



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 09:25 AM EDT

PDB ID : 8DUJ  
EMDB ID : EMD-27721  
Title : Global map in C1 of RyR1 particles in complex with ImperaCalcin  
Authors : Haji-Ghassemi, O.; Van Petegm, F.  
Deposited on : 2022-07-27  
Resolution : 3.70 Å(reported)  
Based on initial model : 6M2W

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

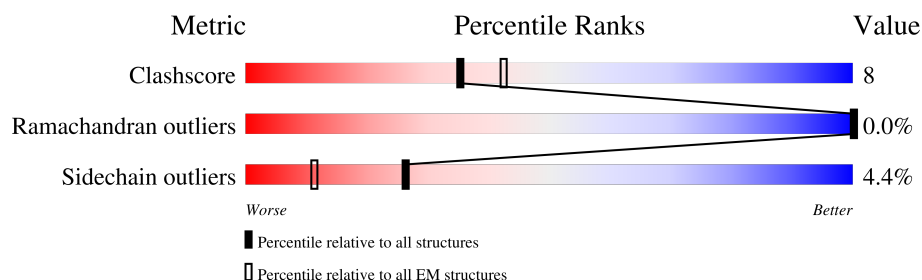
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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  $\geq 3$ , 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	M	33	<div> <div>24%</div> <div>67%</div> <div>33%</div> </div>
2	A	5037	<div> <div>11%</div> <div>64%</div> <div>12%</div> <div>24%</div> </div>
2	D	5037	<div> <div>15%</div> <div>68%</div> <div>8%</div> <div>23%</div> </div>
2	G	5037	<div> <div>8%</div> <div>66%</div> <div>12%</div> <div>22%</div> </div>
2	J	5037	<div> <div>7%</div> <div>67%</div> <div>10%</div> <div>23%</div> </div>
3	B	107	<div> <div>86%</div> <div>13%</div> </div>
3	E	107	<div> <div>12%</div> <div>86%</div> <div>13%</div> </div>
3	H	107	<div> <div>72%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	107	 70% 28% ..
4	C	149	 78% 87% 5% 8%
4	F	149	 76% 89% • 8%
4	I	149	 58% 91% • 7%
4	L	149	 70% 91% • 7%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 106156 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 Imperacalcin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	33	Total	C	N	O	S	33	0
			514	296	116	90	12		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	3933	Total	C	N	O	S	0	0
			26285	16856	4666	4625	138		
2	A	3823	Total	C	N	O	S	1	0
			24845	15885	4439	4407	114		
2	D	3865	Total	C	N	O	S	1	0
			23336	14719	4259	4281	77		
2	J	3892	Total	C	N	O	S	0	0
			25245	16153	4530	4440	122		

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	107	Total	C	N	O	S	0	0
			759	483	134	138	4		
3	B	107	Total	C	N	O	S	0	0
			735	465	130	136	4		
3	E	106	Total	C	N	O	S	0	0
			657	415	115	125	2		
3	K	106	Total	C	N	O	S	0	0
			758	483	135	136	4		

- Molecule 4 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	138	Total	C	N	O	S	0	0
			711	431	139	139	2		

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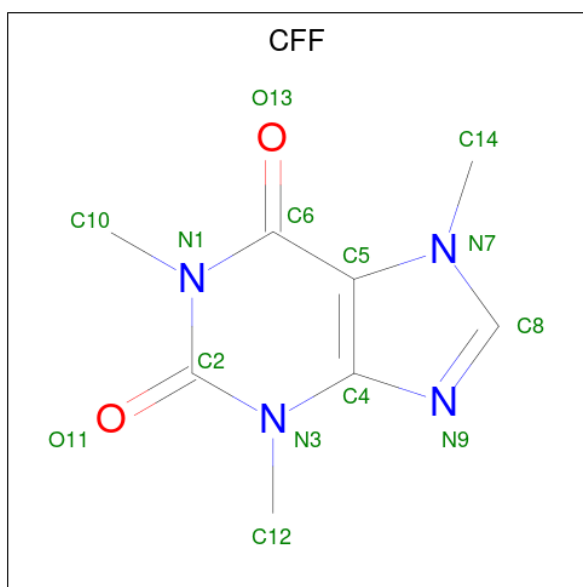
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	137	Total	C	N	O	S	0	0
			707	430	137	139	1		
4	F	137	Total	C	N	O		0	0
			710	434	137	139			
4	L	139	Total	C	N	O	S	0	0
			706	427	139	139	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	J	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

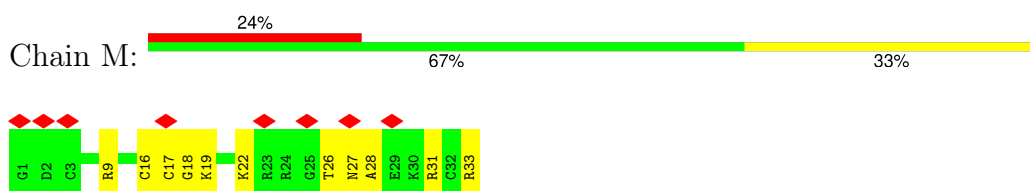
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
8	G	1	Total Zn 1 1	0
8	A	1	Total Zn 1 1	0
8	D	1	Total Zn 1 1	0
8	J	1	Total Zn 1 1	0

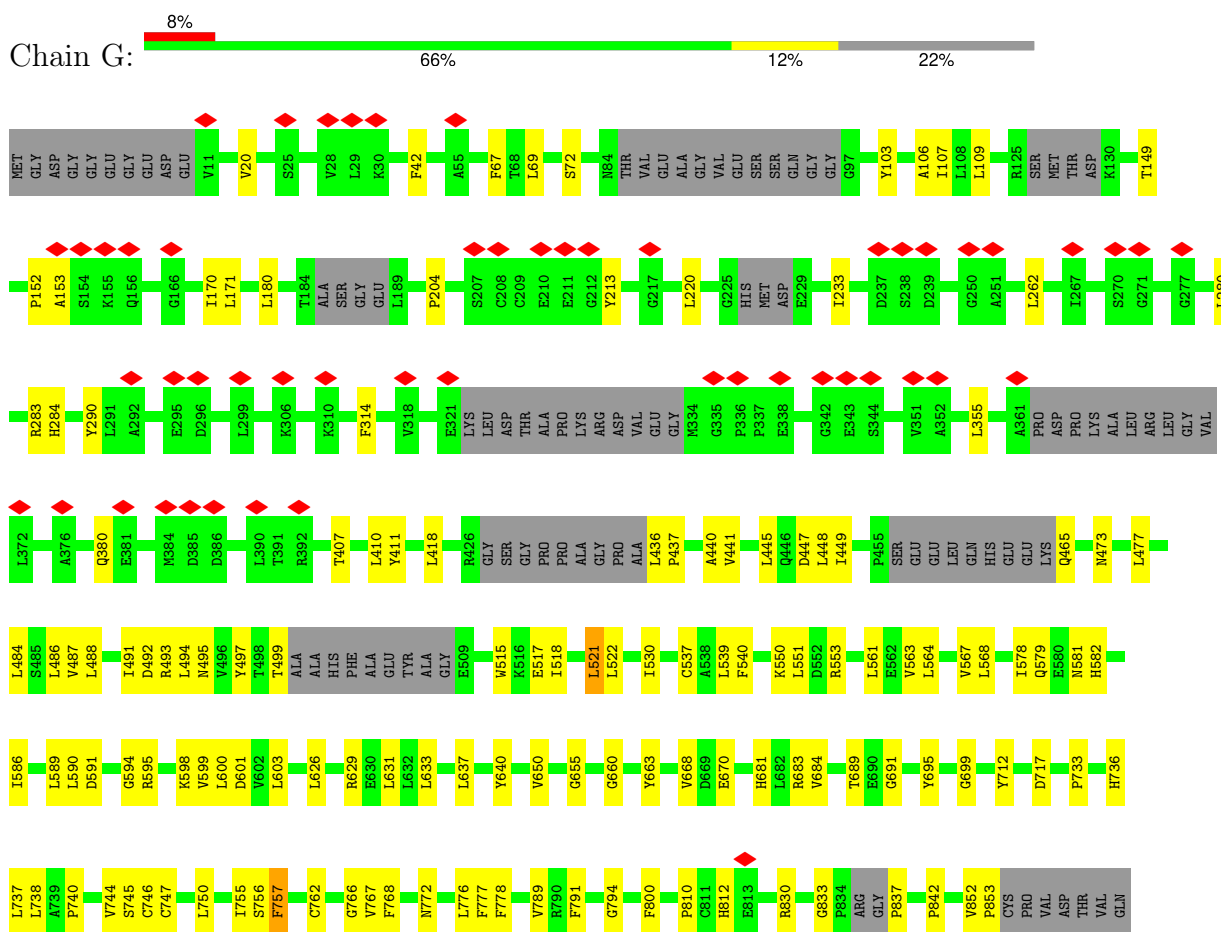
### 3 Residue-property plots [i](#)

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.

