



Full wwPDB EM Validation Report ⓘ

Jun 30, 2025 – 06:28 PM EDT

PDB ID : 9E22 / pdb_00009e22
EMDB ID : EMD-47429
Title : Cryo-EM structure of human cytoplasmic dynein-1 bound to LIS1 in the presence of ATP
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-10-21
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

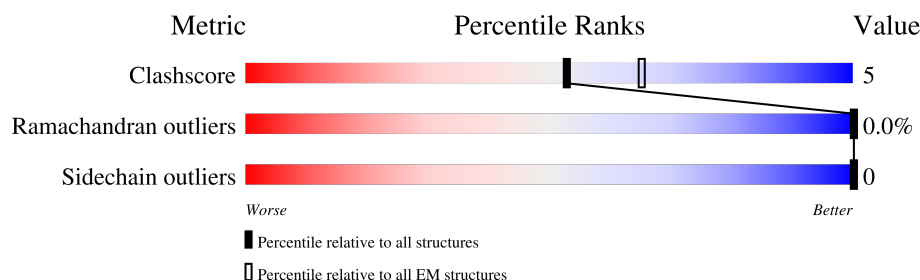
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4843	
2	E	411	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24612 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2925	Total	C	N	O	S	0	0
			22914	14535	3984	4283	112		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-196	GLY	-	expression tag	UNP Q14204
A	-195	ASP	-	expression tag	UNP Q14204
A	-194	TYR	-	expression tag	UNP Q14204
A	-193	ASP	-	expression tag	UNP Q14204
A	-192	ILE	-	expression tag	UNP Q14204
A	-191	PRO	-	expression tag	UNP Q14204
A	-190	THR	-	expression tag	UNP Q14204
A	-189	THR	-	expression tag	UNP Q14204
A	-188	GLU	-	expression tag	UNP Q14204
A	-187	ASN	-	expression tag	UNP Q14204
A	-186	LEU	-	expression tag	UNP Q14204
A	-185	TYR	-	expression tag	UNP Q14204
A	-184	PHE	-	expression tag	UNP Q14204
A	-183	GLN	-	expression tag	UNP Q14204
A	-182	GLY	-	expression tag	UNP Q14204
A	-181	ASP	-	expression tag	UNP Q14204
A	-180	LYS	-	expression tag	UNP Q14204
A	-179	ASP	-	expression tag	UNP Q14204
A	-178	CYS	-	expression tag	UNP Q14204
A	-177	GLU	-	expression tag	UNP Q14204
A	-176	MET	-	expression tag	UNP Q14204
A	-175	LYS	-	expression tag	UNP Q14204
A	-174	ARG	-	expression tag	UNP Q14204
A	-173	THR	-	expression tag	UNP Q14204
A	-172	THR	-	expression tag	UNP Q14204
A	-171	LEU	-	expression tag	UNP Q14204
A	-170	ASP	-	expression tag	UNP Q14204
A	-169	SER	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-168	PRO	-	expression tag	UNP Q14204
A	-167	LEU	-	expression tag	UNP Q14204
A	-166	GLY	-	expression tag	UNP Q14204
A	-165	LYS	-	expression tag	UNP Q14204
A	-164	LEU	-	expression tag	UNP Q14204
A	-163	GLU	-	expression tag	UNP Q14204
A	-162	LEU	-	expression tag	UNP Q14204
A	-161	SER	-	expression tag	UNP Q14204
A	-160	GLY	-	expression tag	UNP Q14204
A	-159	CYS	-	expression tag	UNP Q14204
A	-158	GLU	-	expression tag	UNP Q14204
A	-157	GLN	-	expression tag	UNP Q14204
A	-156	GLY	-	expression tag	UNP Q14204
A	-155	LEU	-	expression tag	UNP Q14204
A	-154	HIS	-	expression tag	UNP Q14204
A	-153	ARG	-	expression tag	UNP Q14204
A	-152	ILE	-	expression tag	UNP Q14204
A	-151	ILE	-	expression tag	UNP Q14204
A	-150	PHE	-	expression tag	UNP Q14204
A	-149	LEU	-	expression tag	UNP Q14204
A	-148	GLY	-	expression tag	UNP Q14204
A	-147	LYS	-	expression tag	UNP Q14204
A	-146	GLY	-	expression tag	UNP Q14204
A	-145	THR	-	expression tag	UNP Q14204
A	-144	SER	-	expression tag	UNP Q14204
A	-143	ALA	-	expression tag	UNP Q14204
A	-142	ALA	-	expression tag	UNP Q14204
A	-141	ASP	-	expression tag	UNP Q14204
A	-140	ALA	-	expression tag	UNP Q14204
A	-139	VAL	-	expression tag	UNP Q14204
A	-138	GLU	-	expression tag	UNP Q14204
A	-137	VAL	-	expression tag	UNP Q14204
A	-136	PRO	-	expression tag	UNP Q14204
A	-135	ALA	-	expression tag	UNP Q14204
A	-134	PRO	-	expression tag	UNP Q14204
A	-133	ALA	-	expression tag	UNP Q14204
A	-132	ALA	-	expression tag	UNP Q14204
A	-131	VAL	-	expression tag	UNP Q14204
A	-130	LEU	-	expression tag	UNP Q14204
A	-129	GLY	-	expression tag	UNP Q14204
A	-128	GLY	-	expression tag	UNP Q14204
A	-127	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-126	GLU	-	expression tag	UNP Q14204
A	-125	PRO	-	expression tag	UNP Q14204
A	-124	LEU	-	expression tag	UNP Q14204
A	-123	MET	-	expression tag	UNP Q14204
A	-122	GLN	-	expression tag	UNP Q14204
A	-121	ALA	-	expression tag	UNP Q14204
A	-120	THR	-	expression tag	UNP Q14204
A	-119	ALA	-	expression tag	UNP Q14204
A	-118	TRP	-	expression tag	UNP Q14204
A	-117	LEU	-	expression tag	UNP Q14204
A	-116	ASN	-	expression tag	UNP Q14204
A	-115	ALA	-	expression tag	UNP Q14204
A	-114	TYR	-	expression tag	UNP Q14204
A	-113	PHE	-	expression tag	UNP Q14204
A	-112	HIS	-	expression tag	UNP Q14204
A	-111	GLN	-	expression tag	UNP Q14204
A	-110	PRO	-	expression tag	UNP Q14204
A	-109	GLU	-	expression tag	UNP Q14204
A	-108	ALA	-	expression tag	UNP Q14204
A	-107	ILE	-	expression tag	UNP Q14204
A	-106	GLU	-	expression tag	UNP Q14204
A	-105	GLU	-	expression tag	UNP Q14204
A	-104	PHE	-	expression tag	UNP Q14204
A	-103	PRO	-	expression tag	UNP Q14204
A	-102	VAL	-	expression tag	UNP Q14204
A	-101	PRO	-	expression tag	UNP Q14204
A	-100	ALA	-	expression tag	UNP Q14204
A	-99	LEU	-	expression tag	UNP Q14204
A	-98	HIS	-	expression tag	UNP Q14204
A	-97	HIS	-	expression tag	UNP Q14204
A	-96	PRO	-	expression tag	UNP Q14204
A	-95	VAL	-	expression tag	UNP Q14204
A	-94	PHE	-	expression tag	UNP Q14204
A	-93	GLN	-	expression tag	UNP Q14204
A	-92	GLN	-	expression tag	UNP Q14204
A	-91	GLU	-	expression tag	UNP Q14204
A	-90	SER	-	expression tag	UNP Q14204
A	-89	PHE	-	expression tag	UNP Q14204
A	-88	THR	-	expression tag	UNP Q14204
A	-87	ARG	-	expression tag	UNP Q14204
A	-86	GLN	-	expression tag	UNP Q14204
A	-85	VAL	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-84	LEU	-	expression tag	UNP Q14204
A	-83	TRP	-	expression tag	UNP Q14204
A	-82	LYS	-	expression tag	UNP Q14204
A	-81	LEU	-	expression tag	UNP Q14204
A	-80	LEU	-	expression tag	UNP Q14204
A	-79	LYS	-	expression tag	UNP Q14204
A	-78	VAL	-	expression tag	UNP Q14204
A	-77	VAL	-	expression tag	UNP Q14204
A	-76	LYS	-	expression tag	UNP Q14204
A	-75	PHE	-	expression tag	UNP Q14204
A	-74	GLY	-	expression tag	UNP Q14204
A	-73	GLU	-	expression tag	UNP Q14204
A	-72	VAL	-	expression tag	UNP Q14204
A	-71	ILE	-	expression tag	UNP Q14204
A	-70	SER	-	expression tag	UNP Q14204
A	-69	TYR	-	expression tag	UNP Q14204
A	-68	SER	-	expression tag	UNP Q14204
A	-67	HIS	-	expression tag	UNP Q14204
A	-66	LEU	-	expression tag	UNP Q14204
A	-65	ALA	-	expression tag	UNP Q14204
A	-64	ALA	-	expression tag	UNP Q14204
A	-63	LEU	-	expression tag	UNP Q14204
A	-62	ALA	-	expression tag	UNP Q14204
A	-61	GLY	-	expression tag	UNP Q14204
A	-60	ASN	-	expression tag	UNP Q14204
A	-59	PRO	-	expression tag	UNP Q14204
A	-58	ALA	-	expression tag	UNP Q14204
A	-57	ALA	-	expression tag	UNP Q14204
A	-56	THR	-	expression tag	UNP Q14204
A	-55	ALA	-	expression tag	UNP Q14204
A	-54	ALA	-	expression tag	UNP Q14204
A	-53	VAL	-	expression tag	UNP Q14204
A	-52	LYS	-	expression tag	UNP Q14204
A	-51	THR	-	expression tag	UNP Q14204
A	-50	ALA	-	expression tag	UNP Q14204
A	-49	LEU	-	expression tag	UNP Q14204
A	-48	SER	-	expression tag	UNP Q14204
A	-47	GLY	-	expression tag	UNP Q14204
A	-46	ASN	-	expression tag	UNP Q14204
A	-45	PRO	-	expression tag	UNP Q14204
A	-44	VAL	-	expression tag	UNP Q14204
A	-43	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	ILE	-	expression tag	UNP Q14204
A	-41	LEU	-	expression tag	UNP Q14204
A	-40	ILE	-	expression tag	UNP Q14204
A	-39	PRO	-	expression tag	UNP Q14204
A	-38	CYS	-	expression tag	UNP Q14204
A	-37	HIS	-	expression tag	UNP Q14204
A	-36	ARG	-	expression tag	UNP Q14204
A	-35	VAL	-	expression tag	UNP Q14204
A	-34	VAL	-	expression tag	UNP Q14204
A	-33	GLN	-	expression tag	UNP Q14204
A	-32	GLY	-	expression tag	UNP Q14204
A	-31	ASP	-	expression tag	UNP Q14204
A	-30	LEU	-	expression tag	UNP Q14204
A	-29	ASP	-	expression tag	UNP Q14204
A	-28	VAL	-	expression tag	UNP Q14204
A	-27	GLY	-	expression tag	UNP Q14204
A	-26	GLY	-	expression tag	UNP Q14204
A	-25	TYR	-	expression tag	UNP Q14204
A	-24	GLU	-	expression tag	UNP Q14204
A	-23	GLY	-	expression tag	UNP Q14204
A	-22	GLY	-	expression tag	UNP Q14204
A	-21	LEU	-	expression tag	UNP Q14204
A	-20	ALA	-	expression tag	UNP Q14204
A	-19	VAL	-	expression tag	UNP Q14204
A	-18	LYS	-	expression tag	UNP Q14204
A	-17	GLU	-	expression tag	UNP Q14204
A	-16	TRP	-	expression tag	UNP Q14204
A	-15	LEU	-	expression tag	UNP Q14204
A	-14	LEU	-	expression tag	UNP Q14204
A	-13	ALA	-	expression tag	UNP Q14204
A	-12	HIS	-	expression tag	UNP Q14204
A	-11	GLU	-	expression tag	UNP Q14204
A	-10	GLY	-	expression tag	UNP Q14204
A	-9	HIS	-	expression tag	UNP Q14204
A	-8	ARG	-	expression tag	UNP Q14204
A	-7	LEU	-	expression tag	UNP Q14204
A	-6	GLY	-	expression tag	UNP Q14204
A	-5	LYS	-	expression tag	UNP Q14204
A	-4	PRO	-	expression tag	UNP Q14204
A	-3	GLY	-	expression tag	UNP Q14204
A	-2	LEU	-	expression tag	UNP Q14204
A	-1	GLY	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q14204
A	1	SER	-	expression tag	UNP Q14204

