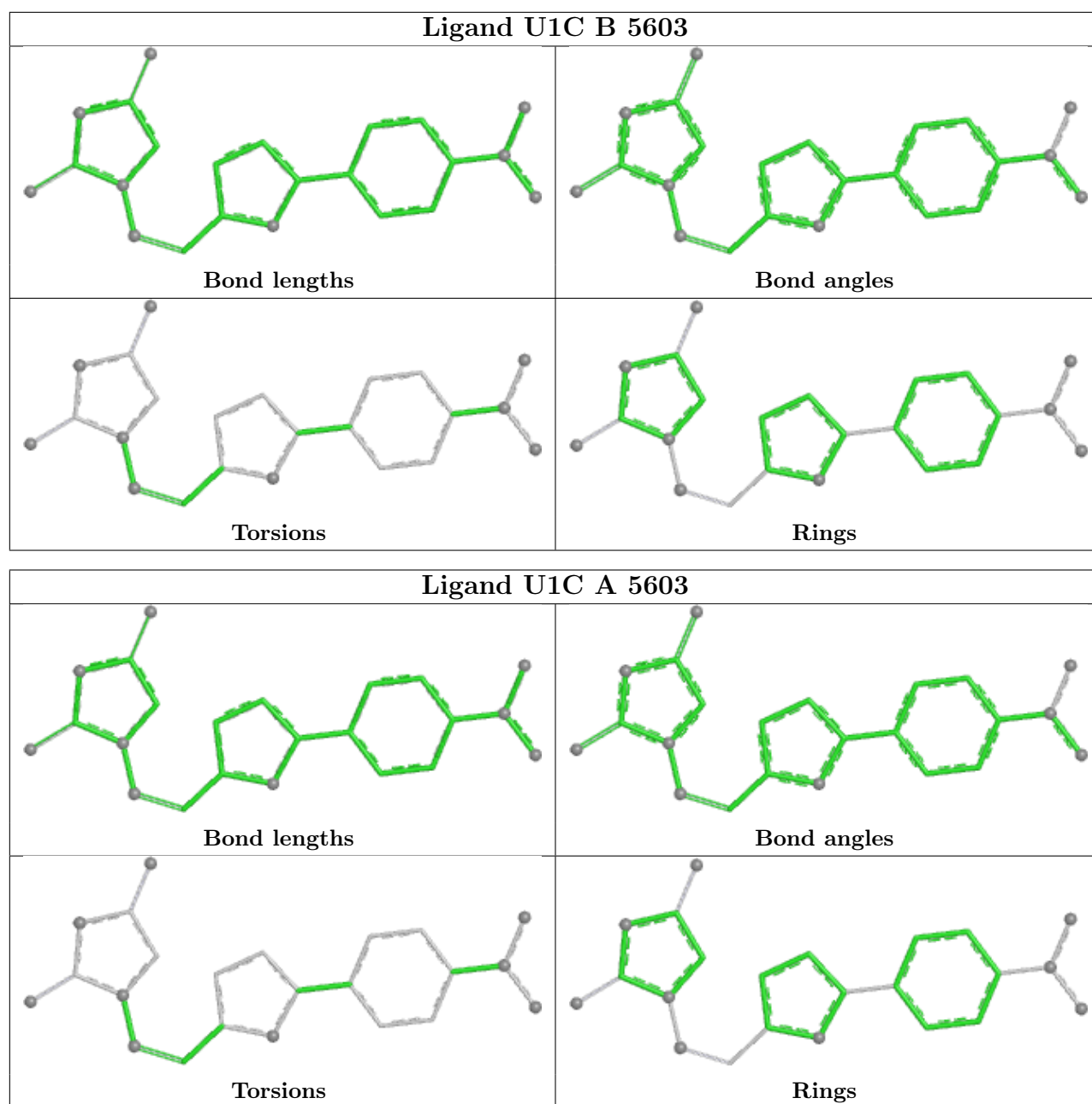


Ligand 43M A 5604



Ligand 43M D 5606





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.

