



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 04:35 PM UTC

PDB ID : 9E0K / pdb_00009e0k
EMDB ID : EMD-47360
Title : Cryo-EM structure of human cytoplasmic dynein-1 in the presence of ATP
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-10-18
Resolution : 3.20 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

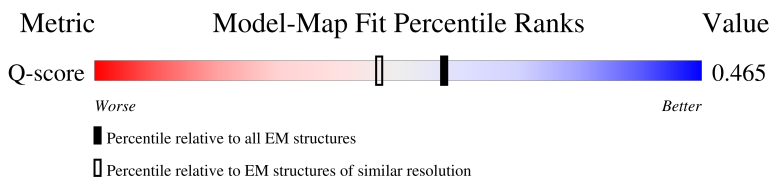
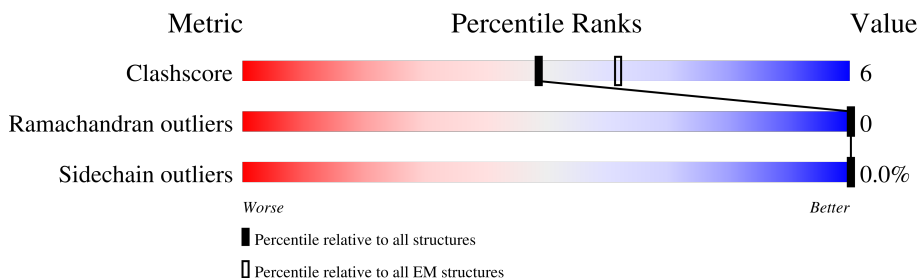
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4843	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22930 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2892	Total	C	N	O	S	0	0
			22816	14568	3944	4193	111		

There are 198 discrepancies between the modelled and reference sequences:

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

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

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

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

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

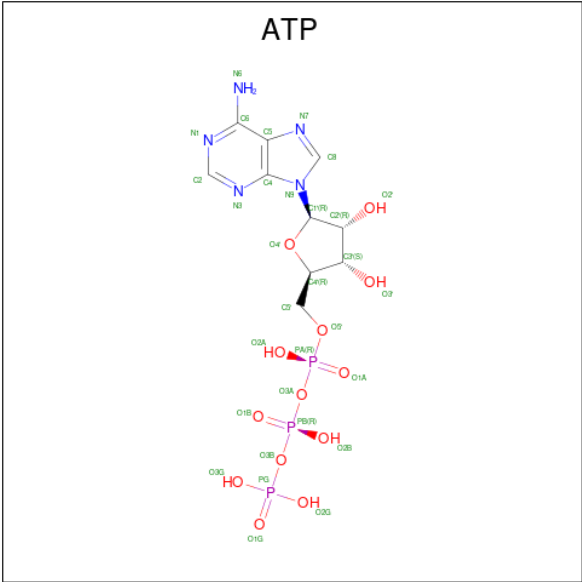
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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q14204
A	1	SER	-	expression tag	UNP Q14204

- # ADP

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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





LYS	ALA	ASN	GLU	VAL	GLN	MET	ILE	ARG	ASP	LEU	GLU	ALA	SER	ILE	ALA	ARG	TYR	LYS	GLU	E3450	E3451	A3452	V3453	L3454	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	L3464	L3465	A3466	A3467	V3468	E3469	A3470	K3471	V3472	N3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	V3489																																																																																					
E3490	K3491	T3492	S3493	E3494	T3495	F3496	K3497	N3498	Q3499	M3500	D3506	A3511	A3512	I3513	A3514	A3515	Y3516	A3517	Y3518	Y3519	M3524	R3525	H3534	R3544	T3545	I3546	I3547	E3551	Y3552	L3553	D3557	E3558	R3559	D3570	N3576	A3577	I3578	R3582	R3585	T3590	T3597	M3601	K3605	K3608	R3611	F3614	L3615	D3616	D3617	A3618	N3622	L3623	E3624	R3628	L3634	E3652	V3653	R3654	R3655	T3656	G3657	G3658	R3659	V3660	D3666	Q3667	D3668	D3669	D3670	L3671	T3681	D3682	D3683	E3687	D3691	N3700	T3704	L3708	L3717	V3724	D3725	E3726	K3727	K3728	S3729	D3730	L3731	L3732	K3733	L3734	Q3735	R3736	E3737	F3738	Q3739	L3740	R3741	L3742	R3743	Q3744	L3745	E3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	L3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	A3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	T3787	D3788	M3791
V3794	E3795	T3796	V3797	S3798	Q3799	C3808	S3809	S3810	I3821	H3822	D3834	I3835	Y3836	N3843	P3844	N3845	L3846	LYS	GLY	V3849	K3861	D3862	F3868	R3869	R3870	R3873	T3882	F3883	I3890	T3895	VAL	G3897	E3898	D3902	Q3906	H3907	R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	L3924	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	V3935	K3945	D3946	L3947	T3948	A3949	Q3952	A3953	L3954	E3955	Q3956	W3960	L3961	P3966	V3974	SER	GLU	T3978	P3979	A3980	D3999	R4000	I4020	M4021	A4022	Q4023	D4026	L4027	E4034	P4040	V4041	L4042	M4043	Y4049																																																			
S4052	E4056	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	I4066	T4067	S4068	I4071	F4077	K4089	R4092	W4093	V4094	M4095	L4096	K4097	W4098	V4099	H4100	L4101	G4104	W4105	L4106	L4124	I4130	G4142	F4147	T4160	R4168	K4171	R4176	A4177	R4178	L4183	H4187	Q4191	D4211	L4212	A4215	C4216	D4217	D4224	D4225	T4226	A4227	K4228	G4229	I4233	D4236	P4239	A4242	A4248	Q4249	S4250	G4253	G4254	R4255	L4269	R4276	S4277	F4278	D4279	C4286	K4287	V4288	D4289	G4290	H4291	P4297	D4298	G4299	I4300	R4301	R4302	E4303	W4308	L4311	D4314	P4318	S4319	M4325	D4336	M4339	M4346	Q4347	M4348	L4349	E4350	ASP	GLU	ASP	ASP	ALA	TYR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	ALA	TRP	MET	ARG	T4379	L4380	H4381	T4382	M4386	W4387	L4388	H4389	L4390	I4391	P4392	Q4393	T4394	L4395	S4396	H4397	L4398	K4399								
R4400	T4401	VAL	E4403	M4404	D4407	P4408	L4409	F4410	R4411	E4414	R4415	E4416	V4417	K4418	A4421	K4422	L4423	L4424	Q4425	D4426	V4427	R4428	Q4429	D4430	D4433	V4434	V4435	D4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443	Q4444	Y4447	L4448	R4449	E4454	K4457	C4458	I4459	S4463	H4466	A4471	C4472	M4473																																																																																																
I4476	Q4477	K4487	M4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	GLY	GLY	ALA	K4502	K4505	K4506	C4510	Q4526	Q4530	A4531	N4532	E4537	E4538	V4543	M4544	V4545	THR	THR	SER	GLN	GLY	ALA	THR	LEU	ASP	ALA	CYS	S4557	G4562	L4563	K4564	N4572	Q4595	THR	ASN	THR	GLU	LYS																																																																																																
E4646	D4617	V4622	T4628	K4629	E4630	D4631	E4646																																																																																																																																									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.519	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/23288	0.34	0/31603

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	22816	0	22641	263	0
2	A	81	0	36	3	0
3	A	2	0	0	0	0
4	A	31	0	12	0	0
All	All	22930	0	22689	263	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 6.

