



wwPDB EM Validation Summary Report ⓘ

Jan 31, 2024 – 03:33 PM EST

PDB ID : 8VK4
EMDB ID : EMD-43304
Title : Structure of mouse RyR1 in complex with S100A1 (high-Ca²⁺/CFF/ATP dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-08
Resolution : 3.56 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

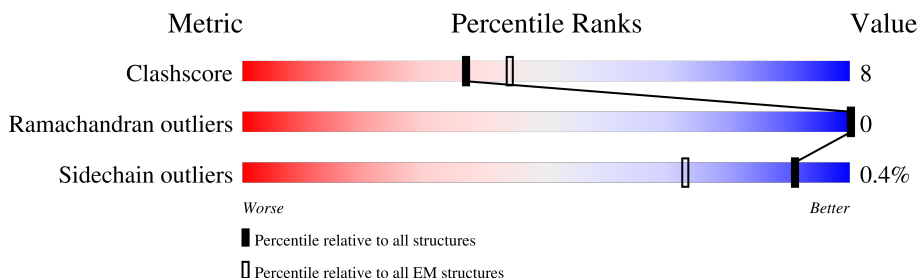
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	108	 86% 13%
1	F	108	 88% 11%
1	G	108	 84% 15%
1	H	108	 85% 14%
2	I	94	 35% 50% 49%
2	J	94	 26% 50% 49%
2	K	94	 36% 50% 49%
2	L	94	 24% 51% 48%

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Mol	Chain	Length	Quality of chain
2	M	94	<p>36% 50% 49%</p>
2	N	94	<p>24% 52% 47%</p>
2	O	94	<p>36% 51% 48%</p>
2	P	94	<p>24% 51% 48%</p>
3	A	5035	<p>10% 71% 16% 13%</p>
3	B	5035	<p>10% 71% 16% 13%</p>
3	C	5035	<p>10% 71% 15% 13%</p>
3	D	5035	<p>10% 72% 15% 13%</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 149304 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
			Total	C	N	O	S		
1	E	107	Total 829	C 526	N 145	O 155	S 3	0	0
1	F	107	Total 829	C 526	N 145	O 155	S 3	0	0
1	G	107	Total 829	C 526	N 145	O 155	S 3	0	0
1	H	107	Total 829	C 526	N 145	O 155	S 3	0	0

- Molecule 2 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	J	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	K	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	L	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	N	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	M	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	O	93	Total 729	C 460	N 114	O 152	S 3	0	0
2	P	93	Total 729	C 460	N 114	O 152	S 3	0	0

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	4379	Total 34849	C 22163	N 5998	O 6451	S 237	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	4379	34849	22163	5998	6451	237	0	0
3	B	4379	34849	22163	5998	6451	237	0	0
3	C	4379	34849	22163	5998	6451	237	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	I	2	Total 2	Ca 2	0
4	J	2	Total 2	Ca 2	0
4	D	1	Total 1	Ca 1	0
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	K	2	Total 2	Ca 2	0
4	L	2	Total 2	Ca 2	0
4	N	2	Total 2	Ca 2	0
4	M	2	Total 2	Ca 2	0
4	O	2	Total 2	Ca 2	0
4	P	2	Total 2	Ca 2	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

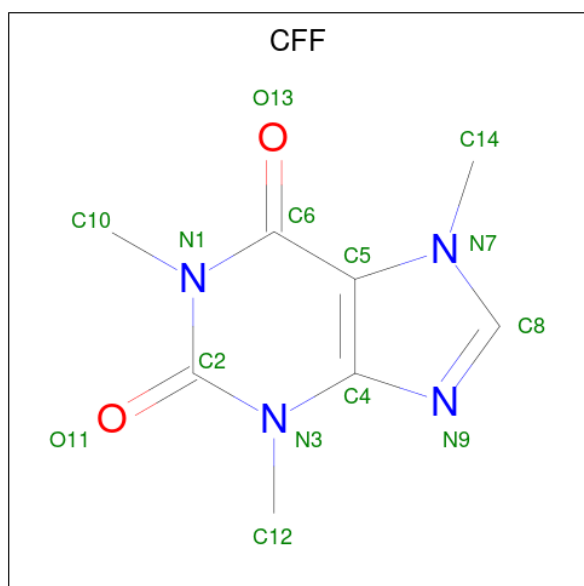
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total 1	Zn 1	0

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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



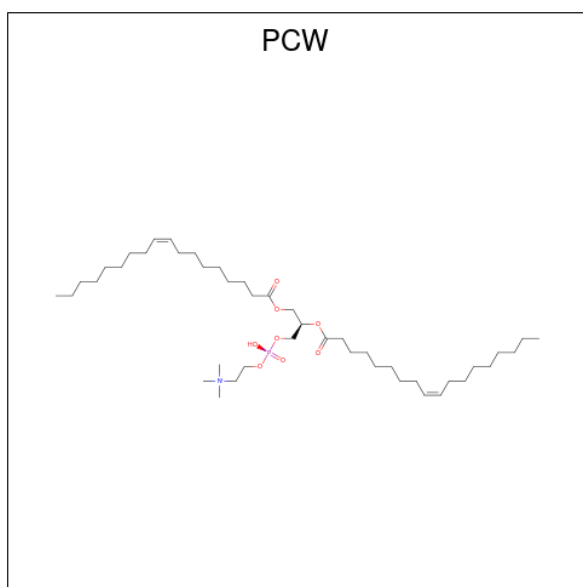
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	4	2	
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

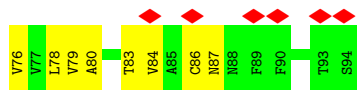
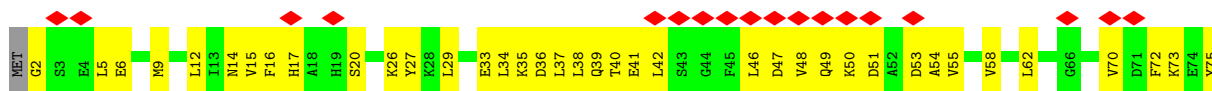
- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



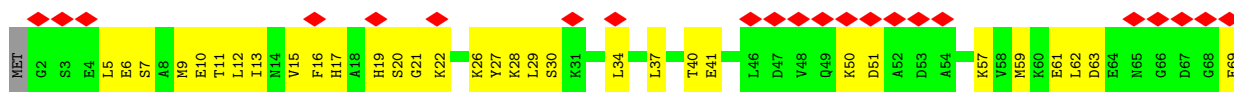
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	D	1	Total 54	44	1	8	1	0
8	D	1	Total 54	44	1	8	1	0
8	A	1	Total 54	44	1	8	1	0
8	A	1	Total 54	44	1	8	1	0
8	B	1	Total 54	44	1	8	1	0
8	B	1	Total 54	44	1	8	1	0
8	C	1	Total 54	44	1	8	1	0
8	C	1	Total 54	44	1	8	1	0



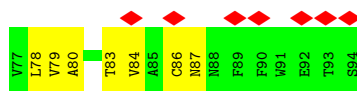
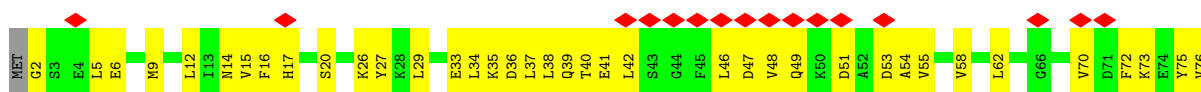
• Molecule 2: Protein S100A1



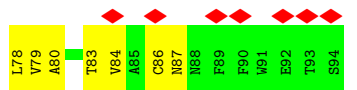
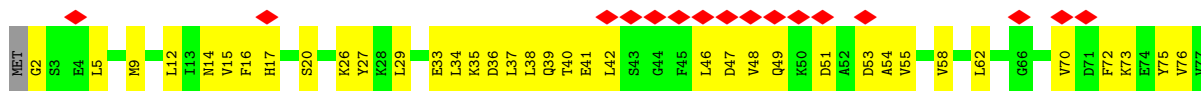
• Molecule 2: Protein S100A1



