



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:42 AM EDT

PDB ID : 9BMF / pdb_00009bmf
EMDB ID : EMD-44697
Title : State-1(phi motor) of full-length human dynein-1 in 5mM ATPVi
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.80 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

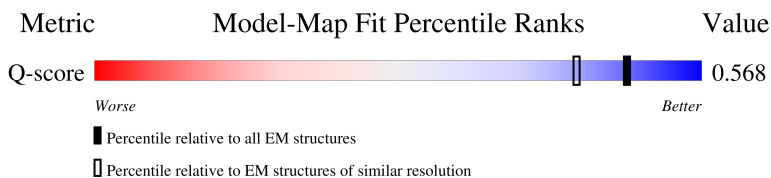
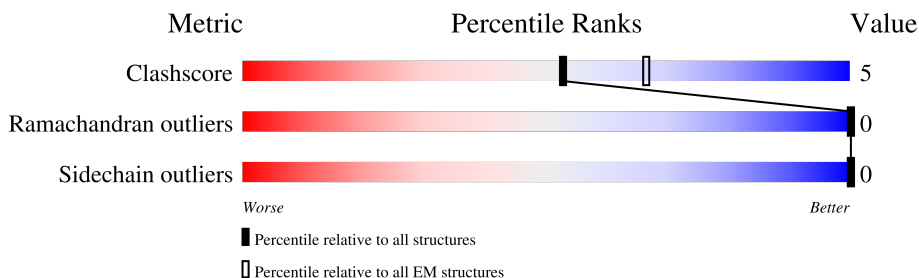
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	

2 Entry composition [i](#)

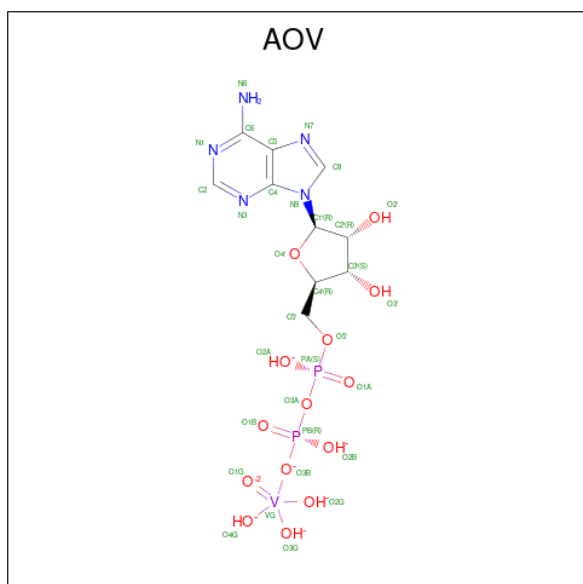
There are 5 unique types of molecules in this entry. The entry contains 23712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

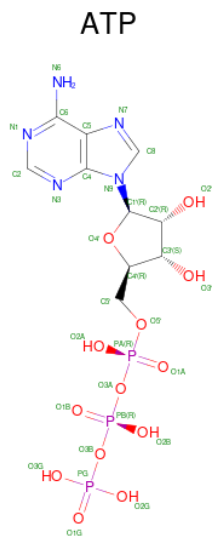
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).



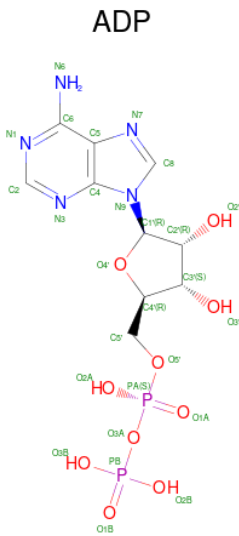
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
2	A	1	32	10	5	14	2	1	0

- 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 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



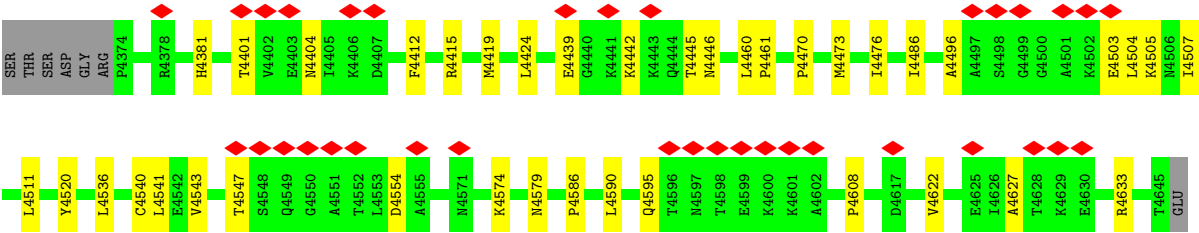
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	A	1	Total 27	C 10	N 5	O 10	P 2	0

- 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 2	Mg 2	0



A4215	A4216	D4217	A4227	R4230	I4251	G4254	D4257	F4260	F4270	R4271	E4281	K4287	V4288	D4289	G4290	H4291	P4297	D4298	W4308	L4312	N4326	K4342	M4346	D4347	NET	LEU	GLU	ASP	GLU	GLU	ASP	ASP	LEU	ALA	TYR	GLU	R4195	K4203	K4204	L4212	THR	THR	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
M4043	C4044	D4050	A4051	S4052	L4058	Q4065	E4075	Q4079	V4088	R4092	M4095	L4096	K4097	N4098	V4099	W4105	L4106	L4116	Q4117	P4118	T4127	I4130	N4137	L4138	I4144	P4150	K4154	T4160	R4168	K4171	R4178	R4195	K4203	K4204	L4212	THR	THR	THR	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	E3930	E3933	K3934	V3935	V3936	R3937	K3945	D3946	L3947	Q3952	A3953	D3954	E3955	Q3956	V3970	E3976	E3977	T3978	P3979	A3980	I3983	R3989	L3990	M4004	V4009	L4013	L4027	P4037	L4042																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L3553	R3782	K3783	V3784	E3785	E3786	T3787	D3788	I3789	V3790	K3791	Q3792	E3793	V3794	E3795	Q3799	S3809	Y3825	Q3830	D3834	I3835	N3838	V3839	E3842	N3843	L3846	Q3709	E3726	L3731	L3732	R3743	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	T3764	I3765	I3767	T3768																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
R3553	R3782	K3783	V3784	E3785	E3786	T3787	D3788	I3789	V3790	K3791	Q3792	E3793	V3794	E3795	Q3799	S3809	Y3825	Q3830	D3834	I3835	N3838	V3839	E3842	N3843	L3846	Q3709	E3726	L3731	L3732	R3743	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	T3764	I3765	I3767	T3768																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
ARG	ASP	LEU	GLU	ALA	SER	ILE	ALA	ARG	TYR	LYS	E3449	E3450	Y3451	A3452	V3453	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	D3464	L3465	A3466	E3469	A3470	K3471	V3472	H3473	R3474	K3480	S3481	K3486	E3487	E3494	H3498	S3510	A3517	Q3523	R3524	R3525	R3544	D3545	I3547																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ASN	TYR	ILE	VAL	ASN	ARG	ALA	ARG	SER	LYS	GLY	CYS	GLY	PRO	VAL	TRP	ALA	ILE	GLN	LEU	ASN	TYR	ALA	A3460	I3461	K3462	D3464	L3465	A3466	E3469	A3470	K3471	V3472	H3473	R3474	K3480	S3481	K3486	E3487	E3494	H3498	S3510	A3517	Q3523	R3524	R3525	R3544	D3545	I3547																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
LYS	LEU	ALA	GLU	GLN	GLU	SER	ILE	CYS	LEU	LEU	GLY	GLU	SER	THR	ASP	LYS	TRP	GLN	ILE	VAL	ASP	MET	ARG	GLU	VAL	ALA	ILE	THR	ILE	VAL	ASN	PHE	GLU	VAL	GLN	LYS	ASP	ALA	ILE	ARG	GLU	LYS	MET	VAL	GLN	ASN	PRO	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
GLN	GLU	ILE	GLN	GLU	GLN	LEU	HIS	LEU	LYS	GLN	H3182	E3210	D3213	Q3214	V3215	E3216	E3217	L3218	R3219	R3220	D3221	L3222	R3223	I3224	K3225	S3226	Q3227	E3228	L3229	E3230	V3231	K3232	N3233	A3234	A3235	A3236	N3237	D3238	K3239	L3240	K3241	K3242	MET	VAL	LYS	ASP	GLN	GLU	ALA	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L2976	L2980	M2984	N2988	V2989	D3001	S3002	E3006	N3014	V3017	L3020	M3043	S3046	E3049	F3054	Q3057	R3060	P3070	S3071	S3072	E3073	D3096	W3097	S3098	T3099	E3100	T3110	D3114	Y3125	V3129	Y3130	K3131	K3132	Q3135	P3136	P3137	R3140	V3149	Y3150	K3151	K3152	Q3153	P3154	P3155	P3156	P3157	P3158	P3159	P3160	P3161	P3162	P3163	P3164	P3165	P3166	P3167	P3168	P3169	P3170	P3171	P3172	P3173	P3174	P3175	P3176	P3177	P3178	P3179	P3180	P3181	P3182	P3183	P3184	P3185	P3186	P3187	P3188	P3189	P3190	P3191	P3192	P3193	P3194	P3195	P3196	P3197	P3198	P3199	P3200	P3201	P3202	P3203	P3204	P3205	P3206	P3207	P3208	P3209	P3210	P3211	P3212	P3213	P3214	P3215	P3216	P3217	P3218	P3219	P3220	P3221	P3222	P3223	P3224	P3225	P3226	P3227	P3228	P3229	P3230	P3231	P3232	P3233	P3234	P3235	P3236	P3237	P3238	P3239	P3240	P3241	P3242	P3243	P3244	P3245	P3246	P3247	P3248	P3249	P3250	P3251	P3252	P3253	P3254	P3255	P3256	P3257	P3258	P3259	P3260	P3261	P3262	P3263	P3264	P3265	P3266	P3267	P3268	P3269	P3270	P3271	