



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 02:48 AM UTC

PDB ID : 6JII / pdb_00006jii
EMDB ID : EMD-9834
Title : Structure of RyR2 (F/A/C/L-Ca²⁺/apo-CaM-M dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-21
Resolution : 4.20 Å(reported)

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

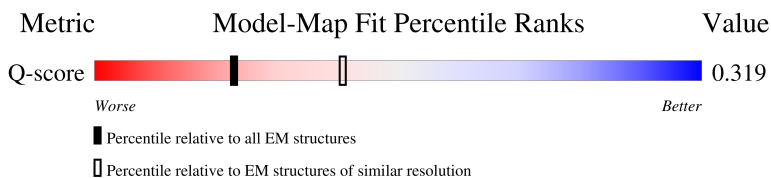
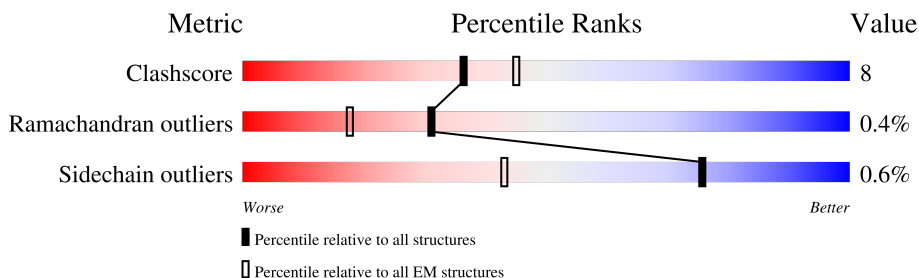
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	 79% 20% .
1	D	108	 77% 22% .
1	G	108	 76% 23% .
1	J	108	 76% 23% .

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Mol	Chain	Length	Quality of chain
2	B	4968	
2	E	4968	
2	H	4968	
2	K	4968	
3	C	149	
3	F	149	
3	I	149	
3	L	149	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CFF	B	6002	-	X	-	-
6	CFF	E	6002	-	X	-	-
6	CFF	H	6002	-	X	-	-
6	CFF	K	6002	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 115028 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	J	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Ryr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	E	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	H	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	K	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	F	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	I	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	L	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

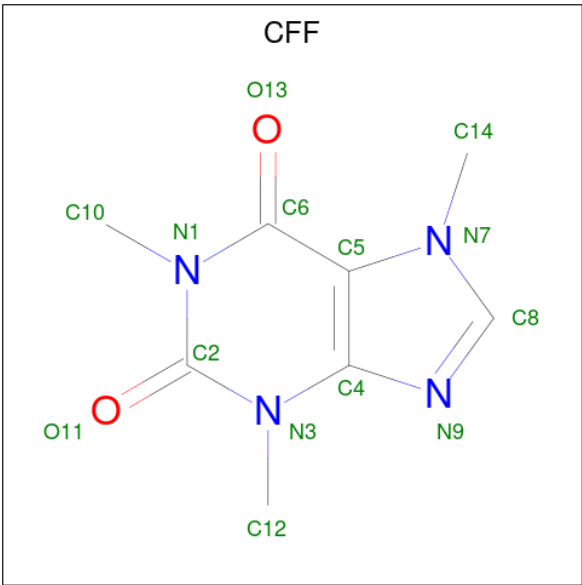
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Zn 1 1	0
4	E	1	Total Zn 1 1	0
4	H	1	Total Zn 1 1	0
4	K	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

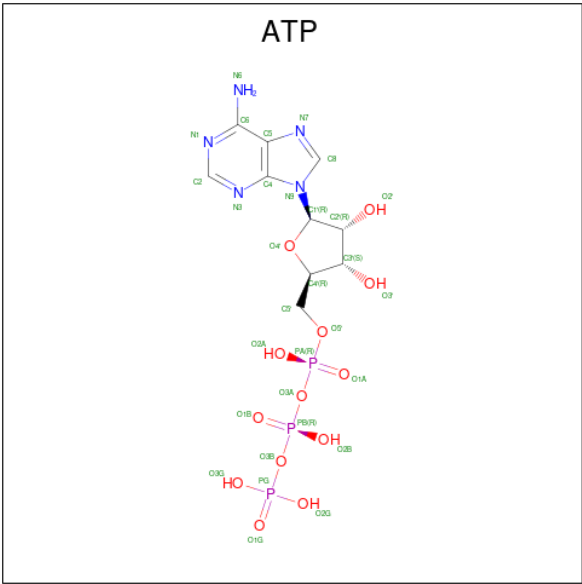
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Ca 1 1	0
5	E	1	Total Ca 1 1	0
5	H	1	Total Ca 1 1	0
5	K	1	Total Ca 1 1	0

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	14	8	4	2	0
6	E	1	14	8	4	2	0
6	H	1	14	8	4	2	0
6	K	1	14	8	4	2	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

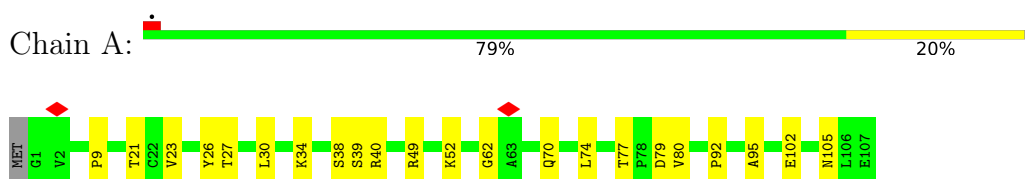


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total 31	C 10	N 5	O 13	P 3	0
7	E	1	Total 31	C 10	N 5	O 13	P 3	0
7	H	1	Total 31	C 10	N 5	O 13	P 3	0
7	K	1	Total 31	C 10	N 5	O 13	P 3	0

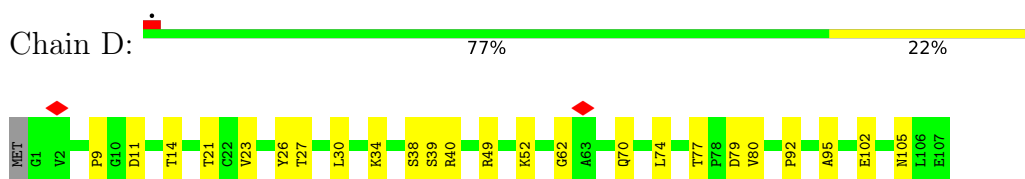
3 Residue-property plots

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.

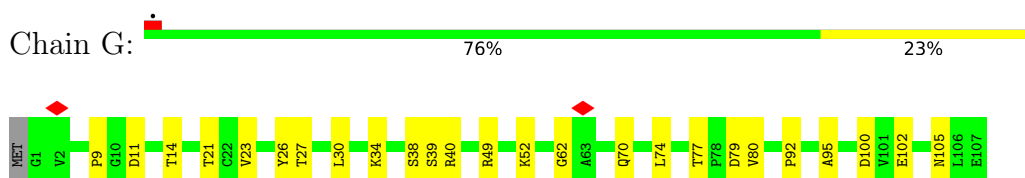
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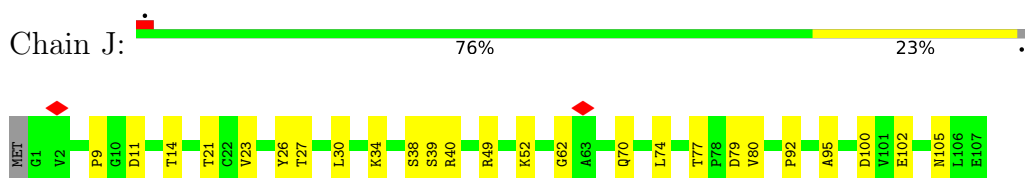
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



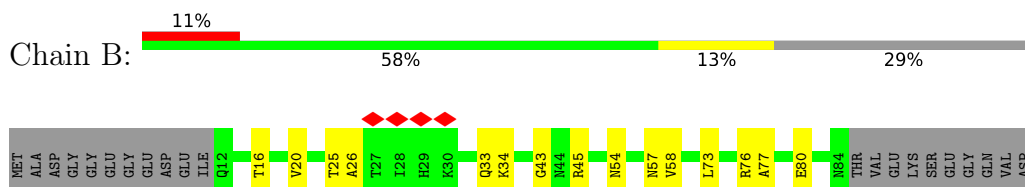
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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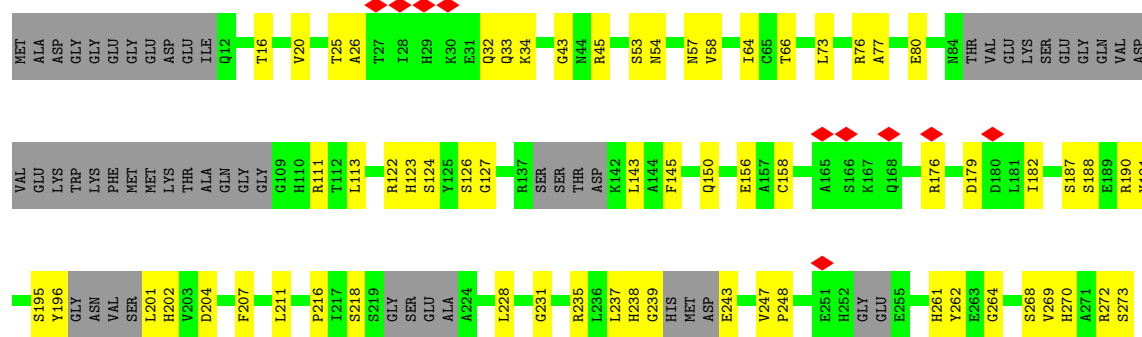
- Molecule 2: Ryr2













