



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:35 AM UTC

PDB ID : 9DH6 / pdb_00009dh6
EMDB ID : EMD-46857
Title : State-2 of the motor domain from full-length human dynein-1 in 5mM
AMPPNP with 5mM Mg²⁺
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 3.40 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.dev132
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) : 2.49

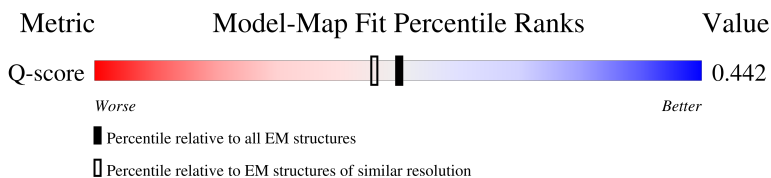
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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 4 unique types of molecules in this entry. The entry contains 23689 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	2935	23575	15017	4067	4374	117	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
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	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Mg 2 2	0





D3946	L3947	L3948	A3949	K3950	V3951	K3952	A3953	L3954	E3955	K3956	F3957	G3958	I3959	K3960	L3961	D3962	P3966	E3967	G3968	T3969	V3970	F3971	V3972	L3973	W3974	S3975	E3976	E3977	T3978	P3979	A3980	T3981	P3982	L3983	G3984	Q3985	R3989	L3990	Q3994	A3995	F3996	D3999	R4000	L4001	L4002	A4003	M4004	V4009	L4013	G4014	E4015	S4016	F4017						
D3879	H3880	L3886	K3890	K3891	L3892	K3893	A3894	T3895	V3896	G3897	E3898	F3899	T3900	T3901	A3902	A3903	E3904	F3905	Q3906	R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	A3918	G3919	E3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	E3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	P3942	A3943	F3944	K3945				
V3784	E3785	E3786	T3787	D3788	K3789	V3790	M3791	Q3792	E3793	V3794	E3795	Q3799	Q3800	V3801	L3802	S3809	E3816	Y3825	Q3830	L3833	D3834	I3835	Y3836	H3837	N3838	L3839	Y3841	E3842	N3843	K3847	G3848	V3849	T3850	D3851	Q3854	R3855	K3861	D3862	L3863	F3864	Q3865	R3870	V3871	A3872	R3873	G3874	M3875	L3876	R3877	V3780	T3781	R3782	K3783						
D3723	V3724	D3725	E3726	K3727	R3728	S3729	D3730	L3731	L3732	K3733	L3734	Q3735	G3736	E3737	F3738	Q3739	L3740	R3741	L3742	Q3743	Q3744	L3745	E3746	K3747	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	D3760	L3761	D3762	D3763	D3764	T3765	I3766	L3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	A3778	E3779	V3780	T3781	R3782	K3783	
Y3641	D3642	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	G3658	R3659	V3660	L3661	I3662	T3663	L3664	G3665	D3666	Q3667	D3668	I3669	D3670	L3671	S3674	T3681	R3682	D3683	P3684	T3685	V3686	E3687	P3690	D3691	L3692	G3693	S3694	R3695	V3696	R3705	S3706	S3707	L3708	Q3711	C3712	E3715	V3716	L3717	K3718	A3719	E3720	R3721	P3722							
A3564	D3570	D3571	E3575	M3579	L3580	K3581	R3582	R3585	L3588	D3591	P3592	S3593	G3594	Q3595	A3596	T3597	E3598	F3599	I3600	K3605	D3606	R3607	K3608	T3609	T3610	R3611	T3612	L3615	D3616	D3617	A3618	F3619	R3620	K3621	N3622	L3623	E3624	L3627	R3628	F3629	G3630	N3631	L3634	V3635	Q3636	D3637	V3638	E3639	S3640										
A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	W3489	E3490	K3491	T3492	S3493	E3494	T3495	F3496	K3497	N3498	Q3499	K3500	S3501	T3502	I3503	D3506	S3510	Y3516	A3517	F3520	D3521	Q3522	K3523	K3524	R3525	Q3537	R3544	T3545	D3546	I3547	A3548	R3549	T3550	E3551	T3552	L3553	D3557	E3558	R3559	Q3563								
GLY	GLY	ILE	SER	ASP	ALA	ILE	ARG	VAL	GLY	VAL	ASN	TYR	MET	ASN	PRO	ALA	SER	VAL	GLY	GLY	GLY	LEU	ALA	CYS	PRO	THR	THR	ILE	ALA	ASP	TRP	LYS	GLN	MET	SER	ARG	ILE	ARG	VAL	L3465	A3466	A3467	V3468	E3469	K3470	K3471	V3472	N3473	R3474	S3475	T3476								
N3237	D3238	K3239	L3240	K3241	LYS	MET	LEU	VAL	LYS	VAL	ARG	LYS	LYS	GLN	GLN	GLN	SER	GLN	GLY	LEU	LEU	LYS	GLN	GLY	GLY	VAL	THR	THR	ALA	ASP	LYS	TRP	LYS	GLN	MET	SER	ARG	ILE	PRO	ALA	VAL	THR	THR	ILE	VAL	GLU	ALA	ASN	ALA	VAL									
A3170	I3171	T3172	P3173	R3174	D3178	F3179	I3180	N3181	H3182	H3188	E3189	K3190	R3191	S3192	E3193	L3194	T3121	V3122	F3123	D3124	V3125	M3126	F3127	L3201	CYS	N3202	L3205	R3206	K3207	I3208	L3133	K3209	E3210	T3211	L3212	D3213	Q3214	V3215	E3216	E3217	ARG	L3218	R3219	R3220	D3221	L3222	R3223	I3224	A3159	R3160	L3161	A3162	K3163	R3164	G3165	G3166	R3167	T3168	K3169



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.222	Depositor
Minimum map value	-0.580	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/24075	0.28	0/32628

