



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:03 PM UTC

PDB ID : 9E1G / pdb_00009e1g
EMDB ID : EMD-47393
Title : Structure of RyR1 in the primed state in the presence of oxypurinol
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.17 Å(reported)
Based on initial model : 7TZC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

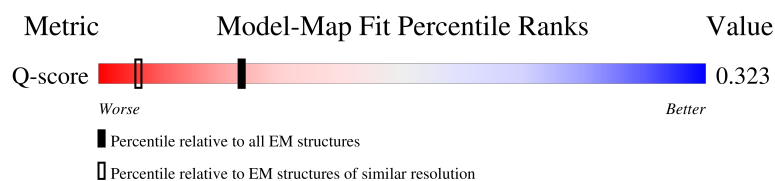
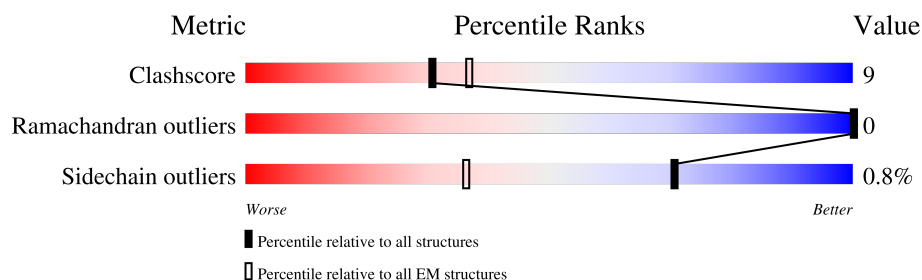
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.17 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	14465 (2.67 - 3.67)

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	5037	40% 70% 17% 13%
1	B	5037	40% 70% 17% 13%
1	C	5037	40% 69% 18% 13%
1	D	5037	40% 69% 18% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	66% 69% 29% ..
2	F	108	66% 77% 21% ..
2	G	108	65% 71% 27% ..
2	H	108	65% 74% 22% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144104 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.

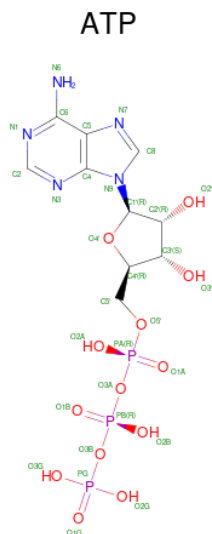
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	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
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

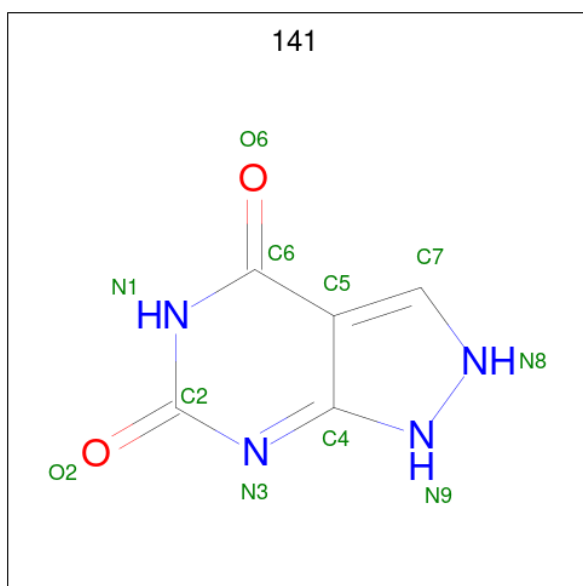
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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

- Molecule 6 is Oxypurinol (CCD ID: 141) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	D	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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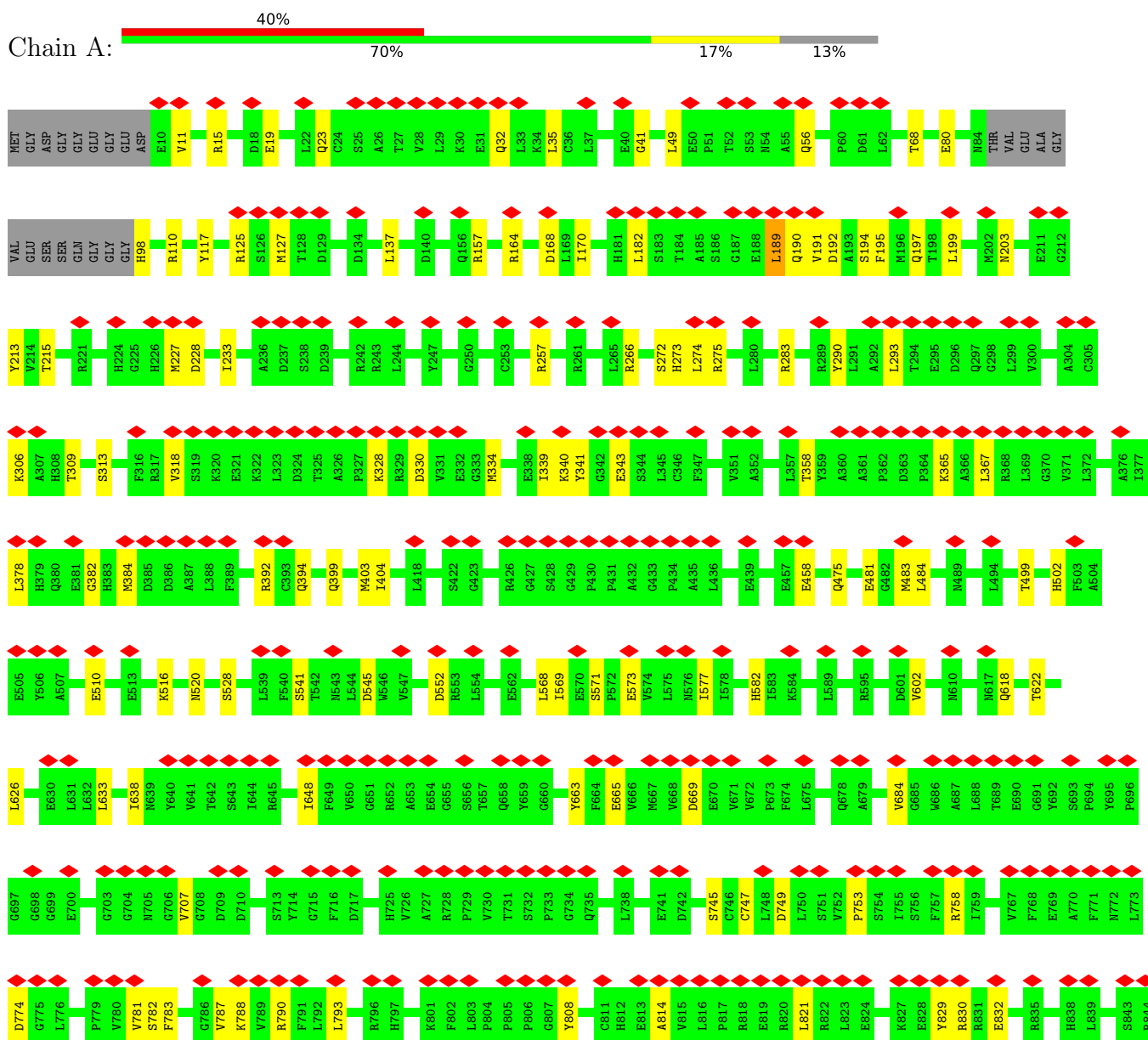
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Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	O	0
			1	1	
7	C	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

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

• Molecule 1: Ryanodine receptor 1



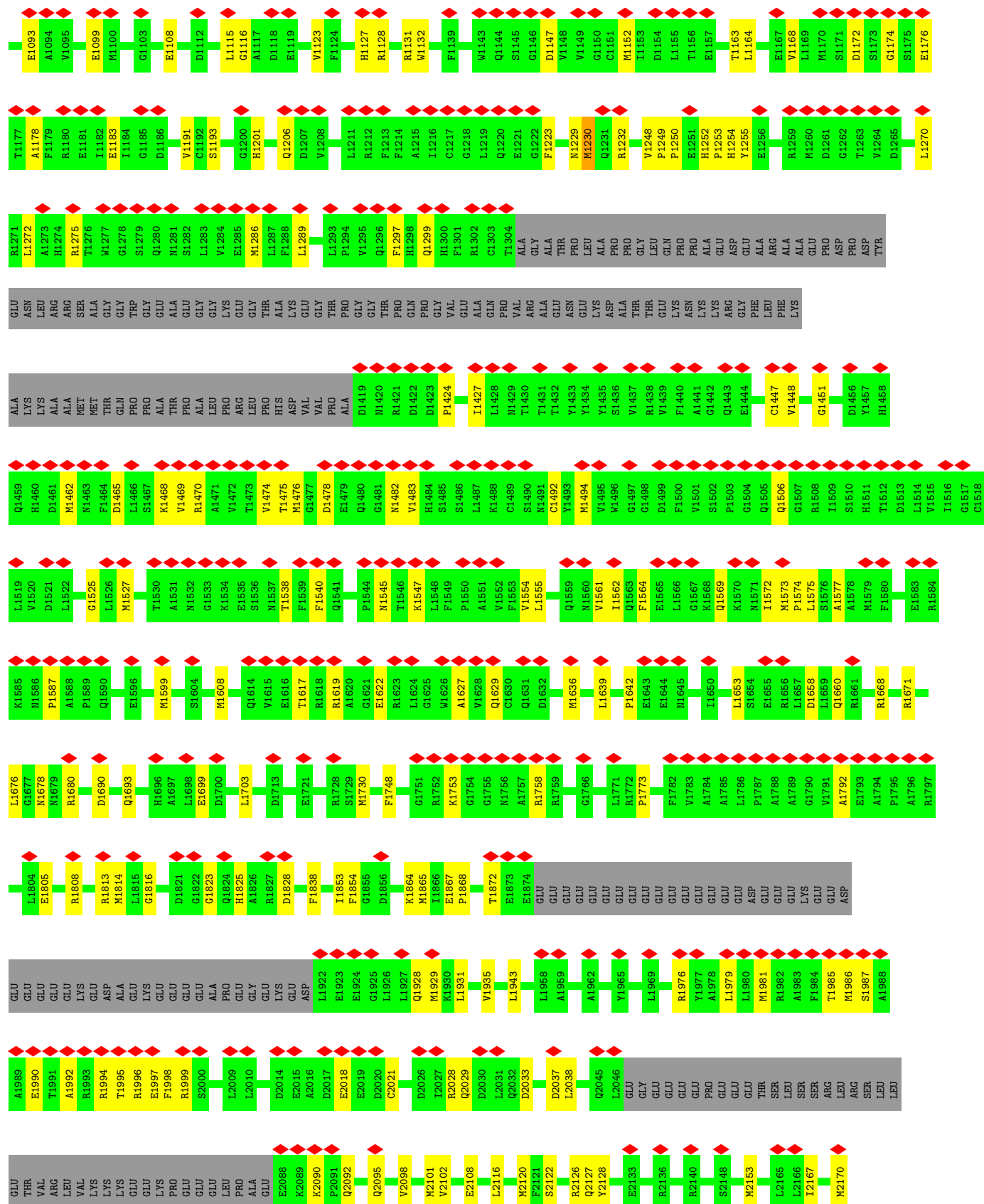
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PROTEIN DATA BANK