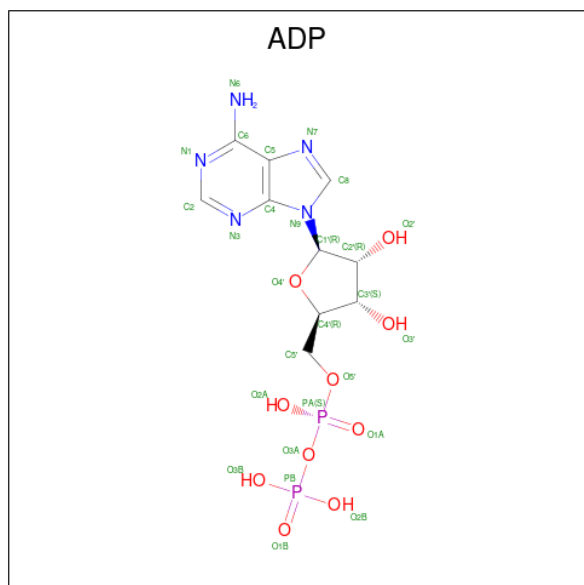
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	320	Total	C	N	O	0	0
			1581	940	320	321		

There are 2 discrepancies between the modelled and reference sequences:

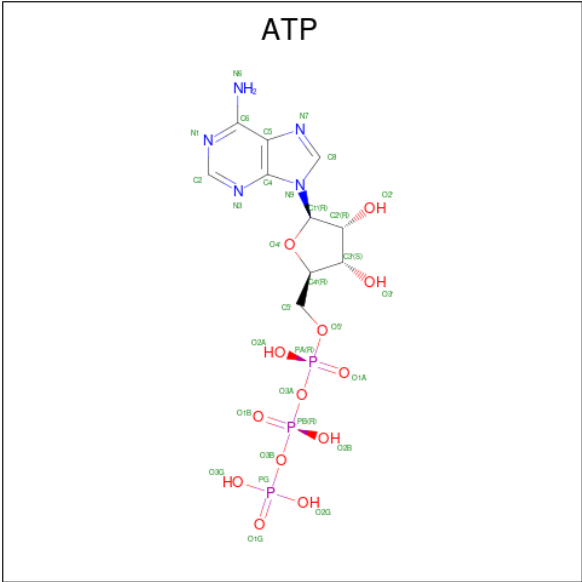
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P43034
E	1	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



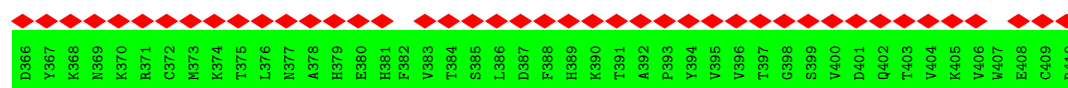
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	



V1975	D1153	F2343	I2532	V2731	G2969	L3091	ALA	SER	GLU	S3475	L3623	V3724
I11978	I2154	E2344	P2533	V2736	E2970	N3092	VAL	ALA	GLU	T3476	E3624	D3725
L11982	L2156	M2361	I2535	M2755	D2971	W3093	SER	ASN	GLU	A3477	S3625	E3726
H11985	L2160	F2364	P2553	M2769	E2974	P3123	LYS	ILE	LYS	L3478	A3626	R3727
K11992	L2161	F2368	P2570	L2769	R2977	M3126	LYS	LYS	ASP	L3479	K3480	R3628
T11993	V2164	L2368	P2581	M2773	T2978	Y3130	HIS	ILE	ALA	S3481	F3629	F3629
S11994	M2176	L2369	L2581	E2775	V2979	K3132	VAL	GLU	ARG	L3482	G3630	G3630
A11995	E2181	P2386	Y2582	T2774	I2990	L3133	GLU	LYS	ASP	S3483	N3631	N3631
W2012	Q2209	R2398	W2584	T2778	A2991	P3134	VAL	GLN	MET	A3484	L3632	L3632
G2021	Q2400	K2399	L2585	T2795	F2992	Q3135	ARG	GLN	LYS	E3485	L3633	L3734
TYR	E2404	G2400	P2590	R2796	I2993	P3137	SER	GLU	ASN	R3486	L3634	Q3735
ALA	E2409	A2409	L2593	R2797	E2996	E3141	ALA	GLU	ASN	E3487	V3638	G3736
GLY	A2408	A2409	G2598	F2807	L3000	L3154	PRO	LYS	PRO	R3488	S3639	E3737
ARG	A2409	A2409	K2601	I2822	L3005	A3157	ALA	VAL	PRO	T3492	S3640	F3738
S2026	L2413	Q2416	L2605	Q2834	E3006	R3160	LYS	GLN	ASN	S3493	Y3641	Q3739
L2039	L2441	Q2416	L2609	L2837	R3007	L3012	GLU	LYS	GLU	E3494	D3642	L3740
A2040	L2444	V2433	M2615	E2838	L3017	V3017	ALA	ILE	ILE	K3491	L3645	R3741
W2041	H2252	L2437	L2620	E2839	P3018	N3019	SER	GLN	VAL	T3492	N3646	L3742
Q2047	A2268	L2437	L2620	A2854	G3019	G3019	ILE	LEU	GLU	S3493	P3647	R3743
L2048	L2259	A2440	L2630	F2858	L3020	L3020	CYS	LYS	LEU	E3494	V3648	Q3744
A2050	N2271	L2443	V2648	D2862	F3021	D3024	LEU	GLN	LEU	T3495	L3649	L3745
L2065	D2277	L2446	V2660	A2866	D3025	G3026	GLY	GLY	CYS	Q3499	E3652	E3746
A2066	G2278	R2451	L2661	L2872	F3026	L3026	THR	THR	VAL	T3502	V3653	K3747
I2069	T2281	Q2464	I2666	F2912	D3029	L3029	ASP	THR	VAL	A3512	R3654	S3748
V2070	H2282	Q2464	I2666	N2913	M3030	G3030	LYS	THR	ASP	F3513	R3655	L3749
F2071	R2292	L2498	Q2677	E2914	T3031	N2913	TRP	TRP	LYS	Y3516	G3657	L3750
F2072	G2293	L2502	L2680	L2920	K3034	D3034	LYS	ILE	ALA	H3535	R3658	A3752
F2073	E2294	S2503	S2681	R2921	D3045	Q3214	GLN	ILE	ALA	A3564	V3660	L3753
L2075	R2298	G2504	F2682	I2922	V3064	V3215	LEU	ARG	GLN	E3575	L3661	K3754
Q2083	Q2299	D2505	I2684	I2925	V3065	E3216	ILE	ASP	ILE	L3586	I3662	E3755
S2084	W2300	M2510	R2684	L2933	M3068	E3217	MET	ASP	ALA	A3596	T3663	V3756
H2085	I2301	E2513	V2687	L2934	N3069	L3218	ARG	GLU	ASP	T3597	L3664	K3757
L2093	D2304	G2515	T2695	L2935	P3070	R3219	GLU	PHE	MET	I3600	G3665	G3758
K2104	L2324	Y2517	V2701	V2958	E3073	G3074	VAL	ILE	ARG	D3606	D3666	R3759
I2136	L2325	L2518	Q2707	K2962	G3074	L3075	THR	THR	ARG	R3607	Q3667	L3760
L2137	R2332	R2519	C2712	K2966	L3076	K3076	ILE	ILE	GLU	L3608	L3668	L3761
P2147	N2338	T2522	R2726	T2967	L3077	D3077	VAL	ASN	LEU	I3609	I3669	L3762
K2148	V2340	L2526		T2968	R3078	R3088	PHE	ASN	ASN	F3614	L3679	D3763
V2150					G3089	G3089				D3616	F3688	D3764
A2151					V3090	V3090				D3617	D3691	D3765
E2152										F3619	D3691	L3766
										R3620	D3691	I3767
										K3621	D3691	T3768
										N3622	D3691	T3769
											D3691	L3770
											D3691	E3771
											D3691	N3772
											D3691	L3773
											D3691	K3774
											D3691	R3775
											D3691	E3776
											D3691	A3777
											D3691	A3778
											D3691	E3779
											D3691	V3780
											D3691	T3781
											D3691	R3782
											D3691	K3783



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.918	Depositor
Minimum map value	-0.525	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.084	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	0.14	0/23382	0.34	0/31728
2	E	0.08	0/1580	0.25	0/2197
All	All	0.14	0/24962	0.34	0/33925