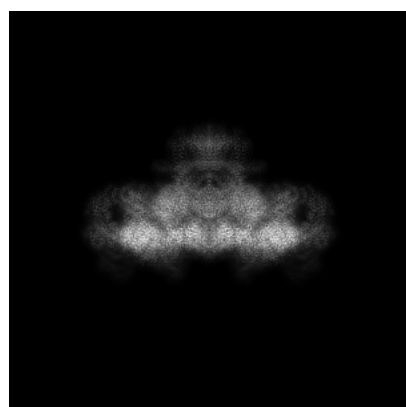
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74436. These allow visual inspection of the internal detail of the map and identification of artifacts.

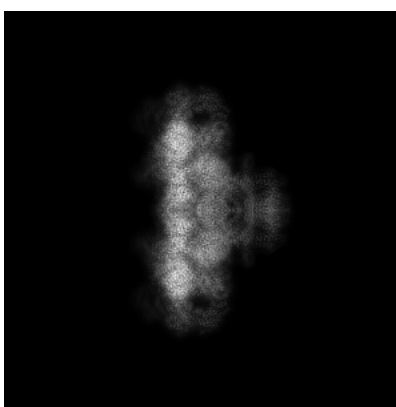
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

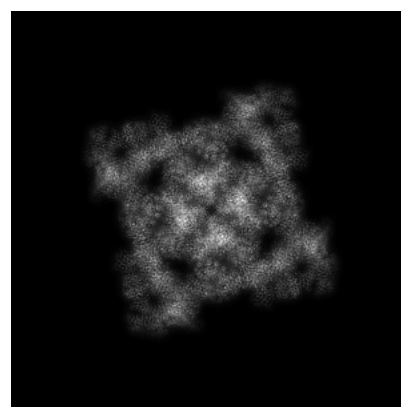
6.1.1 Primary map



X



Y

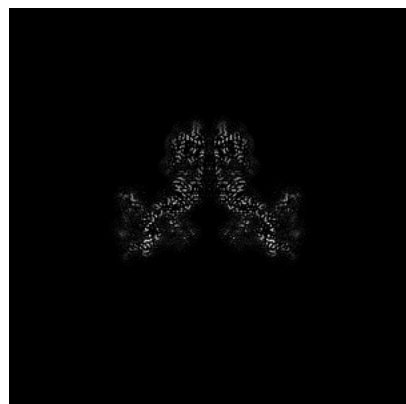


Z

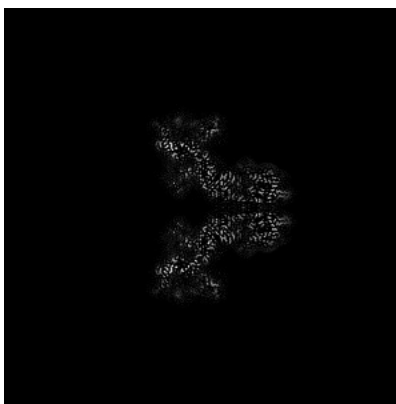
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

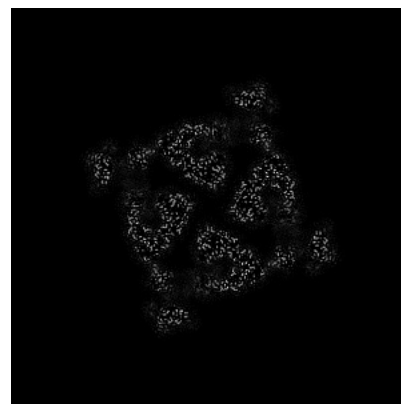
6.2.1 Primary map



X Index: 300



Y Index: 300

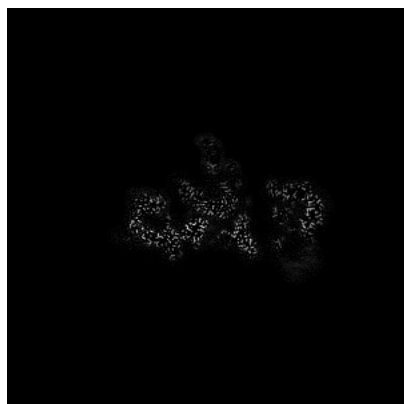


Z Index: 300

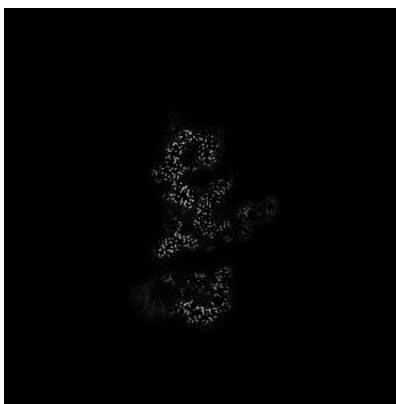
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

