



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:28 AM EDT

PDB ID : 9BM5 / pdb\_00009bm5  
EMDB ID : EMD-44688  
Title : State-6 of motor domain from full-length human dynein-1 in 5 mM ATP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.50 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)

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.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
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)	:	2.42

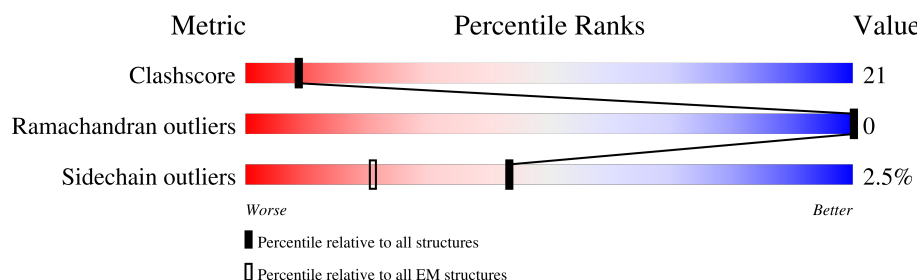
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	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  $\geq 3$ , 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	4646	<div> <div>25%</div> <div>36%</div> <div>22%</div> <div>42%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21780 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
			Total	C	N	O	S		
1	A	2698	21664	13799	3740	4014	111	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	







K3757	D3691	N3631	S3566	F3496	MET	SER	ALA	E3196	Y3125	H3063	S3002	G2937
G3758	L3692	P3632	L3567	K3497	ILE	TYR	VAL	Q3197	M3126	V3064	G3003	V2938
R3759	C3693	L3633	L3567	N3498	ARG	ASN	LYS	Q3198	P3127	V3065	F3004	S2939
I3760	S3694	L3634	D3570	Q3499	LEU	GLU	LEU	K3199	V3128	F3066	L3005	G2942
L3761	R3695	V3635	D3571	M3500	GLU	ILE	LEU	H3200	V3129	T3067	E3006	K2943
D3762	V3696	Q3636	L3572	S3501	ALA	VAL	GLU	L3201	Y3130	K3068	R3007	T2944
D3763	D3699	D3637	E3575	T3502	SER	ASN	GLN	N3202	D3131	N3069	M3008	T2945
D3764	V3699	V3638	A3576	I3503	ILE	ASN	GLN	V3203	K3132	PRO	L3008	L2946
T3765	F3701	E3639	A3577	D3506	ARG	SER	CYS	G3204	L3133	SER	N3009	
L3766	T3702	S3640	L3578	C3507	TYR	LEU	LEU	Q3204	P3134	GLU	T3010	
V3703	V3703	Y3641	M3579	L3508	LYS	LEU	LEU	L2005	G3134	GLY	L3011	F2949
L3767	T3704	D3642	L3580	L3508	GLU	CYS	GLY	R3206	Q3135	LEU	L3012	V2950
T3768	R3705	P3643	K3581	L3514	GLU	GLY	GLU	K3207	Q3135	LYS	A3013	A2951
L3769	S3706	V3644	R3582	A3515	TYR	PRO	SER	N3202	D3131	ASP		
L3770		L3645	R3582	A3515	ALA	ILE	THR	V3203	H3139	ARG	N3014	L2956
E3771	C3712	N3646	R3585	Y3516	VAL	VAL	THR	Q3204	R3140	ASP	L3014	
N3772	L3713	P3647	Y3586	A3517	LEU	LYS	THR	R3209	E3141	ALA	G3015	S2957
L3773	N3714	V3648	P3587	G3518	TRP	TRP	TRP	E3210	A3142	ALA	E3016	V2958
L3774	L3767	L3649	L3588	Y3519	GLU	ILE	LYS	T3211	I3143	THR	V3017	Y2959
L3775	D3642	L3649	L3588	F3520	SER	ALA	GLN	V3212	V3144	SER		
R3776	R3651	N3650	I3589	D3521	GLN	GLN	ILE	D3213	N3145	P3083	P3018	Q2960
E3776	K3718	R3652	S3593	Q3522	ALA	LEU	ARG	D3214	S3146	A3084	G3019	I2961
A3777	A3719	E3652	G3594	M3524	ILE	ASN	ILE	Q3214	V3148	L3085	L3020	K2962
A3778	R3721	V3653	Q3595	R3525	ALA	ALA	MET	V3215	F3149	F3086	F3021	V2963
E3779	P3722	R3654	A3596	Q3526	ASP	ASP	ARG	E3216	V3150	N3087	E3022	H2964
V3780	D3723	R3655	T3597	Q3526	LEU	MET	GLU	E3217	H3151	R3088	R2965	K2965
T3781	V3724	T3656	E3598	L3528	ALA	LEU	ASN	R3219	H3155	V3090	D3024	K2966
R3782	D3725	Q3657	F3599	F3529	VAL	ARG	PHE	R3220	Q3156	L3091	E3025	V2967
K3783	E3726	G3658	I3600		GLU	VAL	PRO	ASP	A3157	N3092	Y3026	T2968
V3784	K3727	R3659	M3601	S3533	ALA	GLU	THR	LEU		F3094	A3027	C2969
E3785	R3728	V3660	N3602	H3534	PRO	LEU	ILE	ARG	R3160	G3095	L3028	E2970
E3786	E3729	L3661	E3603	H3535	ASN	ARG	VAL	ILE	L3161	D3096	L3029	D2971
E3787	S3729	L3662	Y3604	L3536	GLU	ASN	GLN	LYS	A3162	W3097	M3030	F2972
T3788	D3730	T3663	K3605	Q3537	R3474	GLU	SER	GLN	K3163	S3098	T3031	D2973
L3789	L3732	L3664	R3607	Q3538	T3476	LEU	ALA	GLU	R3164	T3099	Q3032	E2974
V3790	K3733	G3665	K3608	F3543	T3476	GLN	ALA	LYS	G3165	E3100	C3033	D2975
M3791	L3734	D3666	I3609	R3544	T3476	LYS	GLU	VAL	G3166	A3101	K3034	L2976
Q3792	Q3735	Q3667	T3610	T3545	A3477	ILE	ILE	LYS	R3167	L3102	E3035	R2977
E3793	G3736	D3668	T3612	I3547	L3478	GLU	ARG	ASN	T3168	Y3103	G3036	T2978
V3794	E3737	I3669	S3613	A3548	L3479	SER	LYS	ASP	M3169	Q3104	A3037	V2979
E3795	F3738	D3670	F3614	R3549	L3479	GLU	ASP	ALA	A3170	V3105	L3038	L2980
T3796	Q3739	L3671	L3615	Y3552	R3480	ASN	ALA	ALA	K3107	G3106	Q3038	R2981
V3797	L3740	S3672	D3616	L3553	L3481	GLN	ILE	ALA	E3108	K3107	K3039	R2982
S3798	R3741	P3673	D3617	L3563	L3482	LYS	LYS	ASP	F3109	E3108	E3040	S2983
Q3799	L3742	S3674	D3617	S3554	E3485	ALA	ASN	LYS	T3110	G3041	G3041	C2984
Q3800	R3743	F3675	D3618	N3555	E3485	ASN	THR	VAL	S3111	L3042	M3043	C2985
Y3801	Q3744	V3676	F3619	A3556	E3487	GLU	MET	ASN	K3112	R2986	K2986	K2986
L3802	L3745	V3677	R3620	D3557	E3487	VAL	SER	GLN	M3113	L3044	N2987	N2987
P3803	E3746	F3678	K3621	E3558	R3488	GLU	ASN	VAL	D3114	D3045	L3045	E2988
L3804	K3747	Y3679	N3622	R3559	W3489	GLU	PRO	ALA	L3115	S3046	H3047	K2989
A3807	S3748	L3679	L3623	L3560	K3491	VAL	SER	PRO	E3116	E3049	A2991	I2993
C3808	L3749	S3680	E3624	R3561	T3492	GLU	ASN	ALA	N3119	E3049	L3050	L2993
F3813	L3750	R3681	S3625	Q3563	S3493	GLN	GLN	ALA	K3117	E3048	Y3051	M2994
T3814	Q3751	D3683	A3626	W3562	S3494	LYS	LYS	LYS	F3118	E3048	K3052	D2995
M3815	A3752	T3685	L3627	A3564	E3494	VAL	VAL	VAL	N3120	F3053	E2996	E2996
E3816	L3753	V3686	R3628	S3565	T3495	GLU	PRO	ALA	D3124	F3054	S2997	S2997
S3817	N3754	E3687	F3629			GLN					Q3057	N2998
L3818	E3755	F3688									V3058	V2999
K3819	V3756	P3689									L3059	L3000
Q3820											R3060	I3001
											N3061	L3062



