



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 06:23 PM JST

PDB ID : 6JIU  
EMDB ID : EMD-9836  
Title : Structure of RyR2 (F/A/C/L-Ca<sup>2+</sup>/Ca<sup>2+</sup>+CaM dataset)  
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.  
Deposited on : 2019-02-23  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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



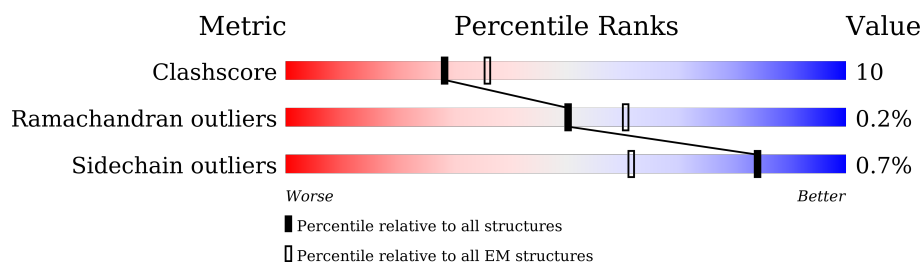
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4968	 6% 54% 16% 30%
1	D	4968	 6% 54% 16% 30%
1	G	4968	 6% 54% 16% 30%
1	J	4968	 6% 54% 16% 30%
2	B	108	 79% 19% ..
2	E	108	 79% 19% ..
2	H	108	 80% 19% ..
2	K	108	 80% 19% ..

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Mol	Chain	Length	Quality of chain
3	C	149	<div><div>42%</div><div><div></div><div></div><div></div></div><div>38%7%54%</div></div>
3	F	149	<div><div>42%</div><div><div></div><div></div><div></div></div><div>39%7%54%</div></div>
3	I	149	<div><div>42%</div><div><div></div><div></div><div></div></div><div>39%7%54%</div></div>
3	L	149	<div><div>42%</div><div><div></div><div></div><div></div></div><div>39%7%54%</div></div>



## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 112212 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	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	D	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	G	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	J	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		

- 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	E	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		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	F	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	I	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	L	68	Total	C	N	O	S	0	0
			524	326	83	110	5		

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



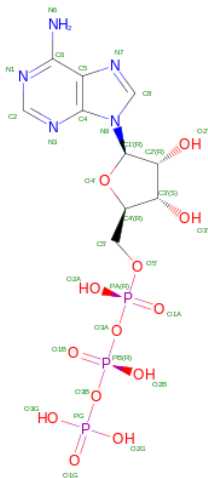
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

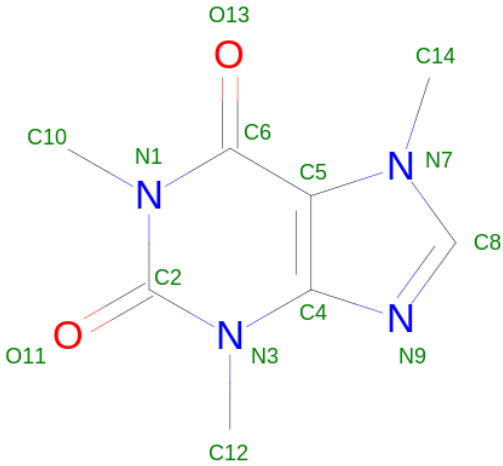
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





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

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula:  $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ ).





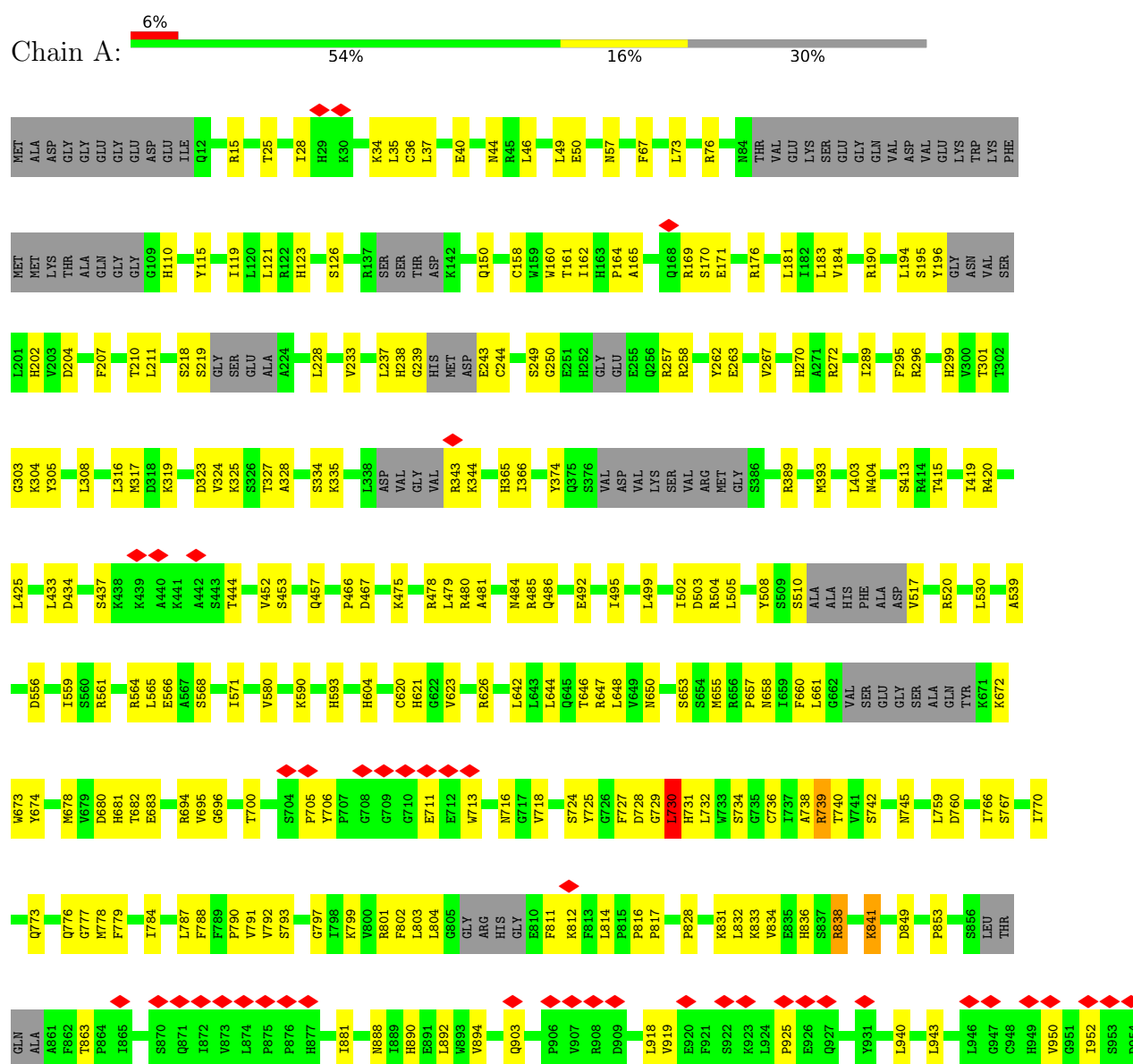
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0