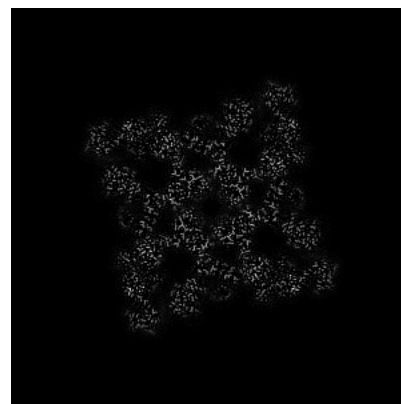
6.3.1 Primary map



X Index: 358



Y Index: 358

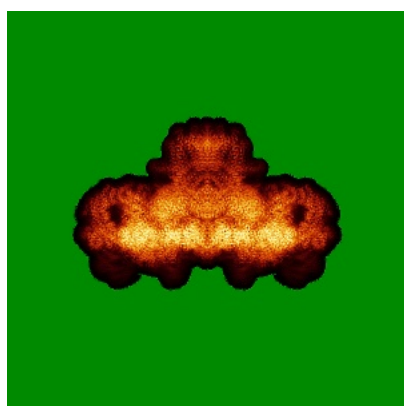


Z Index: 266

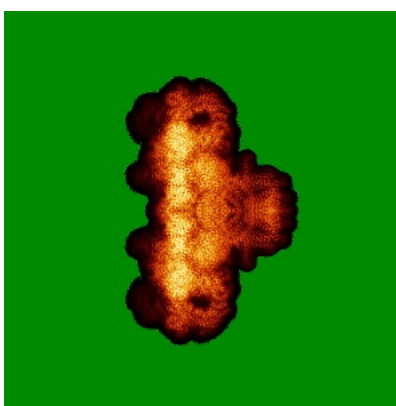
The images above show the largest variance slices of the map in three orthogonal directions.

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

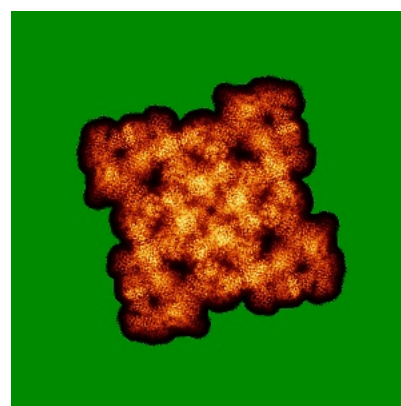
6.4.1 Primary map



X



Y

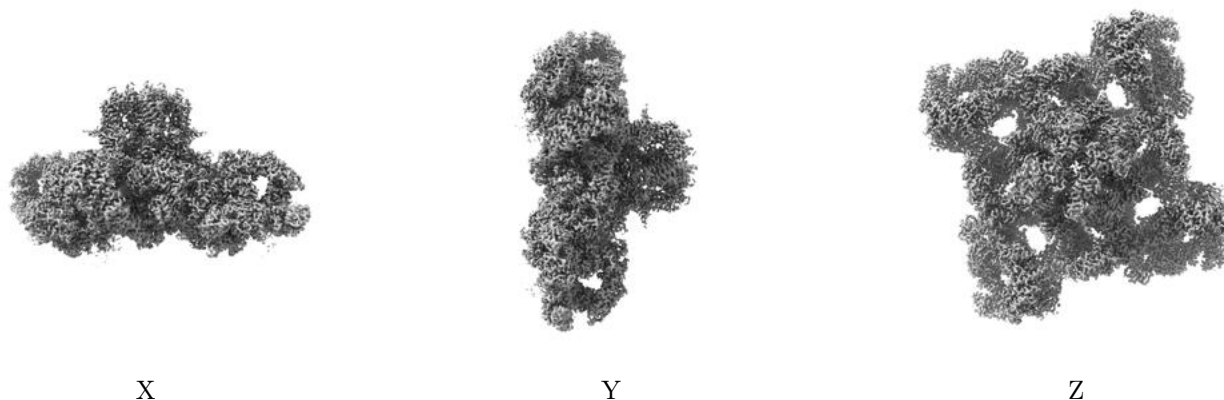


Z

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 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