P3272	P3273	P3274	P3275	P3276	P3277	P3278	P3279	P3280	P3281	P3282	P3283	P3284	P3285	P3286	P3287	P3288	P3289	P3290	P3291	P3292	P3293	P3294	P3295	P3296	P3297	P3298	P3299	P3300	P3301	P3302	P3303	P3304	P3305	P3306	P3307	P3308	P3309	P3310	P3311	P3312	P3313	P3314	P3315	P3316	P3317	P3318	P3319	P3320	P3321	P3322	P3323	P3324	P3325	P3326	P3327	P3328	P3329	P3330	P3331	P3332	P3333	P3334	P3335	P3336	P3337	P3338	P3339	P3340	P3341	P3342	P3343	P3344	P3345	P3346	P3347	P3348	P3349	P3350	P3351	P3352	P3353	P3354	P3355	P3356	P3357	P3358	P3359	P3360	P3361	P3362	P3363	P3364	P3365	P3366	P3367	P3368	P3369	P3370	P3371	P3372	P3373	P3374	P3375	P3376	P3377	P3378	P3379	P3380	P3381	P3382	P3383	P3384	P3385	P3386	P3387	P3388	P3389	P3390	P3391	P3392	P3393	P3394	P3395	P3396	P3397	P3398	P3399	P3400	P3401	P3402	P3403	P3404	P3405	P3406	P3407	P3408	P3409	P3410	P3411	P3412	P3413	P3414	P3415	P3416	P3417	P3418	P3419	P3420	P3421	P3422	P3423	P3424	P3425	P3426	P3427	P3428	P3429	P3430	P3431	P3432	P3433	P3434	P3435	P3436	P3437	P3438	P3439	P3440	P3441	P3442	P3443	P3444	P3445	P3446	P3447	P3448	P3449	P3450	P3451	P3452	P3453	P3454	P3455	P3456	P3457	P3458	P3459	P3460	P3461	P3462	P3463	P3464	P3465	P3466	P3467	P3468	P3469	P3470	P3471	P3472	P3473	P3474	P3475	P3476	P3477	P3478	P3479	P3480	P3481	P3482	P3483	P3484	P3485	P3486	P3487	P3488	P3489	P3490	P3491	P3492	P3493	P3494	P3495	P3496	P3497	P3498	P3499	P3500	P3501	P3502	P3503	P3504	P3505	P3506	P3507	P3508	P3509	P3510	P3511	P3512	P3513	P3514	P3515	P3516	P3517	P3518	P3519	P3520	P3521	P3522	P3523	P3524	P3525	P3526	P3527	P3528	P3529	P3530	P3531	P3532	P3533	P3534	P3535	P3536	P3537	P3538	P3539	P3540	P3541	P3542	P3543	P3544	P3545	P3546	P3547	P3548	P3549	P3550	P3551	P3552	P3553	P3554	P3555	P3556	P3557	P3558	P3559	P3560	P3561	P3562	P3563	P3564	P3565	P3566	P3567	P3568	P3569	P3570	P3571	P3572	P3573	P3574	P3575	P3576	P3577	P3578	P3579	P3580	P3581	P3582	P3583	P3584	P3585	P3586	P3587	P3588	P3589	P3590	P3591	P3592	P3593	P3594	P3595	P3596	P3597	P3598	P3599	P3600	P3601	P3602	P3603	P3604	P3605	P3606	P3607	P3608	P3609	P3610	P3611	P3612	P3613	P3614	P3615	P3616	P3617	P3618	P3619	P3620	P3621	P3622	P3623	P3624	P3625	P3626	P3627	P3628	P3629	P3630	P3631	P3632	P3633	P3634	P3635	P3636	P3637	P3638	P3639	P3640	P3641	P3642	P3643	P3644	P3645	P3646	P3647	P3648	P3649	P3650	P3651	P3652	P3653	P3654	P3655	P3656	P3657	P3658	P3659	P3660	P3661	P3662	P3663	P3664	P3665	P3666	P3667	P3668	P3669	P3670	P3671	P3672	P3673	P3674	P3675	P3676	P3677	P3678	P3679	P3680	P3681	P3682	P3683	P3684	P3685	P3686	P3687	P3688	P3689	P3690	P3691	P3692	P3693	P3694	P3695	P3696	P3697	P3698	P3699	P3700	P3701	P3702	P3703	P3704	P3705	P3706	P3707	P3708	P3709	P3710	P3711	P3712	P3713	P3714	P3715	P3716	P3717	P3718	P3719	P3720	P3721	P3722	P3723	P3724	P3725	P3726	P3727	P3728	P3729	P3730	P3731	P3732	P3733	P3734	P3735	P3736	P3737	P3738	P3739	P3740	P3741	P3742	P3743	P3744	P3745	P3746	P3747	P3748	P3749	P3750	P3751	P3752	P3753	P3754	P3755	P3756	P3757	P3758	P3759	P3760	P3761	P3762	P3763	P3764	P3765	P3766	P3767	P3768	P3769	P3770	P3771	P3772	P3773	P3774	P3775	P3776	P3777	P3778	P3779	P3780	P3781	P3782	P3783	P3784	P3785	P3786	P3787	P3788	P3789	P3790	P3791	P3792	P3793	P3794	P3795	P3796	P3797	P3798	P3799	P3800	P3801	P3802	P3803	P3804	P3805	P3806	P3807	P3808	P3809	P3810	P3811	P3812	P3813	P3814	P3815	P3816	P3817	P3818	P3819	P3820	P3821	P3822	P3823	P3824	P3825	P3826	P3827	P3828	P3829	P3830	P3831	P3832	P3833	P3834	P3835	P3836	P3837	P3838	P3839	P3840	P3841	P3842	P3843	P3844	P3845	P3846	P3847	P3848	P3849	P3850	P3851	P3852	P3853	P3854	P3855	P3856	P3857	P3858	P3859	P3860	P3861	P3862	P3863	P3864	P3865	P3866	P3867	P3868	P3869	P3870	P3871	P3872	P3873	P3874	P3875	P3876	P3877	P3878	P3879	P3880	P3881	P3882	P3883	P3884	P3885	P3886	P3887	P3888	P3889	P3890	P3891	P3892	P3893	P3894	P3895	P3896	P3897	P3898	P3899	P3900	P3901	P3902	P3903	P3904	P3905	P3906	P3907	P3908	P3909	P3910	P3911	P3912	P3913	P3914	P3915	P3916	P3917	P3918	P3919	P3920	P3921	P3922	P3923	P3924	P3925	P3926	P3927	P3928	P3929	P3930	P3931	P3932	P3933	P3934	P3935	P3936	P3937	P3938	P3939	P3940	P3941	P3942	P3943	P3944	P3945	P3946	P3947	P3948	P3949	P3950	P3951	P3952	P3953	P3954	P3955	P3956	P3957	P3958	P3959	P3960	P3961	P3962	P3963	P3964	P3965	P3966	P3967	P3968	P3969	P3970	P3971	P3972	P3973	P3974	P3975	P3976	P3977	P3978	P3979	P3980	P3981	P3982	P3983	P3984	P3985	P3986	P3987	P3988	P3989	P3990	P3991	P3992	P3993	P3994	P3995	P3996	P3997	P3998	P3999	P4000	P4001	P4002	P4003	P4004	P4005	P4006	P4007	P4008	P4009	P4010	P4011	P4012	P4013	P4014	P4015	P4016	P4017	P4018	P4019	P4020	P4021	P4022	P4023	P4024	P4025	P4026	P4027	P4028	P4029	P4030	P4031	P4032	P4033	P4034	P4035	P4036	P4037	P4038	P4039	P4040	P4041	P4042	P4043	P4044	P4045	P4046	P4047	P4048	P4049	P4050	P4051	P4052	P4053	P4054	P4055	P4056	P4057	P4058	P4059	P4060	P4061	P4062	P4063	P4064	P4065	P4066	P4067	P4068	P4069	P4070	P4071	P4072	P



