



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 05:59 PM JST

PDB ID : 6JI0
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)

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<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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

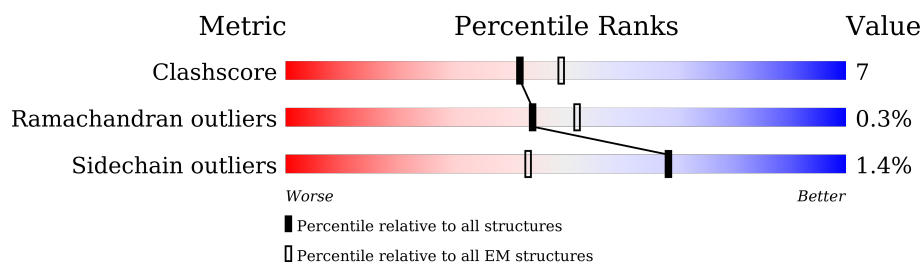
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	C	4968	
1	E	4968	
1	G	4968	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

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 (three-letter code: ZN) (formula: Zn).

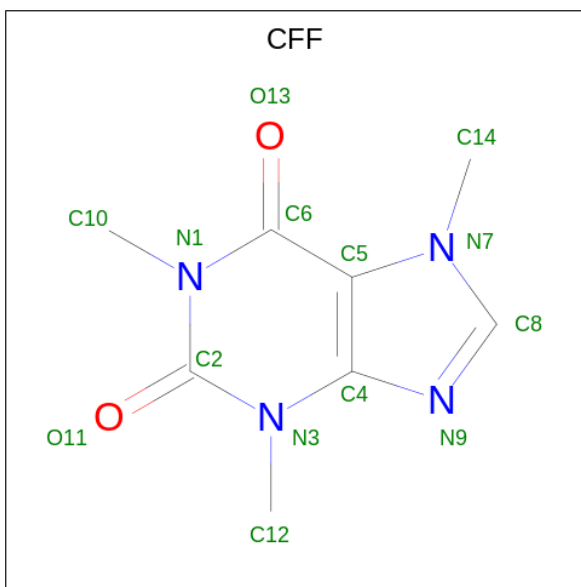
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

ATP

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).