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

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	22914	0	22417	244	0
2	E	1581	0	693	0	0
3	A	54	0	24	1	0
4	A	62	0	24	0	0
5	A	1	0	0	0	0
All	All	24612	0	23158	244	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 5.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:ARG:O	1:A:3725:ASP:HB2	1.74	0.88
1:A:2231:SER:HB3	1:A:2344:GLU:OE2	1.78	0.83
1:A:3645:LEU:O	1:A:3649:LEU:HB2	1.81	0.80
1:A:3624:GLU:O	1:A:3628:ARG:HB2	1.84	0.77
1:A:2601:LYS:HB3	1:A:2736:VAL:HG21	1.70	0.72
1:A:1792:LEU:HD11	1:A:1808:LEU:HD22	1.72	0.72
1:A:1713:LEU:HD11	1:A:1870:PHE:HB3	1.75	0.68
1:A:2503:SER:HB3	1:A:2514:LEU:HD23	1.78	0.66
1:A:1640:ILE:HG12	1:A:1650:LEU:HG	1.78	0.66
1:A:3586:TYR:HD2	1:A:3649:LEU:HD12	1.62	0.64
1:A:3607:ARG:HB3	1:A:3632:PRO:HD3	1.79	0.64
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.80	0.64
1:A:1627:PRO:HB2	1:A:1951:VAL:HB	1.79	0.64
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.79	0.64
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.80	0.63
1:A:1622:GLU:HA	1:A:1699:ASN:HD22	1.64	0.63
1:A:1948:LEU:HD22	1:A:1953:ALA:HB3	1.80	0.63
1:A:2834:GLN:HA	1:A:2837:LEU:HD23	1.80	0.62
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.82	0.62
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.81	0.61
1:A:2838:VAL:HG13	1:A:2839:GLU:HG2	1.83	0.60
1:A:2962:LYS:HE2	1:A:3665:GLY:H	1.67	0.60
1:A:3649:LEU:HD11	1:A:3696:VAL:HG12	1.83	0.60
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.02	0.60
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.83	0.59
1:A:3647:PRO:HG3	1:A:3664:LEU:HB2	1.85	0.59
1:A:4511:LEU:HA	1:A:4514:LEU:HD12	1.85	0.59
1:A:2518:ILE:O	1:A:2522:THR:HB	2.02	0.59
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.84	0.59
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.84	0.58
1:A:2154:ILE:HG13	1:A:2155:PRO:HD3	1.85	0.58
1:A:3012:LEU:HD21	1:A:3064:VAL:HG11	1.85	0.58
1:A:2148:LYS:HG3	1:A:2361:MET:HB2	1.84	0.58
1:A:4068:SER:HA	1:A:4095:MET:HB2	1.85	0.58
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.87	0.57
1:A:1750:VAL:HG12	1:A:1811:LEU:HD11	1.87	0.56
1:A:3840:LEU:HA	1:A:3859:ILE:HD11	1.87	0.56
1:A:3007:ARG:HB2	1:A:3017:VAL:HG11	1.85	0.56
1:A:2769:LEU:HG	1:A:2773:MET:HE2	1.87	0.56
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.86	0.56
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.88	0.56
1:A:2085:HIS:HB2	1:A:2361:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2677:GLN:HB2	1:A:2680:ILE:HG22	1.87	0.56
1:A:3779:GLU:HG2	1:A:3782:ARG:HH12	1.70	0.56
1:A:4628:THR:HG22	1:A:4629:LYS:H	1.71	0.56
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.88	0.56
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.87	0.55
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.87	0.55
1:A:4544:ASN:HA	1:A:4573:ASN:HD21	1.72	0.55
1:A:2992:PHE:HD2	1:A:3064:VAL:HG13	1.70	0.55
1:A:1766:LEU:HA	1:A:1769:MET:HE2	1.88	0.55
1:A:2138:ILE:HG23	1:A:2161:LEU:HD21	1.89	0.55
1:A:4413:PHE:O	1:A:4417:VAL:HB	2.07	0.55
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.87	0.54
1:A:3645:LEU:O	1:A:3649:LEU:CB	2.52	0.54
1:A:3623:LEU:HD22	1:A:3664:LEU:HD23	1.88	0.54
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.73	0.54
1:A:1711:VAL:HG12	1:A:1853:VAL:HG21	1.89	0.54
1:A:2862:ASP:O	1:A:2866:ALA:HB2	2.08	0.54
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.08	0.53
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.90	0.53
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	1.91	0.53
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.90	0.53
1:A:4268:PHE:HE1	1:A:4637:GLU:HG2	1.73	0.53
1:A:2922:ILE:HG12	1:A:2933:LEU:HD21	1.91	0.53
1:A:2222:MET:HG2	1:A:2364:PHE:HE2	1.74	0.53
1:A:2609:LEU:HD11	1:A:2660:VAL:HG11	1.91	0.53
1:A:1708:GLU:HA	1:A:1711:VAL:HG22	1.91	0.52
1:A:1860:GLN:HG2	1:A:1865:LYS:HA	1.92	0.52
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	1.91	0.52
1:A:2083:GLN:HE22	1:A:2150:VAL:HG21	1.75	0.52
1:A:3005:LEU:HD21	1:A:3078:ARG:HD3	1.91	0.52
1:A:4113:LEU:HA	1:A:4116:LEU:HD22	1.91	0.52
1:A:2958:VAL:HA	1:A:2991:ALA:HB3	1.92	0.51
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.92	0.51
1:A:2259:ILE:HD11	1:A:2695:THR:HG22	1.92	0.51
1:A:3767:ILE:HA	1:A:3770:LEU:HD12	1.93	0.51
1:A:2399:LYS:HG3	1:A:2400:GLY:H	1.74	0.50
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.94	0.50
1:A:1899:ARG:HH12	1:A:1982:LEU:HD22	1.76	0.50
1:A:2304:ASP:HA	1:A:2344:GLU:HB3	1.93	0.50
1:A:2464:GLN:HG2	1:A:2583:THR:HA	1.94	0.50
1:A:2150:VAL:HG12	1:A:2152:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:ARG:O	1:A:3725:ASP:CB	2.55	0.50
1:A:4409:LEU:HB3	1:A:4504:LEU:HD21	1.93	0.50
1:A:4211:ASP:HB3	1:A:4252:TYR:HE1	1.76	0.50
1:A:1741:TRP:CZ2	1:A:1750:VAL:HG13	2.47	0.50
1:A:4376:TRP:H	1:A:4376:TRP:CD1	2.29	0.50
1:A:4408:PRO:HB3	1:A:4526:GLN:HE21	1.76	0.50
1:A:2281:THR:HG22	1:A:2325:LEU:HD21	1.94	0.49
1:A:2797:ARG:HH12	1:A:3088:ARG:HD2	1.77	0.49
1:A:2933:LEU:HB3	1:A:3065:VAL:HG22	1.94	0.49
1:A:3691:ASP:O	1:A:3695:ARG:HG2	2.13	0.49
1:A:4444:GLN:HG3	1:A:4449:ARG:HB3	1.95	0.49
1:A:2294:GLU:HA	1:A:2297:LYS:HE3	1.95	0.49
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.94	0.49
1:A:2300:TRP:HE1	1:A:2340:ARG:HD2	1.76	0.48
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.77	0.48
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	1.95	0.48
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.96	0.48
1:A:3624:GLU:O	1:A:3628:ARG:CB	2.59	0.48
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.96	0.48
1:A:2298:ARG:HA	1:A:2338:ASN:HB2	1.95	0.48
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.79	0.48
1:A:4052:SER:HB3	1:A:4097:LYS:HE3	1.96	0.48
1:A:1917:LYS:HG2	1:A:1927:VAL:HG11	1.95	0.47
1:A:2553:PRO:HD2	1:A:2570:PRO:HB2	1.96	0.47
1:A:3626:ALA:HA	1:A:3631:ASN:HD21	1.79	0.47
1:A:1975:VAL:HA	1:A:1978:ILE:HG12	1.96	0.47
1:A:1930:PHE:HZ	1:A:1944:ILE:HG21	1.79	0.47
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.96	0.47
1:A:3973:LEU:HD12	1:A:3992:LEU:HD21	1.96	0.47
1:A:2241:LEU:HB3	1:A:2298:ARG:HH22	1.79	0.47
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.96	0.47
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.80	0.47
1:A:3977:GLU:HG2	1:A:3978:THR:HG23	1.96	0.47
1:A:2221:MET:HB2	1:A:2361:MET:HG2	1.97	0.47
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.49	0.47
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.97	0.47
1:A:1813:THR:HG23	1:A:1880:VAL:HG22	1.95	0.47
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	1.96	0.47
1:A:2872:LEU:HD23	1:A:2920:LEU:HD12	1.97	0.47
1:A:4065:GLN:HB3	1:A:4092:ARG:HD2	1.96	0.47
1:A:2231:SER:HB3	1:A:2344:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.79	0.46
1:A:4544:ASN:HD22	1:A:4591:ARG:HH22	1.62	0.46
1:A:2979:VAL:HG13	1:A:2990:ILE:HD13	1.98	0.46
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.79	0.46
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.97	0.46
1:A:3624:GLU:HA	1:A:3669:ILE:HG22	1.97	0.46
1:A:1713:LEU:HA	1:A:1716:LEU:HG	1.98	0.46
1:A:2519:ARG:HE	1:A:2534:ILE:HD11	1.80	0.46
1:A:2620:LEU:HD11	1:A:2630:LEU:HD21	1.98	0.46
1:A:2775:GLU:HA	1:A:2778:THR:HG22	1.96	0.46
1:A:3730:ASP:HA	1:A:3733:LYS:HD2	1.98	0.46
1:A:4413:PHE:CZ	1:A:4417:VAL:HG21	2.51	0.46
1:A:1814:GLU:O	1:A:1818:GLN:HG2	2.16	0.46
1:A:2581:LEU:O	1:A:2585:LEU:HB2	2.17	0.45
1:A:3874:GLY:HA3	1:A:4144:ILE:HG23	1.97	0.45
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	1.99	0.45
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.97	0.45
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.98	0.45
1:A:3642:ASP:HB3	1:A:3645:LEU:HG	1.99	0.45
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.98	0.45
1:A:1964:GLU:H	1:A:1967:MET:HE3	1.81	0.45
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.52	0.45
1:A:4211:ASP:HB3	1:A:4252:TYR:CE1	2.51	0.45
1:A:3703:VAL:HG11	1:A:3829:LEU:HD22	1.97	0.44
1:A:2075:LEU:HG	1:A:2160:LEU:HD13	1.97	0.44
1:A:2446:ILE:HG22	1:A:2505:ASP:HB2	1.99	0.44
1:A:2935:LEU:HD23	1:A:3092:ASN:HB2	2.00	0.44
1:A:3614:PHE:HE2	1:A:3640:SER:HB2	1.82	0.44
1:A:4066:ILE:HD11	1:A:4095:MET:HG2	2.00	0.44
1:A:4502:LYS:HE2	1:A:4502:LYS:HB2	1.83	0.44
1:A:1985:HIS:CE1	1:A:1992:LYS:HD2	2.52	0.44
1:A:2684:ARG:HD2	1:A:2726:ARG:HB3	1.99	0.44
1:A:2252:HIS:HB2	1:A:2301:ILE:HG12	1.99	0.44
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.52	0.44
1:A:3724:VAL:HA	1:A:3727:LYS:HB2	1.97	0.44
1:A:1729:LYS:HA	1:A:1729:LYS:HD3	1.67	0.44
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	2.00	0.44
1:A:2368:VAL:HG12	1:A:2369:LEU:HD12	2.00	0.44
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	2.00	0.44
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.99	0.44
1:A:4504:LEU:HA	1:A:4507:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2513:GLU:O	1:A:2516:GLU:HG3	2.18	0.44
1:A:4395:LEU:HD22	1:A:4424:LEU:HD12	2.00	0.44
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.98	0.43
1:A:4158:LEU:HD21	1:A:4310:GLU:HG2	1.99	0.43
1:A:1687:LYS:HE3	1:A:1715:LYS:HD2	2.00	0.43
1:A:2104:LYS:HB2	1:A:2136:ILE:HG21	2.01	0.43
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.00	0.43
1:A:1891:THR:HG21	1:A:2039:LEU:HD11	2.00	0.43
1:A:1899:ARG:HH21	1:A:1985:HIS:HB3	1.84	0.43
1:A:3600:ILE:HD13	1:A:3634:LEU:HD13	2.01	0.43
1:A:1800:GLN:H	1:A:1805:ARG:HH22	1.67	0.43
1:A:2996:GLU:HB3	1:A:3068:MET:HB3	2.01	0.43
1:A:3487:GLU:O	1:A:3490:GLU:HG3	2.19	0.43
1:A:3627:LEU:HD23	1:A:3669:ILE:HD12	2.00	0.43
1:A:4408:PRO:HB2	1:A:4523:ALA:HB1	2.00	0.43
1:A:1891:THR:HG22	1:A:4250:SER:HA	2.01	0.42
1:A:3031:THR:HA	1:A:3034:LYS:HG2	2.01	0.42
1:A:2278:GLY:O	1:A:2282:HIS:CB	2.67	0.42
1:A:3513:PHE:HZ	1:A:3575:GLU:HG2	1.84	0.42
1:A:3818:LEU:HA	1:A:4346:MET:HE1	2.01	0.42
1:A:3846:LEU:HD11	1:A:3859:ILE:HD13	2.00	0.42
1:A:2440:ALA:HA	1:A:2443:LEU:HD13	2.00	0.42
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.55	0.42
1:A:2862:ASP:O	1:A:2866:ALA:CB	2.67	0.42
1:A:3588:LEU:HD21	1:A:3688:PHE:CZ	2.54	0.42
1:A:3945:LYS:HA	1:A:3945:LYS:HD3	1.81	0.42
1:A:4246:LEU:HA	1:A:4246:LEU:HD23	1.82	0.42
1:A:2593:LEU:HD11	1:A:2605:LEU:HD13	2.02	0.42
1:A:2838:VAL:HG23	1:A:3093:TRP:CZ2	2.55	0.42
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.34	0.42
1:A:1742:ILE:HG23	1:A:1807:LYS:HD2	2.02	0.42
1:A:2065:LEU:HD12	1:A:2137:LEU:HD22	2.00	0.42
1:A:2755:MET:HG3	1:A:2807:PHE:HD1	1.85	0.42
1:A:2222:MET:HG2	1:A:2364:PHE:CE2	2.55	0.42
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	2.01	0.42
1:A:2440:ALA:HB3	1:A:2502:LEU:HD12	2.02	0.42
1:A:2615:MET:HE2	1:A:2615:MET:HB2	1.99	0.42
1:A:3123:PRO:HG2	1:A:3126:MET:HB2	2.02	0.42
1:A:4631:ASP:HB3	1:A:4634:SER:H	1.85	0.42
1:A:2277:ASP:HB3	1:A:2282:HIS:HB2	2.02	0.42
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4431:LEU:HD12	1:A:4431:LEU:HA	1.89	0.42
1:A:4541:LEU:HD11	1:A:4590:LEU:HD22	2.02	0.42
1:A:2413:LEU:HD23	1:A:2416:GLN:HE21	1.83	0.41
1:A:2072:PHE:HB2	1:A:2164:VAL:HG11	2.02	0.41
1:A:3157:ALA:HA	1:A:3160:ARG:HE	1.84	0.41
1:A:4038:ASN:HB3	1:A:4118:PRO:HG3	2.01	0.41
1:A:3070:PRO:HB3	1:A:3093:TRP:HH2	1.86	0.41
1:A:4408:PRO:HG3	1:A:4527:TYR:HB2	2.03	0.41
1:A:1914:GLU:HG3	3:A:4701:ADP:H3'	2.02	0.41
1:A:2156:LEU:HD11	1:A:4411:ARG:HD3	2.01	0.41
1:A:2993:ILE:HD13	1:A:3065:VAL:HB	2.02	0.41
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.56	0.41
1:A:3662:ILE:H	1:A:3669:ILE:HD11	1.85	0.41
1:A:3819:LYS:HE3	1:A:3819:LYS:HB2	1.88	0.41
1:A:3907:HIS:CG	1:A:3941:LEU:HD11	2.55	0.41
1:A:3597:THR:HA	1:A:3600:ILE:HG22	2.02	0.41
1:A:3740:LEU:HA	1:A:3743:ARG:HG2	2.01	0.41
1:A:4565:LEU:HD12	1:A:4642:VAL:HG22	2.02	0.41
1:A:2175:MET:HE2	1:A:2175:MET:HB3	1.92	0.41
1:A:2181:GLU:HG3	1:A:2244:LEU:HD13	2.01	0.41
1:A:2854:ALA:O	1:A:2858:PHE:HB2	2.21	0.41
1:A:3021:PHE:HB3	1:A:3029:LEU:HD21	2.02	0.41
1:A:3136:PRO:HA	1:A:3137:PRO:HD3	1.92	0.41
1:A:4189:ILE:HD12	1:A:4321:LEU:HA	2.02	0.41
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.03	0.40
1:A:4268:PHE:CE1	1:A:4637:GLU:HG2	2.55	0.40
1:A:2443:LEU:HD23	1:A:2510:MET:HB3	2.02	0.40
1:A:2532:ILE:HD12	1:A:2533:PRO:HD2	2.03	0.40
1:A:2684:ARG:HA	1:A:2687:VAL:HG12	2.03	0.40
1:A:2822:ILE:HD11	1:A:2866:ALA:HB1	2.03	0.40
1:A:4489:LEU:HA	1:A:4492:ILE:HG22	2.04	0.40
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.02	0.40
1:A:2050:ALA:HB2	1:A:2093:LEU:HD21	2.03	0.40
1:A:4492:ILE:HD13	1:A:4507:ILE:HG21	2.02	0.40
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.86	0.40
1:A:3134:PRO:HD2	1:A:3141:GLU:HG2	2.03	0.40
1:A:2661:LEU:HD23	1:A:2661:LEU:HA	1.92	0.40
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2917/4843 (60%)	2833 (97%)	83 (3%)	1 (0%)	100	100
2	E	318/411 (77%)	302 (95%)	16 (5%)	0	100	100
All	All	3235/5254 (62%)	3135 (97%)	99 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1629	PHE

