



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 10:14 AM EDT

PDB ID : 8SEP
EMDB ID : EMD-40424
Title : Cryo-EM Structure of RyR1 + ADP
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.57 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

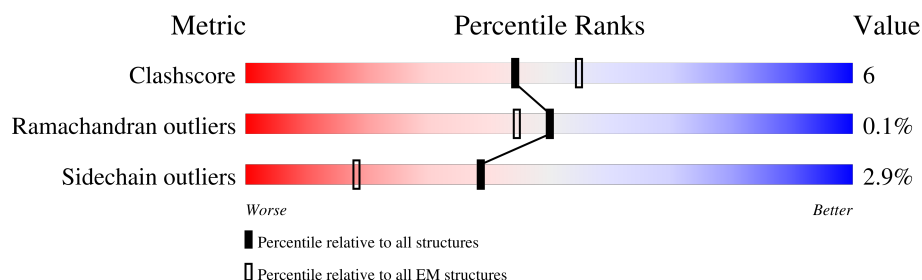
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>13%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	B	5037	<div> <div>13%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	D	5037	<div> <div>13%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
2	E	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>
2	F	350	<div> <div>23%</div> <div>8%</div> <div>69%</div> </div>
2	G	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>
2	H	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 143100 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	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	B	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	C	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	D	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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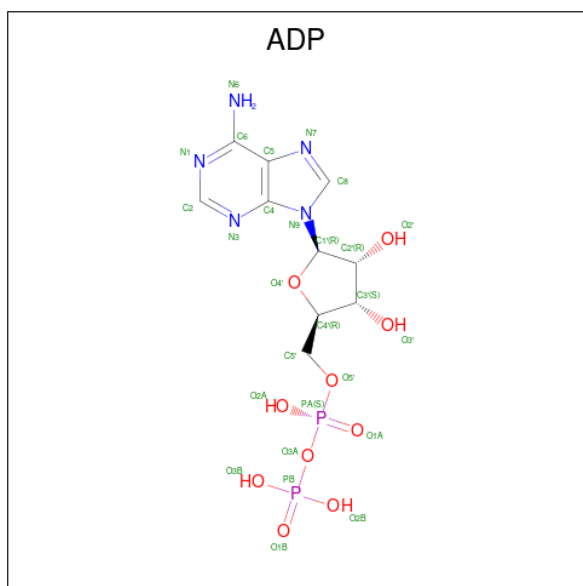
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

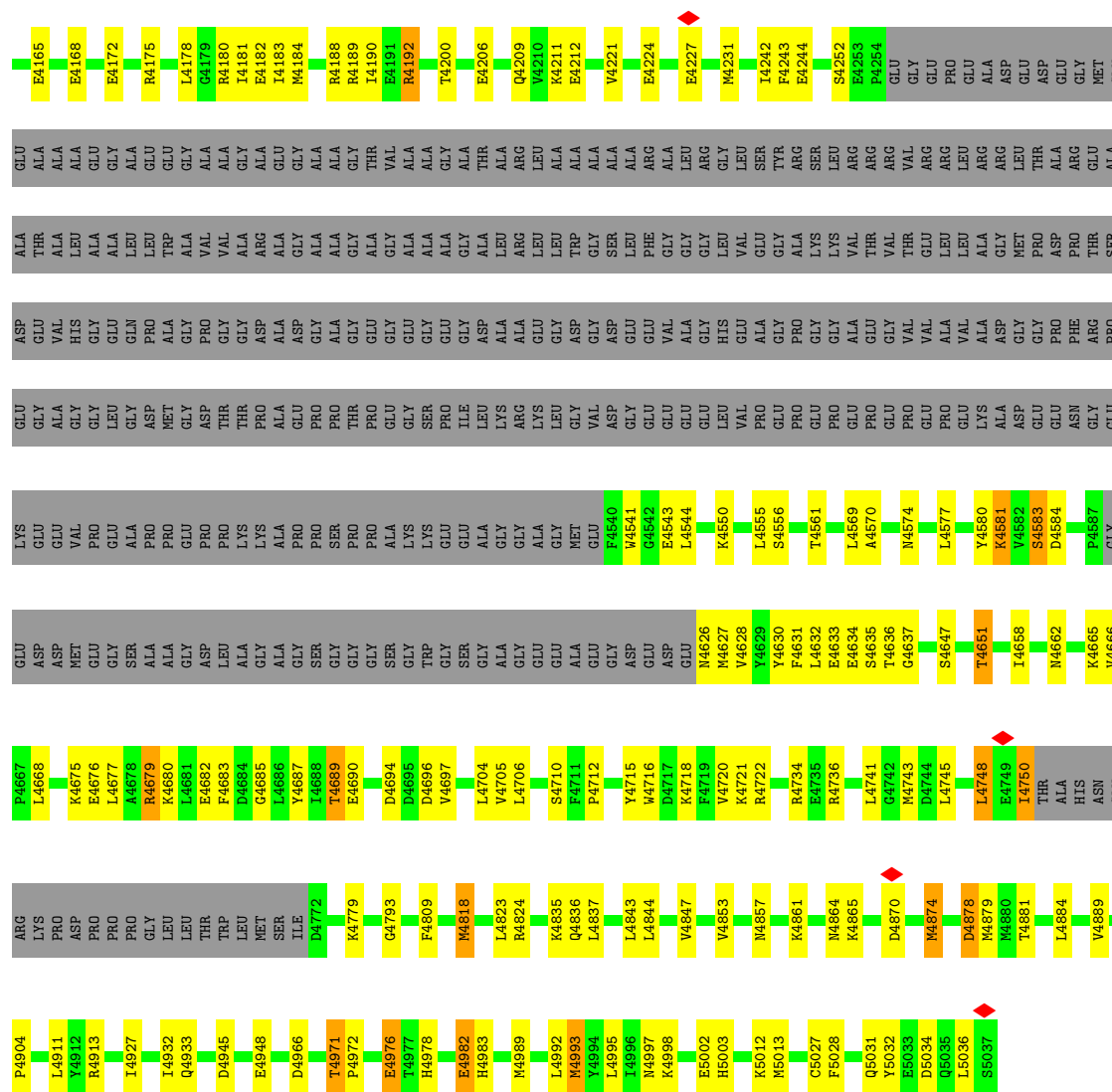
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1