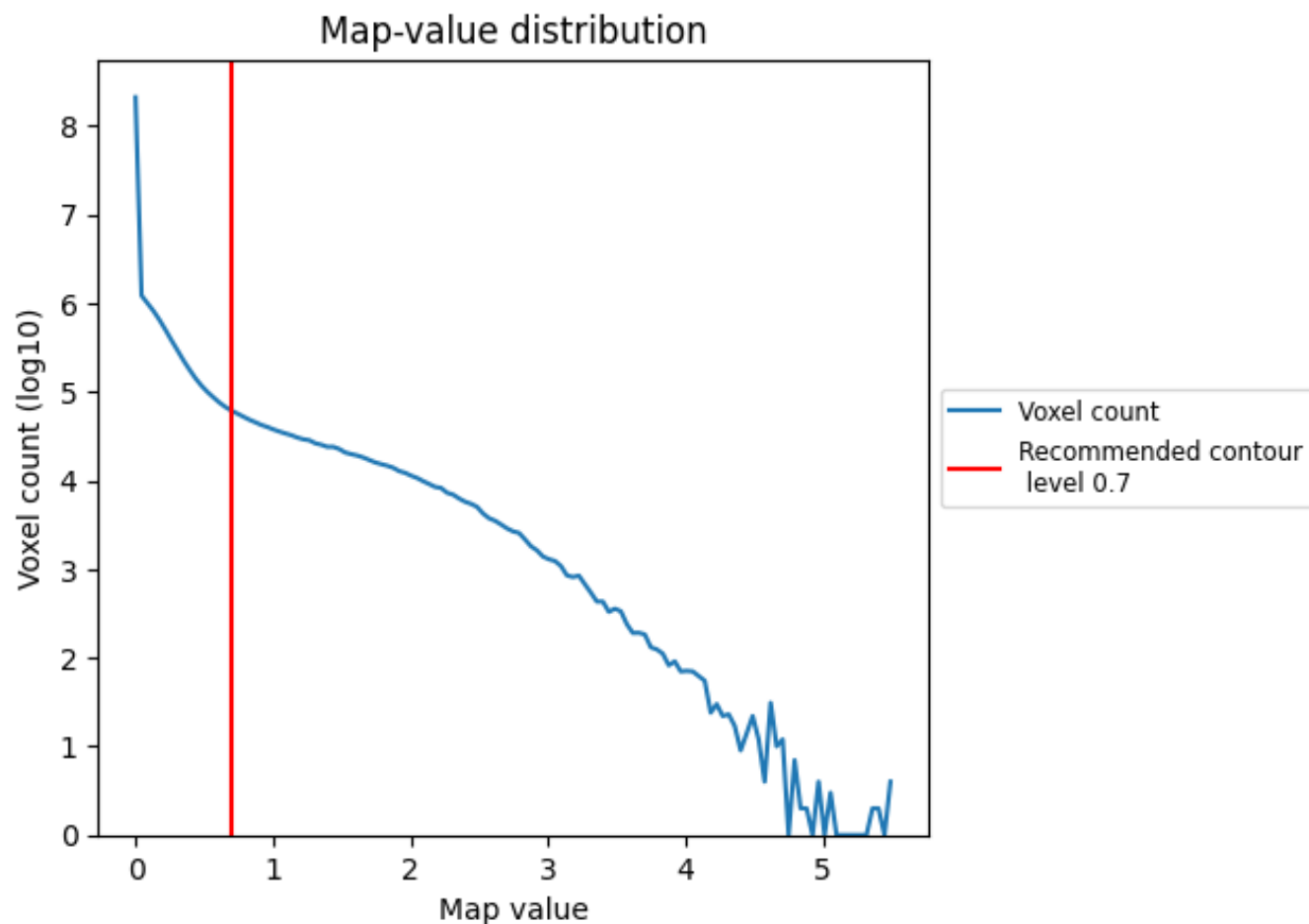
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