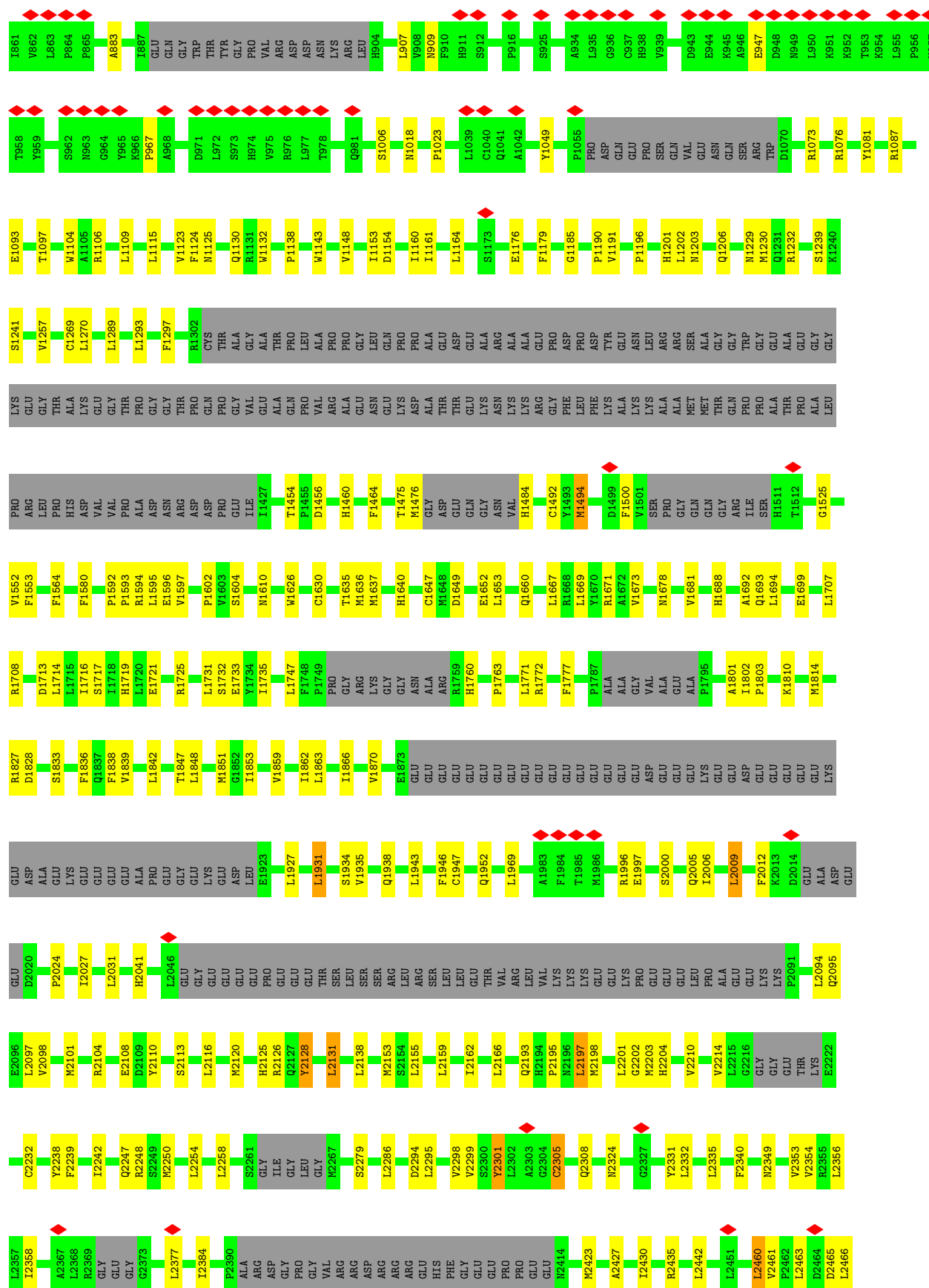
- Molecule 1: Imperacalcin

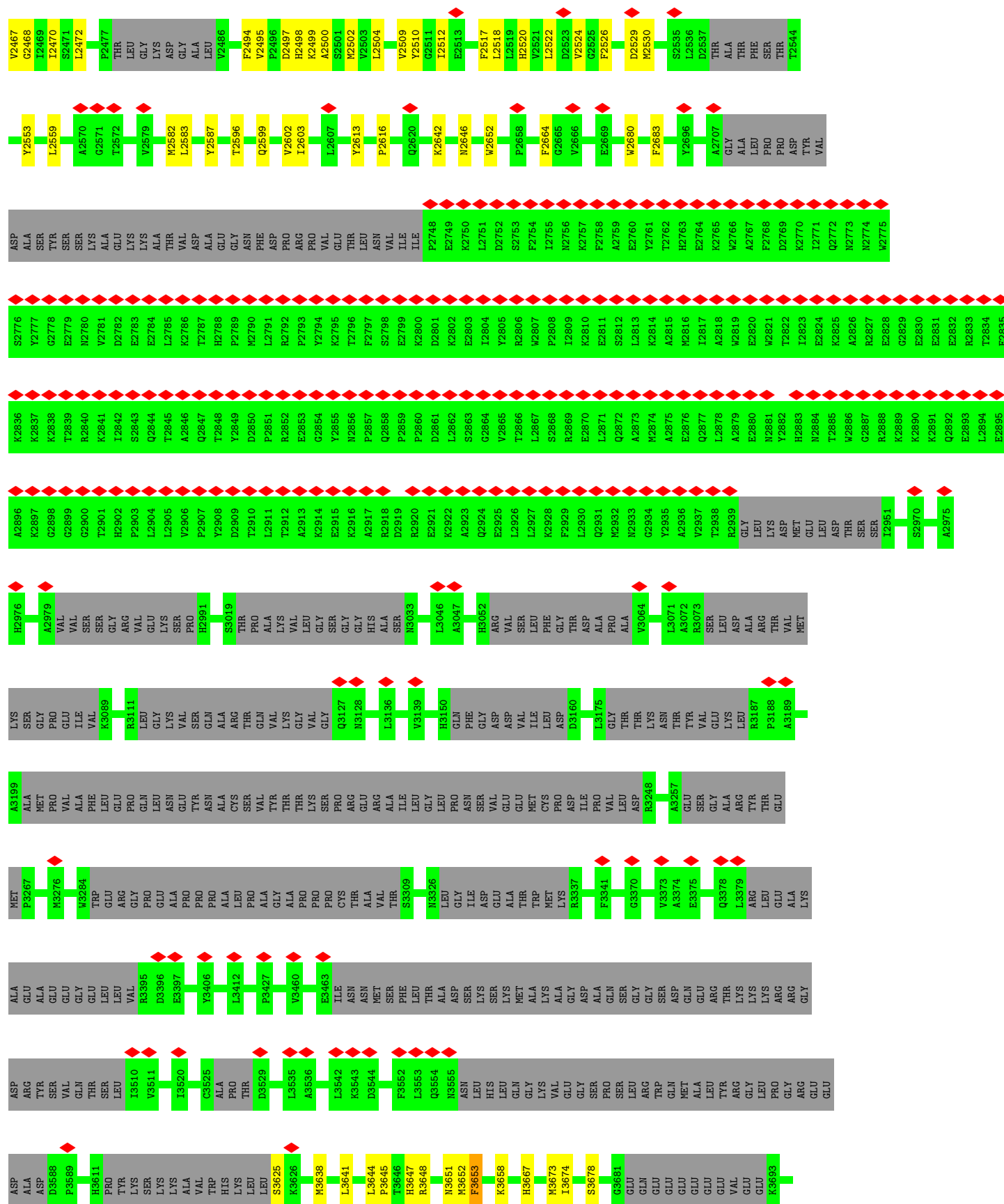


- Molecule 2: Ryanodine receptor 1





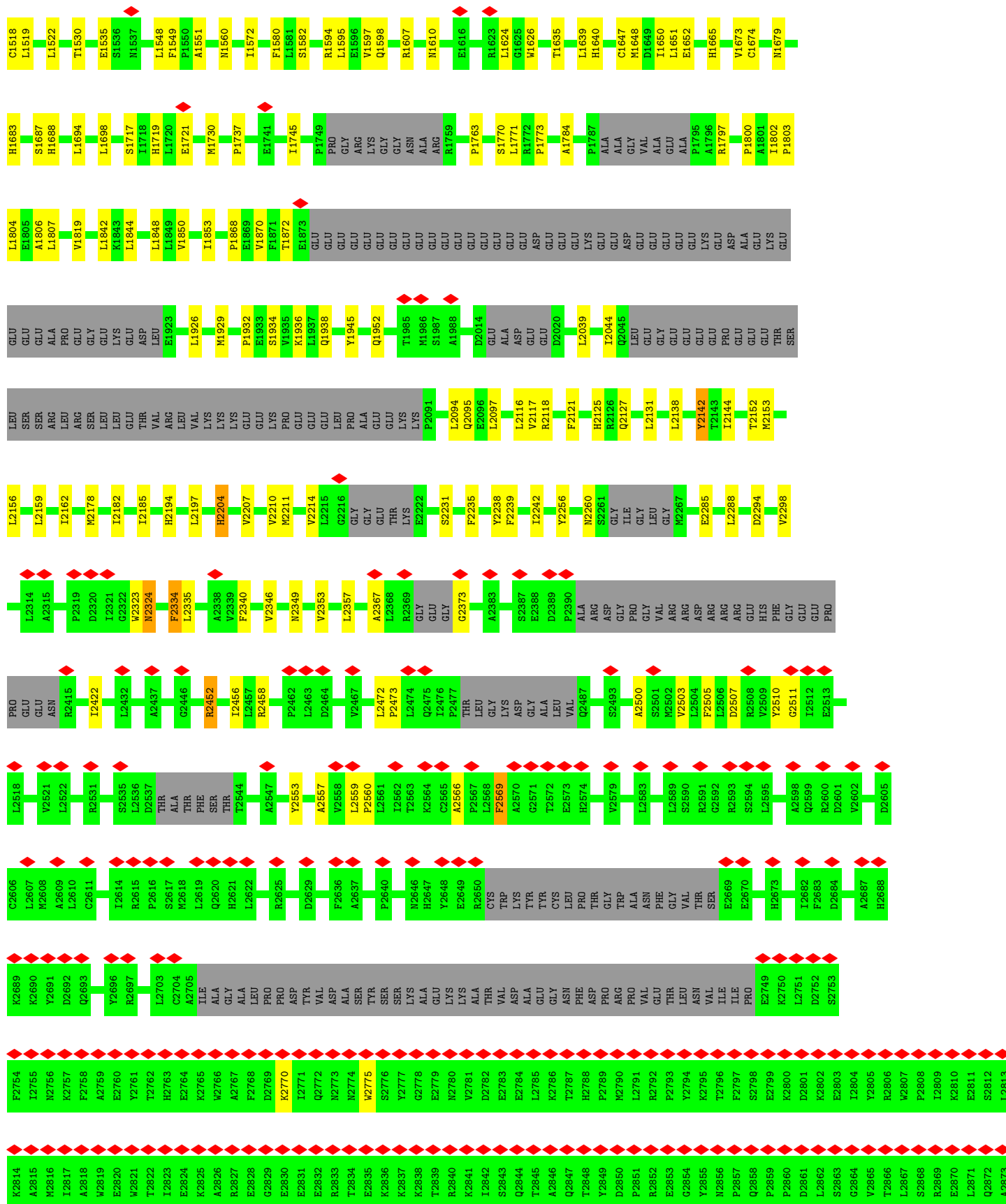




- Molecule 2: Ryanodine receptor 1











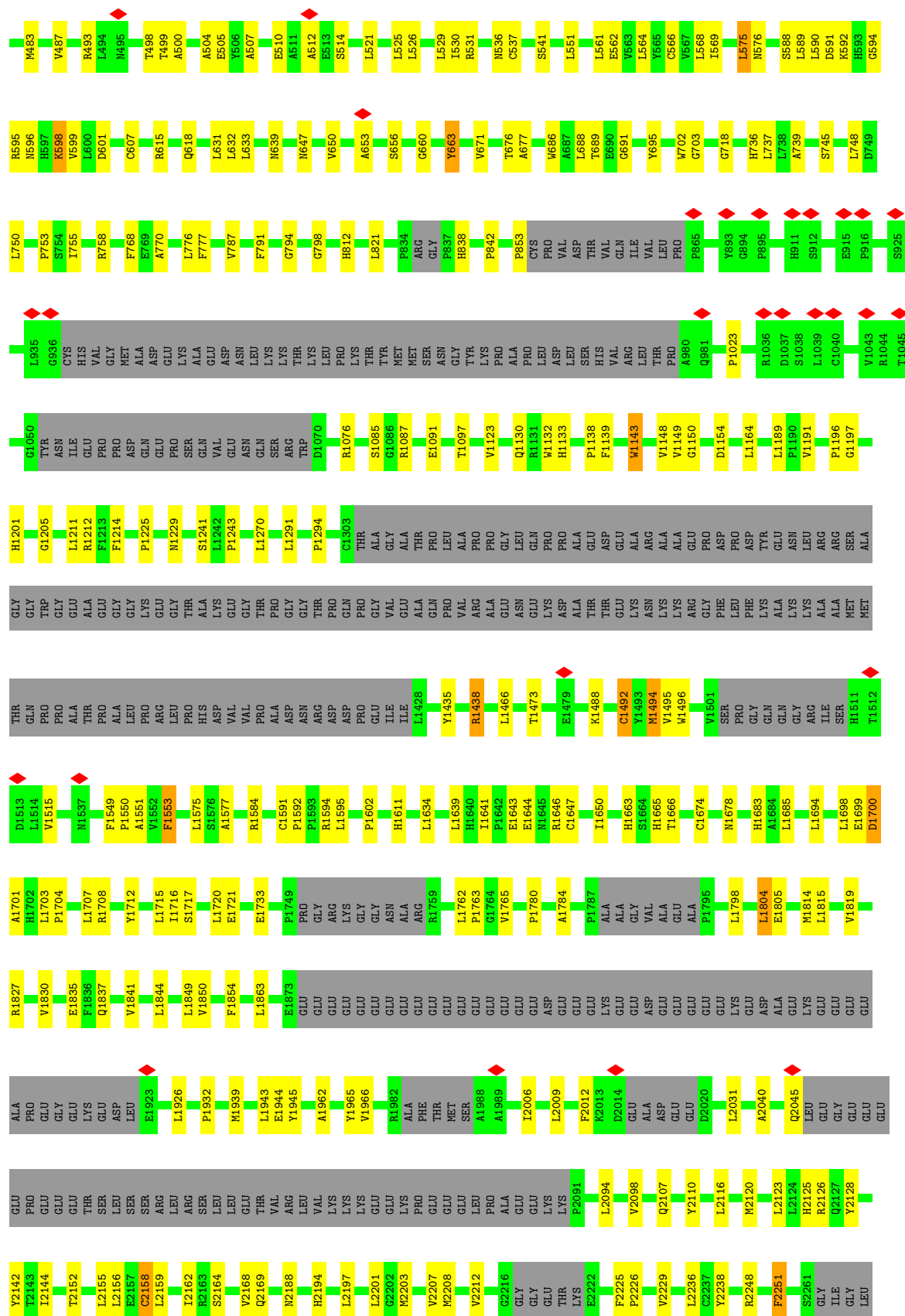












GLY	ASP	ARG	TYR	SER	VAL	GLY	GLY	LEU	VAL	L3510	L3511	L3514	K3515	L3522	A3526	D3529	L3532	L3535	R3539	K3543	D3544	V3549	F3552	L3553	Q3554	N3555	ASN	LEU	HIS	LEU	GLN	GLY	ASP	LYS	VAL	GLY	GLY	SER	PRO	SER	GLU	TRP	GLN	LYS	LYS	ALA	ARG											
M2267	P2272	L2281	D2282	N2283	L2286	A2287	L2288	D2294	L2295	V2298	V2299	C2305	M2312	L2313	L2314	A2315	L2335	R2336	F2337	N2349	V2353	V2354	R2355	L2368	R2369	GLY	GLY	G2373	L2377	A2378	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG																
ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	PRO	GLU	N2414	R2415	L2418	L2422	L2432	L2433	G2434	R2458	G2468	S2471	P2477	T2478	LEU	GLY	LYS	ASP	GLY	ALA	LEU	V2486	Q2487	P2488	K2489	S2493	H2498	K2499	A2500	V2503	L2504	F2505	R2508	V2509	Y2510	D2516												
G2525	A2534	S2535	L2536	D2537	THR	ALA	THR	PHE	SER	THR	T2544	E2545	M2546	Y2553	G2571	T2572	L2589	R2593	S2594	I2614	S2617	F2628	N2634	P2658	A2662	T2667	S2668	E2669	W2680	F2683	R2697	L2703	L2710	P2711	PRO	ASP	TYR	VAL	ASP	ALA	SER																	
TYR	SER	SER	LYS	GLU	ALA	LYS	THR	VAL	ASP	ALA	GLU	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	ASN	VAL	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	N2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778					
E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	H2788	P2789	M2790	L2791	R2792	T2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2802	E2803	L2804	Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	N2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	E2831	E2832	R2833	T2834	E2835	K2836	K2837	K2838
T2839	R2840	K2841	T2842	S2843	Q2844	T2845	A2846	Q2847	T2848	Y2849	D2850	P2851	R2852	E2853	G2854	Y2855	N2856	P2857	Q2858	P2859	T2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900
T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	SER	SER	I2951	S2970	A2979	VAL	VAL	SER	GLY			
ARG	VAL	GLU	LYS	SER	PRO	H2991	E2992	K3000	L3001	L3002	F3017	L3018	S3019	THR	PRO	ALA	LYS	VAL	LEU	GLY	SER	HIS	GLY	ALA	SER	N3033	L3046	H3052	ARG	VAL	SER	PHE	GLY	THR	ALA	ALA	PRO	ALA	Y3064	R3073	SER	LEU	ASP	ALA	ARG	THR	VAL	MET	LYS	SER	GLY	PRO						
GLU	ILE	K3089	E3108	R3111	R3112	R3113	GLY	VAL	VAL	GLN	ALA	ARG	THR	GLN	VAL	LYS	GLY	VAL	GLY	Q3127	Y3131	T3132	T3133	V3134	A3135	L3136	Y3140	H3150	PHE	GLY	ASP	ASP	VAL	ILE	LEU	ASP	D3160	L3175	GLY	THR	THR	LYS	ASN	TYR	THR	VAL	GLU	LYS	R3187									
A3199	ALA	MET	PRO	VAL	ALA	PHE	LEU	PRO	GLN	LEU	ASN	GLU	TYR	ASN	ALA	CYS	VAL	VAL	THR	THR	LYS	PRO	ARG	GLU	ARG	ALA	ILE	LEU	GLY	LEU	PRO	ASN	SER	VAL	GLU	GLY	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	H3248	L3249	M3250	A3251	A3257	GLU	SER	GLY	ALA	ARG			
TYR	THR	GLU	MET	P3267	L3281	W3284	TRP	GLU	ARG	GLY	PRO	GLU	ALA	PRO	PRO	ALA	ALA	ALA	ALA	ALA	GLY	ALA	PRO	PRO	PRO	PRO	CYS	THR	ALA	VAL	THR	S3309	R3326	LEU	GLY	ILE	ASP	GLU	ALA	ALA	THR	TRP	MET	LYS	R3337	A3342	F3351	A3369	Q3378	LEU	ARG	LEU	GLU	ALA				
LYS	ALA	GLU	ALA	GLU	GLY	GLU	LEU	VAL	R3395	D3396	E3397	V3400	L3408	F3435	G3439	E3463	ILE	ASN	ASN	MET	SER	PHE	LEU	THR	ALA	ALA	ASP	ASP	ASP	ASP	ASP	ASN	SER	SER	LYS	SER	LYS	GLY	GLY	ASP	GLN	GLU	THR	LYS	LYS	LYS	LYS	ALA	ARG	ARG								
