



wwPDB EM Validation Summary Report ⓘ

Jul 29, 2025 – 10:46 AM EDT

PDB ID : 9E0Z / pdb_00009e0z
EMDB ID : EMD-47378
Title : Dimeric motor domains from phi-like dynein-1 bound to a Lis1 dimer under Nde1-Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.86 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

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.dev126
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) : 2.45.1

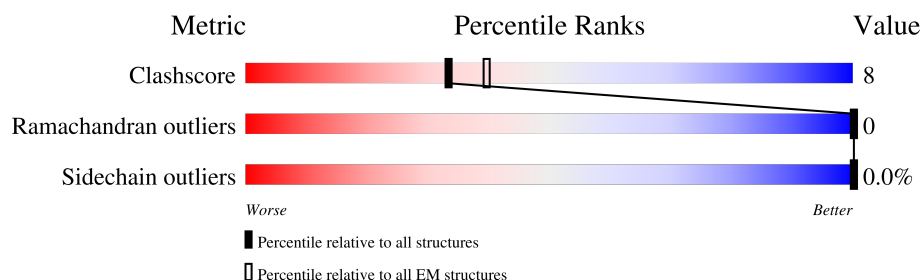
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	4646	<div> <div>15%</div> <div>50%</div> <div>13%</div> <div>37%</div> </div>
1	B	4646	<div> <div>10%</div> <div>51%</div> <div>12%</div> <div>37%</div> </div>
2	C	410	<div> <div>62%</div> <div>16%</div> <div>21%</div> </div>
2	D	410	<div> <div>20%</div> <div>48%</div> <div>29%</div> <div>22%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 52502 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.

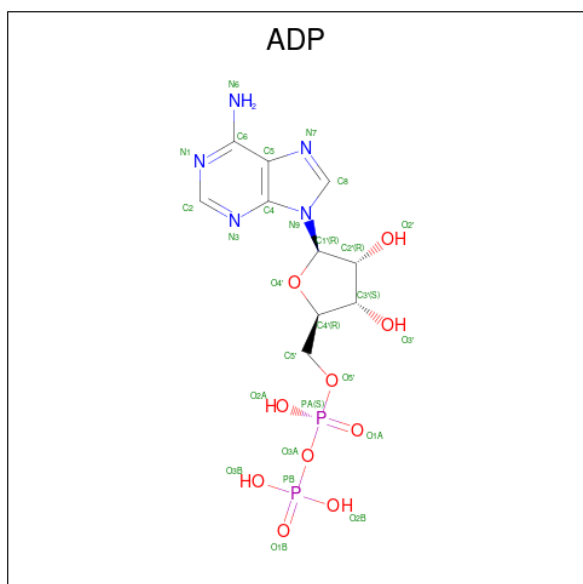
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		
1	B	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		

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

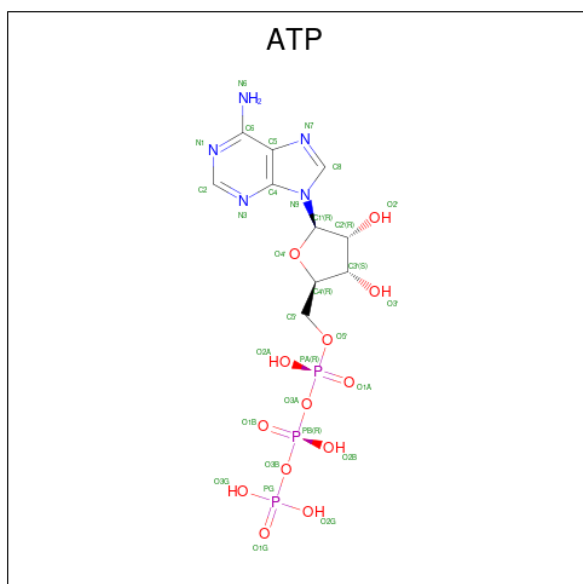
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- 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	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	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	B	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	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	B	2	2	2	0



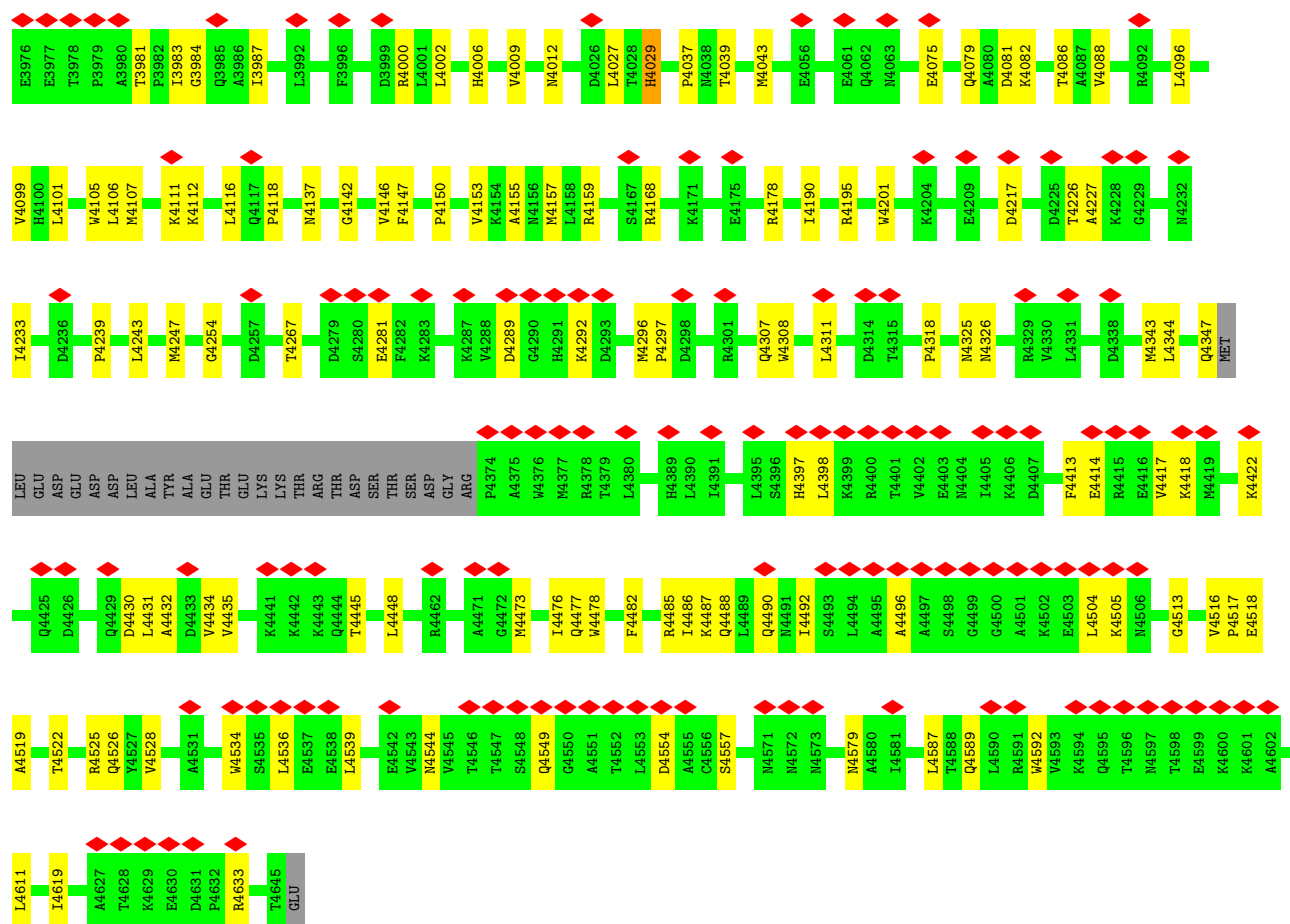
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F3094	D3212	D3213	Q3214	Q3215	E3216	E3217	L3218	R3219	R3220	D3221	L3222	R3223	L3224	K3225	K3226	Q3227	E3228	L3229	E3230	V3231	K3232	K3233	A3234	A3235	P3136	A3037	N3237	D3238	K3239	L3240	V3148	F3149	Q3152	T3153	L3154	R3160	L3161	A3162	K3163	R3164	T3172	P3173	R3174	R3175	D3178	H3182	L3205	R3206	K3207	L3208	T3211
E2996	S2997	N2998	V2999	L3000	D3001	S3002	M3008	L3011	L3012	L3115	E3116	K3117	P3118	R3119	D3124	Y3125	W3126	V3129	Y3130	D3131	K3132	Q3035	Q3036	A3037	Q3038	K3039	E3040	G3041	L3042	M3043	L3044	D3045	S3046	H3047	E3048	E3049	L3050	Y3051	K3052	F3054	R3060	T3067	S3072	E3073	S3077	R3078	L3085	R3088			
D2885	Q2886	E2887	E2888	D2891	K2898	V2899	F2900	Y2901	E2902	E2903	E2904	L2905	D2906	F2912	N2913	E2914	L2920	R2924	R2927	L2934	K2943	A2951	L2956	L2961	K2962	V2963	H2964	K2965	K2966	Y2967	E2970	E2974	L2980	S2983	K2986	N2987	E2988	K2989	I2990	M2994	D2995										
Y2792	L2793	Y2794	R2801	R2804	Q2805	L2806	F2807	E2808	R2811	P2812	L2813	E2814	T2815	L2816	P2817	V2818	E2819	G2820	L2821	R2823	L2824	E2828	R2836	L2837	V2838	E2839	D2840	E2841	E2842	R2843	R2844	D2847	L2855	F2858	N2860	L2861	D2862	R2863	E2864	K2865	S2868	R2869	L2872	L2877	S2878	K2879					
L2661	E2665	L2668	F2682	M2686	G2691	R2694	D2697	V2701	K2702	L2703	E2704	Q2707	P2714	L2723	R2726	R2729	H2730	V2731	P2732	Y2738	P2739	G2740	M2755	L2756	R2757	L2758	I2759	L2762	R2763	T2764	Y2765	E2767	A2772	F2784	T2785	Q2786	V2789	H2791													
L2555	E2557	V2558	T2559	H2560	K2561	V2562	A2563	A2564	P2565	D2566	D2573	T2574	V2575	R2576	H2577	E2578	L2581	V2584	H2588	K2589	P2590	L2591	V2592	P2596	T2604	L2605	F2606	S2607	R2610	E2616	G2619	L2620	F2635	Y2641	R2642	R2643	T2644	P2645	N2646	G2647	V2648	L2650	L2655	K2656	K2657						
S2457	H2463	Q2464	R2467	N2468	Q2471	Y2472	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	L2483	E2484	L2486	E2487	R2492	Y2493	L2494	I2498	L2499	D2505	S2506	R2507	L2508	L2514	G2515	I2521	T2522	T2523	T2528	A2529	P2530	N2531	L2532	P2533	L2534	S2540	I2541	S2542	K2551	Q2554							
M2361	L2369	T2371	F2378	S2384	L2385	P2386	L2387	D2388	E2389	GLY	ASP	GLU	ALA	GLN	ARG	ARG	LYS	GLY	ASP	GLU	GLY	GLU	ALA	S2410	P2411	M2412	Q2416	R2417	D2418	T2422	M2423	F2427	V2433	E2438	T2446	M2447	D2448	L2449	T2450	R2451	L2452	R2453	C2454								
G2224	S2231	W2234	E2242	E2248	K2257	L2268	D2269	M2271	W2275	D2277	R2285	D2289	S2290	L2295	V2302	P2303	D2304	G2305	D2306	V2307	D2308	P2309	E2310	N2314	D2320	D2321	L2324	E2331	S2334	M2342	P2343	Q2346	D2347	T2355	V2356	S2357															
E2120	A2121	V2122	D2123	E2124	G2125	E2126	I2127	A2128	E2129	N2130	L2131	P2132	Q2134	E2135	L2136	I2137	I2138	E2143	K2148	A2151	E2152	L2156	F2165	P2166	G2167	V2168	Q2169	I2170	H2171	R2172	G2173	E2174	M2175	T2176	A2177	L2178	E2179	E2181	K2184	Q2187	E2188	M2189	Y2190	E2198	T2214	L2220	M2221				
D2011	A2023	G2024	R2025	S2026	D2030	L2039	D2045	R2046	Q2047	R2060	T2061	A2066	I2069	V2070	P2071	F2072	F2073	K2074	L2075	C2076	D2077	E2078	Q2079	L2080	D2087	F2088	R2091	K2094	S2095	V2096	N2102	V2103	R2105	E2106	R2107	I2108	Q2109	K2110	I2111	K2112	R2113	E2114	R2115	E2116	E2117	R2118	G2119				

