



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 03:09 PM JST

PDB ID : 7WJI  
EMDB ID : EMD-32544  
Title : Architecture of the human NALCN channelosome  
Authors : Wu, J.P.; Yan, Z.; Zhou, L.; Liu, H.; Zhao, Q.  
Deposited on : 2022-01-06  
Resolution : 4.50 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)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

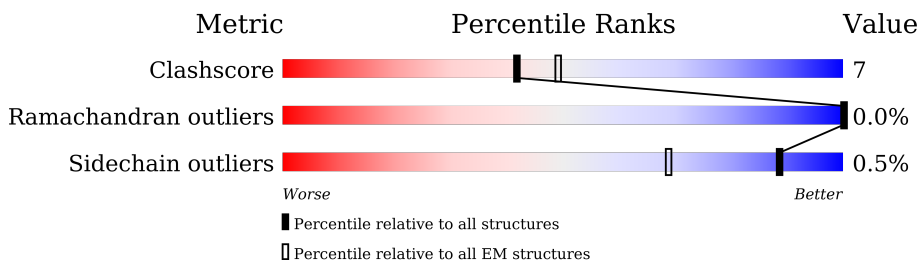
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 4.50 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	3258	
2	B	2658	
3	E	149	
4	C	1992	
5	D	458	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 41173 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 Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1763	14143	9070	2451	2525	97	0	0

- Molecule 2 is a protein called Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1663	13146	8488	2188	2355	115	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2636	ASP	-	expression tag	UNP Q9P2D8
B	2637	GLU	-	expression tag	UNP Q9P2D8
B	2638	VAL	-	expression tag	UNP Q9P2D8
B	2639	ASP	-	expression tag	UNP Q9P2D8
B	2640	ALA	-	expression tag	UNP Q9P2D8
B	2641	GLY	-	expression tag	UNP Q9P2D8
B	2642	SER	-	expression tag	UNP Q9P2D8
B	2643	ASP	-	expression tag	UNP Q9P2D8
B	2644	TYR	-	expression tag	UNP Q9P2D8
B	2645	LYS	-	expression tag	UNP Q9P2D8
B	2646	ASP	-	expression tag	UNP Q9P2D8
B	2647	ASP	-	expression tag	UNP Q9P2D8
B	2648	ASP	-	expression tag	UNP Q9P2D8
B	2649	LYS	-	expression tag	UNP Q9P2D8
B	2650	GLY	-	expression tag	UNP Q9P2D8
B	2651	SER	-	expression tag	UNP Q9P2D8
B	2652	ASP	-	expression tag	UNP Q9P2D8
B	2653	TYR	-	expression tag	UNP Q9P2D8
B	2654	LYS	-	expression tag	UNP Q9P2D8
B	2655	ASP	-	expression tag	UNP Q9P2D8
B	2656	ASP	-	expression tag	UNP Q9P2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2657	ASP	-	expression tag	UNP Q9P2D8
B	2658	LYS	-	expression tag	UNP Q9P2D8

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	126	988	615	160	204	9	0	0

- Molecule 4 is a protein called Sodium leak channel non-selective protein, Extended tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	1394	11413	7523	1877	1926	87	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1739	LEU	-	linker	UNP Q8IZF0
C	1740	GLU	-	linker	UNP Q8IZF0
C	1741	GLY	-	linker	UNP Q8IZF0
C	1742	SER	-	linker	UNP Q8IZF0
C	1743	GLU	-	linker	UNP Q8IZF0
C	1744	ASN	-	linker	UNP Q8IZF0
C	1745	LEU	-	linker	UNP Q8IZF0
C	1746	TYR	-	linker	UNP Q8IZF0
C	1747	PHE	-	linker	UNP Q8IZF0
C	1748	GLN	-	linker	UNP Q8IZF0
C	1749	GLY	-	linker	UNP Q8IZF0
C	1750	GLY	-	linker	UNP Q8IZF0
C	1751	GLY	-	linker	UNP Q8IZF0
C	1752	GLY	-	linker	UNP Q8IZF0
C	1753	SER	-	linker	UNP Q8IZF0

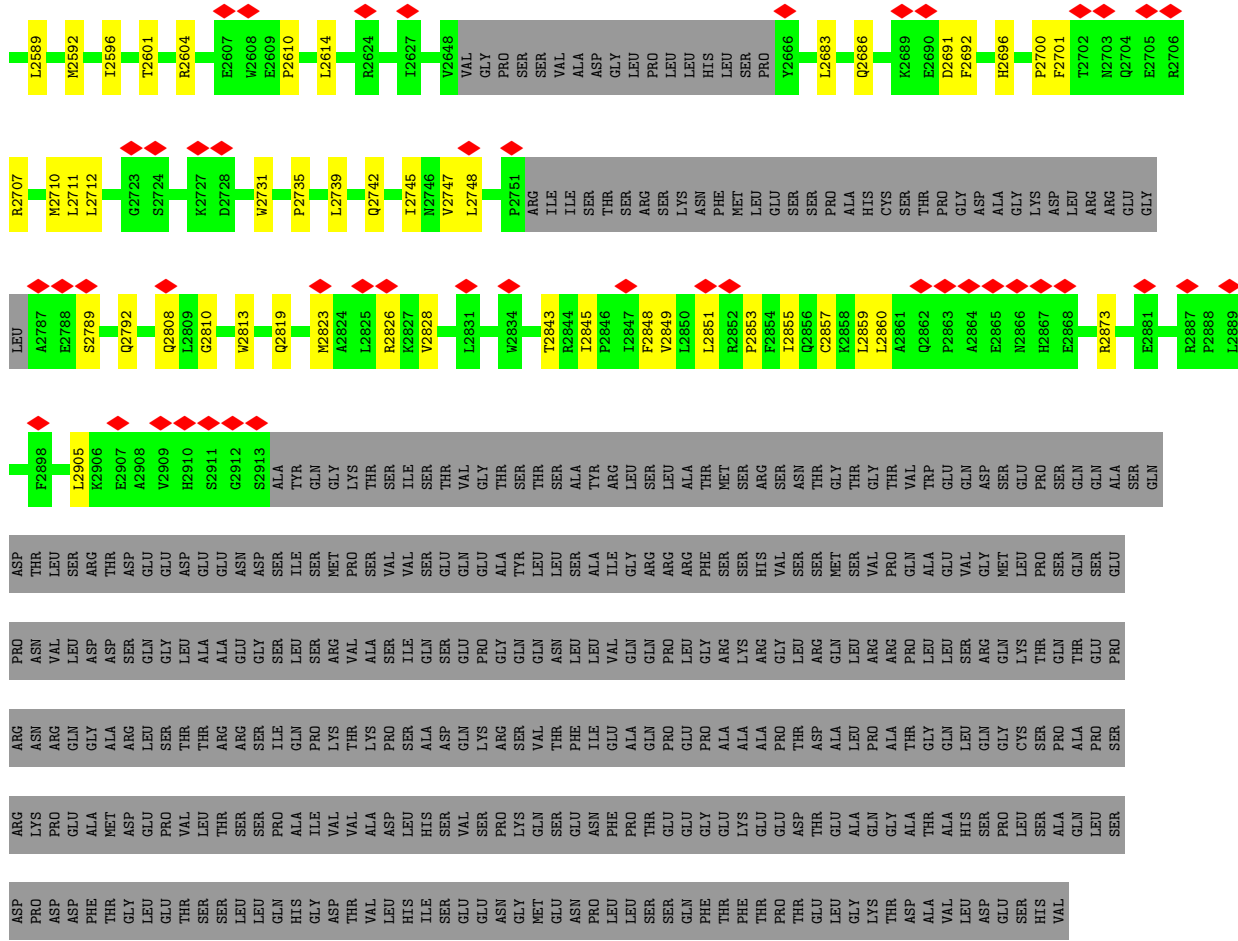
- Molecule 5 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	182	1483	934	243	292	14	0	0