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	2434/4279 (57%)	2434 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1863	ASN
1	A	1979	GLN
1	A	2083	GLN
1	A	2085	HIS
1	A	2109	GLN

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Mol	Chain	Res	Type
1	A	2271	ASN
1	A	2416	GLN
1	A	2464	GLN
1	A	2549	GLN
1	A	2752	ASN
1	A	3047	HIS
1	A	3158	ASN
1	A	3499	GLN
1	A	3534	HIS
1	A	3646	ASN
1	A	4131	ASN
1	A	4291	HIS
1	A	4466	HIS
1	A	4506	ASN
1	A	4573	ASN
1	A	4595	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
3	ADP	A	4705	-	24,29,29	0.89	0	29,45,45	1.32	4 (13%)
4	ATP	A	4702	5	28,33,33	0.70	0	34,52,52	0.61	1 (2%)
4	ATP	A	4704	-	28,33,33	0.67	0	34,52,52	0.65	1 (2%)
3	ADP	A	4701	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)

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
3	ADP	A	4705	-	-	3/12/32/32	0/3/3/3
4	ATP	A	4702	5	-	2/18/38/38	0/3/3/3
4	ATP	A	4704	-	-	6/18/38/38	0/3/3/3
3	ADP	A	4701	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4701	ADP	N3-C2-N1	-3.84	123.45	128.67
3	A	4705	ADP	N3-C2-N1	-3.60	123.79	128.67
3	A	4705	ADP	C4-C5-N7	-2.72	106.46	109.34
3	A	4705	ADP	O4'-C1'-N9	2.45	112.00	108.75
4	A	4702	ATP	C5-C6-N6	2.36	123.91	120.31
3	A	4701	ADP	C4-C5-N7	-2.33	106.87	109.34
4	A	4704	ATP	C5-C6-N6	2.29	123.81	120.31
3	A	4705	ADP	C4'-O4'-C1'	-2.10	108.00	109.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4705	ADP	C5'-O5'-PA-O1A
3	A	4705	ADP	C5'-O5'-PA-O2A
3	A	4705	ADP	C5'-O5'-PA-O3A
4	A	4704	ATP	C5'-O5'-PA-O1A
4	A	4704	ATP	C5'-O5'-PA-O3A
4	A	4704	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	4704	ATP	C3'-C4'-C5'-O5'
3	A	4701	ADP	PB-O3A-PA-O1A
4	A	4702	ATP	PG-O3B-PB-O1B
4	A	4704	ATP	C5'-O5'-PA-O2A
3	A	4701	ADP	PB-O3A-PA-O2A
3	A	4701	ADP	O4'-C4'-C5'-O5'
4	A	4704	ATP	PG-O3B-PB-O2B
4	A	4702	ATP	PG-O3B-PB-O2B

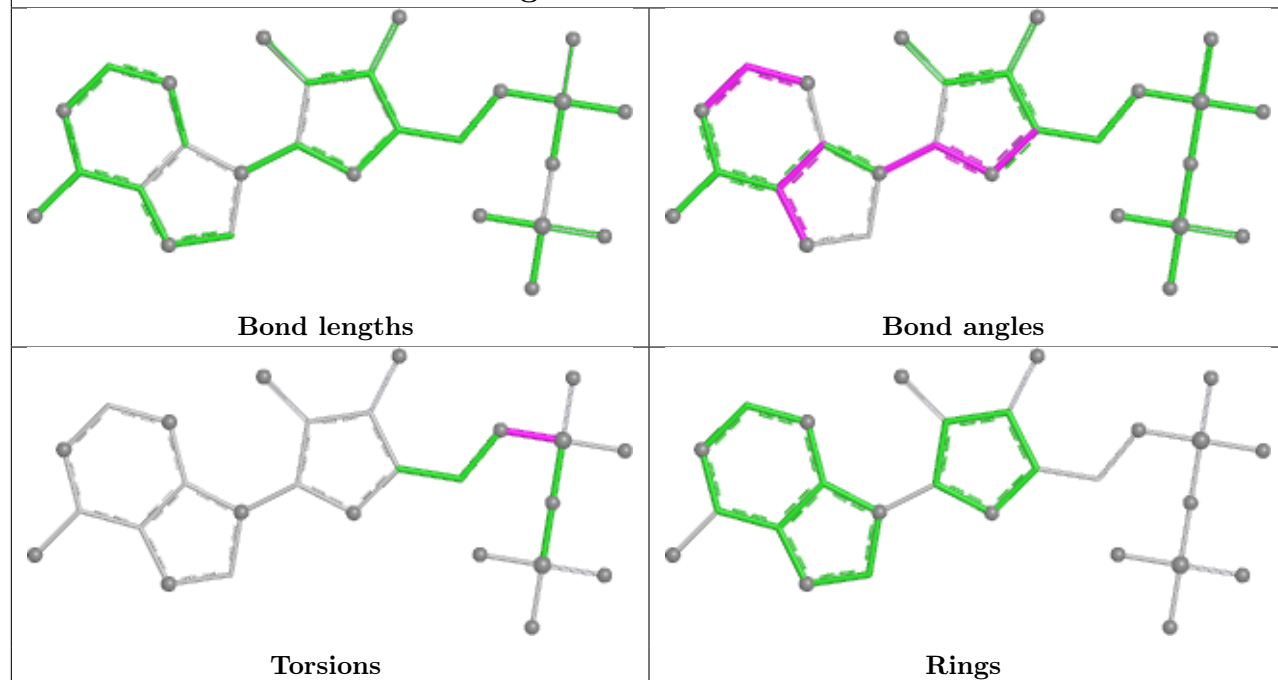
There are no ring outliers.

1 monomer is involved in 1 short contact:

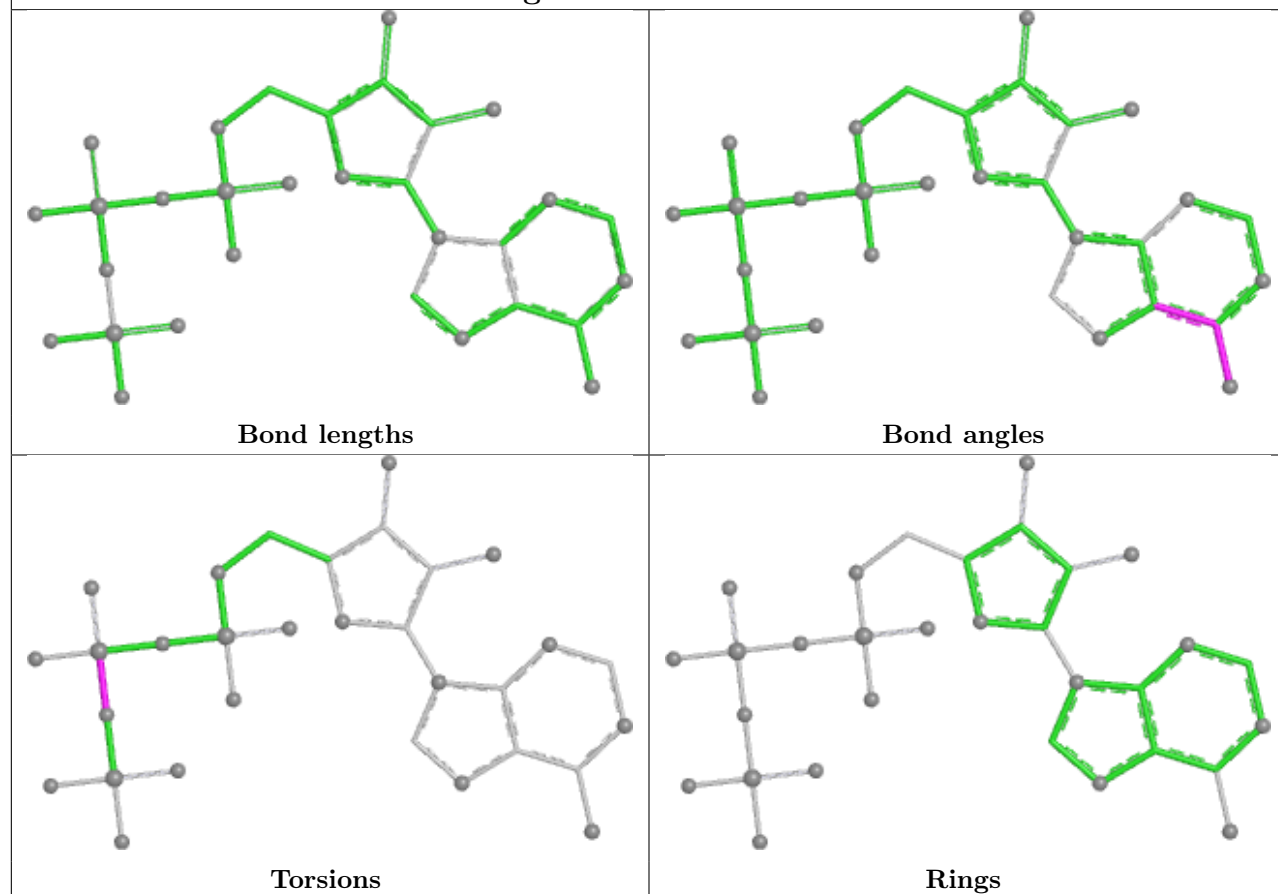
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4701	ADP	1	0