M2829	K2769	T2709	V2615	G2386	N2310	V2133	LYS	PRO	T1733	S1609	L1527
S2830	E2770	S2710	G2627	D2398	N2319	ARG	ASP	CYS	K1734	R1610	S1528
M2831	I2771	N2711	GLU	GLU	MET	GLY	ASP	ALA	F1739	I1611	T1529
T2832	V2772	I2712	TRP	R2402	R2323	GLY	GLY	SER	P1740	R1614	T1530
T2833	V2773	I2713	ASN	G2492	T2326	LYS	ASP	GLU	L1748	Y1531	Y1531
L2834	W2774	I2714	PHE	E2406	R2327	E2138	E1986	SER	G1752	Q1620	P1535
S2835	P2775	P2715	GLY	I2410	E2330	N2153	C1989	ARG	S1636	C1621	S1636
D2837	I2776	E2716	ALA	A2413	CYS	V2155	D2013	LEU	P1541	E1623	P1541
L2838	K2777	K2717	THR	I2418	PHE	G2181	GLY	GLY	Q1546	Q1626	Q1546
H2839	S2779	E2719	ALA	R2419	GLY	GLY	ASP	PRO	F1627	F1627	F1627
A2840	L2780	Y2720	ALA	I2420	PRO	GLY	SER	ALA	M1628	M1628	M1628
M2841	K2781	F2721	LEU	S2425	LEU	SER	LEU	GLU	S1629	S1629	S1629
A2842	T2782	I2722	SER	R2426	ARG	GLY	ASP	GLY	H1631	H1631	H1631
E2843	K2783	N2723	ALA	L2427	GLY	SER	ASN	LYS	I1632	I1632	I1632
M2844	L2784	K2724	LYS	L2432	GLY	GLU	SER	GLY	P1633	P1633	P1633
M2845	A2785	Y2725	Y2658	G2431	GLY	ILE	ASP	GLY	E1634	E1634	E1634
M2846	W2786	A2726	L2665	L2433	GLY	THR	L2024	LYS	I1771	I1771	I1771
E2847	G2787	E2727	L2666	V2436	ASN	P2191	R2029	ARG	M1772	M1772	M1772
N2848	W2788	H2728	L2526	V2436	G2343	Q2212	S2032	PRO	E1781	E1781	E1781
Y2849	K2789	S2729	L2529	I2439	E2349	K2213	Y2039	GLY	K1790	K1790	K1790
H2850	L2790	H2730	ARG	F2440	R2352	L2241	LEU	L1894	L1651	L1651	L1651
M2851	E2791	N2731	ALA	A2441	K2353	S2247	LYS	LYS	H1656	H1656	H1656
T2852	K2792	D2731	LEU	F2441	T2354	V2248	LYS	PRO	L1667	L1667	L1667
W2853	K2793	K2732	PHE	MET	ALA	Q2242	GLN	ALA	G1668	G1668	G1668
W2854	T2794	W2733	A2537	PRO	GLU	N2252	ALA	LEU	K1572	K1572	K1572
K2855	E2795	W2734	ASP	PRO	ASP	N2253	ALA	LEU	V1579	V1579	V1579
K2856	G2796	M2735	V2553	THR	PRO	E2254	LEU	ALA	P1580	P1580	P1580
K2857	G2797	D2736	TYR	ILE	ARG	L2275	GLY	VAL	Q1581	Q1581	Q1581
L2859	MET	K2737	ARG	GLY	ASP	GLN	GLY	GLU	R1585	R1585	R1585
E2860	ALA	L2738	LEU	VAL	GLY	GLN	PRO	THR	L1586	L1586	L1586
L2861	TYR	A2739	ARG	VAL	PRO	SER	ASP	ALA	H1587	H1587	H1587
E2862	ASN	N2740	THR	VAL	THR	GLY	LYS	LYS	V1588	V1588	V1588
S2863	THR	G2741	SER	GLU	GLY	LEU	LYS	THR	Q1589	Q1589	Q1589
K2864	ARG	W2742	MET	ASP	THR	VAL	LYS	LYS	F1590	F1590	F1590
G2865	ARG	I2743	GLU	MET	GLY	SER	SER	THR	L1591	L1591	L1591
G2866	ILE	Y2744	LYS	THR	LYS	VAL	GLY	GLY	S1592	S1592	S1592
G2867	SER	G2745	ILE	GLY	LYS	GLY	ARG	ALA	H1593	H1593	H1593
G2868	SER	E2746	CYS	ALA	PRO	TYR	Q2072	GLY	V1594	V1594	V1594
N2869	SER	I2747	GLN	F2461	THR	PRO	V2075	PRO	D1704	D1704	D1704
P2870	GLN	Y2748	LEU	C2462	GLY	ASP	I2076	GLN	L1705	L1705	L1705
L2871	VAL	M2750	R2582	D2464	GLY	ILE	I2076	GLY	H1710	H1710	H1710
L2872	SER	S2751	GLU	H2465	GLU	TRP	L2081	GLN	L1711	L1711	L1711
L2873	VAL	F2751	GLY	K2466	ASP	P2293	L2088	ILE	Y1714	Y1714	Y1714
P2874	ASP	N2701	HIS	Y2477	ASP	R2298	V2114	ASN	F1601	F1601	F1601
P2875	ASP	F2702	ALA	ILE	THR	F2308	E2115	MET	Q1602	Q1602	Q1602
Y2875	A2819	N2703	K2605	GLY	THR	C2309	T2117	LEU	F1603	F1603	F1603
D2876	H2820	P2704	ILE	V2481	ILE			LEU	K1605	K1605	K1605
T2877	H2821	Q2705	V2612		HIS			ASN	V1606	V1606	V1606
L2878	G2821	Q2706			MET			PHE	D1607	D1607	D1607
T2879	Y2822	P2706							Y1608	Y1608	Y1608
S2880	S2823	L2757									
A2881	P2824	M2758									
K2881	P2825	K2759									
E2882	A2826	P2760									
K2883	I2827	Y2761									
A2884	D2828	K2762									
K2885		L2763									
D2886		L2764									
K2887		S2765									
E2888		K2767									

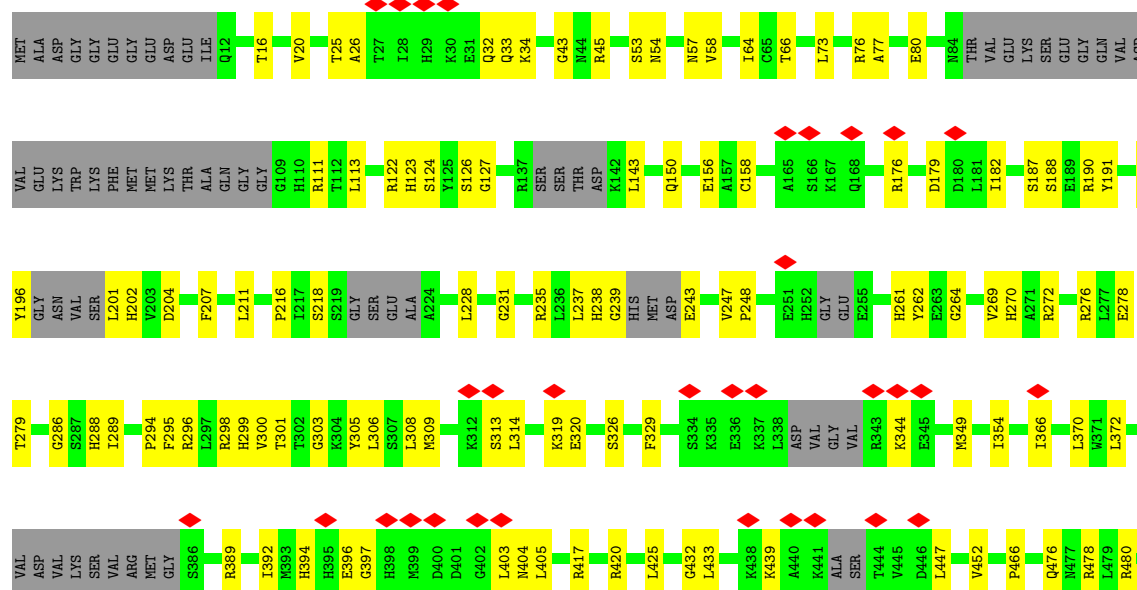






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GLY	LYS	ARG	PRO	LYS	GLU	G1893	L1894	Q1912	D1931	L1953	MET	GLN	SER	ALA	ALA	LYS	THR	ALA	THR	ALA	GLU	ASP	LYS	THR	LYS	PHE	GLU	ALA	ALA	GLY	PRO	GLU	GLN	LYS	ASN	PHE	LYS	PRO	CYS	ALA	SER	GLU	ASP	SER	ARG	LEU	GLU	PRO	ALA	GLU	GLY								
ASN	SER	L2024	L2029	S2032	Y2039	LEU	LYS	LYS	LYS	LYS	GLN	ALA	GLU	GLU	LYS	LEU	VAL	GLU	ASP	SER	SER	LYS	LYS	PHE	SER	SER	GLY	VAL	GLU	ASP	Q2072	V2075	I2076	L2081	L2088	V2114	E2115	D2116	T2117	V2133	ARG	MET	GLY	LYS	E2138	N2153	K2154	V2155	G2181	GLY	GLY	GLU	SER						
LYS	GLU	ILE	THR	PHE	P2191	L2201	Q2212	D2213	L2241	S2247	V2248	N2262	E2263	L2264	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	GLU	ASP	GLN	LYS	GLY	TYR	PRO	ASP	L2076	L2081	L2088	V2114	E2115	D2116	T2117	V2133	ARG	MET	GLY	LYS	E2138	N2153	K2154	V2155	G2181	GLY	GLY	GLU	SER								
LEU	ARG	GLY	GLY	ASN	G2343	E2349	L2352	K2353	I2354	ALA	GLU	ASP	PRO	SER	ARG	GLY	SER	PRO	THR	SER	GLY	SER	SER	GLY	VAL	LYS	GLY	TYR	PRO	ASP	L2076	L2081	L2088	V2114	E2115	D2116	T2117	V2133	ARG	MET	GLY	LYS	E2138	N2153	K2154	V2155	G2181	GLY	GLY	GLU	SER								
I2418	R2419	I2420	R2425	S2426	L2427	G2431	D2432	L2433	V2436	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	F2461	C2462	D2464	H2465	K2466	Y2477	GLY	ILE	V2481	L2488	L2489	VAL	G2492	L2503	ASP	THR	ALA	A2413	E2416	A2417												
LEU	SER	ALA	T2511	A2516	L2521	L2526	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	V2563	TYR	ARG	LEU	SER	K2568	A2565	S2569	S2576	ILE	CYS	GLY	GLN	R2582	N2601	HIS	ALA	K2605	T2612	Y2615	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635															
L2653	SER	GLN	LYS	Y2658	K2664	L2665	A2666	C2669	V2673	A2674	G2675	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	MET	MET	GLU	LYS	GLN	SER	ASP	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719	Y2720											
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K2781	T2782	M2783	L2784	A2785	V2786	G2787	W2788	R2789	I2790	E2791	R2792	L2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	THR	ARG	ARG	ILE	SER	GLN	THR	GLN	VAL	SER	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	D2828	M2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840			
M2841	A2842	E2843	M2844	A2845	A2846	E2847	Y2848	Y2849	H2850	M2851	L2852	A2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	L2899	N2900
G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	ASP	THR	PRO	SER	ILE	GLU	ARG	PHE	ALA	ALA	TYR	SER	PHE	ARG	GLN	VAL	ASP	GLU	ALA	HIS	GLN	TYR	ILE	LEU	GLU	PHE	ASP	GLY	SER	ARG	SER	LYS	GLY	GLU	HIS	PHE	PRO	TYR	GLU	GLN	GLU						