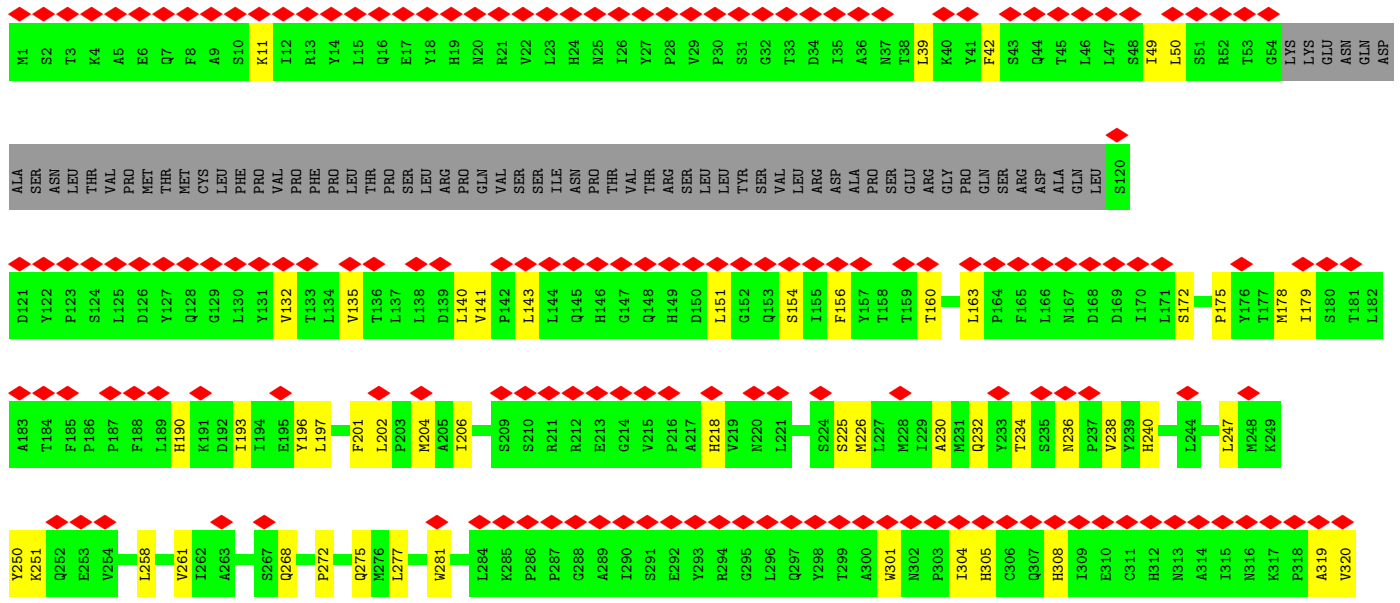




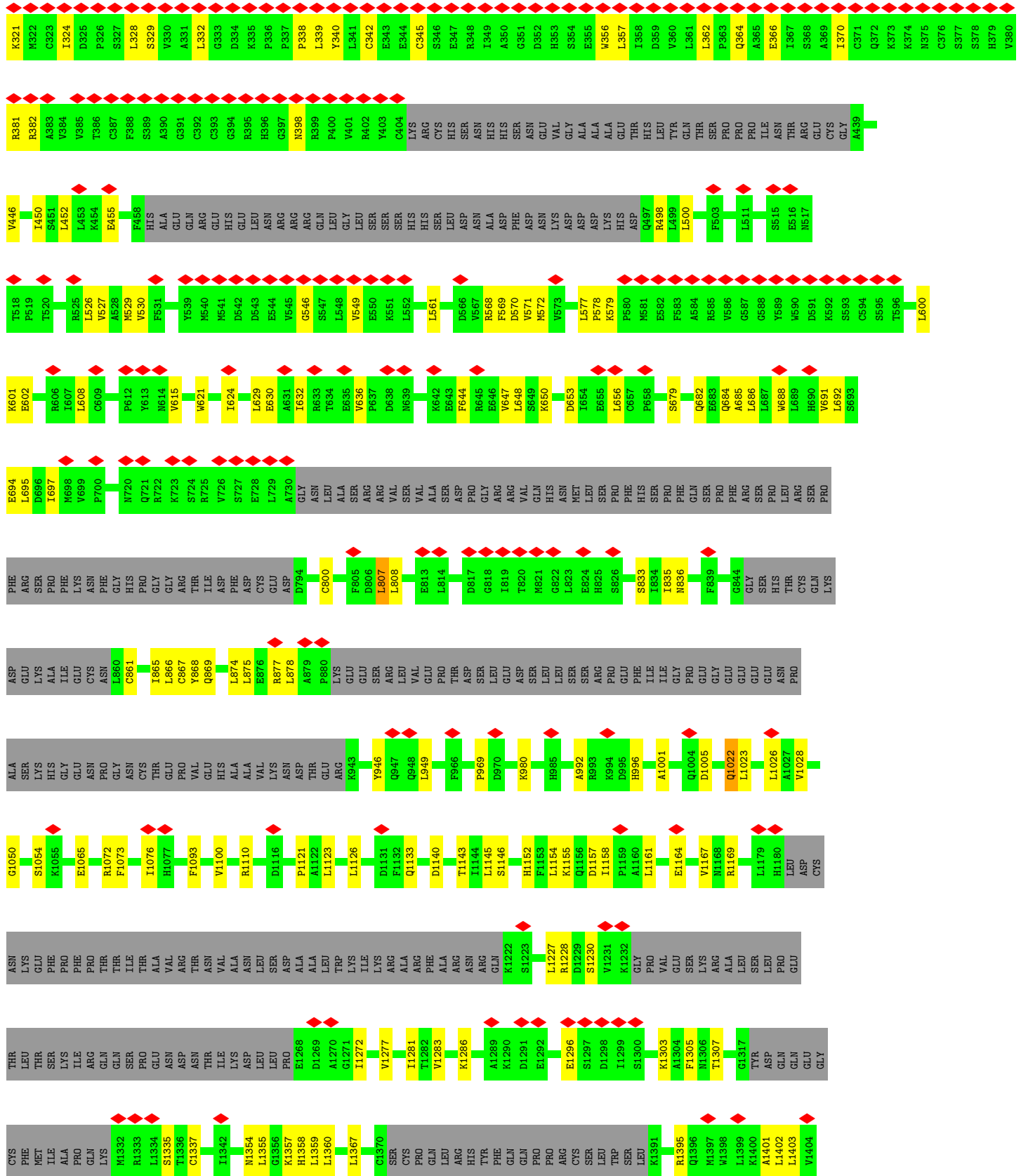




● Molecule 2: Protein unc-79 homolog



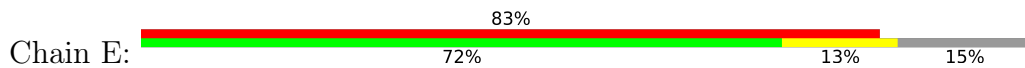




F2331	F2332	A2333	D2334	M2335	H2336	T2337	L2338	L2339	K2340	L2341	K2342	S2343	H2344	M2345	K2346	T2347	C2348	S2349	Q2350	P2351	L2352	H2353	E2354	D2355	F2357	G2358	G2359	H2360	L2361	K2362	V2363	G2364	L2365	A2366	Q2367	A2368	A2369	A2370	D2371	D2372	L2373	S2374	E2375	G2376	M2377	H2378	R2379	D2380	M2381	K2382	A2383	I2385	L2386	R2386	F2387	L2388	F2389	W2390			
K2271	L2272	K2273	S2274	P2275	L2276	P2277	D2278	N2279	N2280	L2281	L2282	L2283	L2284	V2285	Q2286	F2287	I2288	C2289	A2290	D2291	A2292	G2293	T2294	K2296	L2296	A2297	E2298	S2299	T2300	I2301	L2302	S2303	K2304	Q2305	M2306	I2307	A2308	S2309	V2310	P2311	G2312	C2313	G2314	T2315	A2316	A2317	M2318	E2319	C2320	V2321	R2322	Q2323	Y2324	I2325	N2326	E2327	Y2328	L2329	D2330		
M2147	I2148	R2149	C2150	L2151	E2152	N2153	I2154	F2157	M2158	P2162	M2163	D2164	S2165	P2166	S2167	S2168	L2169	W2170	T2171	T2172	L2173	I2174	N2175	Q2176	F2177	Q2178	F2179	F2180	F2181	A2182	K2183	L2184	P2185	C2186	V2187	L2188	P2189	L2190	K2191	C2192	S2193	L2194	D2195	S2196	S2197	L2198	R2199	I2200	M2201	L2204	L2205	K2206	I2207	P2208	S2209	T2210					
M2084	L2085	F2086	L2089	A2090	P2091	G2093	L2094	F2095	E2020	E2021	L2023	G2024	V2029	L2030	S2031	T2032	F2033	I2034	L2040	A2041	P2043	L2044	L2045	L2046	D2047	G2053	R2054	L2055	A2056	S2057	N2120	E2121	L2122	S2123	S2124	I2125	A2126	A2127	L2128	S2129	Q2130	L2131	L2132	E2133	G2134	L2135	M2136	N2137	K2138	K2139	M2140	L2141	P2142	A2143	G2144	G2145	A2146				
GLY	ALA	ILE	GLU	GLY	TYR	ASP	E2020	E2021	L2023	G2024	V2029	L2030	S2031	T2032	F2033	I2034	L2040	A2041	P2043	L2044	L2045	L2046	D2047	G2053	R2054	L2055	A2056	S2057	N2120	E2121	L2122	S2123	S2124	I2125	A2126	A2127	L2128	S2129	Q2130	L2131	L2132	E2133	G2134	L2135	M2136	N2137	K2138	K2139	M2140	L2141	P2142	A2143	G2144	G2145	A2146						
ARG	GLN	CYS	ASN	VAL	PRO	THR	LEU	ASN	PRO	ASP	LEU	ALA	LEU	ARG	GLN	MET	ARG	GLY	ALA	THR	LEU	LYS	THR	SER	GLY	VAL	SER	LEU	LEU	THR	ILE	VAL	MET	PHE	VAL	PRO	THR	ALA	GLN	ASP	THR	LEU	ILE	SER	ASN	THR	TRP	ASP	VAL	THR	GLU	THR	MET	THR	LEU	ASP	ILE	GLN	HIS	PRO	CYS
ASP	ALA	GLY	VAL	PRO	GLU	THR	SER	HIS	ASN	ASP	LEU	ILE	THR	GLN	MET	ARG	GLY	ALA	THR	LEU	LYS	THR	SER	GLY	VAL	SER	LEU	LEU	THR	ILE	VAL	MET	PHE	VAL	PRO	THR	ALA	GLN	ASP	THR	LEU	ILE	SER	ASN	THR	TRP	ASP	VAL	THR	GLU	THR	MET	THR	LEU	ASP	ILE	GLN	HIS	PRO	CYS	
SER	ALA	ILE	THR	LEU	GLY	ASP	PRO	MET	ASP	ALA	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	GLY	ASP	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY	
GLU	THR	GLY	ALA	LEU	GLN	ASP	THR	LEU	ASP	LEU	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY			
LYS	VAL	ASP	PRO	PRO	VAL	LYS	PRO	ALA	LYS	GLY	ASP	PRO	GLY	LEU	SER	SER	GLY	PRO	ASP	GLY	PRO	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY			
PRO	THR	GLN	ALA	LEU	TYR	ILE	ALA	ALA	ALA	ASP	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY			
THR	GLY	ALA	LEU	GLN	TYR	ILE	ALA	ALA	ASP	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY				
THR	GLY	ALA	LEU	GLN	TYR	ILE	ALA	ALA	ASP	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY				
THR	GLY	ALA	LEU	GLN	TYR	ILE	ALA	ALA	ASP	GLY	THR	VAL	SER	LEU	LEU	THR	ASN	PRO	CYS	GLY	THR	ASP	PRO	THR	GLY	THR	GLU	GLY	SER	THR	ALA	VAL	GLY	LEU	GLN	SER	LEU	LEU	THR	THR	THR	GLN	LEU	LEU	THR	THR	VAL	THR	GLY	THR	THR	LEU	ASP	VAL	THR	THR	GLY				