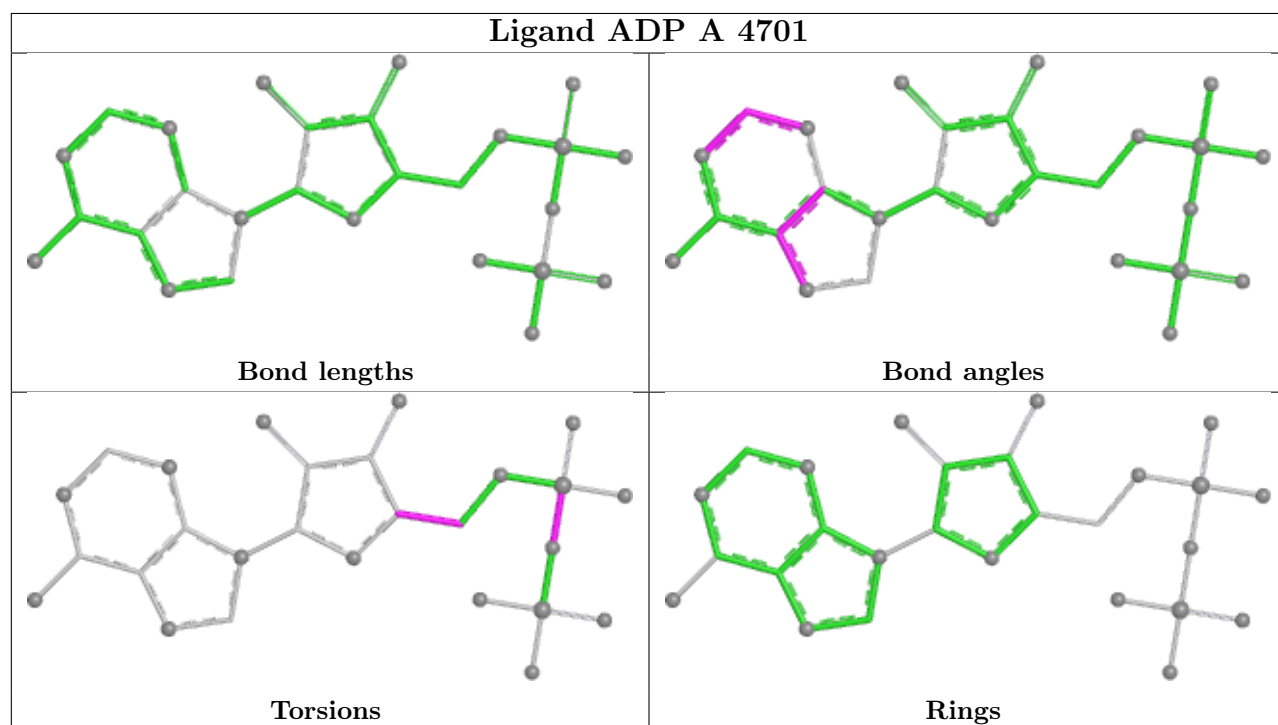
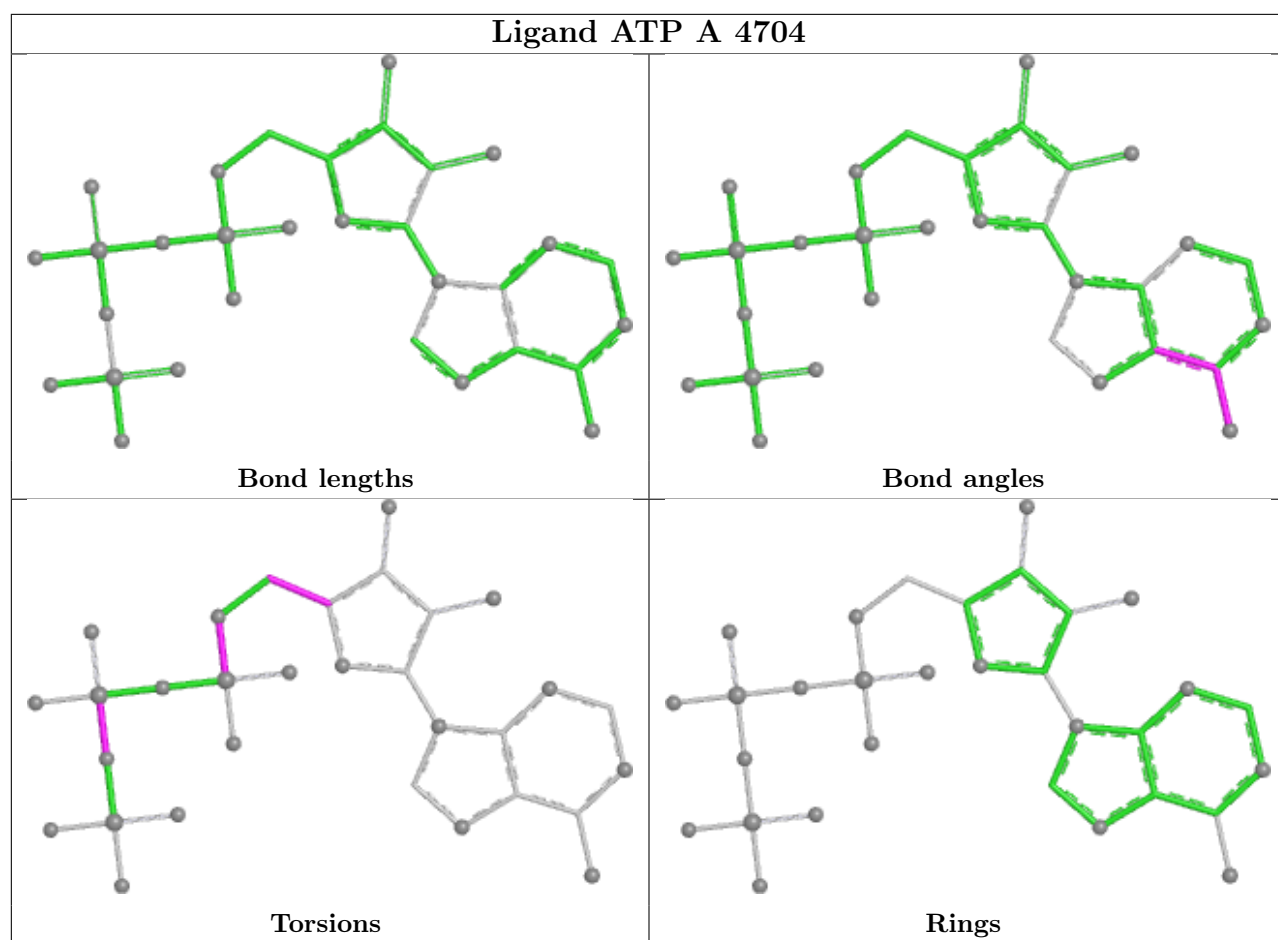
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ADP A 4705



Ligand ATP A 4702





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.

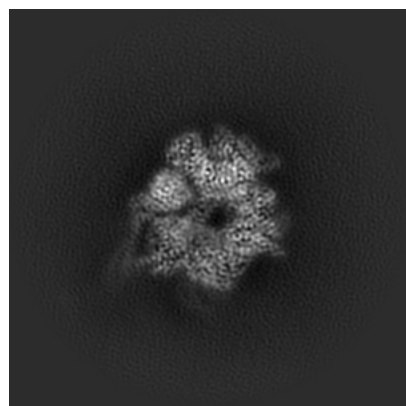
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47429. These allow visual inspection of the internal detail of the map and identification of artifacts.

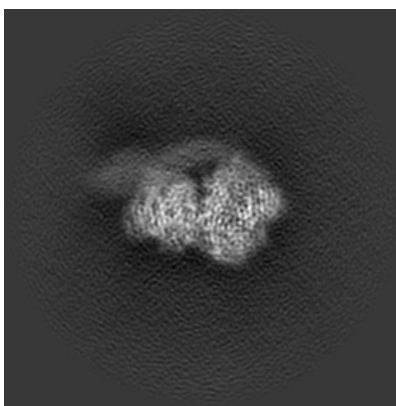
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

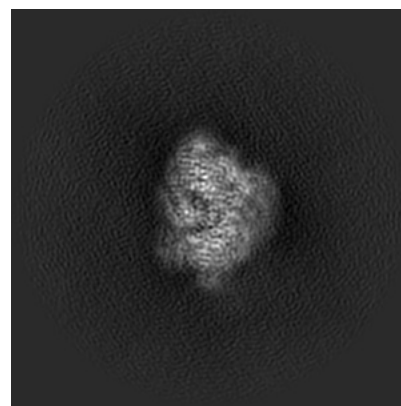
6.1.1 Primary map



X

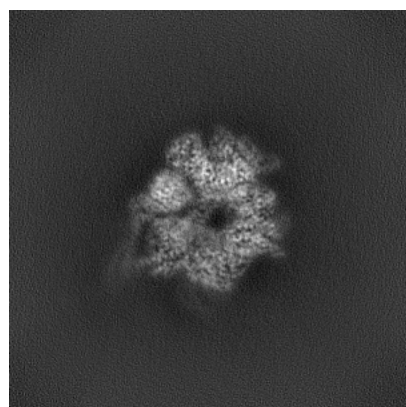


Y

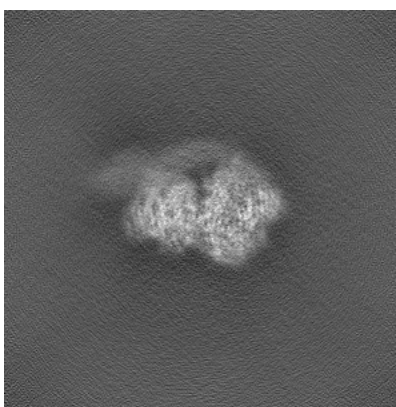


Z

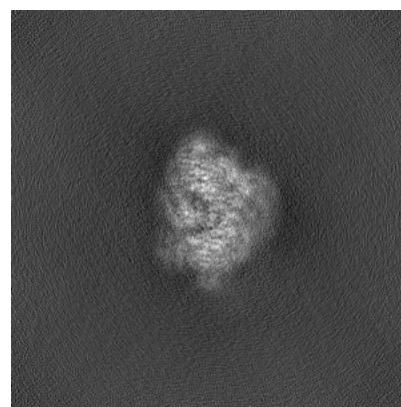
6.1.2 Raw map



X



Y

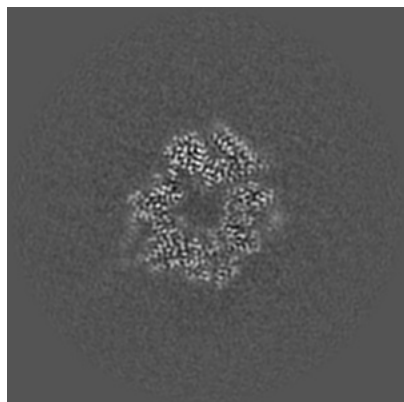


Z

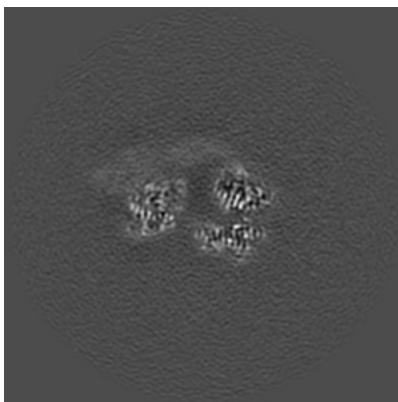
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