THR	THR	THR	ASP	TRP	LYS	GLN	ILE	SER	ASN	ILE	MET	ARG	GLU	ASN	PHE	ILE	PRO	THR	VAL	ASN	PHE	SER	ALA	GLU	GLU	ILE	SER	ASN	TYR	MET	SER	ASN	GLU	TYR	GLU	ILE	VAL	ASN	ARG	ALA	ALA	SER	LEU	ALA	CYS	GLY	PRO							
A4432	D4433	Q4436	V4437	Q4438	E4439	G4440	K4441	K4442	K4443	K4457	L4460	P4461	R4462	S4463	W4464	S4465	H4466	Y4467	T4468	W4469	P4470	A4471	G4472	I4486	K4487	Q4488	L4489	Q4490	N4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	G4499	G4500	A4501	K4502	E4503	L4504	K4505	N4506	I4507	H4508	W4509	E4518	A4519	Y4520	I4521	T4522	R4525	P4608
LYS	LYS	THR	THR	ARG	THR	SER	THR	SER	ASP	GLY	P4374	A4375	W4376	R4378	T4379	L4380	H4381	A4384	H4389	L4390	I4391	L4395	S4396	H4397	L4398	K4399	R4400	T4401	V4402	E4403	N4404	I4405	D4406	D4407	P4408	L4409	F4410	R4411	F4412	F4413	E4414	R4415	W4416	V4417	K4418	L4423	L4424	Q4425	D4426	Q4429	D4430	L4431		
D4257	F4260	D4261	N4266	E4270	R4276	E4281	A4285	K4286	K4287	V4288	D4289	G4290	H4291	K4292	D4293	W4296	P4297	D4298	R4301	R4302	E4303	Q4307	D4314	P4318	N4325	W4326	R4329	W4343	Q4347	LEU	GLU	ASP	GLU	ASP	ASP	LEU	ALA	ALA	TYR	ALA	GLU	THR	GLU											
K4112	L4116	Q4117	P4118	F4125	T4127	I4130	N4137	L4138	R4140	A4141	G4142	V4146	N4156	T4160	K4171	S4172	P4173	N4174	E4175	R4178	Y4205	E4206	L4212	V4219	L4223	D4224	D4225	T4226	A4227	K4228	G4229	R4230	Q4231	N4232	I4233	S4234	K4237	L4243	W4247	I4251														
A3980	T3981	P3982	G3983	V3984	E3913	I3914	V3915	S3917	A3918	G3919	S3920	T3921	P3922	R3923	L3924	Q3925	G3926	L3927	E3930	A3934	S3939	C3940	L3941	F3944	K3945	D3946	L3947	I3948	A3949	K3950	V3951	Q3952	A3953	D3954	E3955	Q3956	F3957	Q3958	I3959	W3960	L3961	D3962	P3966	E3967	Q3968	T3969	Y3972	E3976	E3977	T3978	P3979			
V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	T3789	V3790	M3791	Q3792	E3793	V3794	T3796	Q3799	L3804	S3809	L3824	V3839	N3845	L3846	K3847	G3848	Q3854	T3860	K3861	D3862	L3863	F3868	A3872	M3875	L3876	A3884	A3888	K3891	L3892	T3895	V3896	G3897	E3898	D3902												
S3674	T3681	P3684	D3691	S3694	L3708	Q3709	D3723	V3724	D3725	F3582	N3584	R3585	S3589	L3734	Q3595	A3596	T3597	D3606	R3607	R3611	T3612	S3613	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	P3643	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	R3658	R3659	D3666	Q3667	D3668											
A3452	V3453	L3454	T3455	S3456	E3457	A3458	Q3459	I3461	K3462	A3463	A3466	A3467	V3468	E3469	A3470	K3471	L3734	Q3595	A3596	T3597	D3606	R3607	R3611	T3612	S3613	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	P3643	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	R3658	R3659	D3666	Q3667	D3668								
E3449	E3450	Y3451	E3494	T3495	F3496	K3497	T3502	S3510	Y3516	A3517	D3521	R3525	V3532	Q3542	F3543	R3544																																						

[illegible]

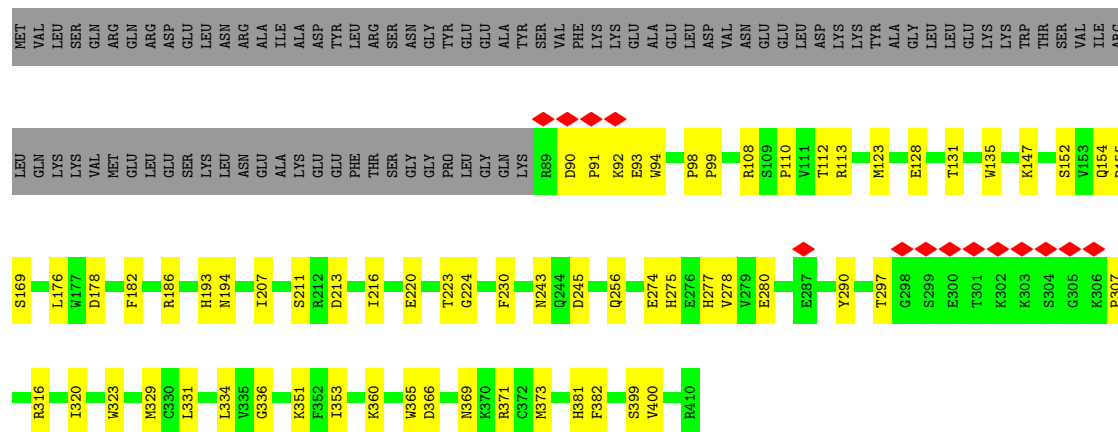






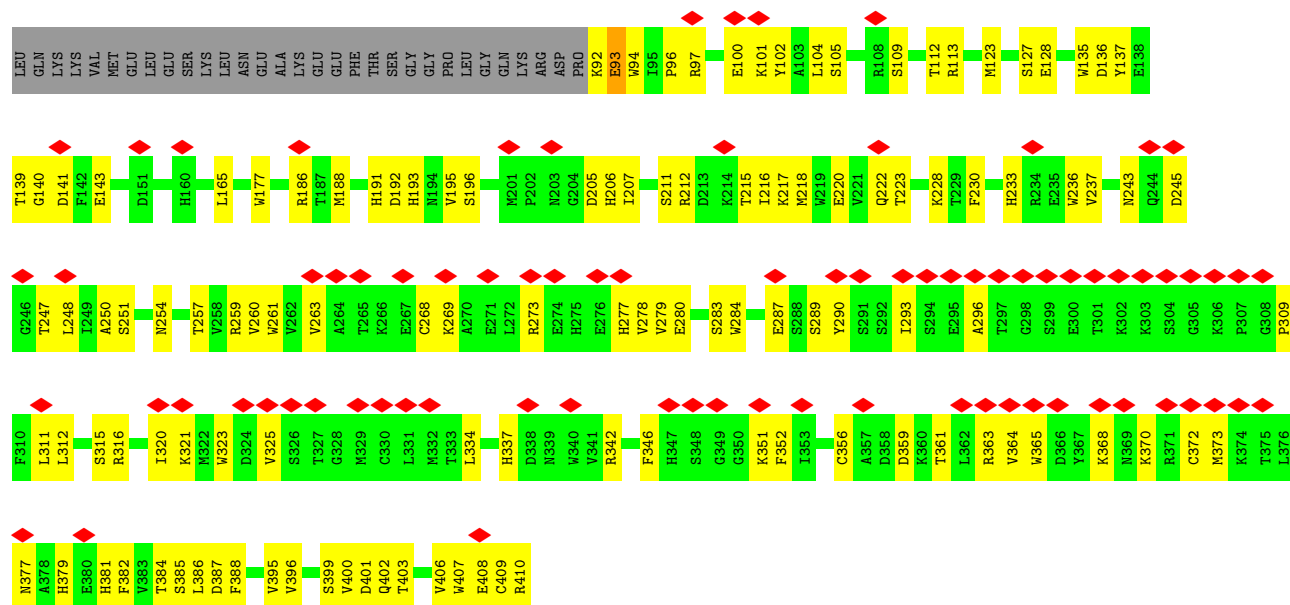
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain C: 62% 16% 21%



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain D: 48% 29% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.498	Depositor
Minimum map value	-0.699	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	0.12	0/24093	0.29	0/32651
1	B	0.12	0/24093	0.29	0/32651
2	C	0.12	0/2624	0.32	0/3555
2	D	0.16	0/2597	0.38	1/3518 (0.0%)
All	All	0.12	0/53407	0.30	1/72375 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	GLU	N-CA-C	-5.10	106.90	112.72

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	23593	0	23658	377	0
1	B	23593	0	23658	351	0
2	C	2557	0	2487	42	0
2	D	2531	0	2463	87	0
3	A	81	0	36	2	0
3	B	81	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	12	1	0
4	B	31	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	52502	0	52362	854	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 854 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:2686:MET:HE2	1:A:2703:LEU:HD11	1.65	0.79
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.64	0.79
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.64	0.79
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.65	0.78
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.49	0.78

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	2929/4646 (63%)	2885 (98%)	44 (2%)	0	100	100
1	B	2929/4646 (63%)	2872 (98%)	57 (2%)	0	100	100
2	C	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
2	D	317/410 (77%)	300 (95%)	17 (5%)	0	100	100
All	All	6495/10112 (64%)	6363 (98%)	132 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2605/4125 (63%)	2604 (100%)	1 (0%)	100	100
1	B	2605/4125 (63%)	2604 (100%)	1 (0%)	100	100
2	C	287/364 (79%)	287 (100%)	0	100	100
2	D	284/364 (78%)	284 (100%)	0	100	100
All	All	5781/8978 (64%)	5779 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4397	HIS
1	B	4029	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4098	ASN
1	B	4191	GLN
2	C	381	HIS
1	A	4012	ASN
1	A	3985	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 12 ligands modelled in this entry, 4 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
3	ADP	B	4703	-	24,29,29	0.88	0	29,45,45	1.23	2 (6%)
3	ADP	A	4701	5	24,29,29	0.89	0	29,45,45	1.22	2 (6%)
3	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.20	2 (6%)
4	ATP	B	4702	5	28,33,33	0.67	0	34,52,52	0.59	1 (2%)
3	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
3	ADP	B	4701	5	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
3	ADP	B	4704	-	24,29,29	0.86	0	29,45,45	1.19	2 (6%)
4	ATP	A	4702	5	28,33,33	0.66	0	34,52,52	0.58	1 (2%)

