



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 02:33 AM JST

PDB ID : 6JRS
EMDB ID : EMD-9880
Title : Structure of RyR2 (*F/A/C/L-Ca2+/Ca2+-CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-04-05
Resolution : 3.70 Å(reported)

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

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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.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

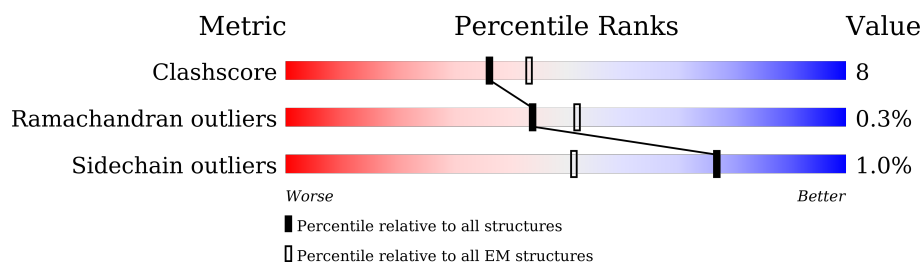
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



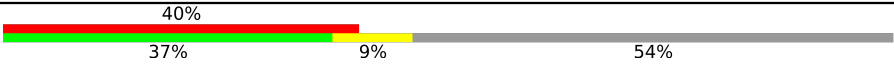



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	D	4968	
1	G	4968	
1	J	4968	
2	B	108	
2	E	108	
2	H	108	
2	K	108	

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Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 112168 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	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	D	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	G	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	J	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		

- 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		

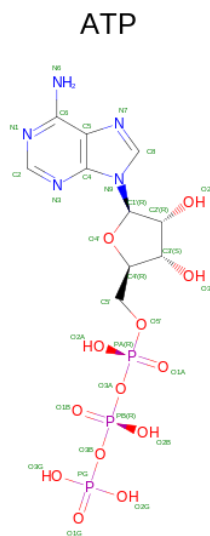
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

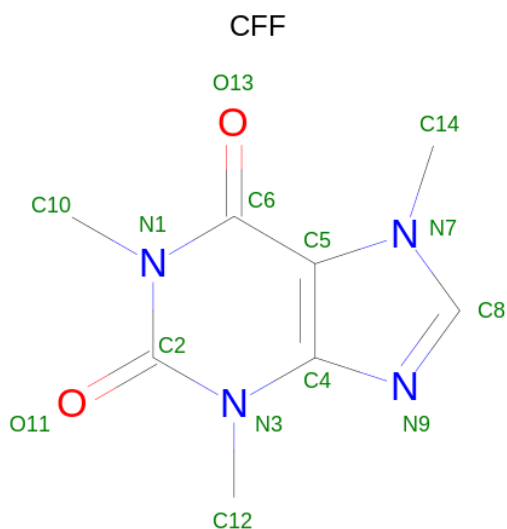
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).