### 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: RyR2









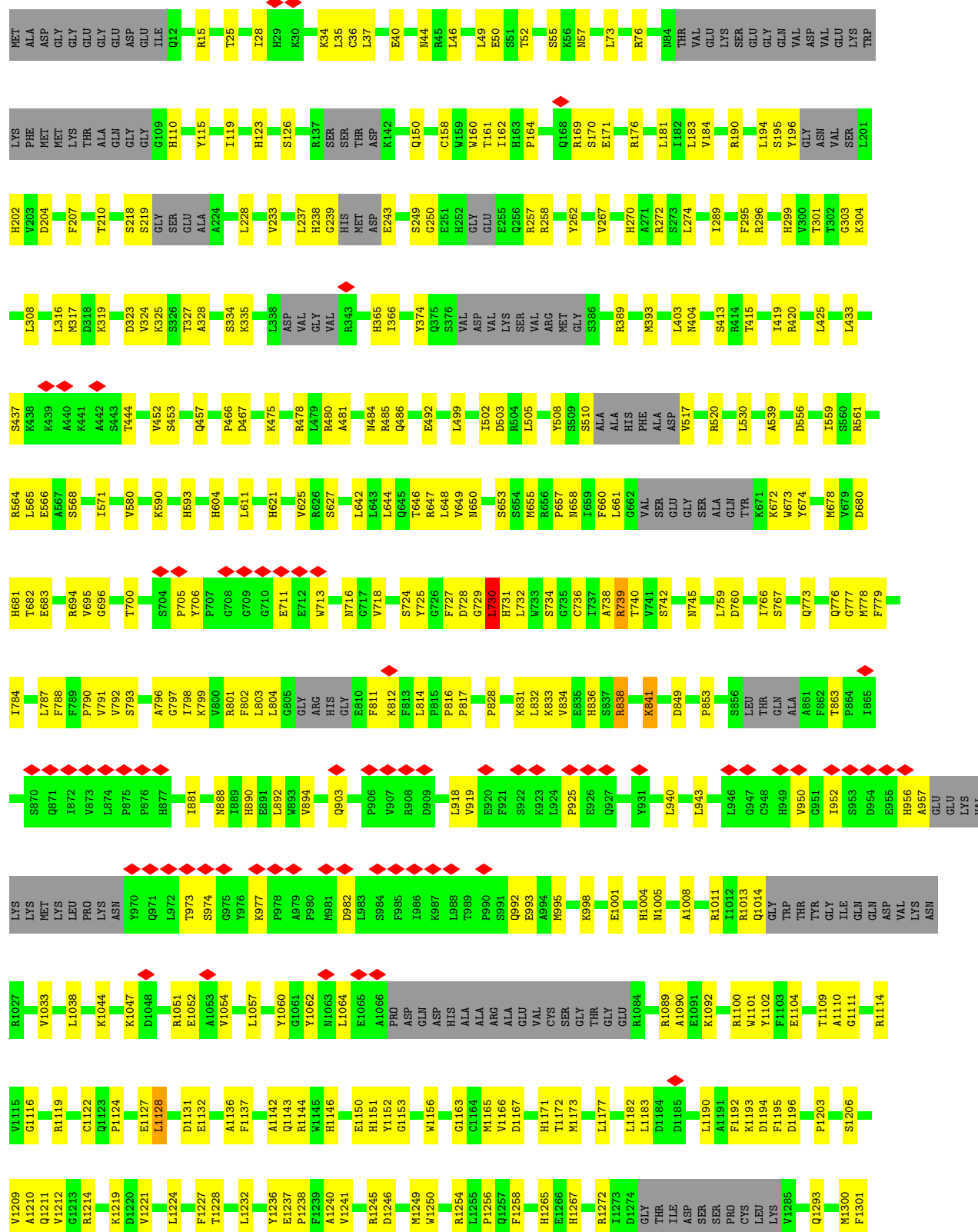
ALA	ARG	ASP	GLN	SER	ILE	W3105	ASP	LEU	ASP	W2853	T2793	GLN	SER	ALA	V2436	GLY	PRO
ARG	ASP	PRO	PRO	THR	TYR	L3106	GLN	THR	TYR	A2854	R2794	GLN	GLN	PRO	GLY	ASN	ALA
TYR	TYR	ILE	ILE	SER	PHE	G3114	PHE	PRO	LYS	K2855	R2795	PRO	TYR	ILE	ASP	ASP	GLU
ALA	ALA	SER	ARG	SER	ASN	Q3115	ASN	ILE	HIS	K2856	R2796	ILE	GLY	GLY	GLY	GLY	GLY
PHE	TYR	SER	TRP	SER	HIS	H3116	HIS	GLU	ASN	K2857	D2797	GLU	ASP	GLY	GLY	GLY	SER
TYR	TYR	ARG	TRP	ARG	ARG	Q3117	ARG	GLU	LEU	K2858	SER	GLU	ASP	GLY	GLY	GLY	SER
PRO	PRO	GLU	GLU	GLU	LEU	F3118	LEU	LEU	LEU	L2859	MET	GLU	ASP	GLY	GLY	GLY	SER
LEU	LEU	ALA	GLY	ALA	GLY	GLY	Y2982	GLU	ASP	L2860	ALA	GLU	ASP	GLY	GLY	GLY	SER
ILE	ILE	LEU	PRO	PRO	ASP	ASP	F2983	ALA	THR	L2861	TYR	TYR	GLU	GLY	GLY	GLY	SER
ARG	ARG	PHE	GLU	GLU	ASN	ILE	K3002	LEU	LEU	L2862	ASN	ASN	GLN	GLY	GLY	GLY	SER
VAL	VAL	VAL	ASN	ASN	LEU	L3124	V3005	LEU	GLN	K2864	ARG	VAL	VAL	GLY	GLY	GLY	SER
ASP	ASP	GLU	PRO	PRO	THR	GLY	THR	GLN	ARG	G2865	ARG	GLN	SER	GLY	GLY	GLY	SER
ASN	ASN	GLU	GLY	GLY	ASN	S3130	SER	GLN	ILE	G2866	ILE	ILE	MET	GLY	GLY	GLY	SER
ARG	ARG	GLU	ARG	ARG	ASN	C3131	LEU	LEU	SER	G2867	GLN	GLN	GLU	GLY	GLY	GLY	SER
ALA	ALA	GLU	GLU	GLU	GLU	Y3132	SER	ILE	SER	N2868	THR	LYS	LYS	GLY	GLY	GLY	SER
LYS	LYS	TRP	GLU	GLU	ASP	R3133	F3009	ARG	THR	G2869	GLN	GLN	GLN	GLY	GLY	GLY	SER
LEU	LEU	LYS	LYS	CYS	VAL	R3134	T3028	VAL	SER	P2870	VAL	VAL	SER	GLY	GLY	GLY	SER
LEU	LEU	LEU	LEU	CYS	PRO	S3137	ILE	GLU	ILE	L2871	SER	VAL	MET	GLY	GLY	GLY	SER
LYS	LYS	GLU	LYS	THR	ILE	L3138	VAL	ALA	ASN	L2872	VAL	SER	ASP	ILE	GLY	GLY	SER
ALA	ALA	ALA	ALA	THR	ALA	L3141	CYS	GLN	CYS	V2873	ASP	GLN	GLY	GLY	GLY	GLY	SER
GLU	GLU	GLU	GLU	SER	LEU	T3142	K3055	ILE	THR	P2874	A2818	GLN	GLY	GLY	GLY	GLY	SER
ASP	ASP	VAL	VAL	HIS	GLU	G3143	SER	LEU	LEU	Y2875	H2819	TYR	TYR	GLY	GLY	GLY	SER
LEU	LEU	VAL	VAL	GLU	LEU	T3144	ALA	GLU	PHE	D2876	H2820	LEU	GLY	GLY	GLY	GLY	SER
PHE	PHE	PHE	SER	GLU	GLU	S3144	LEU	PHE	ASP	T2877	G2821	GLY	GLY	GLY	GLY	GLY	SER
ARG	ARG	ARG	GLU	LEU	LEU	LYS	ARG	GLY	GLY	L2878	Y2822	GLY	GLY	GLY	GLY	GLY	SER
MET	MET	ASP	GLU	LEU	ILE	ILE	ALA	GLY	GLY	T2879	Y2823	GLY	GLY	GLY	GLY	GLY	SER
ASP	ASP	GLU	GLU	LEU	ILE	TYR	F3061	SER	SER	A2880	S2824	GLY	GLY	GLY	GLY	GLY	SER
HIS	HIS	HIS	ASP	GLY	VAL	W3149	L3062	VAL	ARG	K2881	R2825	GLY	GLY	GLY	GLY	GLY	SER
LEU	LEU	LEU	LEU	ILE	ASP	E3150	LEU	LEU	SER	E2882	A2826	GLY	GLY	GLY	GLY	GLY	SER
SER	SER	SER	SER	ALA	ALA	E3158	G3079	GLY	GLY	A2884	L2828	GLY	GLY	GLY	GLY	GLY	SER
VAL	VAL	PHE	GLU	ILE	ALA	GLU	T3082	GLU	GLU	K2885	D2828	GLU	GLY	GLY	GLY	GLY	SER
ILE	ILE	VAL	VAL	SER	GLY	A3161	HIS	HIS	HIS	D2886	M2829	GLU	GLY	GLY	GLY	GLY	SER
ARG	ARG	TRP	ARG	GLY	TYR	A3162	THR	THR	THR	S2830	N2711	THR	THR	THR	GLY	GLY	SER
ASP	ASP	TRP	GLY	ASN	ILE	F3163	ARG	ARG	ARG	E2766	L2712	ALA	ALA	ALA	GLY	GLY	SER
LYS	LYS	SER	ASP	ASN	ILE	A3164	ASN	GLN	TYR	K2767	L2713	ALA	ALA	ALA	GLY	GLY	SER
SER	SER	SER	MET	LEU	TYR	G3165	GLN	GLN	GLU	E2768	L2714	ASN	ASN	ASN	GLY	GLY	SER
HIS	HIS	GLU	GLU	GLY	THR	A3166	PRO	GLN	GLN	K2769	L2715	PHE	PHE	PHE	GLY	GLY	SER
ASN	ASN	PHE	GLU	GLU	MET	PHE	GLY	ILE	ILE	E2770	L2716	ALA	ALA	ALA	GLY	GLY	SER
PHE	PHE	VAL	GLU	PRO	PRO	PRO	VAL	PHE	PHE	S2835	L2717	ALA	ALA	ALA	GLY	GLY	SER
ARG	ARG	ARG	LEU	GLY	HIS	VAL	THR	THR	THR	R2836	K2717	ALA	ALA	ALA	GLY	GLY	SER
GLU	GLU	GLU	LEU	GLY	ALA	A3170	GLN	GLN	GLN	D2837	L2718	GLY	GLY	GLY	GLY	GLY	SER
GLU	GLU	GLU	ILE	TRP	MET	F3171	ILE	ALA	ALA	R2838	E2719	GLY	GLY	GLY	GLY	GLY	SER
GLN	GLN	ASP	GLY	LYS	VAL	F3172	ILE	LYS	LYS	L2838	L2720	GLY	GLY	GLY	GLY	GLY	SER
ASN	ASN	GLU	ARG	VAL	VAL	E3173	ASN	VAL	VAL	H2839	F2721	GLY	GLY	GLY	GLY	GLY	SER
PHE	PHE	PHE	LEU	LEU	LEU	T3174	TYR	LEU	VAL	A2840	L2722	GLY	GLY	GLY	GLY	GLY	SER
VAL	VAL	VAL	PRO	ALA	PRO	H3175	T3098	LEU	LEU	M2841	N2723	GLY	GLY	GLY	GLY	GLY	SER
GLN	GLN	VAL	MET	VAL	MET	L3176	V3100	LEU	LEU	N2842	K2724	GLY	GLY	GLY	GLY	GLY	SER
						S3182				E2843	L2725	GLY	GLY	GLY	GLY	GLY	SER
						S3183				M2845	A2726	GLY	GLY	GLY	GLY	GLY	SER
										E2847	E2727	GLY	GLY	GLY	GLY	GLY	SER
										N2848	H2728	GLY	GLY	GLY	GLY	GLY	SER
										Y2849	S2729	GLY	GLY	GLY	GLY	GLY	SER
										H2850	H2730	GLY	GLY	GLY	GLY	GLY	SER
										R2906	D2731	GLY	GLY	GLY	GLY	GLY	SER
										G2907	K2732	GLY	GLY	GLY	GLY	GLY	SER
										PHE	A2726	GLY	GLY	GLY	GLY	GLY	SER
										LYS	E2727	GLY	GLY	GLY	GLY	GLY	SER
										ASP	H2728	GLY	GLY	GLY	GLY	GLY	SER
										LEU	H2730	GLY	GLY	GLY	GLY	GLY	SER
										LEU	D2731	GLY	GLY	GLY	GLY	GLY	SER
										GLU	K2732	GLY	GLY	GLY	GLY	GLY	SER