T4628	K4629	E4630	D4631	P4632	R4633	S4634	F4635	Y4636	E4637	R4638	V4642	L4643	C4644	T4645	L4541	E4542	V4543	N4544	S4548	Q4549	Q4550	A4551	T4552	L4553	D4554	A4555	G4559	N4571	N4572	L4575	S4576	L4577	S4578	N4579	A4580	T4581	L4590	R4591	K4594	Q4595	T4596	N4597	L4598	E4599	K4600	K4601	A4602	S4603	V4604	T4605	L4606	L4607	P4608	V4609	T4610	L4611	R4615	A4616	D4617	L4618	I4619	D4623	L4536	E4625	L4626	A4627	A4471	Q4472	M4473	T4474	V4475	I4476	Q4477	W4478	V4479	S4480	D4481	F4482	S4483	E4484	R4485	I4486	K4487	Q4488	L4489	Q4490	N4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	G4499	Q4500	A4501	K4502	E4503	L4504	K4505	M4506	I4507	H4508	V4509	C4510	C4512	G4513	L4514	F4515	V4516	P4517	I4521	T4524	S4525	M4532	S4535	L4536	E4537	E4538	K4406	D4407	P4408	L4409	F4410	R4411	F4412	F4413	E4414	R4415	E4416	V4417	G4420	Q4425	D4426	Q4429	D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443	Q4444	T4445	M4446	L4447	L4448	R4449	T4450	L4451	I4452	M4453	E4454	L4455	V4456	K4457	G4458	I4459	L4460	P4461	R4462	S4463	W4464	S4465	H4466	Y4467	T4468	V4469	K4345	M4346	Q4347	MEI	GLU	LEU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	THR	LYS	F4282	E4281	F4282	S4277	R4276	S4277	V4288	D4289	G4290	H4291	K4292	D4293	P4297	D4298	G4299	I4300	R4301	R4302	E4303	E4304	F4305	V4306	Q4307	V4308	V4309	E4310	L4311	L4312	T4315	W4320	L4321	G4322	L4323	P4324	M4325	K4326	D4338	M4339	I4340	S4341	K4342	L4344	K4345	M4346	Q4347	MEI	GLU	LEU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	THR	LYS	F4426	Q4425	D4429	Q4429	D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443	Q4444	T4445	M4446	L4447	L4448	R4449	T4450	L4451	I4452	M4453	E4454	L4455	V4456	K4457	G4458	I4459	L4460	P4461	R4462	S4463	W4464	S4465	H4466	Y4467	T4468	V4469	K4374	A4375	V4376	M4377	R4378	T4379	L4380	H4381	T4382	T4383	A4384	S4385	M4386	W4387	L4388	H4389	I4390	I4391	P4392	Q4393	T4394	L4395	S4396	K4399	R4400	T4401	V4402	E4403	M4404	I4405	K4629	E4630	D4631	P4632	R4633	S4634	F4635	Y4636	E4637	R4638	L4541	E4542	V4543	N4544	S4548	Q4549	Q4550	A4551	T4552	L4553	D4554	A4555	G4559	N4571	N4572	L4575	S4576	L4577	S4578	N4579	A4580	T4581	L4590	R4591	K4594	Q4595	T4596	N4597	L4598	E4599	K4600	K4601	A4602	S4603	V4604	T4605	L4606	L4607	P4608	V4609	T4610	L4611	R4615	A4616	D4617	L4618	I4619	D4623	L4536	E4625	L4626	A4627	I3821	L3824	Y3825	Y3826	Y3827	S3828	L3829	I3835	Y3836	H3837	N3838	Y3839	L3840	Y3841	E3842	L3846	K3847	G3848	Y3849	T3850	D3851	H3852	T3853	G3854	R3855	L3856	I3859	D3862	L3863	A3867	F3868	N3869	R3870	Y3871	A3872	G3873	K3874	K3875	L3876	D3879	H3880	I3881	T3882	F3883	A3884	K3885	L3886	K3893	V3896	G3897	E3898	P3899	T3900	Y3901	D3902	A3903	E3904	F3905	Q3906	H3907	F3908	L3909	R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	G3918	A3919	G3919	S3920	T3921	P3922	I3923	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	E3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	I3942	A3943	F3944	K3945	D3946	L3947	I3948	A3949	K3950	Q3952	A3953	D3954	Q3956	F3957	G3958	I3959	W3960	L3961	D3962	S3963	S3964	S3965	P3966	E3967	V3970	P3971	Y3972	L3973	Y3974	S3975	E3976	E3977	T3978	P3979	A3980	T3981	P3982	L3983	G3984	Q3985	A3986	R3987	H3988	L3989	L3990	L3991	Q3994	A3995	F3996	R3997	P3998	D3999	R4000	L4001	L4002	A4003	M4004	A4005	H4006	V4009	E4015	M4018	S4019	I4020	M4021	E4022	D4026	L4027	T4028	H4029	L4030	V4031	E4034	V4035	K4036	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	Y4049	D4050	G4053	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	L4071	G4072	S4073	A4074	E4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4083	I4084	M4085	T4086	A4087	V4088	K4089	S4090	G4091	D4092	M4095	L4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	L4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	L4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	P4135	L4138	L4139	I4144	F4145	V4146	F4147	E4148	P4151	K4154	T4160	R4168	I4169	C4170	K4171	S4172	I4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	L4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	L4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	P4135	L4138	L4139	I4144	F4145	V4146	F4147	E4148	P4151	K4154	T4160	R4168	I4169	C4170	K4171	S4172	H4029	L4030	V4031	E4034	V4035	K4036	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	Y4049	D4050	G4053	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	L4071	G4072	S4073	A4074	E4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4083	I4084	M4085	T4086	A4087	V4088	K4089	S4090	G4091	D4092	M4095	L4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	L4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	L4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	P4135	L4138	L4139	I4144	F4145	V4146	F4147	E4148	P4151	K4154	T4160	R4168	I4169	C4170	K4171	S4172	I3959	W3960	L3961	D3962	S3963	S3964	S3965	P3966	E3967	V3970	P3971	Y3972	L3973	Y3974	S3975	E3976	E3977	T3978	P3979	A3980	T3981	P3982	L3983	G3984	Q3985	A3986	R3987	H3988	L3989	L3990	L3991	Q3994	A3995	F3996	R3997	P3998	D3999	R4000	L4001	L4002	A4003	M4004	A4005	H4006	V4009	E4015	M4018	S4019	I4020	M4021	E4022	D4026	L4027	T4028	H4029	L4030	V4031	E4034	V4035	K4036	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	Y4049	D4050	G4053	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	L4071	G4072	S4073	A4074	E4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4083	I4084	M4085	T4086	A4087	V4088	K4089	S4090	G4091	D4092	M4095	L4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	L4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	L4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	P4135	L4138	L4139	I4144	F4145	V4146	F4147	E4148	P4151	K4154	T4160	R4168	I4169	C4170	K4171	S4172	I3821	L3824	Y3825	Y3826	Y3827	S3828	L3829	I3835	Y3836	H3837	N3838	Y3839	L3840	Y3841	E3842	L3846	K3847	G3848	Y3849	T3850	D3851	H3852	T3853	G3854	R3855	L3856	I3859	D3862	L3863	A3867	F3868	N3869	R3870	Y3871	A3872	G3873	K3874	K3875	L3876	D3879	H3880	I3881	T3882	F3883	A3884	K3885	L3886	K3893	V3896	G3897	E3898	P3899	T3900	Y3901	D3902	A3903	E3904	F3905	Q3906	H3907	F3908	L3909	R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	G3918	A3919	G3919	S3920	T3921	P3922	I3923	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	E3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	I3942	A3943	F3944	K3945	D3946	L3947	I3948	A3949	K3950	Q3952	A3953	D3954	Q3956	F3957	G3958	I3959	W3960	L3961	D3962	S3963	S3964	S3965	P3966	E3967	V3970	P3971	Y3972	L3973	Y3974	S3975	E3976	E3977	T3978	P3979	A3980	T3981	P3982	L3983	G3984	Q3985	A3986	R3987	H3988	L3989	L3990	L3991	Q3994	A3995	F3996	R3997	P3998	D3999	R4000	L4001	L4002	A4003	M4004	A4005	H4006	V4009	E4015	M4018	S4019	I4020	M4021	E4022	D4026	L4027	T4028	H4029	L4030	V4031	E4034	V4035	K4036	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	Y4049	D4050	G4053	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	L4071	G4072	S4073	A4074	E4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4083	I4084	M4085	T4086	A4087	V4088	K4089	S4090	G4091	D4092	M4095	L4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	L4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	L4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	P4135	L4138	L4139	I4144	F4145	V4146	F4147	E4148	P4151	K4154	T4160	R4168	I4169	C4170	K4171	S4172	I3959	W3960	L3961	D3962	S3963	S3964	S3965	P3966	E3967	V3970	P3971	Y3972	L3973	Y3974	S3975	E3976	E3977	T3978	P3979	A3980	T3981	P3982	L3983	G3984	Q3985	A3986	R3987	H3988	L3989	L3990	L3991	Q3994	A3995	F3996	R3997	P3998	D3999	R4000	L4001	L4002	A4003	M4004	A4005	H4006	V4009	E4015	M4018	S4019	I4020	M4021	E4022	D4026	L4027	T4028	H4029	L4030	V4031	E4034	V4035	K4036	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	Y4049	D4050	G4053	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	L4071	G4072	S4073	A4074	E4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	260931	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.339	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: 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	0.29	2/22127 (0.0%)	0.56	6/29993 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2908	PRO	CB-CG	-9.40	1.02	1.50
1	A	2908	PRO	CG-CD	-8.12	1.23	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2908	PRO	N-CD-CG	-20.03	73.15	103.20
1	A	2908	PRO	CB-CG-CD	18.83	179.94	106.50
1	A	2908	PRO	CA-CB-CG	-17.12	71.48	104.00
1	A	2908	PRO	CA-N-CD	-8.77	99.22	111.50
1	A	2452	LEU	CB-CG-CD2	6.62	122.26	111.00

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	21664	0	21700	899	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	54	0	24	5	0
3	A	62	0	24	1	0
All	All	21780	0	21748	899	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 21.