All (263) 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:3808:CYS:HG	1:A:3836:TYR:HH	1.19	0.90
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.66	0.77
1:A:3808:CYS:SG	1:A:3836:TYR:OH	2.42	0.76
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.68	0.75
1:A:3519:TYR:O	1:A:3700:ASN:ND2	2.24	0.68
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.76	0.68
1:A:2079:GLN:HB3	1:A:4411:ARG:HH12	1.60	0.66
1:A:3681:THR:HG22	1:A:3683:ASP:H	1.61	0.66
1:A:2453:ARG:NH2	1:A:2505:ASP:OD2	2.28	0.66
1:A:2291:VAL:HG23	1:A:2292:ARG:HD2	1.78	0.65
1:A:4564:LYS:HD3	1:A:4646:GLU:HB3	1.79	0.64
1:A:3512:ALA:O	1:A:3516:TYR:HB2	1.97	0.64
1:A:2667:ASN:HB2	1:A:2712:CYS:HB2	1.80	0.63
1:A:3115:LEU:HD13	1:A:3143:ILE:HD11	1.80	0.63
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.81	0.62
1:A:2982:ARG:NH1	1:A:2988:GLU:OE2	2.33	0.61
1:A:3745:LEU:HD13	1:A:3776:GLU:HG3	1.82	0.61
1:A:2069:ILE:HD13	1:A:2137:LEU:HD21	1.81	0.61
1:A:3044:LEU:HD12	1:A:3049:GLU:HG3	1.83	0.60
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.83	0.60
1:A:2507:ARG:HH21	1:A:2509:LYS:HD3	1.65	0.60
1:A:2452:LEU:HD23	1:A:2729:ARG:HD2	1.84	0.60
1:A:4227:ALA:HB2	1:A:4233:ILE:HD11	1.83	0.60
1:A:3113:MET:HE1	1:A:3184:ALA:HA	1.83	0.60
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	1.83	0.60
1:A:1961:ASN:HB3	1:A:2018:MET:HE3	1.85	0.59
1:A:2242:GLU:OE1	1:A:2249:GLY:N	2.35	0.59
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.83	0.59
1:A:3206:ARG:O	1:A:3206:ARG:NH1	2.36	0.59
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.85	0.59
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.36	0.58
1:A:3157:ALA:HB1	1:A:3524:MET:HE1	1.84	0.58
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.20	0.58
1:A:2813:LEU:HD21	1:A:2816:LEU:HB2	1.84	0.58
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.84	0.58
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	1.86	0.57
1:A:3821:ILE:HD11	1:A:4346:MET:HE1	1.86	0.57
1:A:1941:MET:HE3	1:A:1963:LEU:HD21	1.86	0.57
1:A:2965:ARG:HG2	1:A:2966:LYS:HG3	1.86	0.57
1:A:1547:LEU:HD13	1:A:1608:LEU:HD22	1.87	0.56
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.38	0.56
1:A:1899:ARG:O	1:A:1979:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2387:LEU:HD12	1:A:2412:MET:HE3	1.87	0.55
1:A:3158:ASN:OD1	1:A:3168:THR:OG1	2.25	0.55
1:A:2213:ILE:HD12	1:A:2362:VAL:HG22	1.89	0.55
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.88	0.55
1:A:2748:TYR:HH	1:A:2800:THR:HG1	1.54	0.55
1:A:2965:ARG:NH2	1:A:3614:PHE:O	2.40	0.55
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.89	0.55
1:A:4437:VAL:HG21	1:A:4448:LEU:HD21	1.89	0.55
1:A:3618:ALA:O	1:A:3622:ASN:ND2	2.40	0.54
1:A:4543:VAL:HG21	1:A:4622:VAL:HG13	1.88	0.54
1:A:4395:LEU:O	1:A:4428:ARG:NH2	2.41	0.54
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.24	0.54
1:A:3590:ILE:HA	1:A:3681:THR:HB	1.89	0.54
1:A:2107:ARG:NH1	1:A:2135:GLU:OE2	2.37	0.54
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.41	0.54
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.90	0.54
1:A:2906:ASP:OD2	1:A:3655:ARG:NH2	2.39	0.54
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.42	0.53
1:A:2798:GLU:OE2	1:A:2836:ARG:NH2	2.41	0.53
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.89	0.53
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.90	0.53
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.41	0.53
1:A:1905:PHE:HE2	1:A:2038:SER:HB3	1.74	0.53
1:A:1965:GLU:HG3	1:A:2026:SER:HB3	1.90	0.53
1:A:2581:LEU:HD21	1:A:2593:LEU:HD21	1.89	0.53
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.91	0.53
1:A:4020:ILE:HD12	1:A:4023:GLN:HG3	1.91	0.53
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.42	0.53
1:A:1474:GLU:HB2	1:A:1586:PRO:HB2	1.91	0.52
1:A:4052:SER:HA	1:A:4095:MET:HE1	1.90	0.52
1:A:4437:VAL:HG12	1:A:4442:LYS:HB3	1.91	0.52
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.42	0.52
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.43	0.52
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.41	0.52
1:A:1636:ASP:O	1:A:1640:ILE:HG12	2.10	0.52
1:A:3474:ARG:HH21	1:A:3767:ILE:HG21	1.75	0.52
1:A:2370:SER:H	1:A:2373:MET:HE2	1.76	0.51
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.92	0.51
1:A:3570:ASP:OD2	1:A:3704:THR:OG1	2.26	0.51
1:A:4066:ILE:HG12	1:A:4093:TRP:HB2	1.92	0.51
1:A:2265:TYR:HE2	1:A:2311:TRP:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.44	0.51
1:A:2307:VAL:HG23	1:A:2345:VAL:HG11	1.92	0.51
1:A:2320:ASP:OD2	1:A:2358:ARG:NH2	2.43	0.51
1:A:1932:CYS:O	1:A:1962:ARG:NH1	2.44	0.50
1:A:2037:ARG:NH2	1:A:4250:SER:OG	2.44	0.50
1:A:2091:ARG:HG3	2:A:4801:ADP:H4'	1.94	0.50
1:A:3218:LEU:HD22	1:A:3471:LYS:HZ3	1.75	0.50
1:A:3870:ARG:HH12	1:A:4034:GLU:HB3	1.76	0.50
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.44	0.50
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.94	0.50
1:A:4437:VAL:HG11	1:A:4448:LEU:HD21	1.94	0.50
1:A:1946:VAL:HG23	1:A:2006:VAL:HG11	1.94	0.50
1:A:3861:LYS:NZ	1:A:3862:ASP:OD1	2.44	0.50
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.94	0.50
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.94	0.49
1:A:1748:GLN:HG3	1:A:1749:LEU:HD22	1.93	0.49
1:A:1839:LEU:O	1:A:1843:ARG:NH2	2.45	0.49
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.93	0.49
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.45	0.49
1:A:3492:THR:HA	1:A:3495:THR:HG22	1.95	0.49
1:A:2665:GLU:HB3	1:A:2668:LEU:HD23	1.95	0.49
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.12	0.49
1:A:3928:THR:HG23	1:A:3931:GLN:H	1.77	0.49
1:A:4444:GLN:HA	1:A:4448:LEU:HD23	1.94	0.49
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	1.95	0.49
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.77	0.49
1:A:1708:GLU:HA	1:A:1711:VAL:HG22	1.94	0.49
1:A:1964:GLU:O	1:A:1967:MET:N	2.45	0.49
1:A:2670:ASP:HA	1:A:2721:LYS:HE2	1.95	0.48
1:A:3738:PHE:HB3	1:A:3783:LYS:HE2	1.95	0.48
1:A:4286:CYS:O	1:A:4319:SER:OG	2.31	0.48
1:A:2375:PHE:HE1	1:A:2455:LEU:HD11	1.79	0.48
1:A:2713:ASN:HB2	1:A:2720:ARG:HE	1.78	0.48
1:A:1687:LYS:HG3	1:A:1715:LYS:HD3	1.94	0.48
1:A:2783:ARG:HD3	1:A:2845:TRP:NE1	2.28	0.48
1:A:3116:GLU:OE1	1:A:3140:ARG:NH2	2.39	0.48
1:A:2103:VAL:HG13	1:A:2136:ILE:HG23	1.96	0.48
1:A:2188:GLU:OE1	1:A:2243:ARG:NH1	2.39	0.48
1:A:2365:SER:HB3	1:A:2368:VAL:HG23	1.96	0.48
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.96	0.48
1:A:3553:LEU:HD13	1:A:3578:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.96	0.47
1:A:3046:SER:OG	1:A:3047:HIS:N	2.43	0.47
1:A:4171:LYS:HD2	1:A:4176:ARG:HH12	1.79	0.47
1:A:1789:LEU:HD21	1:A:2055:TYR:HE2	1.79	0.47
1:A:1948:LEU:HB3	1:A:2012:MET:HE1	1.97	0.47
1:A:2948:ARG:NH1	1:A:3652:GLU:OE1	2.47	0.47
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.97	0.47
1:A:4187:HIS:NE2	1:A:4191:GLN:OE1	2.48	0.47
1:A:3946:ASP:OD1	1:A:3946:ASP:N	2.44	0.47
1:A:3868:PHE:HA	1:A:3883:PHE:HE2	1.80	0.46
1:A:3551:GLU:HA	1:A:3559:ARG:HH12	1.80	0.46
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.97	0.46
1:A:2430:ASN:HB3	1:A:2435:LYS:HE3	1.98	0.46
1:A:2834:GLN:HE21	1:A:2843:ARG:HB3	1.80	0.46
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.98	0.46
1:A:3175:HIS:CD2	1:A:3585:ARG:HH22	2.32	0.46
1:A:1547:LEU:HD23	1:A:1550:ILE:HD11	1.98	0.46
1:A:2369:LEU:HD21	1:A:2374:ILE:HD11	1.97	0.46
1:A:3544:ARG:NH2	1:A:3546:ASP:OD1	2.48	0.46
1:A:2505:ASP:HB3	1:A:2733:VAL:HG13	1.97	0.46
1:A:3511:ALA:HA	1:A:3514:ILE:HG22	1.96	0.46
1:A:3468:VAL:HA	1:A:3471:LYS:HE3	1.98	0.46
1:A:2457:SER:HB2	1:A:2584:TRP:CH2	2.50	0.46
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.45	0.46
1:A:3728:ARG:O	1:A:3732:LEU:HD12	2.16	0.46
1:A:1931:ASN:ND2	1:A:2313:GLU:O	2.43	0.46
1:A:2854:ALA:O	1:A:2858:PHE:HB2	2.15	0.46
1:A:2957:SER:HB2	1:A:2990:ILE:HD13	1.98	0.46
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.98	0.45
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.50	0.45
1:A:1540:VAL:HG11	1:A:1601:LEU:HD22	1.99	0.45
1:A:1625:SER:OG	1:A:1699:ASN:ND2	2.50	0.45
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.99	0.45
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.51	0.45
1:A:1530:ILE:HG22	1:A:1592:LEU:HD13	1.98	0.45
1:A:2438:GLU:OE2	1:A:2442:GLN:NE2	2.49	0.45
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.48	0.45
1:A:3196:GLU:OE2	1:A:3200:HIS:NE2	2.50	0.45
1:A:4059:ALA:HB2	1:A:4066:ILE:HD12	1.99	0.45
1:A:3043:MET:N	1:A:3043:MET:SD	2.90	0.45
1:A:4398:LEU:HD23	1:A:4421:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:ASP:N	1:A:1491:ASP:OD1	2.50	0.45
1:A:2669:PRO:O	1:A:2677:GLN:NE2	2.48	0.44
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.82	0.44
1:A:1941:MET:HA	1:A:1944:ILE:HG12	2.00	0.44
1:A:1646:ASN:HD22	1:A:1649:LYS:HD2	1.82	0.44
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.83	0.44
1:A:2589:LYS:HG2	1:A:2590:PRO:HD2	1.99	0.44
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.42	0.44
1:A:1680:GLU:HG3	1:A:1875:VAL:HG21	1.99	0.44
1:A:1799:GLU:HG3	1:A:2112:LYS:HE3	1.99	0.44
1:A:2275:TRP:CG	1:A:2329:ASN:HD21	2.35	0.44
1:A:2295:LEU:HD23	1:A:2295:LEU:HA	1.87	0.44
1:A:2138:ILE:HD11	1:A:2165:PHE:CD1	2.53	0.44
1:A:2415:ILE:HD11	1:A:2473:ASN:HD22	1.83	0.44
1:A:4379:THR:O	1:A:4382:THR:OG1	2.36	0.44
1:A:2933:LEU:HB2	1:A:3065:VAL:HG22	2.00	0.44
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.51	0.44
1:A:2831:ARG:HD3	1:A:2831:ARG:HA	1.78	0.43
1:A:2505:ASP:OD1	1:A:2505:ASP:N	2.52	0.43
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	1.99	0.43
1:A:2413:LEU:HD12	1:A:2413:LEU:HA	1.89	0.43
1:A:3822:HIS:HE1	1:A:4130:ILE:HG21	1.83	0.43
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	2.01	0.43
1:A:3717:LEU:HD11	1:A:3797:VAL:HG21	2.01	0.43
1:A:3774:LYS:HD3	1:A:3774:LYS:HA	1.81	0.43
1:A:1806:ARG:HH12	1:A:1875:VAL:HG21	1.83	0.43
1:A:3776:GLU:O	1:A:3779:GLU:HG3	2.19	0.43
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.01	0.43
1:A:1621:ARG:O	1:A:1624:SER:OG	2.37	0.43
1:A:1974:GLN:O	1:A:1978:ILE:HG12	2.19	0.43
1:A:3189:GLU:OE2	1:A:3582:ARG:NH2	2.50	0.43
1:A:3873:ARG:HA	1:A:3873:ARG:HD3	1.82	0.43
1:A:2889:LEU:HD11	1:A:2920:LEU:HD21	2.00	0.43
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.88	0.42
1:A:3747:LYS:HD2	1:A:3747:LYS:HA	1.81	0.42
1:A:1805:ARG:NH1	1:A:2105:ARG:HD3	2.34	0.42
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	2.01	0.42
1:A:3557:ASP:OD1	1:A:3743:ARG:NH2	2.42	0.42
1:A:1671:SER:HB2	1:A:1693:THR:HB	2.00	0.42
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.00	0.42
1:A:2478:ASP:OD1	1:A:2478:ASP:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2837:LEU:HD11	1:A:2846:THR:HG21	2.02	0.42
1:A:1483:LYS:HB2	1:A:1483:LYS:HE2	1.94	0.42
1:A:4068:SER:HB3	1:A:4097:LYS:HE2	2.02	0.42
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.54	0.42
1:A:2241:LEU:HD23	1:A:2241:LEU:HA	1.90	0.42
1:A:4392:PRO:HA	1:A:4395:LEU:HD13	2.02	0.42
1:A:1775:ALA:O	1:A:1779:HIS:ND1	2.42	0.42
1:A:2138:ILE:HD13	1:A:2138:ILE:HA	1.92	0.41
1:A:2527:PRO:HD3	1:A:2545:TRP:CG	2.55	0.41
1:A:3723:ASP:N	1:A:3723:ASP:OD1	2.52	0.41
1:A:3777:ALA:HA	1:A:3780:VAL:HG12	2.01	0.41
1:A:1982:LEU:HD21	1:A:2012:MET:HB3	2.02	0.41
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	2.02	0.41
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	2.02	0.41
1:A:2580:LEU:HD11	1:A:2584:TRP:CZ2	2.56	0.41
1:A:2810:LEU:HD21	1:A:2816:LEU:HD22	2.02	0.41
1:A:2832:LEU:HD23	1:A:2832:LEU:HA	1.91	0.41
1:A:4027:LEU:HD11	1:A:4043:MET:HE2	2.01	0.41
1:A:4288:VAL:HG12	1:A:4290:GLY:H	1.84	0.41
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	2.01	0.41
1:A:1691:SER:HB2	1:A:1693:THR:HG22	2.02	0.41
1:A:1962:ARG:H	1:A:1962:ARG:HG2	1.74	0.41
1:A:2778:THR:O	1:A:2782:GLU:HG2	2.20	0.41
1:A:2840:ASP:OD1	1:A:2840:ASP:N	2.54	0.41
1:A:4099:VAL:HG12	1:A:4106:LEU:HD11	2.02	0.41
1:A:2028:LEU:HB3	1:A:2033:LYS:HG3	2.02	0.41
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	2.02	0.41
1:A:4049:TYR:CE2	1:A:4147:PHE:HB3	2.56	0.41
1:A:2703:LEU:HD22	1:A:2706:ILE:HG13	2.01	0.41
1:A:1927:VAL:HG12	1:A:1954:TRP:HB2	2.02	0.41
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.02	0.41
1:A:2094:LYS:HD2	2:A:4801:ADP:H1'	2.03	0.41
1:A:2060:ARG:HH12	1:A:2130:ASN:HA	1.86	0.41
1:A:2076:CYS:HA	1:A:2080:LEU:HD23	2.03	0.41
1:A:2184:LYS:HD2	1:A:2243:ARG:HH21	1.86	0.41
1:A:2781:GLN:HG3	1:A:2794:TYR:HB2	2.03	0.41
1:A:3794:VAL:HA	1:A:3797:VAL:HG12	2.03	0.41
1:A:4408:PRO:HG3	1:A:4526:GLN:HG2	2.03	0.41
1:A:1687:LYS:NZ	1:A:1719:GLU:OE2	2.50	0.41
1:A:1933:ASP:CG	1:A:2314:ASN:HD21	2.28	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3201:LEU:HD21	1:A:3492:THR:OG1	2.21	0.41
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.56	0.40
1:A:1720:SER:O	1:A:1724:VAL:HG23	2.21	0.40
1:A:1968:LEU:HD21	1:A:2028:LEU:HD22	2.03	0.40
1:A:2600:GLY:HA2	2:A:4805:ADP:H5'2	2.03	0.40
1:A:2948:ARG:HG2	1:A:2958:VAL:HG11	2.03	0.40
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.85	0.40
1:A:1537:TRP:HA	1:A:1540:VAL:HG12	2.04	0.40
1:A:2576:ARG:HE	1:A:2576:ARG:HB2	1.71	0.40
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.85	0.40
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.54	0.40
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.40
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.83	0.40
1:A:2759:ILE:HD13	1:A:2810:LEU:HD22	2.02	0.40
1:A:3978:THR:HA	1:A:3979:PRO:HD3	1.97	0.40
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.56	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	2864/4843 (59%)	2760 (96%)	104 (4%)	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	2459/4279 (58%)	2458 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2578	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1482	ASN
1	A	1595	GLN
1	A	1646	ASN
1	A	1748	GLN
1	A	1790	ASN
1	A	1855	GLN
1	A	1876	GLN
1	A	2346	GLN
1	A	2414	GLN
1	A	2464	GLN
1	A	2621	ASN
1	A	3014	ASN
1	A	3459	GLN
1	A	3535	HIS
1	A	3563	GLN
1	A	3751	GLN
1	A	3830	GLN
1	A	3843	ASN
1	A	4012	ASN
1	A	4232	ASN
1	A	4262	GLN
1	A	4266	ASN
1	A	4508	HIS

