



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:34 AM UTC

PDB ID : 6JI0 / pdb_00006ji0
EMDB ID : EMD-9831
Title : Structure of RyR2 (F/A/C/Ca²⁺ dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-19
Resolution : 4.20 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:

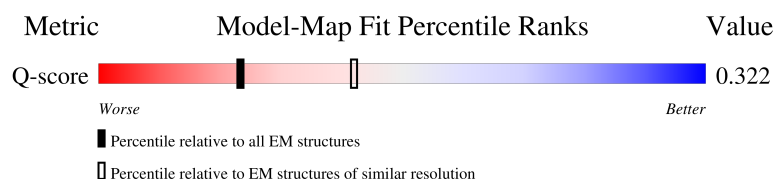
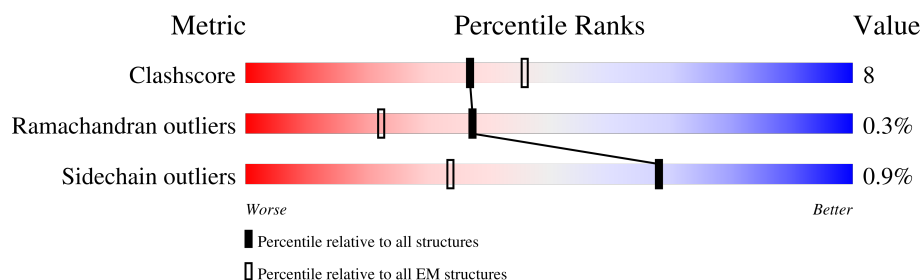
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



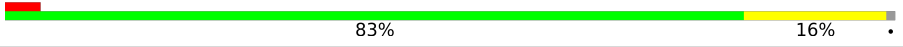
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	4968	16% 57% 13% 30%
1	C	4968	16% 57% 13% 30%
1	E	4968	16% 57% 13% 30%
1	G	4968	16% 57% 13% 30%

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Mol	Chain	Length	Quality of chain
2	B	108	 81% 19%
2	D	108	 82% 17%
2	F	108	 83% 16%
2	H	108	 83% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CFF	A	5103	-	X	-	-
6	CFF	C	5103	-	X	-	-
6	CFF	E	5103	-	X	-	-
6	CFF	G	5103	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 109772 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	C	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	E	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	G	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		

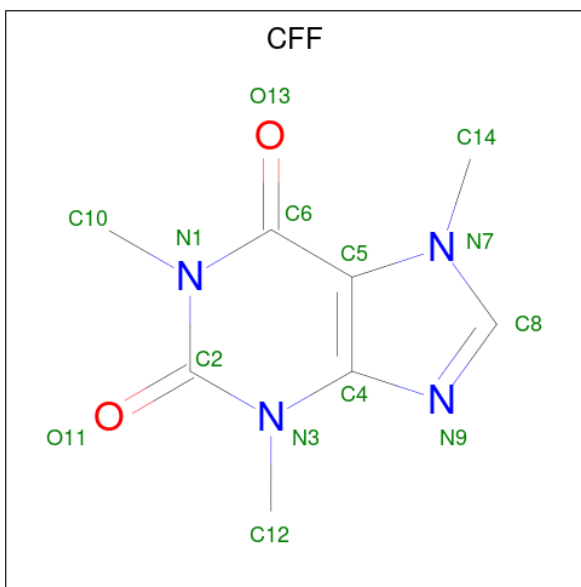
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

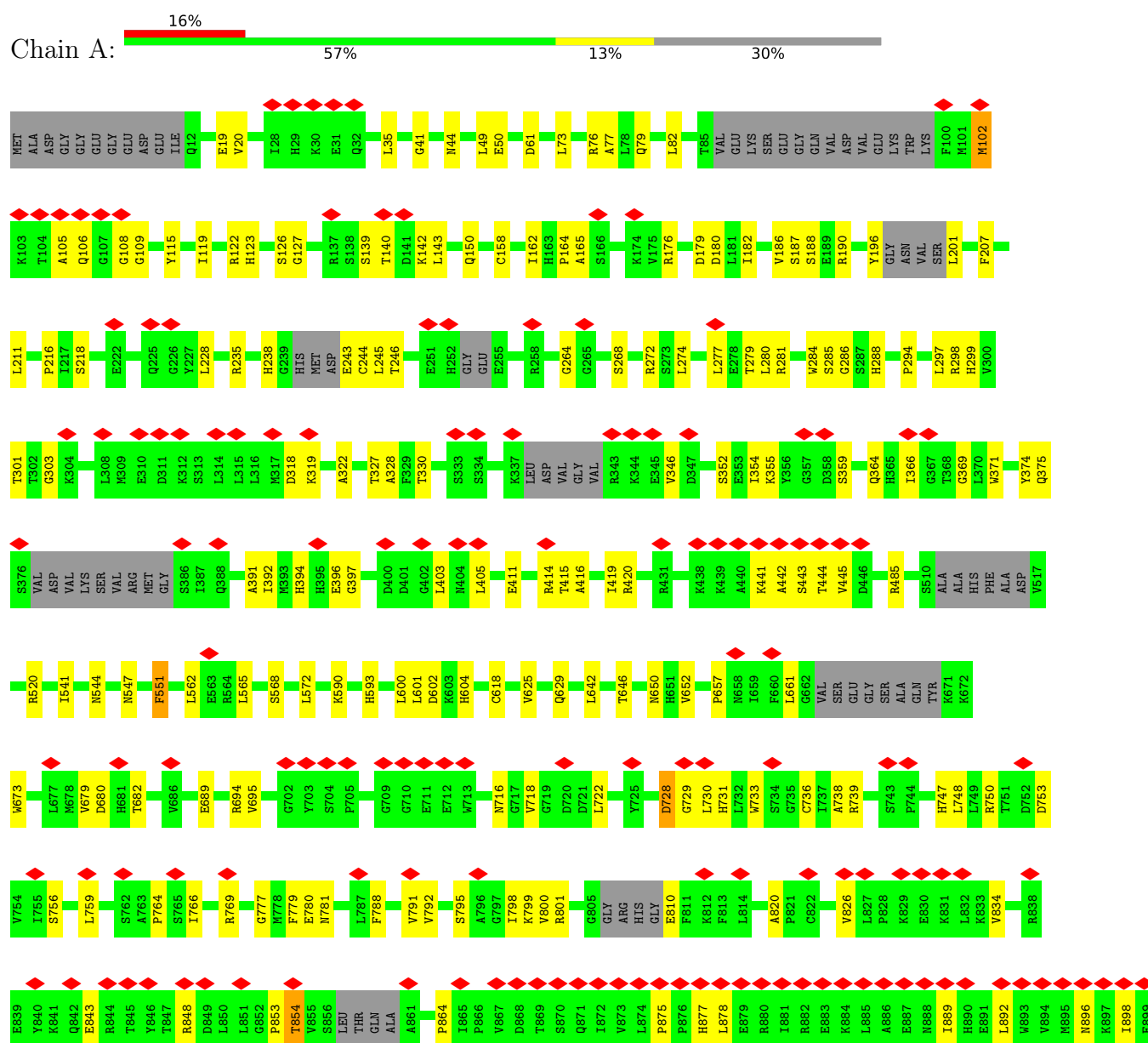


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

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 sequence, but not in the model, are shown in grey.