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266214	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)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.110	Depositor
Minimum map value	-1.492	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: AOV, ADP, ATP, MG

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	0.09	0/24093	0.24	0/32651

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23593	0	23658	249	0
2	A	32	0	12	3	0
3	A	31	0	12	1	0
4	A	54	0	24	0	0
5	A	2	0	0	0	0
All	All	23712	0	23706	249	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 (249) 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:1490:TRP:HH2	1:A:1537:TRP:HD1	1.36	0.72
1:A:2507:ARG:HE	1:A:2509:LYS:HE2	1.58	0.69
1:A:1564:GLU:HG3	1:A:1567:ARG:HH21	1.56	0.68
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.24	0.68
1:A:2239:LYS:HZ2	1:A:2243:ARG:HE	1.41	0.67
1:A:3838:ASN:ND2	1:A:3842:GLU:HB2	2.10	0.66
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.78	0.66
1:A:1558:LYS:HG3	1:A:1565:THR:HG21	1.78	0.66
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.79	0.64
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.78	0.64
1:A:1797:LEU:HD21	1:A:2060:ARG:HD3	1.80	0.63
1:A:3560:LEU:HD11	1:A:3743:ARG:HH22	1.63	0.63
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.80	0.63
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.32	0.63
1:A:1574:GLU:OE2	1:A:1603:ARG:NH2	2.31	0.63
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.17	0.63
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	1.81	0.63
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.81	0.62
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.32	0.62
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.33	0.61
1:A:2188:GLU:OE1	1:A:2243:ARG:NH2	2.33	0.61
1:A:3474:ARG:HH22	1:A:3768:THR:HG22	1.66	0.61
1:A:1537:TRP:HE3	1:A:1601:LEU:HD21	1.65	0.61
1:A:1537:TRP:CE3	1:A:1601:LEU:HD21	2.35	0.61
1:A:2312:VAL:HG13	1:A:2355:THR:HG21	1.83	0.60
1:A:1855:GLN:OE1	1:A:1867:ASN:ND2	2.35	0.60
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.20	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.84	0.59
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.32	0.59
1:A:3838:ASN:HD22	1:A:3842:GLU:HB2	1.68	0.58
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.84	0.58
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.84	0.58
1:A:4095:MET:HE3	1:A:4097:LYS:HE2	1.85	0.58
1:A:4043:MET:HB3	1:A:4051:ALA:HB3	1.85	0.58
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.85	0.57
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.86	0.57
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.37	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.84	0.57
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.87	0.57
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.86	0.56
1:A:1490:TRP:HH2	1:A:1537:TRP:CD1	2.20	0.56
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.87	0.56
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.41	0.55
1:A:2222:MET:HE1	1:A:2234:TRP:CD1	2.41	0.55
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.21	0.55
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.24	0.55
1:A:3229:LEU:HD12	1:A:3465:LEU:HD13	1.89	0.55
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.88	0.55
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.89	0.55
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.88	0.54
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.89	0.54
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.90	0.54
1:A:2488:ARG:NH2	1:A:2542:SER:O	2.40	0.54
1:A:2686:MET:HE3	1:A:2708:PHE:CZ	2.43	0.54
1:A:2172:ARG:NH1	1:A:2205:GLU:OE1	2.41	0.54
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.89	0.53
1:A:4168:ARG:HA	1:A:4171:LYS:HE2	1.91	0.53
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.29	0.53
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.41	0.53
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.90	0.53
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.40	0.53
1:A:3544:ARG:HH21	1:A:3547:ILE:HG21	1.73	0.53
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.41	0.53
1:A:4470:PRO:HG2	1:A:4473:MET:HE3	1.91	0.53
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.91	0.52
1:A:4424:LEU:HD13	1:A:4486:ILE:HG13	1.91	0.52
1:A:3846:LEU:HD21	1:A:3855:ARG:HA	1.92	0.52
1:A:2909:LEU:HD11	1:A:2945:THR:HG21	1.92	0.52
1:A:2826:ALA:HB2	1:A:2867:MET:HE1	1.91	0.52
1:A:2239:LYS:NZ	1:A:2243:ARG:HE	2.07	0.52
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.92	0.52
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.10	0.52
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.92	0.51
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.93	0.51
1:A:2091:ARG:NH1	2:A:4701:AOV:O1G	2.44	0.51
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.92	0.51
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.27	0.51
1:A:2091:ARG:HG3	2:A:4701:AOV:H4'	1.93	0.50
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.38	0.50
1:A:4415:ARG:O	1:A:4419:MET:HG3	2.11	0.50
1:A:1912:LYS:HE2	1:A:2017:THR:HG23	1.93	0.50
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.44	0.50
1:A:3100:GLU:OE2	1:A:3130:TYR:OH	2.27	0.50
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.94	0.50
1:A:2869:ARG:HB3	1:A:2870:PRO:HD3	1.94	0.50
1:A:1825:LEU:HA	1:A:1830:ILE:HD13	1.93	0.49
1:A:2914:GLU:OE2	1:A:3098:SER:OG	2.26	0.49
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.22	0.49
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.95	0.49
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.45	0.49
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.77	0.49
1:A:4401:THR:H	1:A:4404:ASN:HB2	1.75	0.49
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.94	0.49
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.78	0.49
1:A:3910:ARG:NH1	1:A:3913:GLU:OE2	2.45	0.49
1:A:4215:ALA:HA	1:A:4251:ILE:HD13	1.94	0.49
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.31	0.48
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.77	0.48
1:A:3732:LEU:HD12	1:A:3791:MET:HE1	1.94	0.48
1:A:3843:ASN:HD21	1:A:3858:ILE:HG22	1.78	0.48
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.45	0.48
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.95	0.48
1:A:3752:ALA:O	1:A:3756:VAL:HG23	2.13	0.48
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.94	0.48
1:A:2510:MET:HA	1:A:2513:GLU:HB2	1.95	0.48
1:A:3839:VAL:O	1:A:3843:ASN:HB2	2.13	0.48
1:A:1882:THR:HB	1:A:2045:ASP:HB2	1.96	0.47
1:A:4227:ALA:HA	1:A:4230:ARG:HD3	1.96	0.47
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.96	0.47
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.47	0.47
1:A:3471:LYS:HE2	1:A:3761:LEU:HD23	1.94	0.47
1:A:2498:ILE:HG23	1:A:2502:LEU:HD12	1.96	0.47
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.47	0.47
1:A:1508:LYS:HG2	1:A:1513:TYR:CZ	2.49	0.47
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.95	0.47
1:A:1985:HIS:CD2	1:A:2010:PRO:HB3	2.50	0.47
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.97	0.47
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.80	0.47
1:A:3209:LYS:HB2	1:A:3209:LYS:HE2	1.77	0.47
1:A:2221:MET:SD	1:A:2348:LEU:HD11	2.54	0.46
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.15	0.46
1:A:4540:CYS:HB2	1:A:4595:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.43	0.46
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.49	0.46
1:A:3057:GLN:OE1	1:A:3060:ARG:NH1	2.49	0.46
1:A:2139:GLN:HG3	1:A:2170:TYR:CE1	2.50	0.46
1:A:2446:ILE:HG22	1:A:2505:ASP:HB2	1.98	0.46
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.48	0.46
1:A:4050:ASP:OD2	1:A:4052:SER:OG	2.33	0.46
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.97	0.46
1:A:3046:SER:HB3	1:A:3049:GLU:HG3	1.96	0.46
1:A:3933:GLU:HG2	1:A:3937:ARG:HE	1.81	0.46
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.15	0.45
1:A:2164:VAL:HG23	1:A:4536:LEU:HD12	1.98	0.45
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.15	0.45
1:A:3825:TYR:CE1	1:A:3875:MET:HG2	2.51	0.45
1:A:1782:LEU:HD13	1:A:1822:THR:HB	1.98	0.45
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.51	0.45
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.99	0.45
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.51	0.45
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.98	0.45
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.98	0.45
1:A:3523:GLN:CD	1:A:3523:GLN:H	2.25	0.45
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.49	0.45
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.98	0.45
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.50	0.45
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.97	0.45
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	1.99	0.45
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.99	0.45
1:A:2683:ILE:HA	1:A:2686:MET:HE2	1.99	0.45
1:A:2358:ARG:NH2	2:A:4701:AOV:O3G	2.48	0.45
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.51	0.44
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.82	0.44
1:A:2585:LEU:HG	1:A:2591:LEU:HD21	1.99	0.44
1:A:2921:ARG:O	1:A:2924:ARG:HG2	2.17	0.44
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.98	0.44
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.99	0.44
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.28	0.44
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.98	0.44
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.28	0.44
1:A:1563:VAL:O	1:A:1567:ARG:HG3	2.17	0.44
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	2.00	0.44
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2509:LYS:HE3	1:A:2510:MET:HE3	2.00	0.44
1:A:4381:HIS:CD2	1:A:4439:GLU:HG3	2.53	0.44
1:A:2109:GLN:O	1:A:2113:ARG:HG3	2.18	0.43
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.99	0.43
1:A:1487:ILE:HD12	1:A:1537:TRP:NE1	2.33	0.43
1:A:2046:ARG:HH21	1:A:2093:LEU:HD13	1.83	0.43
1:A:2713:ASN:HB2	1:A:2720:ARG:HE	1.83	0.43
1:A:4154:LYS:HD2	1:A:4312:LEU:HB2	1.99	0.43
1:A:2812:PRO:HG2	1:A:2813:LEU:HD12	2.00	0.43
1:A:4547:THR:HA	1:A:4586:PRO:HG2	2.00	0.43
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.99	0.43
1:A:1601:LEU:HA	1:A:1601:LEU:HD23	1.81	0.43
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	2.00	0.43
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.50	0.43
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.54	0.43
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	2.01	0.43
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.88	0.43
1:A:2324:LEU:HD21	1:A:2332:ARG:HH11	1.84	0.43
1:A:2616:GLU:HG3	1:A:2659:LEU:HD12	2.00	0.43
1:A:2894:LYS:HE3	1:A:2894:LYS:HB2	1.90	0.43
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.52	0.43
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.54	0.43
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.52	0.42
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.38	0.42
1:A:3232:LYS:HA	1:A:3232:LYS:HD3	1.76	0.42
1:A:4065:GLN:HB3	1:A:4092:ARG:HD2	2.00	0.42
1:A:4271:ARG:HD3	1:A:4633:ARG:NH1	2.34	0.42
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.01	0.42
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.02	0.42
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.54	0.42
1:A:4342:LYS:O	1:A:4346:MET:HG2	2.19	0.42
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.02	0.42
1:A:2962:LYS:HA	1:A:2962:LYS:HD3	1.92	0.42
1:A:3872:ALA:HA	1:A:3875:MET:HE2	2.00	0.42
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.84	0.42
1:A:2306:ASP:OD2	1:A:2676:THR:OG1	2.36	0.42
1:A:3916:LEU:HD12	1:A:3933:GLU:HG3	2.02	0.42
1:A:2560:HIS:CD2	1:A:2561:LYS:HG3	2.55	0.41
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.20	0.41
1:A:1555:ALA:HA	1:A:1558:LYS:NZ	2.35	0.41
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4042:LEU:HD12	1:A:4144:ILE:HG12	2.02	0.41
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	2.01	0.41
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.02	0.41
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.95	0.41
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.88	0.41
1:A:1932:CYS:O	1:A:1962:ARG:NH1	2.52	0.41
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.20	0.41
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.35	0.41
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	2.02	0.41
1:A:2007:LYS:HE3	1:A:2007:LYS:HB3	1.73	0.41
1:A:2285:ARG:NH1	1:A:2331:GLU:OE1	2.26	0.41
1:A:2994:MET:HE2	1:A:2999:VAL:HG22	2.03	0.41
1:A:4075:GLU:O	1:A:4079:GLN:HG3	2.20	0.41
1:A:4476:ILE:HD12	1:A:4476:ILE:H	1.85	0.41
1:A:2134:GLN:HE21	1:A:2165:PHE:HB3	1.86	0.41
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.45	0.41
1:A:2980:LEU:HB3	1:A:3054:PHE:HZ	1.86	0.41
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.02	0.41
1:A:4203:LYS:NZ	1:A:4257:ASP:OD1	2.46	0.41
1:A:1594:ILE:HB	1:A:1597:VAL:HB	2.02	0.41
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	2.02	0.41
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	2.03	0.41
1:A:3709:GLN:HG3	1:A:3809:SER:HB3	2.03	0.41
1:A:2316:ASN:O	1:A:2320:ASP:HB2	2.20	0.41
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	2.03	0.41
1:A:3842:GLU:H	1:A:3842:GLU:HG3	1.73	0.41
1:A:2132:PRO:HB2	1:A:2135:GLU:HB2	2.03	0.40
1:A:2213:ILE:HG22	1:A:2220:LEU:HG	2.02	0.40
1:A:1526:LYS:HD2	1:A:1589:MET:HE1	2.03	0.40
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.20	0.40
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.56	0.40
1:A:2499:LEU:O	1:A:2503:SER:OG	2.34	0.40
1:A:2767:GLU:CD	1:A:2767:GLU:H	2.29	0.40
1:A:3474:ARG:NH2	1:A:3768:THR:HG22	2.34	0.40
1:A:2131:LEU:HD12	1:A:2131:LEU:HA	1.95	0.40
1:A:2324:LEU:HD21	1:A:2332:ARG:HD3	2.03	0.40
1:A:3621:LYS:HE3	1:A:3621:LYS:HB3	1.78	0.40
1:A:3922:PRO:HG2	1:A:3924:ILE:HD11	2.02	0.40
1:A:1488:ARG:HD2	1:A:1489:GLY:N	2.37	0.40
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.22	0.40
1:A:2716:THR:HB	1:A:4445:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3788:ASP:O	1:A:3792:GLN:HG2	2.20	0.40
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	2.04	0.40

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%)	2887 (99%)	42 (1%)	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%)	2605 (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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1479	ASN
1	A	1593	ASN

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Mol	Chain	Res	Type
1	A	1856	GLN
1	A	1921	HIS
1	A	2005	GLN
1	A	2057	GLN
1	A	2109	GLN
1	A	2134	GLN
1	A	2212	GLN
1	A	2464	GLN
1	A	2485	GLN
1	A	2549	GLN
1	A	2730	HIS
1	A	2834	GLN
1	A	3014	ASN
1	A	3038	GLN
1	A	3119	ASN
1	A	3622	ASN
1	A	3754	ASN
1	A	4038	ASN
1	A	4114	HIS
1	A	4156	ASN
1	A	4174	ASN
1	A	4231	GLN
1	A	4335	GLN
1	A	4347	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 6 ligands modelled in this entry, 2 are 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	ATP	A	4702	5	32,33,33	0.27	0	48,52,52	0.27	0
4	ADP	A	4703	-	28,29,29	1.42	4 (14%)	43,45,45	1.87	8 (18%)
2	AOV	A	4701	5	32,34,34	5.04	7 (21%)	42,56,56	2.28	13 (30%)
4	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

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	-	4/22/38/38	0/3/3/3
4	ADP	A	4703	-	-	5/16/32/32	0/3/3/3
2	AOV	A	4701	5	-	0/16/39/39	0/3/3/3
4	ADP	A	4704	-	-	1/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	AOV	O1G-VG	27.31	2.09	1.61
4	A	4703	ADP	C5-C4	4.76	1.47	1.39
4	A	4704	ADP	C5-C4	4.71	1.47	1.39
2	A	4701	AOV	C5-C4	4.59	1.47	1.39
4	A	4703	ADP	C5-C6	2.73	1.48	1.41
4	A	4704	ADP	C5-C6	2.73	1.48	1.41
2	A	4701	AOV	C5-C6	2.73	1.48	1.41
2	A	4701	AOV	C8-N9	-2.67	1.33	1.37
2	A	4701	AOV	PA-O3A	-2.62	1.56	1.59
2	A	4701	AOV	C5-N7	-2.62	1.34	1.39
4	A	4704	ADP	C8-N7	2.33	1.36	1.31
4	A	4703	ADP	C5-N7	-2.29	1.34	1.39
4	A	4703	ADP	C8-N7	2.28	1.36	1.31
4	A	4704	ADP	C5-N7	-2.27	1.34	1.39
2	A	4701	AOV	C8-N7	2.22	1.36	1.31