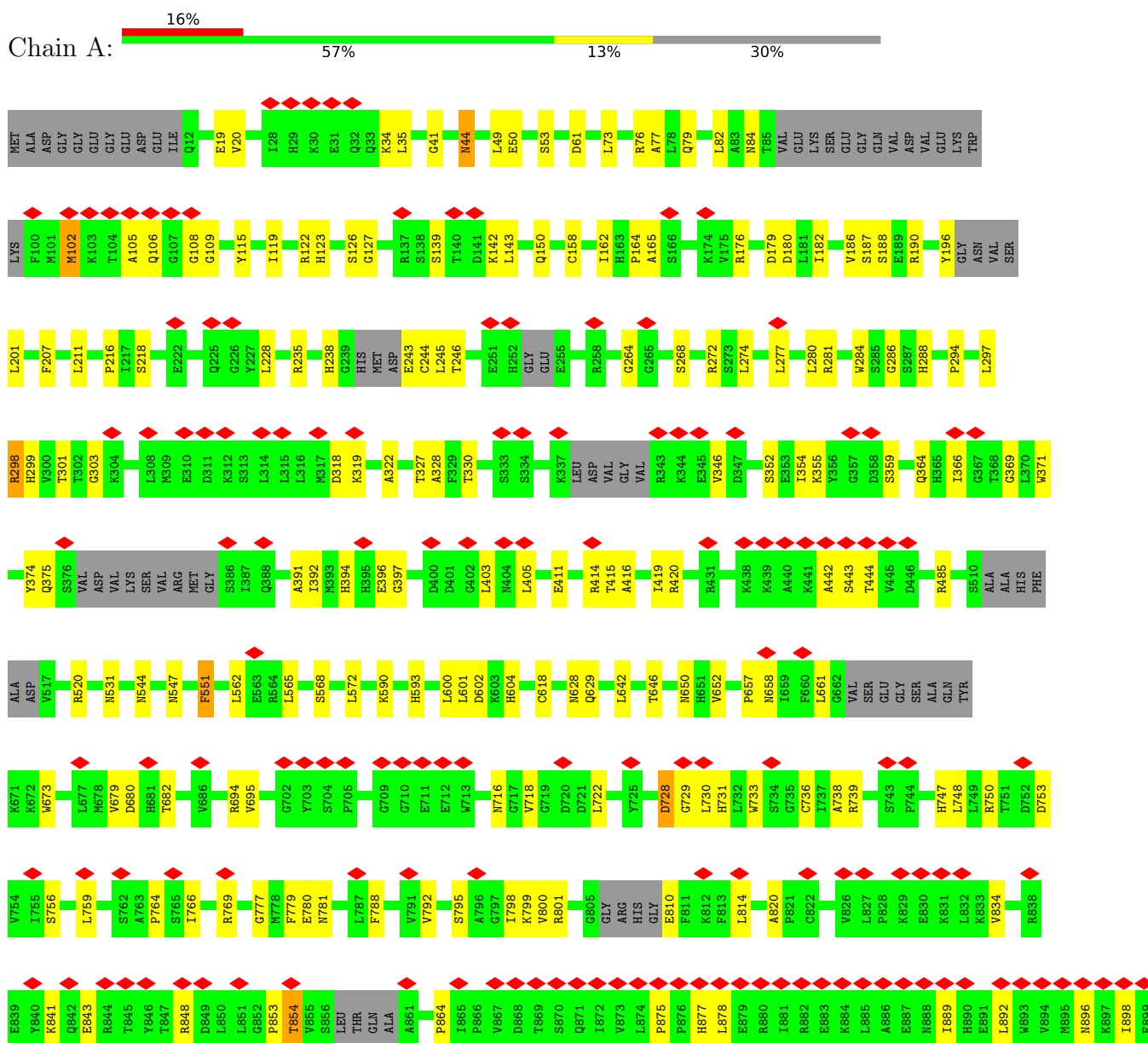


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

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

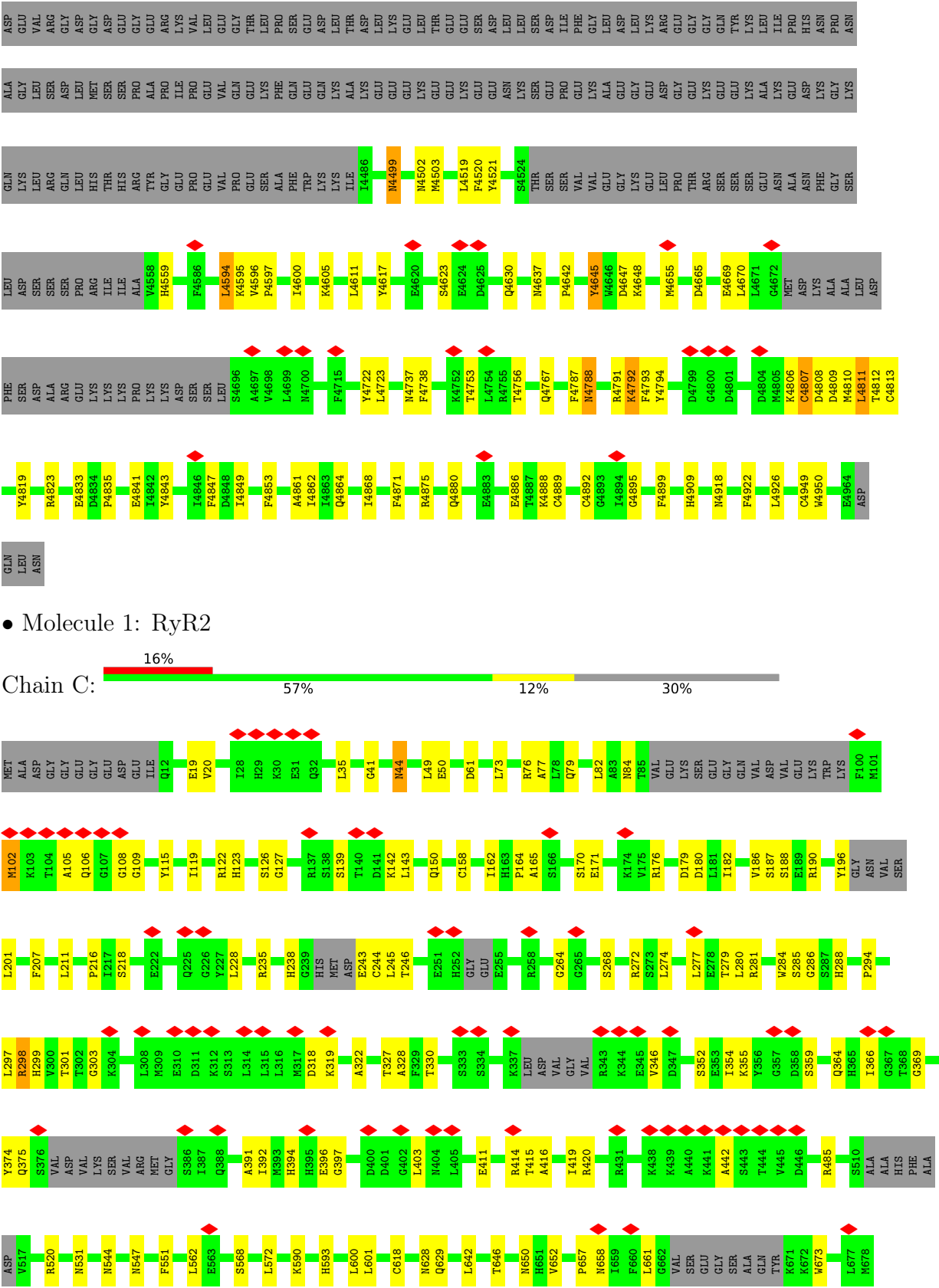
• Molecule 1: RyR2











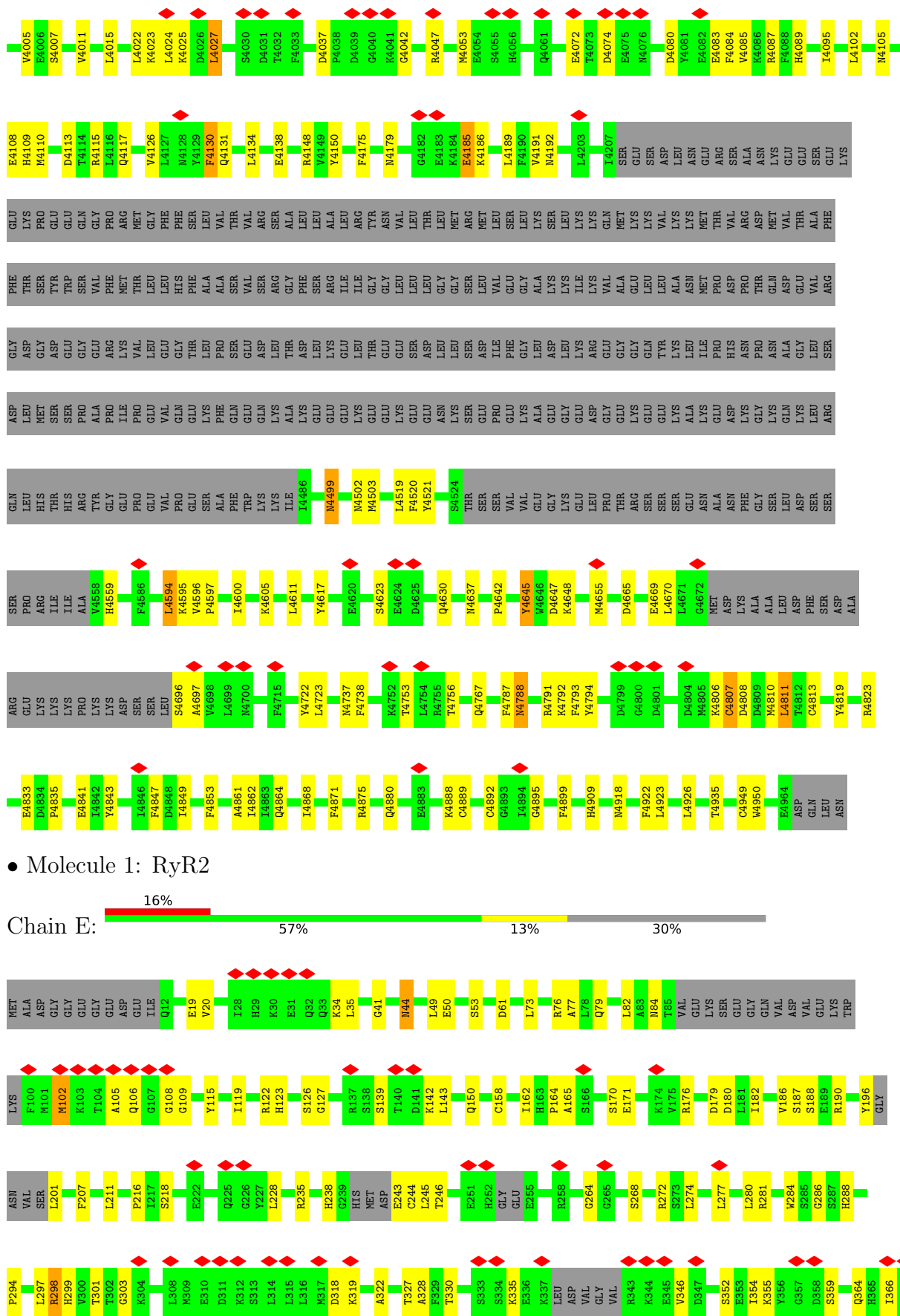
• Molecule 1: RyR2





I1641	L1642	E1643	L1644	T1645	L1651	R1671	S1678	E1682	P1683	Q1684	L1685	I1689	E1690	P1695	Y1703	R1718	L1738	F1739	P1740	D1741	GLU	ASN	LYS	LYS	HIS	G1747	I1751	G1752	L1753	L1757	R1758	P1759	R1760	F1768	N1773	Y1776	Q1777	D1785	K1788	A1789	K1790	R1807																
D1808	P1809	V1810	P1820	I1830	H1835	K1840	Q1844	L1845	I1846	E1847	P1848	S1849	VAL	PHE	LYS	GLU	ALA	ALA	GLY	PRO	GLU	GLU	LYS	GLN	GLU	ASP	GLU	CYS	ALA	GLU	SER	ASP	ARG	LEU	GLY	PRO	ALA	GLU	LYS	SER	LYS	GLY	LYS	ARG	PRO	LYS												
GLU	G1893	L1894	L1905	R1920	H1921	R1922	F1929	Q1938	R1942	V1948	MET	GLN	ALA	GLY	ASN	GLU	LEU	ASN	MET	SER	ALA	ALA	LEU	THR	ALA	ARG	LYS	THR	PRO	PRO	GLN	ILE	ASN	MET	LEU	LEU	ASN	PHE	LYS	ASP	ASP	LYS	SER	LYS	GLY	PRO	CYS	PRO	PRO	GLU								
GLU	I1994	H2007	I2010	E2011	L2012	D2013	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	S2022	T2025	I2026	R2027	G2028	R2029	L2030	L2033	Y2039	LEU	LYS	LYS	LYS	PHE	GLN	ALA	GLU	VAL	GLU	SER	T2058	Q2072	V2075	I2076	E2077	L2081	V2082	R2083																
Y2093	D2116	T2117	T2118	L2124	T2127	M2143	K2154	M2161	R2164	V2177	G2181	GLY	GLY	SER	LYS	GLU	ILE	THR	F2190	P2191	K2192	M2196	N2211	D2217	Y2221	S2226	L2230	A2231	S2232	P2233	R2236	L2241	G2274	LEU	GLN	SER	CYS	GLY	MET	LEU																		
VAL	SER	LYS	GLY	TYR	PRO	ASP	ILE	TRP	ASN	P2293	D2301	R2304	F2308	S2313	V2314	E2315	L2324	L2325	L2326	R2327	R2328	PRO	GLU	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	G2343	L2344	L2345	N2348	E2349	L2354	ALA	GLU	ASP	PRO	GLN	ARG	ASP	GLY	PRO	SER											
PRO	THR	SER	GLY	SER	SER	LYS	MET	PRO	ASP	THR	GLU	GLY	ASP	THR	ILE	HIS	A2404	PRO	GLU	MET	HIS	LEU	ILE	ALA	ALA	LYS	GLY	E2416	R2419	L2420	R2421	S2422	R2425	SER	LEU	ILE	PRO	LEU	G2431	V2434	G2435	V2436	L2437	S2438	I2439	Q2442	PRO											
THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	ALA	F2461	C2462	P2463	R2464	R2465	R2466	R2475	V2476	Y2477	ILE	ILE	GLU	V2481	L2485	L2486	H2487	L2488	L2489	VAL	G2492	F2493	D2496	A2500	L2503	ASP	THR	ALA	ALA	LEU	SER	GLU	HIS	ALA	K2605	L2608	K2609	L2610	L2611						
L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	F2536	A2537	G2538	E2540	L2549	V2553	TYR	ARG	LEU	SER	K2558	Q2566	R2567	L2574	L2575	S2576	ILE	CYS	GLY	GLN	LEU	R2582	P2583	S2584	M2585	M2586	Q2587	H2588	L2589	L2590	L2593	D2596	V2597	P2598	N2601	GLU	HIS	ALA	K2605	L2608	K2609	L2610	L2611								
T2612	N2613	H2614	Y2621	Y2622	C2623	L2624	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	H2640	L2641	K2644	L2645	F2646	F2650	D2651	A2652	L2653	SER	L2658	E2659	F2663	K2664	L2665	P2668	C2669	L2670	S2671	A2672	V2673	A2674	P2678	P2679	TYR	MET	GLU	SER	ASN	TYR											
VAL	SER	MET	GLU	LYS	GLN	SER	MET	ASP	SER	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	L2712	L2713	L2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	L2722	N2723	K2724	Y2725	L2726	E2727	H2728	S2729	H2730	D2731	K2732	L2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	L2743	Y2744	G2745	E2746	
L2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	S2765	E2766	K2767	E2768	K2769	E2770	L2771	Y2772	K2773	W2774	P2775	L2776	K2777	E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	W2786	D2787	W2788	R2789	I2790	E2791	R2792	L2793	R2794	E2795	Q2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	
ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	L2827	D2828	N2829	S2830	N2831	Y2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840	N2841	A2842	E2843	N2844	N2845	A2846	E2847	N2848	Y2849	H2850	N2851	L2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	Q2866