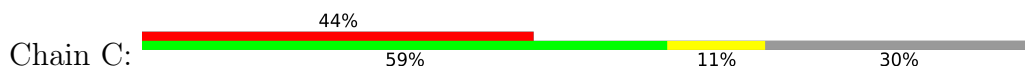
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Y2392	I2452	F2512	S2572	F2632
H2393	V2453	W2513	A2573	Y2633
P2394	I2454	S2514	Q2574	P2634
S2395	L2455	R2515	L2575	L2635
S2396	I2456	W2516	Q2576	ASP
A2397	G2457	T2517	L2577	GLU
H2398	F2458	P2518	R2578	VAL
Q2399	P2459	S2519	L2579	ASP
Q2400	E2460	I2520	Q2580	ALA
G2401	Q2461	L2521	A2581	GLY
P2402	S2462	Q2522	I2582	SER
K2403	K2463	L2523	Q2583	TYR
E2404	T2464	M2524	Q2584	LYS
F2405	S2465	A2525	H2585	ASP
I2406	S2466	H2526	V2586	ASP
E2407	L2467	M2527	M2587	GLY
C2408	H2468	K2528	H2588	SER
V2409	M2469	V2529	H2589	ASP
S2410	C2470	M2530	S2590	TYR
H2411	S2471	L2531	L2591	LYS
I2412	L2472	E2532	R2592	ASP
R2413	F2473	M2533	T2593	ASP
L2414	H2474	V2534	L2594	LYS
L2415	A2475	C2535	P2595	GLY
S2416	F2476	L2536	Q2596	THR
W2417	I2477	H2537	S2597	I28
L2418	F2478	V2538	Q2598	T29
L2419	A2479	I2539	Q2599	T30
L2420	Q2480	S2540	S2600	K31
G2421	L2481	L2541	S2601	L33
S2422	W2482	M2542	A2602	E32
L2423	T2483	E2543	G2603	G34
T2424	V2484	A2544	L2604	T35
H2425	Y2485	L2545	A2605	V36
I2426	C2486	Q2546	A2606	M37
A2427	E2487	E2547	L2607	R38
V2428	Q2488	C2548	R2608	S39
C2429	S2489	M2549	K2609	L40
P2430	A2490	S2550	W2610	G41
H2431	V2491	T2551	L2611	Q42
A2432	A2492	I2552	Q2612	M43
S2433	T2493	F2553	C2613	P44
S2434	N2494	V2554	T2614	T45
P2435	L2495	K2555	Q2615	E46
C2436	Q2496	L2556	F2616	A47
L2437	N2497	I2557	K2617	E48
P2438	Q2498	P2558	M2618	L49
I2439	N2499	M2559	A2619	Q50
P2440	E2500	W2560	W2620	D51
L2441	F2501	L2561	V2621	M52
D2442	S2502	P2562	E2622	I53
A2443	F2503	L2563	I2623	M54
G2444	T2504	M2564	Q2624	E55
S2445	A2505	Q2565	S2625	V56
H2446	I2506	S2566	S2626	ASP
V2447	L2507	N2567	E2627	ALA
D2448	T2508	I2568	A2628	ASP
D2449	A2509	K2569	S2629	GLY
D2450	L2510	H2570	S2630	

Molecule 3: Calmodulin-1

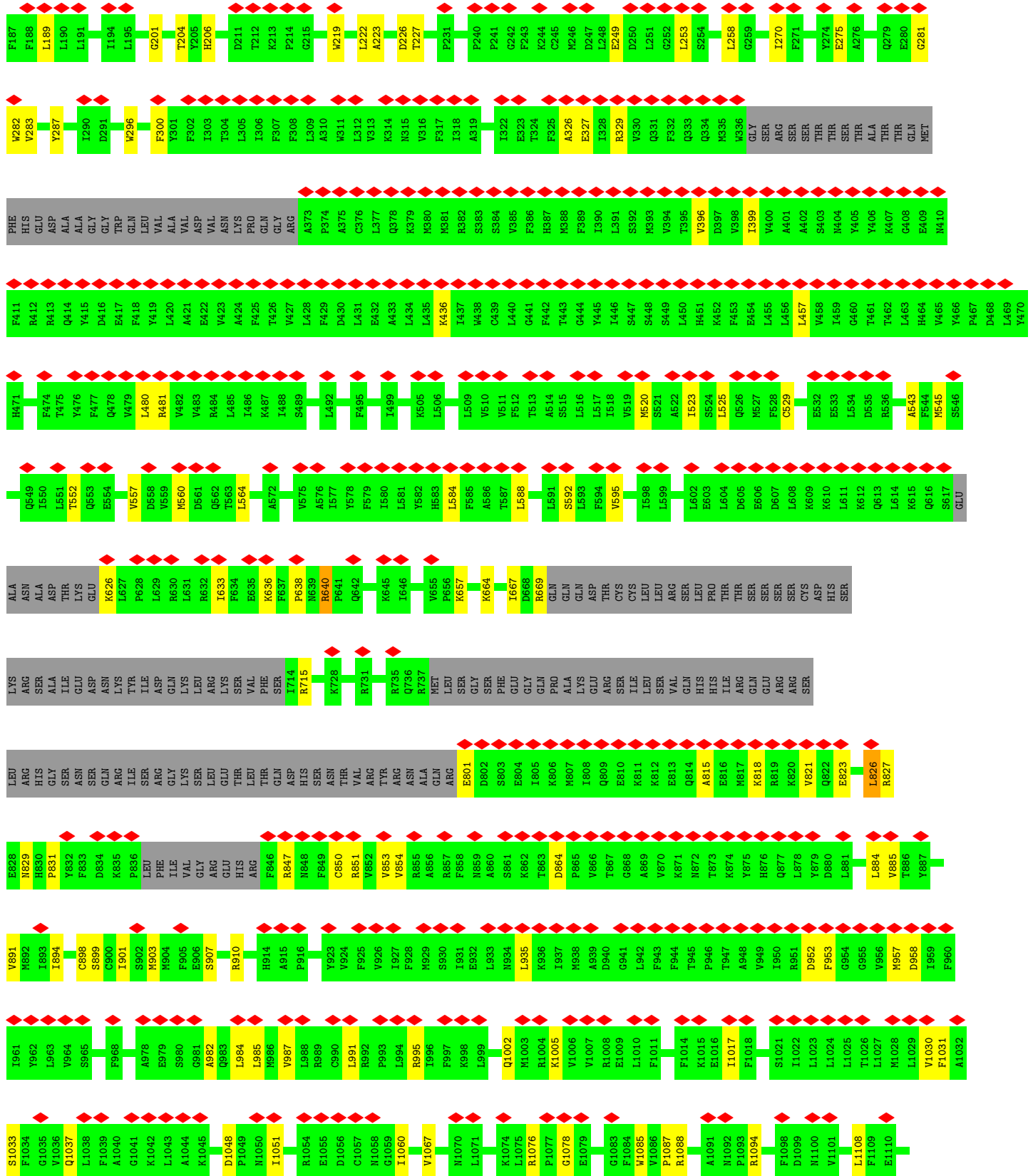


MET	ASN	E121	L28
ALA	G62	V122	T29
ASP	T63	D123	T30
GLN	I64	E124	K31
L5	D65	M125	L33
T6	F66	I126	E32
E7	P67	R127	G34
E8	E68	E128	A95
Q9	F69	A129	D96
I10	L70	D130	G97
A11	T71	I131	N98
E12	M72	D132	G99
F13	M73	G133	I101
K14	A74	D134	S102
E15	R75	G135	L106
A16	K76	Q136	H108
F17	M77	V137	E48
S18	LYS	M138	M110
L19	THR	Y139	T111
F20	ASP	E140	M112
D21	SER	E141	L113
LYS	GLU	F142	G114
ASP	GLU	V143	E115
GLY	I86	Q144	K116
THR	H87	M145	L117
I28	E88	M146	T118
T29	A89	T147	D119
T30	F90	K148	E120
K31	R91	K149	
L33	V92		
E32	F93		
G34	D94		
T35	A95		
V36	D96		
M37	G97		
R38	N98		
S39	G99		
L40	I101		
G41	S102		
Q42	L106		
M43	H108		
P44	E48		
T45	M110		
E46	T111		
A47	M112		
E48	L113		
L49	G114		
Q50	E115		
D51	K116		
M52	L117		
I53	T118		
M54	D119		
E55	E120		