● Molecule 1: RyR2



















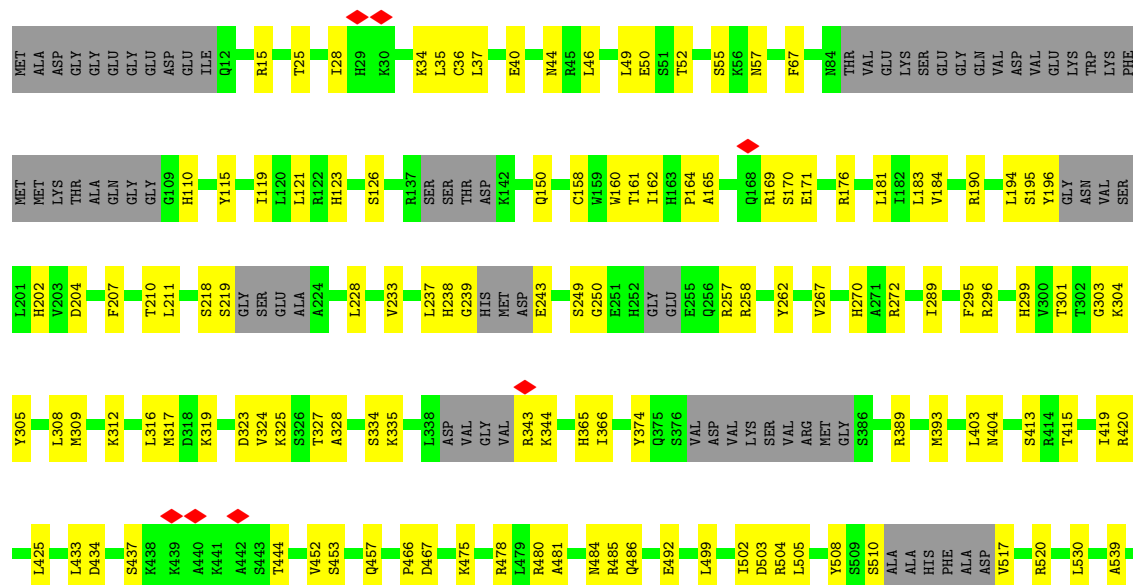
















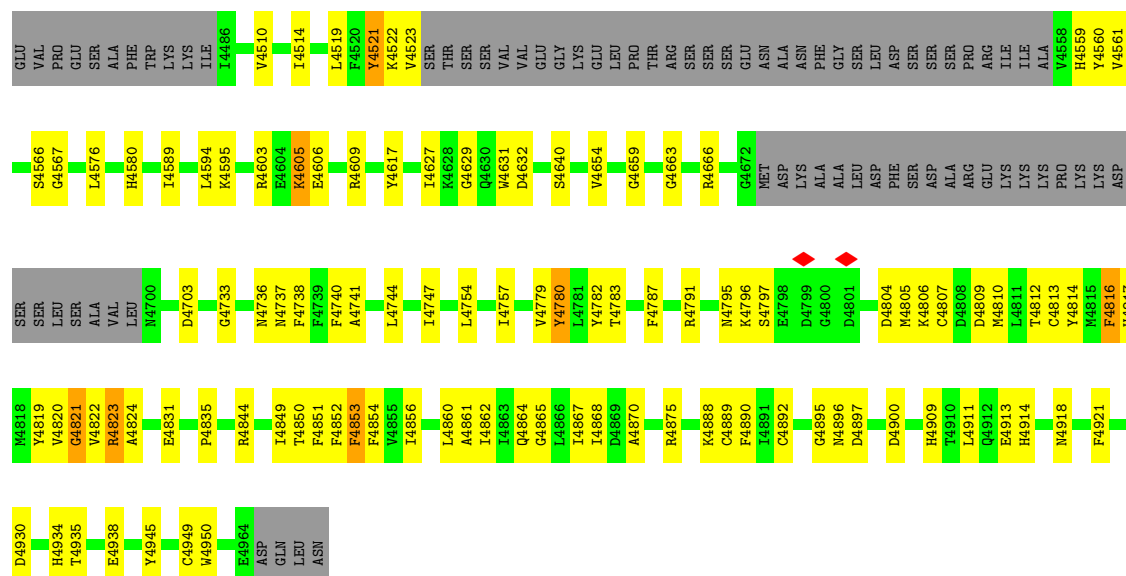






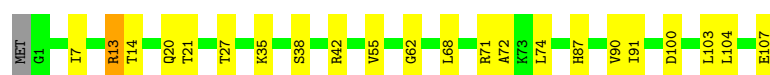






• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 79% 19% ..



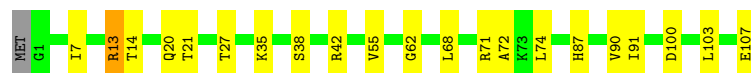
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 79% 19% ..



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

Chain H: 80% 19% ..



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

Chain K: 80% 19% ..



• Molecule 3: Calmodulin-1

Chain C: 42% 38% 7% 54%

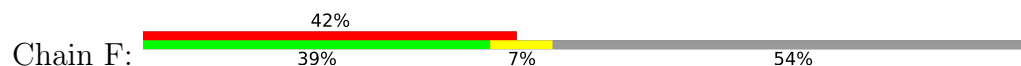


MET	ALA	ASP	GLN	LEU	THR	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	I27	T28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	G60
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N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	A73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	ILE	SER	ALA	ALA	GLU	LEU	Q42	HIS	VAL	MET	THR	ASN	LEU	GLY	E48	L49	LYS	LEU	THR	ASP	GLU
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GLU	VAL	ASP	GLU	MET	ILE	ARG	ALA	ASP	ASP	ILE	ASP	GLY	ASP	GLY	GLN	VAL	ASN	TYR	GLU	K76	PHE	VAL	GLN	MET	THR	ALA	LYS
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- Molecule 3: Calmodulin-1

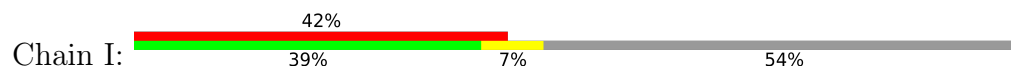


MET	ALA	ASP	GLN	LEU	THR	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	I27	T28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	G60
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N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	A73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	ILE	SER	ALA	ALA	GLU	LEU	Q42	HIS	VAL	MET	THR	ASN	LEU	GLY	E48	L49	LYS	LEU	THR	ASP	GLU
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GLU	VAL	ASP	GLU	MET	ILE	ARG	ALA	ASP	ASP	ILE	ASP	GLY	ASP	GLY	GLN	VAL	ASN	TYR	GLU	K76	PHE	VAL	GLN	MET	THR	ALA	LYS
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- Molecule 3: Calmodulin-1

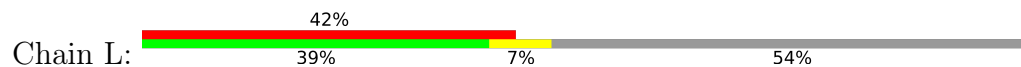


MET	ALA	ASP	GLN	LEU	THR	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	I27	T28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	G60
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N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	A73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	ILE	SER	ALA	ALA	GLU	LEU	Q42	HIS	VAL	MET	THR	ASN	LEU	GLY	E48	L49	LYS	LEU	THR	ASP	GLU
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GLU	VAL	ASP	GLU	MET	ILE	ARG	ALA	ASP	ASP	ILE	ASP	GLY	ASP	GLY	GLN	VAL	ASN	TYR	GLU	K76	PHE	VAL	GLN	MET	THR	ALA	LYS
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- Molecule 3: Calmodulin-1



MET	ALA	ASP	GLN	LEU	THR	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	I27	T28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	G60
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N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	A73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	ILE	SER	ALA	ALA	GLU	LEU	Q42	HIS	VAL	MET	THR	ASN	LEU	GLY	E48	L49	LYS	LEU	THR	ASP	GLU
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GLU	VAL	ASP	GLU	MET	ILE	ARG	ALA	ASP	ASP	ILE	ASP	GLY	ASP	GLY	GLN	VAL	ASN	TYR	GLU	K76	PHE	VAL	GLN	MET	THR	ALA	LYS
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	77092	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 ( $e^-/\text{\AA}^2$ )	45.6	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	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	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, ZN, 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	0.35	2/27161 (0.0%)	0.55	7/36737 (0.0%)
1	D	0.34	0/27161	0.55	9/36737 (0.0%)
1	G	0.34	0/27161	0.55	5/36737 (0.0%)
1	J	0.34	0/27161	0.55	6/36737 (0.0%)
2	B	0.33	0/835	0.53	0/1123
2	E	0.33	0/835	0.53	0/1123
2	H	0.33	0/835	0.53	0/1123
2	K	0.33	0/835	0.53	0/1123
3	C	0.29	0/530	0.49	0/711
3	F	0.29	0/530	0.49	0/711
3	I	0.29	0/530	0.49	0/711
3	L	0.29	0/530	0.49	0/711
All	All	0.34	2/114104 (0.0%)	0.55	27/154284 (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	23
1	D	0	23
1	G	0	23
1	J	0	23
All	All	0	92

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4521	TYR	N-CA	7.55	1.61	1.46
1	A	4522	LYS	CA-C	-6.22	1.36	1.52



The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4823	ARG	N-CA-C	10.38	139.02	111.00
1	D	4823	ARG	CB-CA-C	-7.98	94.43	110.40
1	A	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	D	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	G	730	LEU	CA-CB-CG	6.89	131.16	115.30

There are no chirality outliers.

5 of 92 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	PHE	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	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	26661	0	25136	600	0
1	D	26661	0	25136	589	0
1	G	26661	0	25136	605	0
1	J	26661	0	25136	598	0
2	B	819	0	824	15	0
2	E	819	0	824	15	0
2	H	819	0	824	14	0
2	K	819	0	824	14	0
3	C	524	0	504	8	0
3	F	524	0	504	7	0
3	I	524	0	504	7	0
3	L	524	0	504	7	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	0	0
6	G	31	0	12	0	0
6	J	31	0	12	0	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	112212	0	105944	2282	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 10.