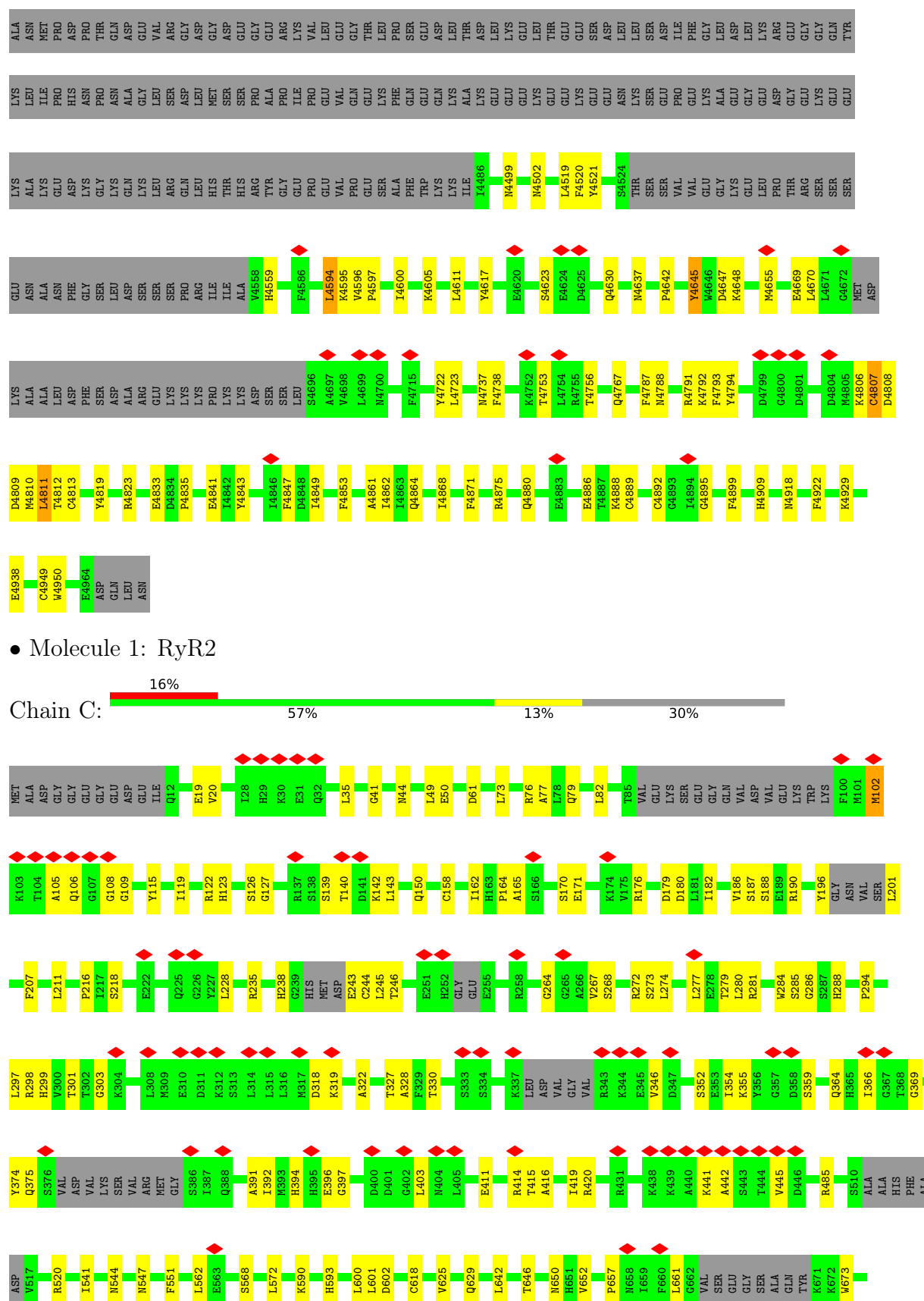
• Molecule 1: RyR2







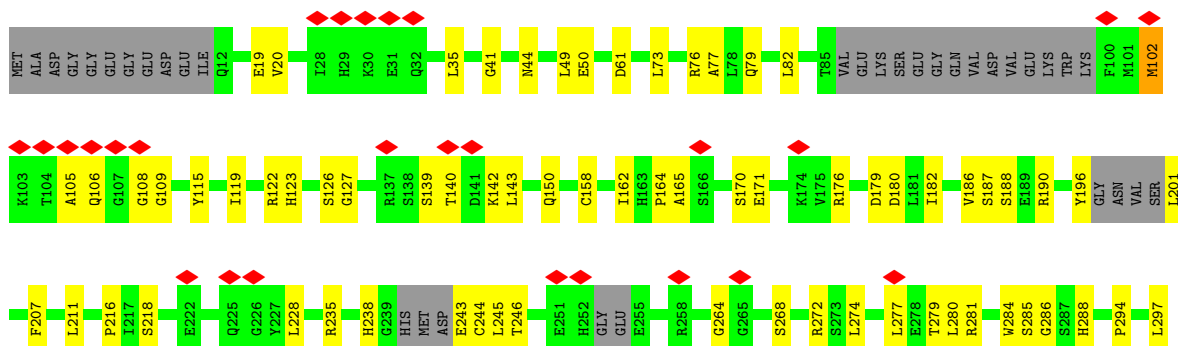




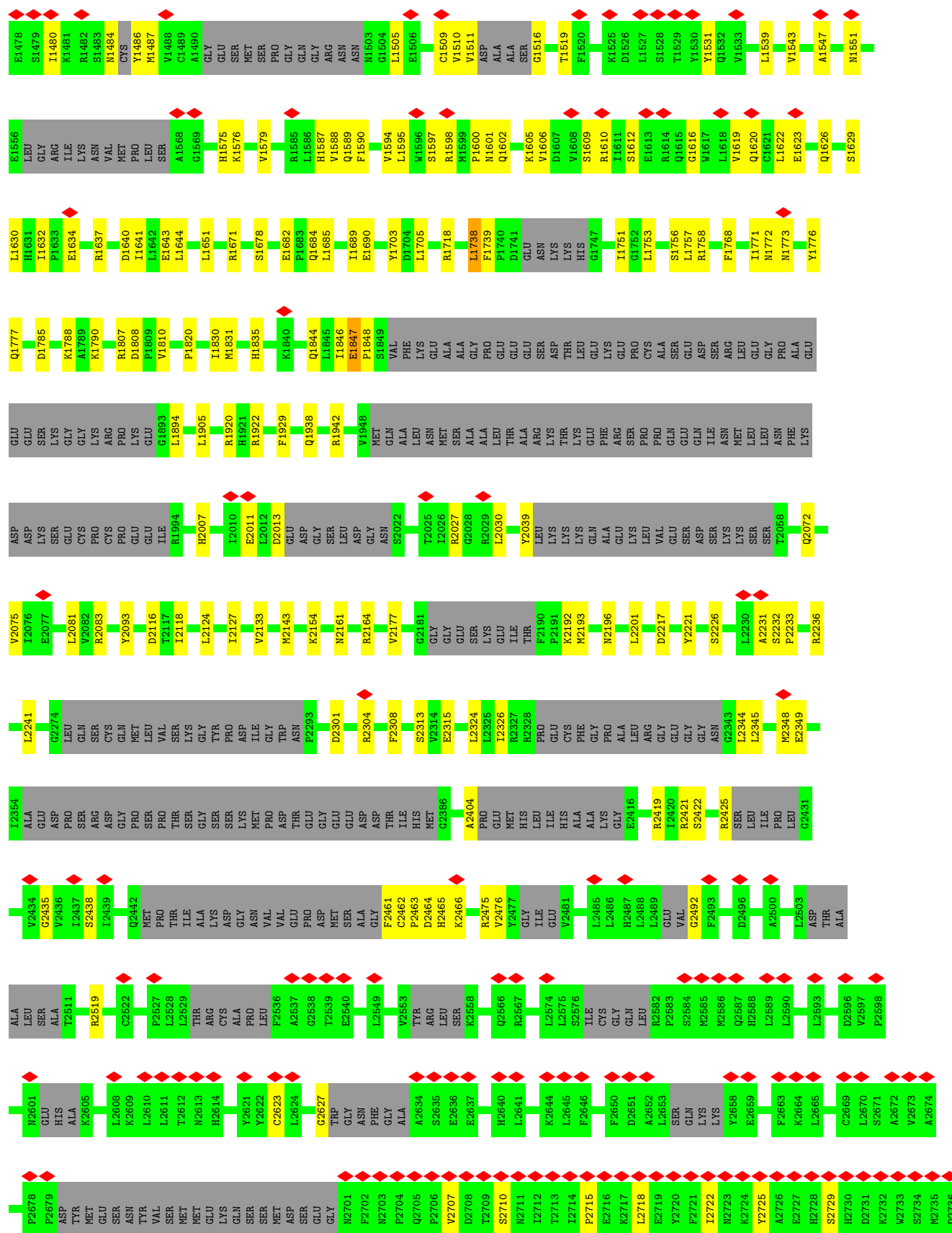














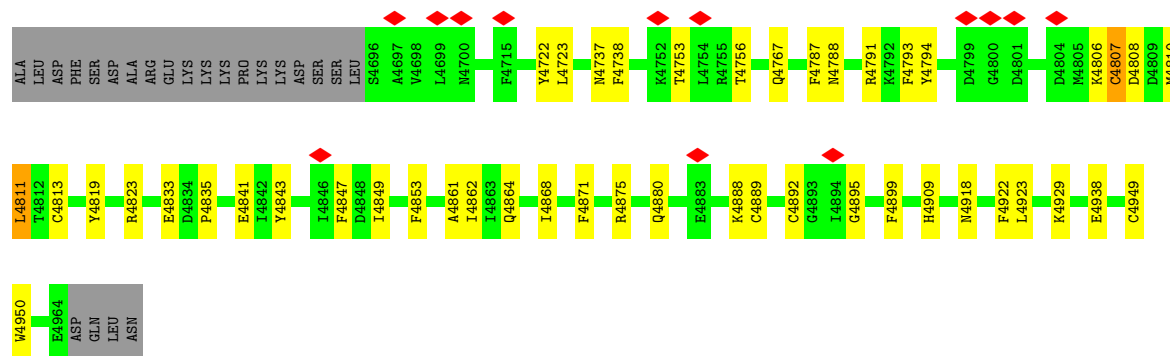






TYR	THR	GLN	MET	PRO	PRO	HIS	VAL	MET	VAL	VAL	GLU	PRO	ASP	MET	SER	ALA	GLY	Q2442	Q2442	P2527	L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	F2536	F2537	G2538	T2539	E2540	H2541	L2549	V2553	TYR	ARG	LEU	SER	K2558	Q2566	R2567	L2574	L2575	S2576	ILE	CYS	GLY	GLN	L2485	L2486	H2487	L2488	L2489	GLU	VAL	Q2492	F2493	D2496	A2500	L2503	ASP	THR	ALA	ALA	LEU	SER	ALA	T2511	C2522
L2610	L2611	T2612	N2613	H2614	Y2621	Y2622	C2623	L2624	Y2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	H2640	L2641	K2644	L2645	F2646	F2650	D2651	A2652	L2653	SER	GLN	LYS	Y2658	E2659	F2663	K2664	L2665	C2669	L2670	S2671	A2672	V2673	A2674	P2678	P2679	ASP	TYR	MET	GLU	ASN	N2601	HIS	ALA	K2605	L2608	K2609																
TYR	VAL	SER	MET	MET	GLU	LYS	GLN	SER	SER	MET	ASP	SER	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	H2730	D2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	Y2744	G2745												
E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	K2758	P2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	E2778	L2780	K2781	T2782	M2783	L2784	A2785	W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	L2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR													
ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	K2828	A2829	D2828	W2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840	W2841	A2842	E2843	M2844	W2845	E2846	N2848	Y2849	H2850	W2851	I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	Q2865												
G2866	G2867	N2868	H2869	P2870	L2871	L2872	P2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	L2893	K2894	K2895	F2896	Q2897	L2898	N2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	ASP	ASP	THR	PRO	SER	ILE	GLU	ARG	PHE	ALA	TYR	SER													
PHE	LEU	GLN	GLN	LEU	ILE	ARG	TYR	VAL	VAL	ALA	HIS	GLN	TYR	ILE	GLU	PHE	ASP	GLY	GLY	ARG	SER	SER	LYS	GLY	GLU	HIS	PRO	TYR	GLU	GLN	ILE	LYS	PHE	ALA	LYS	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	ASN	HIS	ARG	LEU	Y2982	F2983	L2984	S2985																				
S2988	R2989	P2990	L2991	G2994	G2995	H2996	A2997	S2998	N2999	K3000	E3001	K3002	E3003	M3004	V3005	THR	SER	LEU	F3009	C3010	K3011	L3012	V3014	L3015	L3016	K3017	H3018	R3019	F3081	L3020	S3021	L3022	F3023	G3024	N3025	D3026	A3027	T3028	SER	ILE	VAL	ASN	CYS	L3034	H3035	I3036	L3037	T3040	L3041	D3042	A3043	R3044	T3045	V3046	M3047	K3048															
T3049	G3050	L3051	E3052	S3053	K3055	SER	ALA	ALA	LEU	ARG	ALA	F3061	L3062	D3063	N3064	A3065	A3066	E3067	D3068	L3069	E3070	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3078	G3079	Q3080	F3081	L3082	HIS	THR	ARG	ASN	PRO	GLN	LYS	GLY	VAL	THR	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108											
L3109	F3110	E3111	H3112	L3113	G3114	Q3115	H3116	Q3117	F3118	GLY	GLU	ASP	LEU	ILE	L3124	E3125	D3126	V3127	Q3128	V3129	S3130	C3131	R3132	A3133	L3134	L3135	L3136	S3137	L3138	Y3139	A3140	L3141	G3142	T3143	S3144	LYS	SER	ILE	TYR	V3149	E3150	R3151	Q3152	R3153	S3154	A3155	L3156	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO												
VAL	A3170	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	L3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	THR	LYS	SER	SER	GLY	PRO	ARG	GLU	ASN	ALA	ALA	GLY	ASN	ARG	GLU	PRO	THR	VAL	GLU	ASP	GLY	LEU	LEU	GLY	ASN	MET	GLU	GLU	ILE	ILE	VAL	ASP	LEU	ALA	GLU	SER	GLY	ILE	ARG														
TYR	THR	GLN	MET	PRO	PRO	HIS	VAL	MET	VAL	VAL	LEU	PRO	MET	SER	GLY	ARG	ASN	THR	THR	LYS	SER	SER	GLY	PRO	ARG	GLU	ASN	ALA	ALA	GLY	ASN	ARG	GLU	PRO	THR	VAL	GLU	ASP	GLY	LEU	LEU	GLY	ASN	MET	GLU	GLU	ILE	ILE	VAL	ASP	LEU	ALA	GLU	SER	GLY	ILE	ARG														





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

Chain B: 81% 19%



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

Chain D: 82% 17%



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

Chain F: 83% 16%



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

Chain H: 83% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	78841	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ATP, CA, 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	0.32	0/27073	0.65	16/36605 (0.0%)