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	B	4703	-	-	5/12/32/32	0/3/3/3
3	ADP	A	4701	5	-	0/12/32/32	0/3/3/3
3	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
4	ATP	B	4702	5	-	4/18/38/38	0/3/3/3
3	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
3	ADP	B	4701	5	-	3/12/32/32	0/3/3/3
3	ADP	B	4704	-	-	1/12/32/32	0/3/3/3
4	ATP	A	4702	5	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4703	ADP	N3-C2-N1	-3.73	123.61	128.67
3	A	4701	ADP	N3-C2-N1	-3.72	123.62	128.67
3	A	4703	ADP	N3-C2-N1	-3.69	123.66	128.67
3	B	4704	ADP	N3-C2-N1	-3.68	123.67	128.67
3	A	4704	ADP	N3-C2-N1	-3.68	123.67	128.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

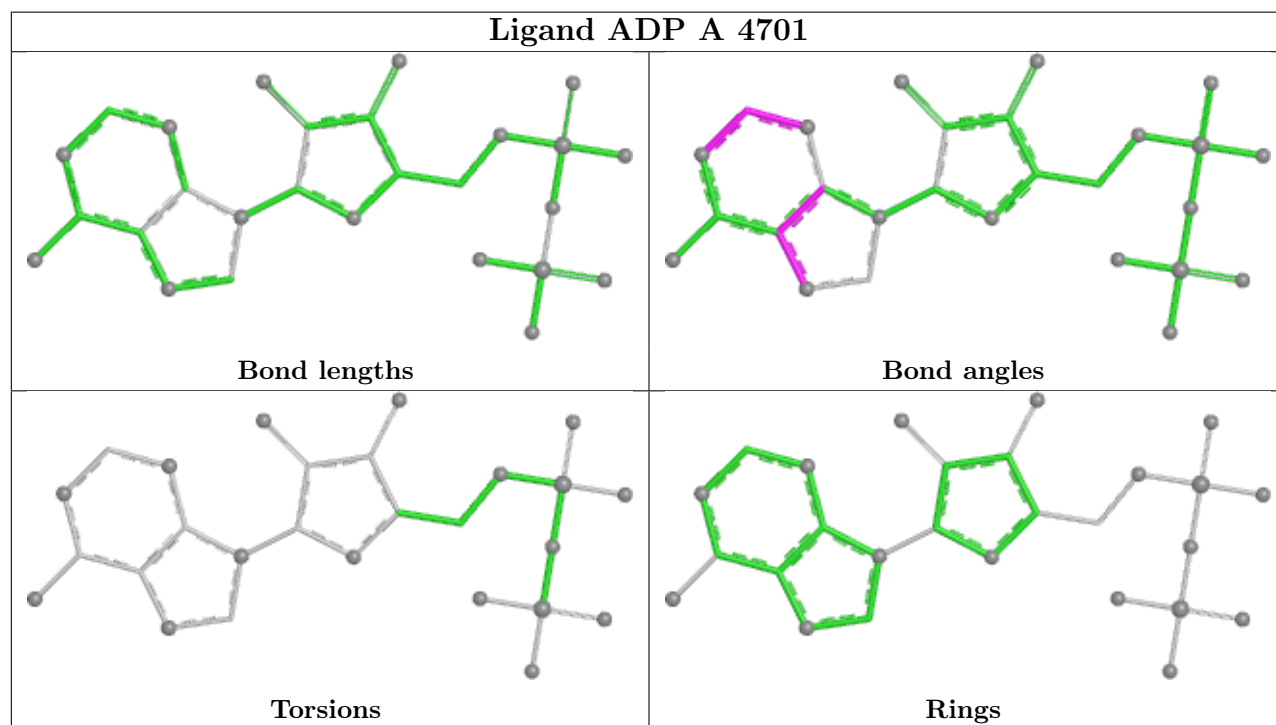
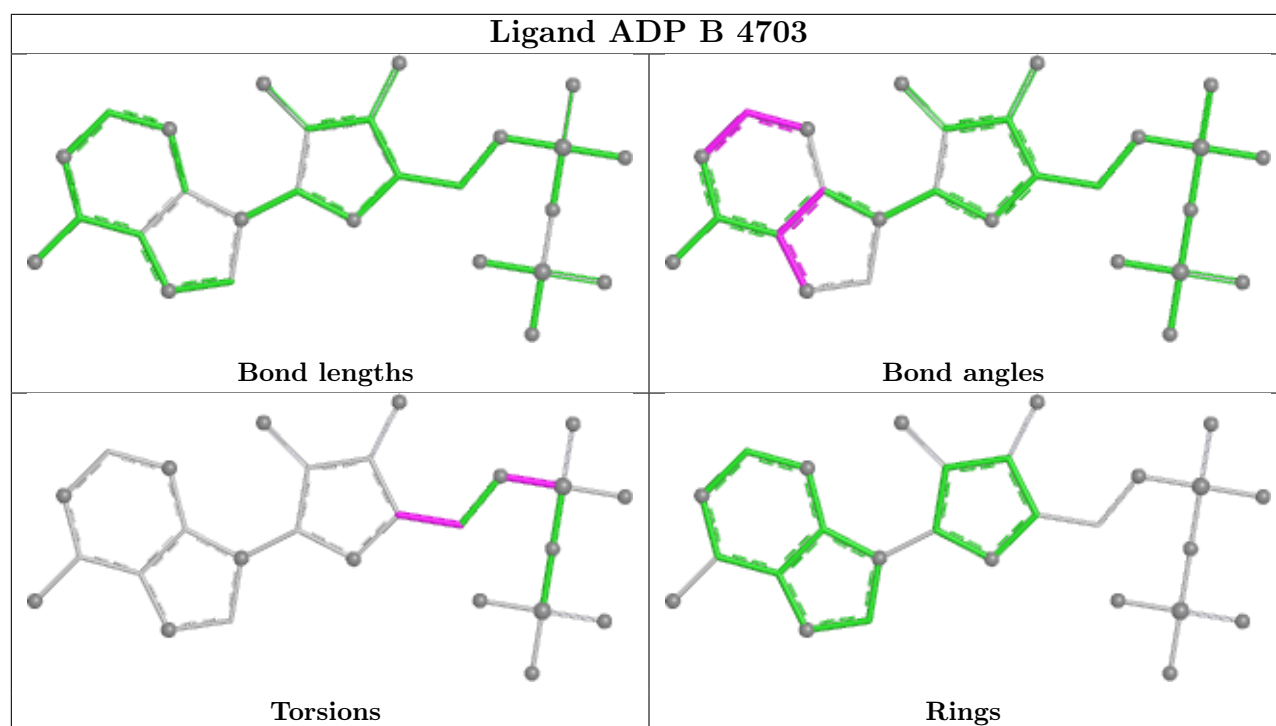
Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	C5'-O5'-PA-O1A
3	A	4703	ADP	C5'-O5'-PA-O3A
3	B	4701	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O2A
3	B	4701	ADP	C5'-O5'-PA-O3A

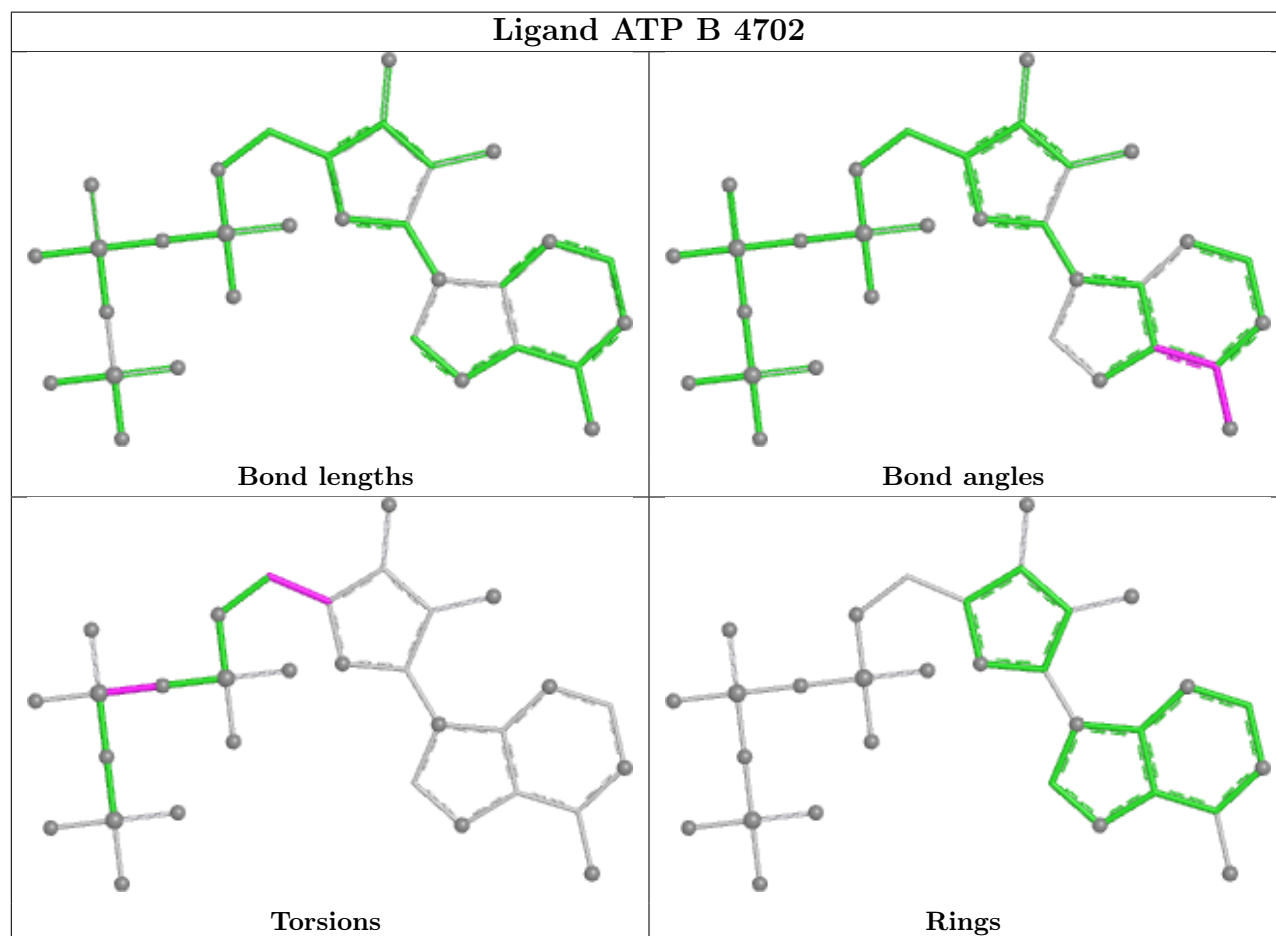
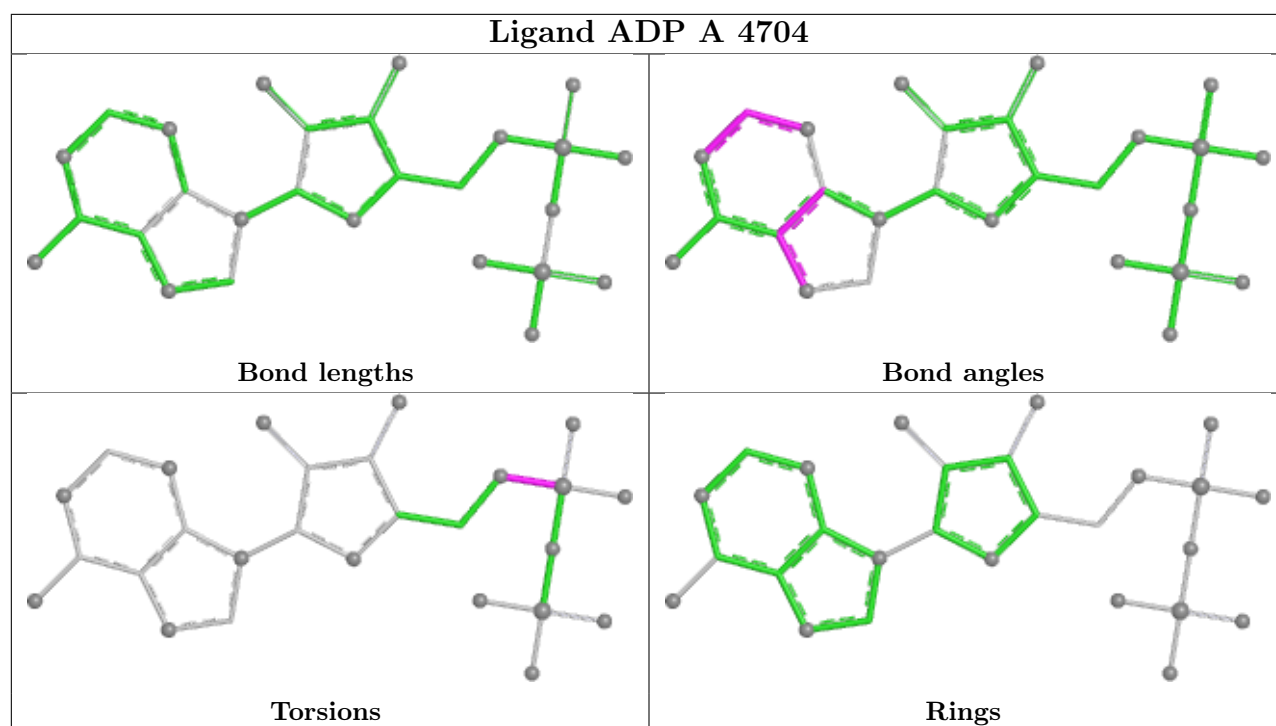
There are no ring outliers.

