



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 04:16 PM JST

PDB ID : 27PZ / pdb_000027pz
EMDB ID : EMD-81336
Title : Dictyostelium discoideum cytoplasmic dynein motor domain in the presence of ADP (ADP state 2)
Authors : Shimo-Kon, R.; Tokita, H.; Imai, H.; Maeshima, T.; Kon, T.
Deposited on : 2026-06-09
Resolution : 3.20 Å(reported)
Based on initial model : 3VKG

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

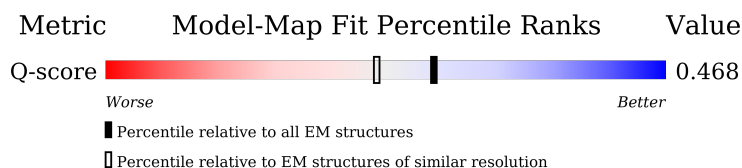
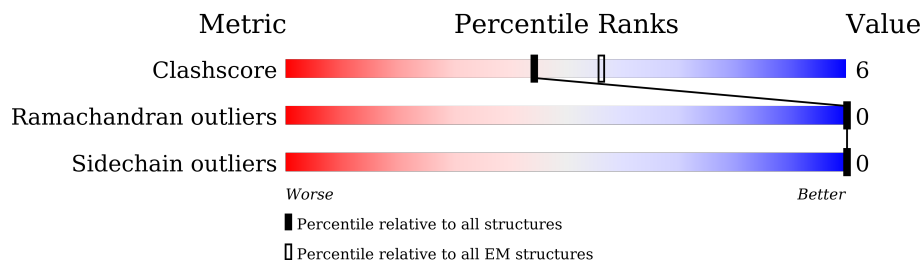
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	3367	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24643 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.

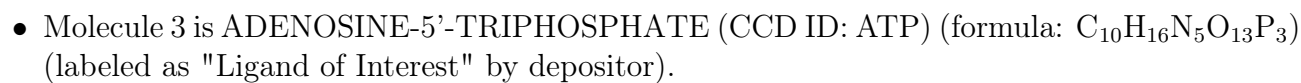
- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3048	Total	C	N	O	S	0	0
			24530	15649	4182	4602	97		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	initiating methionine	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

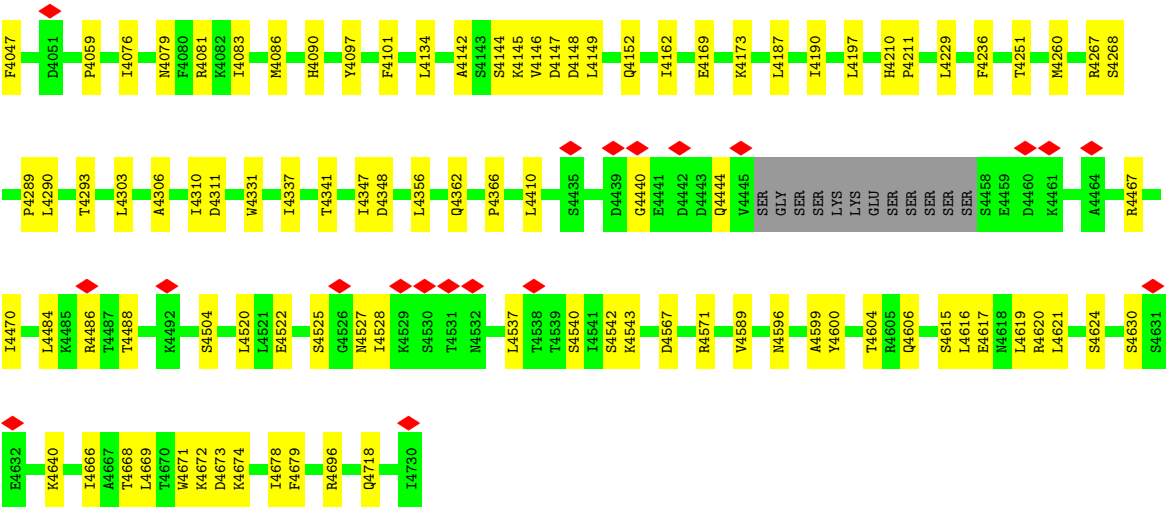


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

K3860	T3766	E3643	THR	GLN	Q3298	T3160	S3081	D3002	L2492
R3767	R3768	W3647	LEU	LYS	V3299	S3161	S3082	R3003	P2508
P3769	P3770	D3655	ARG	VAL	K3300	F3162	F3083	V3004	T2525
I3865	I3866	D3656	THR	ALA	D3301	L3163	L3084	R3006	L2531
L3867	L3868	E3660	GLU	THR	Q3302	N3166	L3090	Q3007	L2535
L3869	L3870	N3661	GLN	ASP	Q3303	R3167	L3091	P3008	L2539
L3871	L3872	N3662	THR	LYS	V3304	C3168	A3092	Q3009	N2542
L3873	L3874	N3663	GLU	GLU	S3305	V3169	G3098	G3010	R2543
L3875	L3876	L3665	PRO	LYS	L3306	L3170	G3098	H3011	S2544
F3786	F3787	K3666	ASN	LYS	A3307	E3187	G3098	A3012	V2546
F3788	F3789	D3676	GLU	GLU	Q3308	E3188	E3101	L3013	
R3813	R3814	A3681	PRO	PRO	Q3308	L3192	E3101	L3014	
D3815	D3816	S3682	THR	ALA	K3309	D3193	G3102	L3015	
L3817	L3818	N3686	THR	ILE	N3310	P3203	E3103	S3023	
K3819	K3820	Y3689	LYS	ILE	ARG	Q3207	E3104	V3024	
Q3821	Q3822	K3692	GLU	GLU	LEU	F3207	F3105	L3025	
G3823	G3824	I3694	VAL	ALA	ASP	I3211	T3106	S3026	
E3825	E3826	F3696	THR	GLN	VAL	N3215	A3107	R3027	
F3827	F3828	P3699	LYS	LYS	LYS	I3219	A3108	L3035	
L3830	L3831	K3706	THR	THR	ASN	F3220	L3109	T3039	
K3832	K3833	N3707	LEU	THR	GLN	P3227	H3110	K3041	
L3835	L3836	L3708	ARG	ILE	LYS	I3234	A3111	V3042	
N3837	N3838	F3714	GLU	ALA	ASN	I3238	C3112	N3044	
Q3839	Q3840	P3717	LYS	LYS	GLN	I3241	K3113	T2925	
A3841	A3842	V3723	GLY	LEU	LEU	A3241	E3114	N3045	
G3843	G3844	I3726	THR	ASP	LYS	S3230	T3115	Y3046	
N3844	N3845	D3727	LEU	PRO	ALA	L3231	A3116	K3047	
I3846	I3847	N3735	ILE	PRO	ALA	I3234	Q3117	S3048	
D3848	D3849	I3738	LYS	LYS	GLN	I3259	R3118	S3049	
S3849	S3850	K3741	ASP	GLY	ASP	I3260	N3119	D3050	
V3851	V3852	R3744	THR	VAL	GLN	I3264	G3120	F3051	
I3852	I3853	I3745	ASN	ALA	LEU	I3271	E3126	R2959	
S3854	S3855	D3751	VAL	CYS	GLN	I3275	E3127	N2964	
L3856	L3857	D3755	ARG	VAL	GLN	Q3282	E3128	R2965	
K3858	K3859	F3760	THR	LEU	VAL	K3290	T3134	N2966	
E3860	E3861	L3764	LYS	LYS	ASP	R3293	Q3135	L2976	
L3862	L3863	F3765	GLY	GLY	VAL	D3294	Q3136	L2977	
K3864	K3865		PRO	LYS	ASN	I3295	R3137	V2978	
E3866	E3867		LEU	LEU	GLU	E3296	R3138	F2979	
F3868	F3869		ALA	ALA	ILE	A3297	N3140	Y2980	
L3870	L3871		VAL	CYS	ALA		V3143	E2981	
K3872	K3873		THR	THR	LYS		V3144	L2984	
S3874	S3875		LYS	LYS	ASP		P3149	L2888	
T3876	T3877		GLY	GLY	VAL		A3150	V2989	
F3878	F3879		ASN	ASN	ASP		S3076	V2994	
L3880	L3881		VAL	VAL	LYS		N3077	H2997	
K3882	K3883		GLN	GLN	GLU		V3078	I3001	
E3884	E3885		PRO	PRO	ILE		L3079		
L3886	L3887		ALA	ALA	ALA		E3080		
K3888	K3889		VAL	VAL	VAL				
L3890	L3891		THR	THR	THR				
S3892	S3893		LYS	LYS	LYS				
F3894	F3895		ASP	ASP	ASP				
K3896	K3897		THR	THR	THR				
L3898	L3899		LYS	LYS	LYS				
M3900	M3901		GLY	GLY	GLY				
E3902	E3903		VAL	VAL	VAL				
Y3904	Y3905		ALA	ALA	ALA				
G3906	G3907		THR	THR	THR				
E3908	E3909		LYS	LYS	LYS				
F3910	F3911		GLU	GLU	GLU				
F3912	F3913		VAL	VAL	VAL				
L3914	L3915		LYS	LYS	LYS				
I3916	I3917		THR	THR	THR				
I3918	I3919		ASN	ASN	ASN				
L3920	L3921		LEU	LEU	LEU				
D3922	D3923		GLY	GLY	GLY				
F3924	F3925		LYS	LYS	LYS				
L3926	L3927		THR	THR	THR				
K3928	K3929		VAL	VAL	VAL				
E3930	E3931		GLN	GLN	GLN				
F3932	F3933		LYS	LYS	LYS				
I3934	I3935		THR	THR	THR				
T3936	T3937		ASP	ASP	ASP				
R3938	R3939		LYS	LYS	LYS				
V3940	V3941		GLU	GLU	GLU				
T3942	T3943		ILE	ILE	ILE				
L3944	L3945		VAL	VAL	VAL				
S3946	S3947		ALA	ALA	ALA				
L3948	L3949		THR	THR	THR				
I3950	I3951		ILE	ILE	ILE				
G3952	G3953		LYS	LYS	LYS				
K3954	K3955		ASP	ASP	ASP				
V3956	V3957		THR	THR	THR				
L3958	L3959		LYS	LYS	LYS				
I3960	I3961		VAL	VAL	VAL				
E3962	E3963		ASN	ASN	ASN				
T3964	T3965		VAL	VAL	VAL				
S3966	S3967		ARG	ARG	ARG				
L3968	L3969		GLU	GLU	GLU				
I3970	I3971		LEU	LEU	LEU				
G3972	G3973		VAL	VAL	VAL				
E3974	E3975		LYS	LYS	LYS				
F3976	F3977		THR	THR	THR				
L3978	L3979		LYS	LYS	LYS				
S3980	S3981		ASP	ASP	ASP				
N3982	N3983		THR	THR	THR				
E3984	E3985		LYS	LYS	LYS				
T3986	T3987		VAL	VAL	VAL				
S4010	S4011		ALA	ALA	ALA				
L4012	L4013		GLY	GLY	GLY				
D4043	D4044		LYS	LYS	LYS				
			PRO	PRO	PRO				
			LEU	LEU	LEU				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLU	GLU	GLU				
			ILE	ILE	ILE				
			ALA	ALA	ALA				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP				
			GLN	GLN	GLN				
			LEU	LEU	LEU				
			VAL	VAL	VAL				
			THR	THR	THR				
			LYS	LYS	LYS				
			ASP	ASP	ASP</				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	596990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF parameters were estimated using Patch CTF estimation in cryoSPARC and further refined by global and local CTF refinement.	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.676	Depositor
Minimum map value	-1.199	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	261.9, 261.9, 261.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.87299997, 0.87299997, 0.87299997	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	0.15	0/25053	0.30	1/33939 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2396	GLU	N-CA-CB	5.55	119.20	110.71