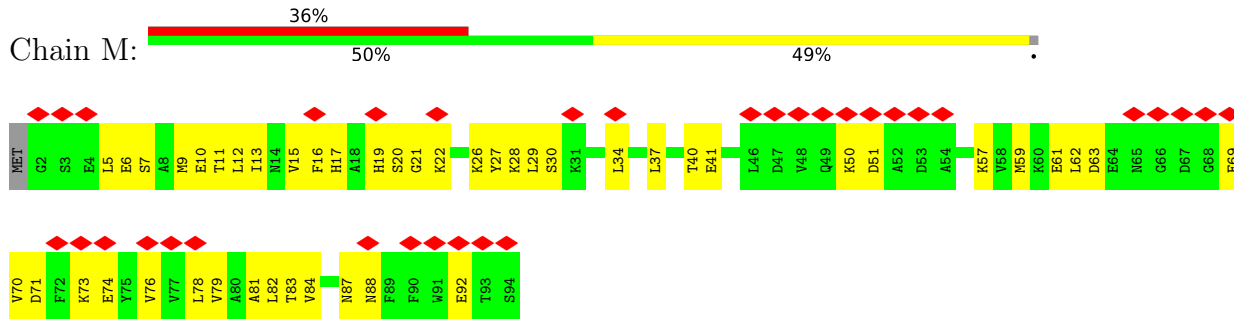
• Molecule 2: Protein S100A1



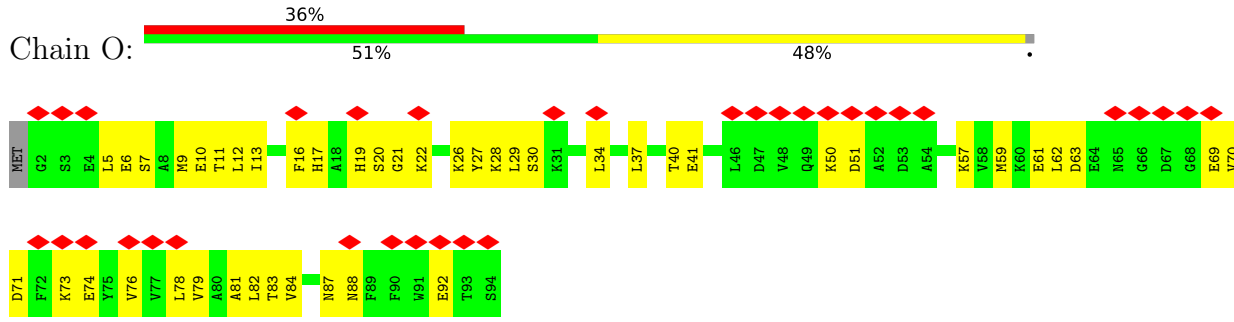
• Molecule 2: Protein S100A1



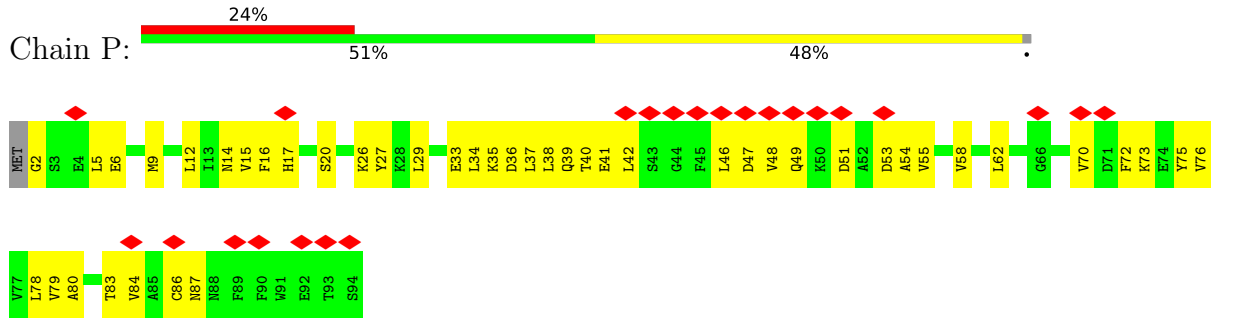
• Molecule 2: Protein S100A1



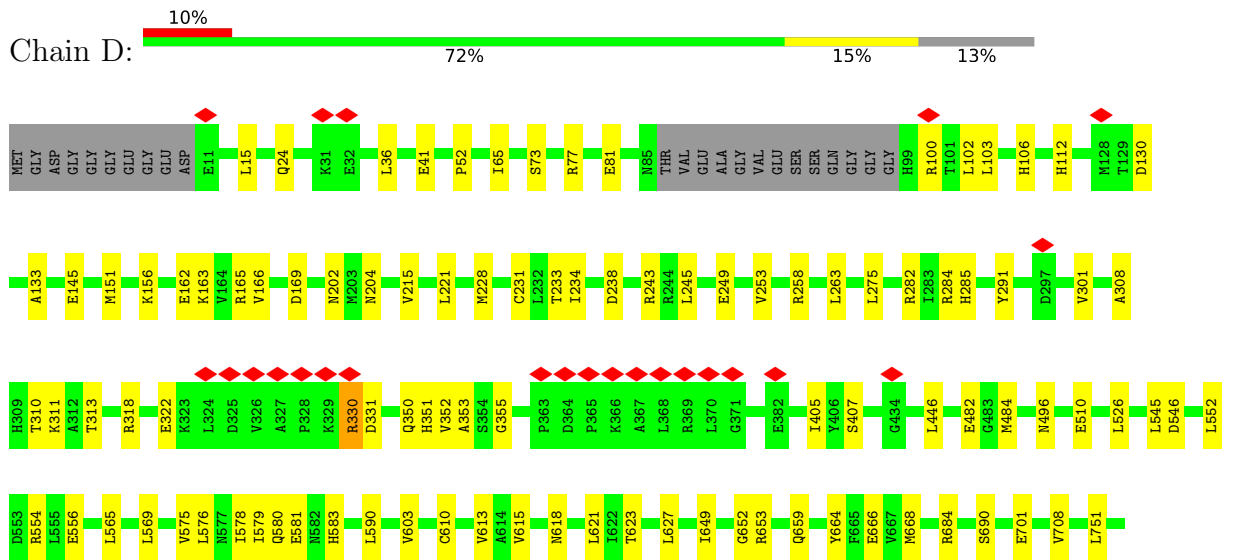
• Molecule 2: Protein S100A1

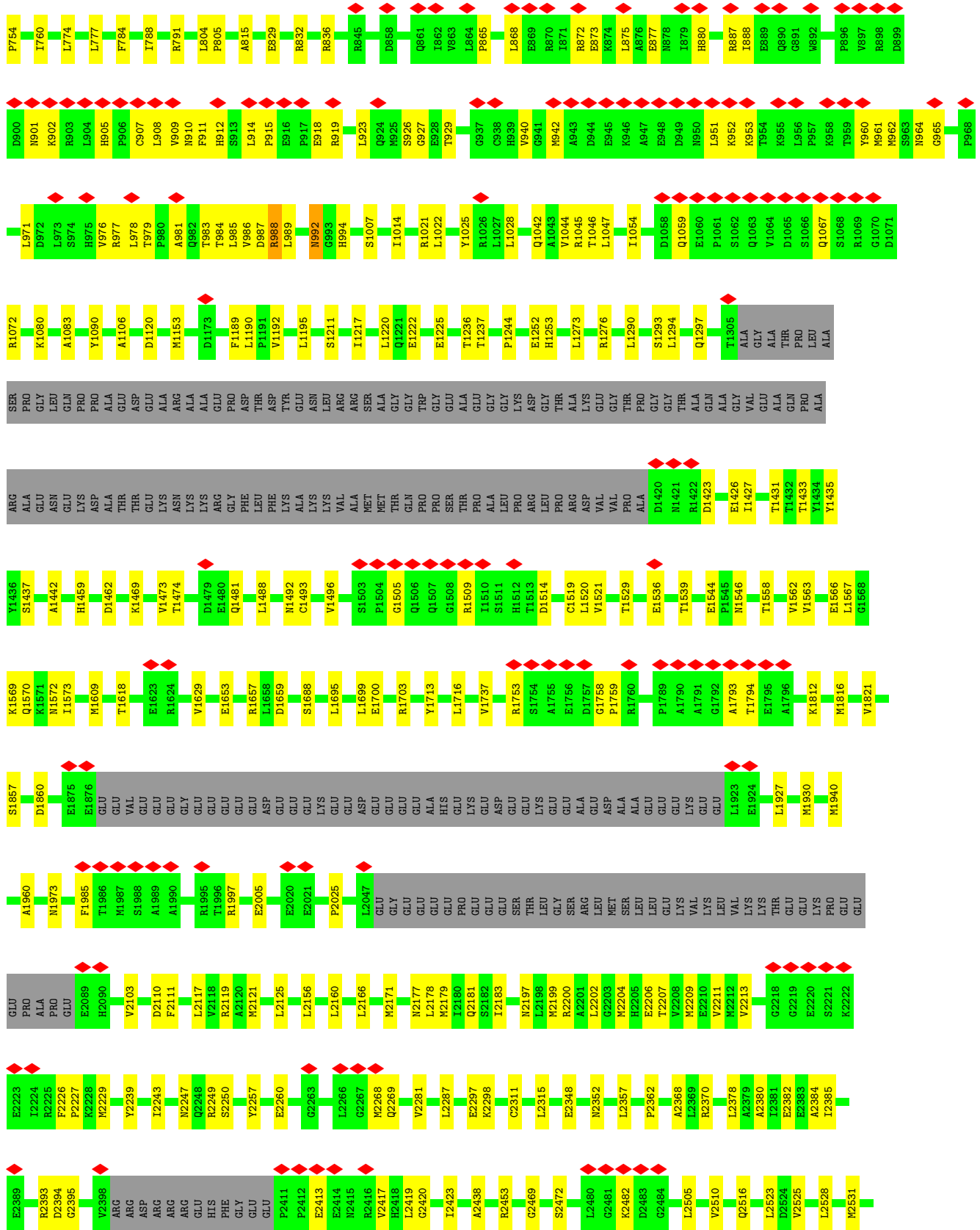


• Molecule 2: Protein S100A1

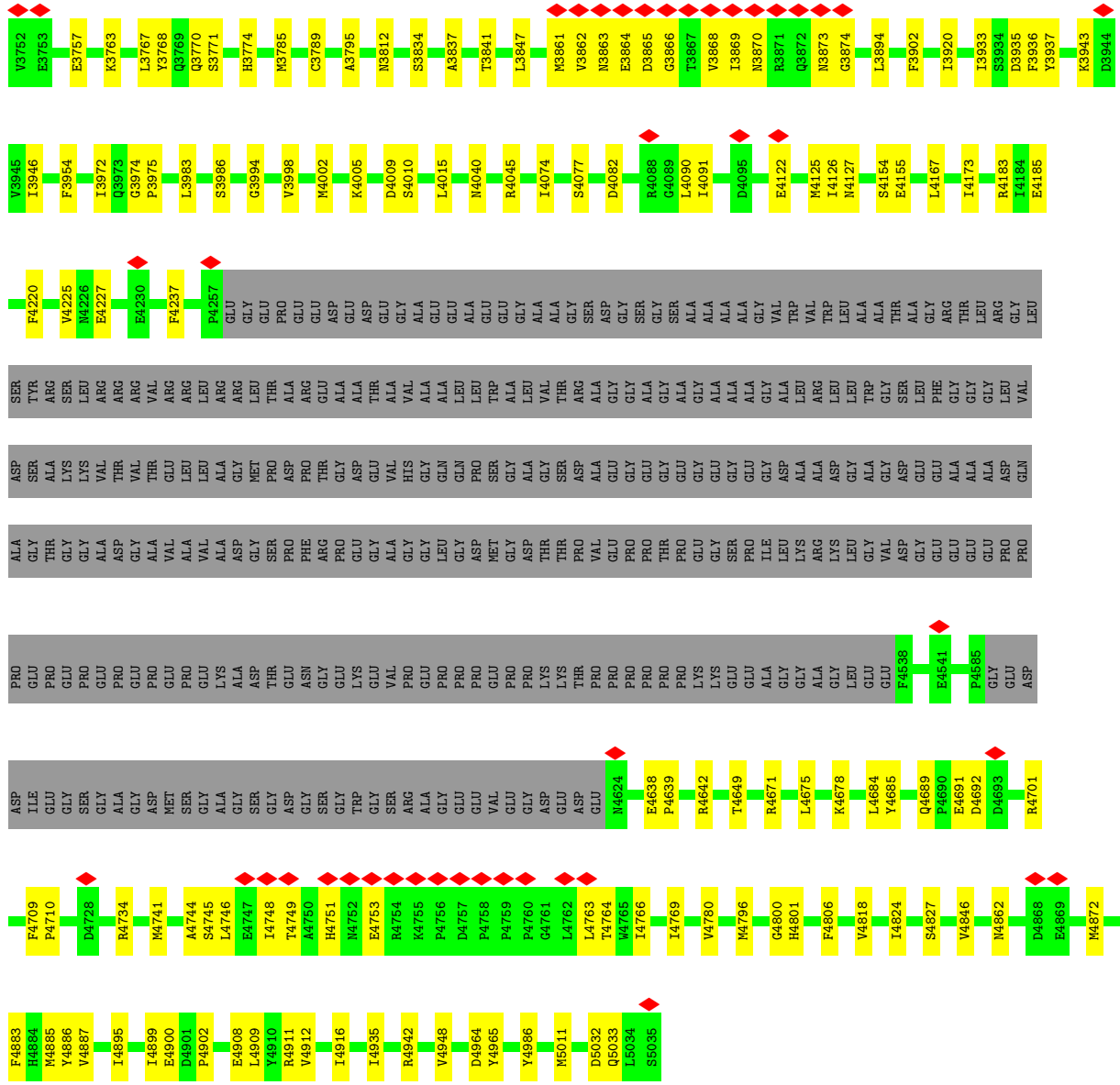


• Molecule 3: Ryanodine receptor 1

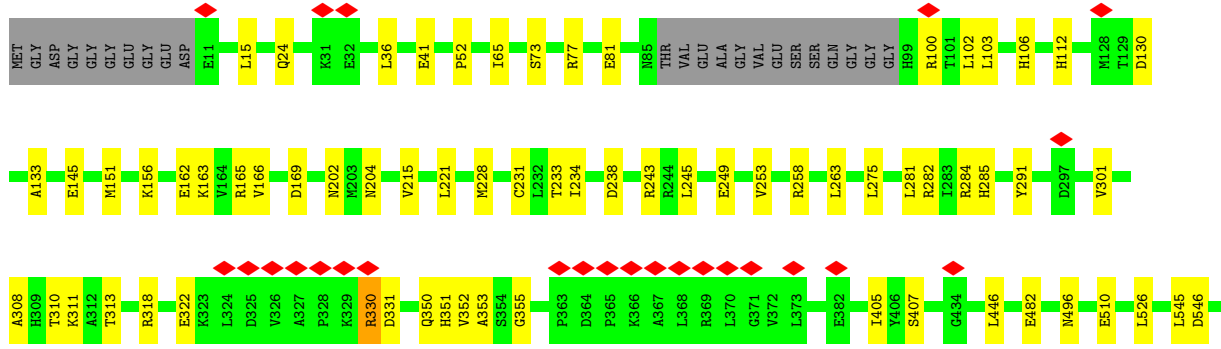


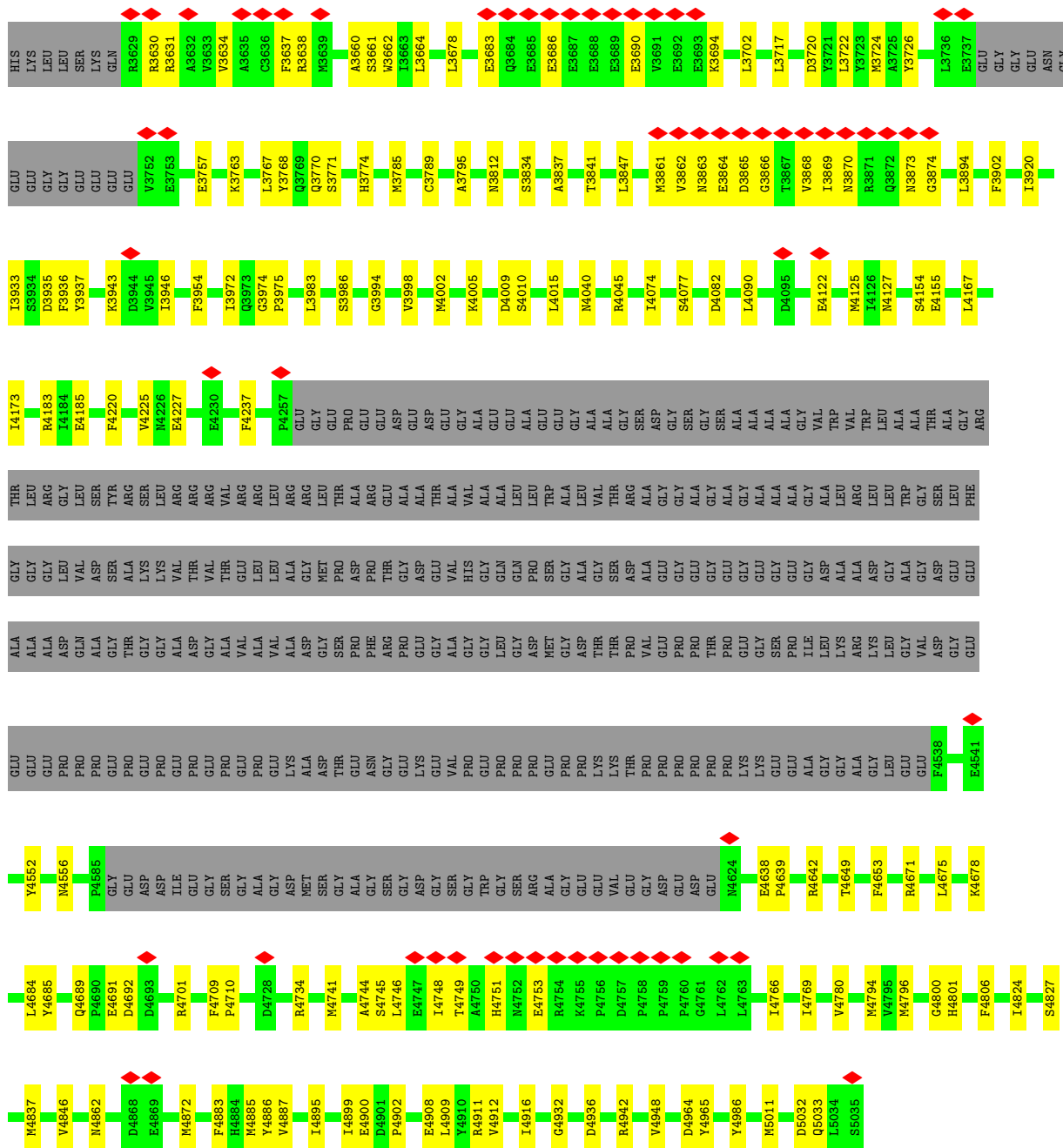


R3629	R3630	R3631	V3634	A3635	C3636	F3637	R3638	R3639	A3660	S3661	R3662	R3663	L3664	L3678	E3683	Q3684	E3685	E3686	E3687	E3688	E3689	E3690	V3691	E3692	E3693	K3694	L3702	L3717	D3720	V3721	L3722	V3723	K3724	A3725	Y3726	L3736	E3737	GLU	GLY	GLU	GLU	GLN																
V3550	R3551	M3557	L3558	M3559	L3560	Q3561	G3562	K3563	V3564	E3565	G3566	L3576	Y3577	R3578	G3579	V3580	R3583	E3584	E3585	D3586	A3587	D3588	I3589	R3590	R3591	R3592	R3593	R3594	R3595	R3596	V3597	F3598	V3599	V3600	V3603	L3604	L3607	E3611	R3612	P3613	TYR	LYS	SER	GLU	ASN	LYS	ALA	VAL	TRP	HIS	GLY	GLU	LEU	SER	LYS	GLN		
E3392	L3393	L3394	V3395	R3396	D3397	E3398	F3399	S3400	F3401	L3402	C3403	R3404	D3405	L3406	F3407	A3408	L3409	Y3410	F3411	L3412	L3413	F3414	R3415	R3421	M3431	A3432	G3440	F3441	F3442	F3443	I3444	S3447	M3451	F3452	K3453	R3454	E3455	E3456	Q3457	M3458	Q3462	M3463	E3464	I3465	M3466	M3467	M3468	S3469	F3470	L3471	L3472	ALA	ASP					
G3300	A3301	T3309	S3310	D3311	H3312	L3316	L3317	G3318	N3319	I3320	L3321	R3322	I3323	I3324	V3325	I3330	D3331	E3332	M3336	K3337	A3343	Q3344	R3345	I3346	V3347	E3353	L3354	L3355	R3356	I3360	R3367	V3373	V3374	A3375	E3376	C3377	E3378	Q3379	L3380	R3381	L3382	E3383	A3384	K3385	A3386	E3387	A3388	E3389	E3390	G3391								
E3208	M3212	E3213	V3219	Y3220	R3226	E3227	R3228	A3229	I3230	L3233	F3234	N3235	S3236	V3237	E3238	E3239	D3243	E3253	I3254	Q3255	L3256	L3257	A3262	A3263	R3263	K3267	F3268	H3269	I3271	E3272	L3275	P3276	L3277	K3278	D3279	S3280	Y3281	L3282	R3288	E3291	A3292	P3293	P3294	P3295	A3296	L3297	P3298	A3299										
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E2854	L2855	E2856	A2857	K2858	G2859	G2860	G2861	S2862	H2863	P2864	L2865	L2866	V2867	E2868	K2869	F2869	L3003	L3004	P3005	S3028	K3035	R3039	L3047	L3050	R3053	R3054	V3055	V3065	L3069	L3076	D3077	A3078	R3079	M3082	P3086	V3089	K3090	D3103	I3104	E3105	T2939	R2940	G2941	L2942	K2943	D2944	M2945	E2946	L2947	K2948	T2949	I2952	S2971					
E2844	L2845	E2846	A2847	K2848	G2849	G2850	G2851	S2852	H2853	P2854	L2855	L2856	V2857	E2858	K2859	F2859	L3003	L3004	P3005	S3028	K3035	R3039	L3047	L3050	R3053	R3054	V3055	V3065	L3069	L3076	D3077	A3078	R3079	M3082	P3086	V3089	K3090	D3103	I3104	E3105	T2939	R2940	G2941	L2942	K2943	D2944	M2945	E2946	L2947	K2948	T2949	I2952	S2971					
E2834	L2835	E2836	A2837	K2838	G2839	G2840	G2841	S2842	H2843	P2844	L2845	L2846	V2847	E2848	K2849	F2849	L3003	L3004	P3005	S3028	K3035	R3039	L3047	L3050	R3053	R3054	V3055	V3065	L3069	L3076	D3077	A3078	R3079	M3082	P3086	V3089	K3090	D3103	I3104	E3105	T2939	R2940	G2941	L2942	K2943	D2944	M2945	E2946	L2947	K2948	T2949	I2952	S2971					
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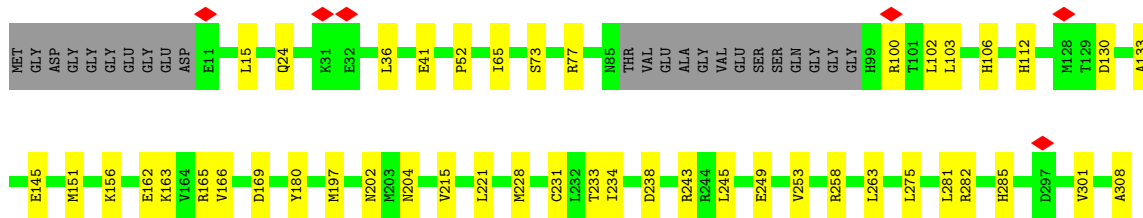