1	C	0.32	0/27073	0.65	16/36605 (0.0%)
1	E	0.32	0/27073	0.65	16/36605 (0.0%)
1	G	0.32	0/27073	0.65	16/36605 (0.0%)
2	B	0.25	0/835	0.51	0/1123
2	D	0.25	0/835	0.51	0/1123
2	F	0.25	0/835	0.51	0/1123
2	H	0.25	0/835	0.51	0/1123
All	All	0.32	0/111632	0.65	64/150912 (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	25
1	C	0	25
1	E	0	25
1	G	0	25
All	All	0	100

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	CA-C-N	7.16	134.58	121.70
1	A	139	SER	C-N-CA	7.16	134.58	121.70
1	C	139	SER	CA-C-N	7.16	134.58	121.70
1	C	139	SER	C-N-CA	7.16	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	139	SER	CA-C-N	7.16	134.58	121.70

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Peptide
1	A	142	LYS	Peptide
1	A	520	ARG	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26577	0	25112	456	0
1	C	26577	0	25112	439	0
1	E	26577	0	25113	439	0
1	G	26577	0	25113	431	0
2	B	819	0	824	12	0
2	D	819	0	824	11	0
2	F	819	0	824	12	0
2	H	819	0	824	10	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	31	0	12	2	0
4	C	31	0	12	1	0
4	E	31	0	12	1	0
4	G	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
All	All	109772	0	103834	1614	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 1614 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:E:4853:PHE:CZ	1:G:4823:ARG:HA	1.53	1.43
1:A:4823:ARG:HA	1:G:4853:PHE:CZ	1.54	1.42
1:C:4853:PHE:CZ	1:E:4823:ARG:HA	1.54	1.41
1:A:4853:PHE:CZ	1:C:4823:ARG:HA	1.54	1.40
1:A:4794:TYR:HD2	1:A:4807:CYS:CB	1.46	1.27

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	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	36	71
1	C	3356/4968 (68%)	2915 (87%)	432 (13%)	9 (0%)	36	71
1	E	3356/4968 (68%)	2910 (87%)	437 (13%)	9 (0%)	36	71
1	G	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	36	71
2	B	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13844/20304 (68%)	12025 (87%)	1783 (13%)	36 (0%)	37	71

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4595	LYS
1	A	4645	TYR
1	C	4595	LYS
1	C	4645	TYR
1	E	4595	LYS

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	2681/4355 (62%)	2654 (99%)	27 (1%)	68	75
1	C	2680/4355 (62%)	2656 (99%)	24 (1%)	70	75
1	E	2682/4355 (62%)	2656 (99%)	26 (1%)	68	75
1	G	2681/4355 (62%)	2655 (99%)	26 (1%)	68	75
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	11076/17776 (62%)	10973 (99%)	103 (1%)	68	75

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	907	VAL
1	E	3847	LEU
1	G	4185	GLU
1	E	950	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1632	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 251 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4499	ASN
1	G	1921	HIS
1	E	747	HIS
1	G	1844	GLN
1	G	3990	ASN

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	$\# Z > 2$
6	CFF	E	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)
6	CFF	A	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	C	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	A	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	E	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	G	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
6	CFF	C	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)
6	CFF	G	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	E	5103	-	-	-	0/2/2/2
6	CFF	A	5103	-	-	-	0/2/2/2
4	ATP	C	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	A	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	E	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5101	ATP	C5-C4	4.27	1.46	1.39
4	C	5101	ATP	C5-C4	4.27	1.46	1.39
4	E	5101	ATP	C5-C4	4.27	1.46	1.39
4	G	5101	ATP	C5-C4	4.27	1.46	1.39
6	G	5103	CFF	C6-N1	-4.22	1.31	1.40

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	CFF	C14-N7-C8	-7.76	111.77	126.28
6	G	5103	CFF	C14-N7-C8	-7.75	111.77	126.28
6	E	5103	CFF	C14-N7-C8	-7.74	111.80	126.28
6	C	5103	CFF	C14-N7-C8	-7.73	111.82	126.28
4	A	5101	ATP	C5-C4-N3	-6.11	118.31	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

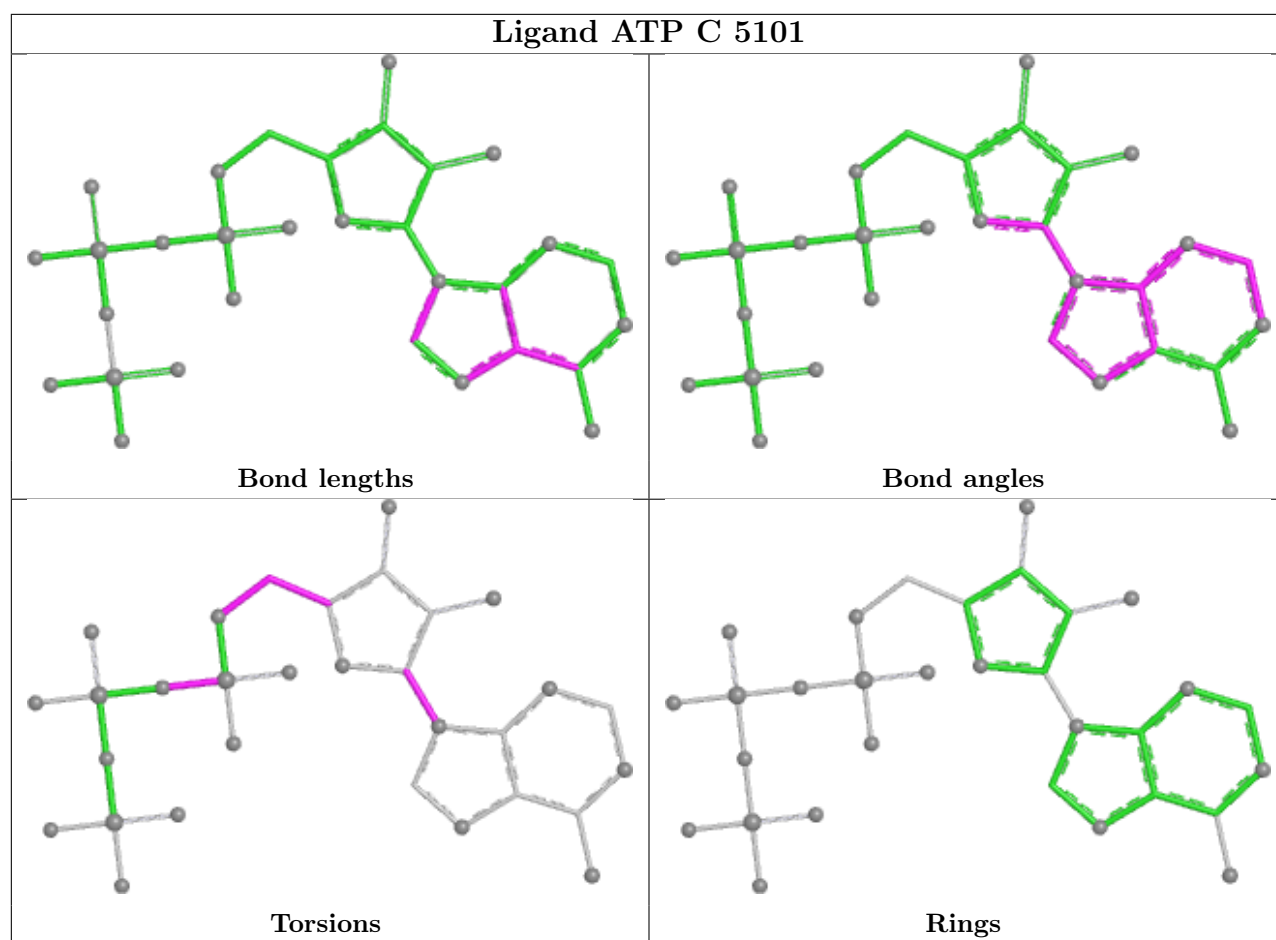
Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	O4'-C1'-N9-C8
4	A	5101	ATP	O4'-C1'-N9-C4
4	C	5101	ATP	O4'-C1'-N9-C8
4	C	5101	ATP	O4'-C1'-N9-C4
4	E	5101	ATP	O4'-C1'-N9-C8