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	24530	0	24573	316	0
2	A	81	0	36	1	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	24643	0	24621	316	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 (316) 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:3271:ILE:HG13	1:A:3592:VAL:HG11	1.63	0.81
1:A:3919:ILE:HD11	1:A:3954:ARG:HD2	1.64	0.80
1:A:1872:ARG:HH12	1:A:2164:ARG:HD2	1.51	0.76
1:A:3044:ASN:ND2	1:A:3751:ASP:OD2	2.19	0.76
1:A:2440:ASP:HB2	1:A:2443:GLU:HG2	1.68	0.75
1:A:3039:THR:HG22	1:A:3072:ILE:HB	1.69	0.75
1:A:1929:MET:HG2	1:A:1930:ALA:H	1.53	0.73
1:A:2200:ASN:ND2	1:A:2229:GLN:O	2.22	0.73
1:A:2337:ARG:HB2	1:A:2385:LEU:HD11	1.71	0.72
1:A:1578:SER:HB3	1:A:3714:PHE:HB3	1.71	0.71
1:A:2105:ARG:HG2	1:A:2149:LEU:HD21	1.73	0.70
1:A:2398:GLN:HB2	1:A:2806:ARG:HD2	1.72	0.69
1:A:3004:VAL:HG11	1:A:3012:ALA:HB2	1.76	0.68
1:A:3023:SER:OG	1:A:3027:ARG:NH1	2.26	0.68
1:A:3158:SER:HB3	1:A:3161:SER:HB2	1.76	0.68
1:A:1982:GLU:HG3	2:A:5001:ADP:H2'	1.76	0.68
1:A:2406:ALA:O	1:A:2410:ARG:NH1	2.26	0.68
1:A:3072:ILE:HG12	1:A:3144:VAL:HB	1.76	0.68
1:A:2525:ILE:HB	1:A:2815:LEU:HD12	1.76	0.67
1:A:1864:LEU:HA	1:A:2164:ARG:HH12	1.59	0.67
1:A:2273:MET:HA	1:A:2395:PHE:HB2	1.76	0.66
1:A:3066:GLU:H	1:A:3069:ILE:HD11	1.59	0.66
1:A:4672:LYS:HG3	1:A:4678:ILE:HD11	1.78	0.66
1:A:4467:ARG:NH2	1:A:4525:SER:OG	2.29	0.65
1:A:4624:SER:HB2	1:A:4668:THR:HG23	1.79	0.65
1:A:2618:SER:OG	1:A:2621:ASP:OD1	2.14	0.65
1:A:2729:VAL:HG12	1:A:2782:LYS:HB3	1.77	0.65
1:A:3643:GLU:OE2	1:A:3666:LYS:NZ	2.29	0.65
1:A:1792:PHE:HD2	1:A:1822:VAL:HG21	1.63	0.64
1:A:2241:GLN:HG2	1:A:2251:THR:HG21	1.81	0.63
1:A:2525:ILE:HD11	1:A:2794:PRO:HG3	1.78	0.63
1:A:3238:ILE:HD11	1:A:3617:TRP:HZ2	1.64	0.62
1:A:3570:GLU:OE2	1:A:3573:ARG:NH2	2.32	0.62
1:A:3694:ILE:HG12	1:A:3717:PRO:HB2	1.80	0.62
1:A:3295:THR:HG21	1:A:3838:LEU:HD11	1.81	0.62
1:A:3689:TYR:HD2	1:A:3692:LYS:HD2	1.65	0.62
1:A:4606:GLN:HG2	1:A:4616:LEU:HD22	1.80	0.62
1:A:2535:ASN:ND2	1:A:2809:ARG:O	2.33	0.62
1:A:3813:ARG:HD3	1:A:3879:ILE:HG13	1.82	0.62
1:A:2908:GLU:OE1	1:A:3003:ARG:NH1	2.33	0.62
1:A:3900:MET:HE2	1:A:3951:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:GLY:O	1:A:1627:GLN:NE2	2.30	0.61
1:A:2669:PRO:HG3	1:A:2767:VAL:HG21	1.82	0.60
1:A:3830:LEU:HB3	1:A:3858:LEU:HD11	1.84	0.60
1:A:2598:GLN:NE2	1:A:2606:PRO:O	2.35	0.59
1:A:1828:ASP:OD1	1:A:1906:TRP:NE1	2.33	0.59
1:A:4522:GLU:HG3	1:A:4527:ASN:HB2	1.84	0.59
1:A:4337:ILE:O	1:A:4341:THR:OG1	2.14	0.59
1:A:1605:TRP:HH2	1:A:1650:VAL:HG21	1.67	0.59
1:A:1845:LEU:HD12	1:A:1889:VAL:HG13	1.84	0.59
1:A:2101:ILE:HD12	1:A:4348:ASP:HB2	1.84	0.59
1:A:2635:GLU:OE2	1:A:2833:ARG:NH1	2.34	0.59
1:A:3258:ARG:NH1	1:A:3735:ASN:OD1	2.36	0.59
1:A:2539:SER:OG	1:A:2668:ARG:NE	2.34	0.58
1:A:3015:ILE:HG23	1:A:3149:PRO:HD2	1.86	0.58
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.85	0.58
1:A:3193:ASP:O	1:A:3275:ARG:NH1	2.31	0.58
1:A:2327:TRP:NE1	1:A:2329:ASP:OD1	2.35	0.58
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.85	0.57
1:A:3113:LYS:HG2	1:A:3114:GLU:HG2	1.86	0.57
1:A:2797:ASP:HB3	1:A:2800:ARG:HD3	1.85	0.57
1:A:3987:GLU:OE2	1:A:4081:ARG:NE	2.37	0.57
1:A:2278:SER:OG	1:A:2809:ARG:HD3	2.05	0.57
1:A:2873:ILE:HD11	1:A:3165:PHE:HB2	1.86	0.56
1:A:4169:GLU:OE2	1:A:4173:LYS:NZ	2.38	0.56
1:A:3647:TRP:HZ2	1:A:3666:LYS:HD3	1.70	0.56
1:A:2964:ASN:ND2	1:A:2966:SER:OG	2.38	0.56
1:A:1967:ARG:HB3	1:A:2051:LYS:HA	1.88	0.56
1:A:2994:VAL:HG13	1:A:3025:LEU:HD21	1.87	0.56
1:A:3594:LEU:HD21	1:A:3618:MET:HG2	1.86	0.56
1:A:3661:ASN:ND2	1:A:3785:ASN:O	2.37	0.56
1:A:3055:LEU:HD21	1:A:3090:LEU:HD11	1.88	0.55
1:A:1910:MET:HE3	1:A:1929:MET:HE3	1.87	0.55
1:A:1744:MET:HE1	1:A:1777:MET:HG3	1.89	0.55
1:A:2025:PHE:HB2	1:A:2075:VAL:HG12	1.88	0.55
1:A:3241:ALA:HB2	1:A:3613:LEU:HD21	1.89	0.54
1:A:3726:ILE:HG21	1:A:3777:LEU:HD22	1.89	0.54
1:A:1607:ASP:OD1	1:A:1610:ARG:NH2	2.39	0.54
1:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.89	0.54
1:A:3042:VAL:HG23	1:A:3043:ASN:H	1.72	0.54
1:A:4522:GLU:HG2	1:A:4528:ILE:HG22	1.88	0.54
1:A:1817:LEU:HD11	1:A:1936:TYR:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3065:LYS:HB3	1:A:3069:ILE:HD13	1.89	0.54
1:A:1698:TYR:O	1:A:2011:ARG:NH1	2.32	0.54
1:A:2766:MET:HE2	1:A:2783:LEU:HD11	1.89	0.54
1:A:2711:LEU:HD23	1:A:2714:PHE:HD2	1.73	0.54
1:A:2274:MET:HB3	1:A:2416:PHE:CE1	2.43	0.53
1:A:2027:GLU:HG3	1:A:2030:ARG:HG2	1.90	0.53
1:A:2989:VAL:HG13	1:A:3187:GLU:HG3	1.89	0.53
1:A:3566:ASN:HB3	1:A:3855:LEU:HD23	1.90	0.53
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.74	0.53
1:A:2424:GLN:HG3	1:A:2508:PRO:HG3	1.92	0.52
1:A:4306:ALA:O	1:A:4310:ILE:HG12	2.09	0.52
1:A:3227:VAL:O	1:A:3231:LEU:HG	2.09	0.52
1:A:2136:GLN:O	1:A:2137:GLU:HG2	2.09	0.52
1:A:2438:PRO:HG2	1:A:2447:GLN:HG2	1.92	0.52
1:A:2919:GLU:HG2	1:A:2922:GLU:HG3	1.91	0.52
1:A:3219:ILE:HG23	1:A:3220:PRO:HD3	1.92	0.52
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.91	0.52
1:A:2006:LEU:HD21	1:A:2035:ILE:HG23	1.90	0.52
1:A:3011:HIS:ND1	1:A:3143:VAL:HG12	2.25	0.52
1:A:1929:MET:HE1	1:A:1957:TYR:HB3	1.91	0.52
1:A:3738:ILE:HG23	1:A:3745:ILE:HG23	1.92	0.52
1:A:4486:ARG:HB3	1:A:4488:THR:HG23	1.92	0.52
1:A:2302:GLU:OE2	1:A:2304:HIS:NE2	2.36	0.52
1:A:2158:SER:O	1:A:2162:ILE:HG12	2.10	0.52
1:A:3741:LYS:O	1:A:3744:ARG:HG2	2.10	0.52
1:A:1413:SER:O	1:A:1417:THR:OG1	2.27	0.52
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	1.92	0.51
1:A:4621:LEU:HD11	1:A:4669:LEU:HB3	1.92	0.51
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	1.91	0.51
1:A:2208:VAL:HG12	1:A:2415:TRP:CE2	2.46	0.51
1:A:3084:LEU:HD13	1:A:3158:SER:HA	1.91	0.51
1:A:3259:HIS:CE1	1:A:3779:SER:HA	2.46	0.51
1:A:2377:LEU:N	1:A:2385:LEU:O	2.40	0.50
1:A:3049:SER:O	1:A:3054:ASP:HB2	2.11	0.50
1:A:2232:GLN:HG3	1:A:2233:MET:H	1.75	0.50
1:A:2793:ASN:HB2	1:A:2800:ARG:HE	1.76	0.50
1:A:3040:ILE:O	1:A:3042:VAL:HG13	2.11	0.50
1:A:1967:ARG:HH22	1:A:2069:GLN:HB3	1.76	0.50
1:A:4362:GLN:OE1	1:A:4718:GLN:NE2	2.44	0.50
1:A:2275:VAL:HG13	1:A:2397:VAL:HG23	1.92	0.50
1:A:2375:LYS:NZ	1:A:2389:ASN:OD1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ILE:HD12	1:A:1665:ILE:HD12	1.94	0.49
1:A:1975:PRO:HD2	1:A:2101:ILE:HG12	1.94	0.49
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.13	0.49
1:A:2381:ASN:OD1	1:A:2382:GLY:N	2.45	0.49
1:A:2273:MET:HG3	1:A:2411:CYS:SG	2.53	0.49
1:A:1768:GLU:C	1:A:1770:LEU:H	2.20	0.49
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.78	0.49
1:A:4630:SER:H	1:A:4668:THR:HG21	1.77	0.49
1:A:3230:SER:O	1:A:3234:ILE:HG12	2.12	0.49
1:A:3699:PHE:CZ	1:A:3726:ILE:HA	2.47	0.49
1:A:3708:LEU:HD11	1:A:3760:PHE:HZ	1.77	0.49
1:A:2872:TYR:OH	1:A:2922:GLU:OE1	2.20	0.49
1:A:3238:ILE:HG13	1:A:3601:TYR:CG	2.48	0.49
1:A:1543:LEU:HD22	1:A:1555:VAL:HG21	1.94	0.48
1:A:3192:LEU:HD21	1:A:3271:ILE:HD12	1.93	0.48
1:A:4440:GLY:O	1:A:4444:GLN:NE2	2.46	0.48
1:A:2848:ASN:ND2	1:A:2937:HIS:O	2.39	0.48
1:A:3776:ASP:OD1	1:A:3780:ARG:NH1	2.46	0.48
1:A:1709:ILE:HG12	1:A:1766:ILE:HG21	1.95	0.48
1:A:3655:ASP:OD1	1:A:3656:GLU:N	2.46	0.48
1:A:4615:SER:OG	1:A:4617:GLU:OE1	2.31	0.48
1:A:2422:THR:O	1:A:2425:MET:HG2	2.13	0.48
1:A:2582:GLY:HA2	1:A:2585:MET:HE3	1.95	0.48
1:A:1456:ASN:O	1:A:1460:ILE:HG12	2.13	0.48
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.49	0.48
1:A:3003:ARG:NH1	1:A:3007:GLN:OE1	2.47	0.48
1:A:3011:HIS:CD2	1:A:3167:ARG:HH12	2.32	0.48
1:A:4197:LEU:HD12	1:A:4229:LEU:HD22	1.95	0.48
1:A:2014:VAL:HG23	1:A:2065:ILE:HG21	1.95	0.47
1:A:2444:LYS:O	1:A:2447:GLN:HG3	2.14	0.47
1:A:3897:TYR:HB2	1:A:3916:PHE:CD2	2.49	0.47
1:A:2856:PHE:CE2	1:A:2909:ALA:HB1	2.50	0.47
1:A:2749:PRO:HG2	1:A:2759:VAL:HG11	1.95	0.47
1:A:3042:VAL:HG23	1:A:3043:ASN:N	2.29	0.47
1:A:4148:ASP:O	1:A:4152:GLN:N	2.45	0.47
1:A:4290:LEU:HG	1:A:4410:LEU:HD22	1.96	0.47
1:A:2274:MET:HB3	1:A:2416:PHE:HE1	1.78	0.47