• Molecule 3: Ryanodine receptor 1

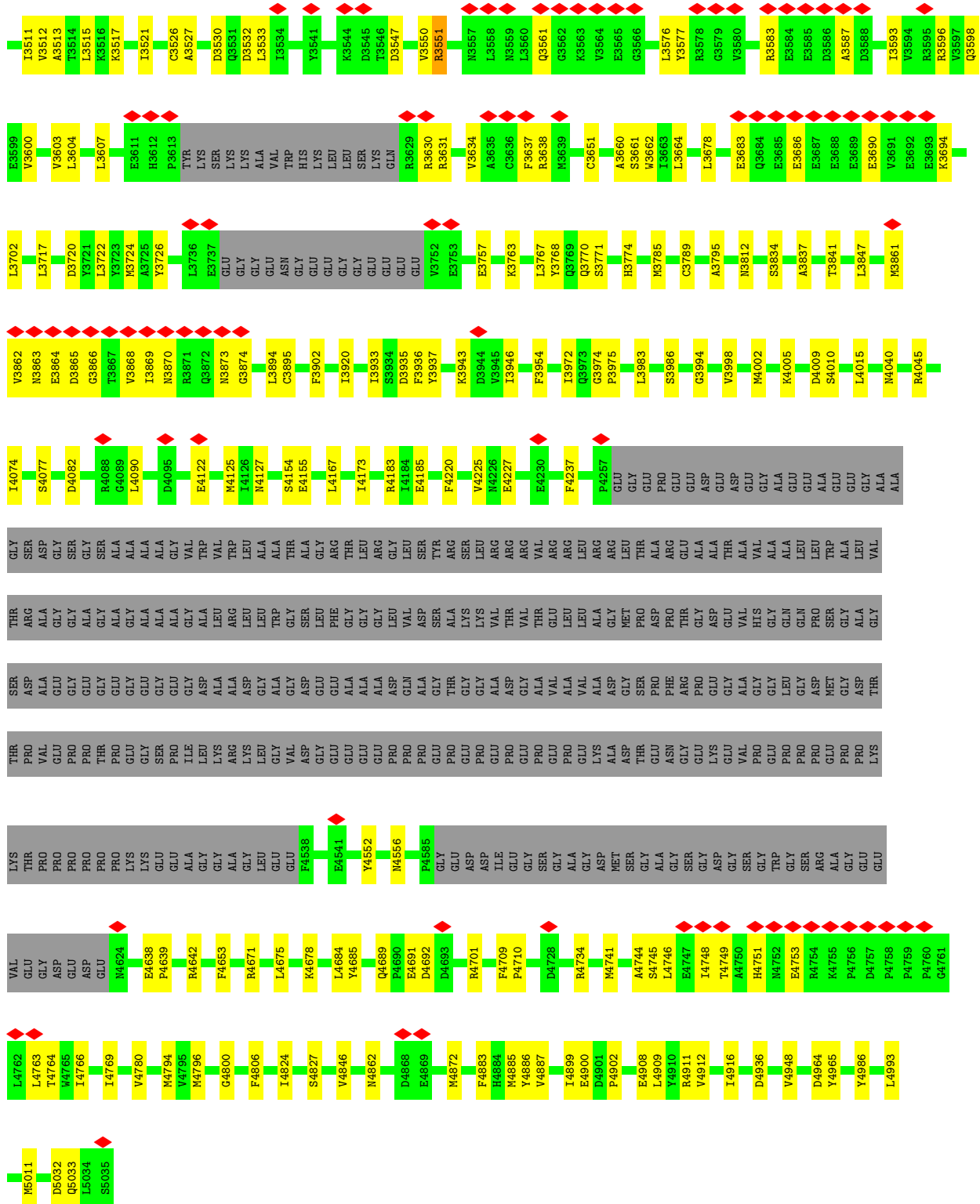




• Molecule 3: Ryanodine receptor 1

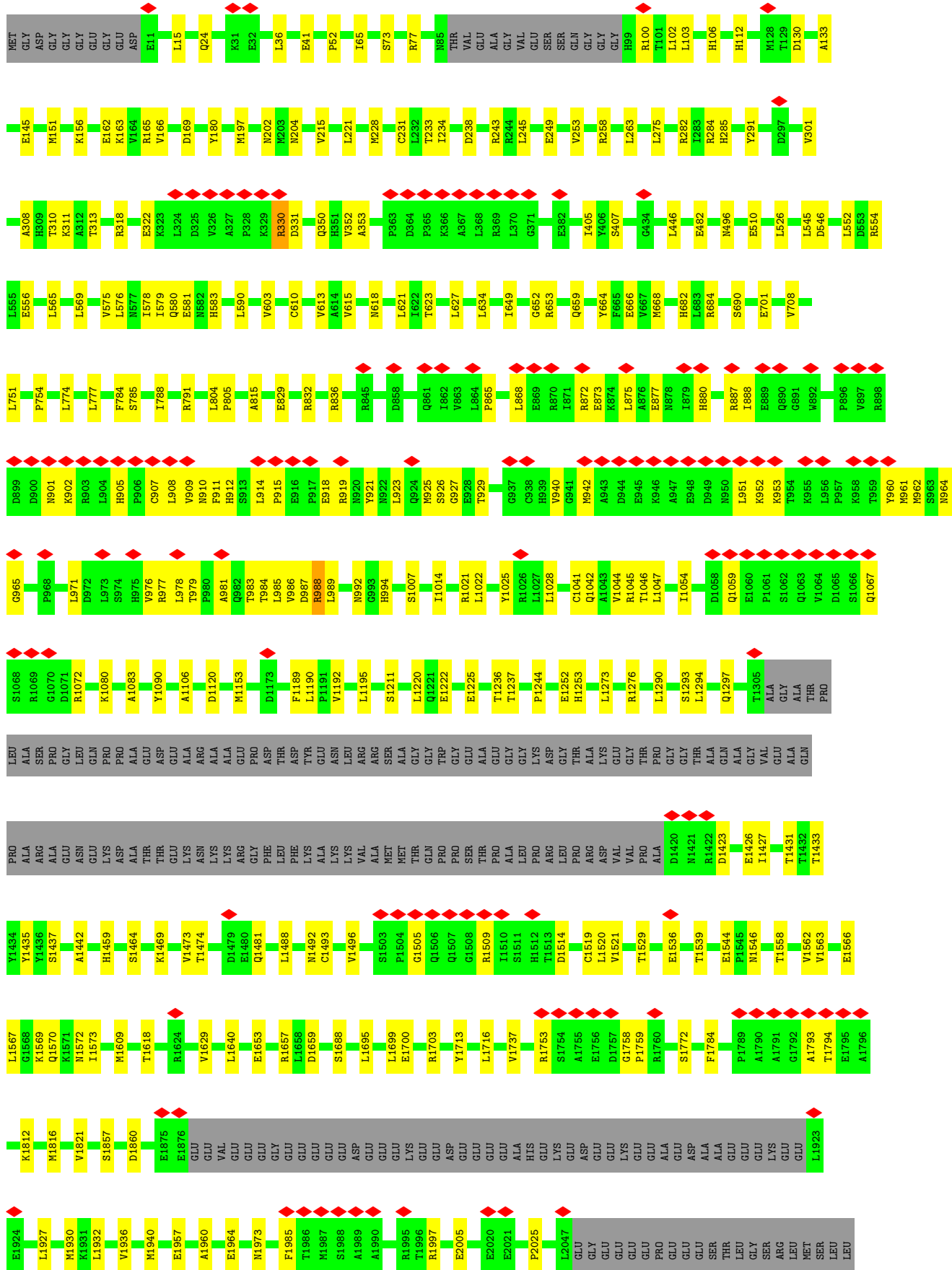


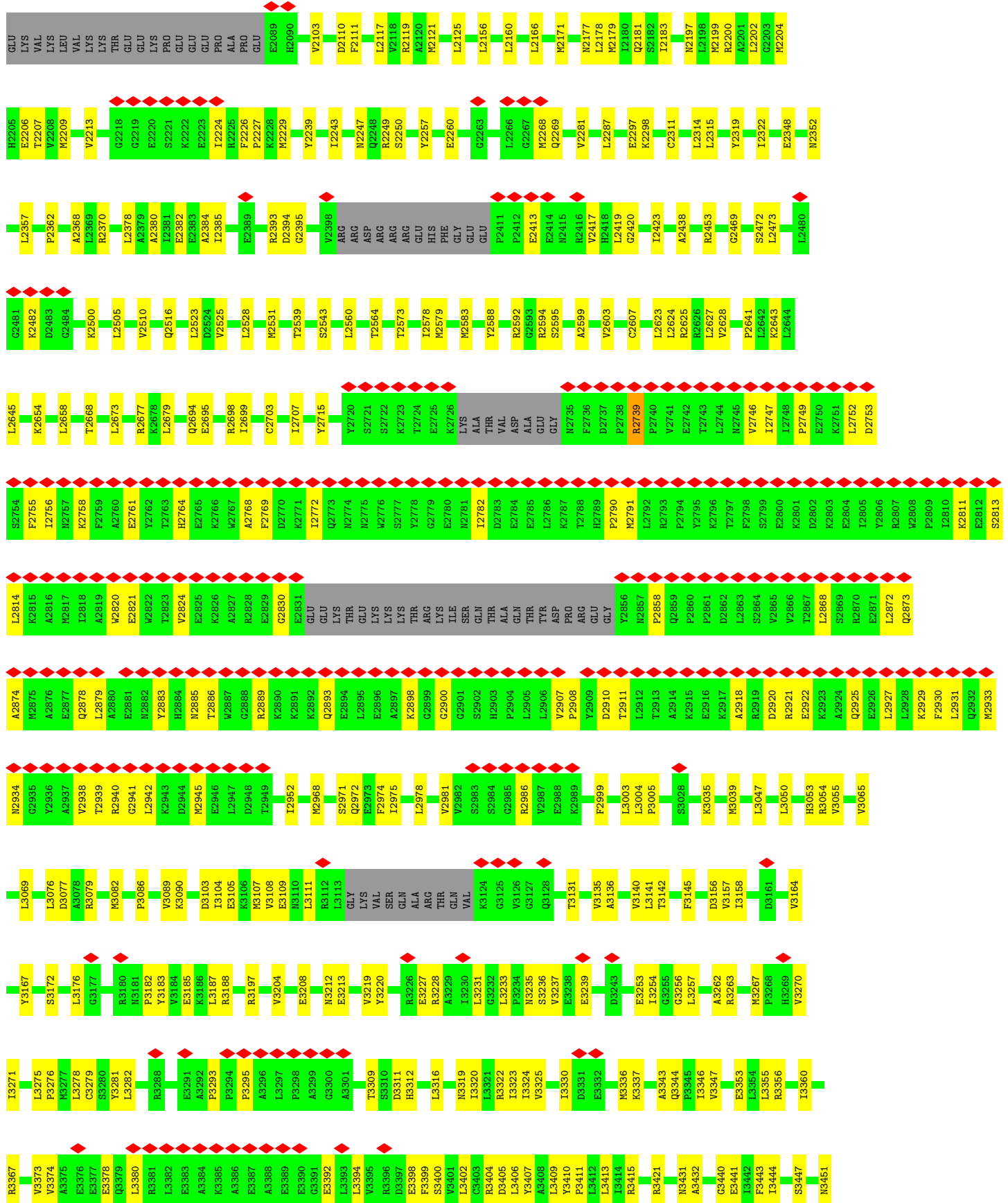
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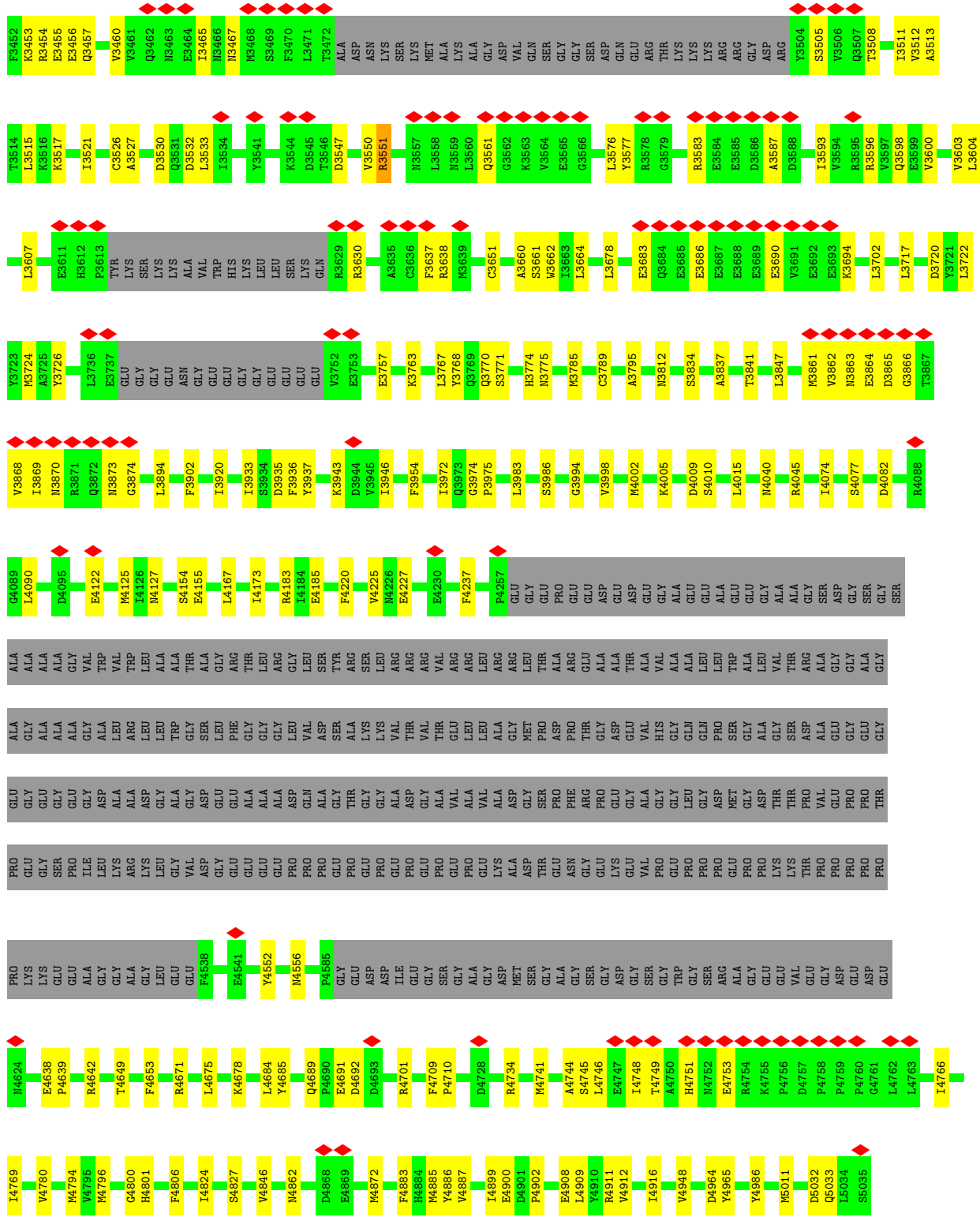


• Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN 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	0.547	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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, ZN, CFF, PCW, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.30	0/847	0.50	0/1142
1	F	0.30	0/847	0.50	0/1142
1	G	0.30	0/847	0.50	0/1142
1	H	0.30	0/847	0.50	0/1142
2	I	0.26	0/739	0.43	0/992
2	J	0.31	0/739	0.53	0/992
2	K	0.26	0/739	0.43	0/992
2	L	0.31	0/739	0.52	0/992
2	M	0.26	0/739	0.43	0/992
2	N	0.31	0/739	0.53	0/992
2	O	0.27	0/739	0.43	0/992
2	P	0.31	0/739	0.53	0/992
3	A	0.29	0/35638	0.49	0/48272
3	B	0.29	0/35638	0.49	0/48272
3	C	0.29	0/35638	0.49	0/48272
3	D	0.29	0/35638	0.49	0/48272
All	All	0.29	0/151852	0.49	0/205592

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

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	829	0	826	10	0
1	F	829	0	826	9	0
1	G	829	0	826	11	0
1	H	829	0	826	10	0
2	I	729	0	705	50	0
2	J	729	0	705	53	0
2	K	729	0	705	51	0
2	L	729	0	705	52	0
2	M	729	0	705	51	0
2	N	729	0	705	51	0
2	O	729	0	705	49	0
2	P	729	0	705	52	0
3	A	34849	0	34448	540	0
3	B	34849	0	34448	543	0
3	C	34849	0	34448	538	0
3	D	34849	0	34448	532	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
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	14	0	10	0	0
6	B	14	0	10	0	0
6	C	14	0	10	0	0
6	D	14	0	10	0	0
7	A	62	0	24	2	0
7	B	62	0	24	2	0
7	C	62	0	24	3	0
7	D	62	0	24	3	0
8	A	108	0	167	6	0
8	B	108	0	167	6	0
8	C	108	0	167	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	108	0	167	5	0
All	All	149304	0	147540	2468	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 8.

The worst 5 of 2468 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:I:10:GLU:OE2	3:A:2694:GLN:NE2	1.72	1.23
3:C:2694:GLN:NE2	2:M:10:GLU:OE2	1.72	1.23
3:D:2694:GLN:NE2	2:O:10:GLU:OE2	1.72	1.22
3:B:2694:GLN:NE2	2:K:10:GLU:OE2	1.72	1.21
3:A:875:LEU:HD11	3:A:1047:LEU:HD21	1.41	1.02

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%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
1	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
1	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	I	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	J	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	K	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	L	91/94 (97%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	N	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	O	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	P	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
3	A	4351/5035 (86%)	4238 (97%)	113 (3%)	0	100	100
3	B	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
3	C	4351/5035 (86%)	4241 (98%)	110 (2%)	0	100	100
3	D	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
All	All	18552/21324 (87%)	18032 (97%)	520 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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	I	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	J	80/81 (99%)	80 (100%)	0	100	100
2	K	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	L	80/81 (99%)	80 (100%)	0	100	100
2	M	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	N	80/81 (99%)	80 (100%)	0	100	100
2	O	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	P	80/81 (99%)	80 (100%)	0	100	100
3	A	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
3	C	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
3	D	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
All	All	16240/18192 (89%)	16180 (100%)	60 (0%)	91	97

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	330	ARG
2	K	57	LYS
3	B	2739	ARG
2	K	22	LYS
2	O	57	LYS

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

Mol	Chain	Res	Type
3	B	2128	GLN
3	C	106	HIS
3	B	3181	ASN
3	C	726	HIS
3	A	726	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 24 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
6	CFF	B	8002	-	8,15,15	0.91	0	8,23,23	2.82	2 (25%)
8	PCW	B	8006	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
7	ATP	D	8005	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
7	ATP	C	5106	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
8	PCW	A	8006	-	53,53,53	1.13	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	C	5101	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
8	PCW	A	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
6	CFF	D	8002	-	8,15,15	0.92	0	8,23,23	2.83	2 (25%)
8	PCW	B	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
7	ATP	B	8003	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
7	ATP	A	8005	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
7	ATP	B	8005	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
6	CFF	A	8002	-	8,15,15	0.90	0	8,23,23	2.79	2 (25%)
7	ATP	C	5104	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
8	PCW	C	5107	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	D	8006	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	D	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
7	ATP	A	8003	-	26,33,33	0.68	0	31,52,52	0.71	1 (3%)
6	CFF	C	5103	-	8,15,15	0.91	0	8,23,23	2.80	2 (25%)
7	ATP	D	8003	-	26,33,33	0.68	0	31,52,52	0.71	1 (3%)

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
6	CFF	B	8002	-	-	-	0/2/2/2
8	PCW	B	8006	-	-	21/57/57/57	-
7	ATP	D	8005	-	-	5/18/38/38	0/3/3/3
7	ATP	C	5106	-	-	5/18/38/38	0/3/3/3
8	PCW	A	8006	-	-	21/57/57/57	-
8	PCW	C	5101	-	-	20/57/57/57	-
8	PCW	A	8007	-	-	20/57/57/57	-
6	CFF	D	8002	-	-	-	0/2/2/2
8	PCW	B	8007	-	-	20/57/57/57	-
7	ATP	B	8003	-	-	7/18/38/38	0/3/3/3
7	ATP	A	8005	-	-	5/18/38/38	0/3/3/3
7	ATP	B	8005	-	-	5/18/38/38	0/3/3/3
6	CFF	A	8002	-	-	-	0/2/2/2
7	ATP	C	5104	-	-	7/18/38/38	0/3/3/3
8	PCW	C	5107	-	-	21/57/57/57	-
8	PCW	D	8006	-	-	21/57/57/57	-
8	PCW	D	8007	-	-	20/57/57/57	-
7	ATP	A	8003	-	-	7/18/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
7	ATP	D	8003	-	-	7/18/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	8006	PCW	O3-C11	3.07	1.42	1.33
8	A	8006	PCW	O3-C11	3.07	1.42	1.33
8	B	8006	PCW	O3-C11	3.07	1.42	1.33
8	C	5107	PCW	O3-C11	3.07	1.42	1.33
8	A	8007	PCW	O3-C11	3.03	1.42	1.33

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	8006	PCW	C8-N-C6	11.85	139.44	108.97
8	C	5107	PCW	C8-N-C6	11.85	139.44	108.97
8	D	8006	PCW	C8-N-C6	11.84	139.42	108.97
8	B	8006	PCW	C8-N-C6	11.84	139.42	108.97
8	B	8007	PCW	C8-N-C6	11.22	137.81	108.97

There are no chirality outliers.

5 of 212 torsion outliers are listed below:

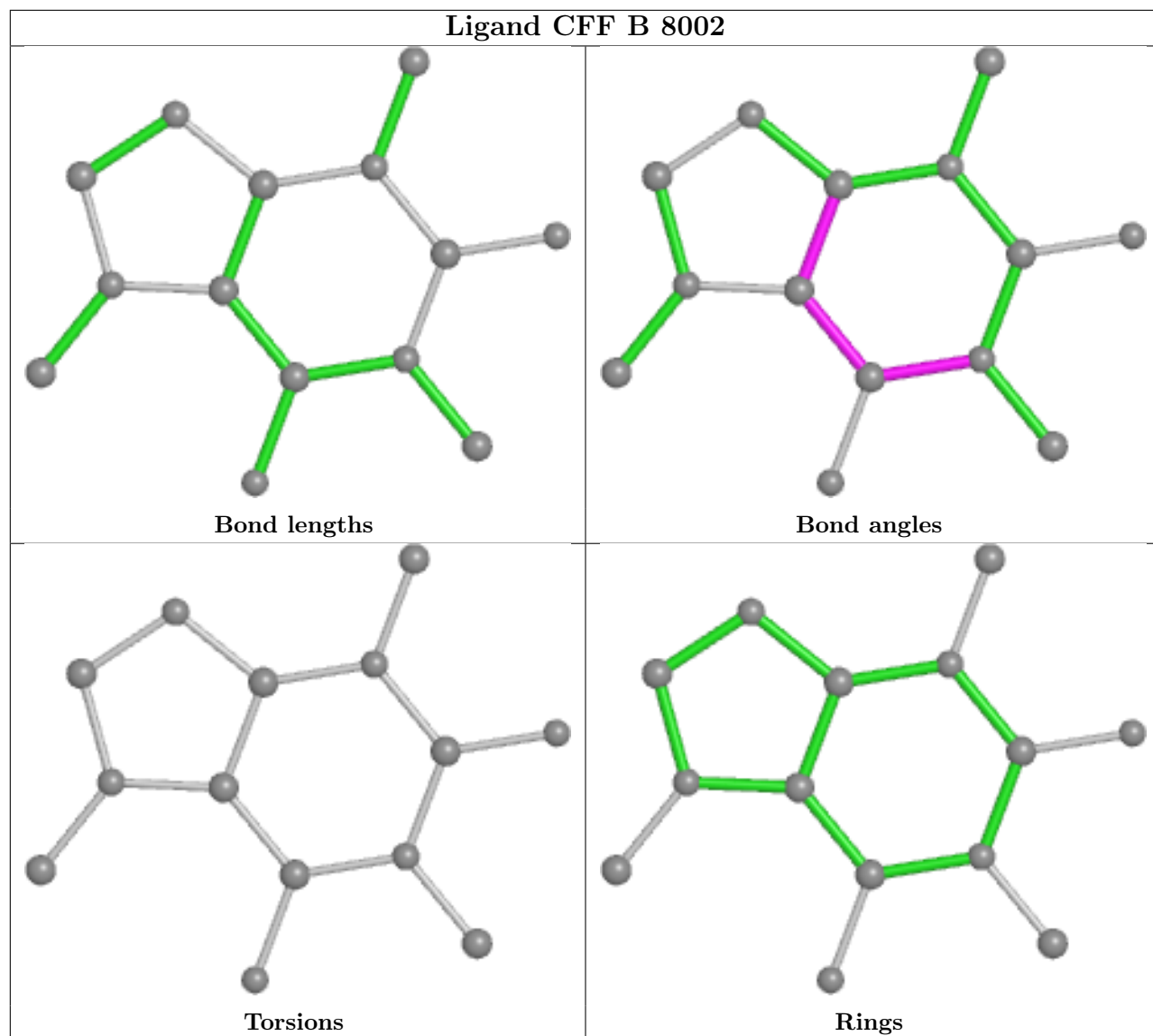
Mol	Chain	Res	Type	Atoms
7	D	8003	ATP	C5'-O5'-PA-O1A
7	D	8005	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O1A
7	A	8005	ATP	C5'-O5'-PA-O1A
7	B	8003	ATP	C5'-O5'-PA-O1A

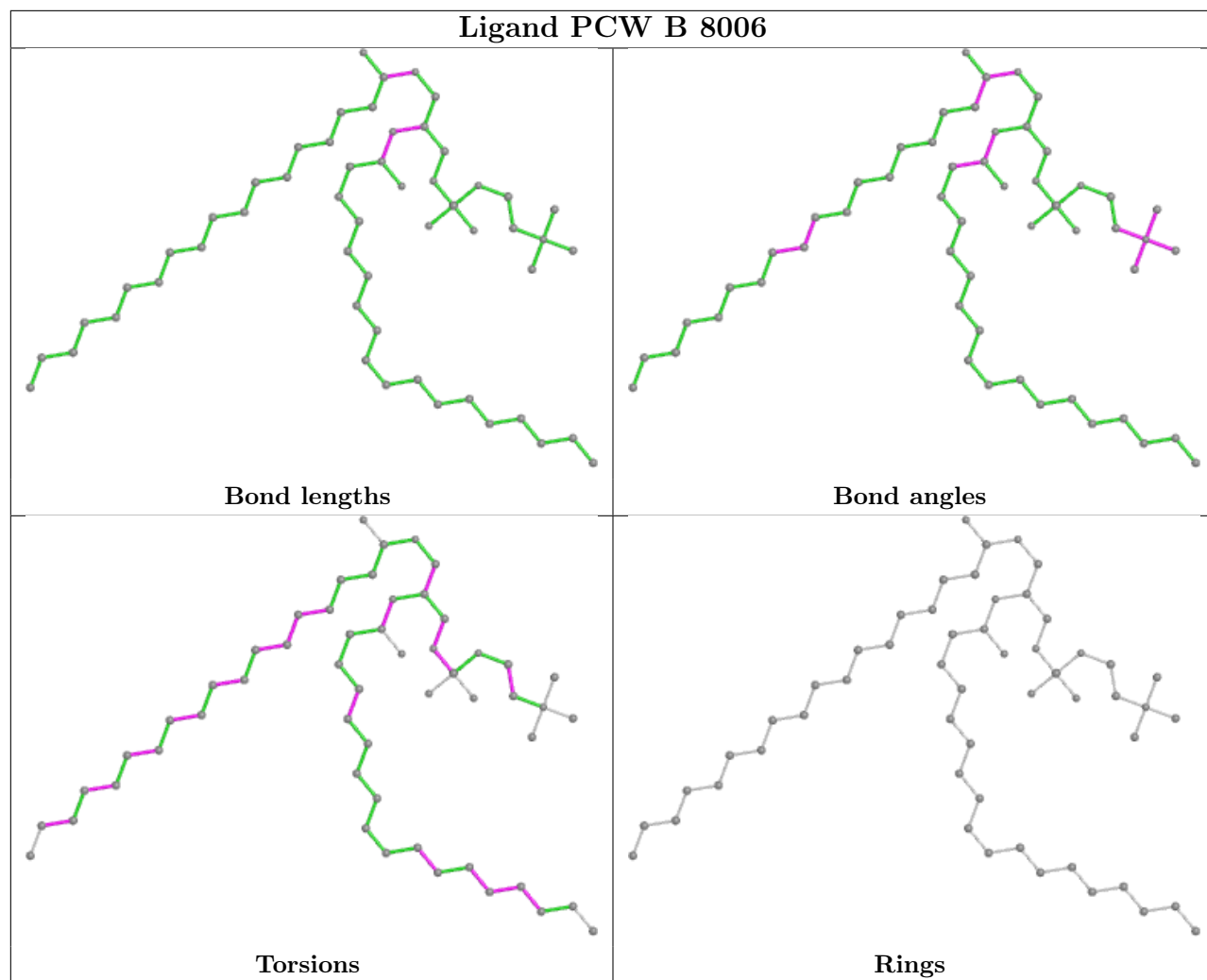
There are no ring outliers.