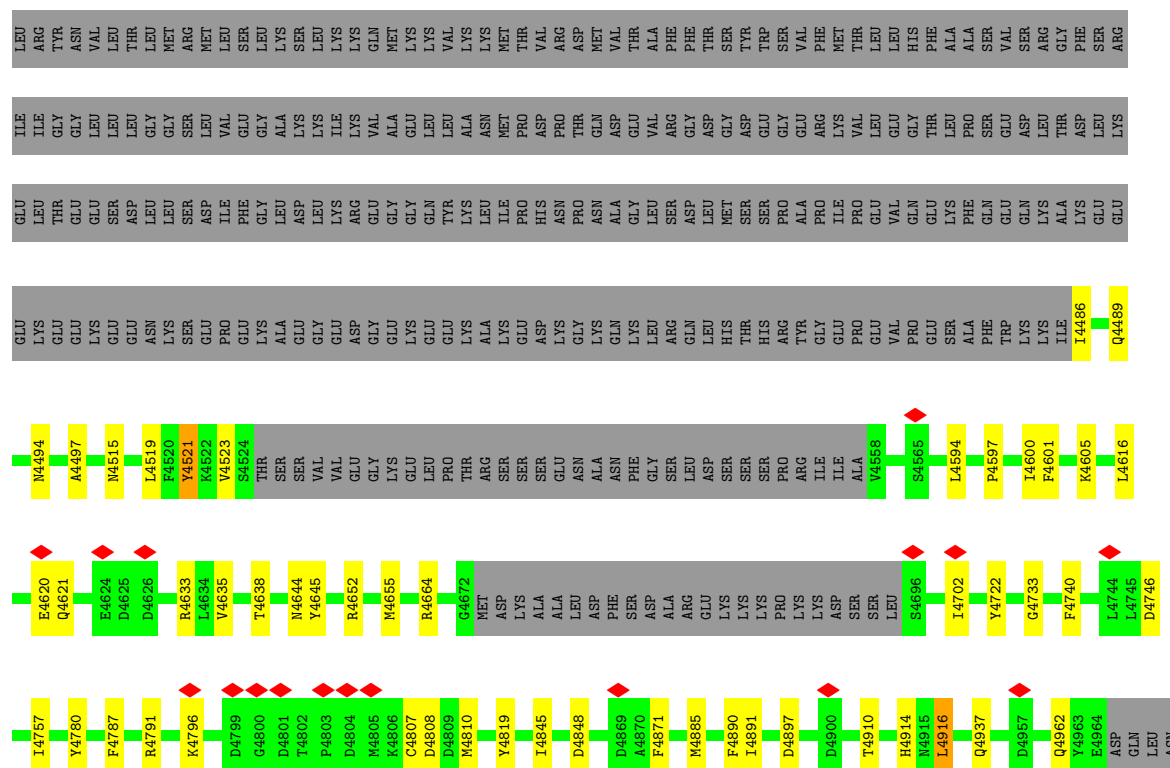




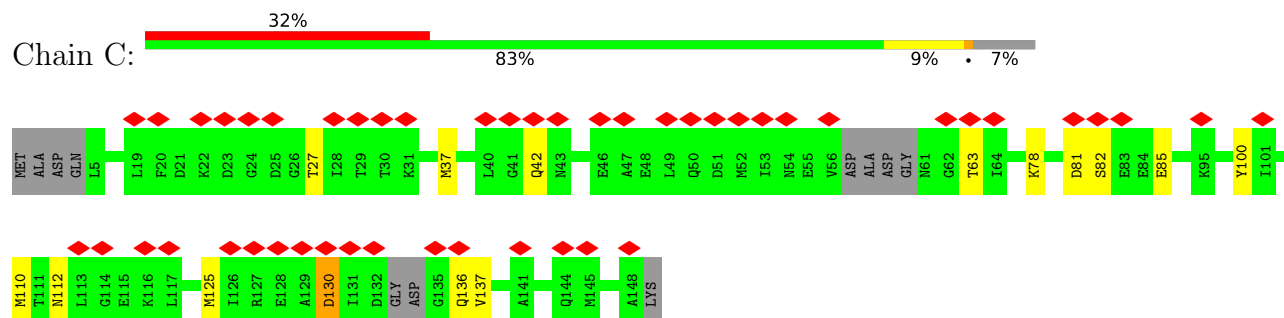


Q1620	C1621	L1622	E1623	Q1626	F1627	M1628	S1629	L1630	H1631	I1632	P1633	E1634	D1640	I1641	L1642	E1643	L1644	L1651	L1667	G1668	N1669	L1676	V1680	E1847	P1848	S1849	VAL	PHE	L1686	Y1687	H1688	I1689	Y1703	H1710	L1711	Y1714	I1726	T1730	E1731	E1732	T1733	K1734	S1735	L1748	G1752	L1753	S1754	T1755										
S1756	L1757	R1758	M1761	Q1762	F1763	I1771	S1772	N1773	H1781	E1781	D1785	K1788	R1807	D1808	P1809	N1836	L1839	L1843	I1846	E1847	P1848	S1849	VAL	PHE	L1686	Y1687	H1688	I1689	Y1703	H1710	L1711	Y1714	I1726	T1730	E1731	E1732	T1733	K1734	S1735	L1748	G1752	L1753	S1754	T1755														
GLY	PRO	ALA	GLU	GLU	SER	LYS	GLY	LYS	ARG	PRO	LYS	GLU	L1893	L1894	Q1912	D1931	N1953	MET	SER	LYS	ALA	VAL	GLU	THR	ALA	ARG	LYS	THR	LYS	PHE	GLU	ALA	ALA	ASN	TLE	ASN	MET	LEU	GLU	LYS	PHE	LYS	ASP	ARG	LEU	GLU												
GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	ASN	L2024	R2029	S2032	Y2039	LEU	LYS	LYS	GLN	ALA	GLU	LYS	LYS	VAL	GLU	THR	ALA	ARG	LYS	THR	LYS	LYS	SER	PHE	GLU	ALA	ALA	ASN	TLE	ASN	MET	LEU	GLU	LYS	PHE	LYS	ASP	ARG	LEU	GLU											
V2155	M2168	G2181	GLY	GLY	GLU	SER	LYS	ILE	THR	PHE	F2191	Q2212	K2213	L2241	S2247	W2248	N2252	E2253	L2254	L2275	GLN	SER	CYS	GLN	MET	VAL	VAL	LYS	GLY	TYR	PRO	ASP	ILE	TRP	P2293	R2298	F2308	G2309	N2310	N2319	R2323	I2326	R2327															
E2330	CYS	PHE	PRO	ALA	LEU	ARG	GLY	GLU	GLY	ASN	G2343	E2349	L2352	K2353	ALA	GLU	ASP	PRO	SER	ARG	ASP	GLY	PRO	GLY	GLY	SER	SER	LYS	MET	PRO	ASP	THR	GLY	GLU	ASP	THR	ILE	ILE	MET	G2386	D2398	R2402	E2406															
I2410	A2413	E2416	A2417	I2418	R2419	I2420	R2425	S2426	L2427	G2431	D2432	L2433	V2436	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	PRO	ASP	SER	GLY	F2461	C2462	P2463	D2464	H2465	K2466	Y2477	GLY	ILE	V2481	L2488	L2489	VAL	G2492												
L2503	ASP	THR	ALA	ALA	LEU	SER	ALA	T2511	A2516	L2521	L2526	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	V2553	TYR	ARG	GLU	SER	GLY	ASN	VAL	VAL	MET	GLY	S2576	ILE	CYS	GLY	GLN	R2582	N2601	GLU	HIS	K2605	T2612	Y2615	G2627	TRP	GLY	ASN											
PHE	GLY	ALA	A2634	S2635	L2653	SER	GLN	LYS	Y2658	K2664	L2665	A2666	C2669	V2673	A2674	G2675	P2678	P2679	ASP	TYR	MET	GLU	SER	GLY	ASN	VAL	VAL	MET	GLY	LYS	GLN	SER	MET	ASP	SER	GLU	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	I2711	I2712	I2713	I2714								
P2715	E2716	K2717	L2718	E2719	Y2720	F2721	L2722	M2723	K2724	Y2725	A2726	H2727	S2729	H2730	D2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	G2745	E2746	I2747	Y2748	MET	ASP	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	N2758	K2759	P2760	Y2761	K2762	L2763	S2765	E2766	K2767	E2768	K2769	E2770	I2771	L2772	R2773	W2774	
P2775	I2776	K2777	E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	W2786	G2787	R2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ILE	SER	GLN	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	D2828	M2829	S2830	N2831	V2832	T2833	L2834		
S2835	R2836	D2837	L2838	H2839	A2840	M2841	A2842	E2843	M2844	M2845	A2846	E2847	Y2849	H2850	T2851	A2852	K2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	K2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	T2893	L2894
K2895	F2896	L2897	Q2898	L2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	LEU	ASP	THR	PRO	SER	ILE	GLU	LYS	ARG	PHE	ALA	TYR	SER	PHE	LEU	GLN	GLN	VAL	ASP	GLU	HIS	TYR	ILE	LEU	GLY	PHE	ASP	GLY	GLY	SER	ARG	SER	LYS	GLY	GLY	HIS						

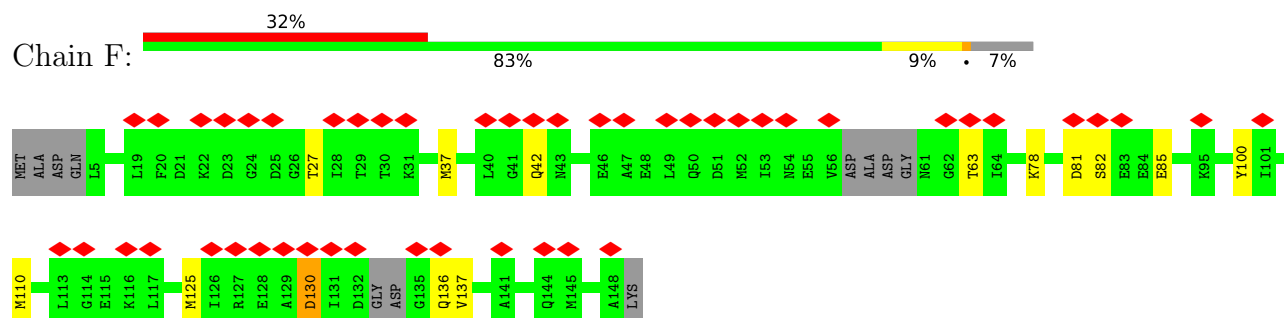




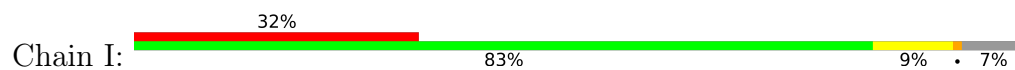
- Molecule 3: Calmodulin-1

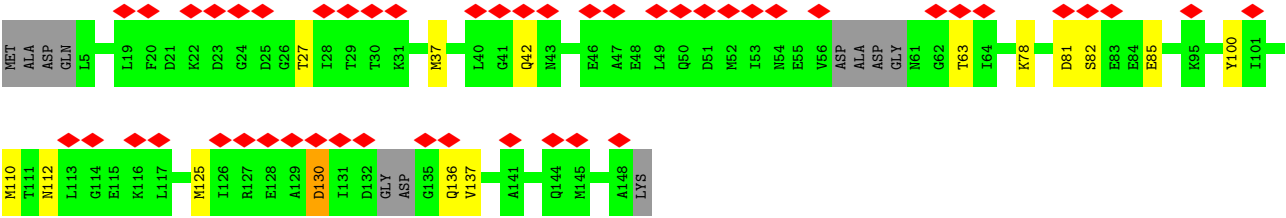


- Molecule 3: Calmodulin-1

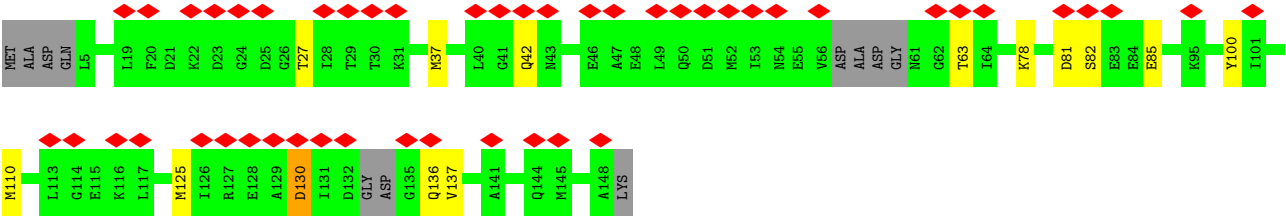
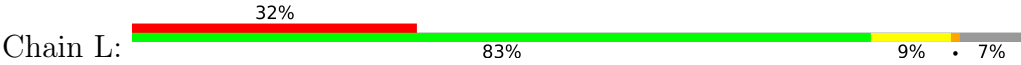