The worst 5 of 2282 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:A:4852:PHE:CZ	1:D:4823:ARG:HA	1.59	1.37
1:G:4861:ALA:CB	1:J:4864:GLN:HE21	1.53	1.22
1:D:4861:ALA:CB	1:G:4864:GLN:HE21	1.52	1.22
1:A:4861:ALA:CB	1:D:4864:GLN:HE21	1.52	1.21
1:A:4782:TYR:CD2	1:A:4851:PHE:CD1	2.30	1.20

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	3374/4968 (68%)	3009 (89%)	357 (11%)	8 (0%)	47	80
1	D	3374/4968 (68%)	3012 (89%)	355 (10%)	7 (0%)	47	80
1	G	3374/4968 (68%)	3012 (89%)	354 (10%)	8 (0%)	47	80
1	J	3374/4968 (68%)	3010 (89%)	355 (10%)	9 (0%)	41	76
2	B	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	K	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
3	C	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	F	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
All	All	14180/20900 (68%)	12694 (90%)	1454 (10%)	32 (0%)	50	80

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4823	ARG
1	J	4823	ARG
1	G	4823	ARG
1	A	730	LEU
1	A	853	PRO

### 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	2672/4355 (61%)	2653 (99%)	19 (1%)	84	90
1	D	2671/4355 (61%)	2650 (99%)	21 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	2671/4355 (61%)	2651 (99%)	20 (1%)	84	90
1	J	2671/4355 (61%)	2653 (99%)	18 (1%)	84	90
2	B	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	E	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	K	88/89 (99%)	87 (99%)	1 (1%)	73	84
3	C	57/127 (45%)	57 (100%)	0	100	100
3	F	57/127 (45%)	57 (100%)	0	100	100
3	I	57/127 (45%)	57 (100%)	0	100	100
3	L	57/127 (45%)	57 (100%)	0	100	100
All	All	11265/18284 (62%)	11183 (99%)	82 (1%)	84	90

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	4780	TYR
1	J	1683	PRO
1	G	4818	MET
1	J	841	LYS
1	J	2836	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3993	ASN
1	J	2196	ASN
1	G	4864	GLN
1	J	604	HIS
1	J	3852	ASN

### 5.3.3 RNA ⓘ

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 24 ligands modelled in this entry, 16 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$
7	CFF	G	6003	-	8,15,15	2.61	4 (50%)	8,23,23	1.31	1 (12%)
7	CFF	A	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
6	ATP	A	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	D	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
7	CFF	D	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
6	ATP	G	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	J	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
7	CFF	J	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	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
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	D	6002	-	-	7/18/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	G	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	J	6002	-	-	7/18/38/38	0/3/3/3
7	CFF	J	6003	-	-	-	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	6003	CFF	C5-C4	-4.65	1.33	1.39
7	D	6003	CFF	C5-C4	-4.63	1.33	1.39
7	A	6003	CFF	C5-C4	-4.61	1.33	1.39
7	J	6003	CFF	C5-C4	-4.61	1.33	1.39
7	A	6003	CFF	C6-N1	-4.27	1.32	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	D	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	G	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	J	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	A	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	C5'-O5'-PA-O2A

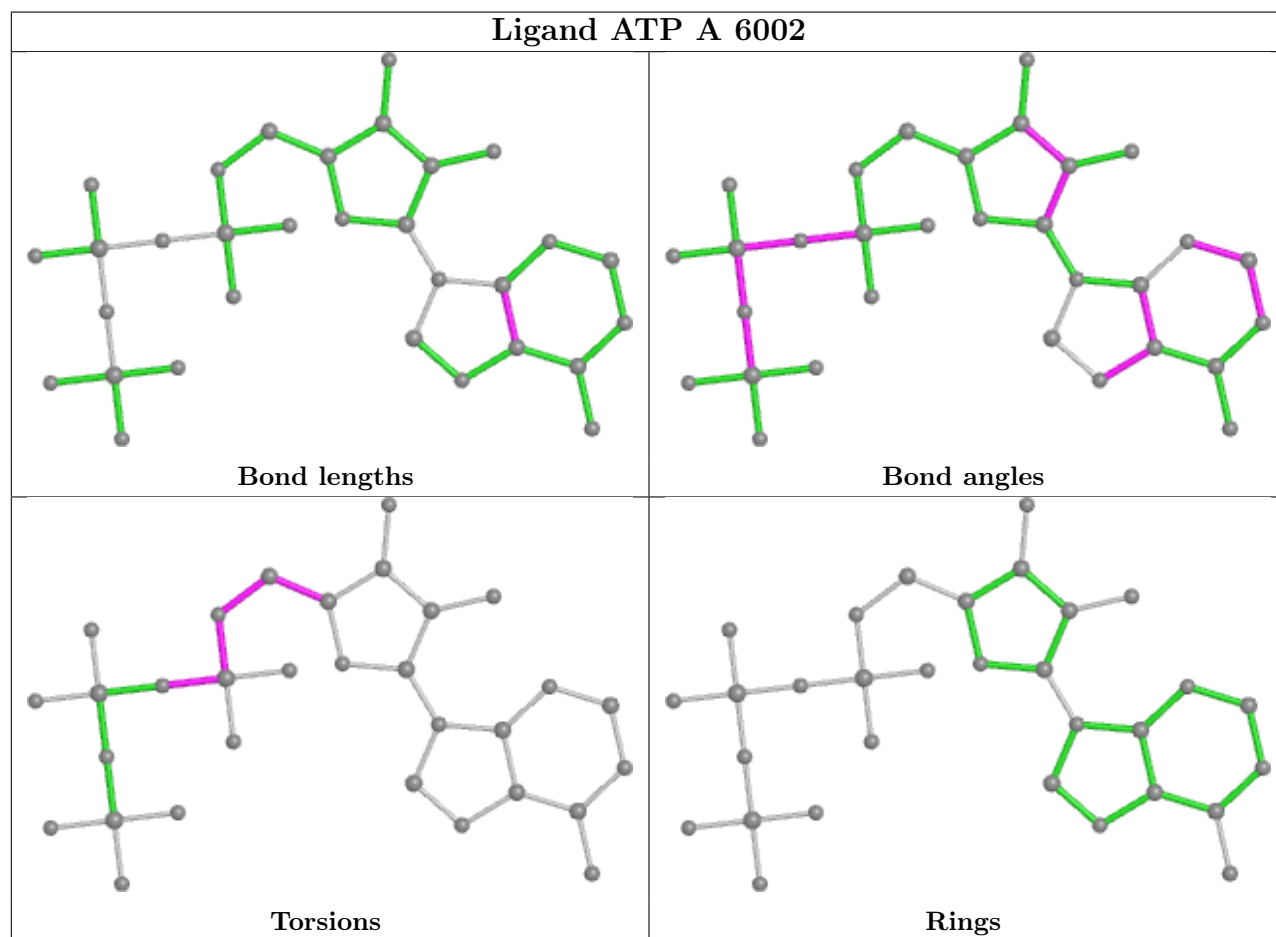
There are no ring outliers.

4 monomers are involved in 4 short contacts:

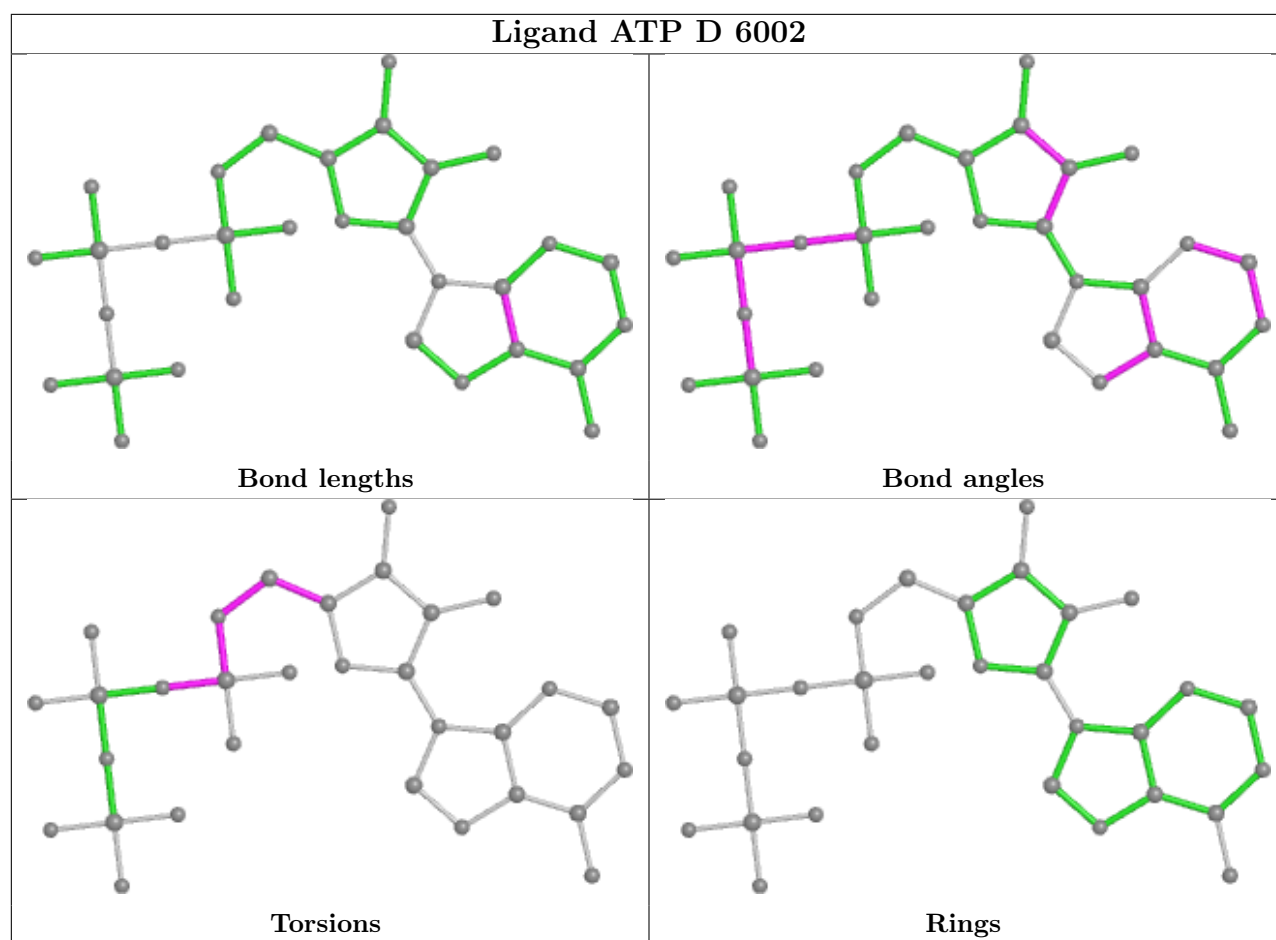
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	6003	CFF	1	0
7	A	6003	CFF	1	0
7	D	6003	CFF	1	0
7	J	6003	CFF	1	0