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	23575	0	23639	376	0
2	A	81	0	36	5	0
3	A	31	0	12	0	0
4	A	2	0	0	0	0
All	All	23689	0	23687	376	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (376) 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:1497:VAL:HG13	1:A:1527:LEU:HD22	1.59	0.85
1:A:2156:LEU:HG	1:A:4411:ARG:HD2	1.59	0.83
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.62	0.81
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.65	0.79
1:A:1810:HIS:HD2	1:A:1878:LYS:HG3	1.48	0.78
1:A:2092:ALA:HB1	1:A:2145:MET:HE1	1.64	0.78
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.67	0.77
1:A:4260:PHE:HD1	1:A:4263:ARG:HH21	1.36	0.74
1:A:1526:LYS:HA	1:A:1529:ARG:HD3	1.68	0.74
1:A:3488:ARG:NH2	1:A:3746:GLU:OE1	2.21	0.74
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.70	0.73
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.21	0.73
1:A:1652:LYS:HG3	1:A:1653:HIS:HD2	1.52	0.73
1:A:4413:PHE:CZ	1:A:4492:ILE:HG23	2.24	0.72
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.71	0.72
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.71	0.71
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.72	0.71
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.73	0.69
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.74	0.69
1:A:4393:GLN:HG3	1:A:4428:ARG:HH12	1.58	0.68
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.74	0.68
1:A:1806:ARG:O	1:A:1810:HIS:ND1	2.21	0.68
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.27	0.68
1:A:3487:GLU:OE1	1:A:3491:LYS:NZ	2.27	0.67
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.78	0.65
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.78	0.65
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.30	0.65
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.77	0.64
1:A:3481:SER:O	1:A:3774:LYS:NZ	2.30	0.64
1:A:3731:LEU:HD21	1:A:3790:VAL:HB	1.80	0.64
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.31	0.63
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.78	0.63
1:A:3499:GLN:O	1:A:3503:ILE:HG13	1.99	0.62
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.79	0.62
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.63	0.62
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.65	0.62
1:A:2382:LEU:HD12	1:A:2416:GLN:HE21	1.65	0.62
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.32	0.62
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.35	0.62
1:A:2172:ARG:NH1	1:A:2205:GLU:OE2	2.33	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.83	0.61
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.81	0.61
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.83	0.61
1:A:2172:ARG:NH2	1:A:2212:GLN:OE1	2.35	0.60
1:A:1543:ARG:HA	1:A:1546:TYR:CE1	2.37	0.60
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.83	0.60
1:A:1504:VAL:HG11	1:A:1524:GLU:HG3	1.84	0.60
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.83	0.59
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.82	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.82	0.59
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.35	0.59
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.36	0.59
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.36	0.59
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.20	0.59
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.84	0.59
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.36	0.59
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.85	0.59
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.34	0.59
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.68	0.59
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.85	0.58
1:A:1639:GLU:OE2	1:A:1643:ASN:ND2	2.36	0.58
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.85	0.58
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.37	0.58
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.86	0.58
1:A:2410:SER:HB3	1:A:2413:LEU:HD23	1.87	0.57
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.83	0.57
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.85	0.57
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.36	0.57
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.38	0.57
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.86	0.57
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.87	0.57
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.36	0.57
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.36	0.57
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.34	0.57
1:A:2519:ARG:HG3	1:A:2526:LEU:HD22	1.86	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:3779:GLU:O	1:A:3783:LYS:HG2	2.04	0.57
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	1.86	0.56
1:A:1887:ARG:HD2	1:A:4249:GLN:HG2	1.87	0.56
1:A:1987:ASN:OD1	1:A:1989:ASN:ND2	2.38	0.56
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.88	0.56
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.39	0.55
1:A:1589:MET:SD	1:A:1589:MET:N	2.80	0.55
1:A:3875:MET:HE3	1:A:3880:HIS:HA	1.88	0.55
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.40	0.55
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.35	0.55
1:A:1763:GLU:OE1	1:A:1838:TRP:NE1	2.34	0.54
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.71	0.54
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.88	0.54
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.36	0.54
1:A:3967:GLU:HB2	1:A:4004:MET:HE2	1.88	0.54
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.88	0.54
1:A:3960:TRP:HD1	1:A:3969:THR:HG23	1.72	0.54
1:A:4489:LEU:HD23	1:A:4492:ILE:HD12	1.88	0.54
1:A:2080:LEU:HD11	1:A:2157:LEU:HD12	1.89	0.54
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.89	0.54
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.90	0.54
1:A:4518:GLU:OE1	1:A:4518:GLU:N	2.33	0.54
1:A:4398:LEU:HD12	1:A:4414:GLU:HA	1.89	0.53
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.39	0.53
1:A:4409:LEU:O	1:A:4413:PHE:HB2	2.08	0.53
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.41	0.53
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.43	0.53
1:A:3653:VAL:HG12	1:A:3662:ILE:HB	1.88	0.53
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.90	0.53
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.90	0.53
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.26	0.53
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.91	0.52
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.91	0.52
1:A:4194:LEU:HD11	1:A:4204:LYS:HA	1.91	0.52
1:A:4605:VAL:HG23	1:A:4636:TYR:HE1	1.75	0.52
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.90	0.52
1:A:3216:GLU:HG2	1:A:3219:ARG:HH21	1.74	0.52
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.91	0.52
1:A:2654:GLN:NE2	1:A:3048:GLU:OE2	2.43	0.52
1:A:4474:THR:HG22	1:A:4476:ILE:H	1.75	0.52
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.58	0.51
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.93	0.51
1:A:2363:TRP:NE1	1:A:2365:SER:OG	2.43	0.51
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.09	0.51
1:A:2440:ALA:HB2	1:A:2502:LEU:HD23	1.92	0.51
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.11	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.93	0.51
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.51
1:A:1847:ASP:N	1:A:1856:GLN:O	2.41	0.51
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.45	0.51
1:A:3720:GLU:OE1	1:A:3855:ARG:NE	2.43	0.51
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.44	0.51
1:A:1527:LEU:HD23	1:A:1530:ILE:HD12	1.92	0.50
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.23	0.50
1:A:3160:ARG:HE	1:A:3164:ARG:HH21	1.60	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.44	0.50
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.28	0.50
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.92	0.50
1:A:2481:MET:HE2	1:A:2485:GLN:HB3	1.94	0.50
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.94	0.50
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.94	0.50
1:A:4408:PRO:HG3	1:A:4526:GLN:HB3	1.92	0.50
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.75	0.50
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.11	0.50
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.93	0.50
1:A:1941:MET:HE3	1:A:1971:VAL:HG11	1.94	0.49
1:A:1535:ASP:O	1:A:2292:ARG:NH2	2.45	0.49
1:A:2485:GLN:NE2	1:A:2542:SER:O	2.45	0.49
1:A:2507:ARG:HH22	1:A:2510:MET:HE2	1.78	0.49
1:A:4392:PRO:O	1:A:4428:ARG:NH1	2.45	0.49
1:A:4192:GLU:HB2	1:A:4321:LEU:HD21	1.95	0.49
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.95	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.49
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.47	0.49
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.13	0.49
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.93	0.49
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.13	0.48
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.13	0.48
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.30	0.48
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.48
1:A:2291:VAL:HG13	1:A:2292:ARG:HG3	1.95	0.48
1:A:3775:ARG:O	1:A:3779:GLU:HG2	2.12	0.48
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.14	0.48
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3160:ARG:HE	1:A:3164:ARG:NH2	2.11	0.48
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.46	0.48
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.41	0.48
1:A:4525:ARG:HG3	1:A:4592:TRP:CH2	2.48	0.48
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.46	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.47	0.48
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	1.94	0.48
1:A:3030:MET:HA	1:A:3030:MET:HE3	1.96	0.48
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.95	0.47
1:A:1980:GLU:O	1:A:1984:GLU:HG2	2.14	0.47
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	1.96	0.47
1:A:1912:LYS:NZ	2:A:4701:ADP:O3B	2.33	0.47
1:A:1985:HIS:CE1	1:A:2010:PRO:HG3	2.49	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.48	0.47
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.94	0.47
1:A:2605:LEU:HD13	1:A:2709:VAL:HG11	1.96	0.47
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.14	0.47
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.96	0.47
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.97	0.47
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.14	0.47
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.96	0.47
1:A:3872:ALA:HA	1:A:3875:MET:HE2	1.97	0.47
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.31	0.47
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.97	0.47
1:A:2463:HIS:O	1:A:2467:ARG:HG3	2.14	0.47
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.14	0.47
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.25	0.47
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.48	0.47
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.30	0.47
1:A:4509:VAL:HG11	1:A:4514:LEU:HD11	1.96	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.50	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.33	0.47
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.96	0.47
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.48	0.47
1:A:3960:TRP:CD1	1:A:3969:THR:HG23	2.49	0.47
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.97	0.47
1:A:2075:LEU:HD13	1:A:2160:LEU:HD11	1.96	0.46
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.48	0.46
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.16	0.46
1:A:4413:PHE:O	1:A:4417:VAL:HG23	2.14	0.46
1:A:1738:TYR:CE2	1:A:1792:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3109:PHE:HD2	1:A:3180:ILE:HG22	1.80	0.46
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.15	0.46
1:A:3728:ARG:HG3	1:A:3791:MET:HE1	1.97	0.46
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.79	0.46
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.97	0.46
1:A:3791:MET:O	1:A:3795:GLU:HG3	2.14	0.46
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.49	0.46
1:A:1490:TRP:HZ3	1:A:1534:PHE:HD1	1.64	0.46
1:A:1903:SER:HA	1:A:2016:ILE:O	2.15	0.46
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.46
1:A:1467:ARG:HB2	1:A:1523:TRP:HH2	1.80	0.46
1:A:1550:ILE:O	1:A:1554:SER:OG	2.29	0.46
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.98	0.46
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.98	0.46
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.81	0.46
1:A:2446:ILE:HG13	1:A:2735:TYR:CD1	2.51	0.46
1:A:1508:LYS:HA	1:A:1513:TYR:CG	2.51	0.45
1:A:3100:GLU:HG2	1:A:3130:TYR:HE1	1.80	0.45
1:A:2983:SER:HB2	1:A:2990:ILE:HD12	1.99	0.45
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.81	0.45
1:A:2606:PHE:HE1	1:A:2617:VAL:HG21	1.81	0.45
1:A:2018:MET:HE2	1:A:2018:MET:HB3	1.88	0.45
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.16	0.45
1:A:4412:PHE:CZ	1:A:4514:LEU:HD13	2.51	0.45
1:A:2104:LYS:HG3	1:A:2131:LEU:HD21	1.99	0.45
1:A:3843:ASN:ND2	1:A:3862:ASP:OD2	2.48	0.45
1:A:4410:PHE:HA	1:A:4413:PHE:HB3	1.99	0.45
1:A:2624:SER:HB3	1:A:3081:THR:HA	1.98	0.45
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.17	0.45
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.50	0.45
1:A:4409:LEU:HA	1:A:4523:ALA:HB1	1.99	0.45
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.98	0.45
1:A:1507:MET:O	1:A:1510:SER:OG	2.29	0.45
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.17	0.45
1:A:2257:LYS:HZ3	1:A:2308:ASP:CG	2.24	0.45
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.17	0.45
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.48	0.45
1:A:2103:VAL:HA	1:A:2106:GLU:HG2	1.99	0.45
1:A:3551:GLU:HA	1:A:3559:ARG:NH1	2.32	0.45
1:A:4489:LEU:HA	1:A:4492:ILE:HD12	1.98	0.45
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2671:MET:HE2	1:A:2675:GLY:HA2	1.99	0.45
1:A:1640:ILE:HA	1:A:1650:LEU:HD22	2.00	0.44
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.17	0.44
1:A:3837:HIS:CE1	1:A:3841:TYR:HD2	2.35	0.44
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.53	0.44
1:A:2965:ARG:HH12	1:A:3640:SER:HB3	1.81	0.44
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.33	0.44
1:A:1572:SER:O	1:A:1576:LEU:HG	2.18	0.44
1:A:2324:LEU:HD23	1:A:2334:SER:HA	1.99	0.44
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.53	0.44
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.16	0.44
1:A:4488:GLN:O	1:A:4492:ILE:HG13	2.18	0.44
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.99	0.44
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.98	0.44
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	2.00	0.44
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.51	0.44
1:A:1568:PHE:HB2	1:A:1611:ILE:HD13	1.99	0.43
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.53	0.43
1:A:1623:ARG:HA	1:A:1629:PHE:HB2	2.01	0.43
1:A:2159:SER:OG	1:A:4411:ARG:NH1	2.52	0.43
1:A:2527:PRO:HD3	1:A:2545:TRP:CD2	2.54	0.43
1:A:2816:LEU:HD21	1:A:2821:LEU:N	2.33	0.43
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.00	0.43
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.43
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.82	0.43
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.19	0.43
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.18	0.43
1:A:4626:ILE:HD12	1:A:4630:GLU:O	2.18	0.43
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.45	0.43
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.00	0.43
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.86	0.43
1:A:1558:LYS:HD3	1:A:1565:THR:HG21	2.00	0.43
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.54	0.43
1:A:4182:LEU:HG	1:A:4296:MET:HE1	2.01	0.43
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.54	0.43
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.18	0.43
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.18	0.43
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.84	0.43
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.81	0.43
1:A:1738:TYR:HE2	1:A:1792:LEU:HD11	1.83	0.43
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1542:ARG:O	1:A:1546:TYR:HD1	2.02	0.43
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.01	0.43
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	2.01	0.42
1:A:2507:ARG:HH21	1:A:2509:LYS:HE2	1.83	0.42
1:A:2936:ILE:O	1:A:3094:PHE:N	2.52	0.42
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.84	0.42
1:A:1933:ASP:OD1	1:A:1935:THR:HG22	2.19	0.42
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.44	0.42
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	2.00	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.85	0.42
1:A:3214:GLN:HB3	1:A:3761:LEU:HD12	2.00	0.42
1:A:3951:VAL:HG12	1:A:3973:LEU:HD21	2.00	0.42
1:A:1543:ARG:HA	1:A:1546:TYR:CD1	2.55	0.42
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	2.00	0.42
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	2.03	0.42
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	2.00	0.42
1:A:3900:THR:HG23	1:A:3902:ASP:H	1.84	0.42
1:A:1814:GLU:OE1	1:A:1878:LYS:NZ	2.52	0.42
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.19	0.42
1:A:4529:ALA:O	1:A:4533:SER:N	2.53	0.42
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.55	0.42
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.78	0.42
1:A:3906:GLN:NE2	1:A:3910:ARG:HD2	2.34	0.42
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	2.02	0.42
1:A:2083:GLN:HE21	1:A:2150:VAL:HG11	1.85	0.42
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.20	0.42
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.47	0.42
1:A:1561:LEU:HB3	1:A:1564:GLU:OE2	2.19	0.42
1:A:1587:LEU:HD12	1:A:1587:LEU:HA	1.94	0.41
1:A:1680:GLU:HG2	1:A:1803:LEU:HD13	2.02	0.41
1:A:2163:ASP:HB3	1:A:4526:GLN:HE21	1.84	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.41
1:A:2686:MET:HE3	1:A:2708:PHE:CZ	2.54	0.41
1:A:4486:ILE:HD13	1:A:4486:ILE:HA	1.90	0.41
1:A:1501:ILE:HG13	1:A:1527:LEU:HD13	2.01	0.41
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.41
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.85	0.41
1:A:4400:ARG:NE	1:A:4414:GLU:OE1	2.53	0.41
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.02	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.03	0.41
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3085:LEU:O	1:A:3089:CYS:HB2	2.21	0.41
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	2.03	0.41
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.21	0.41
1:A:1969:SER:O	1:A:1972:SER:OG	2.35	0.41
1:A:2091:ARG:HH21	2:A:4701:ADP:PA	2.44	0.41
1:A:2766:ALA:O	1:A:2770:THR:HG22	2.21	0.41
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.21	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD2	1.77	0.41
1:A:3608:LYS:HD2	1:A:3608:LYS:HA	1.67	0.41
1:A:2671:MET:HA	1:A:2676:THR:O	2.19	0.41
1:A:2949:PHE:CE2	1:A:2953:MET:HE3	2.56	0.41
1:A:3955:GLU:OE1	1:A:3955:GLU:N	2.52	0.41
1:A:1672:VAL:HG22	1:A:1691:SER:HB3	2.03	0.41
1:A:1810:HIS:CD2	1:A:1878:LYS:HG3	2.39	0.41
1:A:2525:PRO:C	1:A:2526:LEU:HD12	2.45	0.41
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.45	0.41
1:A:2079:GLN:O	1:A:4415:ARG:NH1	2.47	0.41
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	2.01	0.41
1:A:2541:ILE:HD12	1:A:2541:ILE:HA	1.95	0.41
1:A:3550:THR:HG22	1:A:3575:GLU:HG3	2.03	0.41
1:A:3723:ASP:O	1:A:3726:GLU:HG2	2.21	0.41
1:A:4260:PHE:CZ	1:A:4608:PRO:HB3	2.55	0.41
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.86	0.41
1:A:3570:ASP:OD2	1:A:3707:SER:HB3	2.21	0.41
1:A:3612:THR:O	1:A:3635:VAL:HA	2.20	0.41
1:A:3718:LYS:HB2	1:A:3725:ASP:OD2	2.20	0.41
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.20	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4418:LYS:HE3	1:A:4418:LYS:HB2	1.88	0.41
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.89	0.41
1:A:2697:ASP:N	1:A:2697:ASP:OD1	2.50	0.40
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.53	0.40
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.21	0.40
1:A:4002:LEU:HD23	1:A:4002:LEU:HA	1.92	0.40
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.56	0.40
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.94	0.40
1:A:1467:ARG:HB2	1:A:1523:TRP:CH2	2.57	0.40
1:A:1564:GLU:HA	1:A:1567:ARG:HB2	2.04	0.40
1:A:1941:MET:HE1	1:A:1960:PHE:HE1	1.86	0.40
1:A:2029:PRO:HB2	1:A:2031:ASN:OD1	2.22	0.40
1:A:2075:LEU:HB3	1:A:2160:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4158:LEU:HD21	1:A:4310:GLU:HG3	2.03	0.40
1:A:4605:VAL:HG23	1:A:4636:TYR:CE1	2.55	0.40
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.85	0.40
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.86	0.40
1:A:3485:GLU:HG3	1:A:3488:ARG:HH21	1.86	0.40
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	2.03	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	2927/4646 (63%)	2883 (98%)	44 (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	2603/4125 (63%)	2603 (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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1465	GLN
1	A	1612	GLN
1	A	1643	ASN
1	A	1653	HIS
1	A	1755	GLN
1	A	1856	GLN
1	A	1922	GLN
1	A	1976	GLN
1	A	1989	ASN
1	A	2057	GLN
1	A	2067	ASN
1	A	2171	HIS
1	A	2218	HIS
1	A	2416	GLN
1	A	2588	HIS
1	A	2752	ASN
1	A	2827	HIS
1	A	2960	GLN
1	A	3200	HIS
1	A	3237	ASN
1	A	3526	GLN
1	A	3711	GLN
1	A	3754	ASN
1	A	3799	GLN
1	A	3820	GLN
1	A	3838	ASN
1	A	4029	HIS
1	A	4054	HIS
1	A	4114	HIS
1	A	4156	ASN
1	A	4191	GLN
1	A	4307	GLN
1	A	4335	GLN
1	A	4429	GLN
1	A	4526	GLN

