



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 10:31 AM EDT

PDB ID : 7T65
EMDB ID : EMD-25710
Title : Rabbit RyR1 disease mutant Y523S in complex with FKBP12.6 embedded in lipidic nanodisc in the open state
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on : 2021-12-13
Resolution : 4.05 Å(reported)
Based on initial model : 6WOT

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

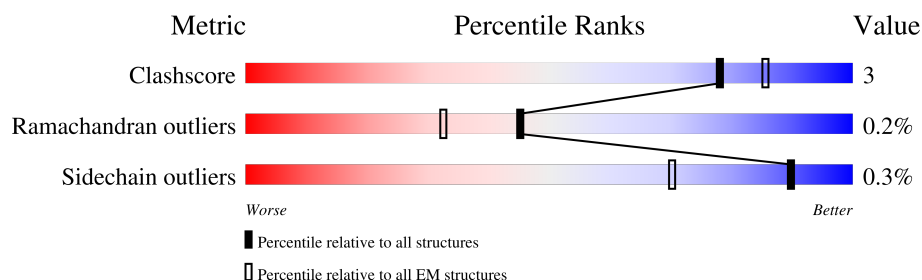
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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>17%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
1	B	5037	<div> <div>18%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
1	C	5037	<div> <div>17%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
1	D	5037	<div> <div>18%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
2	E	107	<div> <div>97%</div> <div>5%</div> </div>
2	F	107	<div> <div>95%</div> <div>5%</div> </div>
2	G	107	<div> <div>95%</div> <div>5%</div> </div>
2	H	107	<div> <div>95%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 135328 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	4252	Total 32981	C 20992	N 5666	O 6114	S 209	0	0
1	B	4252	Total 32981	C 20992	N 5666	O 6114	S 209	0	0
1	C	4252	Total 32981	C 20992	N 5666	O 6114	S 209	0	0
1	D	4252	Total 32981	C 20992	N 5666	O 6114	S 209	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
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	C	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

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

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

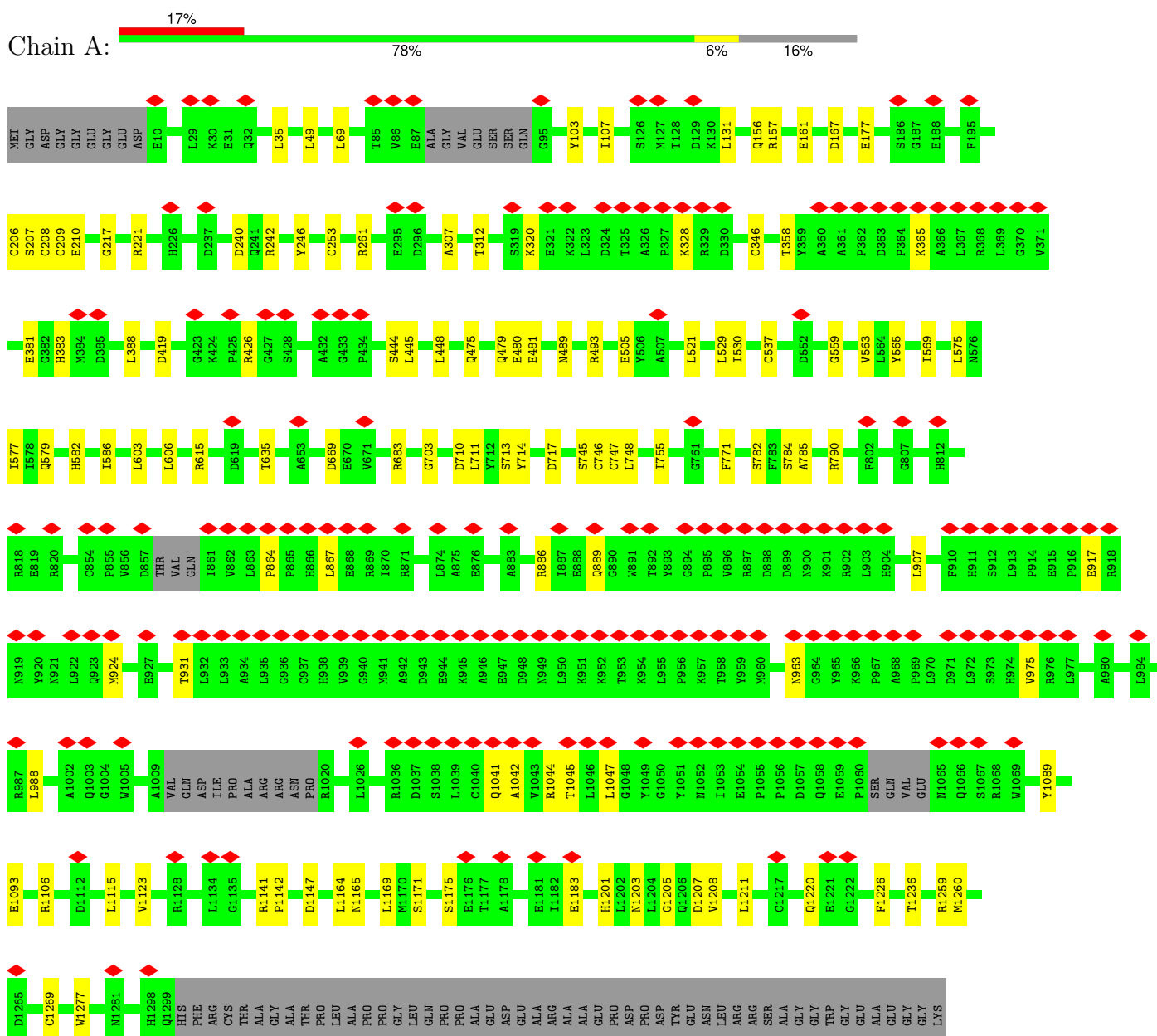
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

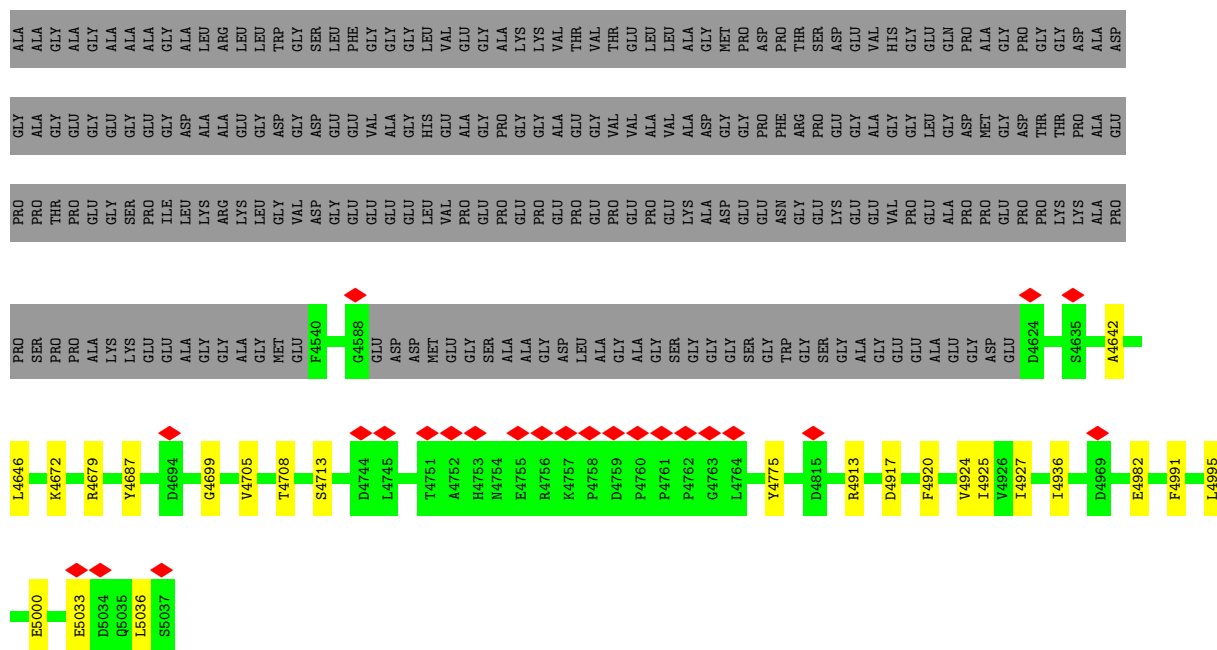
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