1:A:2217:SER:C	1:A:2219:LEU:H	2.21	0.47
1:A:4620:ARG:N	1:A:4672:LYS:O	2.39	0.47
1:A:1988:GLY:HA3	1:A:1995:VAL:HG21	1.97	0.47
1:A:2112:MET:O	1:A:2116:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3040:ILE:HG12	1:A:3083:PHE:HE2	1.80	0.47
1:A:3681:ALA:HB2	1:A:3786:PHE:CG	2.49	0.47
1:A:1792:PHE:CD2	1:A:1822:VAL:HG21	2.47	0.47
1:A:2370:LEU:HD13	1:A:2377:LEU:HB2	1.97	0.47
1:A:2370:LEU:HD21	1:A:2387:LEU:HD13	1.98	0.47
1:A:3013:LEU:HD22	1:A:3170:LEU:HD22	1.97	0.47
1:A:1908:TYR:CE1	1:A:1958:LEU:HD22	2.49	0.46
1:A:4210:HIS:CG	1:A:4211:PRO:HD2	2.49	0.46
1:A:4293:THR:HG23	1:A:4696:ARG:HB3	1.96	0.46
1:A:4604:THR:HG23	1:A:4671:TRP:HE1	1.80	0.46
1:A:1929:MET:SD	1:A:1958:LEU:HA	2.56	0.46
1:A:2058:GLU:OE1	1:A:2064:ASN:ND2	2.48	0.46
1:A:1909:HIS:O	1:A:1911:ARG:NH1	2.49	0.46
1:A:1520:ALA:HA	1:A:1580:TYR:CE1	2.51	0.46
1:A:4347:ILE:HD12	1:A:4356:LEU:HD22	1.97	0.46
1:A:4540:SER:HA	1:A:4543:LYS:HE2	1.98	0.46
1:A:2705:THR:HG23	1:A:2709:LEU:HD22	1.98	0.46
1:A:3923:LEU:HD22	1:A:3947:ILE:HD13	1.97	0.46
1:A:4484:LEU:HD11	1:A:4504:SER:HB2	1.97	0.46
1:A:2438:PRO:HG3	1:A:2492:LEU:HD13	1.99	0.45
1:A:3079:LEU:O	1:A:3080:GLU:HB2	2.16	0.45
1:A:3203:PRO:O	1:A:3207:GLN:HG2	2.17	0.45
1:A:4076:ILE:HG23	1:A:4101:PHE:HE1	1.81	0.45
1:A:4086:MET:HE3	1:A:4097:TYR:CE1	2.50	0.45
1:A:1800:HIS:CD2	1:A:1858:ASN:HB3	2.51	0.45
1:A:2544:SER:HB3	1:A:2572:ARG:HG2	1.97	0.45
1:A:2660:LEU:HD11	1:A:2672:LEU:HD21	1.99	0.45
1:A:1642:GLU:OE1	1:A:1671:ARG:NH1	2.33	0.45
1:A:2888:GLU:HG3	1:A:3008:PRO:HD3	1.98	0.45
1:A:4010:SER:O	1:A:4012:LEU:N	2.47	0.45
1:A:4673:ASP:OD1	1:A:4674:LYS:N	2.49	0.45
1:A:2824:LEU:HD21	1:A:2876:PRO:HG3	1.98	0.45
1:A:4470:ILE:HD11	1:A:4520:LEU:HD23	1.99	0.45
1:A:2308:PRO:HD2	1:A:2357:GLY:HA3	1.98	0.45
1:A:2839:LEU:HD11	1:A:2890:ILE:HD12	1.97	0.45
1:A:3744:ARG:NH2	1:A:3755:ASP:OD1	2.50	0.45
1:A:3956:THR:O	1:A:3964:LYS:NZ	2.50	0.45
1:A:4142:ALA:O	1:A:4145:LYS:HB2	2.17	0.45
1:A:4146:VAL:HG23	1:A:4149:LEU:HD23	1.99	0.45
1:A:2100:MET:HE3	1:A:2100:MET:HB3	1.89	0.44
1:A:2130:PRO:HG2	1:A:4617:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2542:ASN:O	1:A:2546:VAL:HG23	2.17	0.44
1:A:3035:LEU:HD23	1:A:3070:CYS:HB2	1.99	0.44
1:A:4589:VAL:HG11	1:A:4600:TYR:CZ	2.52	0.44
1:A:2145:TYR:OH	1:A:2211:ASP:OD2	2.22	0.44
1:A:3003:ARG:HA	1:A:3006:ARG:HG2	1.98	0.44
1:A:1764:PRO:HG2	1:A:1769:TRP:CD1	2.53	0.44
1:A:2882:TRP:CZ2	1:A:2909:ALA:HB2	2.53	0.44
1:A:3008:PRO:O	1:A:3010:GLY:N	2.51	0.44
1:A:4672:LYS:HB2	1:A:4679:PHE:CE2	2.52	0.44
1:A:2800:ARG:HH22	1:A:3160:THR:HG23	1.82	0.43
1:A:2697:VAL:HG23	1:A:2739:LEU:HD11	2.01	0.43
1:A:2714:PHE:CE2	1:A:2766:MET:HE1	2.52	0.43
1:A:4047:PHE:O	1:A:4090:HIS:NE2	2.36	0.43
1:A:2897:THR:HG23	1:A:2900:GLY:H	1.83	0.43
1:A:3163:ALA:O	1:A:3167:ARG:HB3	2.18	0.43
1:A:3244:ARG:NH1	1:A:3612:ASP:OD2	2.51	0.43
1:A:3815:ASP:C	1:A:3817:LEU:H	2.27	0.43
1:A:4537:LEU:O	1:A:4542:SER:OG	2.31	0.43
1:A:1694:PHE:CE2	1:A:1696:ARG:HB2	2.54	0.43
1:A:4134:LEU:HD23	1:A:4236:PHE:HB2	2.00	0.43
1:A:3001:ILE:HD11	1:A:3014:LEU:HD21	2.01	0.43
1:A:3898:PHE:O	1:A:3902:GLU:HG2	2.18	0.43
1:A:4596:ASN:HD21	1:A:4599:ALA:HB2	1.83	0.43
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.53	0.43
1:A:3293:ARG:O	1:A:3296:GLU:HG3	2.19	0.43
1:A:3689:TYR:HB2	1:A:3694:ILE:CD1	2.49	0.43
1:A:2012:ILE:O	1:A:2016:LEU:HG	2.19	0.43
1:A:2370:LEU:HD11	1:A:2387:LEU:HB2	2.01	0.43
1:A:1590:HIS:CE1	1:A:1594:ARG:HD2	2.54	0.43
1:A:1971:ASN:HA	1:A:2075:VAL:O	2.19	0.43
1:A:2058:GLU:HB3	1:A:2062:GLY:HA2	2.01	0.43
1:A:3207:GLN:O	1:A:3211:ILE:HG12	2.19	0.43
1:A:4086:MET:HE3	1:A:4097:TYR:CZ	2.54	0.43
1:A:1908:TYR:HE1	1:A:1958:LEU:HD22	1.84	0.43
1:A:2531:LEU:HD23	1:A:2809:ARG:HH11	1.84	0.43
1:A:3295:THR:O	1:A:3298:GLN:HG3	2.18	0.43
1:A:3676:ASP:HB3	1:A:3786:PHE:HB2	2.01	0.43
1:A:1785:LEU:HD12	1:A:1814:LEU:HD22	2.00	0.42
1:A:2233:MET:HE1	1:A:2263:HIS:HD2	1.84	0.42
1:A:3282:GLN:NE2	1:A:3582:ASN:OD1	2.45	0.42
1:A:3816:LEU:O	1:A:3820:GLN:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4210:HIS:CD2	1:A:4211:PRO:HD2	2.54	0.42
1:A:4540:SER:HA	1:A:4543:LYS:HG2	2.00	0.42
1:A:1428:ARG:NH2	1:A:2984:LEU:O	2.52	0.42
1:A:2017:CYS:SG	1:A:2067:LEU:HA	2.60	0.42
1:A:2543:ARG:HH11	1:A:2665:SER:HB2	1.84	0.42
1:A:1537:PHE:CE1	1:A:1564:LYS:HG2	2.54	0.42
1:A:2000:CYS:HB3	1:A:2031:LEU:HD13	2.00	0.42
1:A:2283:THR:HG23	1:A:2286:TRP:CZ2	2.54	0.42
1:A:2663:TRP:HZ3	1:A:2814:LEU:HB2	1.84	0.42
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.55	0.42
1:A:3979:THR:HG23	1:A:3981:ASN:H	1.85	0.42
1:A:2189:GLN:O	1:A:2192:ILE:HB	2.20	0.42
1:A:2273:MET:HE2	1:A:2273:MET:HB3	1.80	0.42
1:A:2265:ILE:HG22	1:A:2272:VAL:HG22	2.02	0.42
1:A:2160:GLY:O	1:A:2164:ARG:HG2	2.18	0.42
1:A:3823:PHE:CE1	1:A:3865:ILE:HG13	2.55	0.42
1:A:3909:TYR:OH	1:A:3963:ASP:OD2	2.31	0.42
1:A:4079:ASN:O	1:A:4083:ILE:HG13	2.20	0.42
1:A:3167:ARG:HD3	1:A:3168:CYS:SG	2.60	0.42
1:A:1642:GLU:OE2	1:A:1671:ARG:NH2	2.46	0.42
1:A:2336:LEU:HA	1:A:2340:ILE:HD12	2.02	0.42
1:A:2866:PRO:HA	1:A:2869:GLN:O	2.20	0.42
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	2.02	0.42
1:A:4144:SER:HA	1:A:4147:ASP:HB2	2.02	0.42
1:A:4260:MET:O	1:A:4268:SER:OG	2.30	0.42
1:A:4619:LEU:HD23	1:A:4673:ASP:HA	2.02	0.42
1:A:2207:LEU:HD23	1:A:2211:ASP:HB3	2.01	0.41
1:A:2976:LEU:HD12	1:A:2988:LEU:HB3	2.01	0.41
1:A:3040:ILE:HG23	1:A:3041:LYS:N	2.35	0.41
1:A:3238:ILE:HD11	1:A:3617:TRP:CZ2	2.50	0.41
1:A:3723:VAL:HG11	1:A:3764:LEU:HB3	2.01	0.41
1:A:2293:ILE:HG13	1:A:2350:ARG:HH22	1.85	0.41
1:A:3054:ASP:HA	1:A:3057:MET:HB2	2.01	0.41
1:A:3770:THR:HG22	1:A:3770:THR:O	2.19	0.41
1:A:3706:LYS:C	1:A:3706:LYS:HD3	2.45	0.41
1:A:2315:GLN:HB3	1:A:2775:THR:HG21	2.03	0.41
1:A:2746:ILE:O	1:A:2760:ILE:HD11	2.21	0.41
1:A:4251:THR:HG23	1:A:4303:LEU:HD21	2.02	0.41
1:A:1531:LEU:HD11	1:A:1575:MET:HE1	2.02	0.41
1:A:3664:MET:HE2	1:A:3664:MET:HB3	1.93	0.41
1:A:2009:MET:HG3	1:A:2013:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2438:PRO:HG2	1:A:2444:LYS:HA	2.02	0.41
1:A:2980:TYR:HA	1:A:2984:LEU:HB2	2.03	0.41
1:A:4640:LYS:HB3	1:A:4666:ILE:HD12	2.02	0.41
1:A:3660:GLU:O	1:A:3664:MET:HG3	2.20	0.41
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	2.03	0.41
1:A:1470:ASP:HB3	1:A:1518:ILE:HG21	2.03	0.41
1:A:1519:THR:HG22	1:A:1580:TYR:OH	2.21	0.41
1:A:1813:GLN:HE21	1:A:1936:TYR:HE2	1.68	0.41
1:A:3134:THR:O	1:A:3138:ARG:HG2	2.21	0.41
1:A:4162:ILE:HD11	1:A:4187:LEU:HG	2.02	0.41
1:A:4567:ASP:O	1:A:4571:ARG:HG3	2.20	0.41
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.20	0.41
1:A:2275:VAL:HG21	1:A:2400:LEU:HD23	2.02	0.41
1:A:2978:VAL:O	1:A:2981:GLU:HG2	2.21	0.41
1:A:1748:GLU:HG3	1:A:1943:ILE:HB	2.03	0.40
1:A:2997:HIS:O	1:A:3001:ILE:HG12	2.21	0.40
1:A:3040:ILE:HG23	1:A:3041:LYS:H	1.85	0.40
1:A:3136:GLN:HG3	1:A:3140:ASN:HD22	1.86	0.40
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.21	0.40
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.56	0.40
1:A:2543:ARG:HG2	1:A:2662:ALA:HA	2.04	0.40
1:A:3164:LEU:HD23	1:A:3167:ARG:HD2	2.02	0.40
1:A:3686:MET:HG3	1:A:3696:LYS:HE3	2.03	0.40
1:A:4083:ILE:HD11	1:A:4101:PHE:CB	2.52	0.40
1:A:1437:LYS:O	1:A:1438:LEU:HB3	2.22	0.40
1:A:2894:ASP:OD1	1:A:2894:ASP:N	2.53	0.40
1:A:2924:GLU:C	1:A:2926:THR:H	2.29	0.40
1:A:3640:LYS:HE2	1:A:3642:GLU:OE2	2.21	0.40
1:A:4267:ARG:NH2	1:A:4311:ASP:OD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	3040/3367 (90%)	2920 (96%)	120 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	2747/3028 (91%)	2747 (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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1690	GLN
1	A	1767	HIS
1	A	1813	GLN
1	A	1820	GLN
1	A	1928	HIS
1	A	2018	GLN
1	A	2047	GLN
1	A	2264	GLN
1	A	2269	ASN
1	A	2315	GLN
1	A	2429	ASN
1	A	2592	ASN
1	A	2700	ASN
1	A	2717	HIS
1	A	2778	HIS
1	A	2787	GLN
1	A	2961	GLN
1	A	2964	ASN
1	A	3045	ASN
1	A	3140	ASN
1	A	3214	ASN