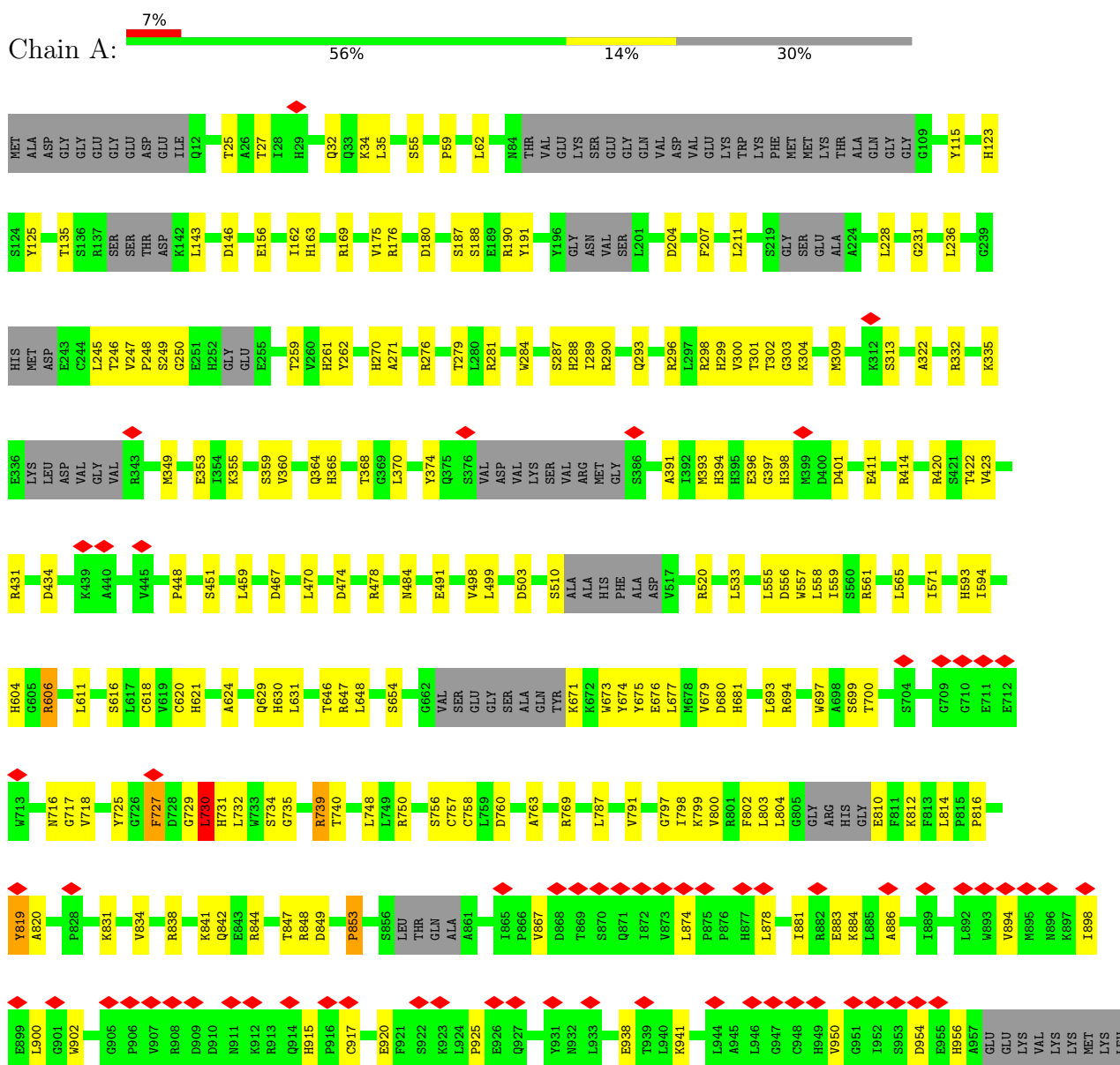


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

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

















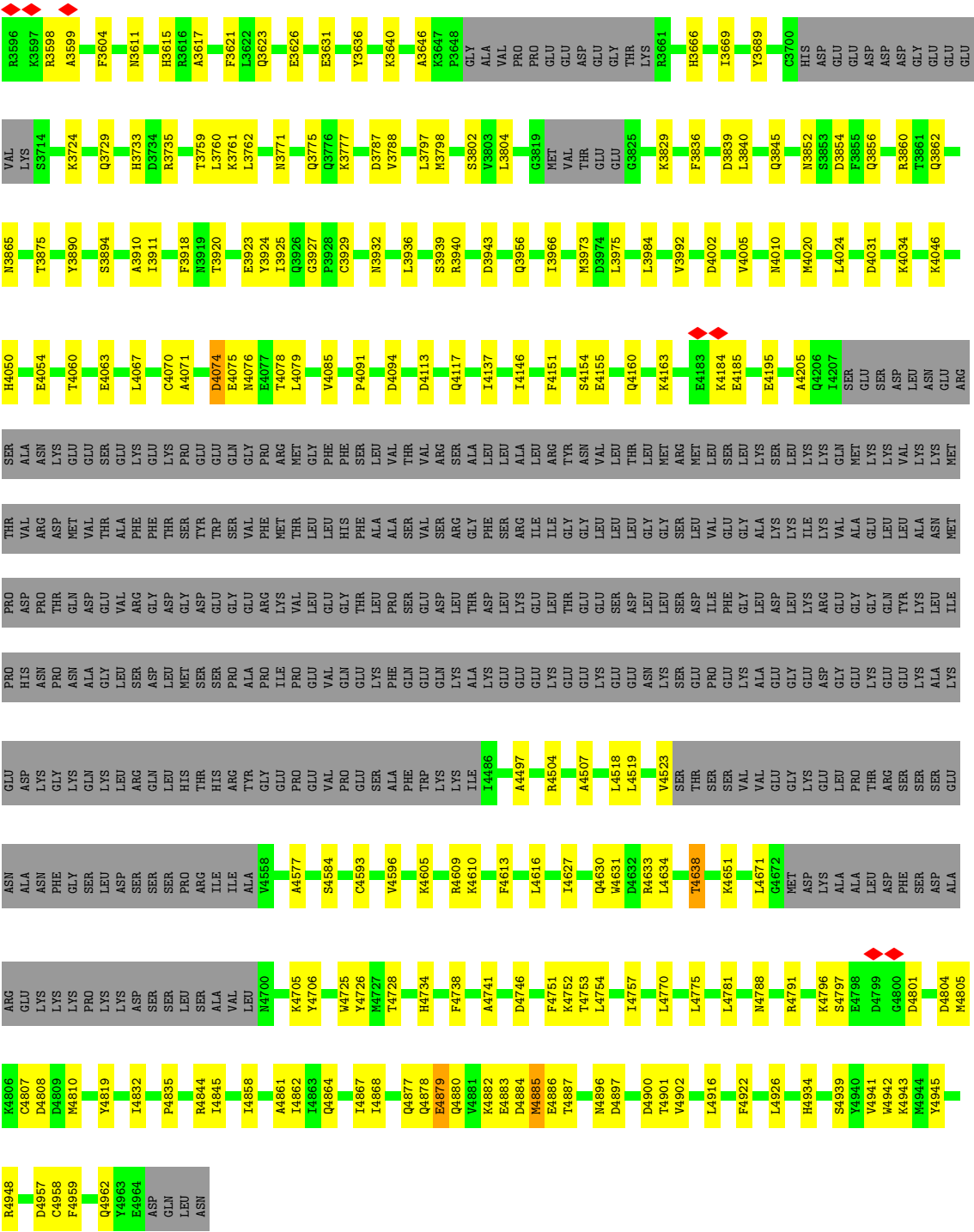
GLU	LYS	GLU	PRO	CYS	ALA	SER	GLU	ASP	SER	SER	ARG	LEU	GLU	GLY	PRO	ALA	GLU	GLU	SER	GLY	G1893	L1911	D1916	Q1938	R1942	L1982	ASN	MET	GLN	ALA	GLU	ALA	LEU	THR	VAL	GLU	ASP	ARG	LYS	THR	LYS	GLU	PHE	ARG	SER	PRO	PRO	GLN	GLN									
ILE	ASN	MET	LEU	LEU	ASN	PHE	LYS	ASP	ASP	SER	LYS	SER	GLN	GLU	C1987	P1988	P1989	P1990	D2013	GLU	ASP	GLY	ILE	T2024	T2025	R2029	Y2039	LEU	LYS	LYS	GLN	ALA	GLU	LYS	LEU	VAL	GLU	SER	ASP	LYS	LYS	LYS	THR	VAL	GLY	ASN	Q2061	M2067	L2088									
R2091	L2103	T2106	L2258	Y2107	M2110	V2133	ARG	MET	GLY	E2138	K2141	T2150	F2156	Y2157	M2163	M2168	H2169	G2181	GLY	GLY	GLU	SER	LYS	GLU	ILE	THR	PHE	F2191	Y2203	F2204	K2213	S2227	V2228	GLY	ALA	LEU	ALA	SER	PRO	ARG	GLY	MET	GLY	SER	ASN	T2239												
V2248	L2254	A2257	R2259	L2275	SER	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	LYS	GLY	TRP	ASN	P2293	F2308	C2309	S2313	V2314	N2317	Y2320	V2321	V2322	R2323	L2324	L2325	L2326	R2327	E2330	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLY	ASN	G2343															
L2354	ALA	GLU	ASP	PRO	SER	ARG	ASP	GLY	PRO	SER	PRO	THR	THR	SER	GLY	SER	LYS	MET	PRO	ASP	THR	ILE	HIS	MET	G2386	L2400	G2401	R2402	C2403	H2407	I2423	L2424	R2425	S2426	L2427	L2428	P2429	L2430	V2436	I2437	I2439	A2440	F2441															
Q2442	MET	THR	ILE	LYS	ASP	ASN	VAL	GLU	PRO	GLU	ASP	MET	ALA	ALA	GLY	ILE	GLU	V2481	L2503	ASP	THR	ALA	ALA	LEU	ALA	T2511	D2512	R2519	L2529	THR	ARG	CYS	ALA	PRO	L2585	V2583	TYR	ARG	LEU	SER	K2588	S2576	ILE	CYS														
GLY	GLN	LEU	ARG	P2583	L2589	L2593	V2597	M2601	GLU	HIS	ALA	K2605	G2627	TRP	GLY	ASN	PHE	GLY	ILE	GLU	V2645	L2649	L2653	SER	GLN	LYS	LYS	Y2658	A2672	L2677	P2678	PRO	ASP	TYR	MET	GLU	SER	ASN	VAL	SER	MET	MET	GLU	LYS	GLN	SER	MET											
ASP	SER	GLY	W2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	M2711	L2712	T2713	L2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	N2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	D2730	L2731	K2732	N2733	S2734	M2735	N2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	Y2744	G2745	E2746	L2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	P2756	
L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	L2771	Y2772	R2773	W2774	P2775	L2776	K2777	E2778	L2780	K2781	T2782	M2783	L2784	A2785	W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ILE	SER	GLN	THR	SER	GLN	VAL				
ASP	A2818	A2819	H2820	Q2821	Y2822	S2823	P2824	R2825	P2826	A2826	I2827	D2828	W2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840	W2841	A2842	E2843	W2844	M2845	A2846	E2847	N2848	Y2849	H2850	N2851	I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	W2864	Q2865	Q2866	Q2867	W2868	H2869	P2870	L2871	L2872	Y2875	L2878
T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	I2899	N2900	G2901	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	THR	PRO	ILE	SER	ILE	GLU	LYS	ARG	PHE	ALA	TYR	SER	PHE	GLY	LEU	GLN	GLN	ILE	ARG	TYR	VAL	ASP	GLU	ALA	HIS
GLN	TYR	ILE	GLU	PHE	ASP	GLY	ARG	SER	SER	LYS	GLY	GLU	HIS	PHE	PRO	TYR	GLU	GLN	ILE	PHE	PHE	ALA	LYS	VAL	LEU	PRO	GLY	VAL	ILE	ASP	GLN	TYR	PHE	ASN	HIS	ARG	LEU	Y2982	S2985	S2988	C2992	Y2999	E3003	H3004	V3005	THR	SER	LEU	LEU	ILE	ARG	TYR	VAL	ASP	GLU	ALA	HIS	
T3028	SER	ILE	VAL	ASN	CYS	L3034	S3053	V3054	K3055	SER	ALA	LEU	ARG	ALA	F3061	T3072	L3076	T3082	HIS	THR	ARG	ASN	GLN	PRO	LYS	VAL	GLY	THR	GLN	ILE	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	P3104	S3107	G3114	Q3115	H3116	Q3117	F3118	GLY	GLU	ASP	LEU	ILE	L3124	E3125						





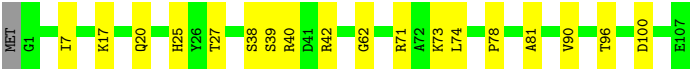







● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 82% 17%




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

Chain E:  82% 17%




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

Chain H:  83% 16%




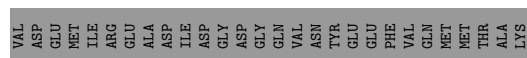
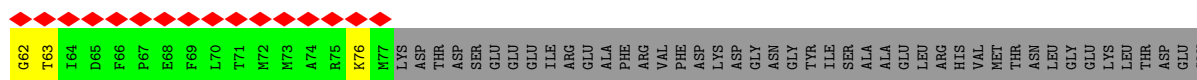
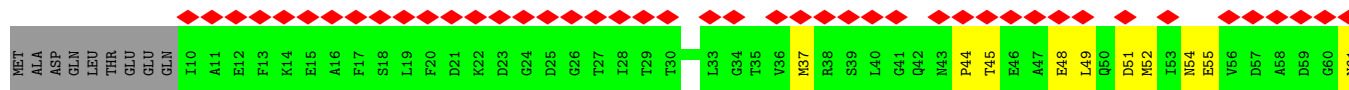
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:  83% 16%




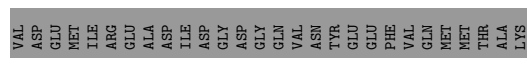
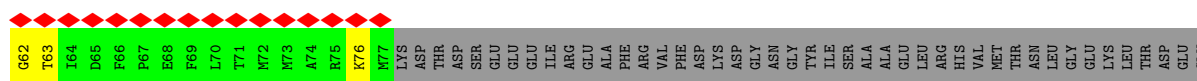
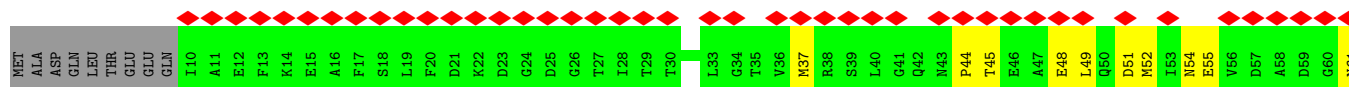
- Molecule 3: Calmodulin-1