- Molecule 3: Calmodulin-1





• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69556	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	0.096	Depositor
Minimum map value	-0.036	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, CA, CFF, ATP

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	0.30	0/835	0.54	0/1123
1	D	0.30	0/835	0.54	0/1123
1	G	0.30	0/835	0.54	0/1123
1	J	0.30	0/835	0.54	0/1123
2	B	0.36	0/27315	0.64	12/36936 (0.0%)
2	E	0.36	0/27315	0.64	12/36936 (0.0%)
2	H	0.36	0/27315	0.64	10/36936 (0.0%)
2	K	0.36	0/27315	0.64	12/36936 (0.0%)
3	C	0.28	0/1088	0.60	0/1459
3	F	0.28	0/1088	0.60	0/1459
3	I	0.28	0/1088	0.60	0/1459
3	L	0.28	0/1088	0.60	0/1459
All	All	0.36	0/116952	0.64	46/158072 (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
2	B	0	24
2	E	0	24
2	H	0	24
2	K	0	24
All	All	0	96

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4165	GLN	N-CA-C	-6.15	107.01	114.75
2	B	4165	GLN	N-CA-C	-6.14	107.02	114.75
2	K	4165	GLN	N-CA-C	-6.14	107.02	114.75
2	E	4165	GLN	N-CA-C	-6.11	107.05	114.75
2	B	2431	GLY	CA-C-N	5.67	128.66	120.38

There are no chirality outliers.

5 of 96 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	685	PHE	Peptide
2	B	729	GLY	Peptide
2	B	748	LEU	Peptide
2	B	791	VAL	Peptide
2	B	816	PRO	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	819	0	824	13	0
1	D	819	0	824	14	0
1	G	819	0	824	15	0
1	J	819	0	824	15	0
2	B	26813	0	25339	463	0
2	E	26813	0	25339	454	0
2	H	26813	0	25339	454	0
2	K	26813	0	25339	451	0
3	C	1078	0	1032	9	0
3	F	1078	0	1032	8	0
3	I	1078	0	1032	9	0
3	L	1078	0	1032	8	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	H	14	0	10	0	0
6	K	14	0	10	0	0
7	B	31	0	12	4	0
7	E	31	0	12	4	0
7	H	31	0	12	5	0
7	K	31	0	12	4	0
All	All	115028	0	108868	1732	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 1732 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)
2:K:1986:GLU:N	2:K:1989:CYS:HG	1.54	1.05
2:B:1986:GLU:N	2:B:1989:CYS:HG	1.54	1.05
2:H:1986:GLU:N	2:H:1989:CYS:HG	1.55	1.03
2:B:4811:LEU:HD13	2:E:4519:LEU:HD21	1.39	1.03
2:E:1986:GLU:N	2:E:1989:CYS:HG	1.56	1.02

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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3386/4968 (68%)	2990 (88%)	383 (11%)	13 (0%)	30	66
2	E	3386/4968 (68%)	2986 (88%)	387 (11%)	13 (0%)	30	66
2	H	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	30	66
2	K	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	30	66
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	I	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
All	All	14492/20900 (69%)	12806 (88%)	1630 (11%)	56 (0%)	31	66

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1477	HIS
2	E	1477	HIS
2	H	1477	HIS
2	K	1477	HIS
2	B	1580	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	88/89 (99%)	88 (100%)	0	100	100
1	D	88/89 (99%)	88 (100%)	0	100	100
1	G	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2698/4355 (62%)	2680 (99%)	18 (1%)	76	78
2	E	2698/4355 (62%)	2680 (99%)	18 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	2699/4355 (62%)	2680 (99%)	19 (1%)	76	78
2	K	2699/4355 (62%)	2680 (99%)	19 (1%)	76	78
3	C	115/123 (94%)	115 (100%)	0	100	100
3	F	115/123 (94%)	115 (100%)	0	100	100
3	I	115/123 (94%)	115 (100%)	0	100	100
3	L	115/123 (94%)	115 (100%)	0	100	100
All	All	11606/18268 (64%)	11532 (99%)	74 (1%)	76	80

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	625	VAL
2	K	4521	TYR
2	K	832	LEU
2	K	1054	VAL
2	E	925	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 260 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	2211	ASN
2	K	2848	ASN
2	E	1996	GLN
2	E	1722	ASN
2	K	3916	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	CFF	H	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.79	9 (39%)
6	CFF	B	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	K	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
6	CFF	K	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	E	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
7	ATP	B	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
6	CFF	E	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	H	6003	-	32,33,33	1.33	6 (18%)	48,52,52	1.77	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	H	6002	-	-	-	0/2/2/2
6	CFF	B	6002	-	-	-	0/2/2/2
7	ATP	K	6003	-	-	8/22/38/38	0/3/3/3
6	CFF	K	6002	-	-	-	0/2/2/2
7	ATP	E	6003	-	-	8/22/38/38	0/3/3/3
7	ATP	B	6003	-	-	8/22/38/38	0/3/3/3
6	CFF	E	6002	-	-	-	0/2/2/2
7	ATP	H	6003	-	-	8/22/38/38	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	6002	CFF	C6-N1	-4.38	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6002	CFF	C6-N1	-4.37	1.31	1.40
6	H	6002	CFF	C6-N1	-4.37	1.31	1.40
6	K	6002	CFF	C6-N1	-4.37	1.31	1.40
7	B	6003	ATP	C5-C4	4.03	1.46	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6002	CFF	C14-N7-C8	-7.63	112.01	126.28
6	H	6002	CFF	C14-N7-C8	-7.63	112.01	126.28
6	E	6002	CFF	C14-N7-C8	-7.61	112.04	126.28
6	K	6002	CFF	C14-N7-C8	-7.61	112.04	126.28
7	B	6003	ATP	C5-C4-N3	-5.49	119.16	126.72

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	6003	ATP	PB-O3B-PG-O2G
7	B	6003	ATP	PB-O3B-PG-O3G
7	B	6003	ATP	C5'-O5'-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O2A
7	B	6003	ATP	C5'-O5'-PA-O3A

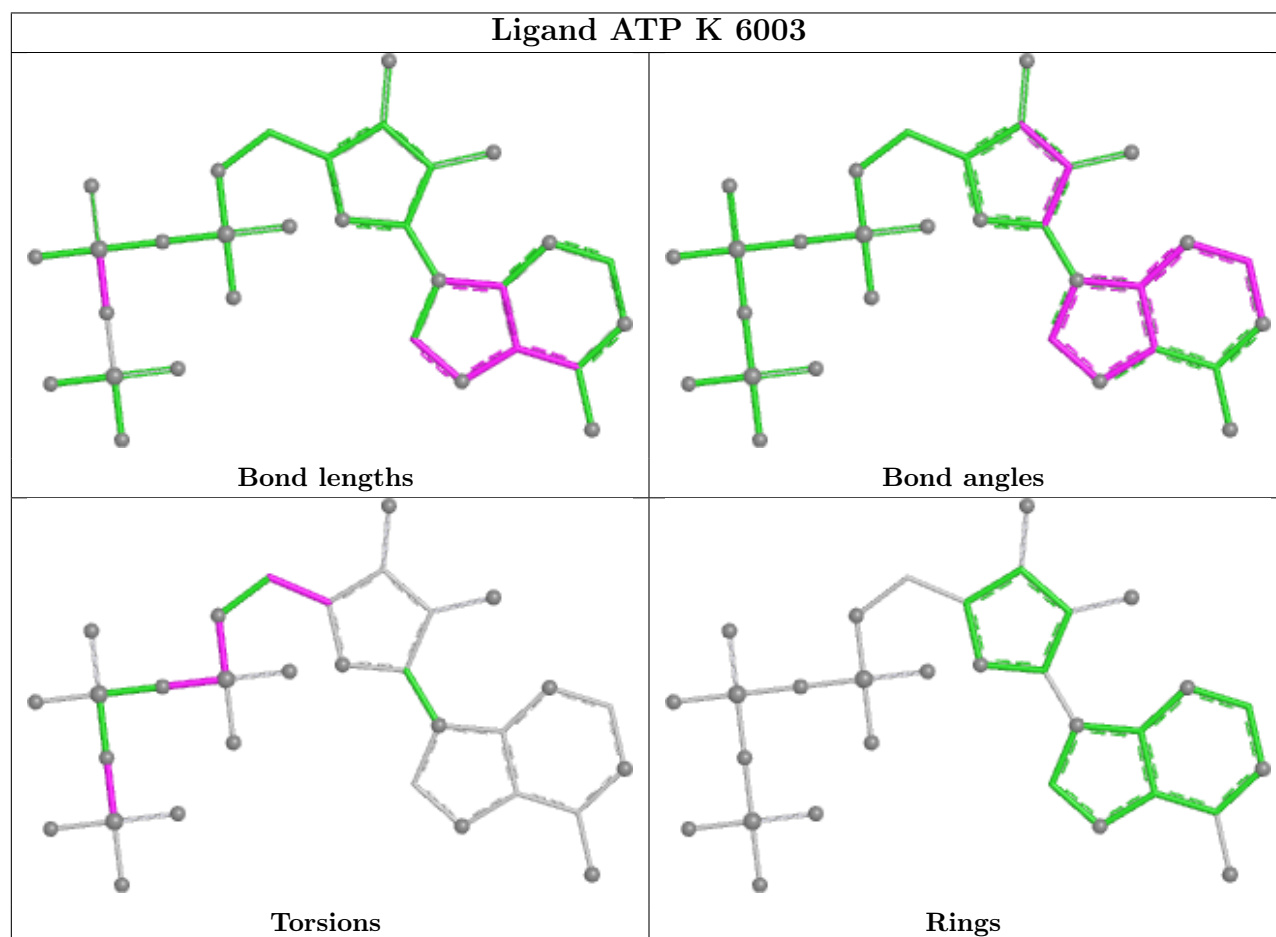
There are no ring outliers.