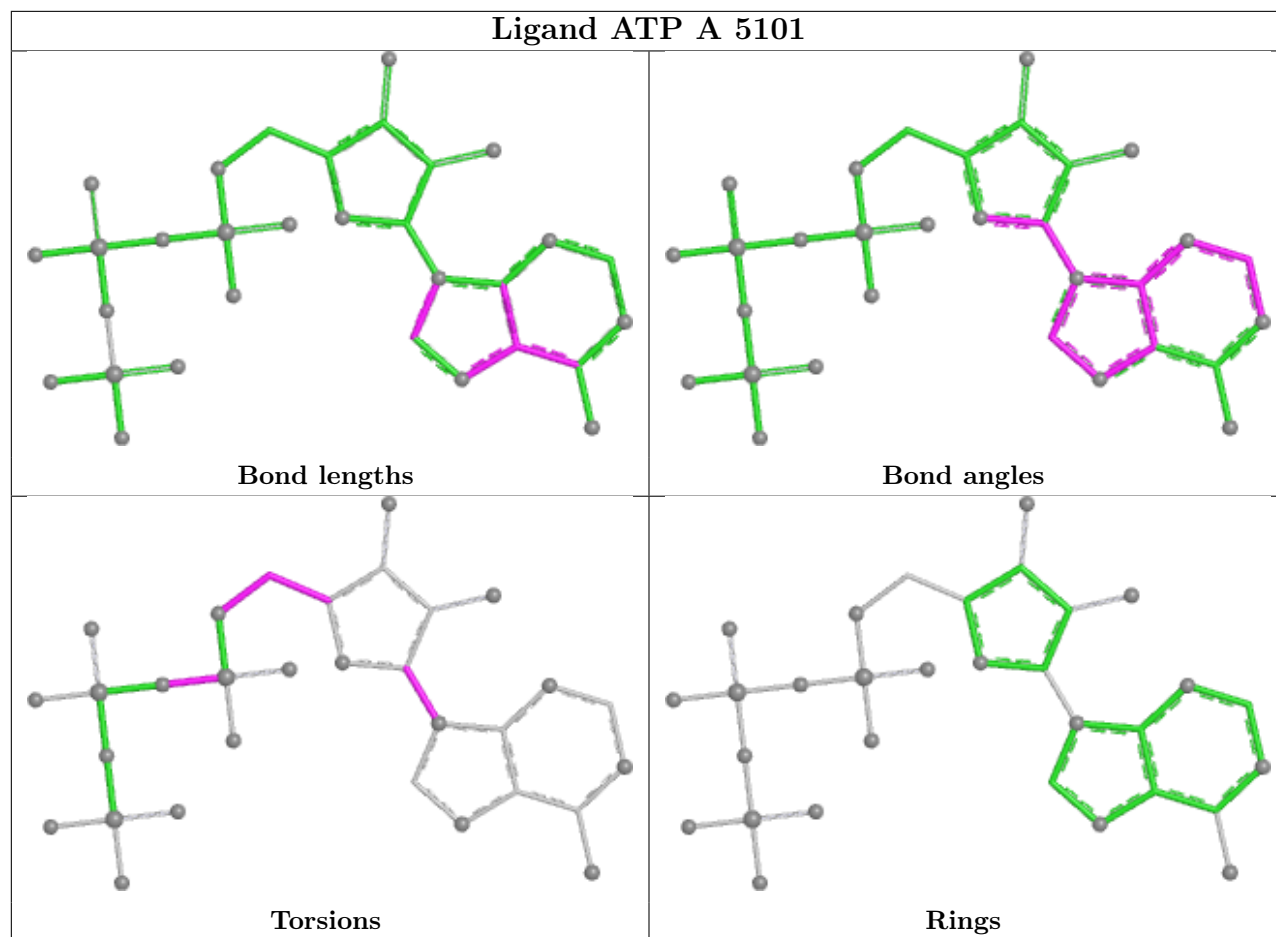
There are no ring outliers.

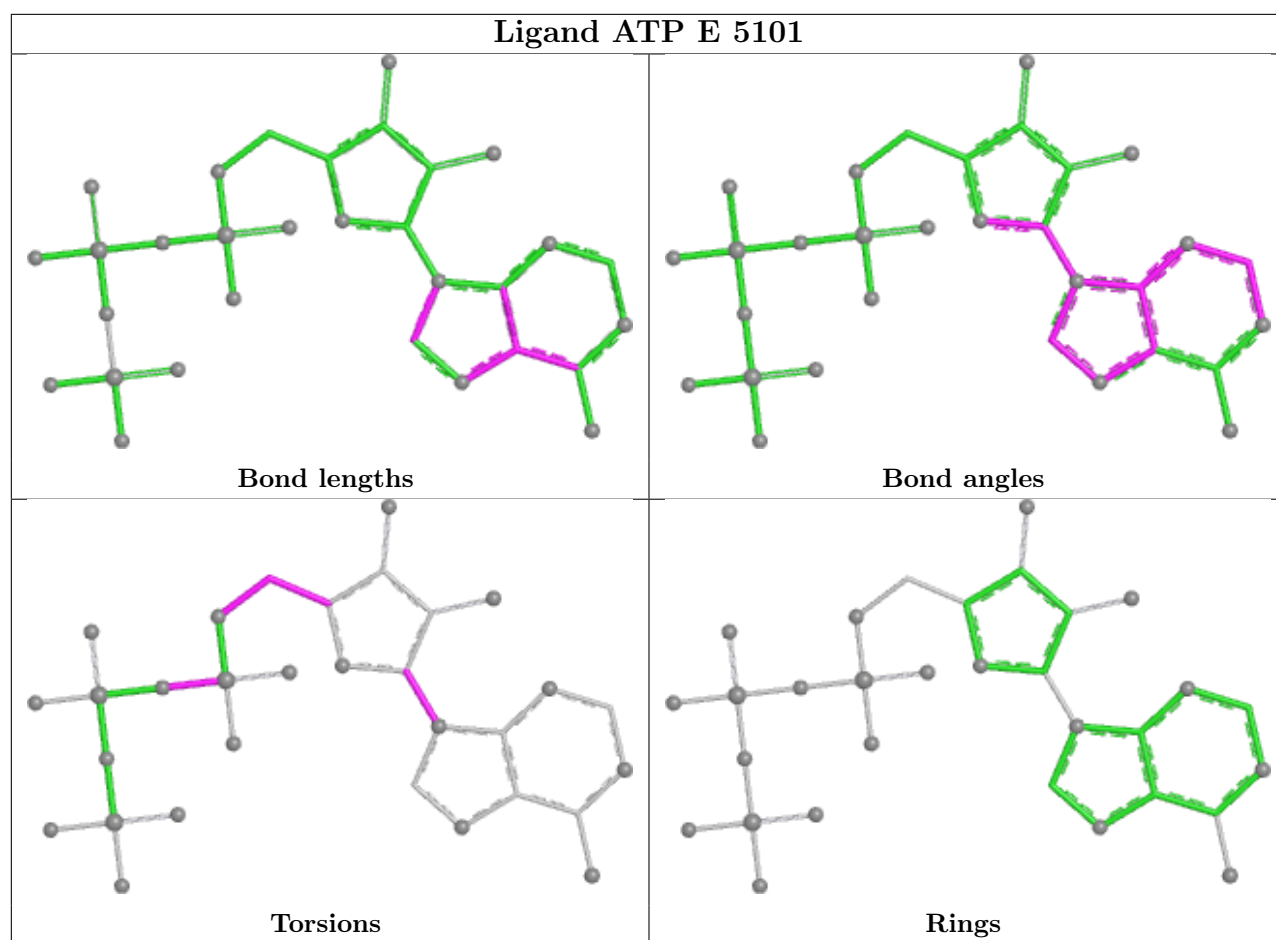
4 monomers are involved in 5 short contacts:

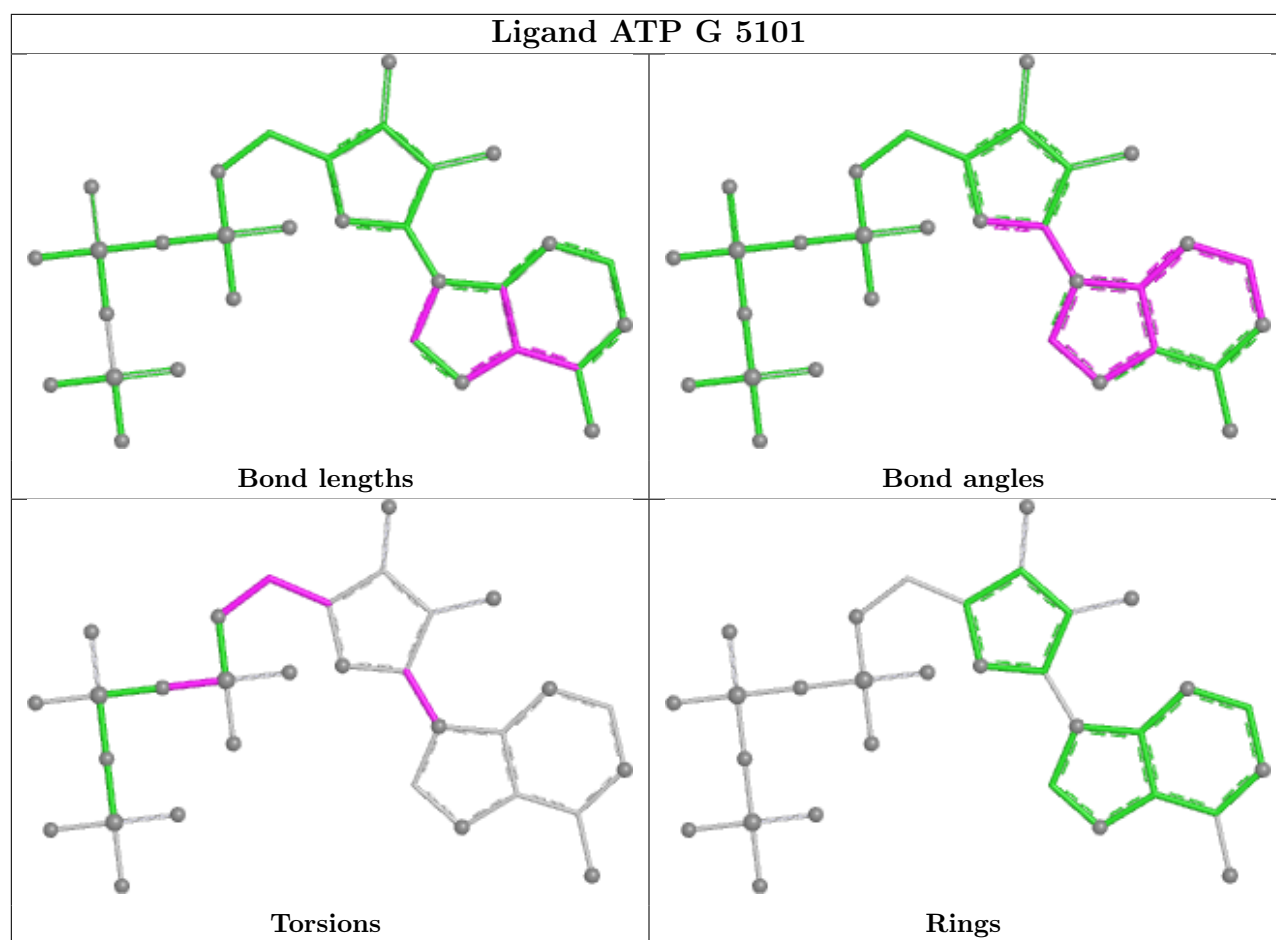
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5101	ATP	1	0
4	A	5101	ATP	2	0
4	E	5101	ATP	1	0
4	G	5101	ATP	1	0

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.

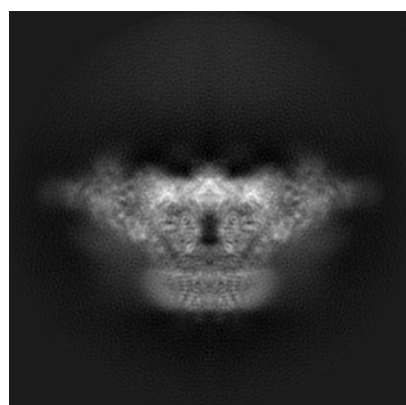
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9831. These allow visual inspection of the internal detail of the map and identification of artifacts.

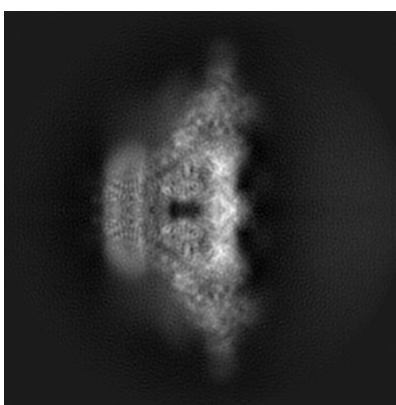
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

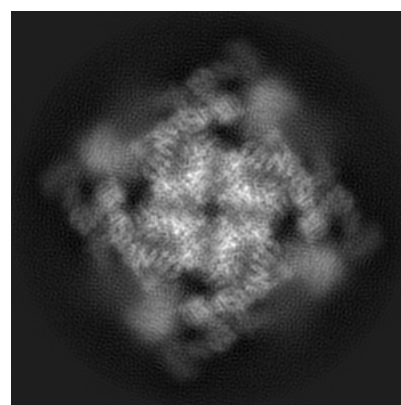
6.1.1 Primary map



X



Y

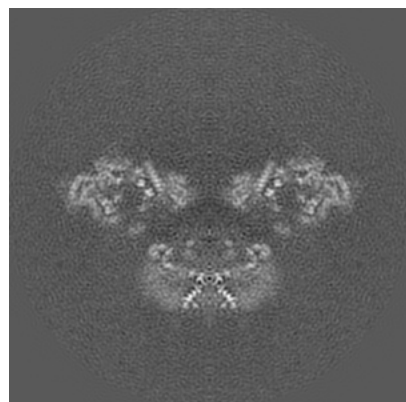


Z

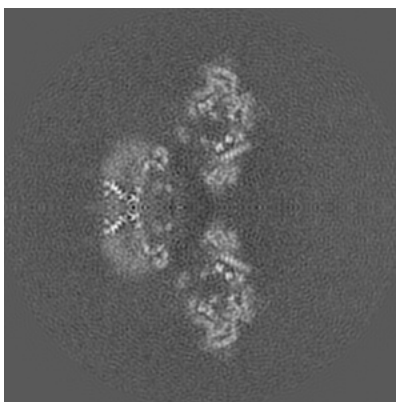
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

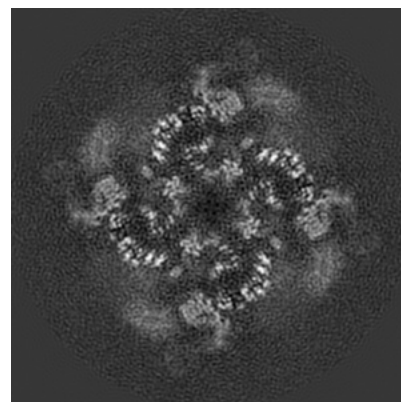
6.2.1 Primary map



X Index: 200



Y Index: 200

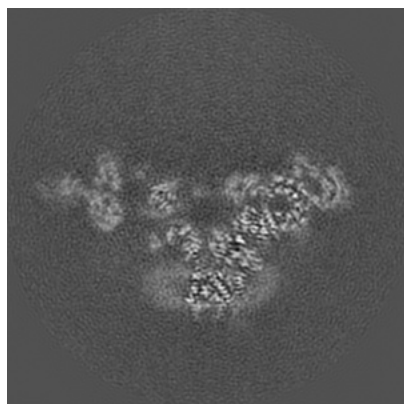


Z Index: 200

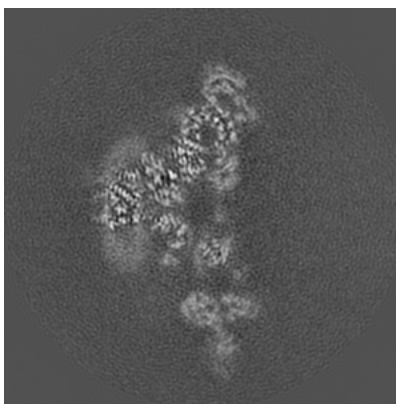
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

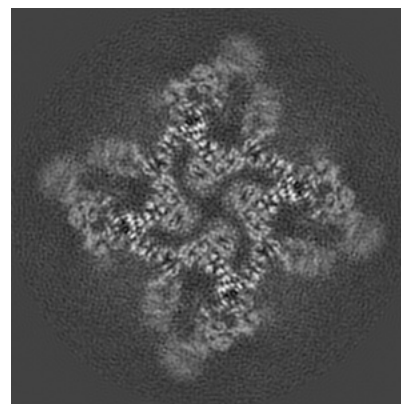
6.3.1 Primary map



X Index: 186



Y Index: 214

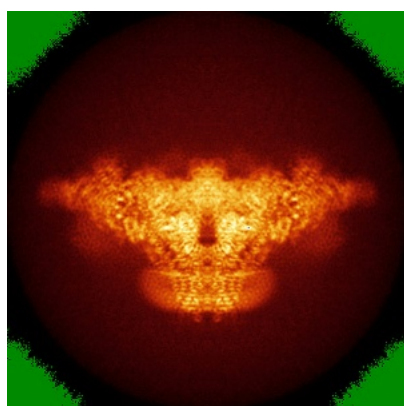


Z Index: 217

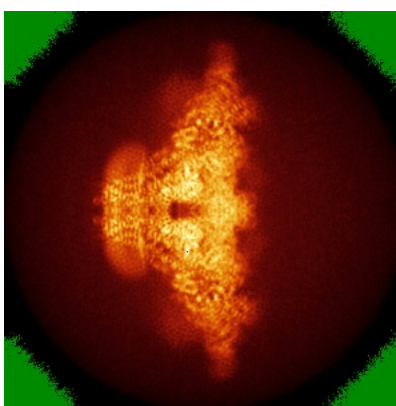
The images above show the largest variance slices of the map in three orthogonal directions.