5.3.3 RNA ⓘ

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
2	ADP	A	4806	-	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
2	ADP	A	4805	-	28,29,29	1.38	4 (14%)	43,45,45	1.89	8 (18%)
2	ADP	A	4801	3	28,29,29	1.38	4 (14%)	43,45,45	1.85	8 (18%)
4	ATP	A	4803	3	32,33,33	0.48	0	48,52,52	0.37	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	4806	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4805	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4801	3	-	3/16/32/32	0/3/3/3
4	ATP	A	4803	3	-	1/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4805	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	4806	ADP	C5-C4	4.57	1.47	1.39
2	A	4801	ADP	C5-C4	4.56	1.47	1.39
2	A	4806	ADP	C5-C6	2.61	1.48	1.41
2	A	4805	ADP	C5-C6	2.58	1.48	1.41
2	A	4801	ADP	C5-C6	2.54	1.48	1.41
2	A	4801	ADP	C5-N7	-2.49	1.34	1.39
2	A	4805	ADP	C5-N7	-2.48	1.34	1.39
2	A	4806	ADP	C5-N7	-2.41	1.34	1.39
2	A	4806	ADP	C8-N7	2.27	1.36	1.31
2	A	4801	ADP	C8-N7	2.20	1.35	1.31
2	A	4805	ADP	C8-N7	2.16	1.35	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4805	ADP	C5-C4-N3	-6.24	118.12	126.72
2	A	4801	ADP	C5-C4-N3	-5.84	118.68	126.72
2	A	4806	ADP	C5-C4-N3	-5.82	118.70	126.72
2	A	4805	ADP	N3-C4-N9	5.06	135.77	127.17
2	A	4801	ADP	N3-C4-N9	4.70	135.16	127.17
2	A	4806	ADP	N3-C4-N9	4.62	135.02	127.17
2	A	4805	ADP	C2-N3-C4	3.85	121.23	111.83
2	A	4806	ADP	C2-N3-C4	3.68	120.83	111.83
2	A	4801	ADP	C2-N3-C4	3.68	120.81	111.83
2	A	4806	ADP	C4-C5-N7	-3.41	106.68	110.58
2	A	4805	ADP	N3-C2-N1	-3.33	123.54	128.58
2	A	4801	ADP	C4-C5-N7	-3.27	106.84	110.58
2	A	4801	ADP	N3-C2-N1	-3.26	123.65	128.58
2	A	4806	ADP	N3-C2-N1	-3.22	123.71	128.58
2	A	4805	ADP	C4-C5-N7	-3.22	106.90	110.58
2	A	4806	ADP	C4-N9-C8	2.63	108.50	105.74
2	A	4801	ADP	C4-N9-C8	2.55	108.42	105.74
2	A	4806	ADP	C3'-C2'-C1'	2.50	106.19	101.46
2	A	4805	ADP	C3'-C2'-C1'	2.49	106.17	101.46
2	A	4806	ADP	C5-N7-C8	2.45	107.31	103.45
2	A	4805	ADP	C5-N7-C8	2.43	107.27	103.45
2	A	4801	ADP	C5-N7-C8	2.41	107.23	103.45
2	A	4805	ADP	C4-N9-C8	2.39	108.25	105.74
2	A	4801	ADP	C3'-C2'-C1'	2.33	105.88	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