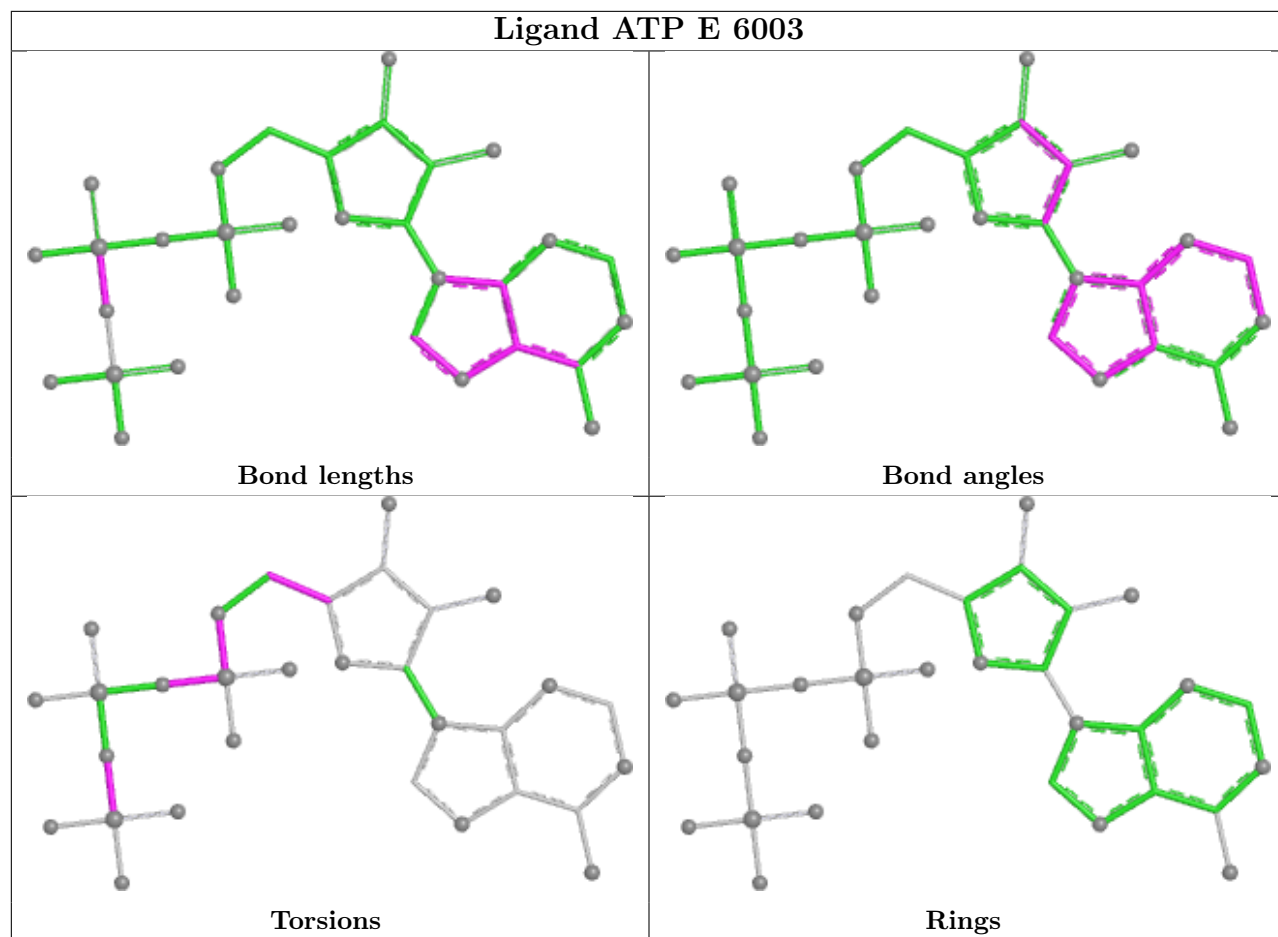
6 monomers are involved in 19 short contacts:

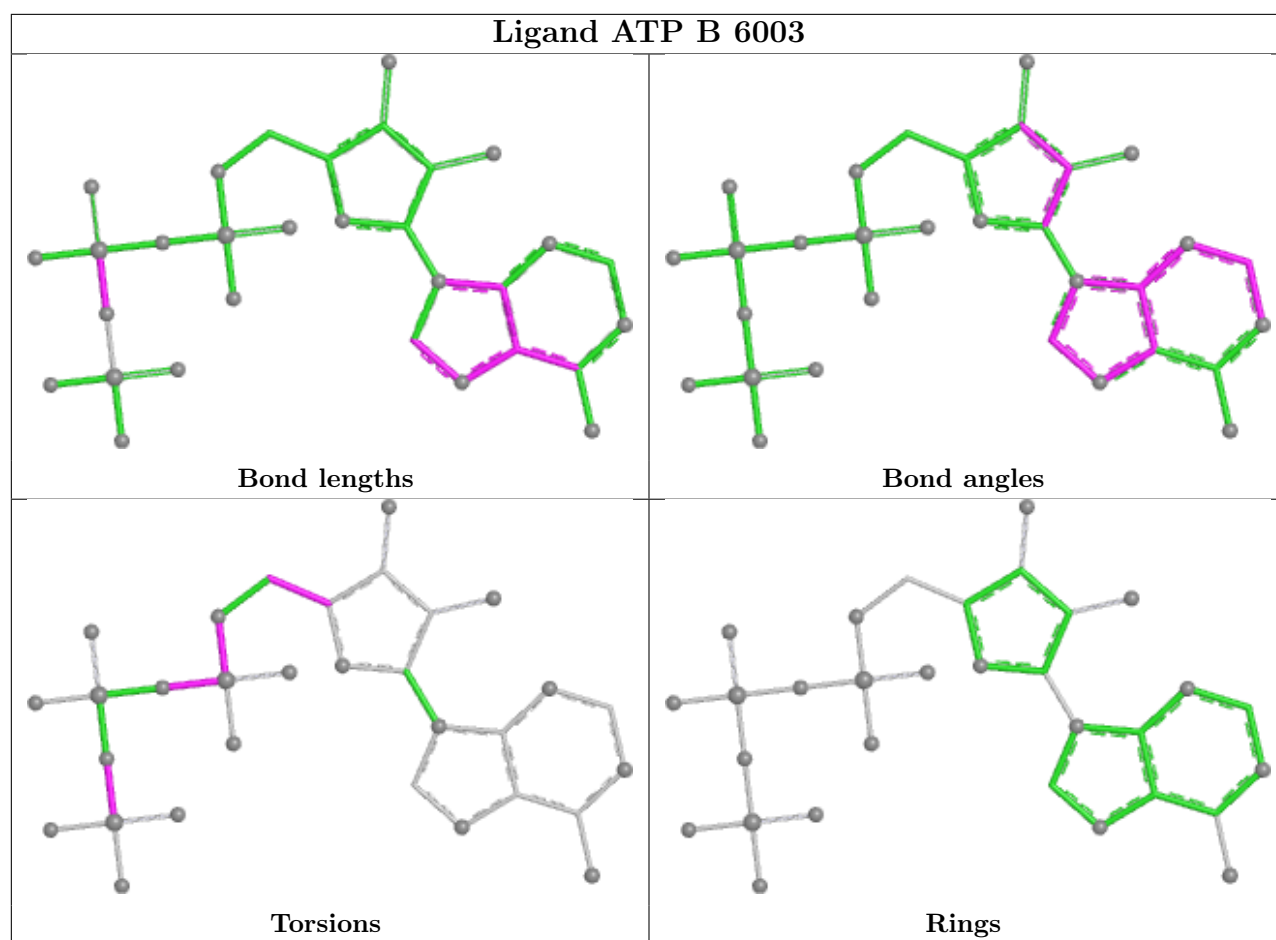
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	6002	CFF	1	0
7	K	6003	ATP	4	0
7	E	6003	ATP	4	0
7	B	6003	ATP	4	0
6	E	6002	CFF	1	0
7	H	6003	ATP	5	0

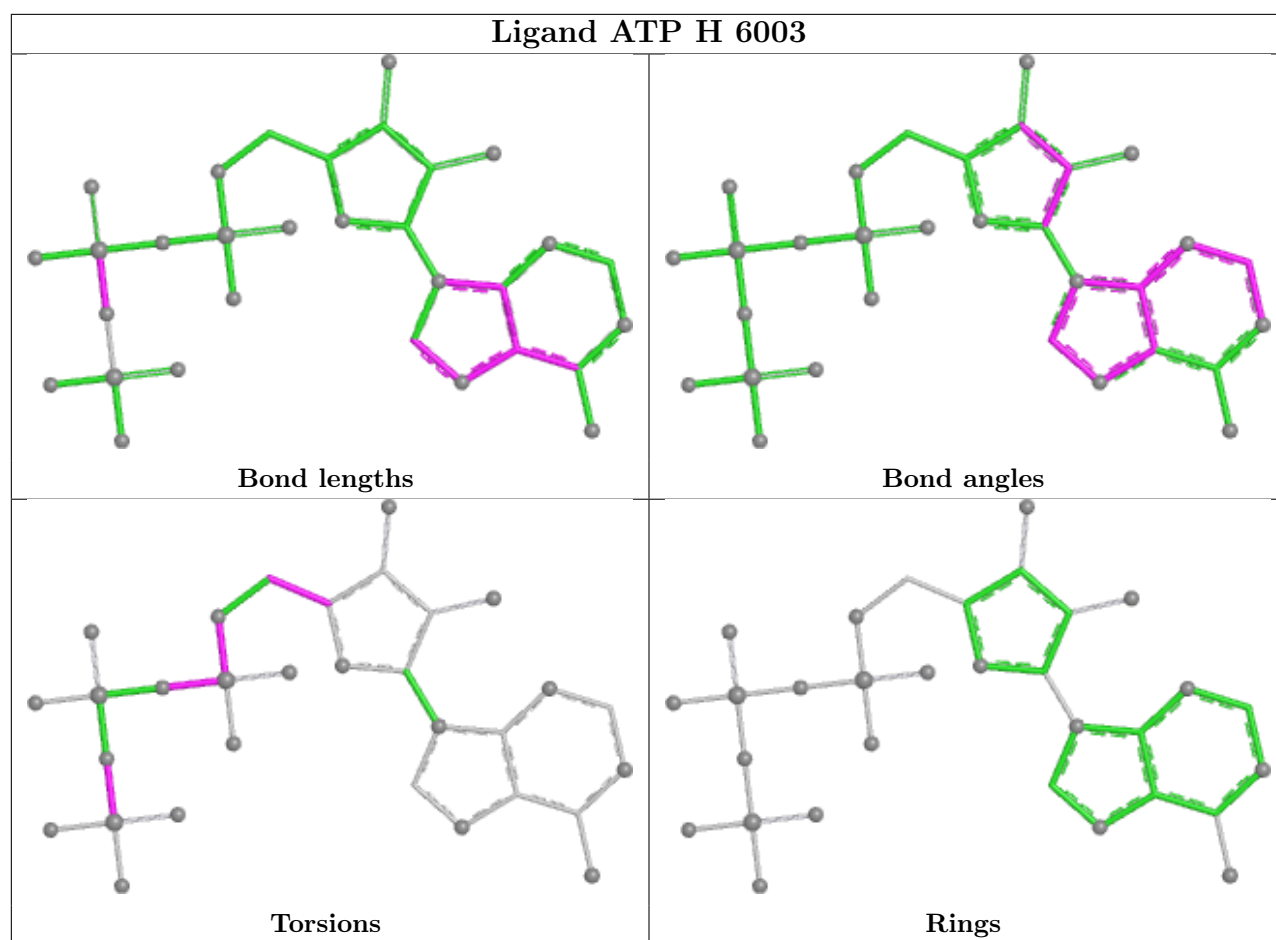
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

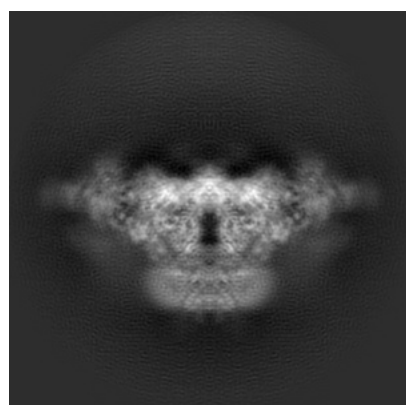
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9834. These allow visual inspection of the internal detail of the map and identification of artifacts.