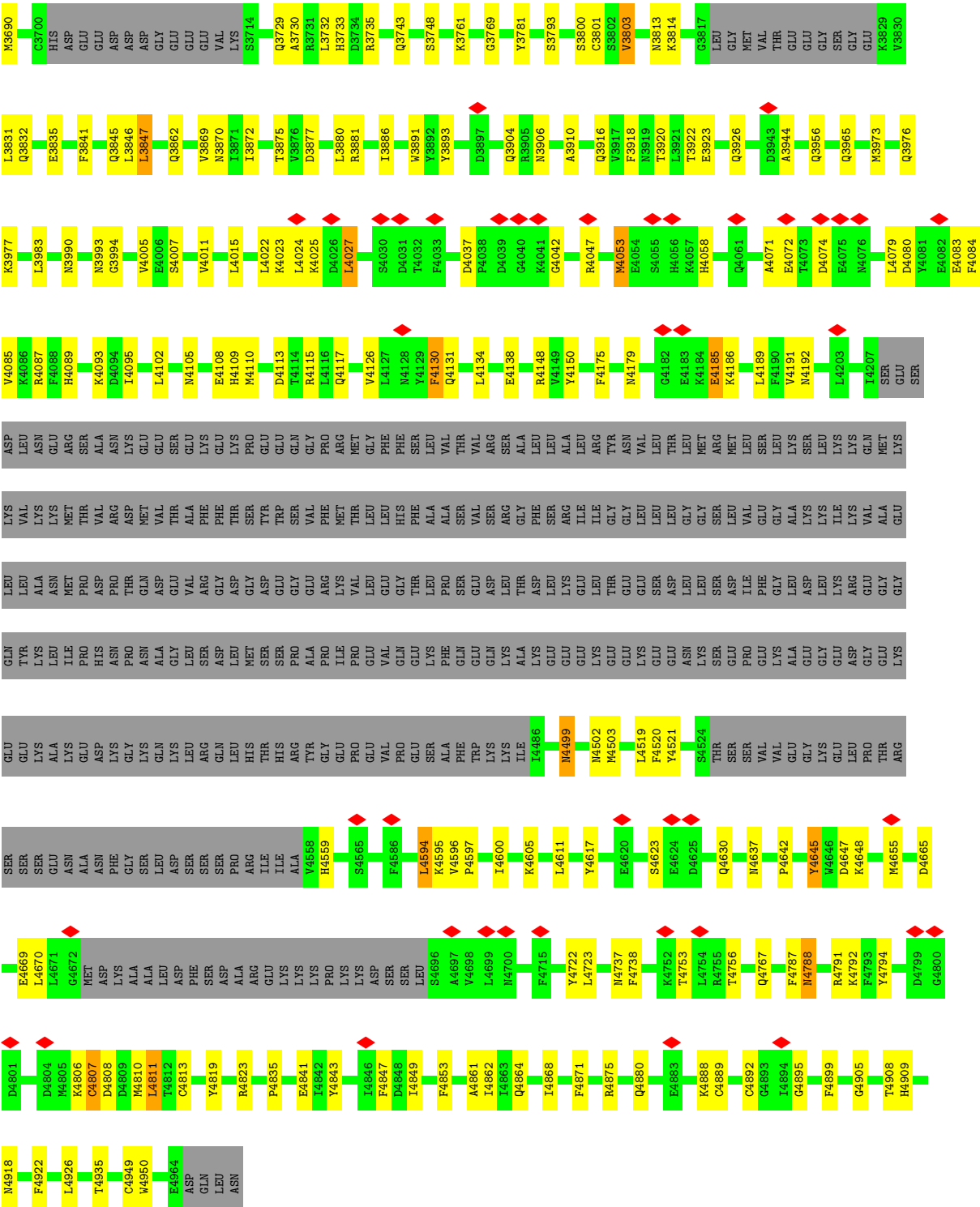












• Molecule 1: RyR2













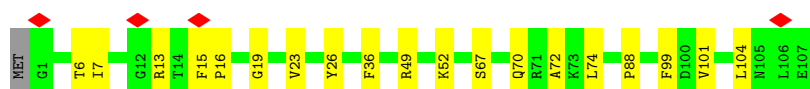
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:  81% 19%




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

Chain D:  81% 18%




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

Chain F:  83% 16%



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

Chain H:  82% 17%



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: ZN, CFF, ATP, CA

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	0.38	0/27073	0.62	12/36605 (0.0%)
1	C	0.38	0/27073	0.62	12/36605 (0.0%)
1	E	0.38	0/27073	0.62	12/36605 (0.0%)
1	G	0.38	0/27073	0.62	12/36605 (0.0%)
2	B	0.32	0/835	0.55	0/1123
2	D	0.32	0/835	0.55	0/1123
2	F	0.32	0/835	0.55	0/1123
2	H	0.32	0/835	0.55	0/1123
All	All	0.38	0/111632	0.62	48/150912 (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 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	C	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	E	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	G	1644	LEU	CA-CB-CG	7.80	133.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3846	LEU	CA-CB-CG	6.67	130.65	115.30

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 [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	26577	0	25112	446	0
1	C	26577	0	25112	426	0
1	E	26577	0	25113	426	0
1	G	26577	0	25113	419	0
2	B	819	0	824	11	0
2	D	819	0	824	11	0
2	F	819	0	824	11	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	1565	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 7.

The worst 5 of 1565 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%)	41	76
1	C	3356/4968 (68%)	2915 (87%)	432 (13%)	9 (0%)	41	76
1	E	3356/4968 (68%)	2910 (87%)	437 (13%)	9 (0%)	41	76
1	G	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	41	76
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%)	44	76

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%)	2641 (98%)	40 (2%)	65	80
1	C	2680/4355 (62%)	2643 (99%)	37 (1%)	67	80
1	E	2682/4355 (62%)	2643 (98%)	39 (2%)	65	80
1	G	2681/4355 (62%)	2642 (98%)	39 (2%)	65	80
2	B	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	D	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	F	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	73	84
All	All	11076/17776 (62%)	10917 (99%)	159 (1%)	68	80

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4792	LYS
1	G	3870	ASN
1	G	44	ASN
1	G	950	VAL

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Mol	Chain	Res	Type
1	G	4185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	745	ASN
1	E	3990	ASN
1	E	1149	ASN
1	E	1941	GLN
1	G	84	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 monosaccharides 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
4	ATP	A	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)
4	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.45	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	C	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)
6	CFF	A	5103	-	8,15,15	2.62	3 (37%)	8,23,23	1.30	1 (12%)
6	CFF	G	5103	-	8,15,15	2.63	3 (37%)	8,23,23	1.30	1 (12%)
6	CFF	C	5103	-	8,15,15	2.61	3 (37%)	8,23,23	1.30	1 (12%)
4	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)
6	CFF	E	5103	-	8,15,15	2.62	3 (37%)	8,23,23	1.29	1 (12%)

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
4	ATP	A	5101	-	-	4/18/38/38	0/3/3/3
4	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	ATP	C	5101	-	-	4/18/38/38	0/3/3/3
6	CFF	A	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	C	5103	-	-	-	0/2/2/2
4	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
6	CFF	E	5103	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	CFF	C5-C4	-4.74	1.33	1.39
6	E	5103	CFF	C5-C4	-4.74	1.33	1.39
6	G	5103	CFF	C5-C4	-4.74	1.33	1.39
6	C	5103	CFF	C5-C4	-4.69	1.33	1.39
6	G	5103	CFF	C6-N1	-4.58	1.31	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	C	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	E	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	G	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	A	5101	ATP	PB-O3B-PG	-3.13	122.08	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