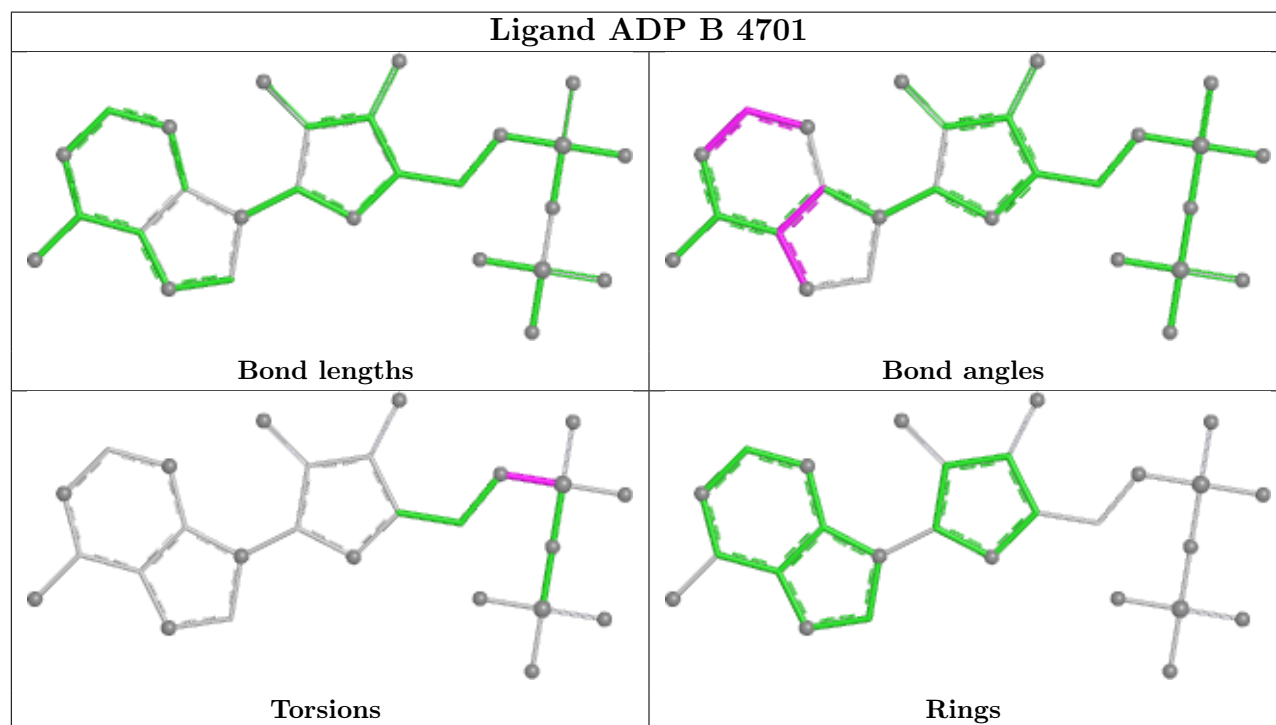
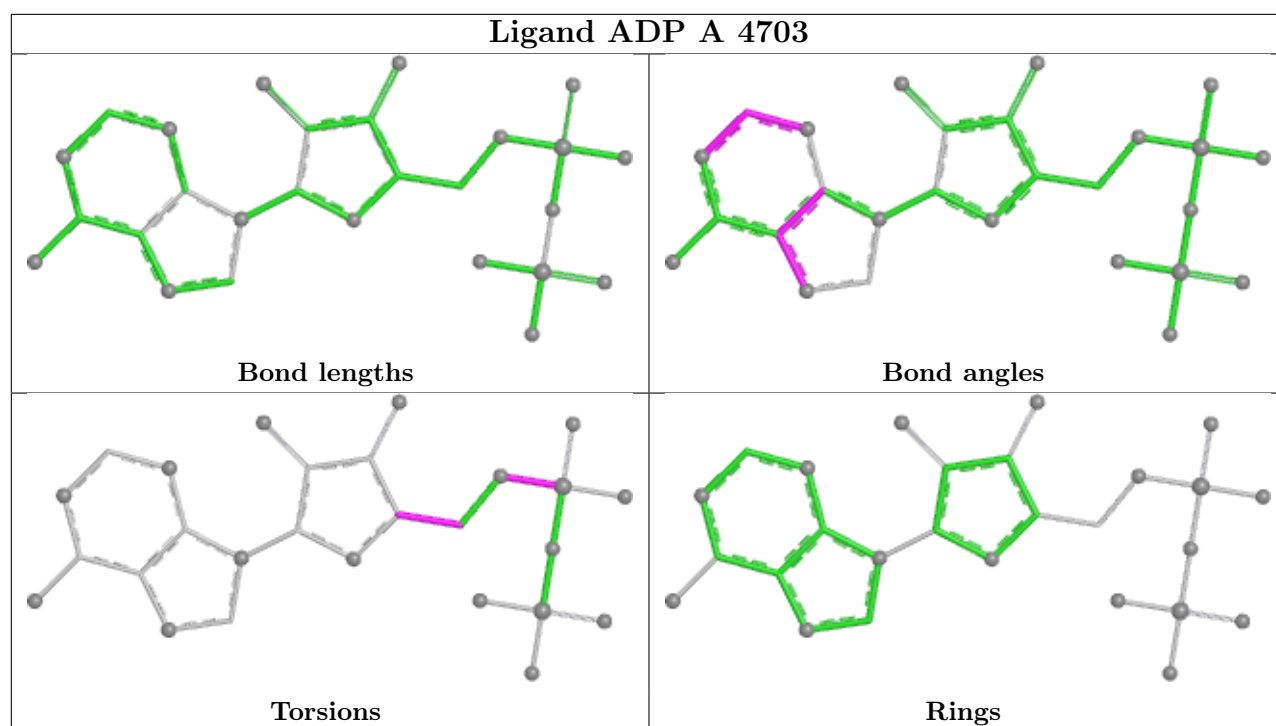
4 monomers are involved in 8 short contacts:

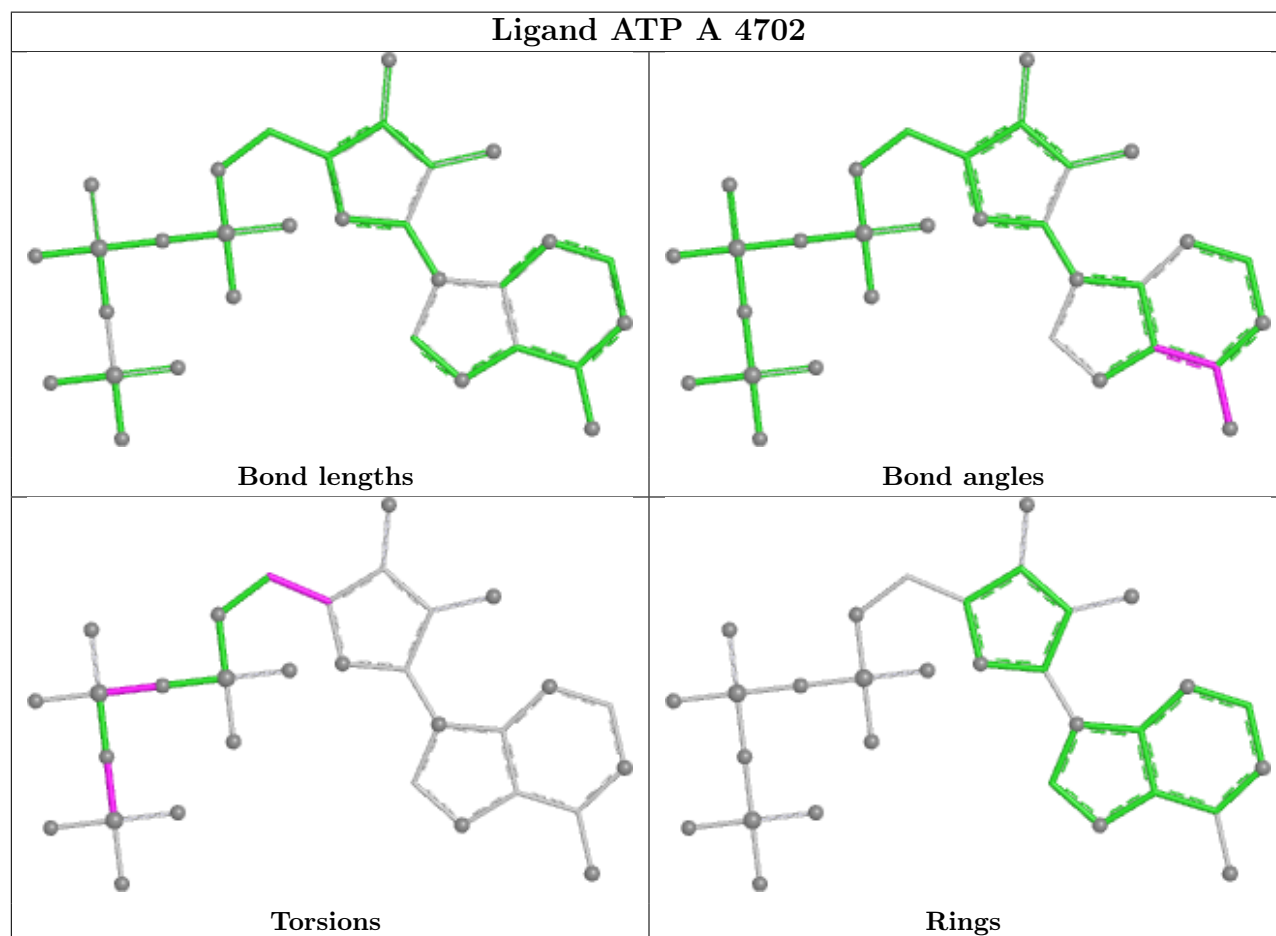
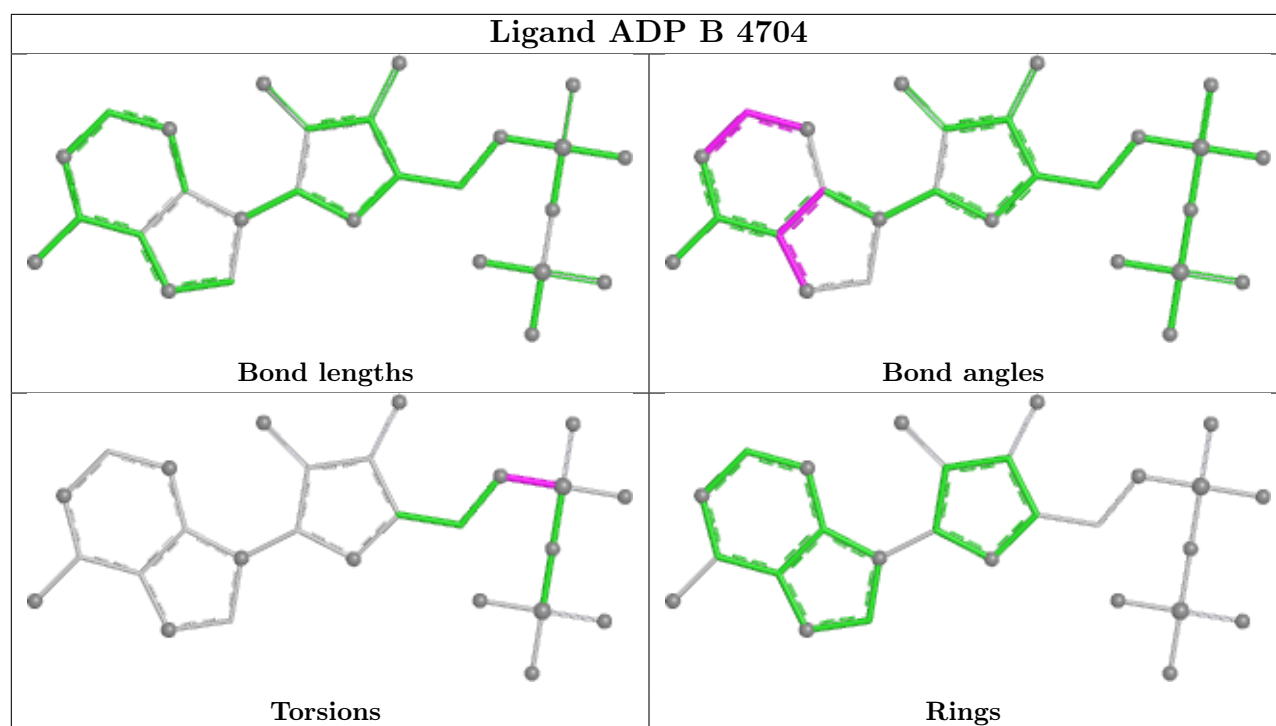
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4703	ADP	2	0
3	A	4701	ADP	2	0
3	B	4701	ADP	3	0
4	A	4702	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

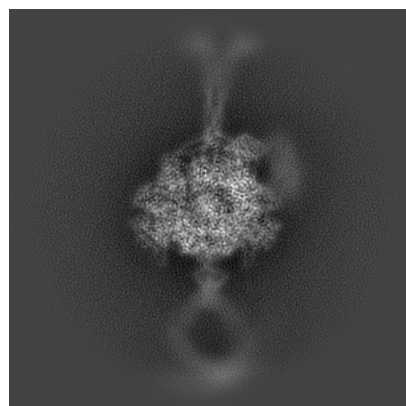
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47378. These allow visual inspection of the internal detail of the map and identification of artifacts.

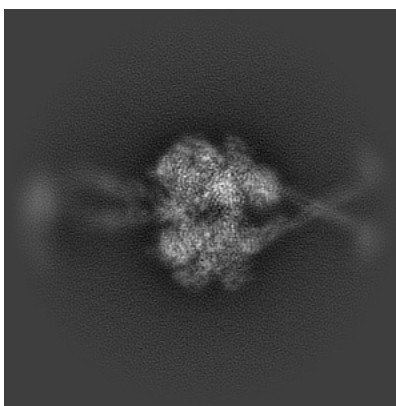
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

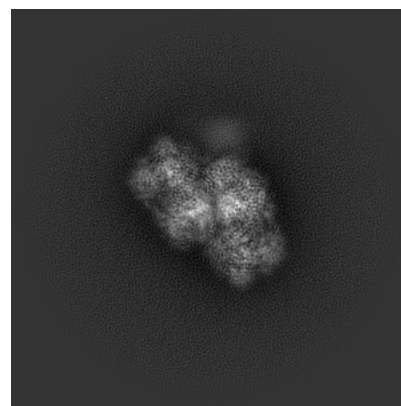
6.1.1 Primary map



X

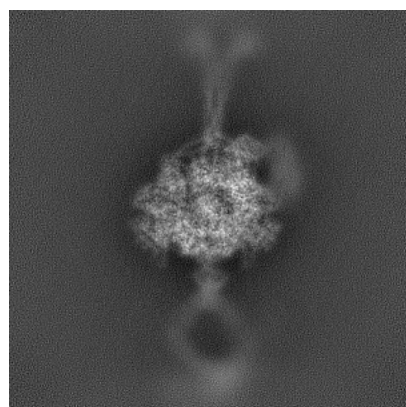


Y

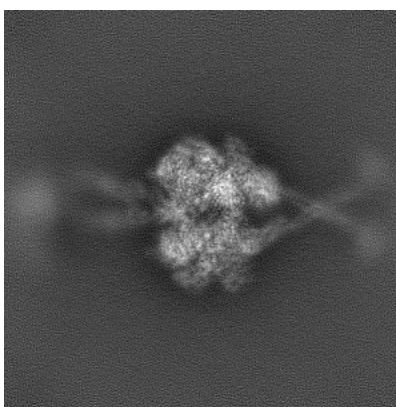


Z

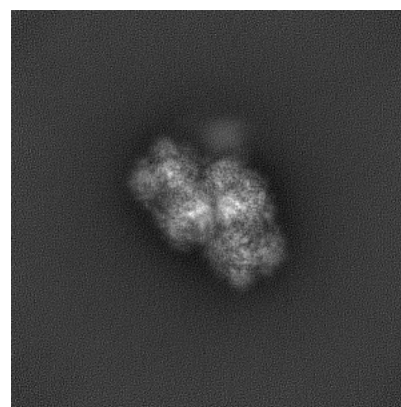
6.1.2 Raw map



X



Y

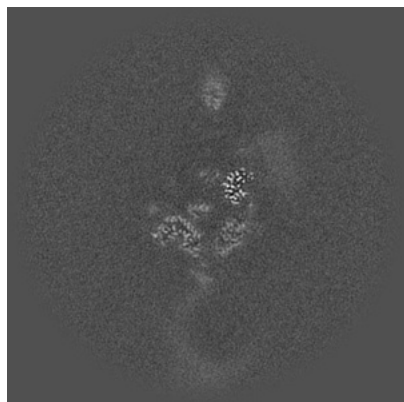


Z

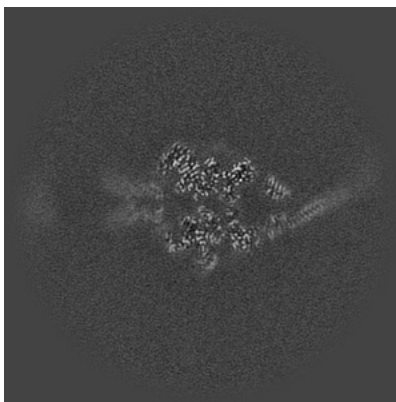
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

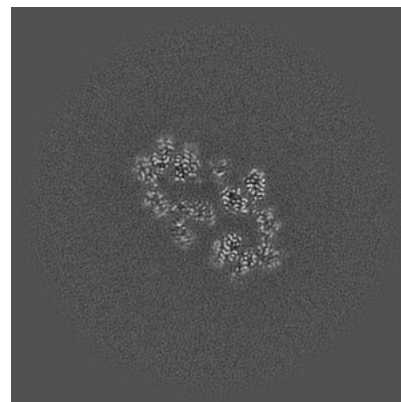
6.2.1 Primary map



X Index: 192

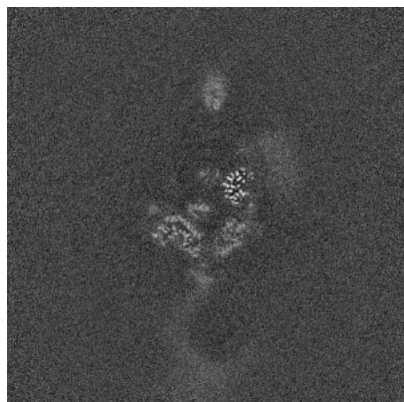


Y Index: 192

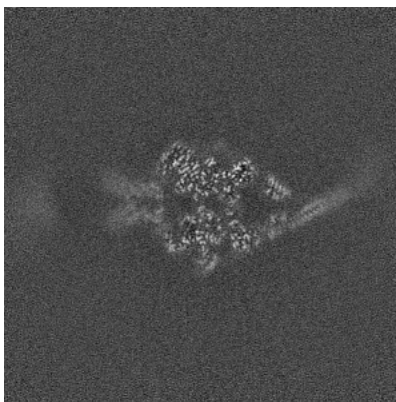


Z Index: 192

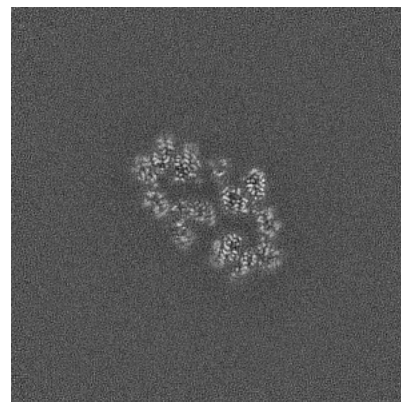
6.2.2 Raw map



X Index: 192



Y Index: 192

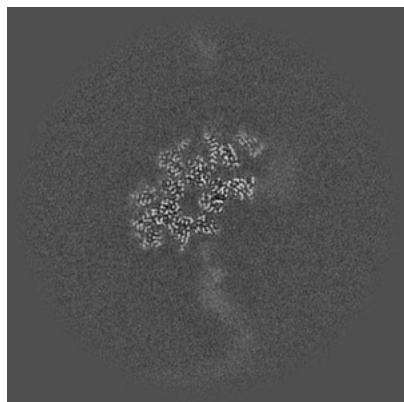


Z Index: 192

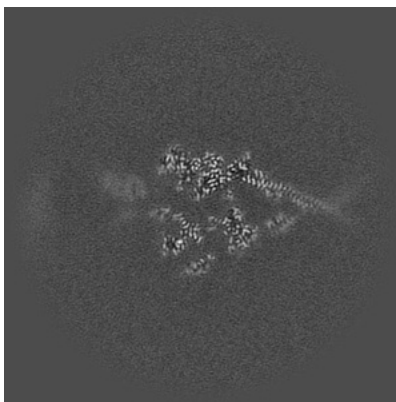
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