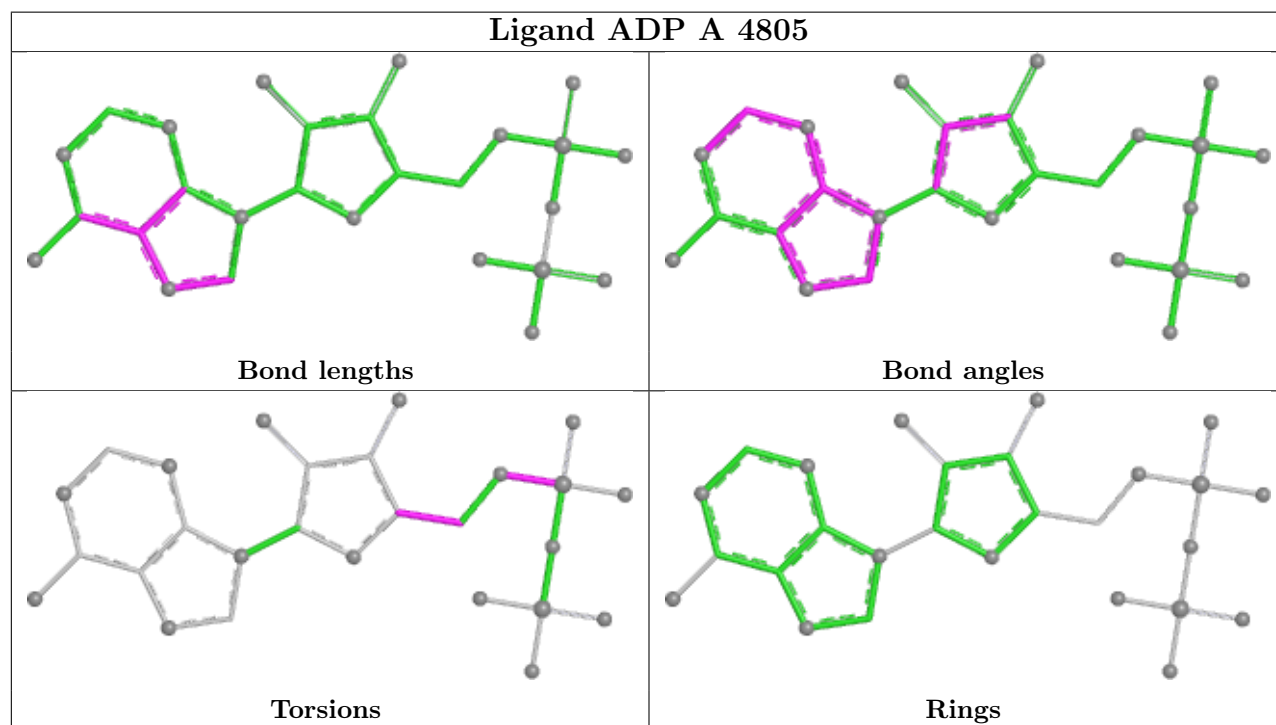
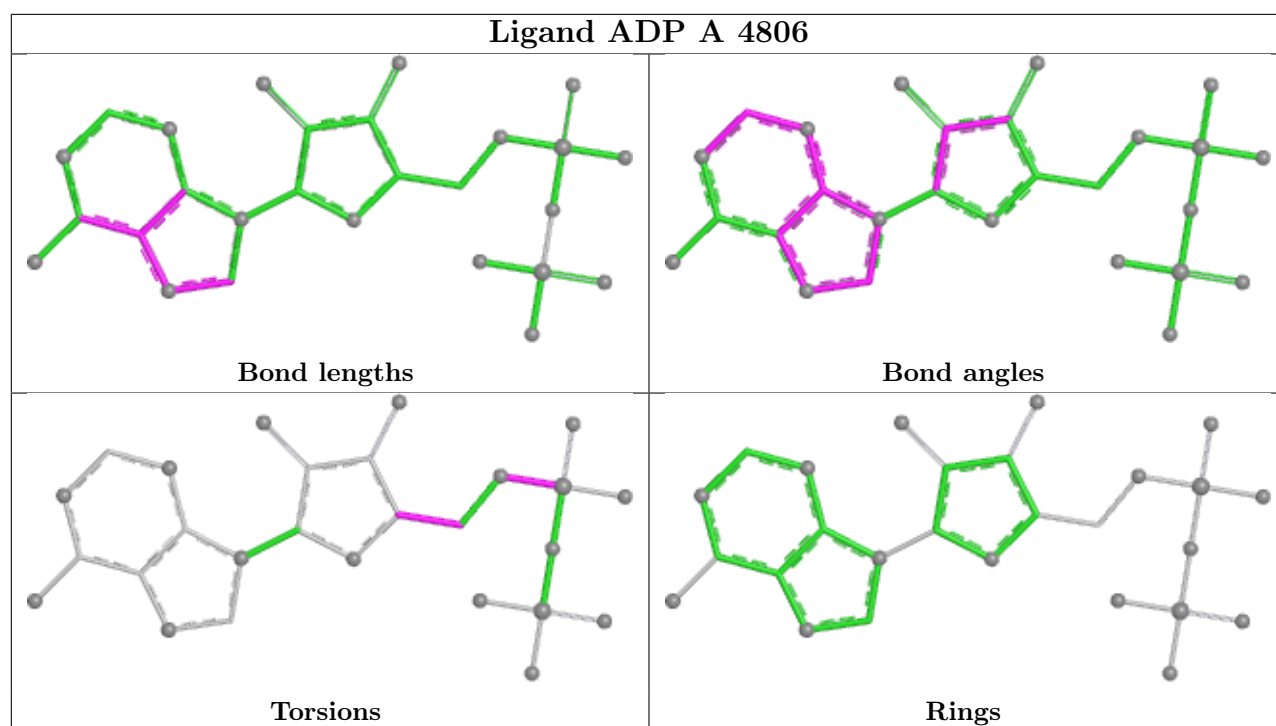
Mol	Chain	Res	Type	Atoms
2	A	4801	ADP	C5'-O5'-PA-O2A
2	A	4801	ADP	C5'-O5'-PA-O3A
2	A	4805	ADP	C5'-O5'-PA-O2A
2	A	4805	ADP	C5'-O5'-PA-O3A
2	A	4806	ADP	C5'-O5'-PA-O1A
2	A	4806	ADP	C5'-O5'-PA-O2A
2	A	4806	ADP	C5'-O5'-PA-O3A
2	A	4805	ADP	C3'-C4'-C5'-O5'
2	A	4805	ADP	O4'-C4'-C5'-O5'
2	A	4801	ADP	O4'-C4'-C5'-O5'
2	A	4806	ADP	C3'-C4'-C5'-O5'
4	A	4803	ATP	PB-O3A-PA-O2A

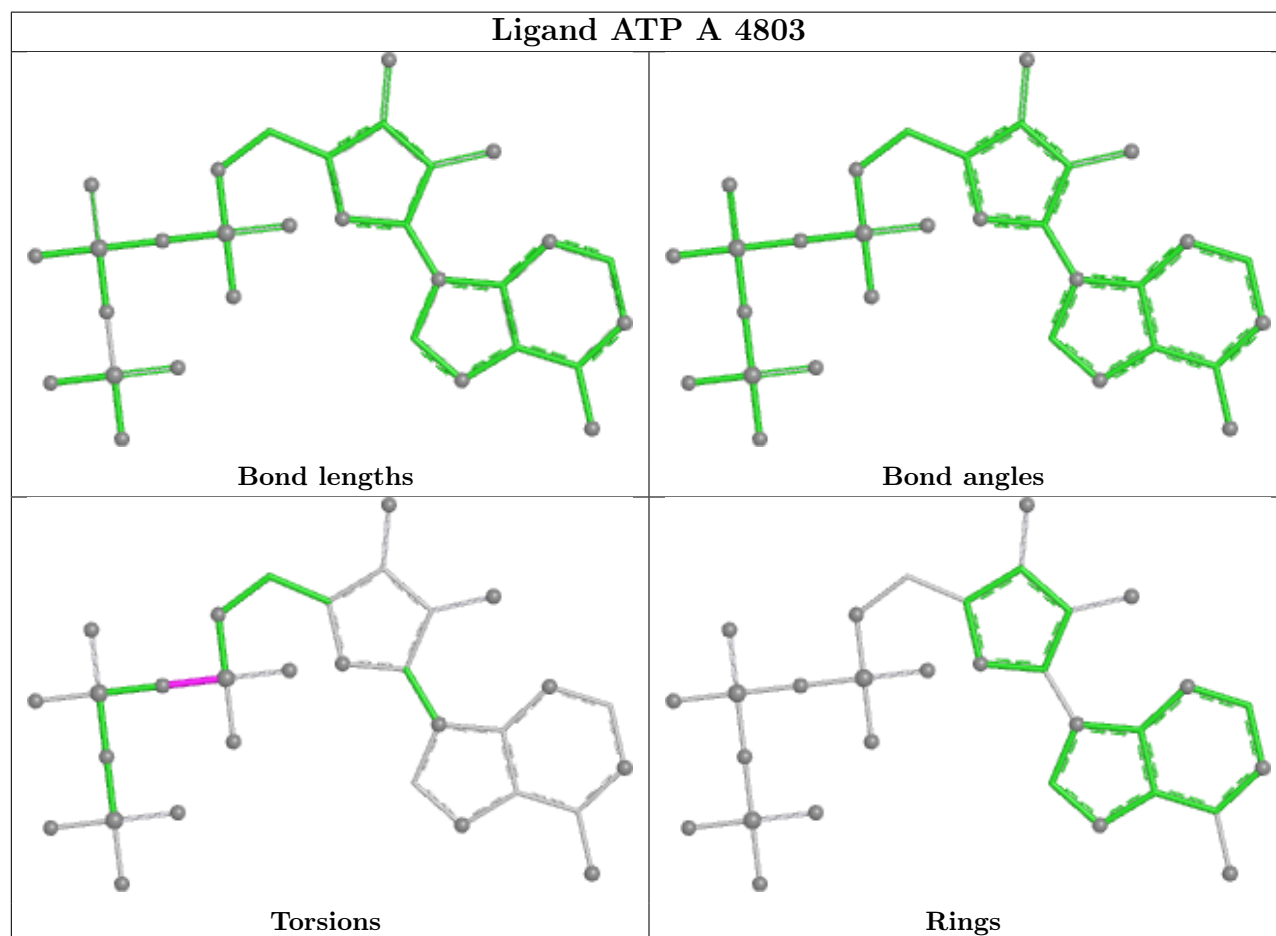
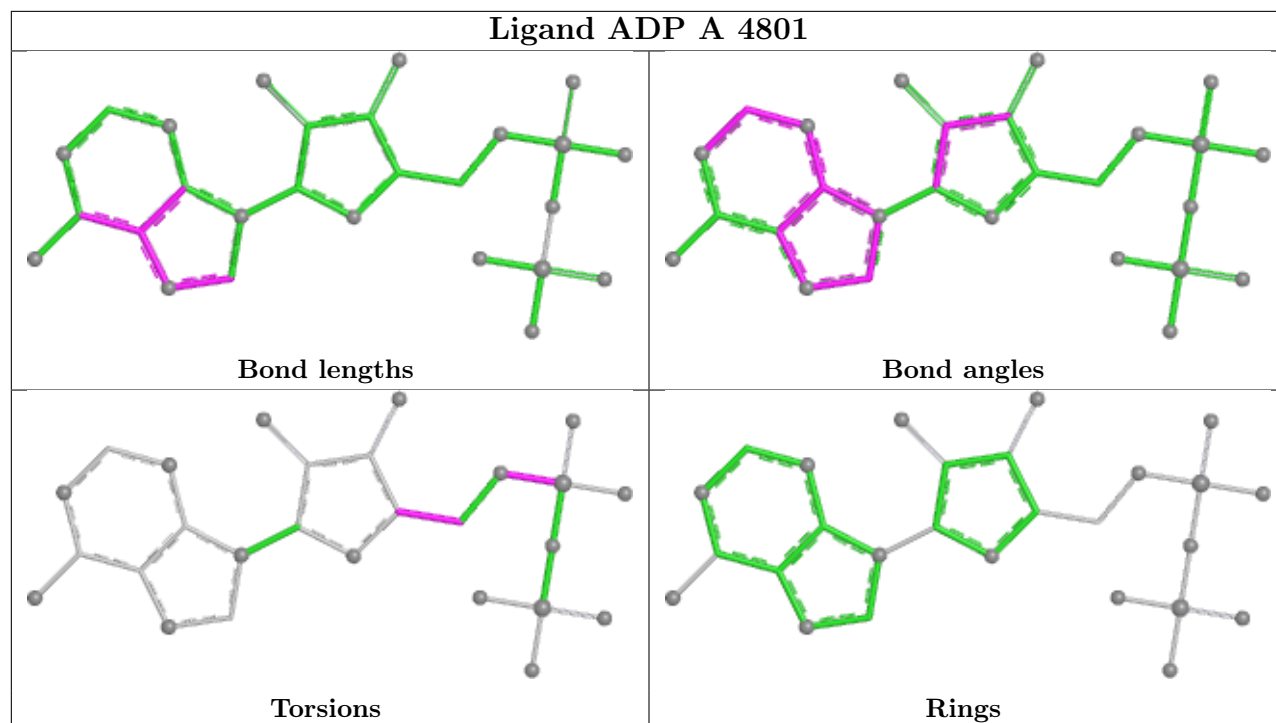
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4805	ADP	1	0
2	A	4801	ADP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

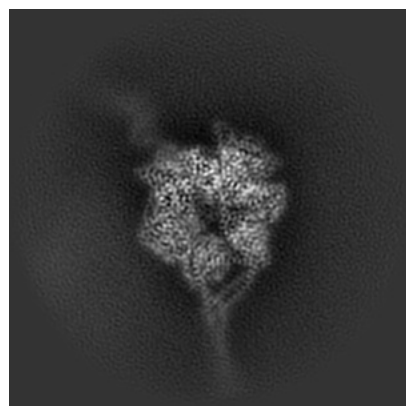
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47360. These allow visual inspection of the internal detail of the map and identification of artifacts.