The worst 5 of 899 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:4027:LEU:CD2	1:A:4058:LEU:HD22	1.26	1.58
1:A:4027:LEU:HD23	1:A:4058:LEU:CD2	1.43	1.43
1:A:4027:LEU:CD2	1:A:4058:LEU:CD2	2.10	1.14
1:A:4027:LEU:HD22	1:A:4058:LEU:HD22	1.24	1.10
1:A:4321:LEU:CD1	1:A:4323:LEU:HD12	1.81	1.10

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	2684/4646 (58%)	2619 (98%)	65 (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	2397/4125 (58%)	2337 (98%)	60 (2%)	42 67

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3051	TYR
1	A	4217	ASP
1	A	3149	PHE
1	A	4171	LYS
1	A	4447	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4100	HIS
1	A	4108	GLN
1	A	4381	HIS
1	A	2930	GLN
1	A	3200	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	ATP	A	4702	-	28,33,33	0.67	0	34,52,52	0.60	1 (2%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.33	3 (10%)
3	ATP	A	4703	-	28,33,33	0.66	0	34,52,52	0.59	1 (2%)
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.24	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	ATP	A	4702	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	3/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.65	123.72	128.67
2	A	4701	ADP	N3-C2-N1	-3.52	123.89	128.67
2	A	4704	ADP	C4-C5-N7	-2.50	106.70	109.34
2	A	4704	ADP	O4'-C1'-N9	2.47	112.03	108.75
2	A	4701	ADP	C4-C5-N7	-2.46	106.74	109.34

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

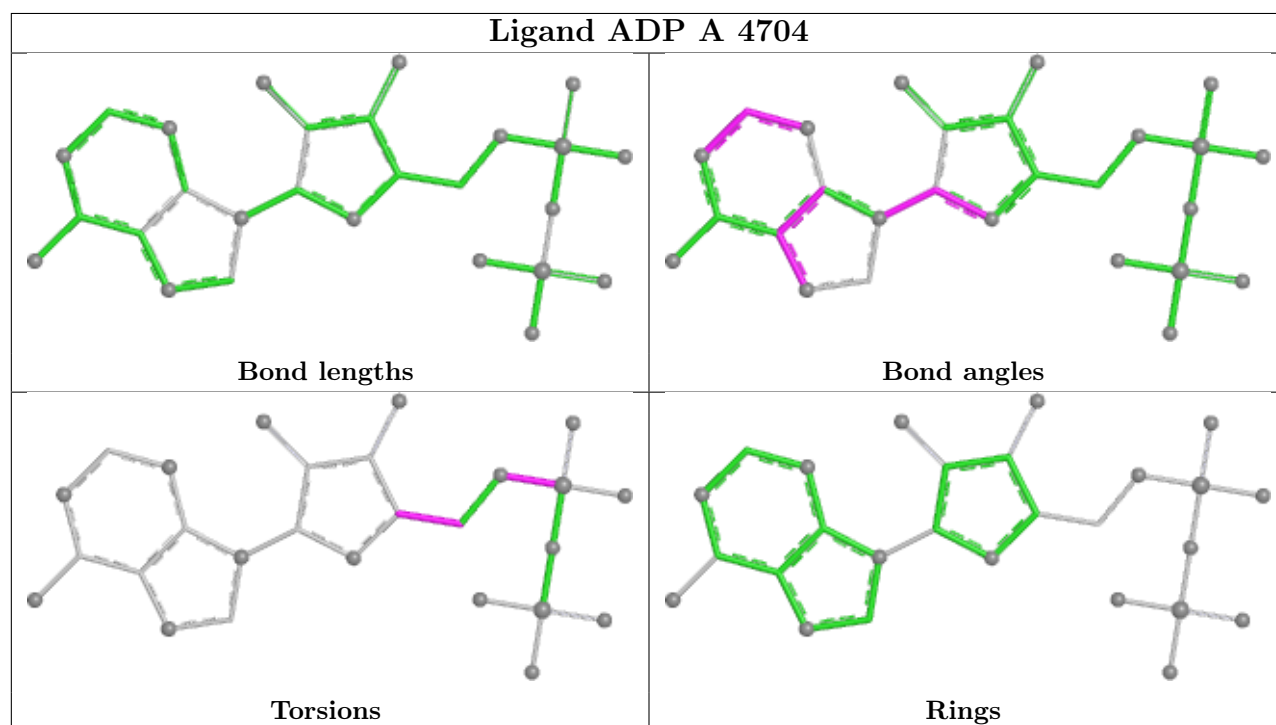
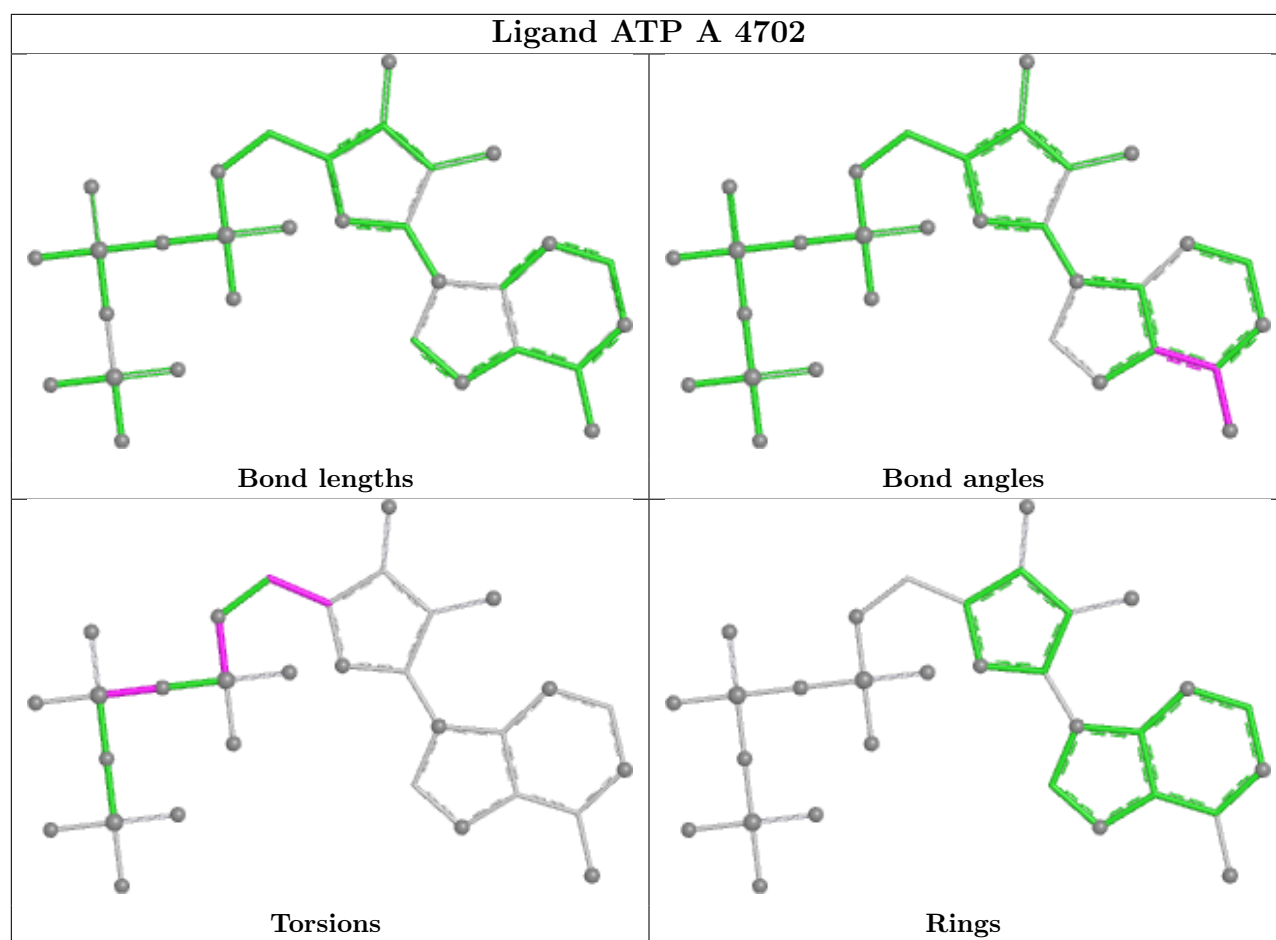
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4703	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