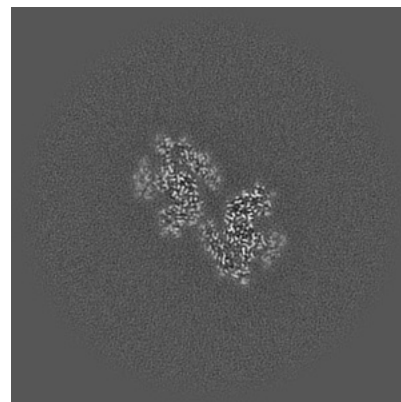
6.3.1 Primary map



X Index: 215

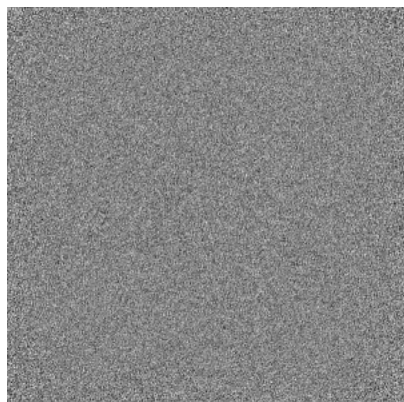


Y Index: 199

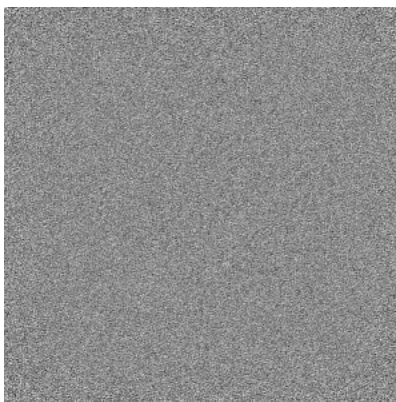


Z Index: 173

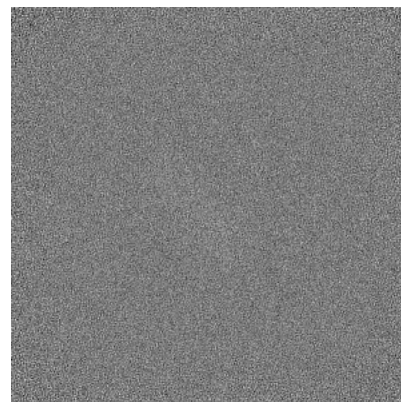
6.3.2 Raw map



X Index: 0



Y Index: 0

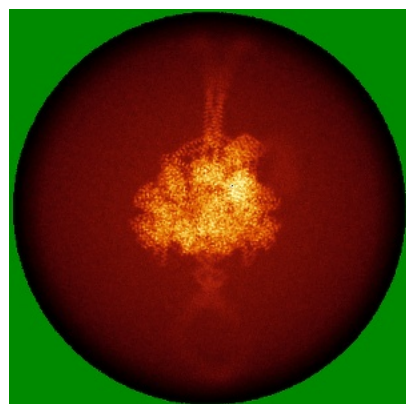


Z Index: 0

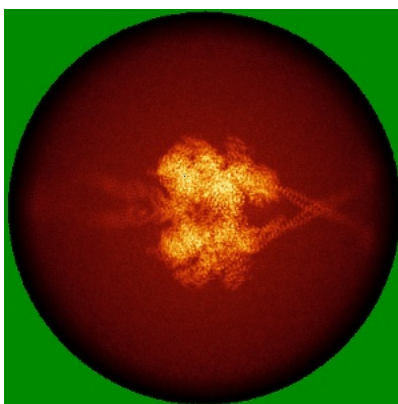
The images above show the largest variance slices of the map in three orthogonal directions.

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

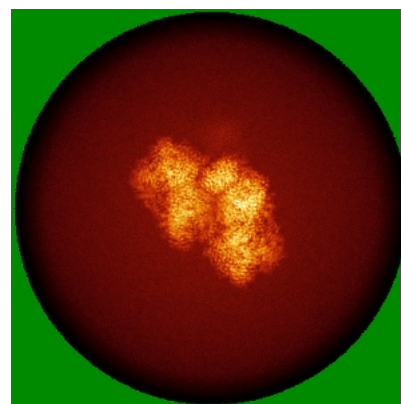
6.4.1 Primary map



X

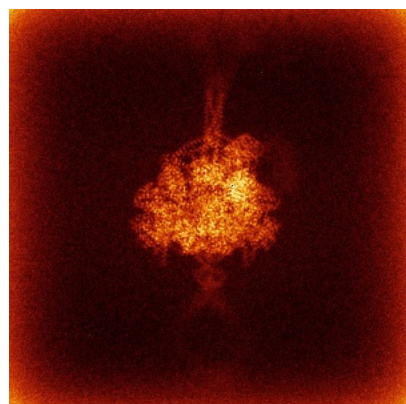


Y

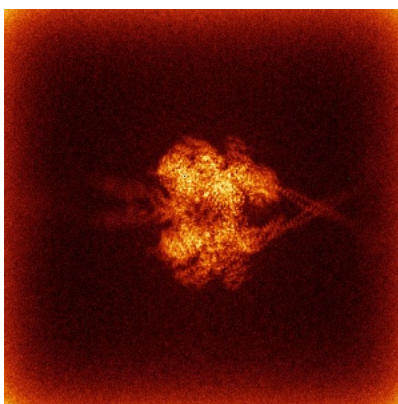


Z

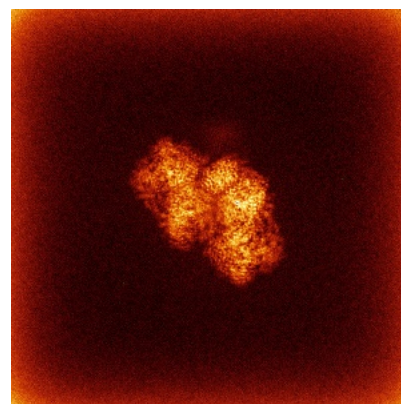
6.4.2 Raw map



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.

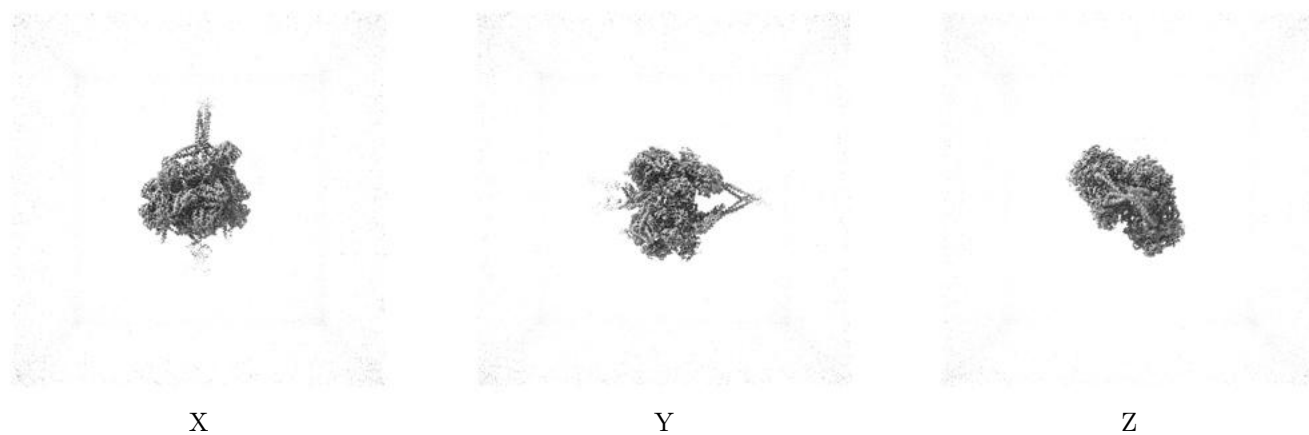
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

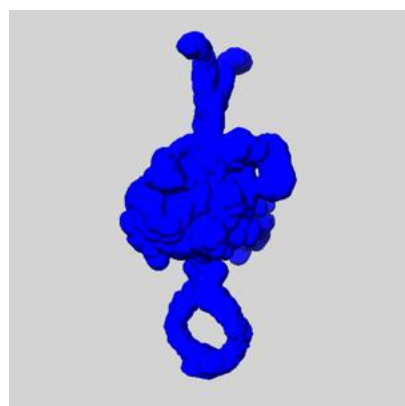
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

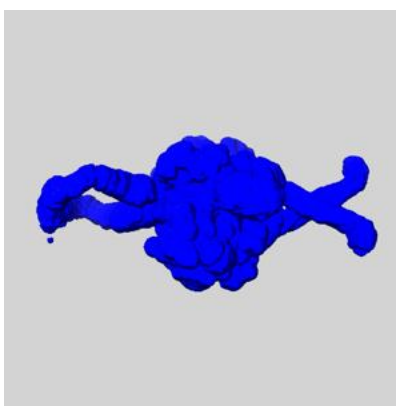
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

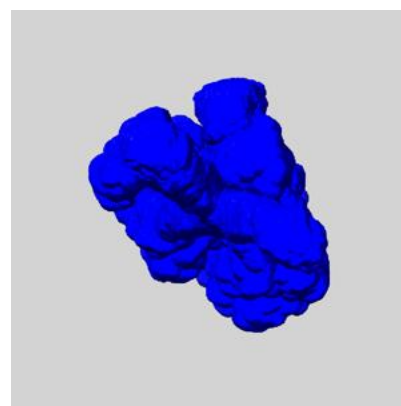
6.6.1 emd_47378_msk_1.map [i](#)