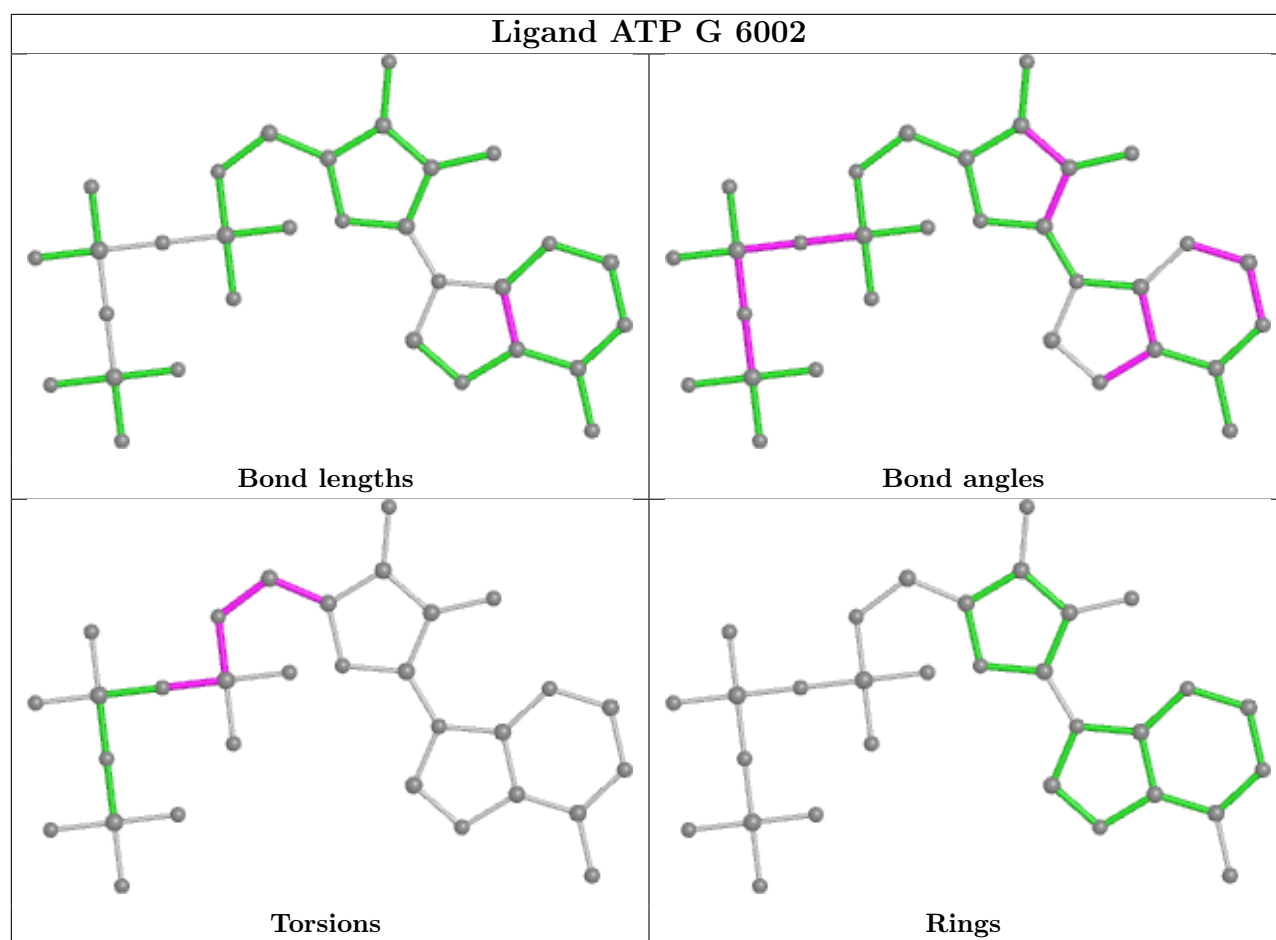
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



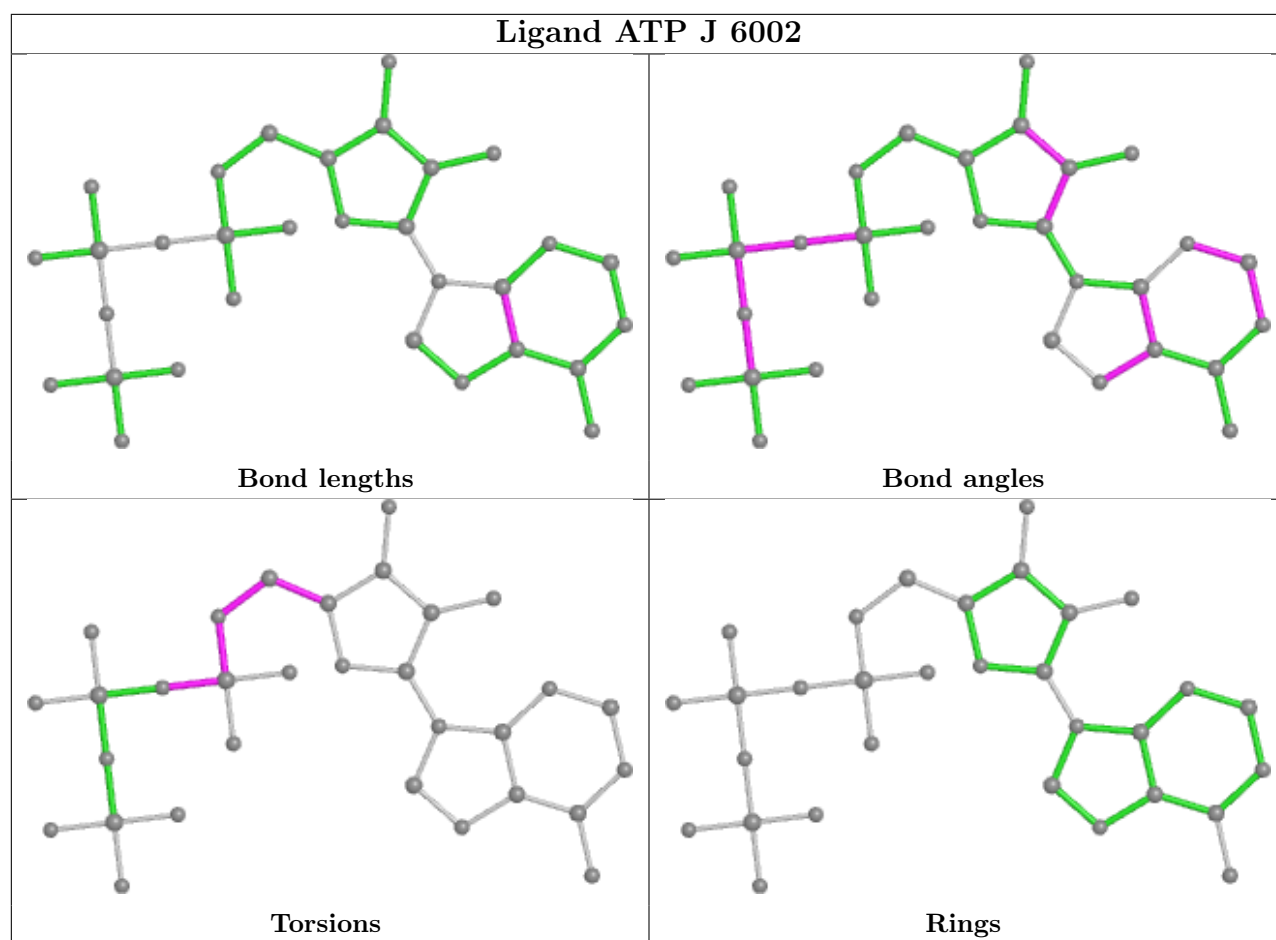












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



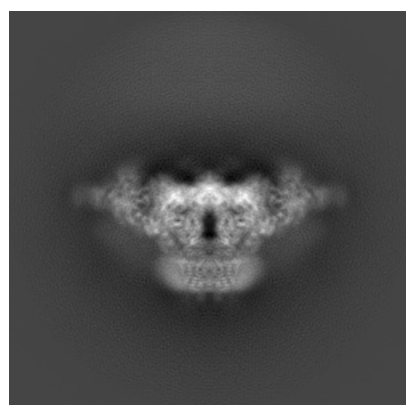
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9836. These allow visual inspection of the internal detail of the map and identification of artifacts.