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Mol	Chain	Res	Type
1	A	3721	GLN
1	A	4040	ASN
1	A	4282	GLN
1	A	4428	ASN
1	A	4596	ASN
1	A	4610	GLN
1	A	4622	HIS
1	A	4638	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	5001	-	27,29,29	0.50	0	42,45,45	0.52	0
2	ADP	A	5004	-	27,29,29	0.50	0	42,45,45	0.49	0
3	ATP	A	5002	-	29,33,33	0.56	0	44,52,52	0.62	0
2	ADP	A	5005	-	27,29,29	0.43	0	42,45,45	0.53	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	5001	-	-	0/16/32/32	0/3/3/3
2	ADP	A	5004	-	-	2/16/32/32	0/3/3/3
3	ATP	A	5002	-	-	2/22/38/38	0/3/3/3
2	ADP	A	5005	-	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

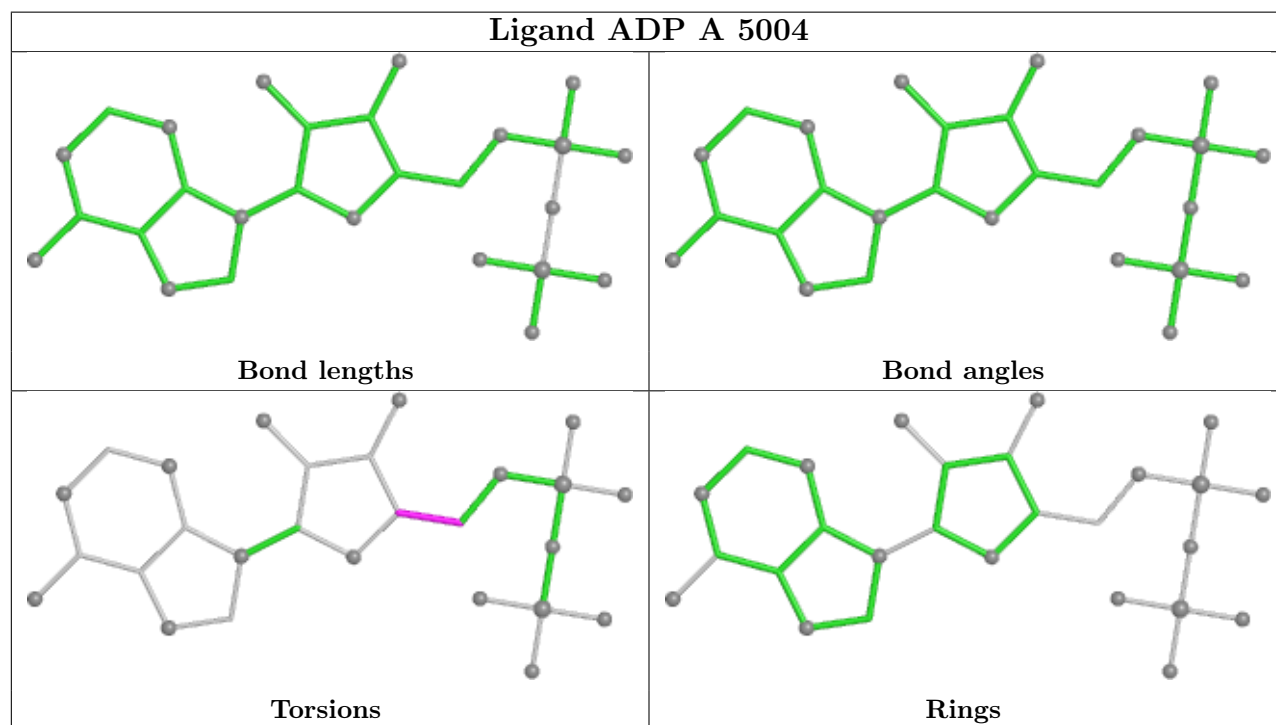
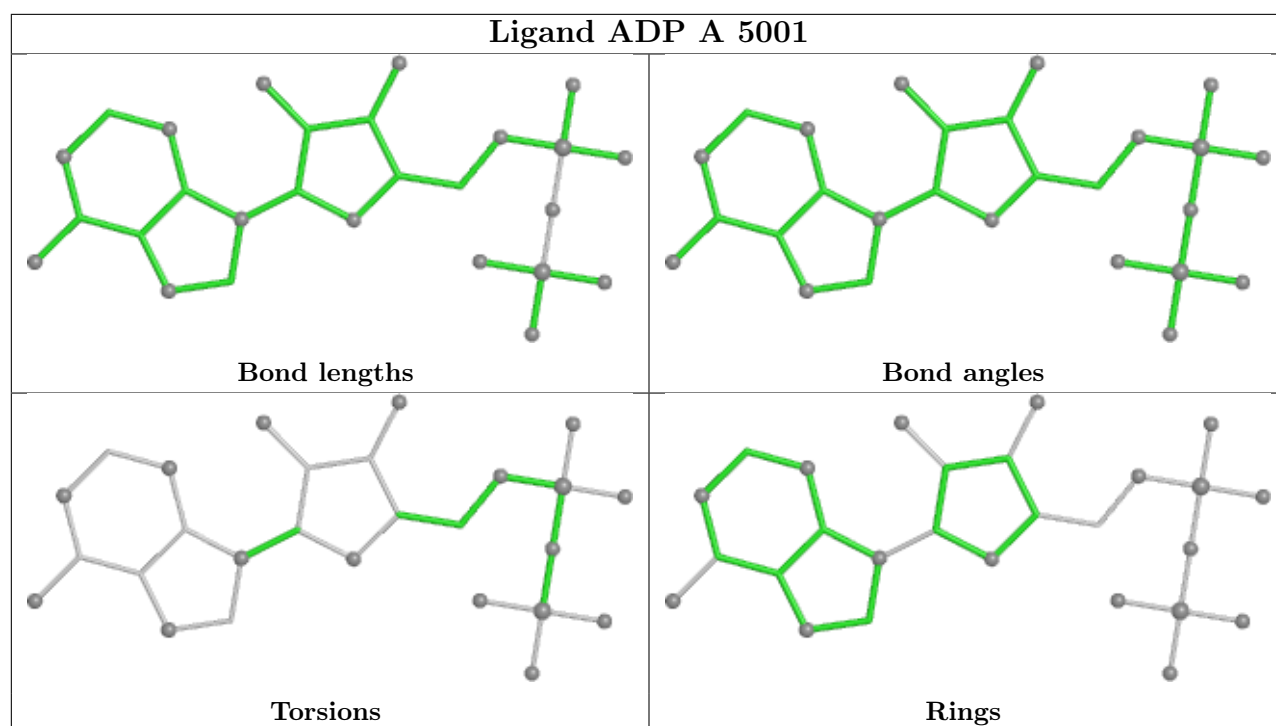
Mol	Chain	Res	Type	Atoms
2	A	5004	ADP	O4'-C4'-C5'-O5'
3	A	5002	ATP	C5'-O5'-PA-O1A
2	A	5004	ADP	C3'-C4'-C5'-O5'
2	A	5005	ADP	PA-O3A-PB-O1B
2	A	5005	ADP	PA-O3A-PB-O2B
2	A	5005	ADP	PA-O3A-PB-O3B
3	A	5002	ATP	O4'-C4'-C5'-O5'