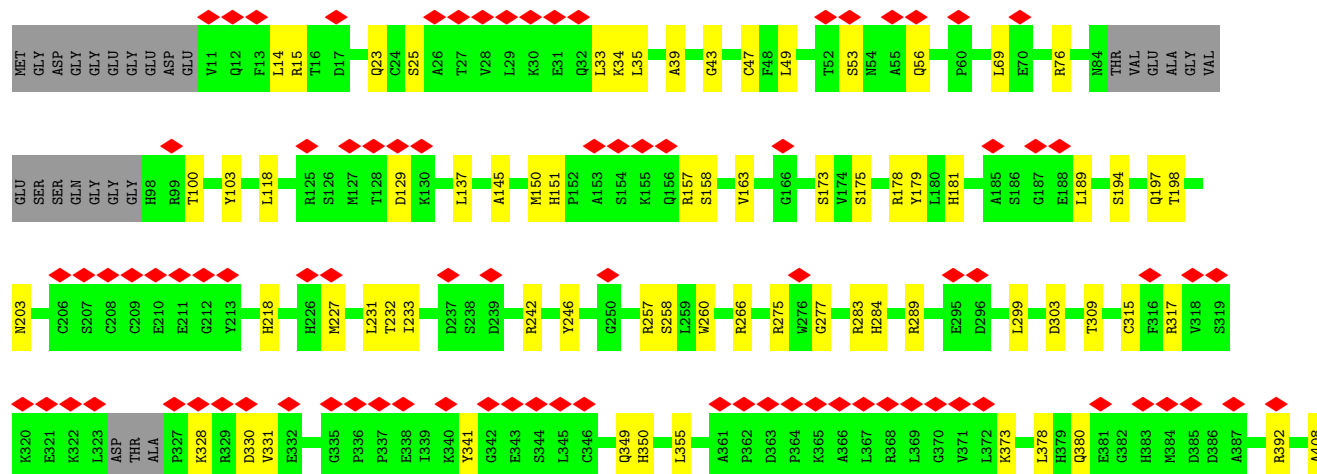








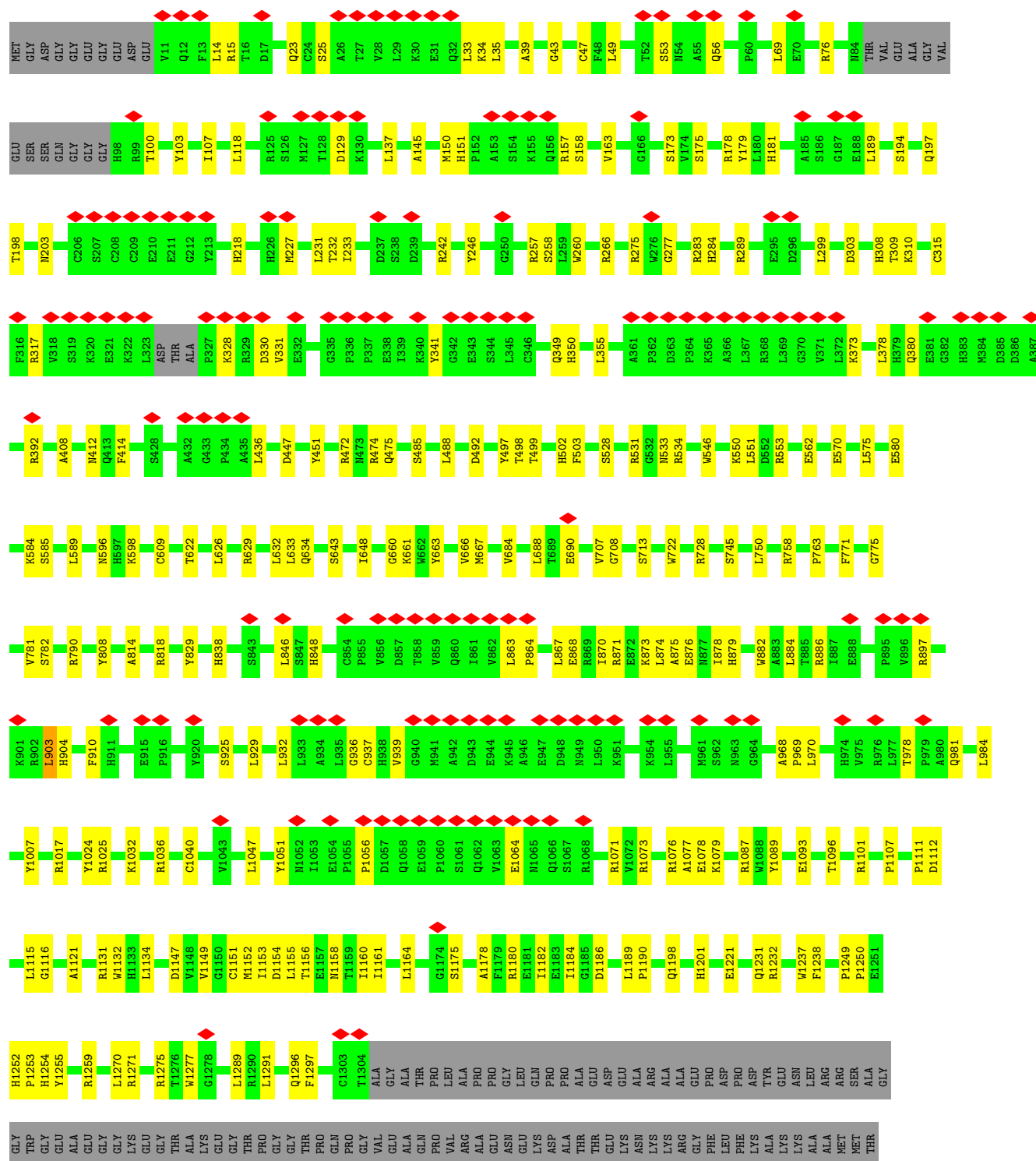
• Molecule 1: Ryanodine receptor 1





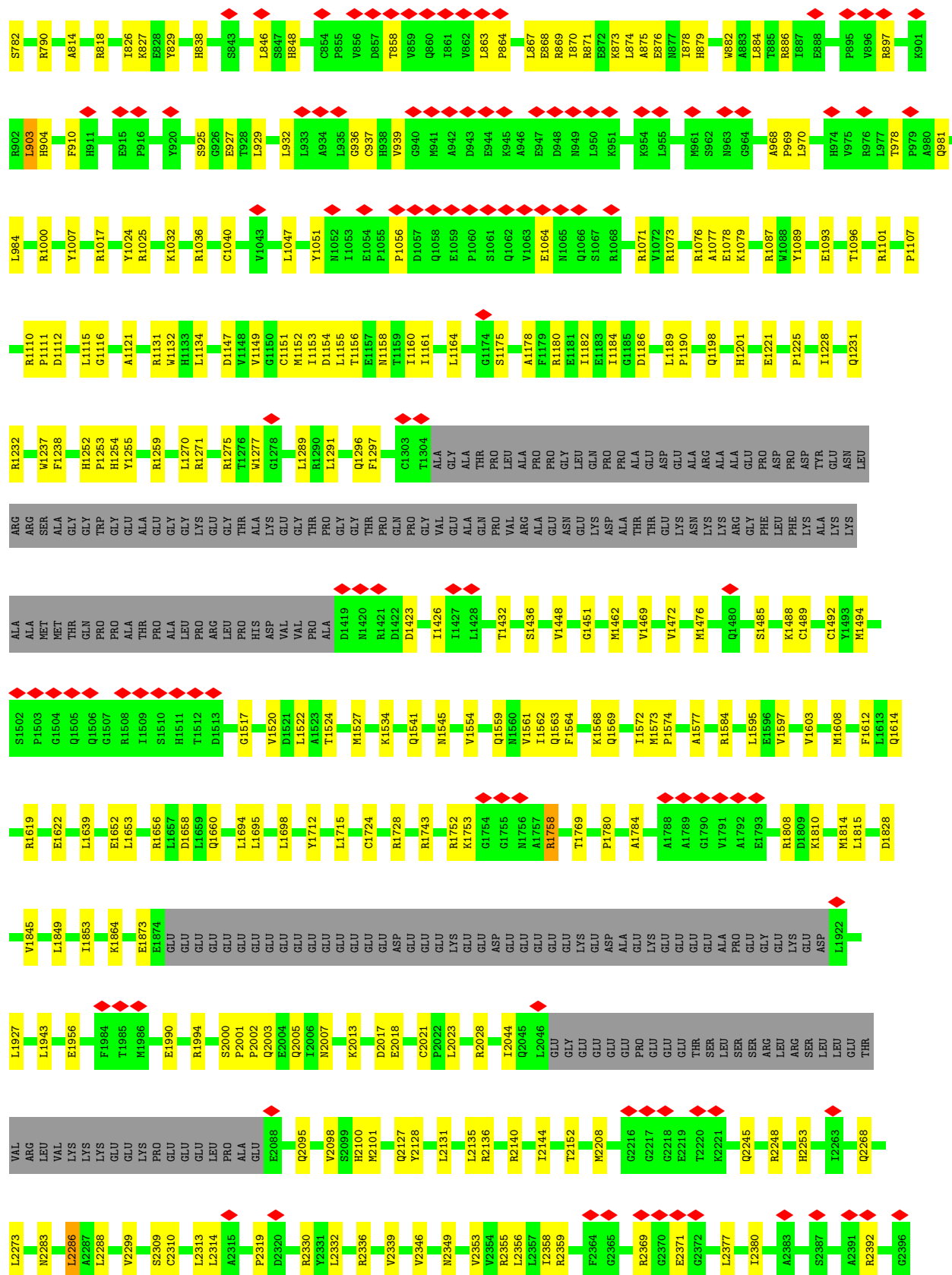




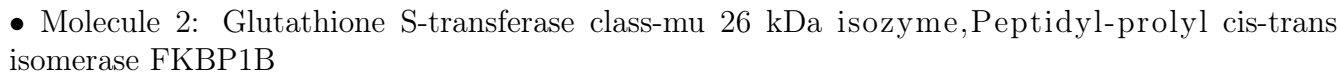


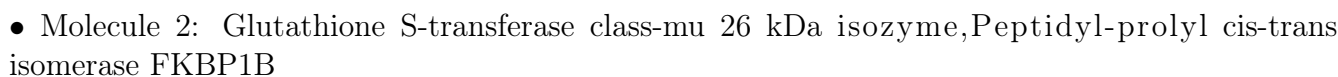






K3571	A3385	L3274	V3156	G3026	G2934	M2874	K2814	S2753	L2841	G3525	V2397
L3579	E3386	L3274	I3157	S3027	Y2935	A2875	A2815	F2754	K2642	F2526	ARG
R3582	A3387	Y3280	L3158	G3028	A2936	E2876	M2816	I2755	K2653	R2531	ARG
E3583	E3388	L3281	V3161	R3033	V2937	Q2877	L2817	N2756	Y2654	A2534	ARG
E3584	E3389	P3282	Q3162	R3033	T2938	L2878	A2818	K2757	L2657	S2535	ARG
D3585	R3395	W3285	S3171	E3037	GLY	E2880	W2819	E2760	P2658	L2536	ARG
A3586	R3403	E3290	N3180	K3045	LEU	Y2881	E2820	Y2761	T2659	G2537	GLU
D3587	D3404	A3291	V3183	L3046	LYS	W2882	W2821	T2762	G2660	T2538	HIS
I3592	L3405	P3292	E3184	L3049	ASP	H2883	T2822	H2763	W2661	A2539	PHE
R3498	L3408	P3293	F3185	V3050	MET	W2884	E2824	E2764	S2668	GLY	GLU
R3499	Y3409	P3294	R3051	R3052	GLU	T2885	K2825	K2765	E2669	Y2553	GLU
G3500	I3413	L3296	L3186	R3053	D2947	W2886	A2826	A2767	K2677	L2561	P2410
D3501	R3414	P3297	L3190	L3056	T2948	Q2887	R2827	I2682	I2682	A2570	P2411
R3502	R3417	A3298	L3194	L3059	S2949	R2888	E2828	F2768	E2677	G2571	E2412
Q3506	N3418	G3299	L3197	T3059	E2982	K2889	Q2829	D2769	I2682	T2572	E2413
K3515	R3420	P3301	F3205	P3062	Q2961	W2890	E2830	K2770	H2688	H2574	W2414
K3516	L3424	P3302	F3206	V3065	L2960	K2891	GLU	I2771	K2689	I2577	A2437
N3623	E3433	P3303	E3207	L3068	Q2962	Q2892	ARG	Q2772	E2694	I2577	I2456
M3524	F3435	P3304	E3210	H3069	L2963	E2893	THR	N2773	D2716	I2583	I2469
D3531	R3436	I3322	Y3213	L3075	L2964	L2894	GLU	N2774	A2717	H2584	I2469
L3532	N3437	V3324	N3214	L3076	R2965	E2895	LYS	W2775	I2577	T2588	L2474
L3533	R3453	M3325	A3215	A3077	W2966	A2896	LYS	S2776	I2577	I2475	I2476
M3534	E3454	L3327	R3078	R3078	M2967	K2897	THR	Y2777	S2720	R2588	I2476
K3537	N3457	G3328	S3217	S3083	S2970	Q2898	THR	Q2778	S2721	S2590	L2479
R3538	F3458	I3329	V3218	E3086	Q2971	Q2899	ALA	E2779	K2722	R2589	K2480
R3539	V3459	D3330	V3219	S2982	Q2971	Q2899	GLN	E2780	A2723	I2589	K2481
Y3540	Q3461	M3335	T3220	S2982	I2974	Q2900	THR	N2781	E2724	R2591	G2482
A3541	N3462	A3339	T3221	S2982	E2978	H2902	ALA	D2782	K2725	L2595	G2483
L3542	R3463	V3340	K3222	S2983	A2979	P2903	GLN	E2783	LYS	R2600	G2484
K3543	I3464	V3340	K3223	S2983	A2979	L2904	THR	E2784	THR	M2608	A2484
E3548	N3465	I3345	P3224	S2985	R2985	V2906	ASP	K2786	ASP	C2611	L2485
V3549	R3466	I3345	R3225	R2985	V2986	P2907	PRO	T2787	ALA	I2614	F2494
E3551	N3467	R3348	A3226	R2987	V2986	D2909	GLU	H2788	N2734	R2615	K2499
N3555	F3469	A3349	I3229	S2988	Q2987	T2910	GLY	P2789	F2735	P2616	A2500
N3556	L3470	R3350	L3230	ARG	K2988	L2911	N2856	L2790	D2736	L2619	V2503
L3557	T3471	P3351	G3231	THR	S2989	A2913	P2857	R2792	P2737	L2622	D2507
H3558	A3472	L3354	L3232	GLN	P2990	K2914	P2859	Y2794	P2739	R2625	R2508
L3559	D3473	F3358	L3233	VAL	H2991	E2915	P2860	K2795	V2740	L2626	L2513
Q3560	S3474	I3362	P3233	K3123	Q2993	K2916	D2861	T2796	E2741	V2630	D2513
G3561	R3475	I3362	E3238	Y3131	Q2993	A2917	L2862	F2797	T2742	N2634	D2516
K3562	K3476	E3377	M3239	H3146	F2997	R2918	S2863	S2798	L2743	F2517	F2517
L3563	K3477	R3380	V3245	H3146	I3001	D2919	G2864	E2799	N2744	K2638	L2518
E3564	N3478	L3381	R3248	Q3149	T3020	R2920	V2865	K2800	V2745	H2639	L2519
G3565	A3479	E3382	S3259	H3150	P3021	E2921	T2866	D2801	I2746	P2640	L2522
S3568	LYS	L3381	S3259	Q3151	A3022	A2923	L2867	K2802	I2747	L2522	D2523
	ALA	E3382	S3259	Q3151	A3022	Q2924	R2869	E2803	P2748	L2522	V2524
	GLY	A3383	S3259	Q3151	A3022	E2925	E2870	I2804	E2749	K2750	
	ASP	K3384	S3259	Q3151	A3022	L2926	L2871	R2806	K2751	L2751	
			I3270			L2927	Q2872	W2807	D2752		
						K2928	A2873	P2808			
						F2929		I2809			
						L2930		K2810			
						Q2931		E2811			
						W2932		S2812			
								L2813			