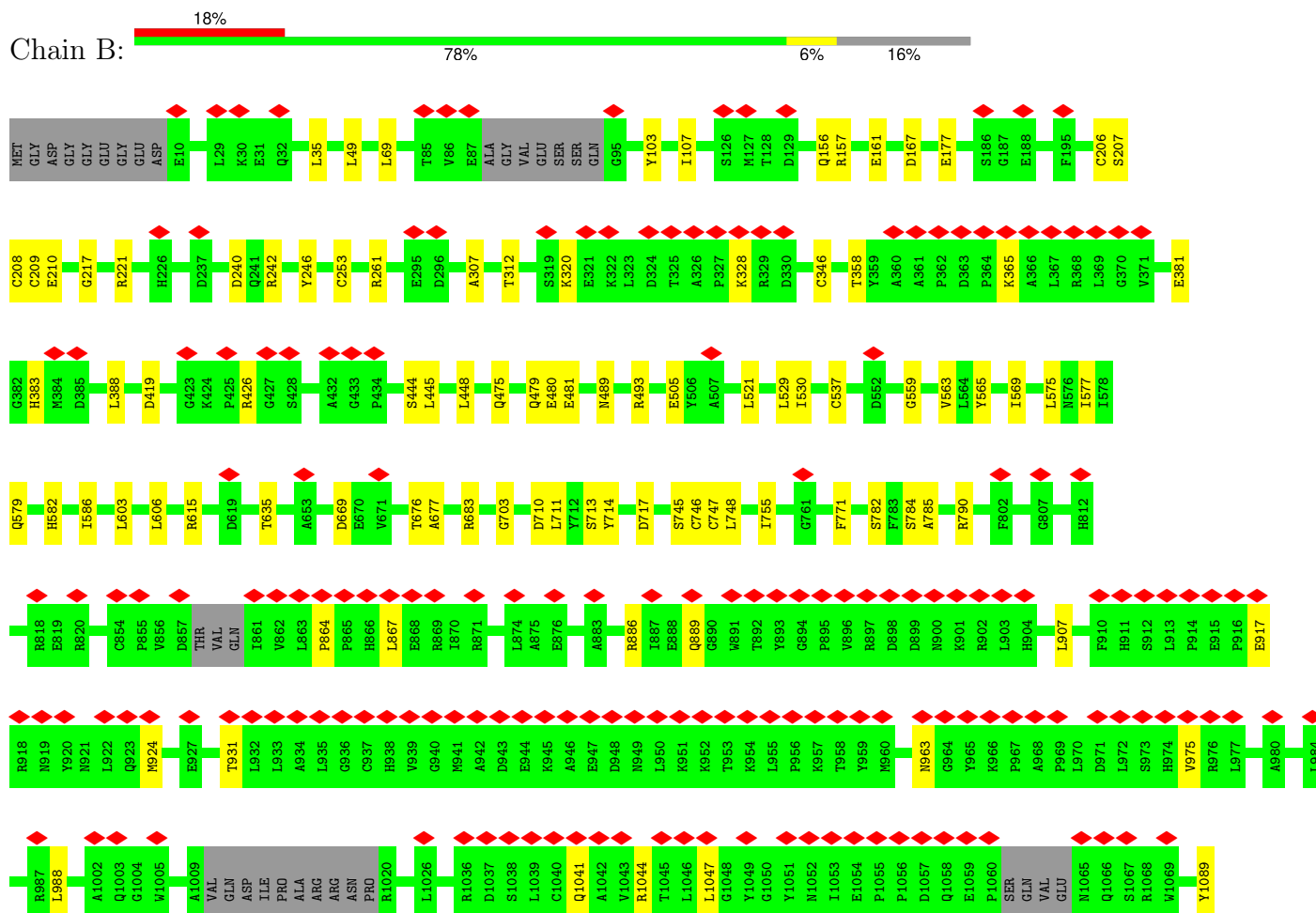




ALA	E4152	Q3869	E3682	L3579	ARG	E3429	H3357	P3293	A3228	D3159	LYS	T2995
GLY	P4155	N3870	Q3683	P3590	ARG	A3429	F3358	PRO	ILE	G	S3083	K2996
THR	D3877	D3877	E3684	G3591	ASP	E4433	I3362	ALA	LEU	Y3166	G3084	F2997
VAL	H4156	D3877	E3685	R3592	ARG	L3434	G3363	LEU	GLY	R3167	A3090	F2998
ALA	D4157	R3886	E3686	R3592	TYR	R3435	R3364	PRO	LEU	L3169	A3090	A2999
ALA	P4158	R3886	E3687	E3593	ARG	R3436	R3365	ALA	PRO	L3169	R3093	K3000
GLY	R4159	E3687	E3688	E3594	SER	R3437	R3366	GLY	PRO	C3170	F3010	K3000
THR	E4165	L3891	E3688	D3595	VAL	M3437	R3366			S3171	E3101	
ALA	F3899	F3899	E3689	A3596		E3440	K3367			T3172	K3105	C3014
ARG	D3941	D3941	V3690	A3597		E3440	R3368			S3173	E3108	F3017
ALA	N3963	N3963	E3691	D3598		W3445	R3369			L3174	N3109	T3020
ALA	M4184	M4184	E3692	P3599		S3446	R3370			G3175	L3110	P3021
ALA	G4185	G4185		E3590		K3447	G3371			G3176	R3111	A3022
ALA	R4188	R4188	H3734	K3591		F3451	E3375			G3177	L3112	K3023
ALA	T3966	T3966	L3735	L3514		R3452	E3376			T3178	G3113	V3024
ALA	A3981	A3981	E3736	K3515		K3453	E3377			T3179	VAL	L3025
ARG	W3986	W3986	E3737	R3595		R3454	E3378			N3180	SER	GLY
ARG	K4002	K4002	G3738	Q3597		E3455	Q3379			T3181	GLN	GLY
GLY	L4003	L4003	G3739	E3598		Q3456	R3380			Y3182	GLY	SER
LEU	L4012	L4012	ASN	E3610		N3457	L3381			VAL	GLY	GLY
TYR	M4026	M4026	GLY	H3611			ALA			GLU	GLY	GLY
ARG	E4056	E4056	ALA	P3612			GLY			K3185	ARG	H3030
ARG	D4070	D4070	GLU	TYR		Q3461	ALA			L3186	THR	A3031
ARG	S4074	S4074	GLU	P3612		N3462	ALA			R3187	GLN	S3032
ARG	D4079	D4079	LYS	L3535		E3463	ALA			A3188	VAL	L3046
ARG	Y4080	Y4080	LYS	T3538		I3464	ALA			A3189	LYS	A3047
ARG	Y4081	Y4081	LYS	R3539		N3465	ALA			G3193	GLY	A3048
ARG	R4085	R4085	ALA	Y3540		N3467	ALA			L3194	GLY	L3049
ARG	G4086	G4086	VAL	A3541		M3468	ALA			G3197	VAL	Y3050
GLY	L4087	L4087	VAL	A3541		M3468	ALA			A3198	ARG	R3053
GLY	Q4102	Q4102	VAL	A3541		F3469	ALA			A3199	ARG	V3054
ALA	F4103	F4103	VAL	A3541		L3470	ALA			M3201	THR	S3055
ALA	T4104	T4104	VAL	A3541		THR	ALA			P3202	THR	L3056
ALA	G4105	G4105	VAL	A3541		ASP	ALA			V3203	THR	F3057
ALA	D4118	D4118	VAL	A3541		SER	ALA			A3204	THR	G3058
LEU	E4119	E4119	VAL	A3541		SER	ALA			F3205	THR	T3059
LEU	N4120	N4120	VAL	A3541		SER	ALA			A3206	THR	D3060
ALA	E4121	E4121	VAL	A3541		GLN	ALA			E3207	THR	A3061
VAL	MET	MET	VAL	A3541		GLY	ALA			P3208	THR	F3062
ALA	N3858	N3858	VAL	A3541		GLY	ALA			Q3209	THR	A3063
ALA	V3859	V3859	VAL	A3541		GLY	ALA			L3210	THR	V3064
ALA	N3860	N3860	VAL	A3541		GLY	ALA			N3211	THR	V3065
ARG	E3861	E3861	VAL	A3541		GLY	ALA			E3212	THR	N3066
ALA	D3862	D3862	VAL	A3541		GLY	ALA			N3213	THR	H3069
GLY	G3863	G3863	VAL	A3541		GLY	ALA			N3214	THR	I3070
GLY	T3864	T3864	VAL	A3541		GLY	ALA			A3215	THR	R3073
GLY	V3865	V3865	VAL	A3541		GLY	ALA			SER	THR	S3074
ALA	V3866	V3866	VAL	A3541		GLY	ALA			V3218	THR	L3075
ALA	N3867	N3867	VAL	A3541		GLY	ALA			Y3219	THR	ASP
ALA	E3868	E3868	VAL	A3541		GLY	ALA			T3220	THR	ALA
										T3221	THR	R3078
										T3222	THR	T3079
										T3223	THR	V3080
										P3224	THR	K3081
										R3225	THR	



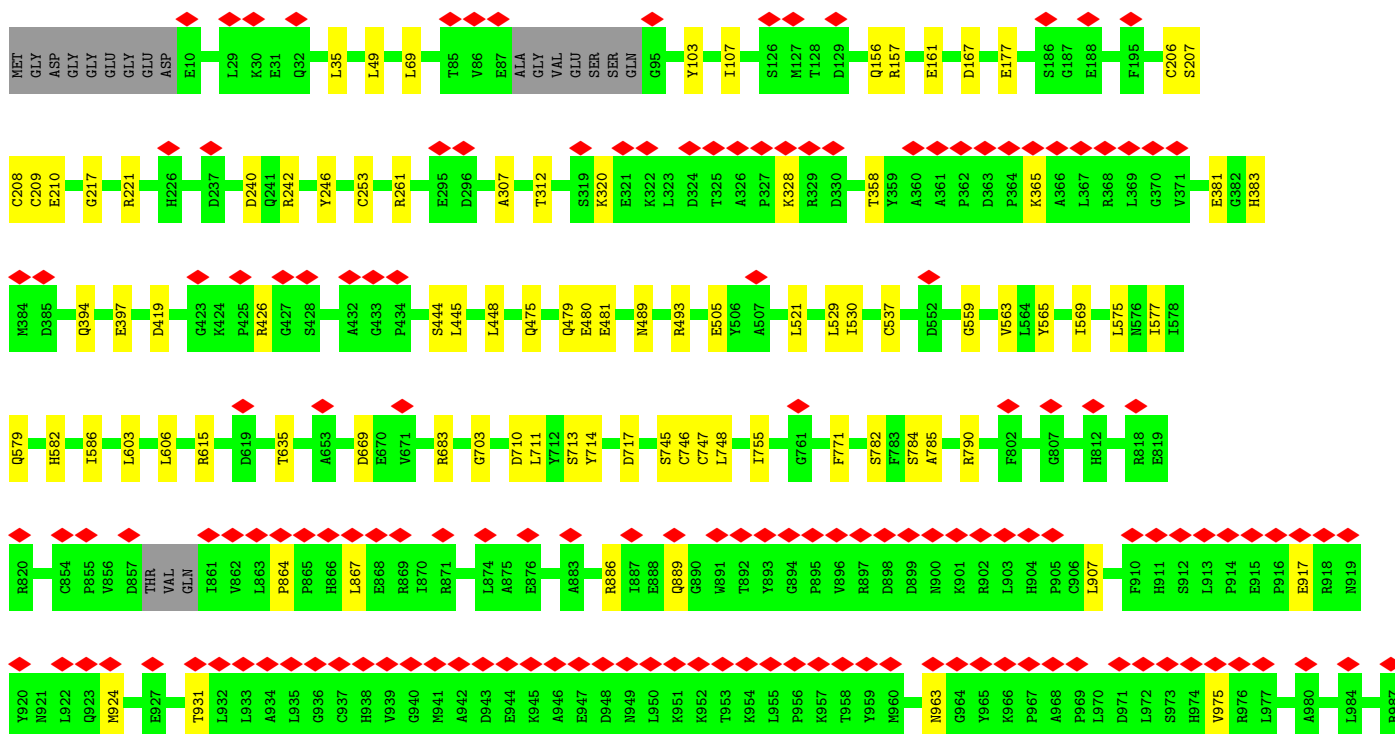
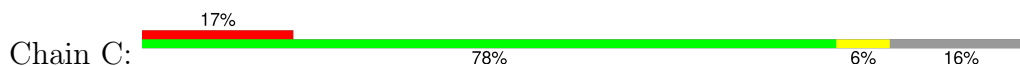
• Molecule 1: Ryanodine receptor 1