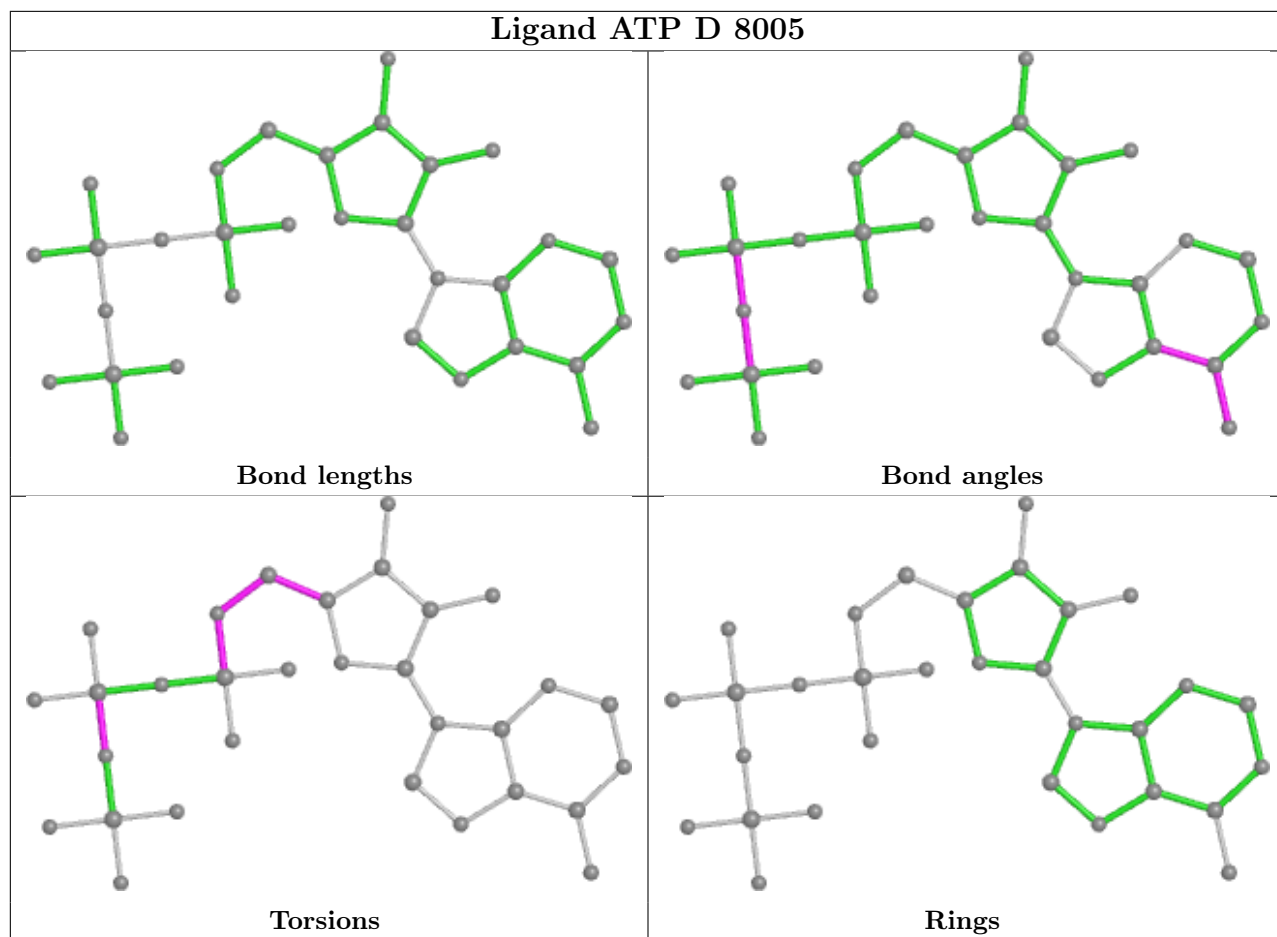
12 monomers are involved in 27 short contacts:

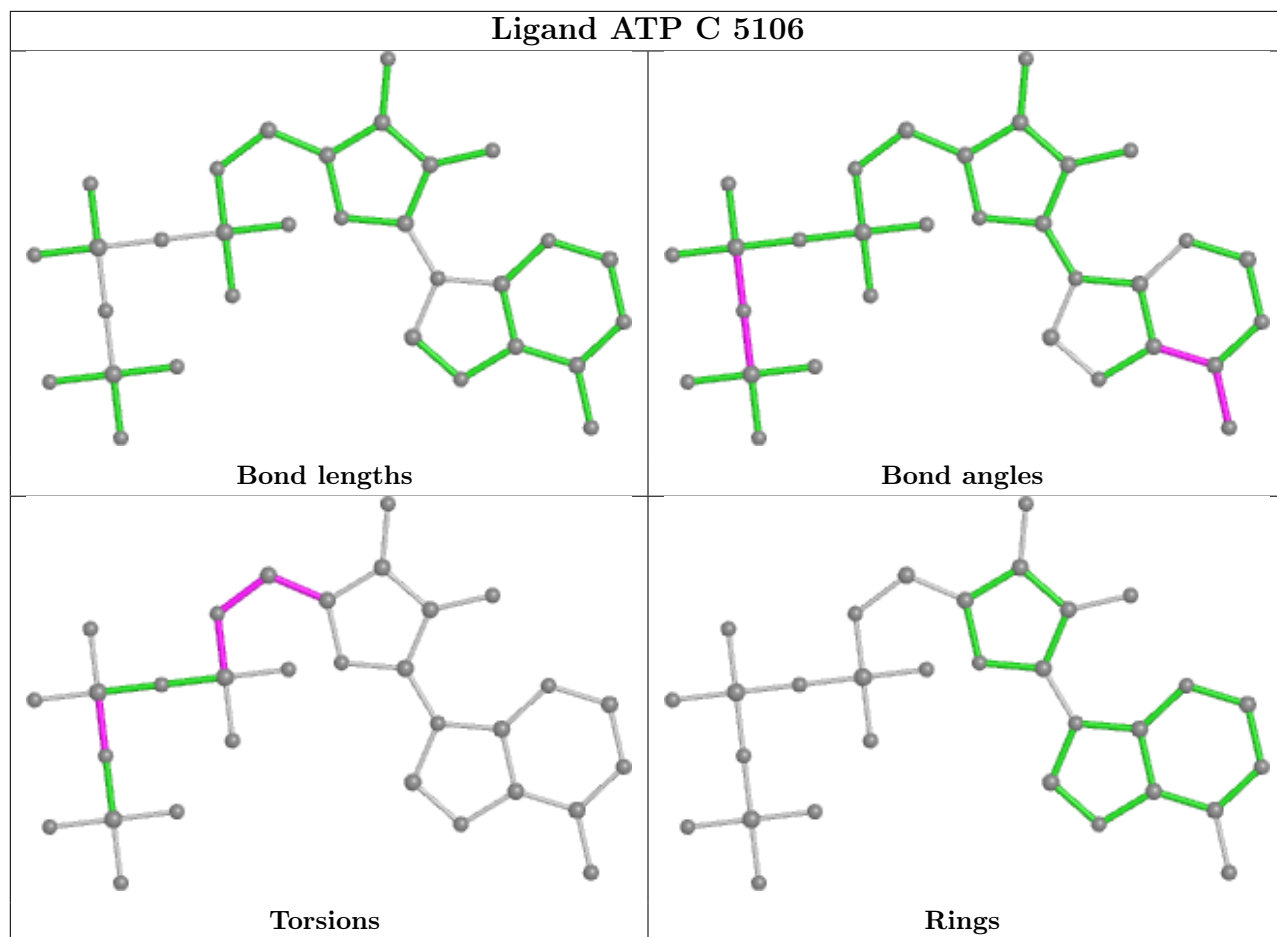
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	8006	PCW	1	0
7	D	8005	ATP	3	0
7	C	5106	ATP	3	0
8	A	8006	PCW	2	0
8	C	5101	PCW	3	0
8	A	8007	PCW	4	0
8	B	8007	PCW	5	0
7	A	8005	ATP	2	0
7	B	8005	ATP	2	0
8	C	5107	PCW	1	0
8	D	8006	PCW	1	0
8	D	8007	PCW	4	0

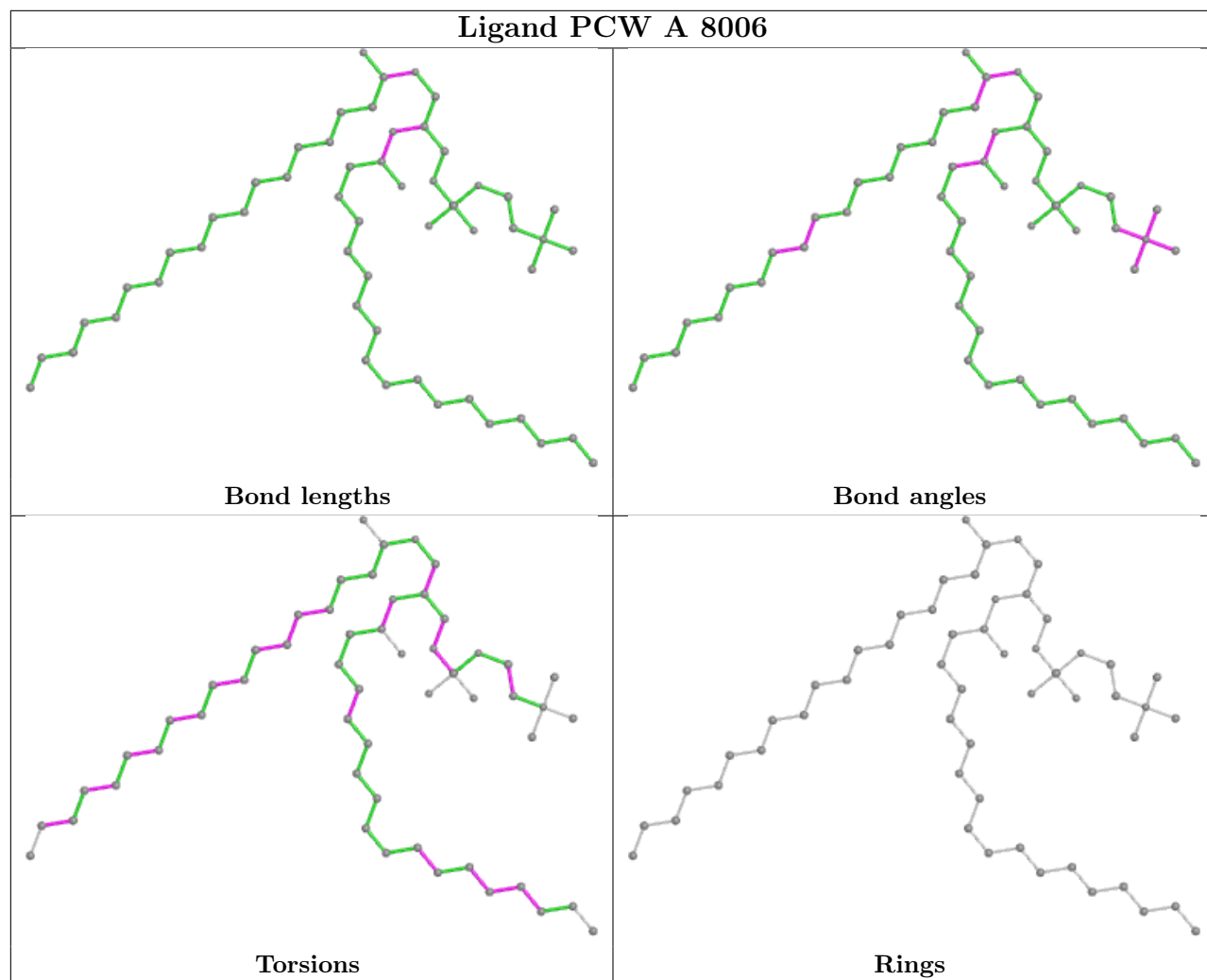
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