- Chain H: 23% 7% 69%

Met	LEU	ARG	Met
LEU	GLY	ILE	CYS
GLY	LEU	ALA	LEU
LEU	GLU	TYR	ASP
PHE	SER	LYS	ALA
PRO	ASP	ASP	PHE
ASN	LEU	PHE	PRO
LEU	GLU	LYS	LYS
PRO	THR	GLY	LEU
THR	LEU	THR	VAL
TYR	LEU	ILE	CYS
GLY	ILE	LYS	PHE
SER	ASP	VAL	LYS
SER	GLY	ASP	LYS
Met	ASP	PHE	ARG
SER	VAL	LEU	ILE
PRO	VAL	SER	GLY
ALA	LYS	ALA	ALA
LEU	LEU	LEU	ILE
THR	THR	PRO	PRO
GLY	GLN	GLU	GLN
TRP	SER	GLY	ILE
LYS	MET	MET	ILE
ILE	LEU	LEU	ASP
ILE	ALA	LYS	LYS
GLY	ILE	MET	TYR
LYS	ARG	PHE	LEU
LEU	TYR	GLY	LYS
VAL	TYR	GLU	LEU
GLN	ILE	ASP	SER
PRO	ALA	ARG	LEU
PRO	ASP	LEU	LYS
THR	ASP	CYS	TYR
ARG	LYS	HIS	ILE
LEU	ASN	LYS	ALA
LEU	MET	THR	TRP
GLU	LEU	TYR	PRO
TYR	GLY	LEU	LEU
LEU	CYS	ASN	GLN
GLY	GLY	GLY	GLY
GLU	PRO	ASP	TRP
LYS	LYS	HIS	GLN
TYR	GLU	VAL	ALA
GLU	ARG	THR	THR
GLU	ALA	HIS	PHE
HIS	GLU	PRO	GLY
LEU	ILE	ASP	GLY
LEU	SER	PHE	GLY
GLU	MET	MET	ASP
ARG	LEU	LEU	HIS
ASP	GLU	TYR	PRO
GLY	GLY	ASP	PRO
ALA	VAL	ALA	LYS
ASP	LEU	LEU	GLY
LYS	LEU	ASP	ILE
TRP	ASP	VAL	GLU
ARG	ILE	VAL	GLU
ASN	ARG	VAL	GLU
LYS	TYR	TYR	ASN
LYS	GLY	MET	LEU
PHE	VAL	ASP	TYR
GLU	SER	PRO	PHE
SER	SER	PRO	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171805	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.602	Depositor
Minimum map value	-0.818	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.263	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	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: ZN, ADP

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	0.33	0/35746	0.66	14/48409 (0.0%)
1	B	0.33	0/35746	0.66	14/48409 (0.0%)
1	C	0.33	0/35746	0.66	14/48409 (0.0%)
1	D	0.33	0/35746	0.66	14/48409 (0.0%)
2	E	0.33	0/834	0.62	0/1123
2	F	0.33	0/834	0.62	0/1123
2	G	0.33	0/834	0.62	0/1123
2	H	0.33	0/834	0.62	0/1123
All	All	0.33	0/146320	0.66	56/198128 (0.0%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4945	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	4945	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	4945	ASP	CB-CG-OD1	7.53	125.07	118.30
1	D	4945	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	903	LEU	CA-CB-CG	6.81	130.97	115.30

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	A	34929	0	34552	426	0
1	B	34929	0	34552	434	0
1	C	34929	0	34552	436	0
1	D	34929	0	34552	442	0
2	E	818	0	824	18	0
2	F	818	0	824	20	0
2	G	818	0	824	20	0
2	H	818	0	824	18	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	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
All	All	143100	0	141552	1777	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1777 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:B:2248:ARG:HB3	1:B:2286:LEU:HD11	1.72	0.71
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.72	0.71
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.72	0.71
1:D:2248:ARG:HB3	1:D:2286:LEU:HD11	1.72	0.71
1:A:2248:ARG:HB3	1:A:2286:LEU:HD11	1.72	0.71

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	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	B	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	C	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	D	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17844/21548 (83%)	17272 (97%)	560 (3%)	12 (0%)	50	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	A	4712	PRO
1	B	3615	SER
1	B	4712	PRO
1	C	3615	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	B	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	C	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	D	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15584/18320 (85%)	15116 (97%)	468 (3%)	39 63

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5027	CYS
1	D	4861	LYS
1	C	4580	TYR
1	D	4818	MET
1	D	4556	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1631	GLN
2	E	20	GLN
1	D	2634	ASN
1	D	3895	HIS
1	B	2872	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	ADP	A	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	B	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	D	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	C	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)

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
3	ADP	A	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	B	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	D	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	C	5101	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	ADP	PA-O3A	2.17	1.61	1.59
3	D	5101	ADP	PA-O3A	2.17	1.61	1.59
3	C	5101	ADP	PA-O3A	2.16	1.61	1.59
3	B	5101	ADP	PA-O3A	2.16	1.61	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	ADP	C4'-O4'-C1'	-3.85	106.40	109.92
3	A	5101	ADP	C4'-O4'-C1'	-3.84	106.40	109.92
3	B	5101	ADP	C4'-O4'-C1'	-3.84	106.41	109.92
3	C	5101	ADP	C4'-O4'-C1'	-3.84	106.41	109.92
3	D	5101	ADP	N3-C2-N1	-3.71	123.63	128.67