GLY	ASP	ARG	TYR	SER	VAL	GLN	THR	SER	L3510	V3511	L3514	K3515	L3522	A3526	D3529	L3532	L3535	R3539	K3543	P3544	V3549	F3552	L3553	Q3554	N3555	ASN	LEU	HIS	LEU	GLN	GLY	LYS	VAL	GLU	GLY	VAL	GLU	GLY	SER	PRO	GLU	LEU	ARG	TRP	GLN	MET	ALA	TYR	ARG	GLY								




- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




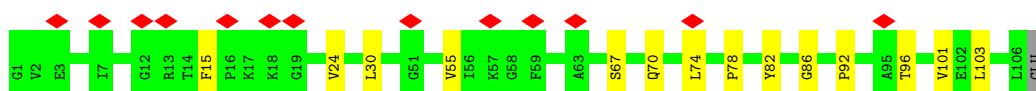
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 



- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 

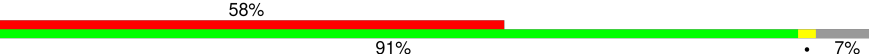


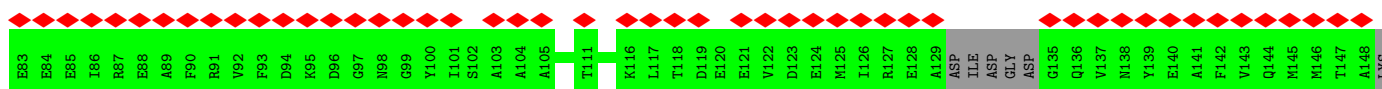
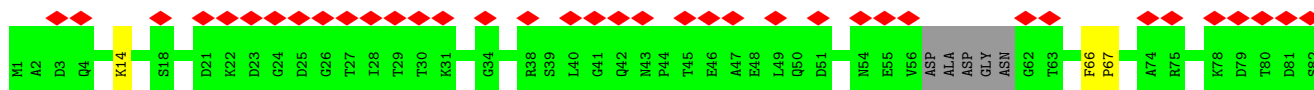
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K: 




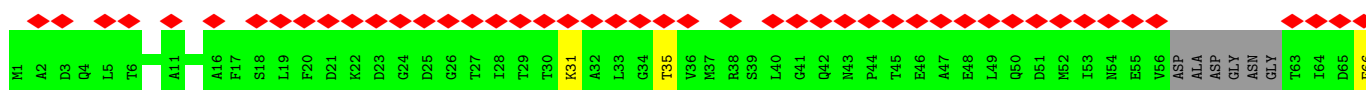
- Molecule 4: Calmodulin-1

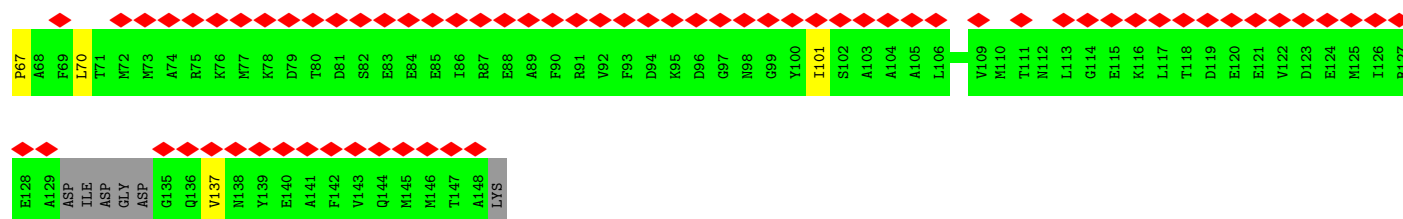
Chain I: 



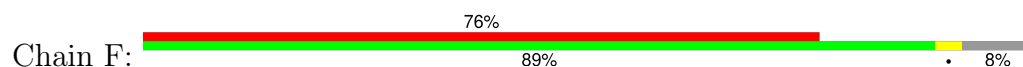
- Molecule 4: Calmodulin-1

Chain C: 

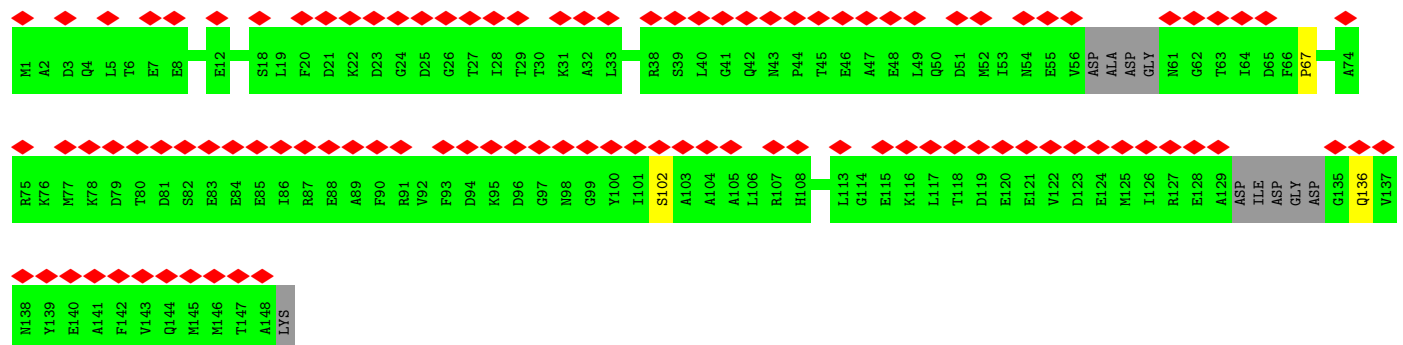




• Molecule 4: Calmodulin-1



• Molecule 4: Calmodulin-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	144529	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.559	Depositor
Minimum map value	-1.060	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, CFF, CA, ATP

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	M	0.25	0/516	0.62	0/672
2	A	0.27	0/25342	0.46	0/34836
2	D	0.27	0/23698	0.43	0/32668
2	G	0.25	0/26809	0.45	0/36763
2	J	0.26	0/25729	0.44	0/35328
3	B	0.26	0/751	0.55	0/1025
3	E	0.24	0/671	0.42	0/926
3	H	0.27	0/775	0.55	0/1054
3	K	0.32	0/774	0.55	0/1051
4	C	0.24	0/707	0.38	0/978
4	F	0.24	0/711	0.35	0/984
4	I	0.23	0/711	0.35	0/981
4	L	0.24	0/706	0.35	0/976
All	All	0.26	0/107900	0.45	0/148242

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	514	0	522	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	24845	0	19916	424	0
2	D	23336	0	16446	294	0
2	G	26285	0	21941	392	0
2	J	25245	0	20257	321	0
3	B	735	0	669	11	0
3	E	657	0	537	7	0
3	H	759	0	724	19	0
3	K	758	0	735	21	0
4	C	707	0	386	5	0
4	F	710	0	386	3	0
4	I	711	0	383	4	0
4	L	706	0	363	2	0
5	A	14	0	10	0	0
5	D	14	0	10	1	0
5	G	14	0	10	0	0
5	J	14	0	10	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	A	31	0	12	2	0
7	D	31	0	12	1	0
7	G	31	0	12	3	0
7	J	31	0	12	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
All	All	106156	0	83353	1461	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 1461 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:A:415:ILE:CD1	2:A:493:ARG:HD2	1.68	1.23
2:A:415:ILE:HD11	2:A:493:ARG:CD	1.68	1.21
2:D:4055:VAL:HG11	2:D:4163:PHE:CZ	1.91	1.05
2:A:4048:LEU:HD11	2:A:4055:VAL:HG21	1.36	1.03
2:A:357:LEU:HB2	2:A:378:LEU:HA	1.45	0.98

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	M	62/33 (188%)	56 (90%)	6 (10%)	0	100	100
2	A	3718/5037 (74%)	3668 (99%)	48 (1%)	2 (0%)	48	78
2	D	3750/5037 (74%)	3701 (99%)	49 (1%)	0	100	100
2	G	3827/5037 (76%)	3774 (99%)	53 (1%)	0	100	100
2	J	3786/5037 (75%)	3726 (98%)	60 (2%)	0	100	100
3	B	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	E	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
3	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	K	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
4	C	131/149 (88%)	131 (100%)	0	0	100	100
4	F	131/149 (88%)	130 (99%)	1 (1%)	0	100	100
4	I	132/149 (89%)	132 (100%)	0	0	100	100
4	L	133/149 (89%)	131 (98%)	2 (2%)	0	100	100
All	All	16088/21205 (76%)	15849 (98%)	237 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4052	SER
2	A	614	VAL