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

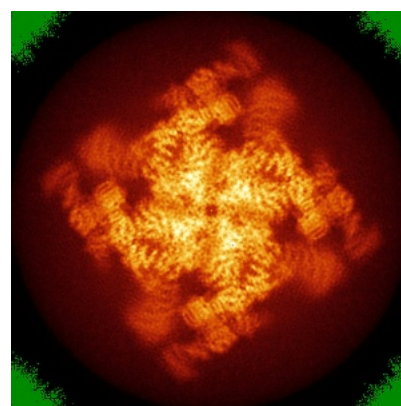
6.4.1 Primary map



X



Y

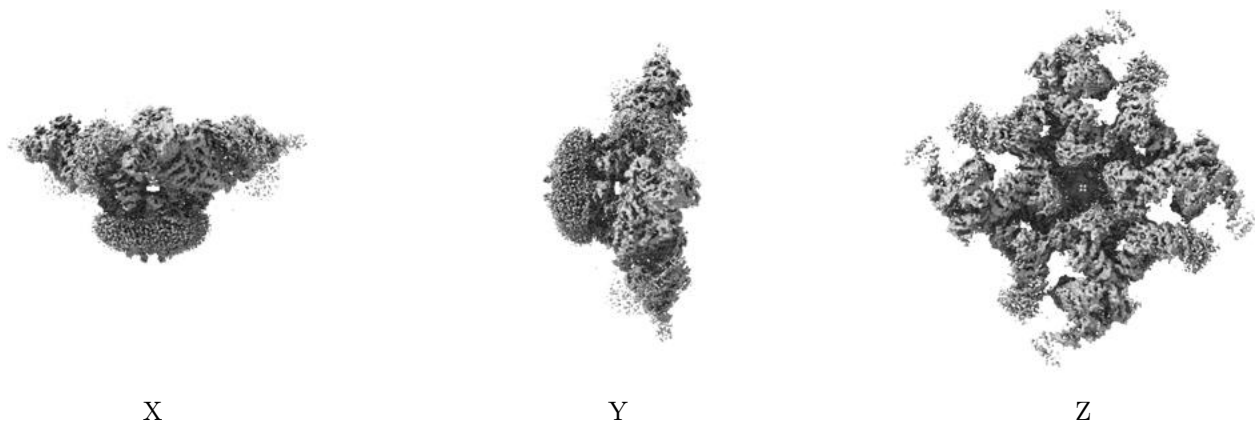


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

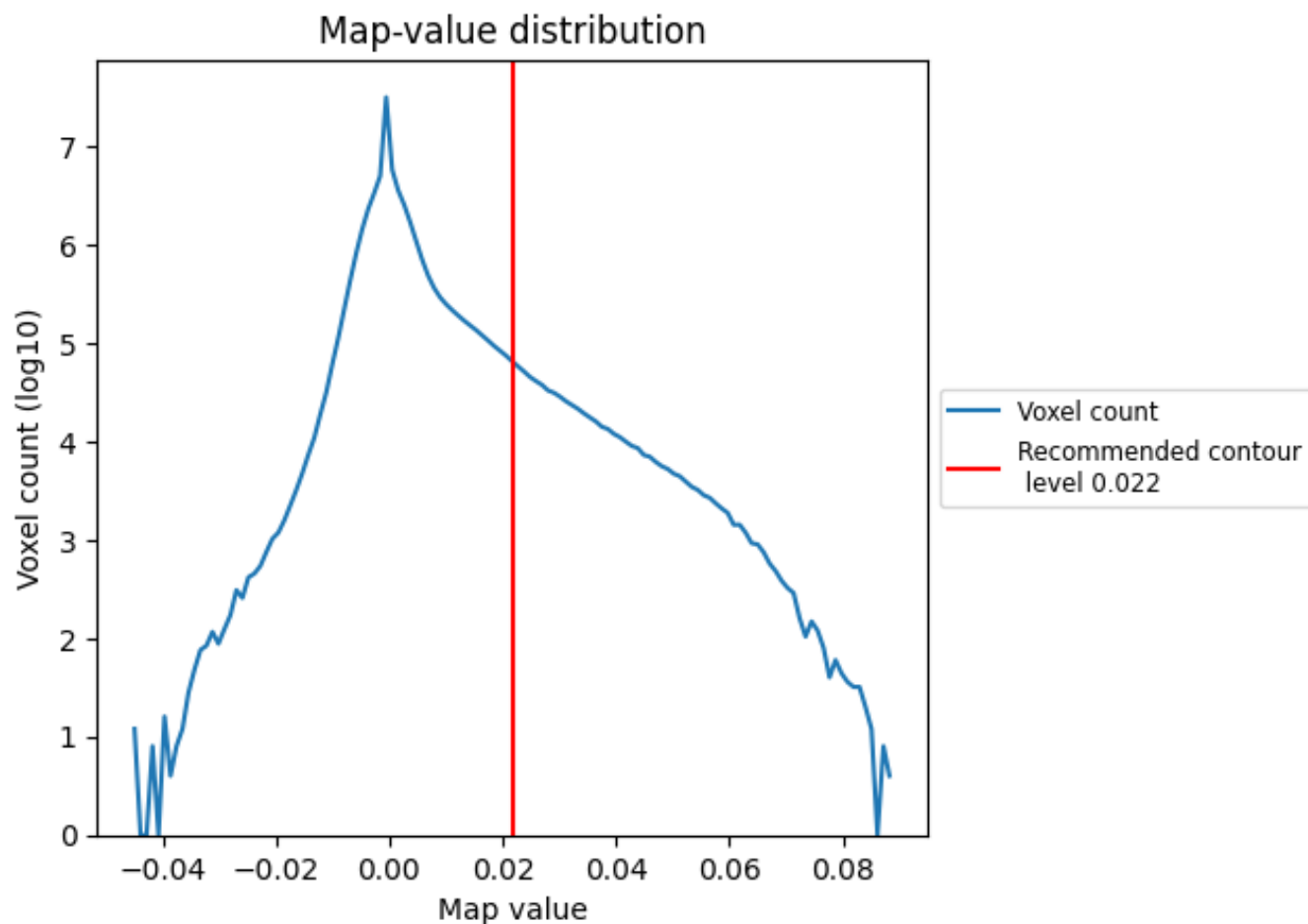
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

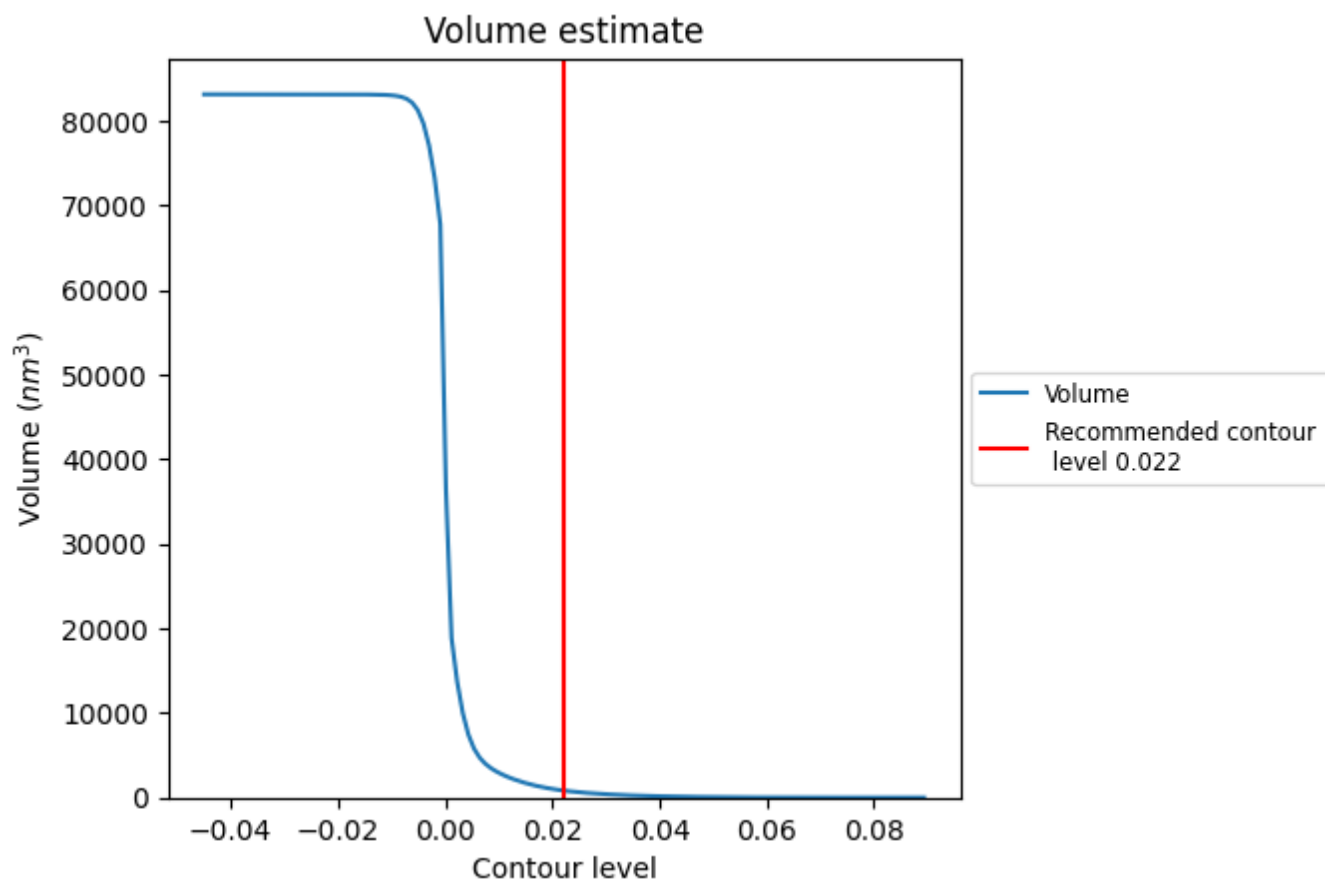
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