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 ⓘ

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$
2	ADP	A	4703	-	28,29,29	1.39	4 (14%)	43,45,45	1.85	8 (18%)
2	ADP	A	4701	4	28,29,29	1.39	5 (17%)	43,45,45	1.82	9 (20%)
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
3	ATP	A	4702	4	32,33,33	0.33	0	48,52,52	0.28	0

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
2	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	7/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.65	1.47	1.39
2	A	4703	ADP	C5-C4	4.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.61	1.47	1.39
2	A	4701	ADP	C5-C6	2.65	1.48	1.41
2	A	4704	ADP	C5-C6	2.65	1.48	1.41
2	A	4703	ADP	C5-C6	2.64	1.48	1.41
2	A	4703	ADP	C5-N7	-2.43	1.34	1.39
2	A	4701	ADP	C5-N7	-2.38	1.34	1.39
2	A	4704	ADP	C5-N7	-2.37	1.34	1.39
2	A	4704	ADP	C8-N7	2.26	1.36	1.31
2	A	4703	ADP	C8-N7	2.26	1.36	1.31
2	A	4701	ADP	C8-N7	2.25	1.36	1.31
2	A	4701	ADP	C4-N9	-2.00	1.33	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-5.96	118.51	126.72
2	A	4704	ADP	C5-C4-N3	-5.92	118.56	126.72
2	A	4701	ADP	C5-C4-N3	-5.70	118.87	126.72
2	A	4703	ADP	N3-C4-N9	4.73	135.21	127.17
2	A	4704	ADP	N3-C4-N9	4.63	135.04	127.17
2	A	4701	ADP	N3-C4-N9	4.52	134.85	127.17
2	A	4703	ADP	C2-N3-C4	3.76	121.02	111.83
2	A	4704	ADP	C2-N3-C4	3.73	120.94	111.83
2	A	4701	ADP	C2-N3-C4	3.63	120.69	111.83
2	A	4704	ADP	C4-C5-N7	-3.46	106.62	110.58
2	A	4703	ADP	C4-C5-N7	-3.36	106.74	110.58
2	A	4701	ADP	C4-C5-N7	-3.33	106.77	110.58
2	A	4703	ADP	N3-C2-N1	-3.24	123.68	128.58
2	A	4701	ADP	N3-C2-N1	-3.18	123.77	128.58
2	A	4704	ADP	N3-C2-N1	-3.17	123.78	128.58
2	A	4701	ADP	C4-N9-C8	2.60	108.47	105.74
2	A	4703	ADP	C3'-C2'-C1'	2.53	106.25	101.46
2	A	4703	ADP	C4-N9-C8	2.47	108.34	105.74
2	A	4703	ADP	C5-N7-C8	2.44	107.28	103.45
2	A	4704	ADP	C4-N9-C8	2.42	108.28	105.74
2	A	4704	ADP	C5-N7-C8	2.42	107.25	103.45
2	A	4701	ADP	C5-N7-C8	2.41	107.24	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.32	105.86	101.46
2	A	4701	ADP	C3'-C2'-C1'	2.18	105.59	101.46
2	A	4701	ADP	C6-C5-N7	2.03	136.01	132.09
2	A	4704	ADP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

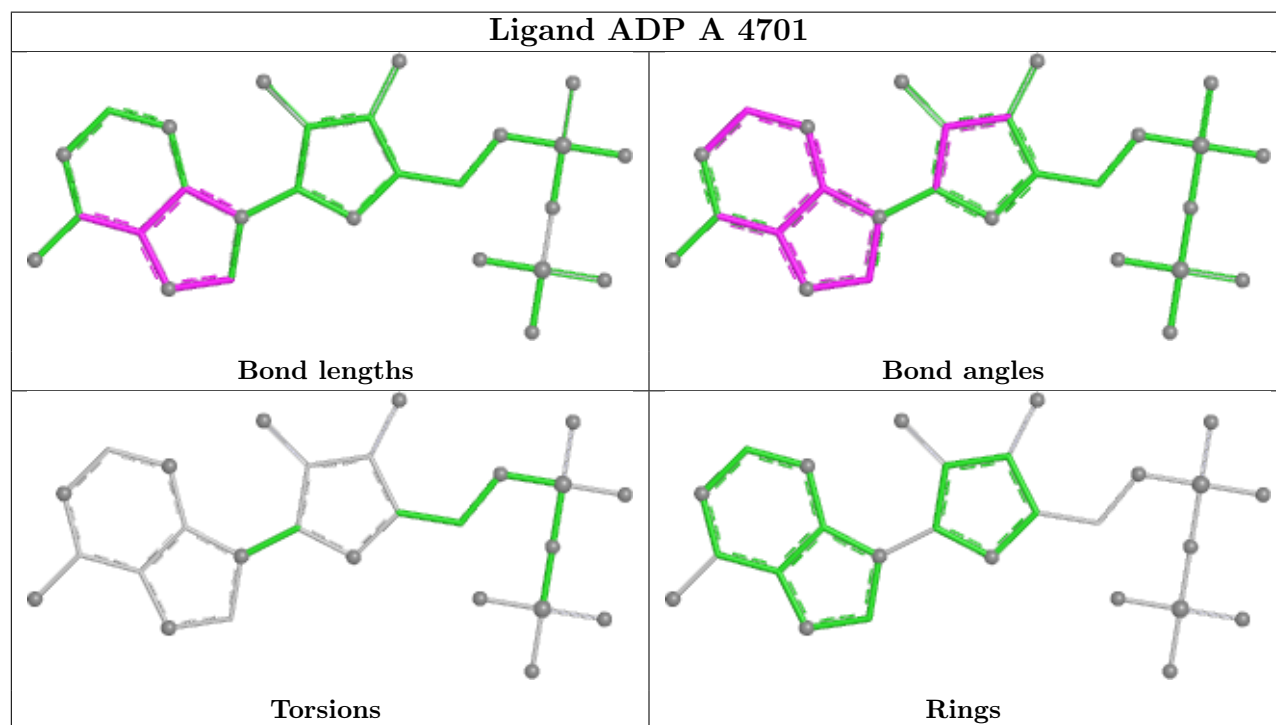
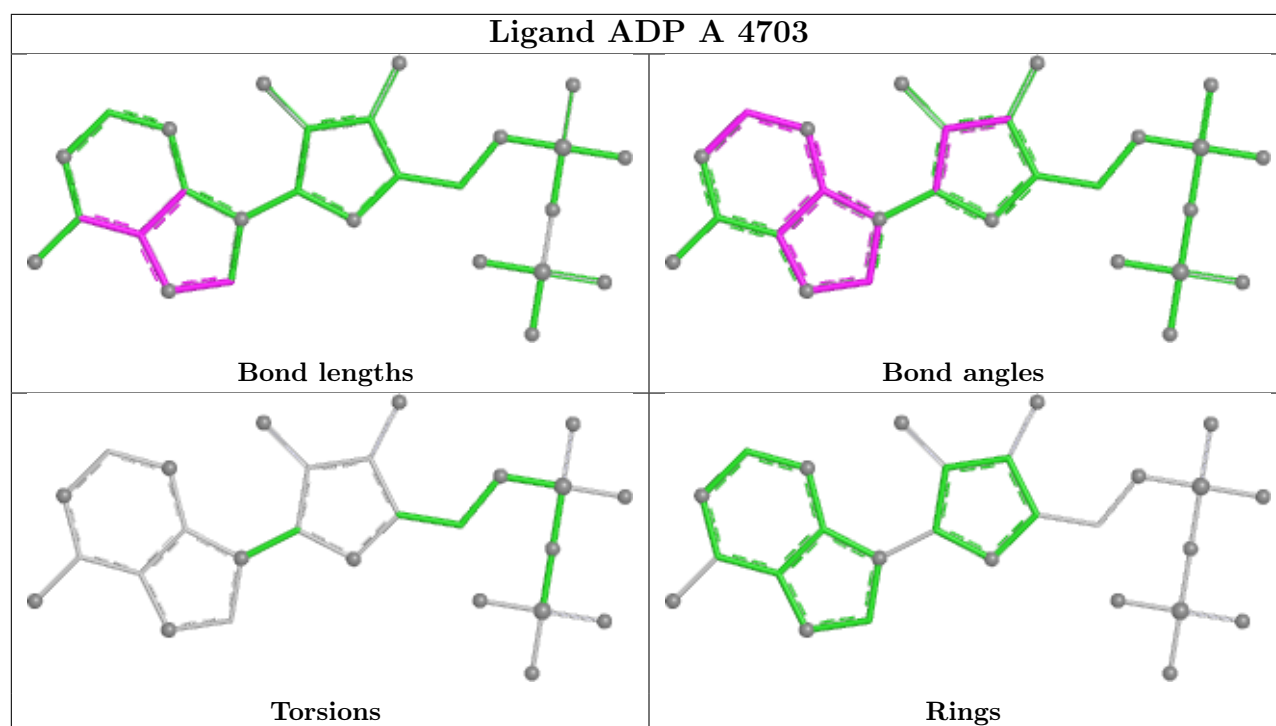
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O2B