Molecule 4: Sodium leak channel non-selective protein, Extended tegument protein pp150



MET	Y64	L131	H39
LEU	P65	L32	D99
LYS	P66	W32	S40
ARG	F69	I33	L41
LYS	F72	K34	L42
GLN	F73	K35	L43
SER	F74	P36	R43
ARG	L74	W37	I44
VAL	D75	V38	C45
GLU	T76	H39	A46
ALA	L77	S40	I47
GLN	L78	L41	I48
PRO	M79	L42	S49
VAL	F80	L43	S52
THR	L81	L44	M56
THR	L82	L45	T57
ASP	F83	L46	F58
PHE	L84	L47	M59
GLY	L85	L48	T60
PRO	Y86	L49	F61
PRO	L87	L50	H62
ASP	L88	L51	H63
ASP	L89	L52	
ASN	M90	L53	
ALA	I91	L54	
ASP	L92	L55	
ILE	R93	L56	
L31	G94	L57	
W32	I95	L58	
I33	V96	L59	
K34	F97	L60	
K35	G98	L61	
P36	D99	L62	
W37	S100	L63	
V38	I101	L64	
H39	F102	L65	
S40	Y102	L66	
L41	V103	L67	
L42	K104	L68	
R43	D105	L69	
I44	I106	L70	
C45	R106	L71	
A46	I107	L72	
I47	W107	L73	
I48	C108	L74	
S49	V109	L75	
S52	F110	L76	
M56	D111	L77	
T57	G112	L78	
F58	F113	L79	
M59	M114	L80	
T60	V115	L81	
F61	T60	L82	
H62	F116	L83	
H63	C117	L84	
	M118	L85	
	W119	L86	
	V120		
	S121		
	L122		
	I123		
	F124		
	L118		
	W119		
	S180		
	V181		
	S182		
	I183		
	F184		
	L185		
	L186		





ALA	ALA	C376	A310	P241	CYS	ARG	GLU	MET
GLN	GLN	C377	M311	N242	PHE	LEU	ALA	THR
ASN	ASN	D378	L312	N243	THR	LEU	LYS	ARG
THR	THR	V379	C313	T243	VAL	SER	LEU	GLY
GLY	GLY	R380	S314	L244	GLU	ALA	THR	ALA
LEU	LEU	R381	Q315	N245	SER	ALA	ARG	TRP
SER	SER	E382	Y316	C246	SER	ALA	ALA	MET
PHE	PHE	GLU	F317	S247	PRO	SER	ARG	CYS
GLY	GLY	LEU	E318	L248	THR	PRO	LYS	ARG
ILE	ILE	LYS	V319	D249	VAL	LEU	GLN	VAL
ASN	ASN	ASN	T320	VAL	VAL	PRO	HIS	ASP
THR	THR	ASN	Q321	VAL	LEU	SER	GLN	ASP
LEU	LEU	PRO	F322	LYS	LEU	GLY	GLN	GLY
GLU	GLU	SER	N323	GLU	LYS	GLY	GLN	LEU
GLU	GLU	LYS	C324	GLY	ASP	GLY	GLN	TRP
ASN	ASN	THR	R325	GLY	TRP	GLY	GLN	LEU
SER	SER	VAL	K326	GLU	GLU	GLY	GLN	ALA
THR	THR	GLU	T327	MET	GLU	GLY	GLN	ALA
ASN	ASN	GLU	K328	T259	A199	GLY	GLN	ALA
GLU	GLU	LYS	T328	T260	A200	GLY	GLN	ALA
GLU	GLU	SER	P329	C261	G201	GLY	GLN	ALA
GLU	GLU	GLY	C330	R262	G202	GLY	GLN	ALA
GLU	GLU	CYS	K331	Q263	D203	ASN	GLN	ALA
GLU	GLU	HIS	Q332	Q264	G204	ARG	GLU	ALA
GLU	GLU	ARG	Y333	C265	Q205	ARG	GLN	ALA
GLU	GLU	THR	C334	V265	E206	LYS	GLN	ALA
GLU	GLU	SER	L335	E266	E207	ASP	GLN	ALA
GLU	GLU	LEU	E336	A267	V207	ASP	GLN	ALA
GLU	GLU	THR		Y268	R208	SER	GLN	ALA
GLU	GLU	VAL		Q269	S209	LEU	GLU	ALA
GLU	GLU	SER			K210	ARG	GLN	ALA
GLU	GLU	SER			H211	GLN	GLN	ALA
GLU	GLU	ALA			P212	ARG	GLN	ALA
GLU	GLU	THR			T213	PHE	GLN	ALA
GLU	GLU	ARG			P214	LEU	GLN	ALA
GLU	GLU	ARG			L215	GLY	GLN	ALA
GLU	GLU	CYS			K216	ASN	GLN	ALA
GLU	GLU	ASN			N217	ALA	GLN	ALA
GLU	GLU	LEU			L218	LYS	GLN	ALA
GLU	GLU	LEU			V219	TRP	PRO	ALA
GLU	GLU	LEU			L218	VAL	ALA	ALA
GLU	GLU	LEU			D220	TRP	ALA	ALA
GLU	GLU	LEU			F221	VAL	LEU	ALA
GLU	GLU	LEU			Y222	VAL	LEU	ALA
GLU	GLU	LEU			L223	THR	LEU	ALA
GLU	GLU	LEU			S224	GLU	LEU	ALA
GLU	GLU	HIS			F225	SER	LEU	ALA
GLU	GLU	THR			C226	THR	LEU	ALA
GLU	GLU	VAL			N227	VAL	LEU	ALA
GLU	GLU	LEU			S228	CYS	LEU	ALA
GLU	GLU	LEU			Y229	THR	LEU	ALA
GLU	GLU	ALA			T230	VAL	LEU	ALA
GLU	GLU	SER			L231	THR	LEU	ALA
GLU	GLU	SER			T232	CYS	LEU	ALA
GLU	GLU	SER			E233	THR	LEU	ALA
GLU	GLU	SER			L234	VAL	LEU	ALA
GLU	GLU	SER			F235	VAL	LEU	ALA
GLU	GLU	SER			S236	THR	LEU	ALA
GLU	GLU	SER			G237	VAL	LEU	ALA
GLU	GLU	SER			L238	CYS	LEU	ALA
GLU	GLU	SER			S239	THR	LEU	ALA
GLU	GLU	SER			S240	VAL	LEU	ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174294	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)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.947	Depositor
Minimum map value	-1.055	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	556.544, 556.544, 556.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.33	0/14450	0.69	0/19574
2	B	0.32	0/13441	0.68	0/18238
3	E	0.33	0/997	0.67	0/1335
4	C	0.34	0/11701	0.72	0/15843
5	D	0.38	0/1522	0.73	0/2065
All	All	0.33	0/42111	0.69	0/57055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	14143	0	14323	208	0
2	B	13146	0	13362	207	0
3	E	988	0	920	12	0
4	C	11413	0	11682	157	0
5	D	1483	0	1374	30	0
All	All	41173	0	41661	601	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 601 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:B:178:MET:SD	2:B:197:LEU:HD22	1.47	1.53
1:A:1460:LEU:HD22	1:A:1463:MET:CE	1.47	1.40
2:B:178:MET:SD	2:B:197:LEU:CD2	2.34	1.15
1:A:1460:LEU:HD22	1:A:1463:MET:HE2	1.31	1.13
3:E:110:MET:HG3	4:C:1576:LEU:HD11	1.30	1.11

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	1739/3258 (53%)	1635 (94%)	104 (6%)	0	100	100
2	B	1639/2658 (62%)	1527 (93%)	112 (7%)	0	100	100
3	E	118/149 (79%)	111 (94%)	7 (6%)	0	100	100
4	C	1382/1992 (69%)	1311 (95%)	71 (5%)	0	100	100
5	D	178/458 (39%)	162 (91%)	15 (8%)	1 (1%)	25	65
All	All	5056/8515 (59%)	4746 (94%)	309 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	214	PRO

### 5.3.2 Protein sidechains [i](#)

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	1563/2853 (55%)	1554 (99%)	9 (1%)	86	92
2	B	1486/2380 (62%)	1477 (99%)	9 (1%)	86	92
3	E	103/127 (81%)	103 (100%)	0	100	100
4	C	1261/1787 (71%)	1255 (100%)	6 (0%)	88	93
5	D	168/397 (42%)	168 (100%)	0	100	100
All	All	4581/7544 (61%)	4557 (100%)	24 (0%)	89	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2110	ARG
2	B	2153	ASN
2	B	2139	LYS
4	C	640	ARG
1	A	2187	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	269	GLN
4	C	1318	HIS
2	B	2425	HIS
2	B	1022	GLN
4	C	1274	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

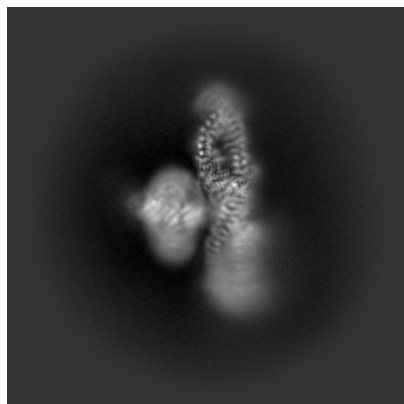
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32544. These allow visual inspection of the internal detail of the map and identification of artifacts.