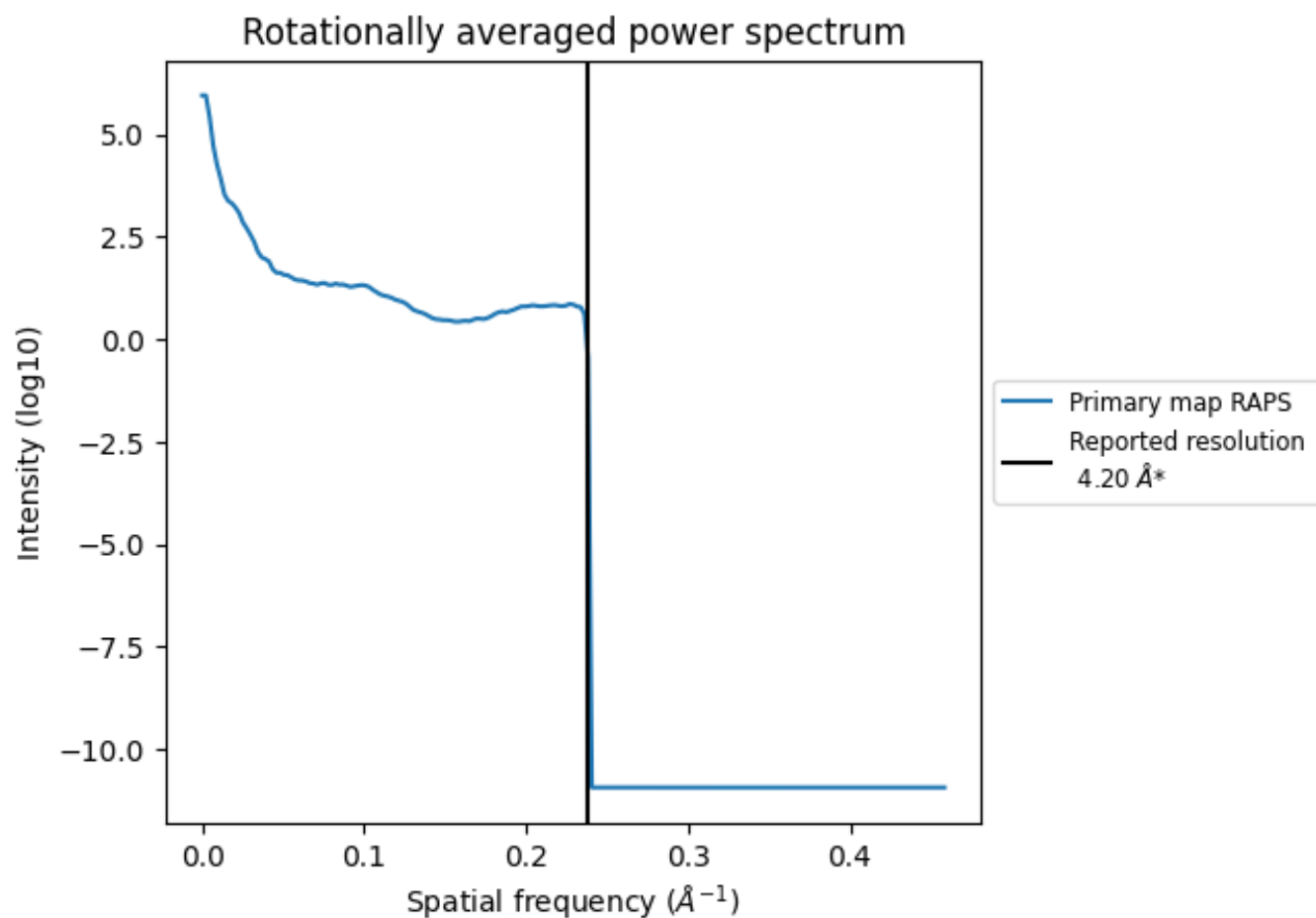
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm³; this corresponds to an approximate mass of 755 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 ⓘ