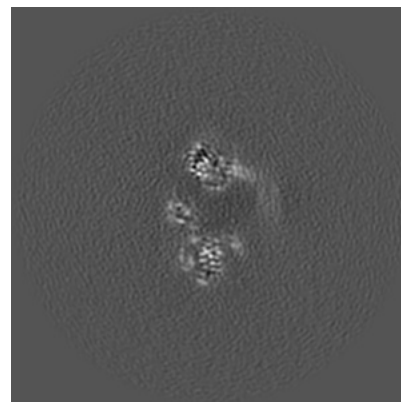
6.2.1 Primary map



X Index: 176

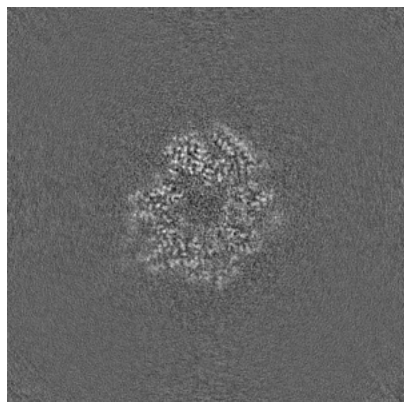


Y Index: 176

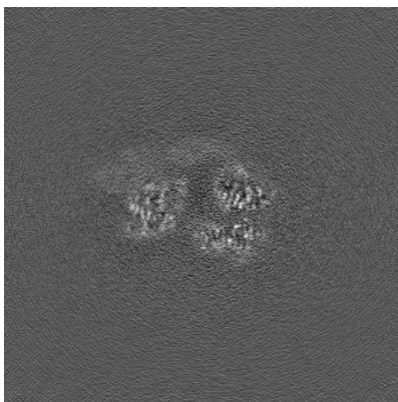


Z Index: 176

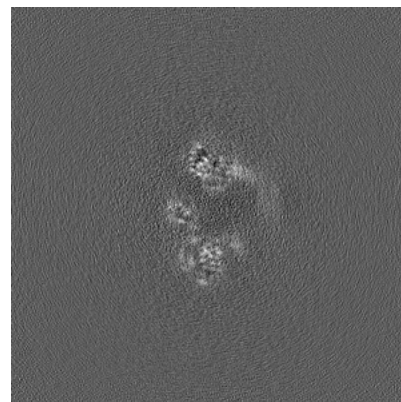
6.2.2 Raw map



X Index: 176



Y Index: 176

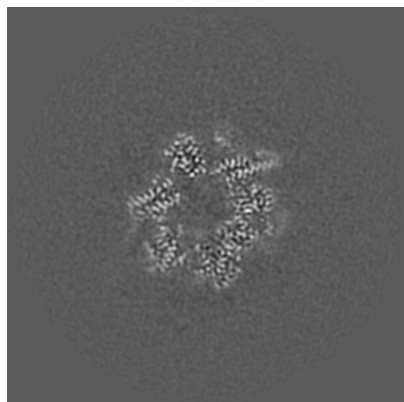


Z Index: 176

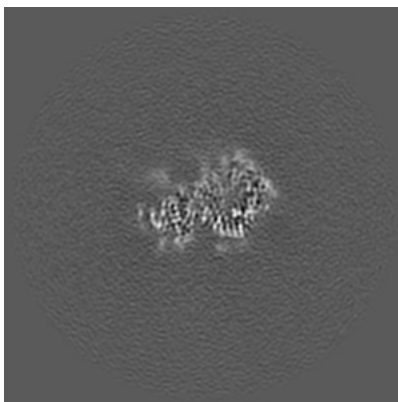
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

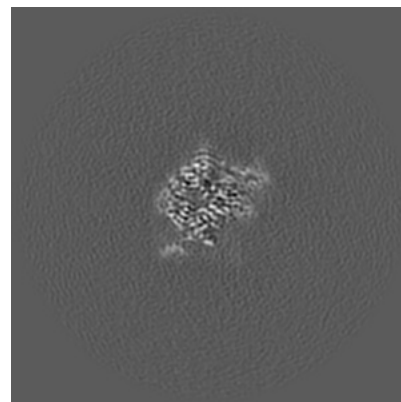
6.3.1 Primary map



X Index: 170

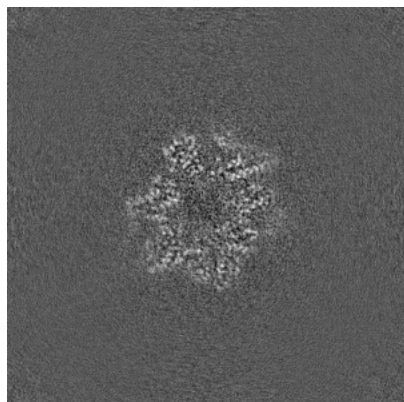


Y Index: 204

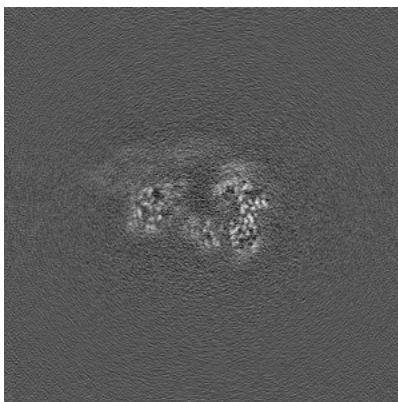


Z Index: 208

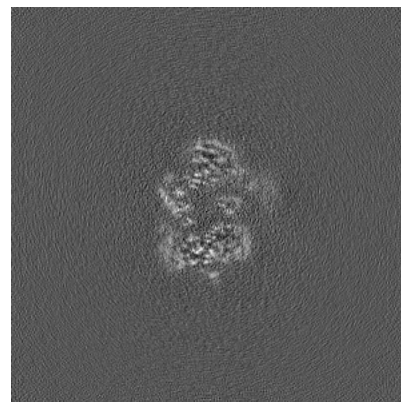
6.3.2 Raw map



X Index: 172



Y Index: 171

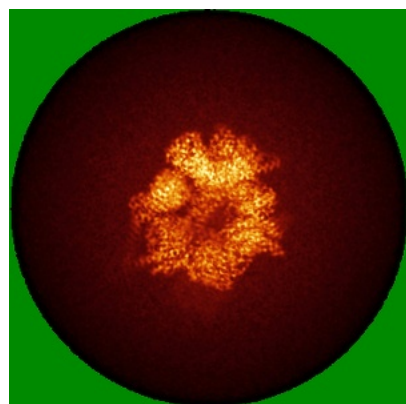


Z Index: 188

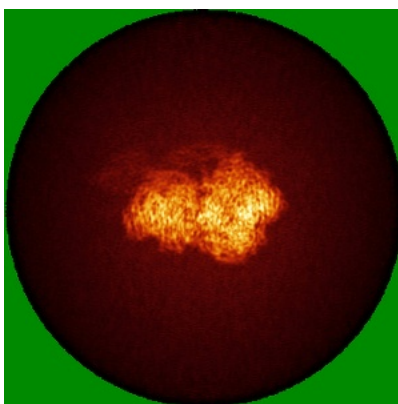
The images above show the largest variance slices of the map in three orthogonal directions.

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

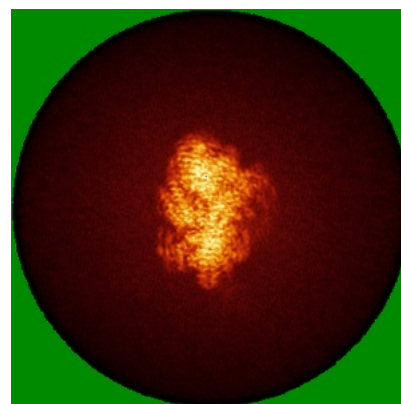
6.4.1 Primary map



X

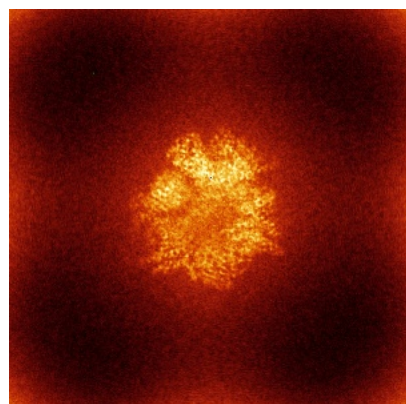


Y

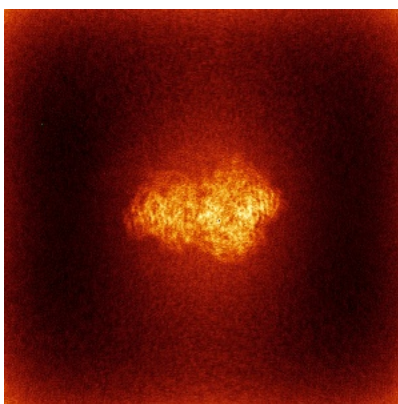


Z

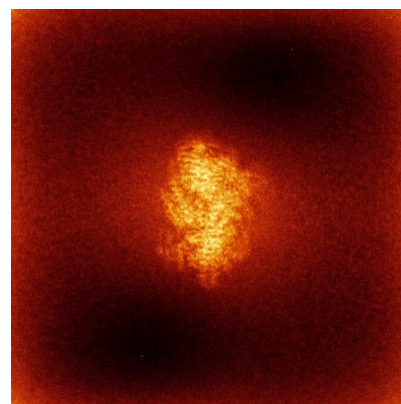
6.4.2 Raw map



X



Y

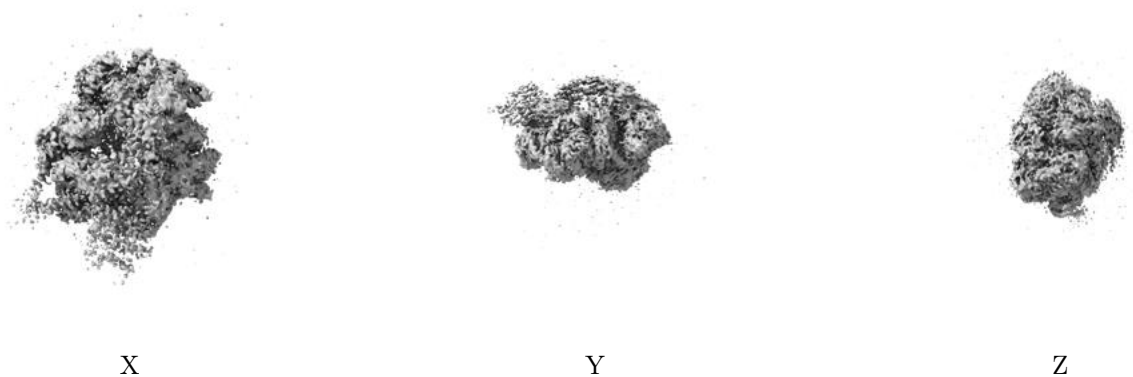


Z

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.

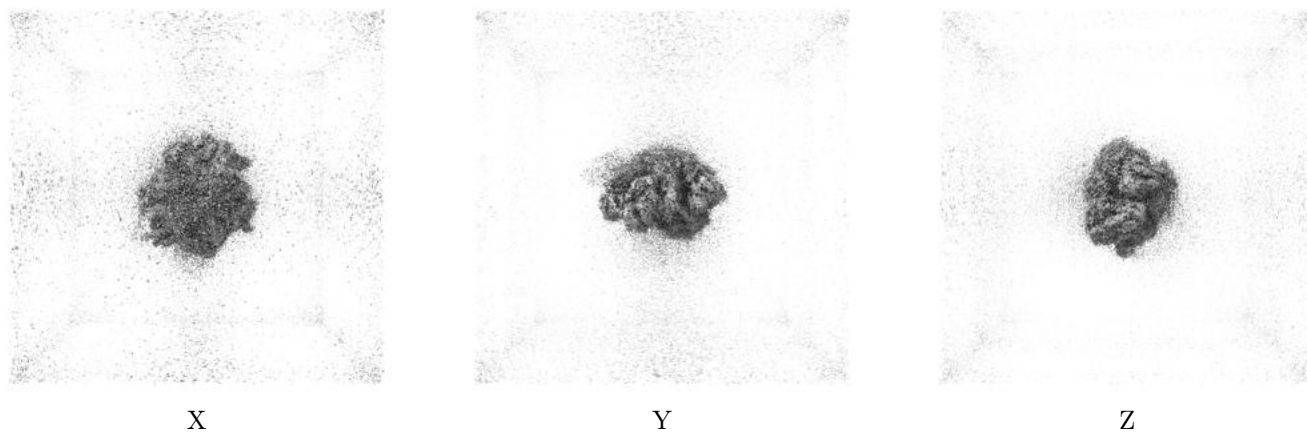
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