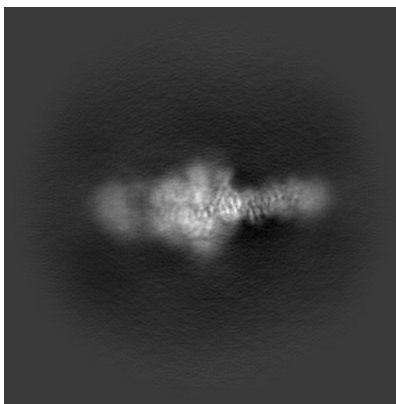
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

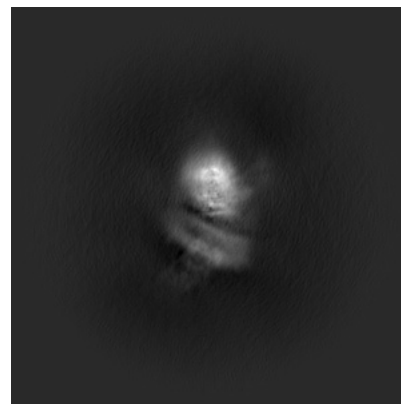
#### 6.1.1 Primary map



X

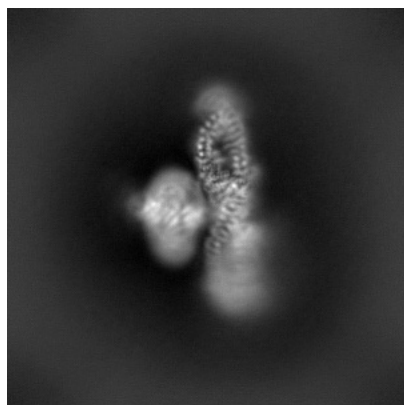


Y

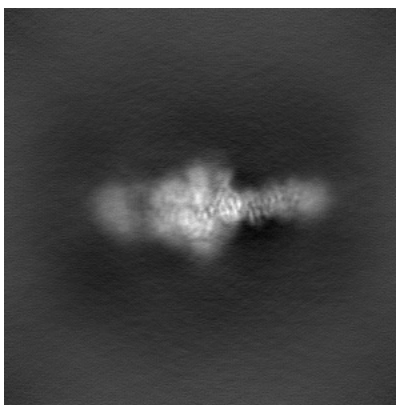


Z

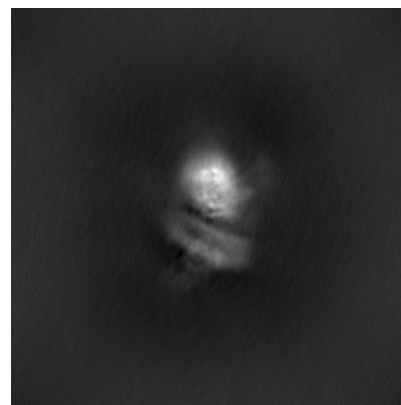
#### 6.1.2 Raw map



X



Y

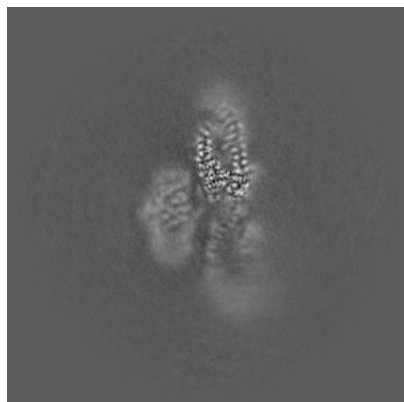


Z

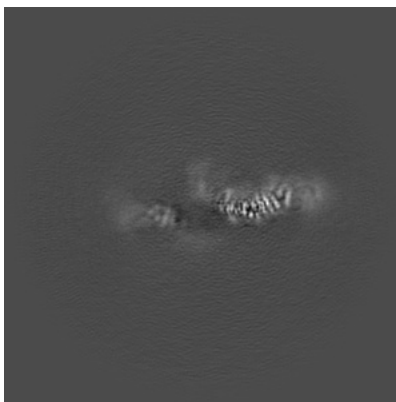
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

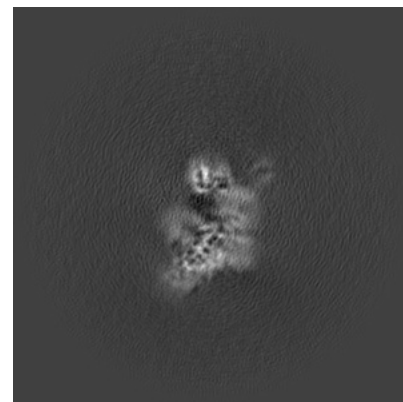
### 6.2.1 Primary map



X Index: 256



Y Index: 256

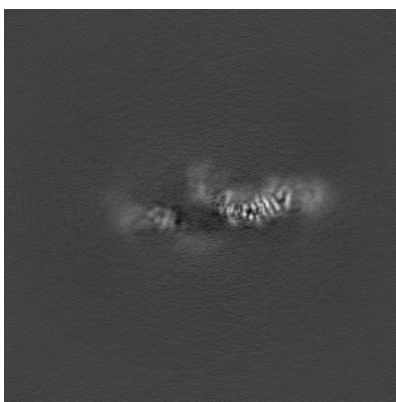


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256

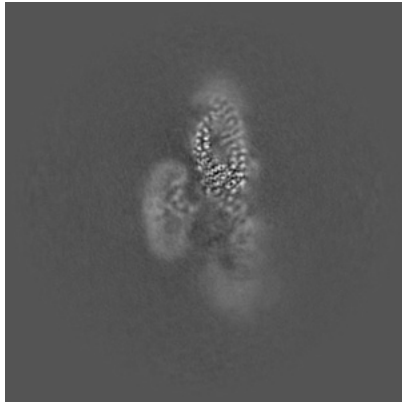


Z Index: 256

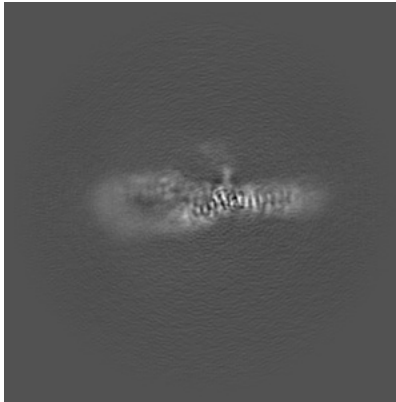
The images above show central slices of the map in three orthogonal directions.