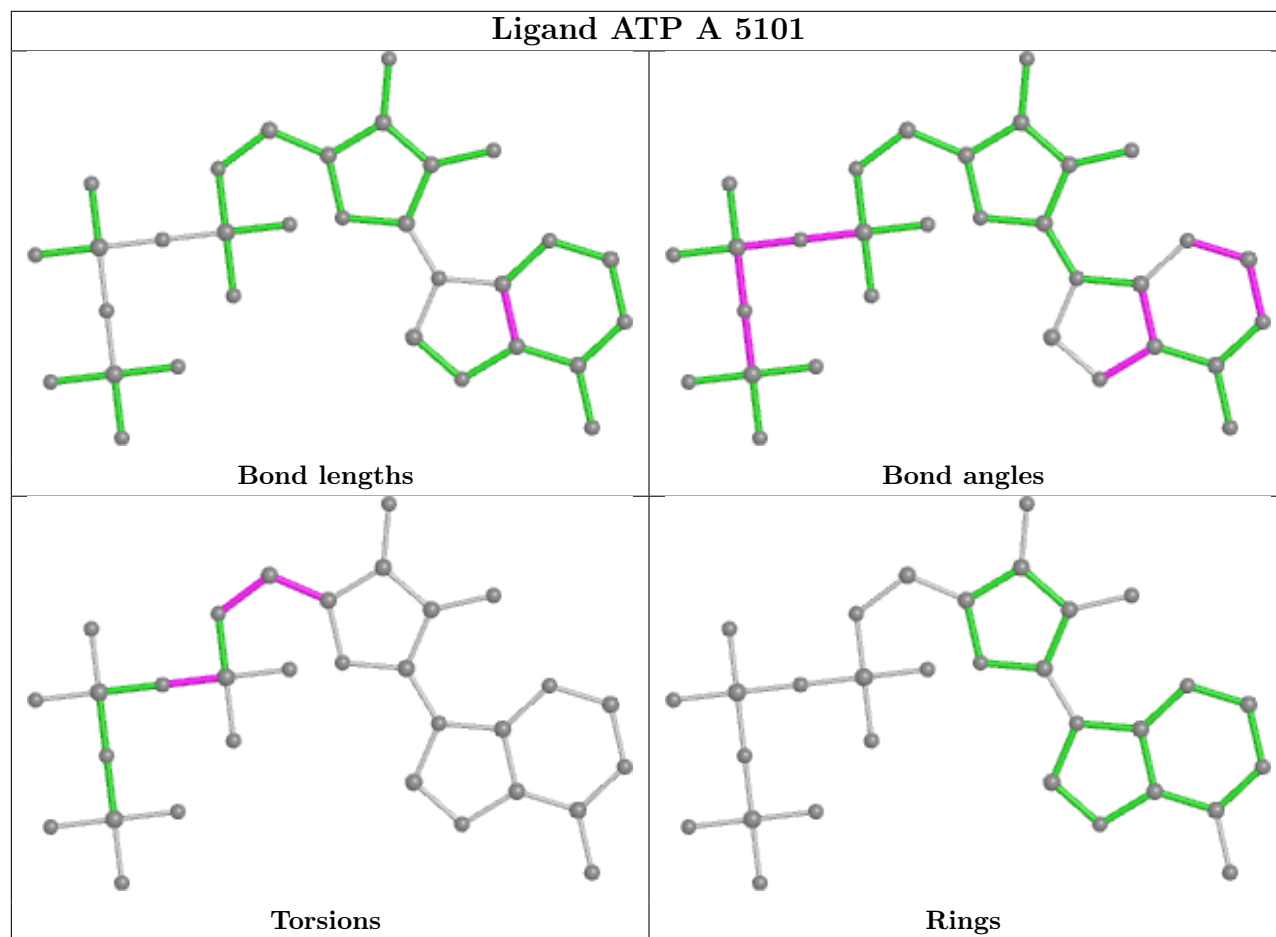
Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	PB-O3A-PA-O1A
4	A	5101	ATP	PB-O3A-PA-O2A
4	C	5101	ATP	PB-O3A-PA-O1A
4	C	5101	ATP	PB-O3A-PA-O2A
4	E	5101	ATP	PB-O3A-PA-O1A

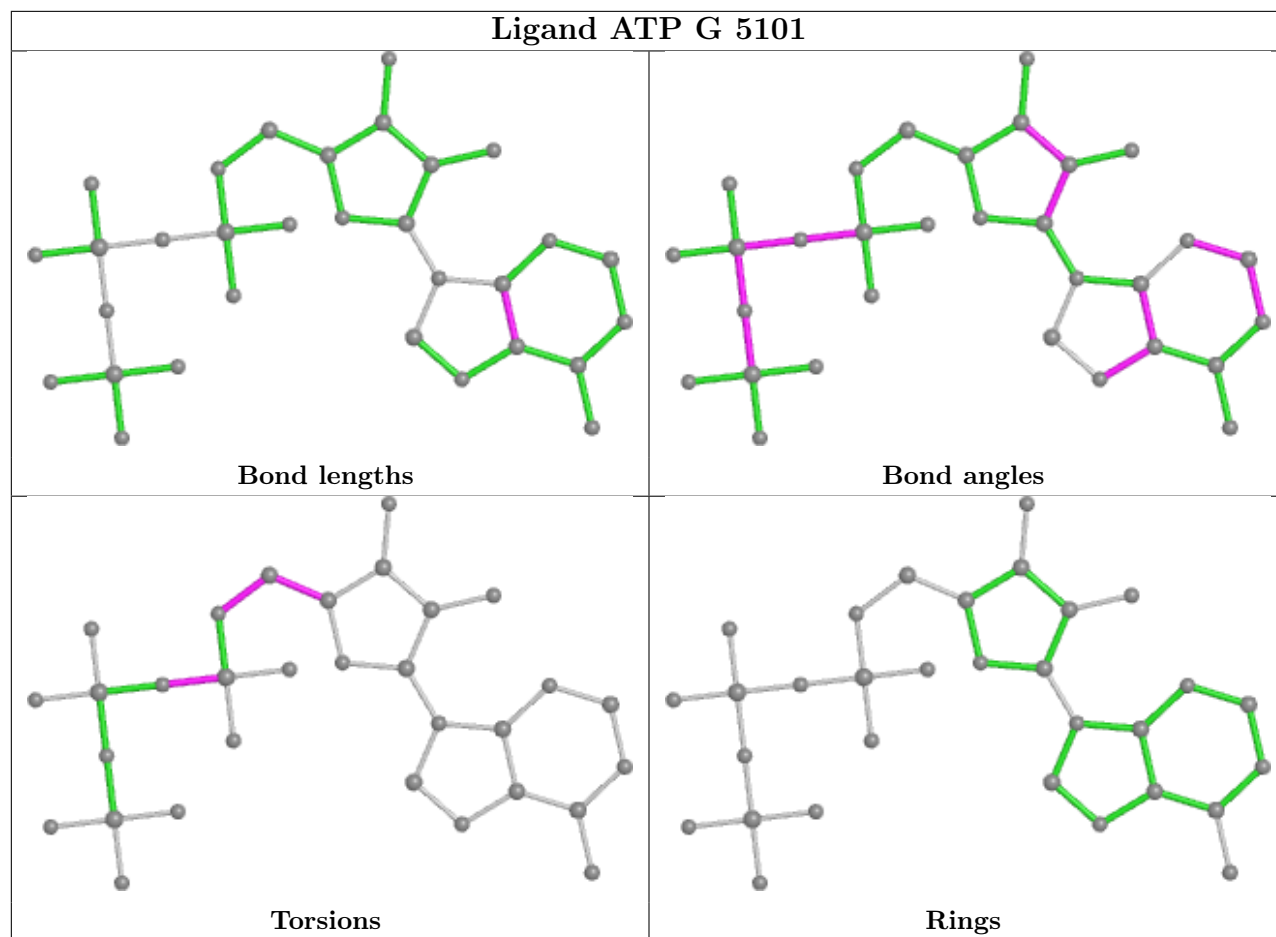
There are no ring outliers.

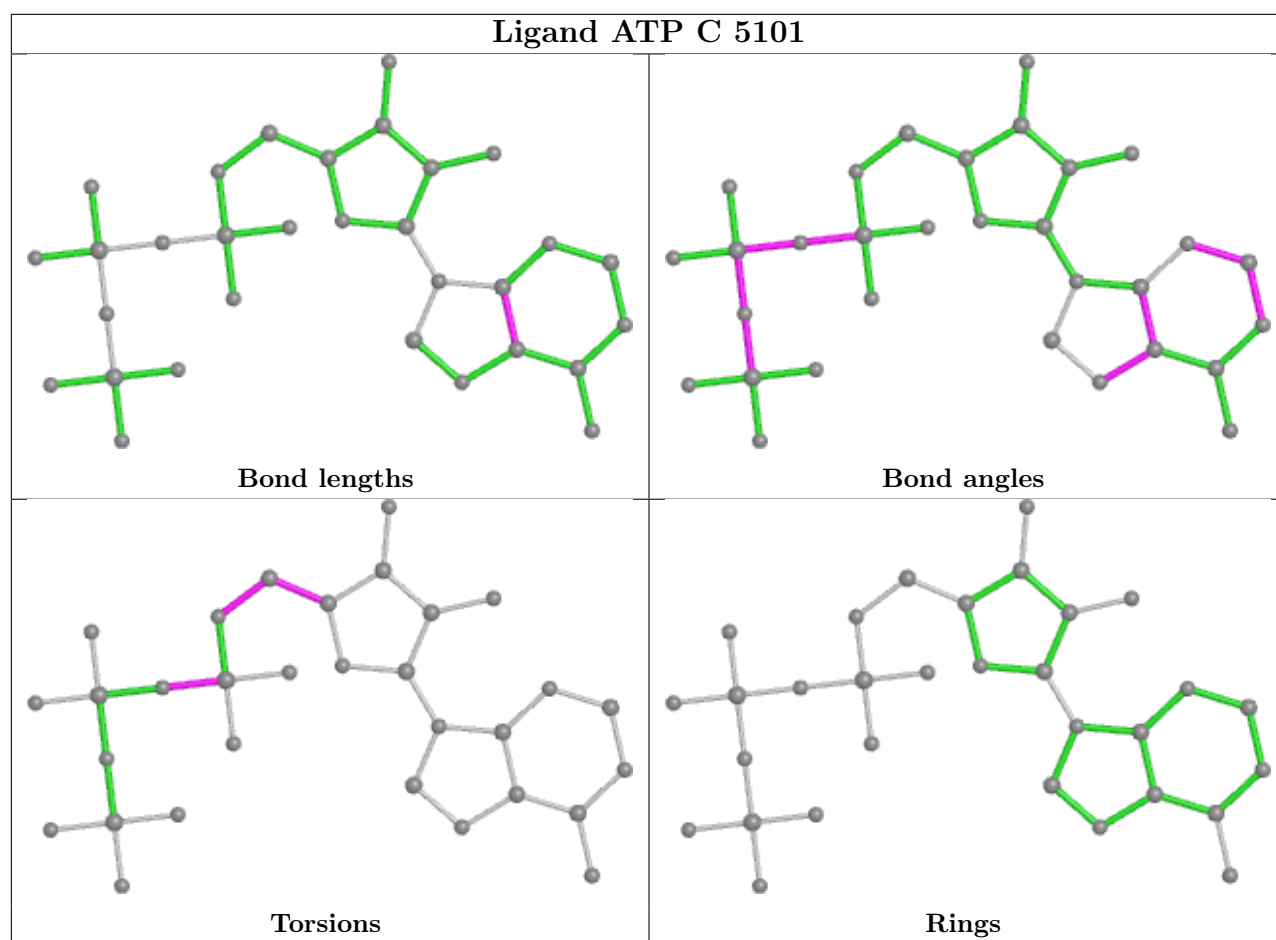
4 monomers are involved in 5 short contacts:

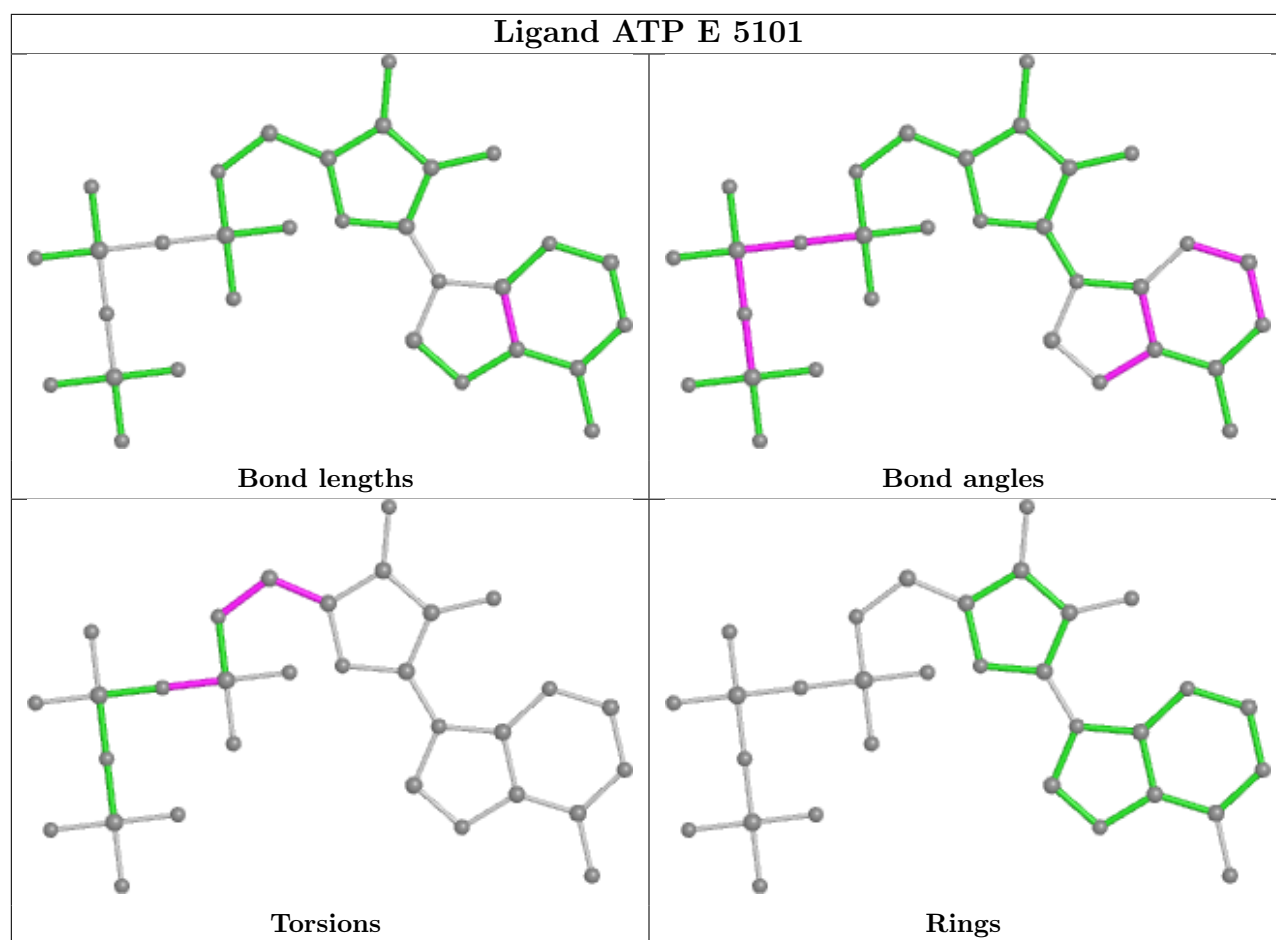
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5101	ATP	2	0
4	G	5101	ATP	1	0
4	C	5101	ATP	1	0
4	E	5101	ATP	1	0

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.

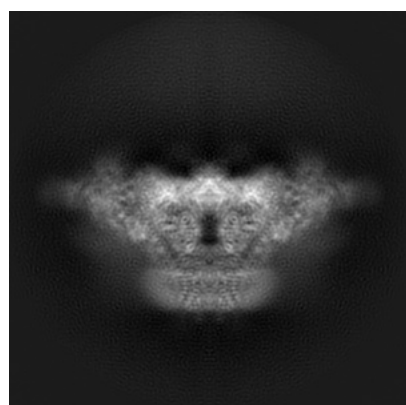
6 Map visualisation [i](#)

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.

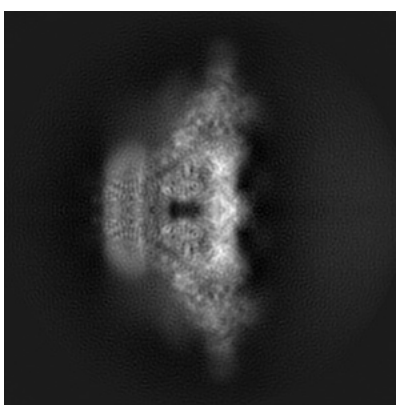
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

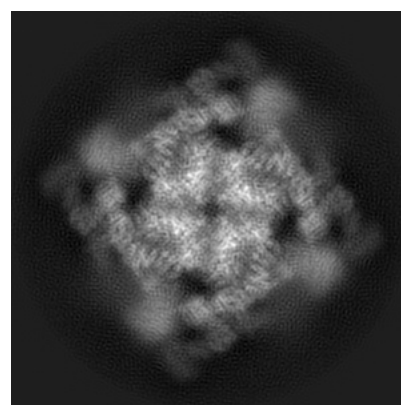
6.1.1 Primary map



X



Y

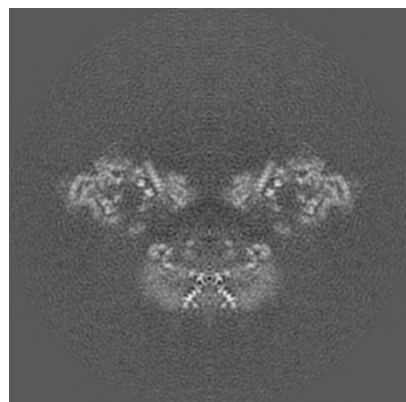


Z

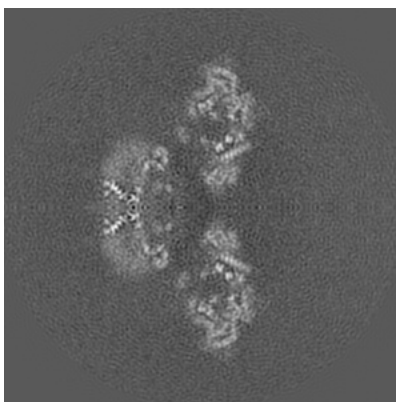
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