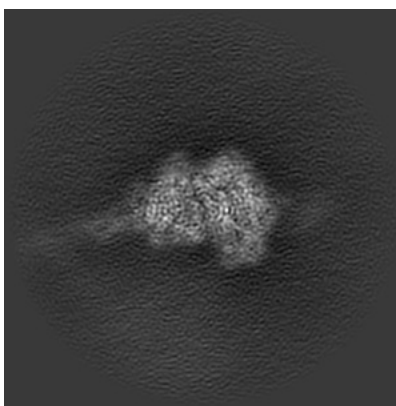
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

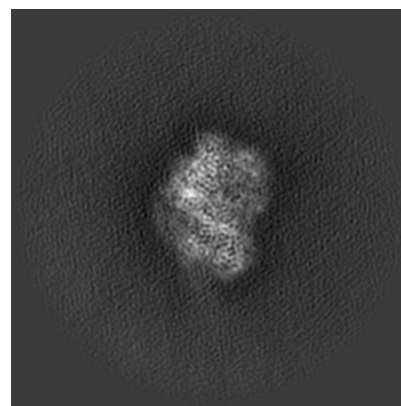
6.1.1 Primary map



X

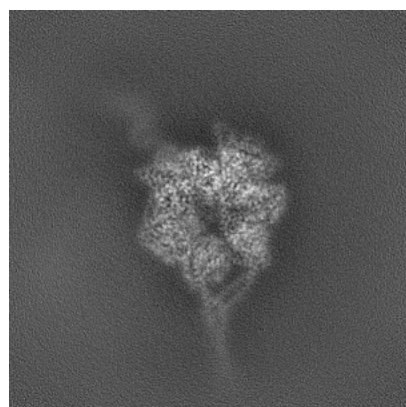


Y

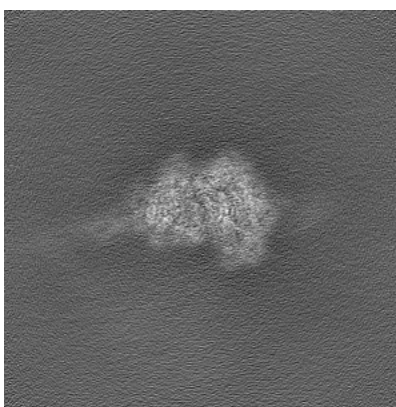


Z

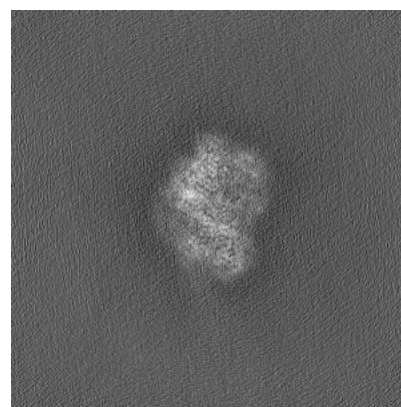
6.1.2 Raw map



X



Y

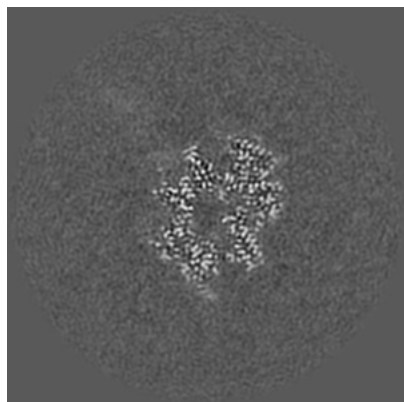


Z

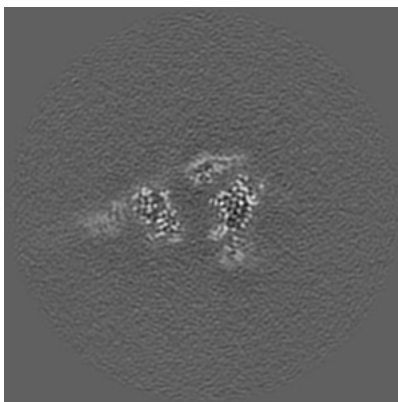
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

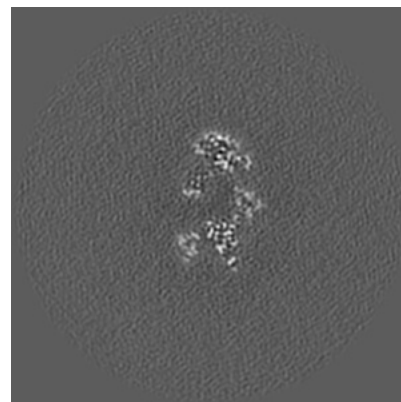
6.2.1 Primary map



X Index: 176

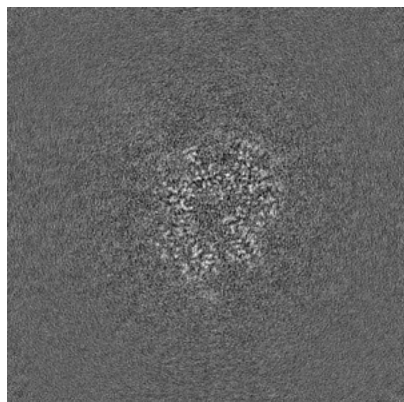


Y Index: 176

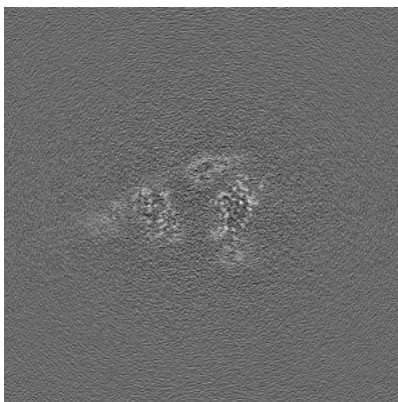


Z Index: 176

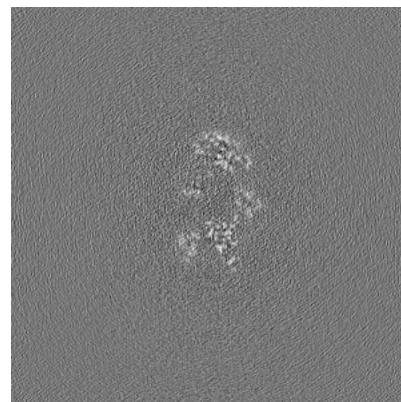
6.2.2 Raw map



X Index: 176



Y Index: 176

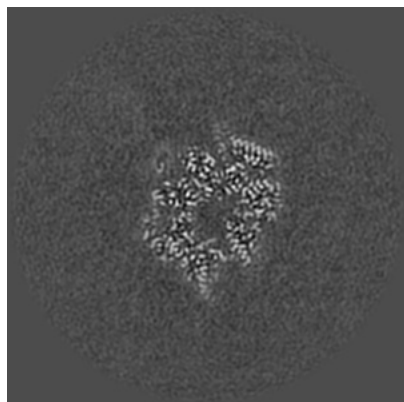


Z Index: 176

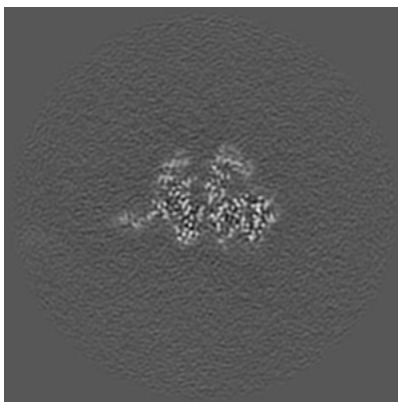
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