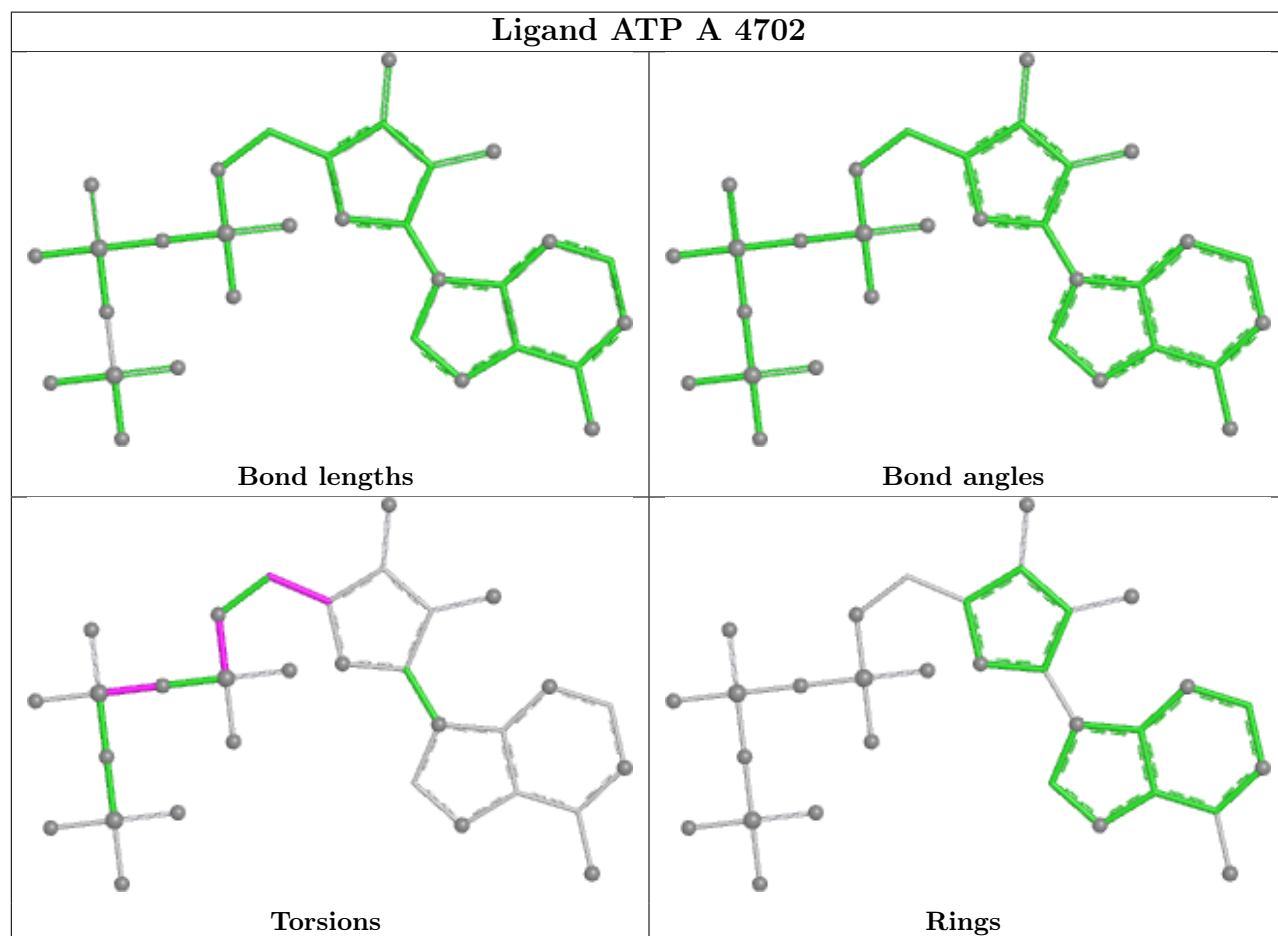
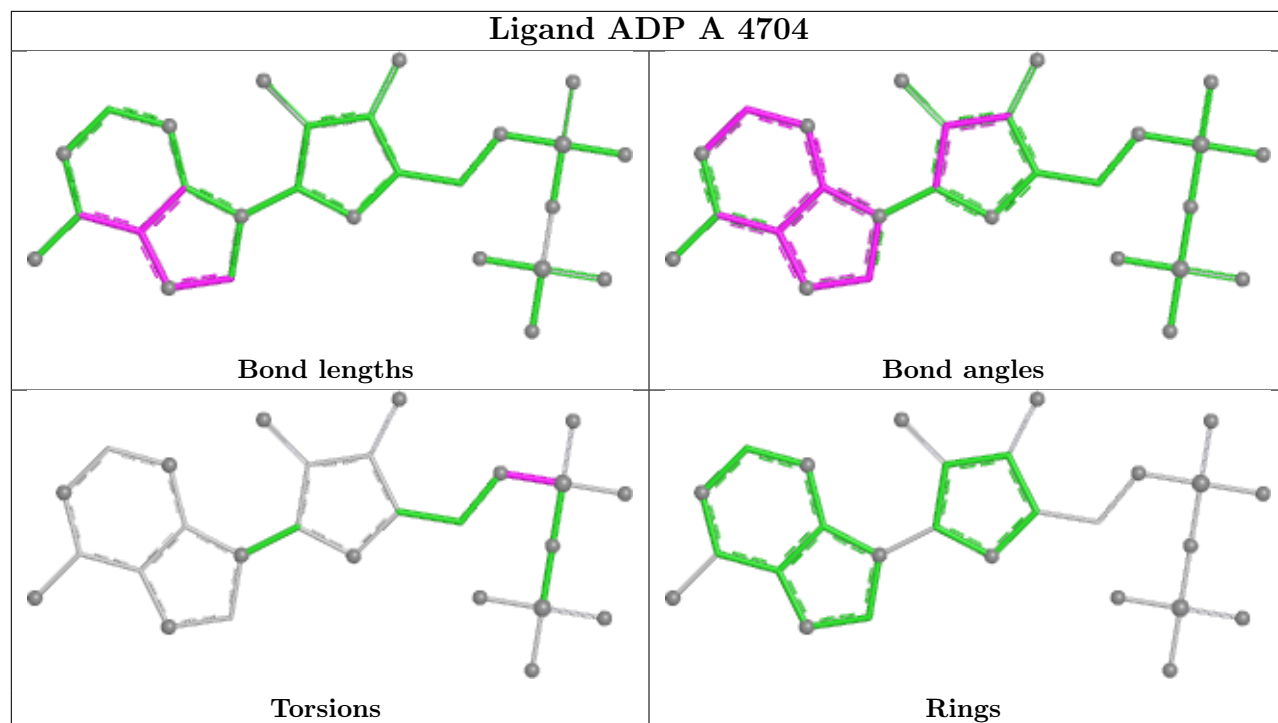
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	5	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

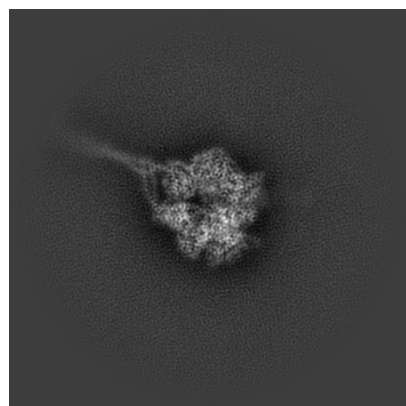
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46857. These allow visual inspection of the internal detail of the map and identification of artifacts.