### 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	M	56/28 (200%)	56 (100%)	0	100	100
2	A	1728/4276 (40%)	1650 (96%)	78 (4%)	23	50
2	D	1204/4276 (28%)	1137 (94%)	67 (6%)	17	45
2	G	1976/4276 (46%)	1902 (96%)	74 (4%)	29	54
2	J	1721/4276 (40%)	1640 (95%)	81 (5%)	22	48
3	B	67/88 (76%)	66 (98%)	1 (2%)	60	75
3	E	49/88 (56%)	48 (98%)	1 (2%)	50	68
3	H	73/88 (83%)	72 (99%)	1 (1%)	62	76
3	K	74/88 (84%)	72 (97%)	2 (3%)	40	61
4	C	9/123 (7%)	9 (100%)	0	100	100
4	F	9/123 (7%)	8 (89%)	1 (11%)	5	24
4	I	8/123 (6%)	8 (100%)	0	100	100
4	L	5/123 (4%)	5 (100%)	0	100	100
All	All	6979/17976 (39%)	6673 (96%)	306 (4%)	26	50

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	493	ARG
2	J	4065	PHE
2	J	702	TRP
2	J	2251	PHE
2	J	5012	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	639	ASN
2	J	4142	ASN
2	A	2127	GLN
2	A	3900	GLN
2	A	4043	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 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$
5	CFF	G	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.66	3 (37%)
7	ATP	D	5103	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
5	CFF	A	5101	-	8,15,15	1.16	1 (12%)	8,23,23	2.63	3 (37%)
5	CFF	D	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.66	3 (37%)
7	ATP	G	5103	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	CFF	J	5101	-	8,15,15	1.17	1 (12%)	8,23,23	2.65	3 (37%)
7	ATP	A	5103	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
7	ATP	J	5103	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CFF	G	5101	-	-	-	0/2/2/2
7	ATP	D	5103	-	-	12/18/38/38	0/3/3/3
5	CFF	A	5101	-	-	-	0/2/2/2
5	CFF	D	5101	-	-	-	0/2/2/2
7	ATP	G	5103	-	-	6/18/38/38	0/3/3/3
7	ATP	A	5103	-	-	6/18/38/38	0/3/3/3
5	CFF	J	5101	-	-	-	0/2/2/2
7	ATP	J	5103	-	-	8/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5101	CFF	C6-N1	2.83	1.42	1.38
5	J	5101	CFF	C6-N1	2.83	1.42	1.38
5	G	5101	CFF	C6-N1	2.82	1.42	1.38
5	A	5101	CFF	C6-N1	2.82	1.42	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5101	CFF	C5-C6-N1	-5.57	112.54	118.20
5	G	5101	CFF	C5-C6-N1	-5.56	112.56	118.20
5	A	5101	CFF	C5-C6-N1	-5.54	112.58	118.20
5	J	5101	CFF	C5-C6-N1	-5.53	112.58	118.20
5	G	5101	CFF	C4-C5-C6	3.89	122.92	119.96

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	5103	ATP	PB-O3B-PG-O2G
7	G	5103	ATP	C5'-O5'-PA-O2A
7	G	5103	ATP	C4'-C5'-O5'-PA
7	A	5103	ATP	PB-O3A-PA-O5'
7	A	5103	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

4 monomers are involved in 7 short contacts:

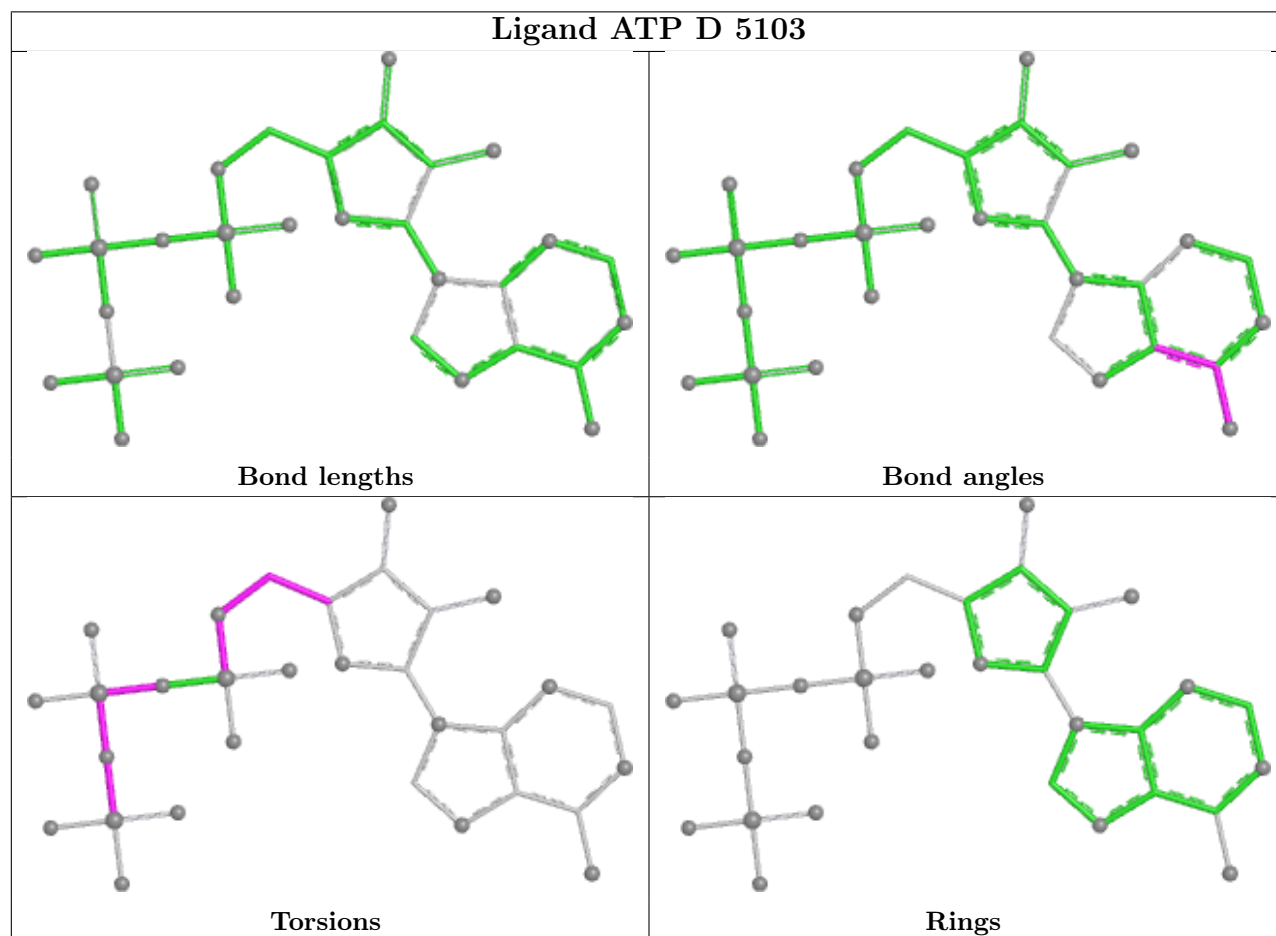
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	5103	ATP	1	0