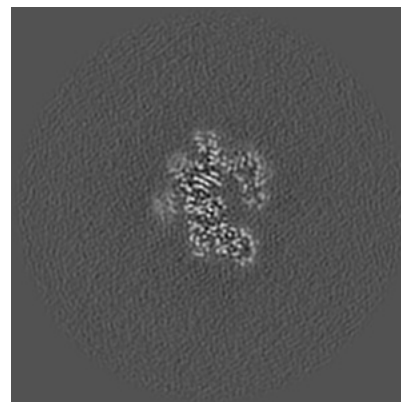
6.3.1 Primary map



X Index: 179

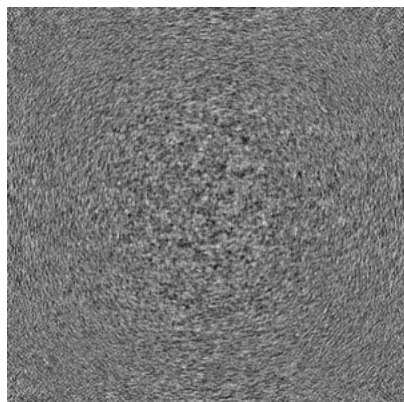


Y Index: 206

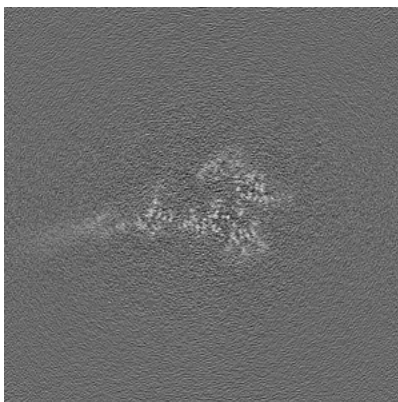


Z Index: 194

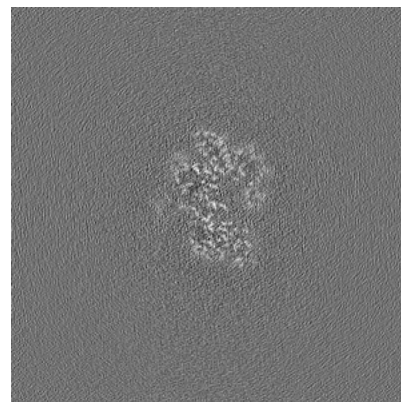
6.3.2 Raw map



X Index: 0



Y Index: 188

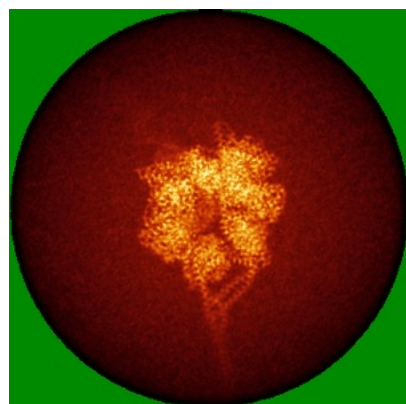


Z Index: 191

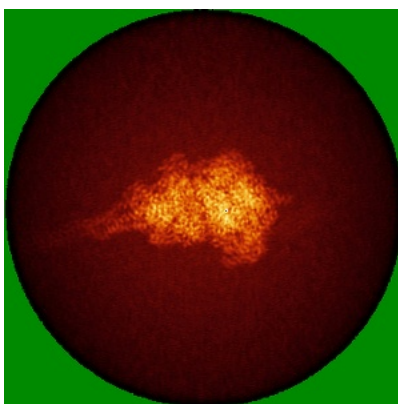
The images above show the largest variance slices of the map in three orthogonal directions.

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

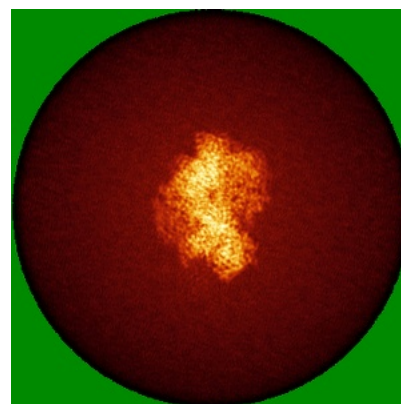
6.4.1 Primary map



X

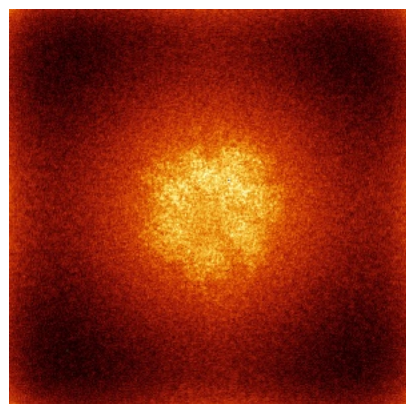


Y

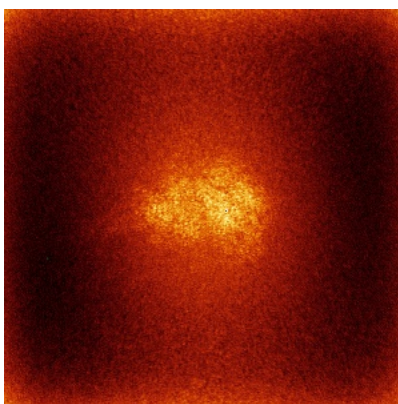


Z

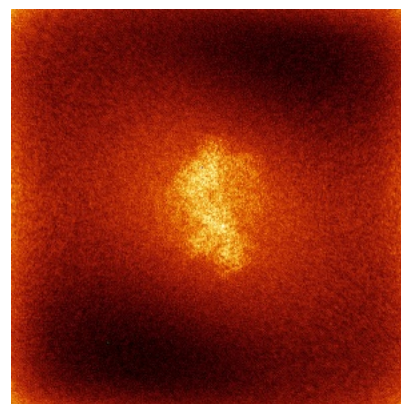
6.4.2 Raw map



X



Y

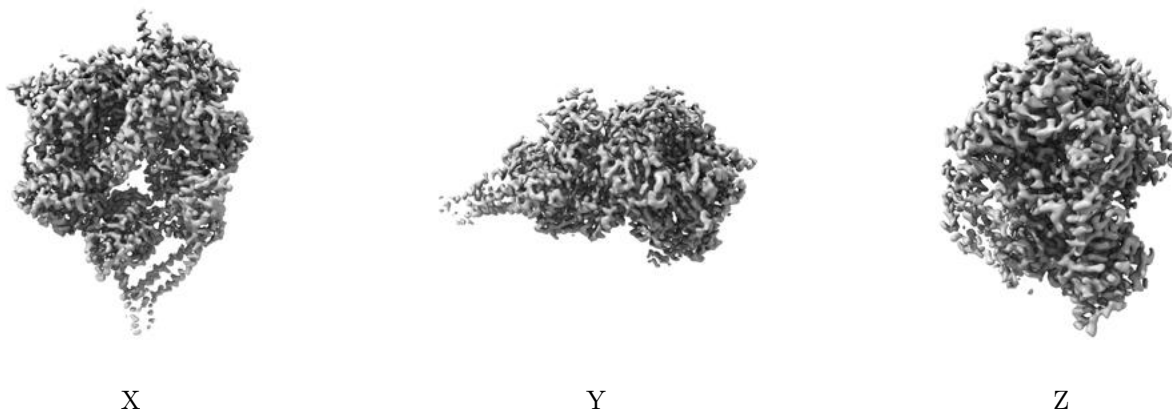


Z

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.

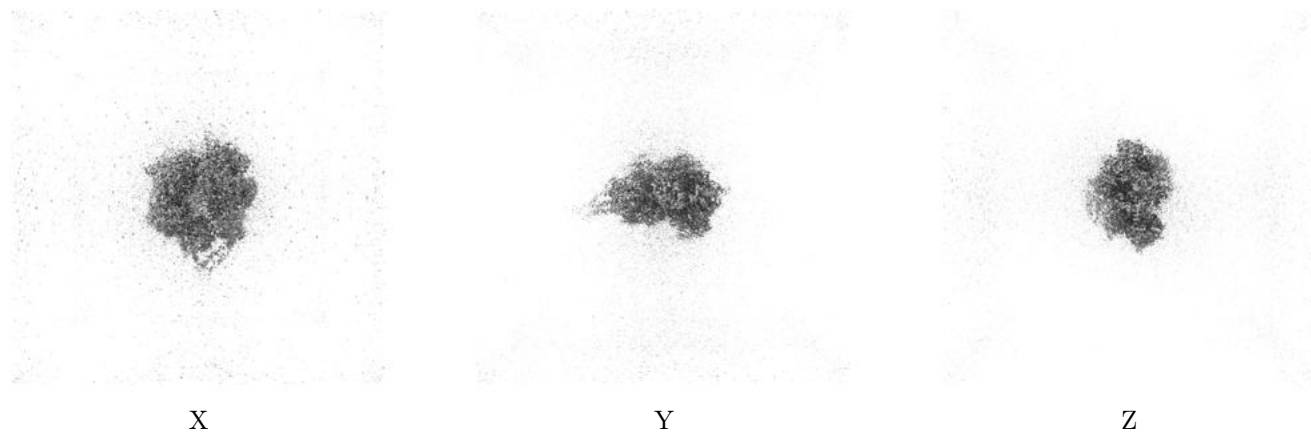
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

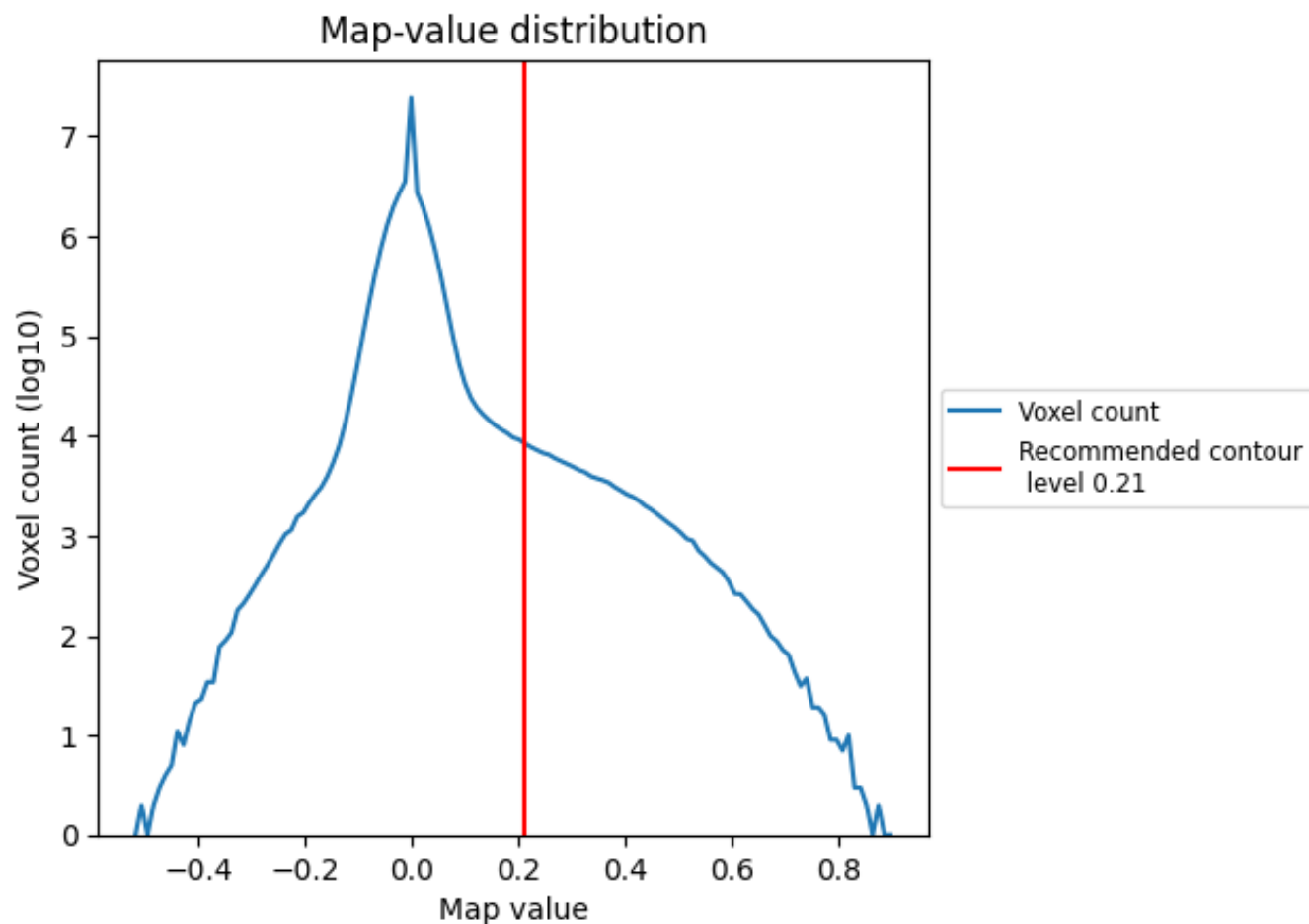
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