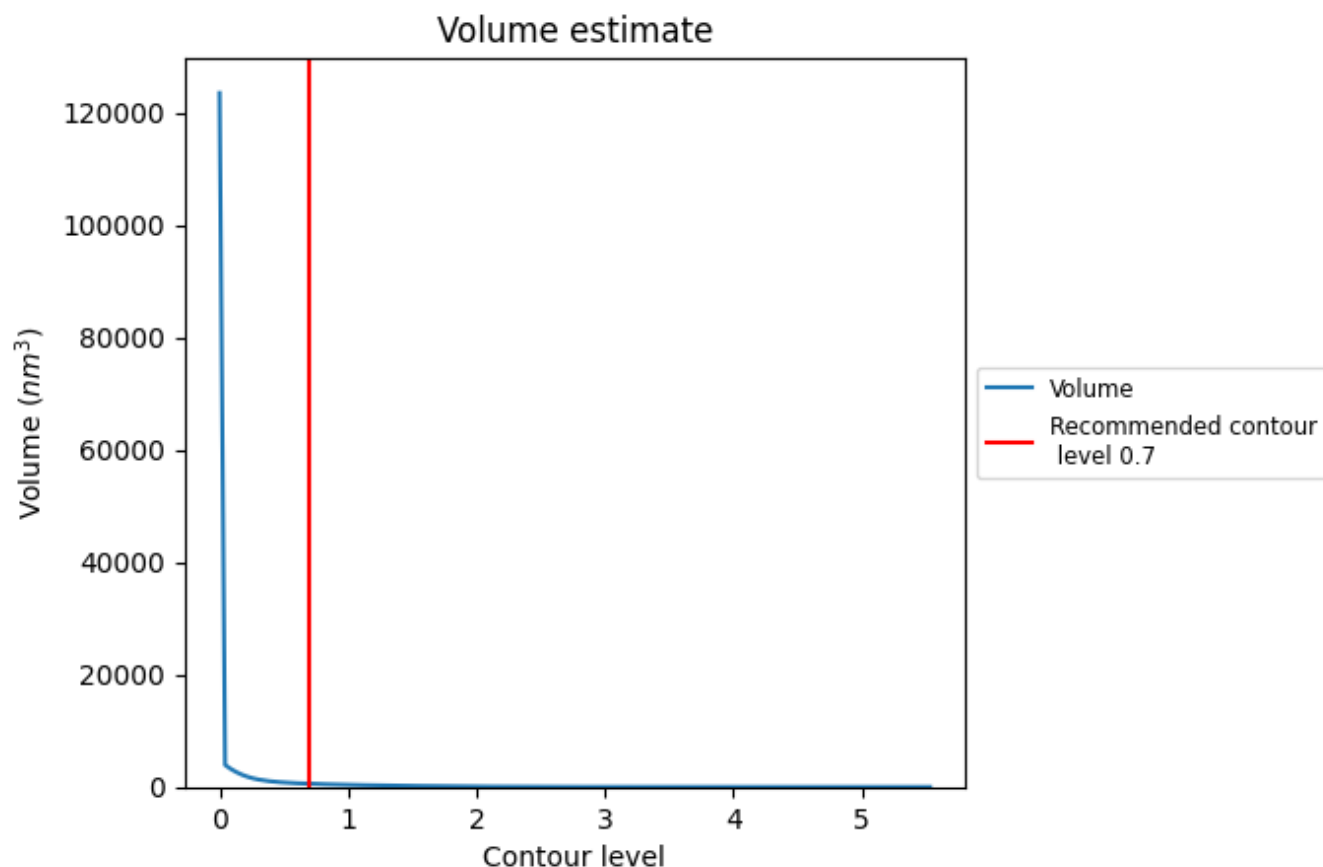
This section contains the results of statistical analysis of the map.

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.