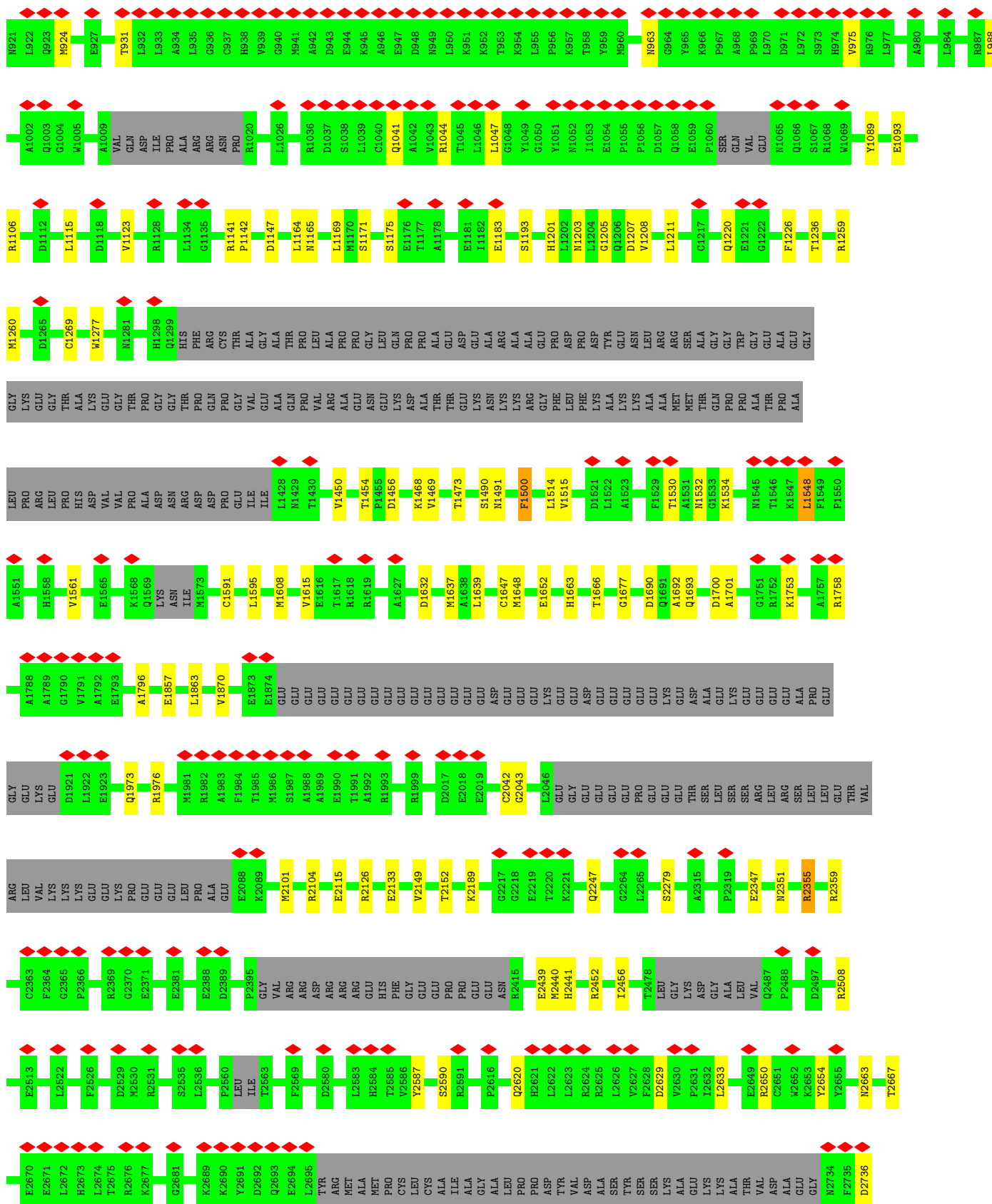
- Molecule 1: Ryanodine receptor 1





K2800	D2801	K2802	E2803	T2804	Y2805	K2806	W2807	P2808	K2809	K2810	E2811	S2812	T2813	K2814	A2815	K2816	A2817	A2818	W2819	E2820	W2821	T2822	T2823	E2824	K2825	A2826	R2827	E2828	E2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	GLU	GLY	Y2855	W2856	P2857	Q2858	P2859	
P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	R2917	R2918	R2919
R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	M2933	G2934	Y2935	A2936	V2937	T2938	R2939	G2940	L2941	K2942	D2943	M2944	E2945	L2946	D2947	T2948	S2949	S2950	T2951	E2952	K2953	R2954	F2955	A2956	F2959	W2966	F2973	T2974	H2902	A2975	H2976	L2977	E2978	ALA	VAL	VAL	SER	GLY	ARG	VAL	GLU	LYS	SER	PRO			
W2991	E2992	T2995	K2996	F2997	F2998	A2999	K3000	F3010	C3014	F3017	T3020	P3021	A3022	K3023	V3024	T2938	R2939	G2940	L2941	K2942	D2943	N2944	E2945	L2946	D2947	T2948	S2949	S2950	T2951	E2952	K2953	R2954	F2955	A2956	F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064	V3065	N3066	H3069	T3070	R3073	S3074	ASP	ALA									
R3078	T3079	V3080	M3081	L3083	G3084	A3090	R3093	E3101	K3105	E3108	N3109	L3110	R3111	L3112	K3113	LYS	VAL	SER	GLN	ALA	ARG	THR	GLN	VAL	LYS	V3125	K3126	Q3127	R3128	L3129	T3130	T3133	V3134	A3135	L3136	L3137	P3138	L3140	T3141	T3142	Q3145	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154											
D3155	V3156	T3157	L3158	D3159	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	K3178	N3180	T3181	V3182	VAL	GLU	K3185	L3186	R3187	P3188	A3189	C3193	L3194	L3197	A3198	A3199	M3201	P3202	V3203	A3204	F3205	L3206	E3207	I3272	P3208	Q3209	L3210	N3211	E3212	V3213	N3214	A3215	C3216	SER	V3218	Y3219	T3220	K3221	K3222				
S3223	P3224	R3225	A3228	ILE	LEU	GLY	LEU	PRO	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	R3247	K3248	L3249	D3252	I3253	G3254	G3255	L3256	A3257	E3258	Y3263	THR	GLU	MET	P3267	H3268	V3269	I3270	E3271	I3272	T3273	L3274	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	G3288							
P3289	E3290	A3291	P3292	P3293	PRO	LEU	LEU	PRO	A3300	P3301	P3302	P3303	C3304	T3305	ALA	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316	T3319	L3320	R3321	L3322	N3325	G3328	L3329	D3330	E3331	W3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	T3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352						
L3353	L3354	H3355	S3356	H3357	F3358	T3362	G3363	R3364	L3365	R3366	K3367	R3368	A3369	G3370	K3371	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	GLU	ALA	LYS	ALA	E3388	E3389	G3390	E3391	L3392	L3393	V3394	D3395	R3396	E3397	W3400	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	T3413	R3414	Y3415	Y3416	D3417	N3418	N3419	R3420							
A3421	H3422	W3423	L3424	A3429	E3433	L3434	F3435	R3436	K3437	E3440	W3445	S3446	K3447	F3451	K3452	R3453	E3454	E3455	Q3456	N3457	Q3461	N3462	I3464	N3465	N3466	M3467	S3468	F3469	L3470	THR	ALA	ASP	SER	LYS	LYS	MET	ALA	LYS	GLY	ASP	ALA	GLN	SER	GLY	SER	ASP	GLN	GLU	ARG										
THR	LYS	LYS	ARG	ARG	GLY	ASP	THR	SER	VAL	Q3506	T3507	S3508	L3509	T3510	T3513	L3514	K3515	K3516	M3517	G3521	L3522	N3523	D3531	L3535	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545	D3546	E3547	E3548	V3549	F3552	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565									
L3575	Y3576	G3577	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	D3586	D3587	P3588	P3589	E3590	K3591	I3592	R3595	W3596	Q3597	E3598	E3610	H3611	P3612	LYS	SER	LYS	LYS	VAL	TRP	HIS	LYS	LEU	LEU	SER	LYS	ARG	ARG	ALA	VAL	VAL	VAL	ALA	CYS	PHE	ARG	MET	T3639	W3661	T3664	E3665	D3666							
H3667	K3679	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	H3734	L3735	E3736	E3737	G3738	G3739	E3740	ASN	GLY	GLU	ALA	GLU	GLU	E3748	V3749	E3750	Q3767	T3772	R3773	C3786	T3802	S3803	L3804	N3805	N3806	K3815	S3831	S3840	G3857	M3858	V3859	N3860	E3861	L3862	G3863												

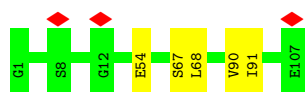




WORLDWIDE
PDB
PROTEIN DATA BANK



Chain G:  95% 5%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	84954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.19	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.769	Depositor
Minimum map value	-0.355	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.176	Depositor
Map size (\AA)	463.54004, 463.54004, 463.54004	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0780001, 1.0780001, 1.0780001	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: CA, ATP, 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	0.35	0/33703	0.66	4/45746 (0.0%)
1	B	0.35	0/33703	0.66	4/45746 (0.0%)
1	C	0.35	1/33703 (0.0%)	0.66	4/45746 (0.0%)
1	D	0.35	1/33703 (0.0%)	0.66	4/45746 (0.0%)
2	E	0.34	0/834	0.70	0/1123
2	F	0.34	0/834	0.70	0/1123
2	G	0.34	0/834	0.70	0/1123
2	H	0.34	0/834	0.70	0/1123
All	All	0.35	2/138148 (0.0%)	0.66	16/187476 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1652	GLU	C-O	-5.06	1.13	1.23
1	D	1652	GLU	C-O	-5.03	1.13	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3056	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	3056	LEU	CA-CB-CG	5.82	128.68	115.30
1	D	3056	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	3056	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	1548	LEU	CA-CB-CG	5.59	128.17	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4253	GLU	Peptide
1	B	4253	GLU	Peptide
1	C	4253	GLU	Peptide
1	D	4253	GLU	Peptide

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	32981	0	31923	181	0
1	B	32981	0	31923	178	0
1	C	32981	0	31923	183	0
1	D	32981	0	31923	181	0
2	E	818	0	824	2	0
2	F	818	0	824	3	0
2	G	818	0	824	3	0
2	H	818	0	824	3	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	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
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	135328	0	131036	721	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 3.

The worst 5 of 721 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:4913:ARG:NH1	1:C:4917:ASP:OD2	2.23	0.72
1:B:4913:ARG:NH1	1:B:4917:ASP:OD2	2.22	0.72
1:A:4913:ARG:NH1	1:A:4917:ASP:OD2	2.22	0.72
1:D:4913:ARG:NH1	1:D:4917:ASP:OD2	2.22	0.71
1:A:3540:TYR:OH	1:A:3597:GLN:OE1	2.11	0.69

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	4188/5037 (83%)	3792 (90%)	385 (9%)	11 (0%)	37	71
1	B	4188/5037 (83%)	3794 (91%)	384 (9%)	10 (0%)	44	76
1	C	4188/5037 (83%)	3794 (91%)	384 (9%)	10 (0%)	44	76
1	D	4188/5037 (83%)	3795 (91%)	383 (9%)	10 (0%)	44	76
2	E	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	G	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
All	All	17172/20576 (84%)	15555 (91%)	1576 (9%)	41 (0%)	45	76

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1548	LEU
1	A	2956	ALA
1	B	1548	LEU
1	B	2956	ALA
1	C	1548	LEU

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	3479/4276 (81%)	3469 (100%)	10 (0%)	91	92
1	B	3479/4276 (81%)	3469 (100%)	10 (0%)	91	92
1	C	3479/4276 (81%)	3469 (100%)	10 (0%)	91	92
1	D	3479/4276 (81%)	3469 (100%)	10 (0%)	91	92
2	E	88/88 (100%)	88 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	G	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
All	All	14268/17456 (82%)	14228 (100%)	40 (0%)	90	92

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3679	LYS
1	D	3111	ARG
1	C	3773	ARG
1	D	1468	LYS
1	D	3595	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 8 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	ATP	D	5101	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
3	ATP	C	5101	-	28,33,33	0.66	0	34,52,52	0.91	1 (2%)
3	ATP	A	5101	-	28,33,33	0.67	0	34,52,52	0.92	1 (2%)
3	ATP	B	5101	-	28,33,33	0.67	0	34,52,52	0.92	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
3	ATP	D	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	C	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	A	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	C5-C6-N6	2.26	123.75	120.31
3	D	5101	ATP	C5-C6-N6	2.24	123.73	120.31
3	A	5101	ATP	C5-C6-N6	2.24	123.72	120.31
3	C	5101	ATP	C5-C6-N6	2.22	123.69	120.31