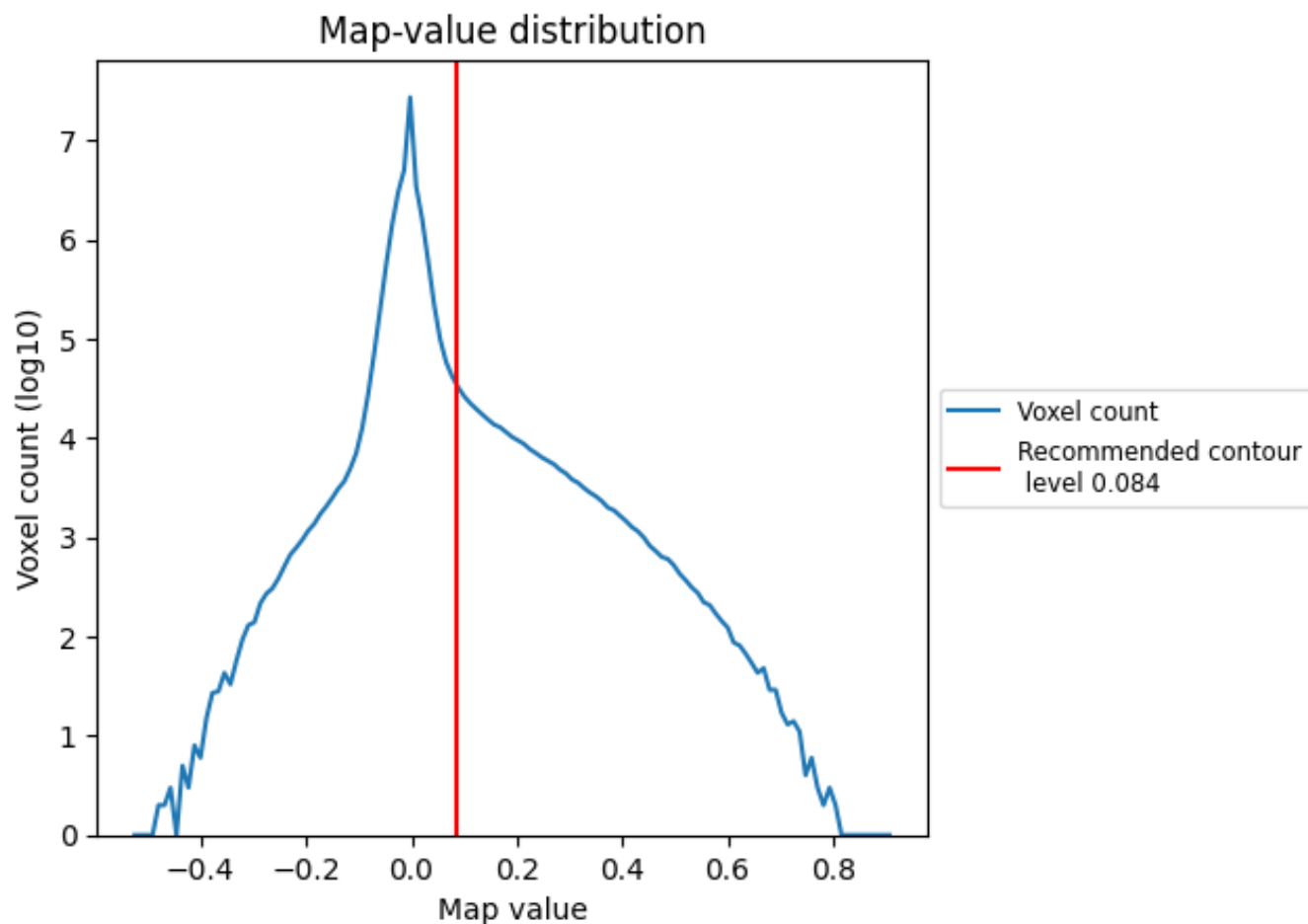
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

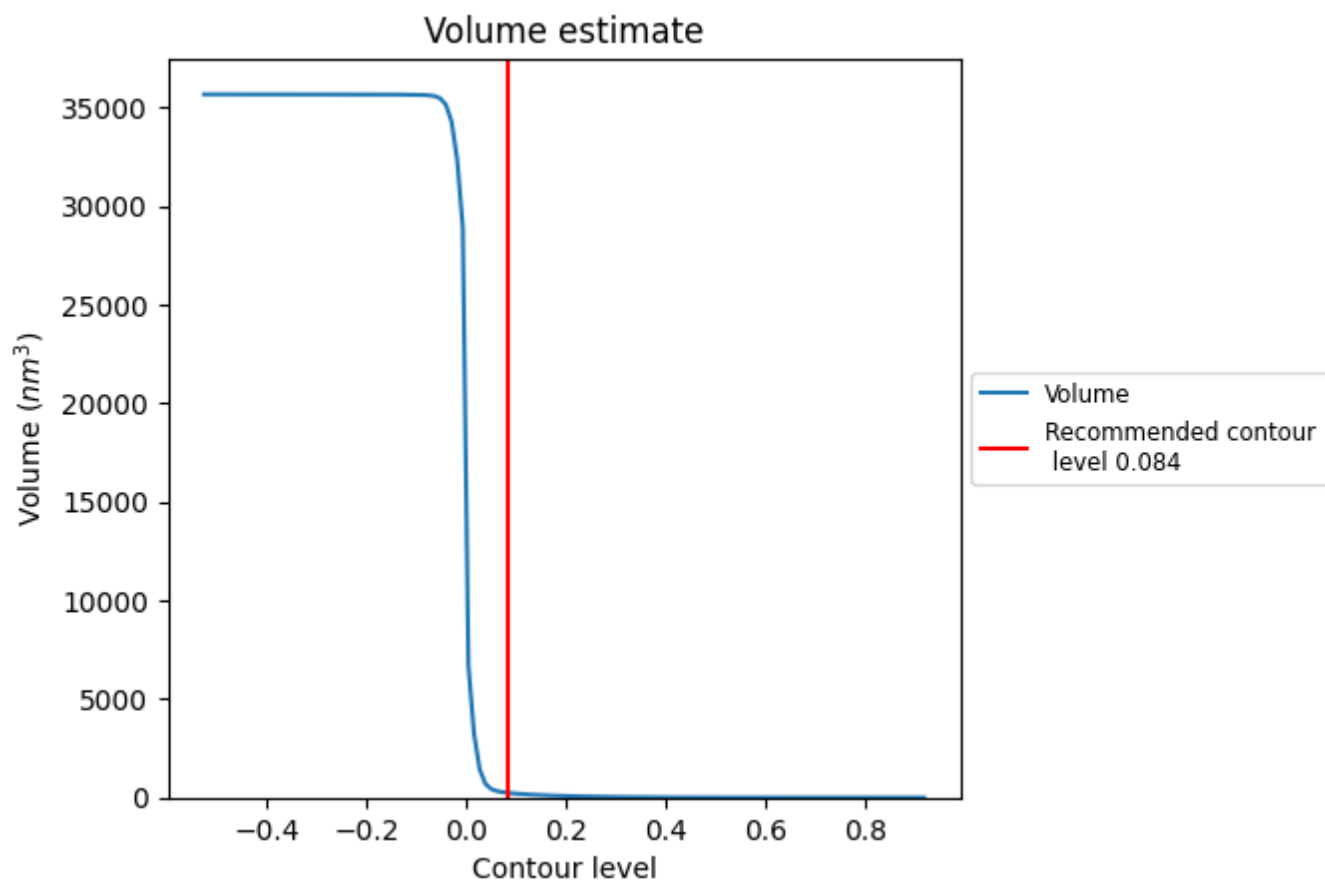
This section contains the results of statistical analysis of the map.

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.

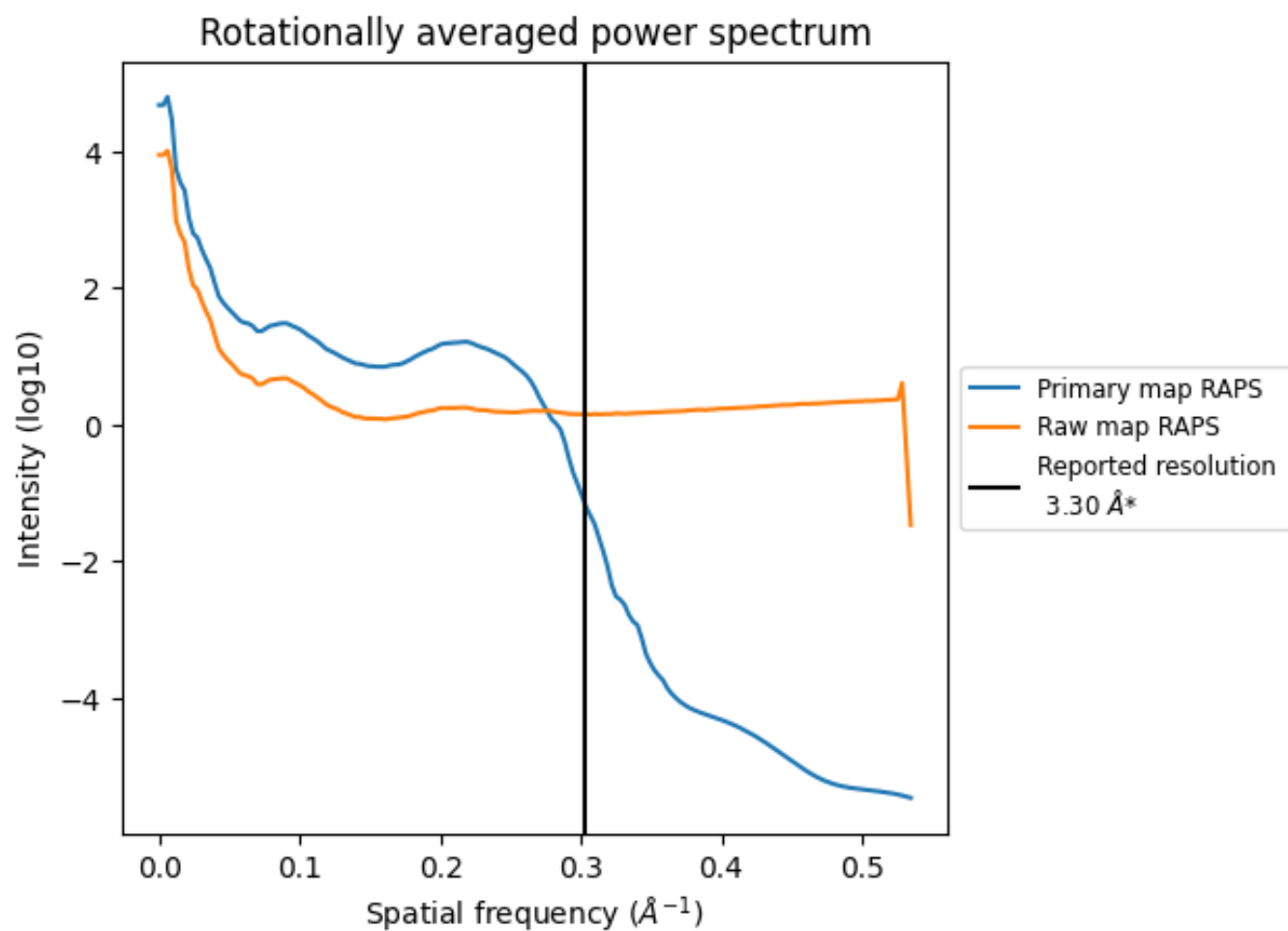
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm³; this corresponds to an approximate mass of 215 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 ⓘ