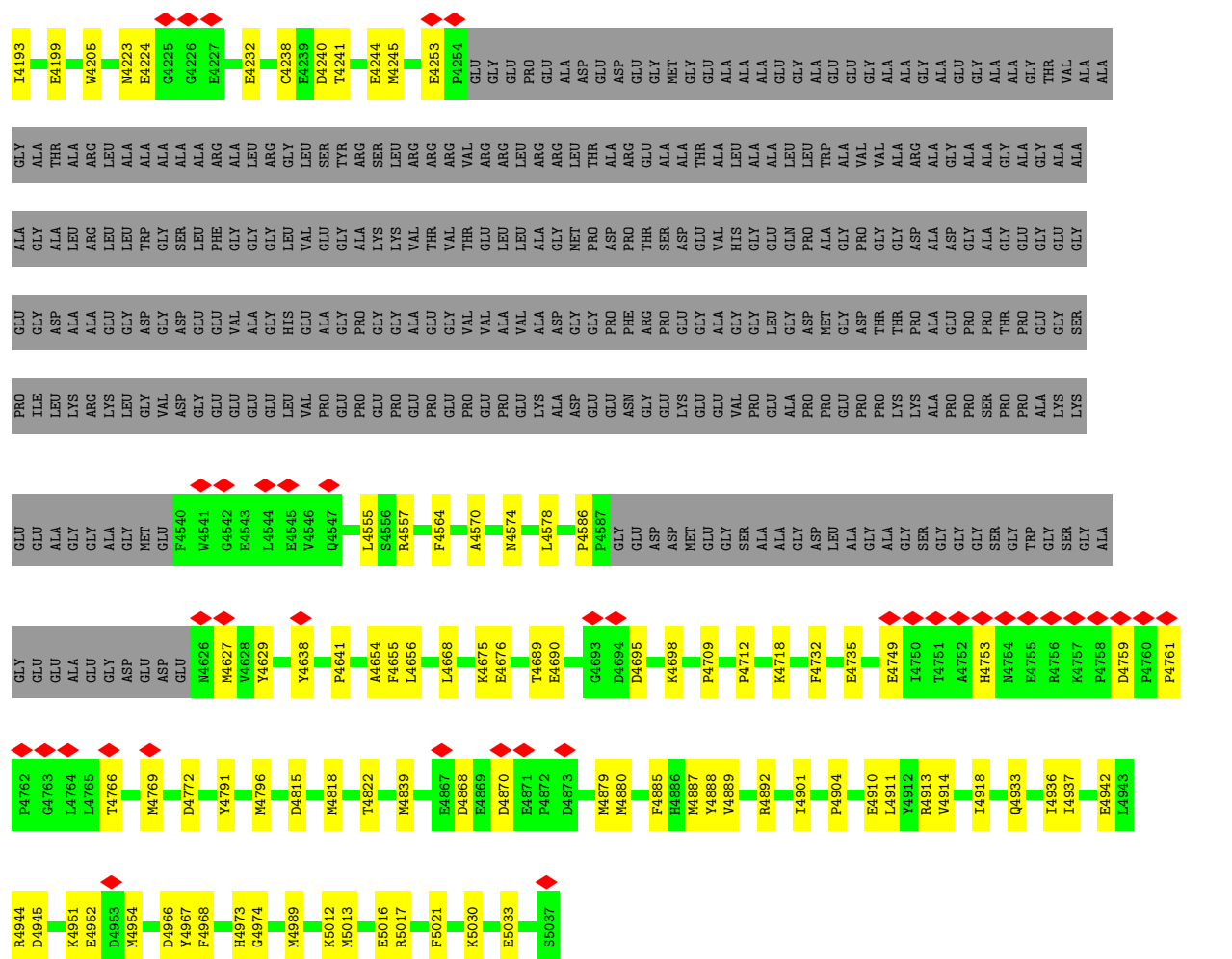




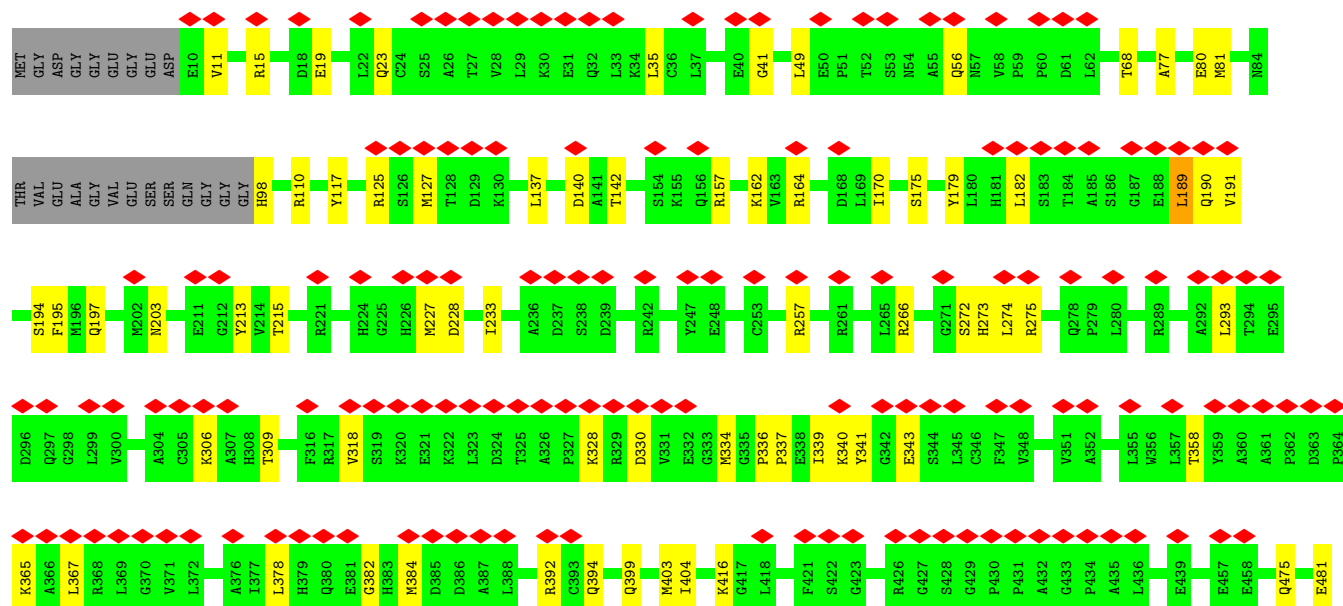
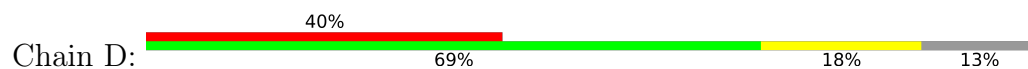


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G3058	P2998	T2937	I2817	F2758	I2817	F2758	R2697	A2637	R2575	P2410	GLU	
T3059	A2999	T2938	W2818	A2759	W2818	E2760	M2698	K2638	I2577	P2411	P2410	
D3060	K3000	R2939	E2820	E2760	E2820	Y2761	M2700	W2639	M2578	E2412	R2228	
A3061	I3001	GLY	W2821	T2762	W2821	T2762	P2701	P2640	I2579	E2413	T2230	
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A3072	T3011	E2952	GLU	Q2772	E2952	Q2772	P2712	C2651	S2590		C2363	
H3073	H3013	K2953	ARG	L2773	K2953	L2773	D2713		R2591		F2364	
S3074	C3014	F2955	THR	M2774	F2955	M2774	G2714	H2520	Q2435		G2365	
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F3017	F3017	G2958	LVS	Y2777	F2958	Y2777	T2718	D2523	P2438		Q2262	
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T3020	T3020	Q2961	LVS	W2780	T2961	W2780	Y2719	F2596	L2442		L2265	
P3021	P3021	Q2962	ILE	V2781	P2962	V2781	R2600	A2598	E2449		L2266	
A3022	A3022	L2963	GLN	D2782	A2963	D2782	L2603	Q2599	L2460		G2372	
K3023	K3023	L2964	THR	E2783	K2964	E2783	E2604	F2596			G2373	
G3024	G3024	R2965	ALA	E2784	G2965	E2784	D2605	G2606			G2374	
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E3086	E3086	M2967	THR	K2786	E2967	K2786	K2725				L2376	
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D4018	L3866	L3735	E3630	L3569	L3509	H3449	E3389	I3329	V3289	Q3209	Q3149	K3089
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F3880	F3640	GLU	F3640	L3579	P3519	V3460	S3399	A3339	S3279	F3219	D3159	A3099
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W3934	D3866	GLU	D3866	T3528	T3528	F3469	L3408	R3348	G3288	A3228	T3168	E3108
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R3769	D3671	GLU	D3671	Q3530	Q3530	T3471	P3410	R3350	E3290	C3170	L3110	L3110
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S3803	G3681	GLU	G3681	R3594	M3534	K3475	R3414	L3354	P3294	M3234	S3174	K3114
D3822	Q3682	GLU	Q3682	R3595	L3535	S3476	Y3415	H3355	A3295	S3235	L3175	V3115
M3836	E3684	GLU	E3684	V3596	A3536	K3477	V3416	S3356	L3296	V3236	G3176	S3116
S3840	E3686	GLU	E3686	Q3597	K3537	N3478	D3417	H3357	P3297	E3237	T3177	ALA
L3841	E3687	GLU	E3687	E3598	T3538	M3479	N3418	F3358	A3298	I3359	R3178	ARG
D3842	E3688	GLU	E3688	R3599	R3539	A3479	N3419	P3360	G3299	K3179	THR	GLN
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L3844	V3607	GLU	V3607	L3603	A3541	GLY	A3421	I3362	P3241	T3181	K3123	K3123
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E3861	L3716	GLU	E3861	E3612	E3551	THR	A3431	K3371	D3310	M3250	G3191	T3132
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V3865	D3717	GLU	V3865	K3617	M3556	G3500	R3436	E3377	L3316	G3255	R3196	L3136
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M3729	M3729	GLU	M3729	W3620	L3559	R3502	E3439	R3380	T3319	E3258	A3198	V3139
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H3734	H3734	GLU	H3734	K3622	G3561	V3505	T3441	E3382	R3321	A3261	A3200	T3141
				L3624	K3562	Q3506	F3442	A3383	T3322	R3262	M3201	T3142
				S3625	V3563	T3507	T3443	K3384	Y3324	Y3263	V3203	L3143
				E3664	E3564	S3508	Y3444	A3385	N3325	T3264	A3204	F3144
				G3565	G3565		W3445	E3386	N3326	E3265	F3205	Q3145
				P3567	P3567		S3446	A3387	L3327	M3266	L3206	H3146
				S3568	S3568		S3447	E3388	G3328	P3267	E3207	T3147
							S3448			H3268	P3208	A3148



• Molecule 1: Ryanodine receptor 1

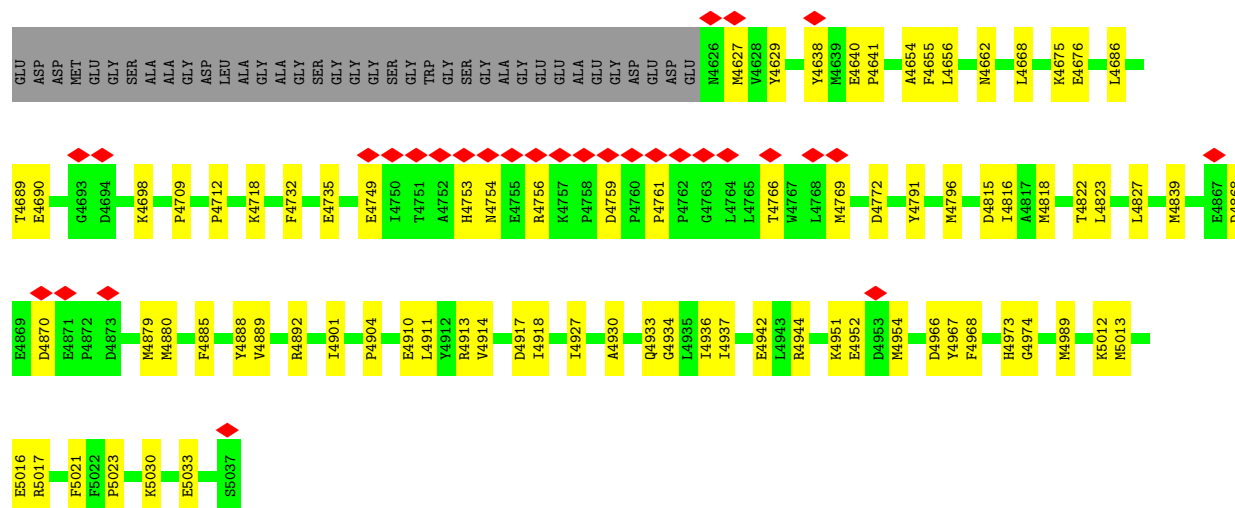




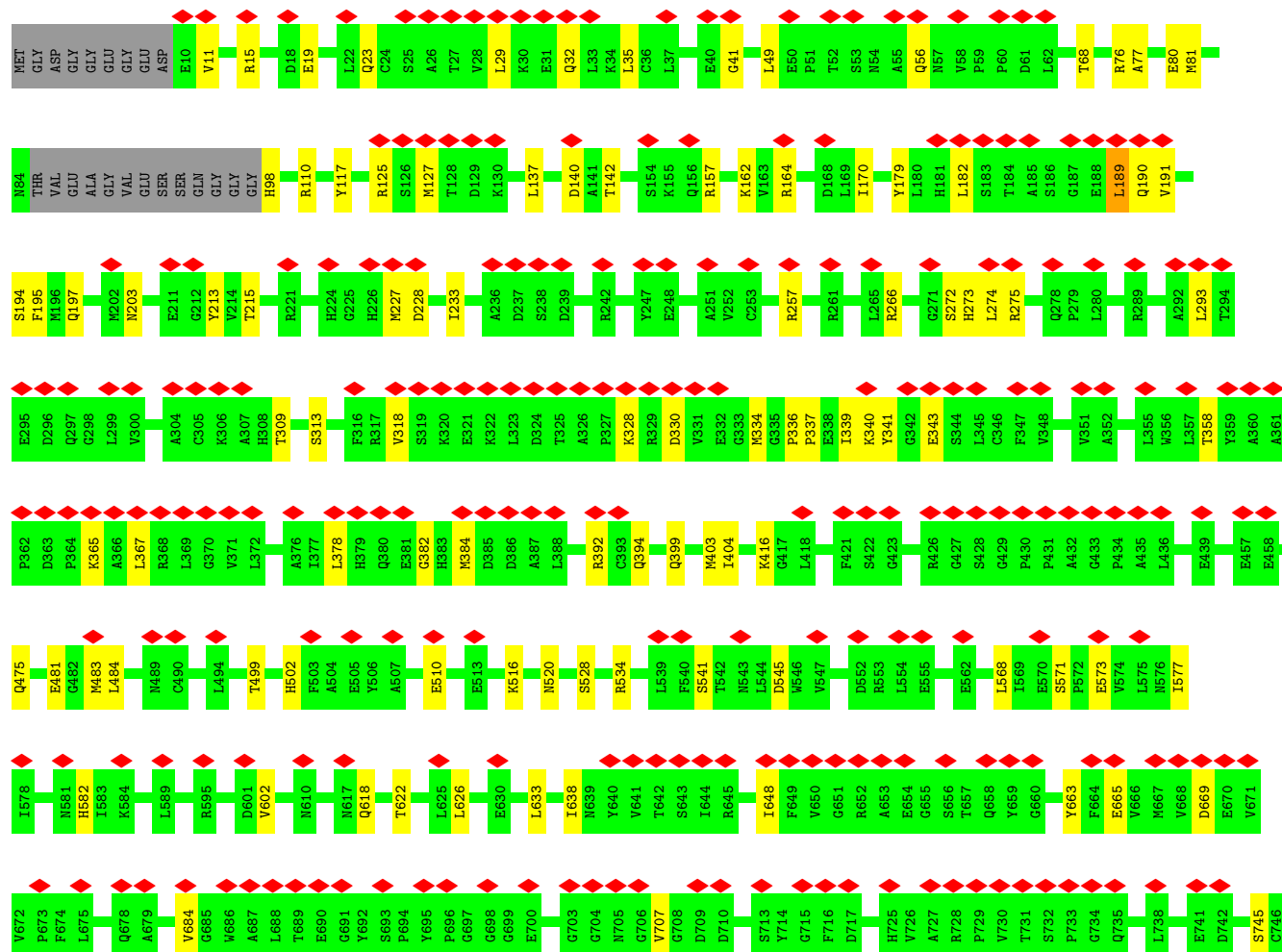
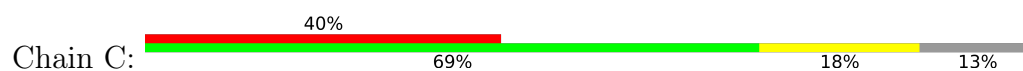
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D2523	A2437	P2366	R2148	GLU	A1788	D1657	S1576	S1510	V1448
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R3287	R3227	V3107	R3167	V3107	A3047	E2987	L2926	Q2872	R2806	T2748	H2688	V2627
G3288	A3228	E3108	L3169	E3108	A3048	K2988	L2927	A2873	W2807	E2749	K2689	F2628
P3289	T3229	N3109	L3170	N3109	L3049	S2989	K2928	M2874	P2808	K2750	K2690	D2629
E3290	G3230	L3110	C3170	L3110	V3050	P2990	F2929	A2875	I2809	L2751	Y2691	V2630
A3291	G3231	R3111	S3171	R3111	R3051	H2991	L2930	E2876	K2810	D2752	P2631	P2631
P3292	L3232	G3112	F3173	G3112	H3052	E2992	Q2931	Q2877	E2811	S2753	Q2693	L2632
L3293	P3233	G3113	V3173	G3113	R3053	Q2993	W2932	L2878	S2812	F2754	E2694	L2633
P3294	N3234	K3114	S3174	K3114	V3054	E2994	G2934	A2879	L2813	I2755	L2695	M2634
A3295	S3235	V3115	L3175	V3115	S3055	I2995	Y2935	N2881	A2815	K2756	Y2696	E2635
L3296	V3236	GLN	G3176	GLN	L3056	K2996	A2936	N2882	M2816	K2757	R2697	F2636
P3297	E3237	ALA	T3177	ALA	F3057	F2997	V2937	H2883	I2817	F2758	M2698	A2637
L3298	G3238	ARG	T3178	ARG	G3058	F2998	T2938	H2884	A2818	A2759	K2638	K2638
G3299	E3239	THR	K3179	THR	T3059	A2999	N2884	T2885	W2819	E2760	M2700	M2639
A3300	M3239	GLN	D3060	GLN	D3060	K3000	GLY	W2886	E2820	Y2761	P2701	P2640
P3301	C3240	VAL	T3181	VAL	A3061	I3001	LEU	T2887	T2762	T2762	C2702	L2641
L3302	P3241	K3123	Y3182	K3123	P3062	L3002	LYS	G2887	H2763	L2703	C2703	K2642
R3303	D3242	G3124	V3183	G3124	A3063	L3003	ASP	R2888	E2764	K2765	C2704	L2643
C3304	I3243	V3125	I3184	V3125	V3064	P3004	MET				A2705	L2644
L3305	P3244	G3126	K3185	G3126	V3065	L3005	GLU				L2706	T2645
S3306	V3245	Q3127	L3186	Q3127	N3066	I3006					A2707	H2646
A3307	L3246	N3128	F3187	N3128	C3067	N3007					G2708	
L3308	D3247	R3248	P3188		L3068	Q3008						