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

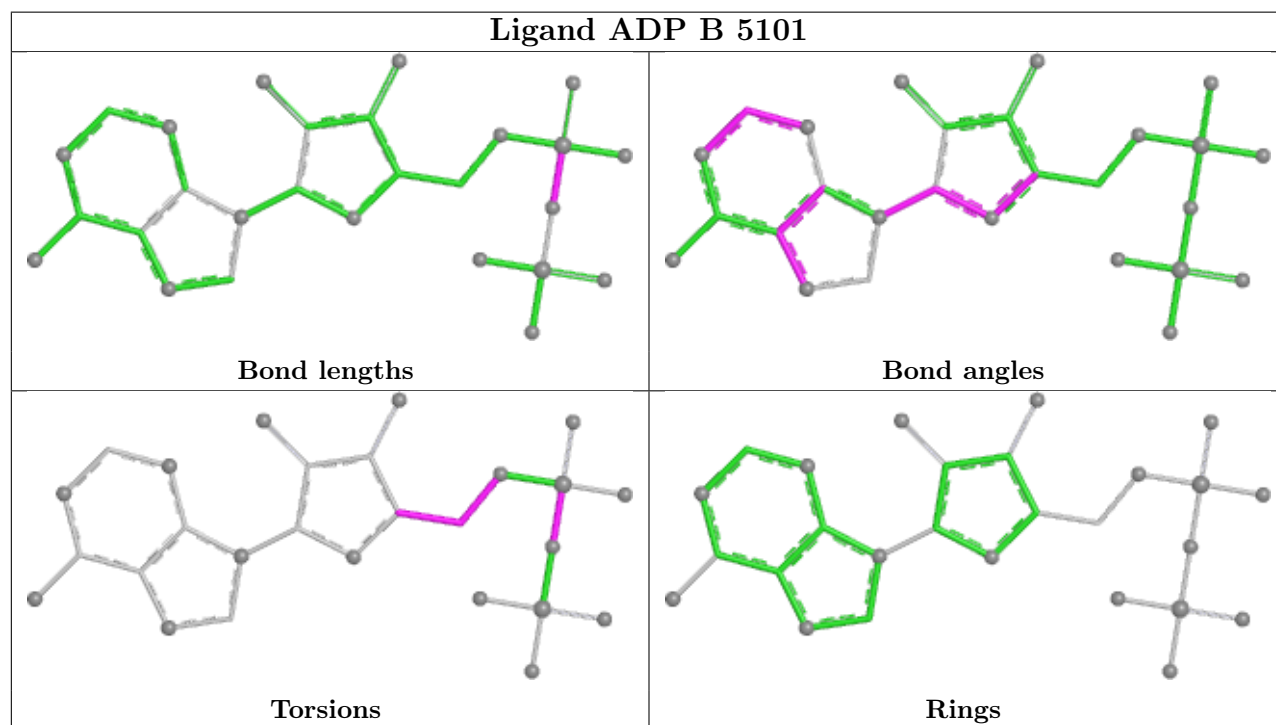
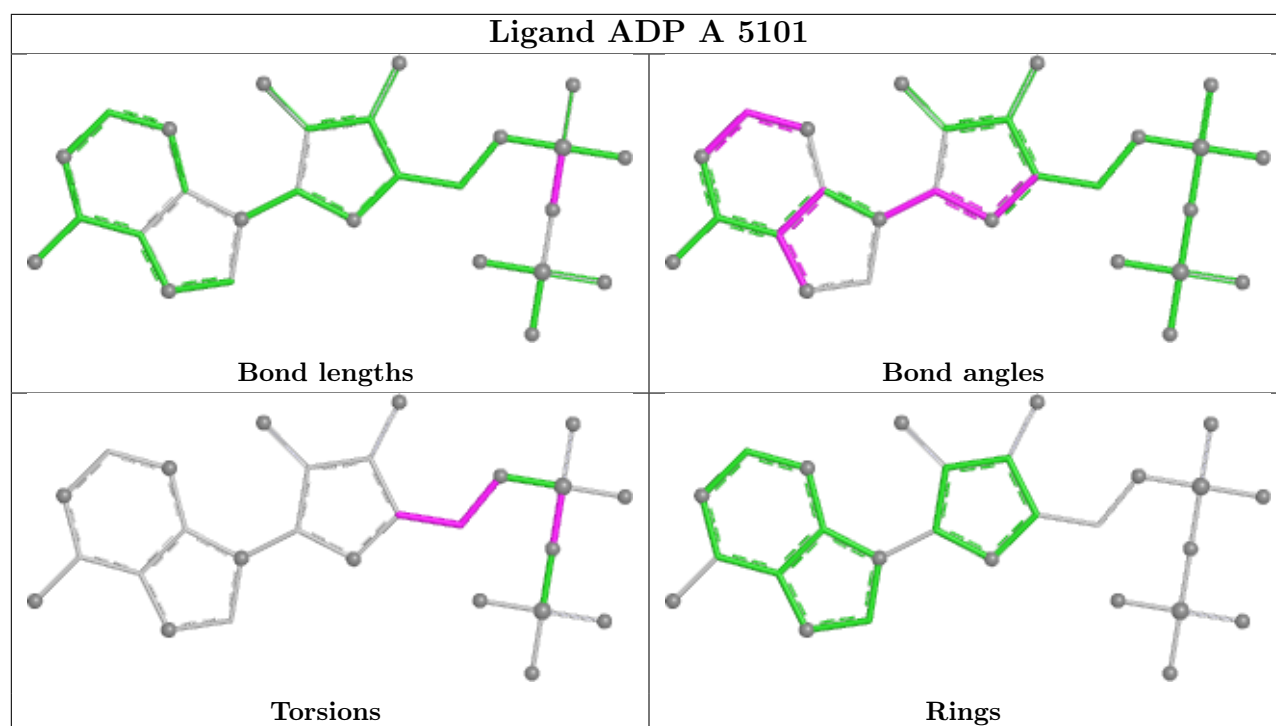
Mol	Chain	Res	Type	Atoms
3	A	5101	ADP	PB-O3A-PA-O5'
3	B	5101	ADP	PB-O3A-PA-O5'
3	C	5101	ADP	PB-O3A-PA-O5'
3	D	5101	ADP	PB-O3A-PA-O5'
3	A	5101	ADP	O4'-C4'-C5'-O5'

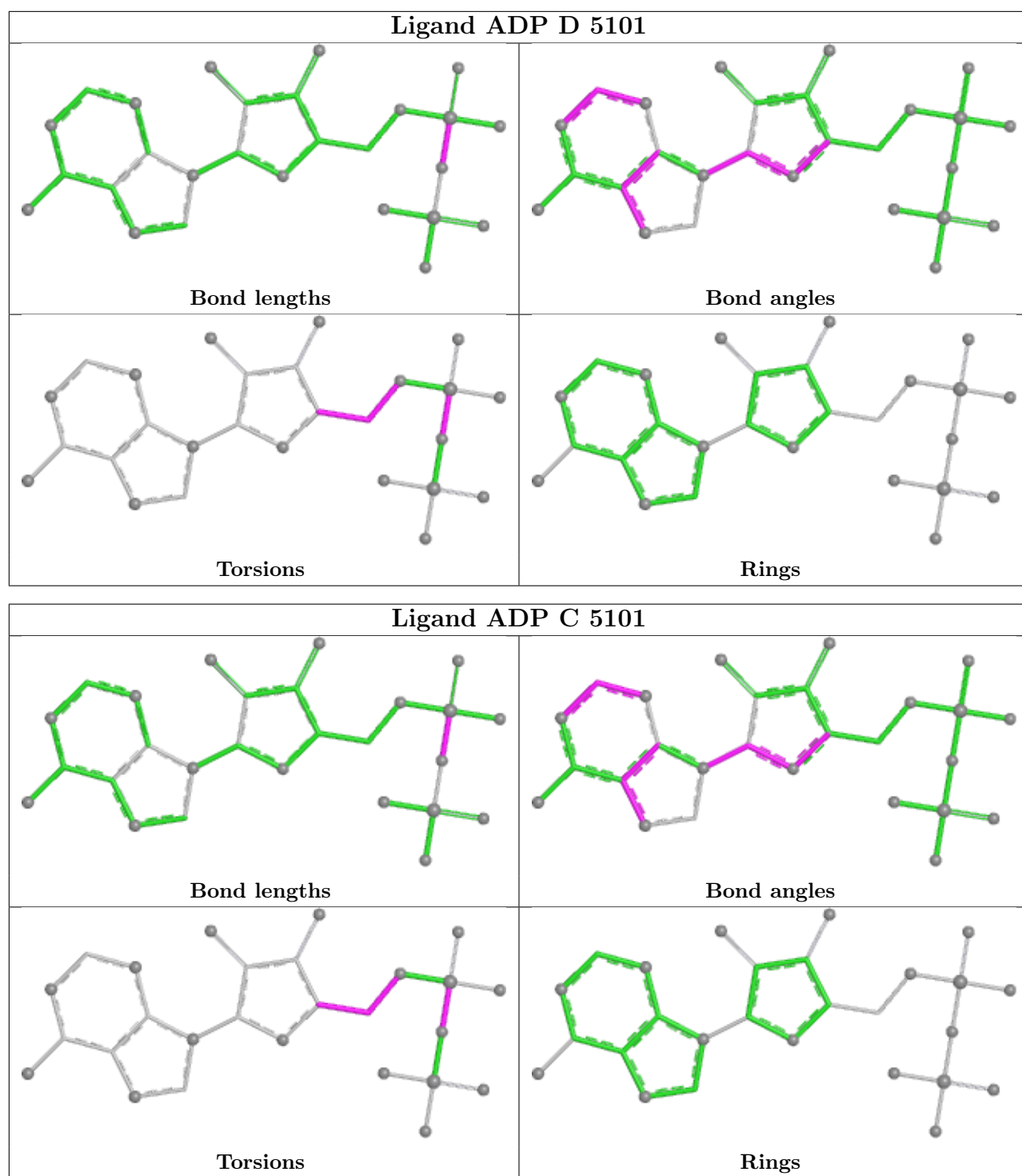
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5101	ADP	1	0
3	B	5101	ADP	1	0
3	D	5101	ADP	1	0
3	C	5101	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

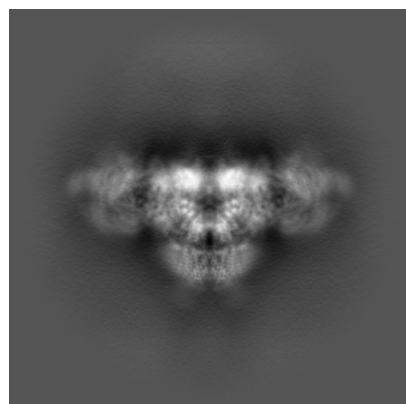
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40424. These allow visual inspection of the internal detail of the map and identification of artifacts.

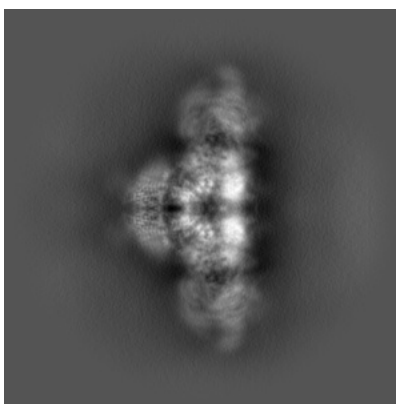
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