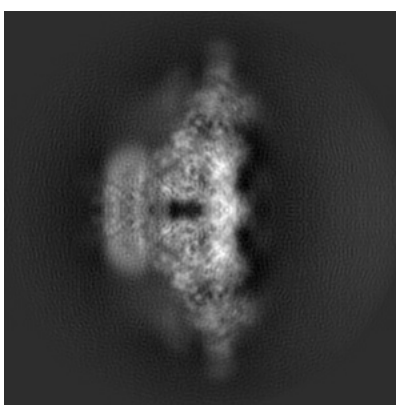
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

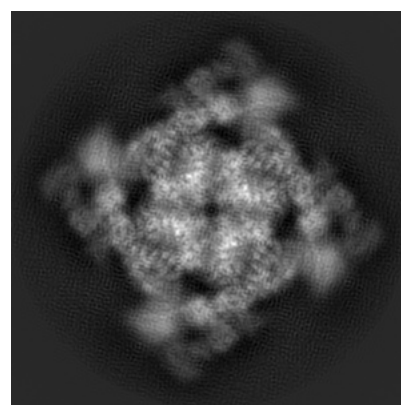
6.1.1 Primary map



X



Y

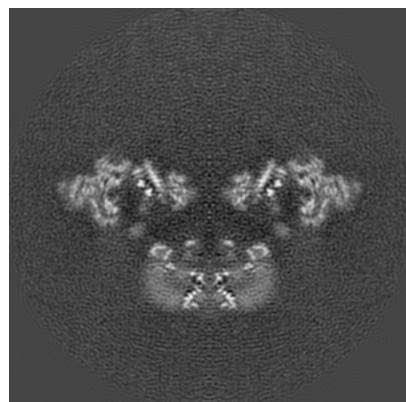


Z

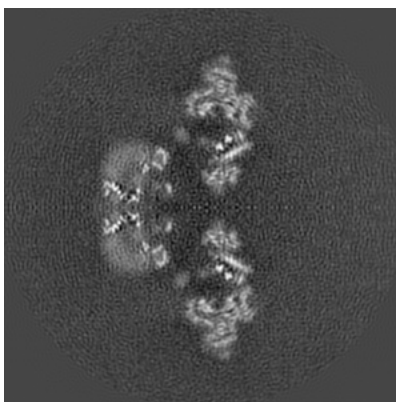
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

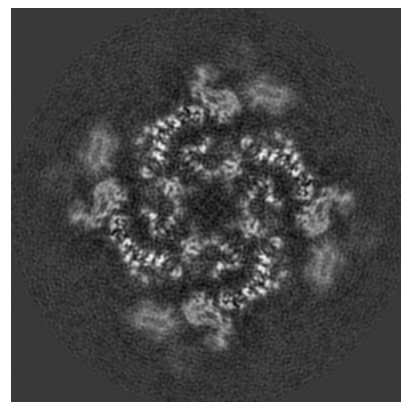
6.2.1 Primary map



X Index: 200



Y Index: 200

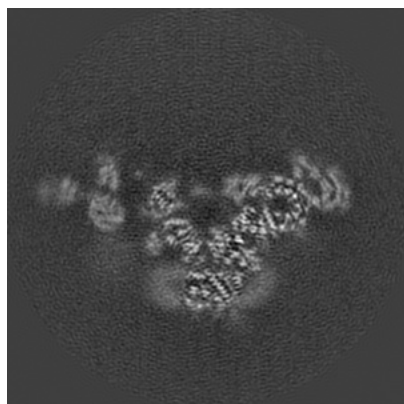


Z Index: 200

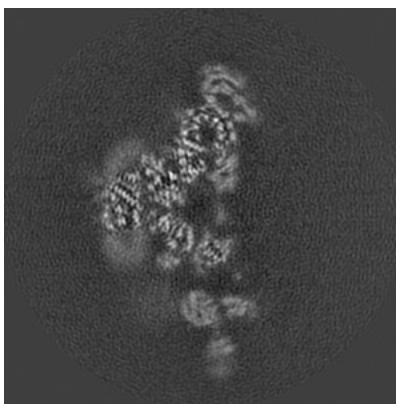
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

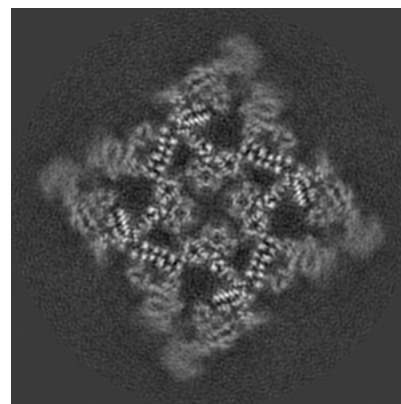
6.3.1 Primary map



X Index: 185



Y Index: 215

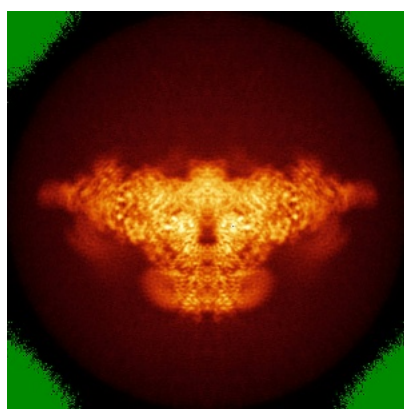


Z Index: 212

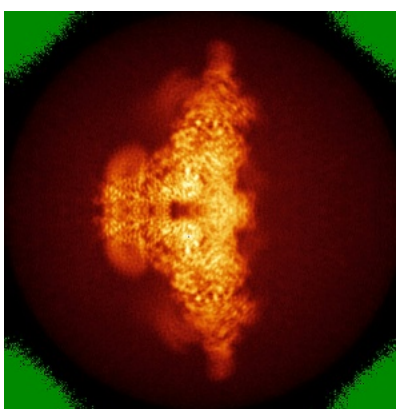
The images above show the largest variance slices of the map in three orthogonal directions.

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

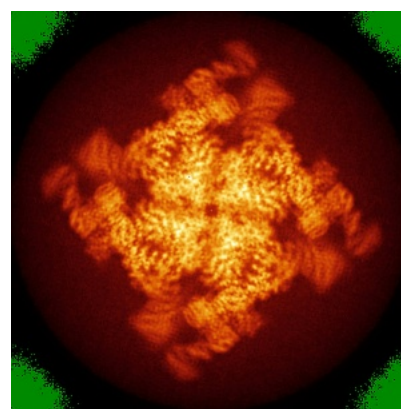
6.4.1 Primary map



X



Y

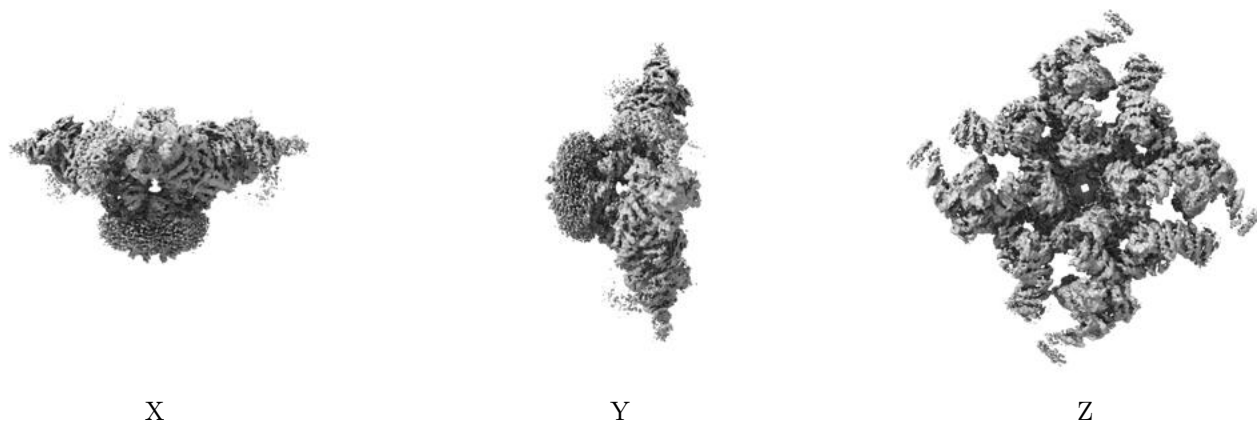


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

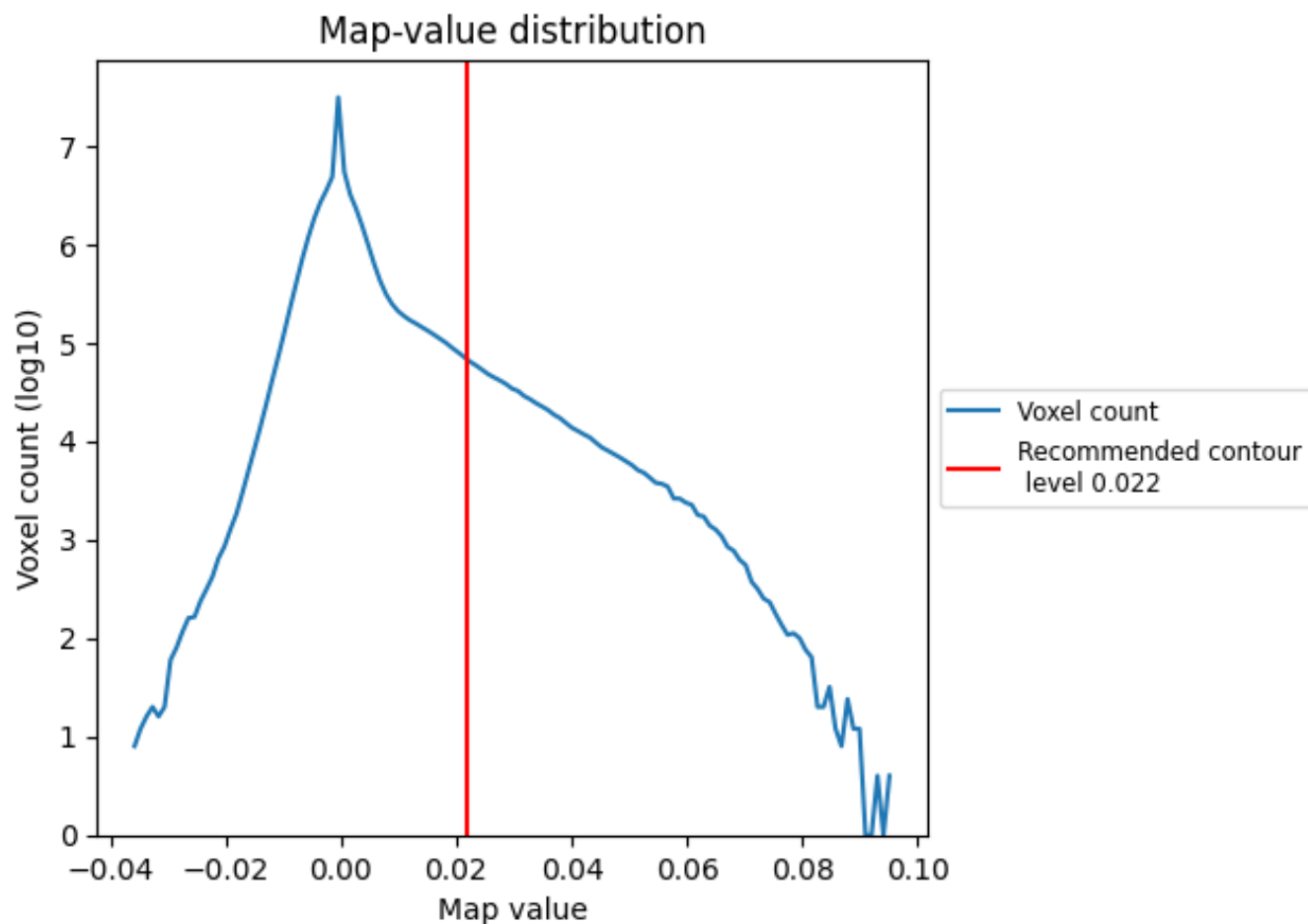
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