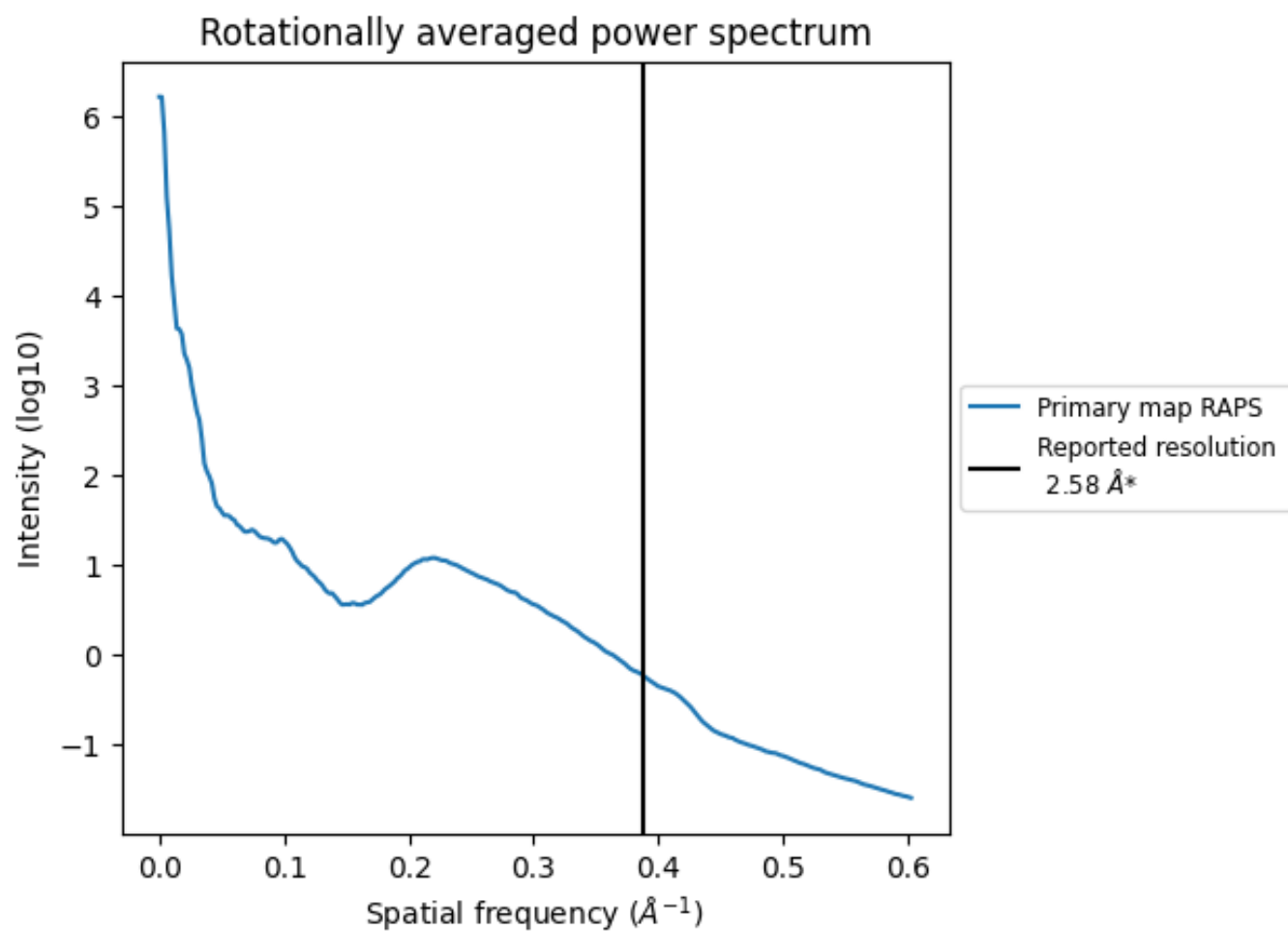
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 574 nm^3 ; this corresponds to an approximate mass of 519 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 0.388 Å⁻¹

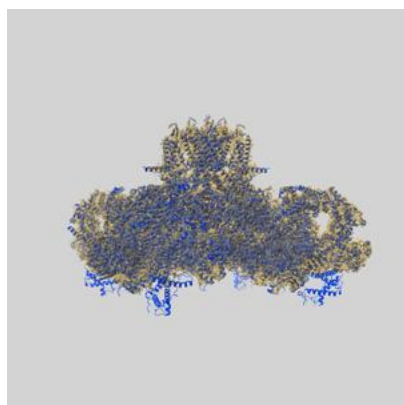
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

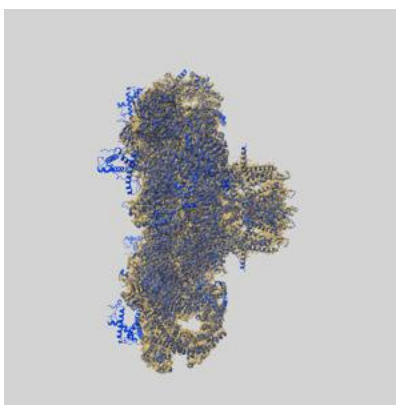
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74436 and PDB model 9ZN6. Per-residue inclusion information can be found in section [3](#) on page [10](#).