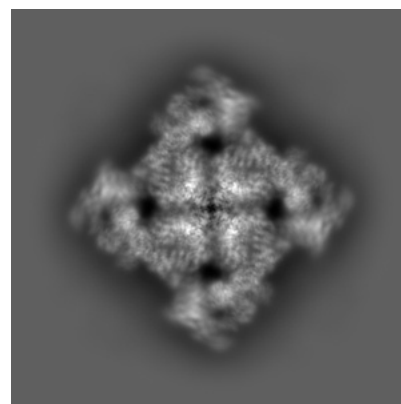
6.1.1 Primary map



X

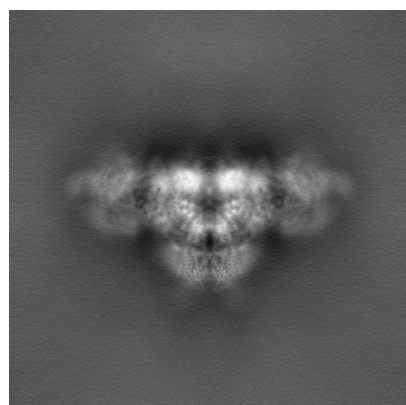


Y

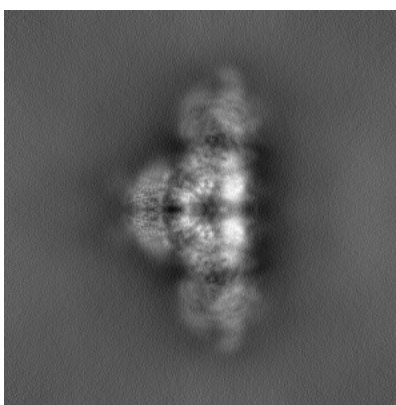


Z

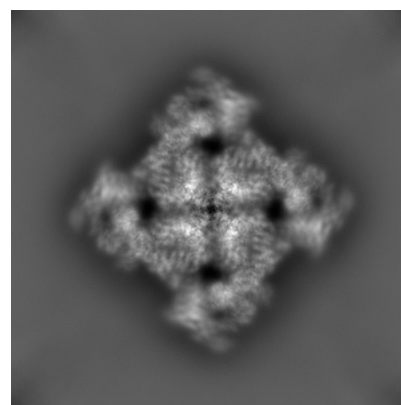
6.1.2 Raw map



X



Y

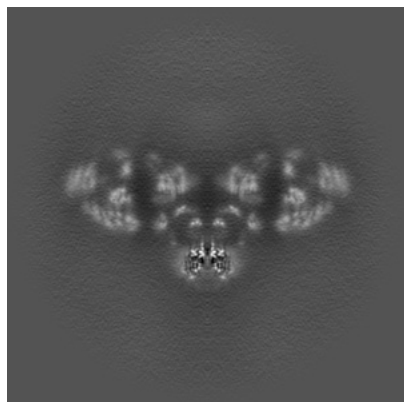


Z

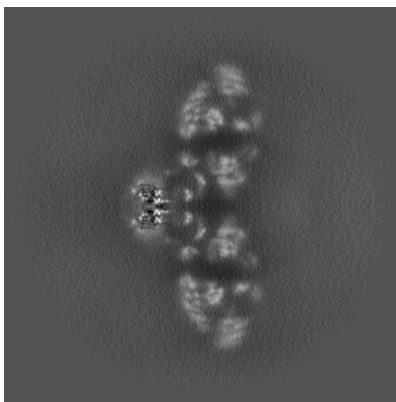
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

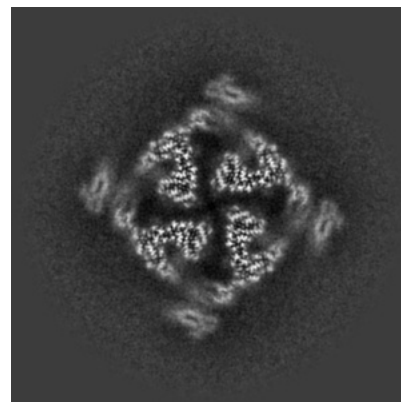
6.2.1 Primary map



X Index: 200

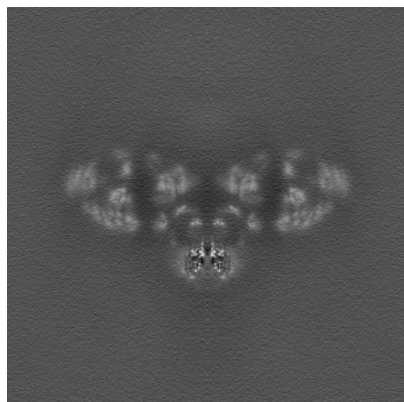


Y Index: 200

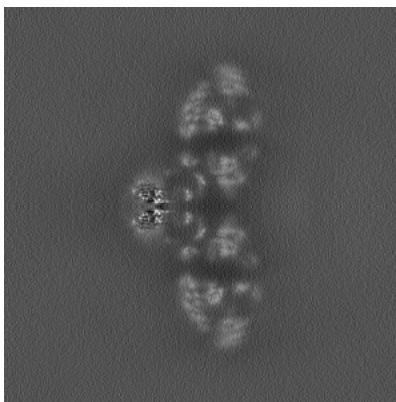


Z Index: 200

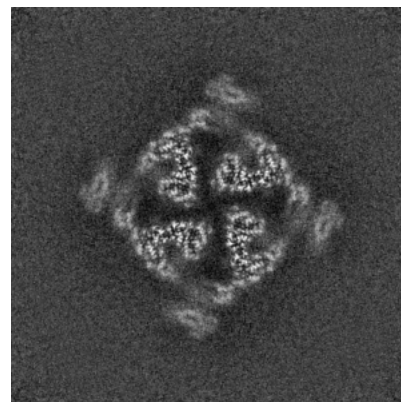
6.2.2 Raw map



X Index: 200



Y Index: 200

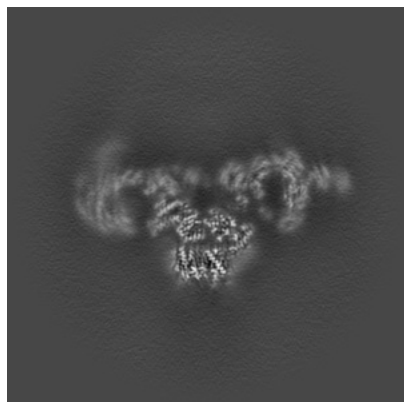


Z Index: 200

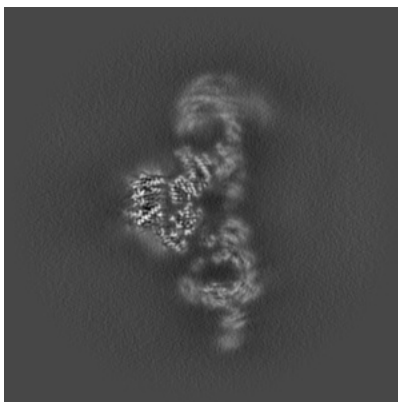
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

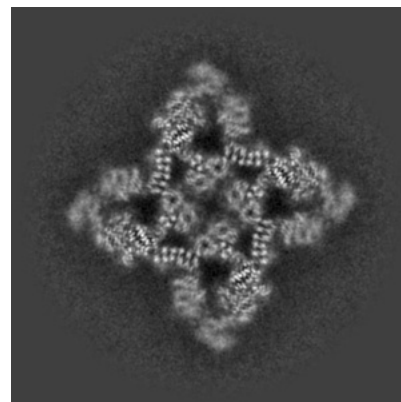
6.3.1 Primary map



X Index: 186

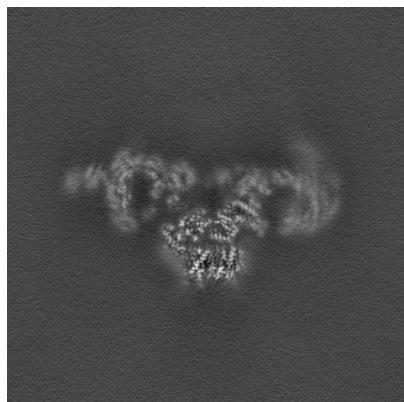


Y Index: 186

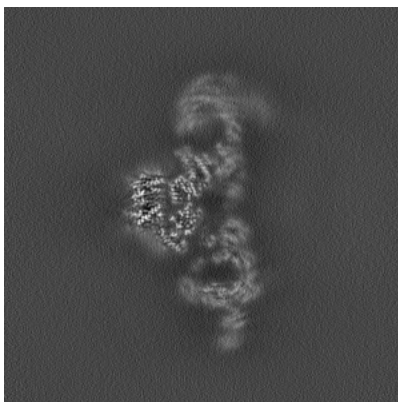


Z Index: 223

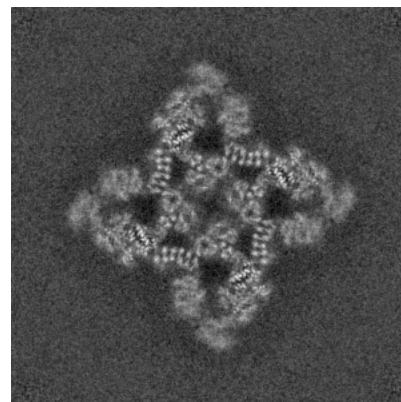
6.3.2 Raw map



X Index: 214



Y Index: 186

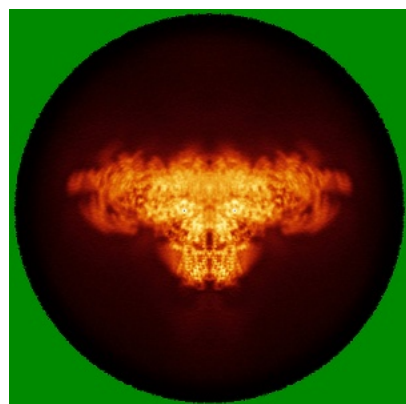


Z Index: 223

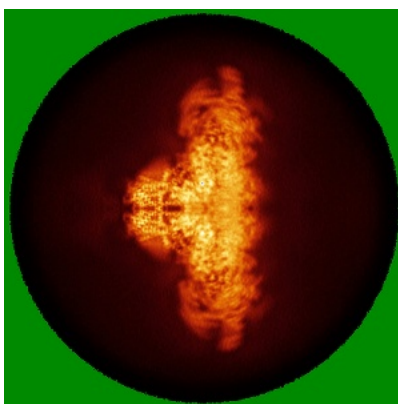
The images above show the largest variance slices of the map in three orthogonal directions.