Chain C:  40% 37% 9% 54%




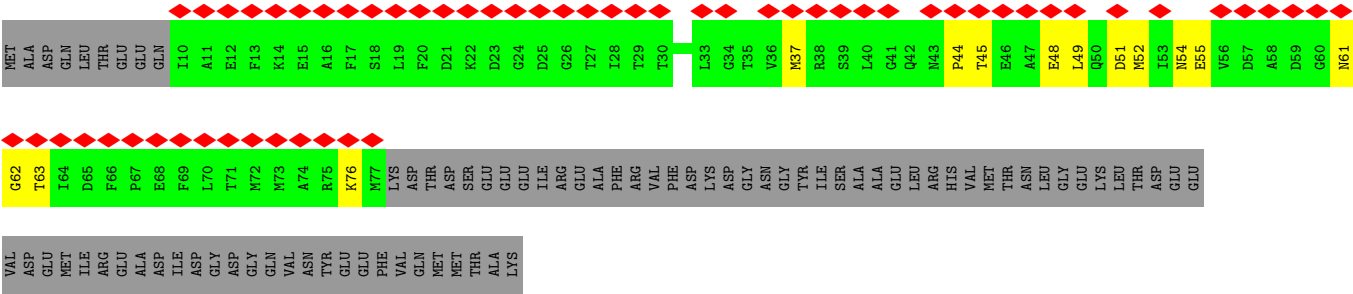
- Molecule 3: Calmodulin-1

Chain F:  40% 37% 9% 54%

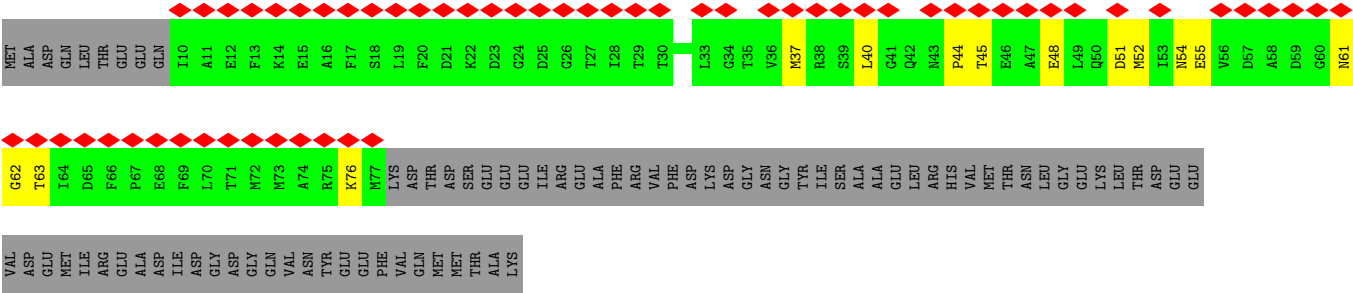
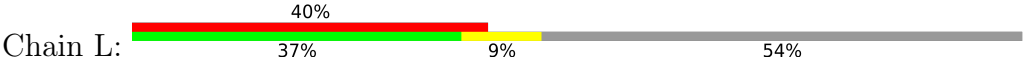


- Molecule 3: Calmodulin-1

Chain I:  40% 37% 9% 54%



● Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	154111	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	0.182	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	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, ATP, CA, CFF

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	0.47	0/27151	0.60	7/36715 (0.0%)
1	D	0.47	0/27151	0.60	7/36715 (0.0%)
1	G	0.47	0/27151	0.60	7/36715 (0.0%)
1	J	0.47	0/27151	0.60	7/36715 (0.0%)
2	B	0.39	0/835	0.56	0/1123
2	E	0.39	0/835	0.56	0/1123
2	H	0.39	0/835	0.56	0/1123
2	K	0.39	0/835	0.56	0/1123
3	C	0.29	0/530	0.54	0/711
3	F	0.29	0/530	0.54	0/711
3	I	0.29	0/530	0.54	0/711
3	L	0.29	0/530	0.54	0/711
All	All	0.46	0/114064	0.60	28/154196 (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	17
1	D	0	17
1	G	0	17
1	J	0	17
All	All	0	68

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	D	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	G	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	J	1608	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	A	2403	CYS	C-N-CA	6.51	137.97	121.70

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	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	26650	0	25168	484	0
1	D	26650	0	25168	493	0
1	G	26650	0	25168	475	0
1	J	26650	0	25168	495	0
2	B	819	0	824	13	0
2	E	819	0	824	12	0
2	H	819	0	824	12	0
2	K	819	0	824	12	0
3	C	524	0	503	8	0
3	F	524	0	503	8	0
3	I	524	0	503	8	0
3	L	524	0	503	8	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
5	A	1	0	0	0	0
5	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
6	D	31	0	12	0	0
6	G	31	0	12	1	0
6	J	31	0	12	1	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	112168	0	106068	1842	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 1842 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:G:143:LEU:HD22	1:J:2427:LEU:CB	1.57	1.34
1:A:2427:LEU:CB	1:J:143:LEU:HD22	1.56	1.33
1:A:143:LEU:HD22	1:D:2427:LEU:CB	1.58	1.33
1:D:143:LEU:HD22	1:G:2427:LEU:CB	1.55	1.33
1:A:2427:LEU:HB3	1:J:143:LEU:CD2	1.60	1.29

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	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	34	69
1	D	3366/4968 (68%)	2927 (87%)	428 (13%)	11 (0%)	41	74
1	G	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	34	69
1	J	3366/4968 (68%)	2927 (87%)	427 (13%)	12 (0%)	34	69
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	K	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
3	C	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	F	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
All	All	14148/20900 (68%)	12344 (87%)	1757 (12%)	47 (0%)	44	74

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2321	VAL
1	A	4901	THR
1	D	2321	VAL
1	D	4901	THR
1	G	2321	VAL

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	2677/4355 (62%)	2650 (99%)	27 (1%)	76	86
1	D	2678/4355 (62%)	2650 (99%)	28 (1%)	76	86
1	G	2677/4355 (62%)	2650 (99%)	27 (1%)	76	86
1	J	2678/4355 (62%)	2650 (99%)	28 (1%)	76	86

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
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	11290/18284 (62%)	11180 (99%)	110 (1%)	77	86

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	606	ARG
1	G	3992	VAL
1	J	4886	GLU
1	J	3992	VAL
1	G	727	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3990	ASN
1	J	1918	GLN
1	G	4490	GLN
1	J	476	GLN
1	J	3623	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [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	2.91	4 (50%)	8,23,23	1.35	1 (12%)
6	ATP	D	6002	-	26,33,33	0.92	0	31,52,52	1.67	5 (16%)
7	CFF	D	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.34	1 (12%)
7	CFF	J	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.35	1 (12%)
6	ATP	A	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)
6	ATP	G	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)
7	CFF	A	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.35	1 (12%)
6	ATP	J	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)

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
6	ATP	D	6002	-	-	6/18/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	6/18/38/38	0/3/3/3
6	ATP	G	6002	-	-	6/18/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	J	6002	-	-	6/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6003	CFF	C5-C4	-5.00	1.32	1.39
7	D	6003	CFF	C5-C4	-5.00	1.32	1.39
7	G	6003	CFF	C5-C4	-5.00	1.32	1.39
7	J	6003	CFF	C5-C4	-5.00	1.32	1.39
7	A	6003	CFF	C6-N1	-4.92	1.31	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	N3-C2-N1	-4.12	122.24	128.68
6	D	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	G	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	J	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	G	6002	ATP	PA-O3A-PB	-3.75	119.94	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C3'-C4'-C5'-O5'
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C3'-C4'-C5'-O5'
6	G	6002	ATP	C5'-O5'-PA-O2A