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	AOV	C5-C4-N3	-7.23	116.77	126.72
4	A	4703	ADP	C5-C4-N3	-6.08	118.35	126.72
4	A	4704	ADP	C5-C4-N3	-5.84	118.67	126.72
2	A	4701	AOV	N3-C4-N9	5.67	136.81	127.17
4	A	4703	ADP	N3-C4-N9	4.87	135.45	127.17
4	A	4704	ADP	N3-C4-N9	4.64	135.06	127.17
2	A	4701	AOV	C4-C5-N7	-4.53	105.40	110.58
2	A	4701	AOV	C2-N3-C4	4.28	122.29	111.83
4	A	4703	ADP	C2-N3-C4	3.81	121.14	111.83
4	A	4704	ADP	C2-N3-C4	3.71	120.89	111.83
2	A	4701	AOV	O2B-PB-O3A	3.63	117.10	107.27
2	A	4701	AOV	N3-C2-N1	-3.56	123.19	128.58
4	A	4704	ADP	C4-C5-N7	-3.45	106.63	110.58
2	A	4701	AOV	C5-N7-C8	3.43	108.84	103.45
4	A	4703	ADP	C4-C5-N7	-3.40	106.69	110.58
4	A	4703	ADP	N3-C2-N1	-3.26	123.65	128.58
4	A	4704	ADP	N3-C2-N1	-3.23	123.69	128.58
2	A	4701	AOV	C4-N9-C8	2.87	108.75	105.74
4	A	4704	ADP	C4-N9-C8	2.59	108.46	105.74
4	A	4703	ADP	C3'-C2'-C1'	2.56	106.31	101.46
4	A	4704	ADP	C5-N7-C8	2.53	107.42	103.45
4	A	4703	ADP	C4-N9-C8	2.52	108.39	105.74
4	A	4703	ADP	C5-N7-C8	2.52	107.40	103.45
4	A	4704	ADP	C3'-C2'-C1'	2.41	106.03	101.46
2	A	4701	AOV	N9-C8-N7	-2.36	110.59	113.94
2	A	4701	AOV	O3A-PA-O1A	-2.26	103.91	110.70
2	A	4701	AOV	C2'-C1'-N9	-2.26	107.69	113.30
2	A	4701	AOV	C6-C5-N7	2.22	136.38	132.09
2	A	4701	AOV	O3A-PB-O1B	-2.12	104.31	110.70
4	A	4704	ADP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O1B
4	A	4703	ADP	O4'-C4'-C5'-O5'
4	A	4703	ADP	C5'-O5'-PA-O2A

Continued on next page...

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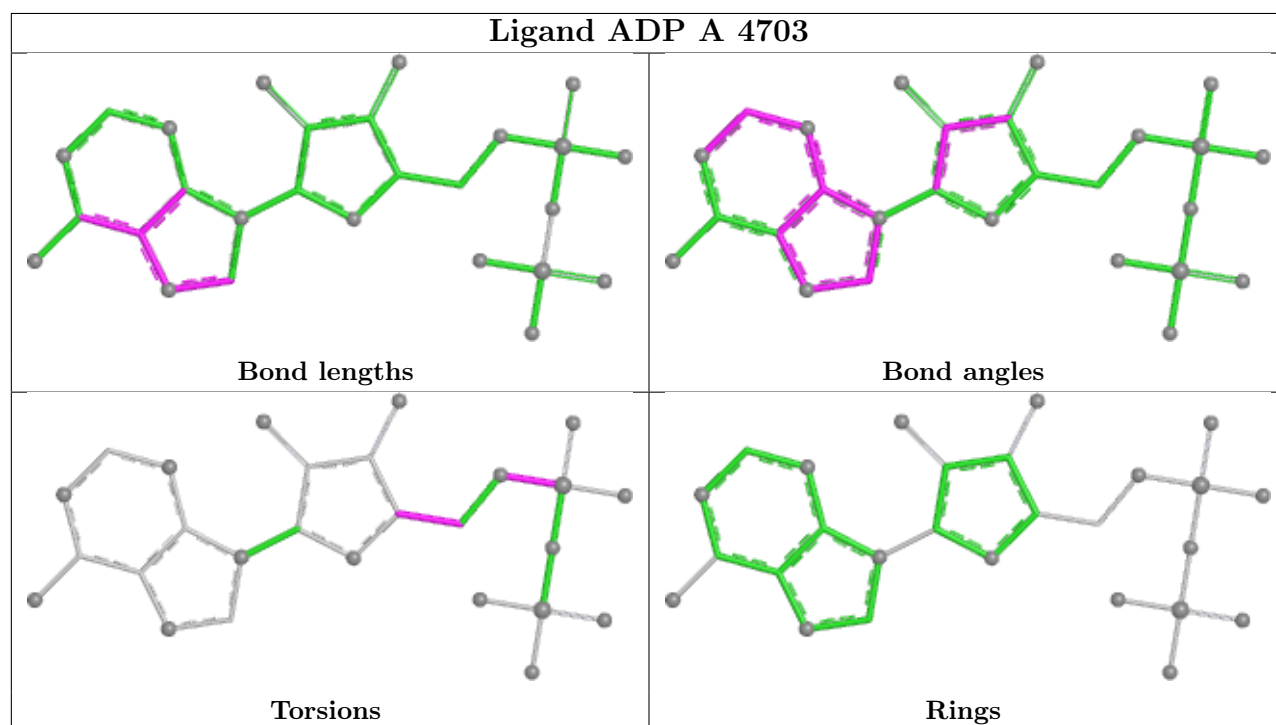
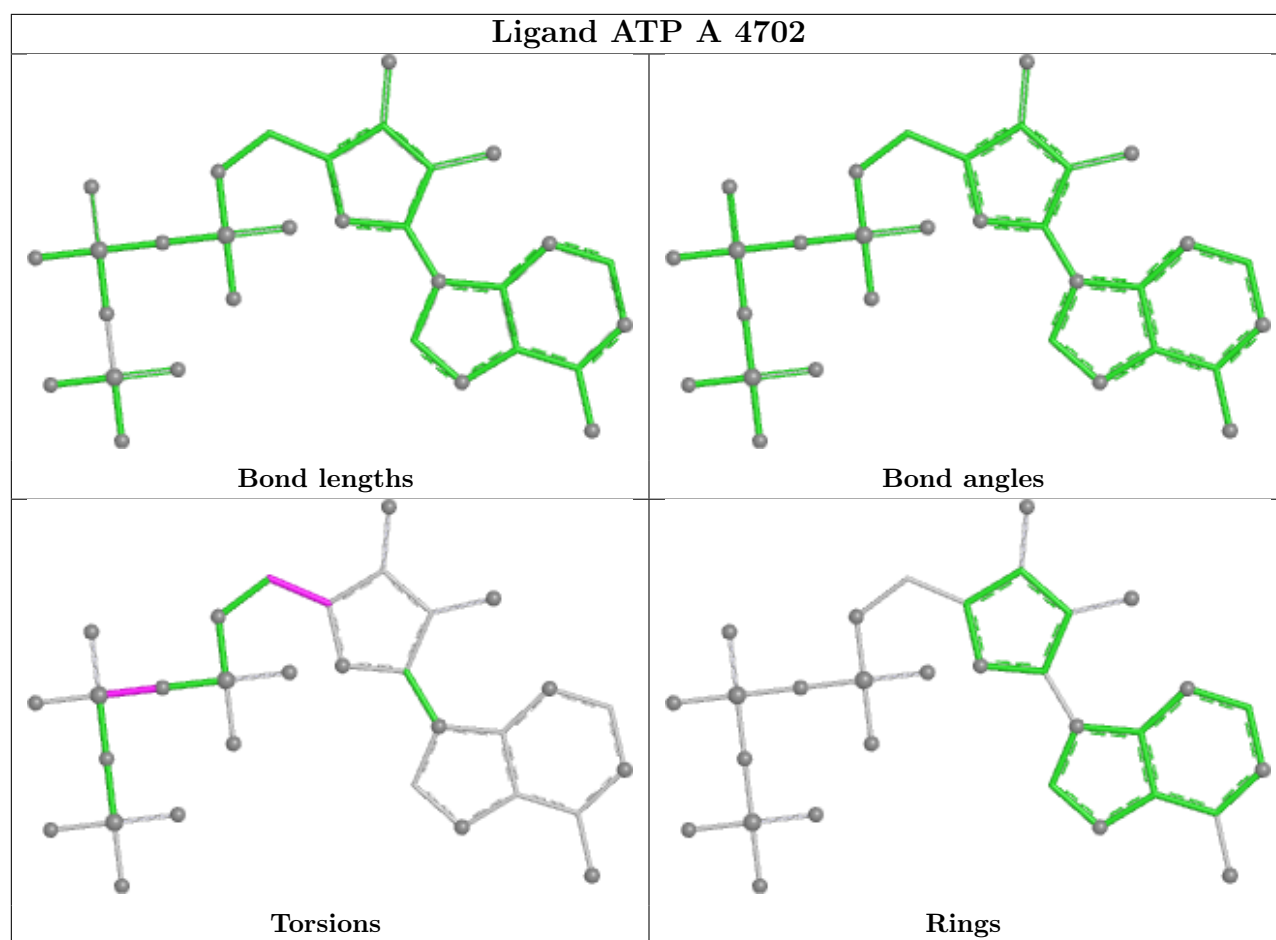
Mol	Chain	Res	Type	Atoms
4	A	4703	ADP	C5'-O5'-PA-O3A
4	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	PA-O3A-PB-O2B
4	A	4703	ADP	C3'-C4'-C5'-O5'