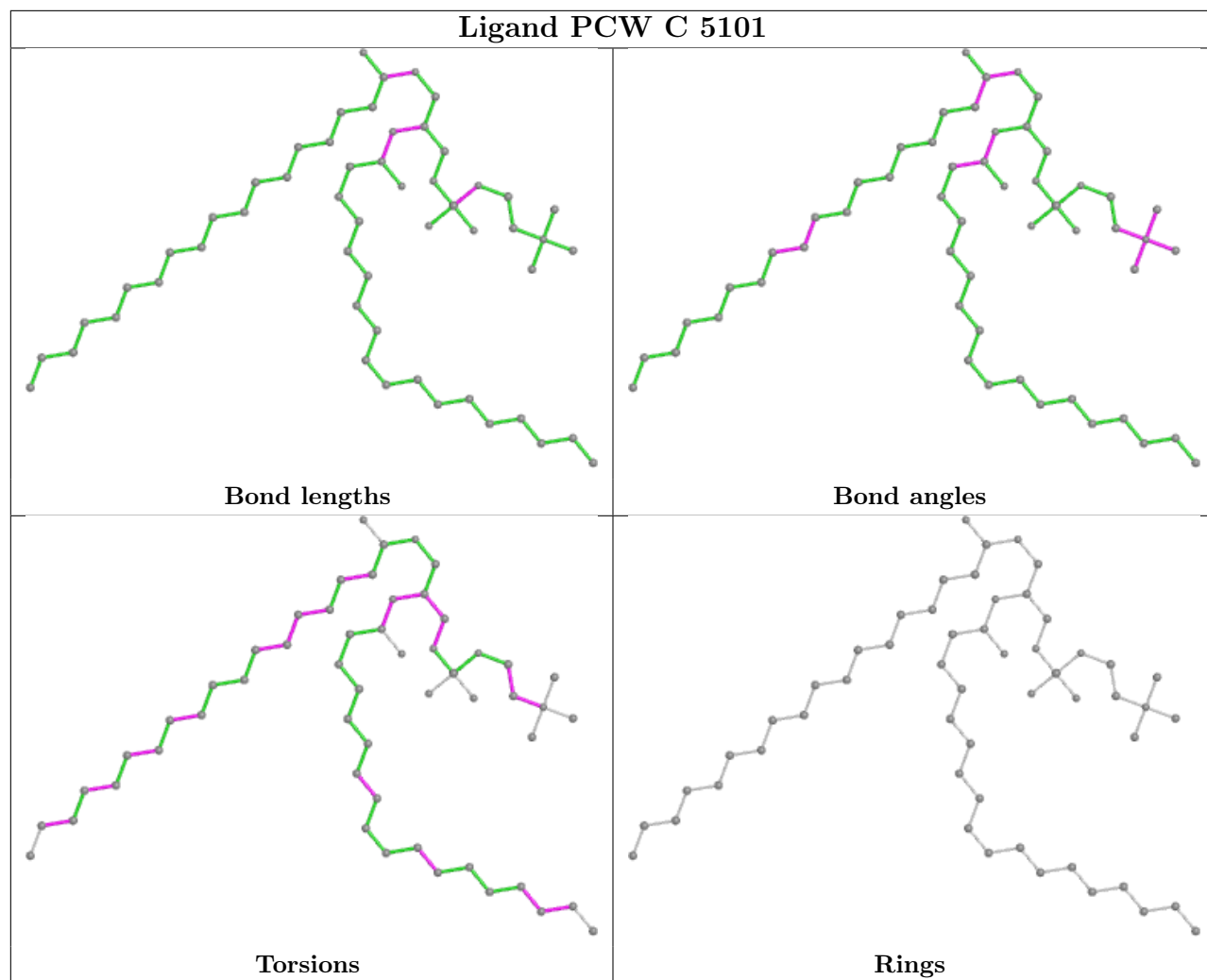


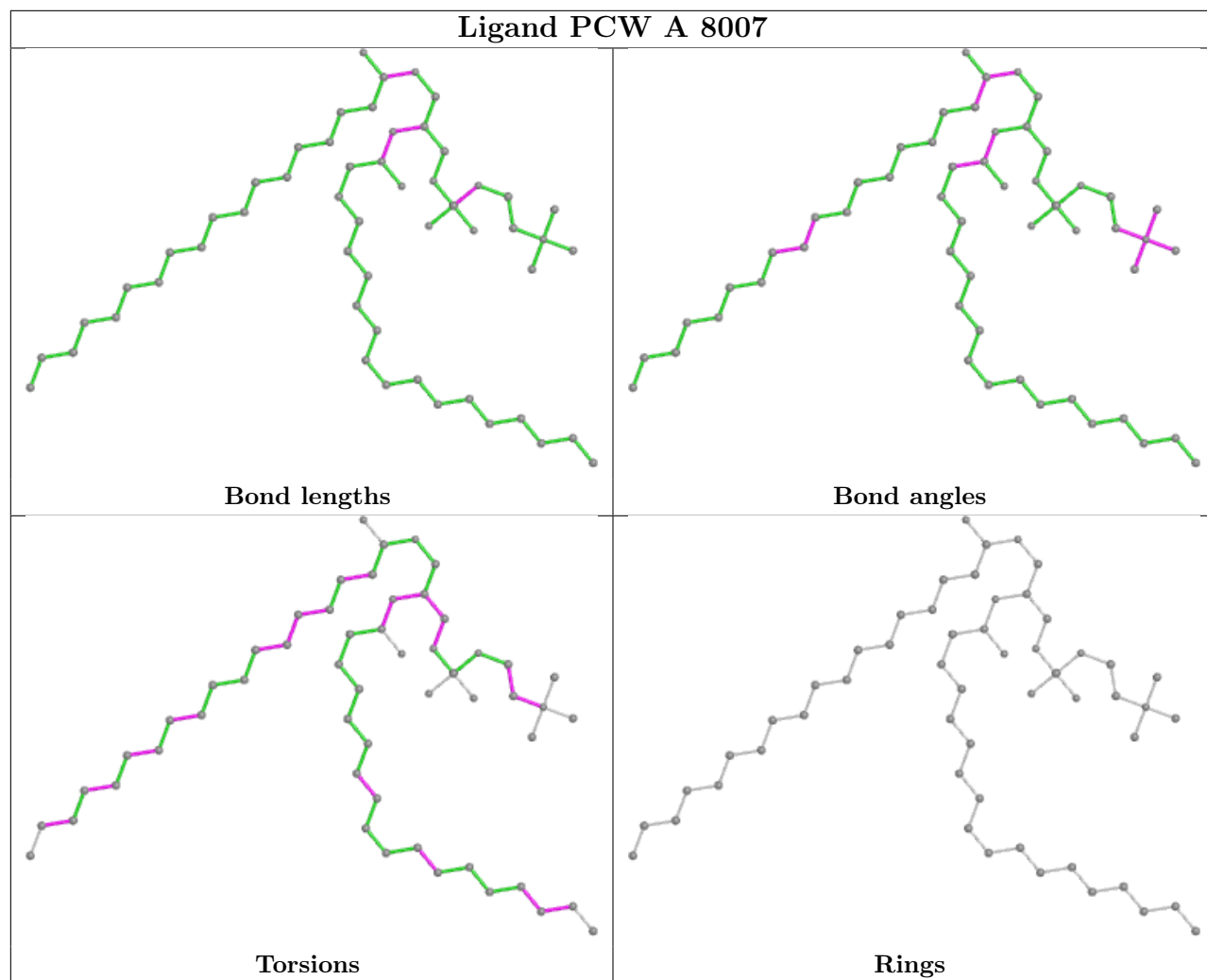


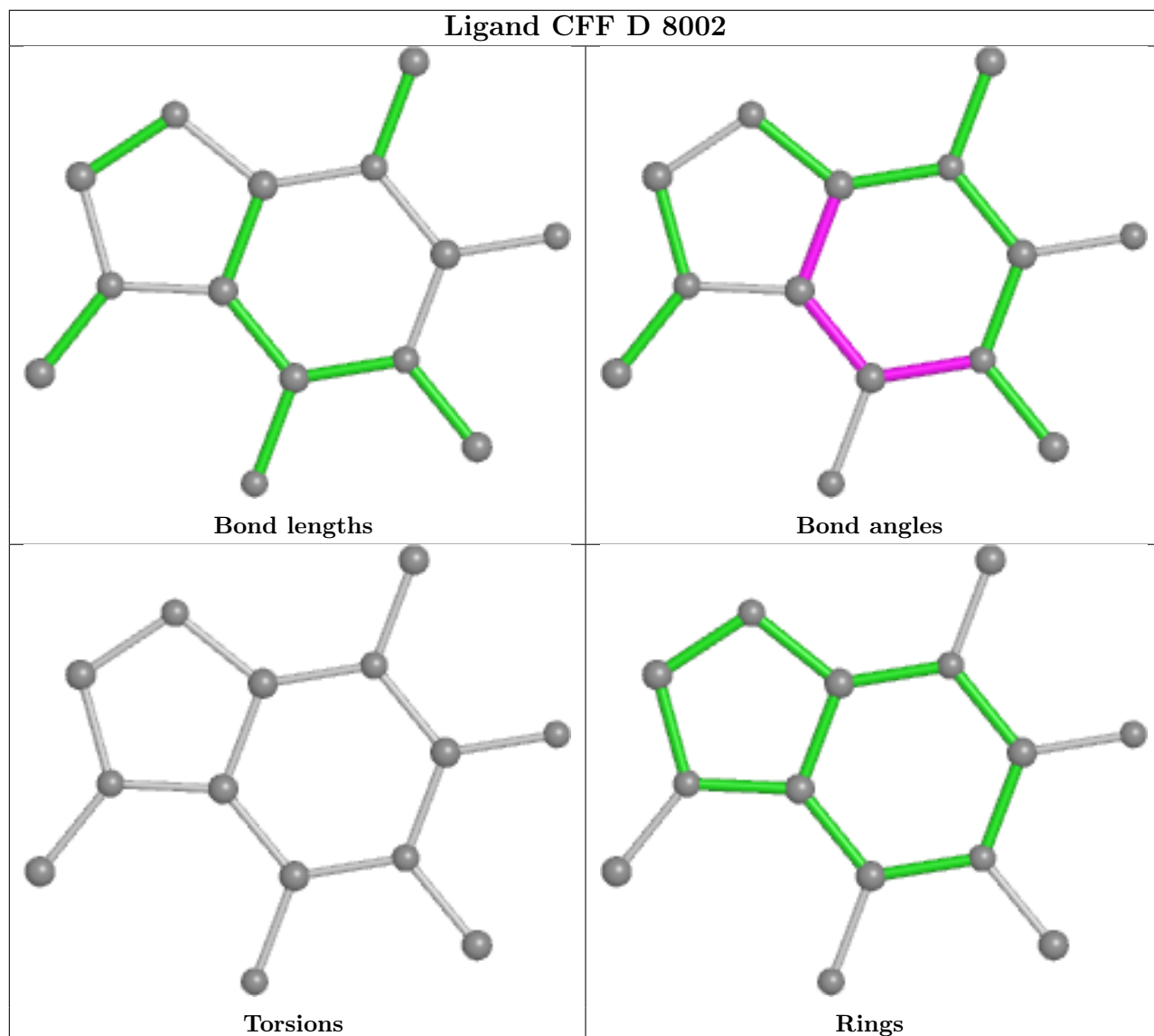


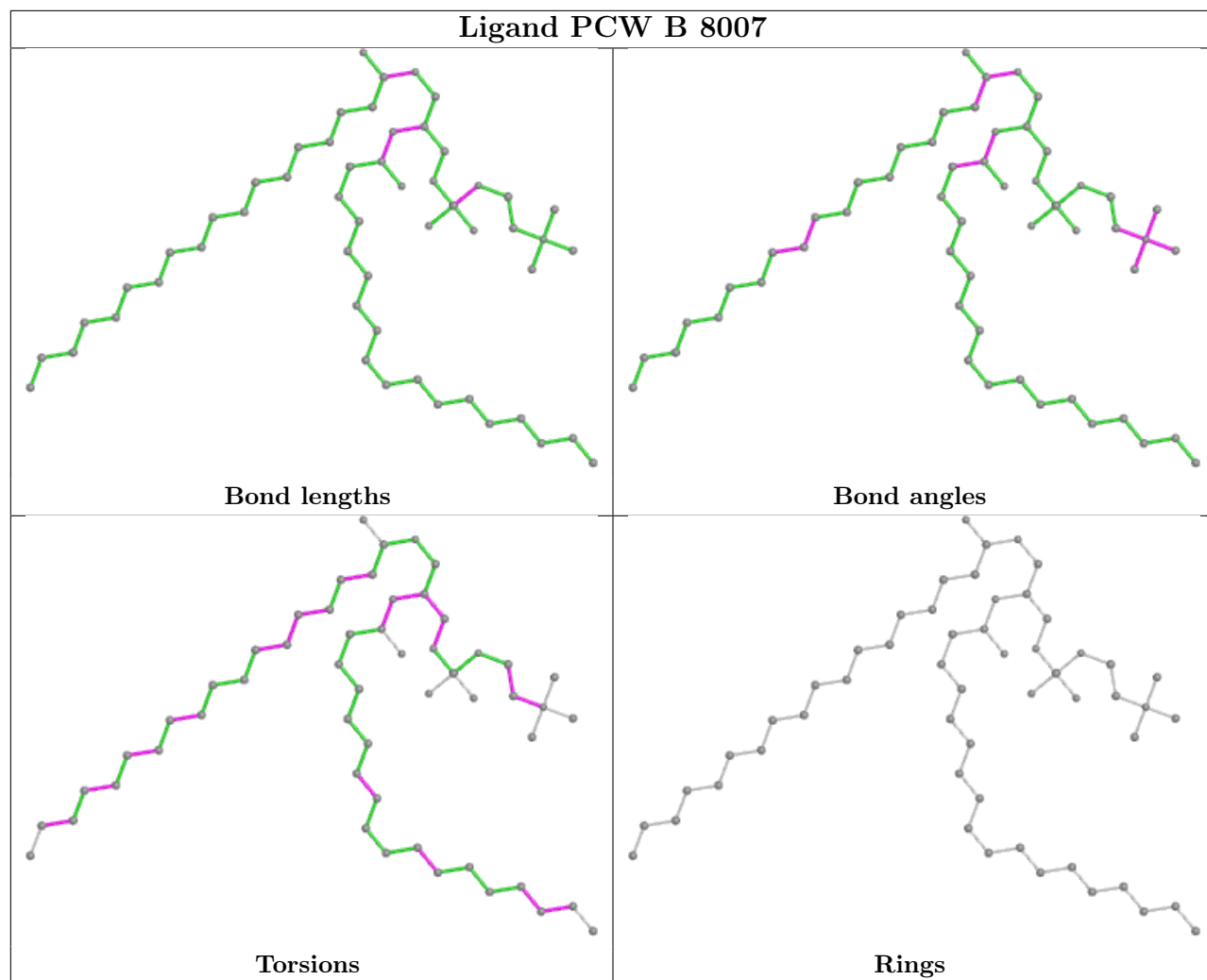


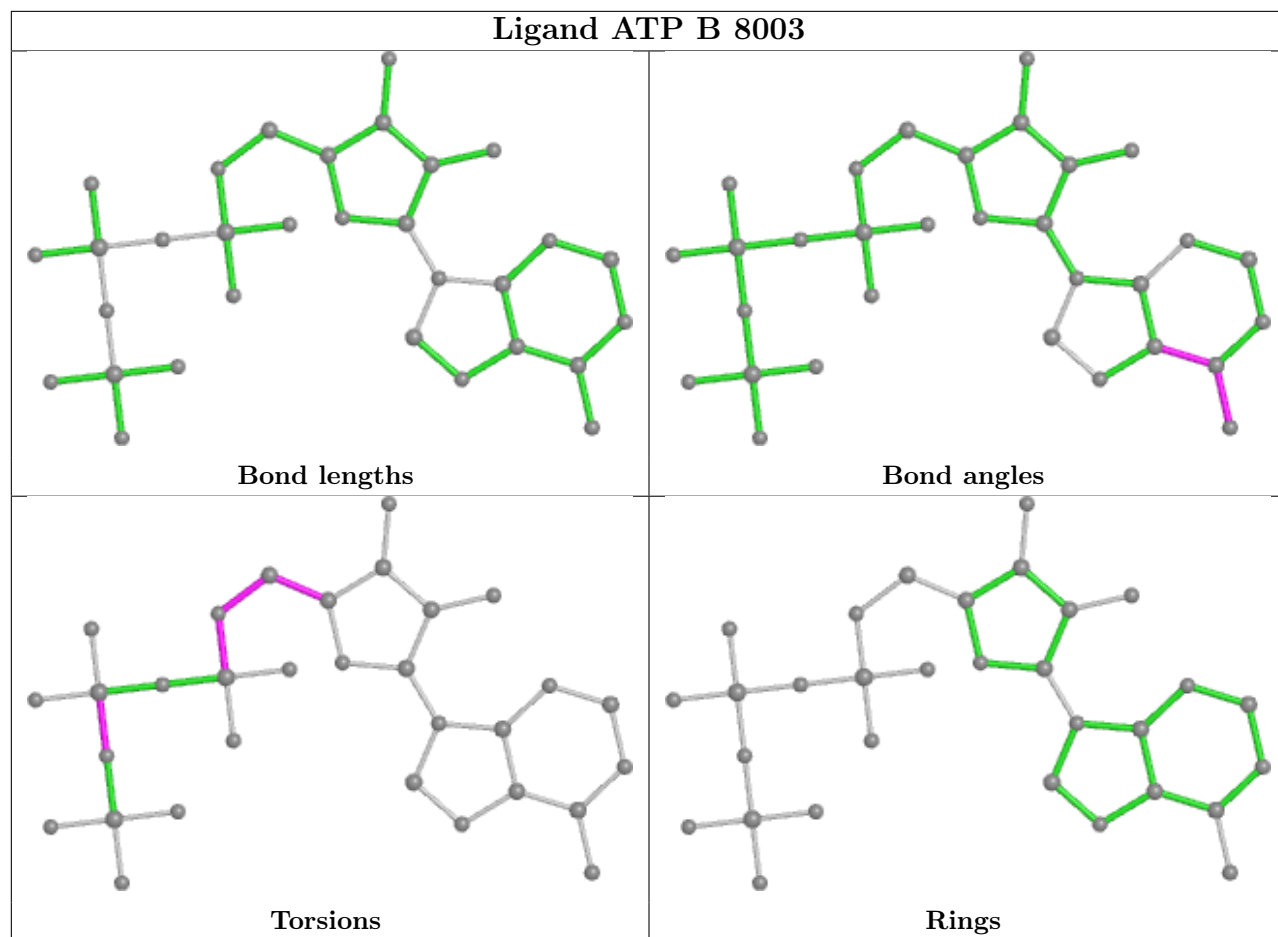


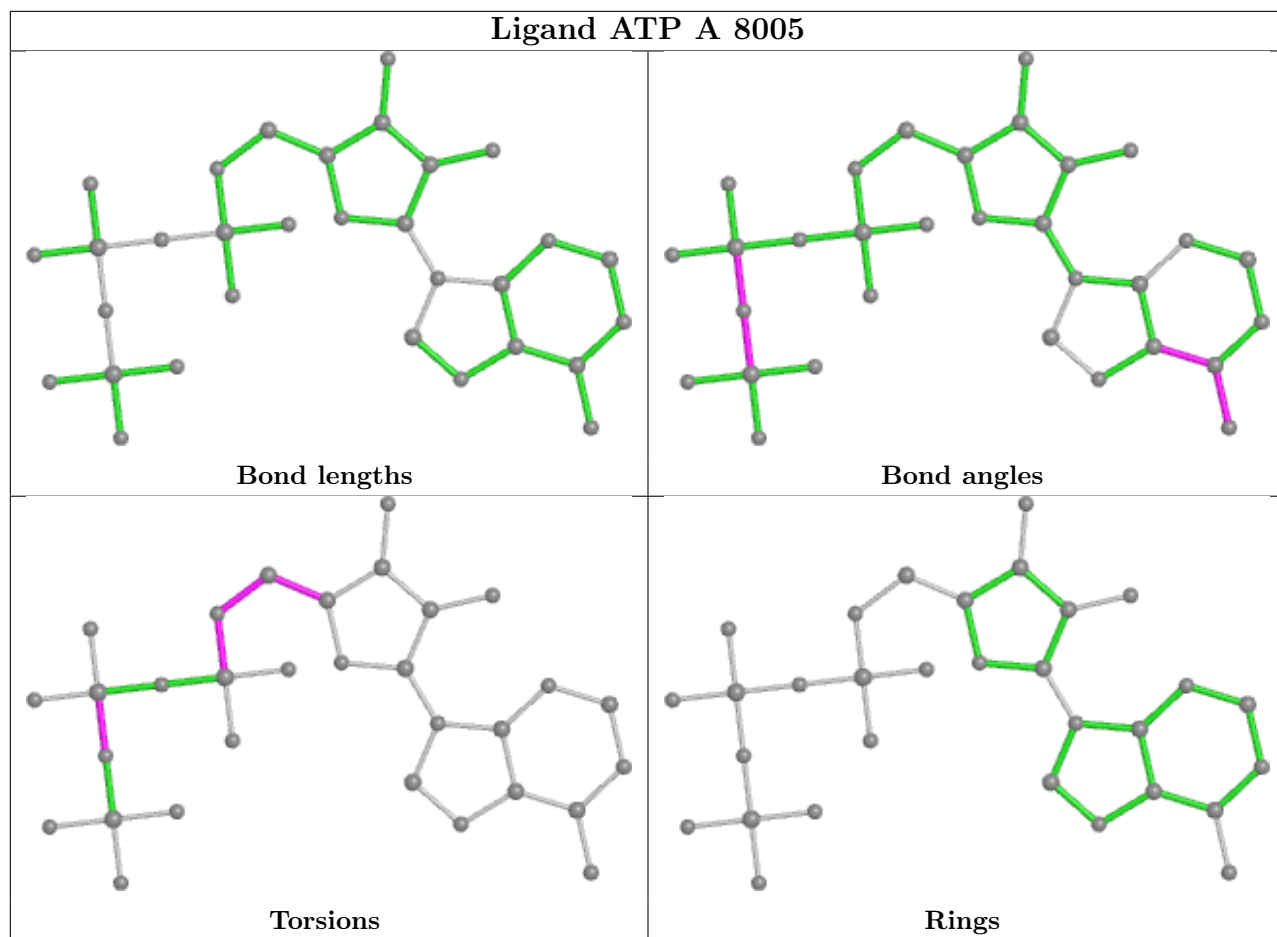


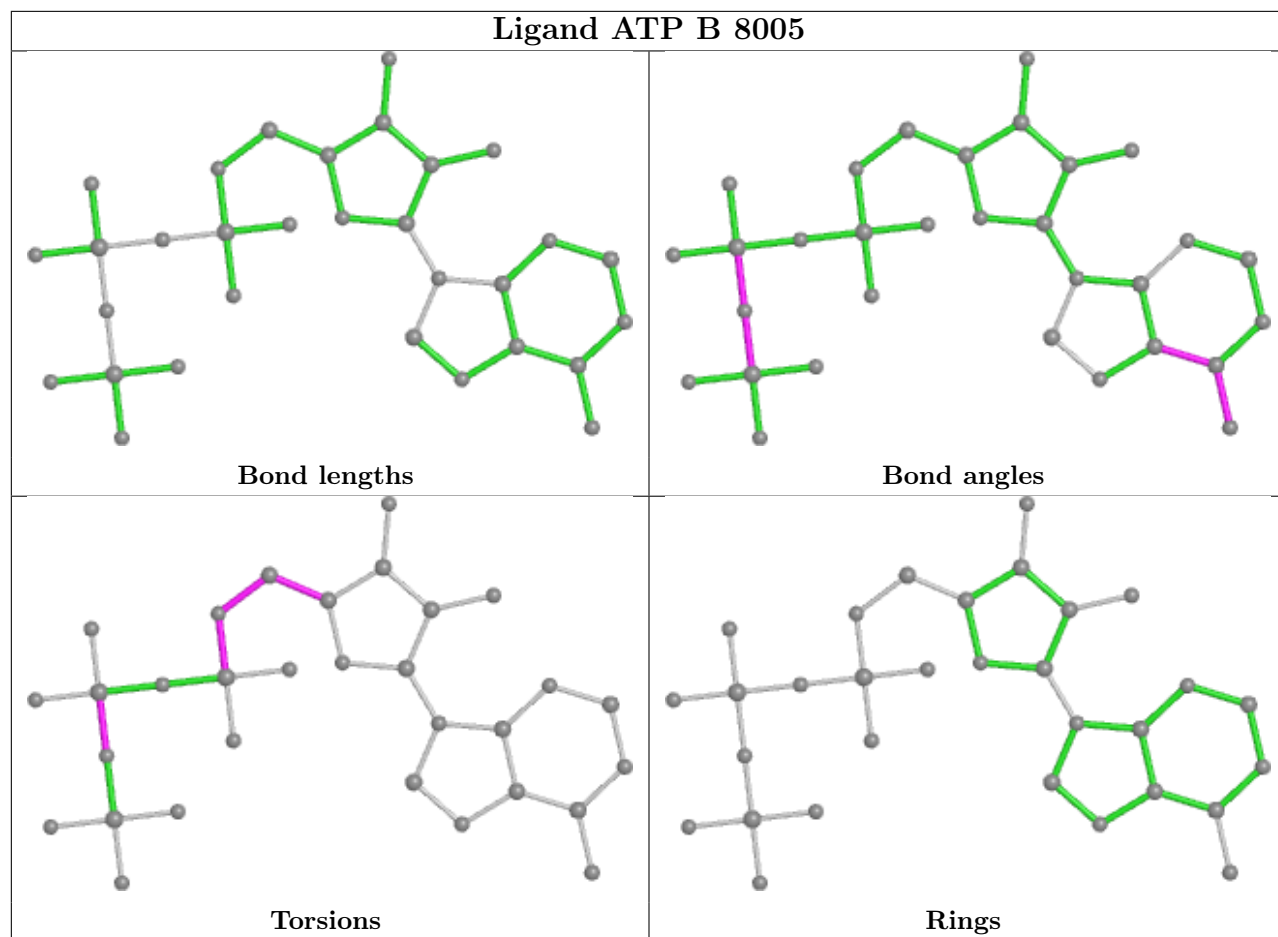


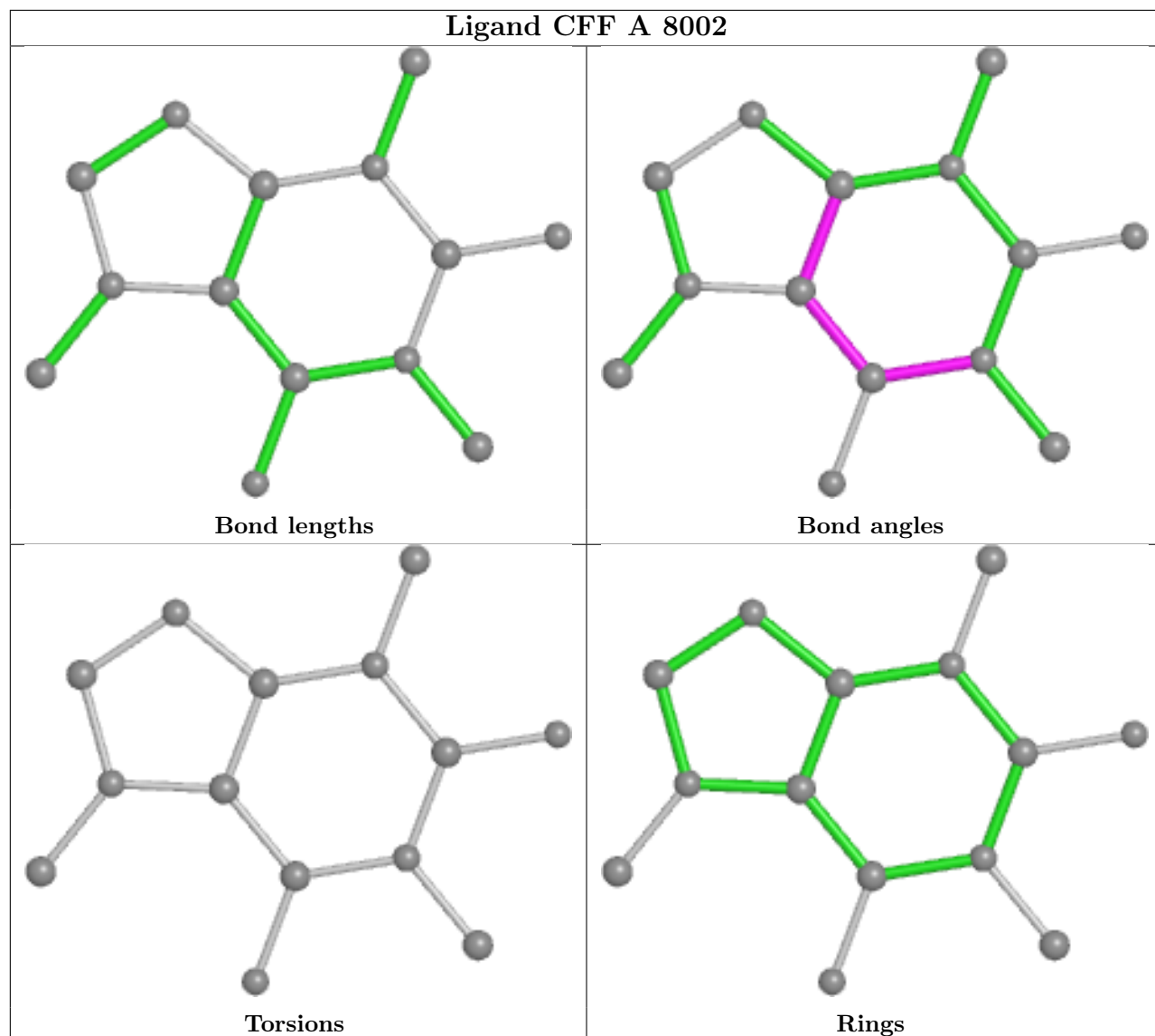


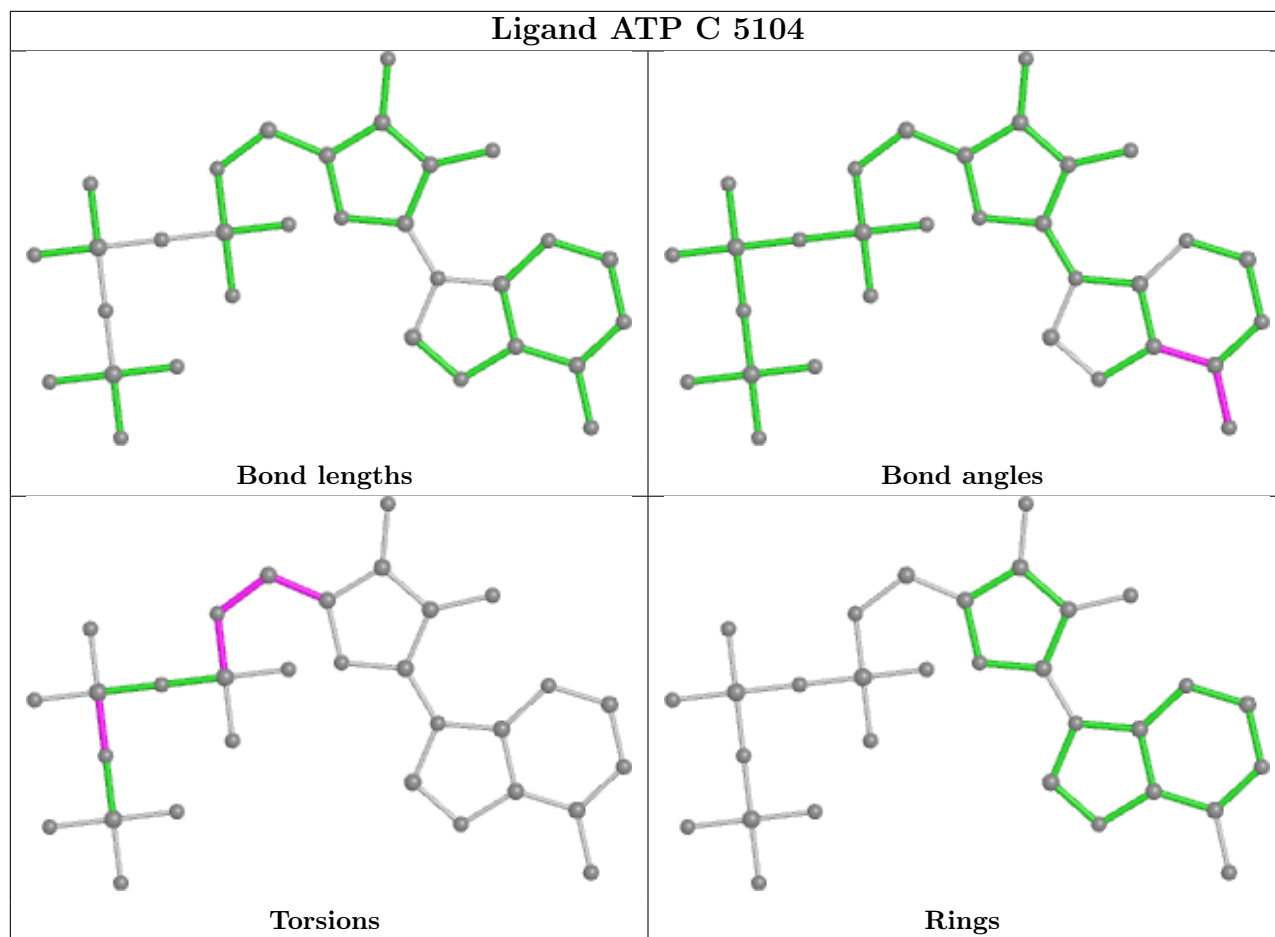


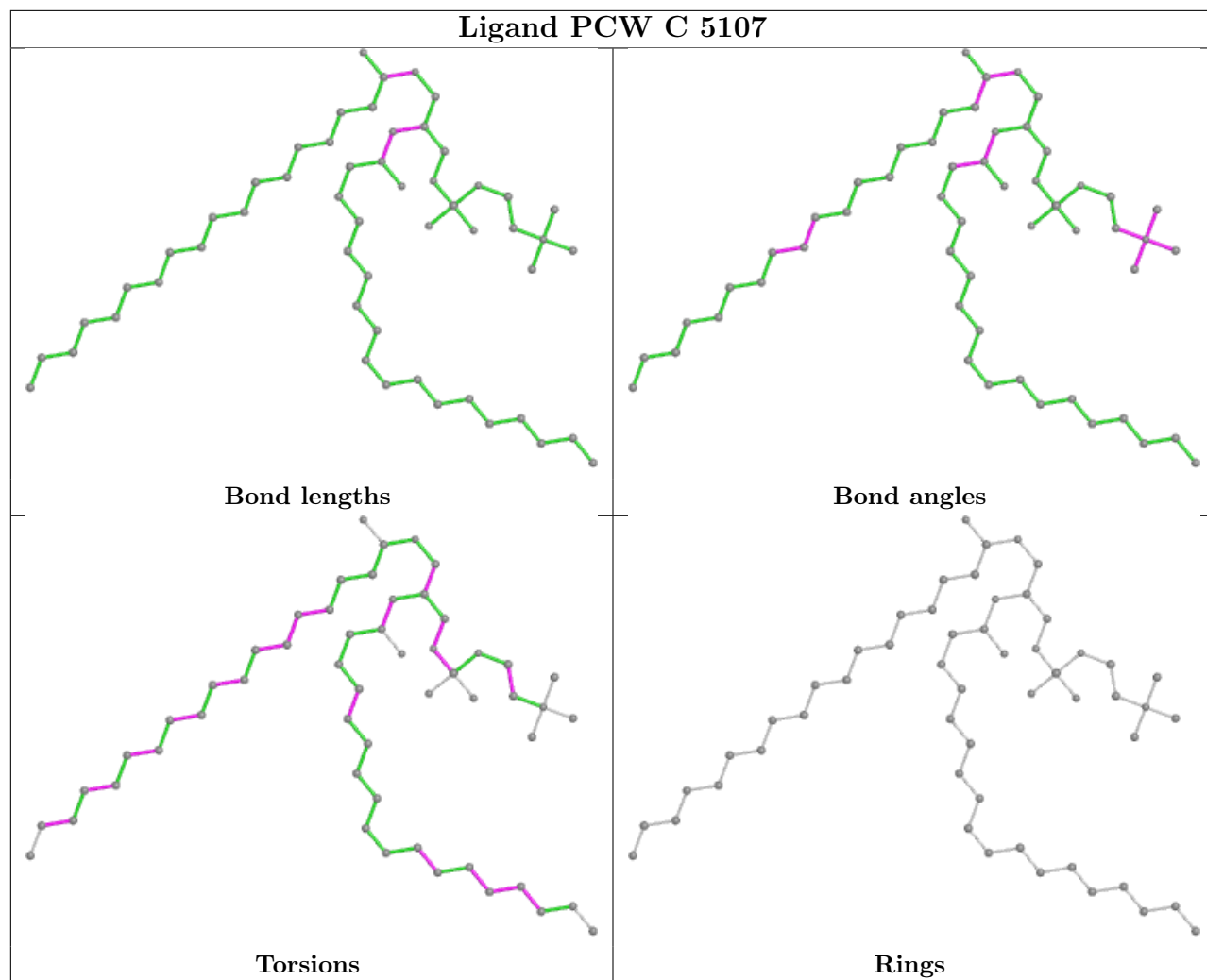


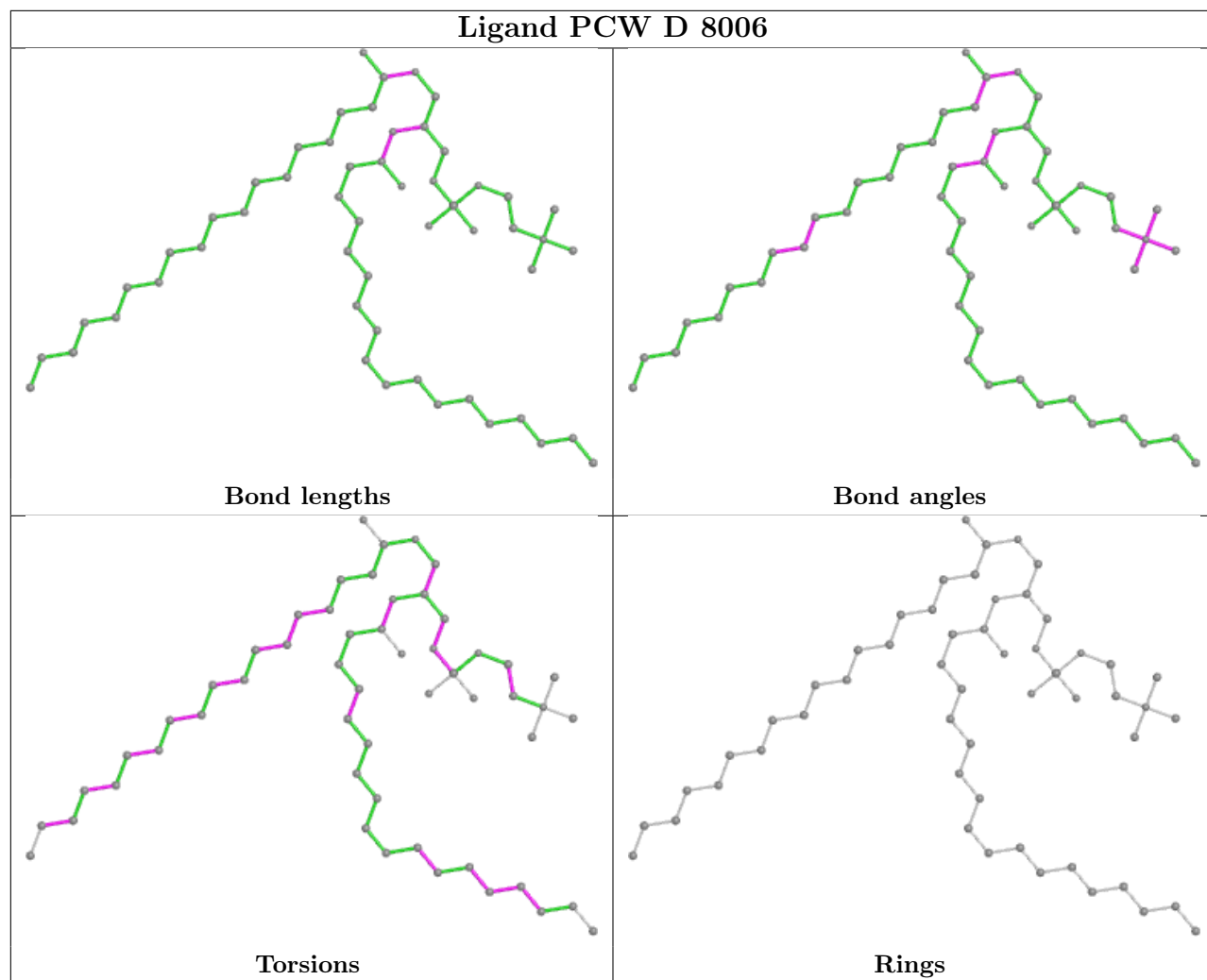


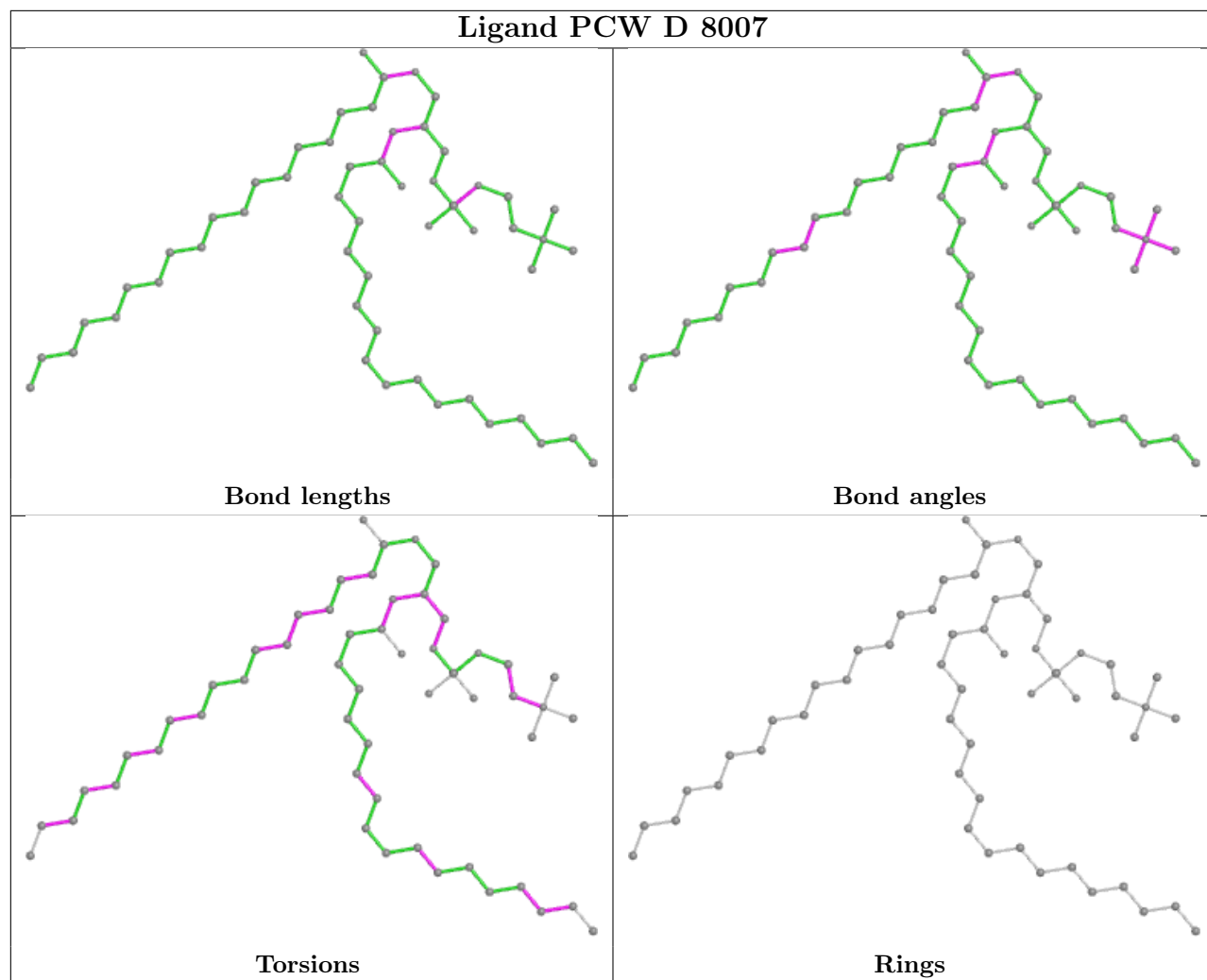


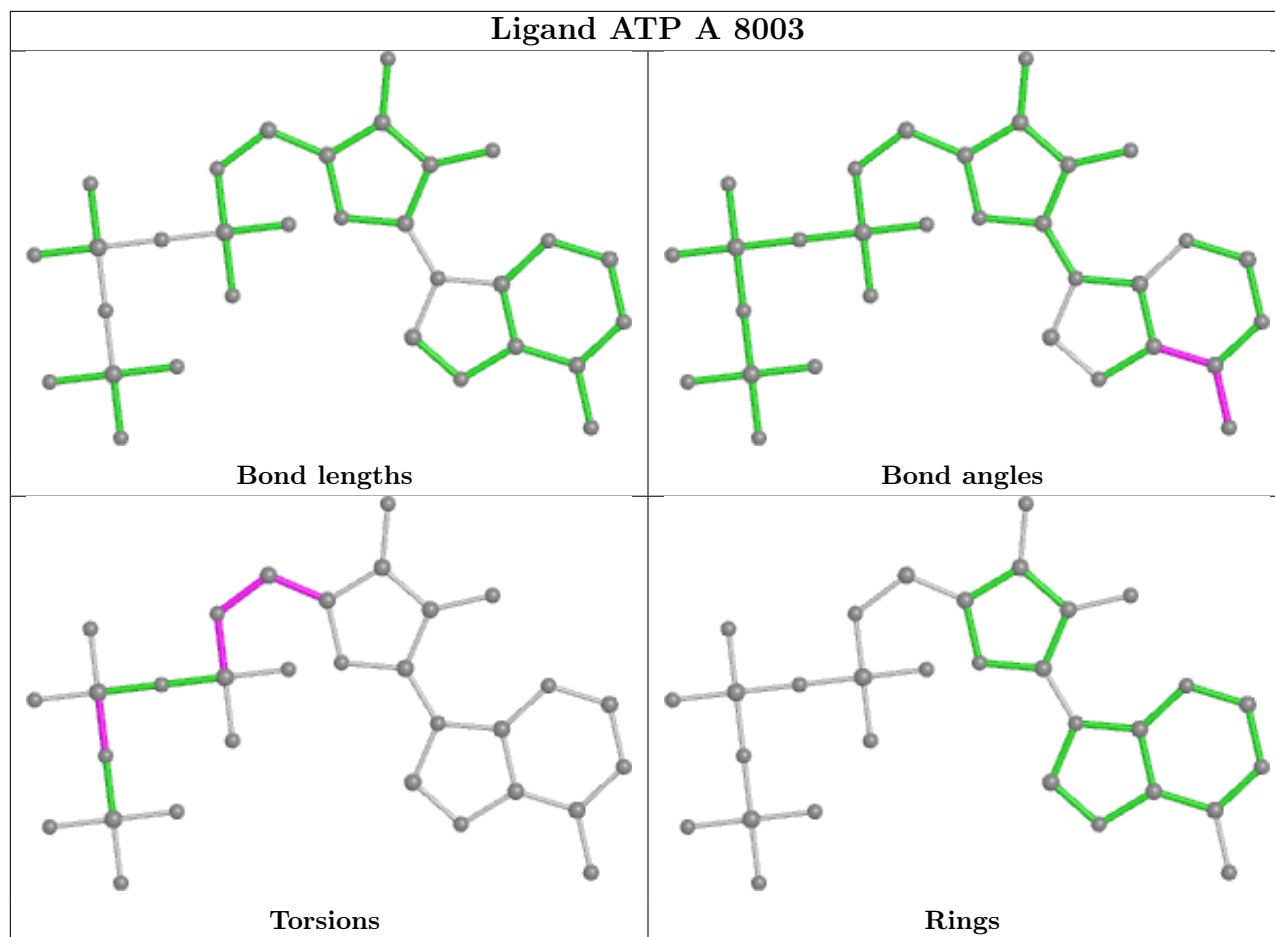


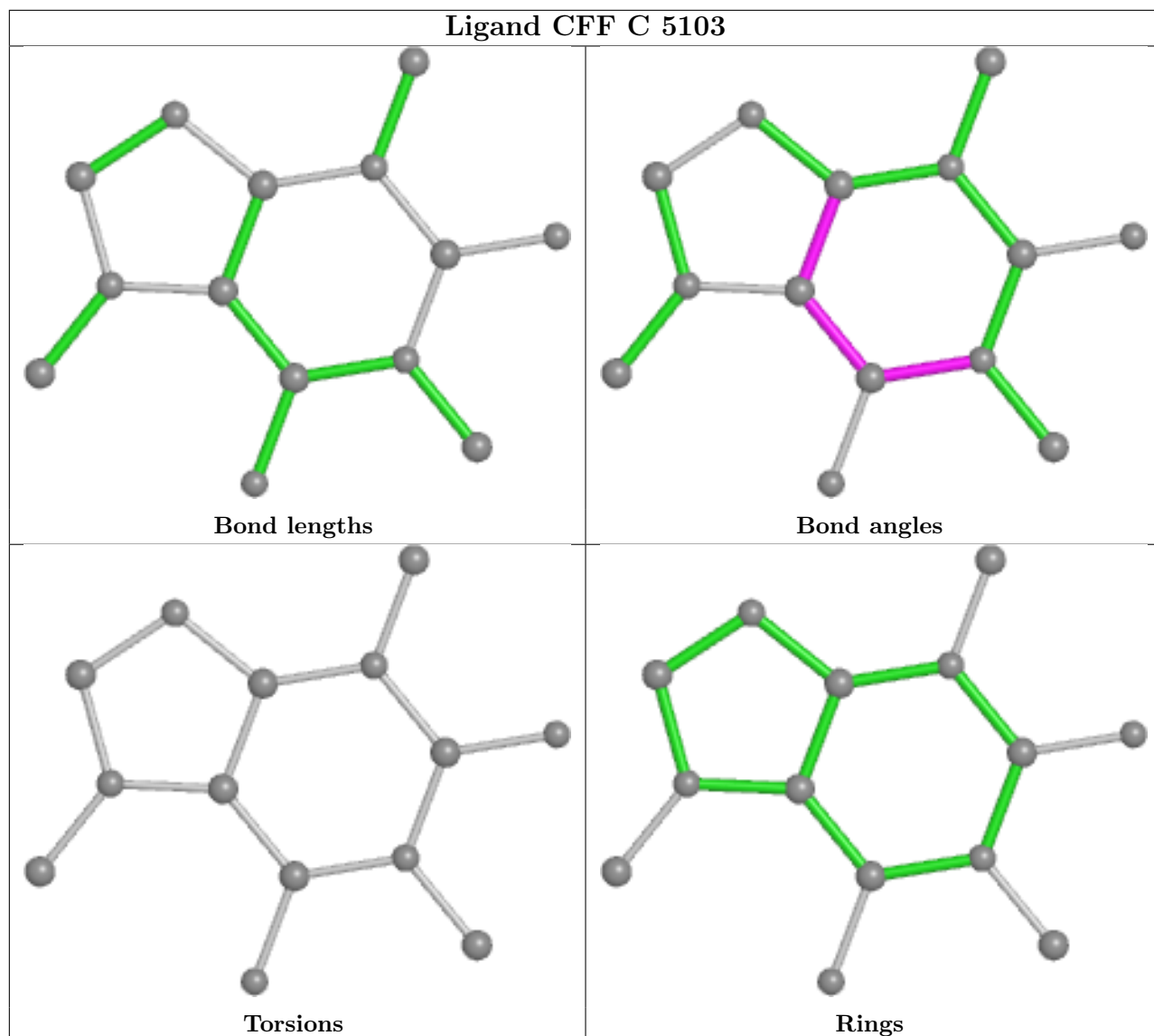


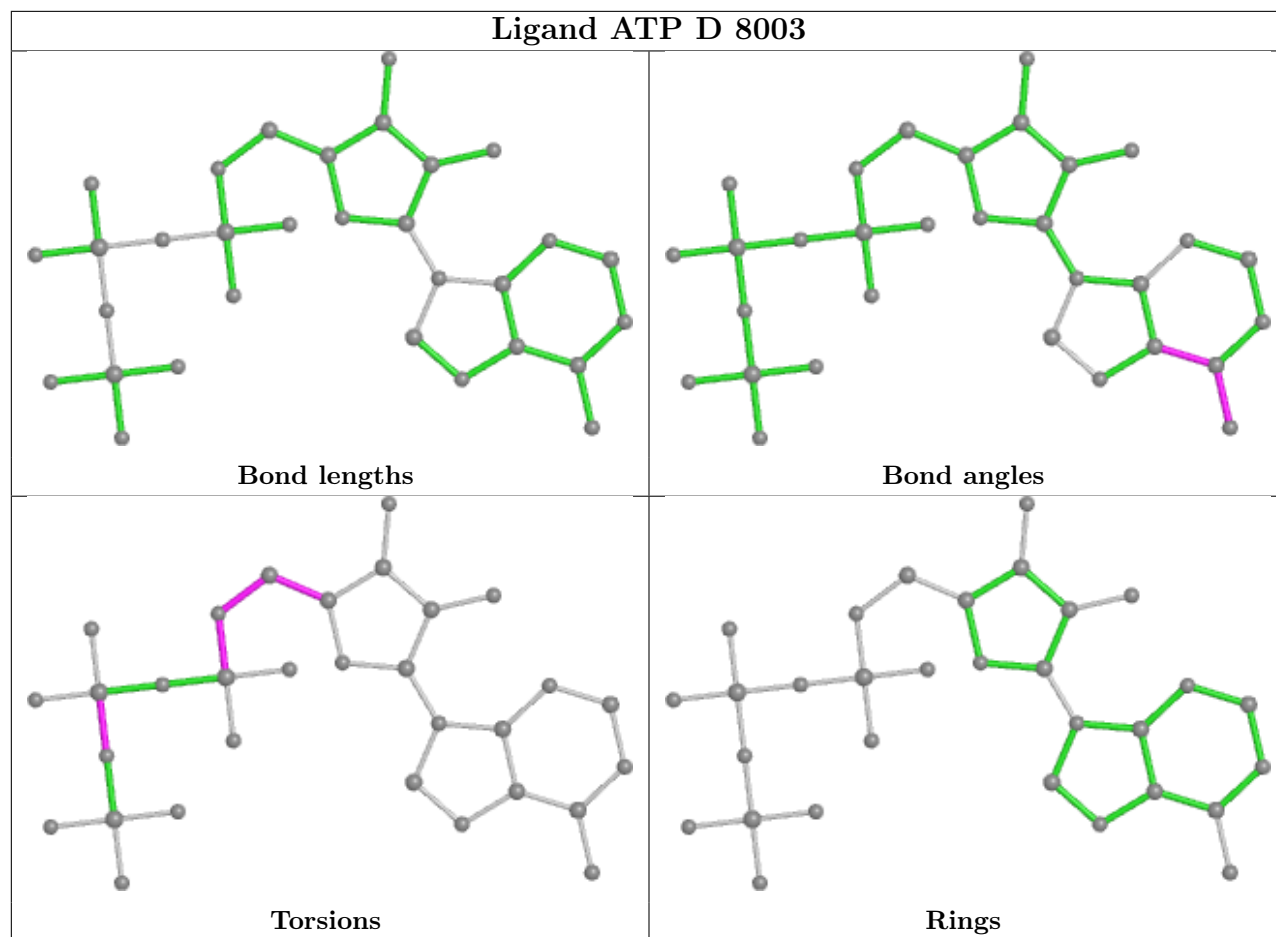












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