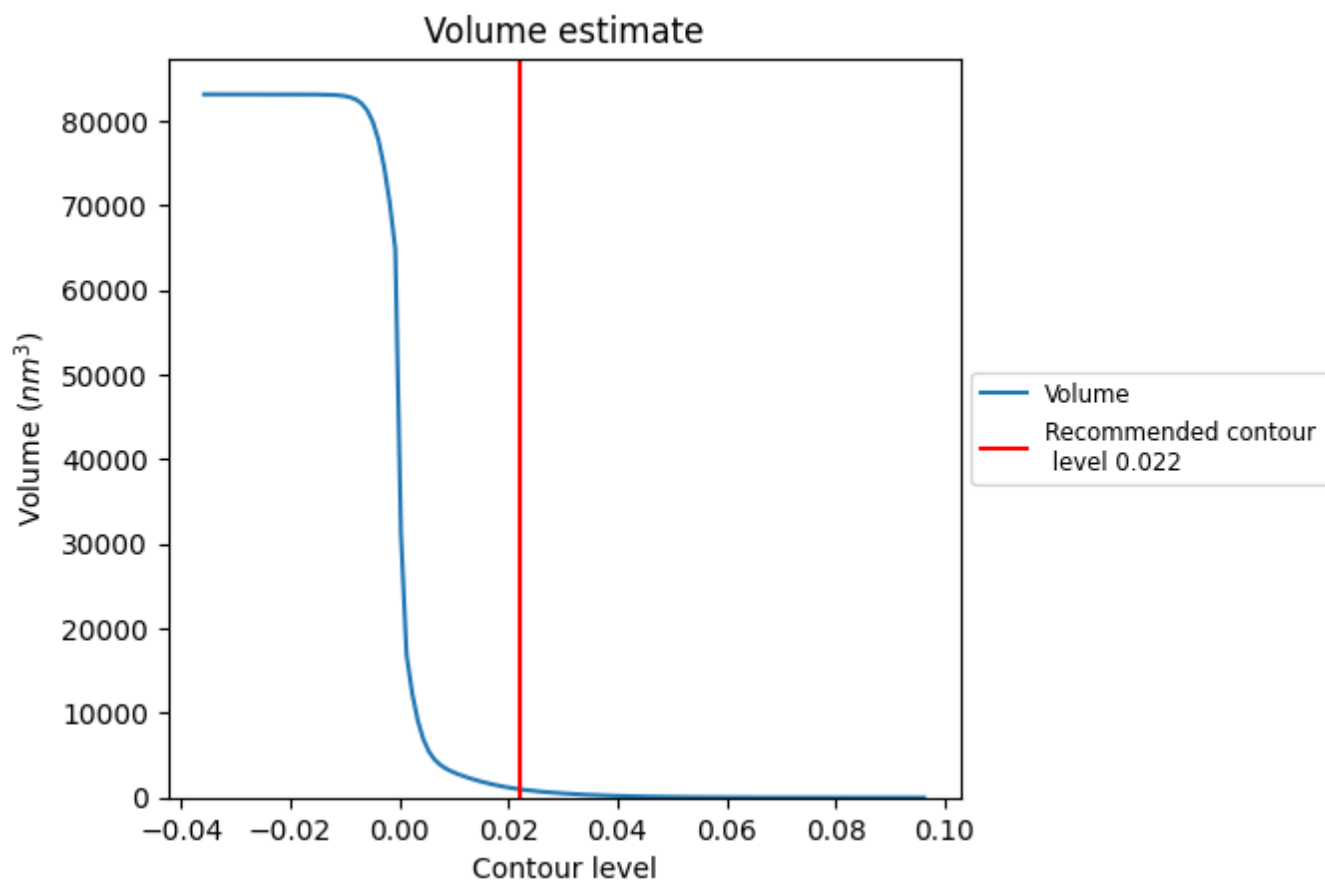
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

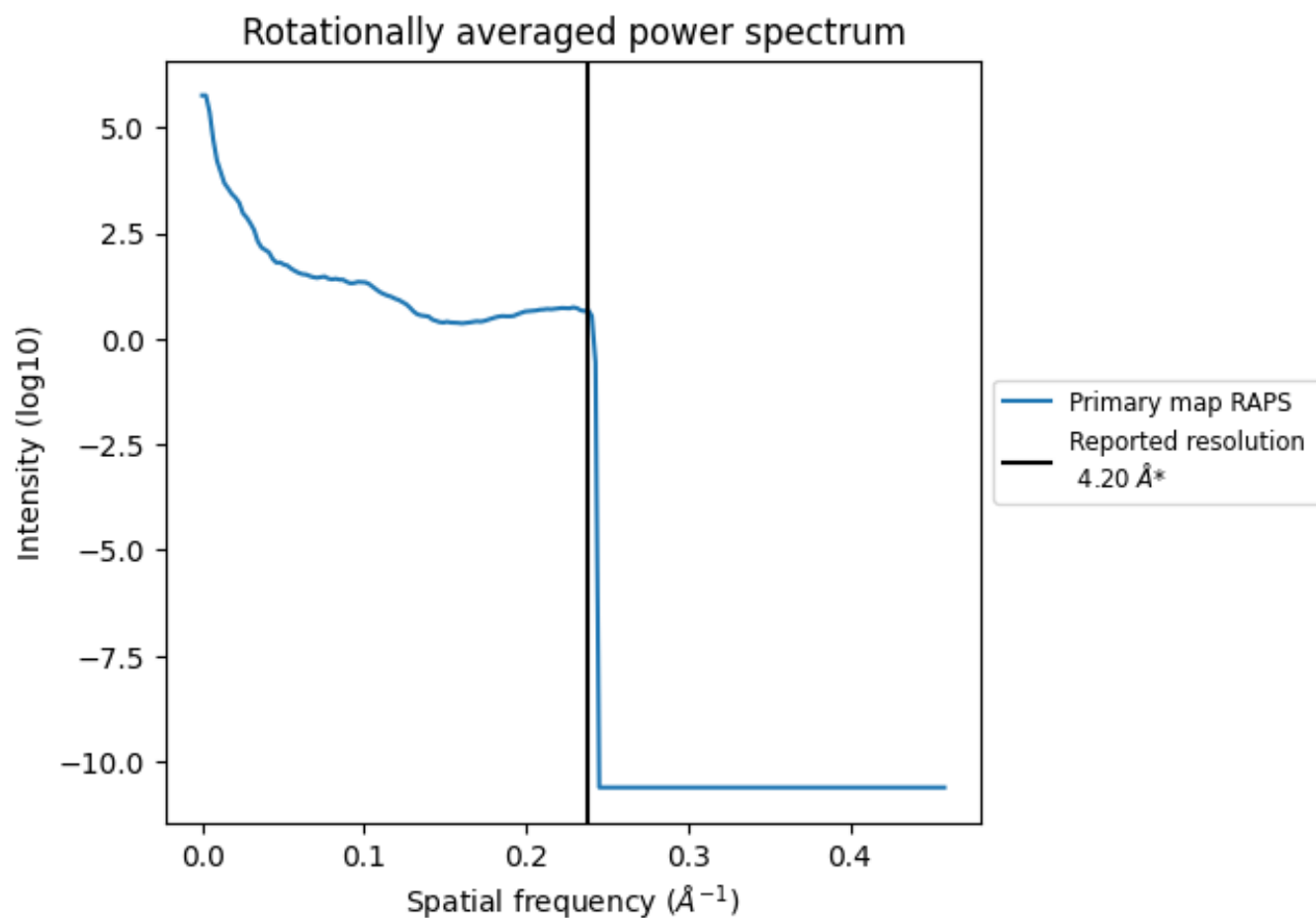
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 992 nm³; this corresponds to an approximate mass of 896 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 ⓘ

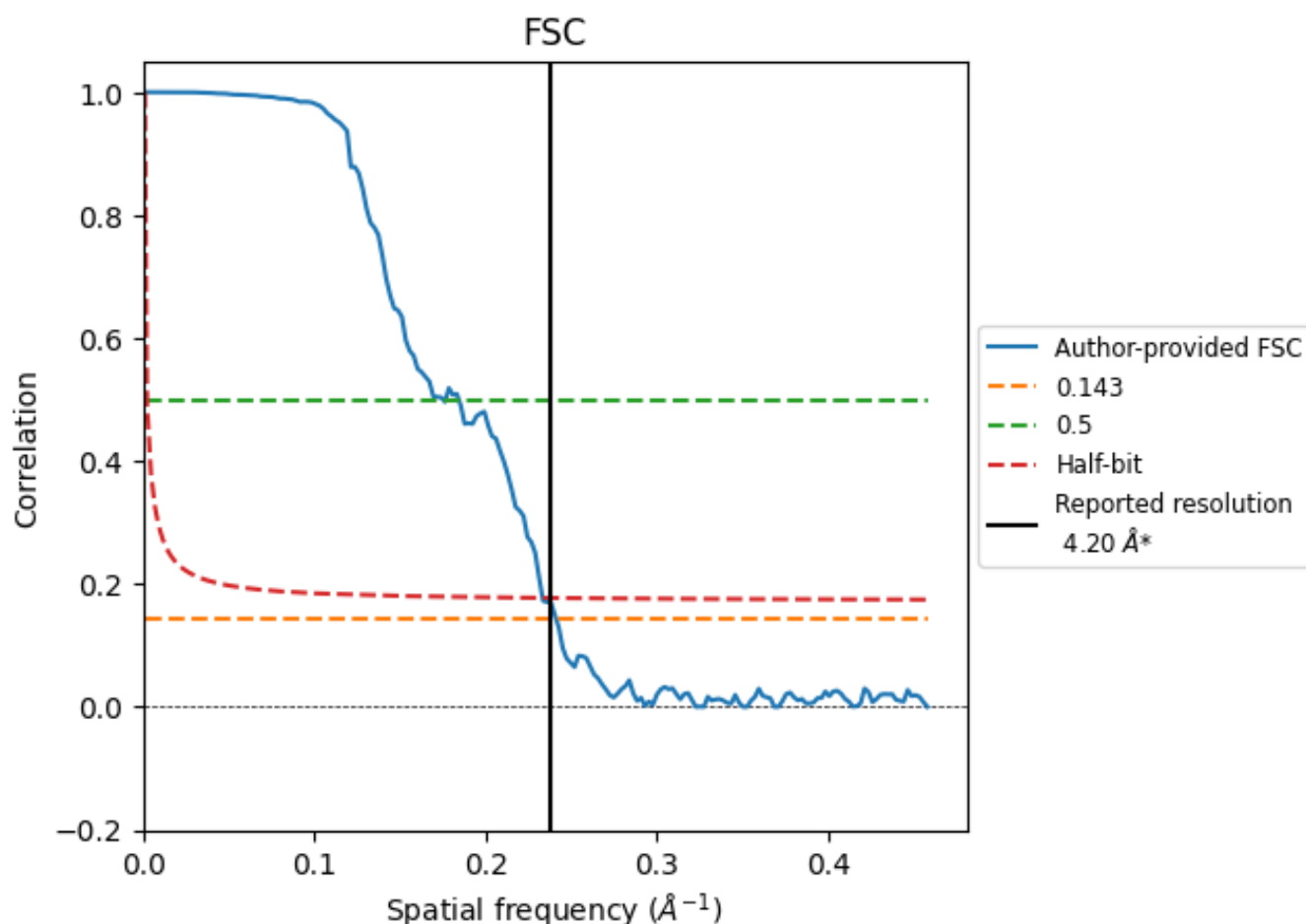


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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](#)