*Continued on next page...*

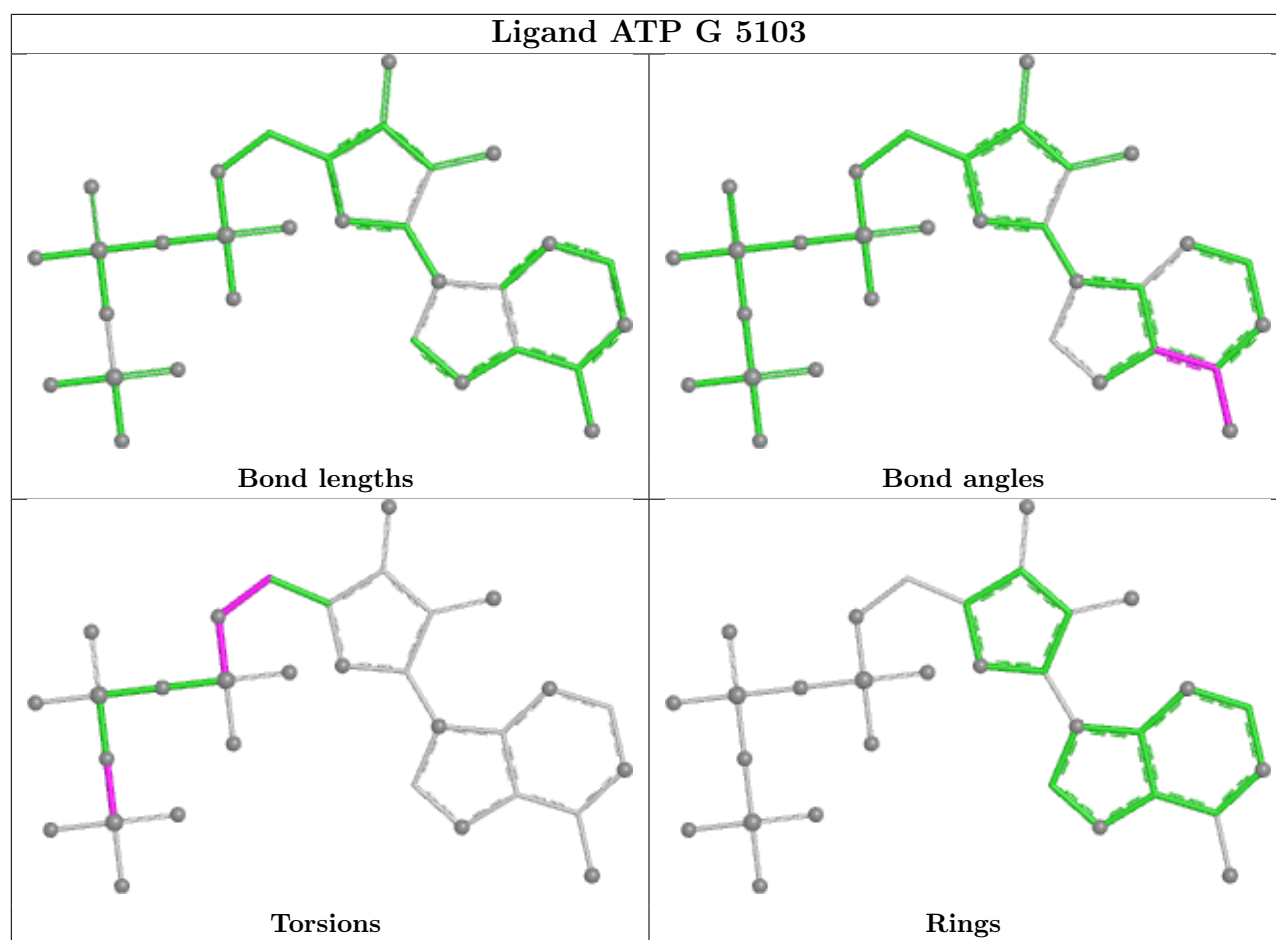
*Continued from previous page...*

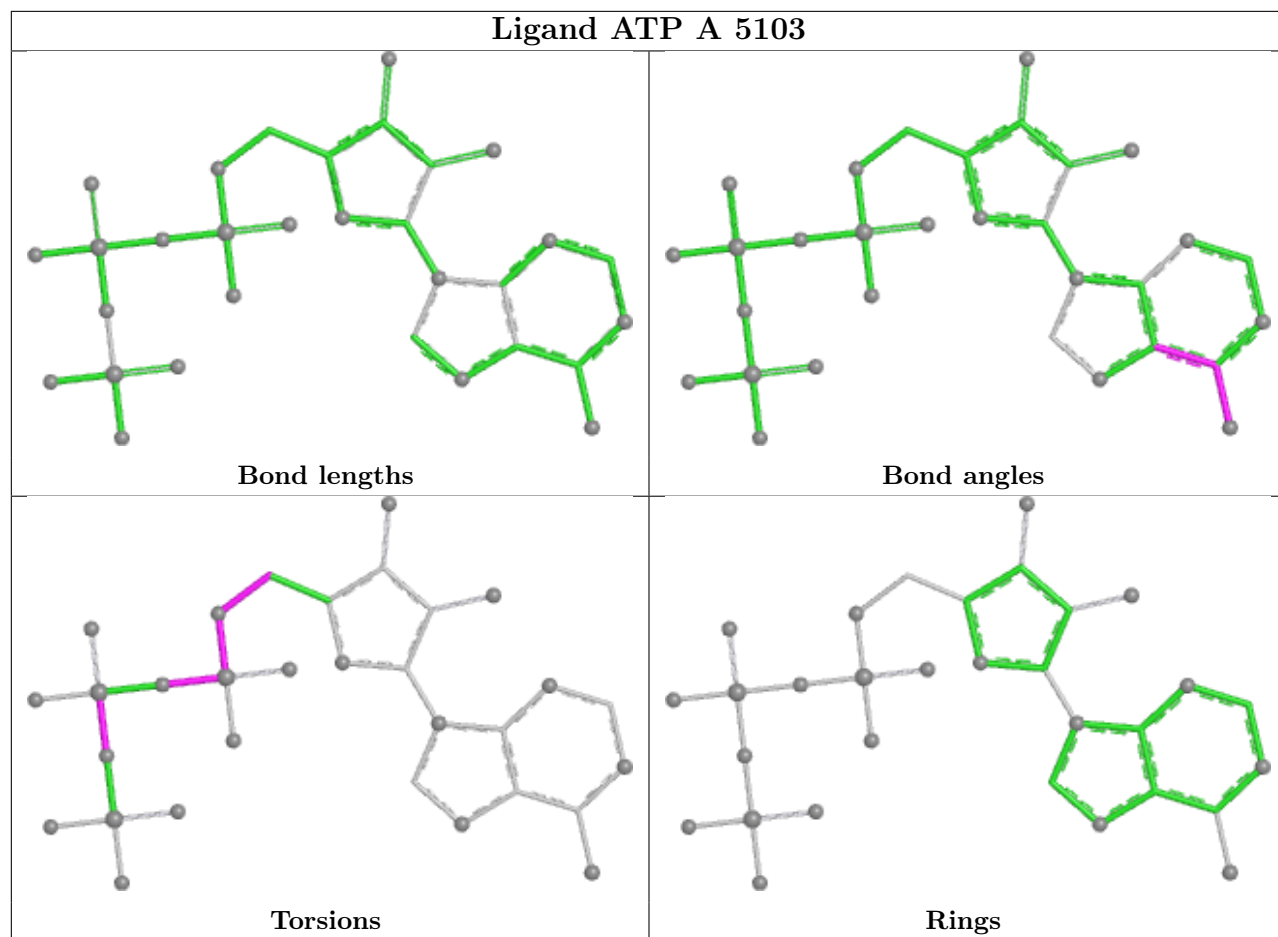
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5101	CFF	1	0
7	G	5103	ATP	3	0
7	A	5103	ATP	2	0

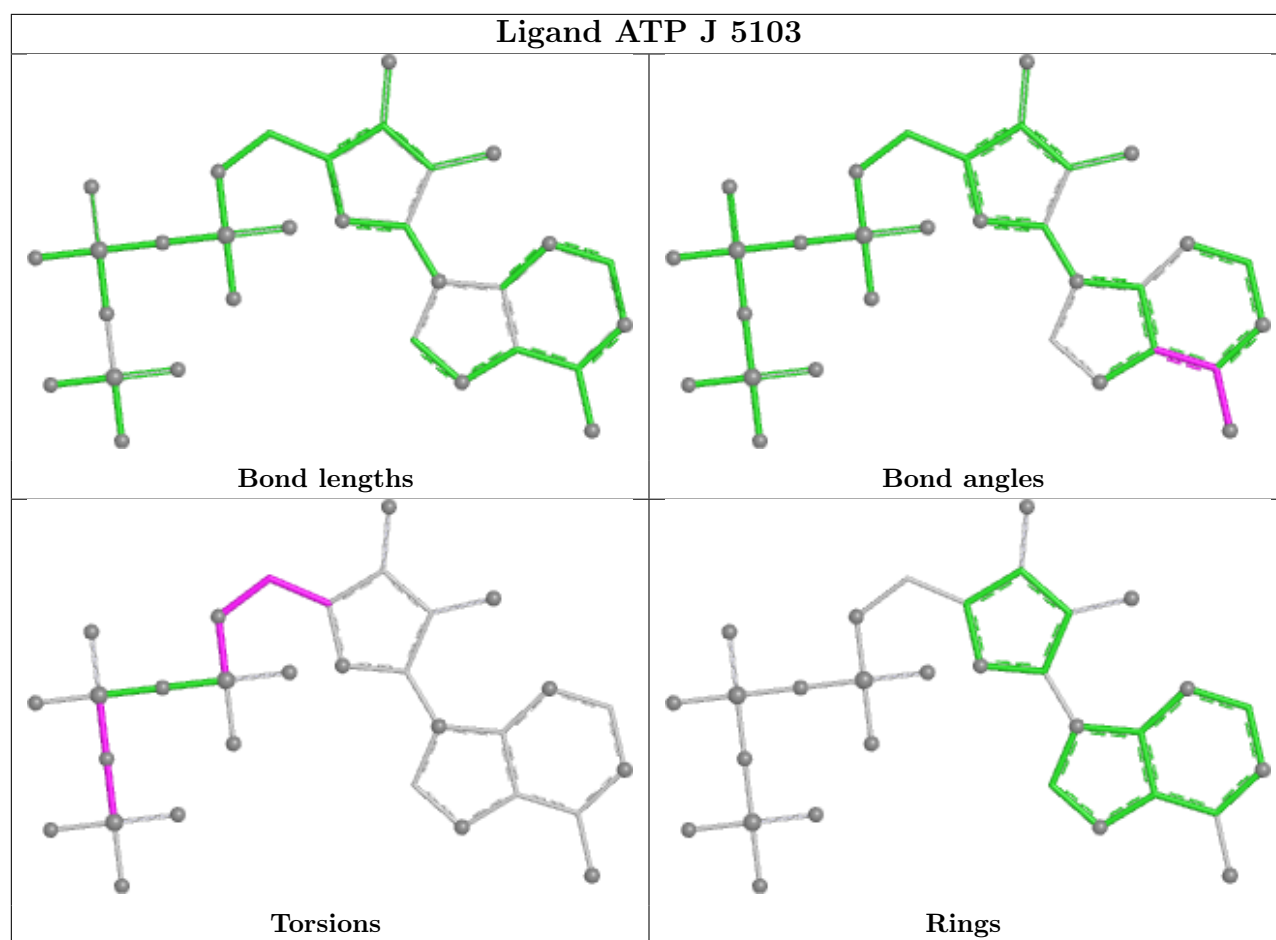
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

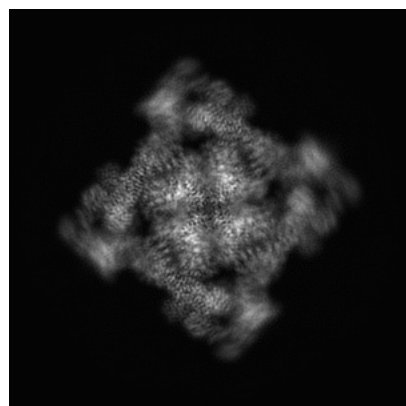
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27721. These allow visual inspection of the internal detail of the map and identification of artifacts.

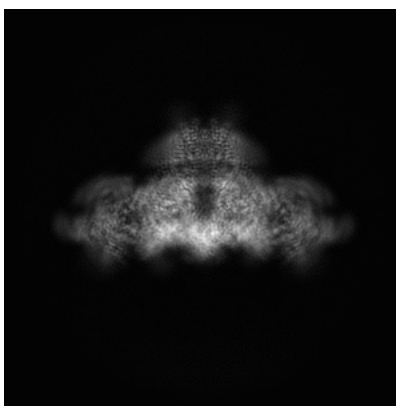
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

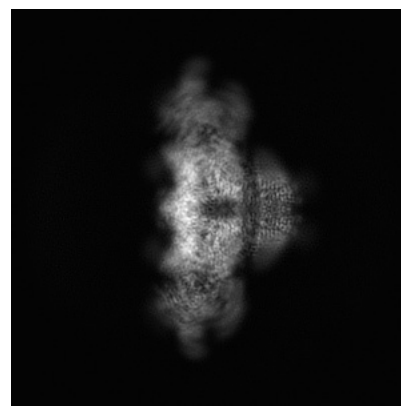
#### 6.1.1 Primary map



X

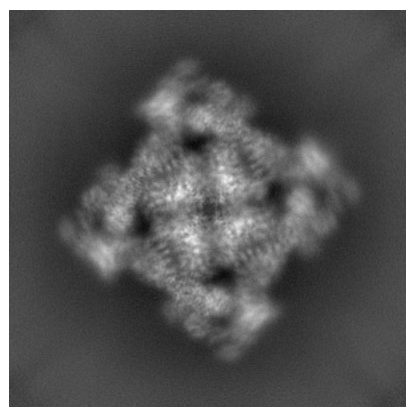


Y

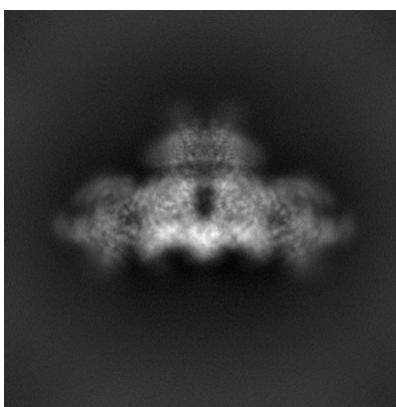


Z

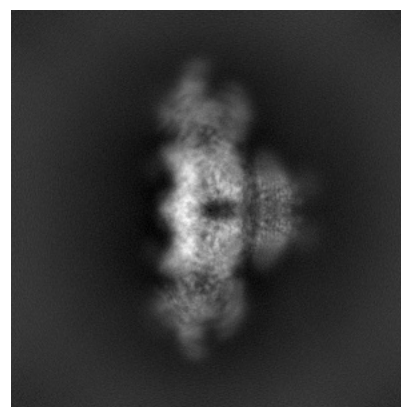
#### 6.1.2 Raw map



X



Y

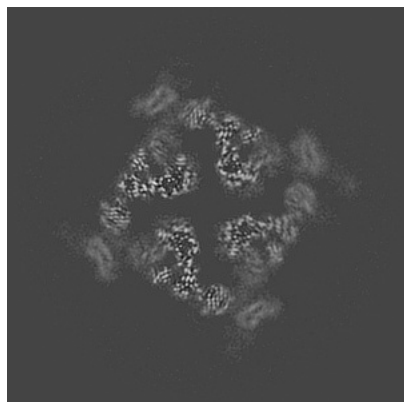


Z

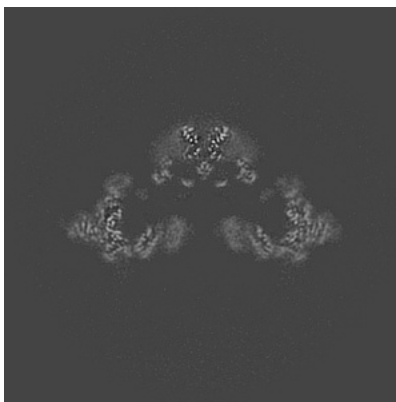
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