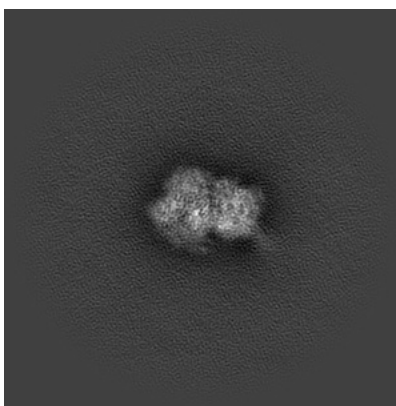
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

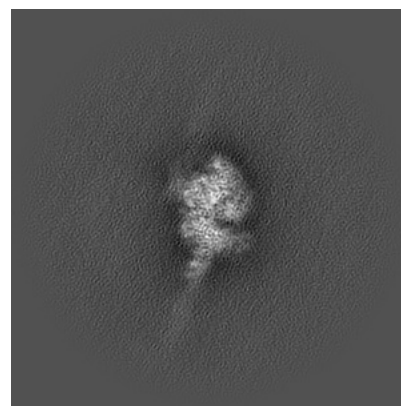
6.1.1 Primary map



X

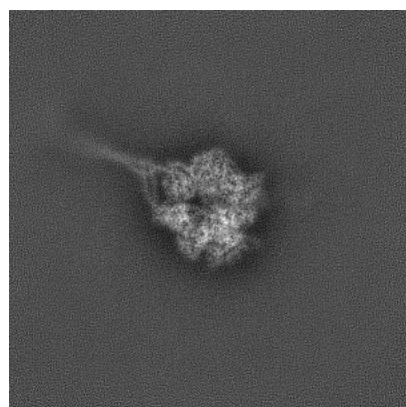


Y

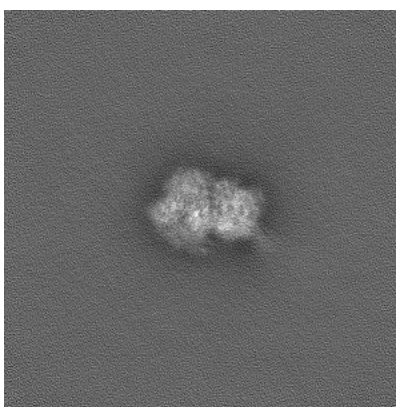


Z

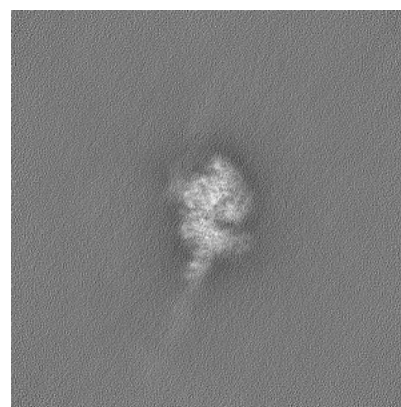
6.1.2 Raw map



X



Y

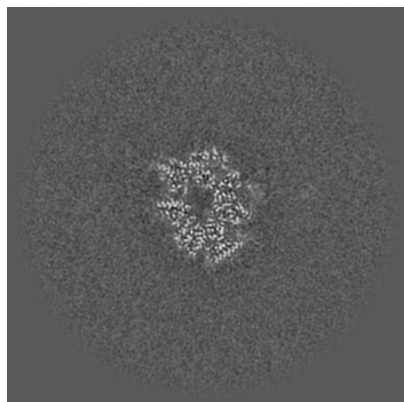


Z

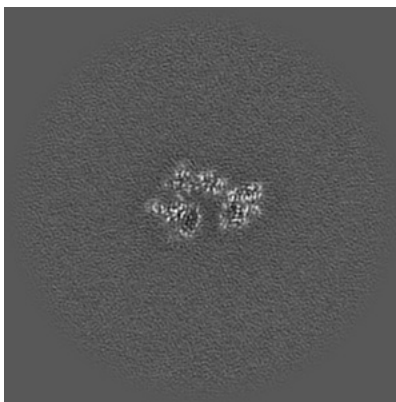
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

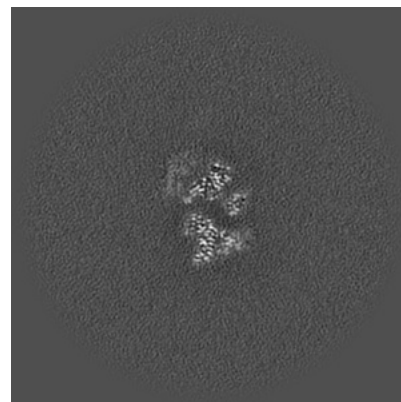
6.2.1 Primary map



X Index: 192

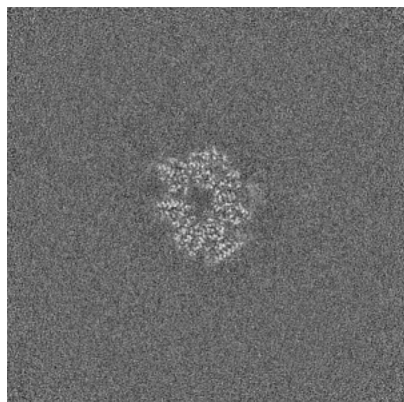


Y Index: 192

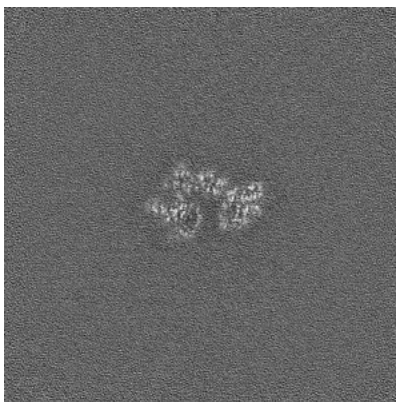


Z Index: 192

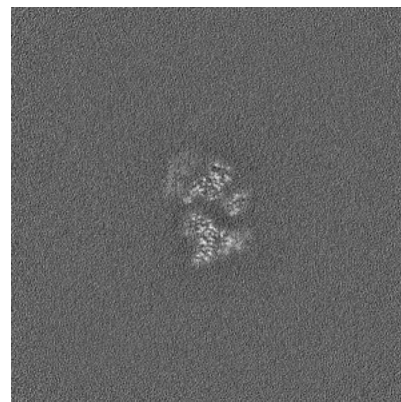
6.2.2 Raw map



X Index: 192



Y Index: 192

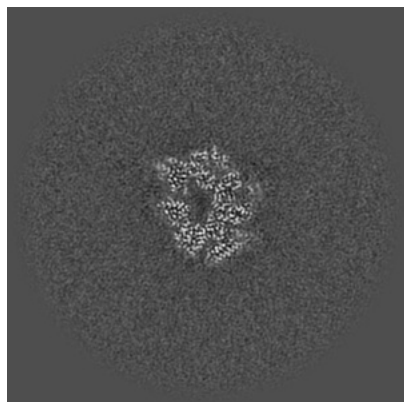


Z Index: 192

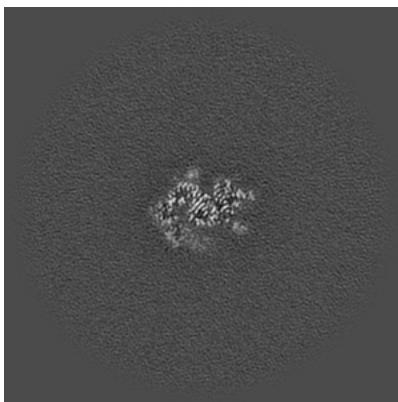
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

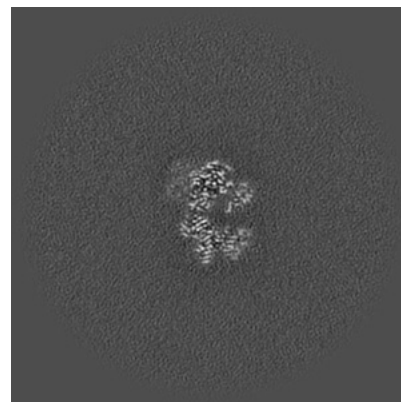
6.3.1 Primary map



X Index: 193

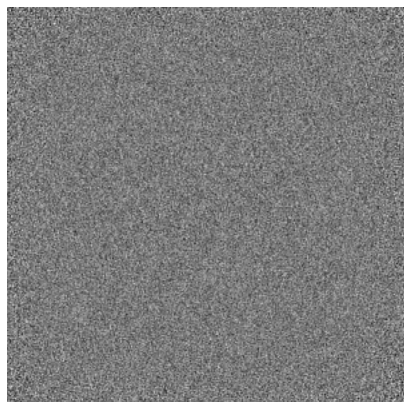


Y Index: 214

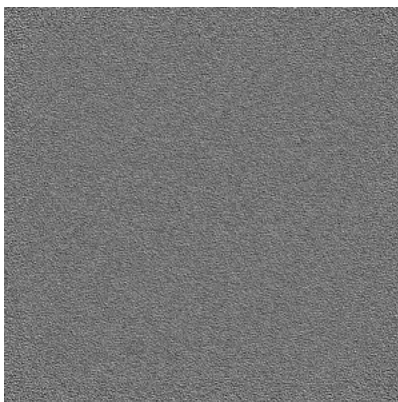


Z Index: 185

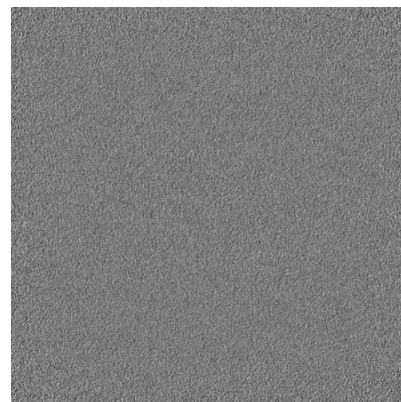
6.3.2 Raw map



X Index: 0



Y Index: 0

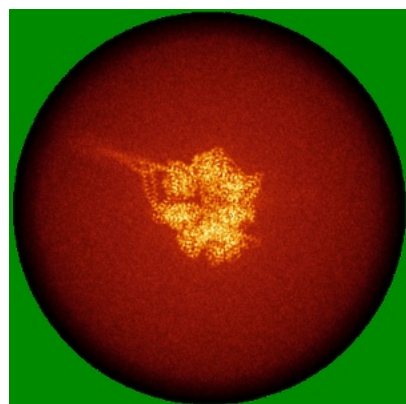


Z Index: 0

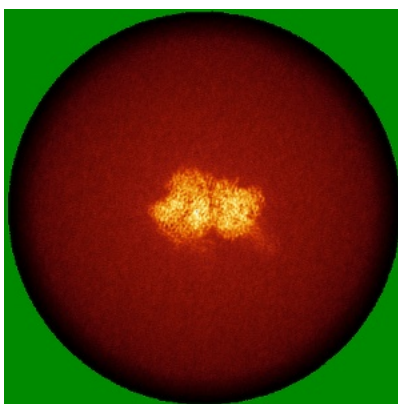
The images above show the largest variance slices of the map in three orthogonal directions.