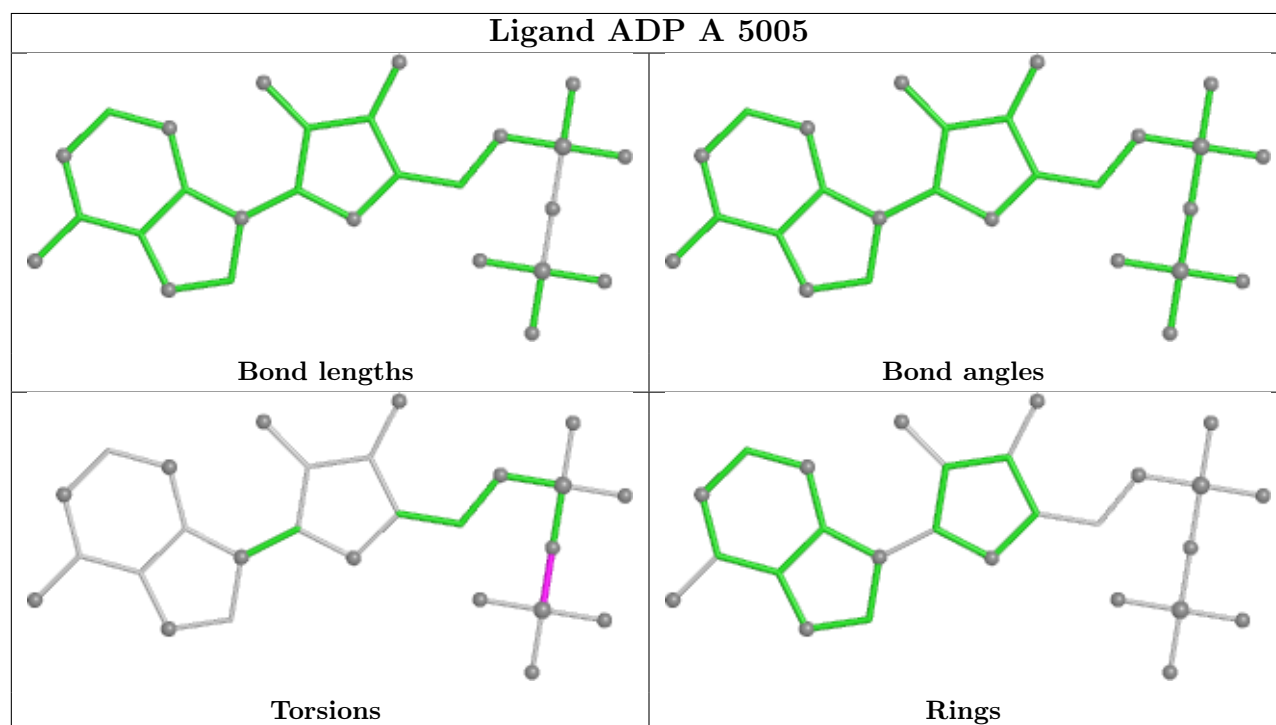
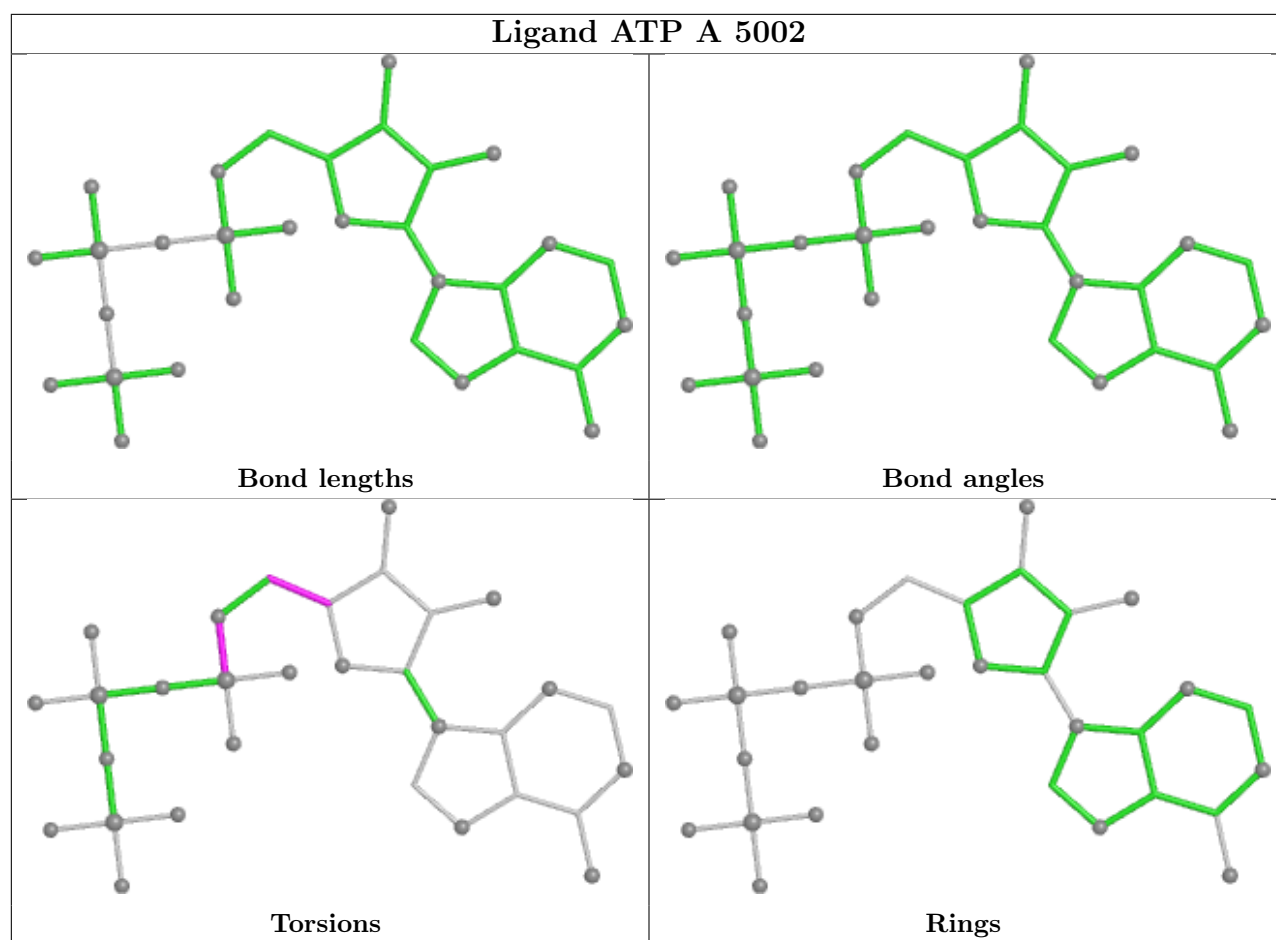
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	ADP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

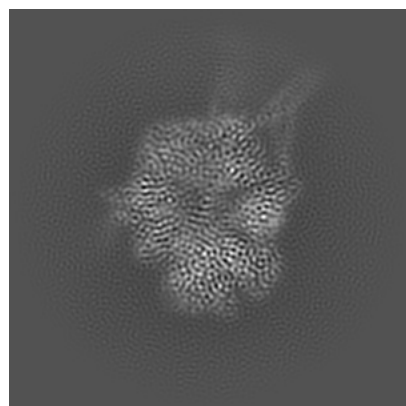
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-81336. These allow visual inspection of the internal detail of the map and identification of artifacts.