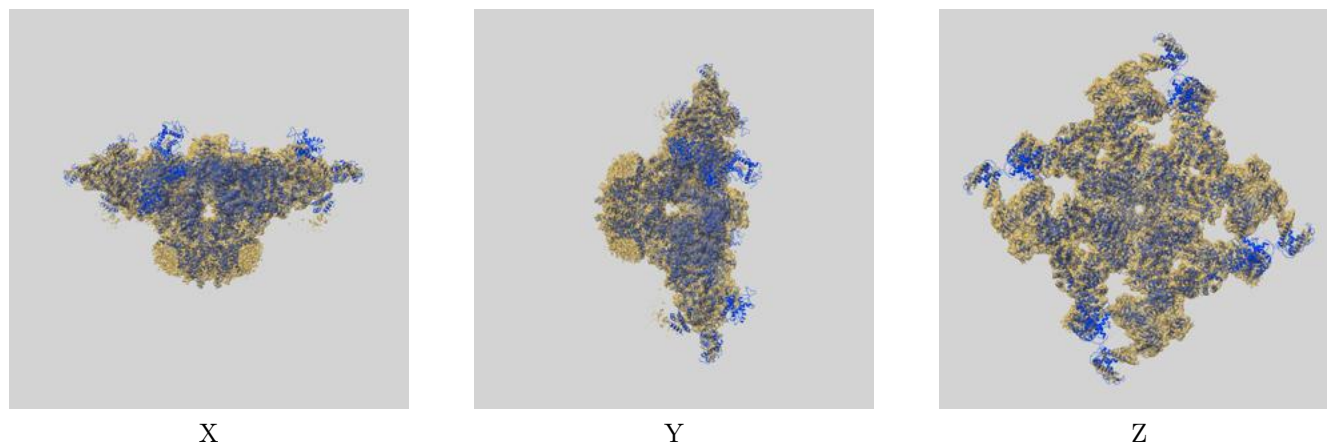
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	5.71	4.28
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

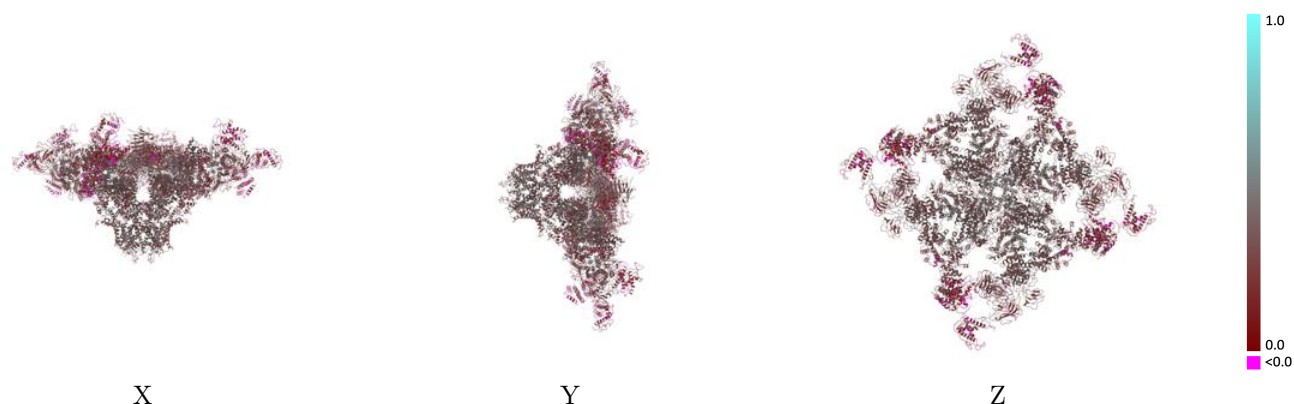
This section contains information regarding the fit between EMDB map EMD-9834 and PDB model 6JII. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



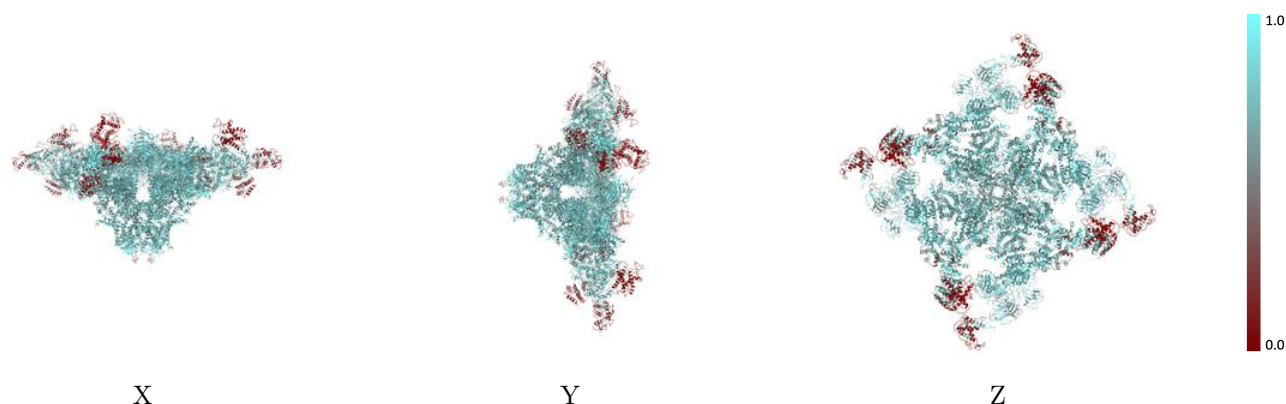
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



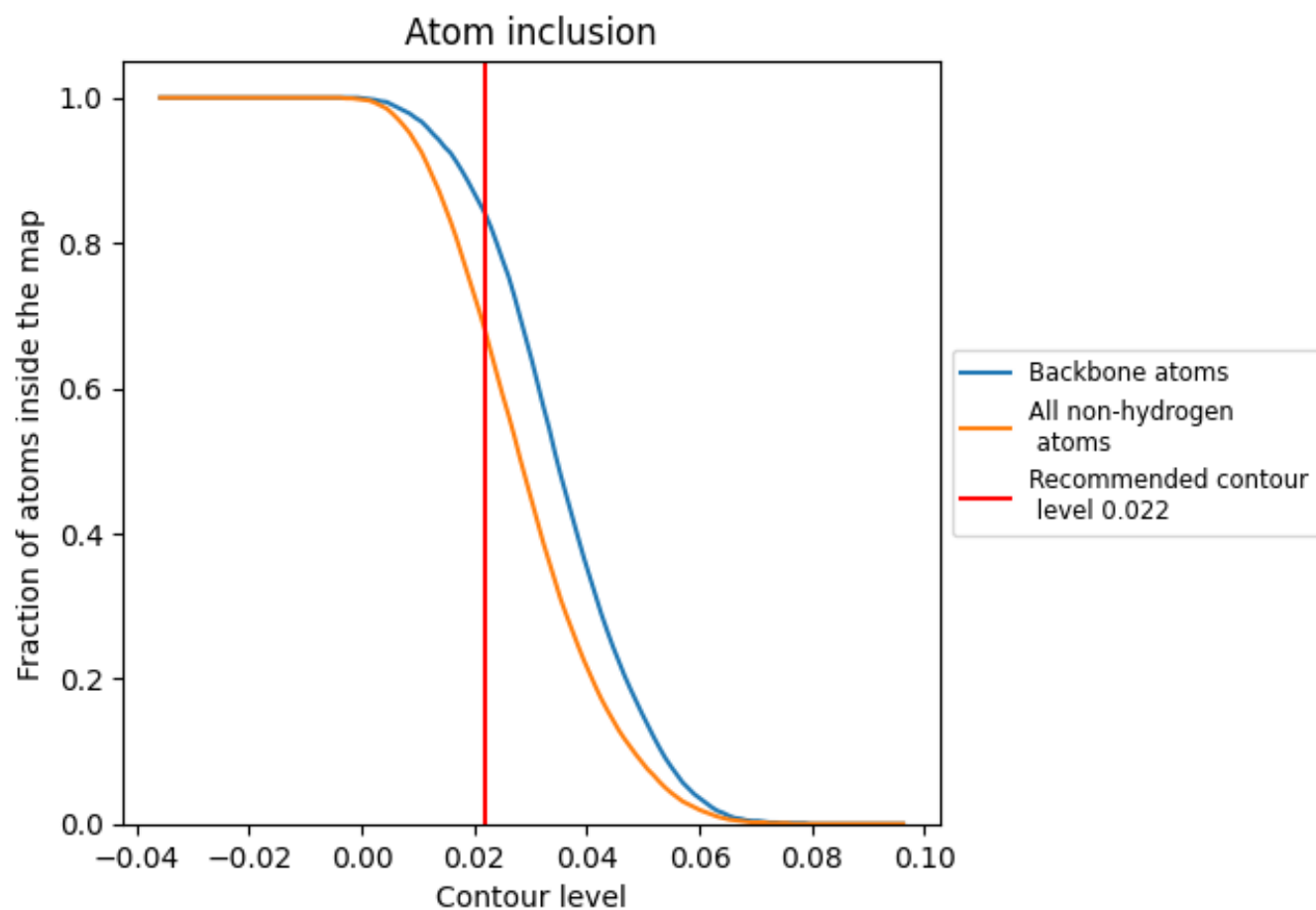
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.3190
A	0.7090	0.3340
B	0.6840	0.3210
C	0.4910	0.2490
D	0.7100	0.3380
E	0.6840	0.3220
F	0.4910	0.2470
G	0.7110	0.3370
H	0.6840	0.3220
I	0.4910	0.2480
J	0.7100	0.3360
K	0.6840	0.3210
L	0.4910	0.2490

1.0

0.0

<0.0