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

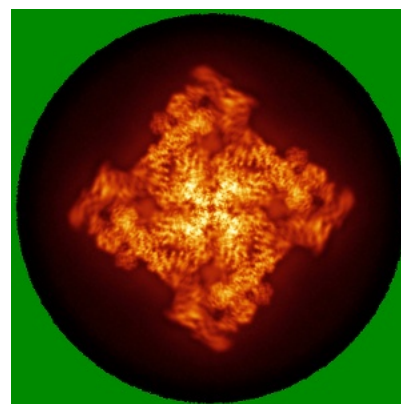
6.4.1 Primary map



X

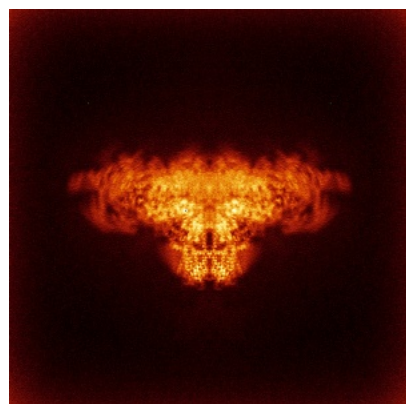


Y

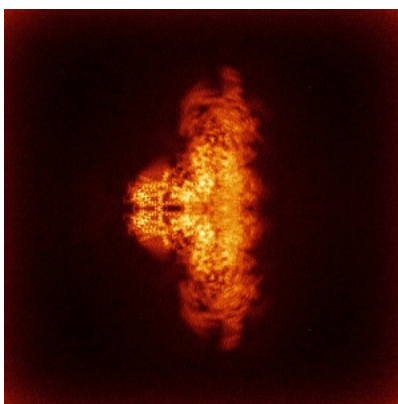


Z

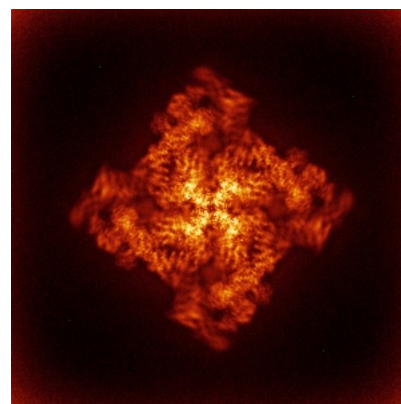
6.4.2 Raw map



X



Y

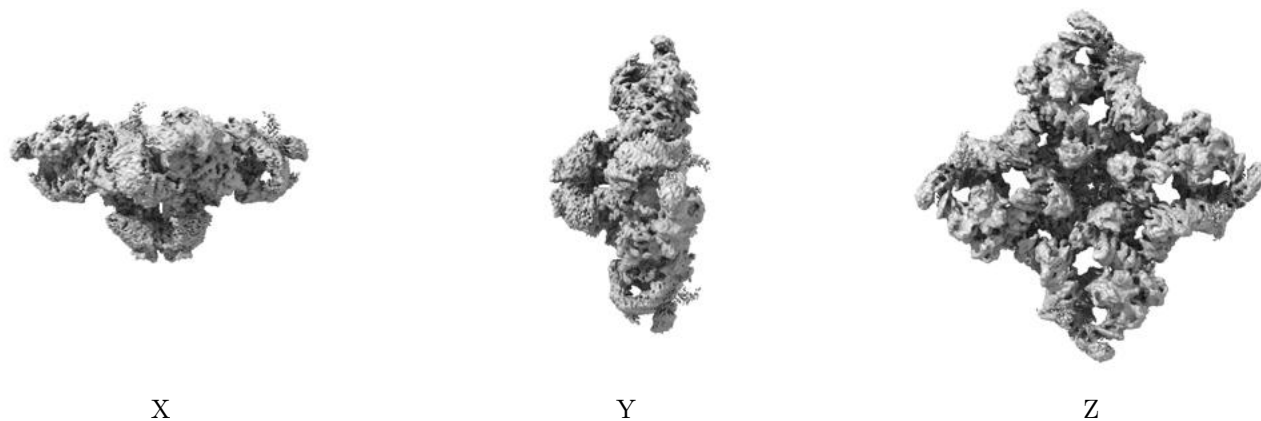


Z

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.

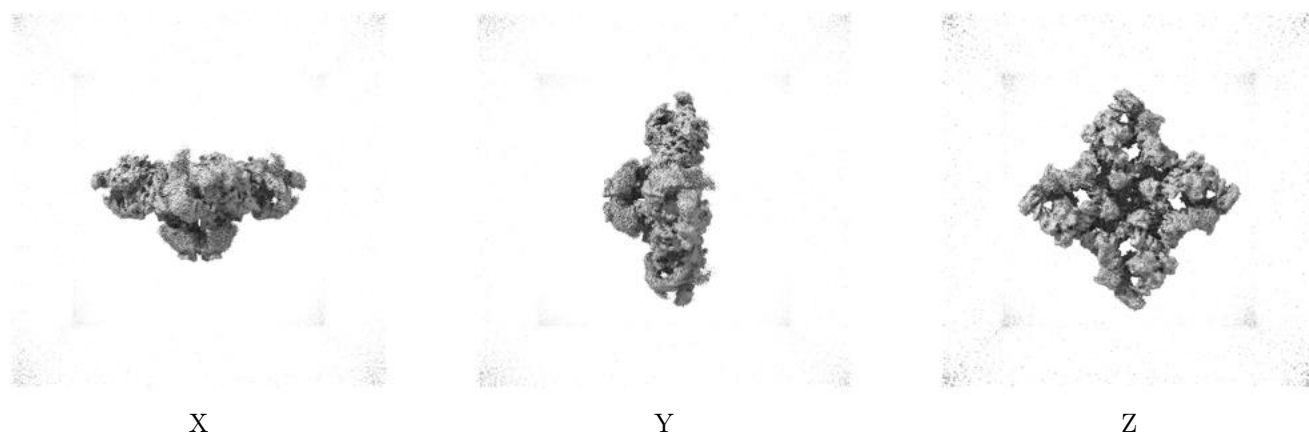
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.263. 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.

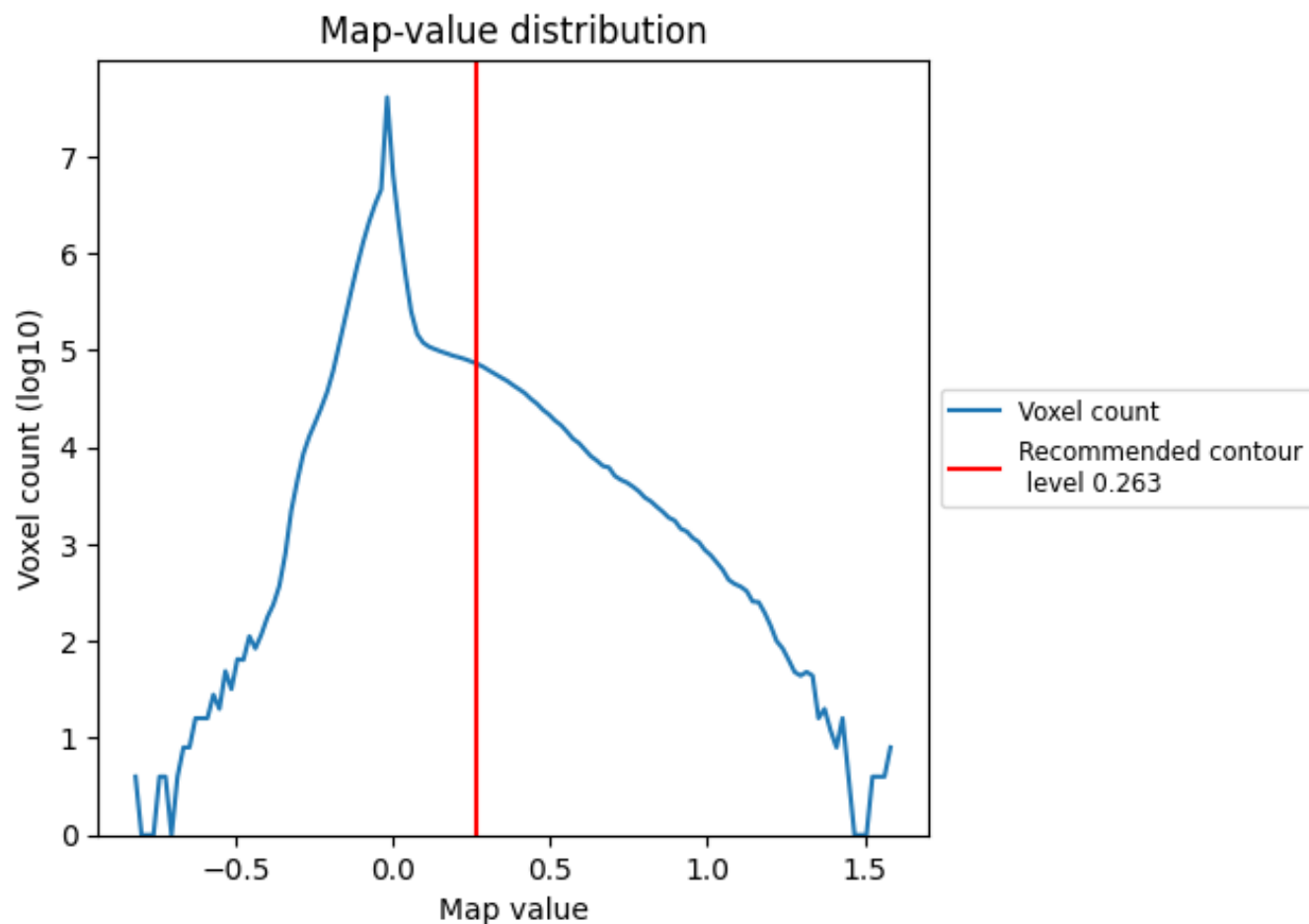
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