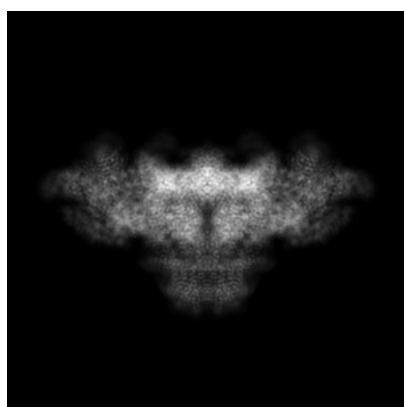
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43304. These allow visual inspection of the internal detail of the map and identification of artifacts.

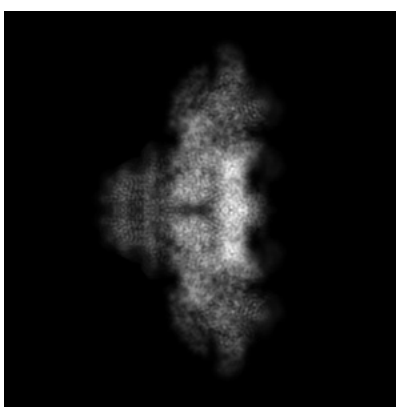
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

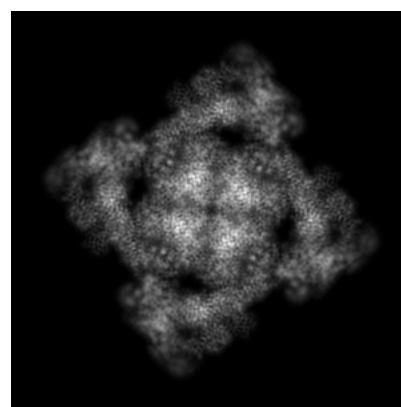
6.1.1 Primary map



X



Y



Z

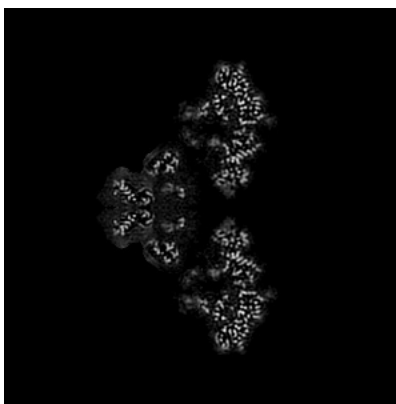
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

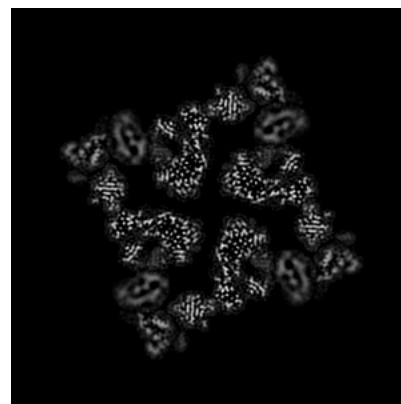
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

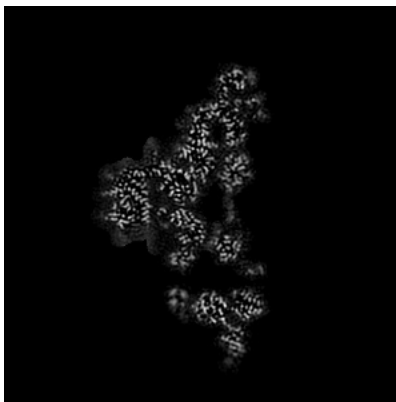
The images above show central slices of the map in three orthogonal directions.