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

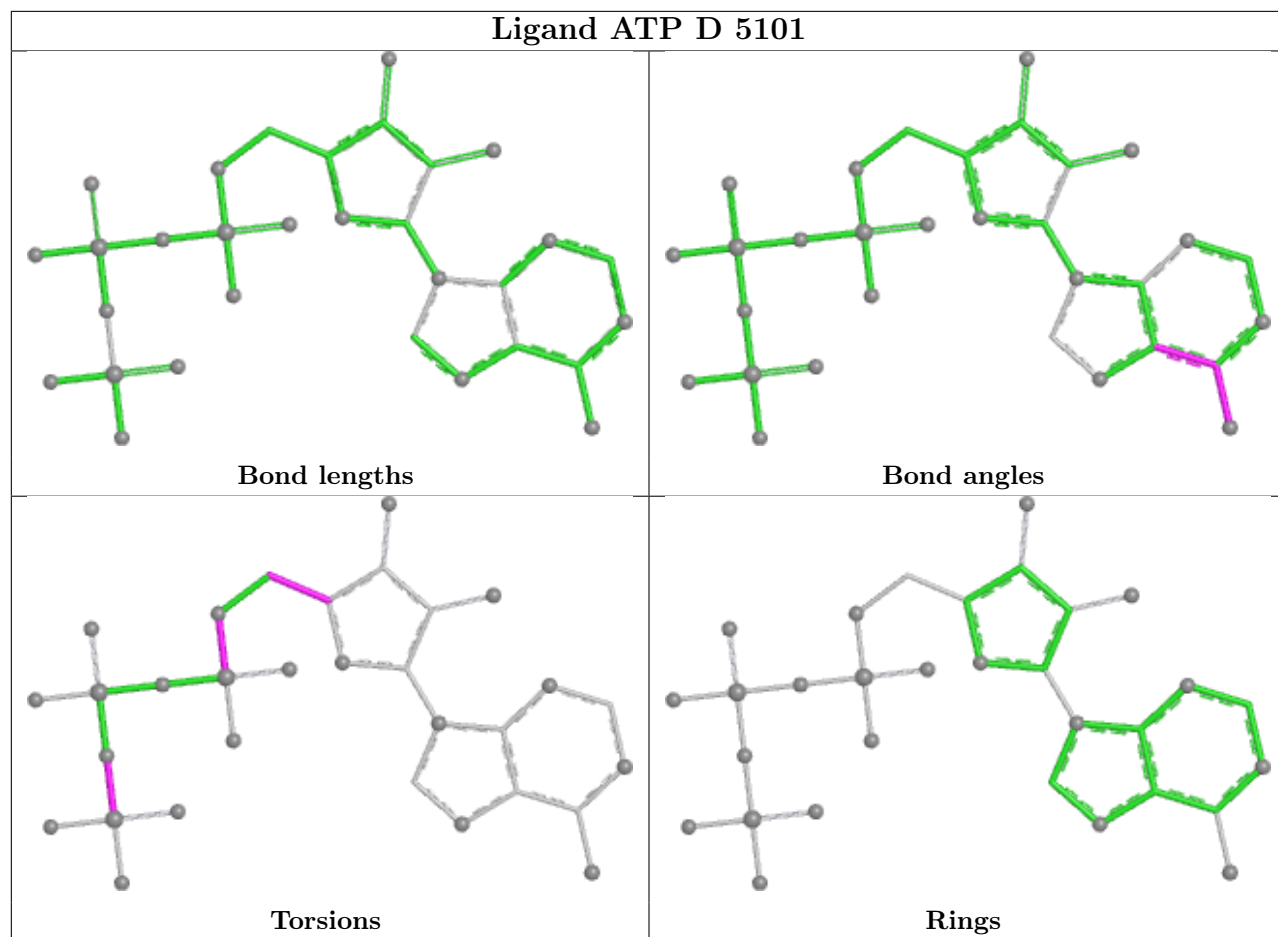
Mol	Chain	Res	Type	Atoms
3	A	5101	ATP	C5'-O5'-PA-O1A
3	A	5101	ATP	C5'-O5'-PA-O2A
3	A	5101	ATP	C5'-O5'-PA-O3A
3	A	5101	ATP	O4'-C4'-C5'-O5'
3	A	5101	ATP	C3'-C4'-C5'-O5'

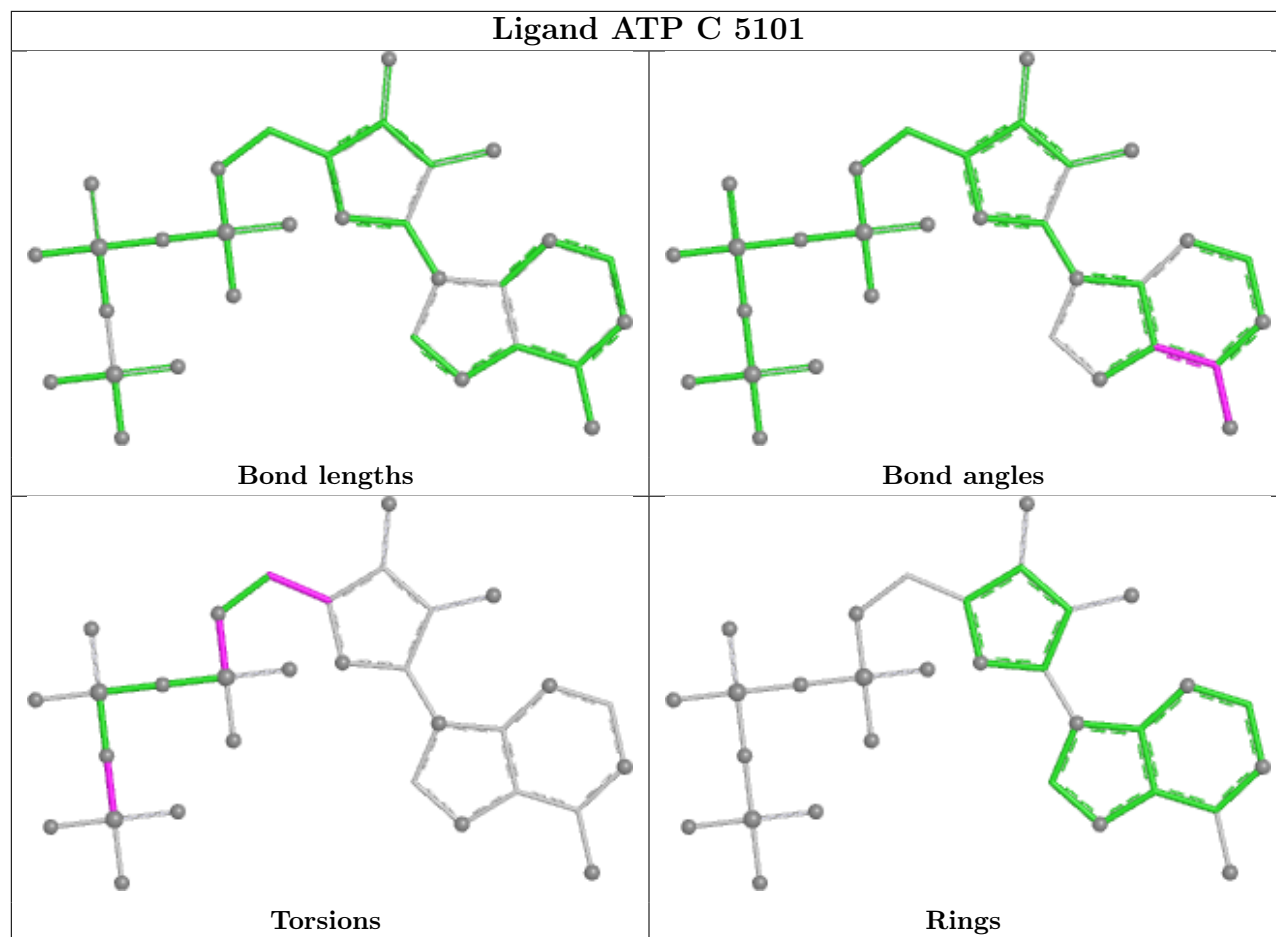
There are no ring outliers.

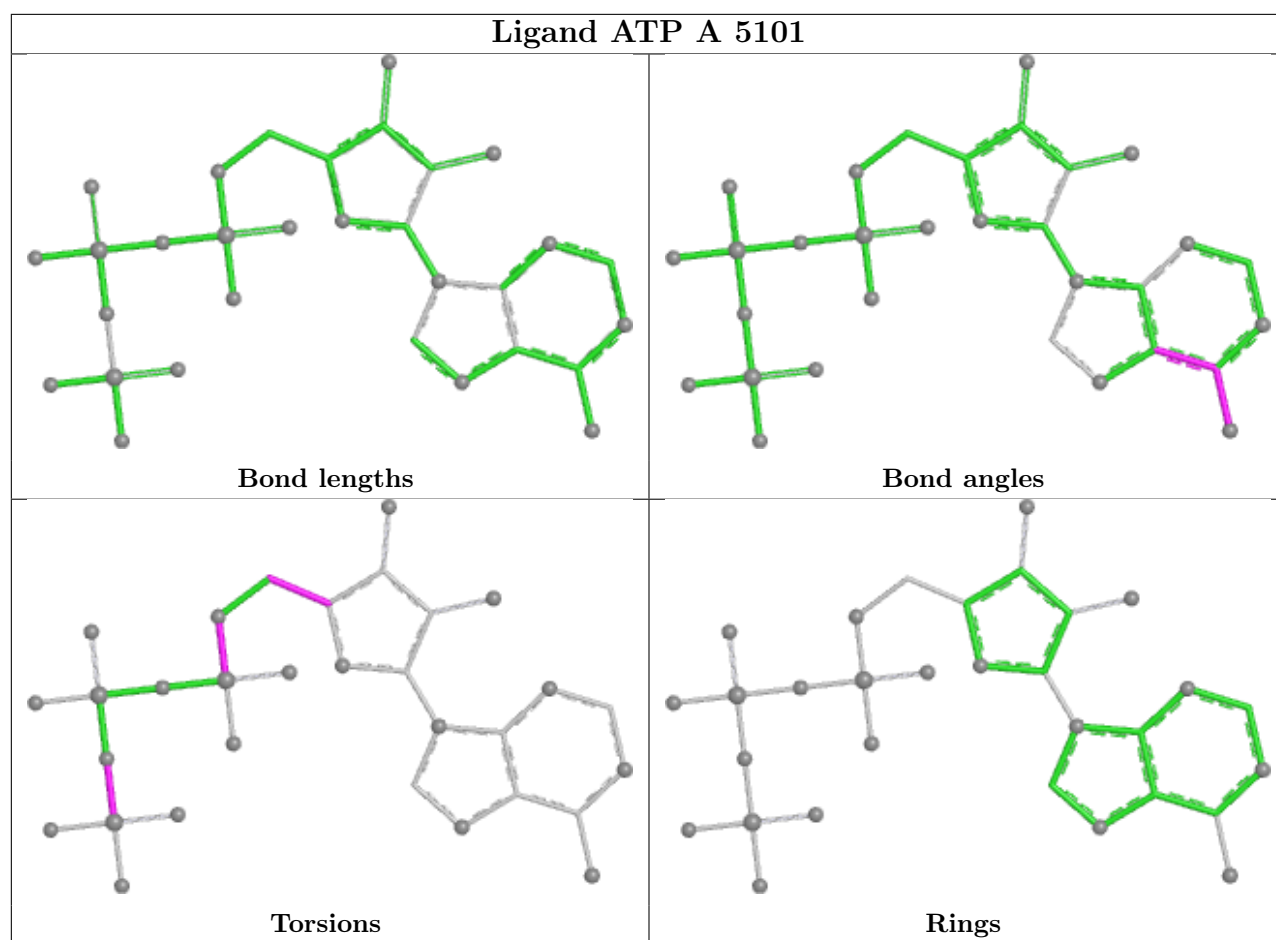
4 monomers are involved in 4 short contacts:

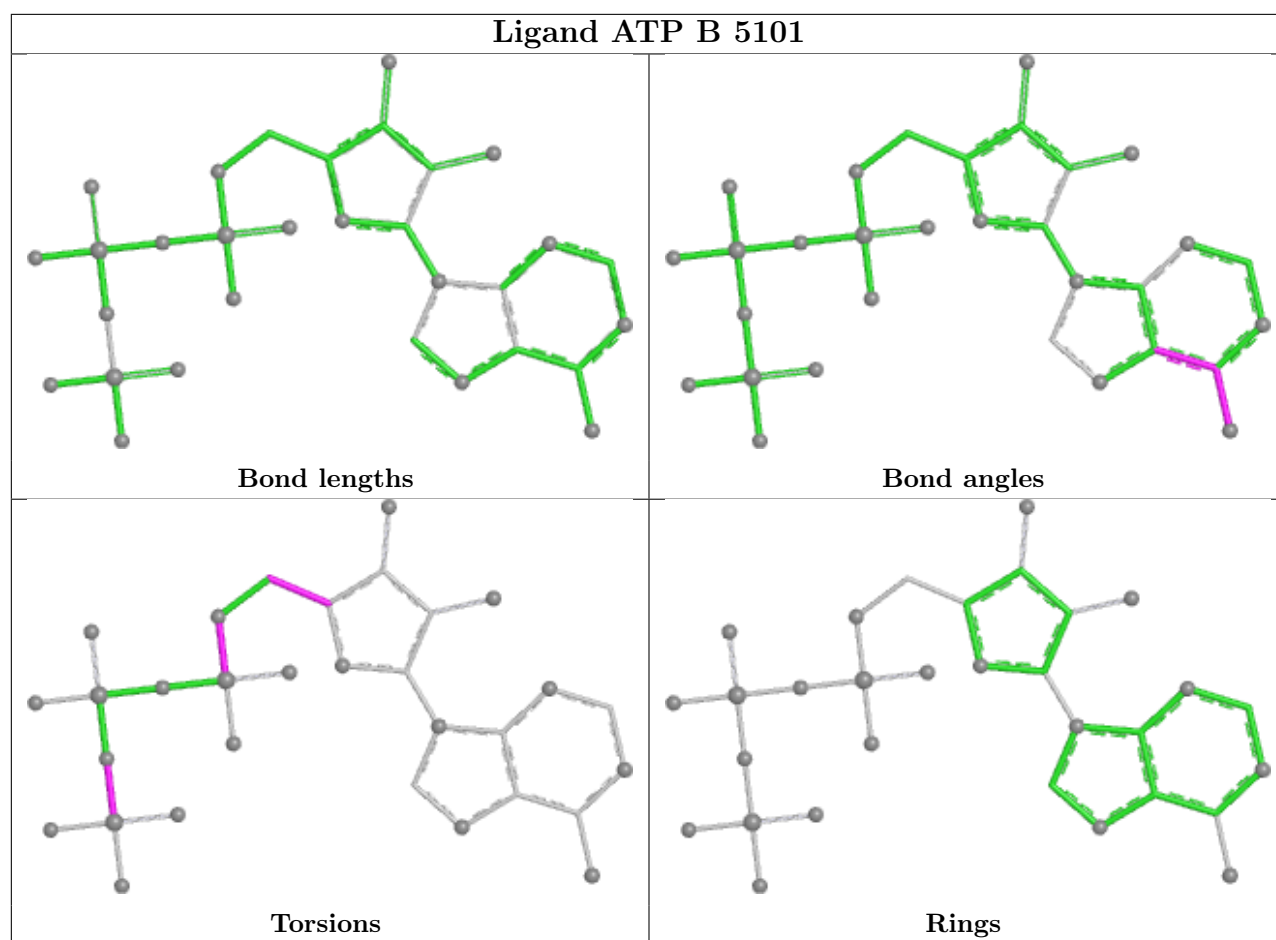
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5101	ATP	1	0
3	C	5101	ATP	1	0
3	A	5101	ATP	1	0
3	B	5101	ATP	1	0

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 [i](#)

There are no chain breaks in this entry.

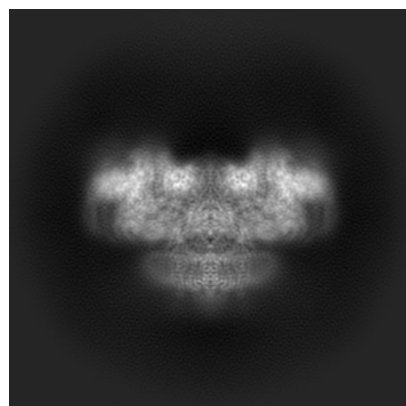
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25710. These allow visual inspection of the internal detail of the map and identification of artifacts.

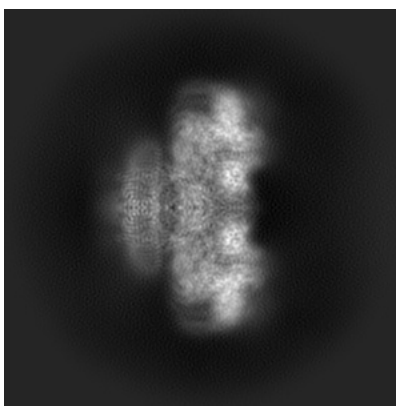
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

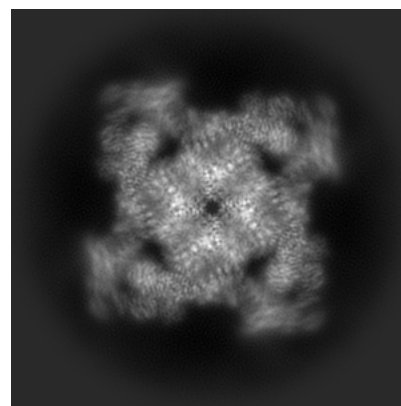
6.1.1 Primary map



X

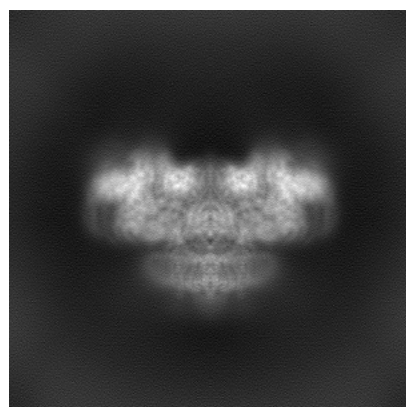


Y

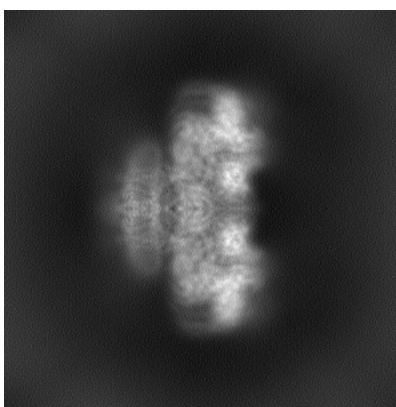


Z

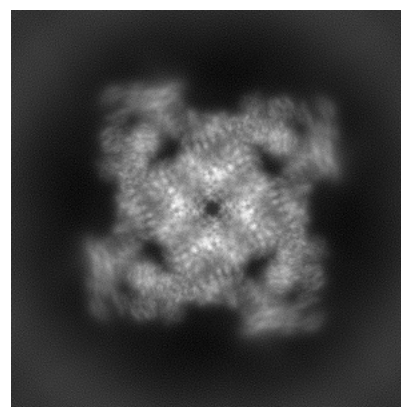
6.1.2 Raw map



X



Y

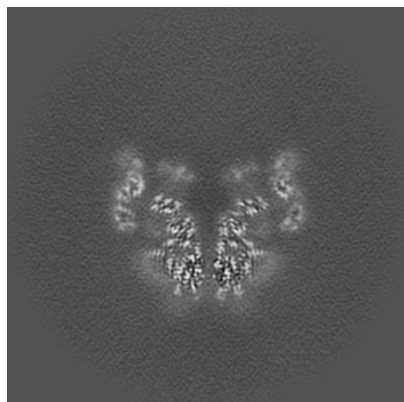


Z

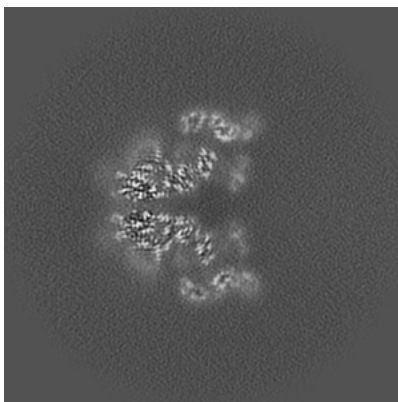
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

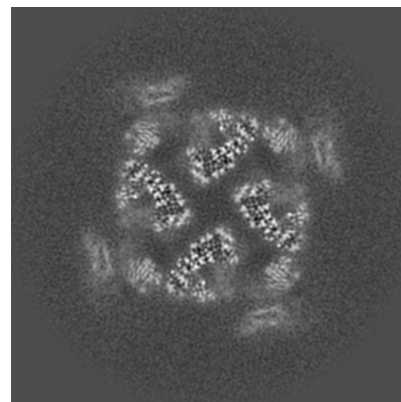
6.2.1 Primary map



X Index: 215

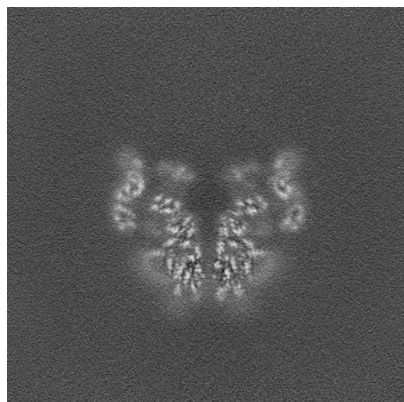


Y Index: 215

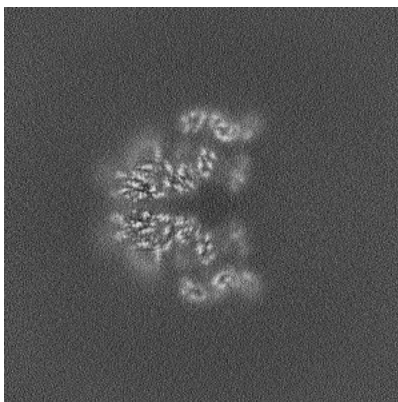


Z Index: 215

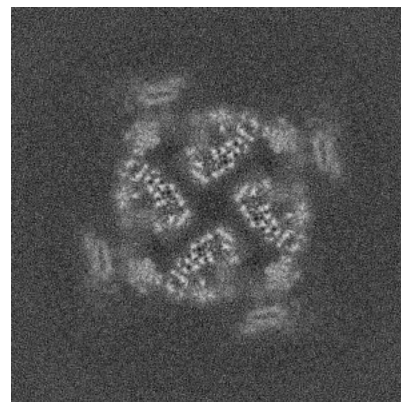
6.2.2 Raw map



X Index: 215



Y Index: 215

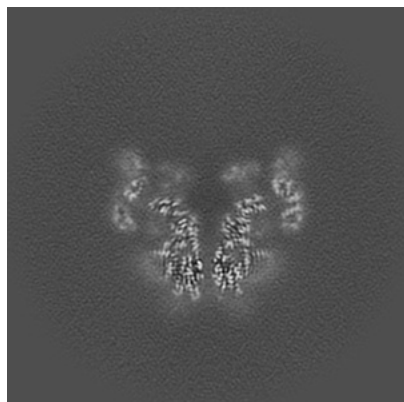


Z Index: 215

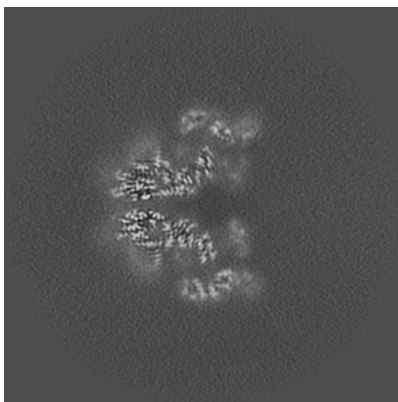
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