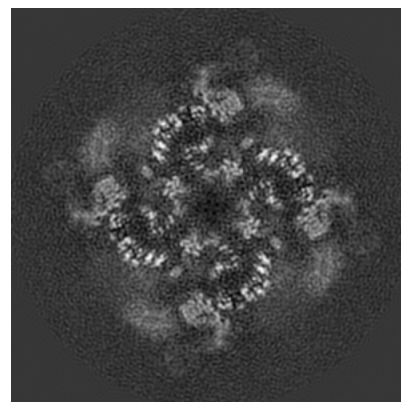
6.2.1 Primary map



X Index: 200



Y Index: 200

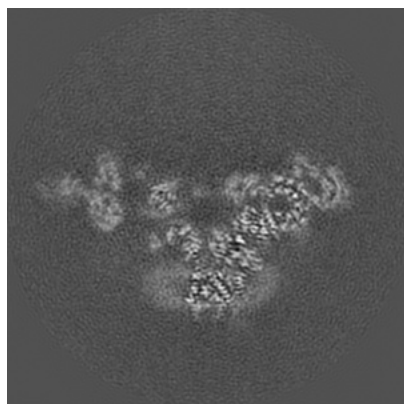


Z Index: 200

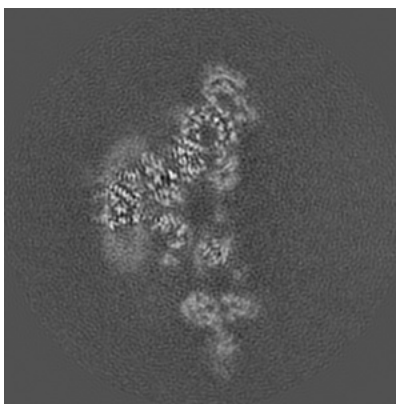
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

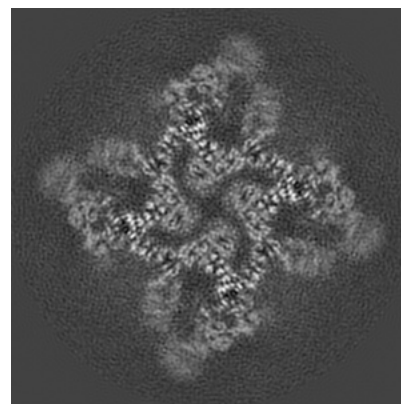
6.3.1 Primary map



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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

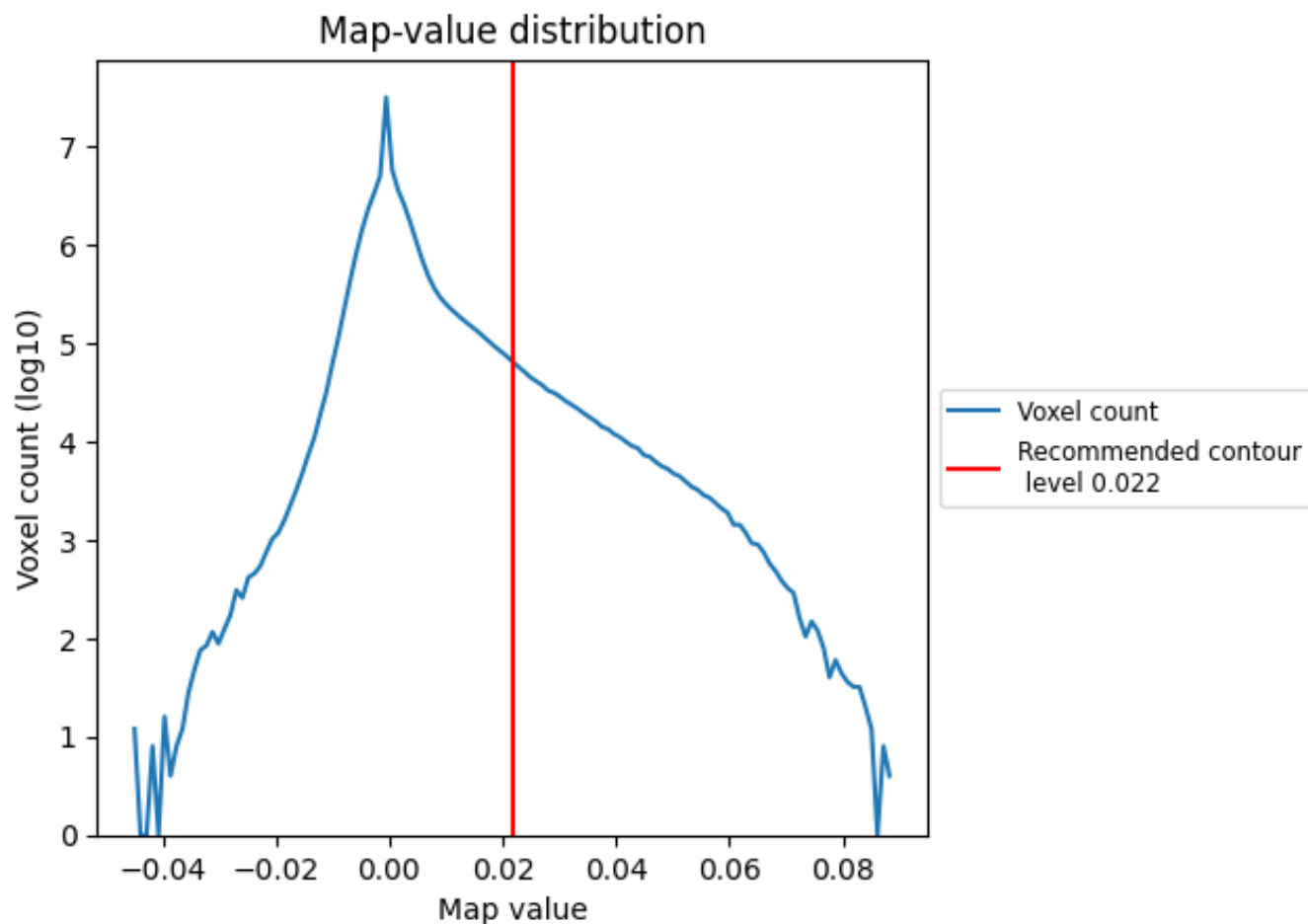
6.5 Mask visualisation

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

7 Map analysis [i](#)

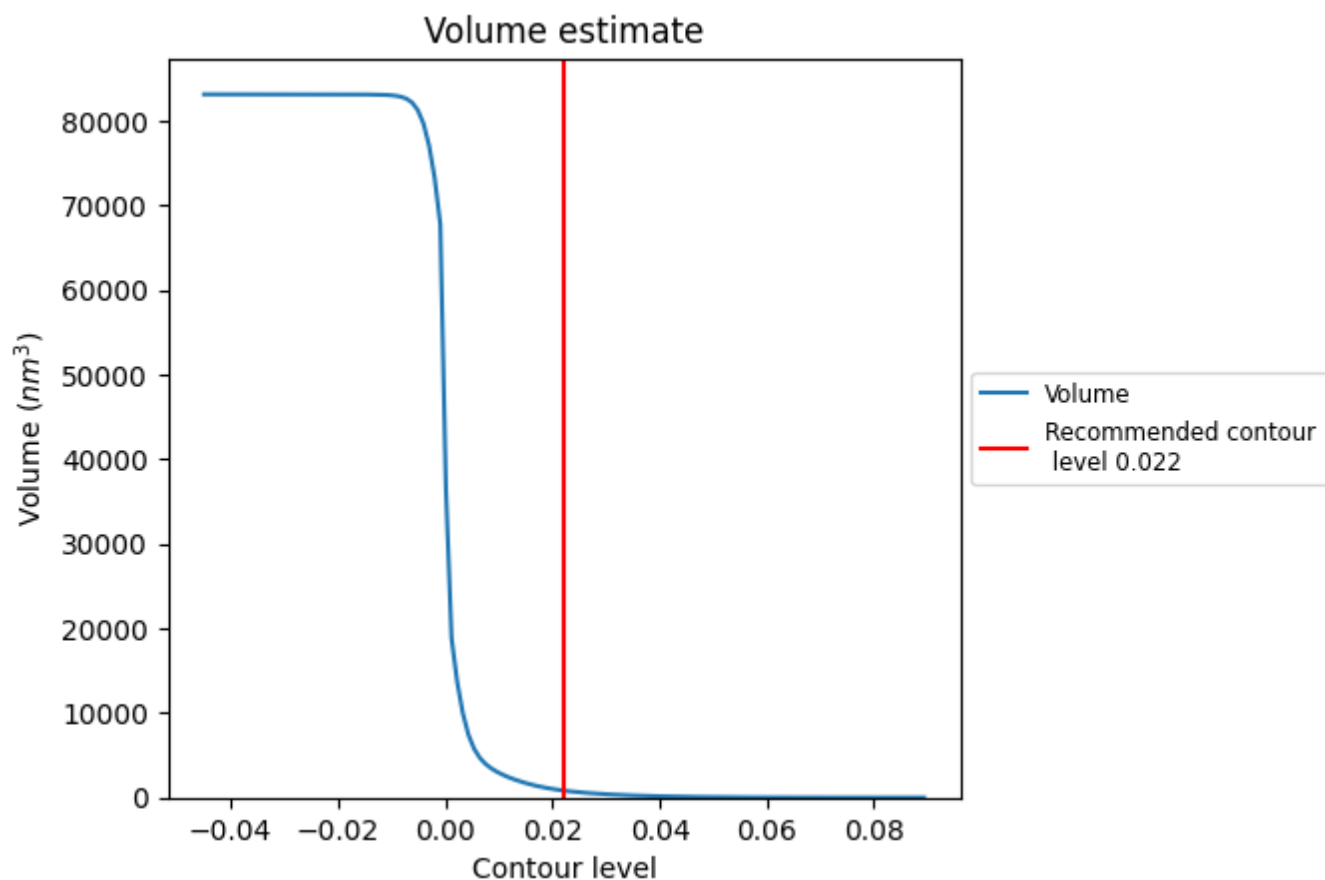
This section contains the results of statistical analysis of the map.