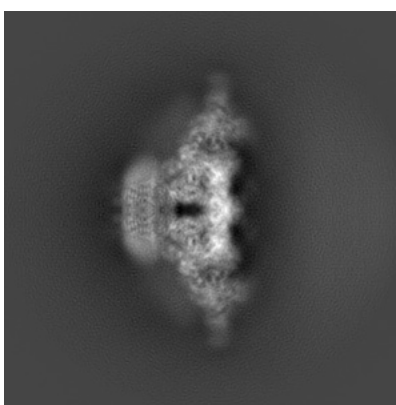
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

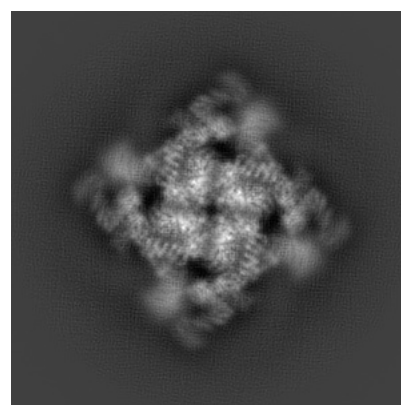
#### 6.1.1 Primary map



X



Y

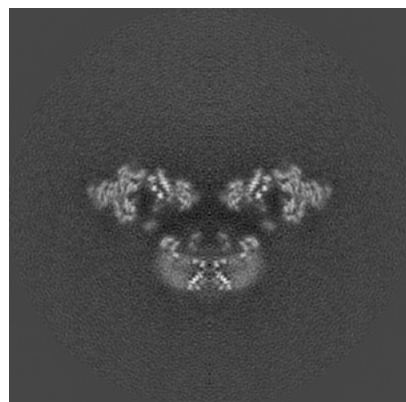


Z

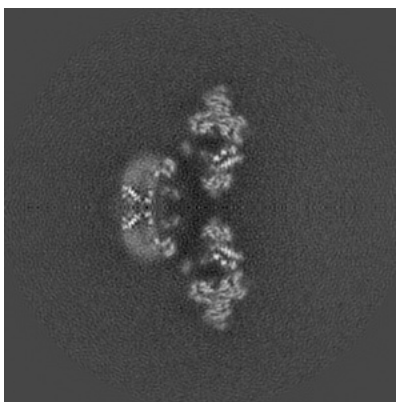
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

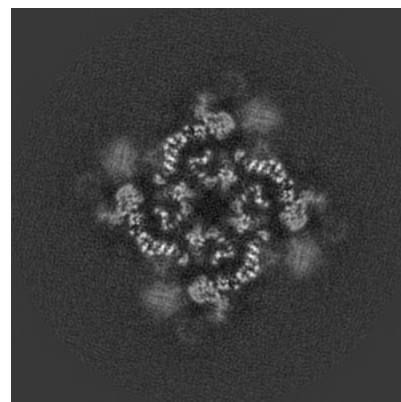
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



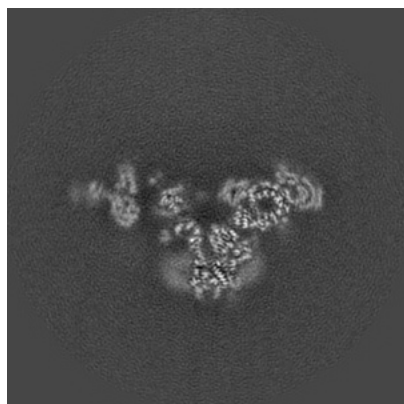
Z Index: 200



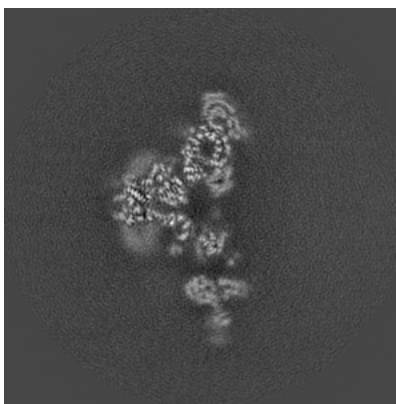
The images above show central slices of the map in three orthogonal directions.

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

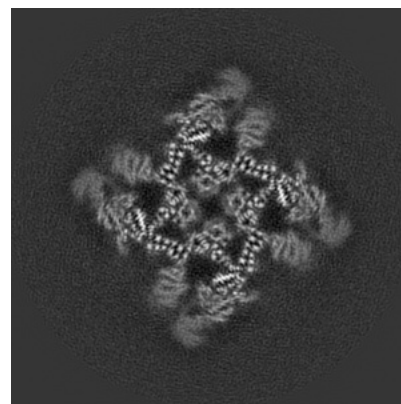
### 6.3.1 Primary map



X Index: 190



Y Index: 210

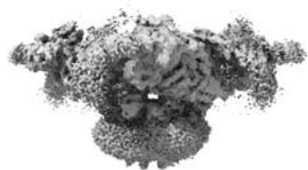


Z Index: 209

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

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

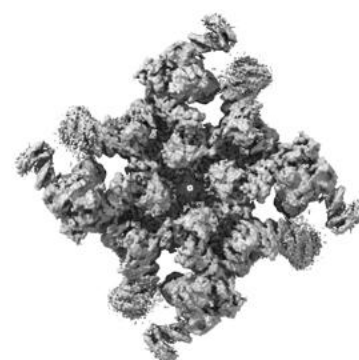
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

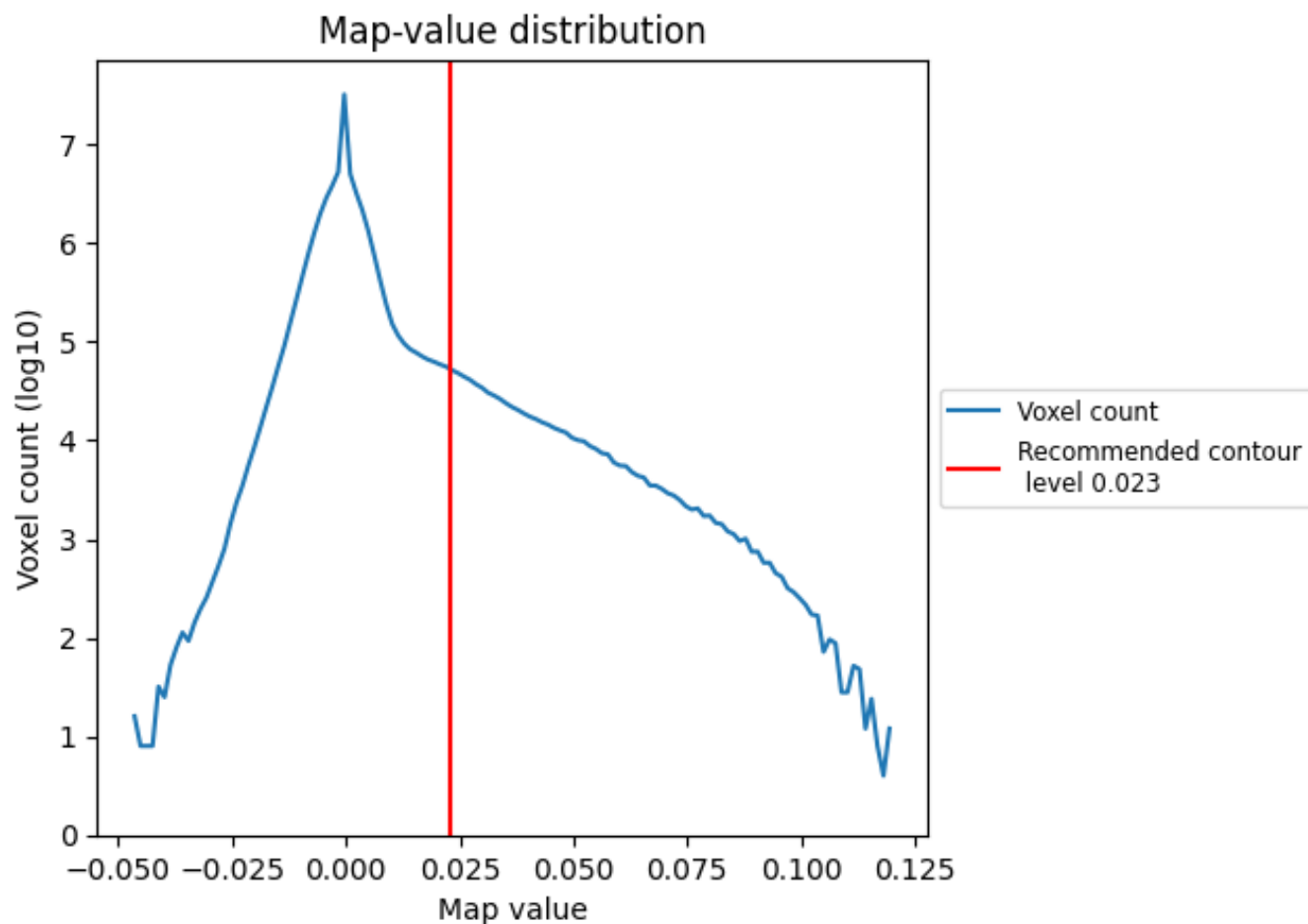
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