• Molecule 1: Ryanodine receptor 1

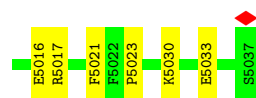




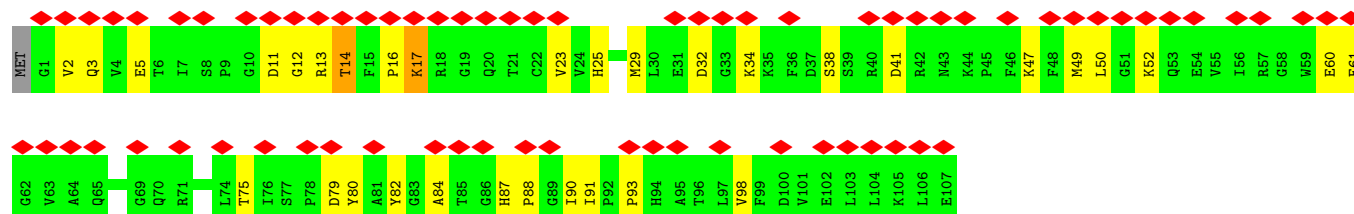




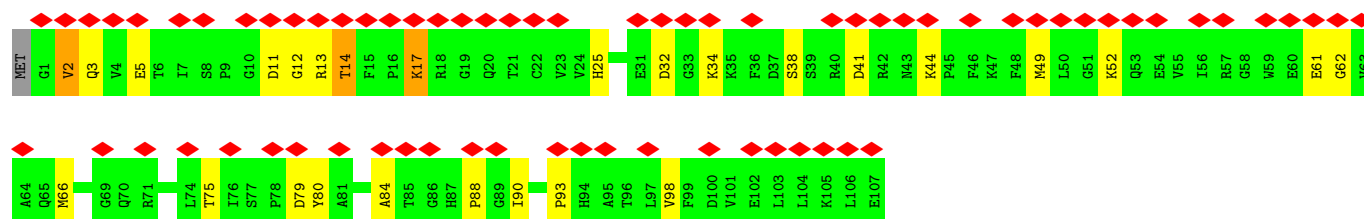
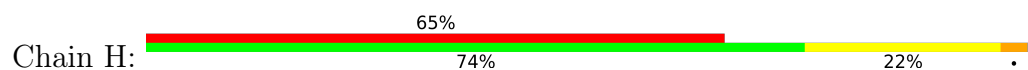




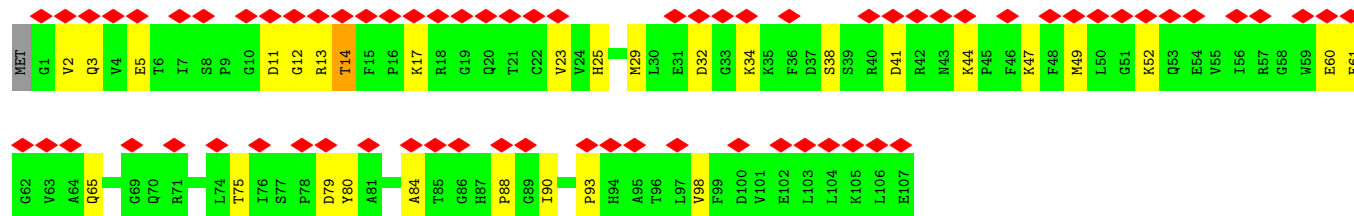
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



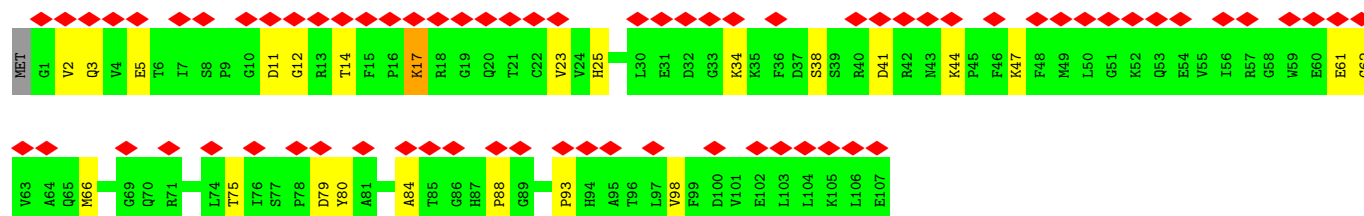
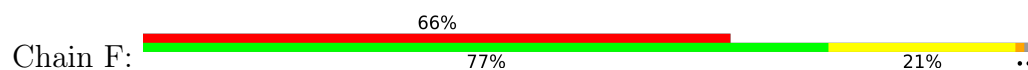
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17393	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	0.436	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.288, 428.288, 428.288	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8365, 0.8365, 0.8365	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, 141, 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	0.29	0/35977	0.38	1/48726 (0.0%)
1	B	0.29	0/35977	0.38	1/48726 (0.0%)
1	C	0.29	0/35977	0.38	1/48726 (0.0%)
1	D	0.29	0/35977	0.38	1/48726 (0.0%)
2	E	0.30	0/850	0.43	0/1146
2	F	0.27	0/850	0.40	0/1146
2	G	0.28	0/850	0.40	0/1146
2	H	0.29	0/850	0.41	0/1146
All	All	0.29	0/147308	0.38	4/199488 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3239	MET	CB-CG-SD	7.01	133.72	112.70
1	A	3239	MET	CB-CG-SD	7.00	133.71	112.70
1	C	3239	MET	CB-CG-SD	7.00	133.69	112.70
1	B	3239	MET	CB-CG-SD	6.99	133.67	112.70

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	A	35150	0	34797	630	0
1	B	35150	0	34797	622	0
1	C	35150	0	34797	648	0
1	D	35150	0	34797	650	0
2	E	831	0	831	25	0
2	F	831	0	831	18	0
2	G	831	0	831	23	0
2	H	831	0	831	21	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	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	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	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144104	0	142576	2538	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2538 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:C:1573:MET:HE3	1:C:1574:PRO:HD2	1.37	1.05
1:A:1573:MET:HE3	1:A:1574:PRO:HD2	1.37	1.03
1:D:1573:MET:HE3	1:D:1574:PRO:HD2	1.37	1.02
1:B:1573:MET:HE3	1:B:1574:PRO:HD2	1.37	1.02
1:B:3467:MET:HE1	1:C:1174:GLY:CA	1.99	0.93

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	4385/5037 (87%)	4246 (97%)	139 (3%)	0	100	100
1	B	4385/5037 (87%)	4245 (97%)	140 (3%)	0	100	100
1	C	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	D	4385/5037 (87%)	4246 (97%)	139 (3%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	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	17960/20580 (87%)	17392 (97%)	568 (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	A	3836/4276 (90%)	3808 (99%)	28 (1%)	76	81
1	B	3836/4276 (90%)	3808 (99%)	28 (1%)	76	81
1	C	3836/4276 (90%)	3808 (99%)	28 (1%)	76	81
1	D	3836/4276 (90%)	3807 (99%)	29 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	83 (93%)	6 (7%)	15	43
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	61
2	G	89/90 (99%)	84 (94%)	5 (6%)	19	48
2	H	89/90 (99%)	85 (96%)	4 (4%)	24	55
All	All	15700/17464 (90%)	15569 (99%)	131 (1%)	70	80

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1979	LEU
1	C	2577	ILE
1	C	4973	HIS
1	B	318	VAL
1	B	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	HIS
1	D	2342	ASN
1	C	3211	ASN
1	D	581	ASN
1	D	1640	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	141	D	5304	-	11,12,12	1.77	3 (27%)	11,17,17	0.97	0
6	141	A	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.97	0
3	ATP	D	5301	-	32,33,33	0.46	0	48,52,52	0.41	0
3	ATP	C	5301	-	32,33,33	0.45	0	48,52,52	0.40	0
6	141	C	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.98	0
3	ATP	B	5301	-	32,33,33	0.45	0	48,52,52	0.41	0
3	ATP	A	5301	-	32,33,33	0.45	0	48,52,52	0.41	0
6	141	B	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.97	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
6	141	D	5304	-	-	-	0/2/2/2
6	141	A	5304	-	-	-	0/2/2/2
3	ATP	D	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/22/38/38	0/3/3/3
6	141	C	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	A	5301	-	-	6/22/38/38	0/3/3/3
6	141	B	5304	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5304	141	C5-C4	-4.04	1.38	1.45
6	A	5304	141	C5-C4	-4.01	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5304	141	C5-C4	-3.99	1.38	1.45
6	D	5304	141	C5-C4	-3.99	1.38	1.45
6	B	5304	141	C7-N8	2.49	1.35	1.33

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

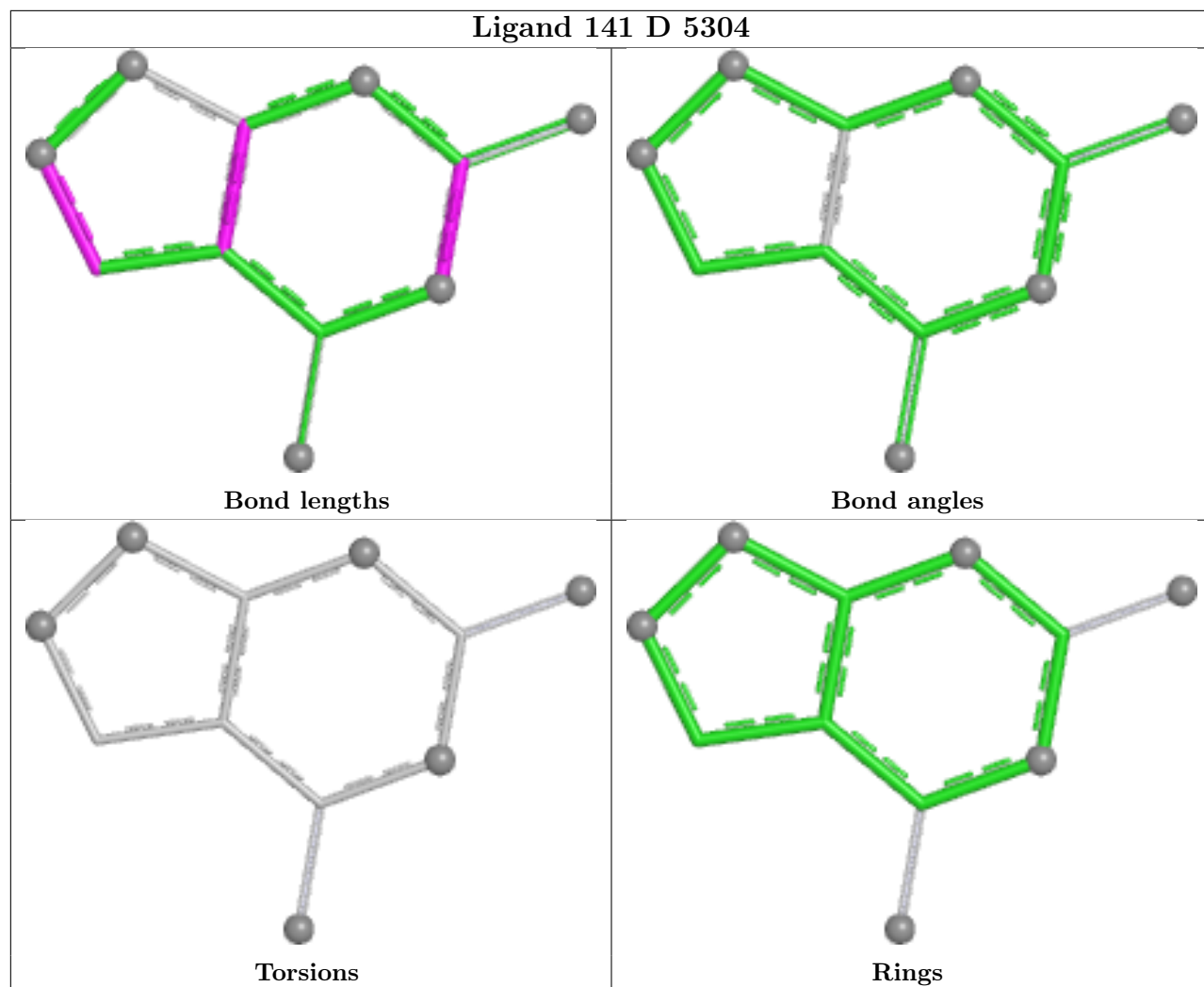
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O2G
3	B	5301	ATP	PB-O3B-PG-O2G
3	D	5301	ATP	PB-O3B-PG-O2G
3	C	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