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

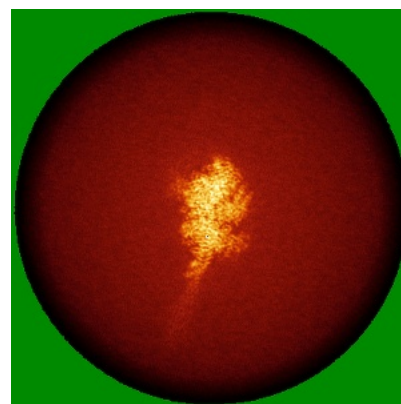
6.4.1 Primary map



X

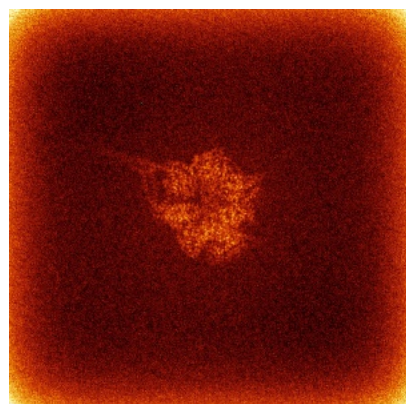


Y

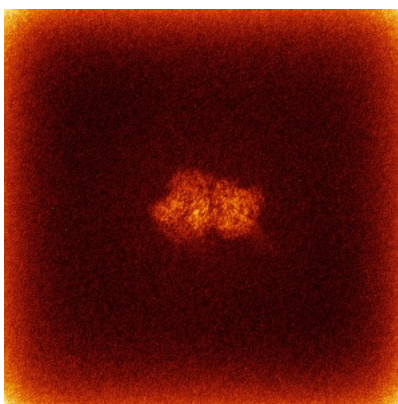


Z

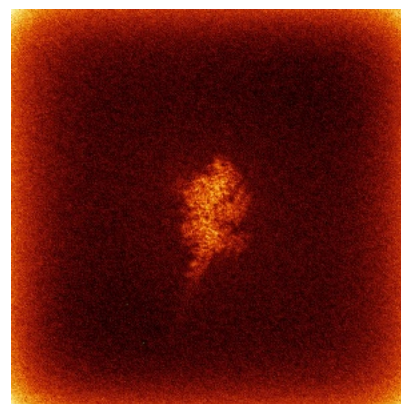
6.4.2 Raw map



X



Y

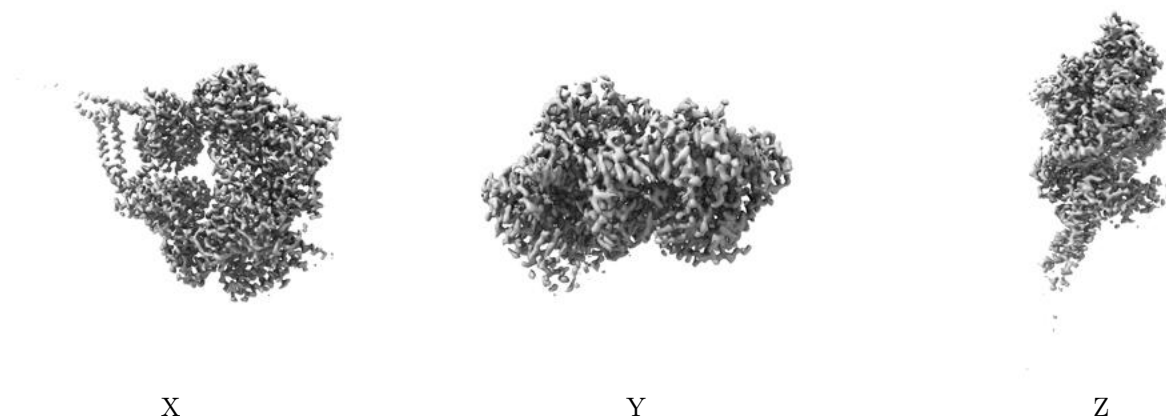


Z

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.

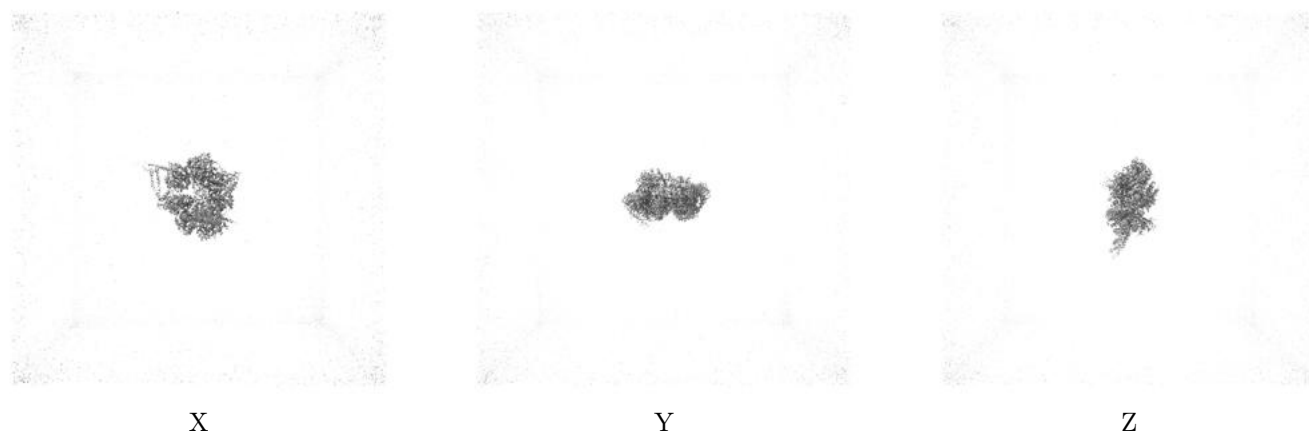
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

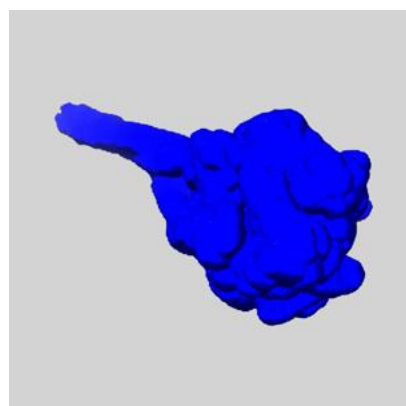
6.6 Mask visualisation [i](#)

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

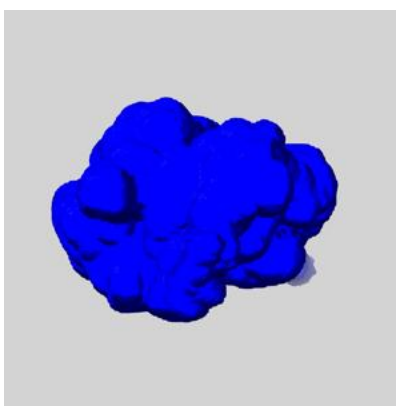
A mask typically either:

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

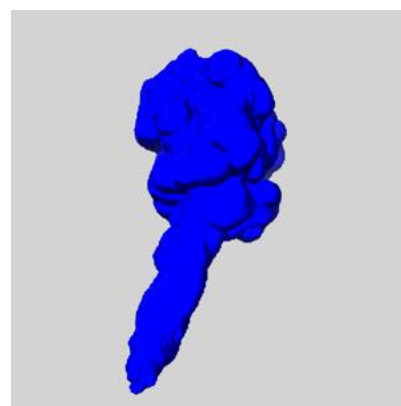
6.6.1 emd_46857_msk_1.map [i](#)