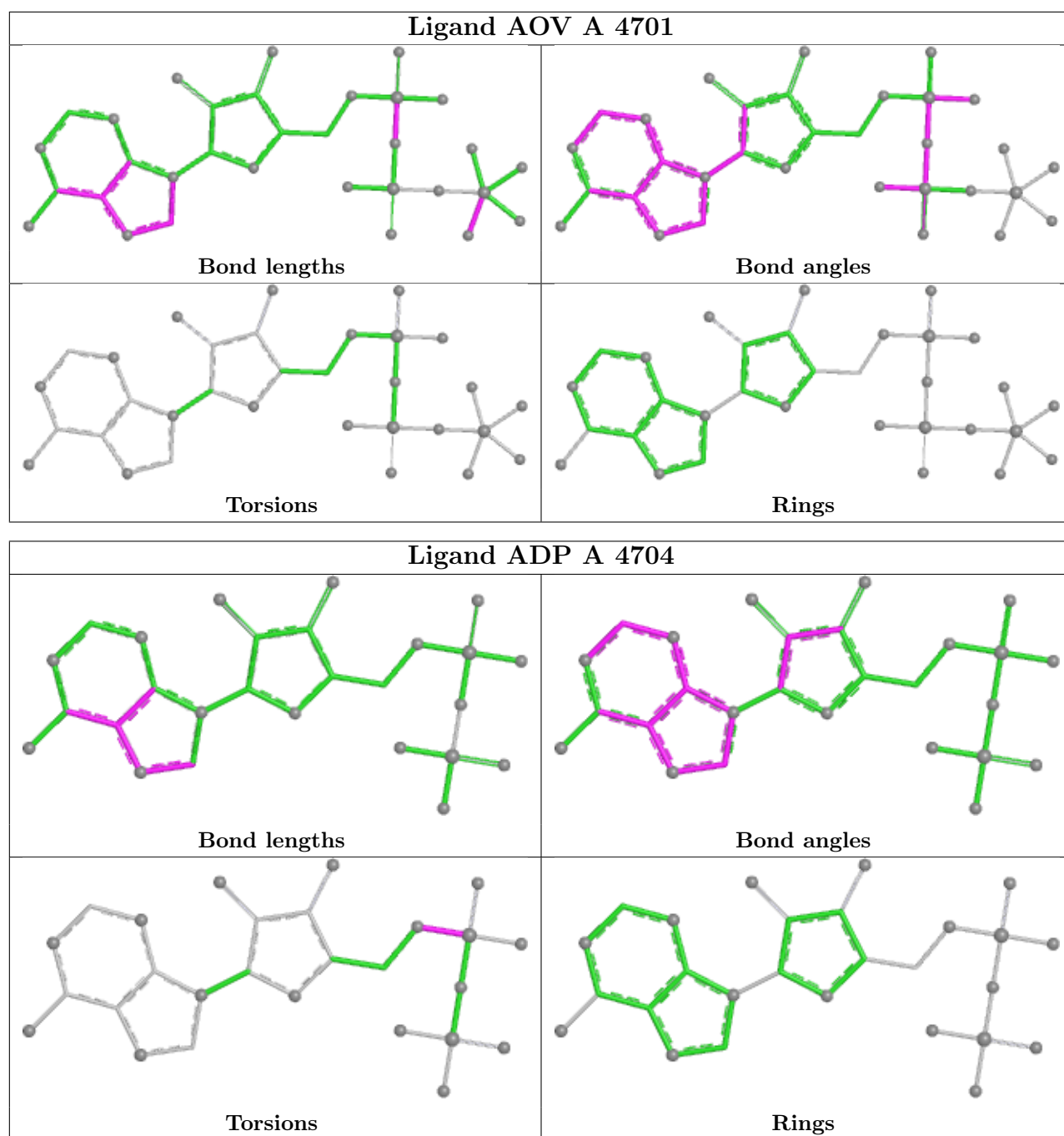
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	1	0
2	A	4701	AOV	3	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.

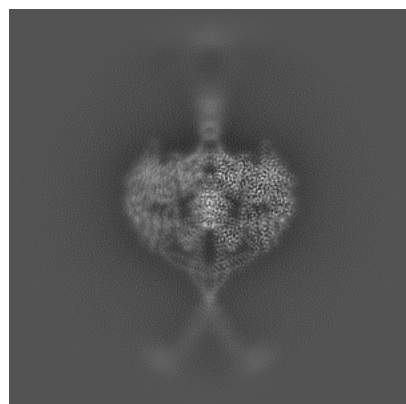
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44697. These allow visual inspection of the internal detail of the map and identification of artifacts.

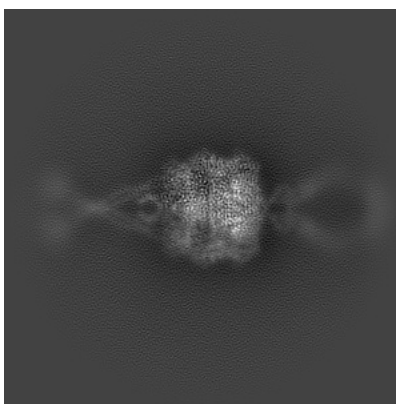
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

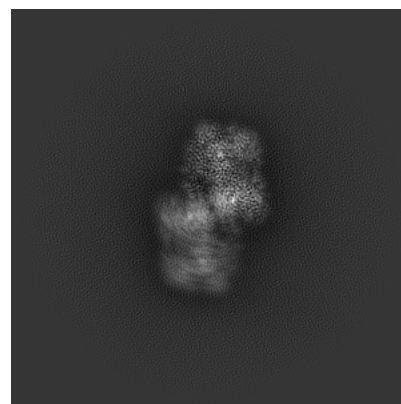
6.1.1 Primary map



X

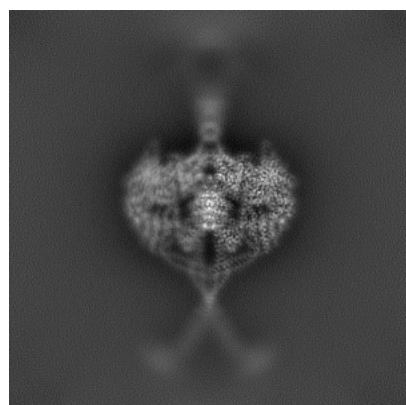


Y

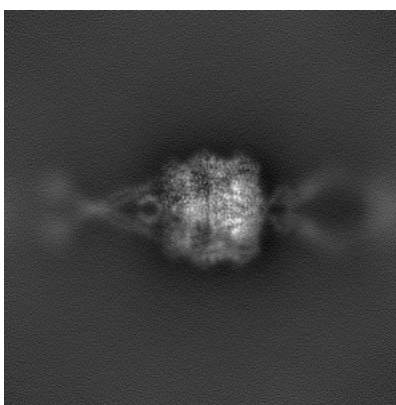


Z

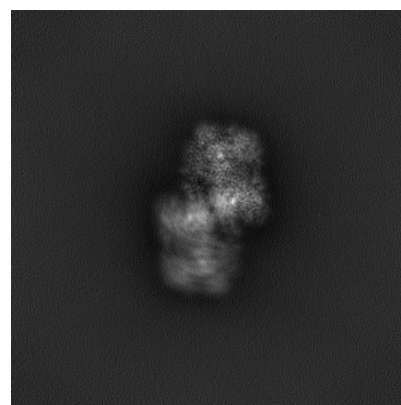
6.1.2 Raw map



X



Y

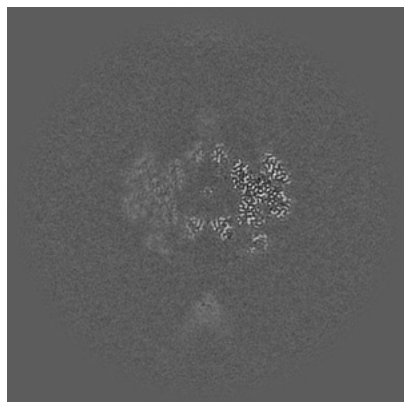


Z

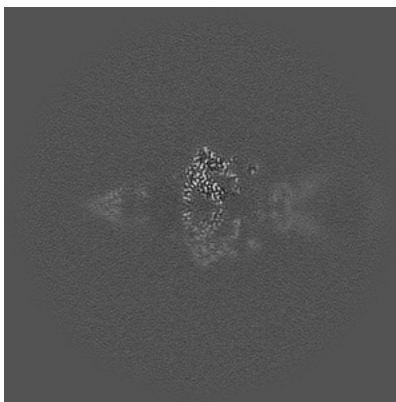
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

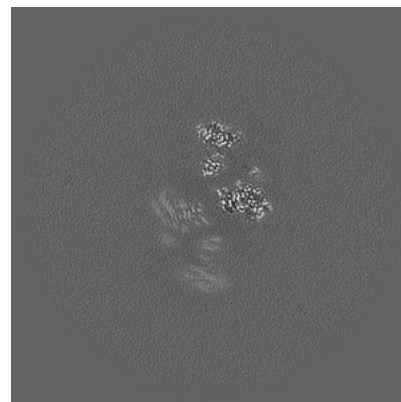
6.2.1 Primary map



X Index: 192

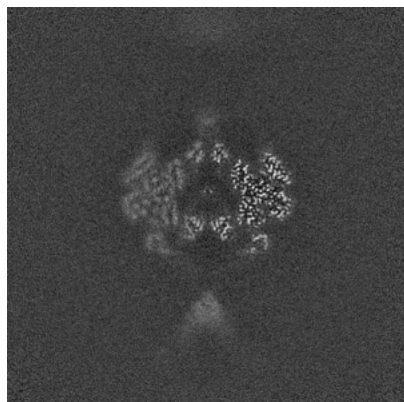


Y Index: 192

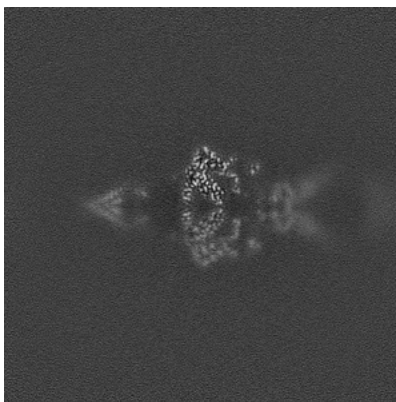


Z Index: 192

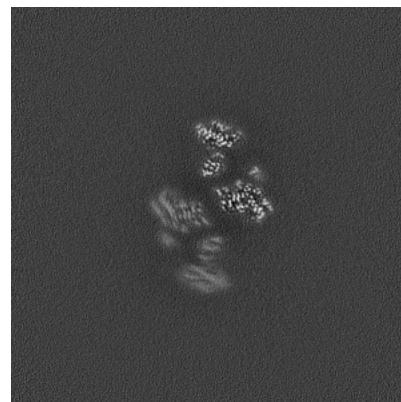
6.2.2 Raw map



X Index: 192



Y Index: 192

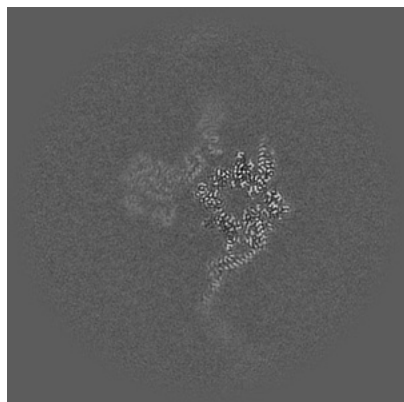


Z Index: 192

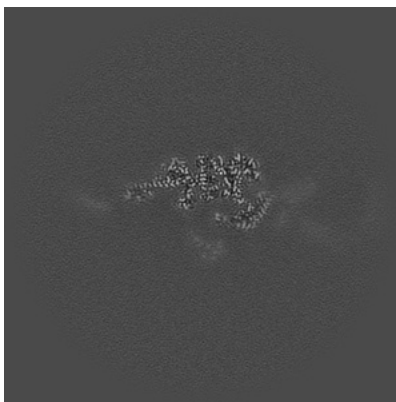
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