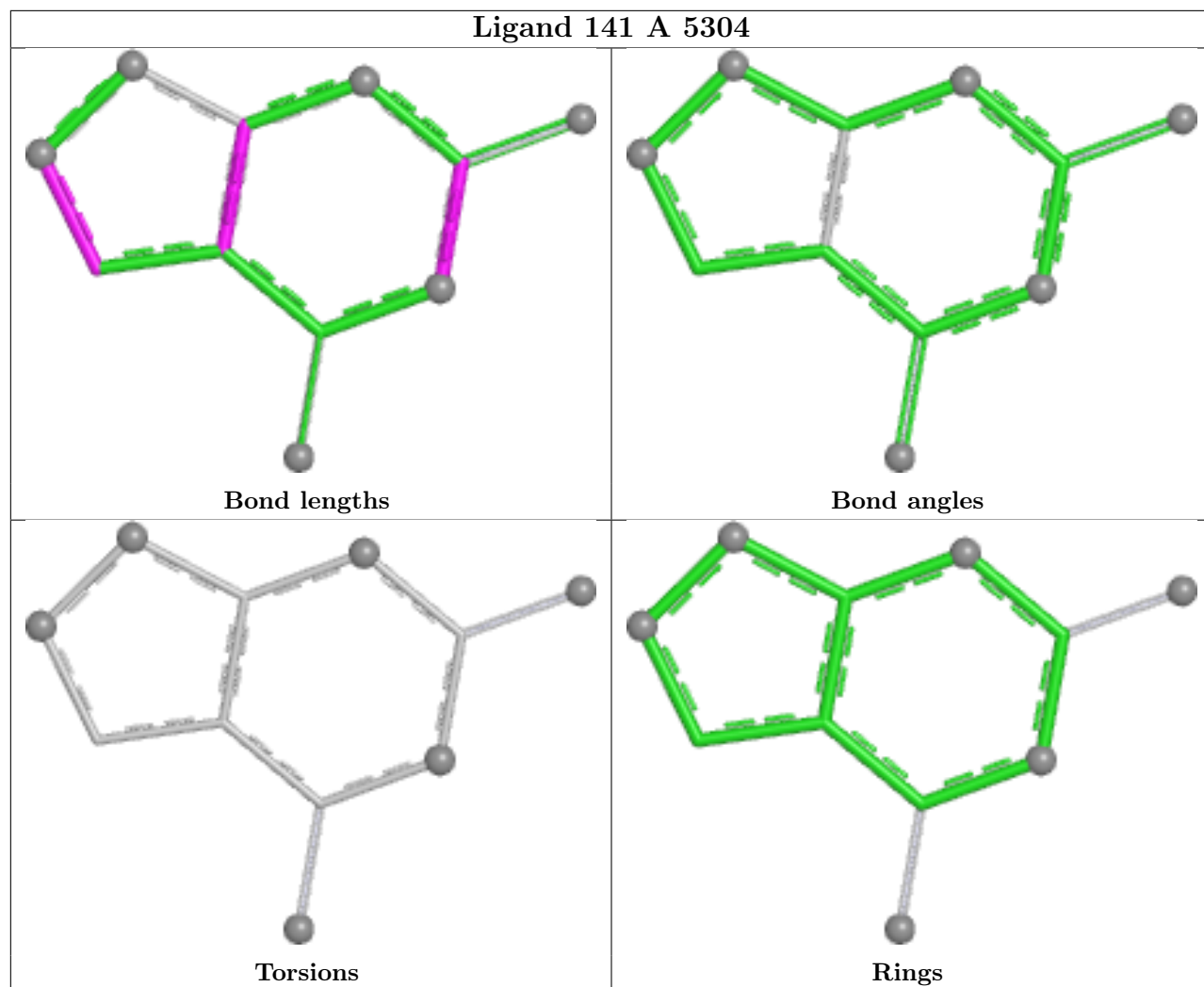
No monomer is involved in short contacts.

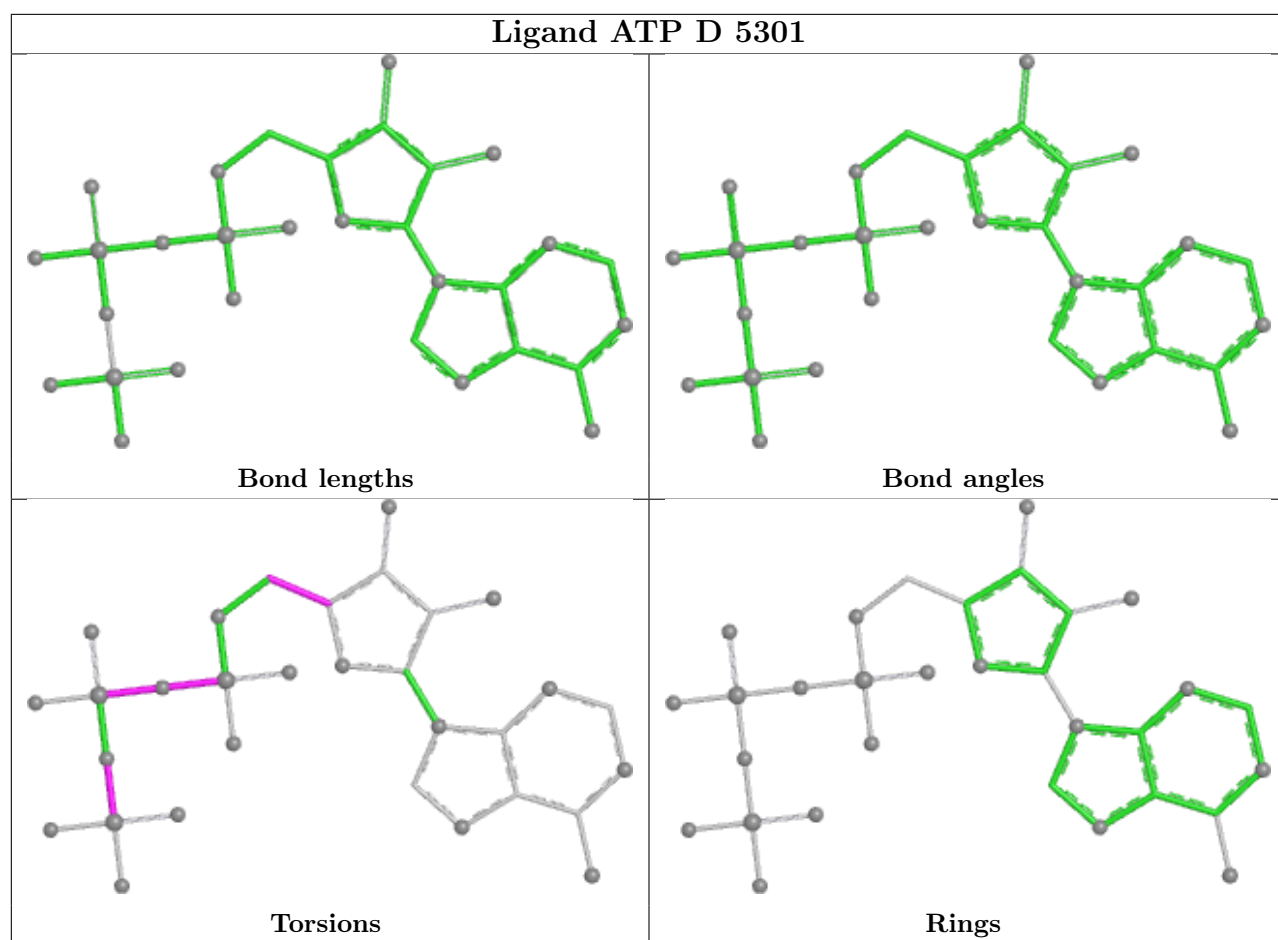
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