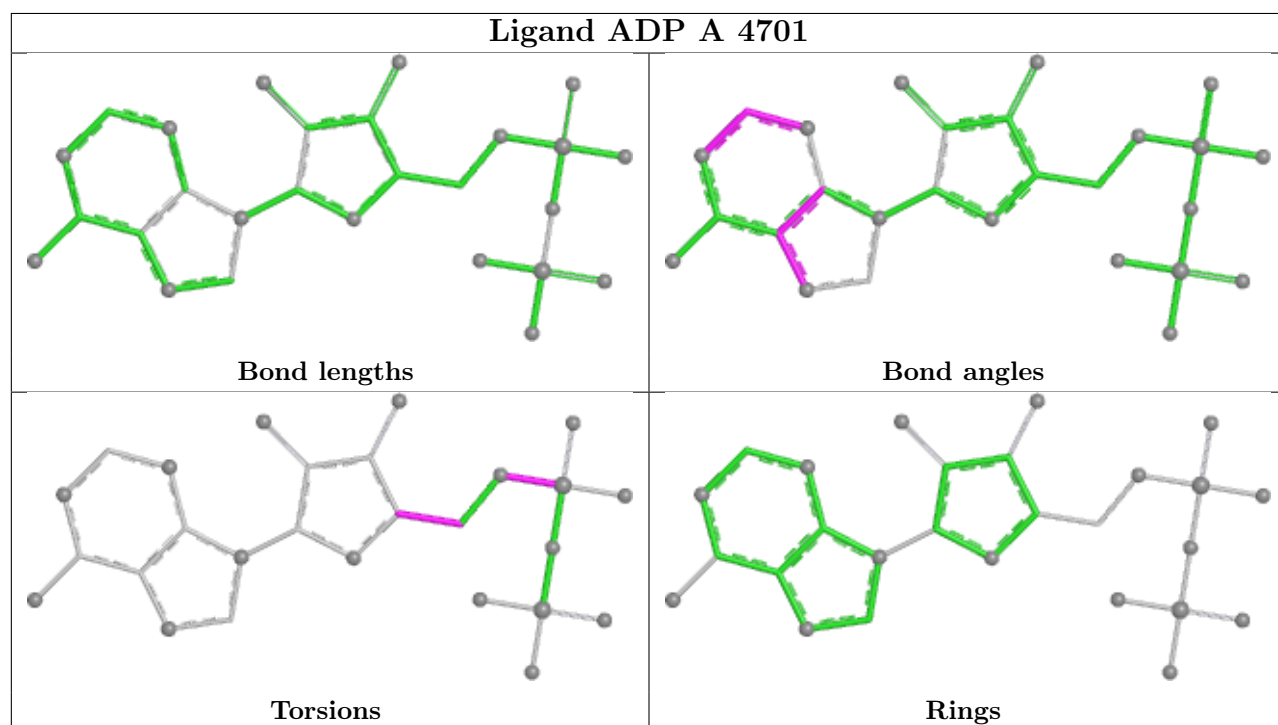
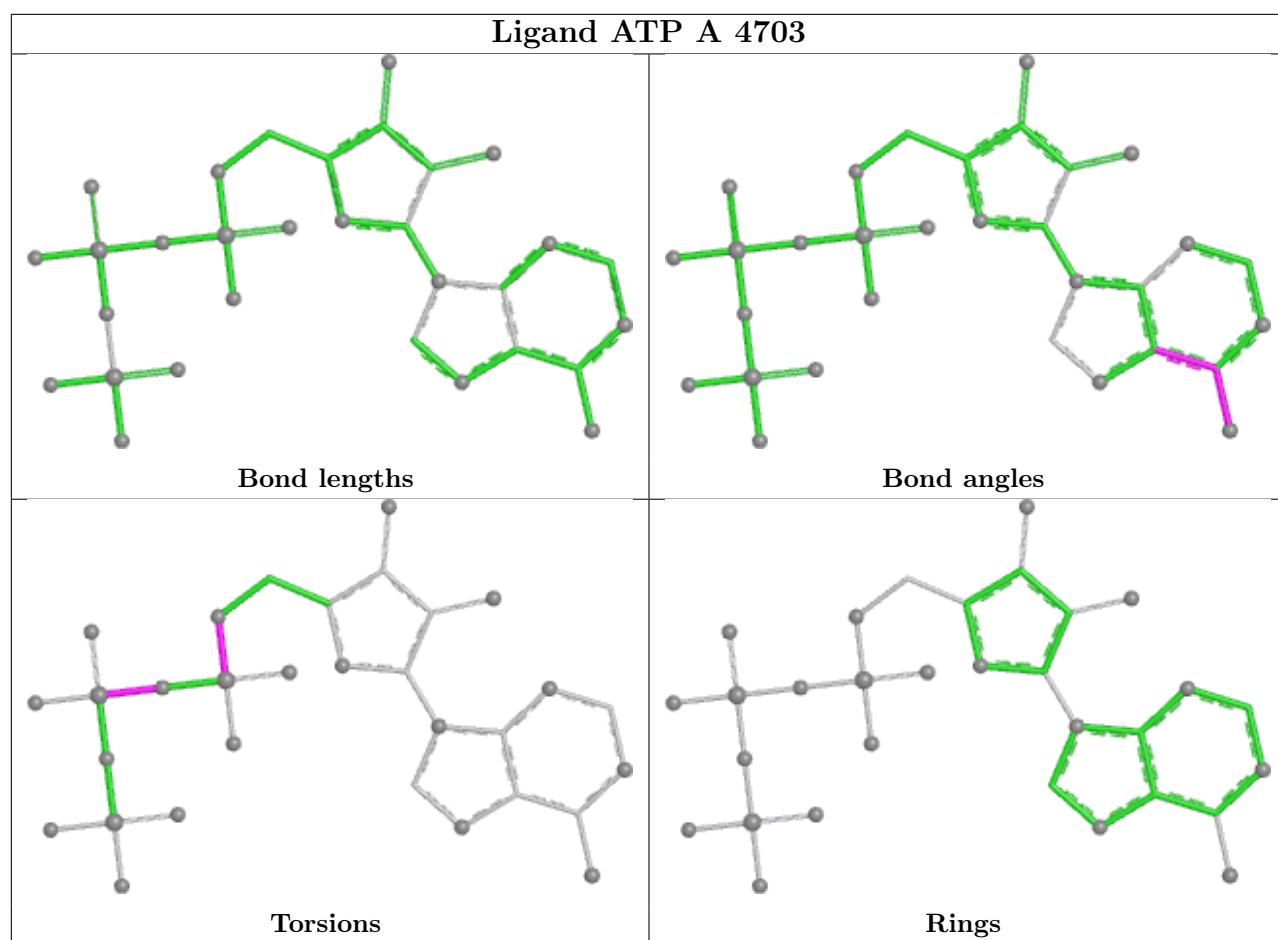
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	3	0
3	A	4703	ATP	1	0
2	A	4701	ADP	2	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.

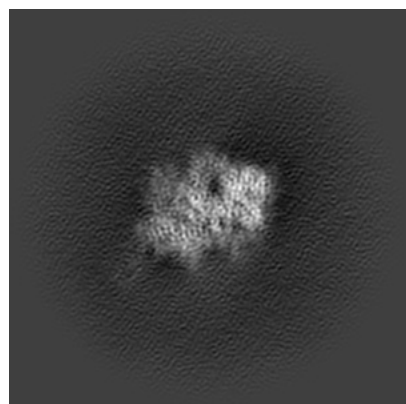
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44688. These allow visual inspection of the internal detail of the map and identification of artifacts.

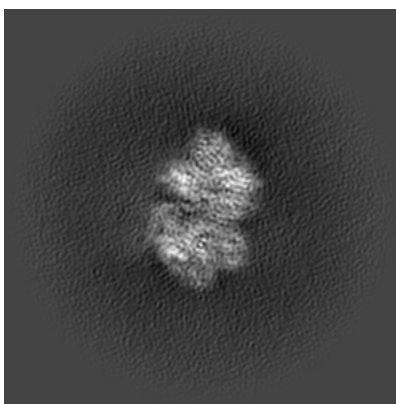
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

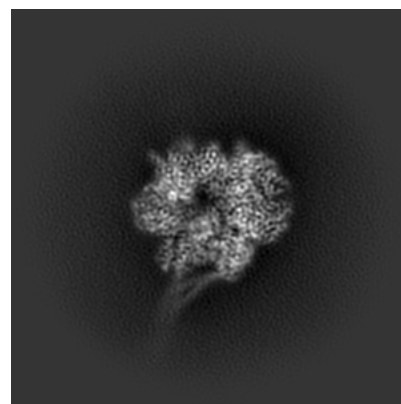
#### 6.1.1 Primary map



X

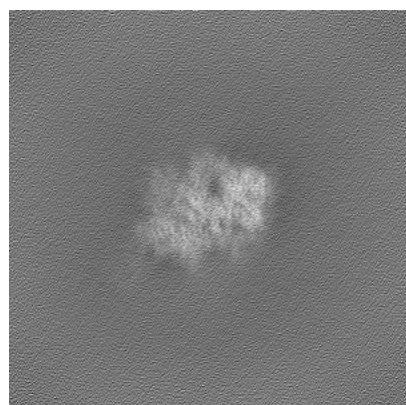


Y

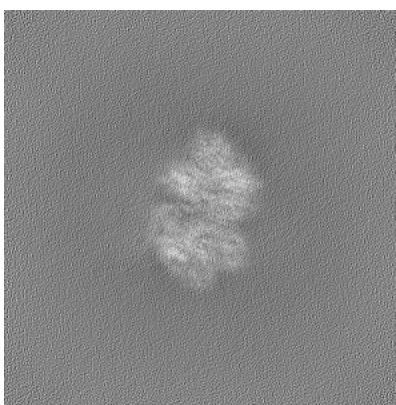


Z

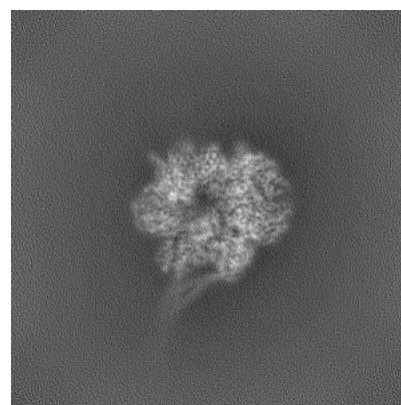
#### 6.1.2 Raw map



X



Y

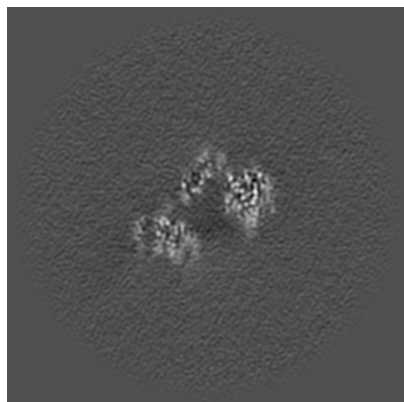


Z

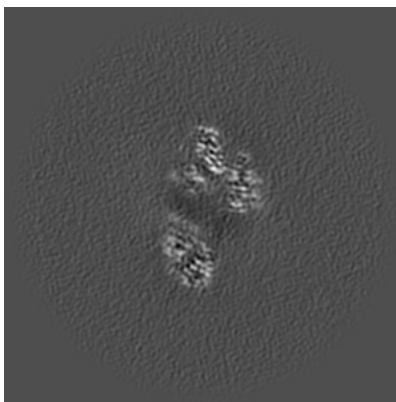
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