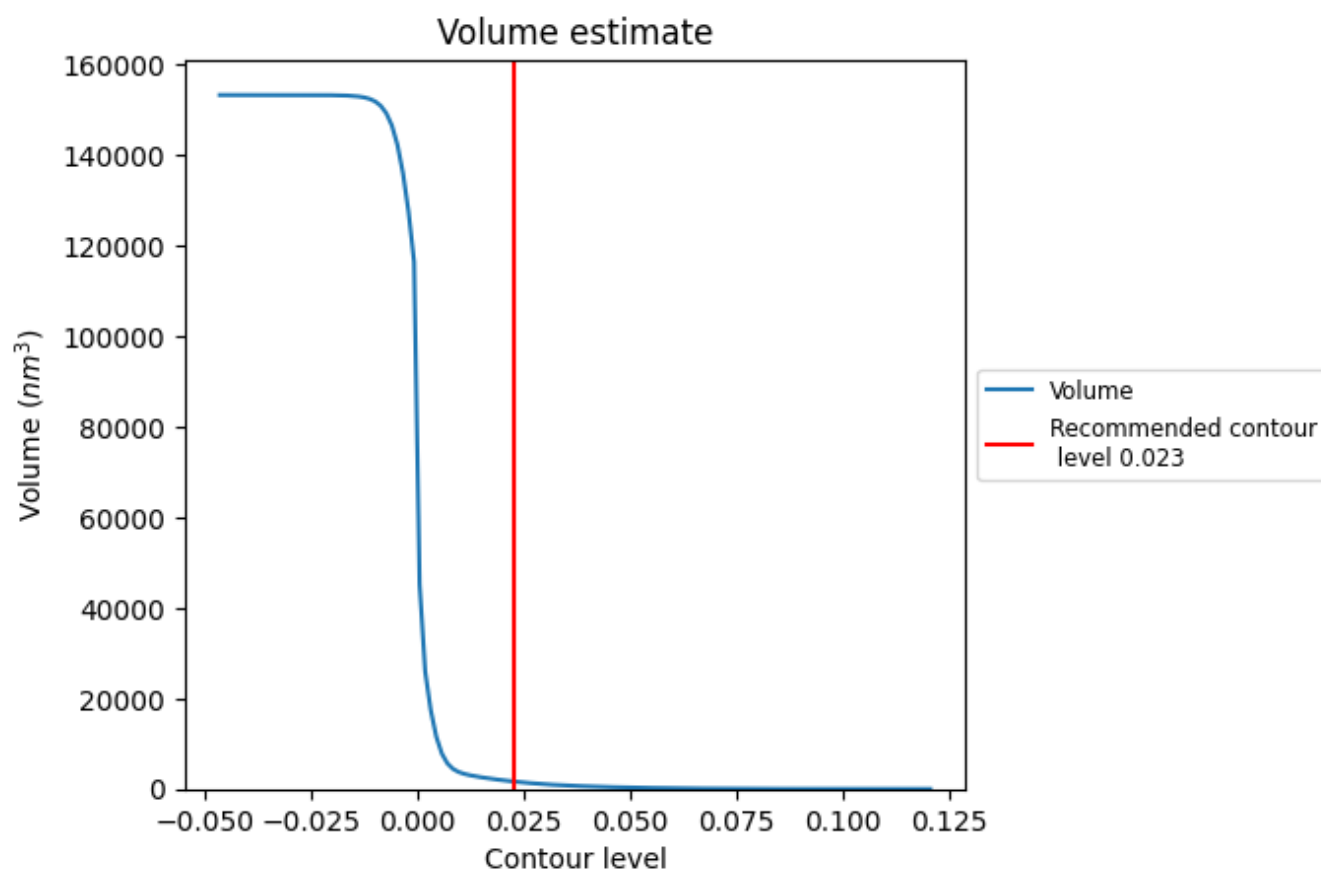
### 7.1 Map-value distribution [i](#)



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](#)

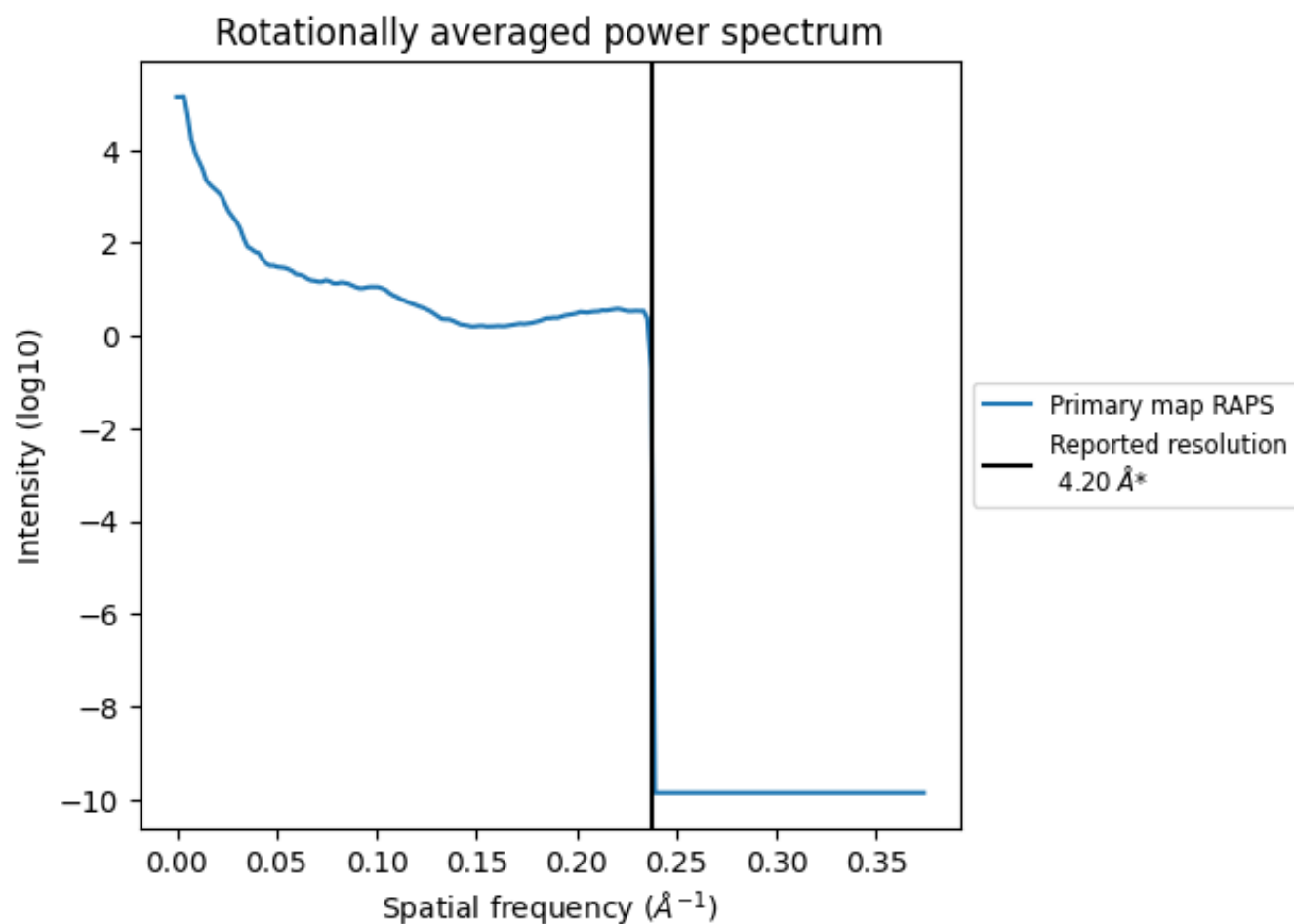


The volume at the recommended contour level is 1619 nm<sup>3</sup>; this corresponds to an approximate mass of 1462 kDa.

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 ⓘ



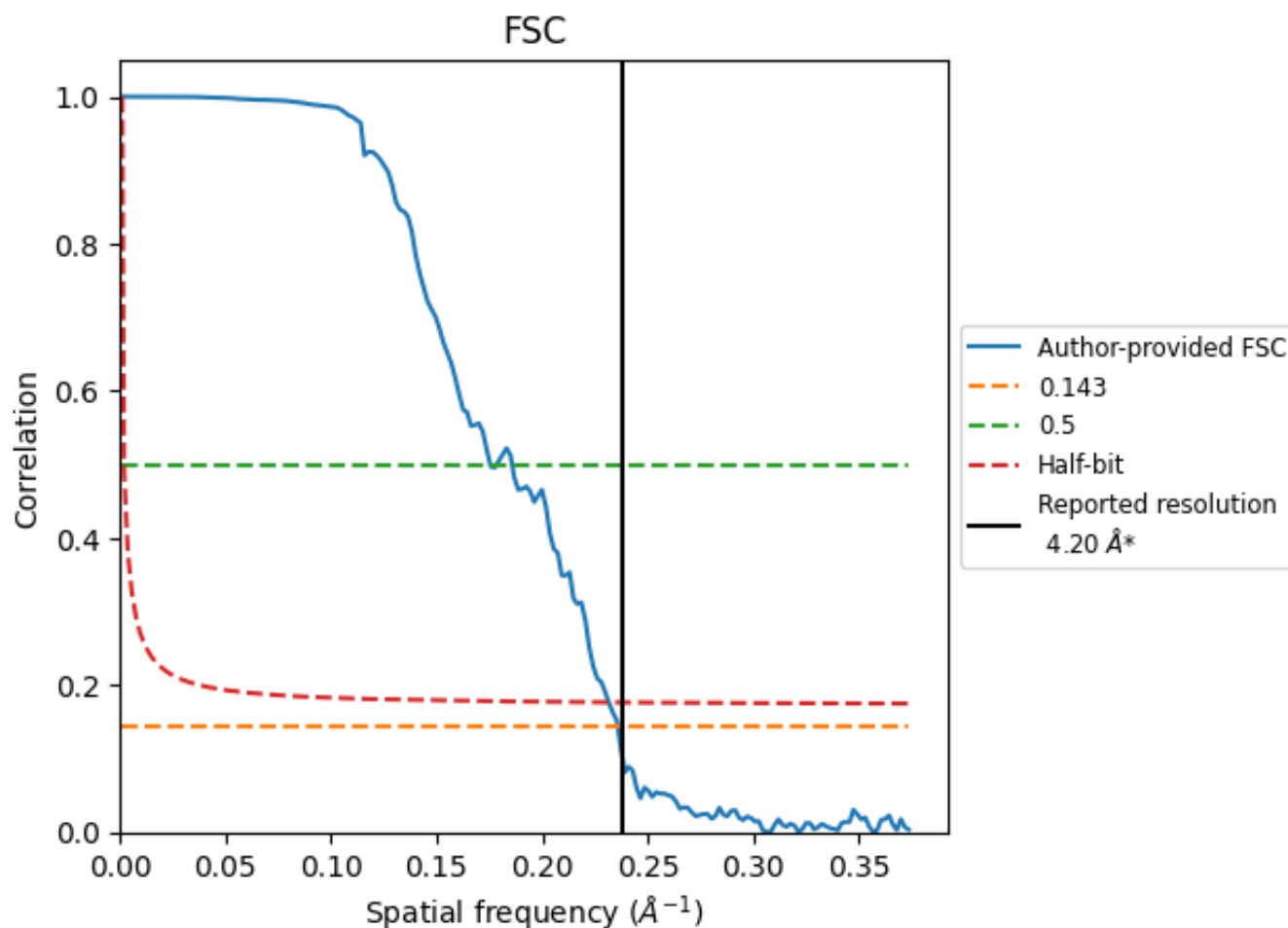
\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.70	4.32
Unmasked-calculated*	-	-	-