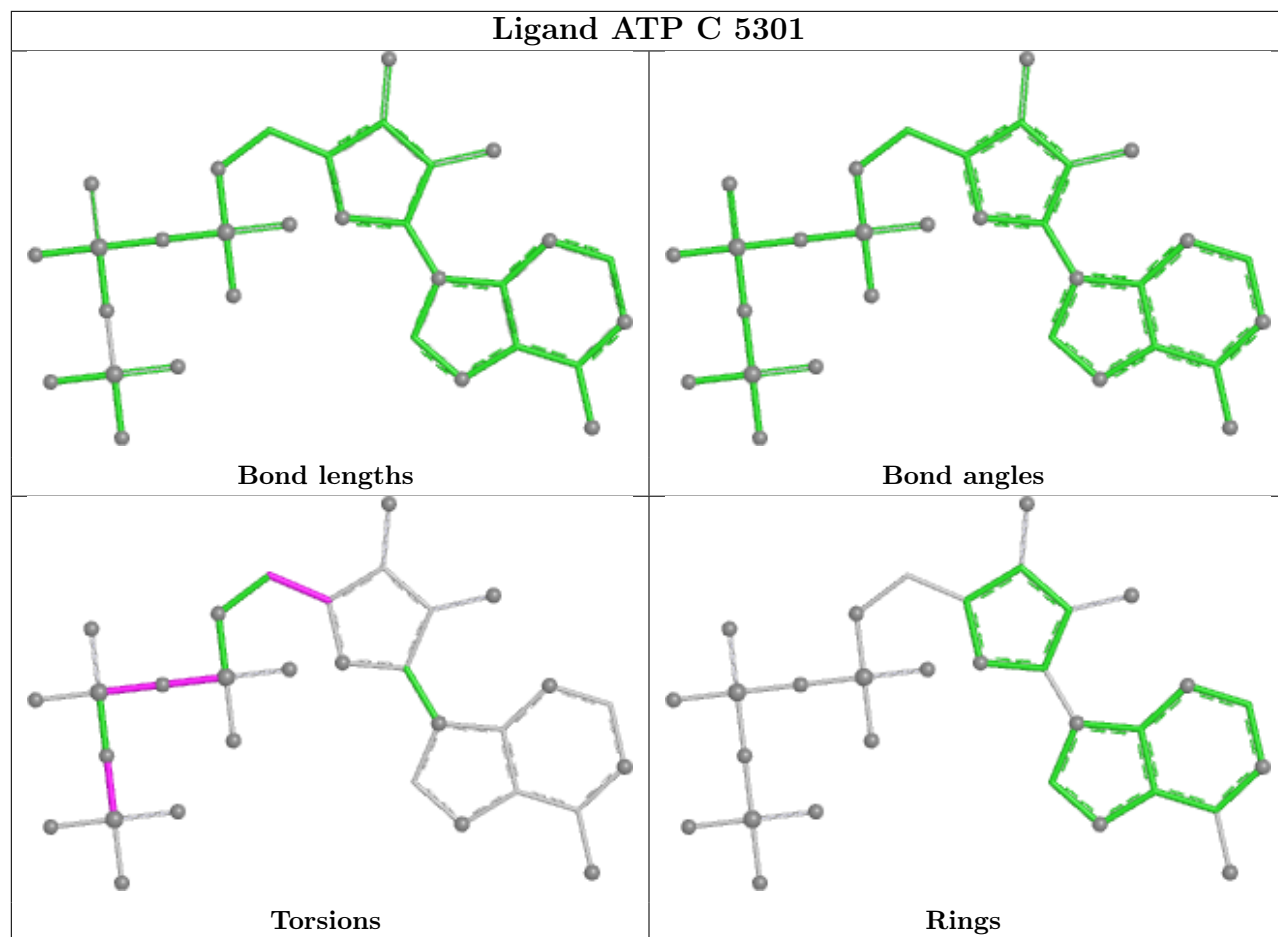
Ligand 141 D 5304



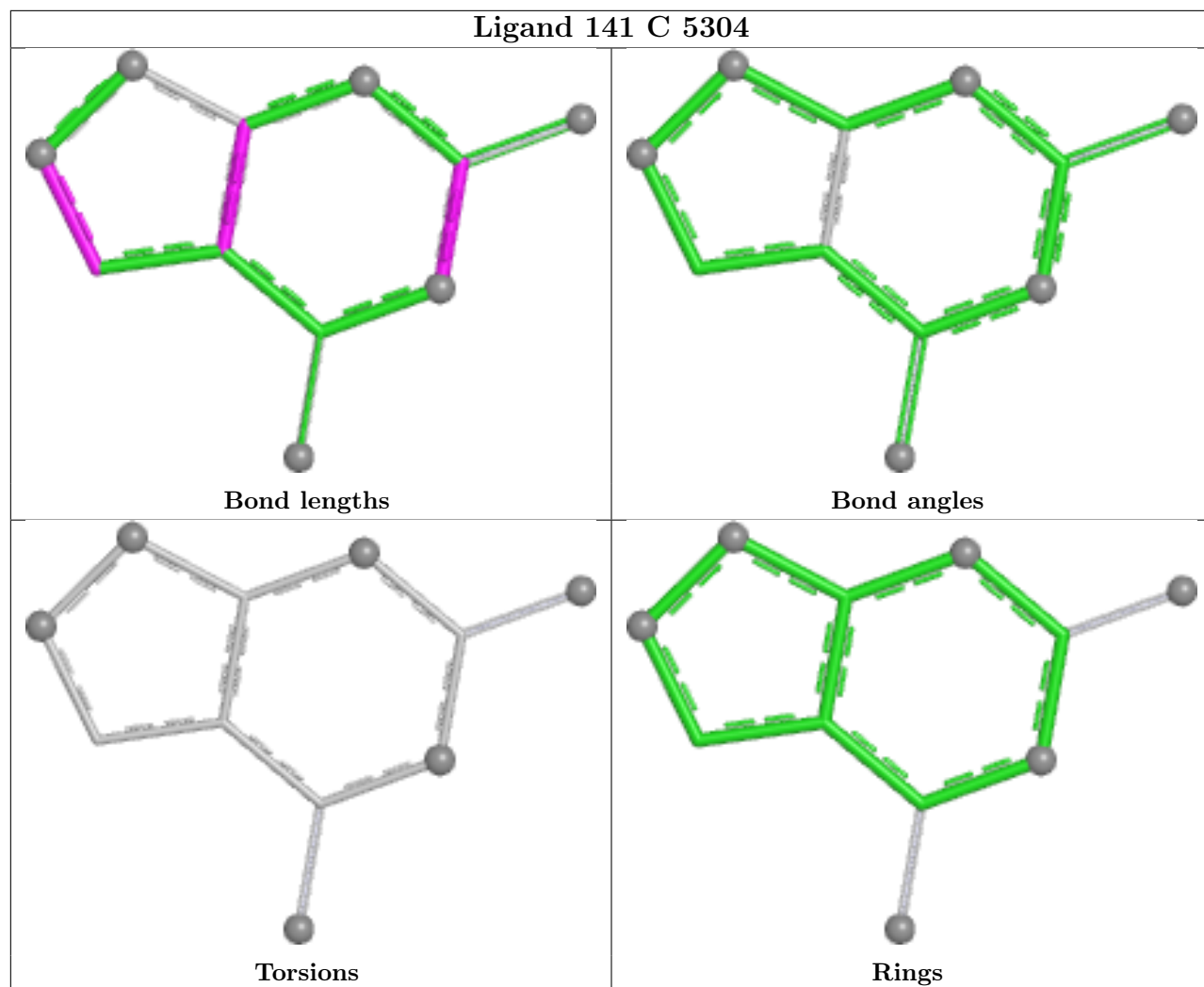
Ligand 141 A 5304

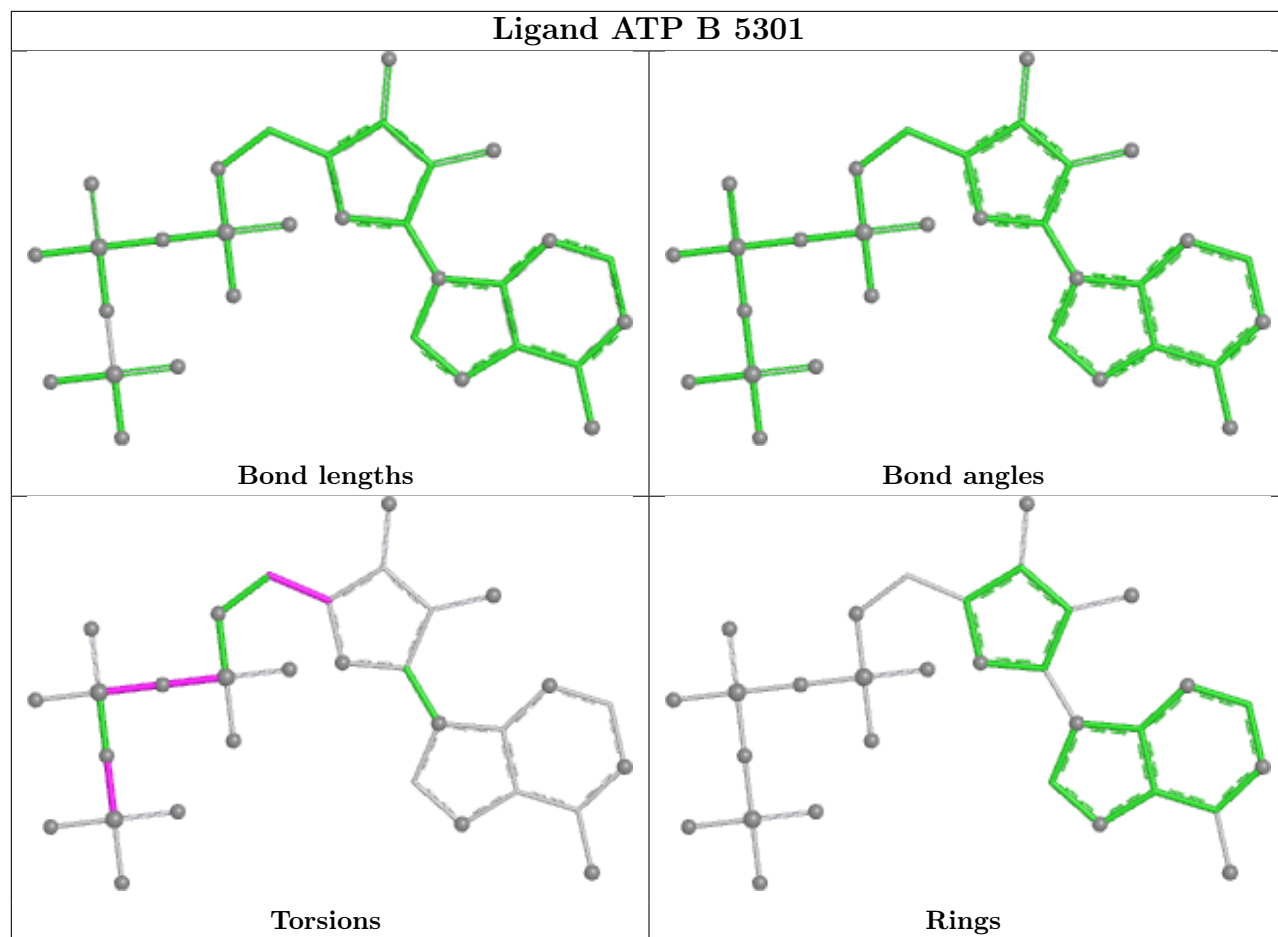


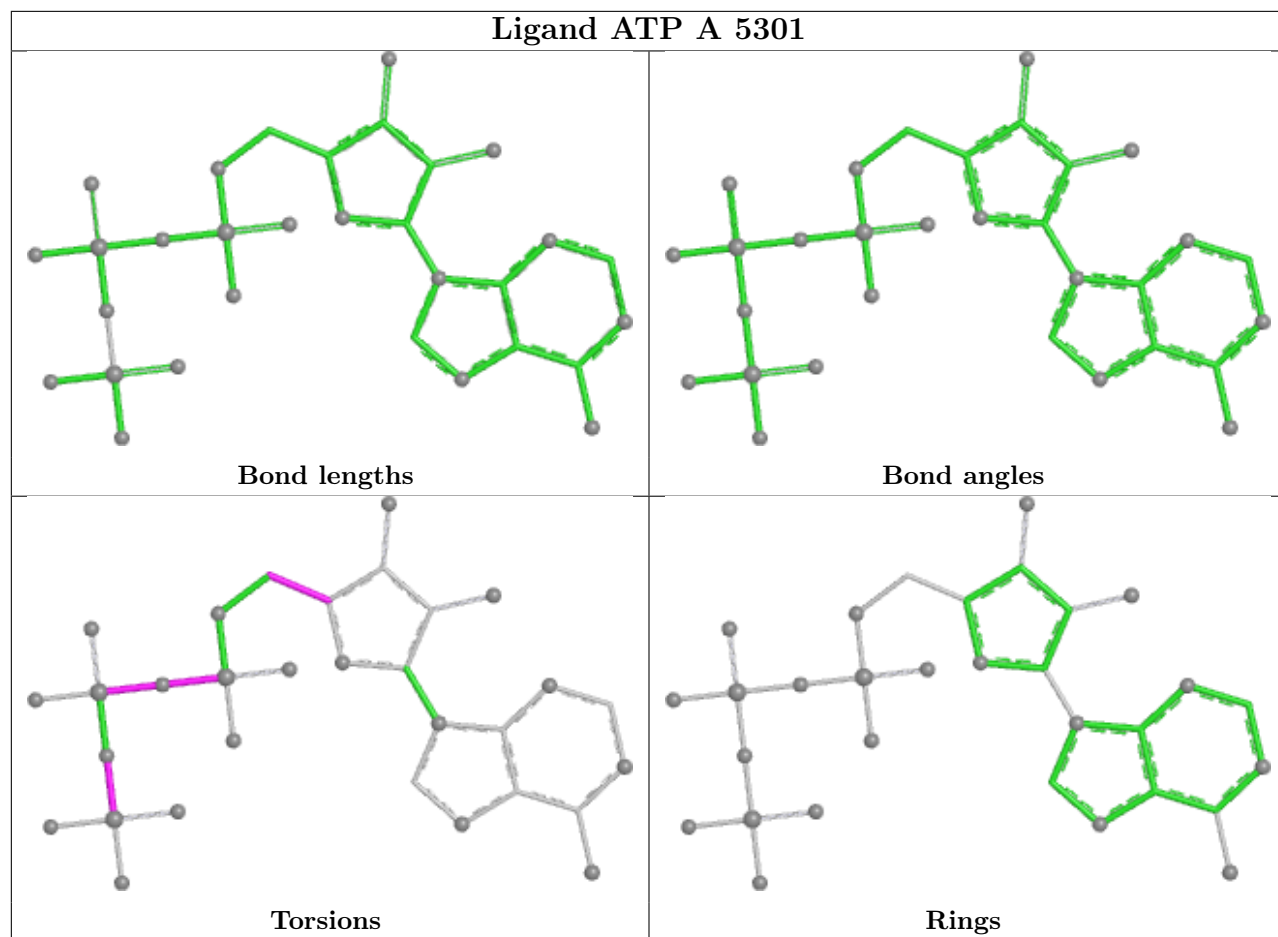


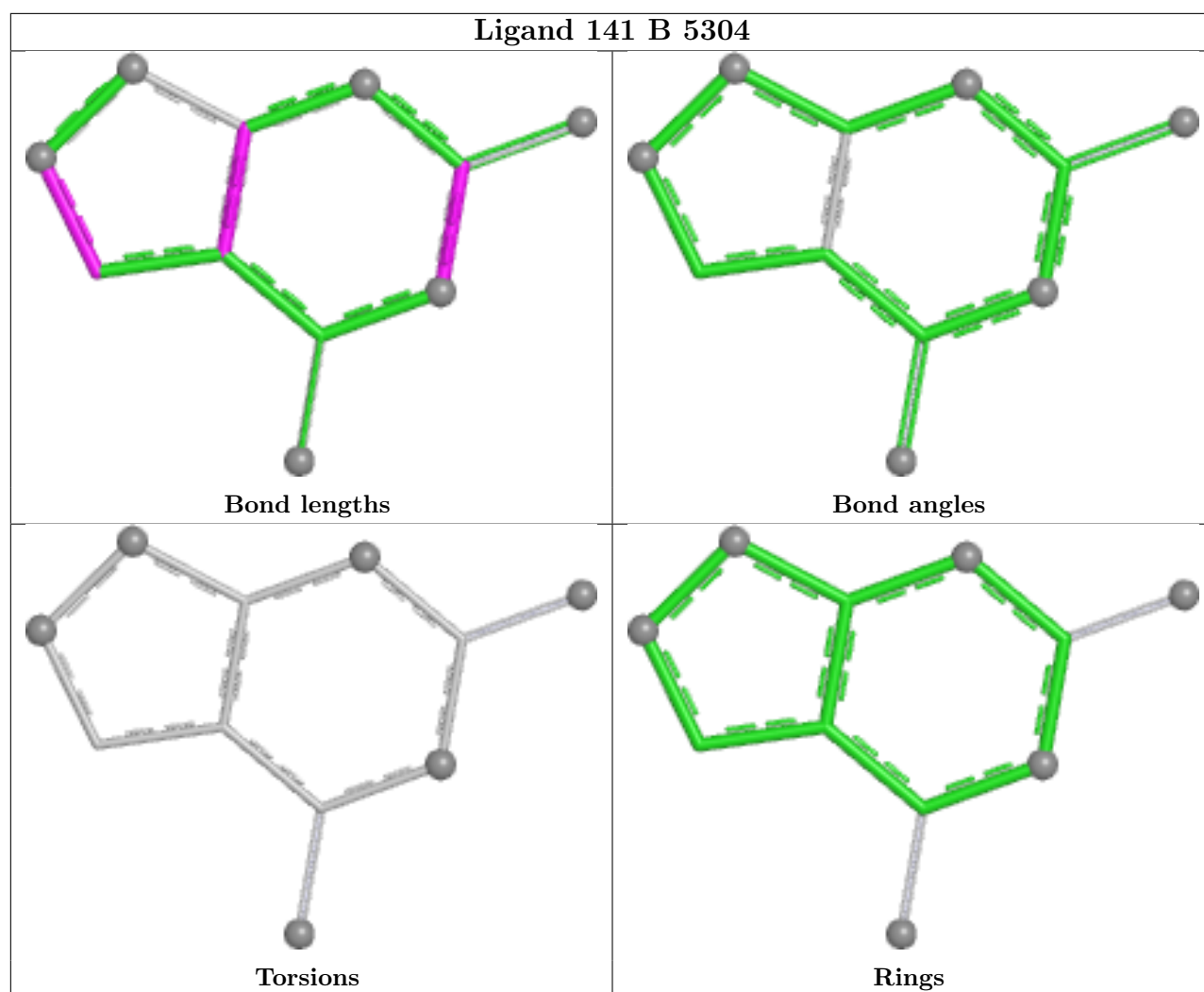


Ligand 141 C 5304









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.