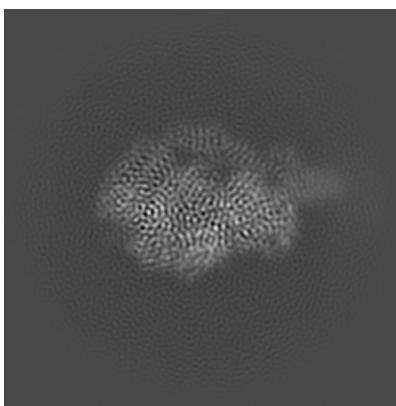
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

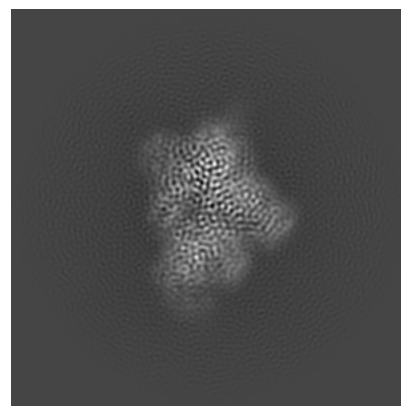
6.1.1 Primary map



X

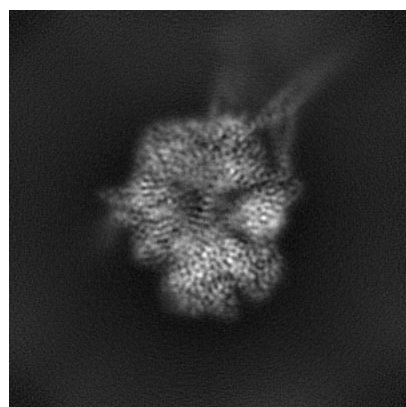


Y

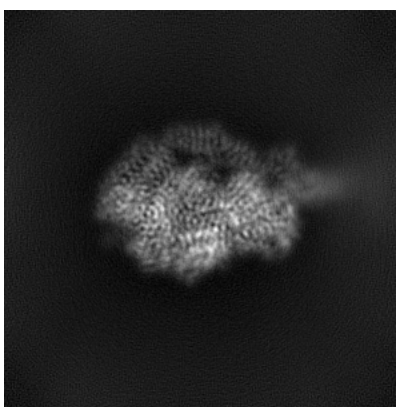


Z

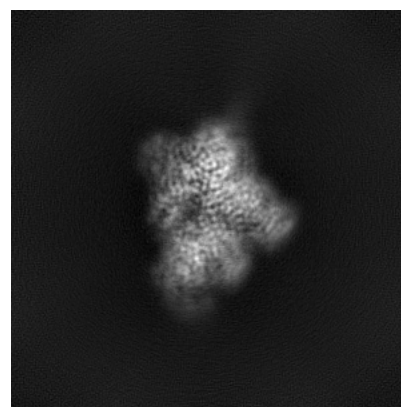
6.1.2 Raw map



X



Y

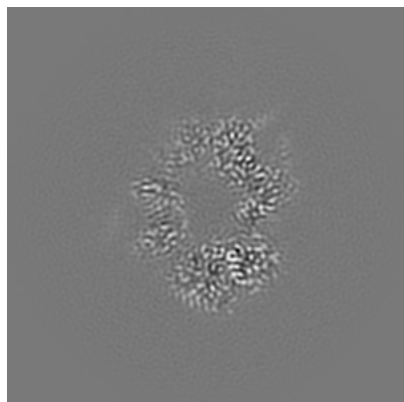


Z

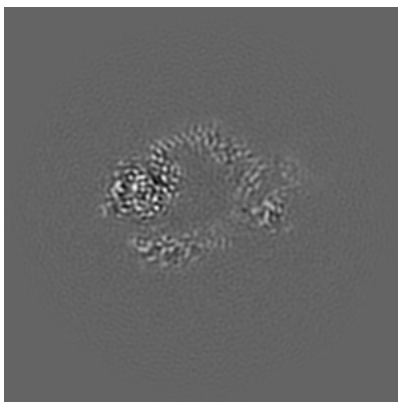
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

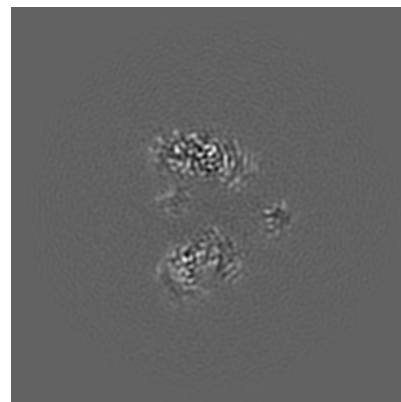
6.2.1 Primary map



X Index: 150

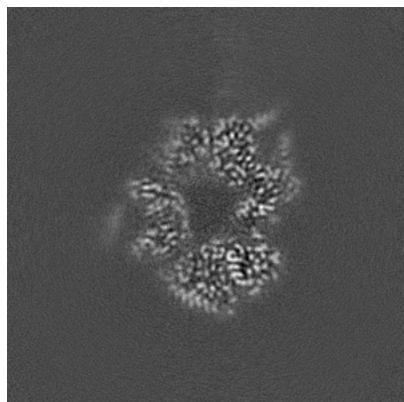


Y Index: 150

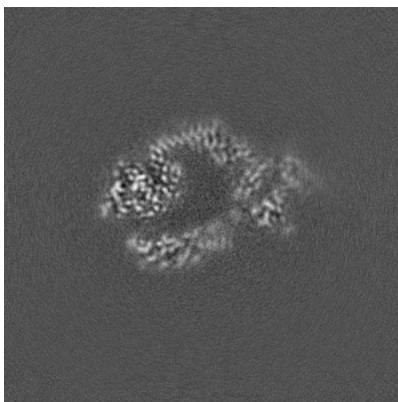


Z Index: 150

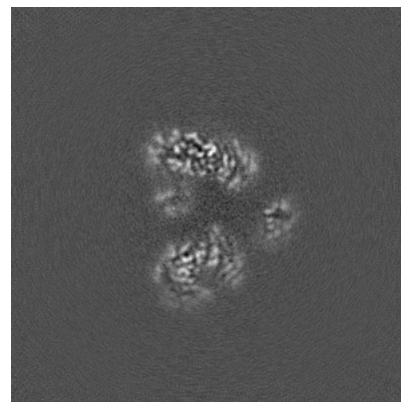
6.2.2 Raw map



X Index: 150



Y Index: 150

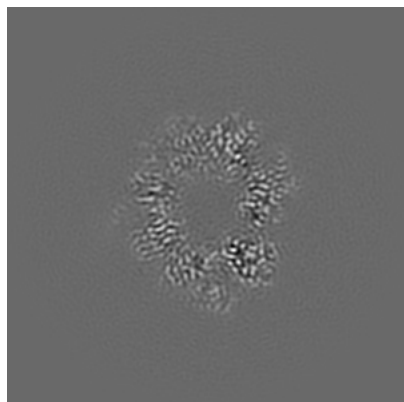


Z Index: 150

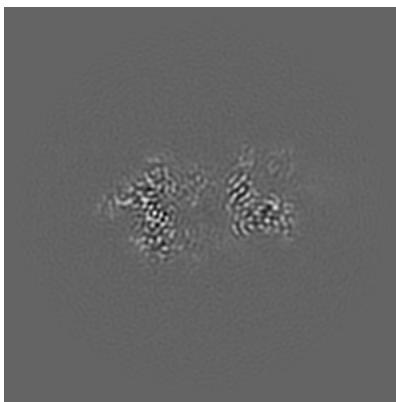
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

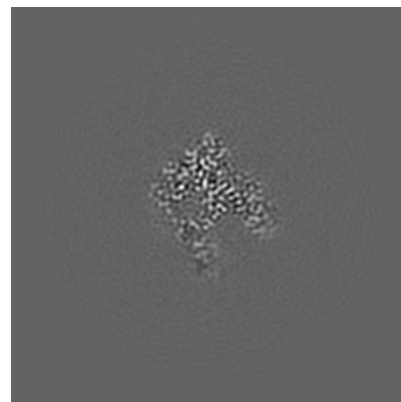
6.3.1 Primary map



X Index: 144

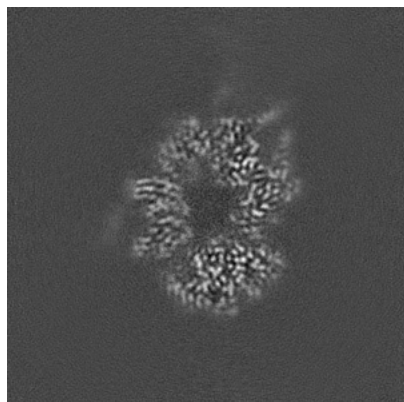


Y Index: 168

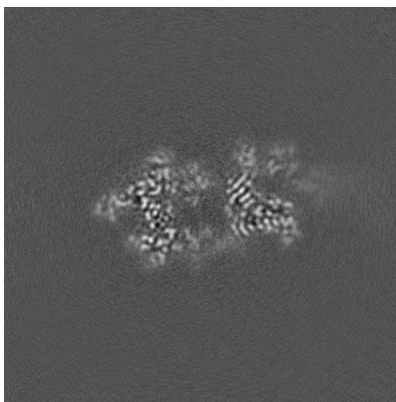


Z Index: 113

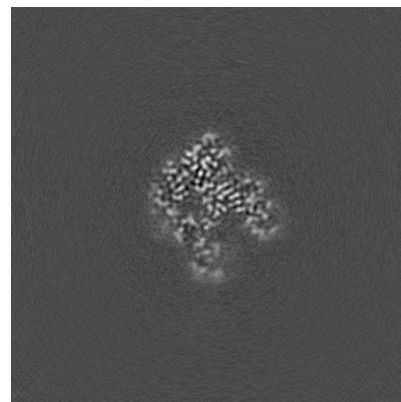
6.3.2 Raw map



X Index: 152



Y Index: 167

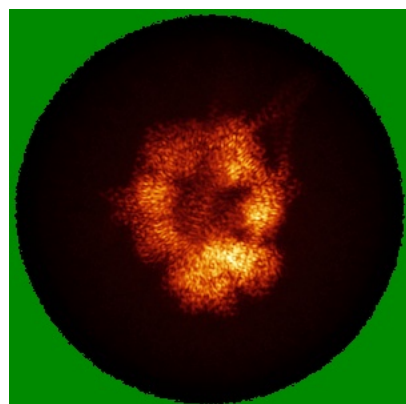


Z Index: 114

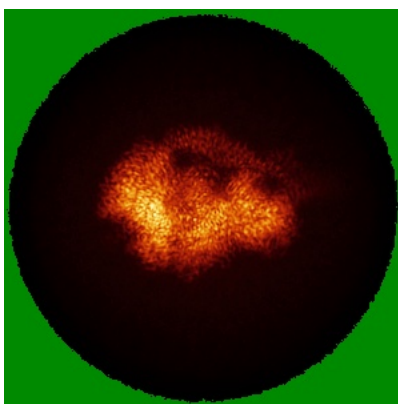
The images above show the largest variance slices of the map in three orthogonal directions.