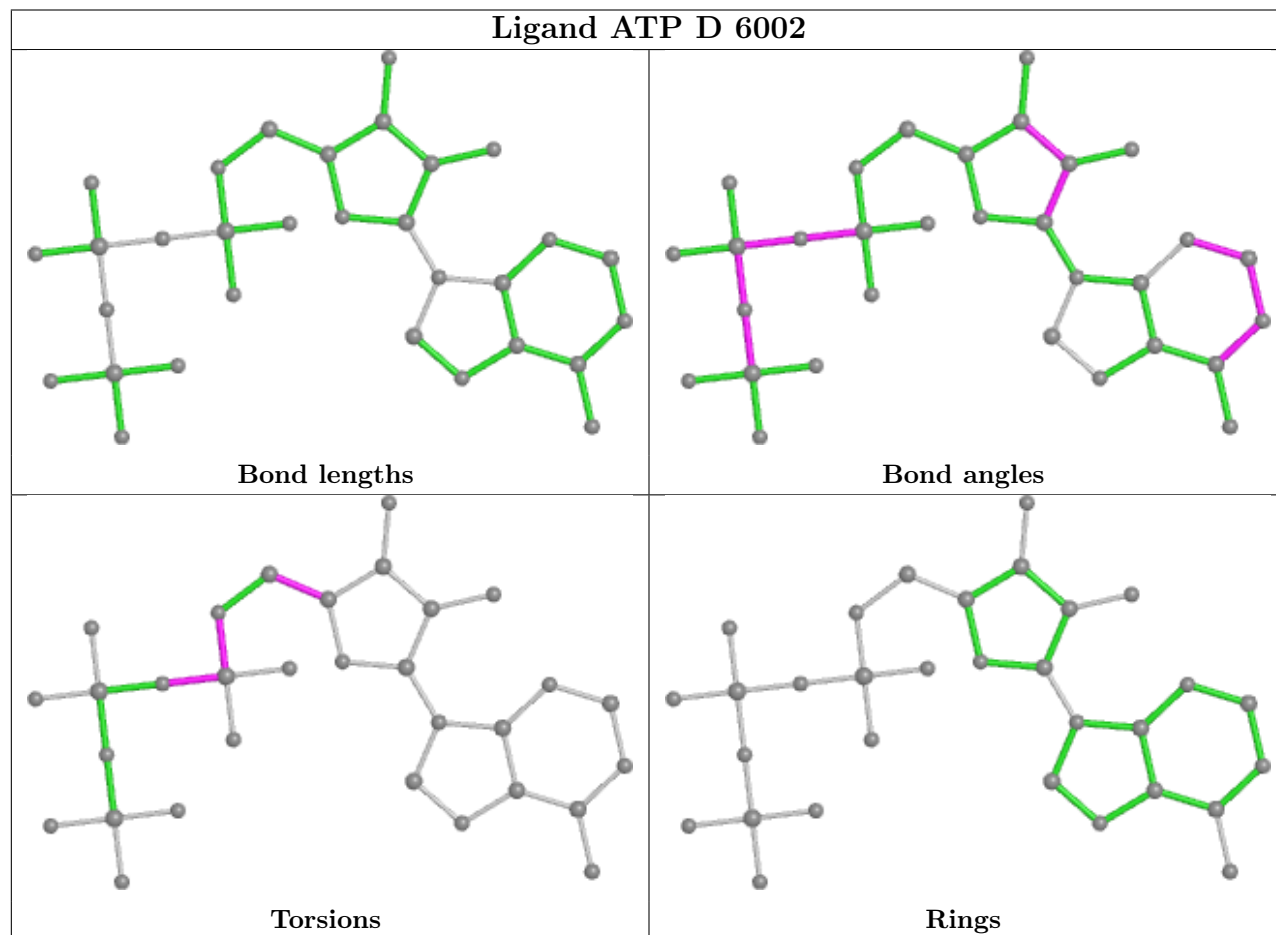
There are no ring outliers.

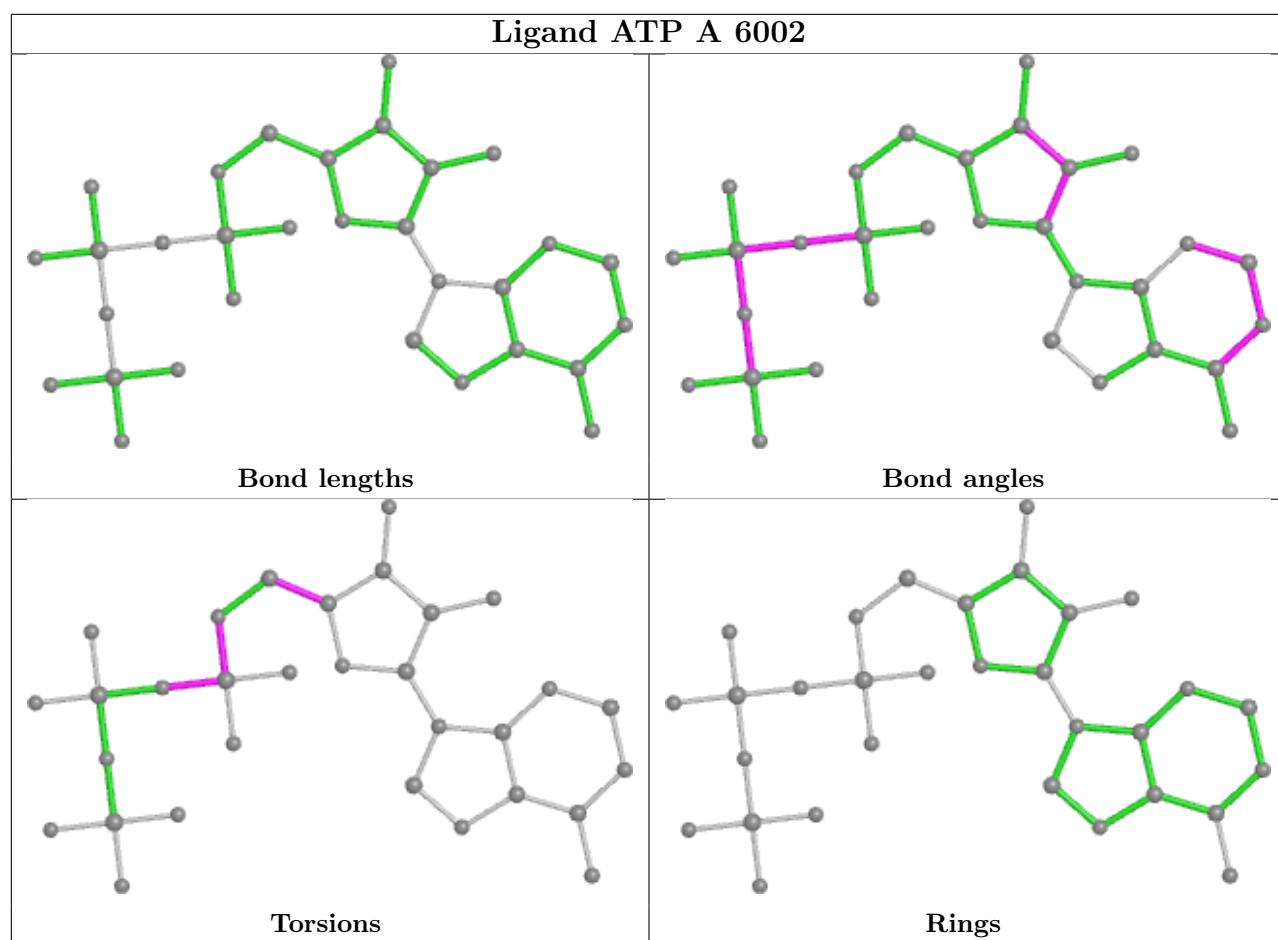
7 monomers are involved in 7 short contacts:

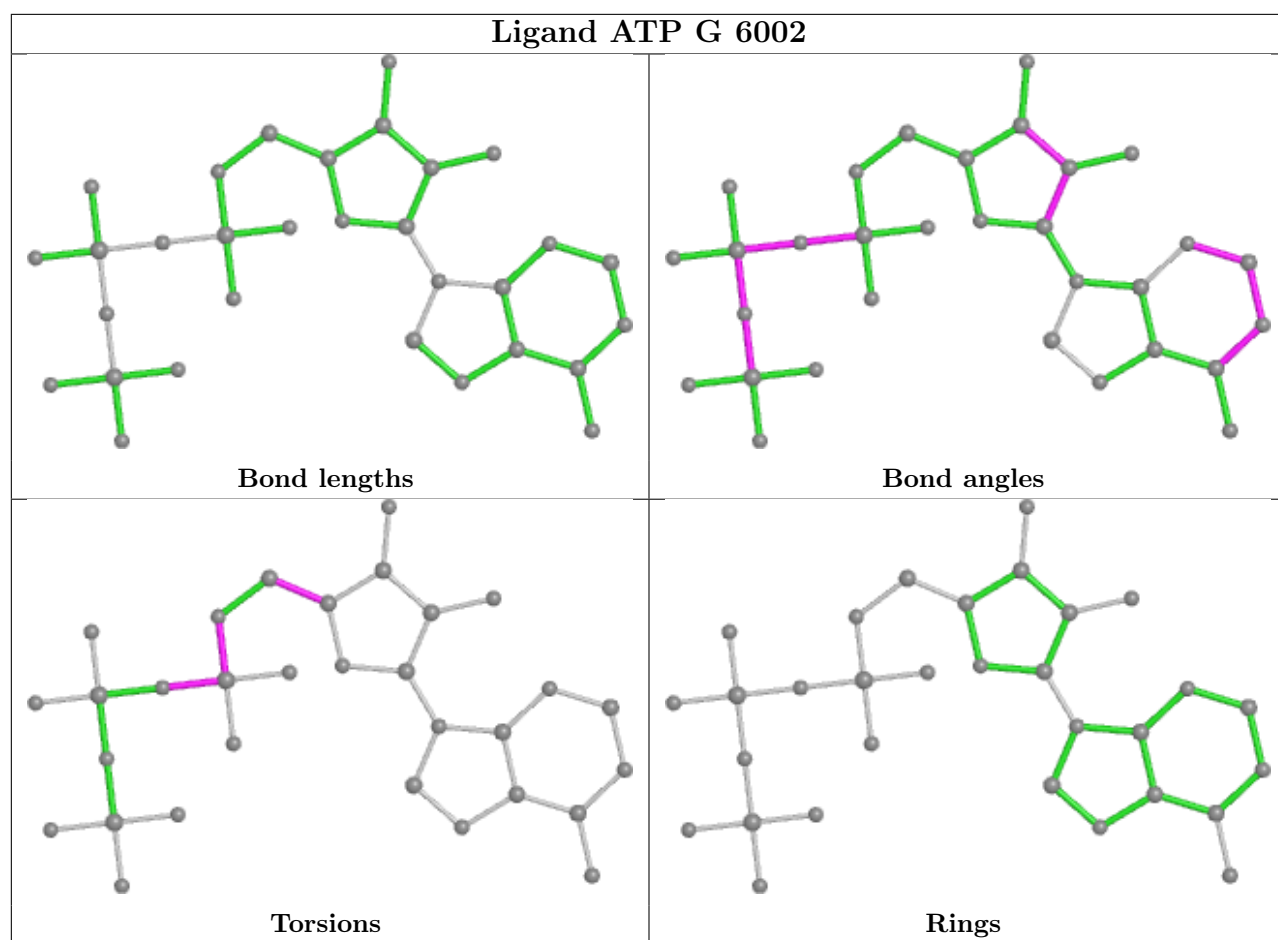
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	6003	CFF	1	0
7	D	6003	CFF	1	0
7	J	6003	CFF	1	0
6	A	6002	ATP	1	0
6	G	6002	ATP	1	0
7	A	6003	CFF	1	0
6	J	6002	ATP	1	0