X



Y

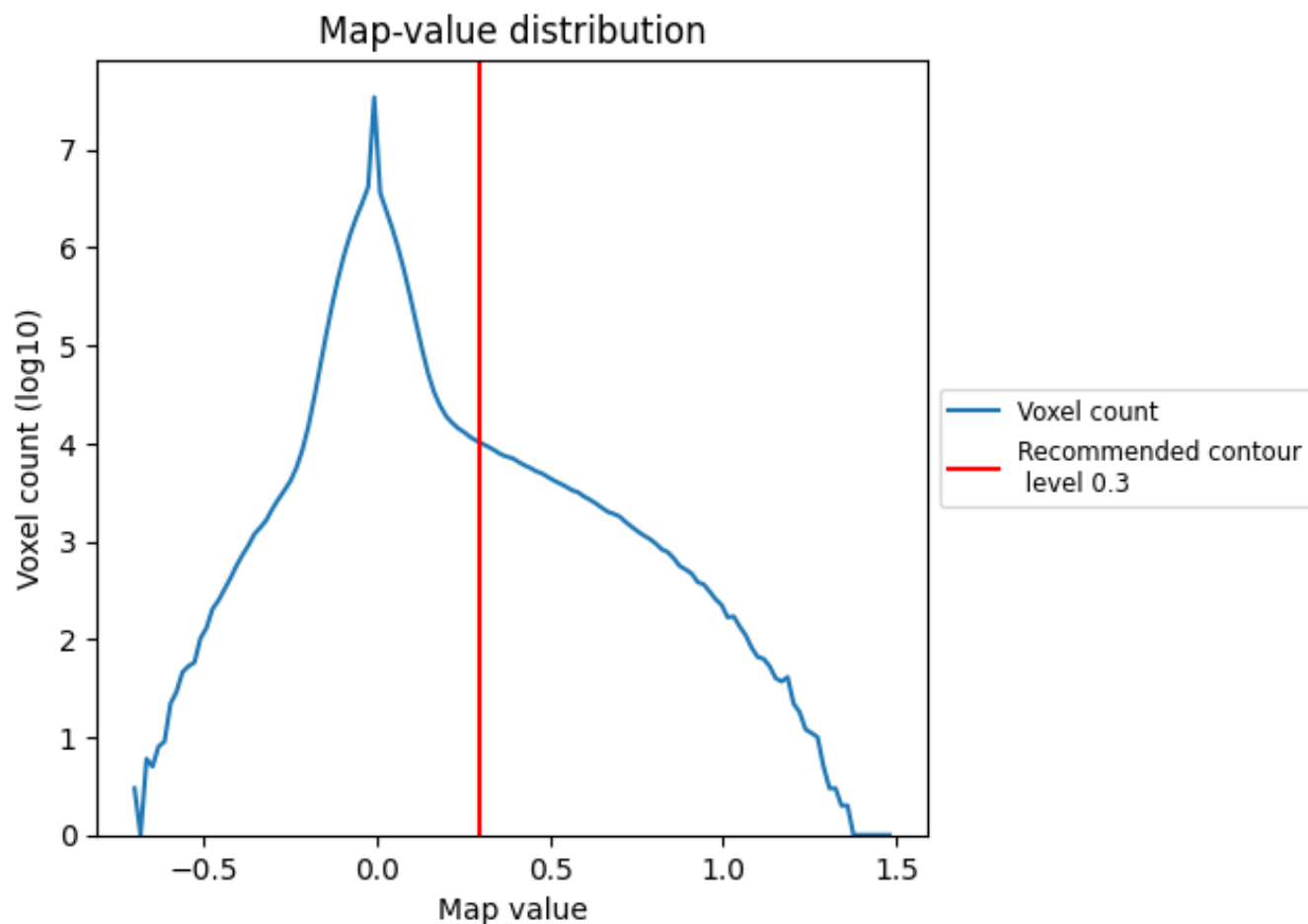


Z

7 Map analysis [i](#)

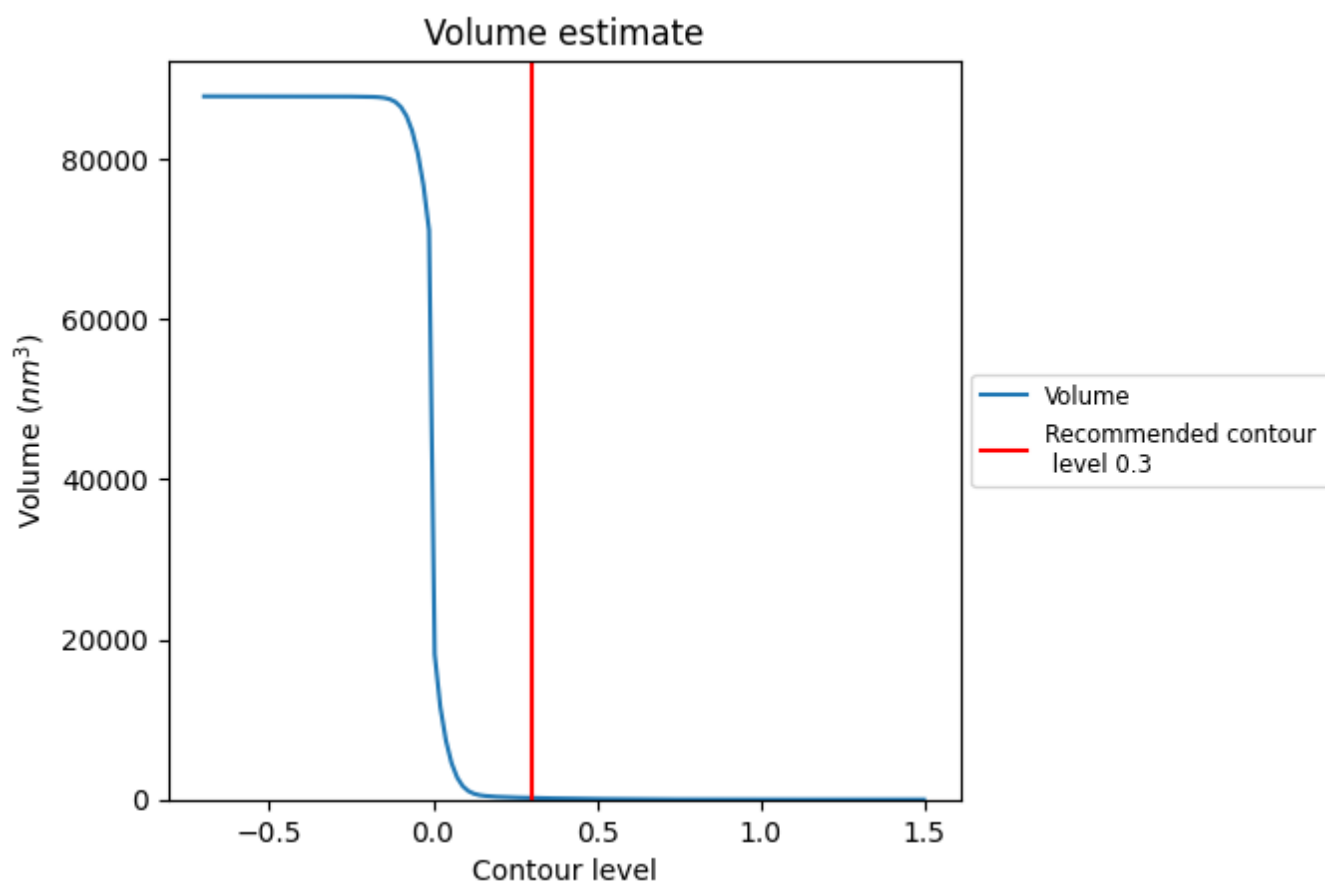
This section contains the results of statistical analysis of the map.

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.

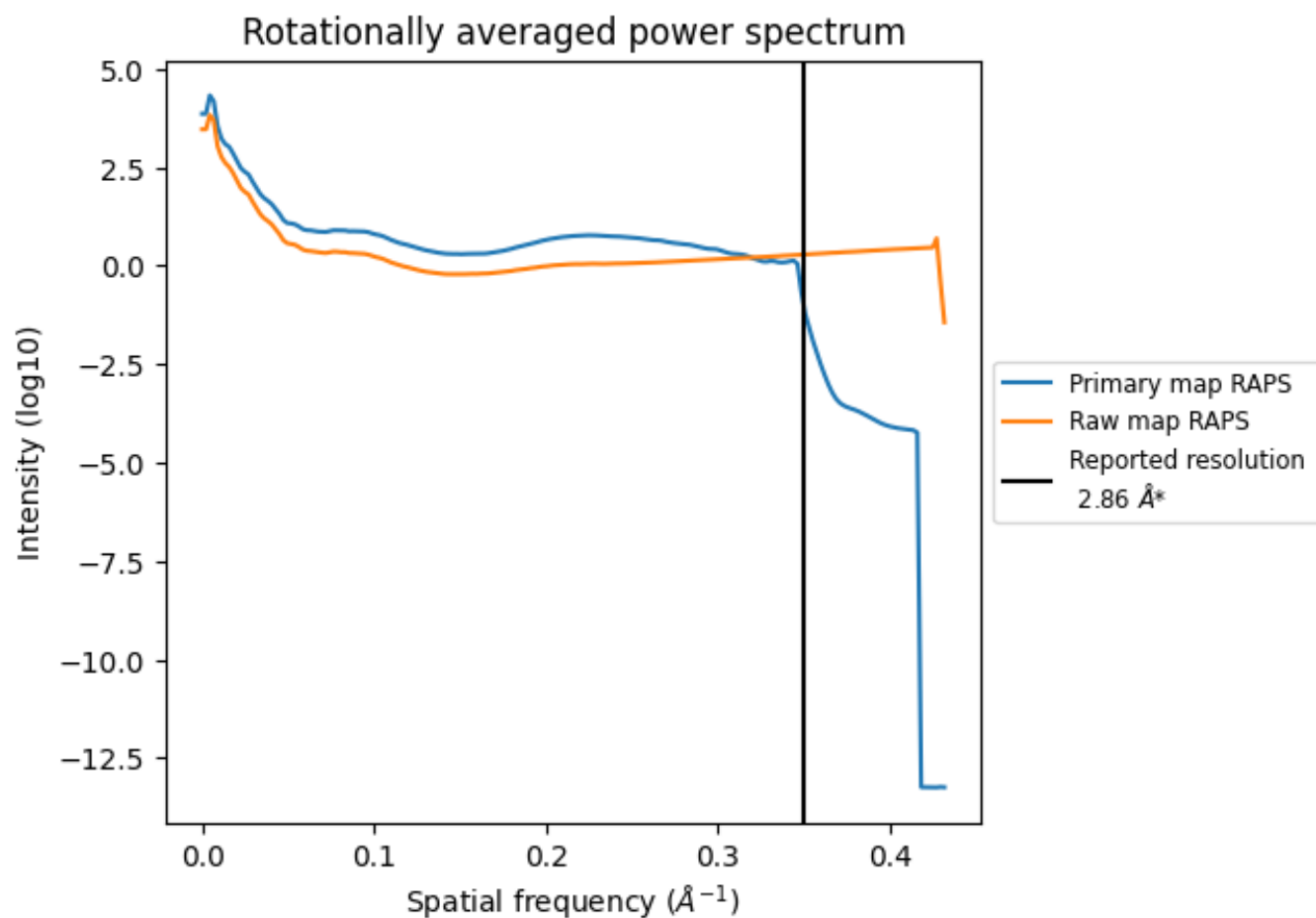
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