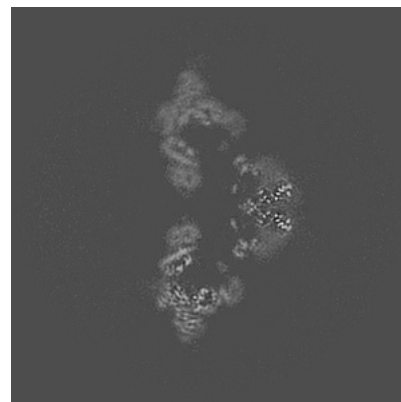
### 6.2.1 Primary map



X Index: 224

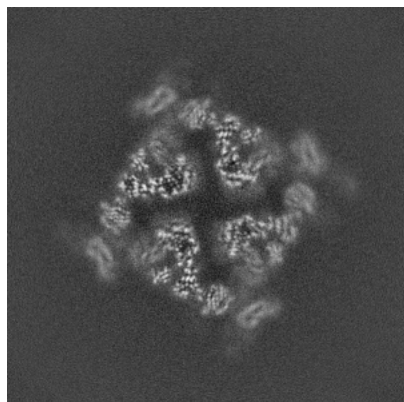


Y Index: 224

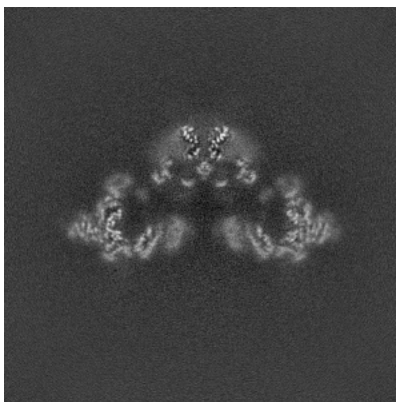


Z Index: 224

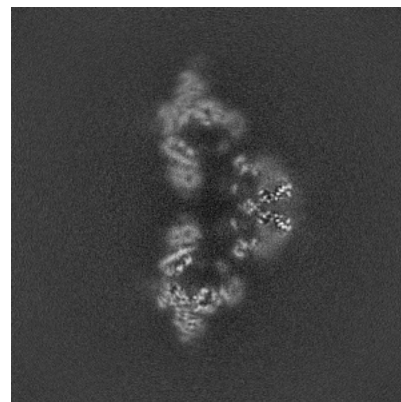
### 6.2.2 Raw map



X Index: 224



Y Index: 224

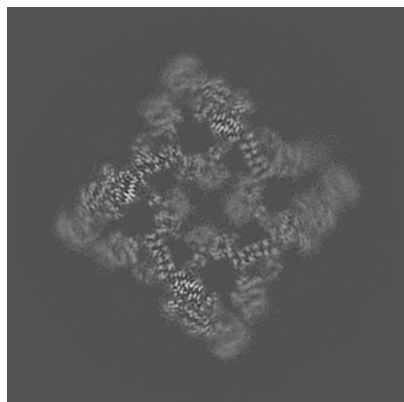


Z Index: 224

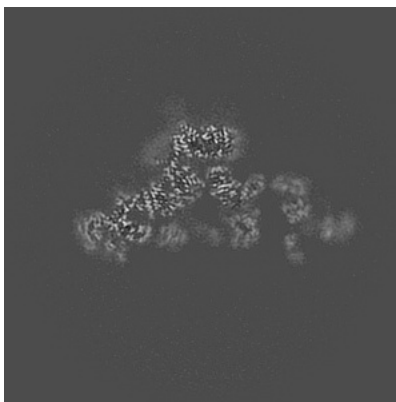
The images above show central slices of the map in three orthogonal directions.

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

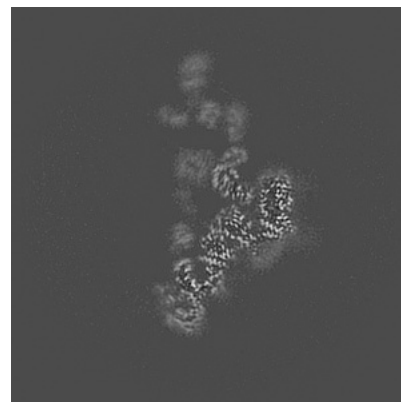
### 6.3.1 Primary map



X Index: 203

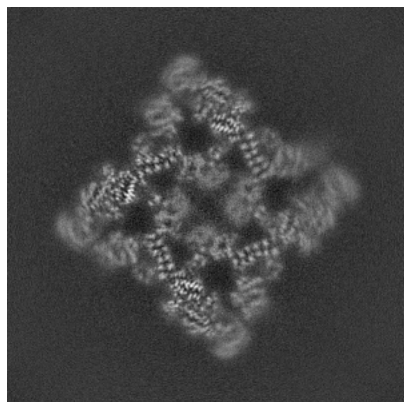


Y Index: 205

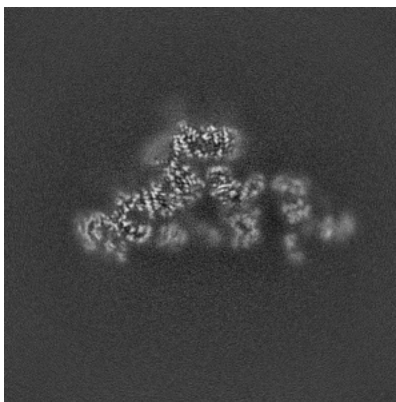


Z Index: 242

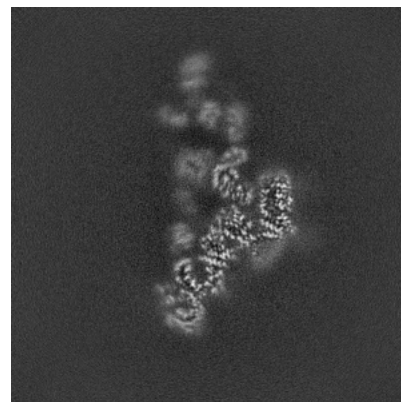
### 6.3.2 Raw map



X Index: 203



Y Index: 205



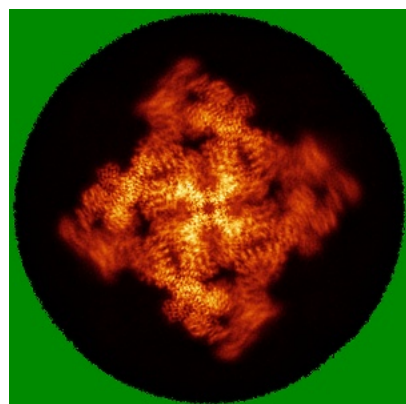
Z Index: 242

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

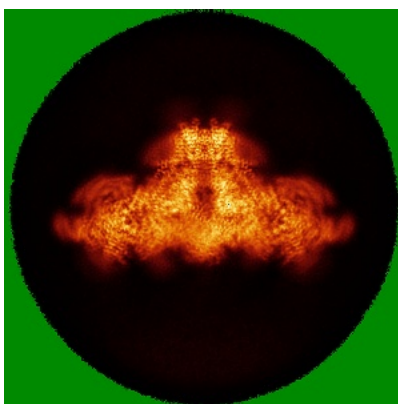


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

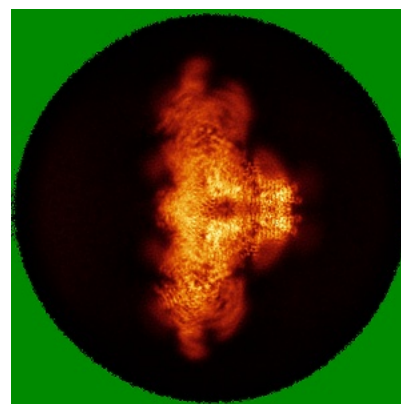
### 6.4.1 Primary map



X

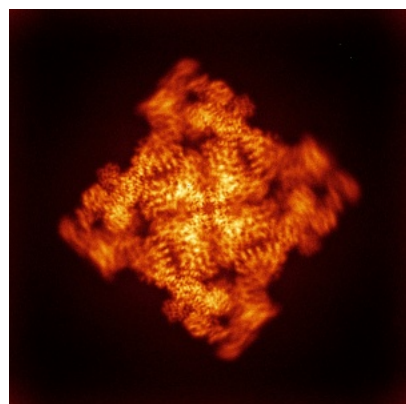


Y

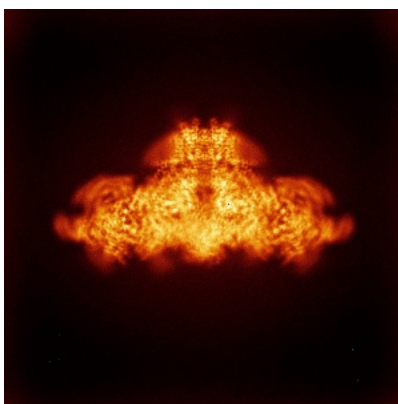


Z

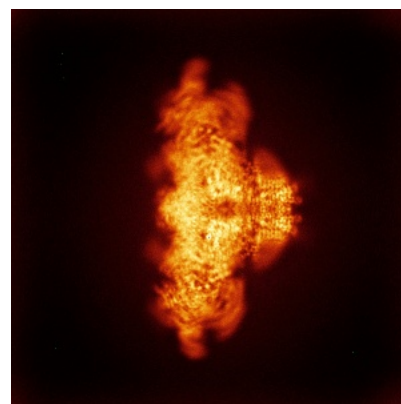
### 6.4.2 Raw map



X



Y

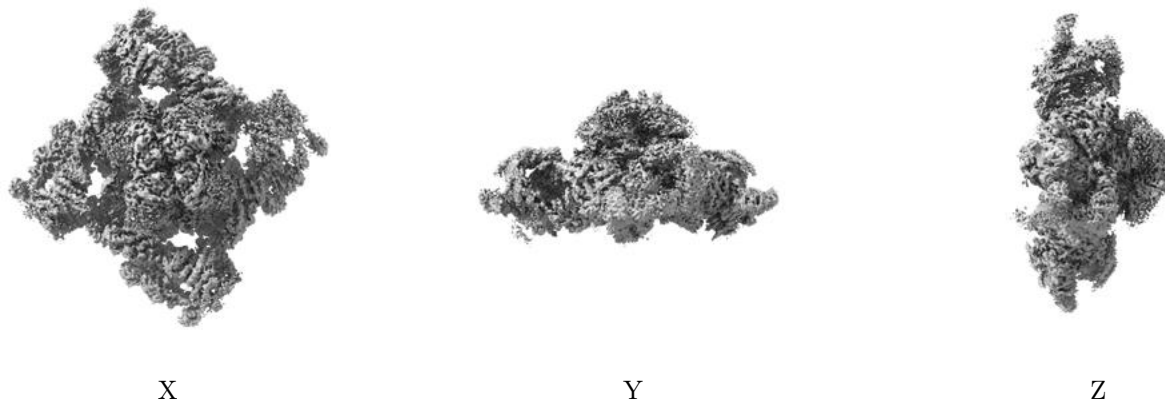


Z

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.

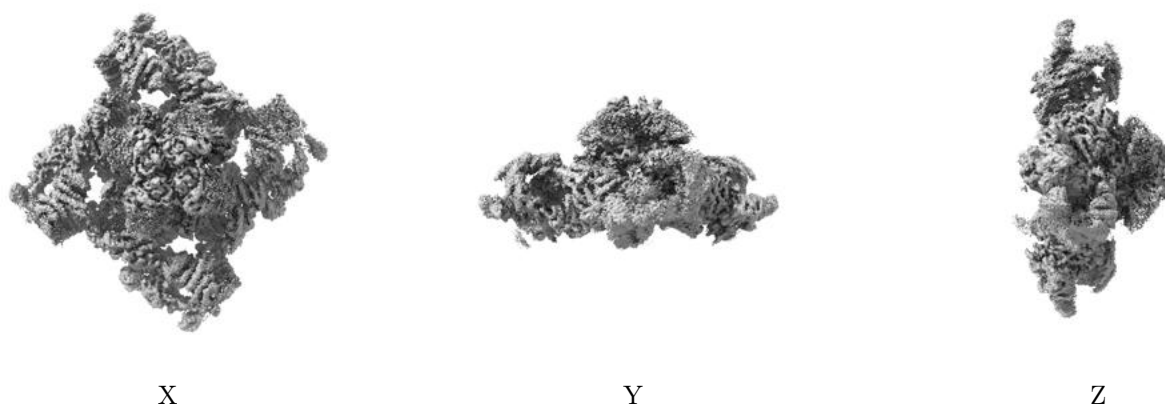
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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](#)