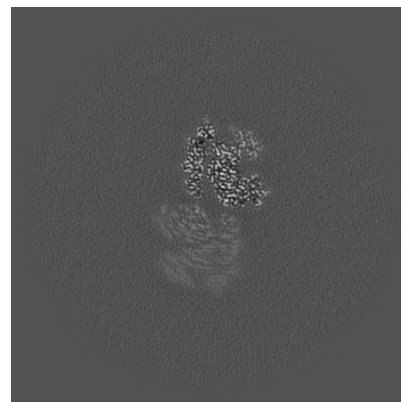
6.3.1 Primary map



X Index: 202

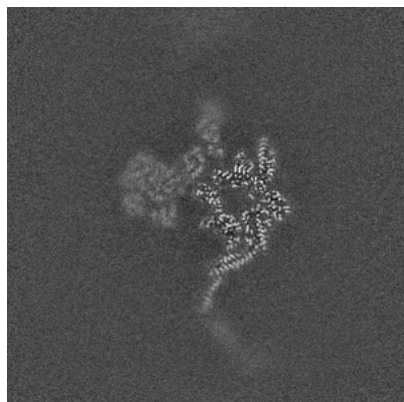


Y Index: 202

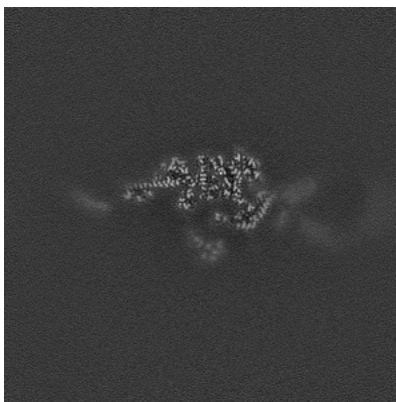


Z Index: 221

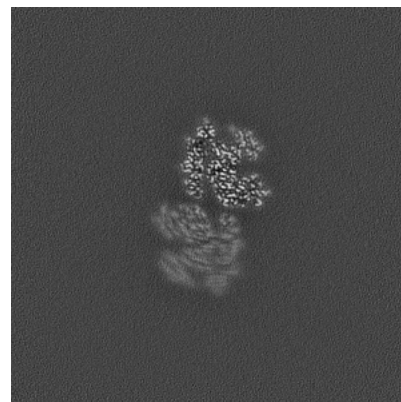
6.3.2 Raw map



X Index: 201



Y Index: 202

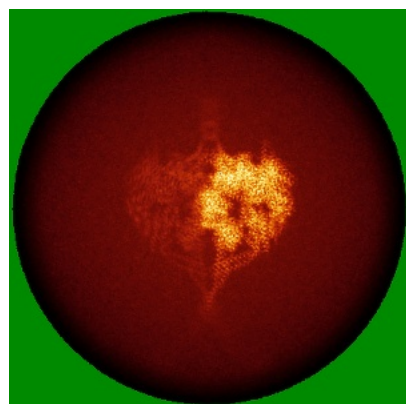


Z Index: 221

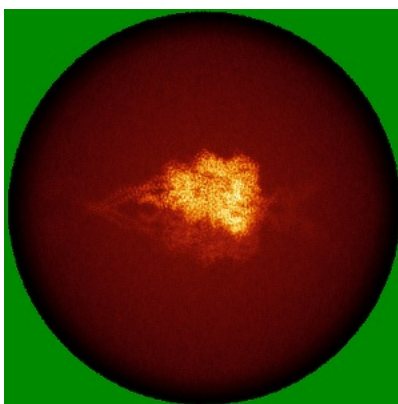
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

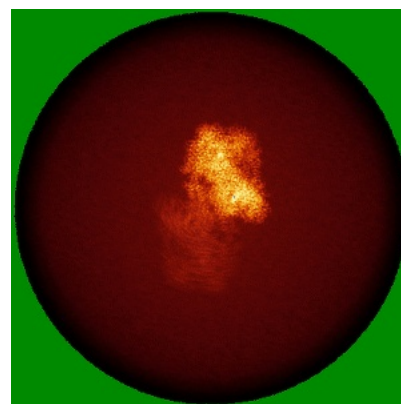
6.4.1 Primary map



X

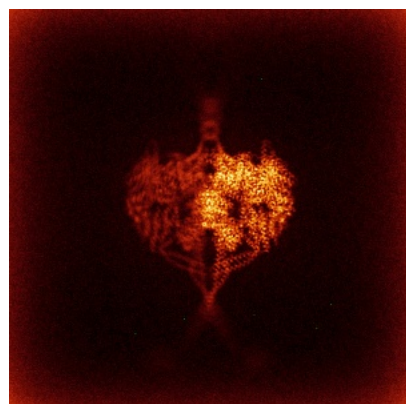


Y

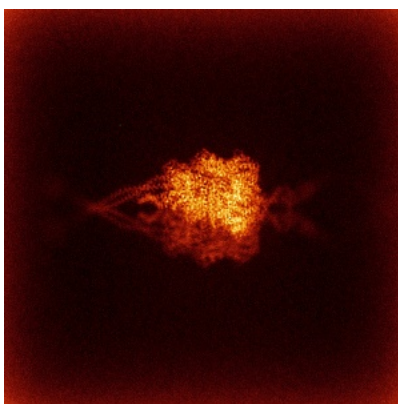


Z

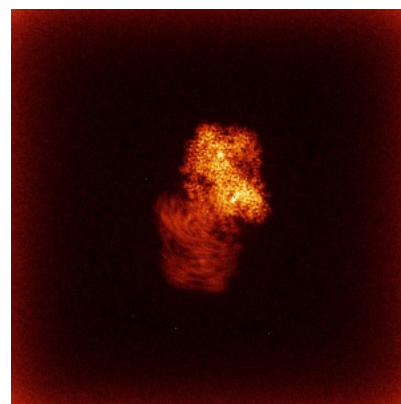
6.4.2 Raw map



X



Y

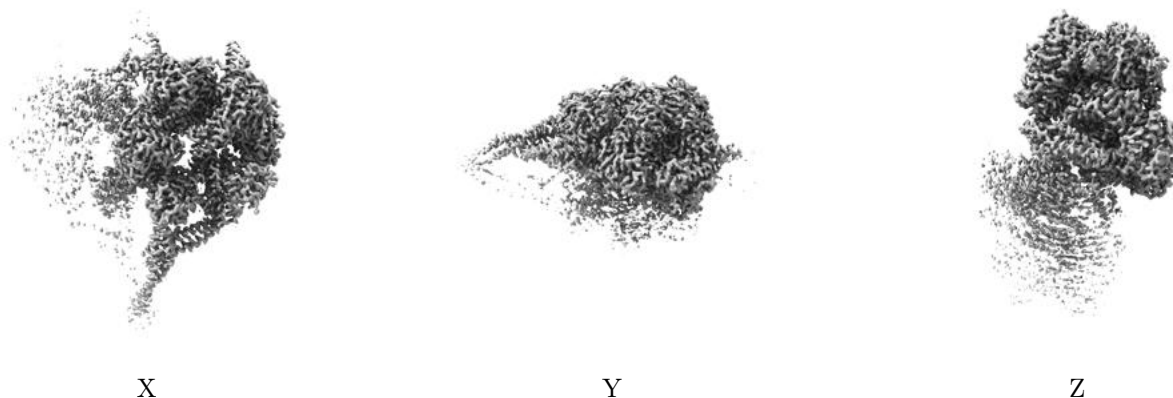


Z

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.

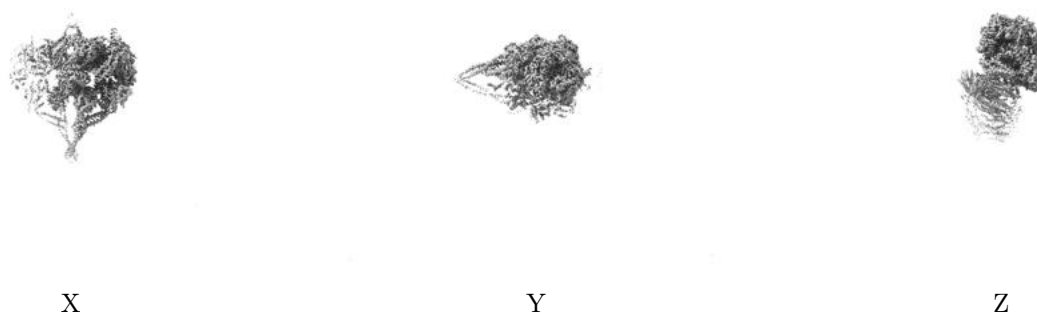
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

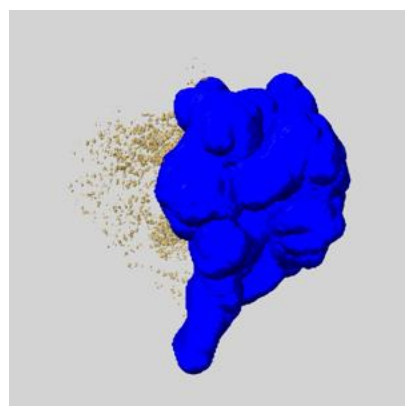
6.6 Mask visualisation [i](#)

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

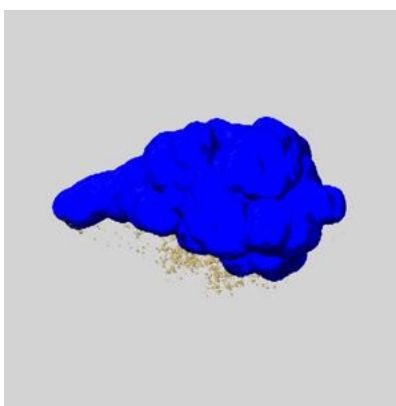
A mask typically either:

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

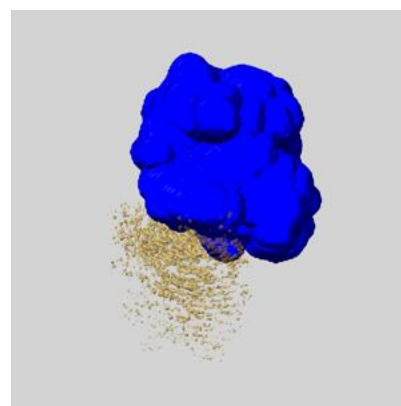
6.6.1 emd_44697_msk_1.map [i](#)