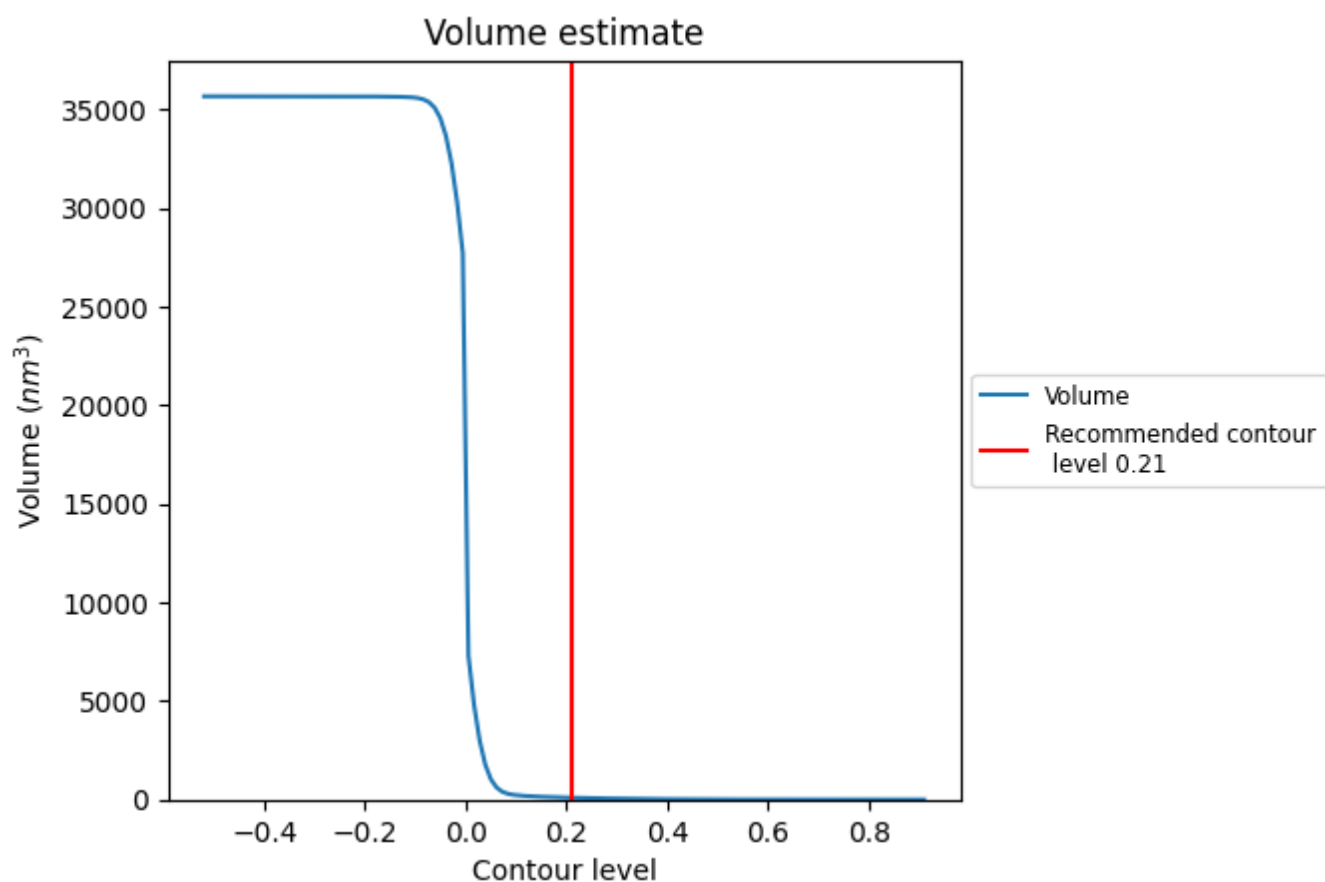
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

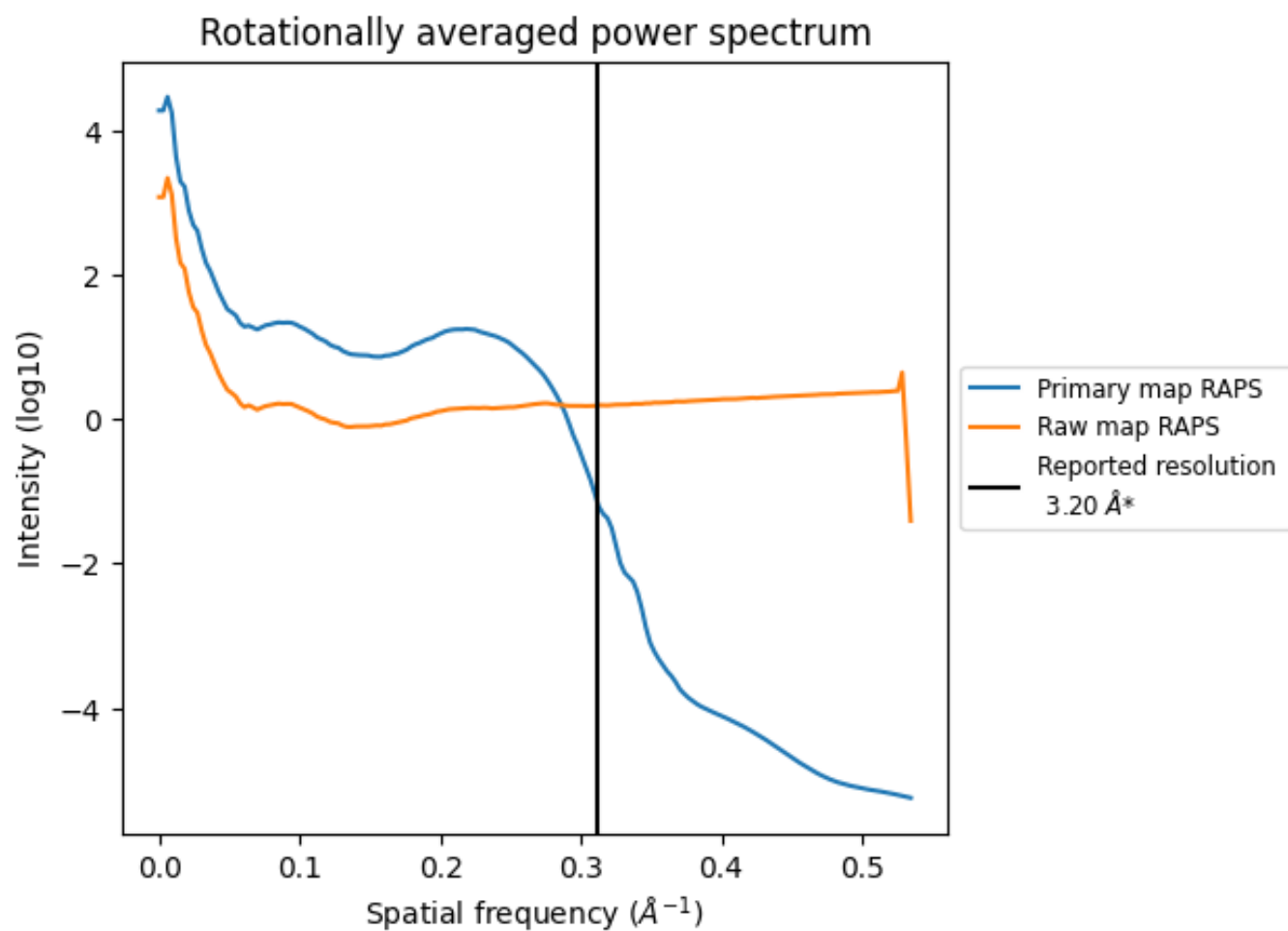
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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 ⓘ