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

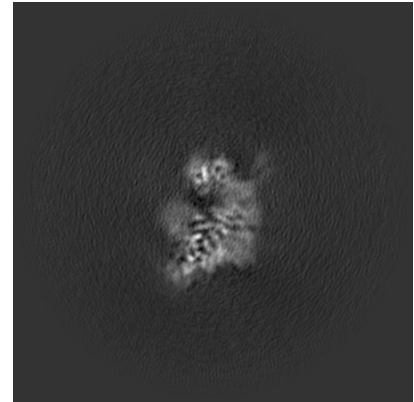
### 6.3.1 Primary map



X Index: 261

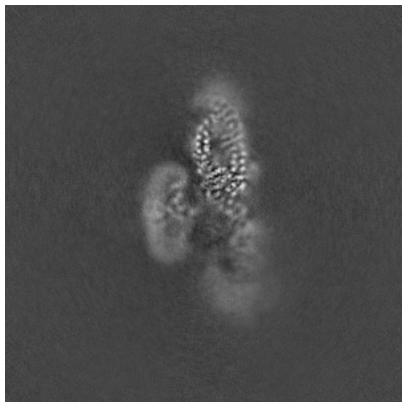


Y Index: 293

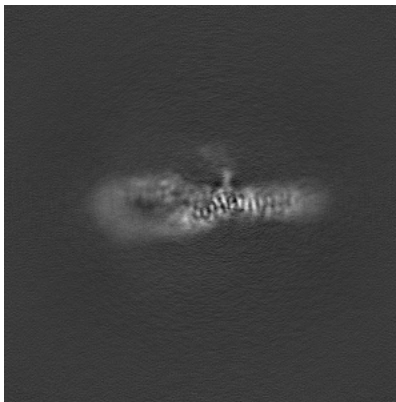


Z Index: 249

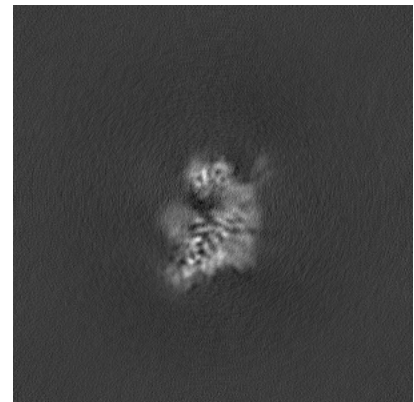
### 6.3.2 Raw map



X Index: 261



Y Index: 293

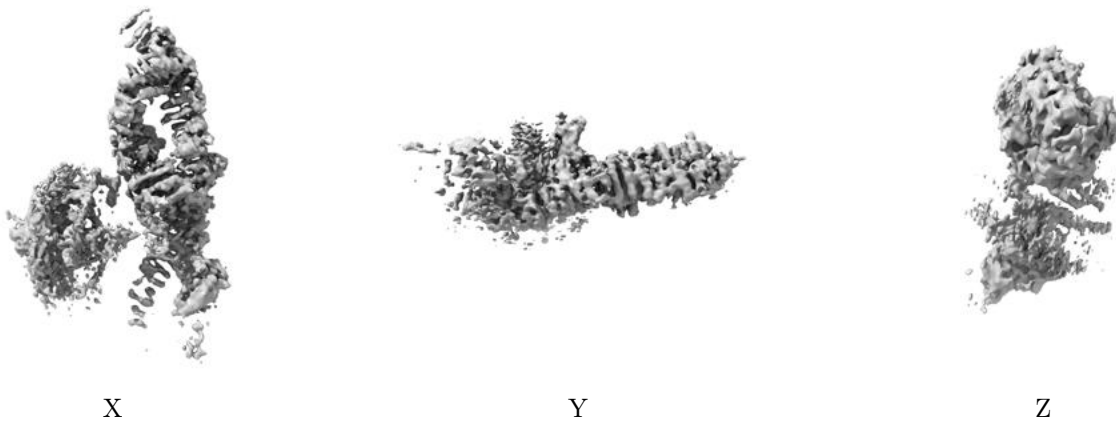


Z Index: 249

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

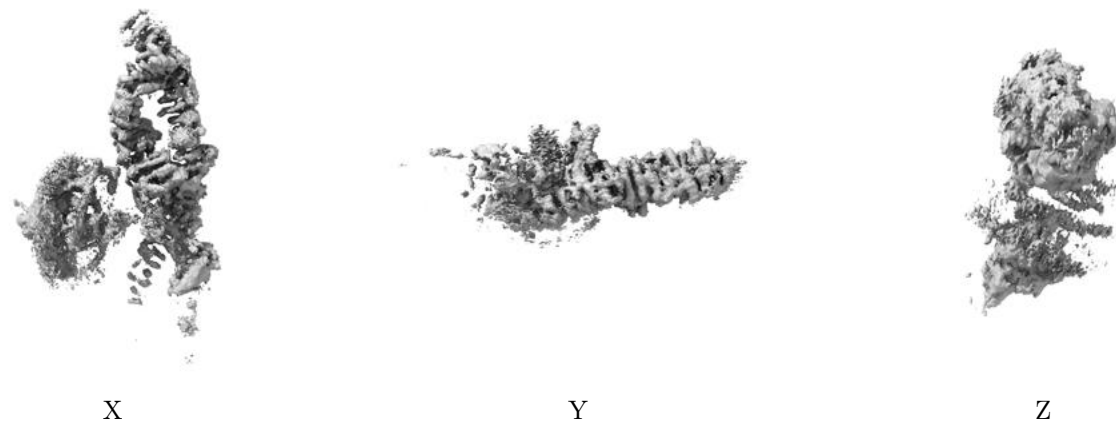
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

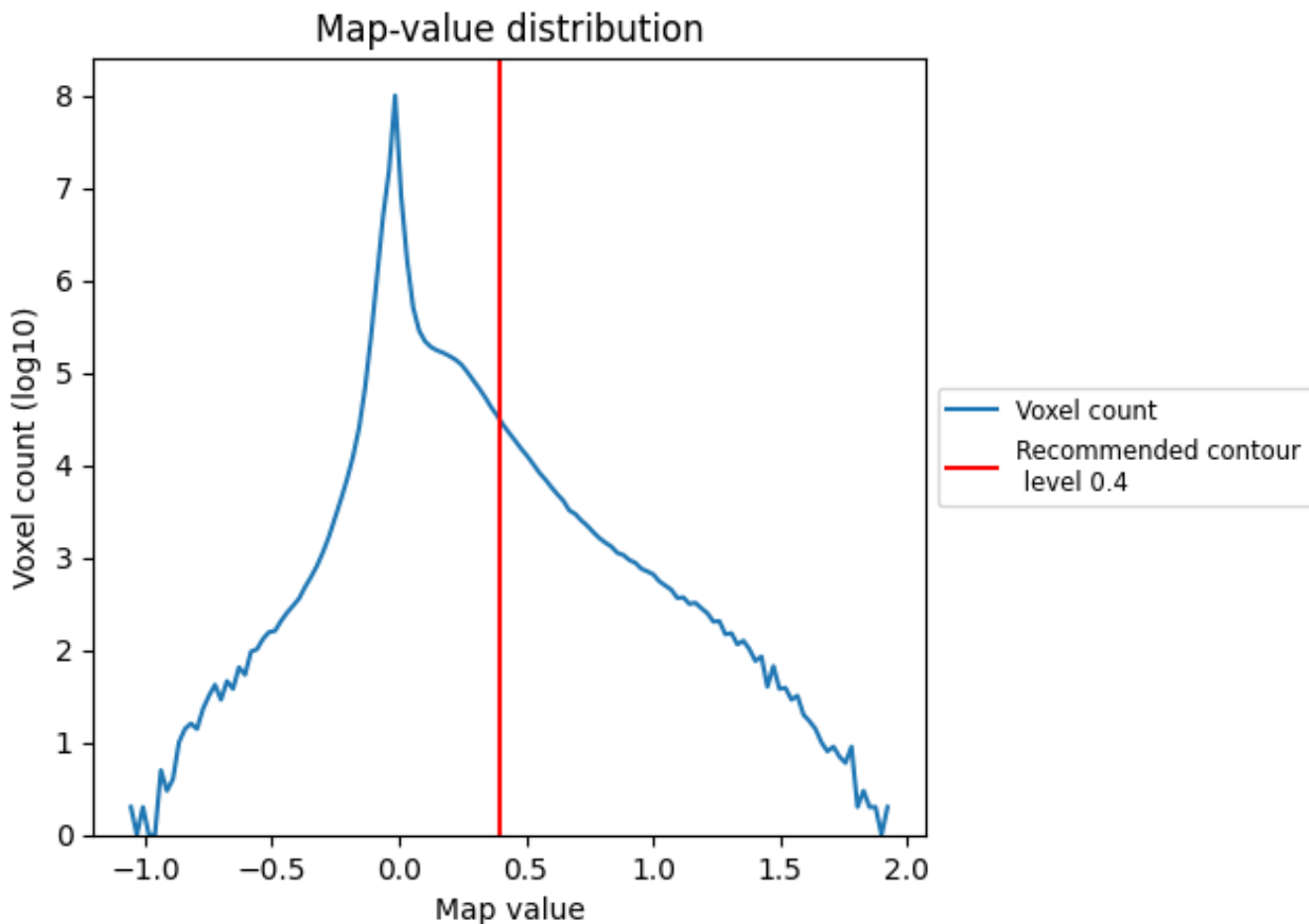
## 6.5 Mask visualisation [i](#)

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.

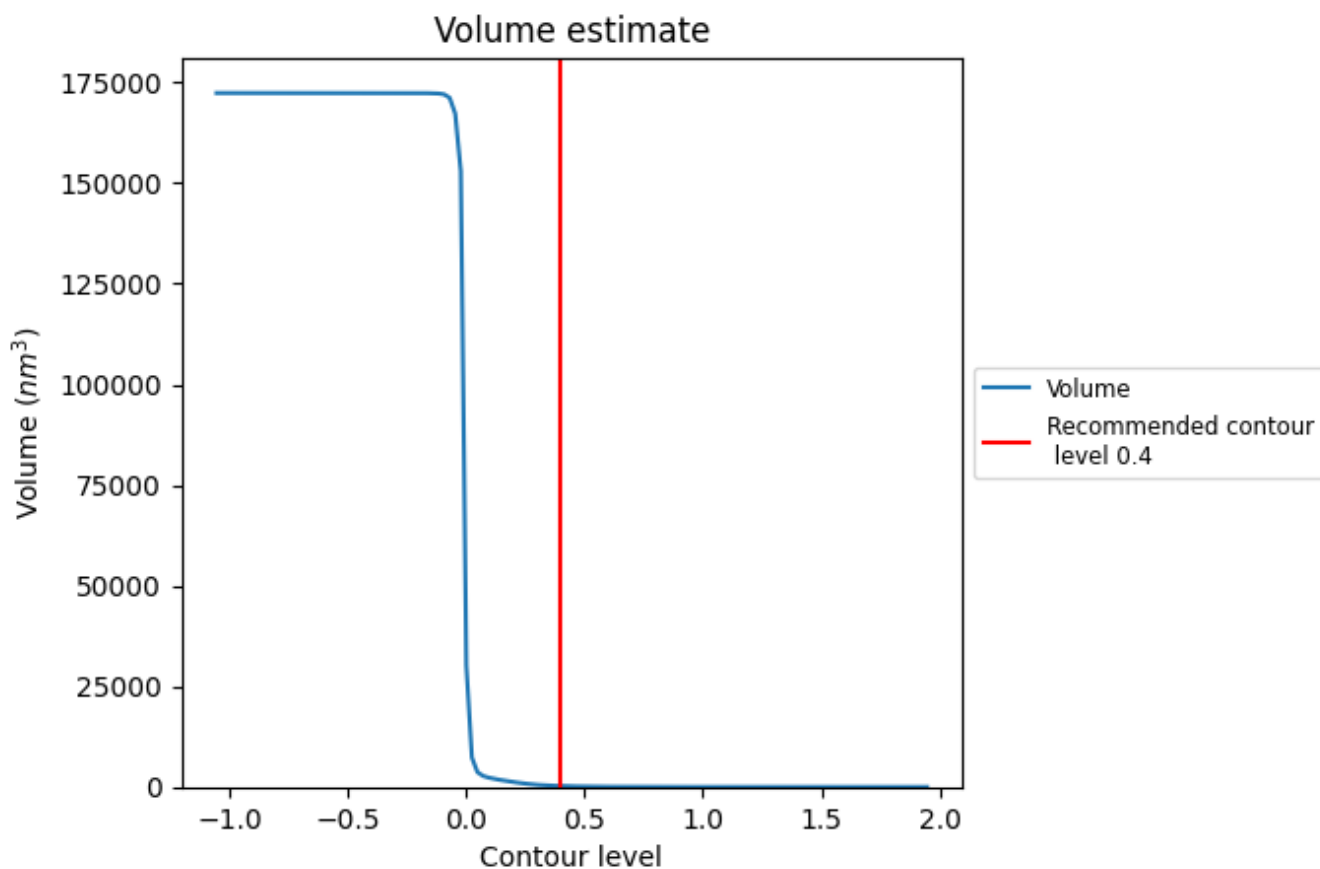
### 7.1 Map-value distribution [i](#)



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.