X



Y

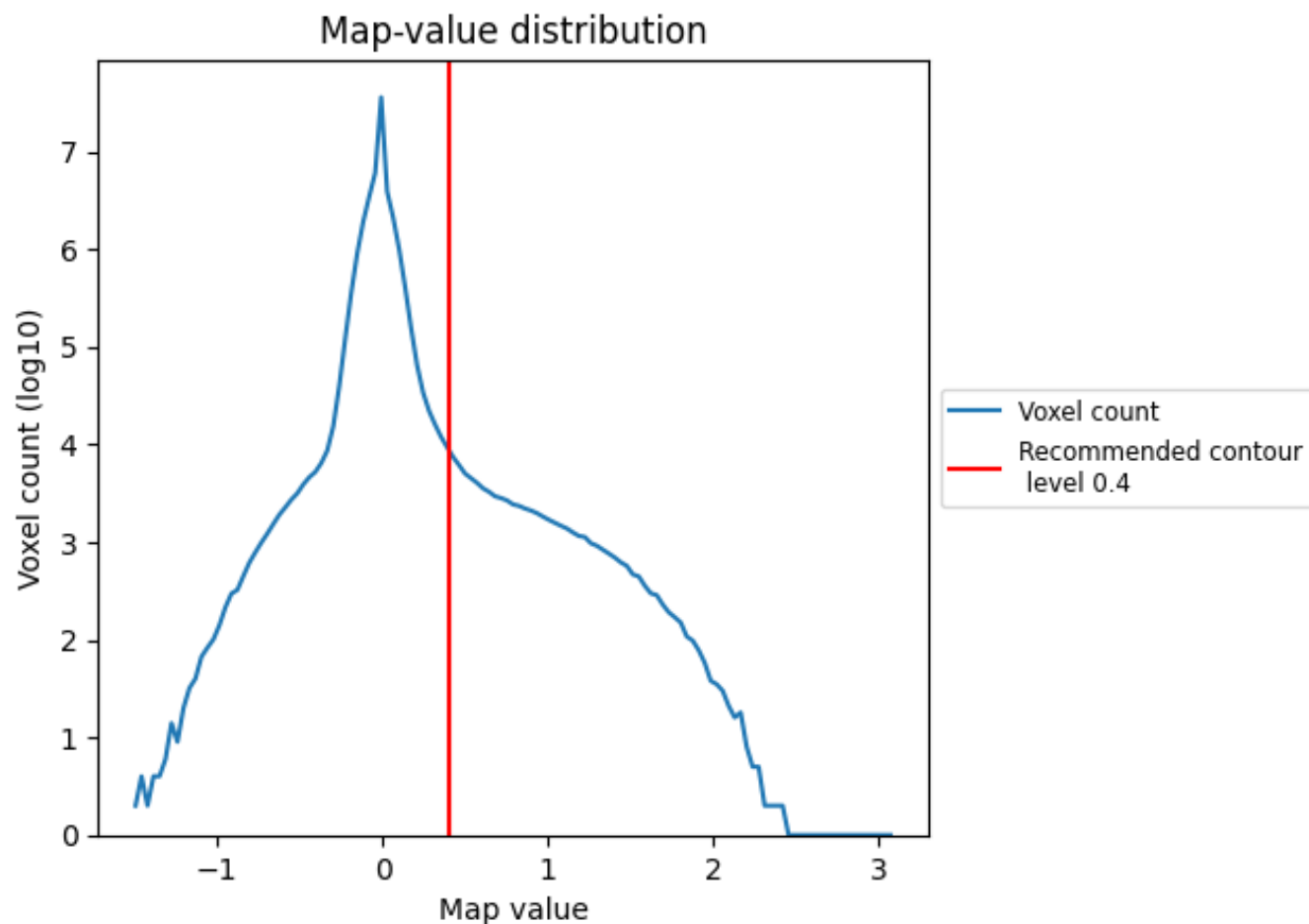


Z

7 Map analysis [i](#)

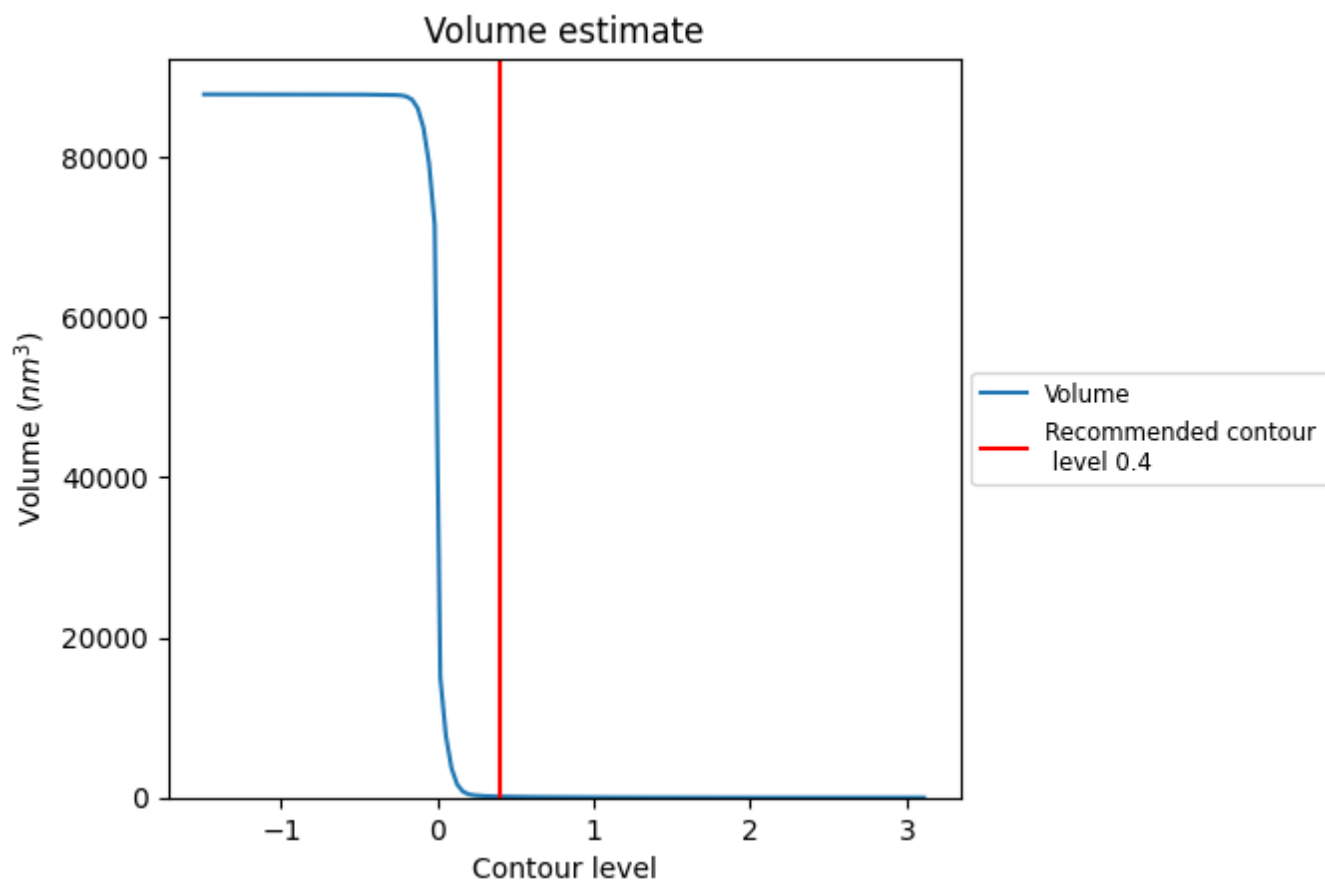
This section contains the results of statistical analysis of the map.

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.

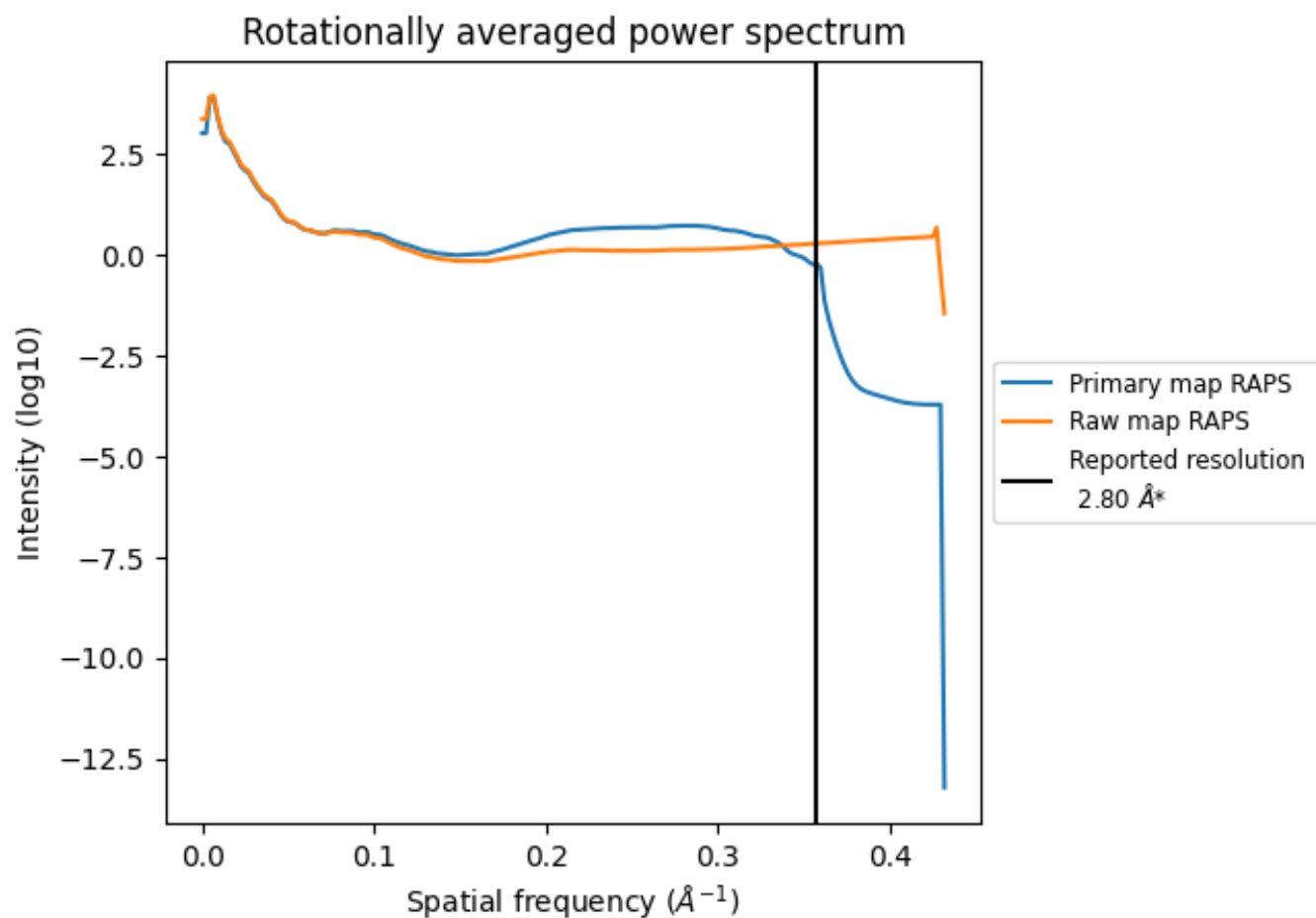
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 113 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 ⓘ