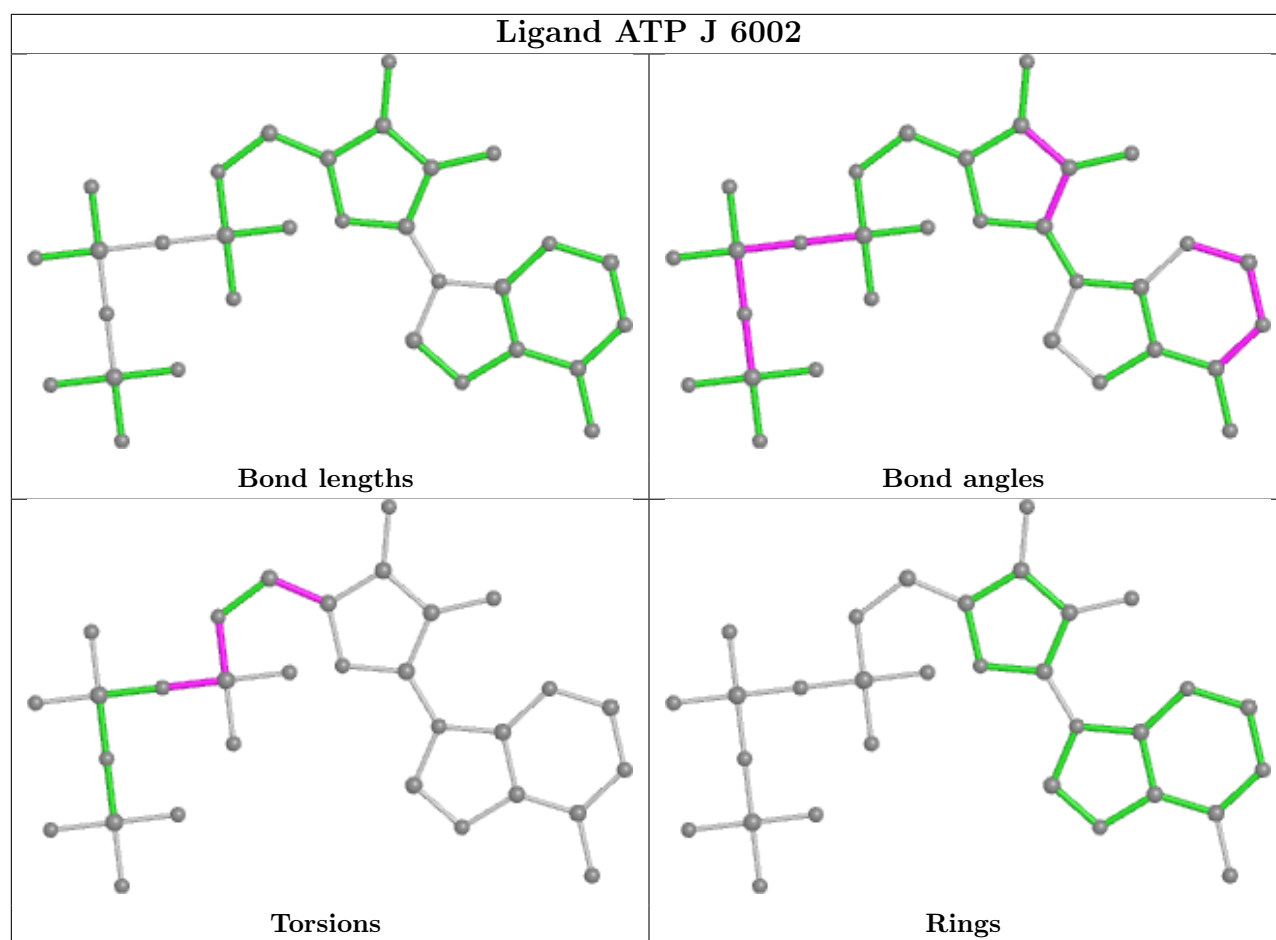
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

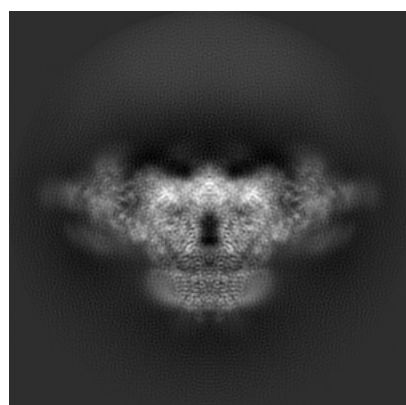
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9880. These allow visual inspection of the internal detail of the map and identification of artifacts.

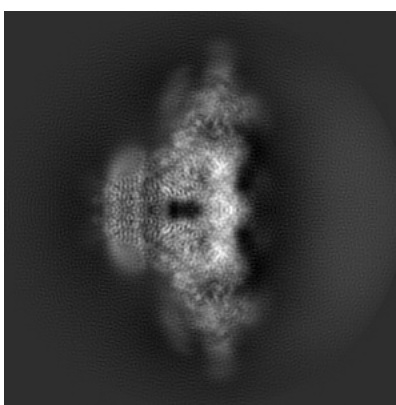
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

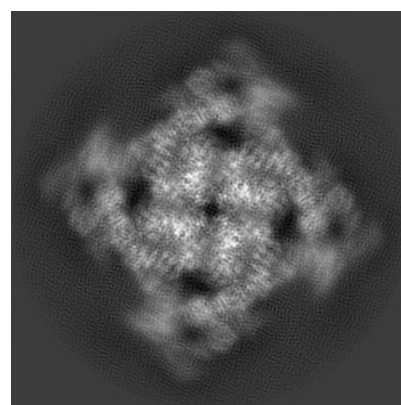
6.1.1 Primary map



X



Y

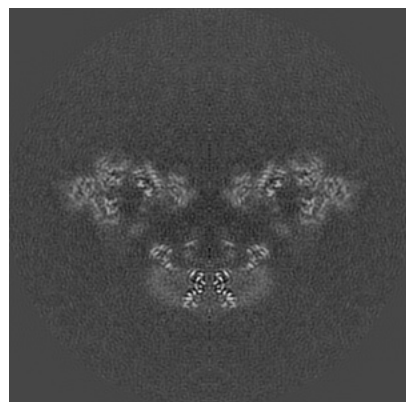


Z

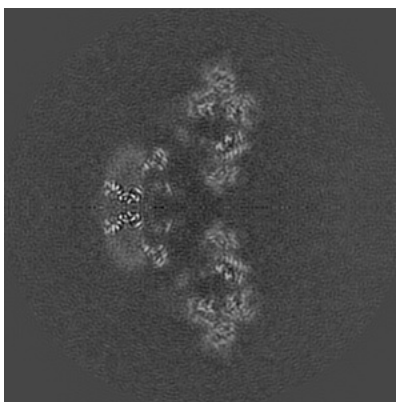
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

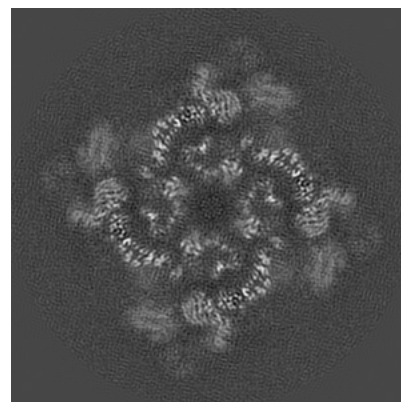
6.2.1 Primary map



X Index: 200



Y Index: 200

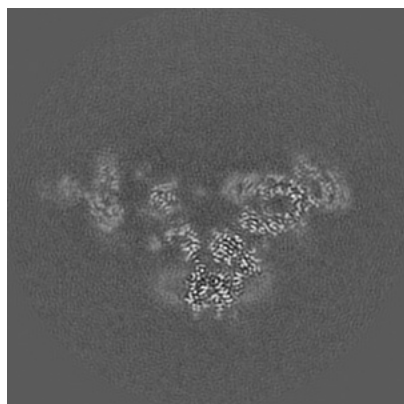


Z Index: 200

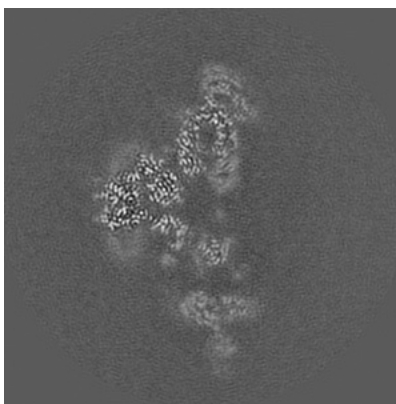
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