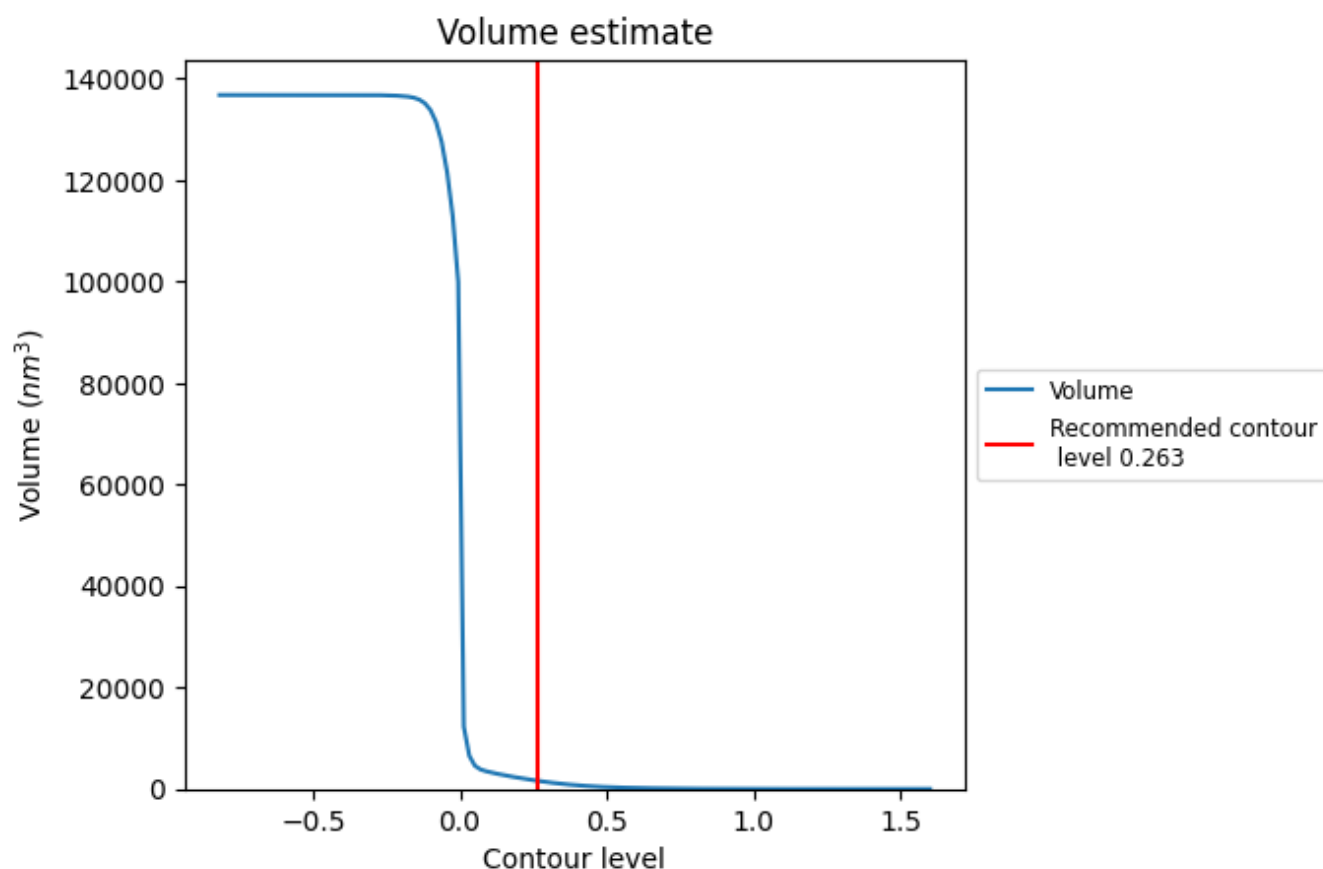
This section contains the results of statistical analysis of the map.

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.

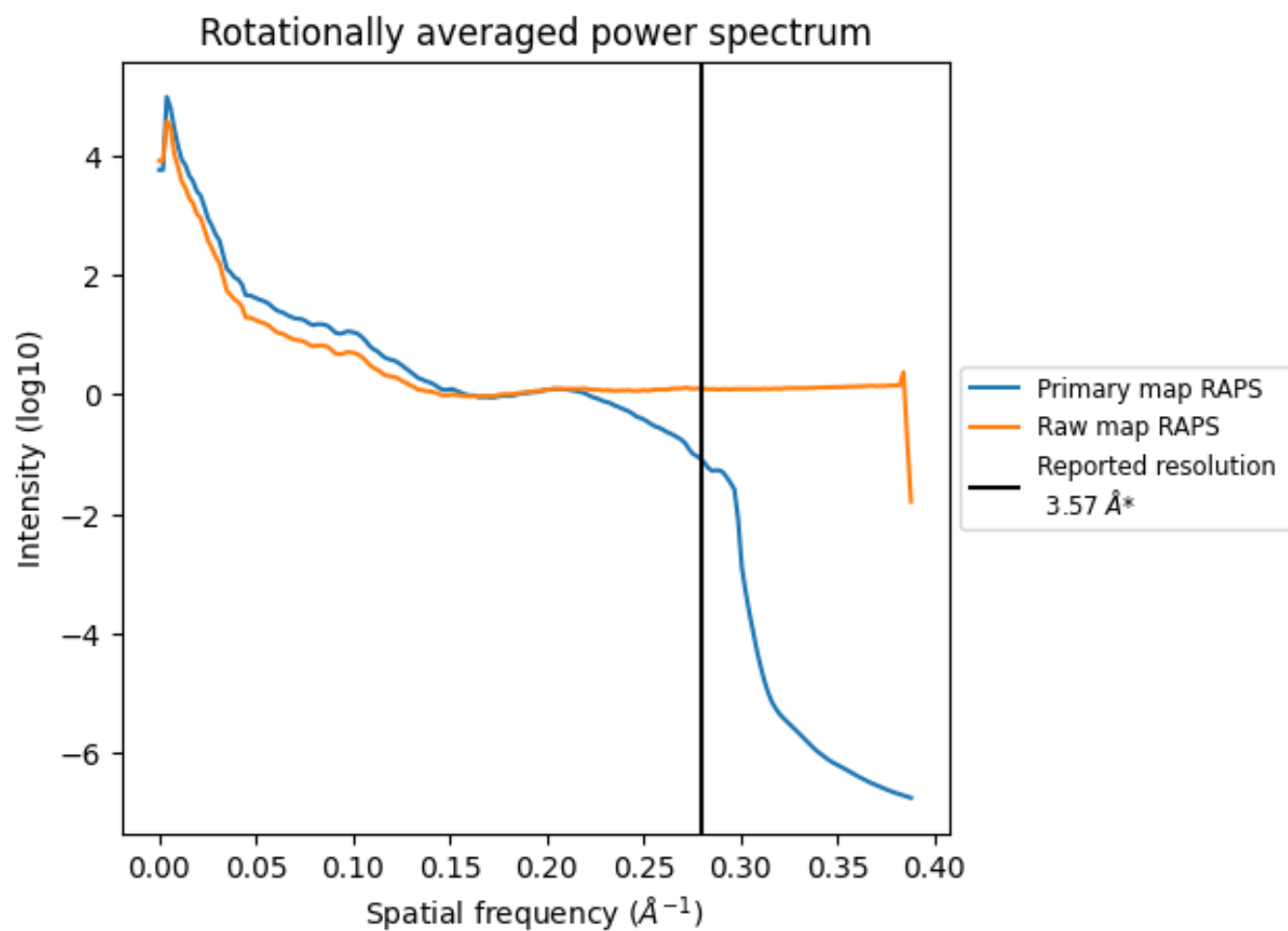
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1622 nm^3 ; this corresponds to an approximate mass of 1465 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 ⓘ