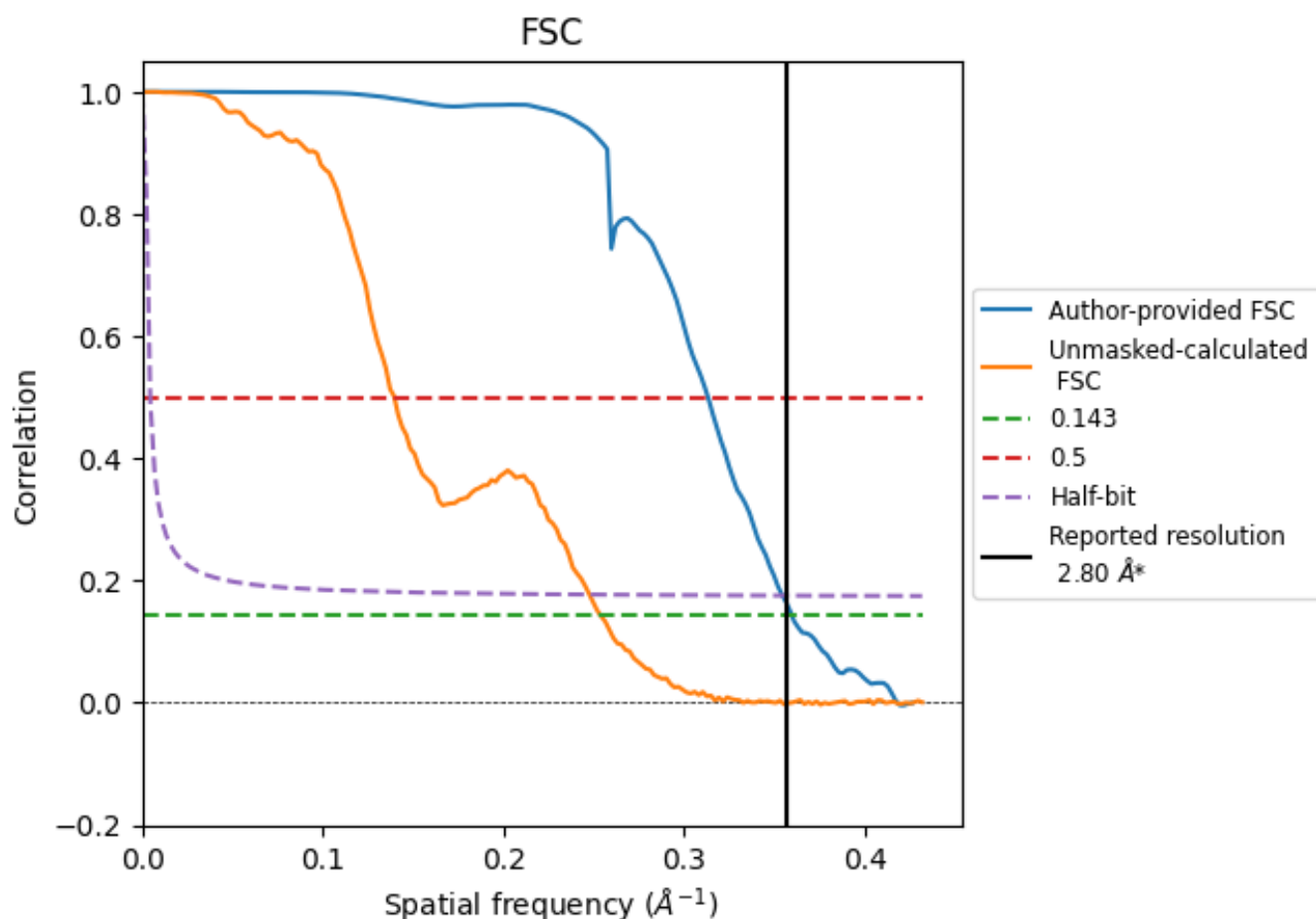


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

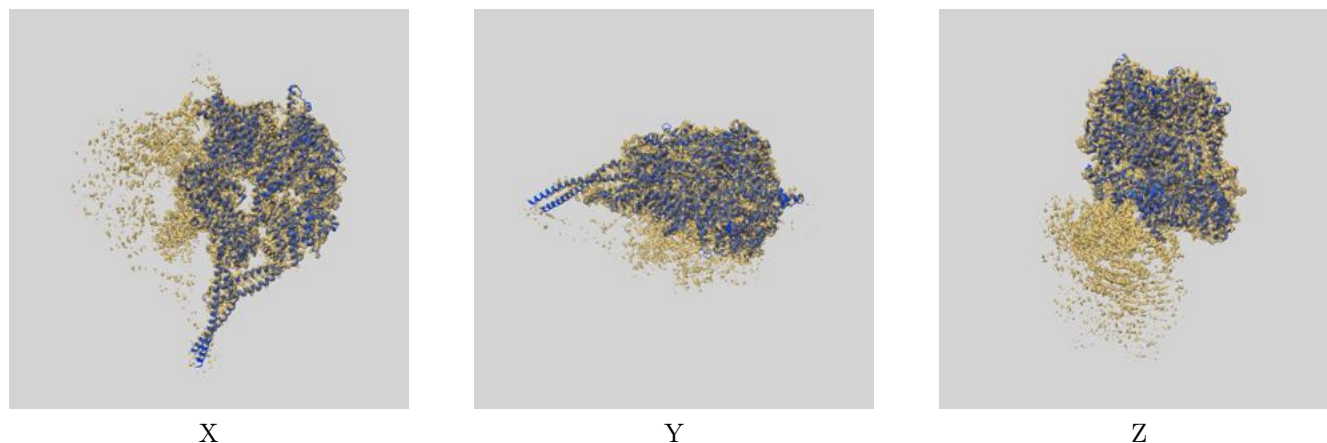
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.78	3.19	2.82
Unmasked-calculated*	3.94	7.16	4.04

*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 3.94 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

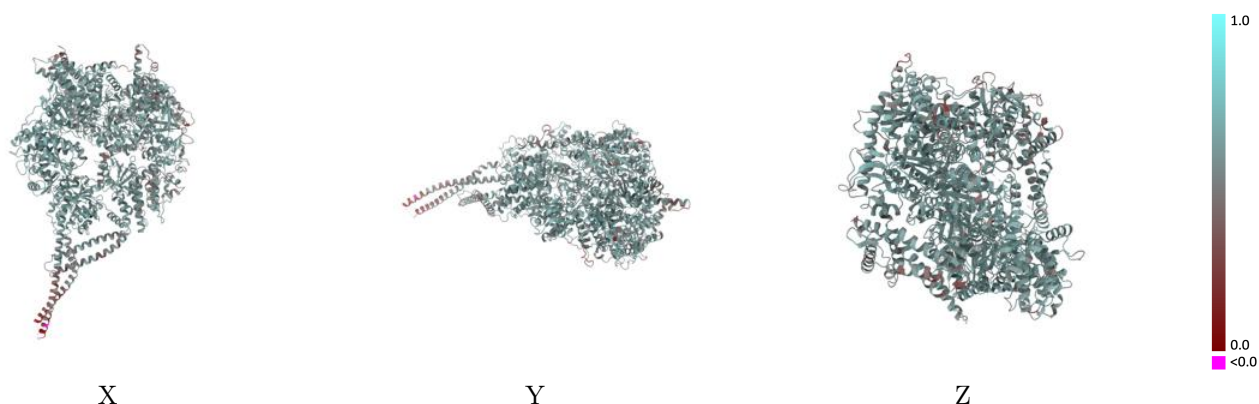
This section contains information regarding the fit between EMDB map EMD-44697 and PDB model 9BMF. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



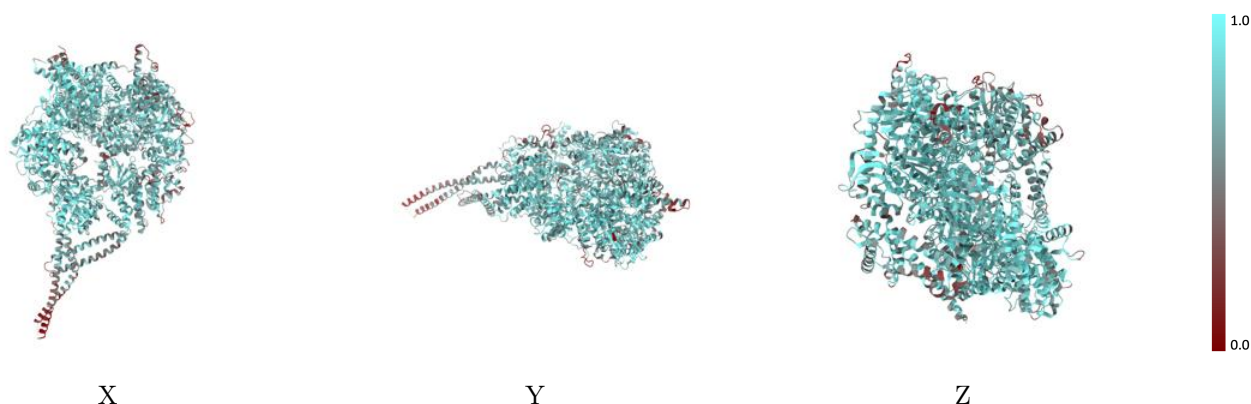
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



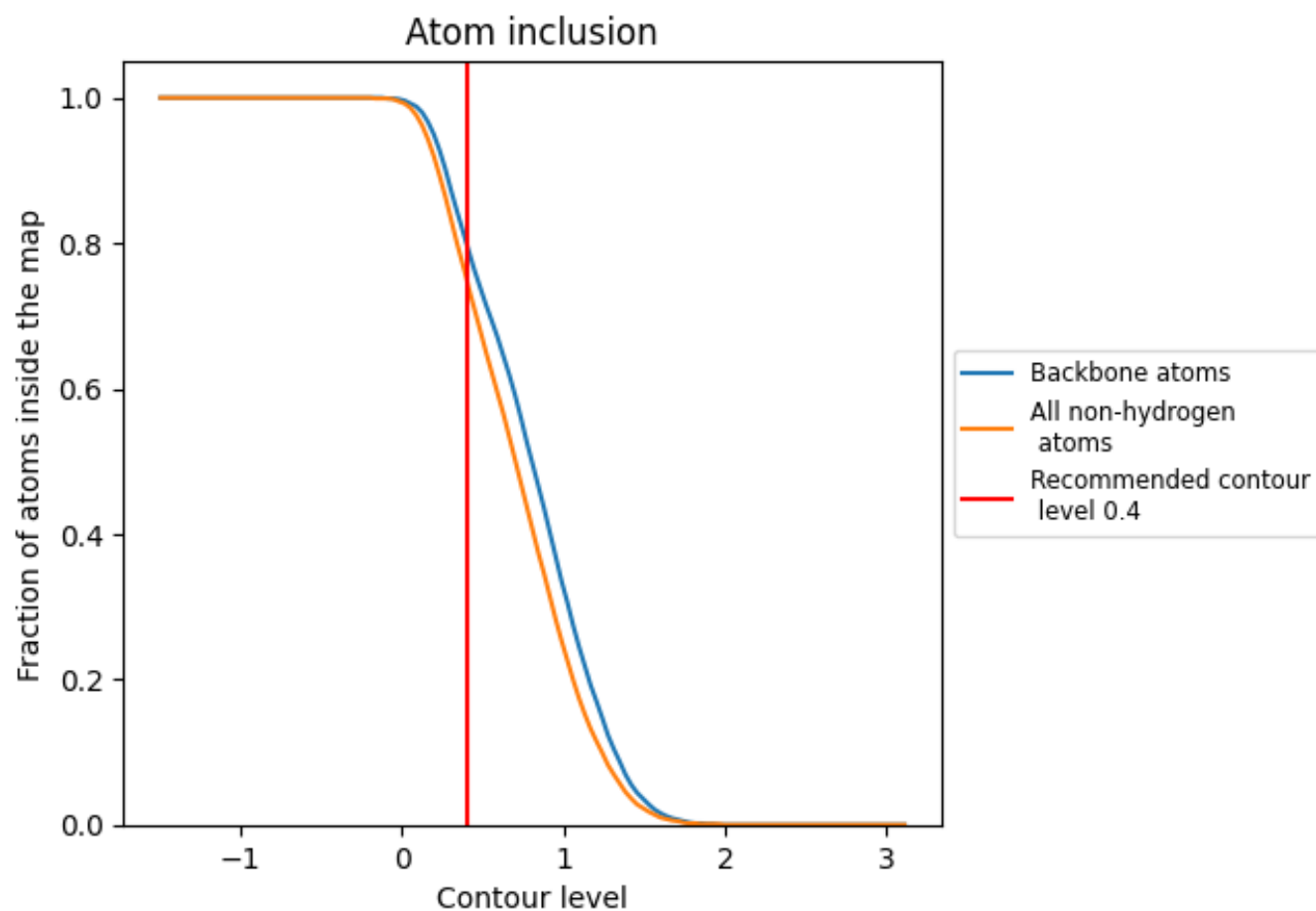
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.5680
A	0.7520	0.5680