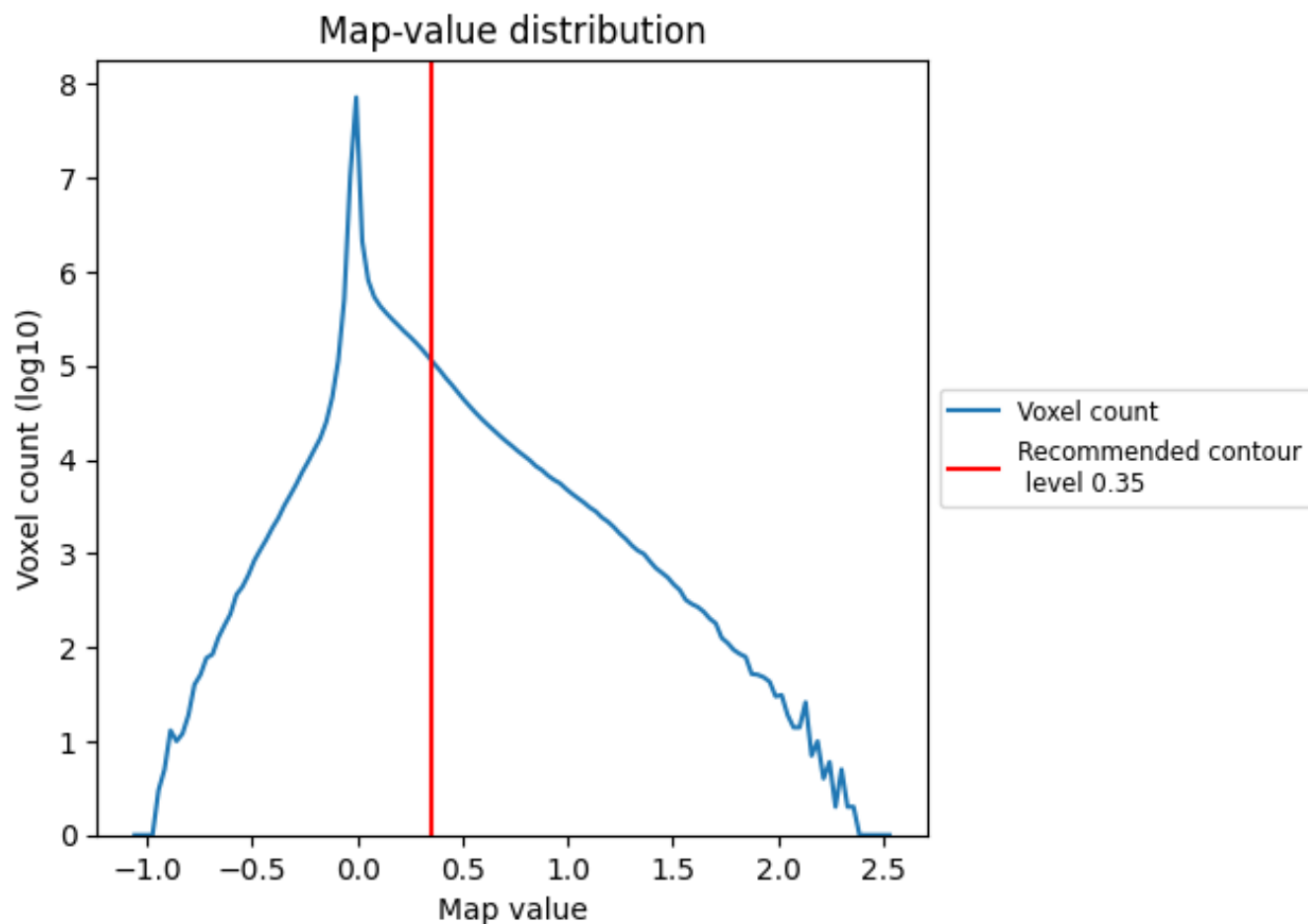
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

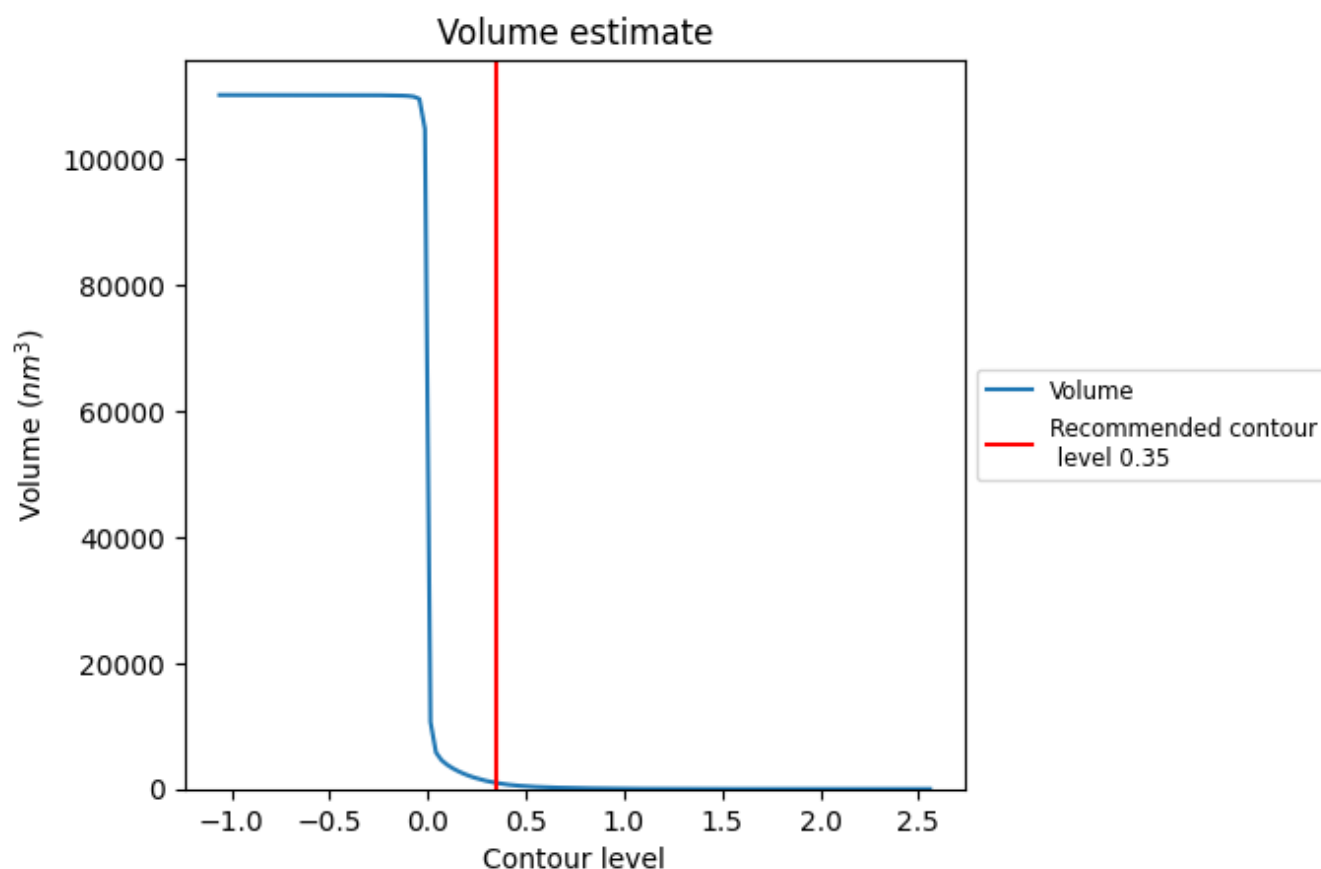
This section contains the results of statistical analysis of the map.

### 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.

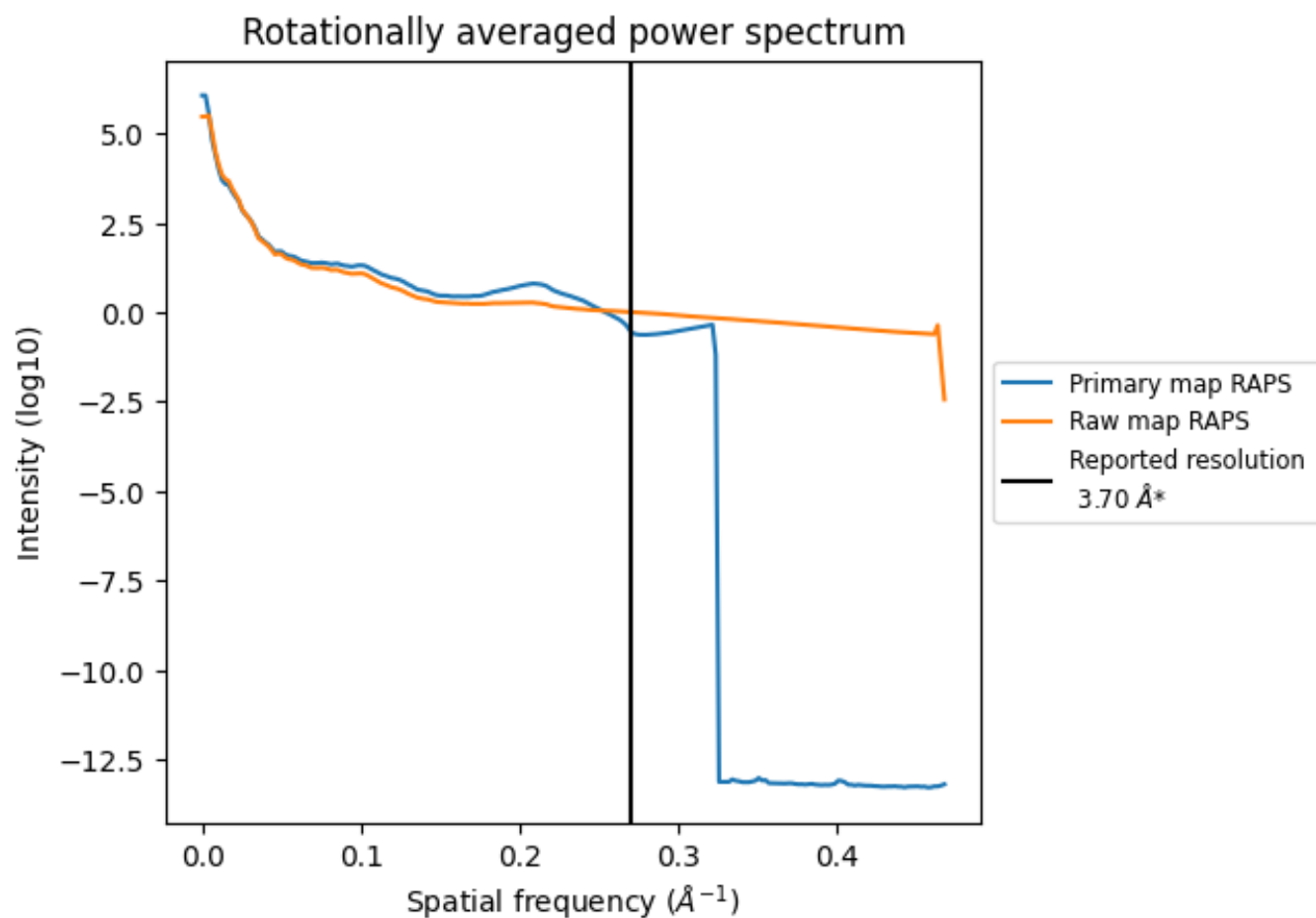
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 957  $\text{nm}^3$ ; this corresponds to an approximate mass of 865 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 ⓘ