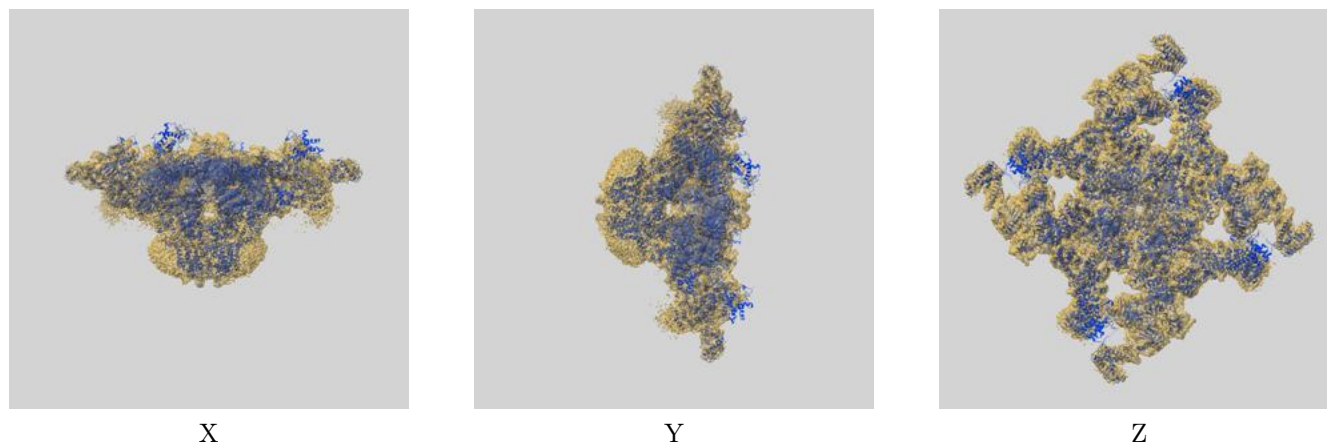
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

This section contains information regarding the fit between EMDB map EMD-9836 and PDB model 6JIU. Per-residue inclusion information can be found in section 3 on page 8.

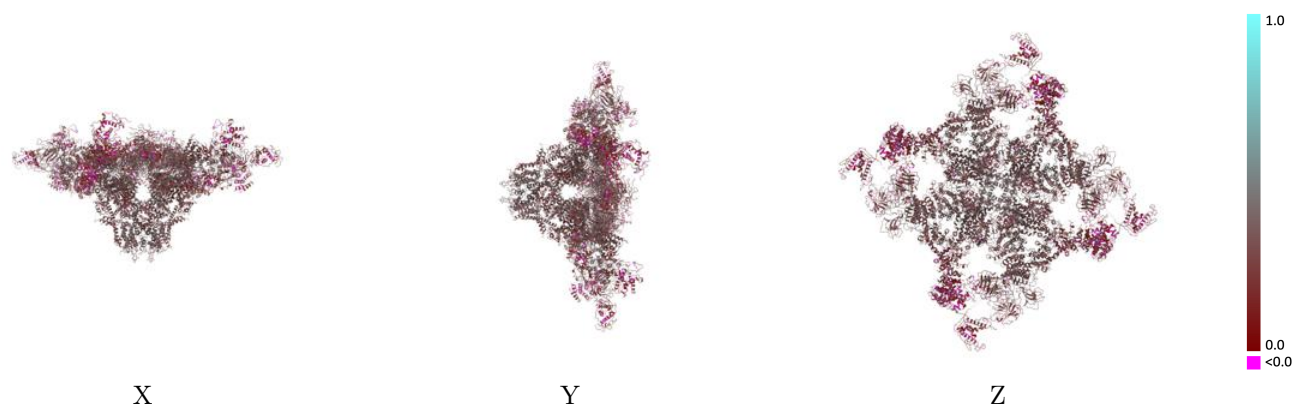
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.023 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.

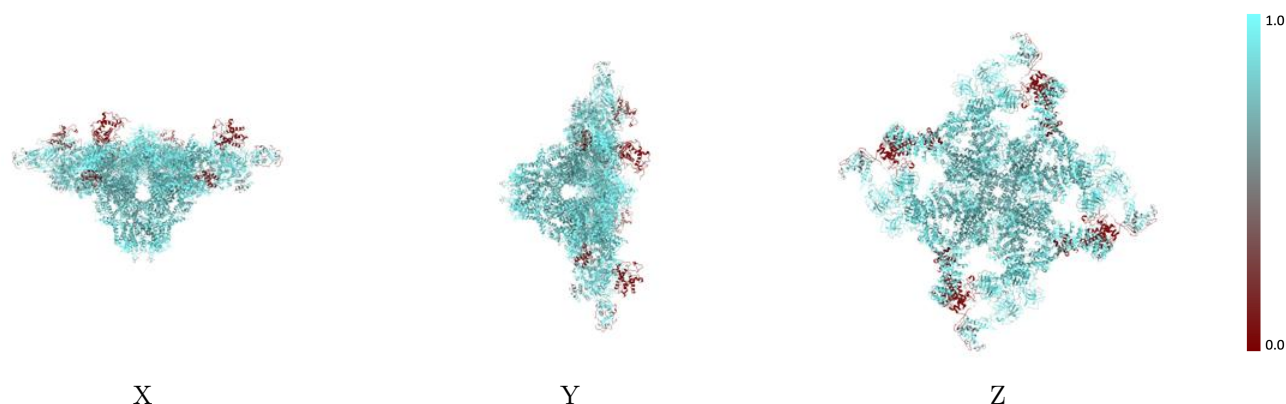


## 9.2 Q-score mapped to coordinate model [i](#)



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.

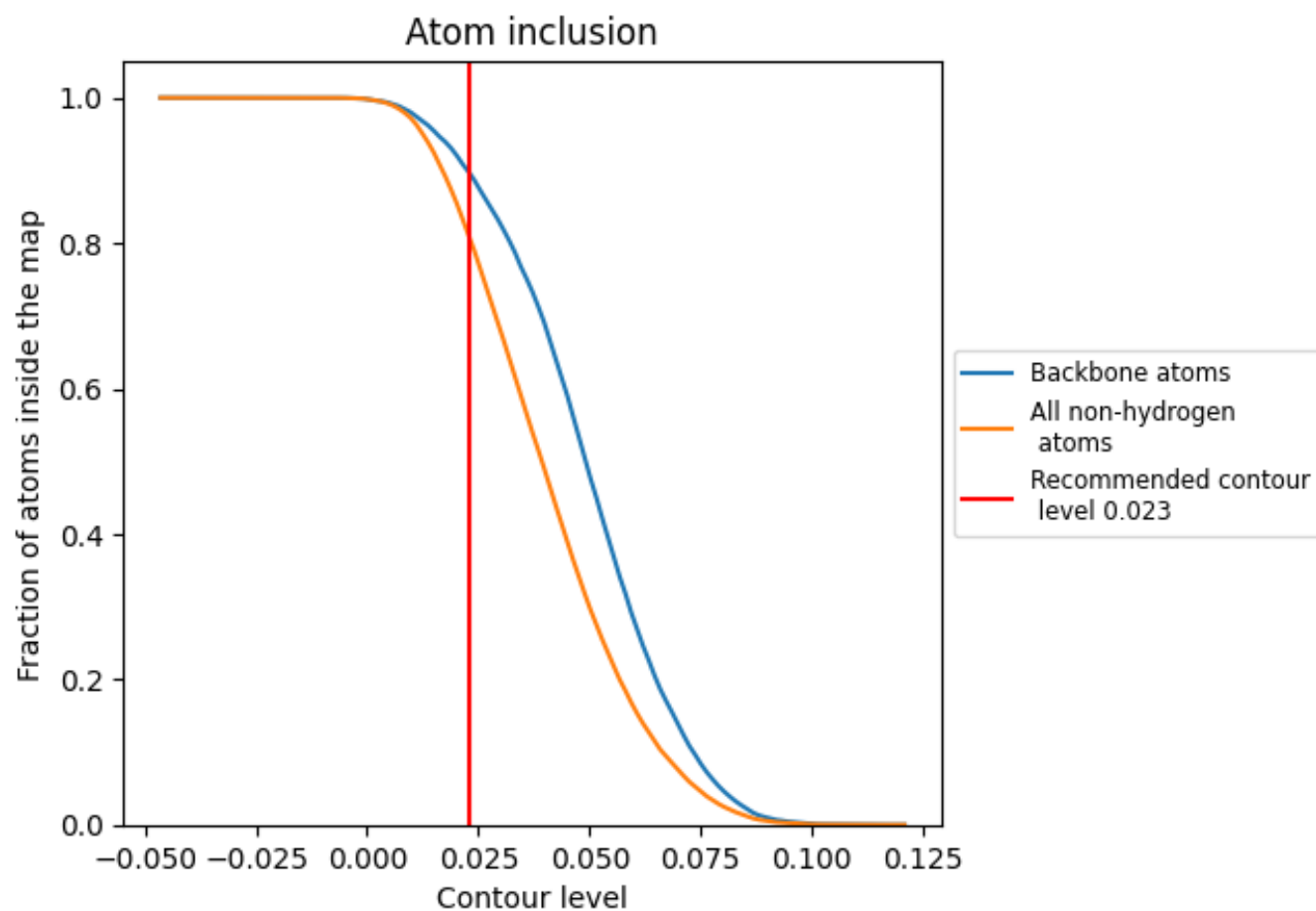
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.023).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8083	<div></div> 0.3030
A	<div></div> 0.8202	<div></div> 0.3050
B	<div></div> 0.8711	<div></div> 0.3450
C	<div></div> 0.1111	<div></div> 0.1780
D	<div></div> 0.8200	<div></div> 0.3050
E	<div></div> 0.8699	<div></div> 0.3430
F	<div></div> 0.1111	<div></div> 0.1750
G	<div></div> 0.8204	<div></div> 0.3040
H	<div></div> 0.8724	<div></div> 0.3420
I	<div></div> 0.1111	<div></div> 0.1790
J	<div></div> 0.8205	<div></div> 0.3040
K	<div></div> 0.8724	<div></div> 0.3420
L	<div></div> 0.1111	<div></div> 0.1800

1.0

0.0

<0.0