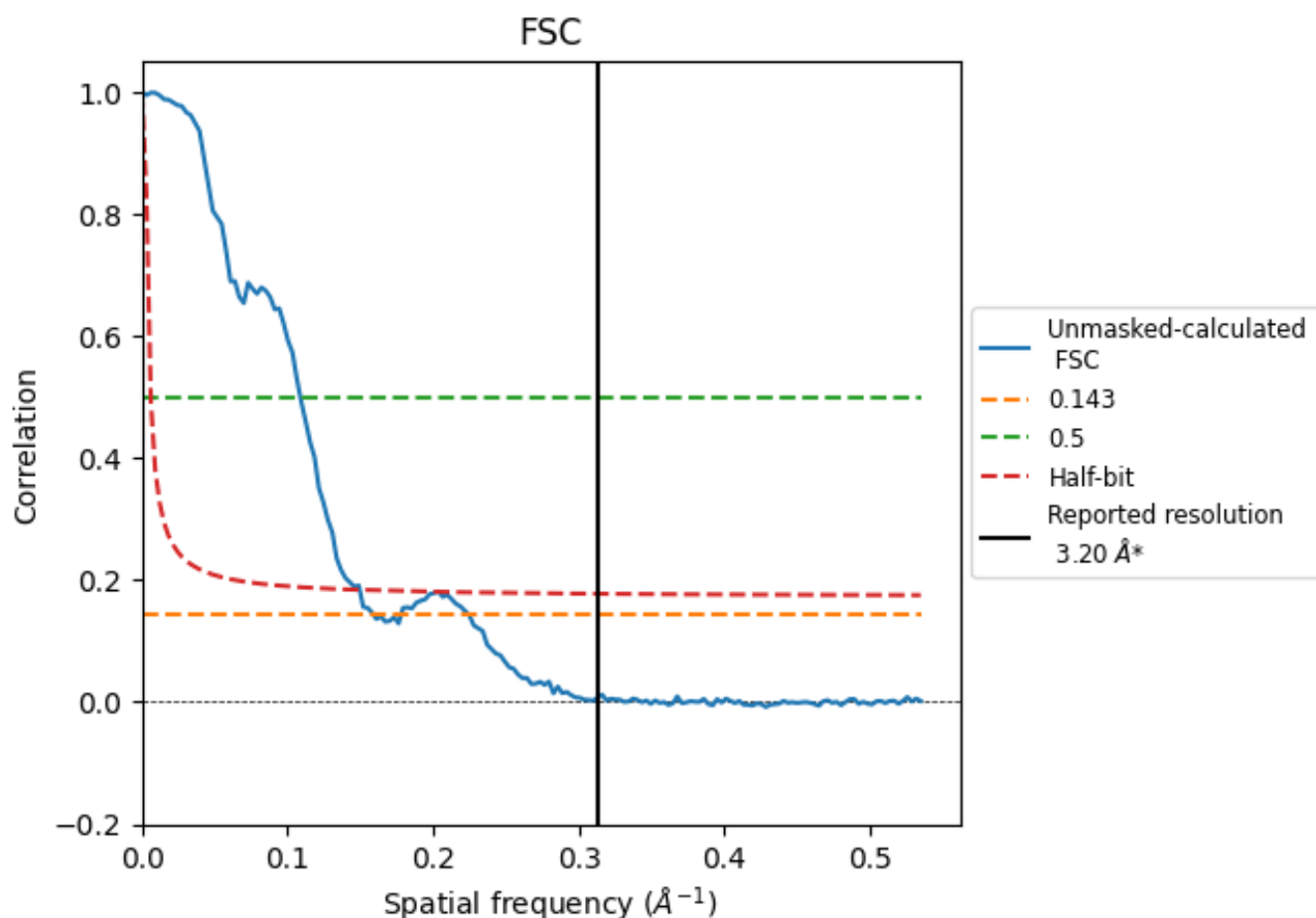


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

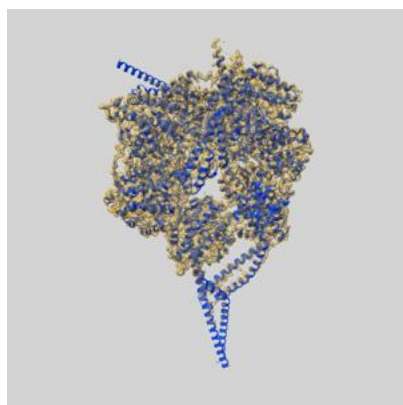
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.29	9.20	6.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 3.2 by more than 10 %

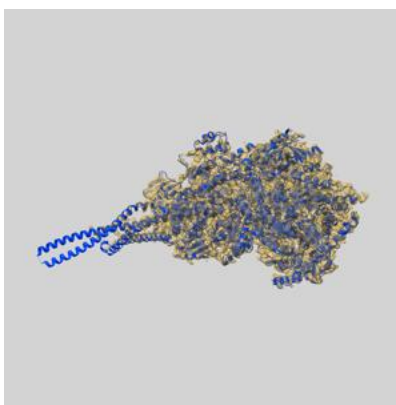
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47360 and PDB model 9E0K. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

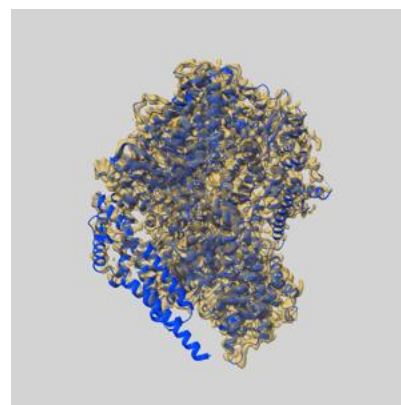
9.1 Map-model overlay [i](#)



X



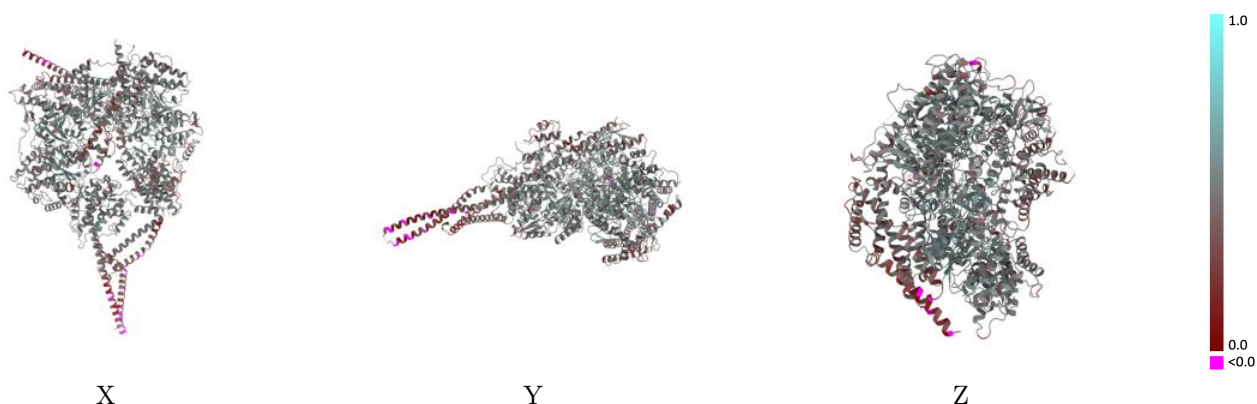
Y



Z

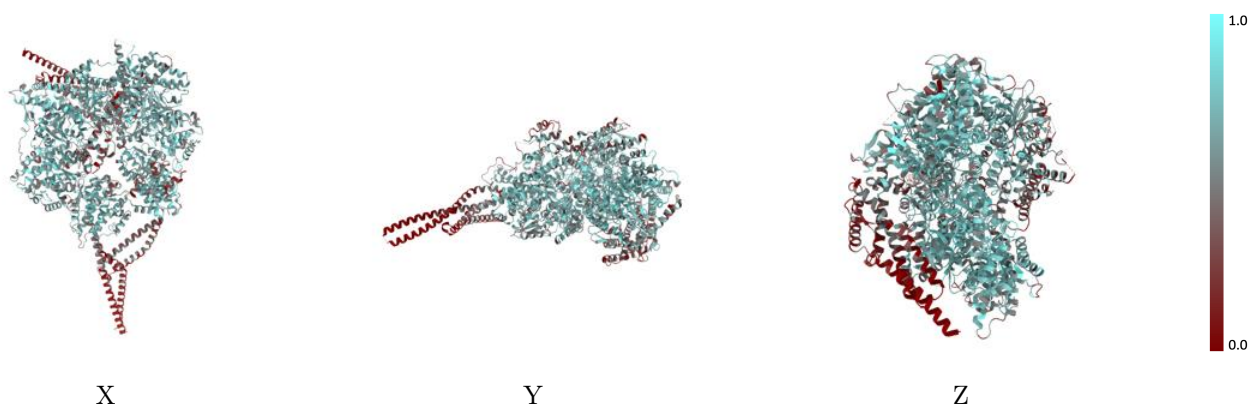
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



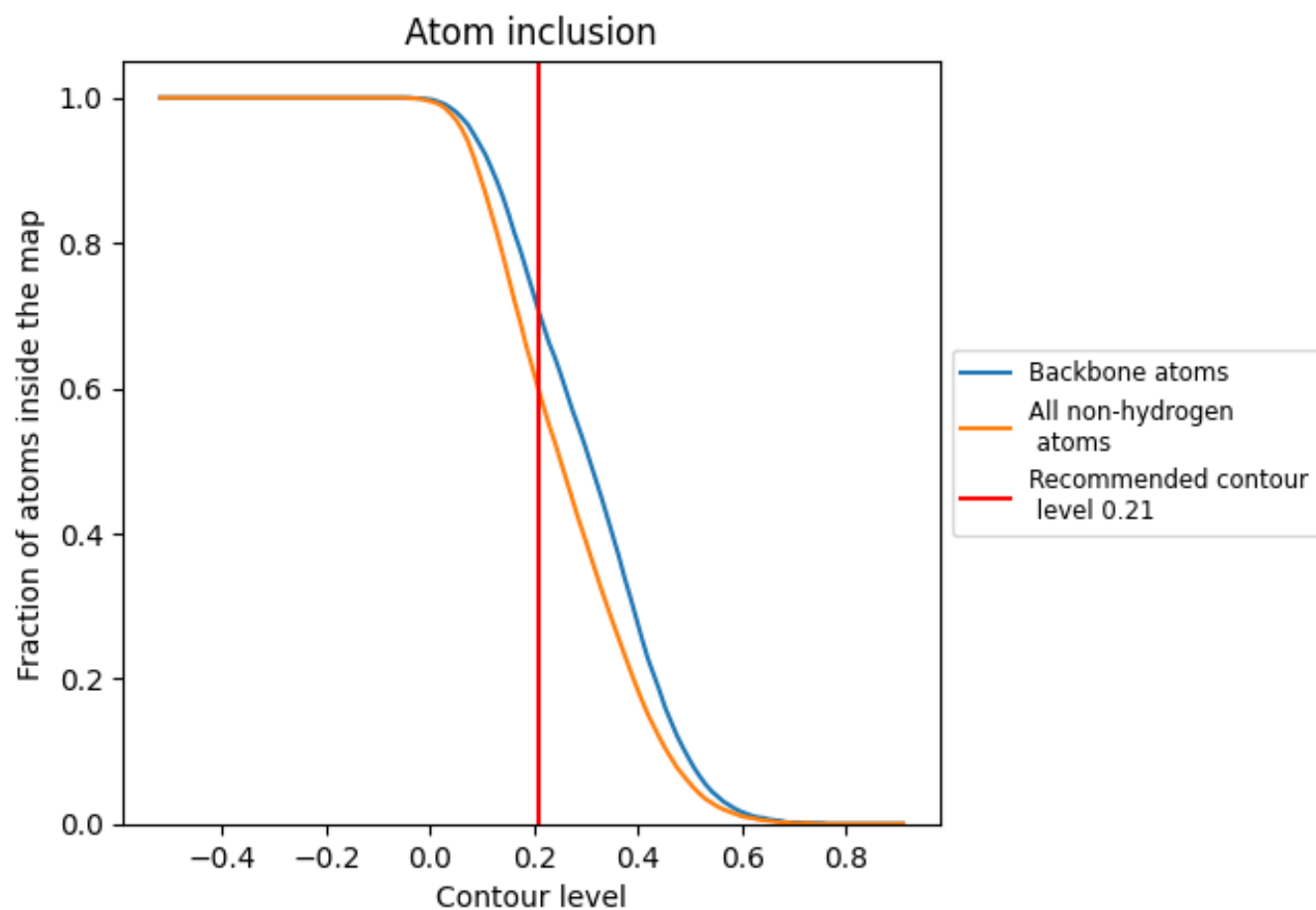
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5940	<div></div> 0.4650
A	<div></div> 0.5940	<div></div> 0.4650