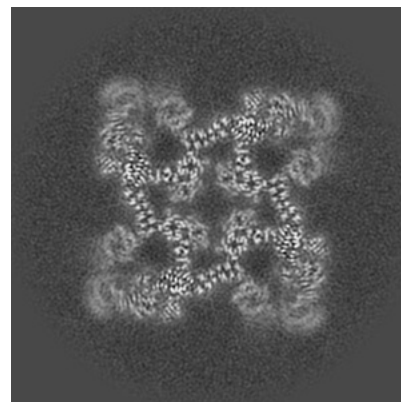
6.3.1 Primary map



X Index: 218

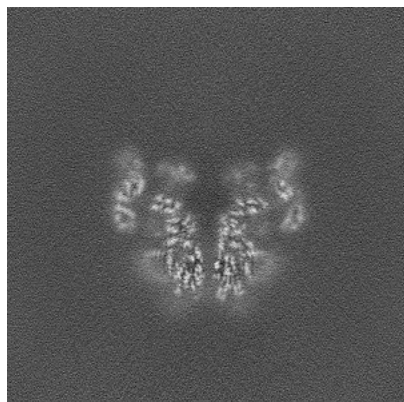


Y Index: 218

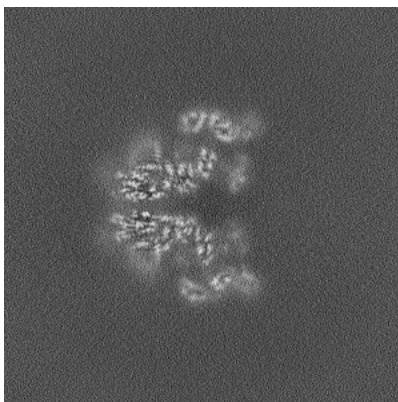


Z Index: 240

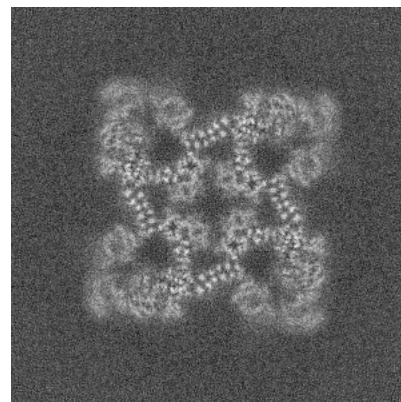
6.3.2 Raw map



X Index: 214



Y Index: 214

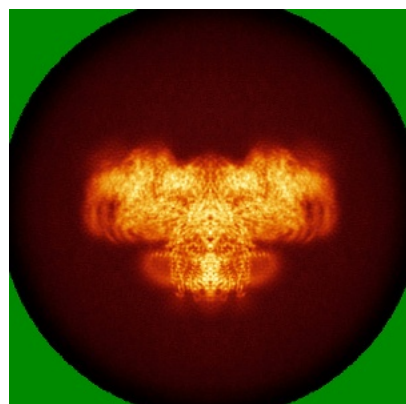


Z Index: 240

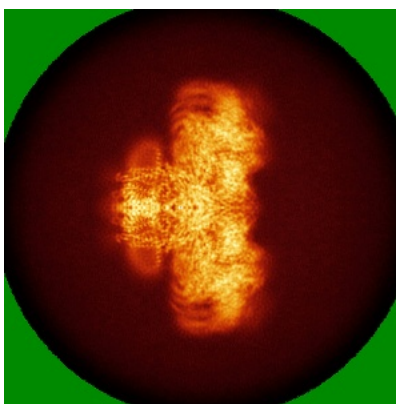
The images above show the largest variance slices of the map in three orthogonal directions.

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

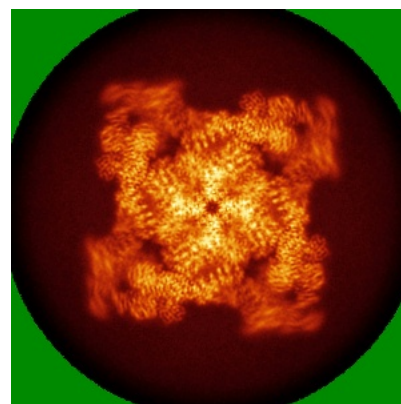
6.4.1 Primary map



X

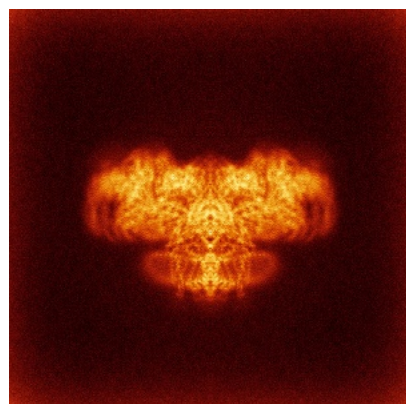


Y

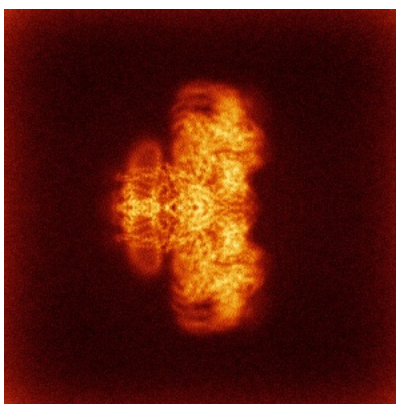


Z

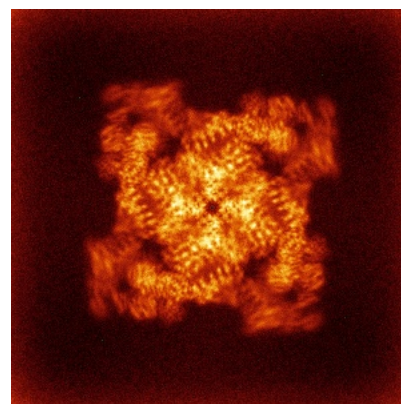
6.4.2 Raw map



X



Y

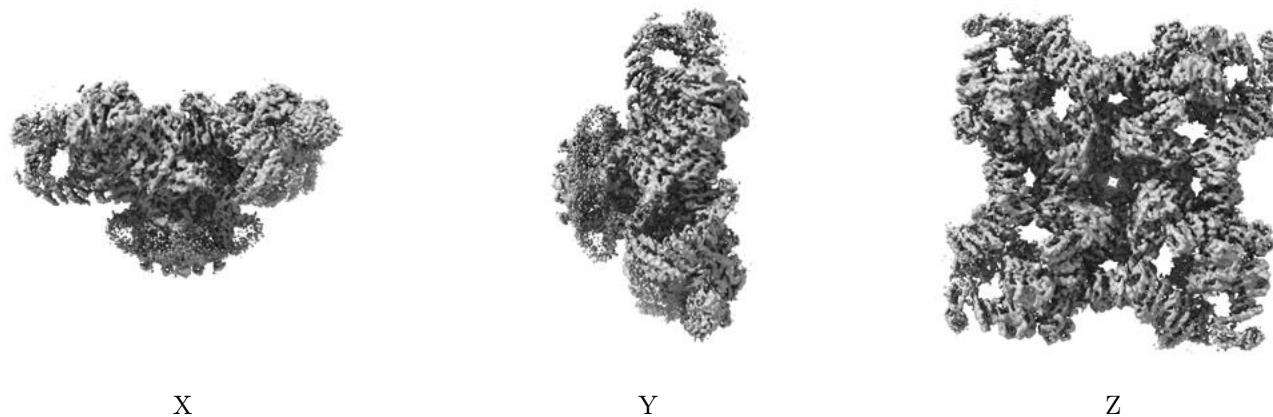


Z

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 0.176. 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.

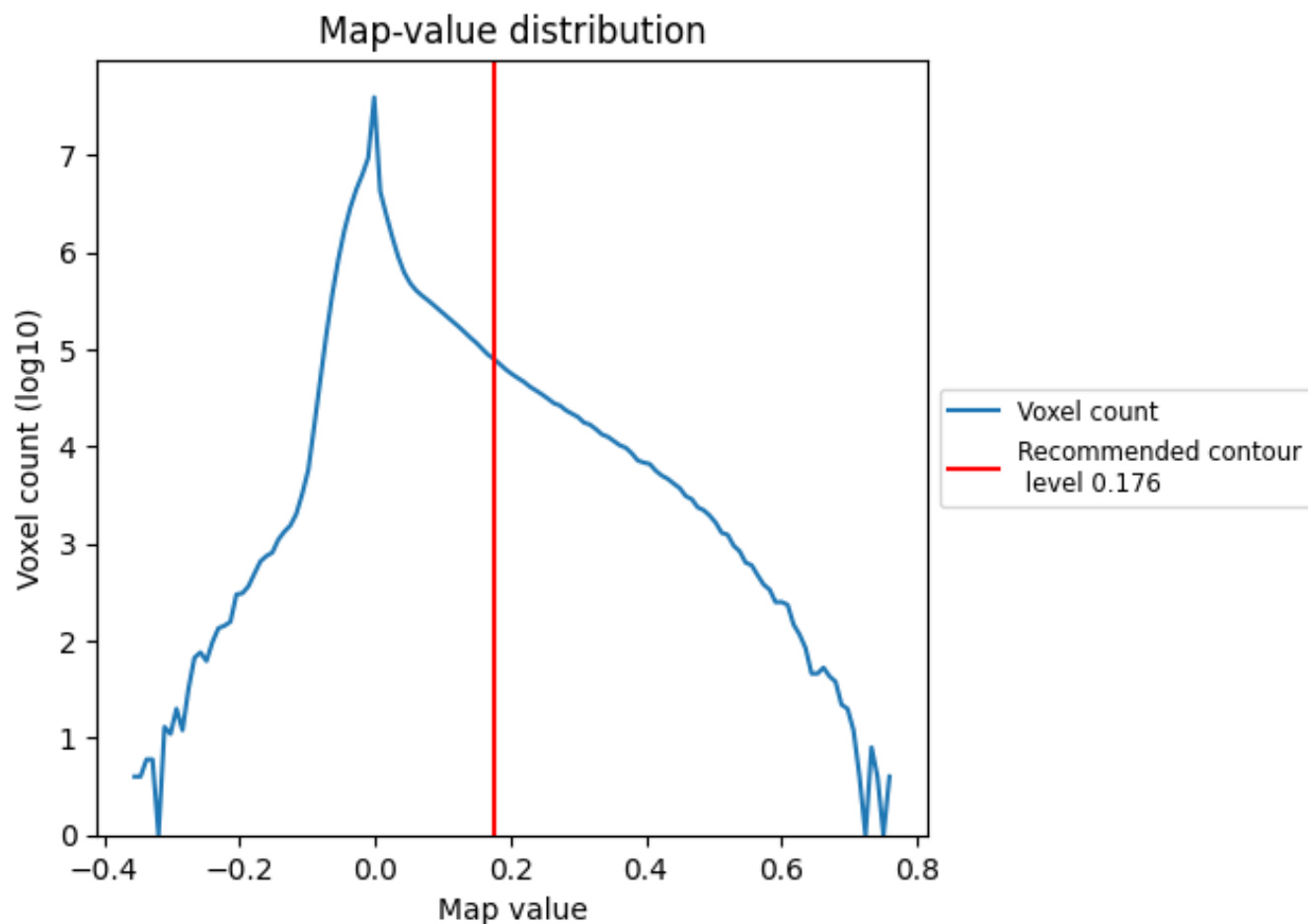
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