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.

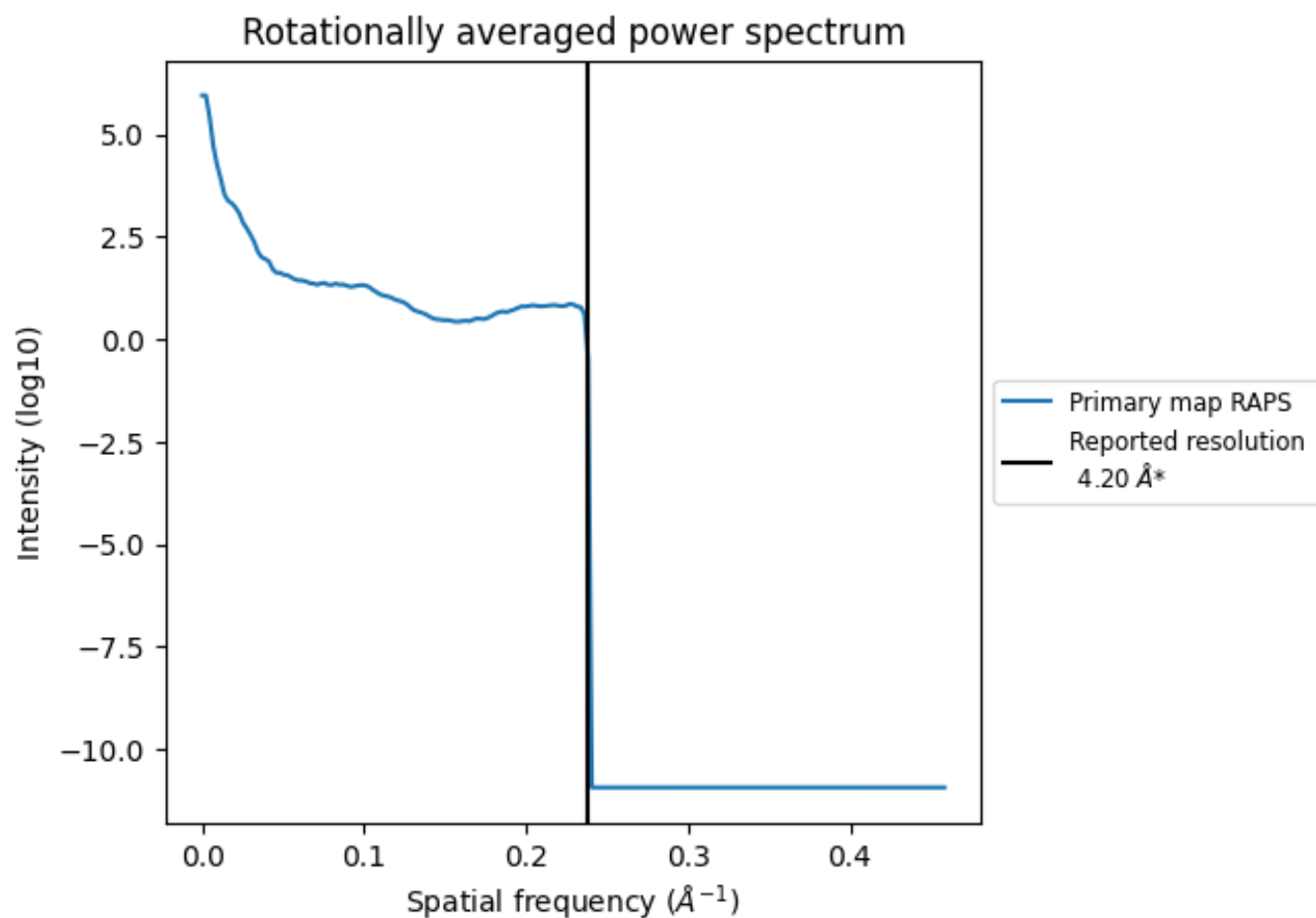
7.2 Volume estimate [i](#)



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 ⓘ

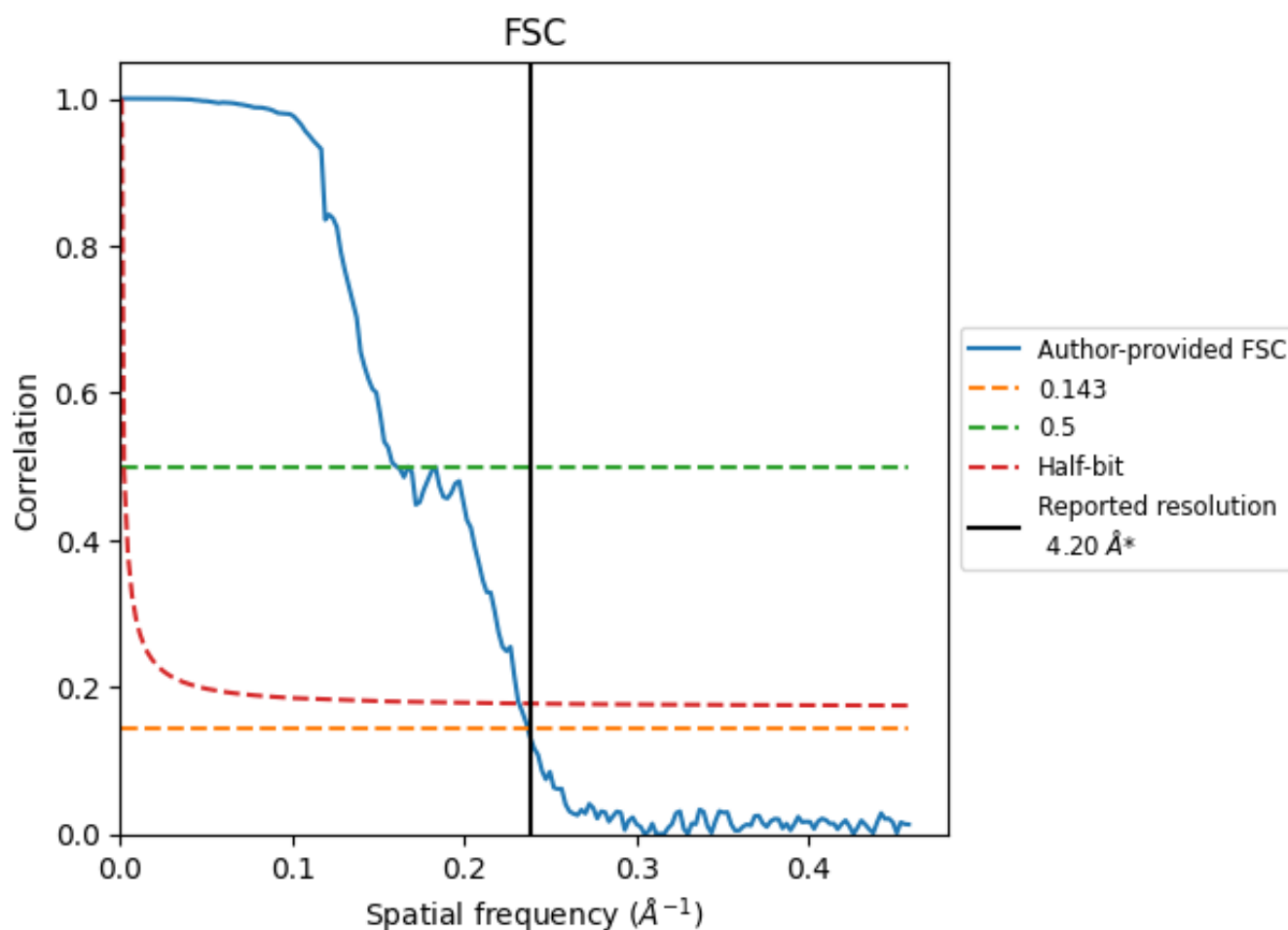


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

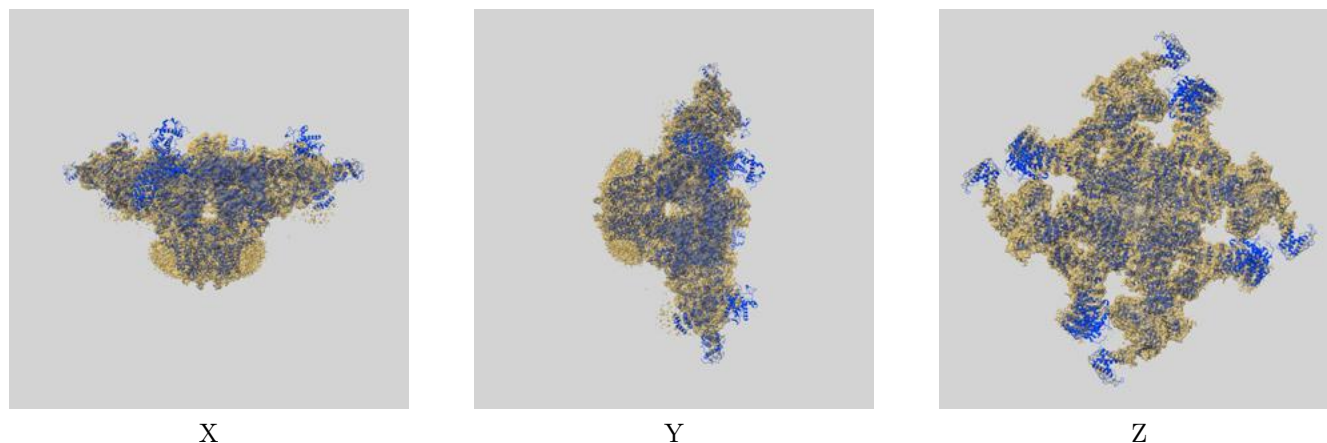
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.23	4.31
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