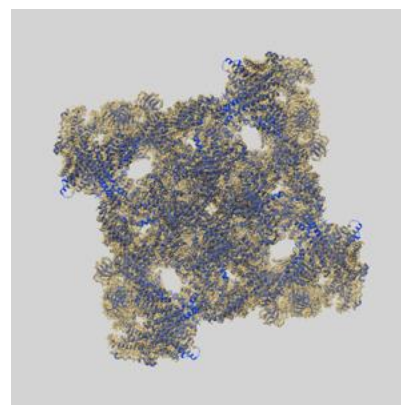
9.1 Map-model overlay [i](#)



X



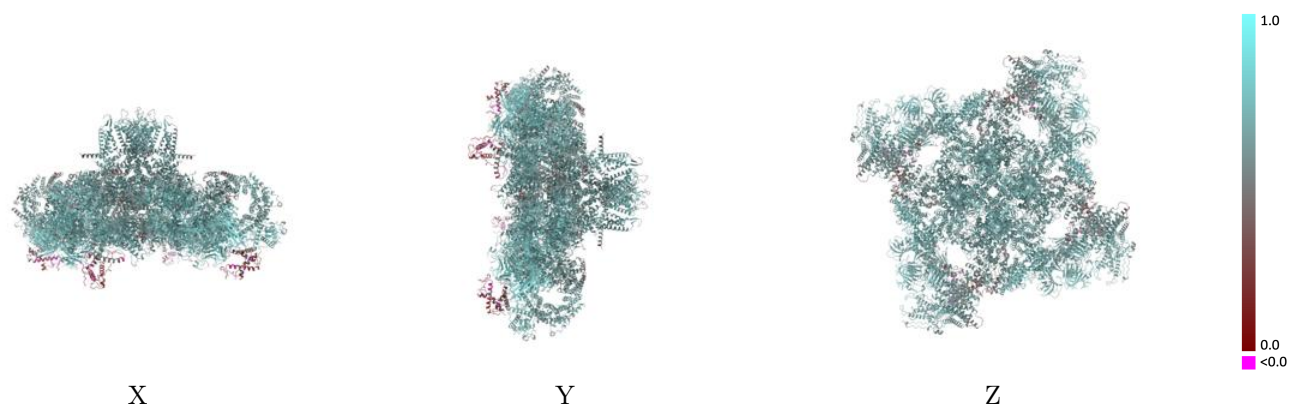
Y



Z

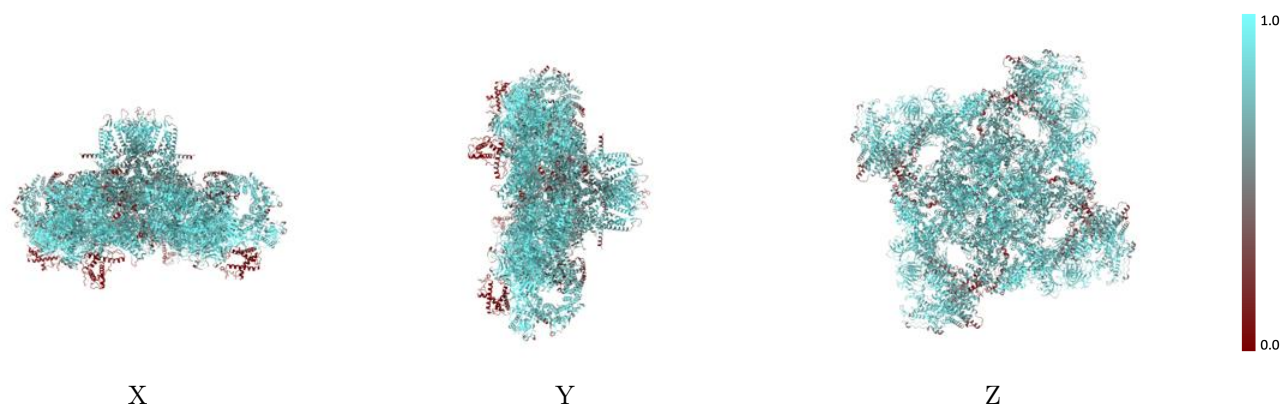
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