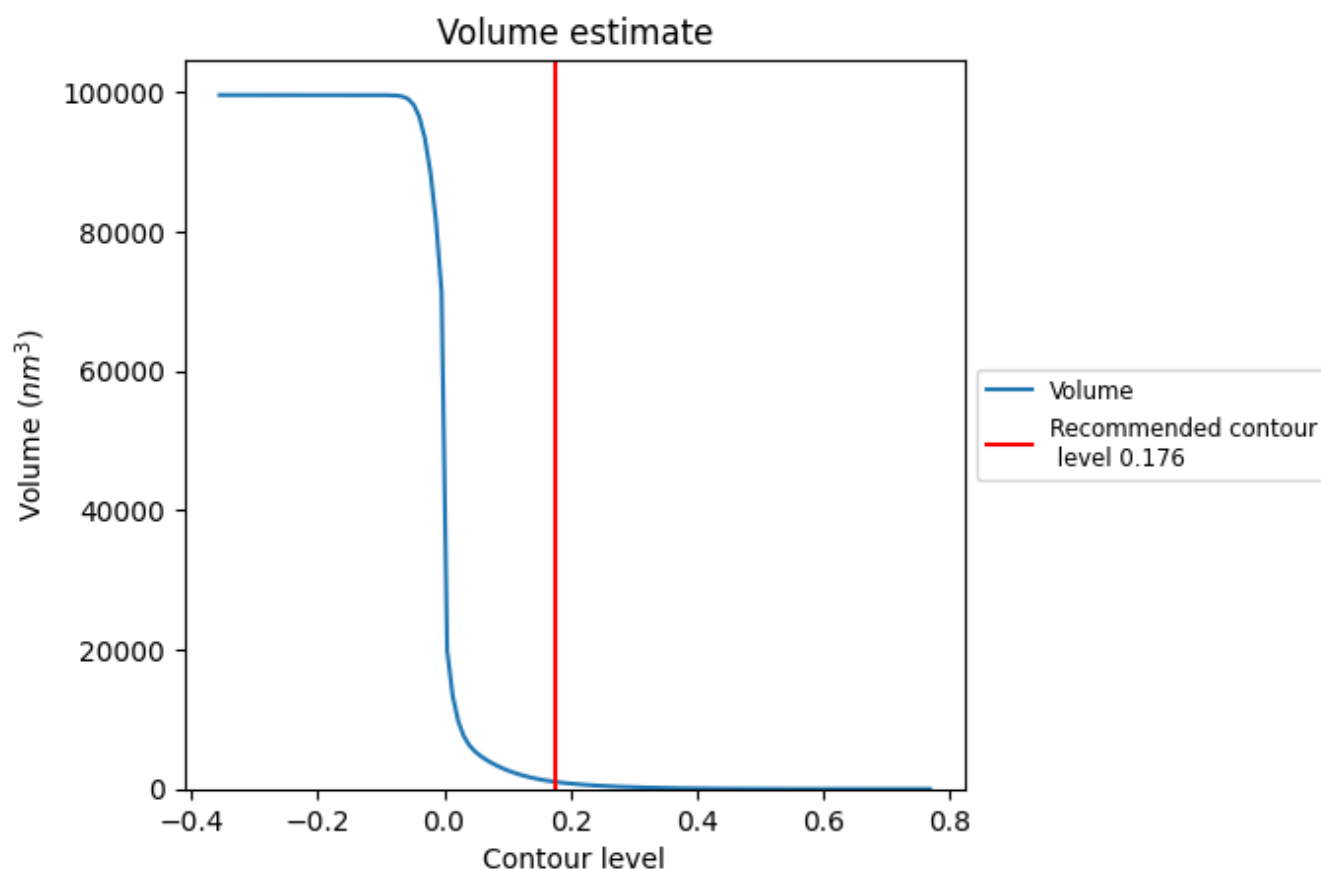
This section contains the results of statistical analysis of the map.

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.

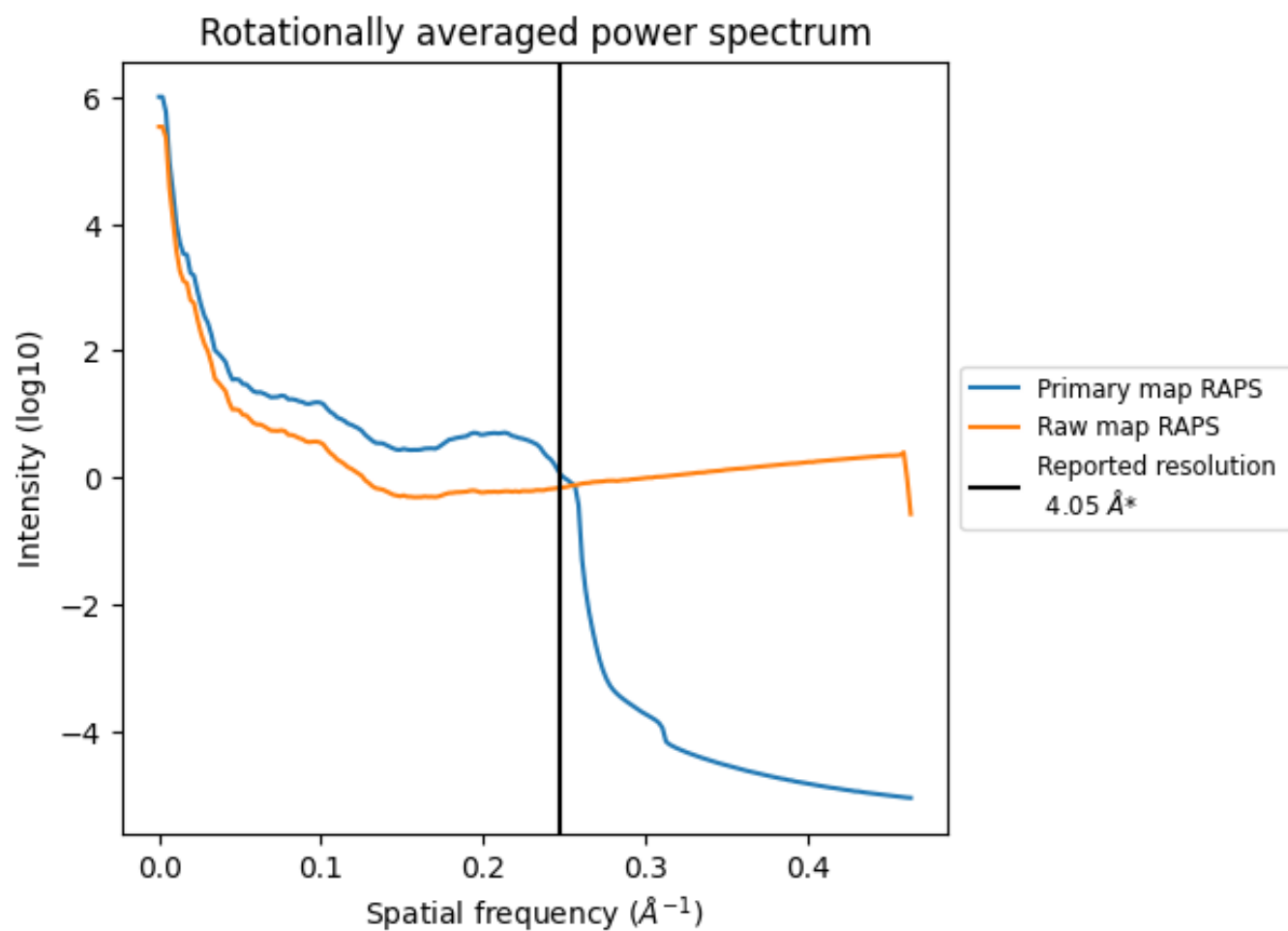
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1017 nm³; this corresponds to an approximate mass of 918 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 ⓘ