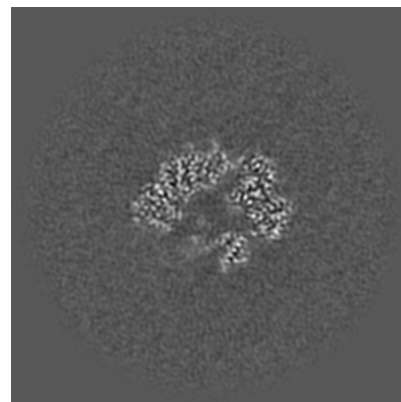
### 6.2.1 Primary map



X Index: 200

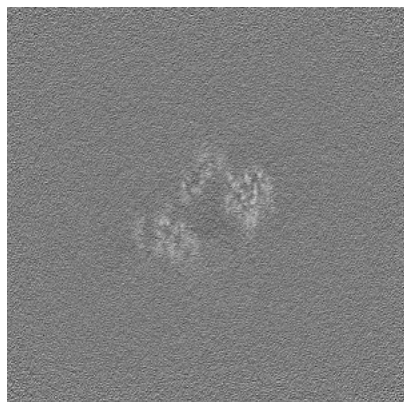


Y Index: 200

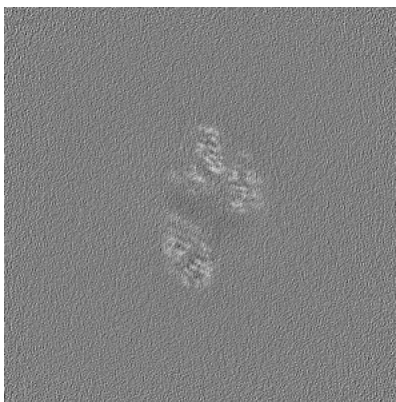


Z Index: 200

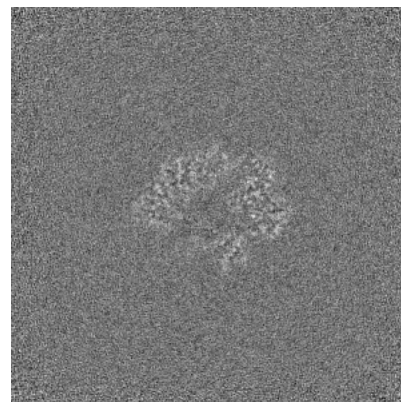
### 6.2.2 Raw map



X Index: 200



Y Index: 200

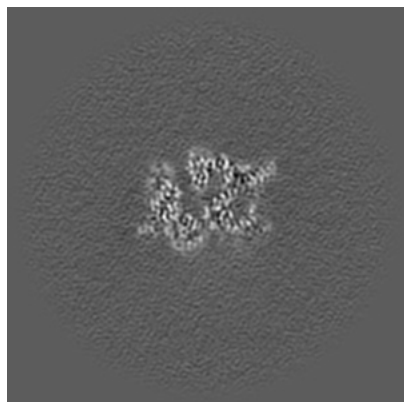


Z Index: 200

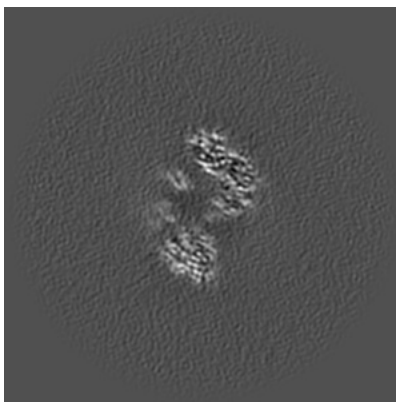
The images above show central slices of the map in three orthogonal directions.

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

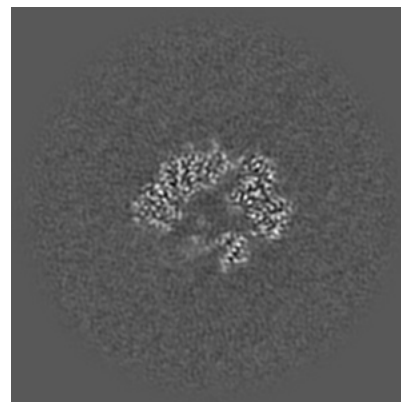
### 6.3.1 Primary map



X Index: 228

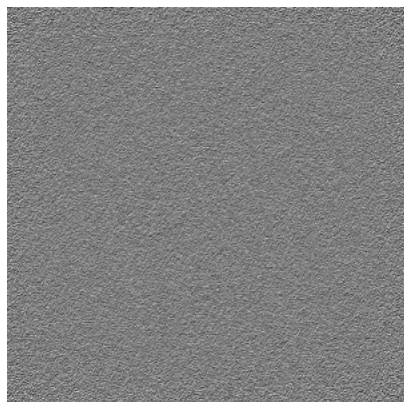


Y Index: 191

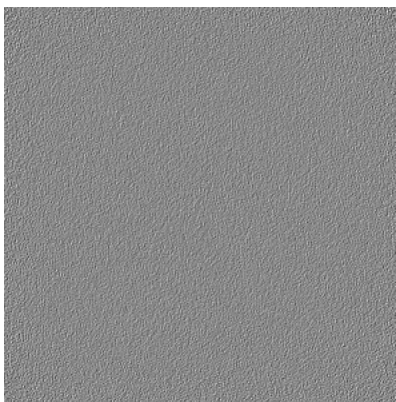


Z Index: 200

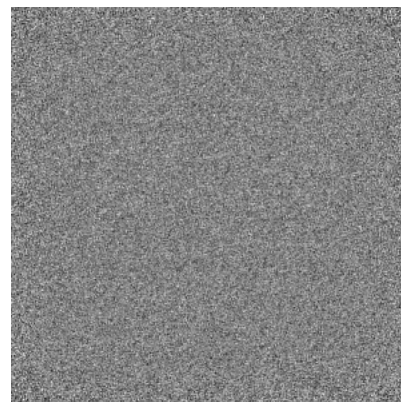
### 6.3.2 Raw map



X Index: 0



Y Index: 0



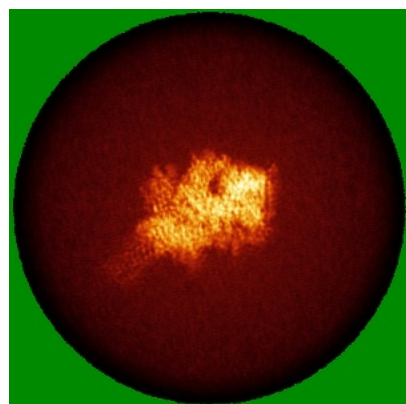
Z Index: 0

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

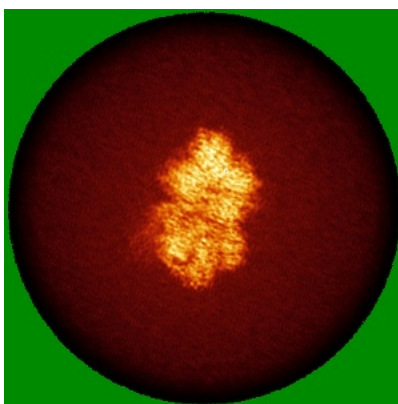


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

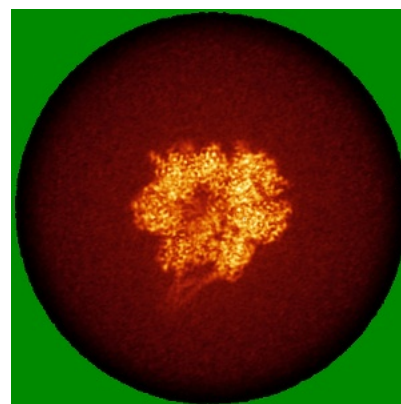
### 6.4.1 Primary map



X

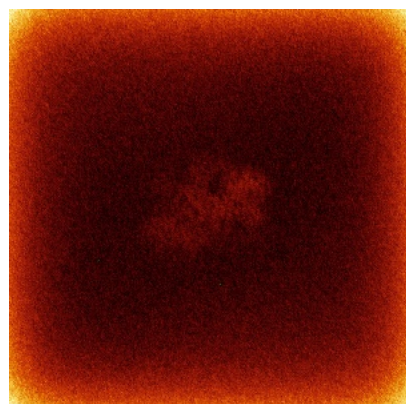


Y

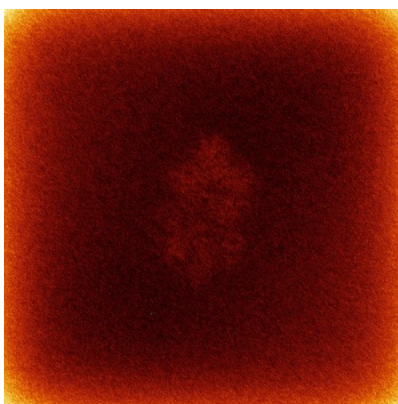


Z

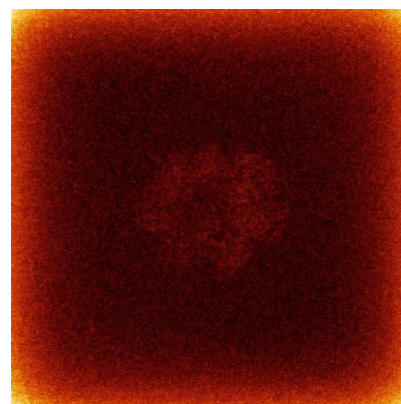
### 6.4.2 Raw map



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.