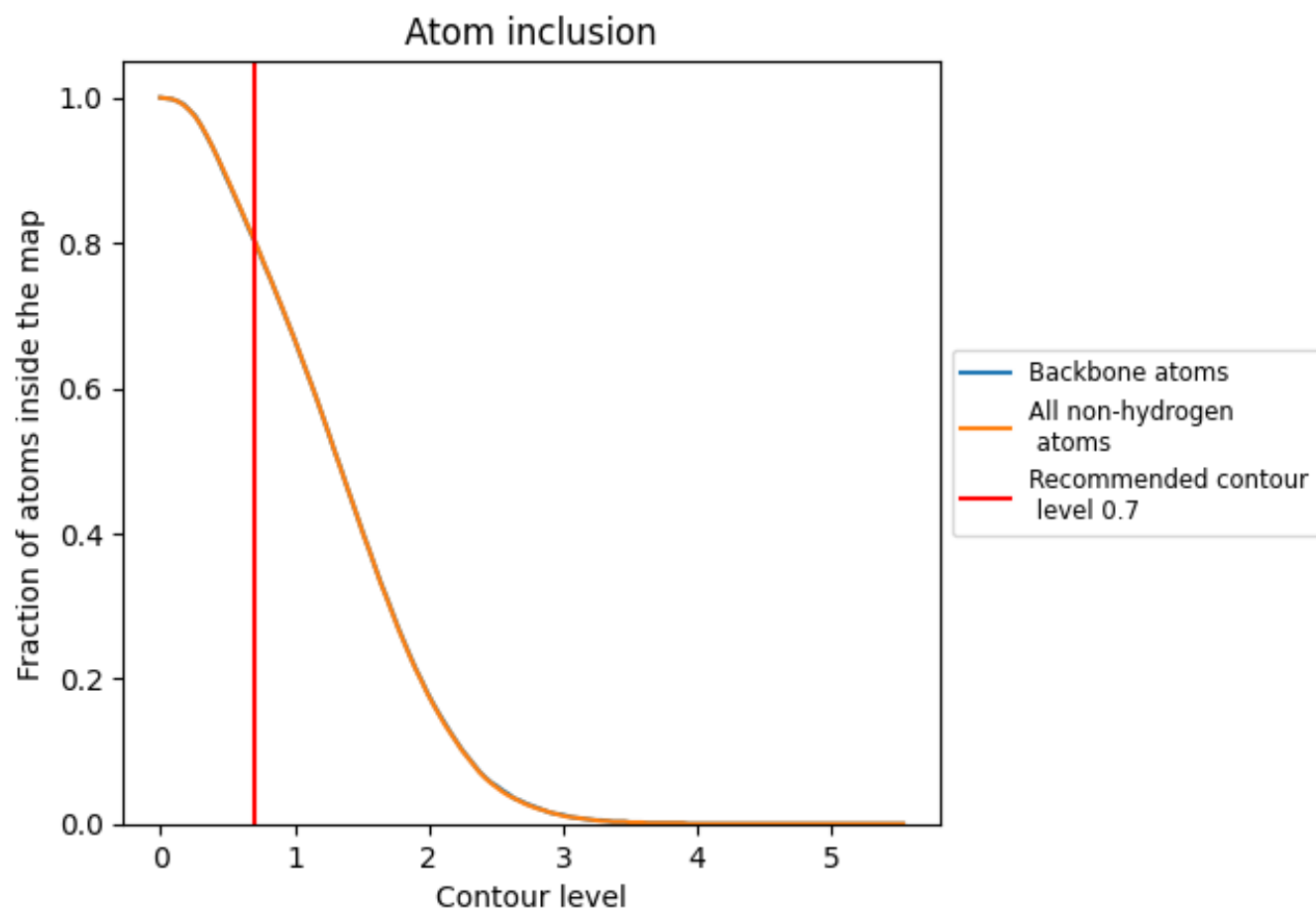
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.6540
A	0.8180	0.6590
B	0.8180	0.6590
C	0.8180	0.6590
D	0.8180	0.6590
E	0.8470	0.6720
F	0.8520	0.6710
G	0.8540	0.6720
H	0.8520	0.6720
I	0.4250	0.4780
J	0.4380	0.4840
K	0.4350	0.4850
L	0.4310	0.4850

1.0

0.0

<0.0