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

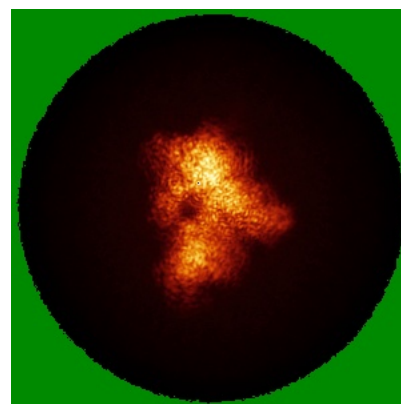
6.4.1 Primary map



X

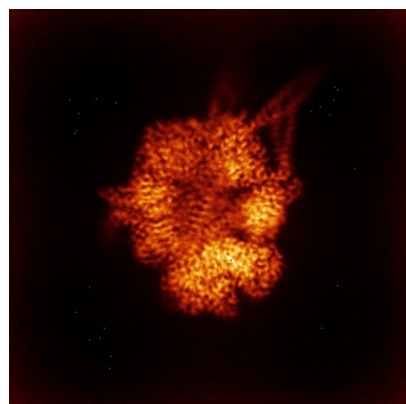


Y

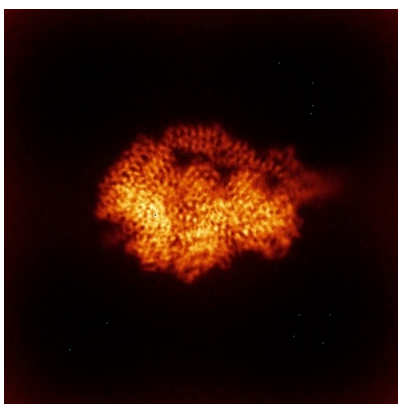


Z

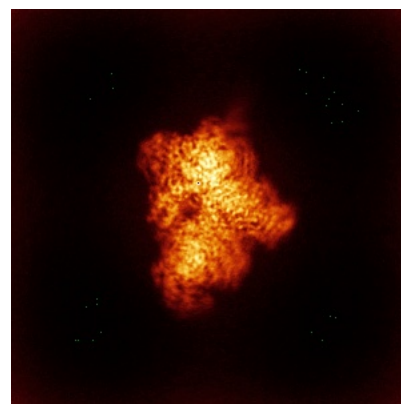
6.4.2 Raw map



X



Y

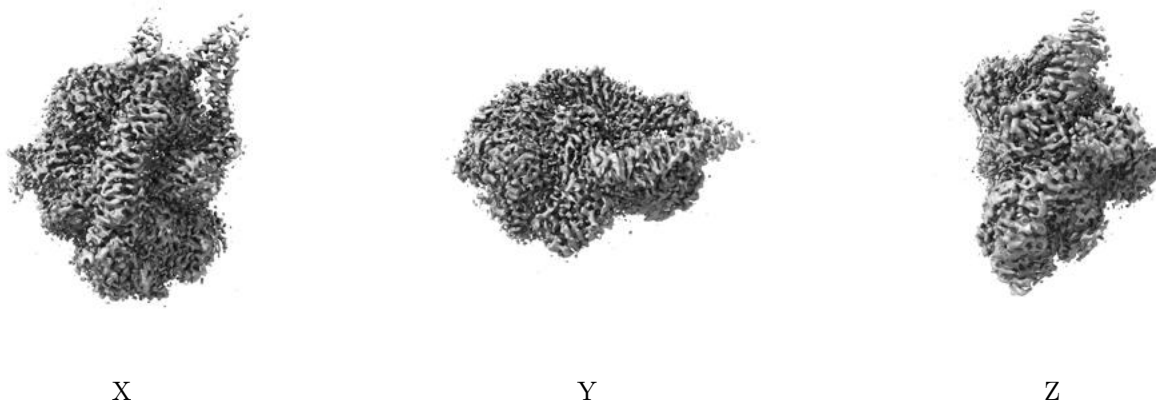


Z

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.

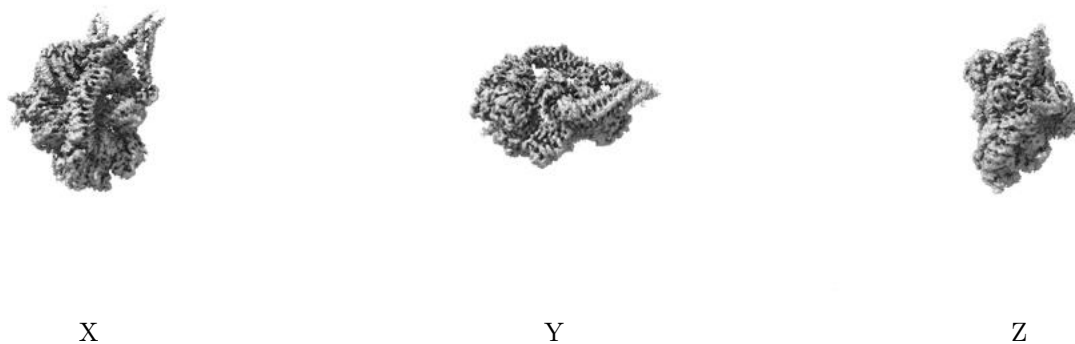
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

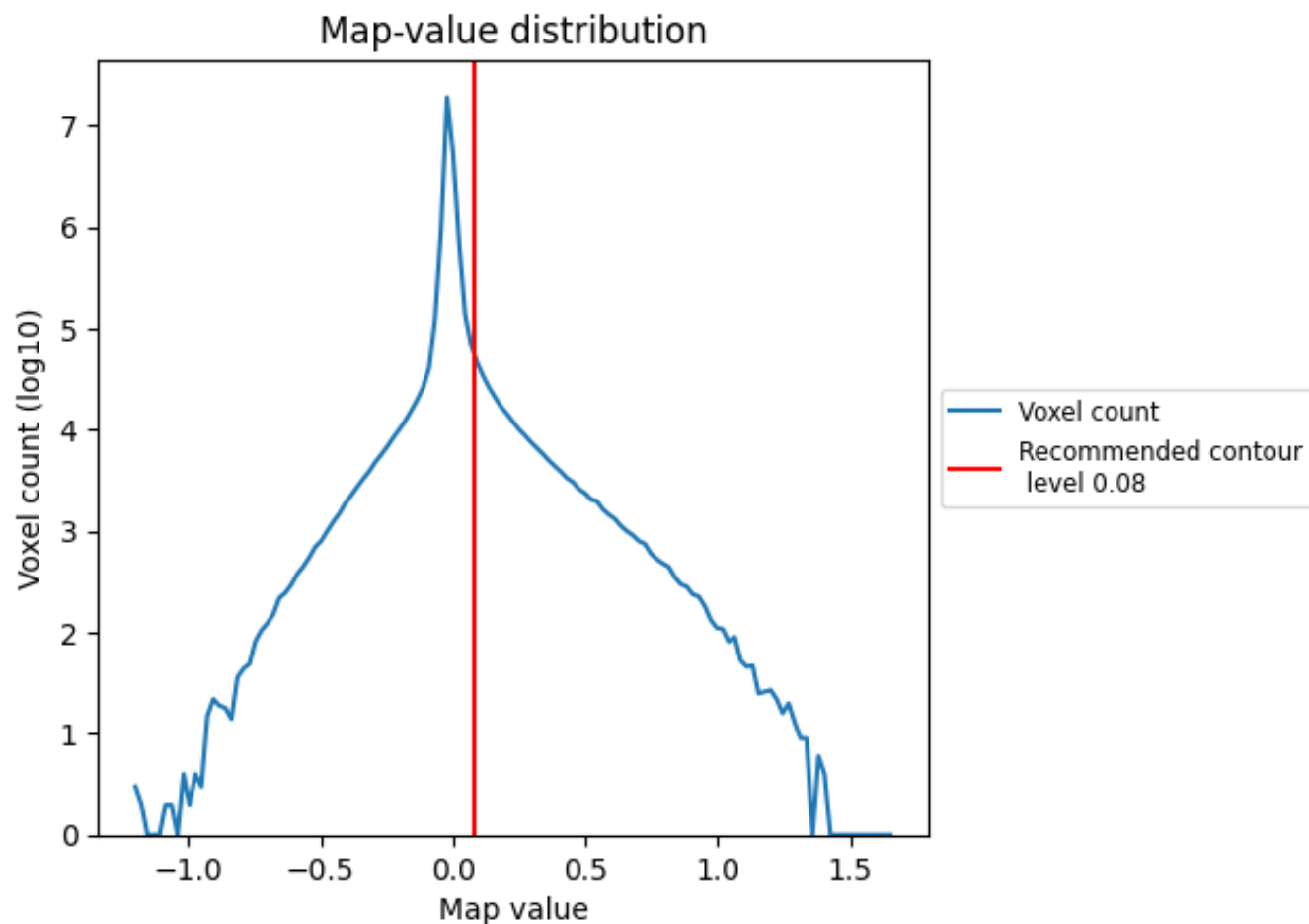
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

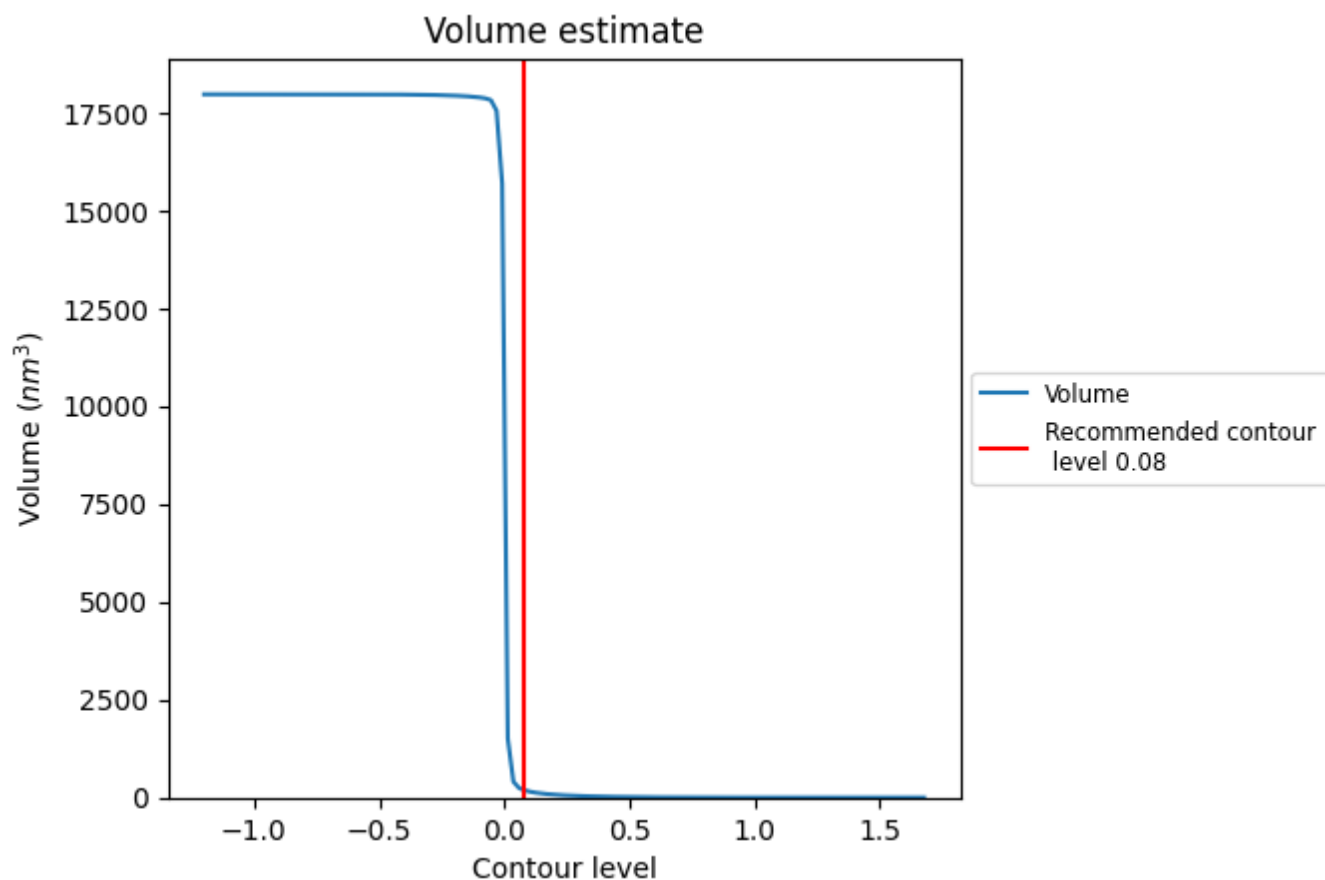
This section contains the results of statistical analysis of the map.