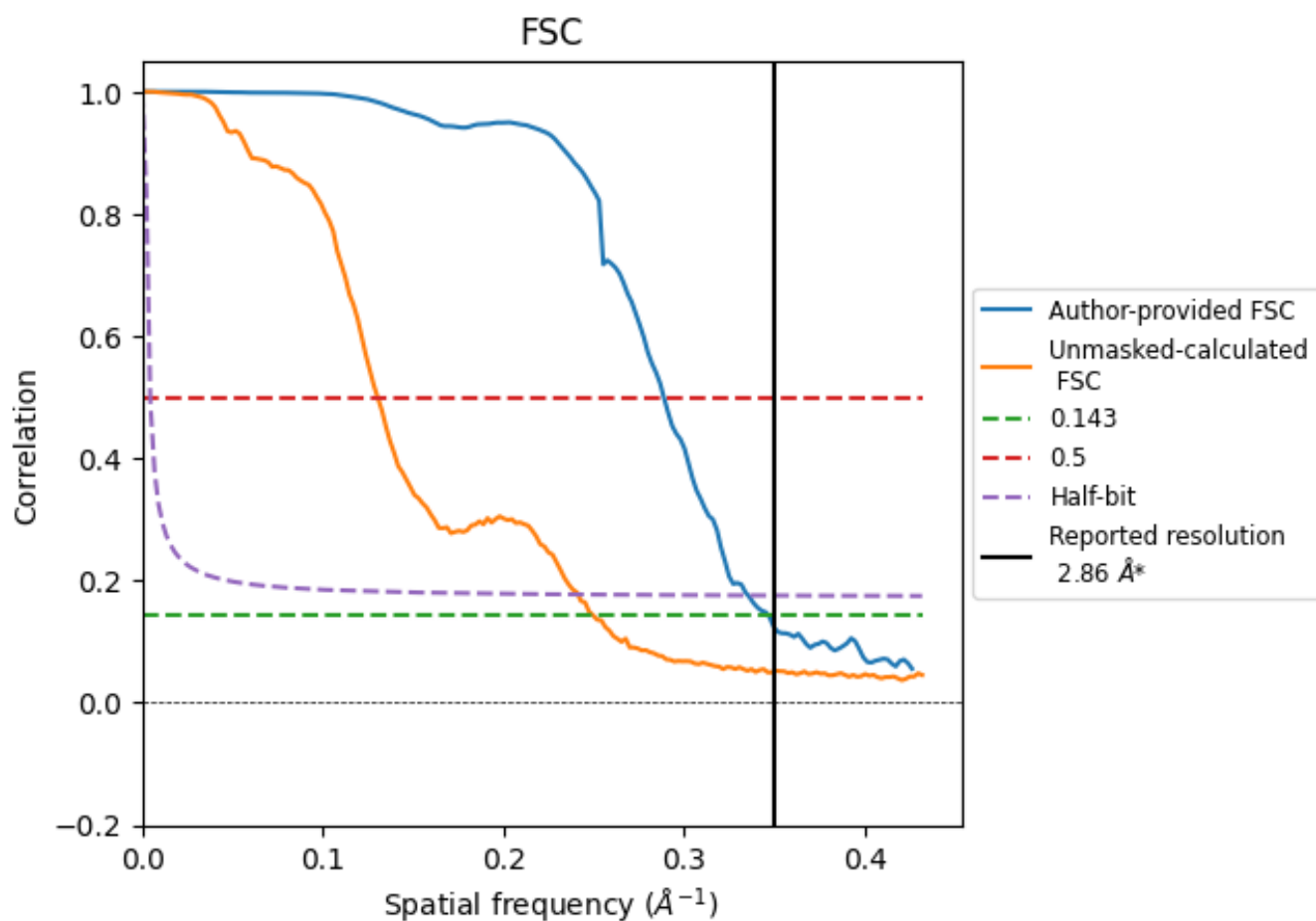


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

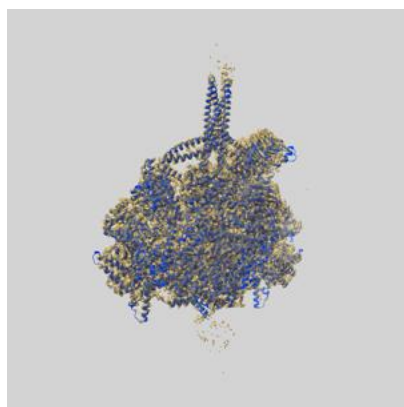
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.88	3.46	2.98
Unmasked-calculated*	4.00	7.67	4.14

*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 4.00 differs from the reported value 2.86 by more than 10 %

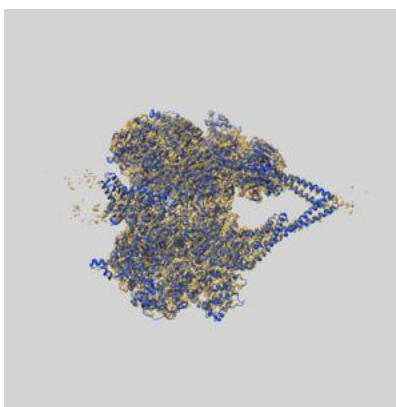
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47378 and PDB model 9E0Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

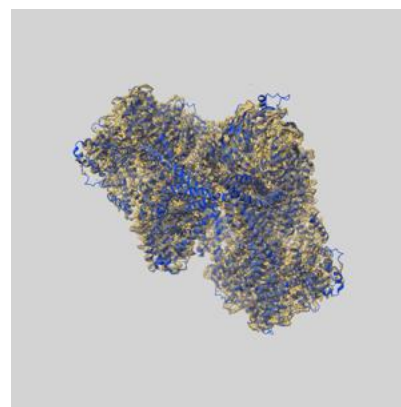
9.1 Map-model overlay [i](#)



X



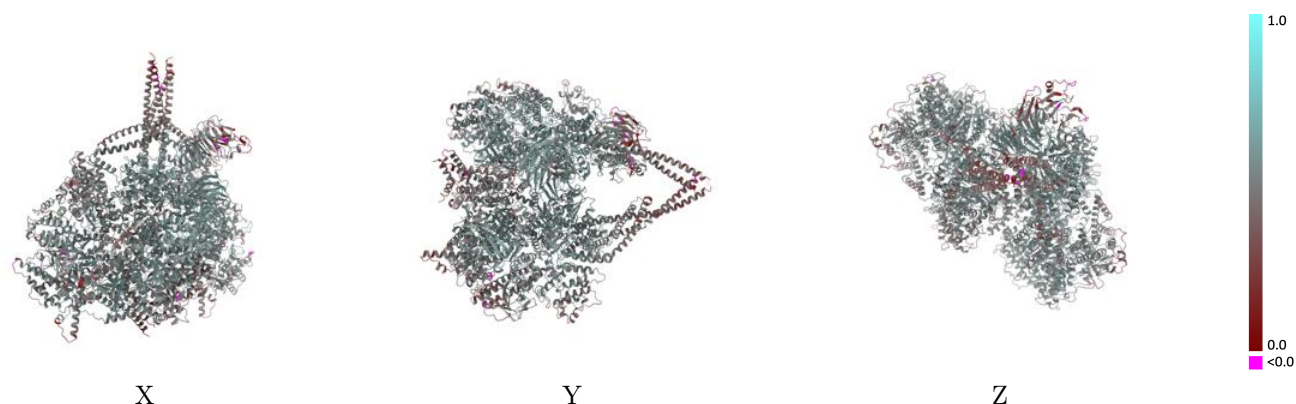
Y



Z

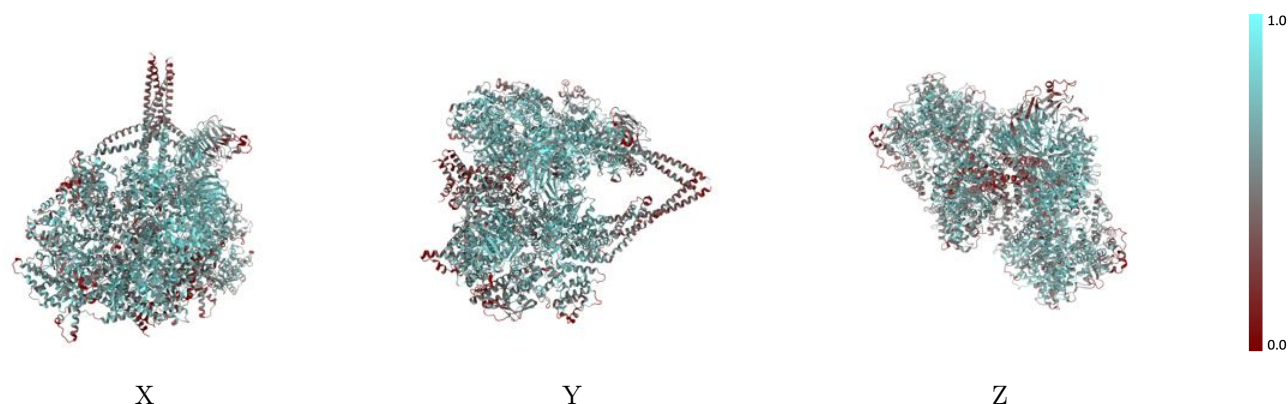
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



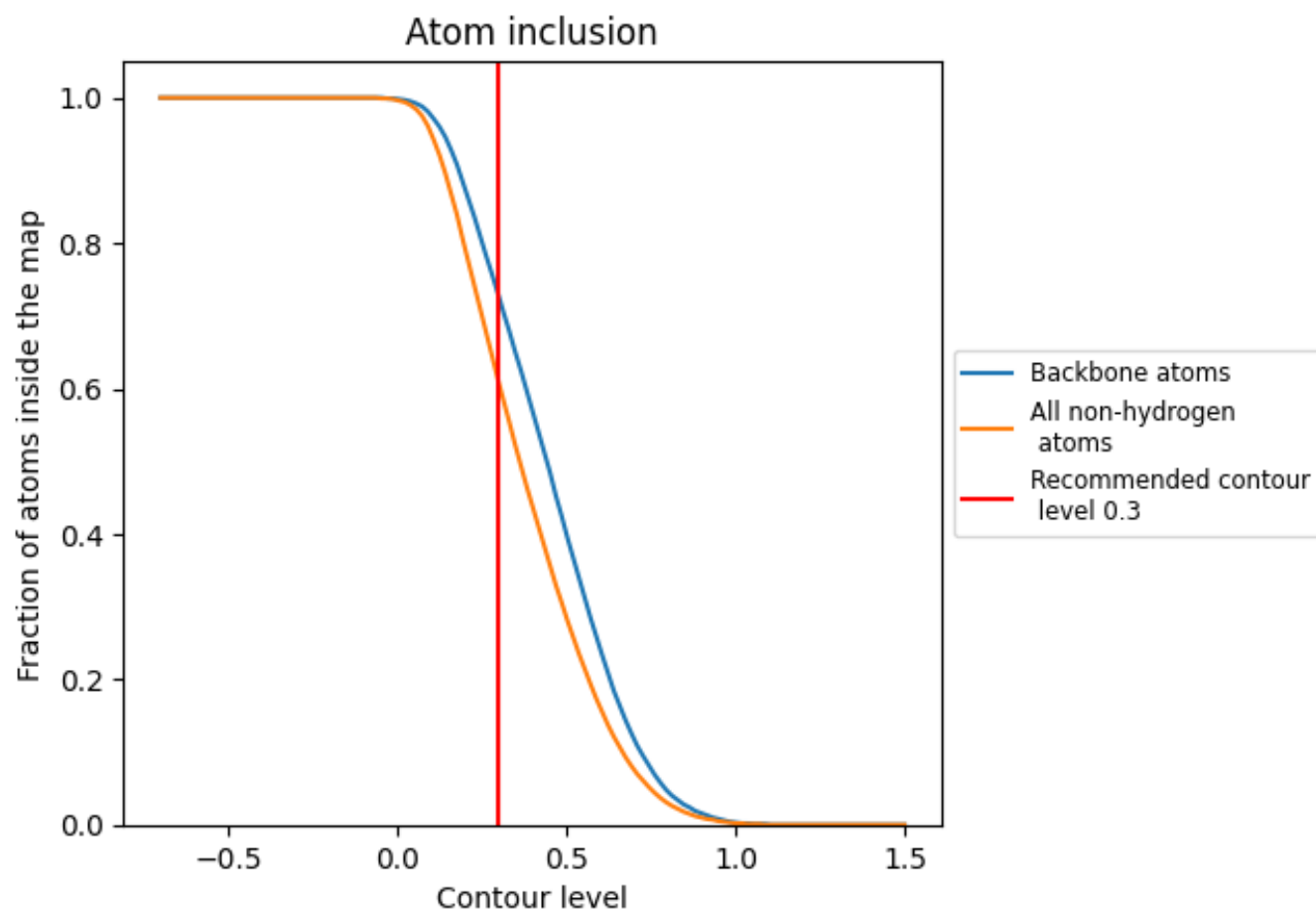
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 61% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6080	<div></div> 0.5020
A	<div></div> 0.5740	<div></div> 0.4920
B	<div></div> 0.6360	<div></div> 0.5130
C	<div></div> 0.7400	<div></div> 0.5600
D	<div></div> 0.5350	<div></div> 0.4330