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

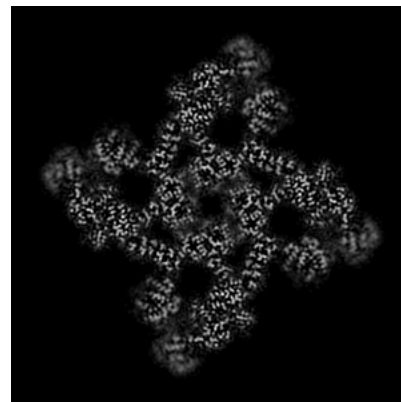
6.3.1 Primary map



X Index: 274



Y Index: 274

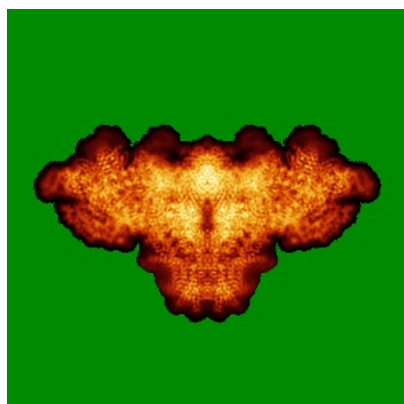


Z Index: 285

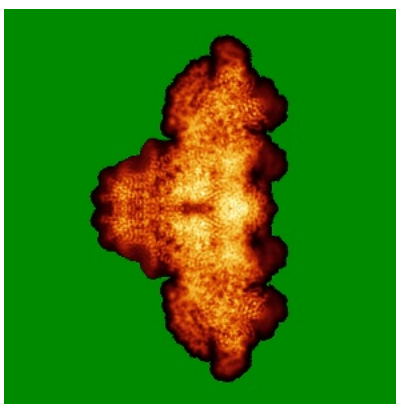
The images above show the largest variance slices of the map in three orthogonal directions.

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

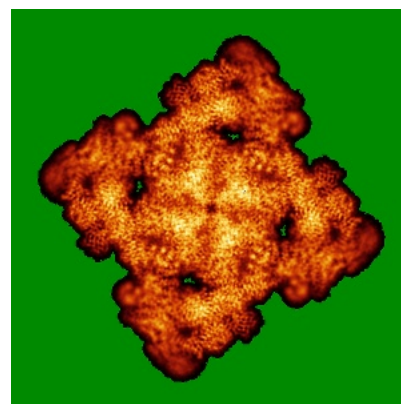
6.4.1 Primary map



X



Y

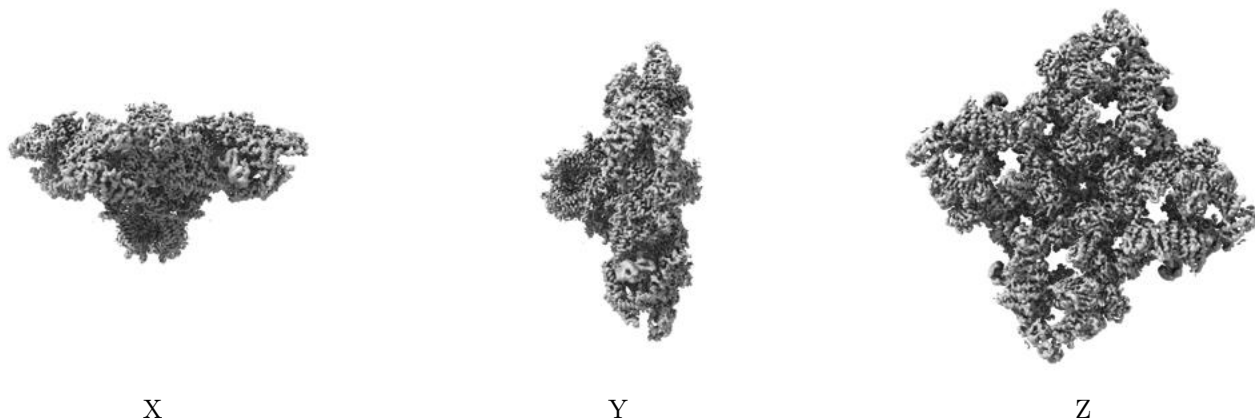


Z

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

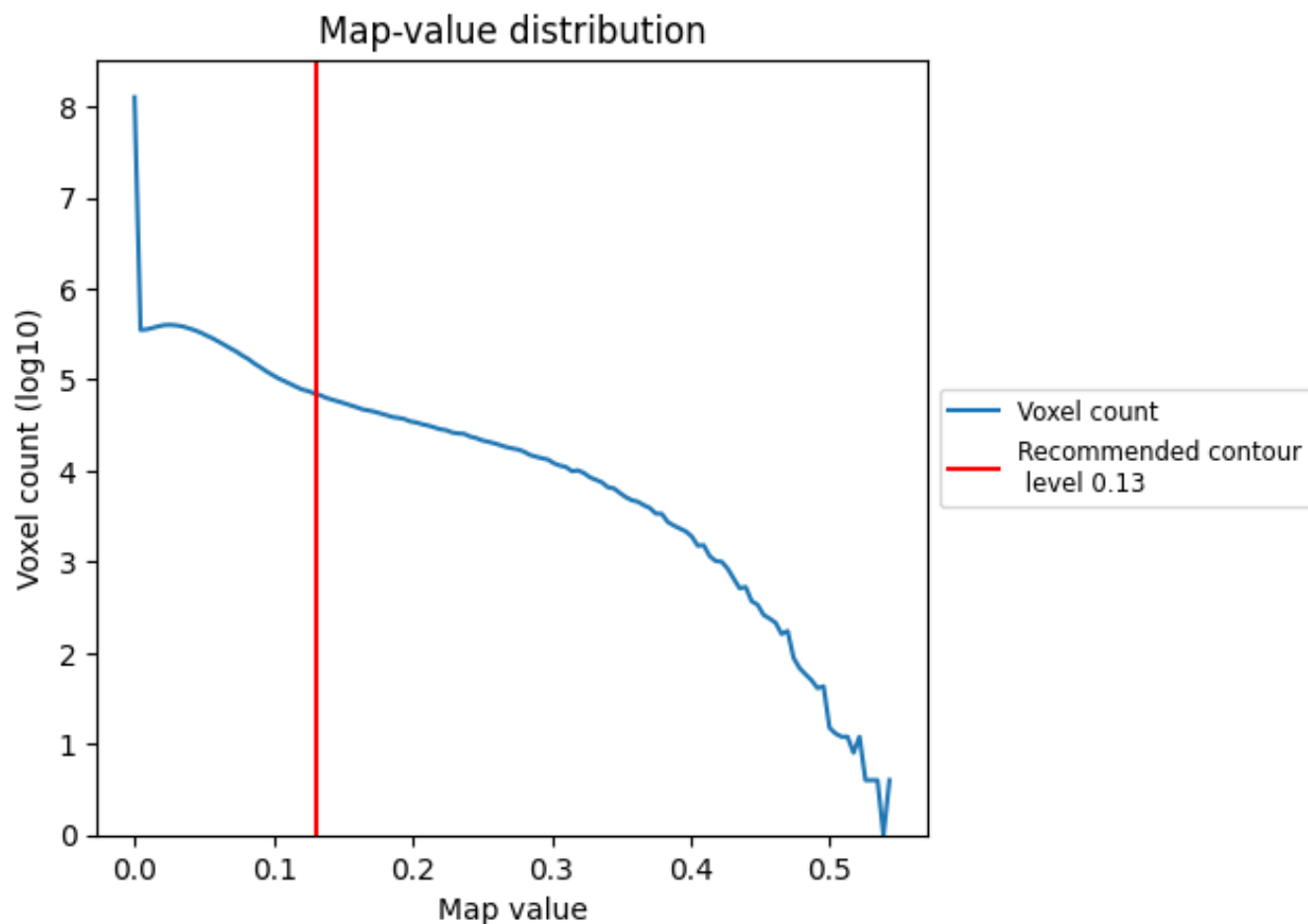
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