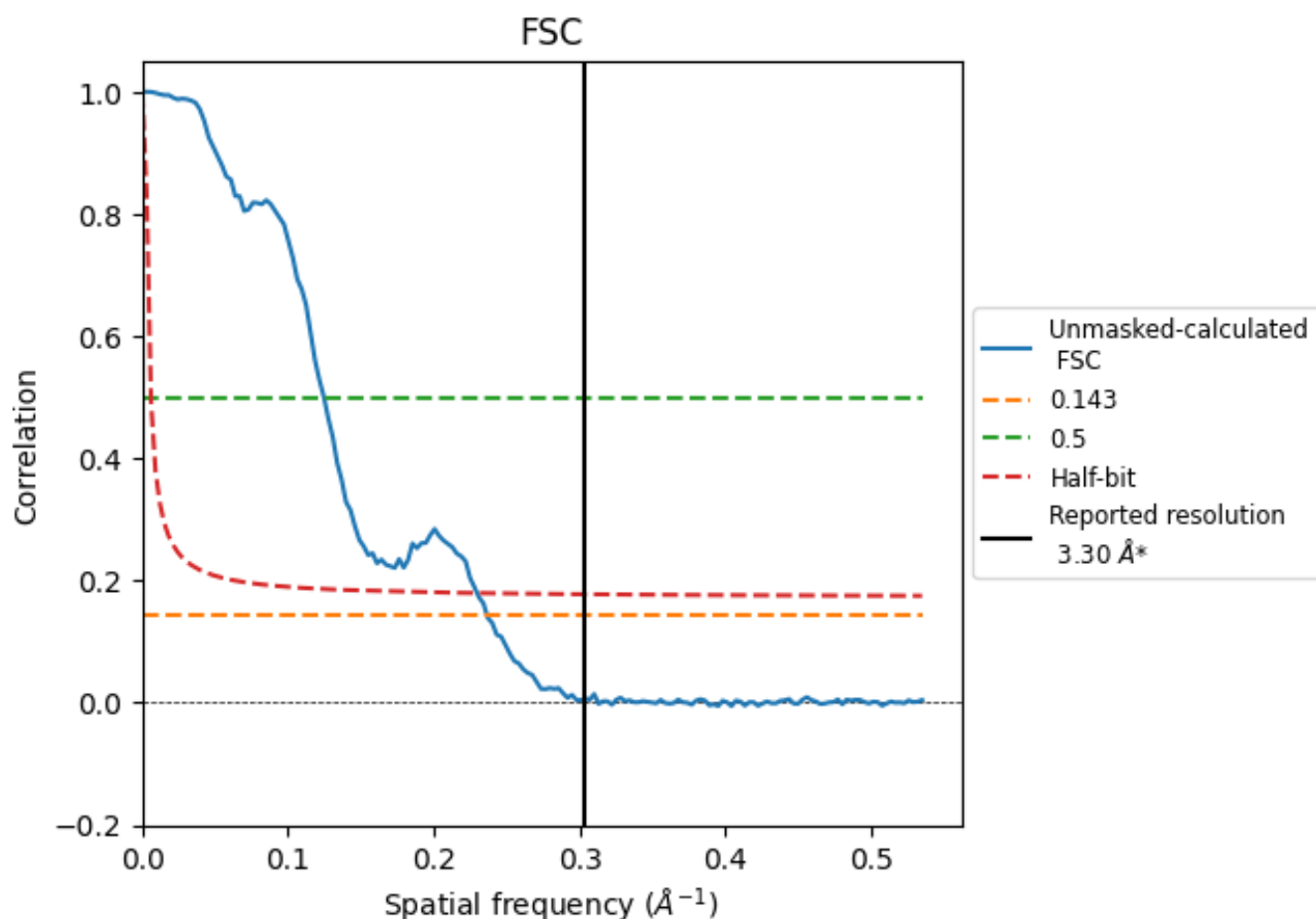


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

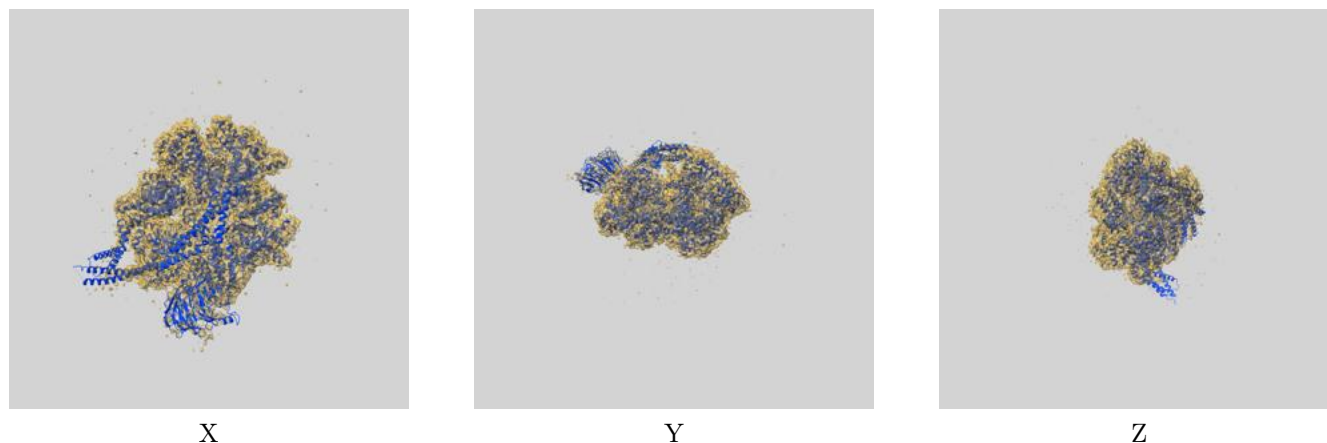
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	8.03	4.36

*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 4.23 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

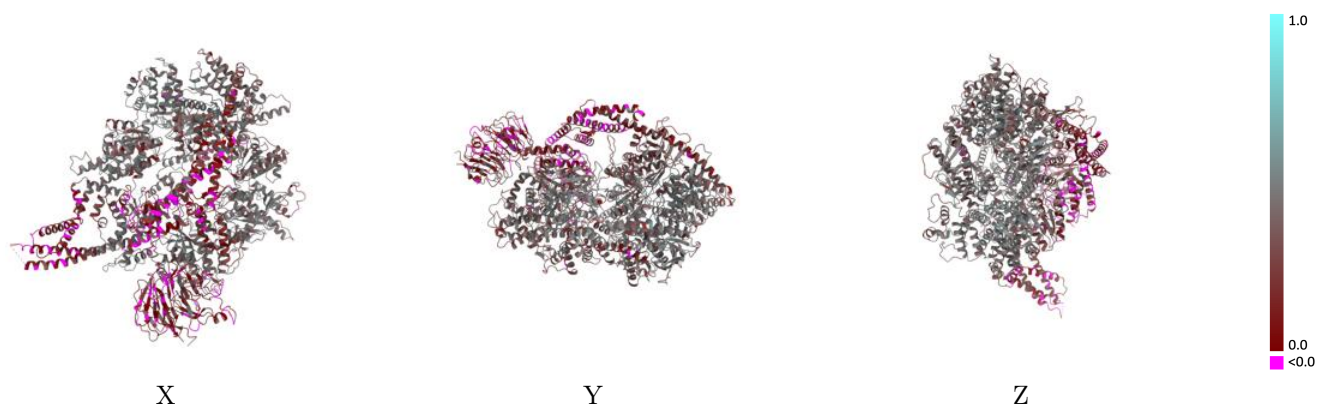
This section contains information regarding the fit between EMDB map EMD-47429 and PDB model 9E22. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



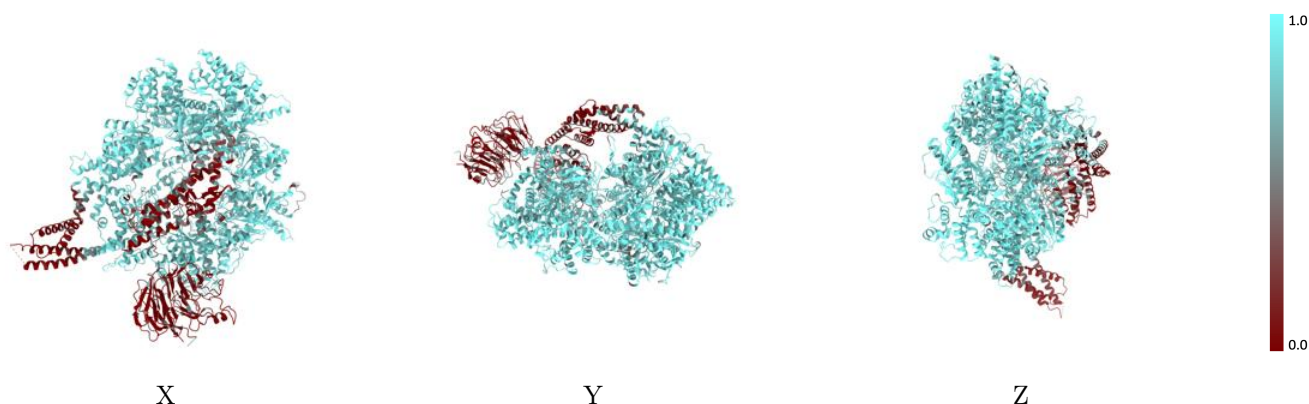
The images above show the 3D surface view of the map at the recommended contour level 0.084 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



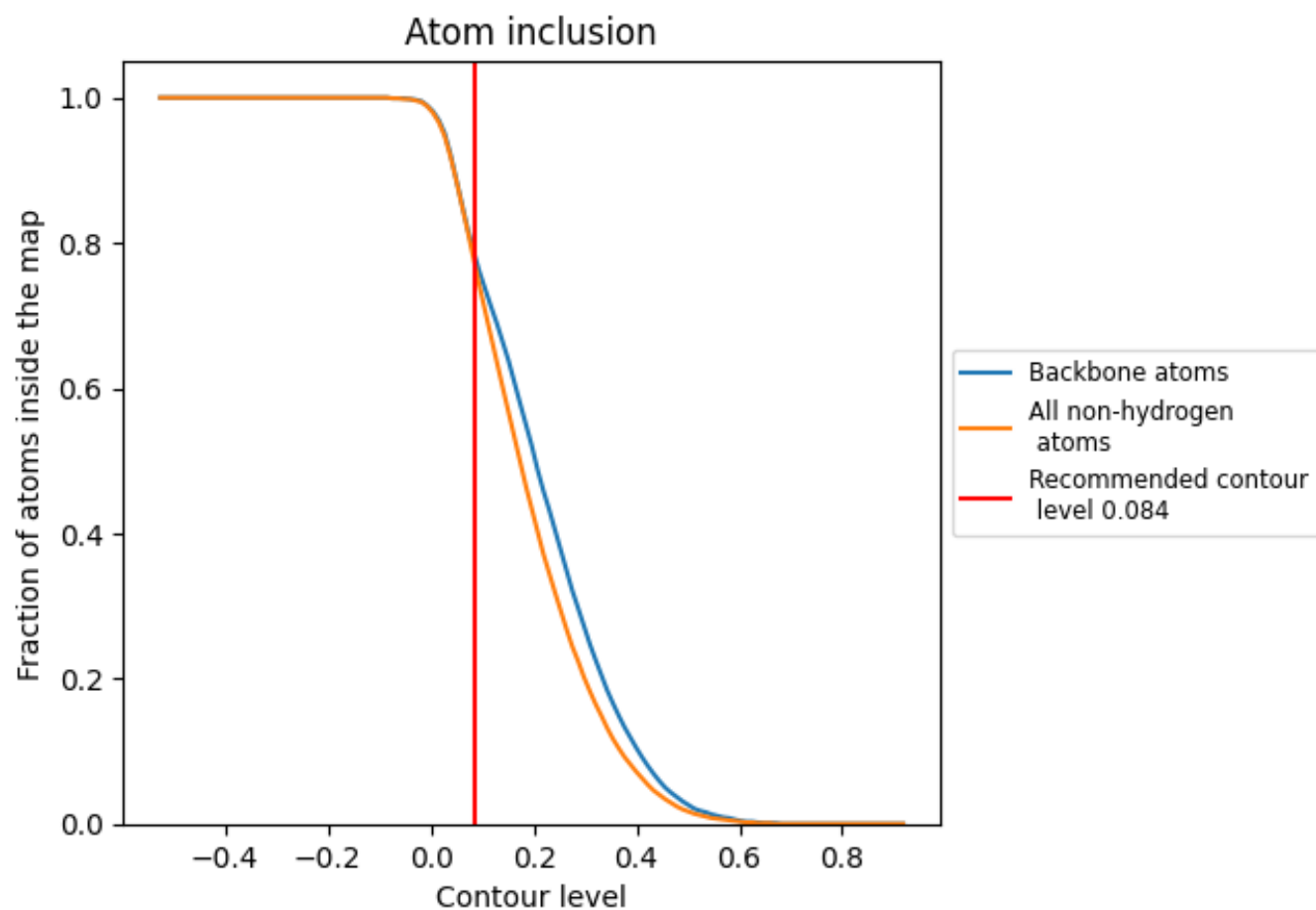
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.084).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7760	<div></div> 0.3650
A	<div></div> 0.8210	<div></div> 0.3770
E	<div></div> 0.1320	<div></div> 0.1830