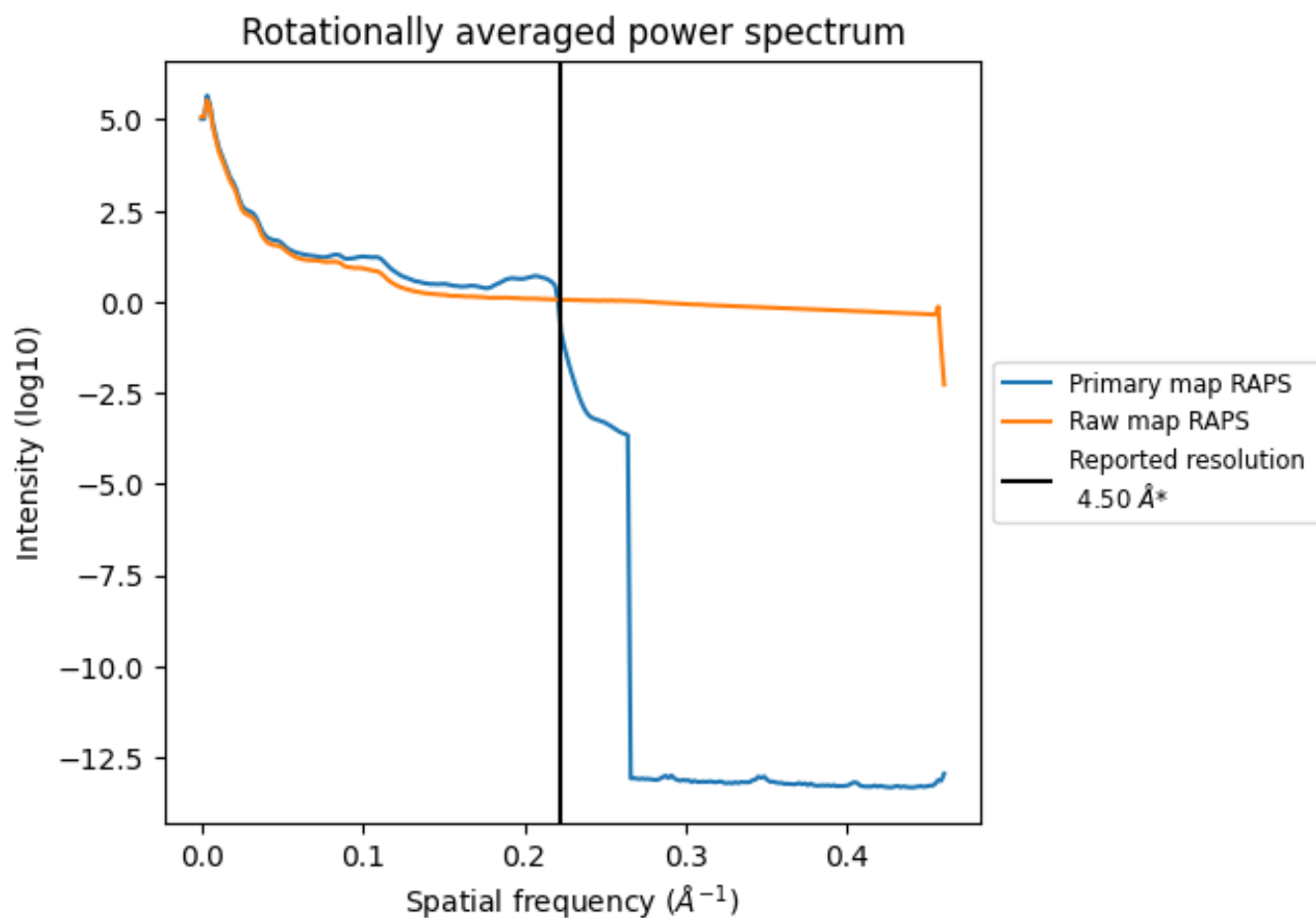
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm<sup>3</sup>; this corresponds to an approximate mass of 207 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 [i](#)

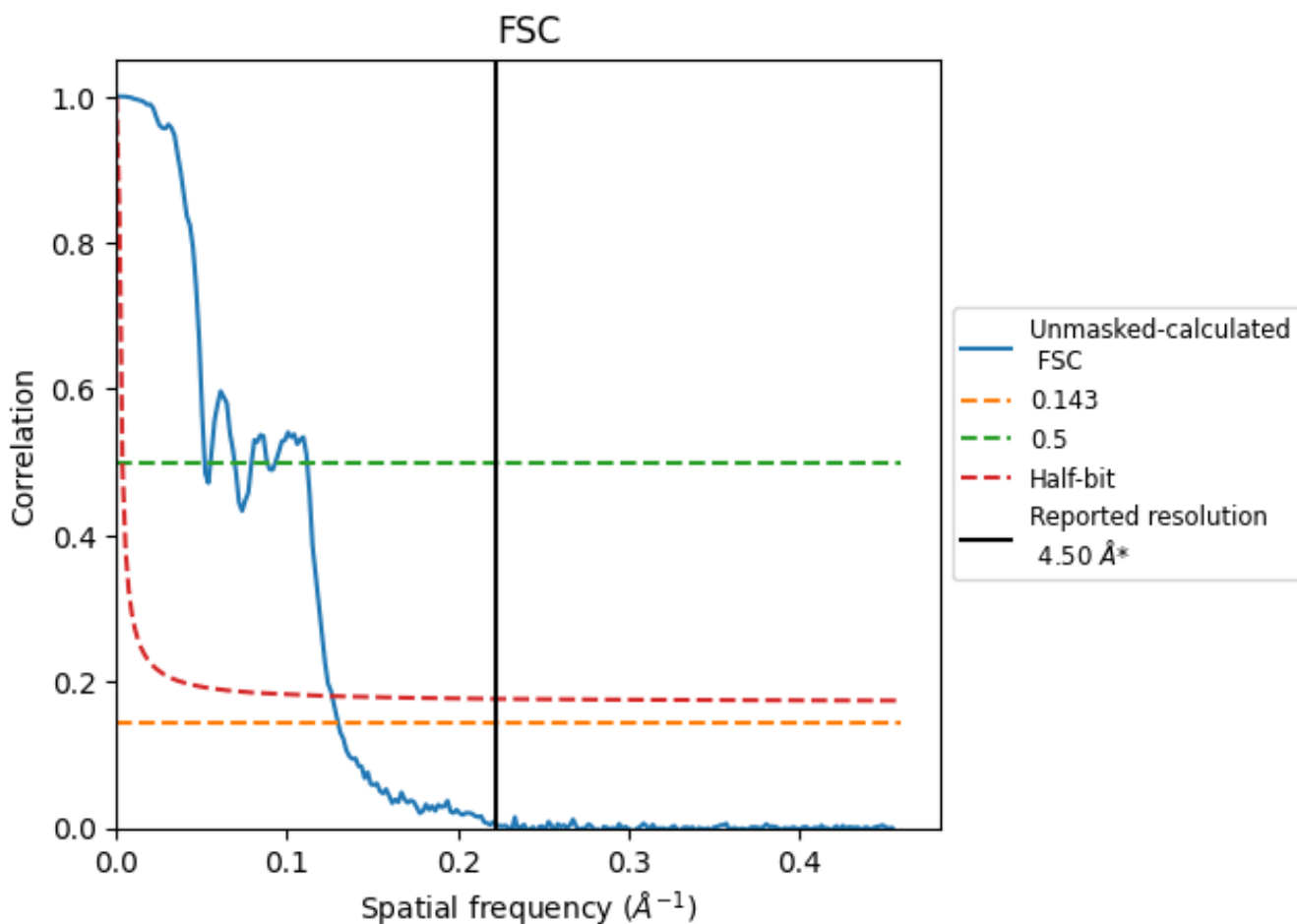


\*Reported resolution corresponds to spatial frequency of  $0.222 \text{ \AA}^{-1}$