X



Y

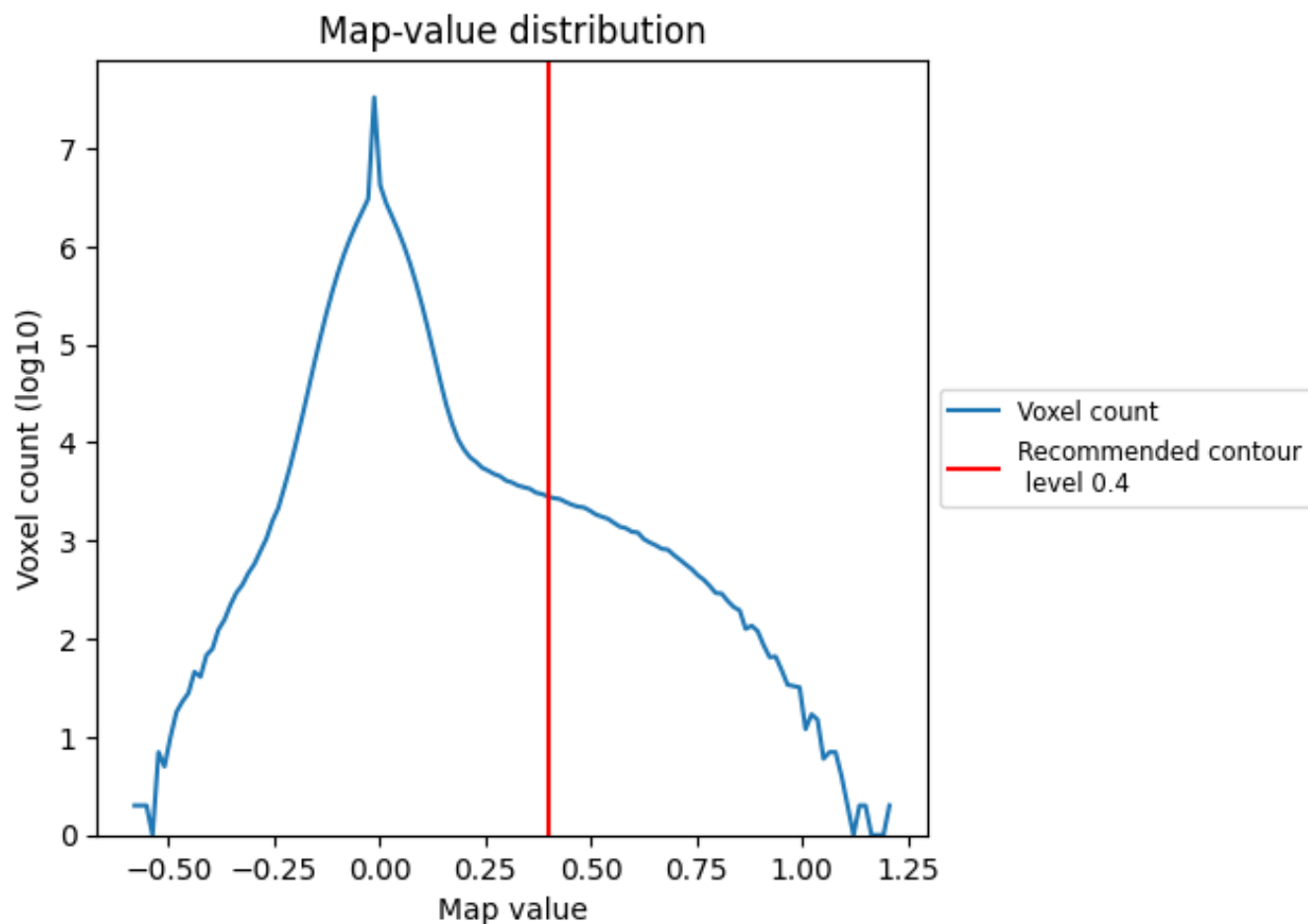


Z

7 Map analysis [i](#)

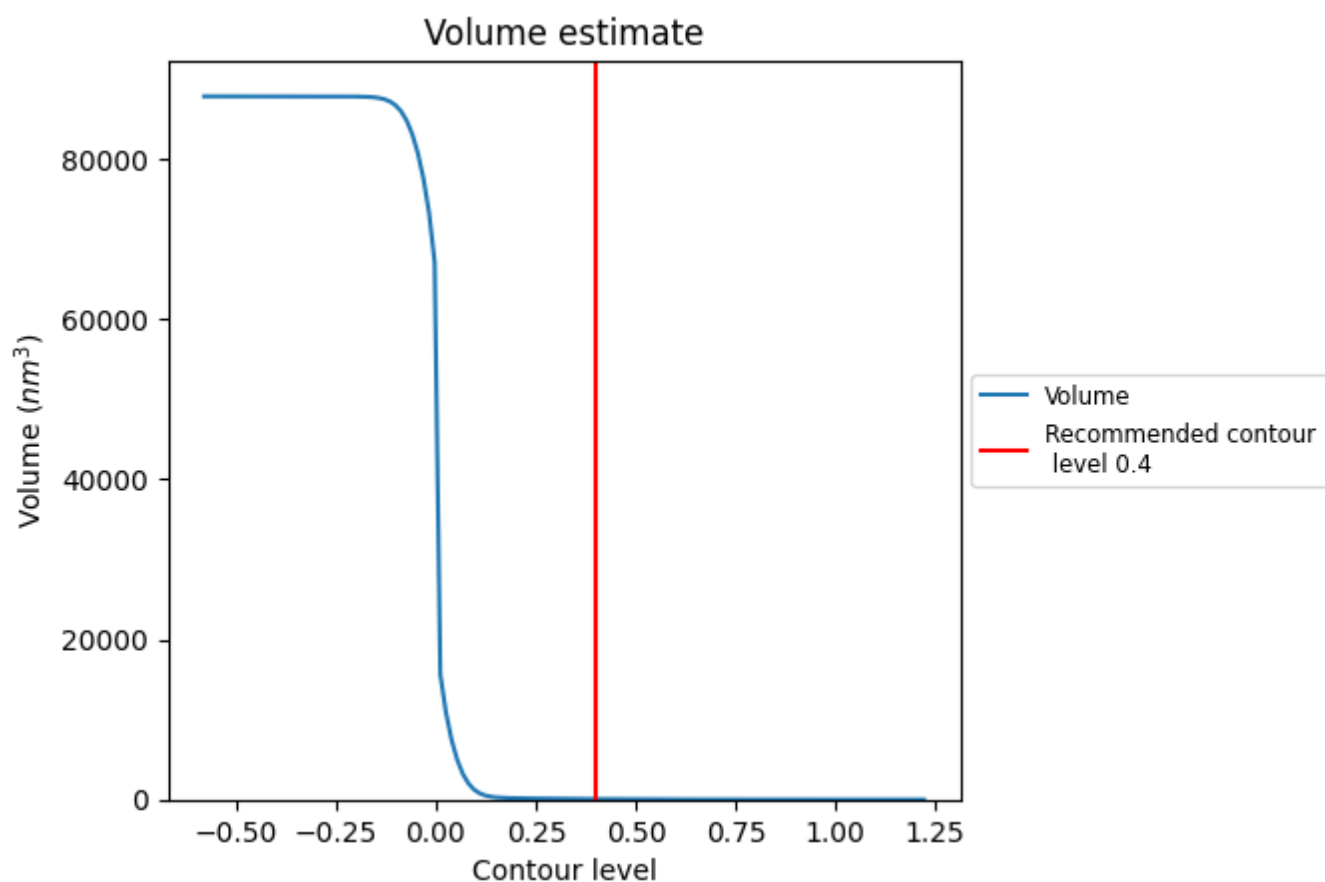
This section contains the results of statistical analysis of the map.

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.

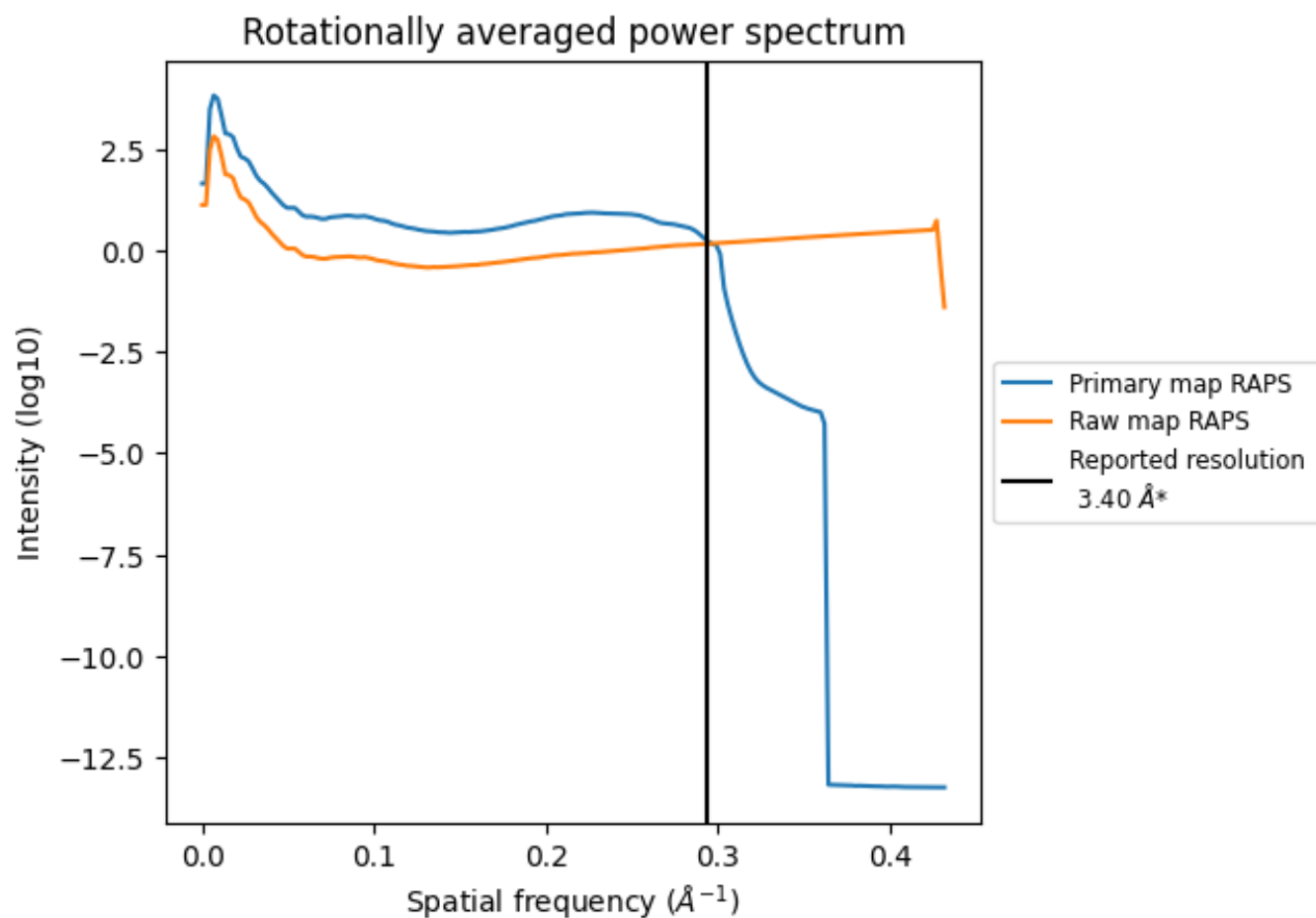
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 ⓘ