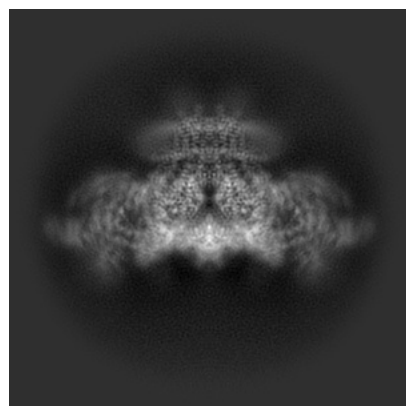
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47393. These allow visual inspection of the internal detail of the map and identification of artifacts.

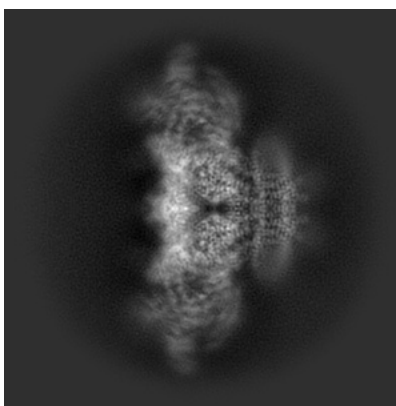
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

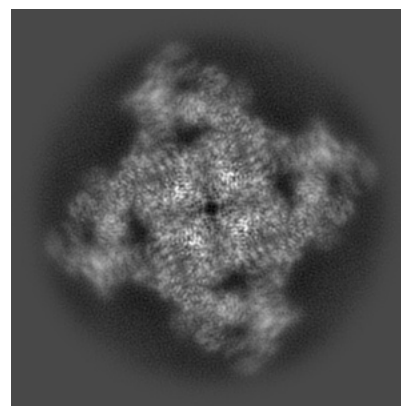
6.1.1 Primary map



X

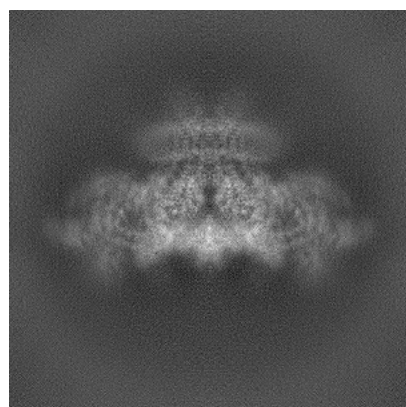


Y

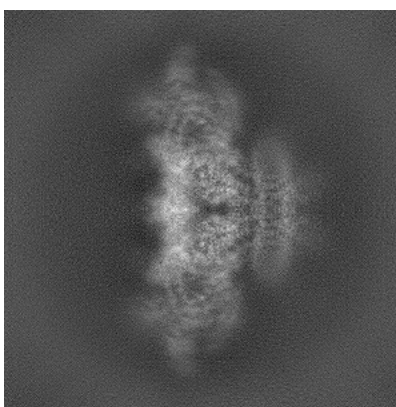


Z

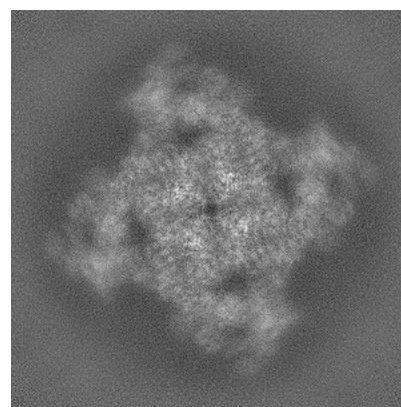
6.1.2 Raw map



X



Y

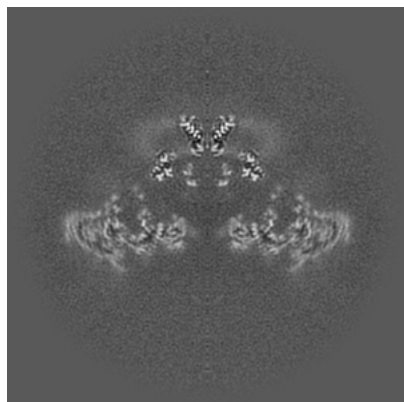


Z

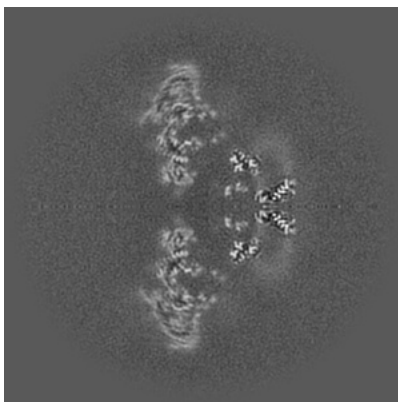
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

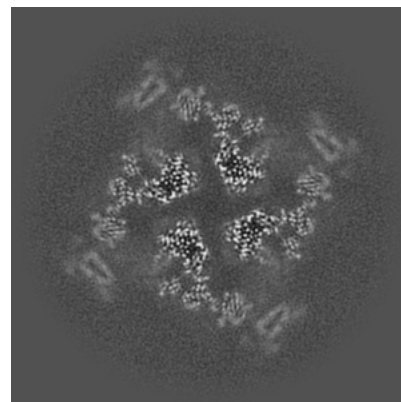
6.2.1 Primary map



X Index: 256

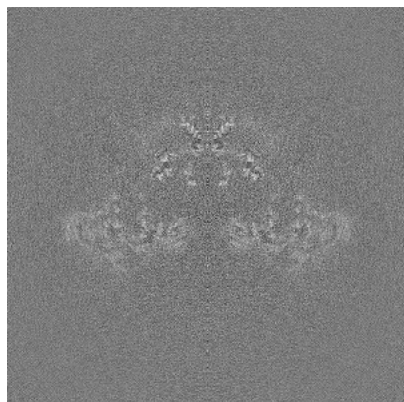


Y Index: 256

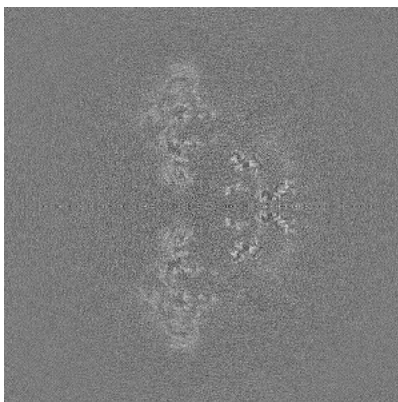


Z Index: 256

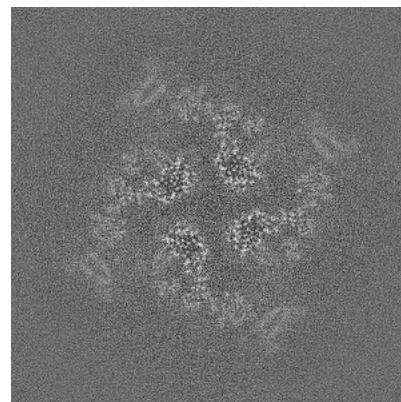
6.2.2 Raw map



X Index: 256



Y Index: 256

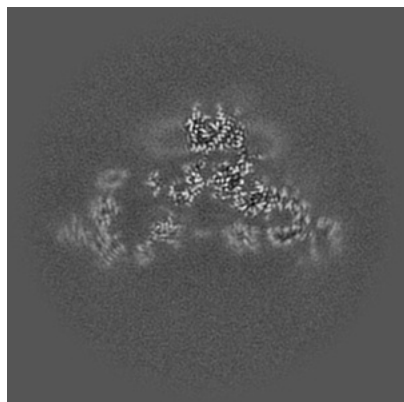


Z Index: 256

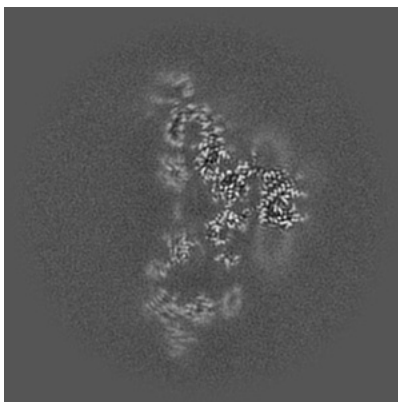
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

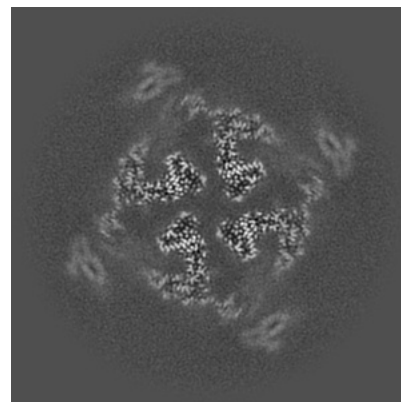
6.3.1 Primary map



X Index: 273

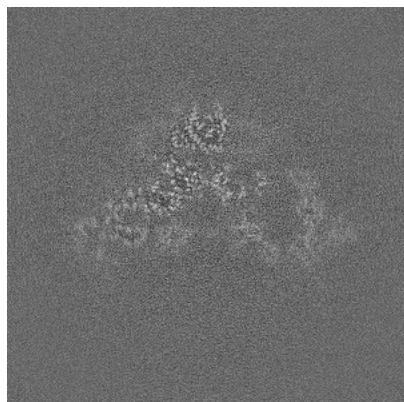


Y Index: 239

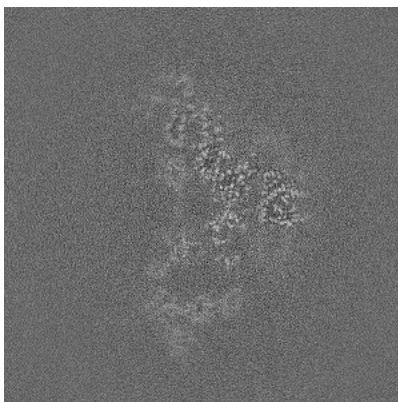


Z Index: 265

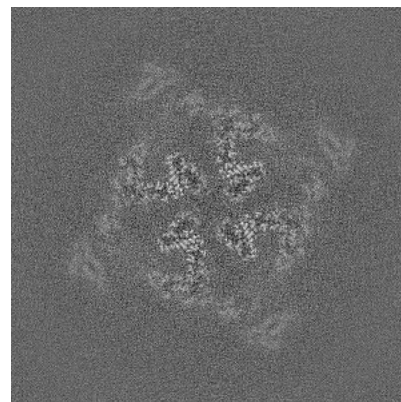
6.3.2 Raw map



X Index: 239



Y Index: 239

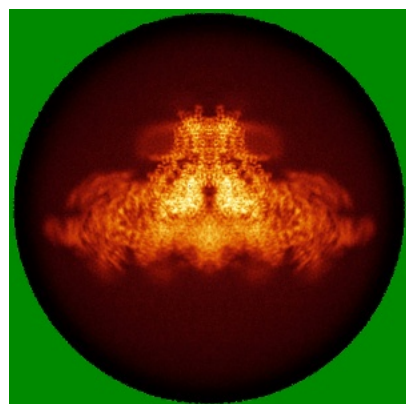


Z Index: 266

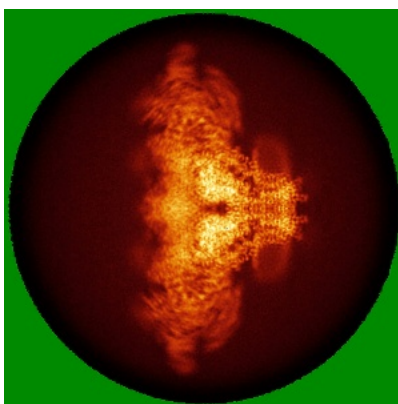
The images above show the largest variance slices of the map in three orthogonal directions.

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

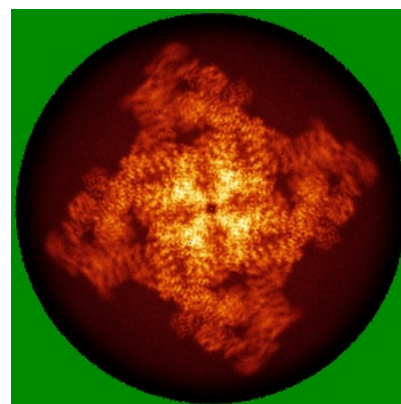
6.4.1 Primary map



X

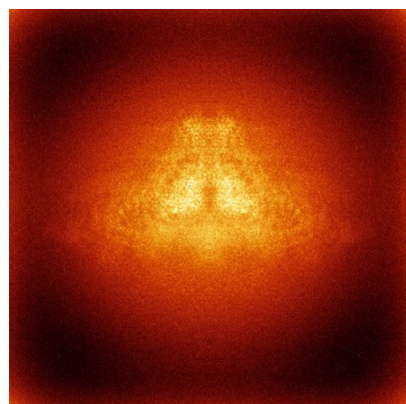


Y

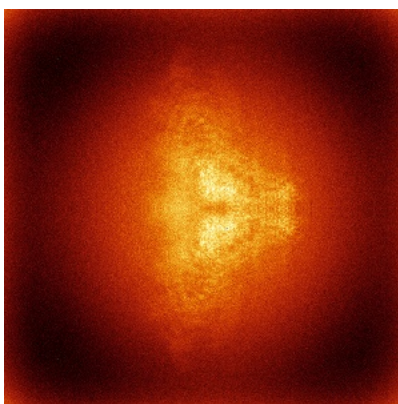


Z

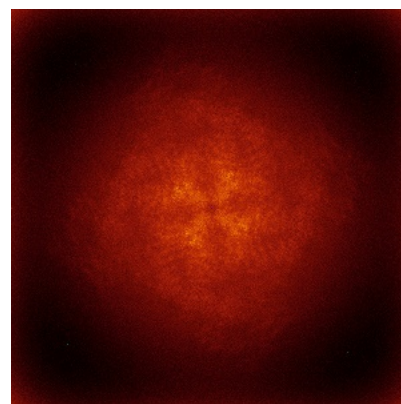
6.4.2 Raw map



X



Y

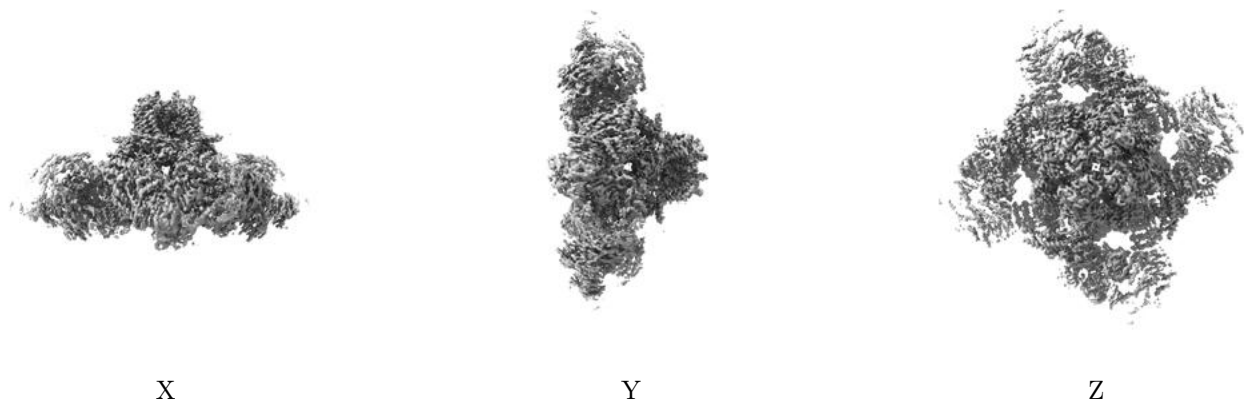


Z

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.