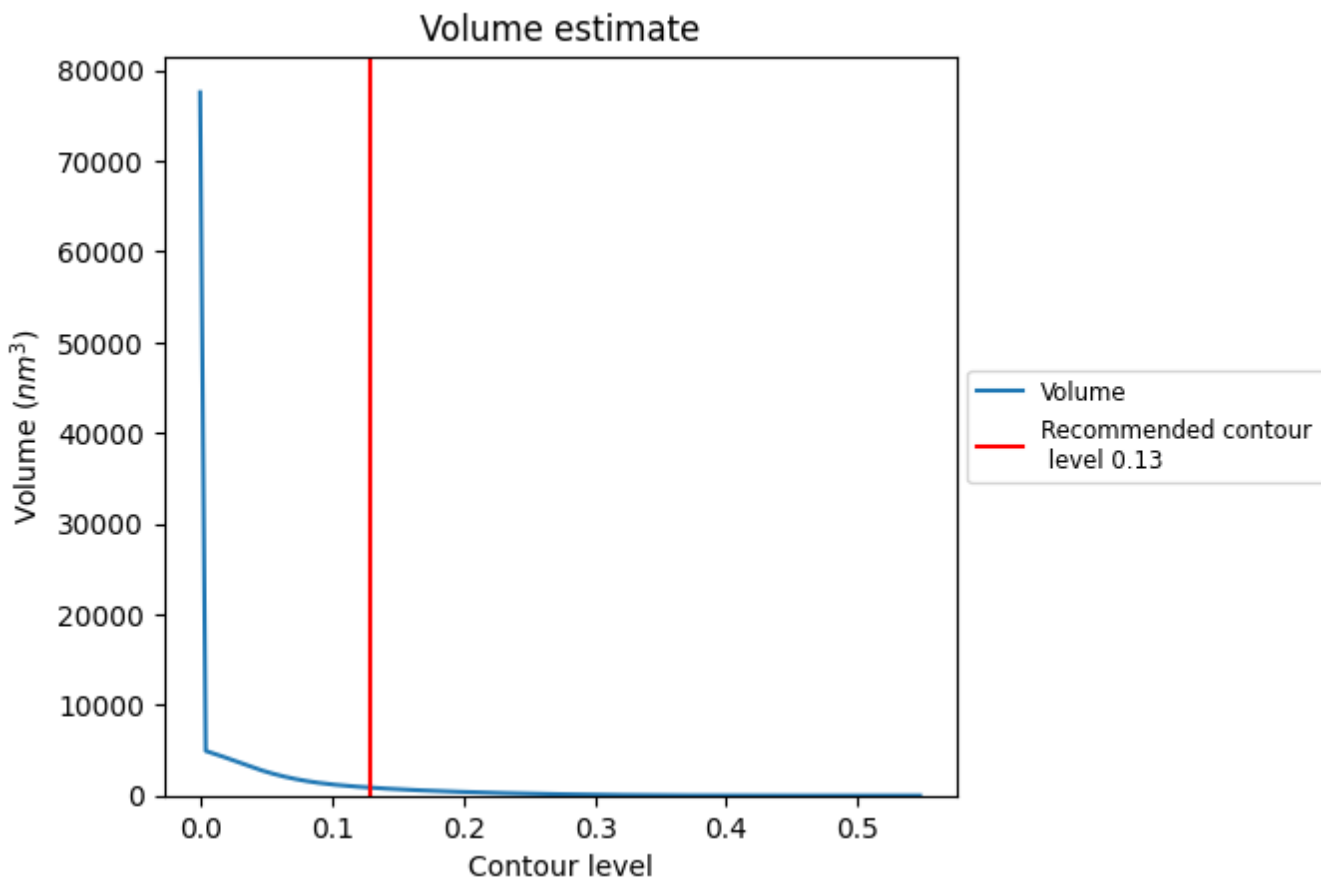
This section contains the results of statistical analysis of the map.

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.

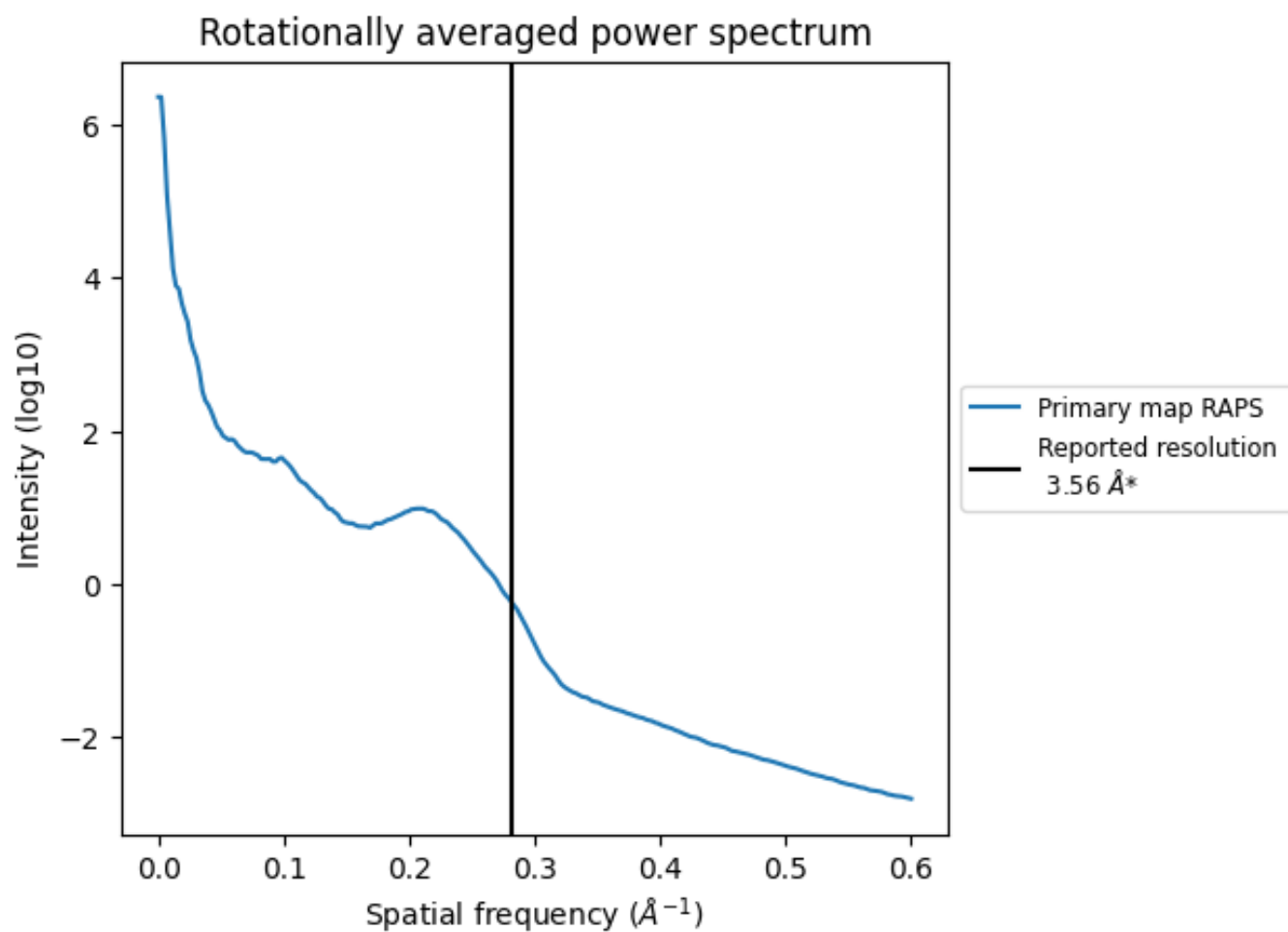
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 870 nm³; this corresponds to an approximate mass of 786 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

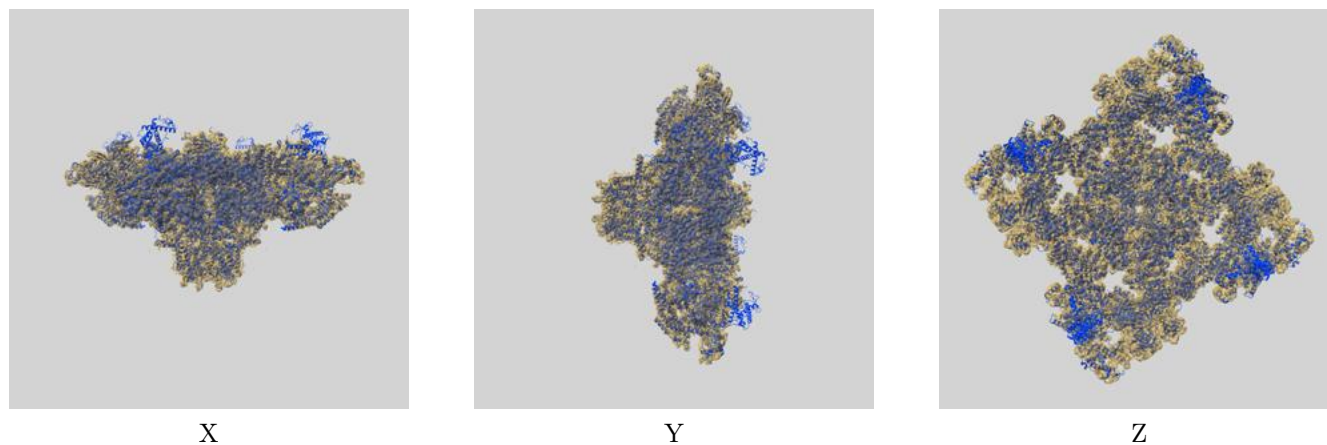
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

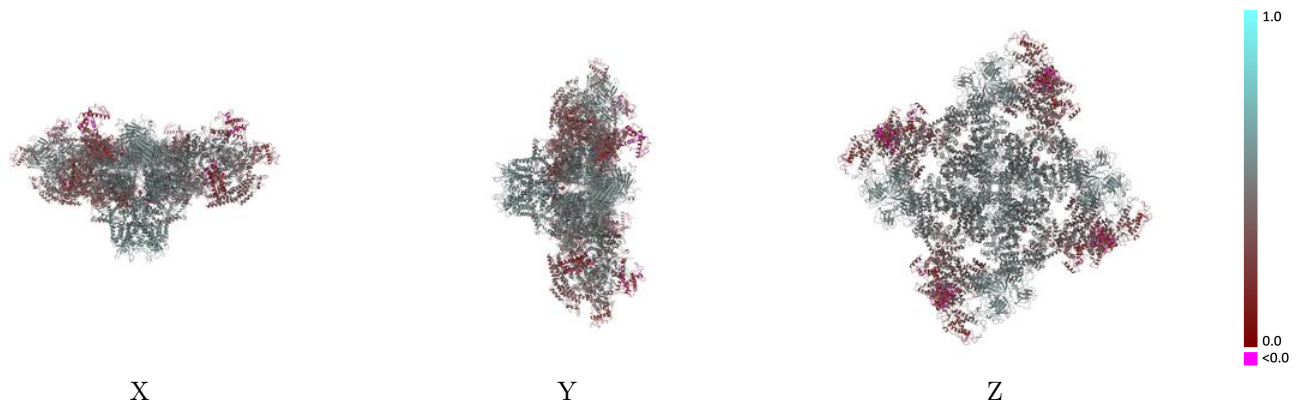
This section contains information regarding the fit between EMDB map EMD-43304 and PDB model 8VK4. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



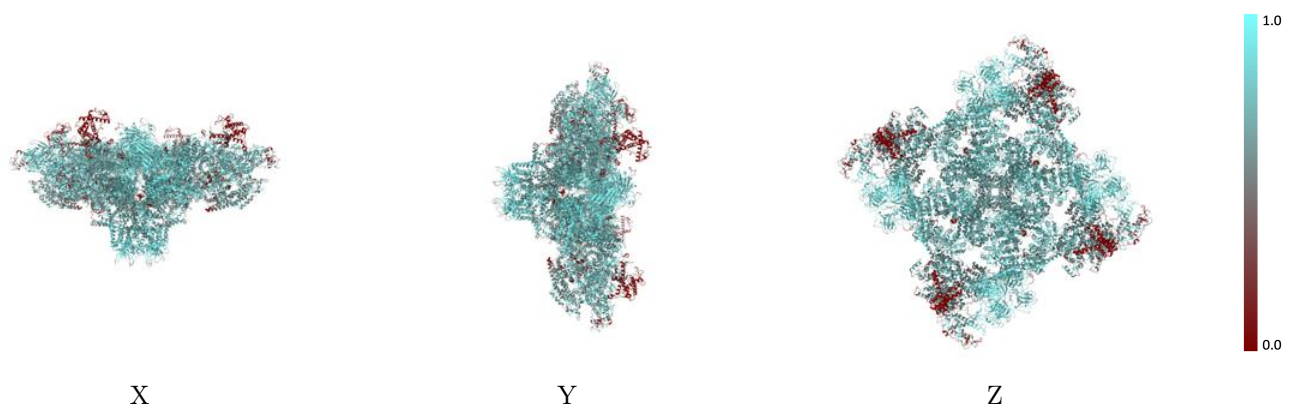
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



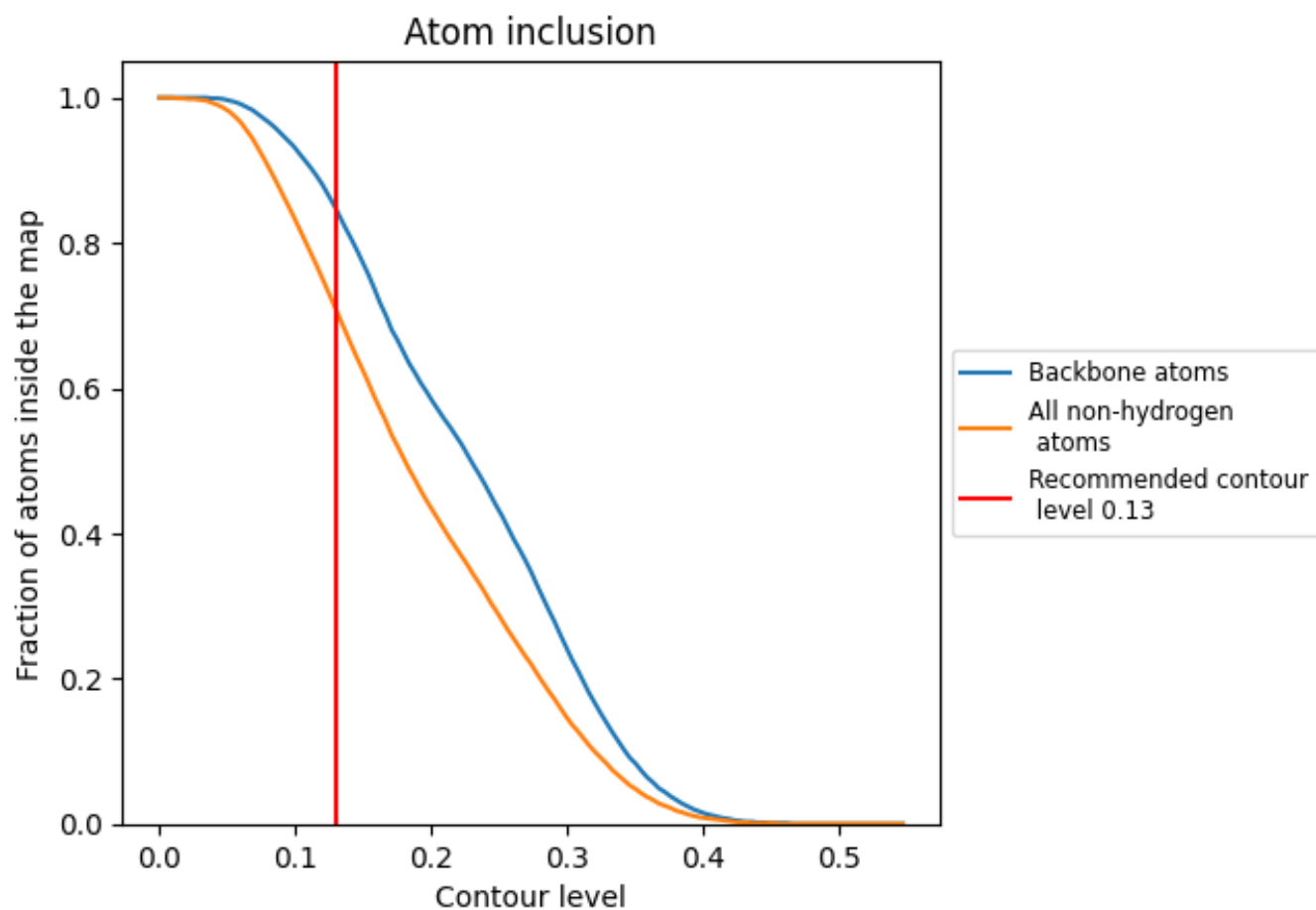
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4400
A	 0.7140	 0.4500
B	 0.7140	 0.4490
C	 0.7140	 0.4500
D	 0.7140	 0.4500
E	 0.7630	 0.5070
F	 0.7700	 0.5060
G	 0.7670	 0.5050
H	 0.7690	 0.5070
I	 0.4960	 0.1660
J	 0.5800	 0.1760
K	 0.4990	 0.1680
L	 0.5820	 0.1770
M	 0.5000	 0.1690
N	 0.5820	 0.1790
O	 0.4970	 0.1650
P	 0.5810	 0.1770