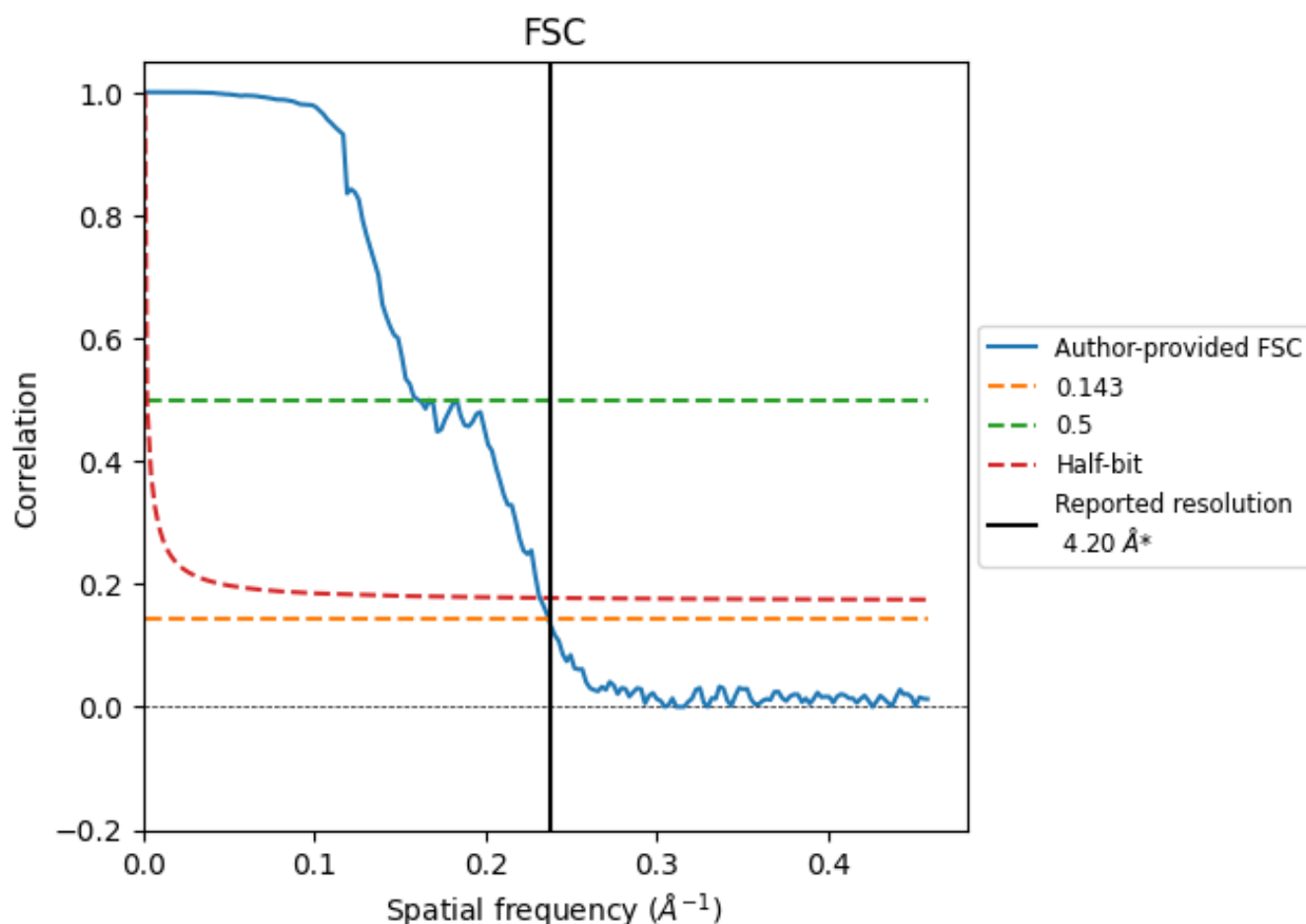


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

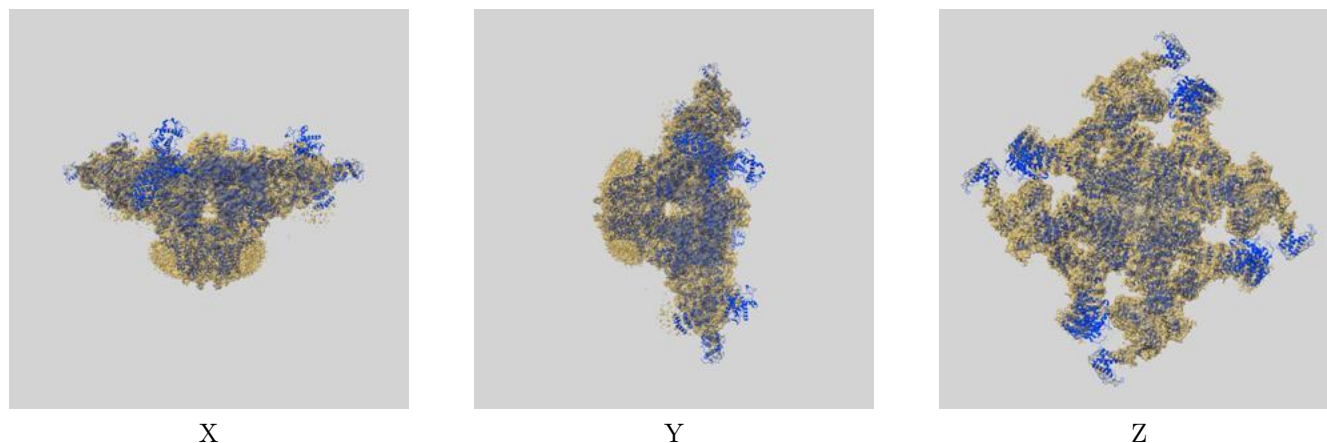
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.23	4.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

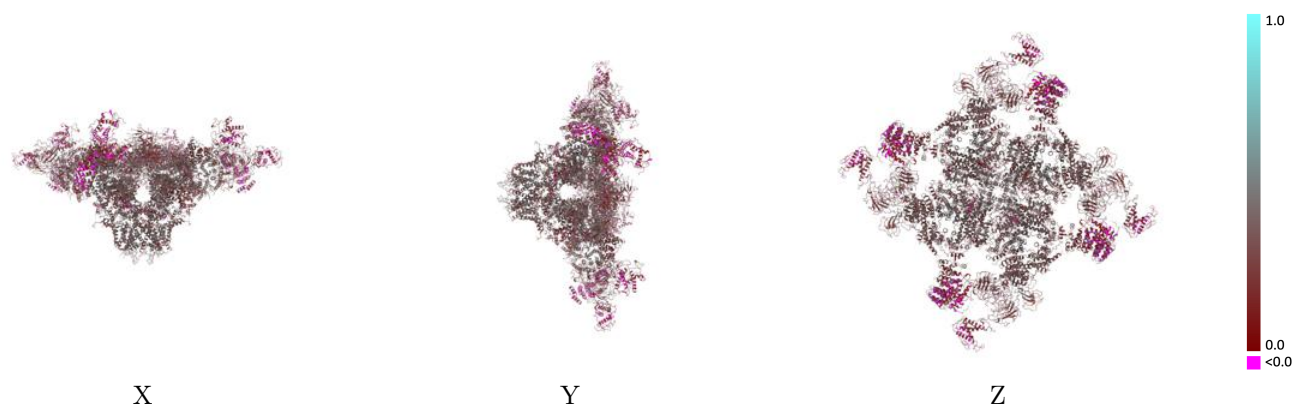
This section contains information regarding the fit between EMDB map EMD-9831 and PDB model 6JI0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



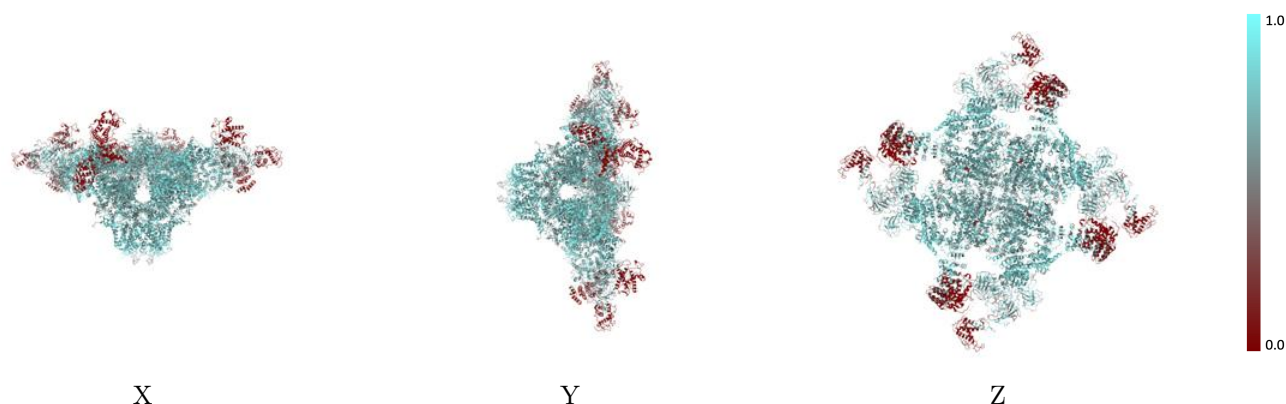
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



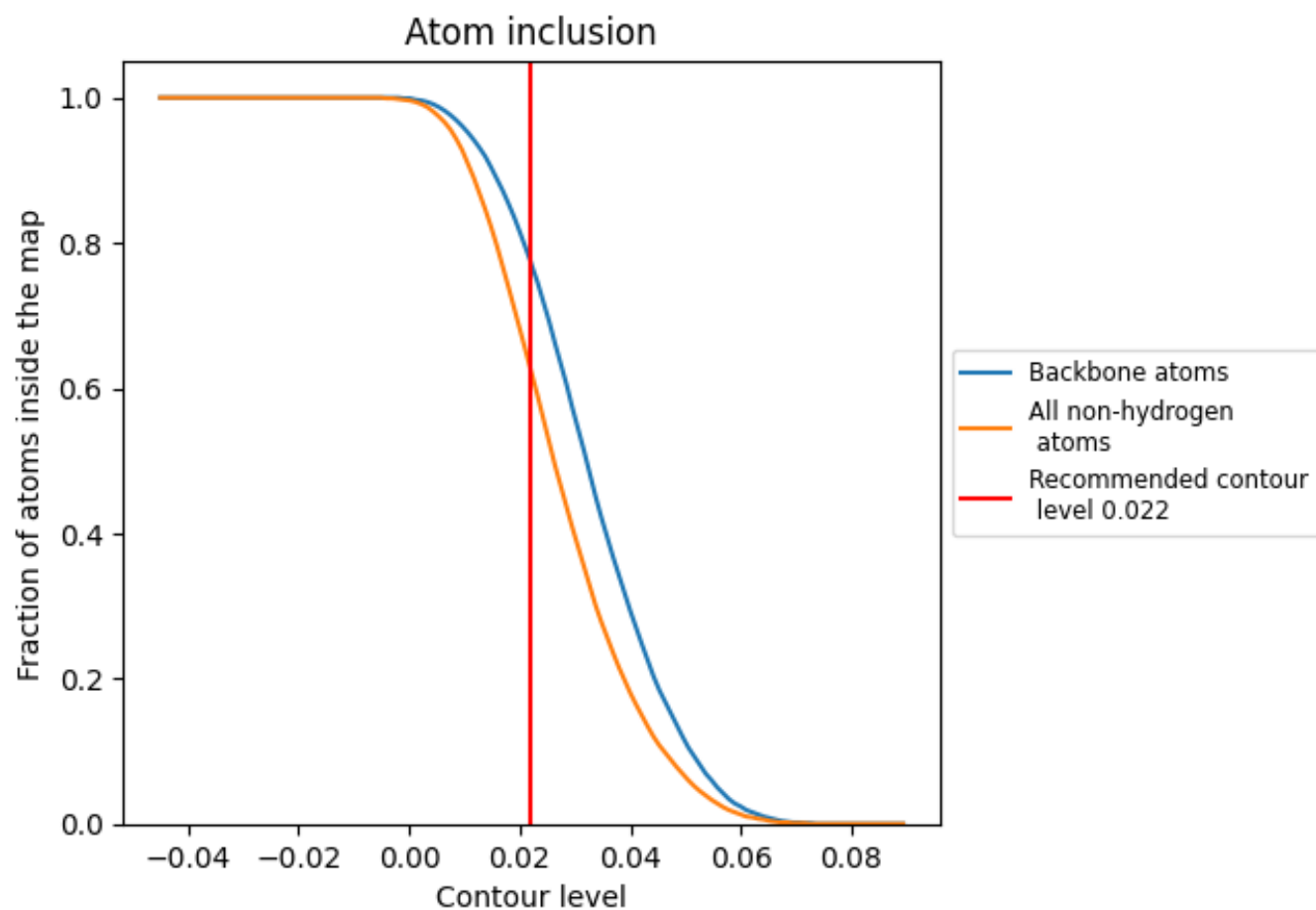
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.3220
A	0.6250	0.3220
B	0.6630	0.3270
C	0.6250	0.3220
D	0.6630	0.3280
E	0.6250	0.3210
F	0.6630	0.3250
G	0.6250	0.3210
H	0.6650	0.3240

1.0

0.0

<0.0