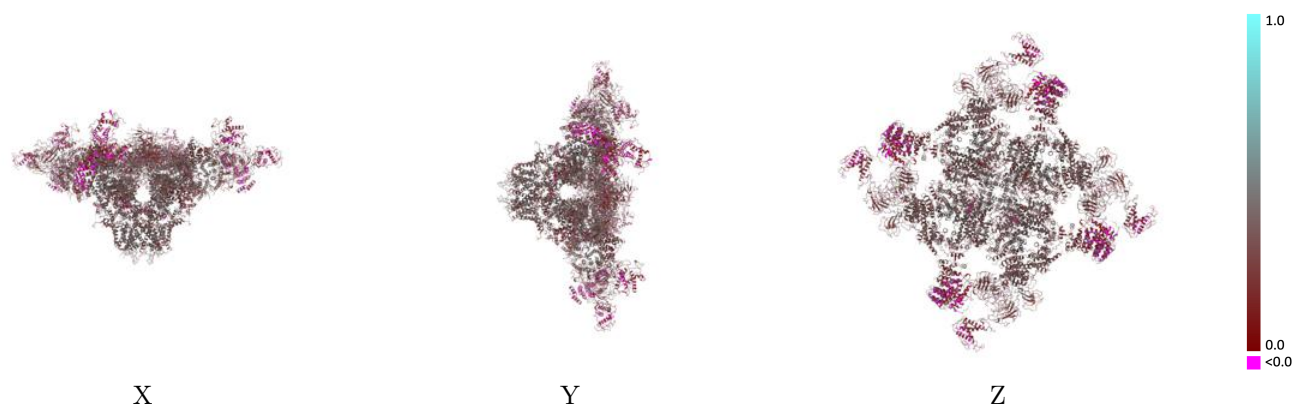
This section contains information regarding the fit between EMDB map EMD-9831 and PDB model 6JI0. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



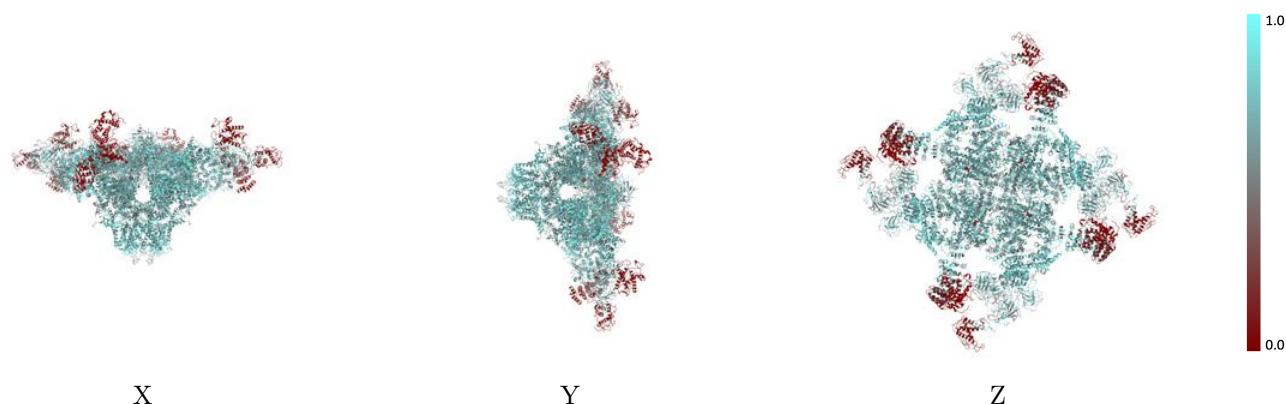
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



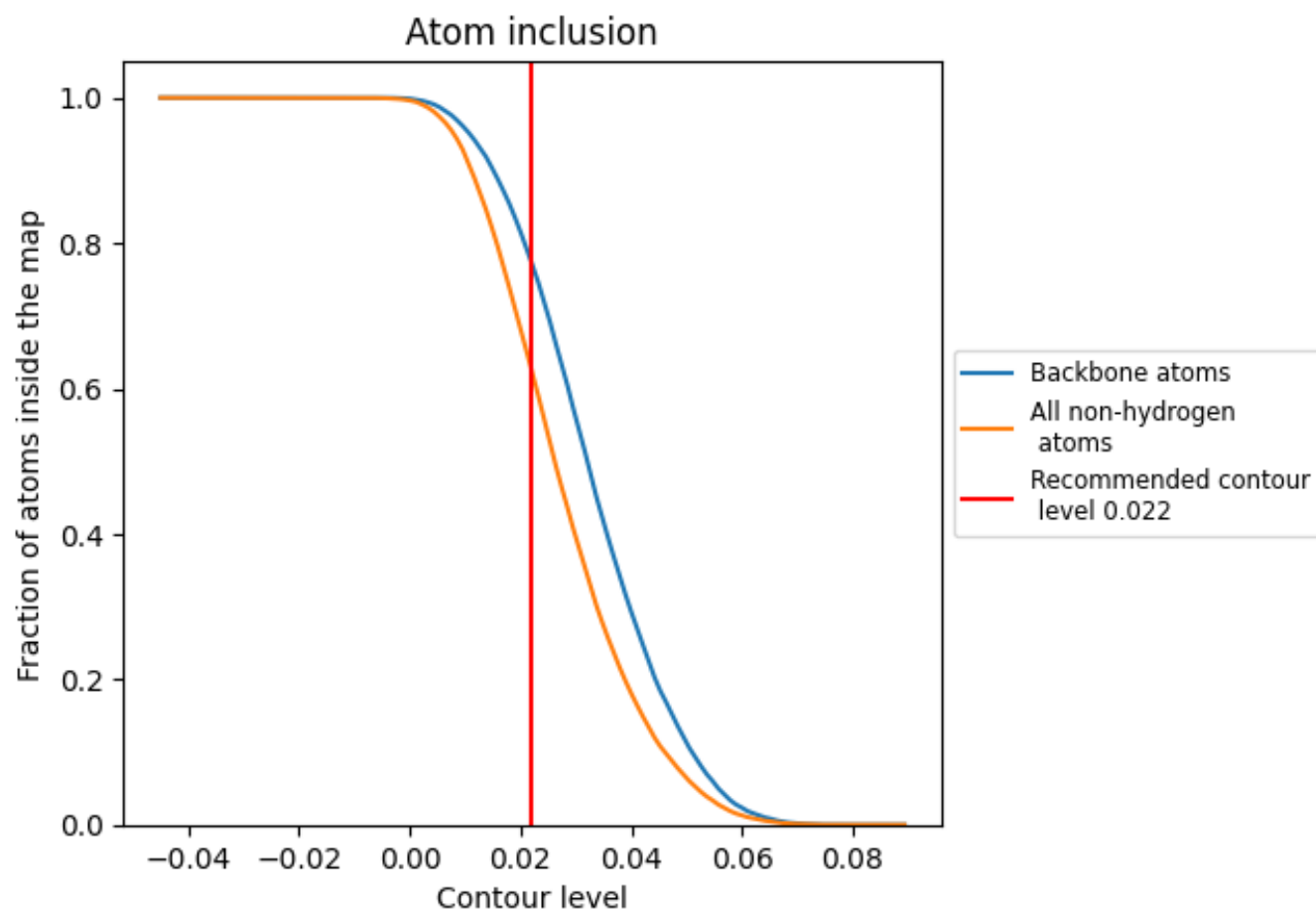
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.6260	<div></div> 0.3220
A	<div></div> 0.6245	<div></div> 0.3220
B	<div></div> 0.6629	<div></div> 0.3270
C	<div></div> 0.6251	<div></div> 0.3220
D	<div></div> 0.6629	<div></div> 0.3280
E	<div></div> 0.6250	<div></div> 0.3210
F	<div></div> 0.6629	<div></div> 0.3250
G	<div></div> 0.6247	<div></div> 0.3210
H	<div></div> 0.6654	<div></div> 0.3240