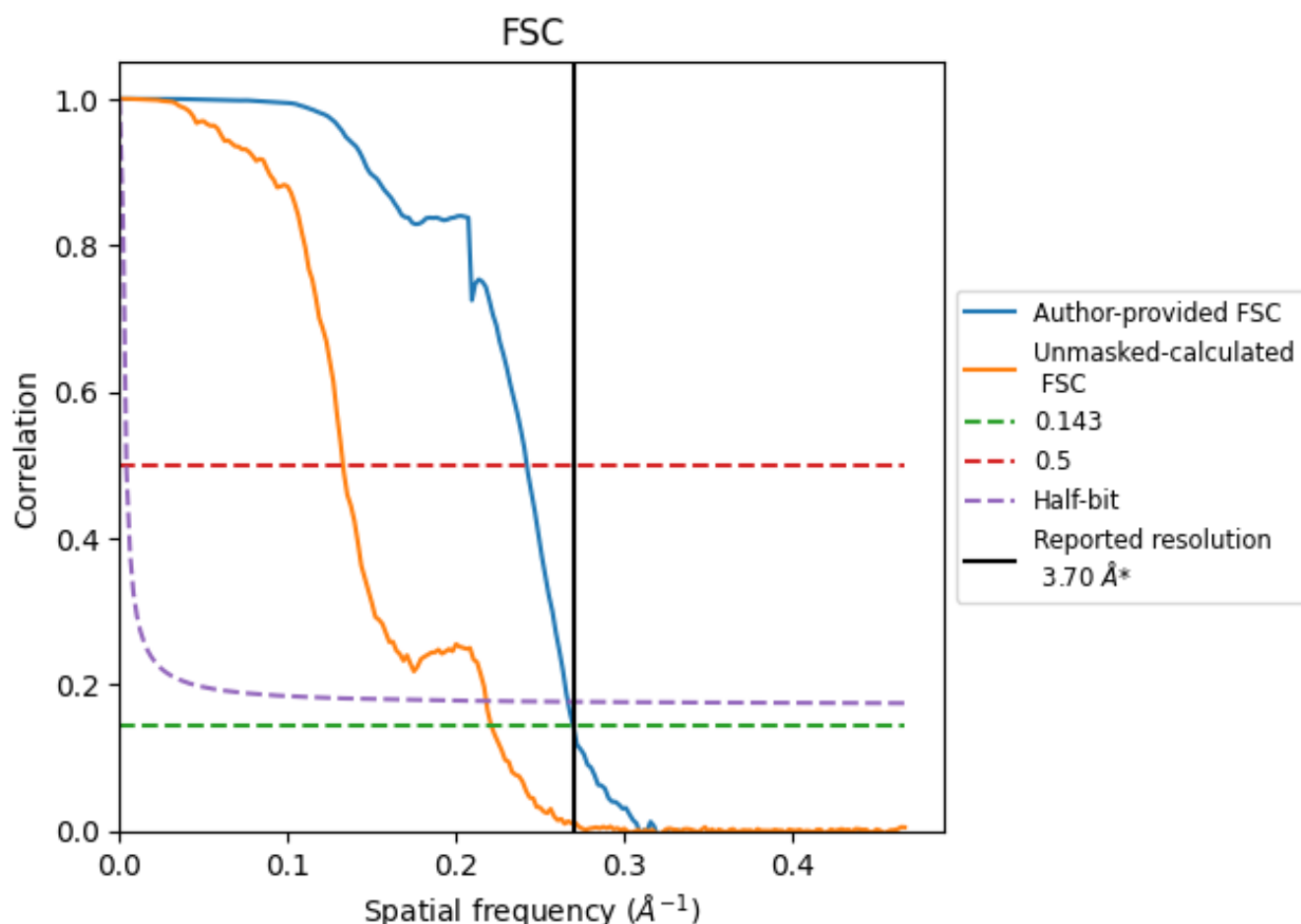


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

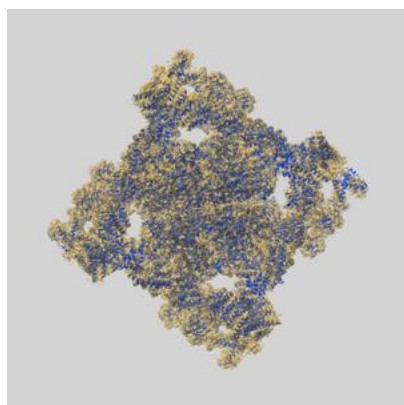
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.13	3.75
Unmasked-calculated*	4.52	7.52	4.58

\*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 4.52 differs from the reported value 3.7 by more than 10 %

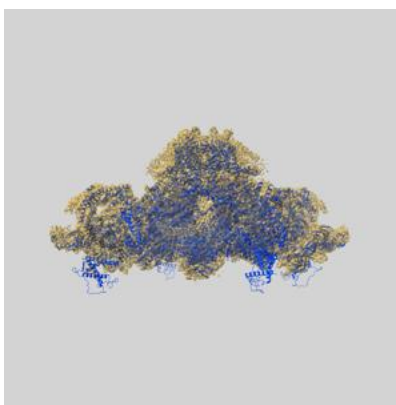
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27721 and PDB model 8DUJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

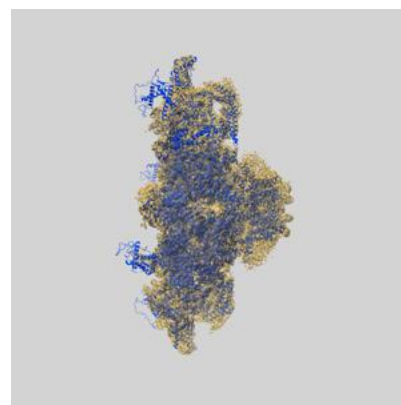
### 9.1 Map-model overlay [i](#)



X



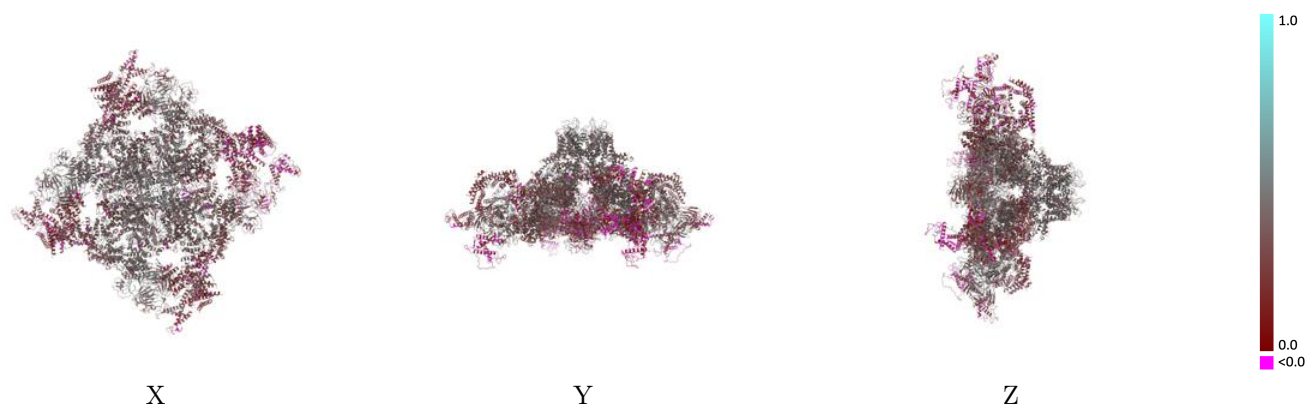
Y



Z

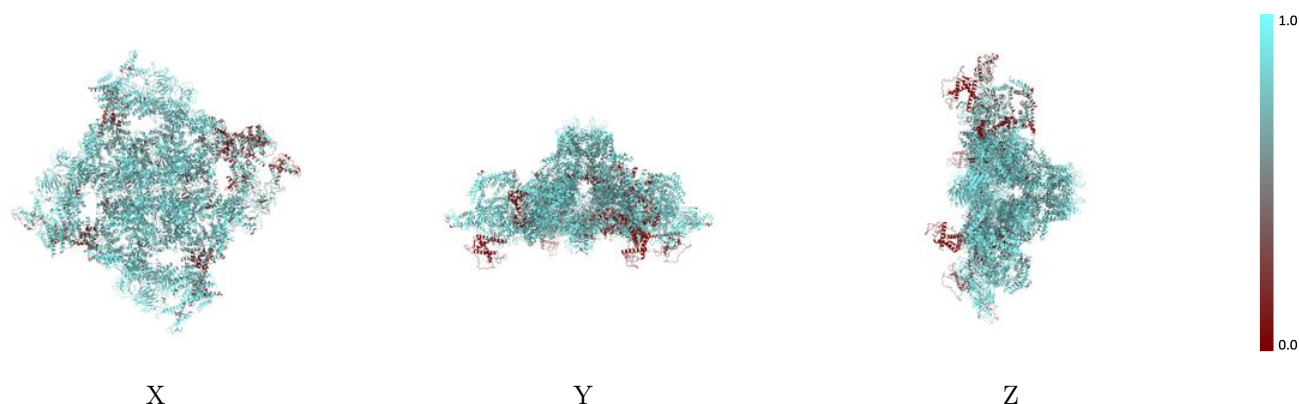
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



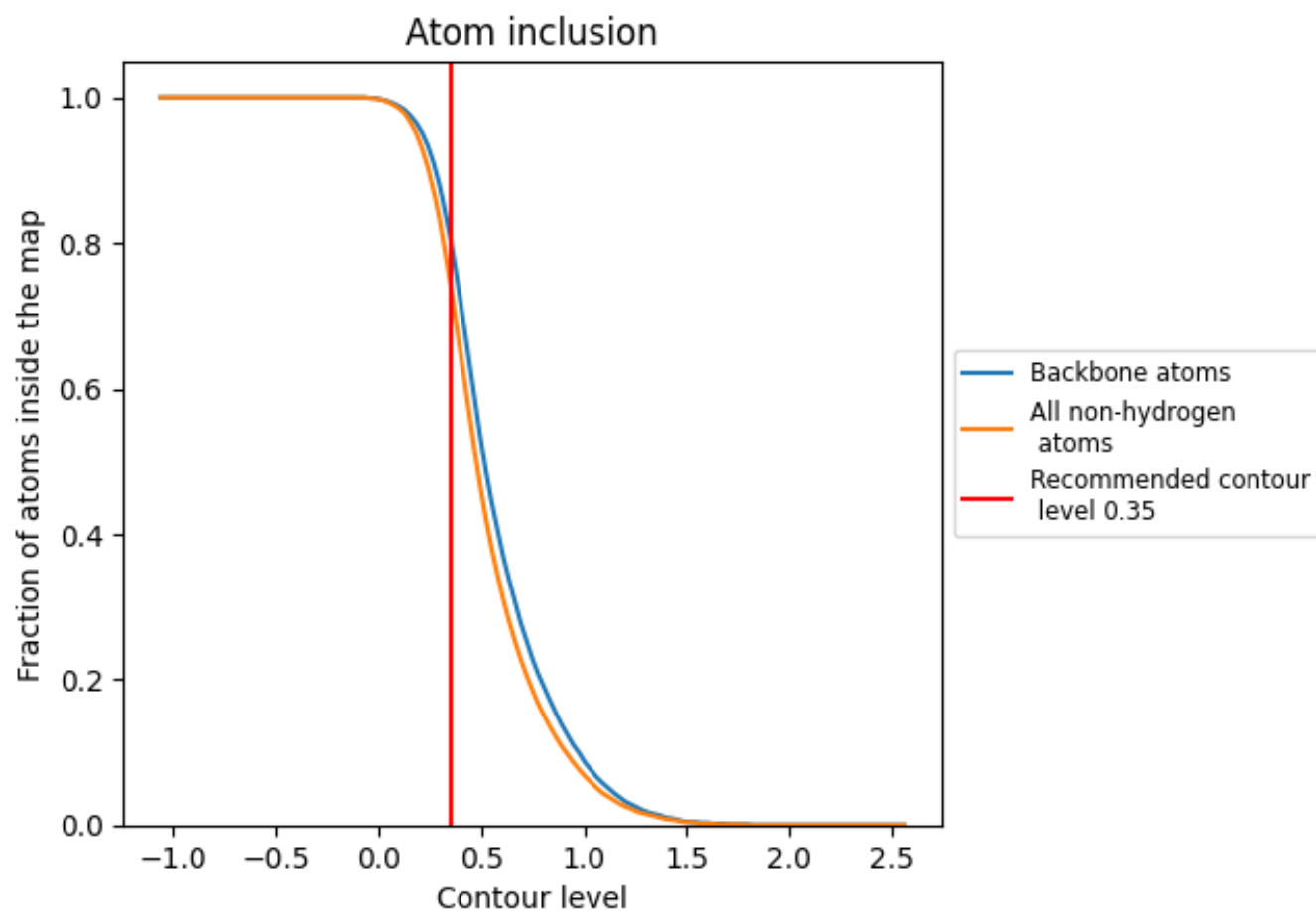
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7430	<div></div> 0.3450
A	<div></div> 0.7390	<div></div> 0.3470
B	<div></div> 0.8290	<div></div> 0.3980
C	<div></div> 0.1920	<div></div> 0.2430
D	<div></div> 0.7080	<div></div> 0.3050
E	<div></div> 0.7030	<div></div> 0.2960
F	<div></div> 0.1970	<div></div> 0.2240
G	<div></div> 0.7760	<div></div> 0.3660
H	<div></div> 0.8610	<div></div> 0.4330
I	<div></div> 0.3760	<div></div> 0.2800
J	<div></div> 0.7910	<div></div> 0.3640
K	<div></div> 0.8640	<div></div> 0.4400
L	<div></div> 0.2950	<div></div> 0.2410
M	<div></div> 0.6070	<div></div> 0.3960

1.0

0.0

<0.0