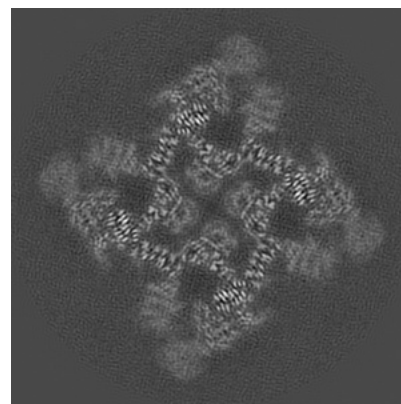
6.3.1 Primary map



X Index: 187



Y Index: 213

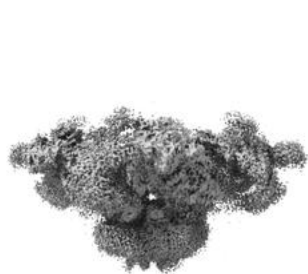


Z Index: 212

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

6.4 Orthogonal surface views [i](#)

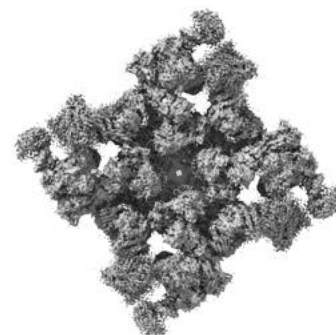
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

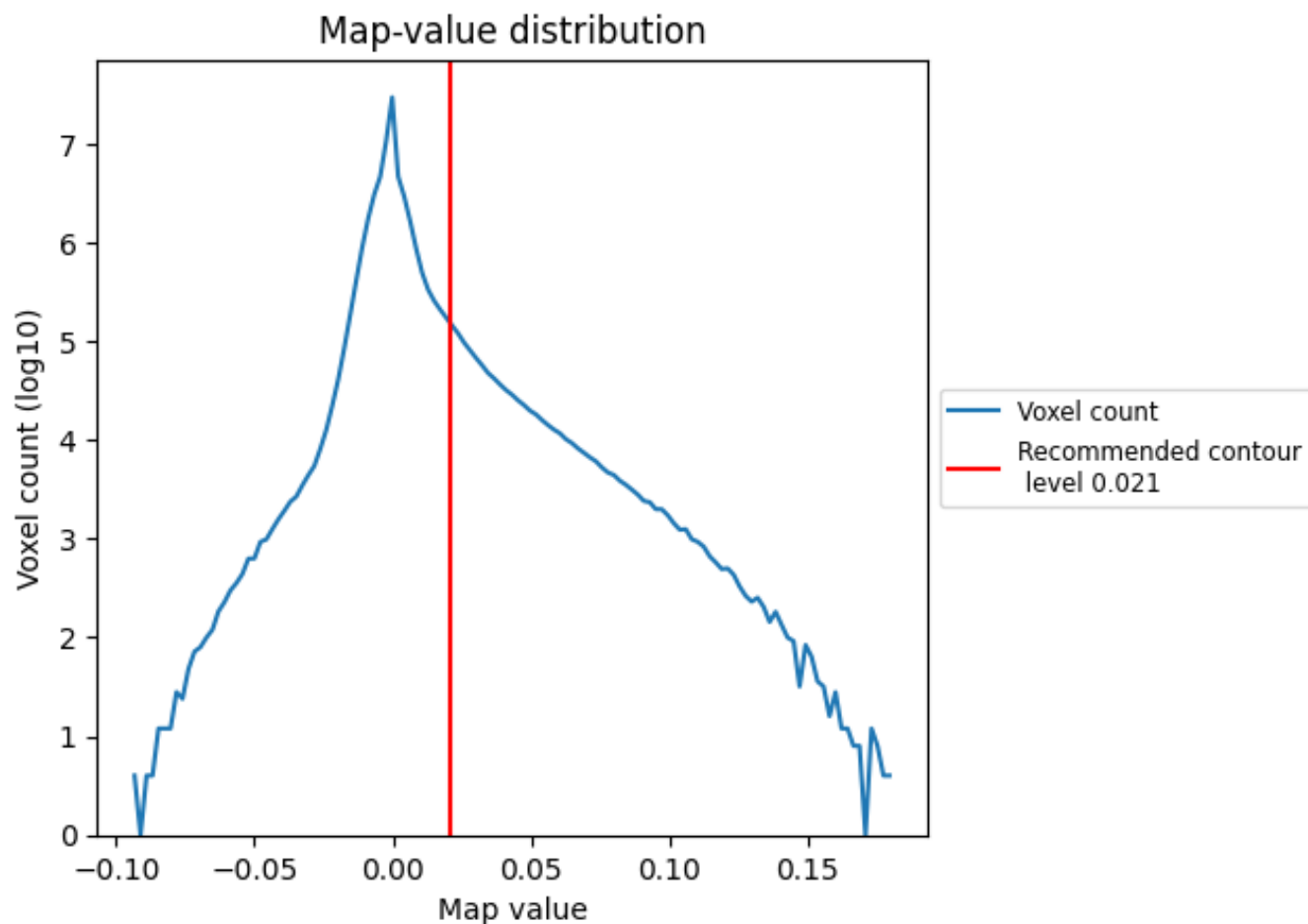
6.5 Mask visualisation

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

7 Map analysis [i](#)

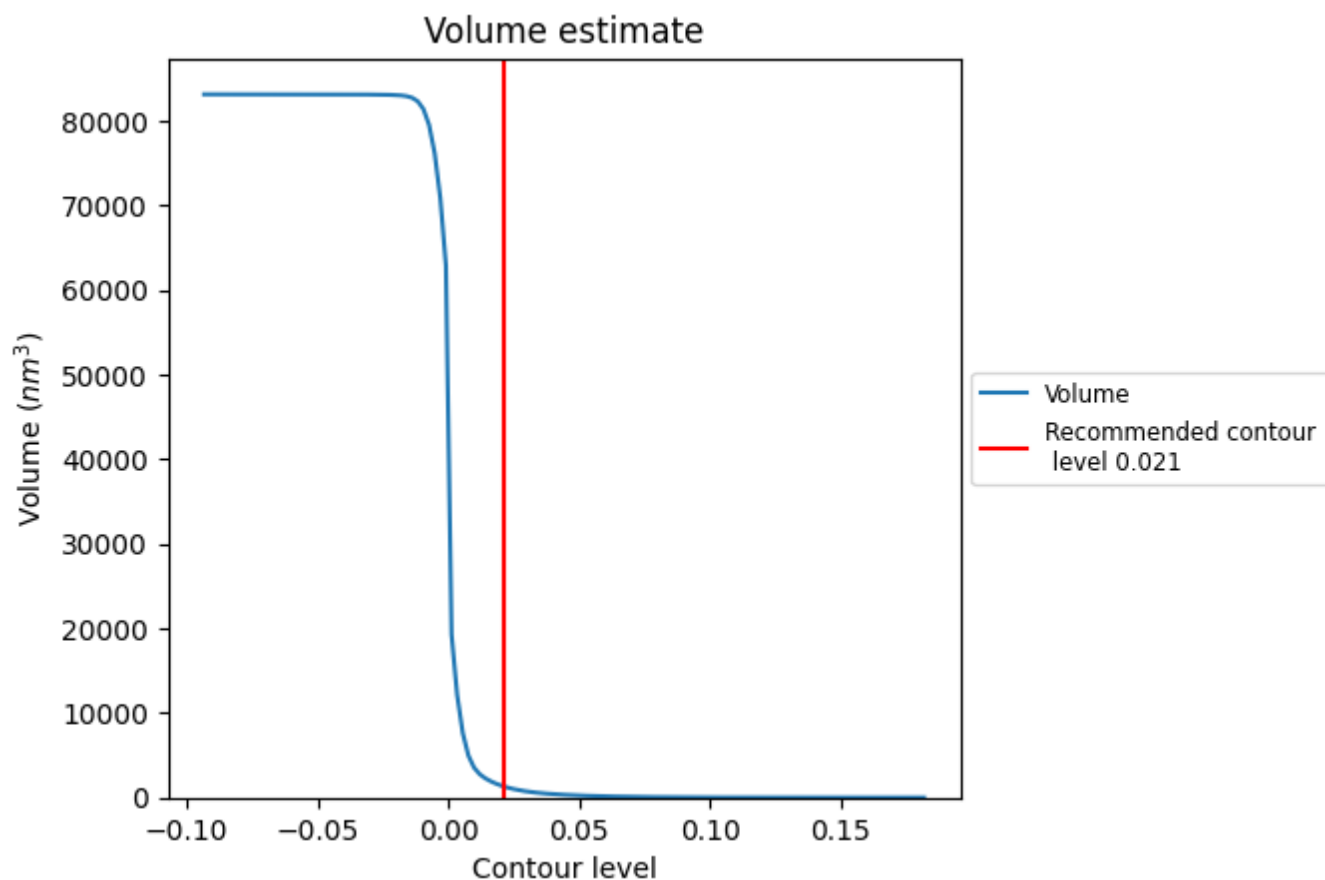
This section contains the results of statistical analysis of the map.