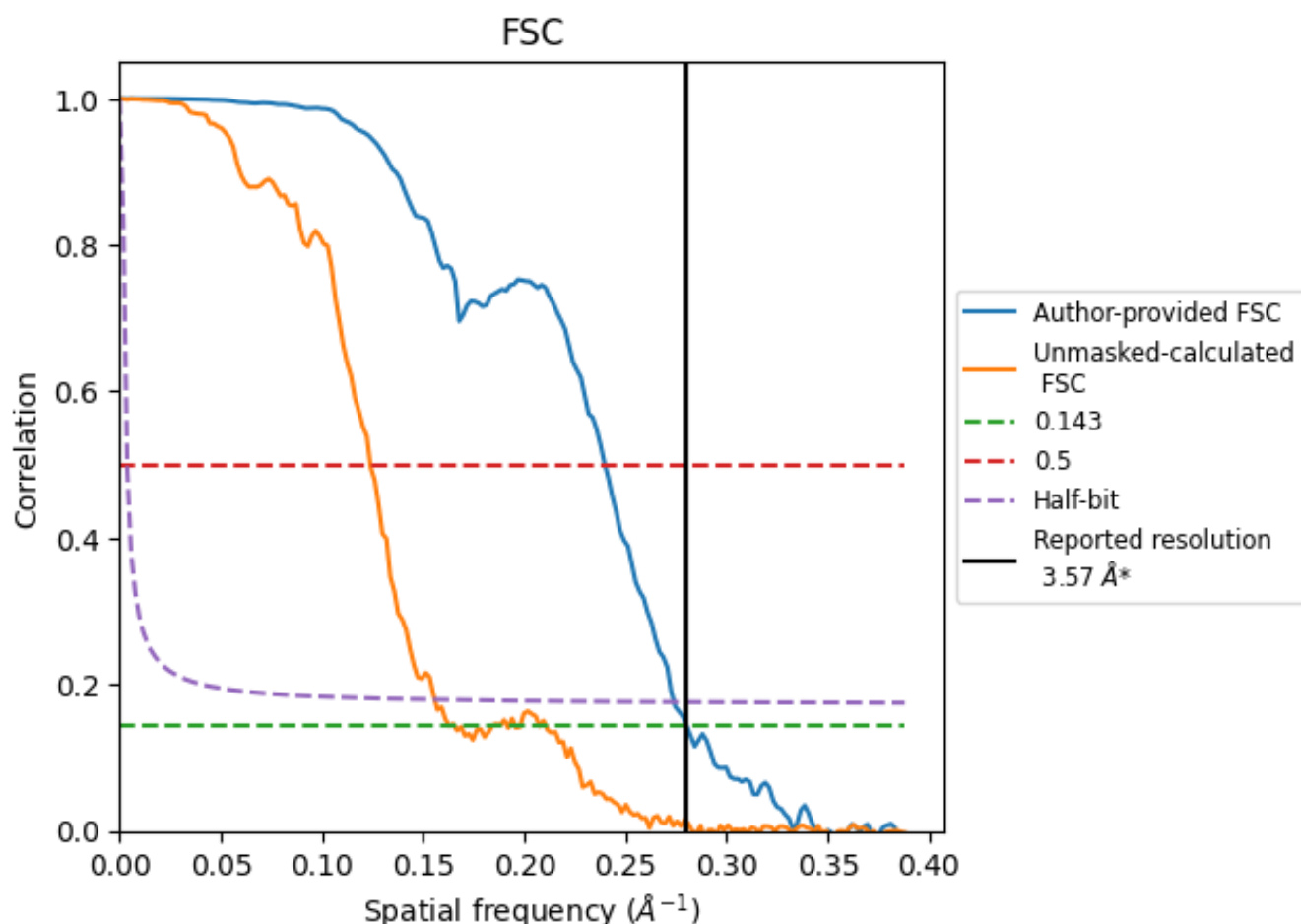


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

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 0.280 \AA^{-1}

8.2 Resolution estimates [i](#)

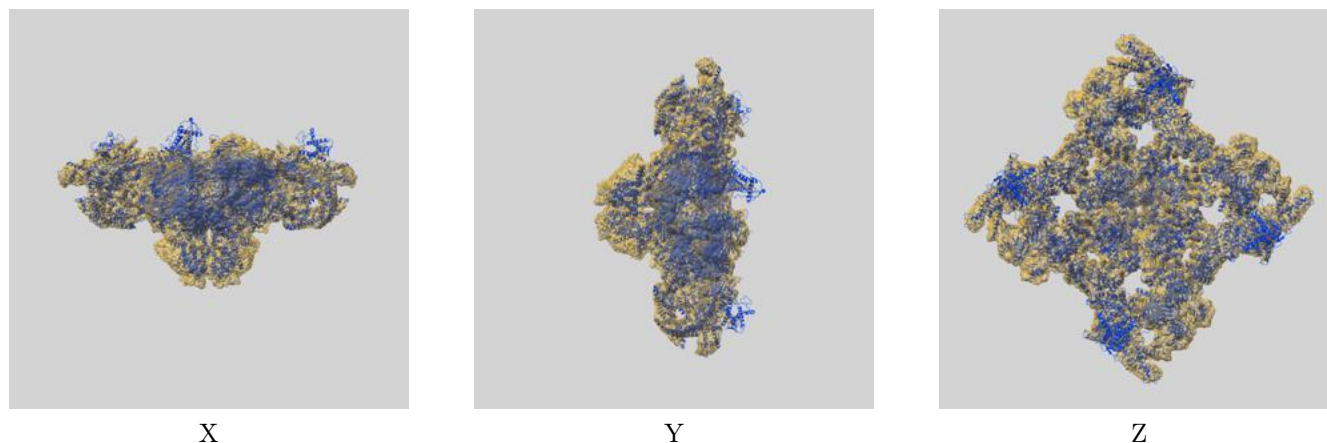
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.17	3.65
Unmasked-calculated*	6.04	8.06	6.41

*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 6.04 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

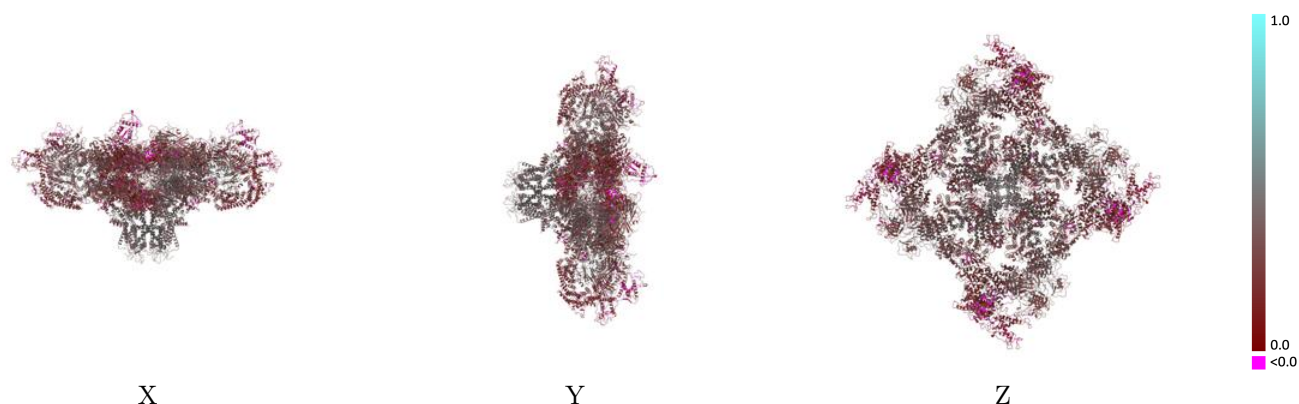
This section contains information regarding the fit between EMDB map EMD-40424 and PDB model 8SEP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



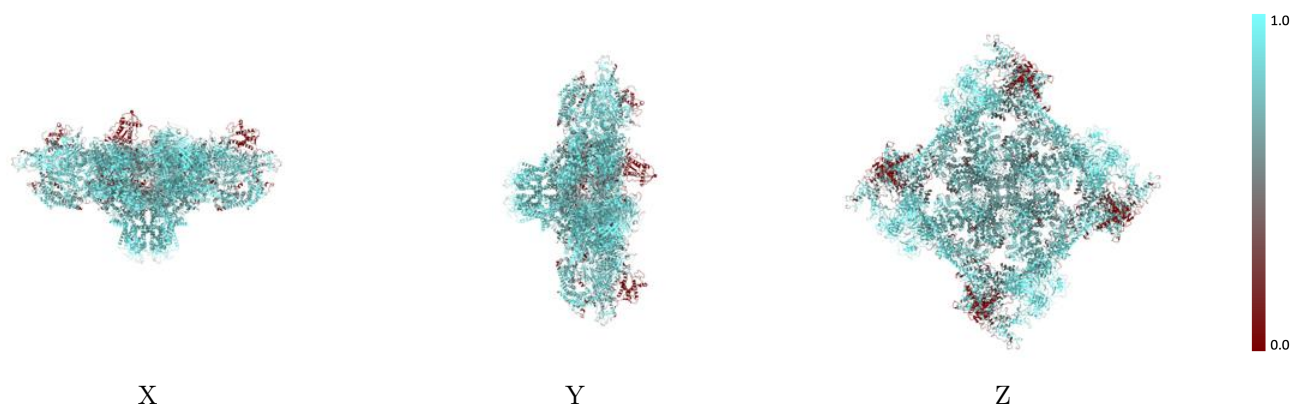
The images above show the 3D surface view of the map at the recommended contour level 0.263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



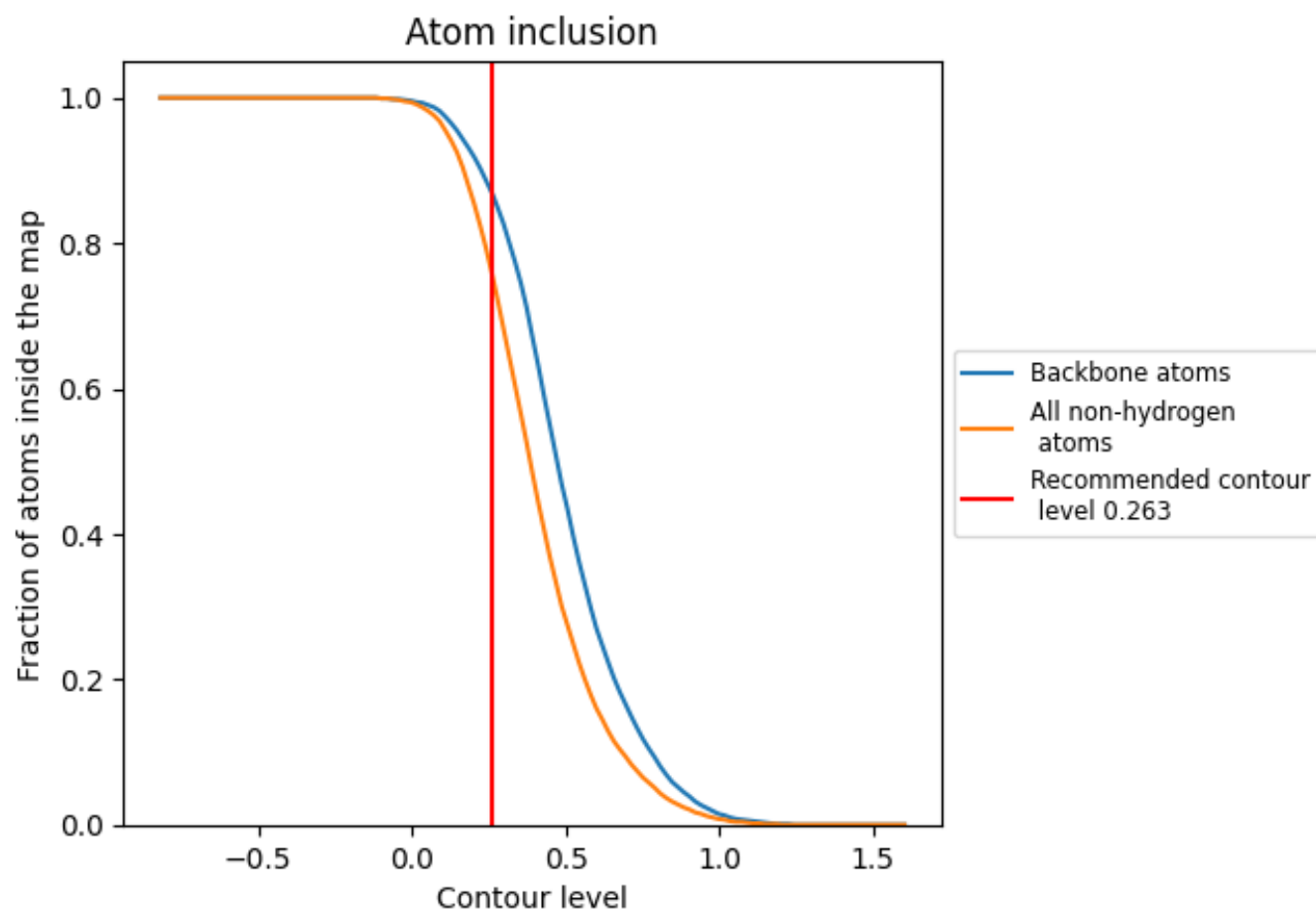
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.263).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7520	<div></div> 0.2890
A	<div></div> 0.7480	<div></div> 0.2870
B	<div></div> 0.7490	<div></div> 0.2880
C	<div></div> 0.7490	<div></div> 0.2880
D	<div></div> 0.7490	<div></div> 0.2880
E	<div></div> 0.9160	<div></div> 0.3620
F	<div></div> 0.9160	<div></div> 0.3620
G	<div></div> 0.9160	<div></div> 0.3620
H	<div></div> 0.9160	<div></div> 0.3620

1.0

0.0

<0.0