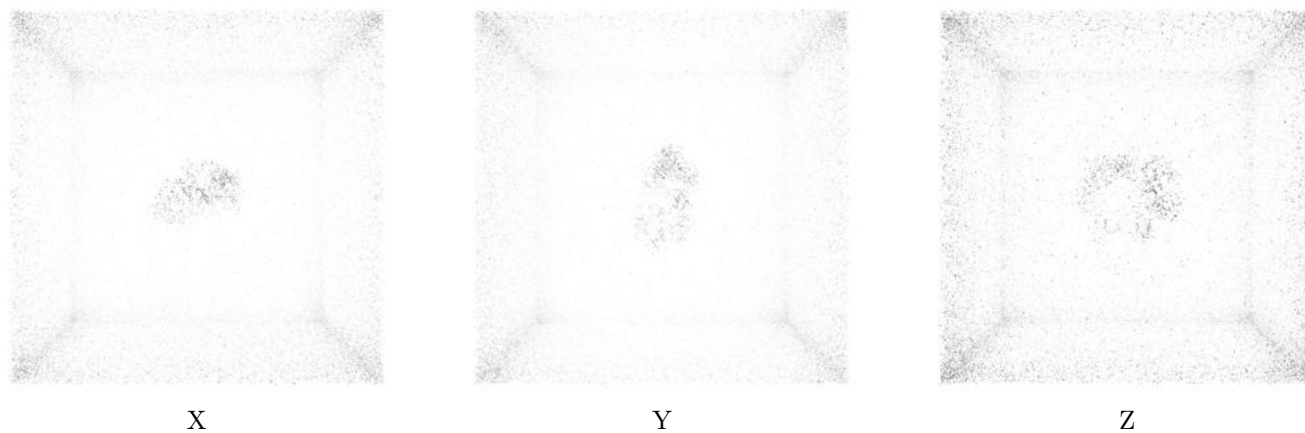
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

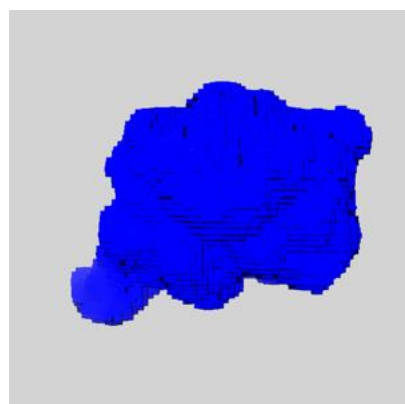
## 6.6 Mask visualisation [i](#)

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

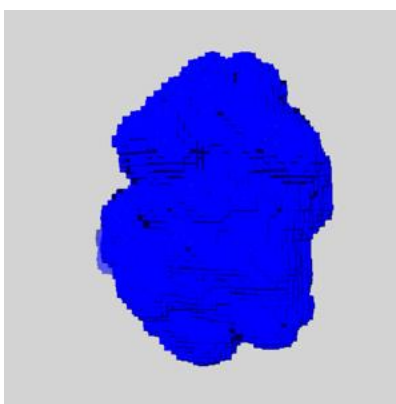
A mask typically either:

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

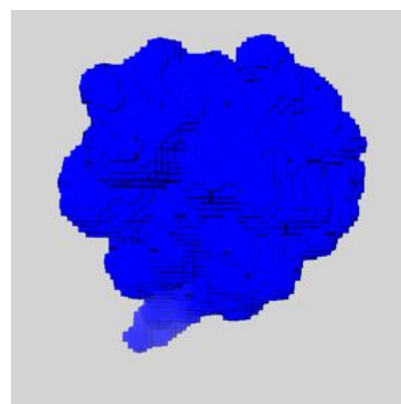
### 6.6.1 emd\_44688\_msk\_1.map [i](#)