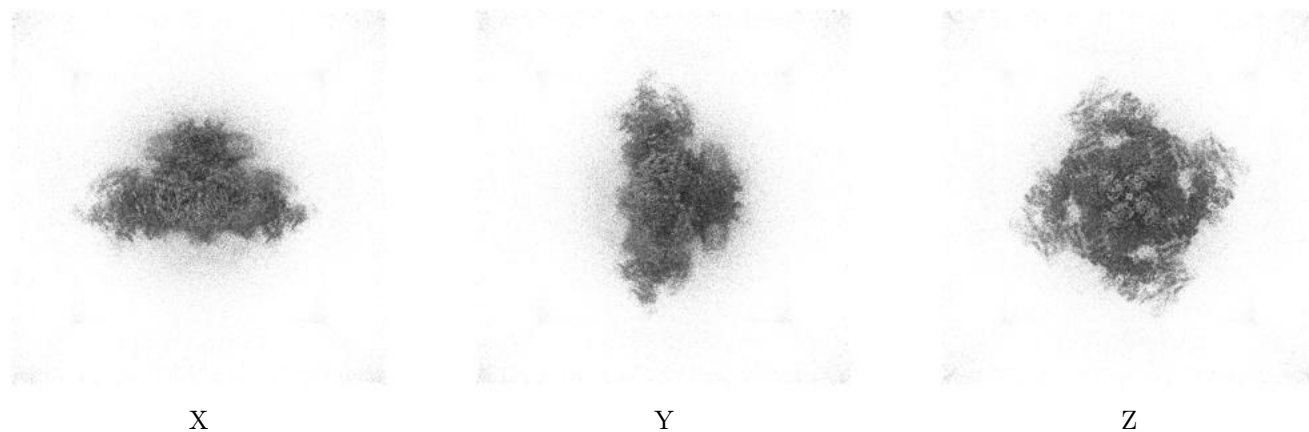
6.5 Orthogonal surface views [i](#)

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.

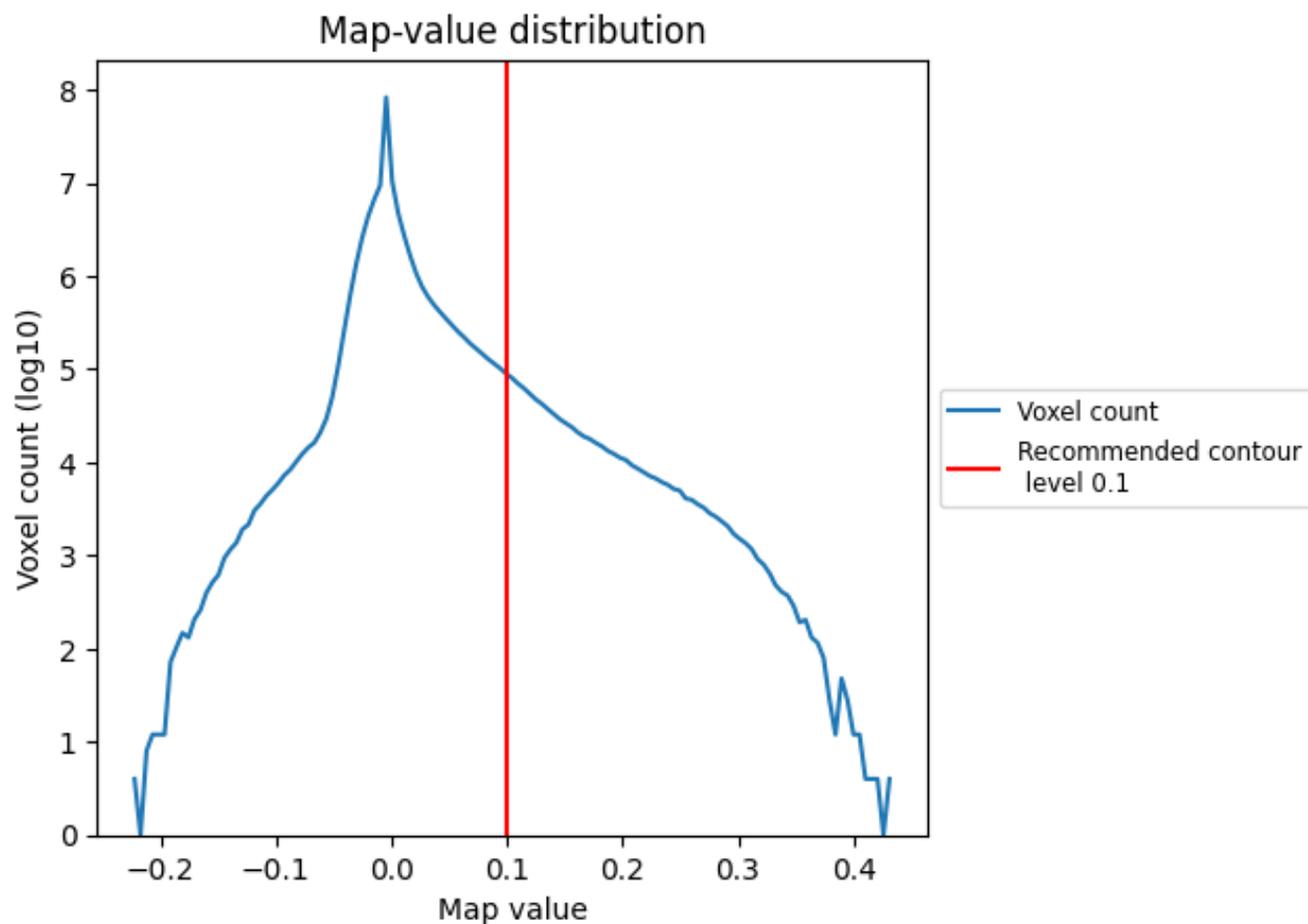
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

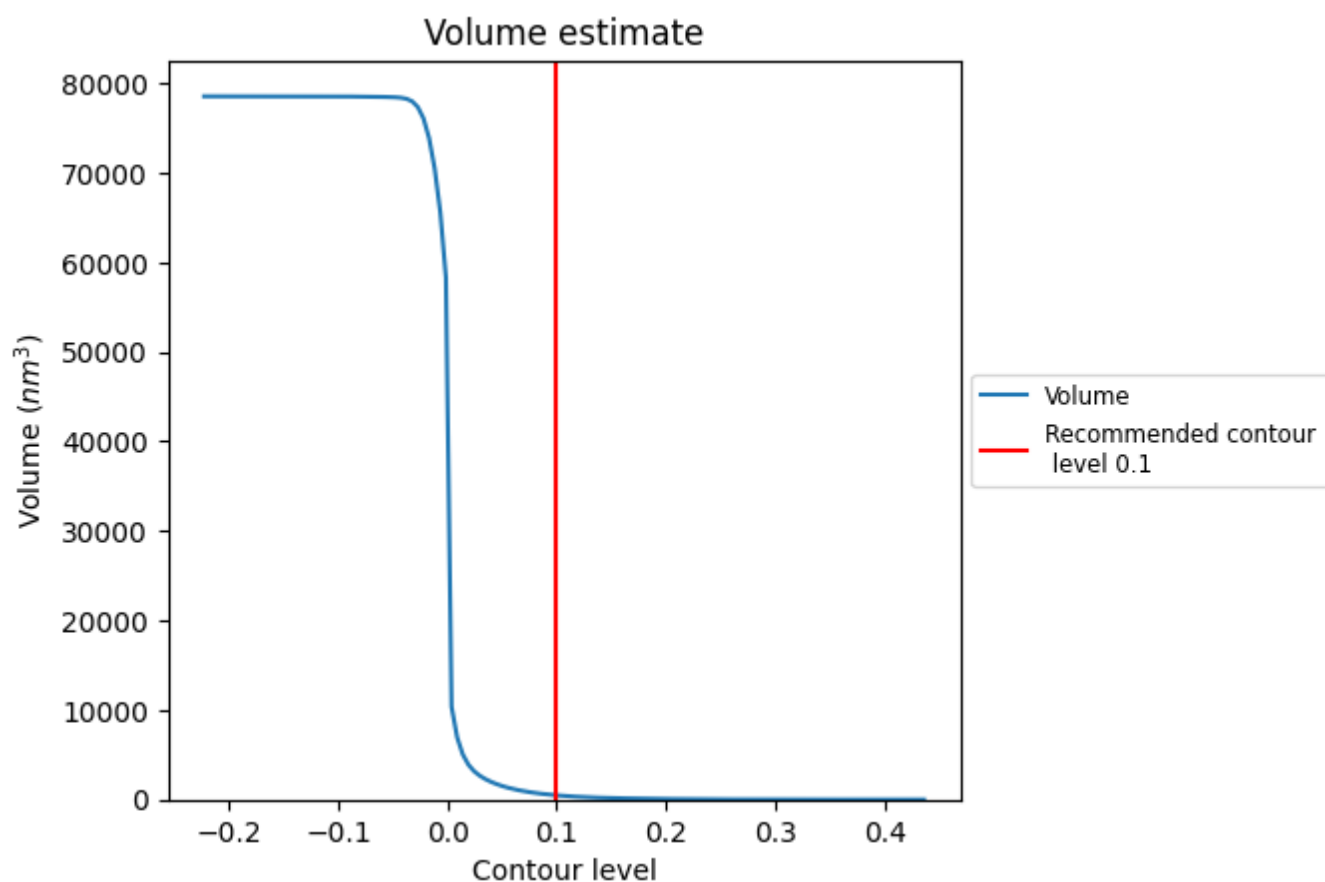
This section contains the results of statistical analysis of the map.

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.

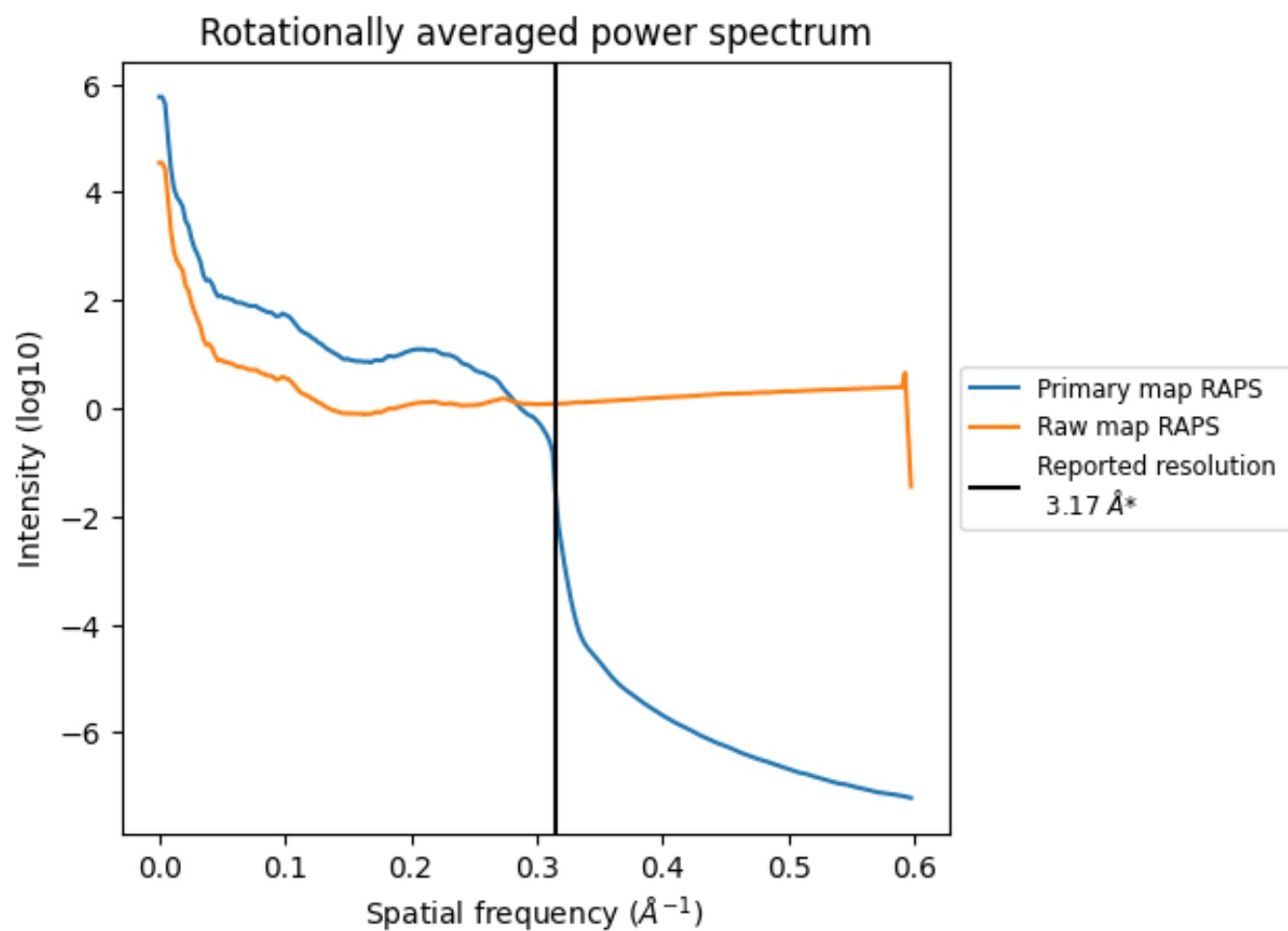
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm^3 ; this corresponds to an approximate mass of 431 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 ⓘ