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.

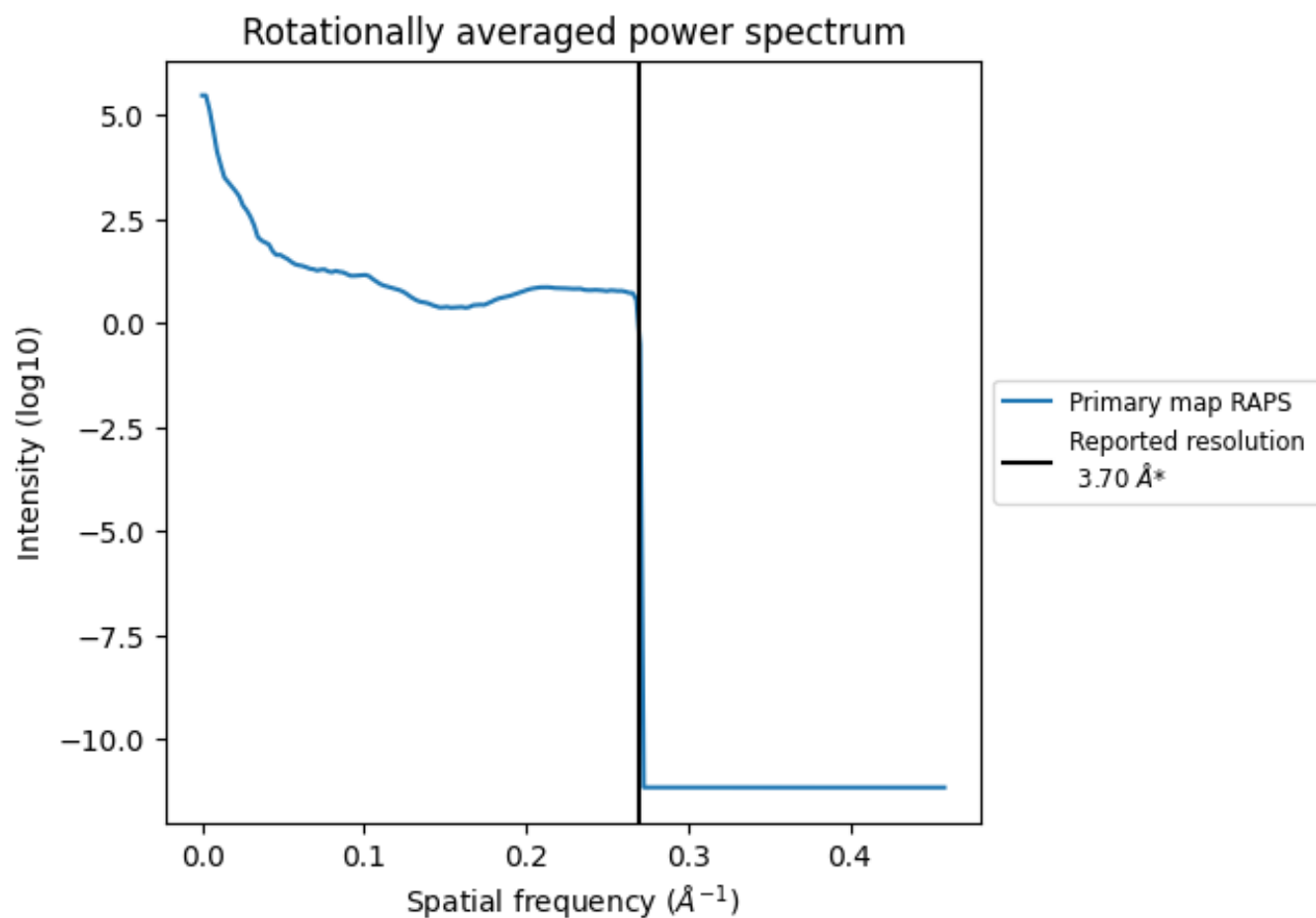
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1340 nm³; this corresponds to an approximate mass of 1210 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

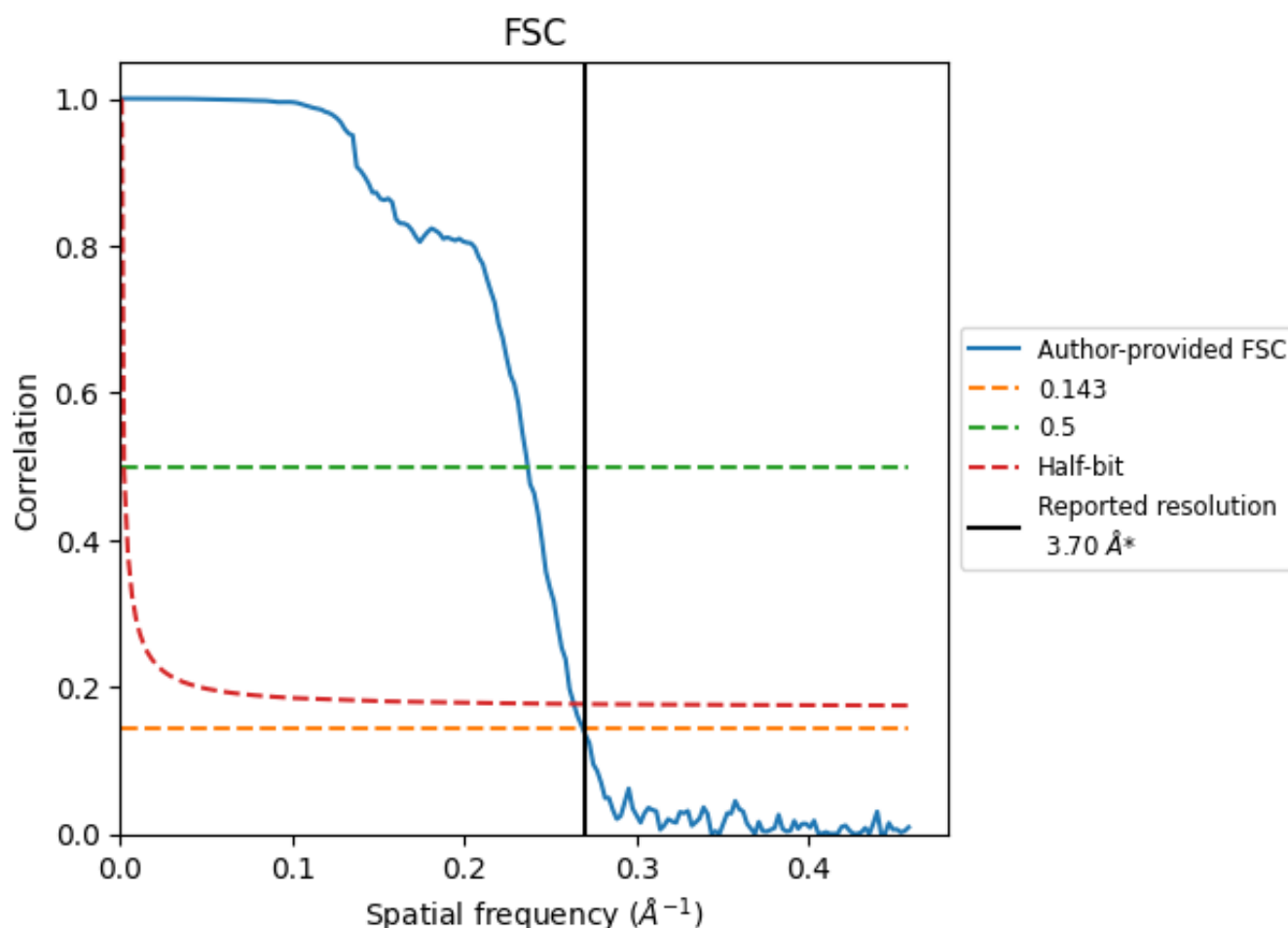


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

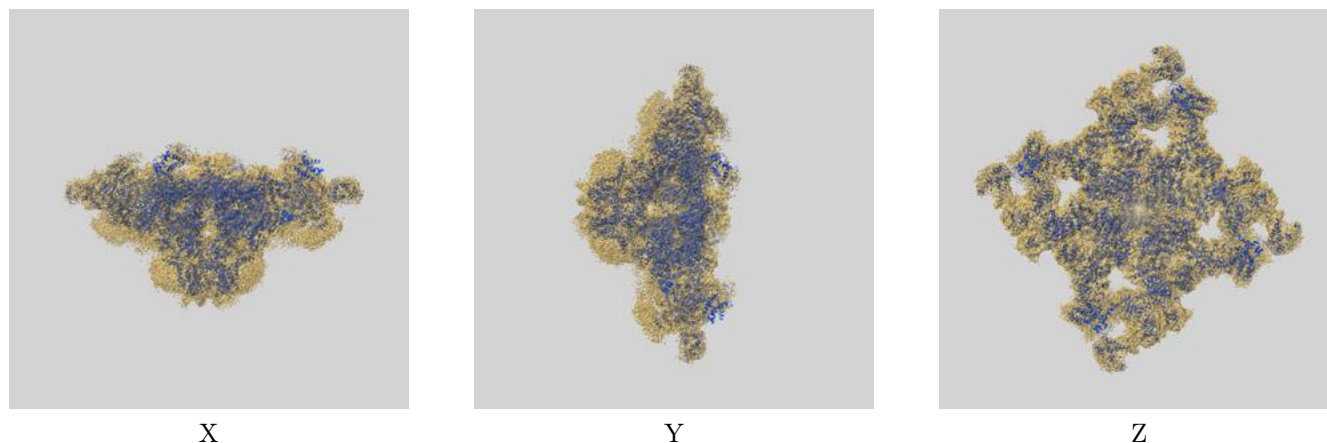
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.22	3.79
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