## 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 0.222 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

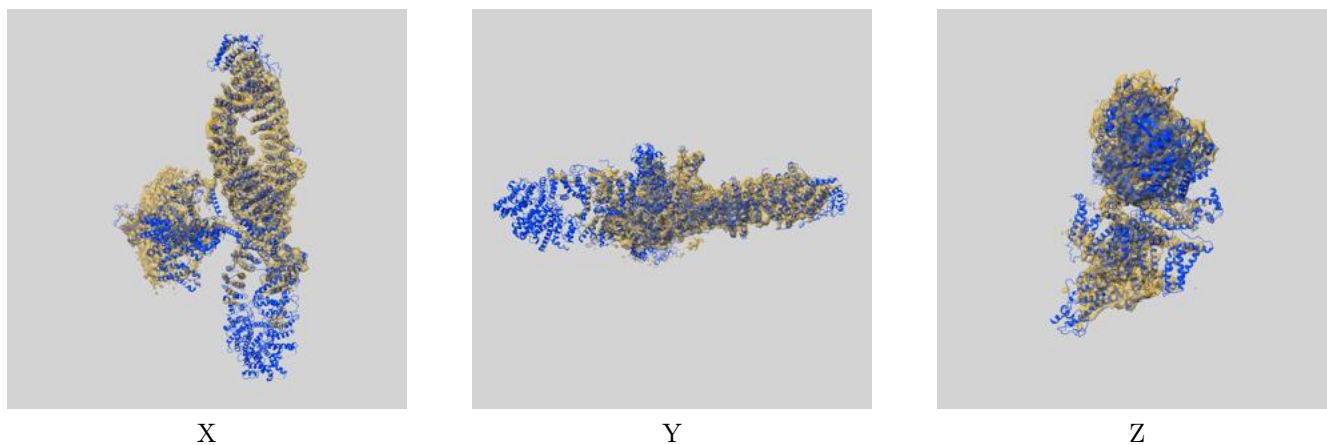
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.70	19.31	7.91

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.70 differs from the reported value 4.5 by more than 10 %

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

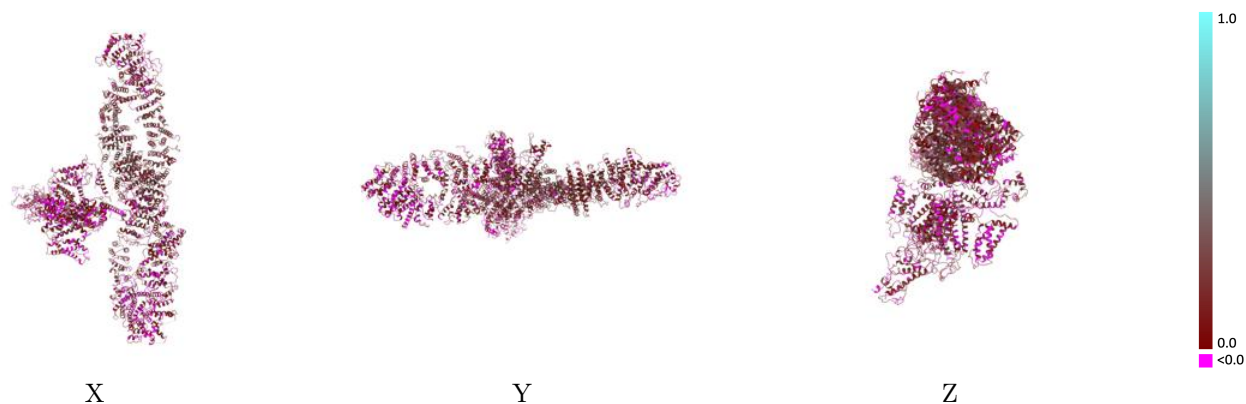
This section contains information regarding the fit between EMDB map EMD-32544 and PDB model 7WJI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



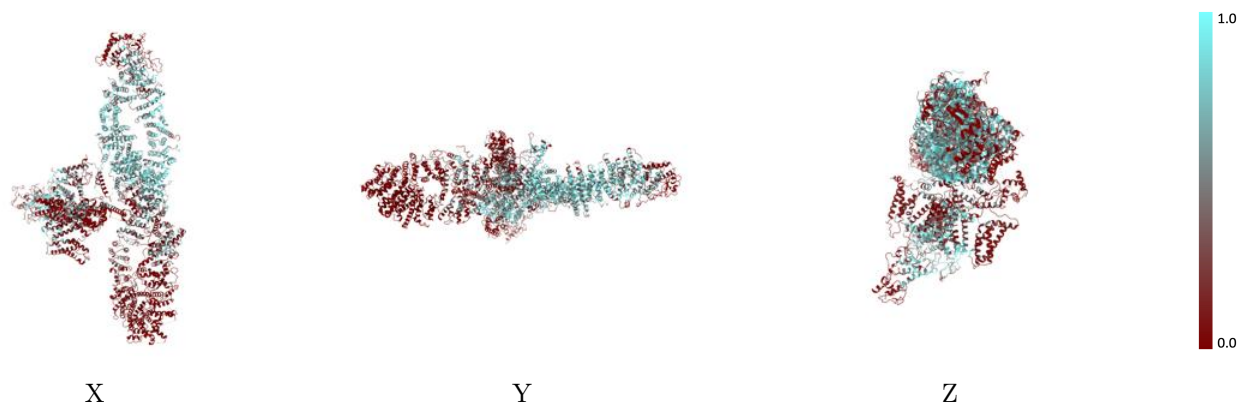
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



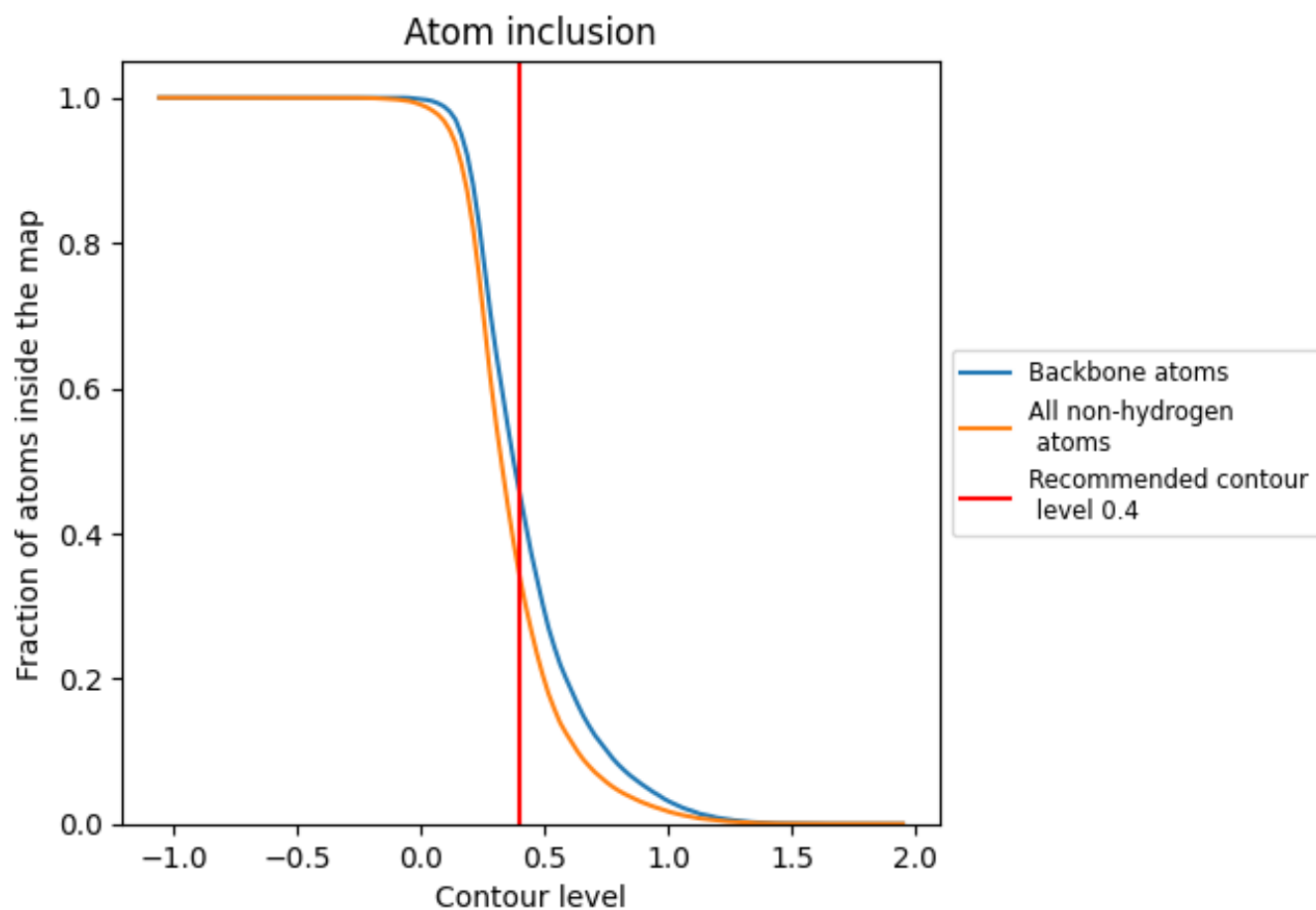
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3406	 0.1390
A	 0.3790	 0.1700
B	 0.3525	 0.1440
C	 0.3141	 0.0990
D	 0.2646	 0.1070
E	 0.0534	 0.1160