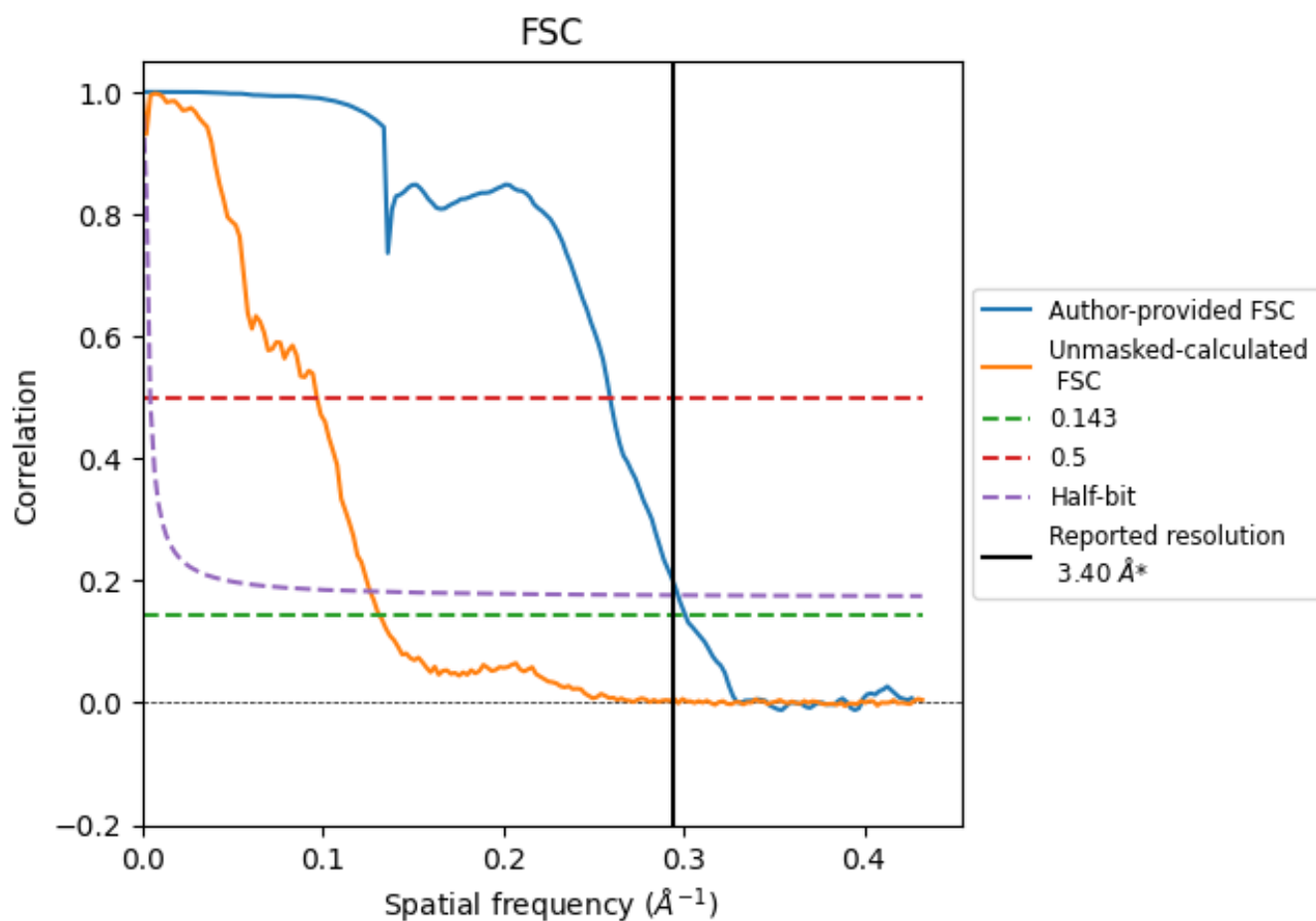


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

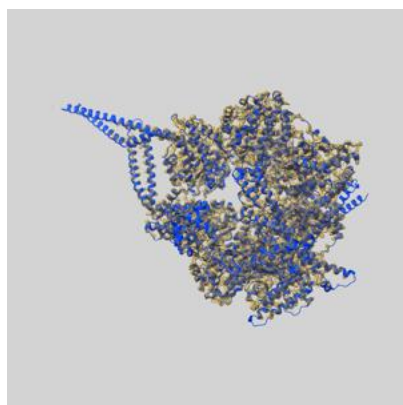
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.32	3.86	3.37
Unmasked-calculated*	7.60	10.33	7.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.60 differs from the reported value 3.4 by more than 10 %

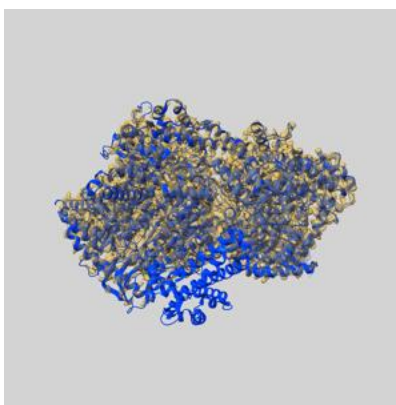
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46857 and PDB model 9DH6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

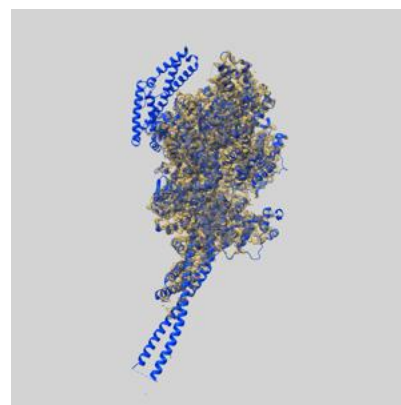
9.1 Map-model overlay [i](#)



X



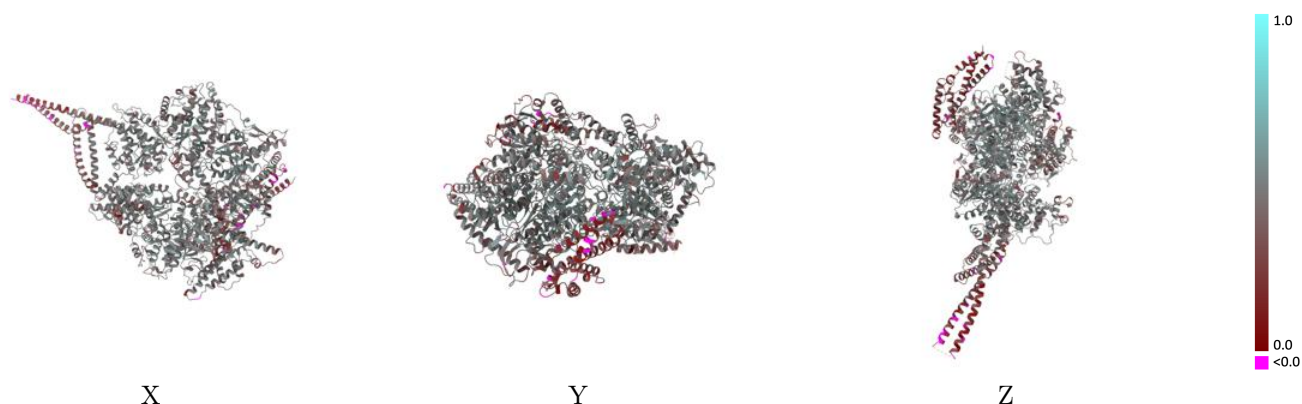
Y



Z

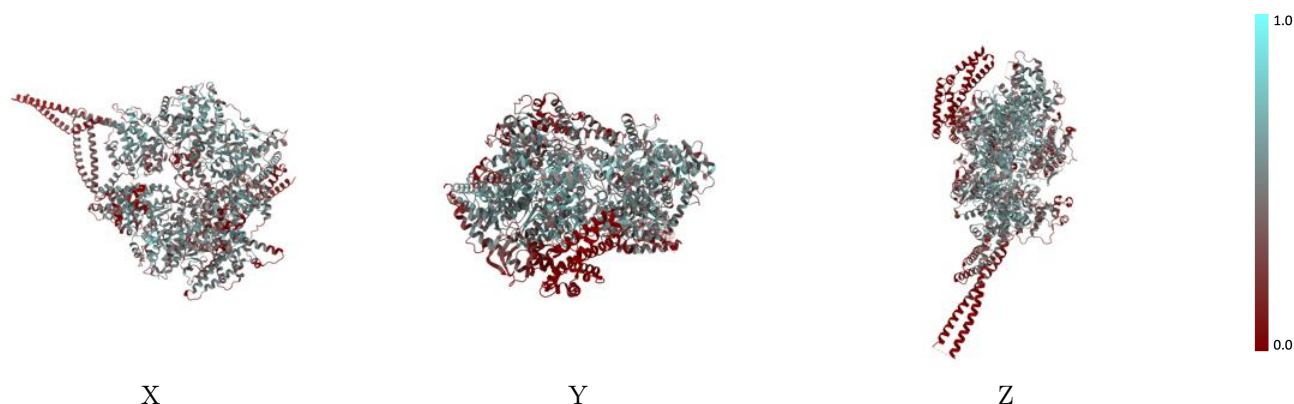
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



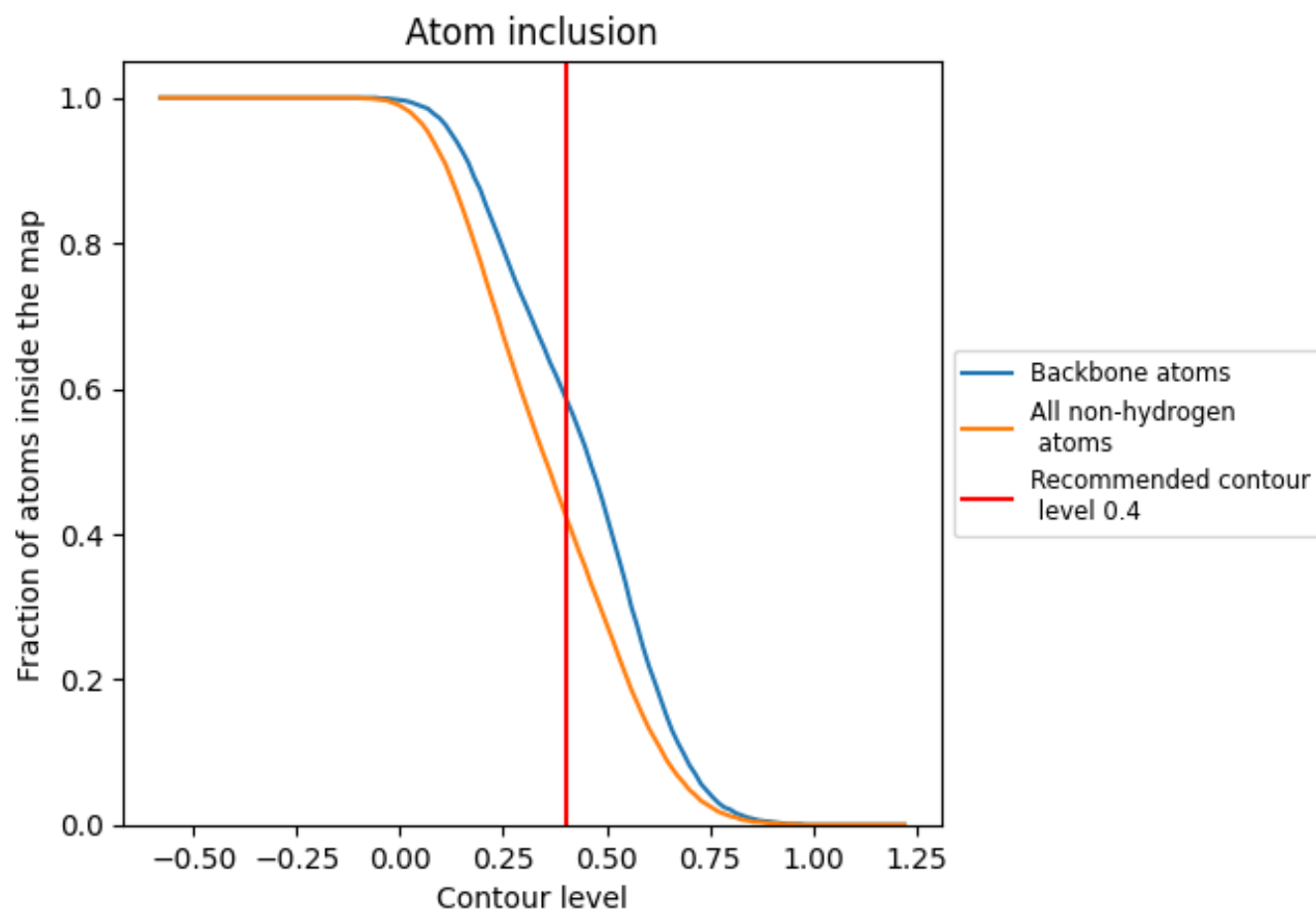
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 59% of all backbone atoms, 43% 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	0.4270	0.4420
A	0.4270	0.4420