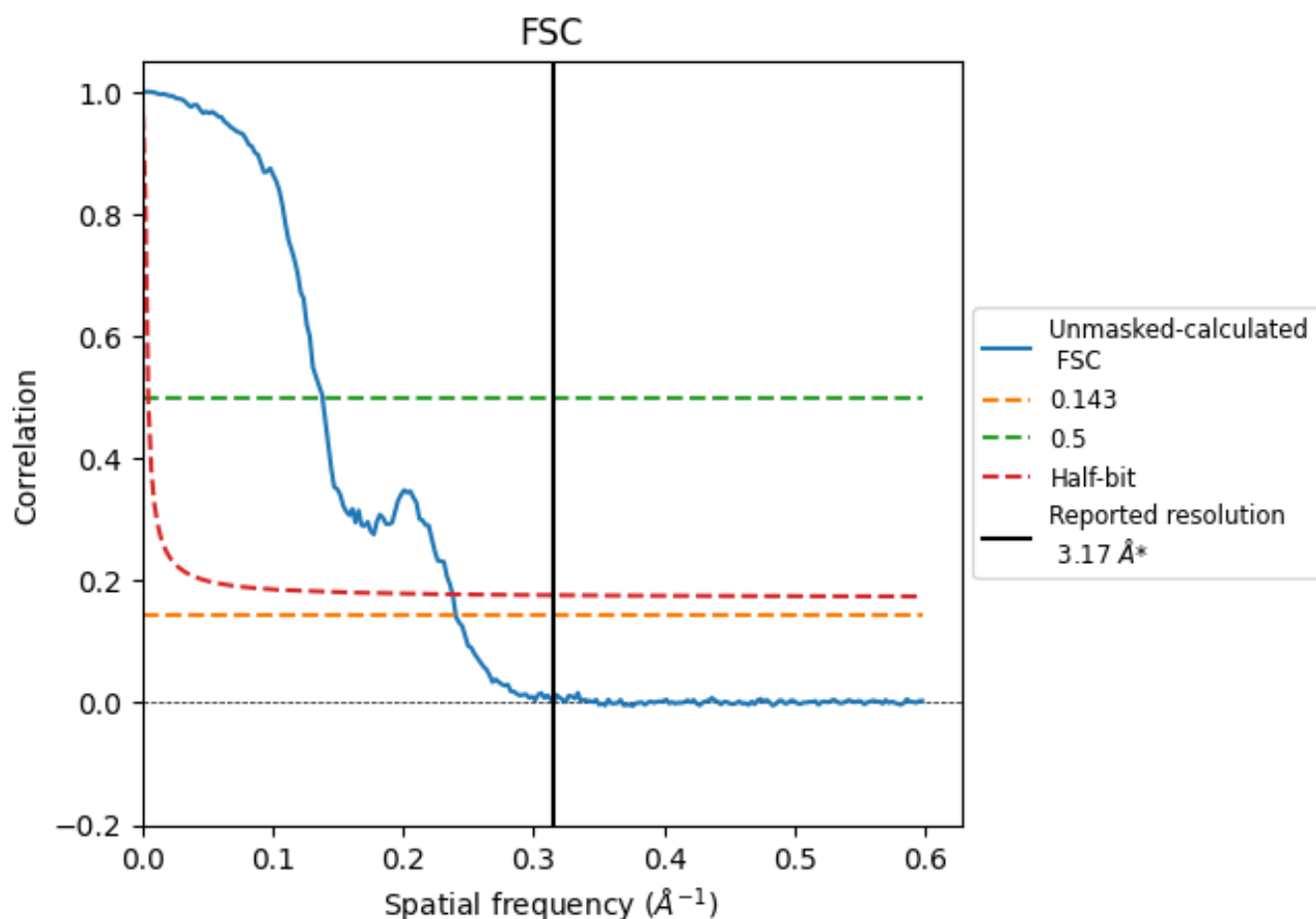


*Reported resolution corresponds to spatial frequency of 0.315 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

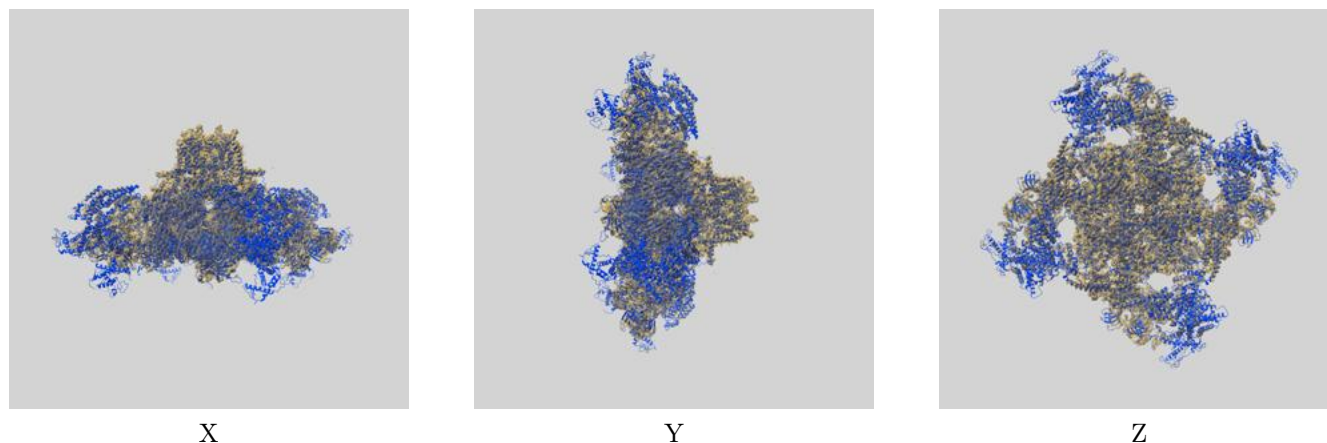
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.24	4.21

*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 4.16 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

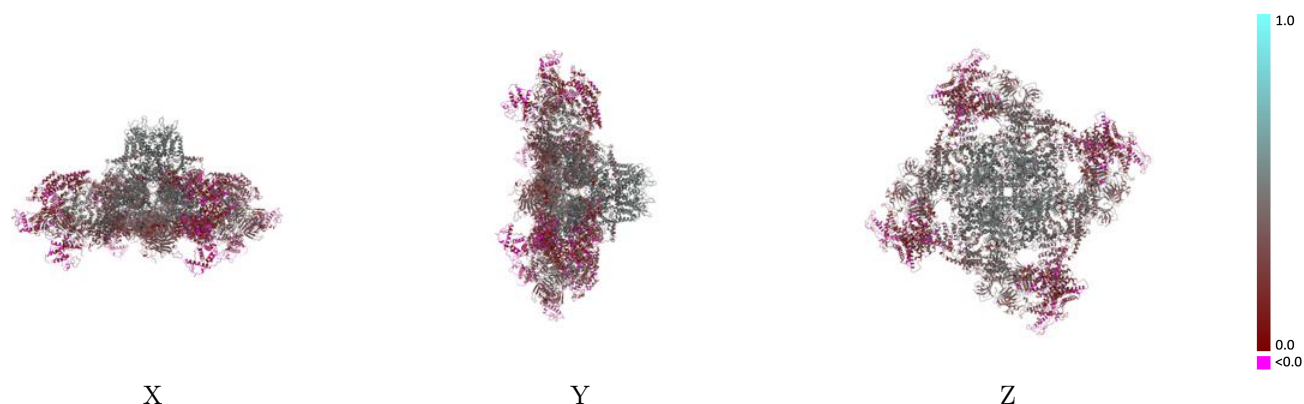
This section contains information regarding the fit between EMDB map EMD-47393 and PDB model 9E1G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



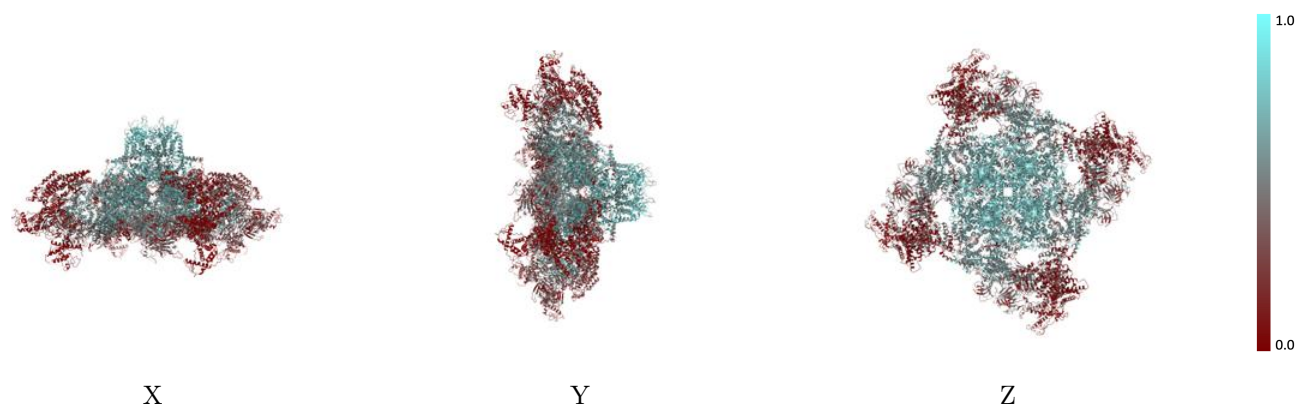
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



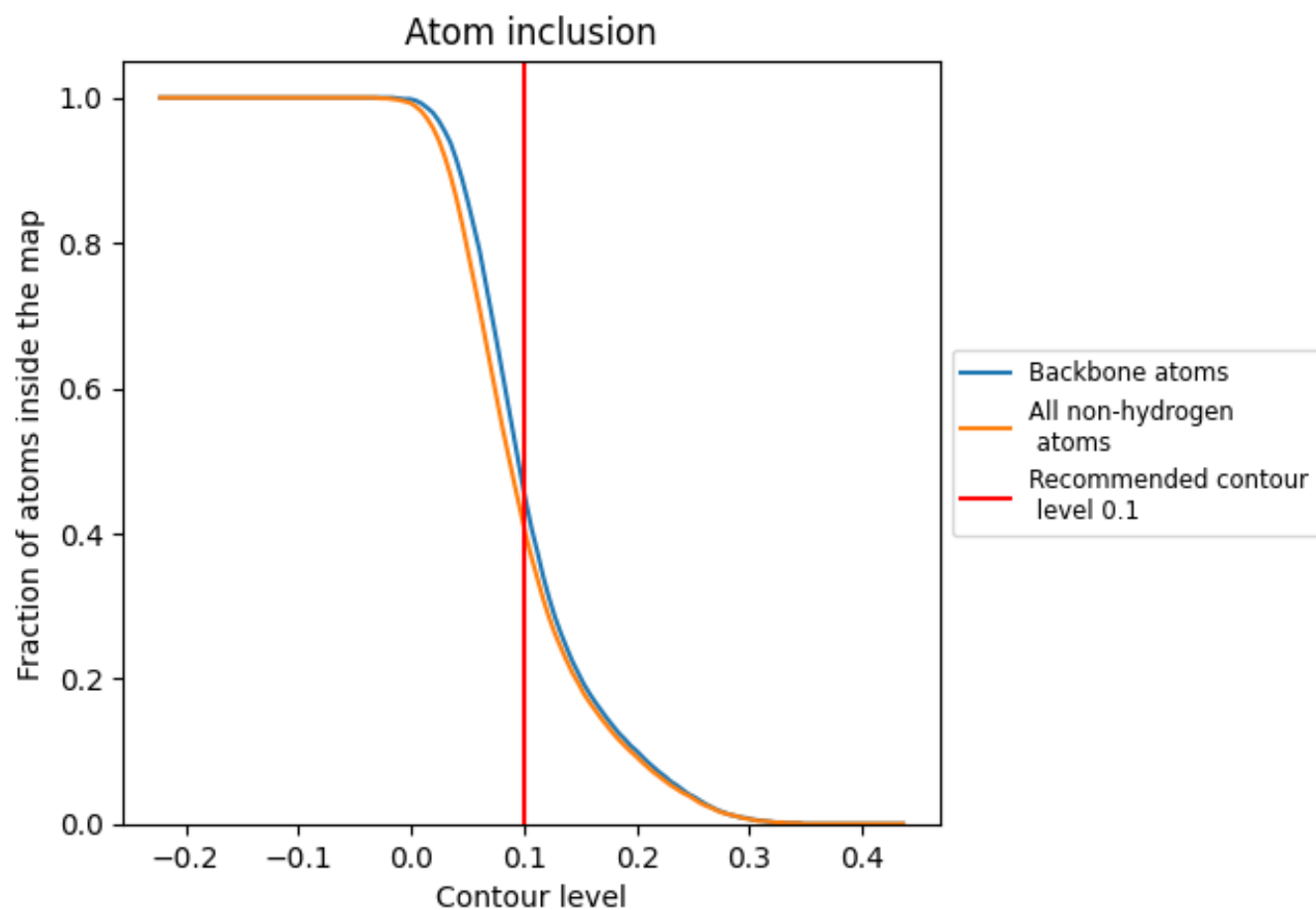
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 41% 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	0.4080	0.3230
A	0.4200	0.3260
B	0.4200	0.3210
C	0.4200	0.3210
D	0.4200	0.3210
E	0.2860	0.3640
F	0.2850	0.3620
G	0.2850	0.3570
H	0.2860	0.3640

1.0

0.0

<0.0