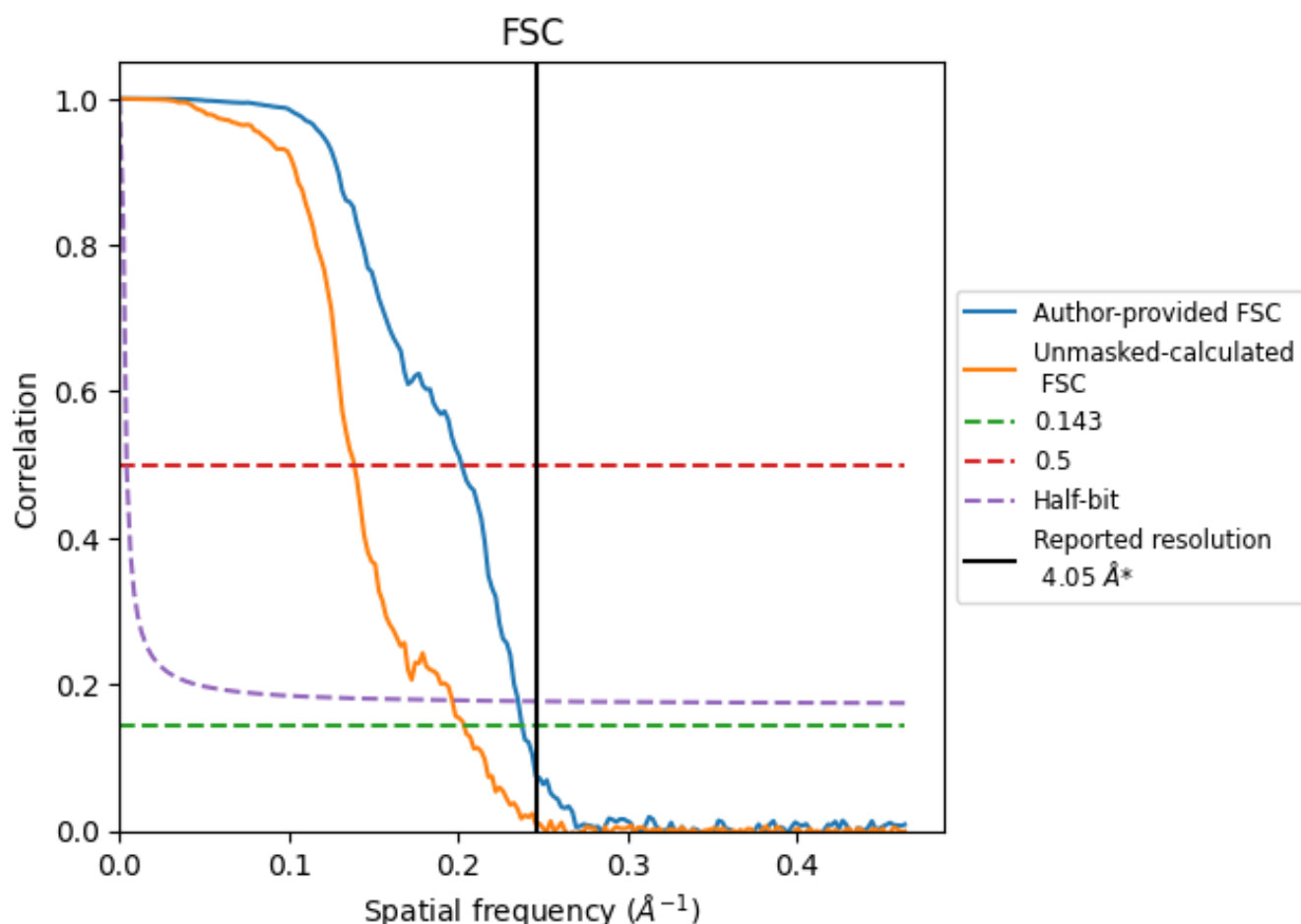


*Reported resolution corresponds to spatial frequency of 0.247 \AA^{-1}

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 0.247 \AA^{-1}

8.2 Resolution estimates [i](#)

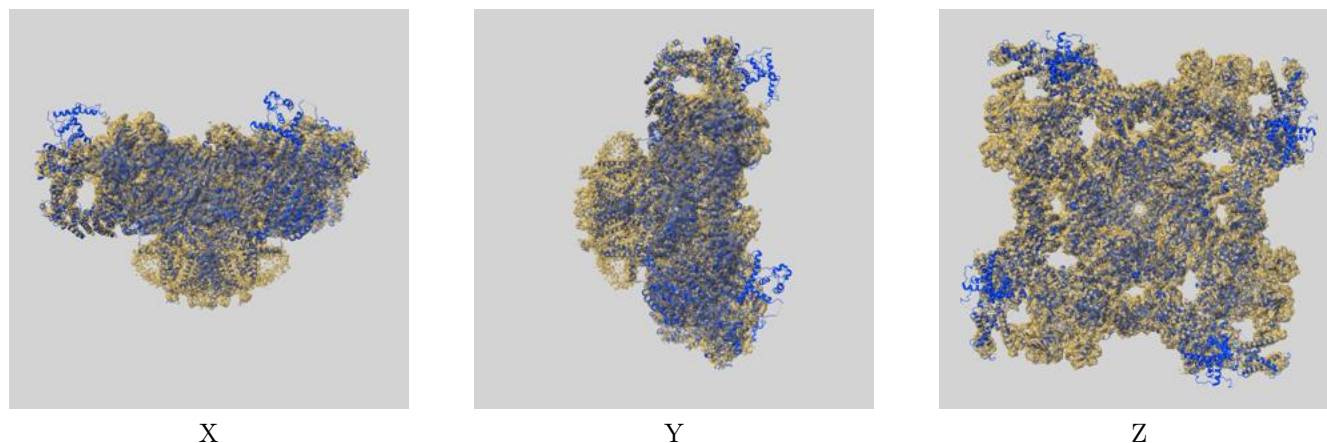
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.21	4.95	4.25
Unmasked-calculated*	4.91	7.22	5.09

*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 4.91 differs from the reported value 4.05 by more than 10 %

9 Map-model fit [i](#)

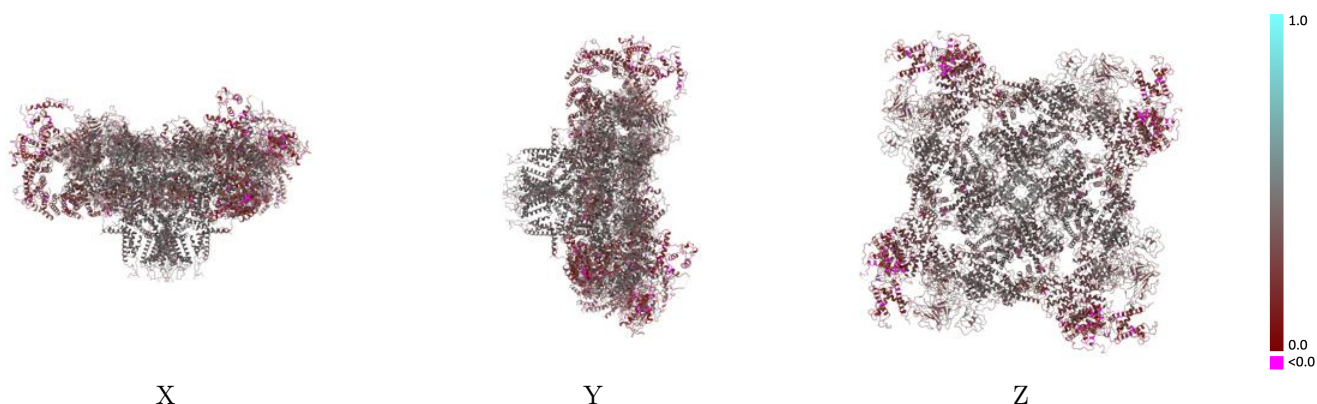
This section contains information regarding the fit between EMDB map EMD-25710 and PDB model 7T65. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



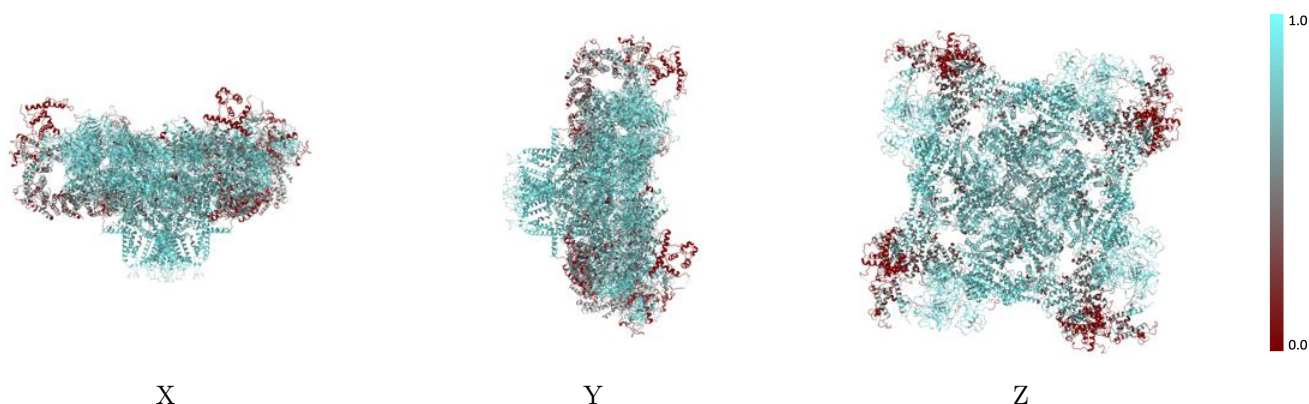
The images above show the 3D surface view of the map at the recommended contour level 0.176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



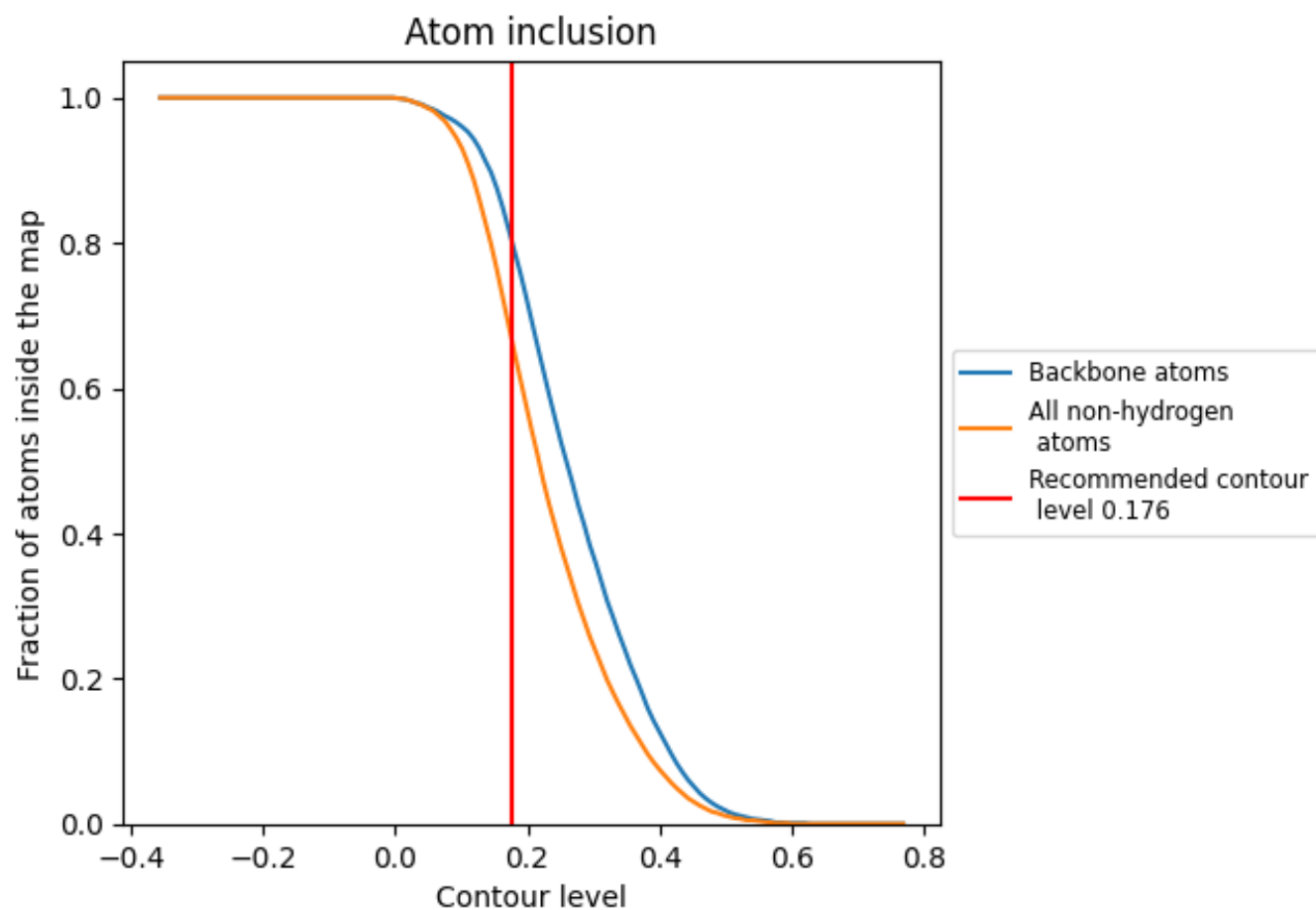
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.176).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 67% 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 (0.176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6680	<div></div> 0.3480
A	<div></div> 0.6650	<div></div> 0.3460
B	<div></div> 0.6650	<div></div> 0.3470
C	<div></div> 0.6650	<div></div> 0.3460
D	<div></div> 0.6650	<div></div> 0.3460
E	<div></div> 0.7840	<div></div> 0.3990
F	<div></div> 0.7840	<div></div> 0.4000
G	<div></div> 0.7870	<div></div> 0.3980
H	<div></div> 0.7850	<div></div> 0.3970

1.0

0.0

<0.0