X



Y



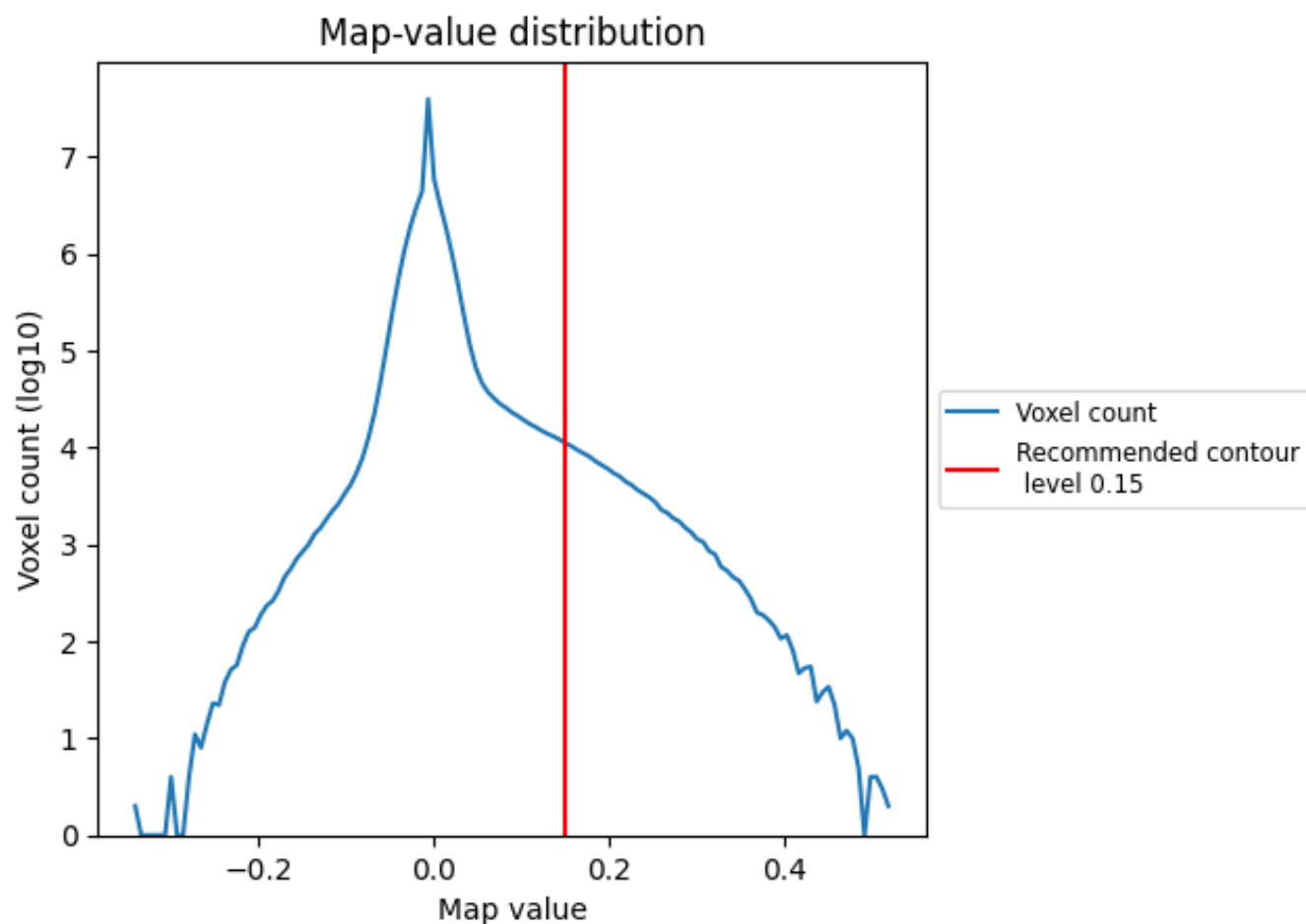
Z



## 7 Map analysis [i](#)

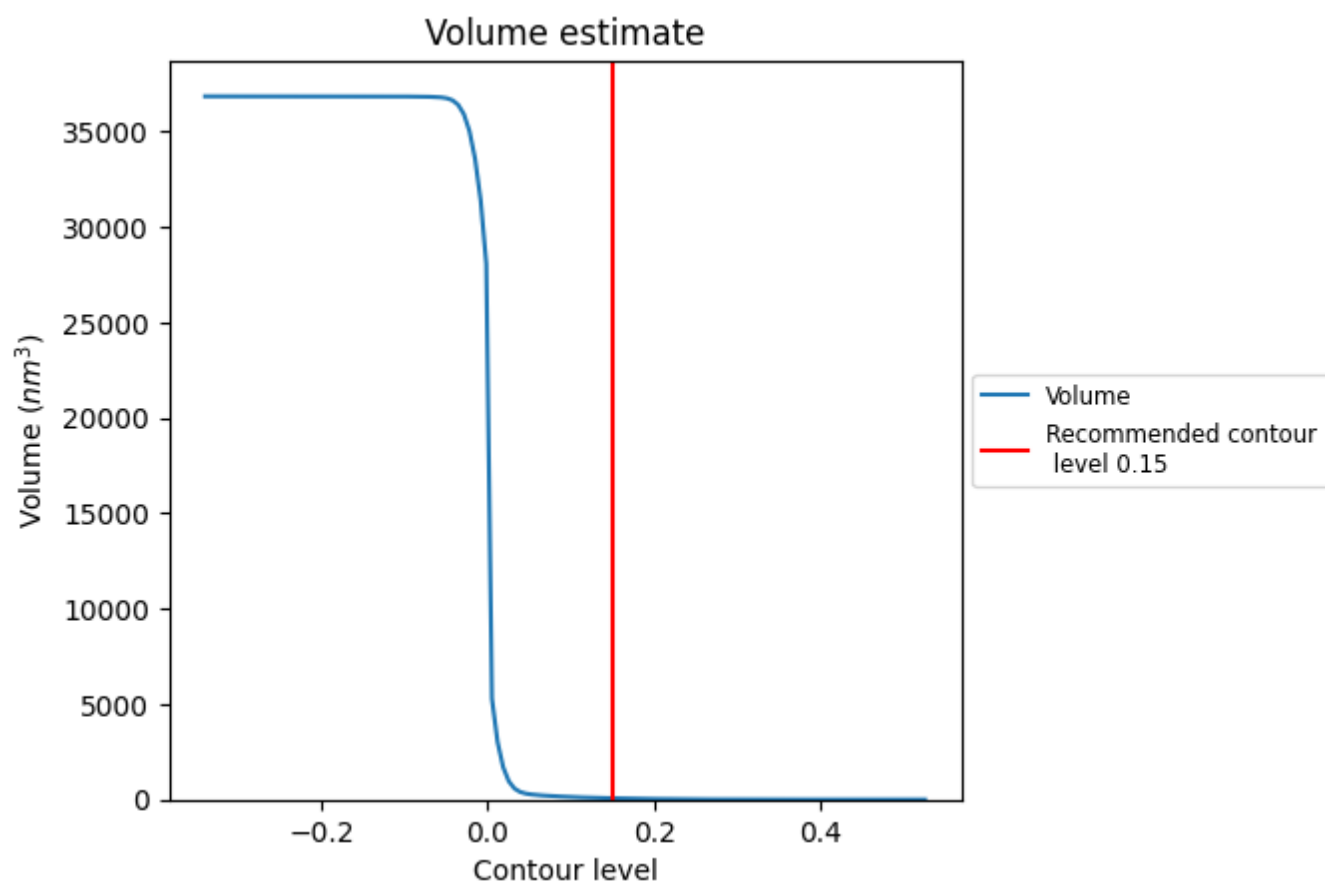
This section contains the results of statistical analysis of the map.

### 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.

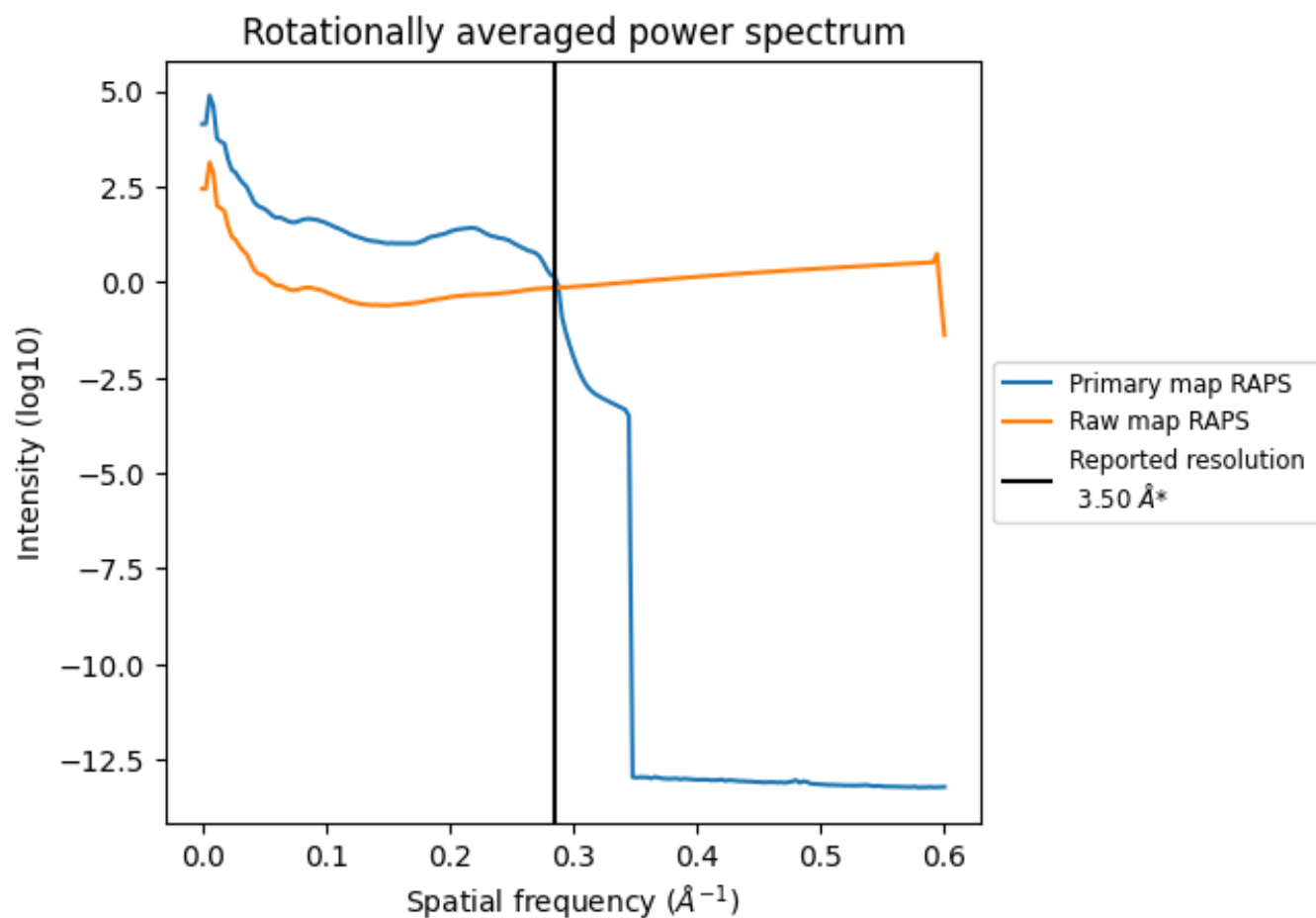
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm<sup>3</sup>; this corresponds to an approximate mass of 62 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 ⓘ

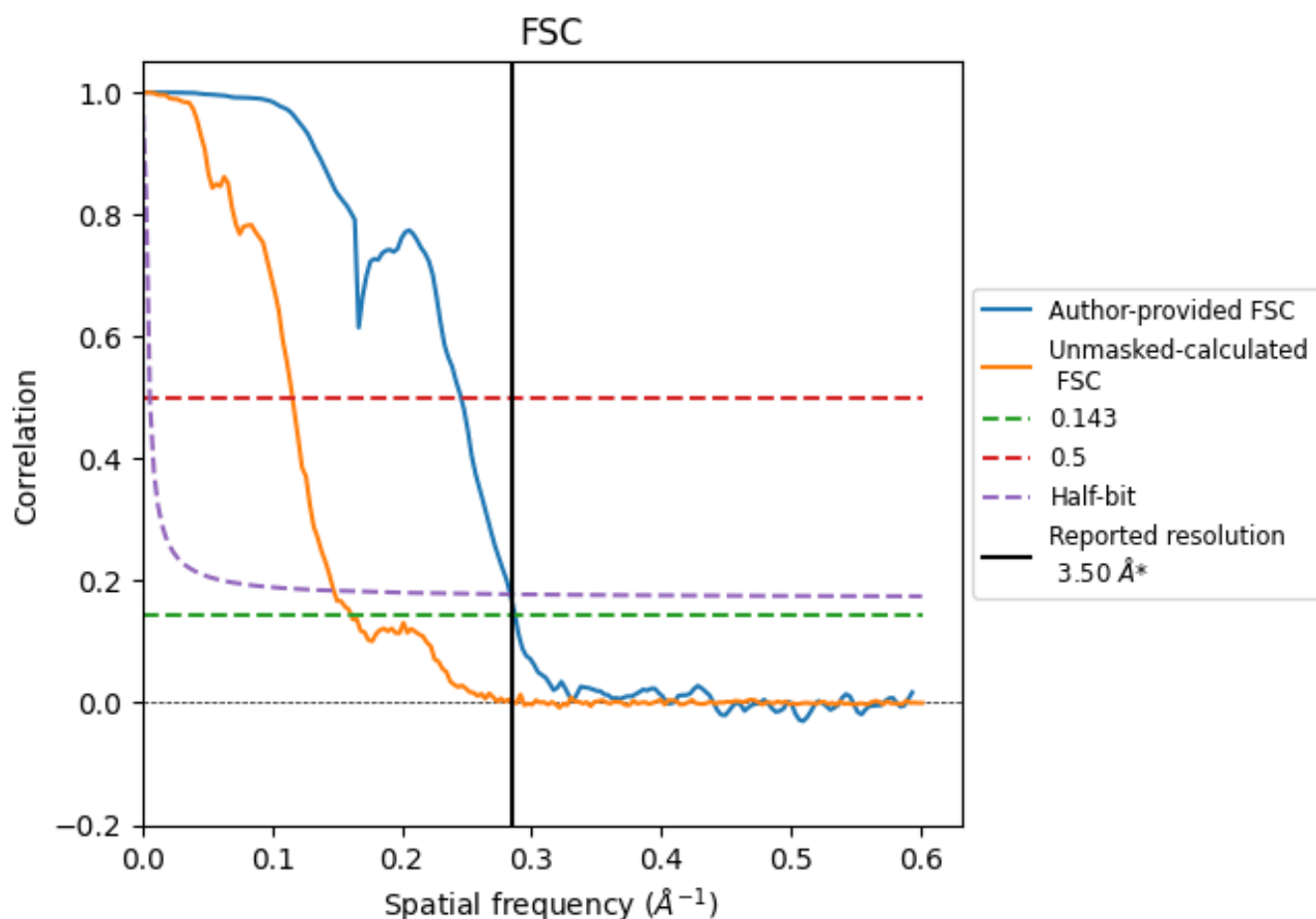


\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

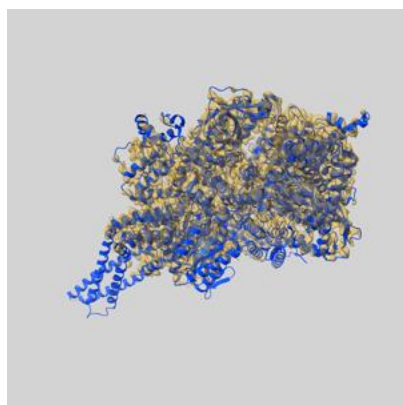
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.07	3.53
Unmasked-calculated*	6.21	8.64	6.77