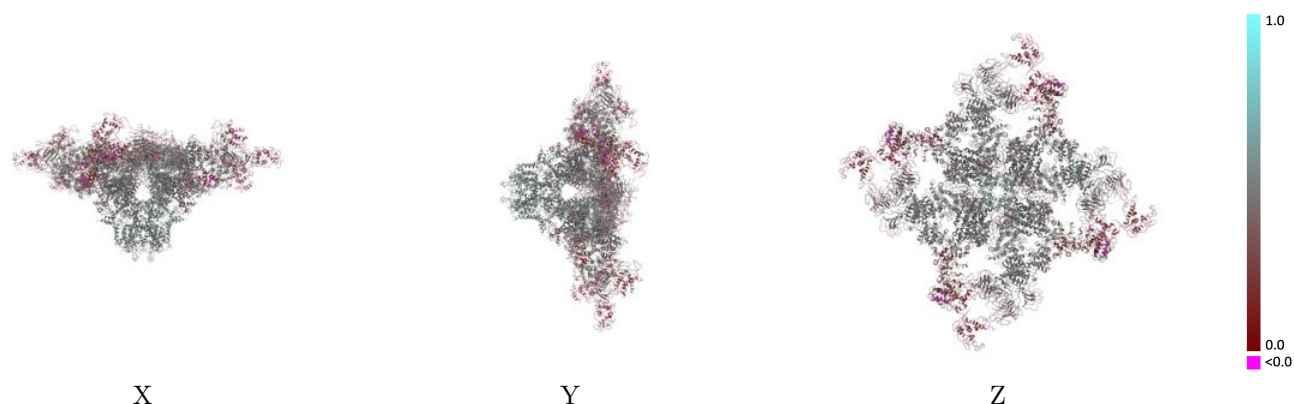
This section contains information regarding the fit between EMDB map EMD-9880 and PDB model 6JRS. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



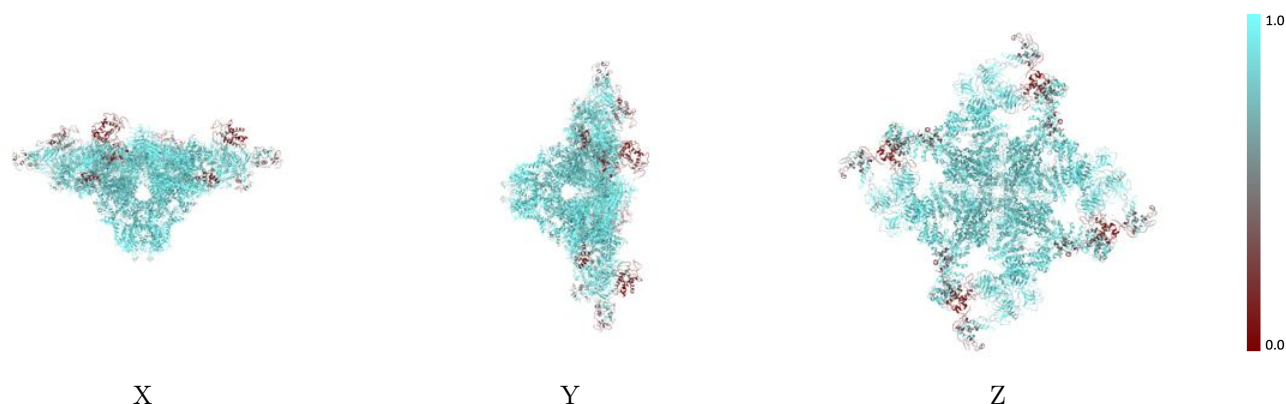
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



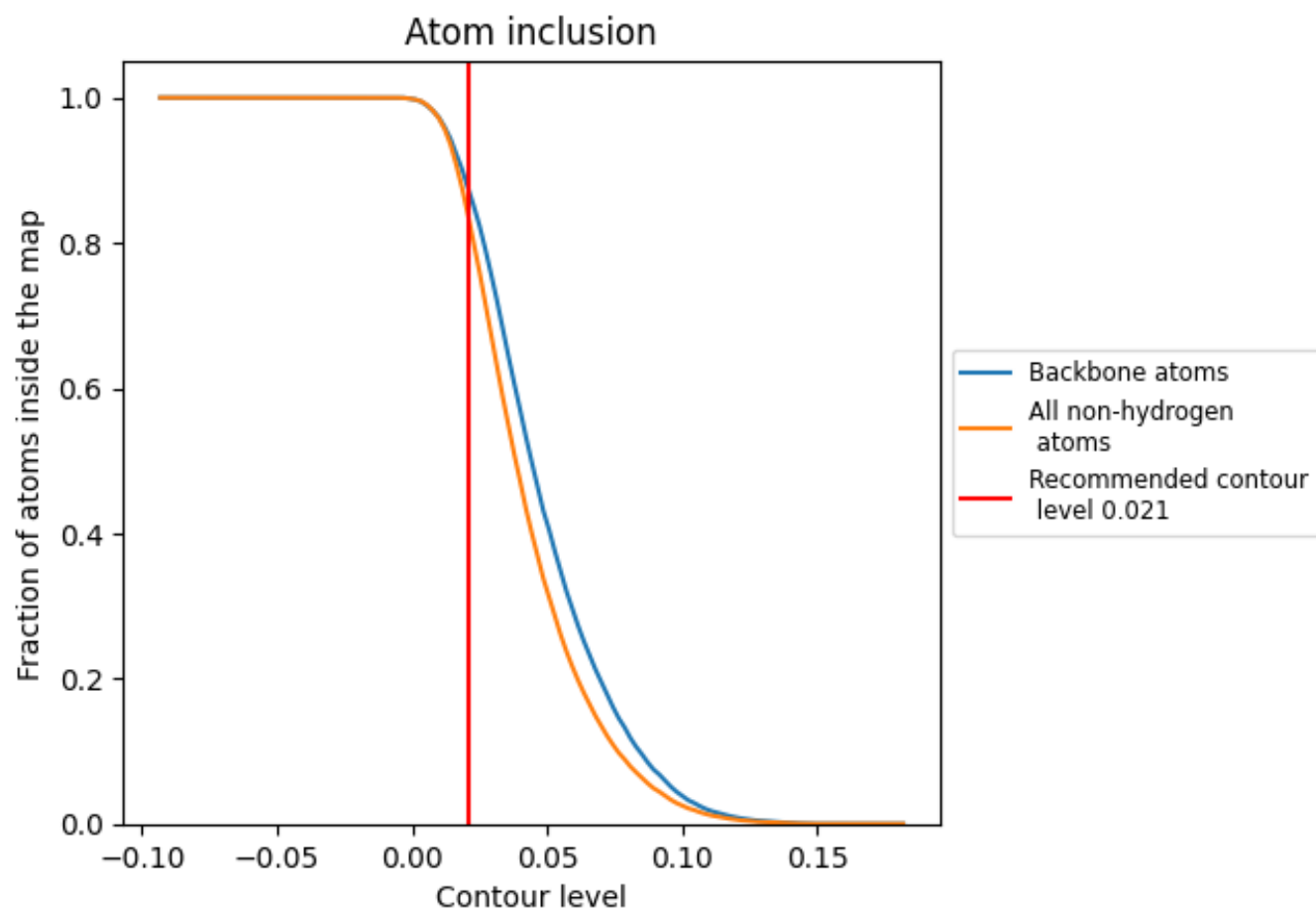
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8321	<div></div> 0.4210
A	<div></div> 0.8424	<div></div> 0.4240
B	<div></div> 0.9009	<div></div> 0.4500
C	<div></div> 0.2031	<div></div> 0.2530
D	<div></div> 0.8427	<div></div> 0.4240
E	<div></div> 0.9009	<div></div> 0.4470
F	<div></div> 0.2050	<div></div> 0.2570
G	<div></div> 0.8422	<div></div> 0.4240
H	<div></div> 0.9058	<div></div> 0.4470
I	<div></div> 0.2050	<div></div> 0.2560
J	<div></div> 0.8427	<div></div> 0.4230
K	<div></div> 0.8996	<div></div> 0.4460
L	<div></div> 0.2011	<div></div> 0.2520