\*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 6.21 differs from the reported value 3.5 by more than 10 %

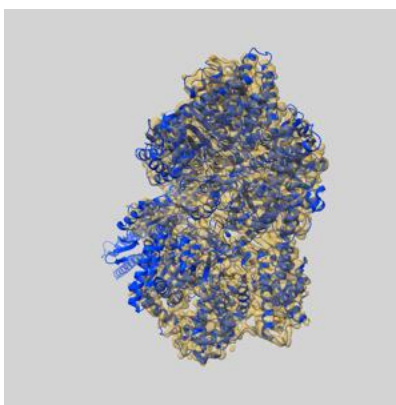
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44688 and PDB model 9BM5. Per-residue inclusion information can be found in section 3 on page 5.

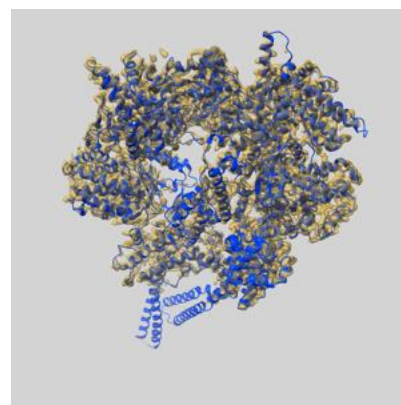
### 9.1 Map-model overlay [i](#)



X



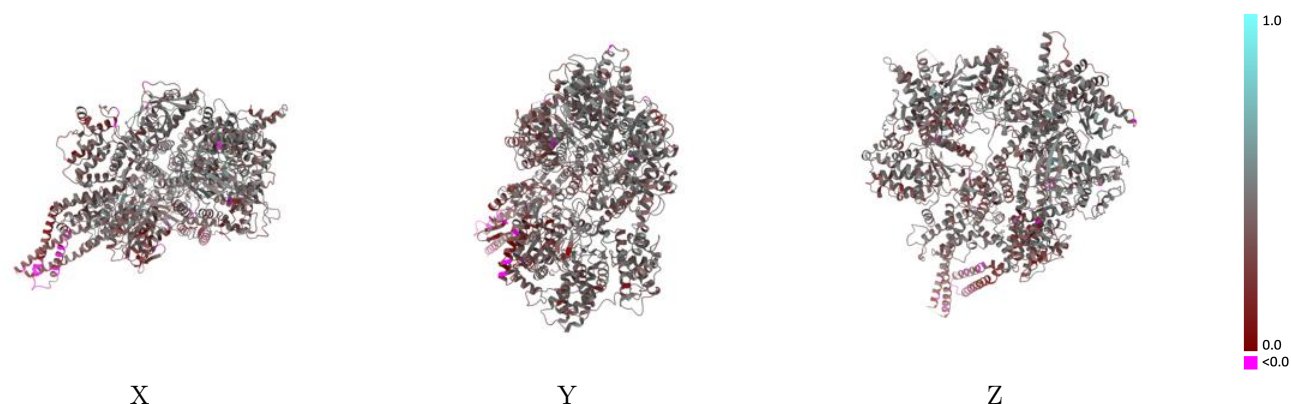
Y



Z

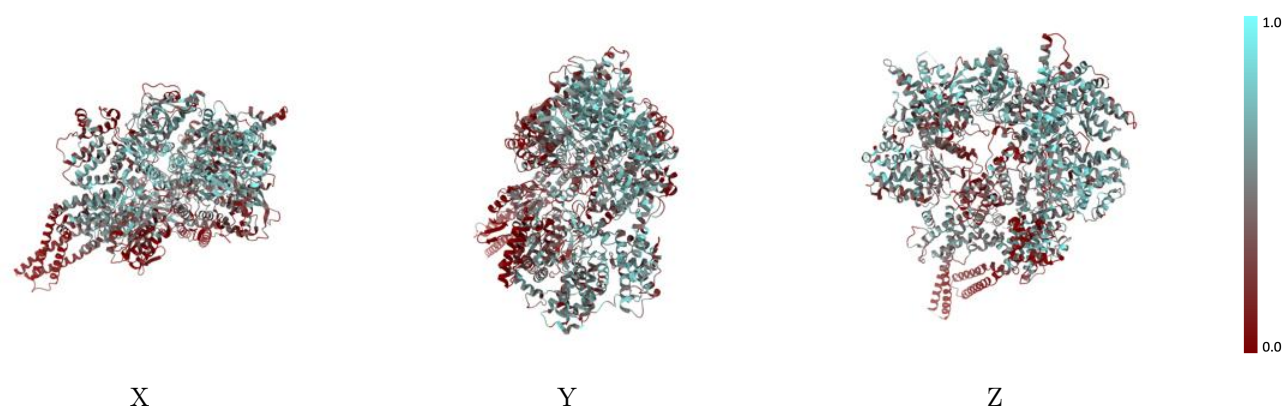
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



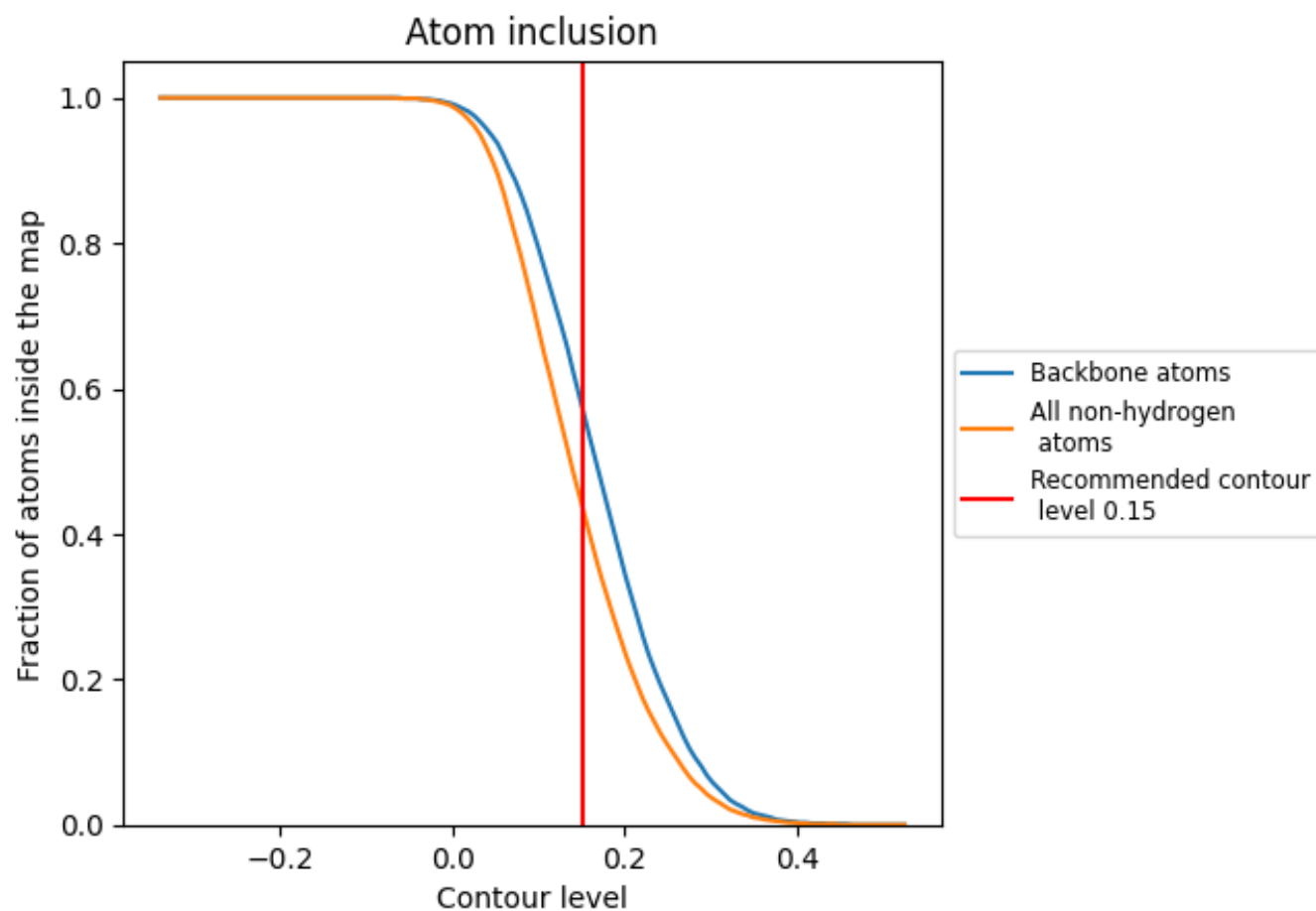
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 44% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4400	<div></div> 0.3910
A	<div></div> 0.4400	<div></div> 0.3910