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.

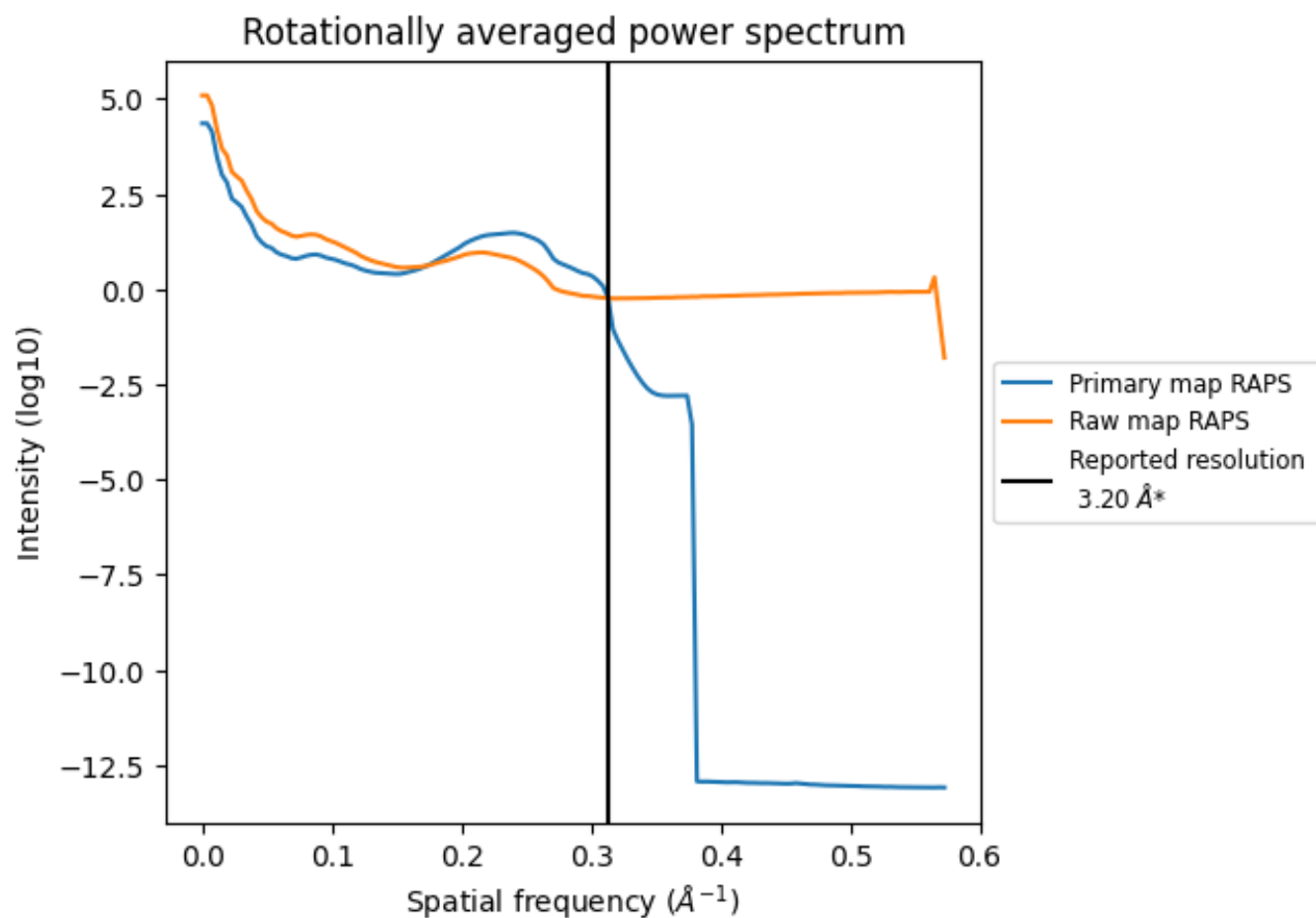
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 170 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 ⓘ

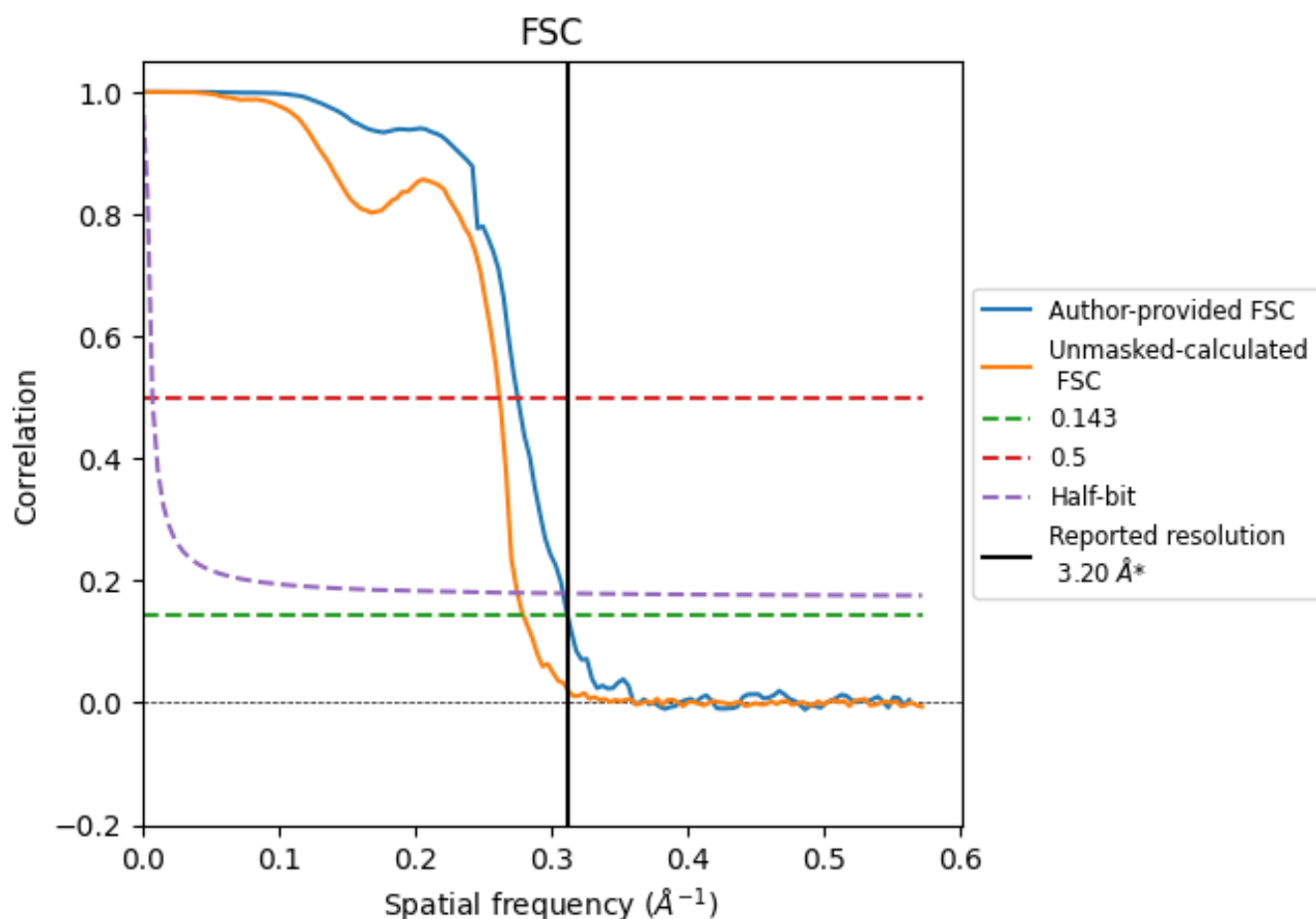


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

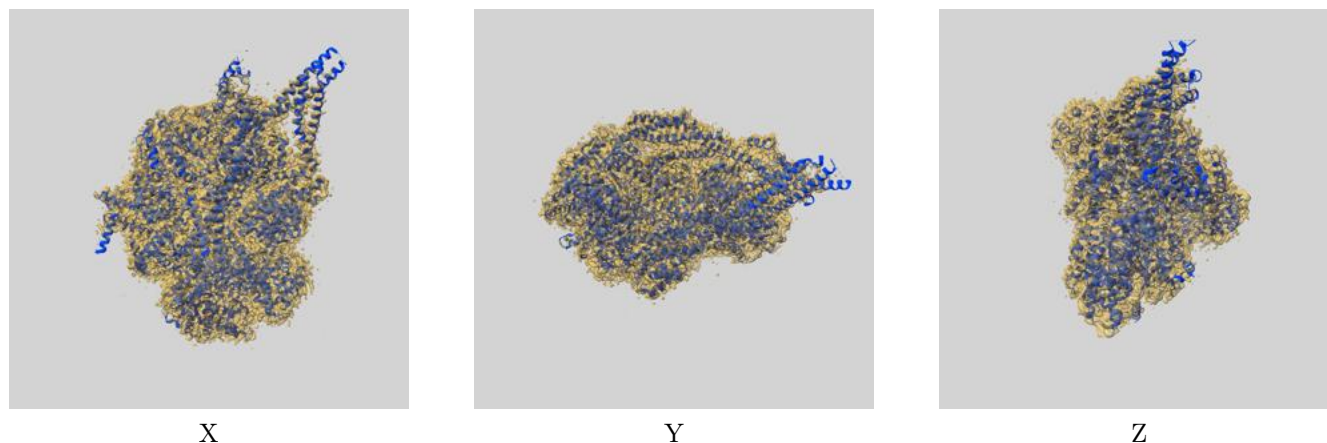
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.63	3.24
Unmasked-calculated*	3.57	3.81	3.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

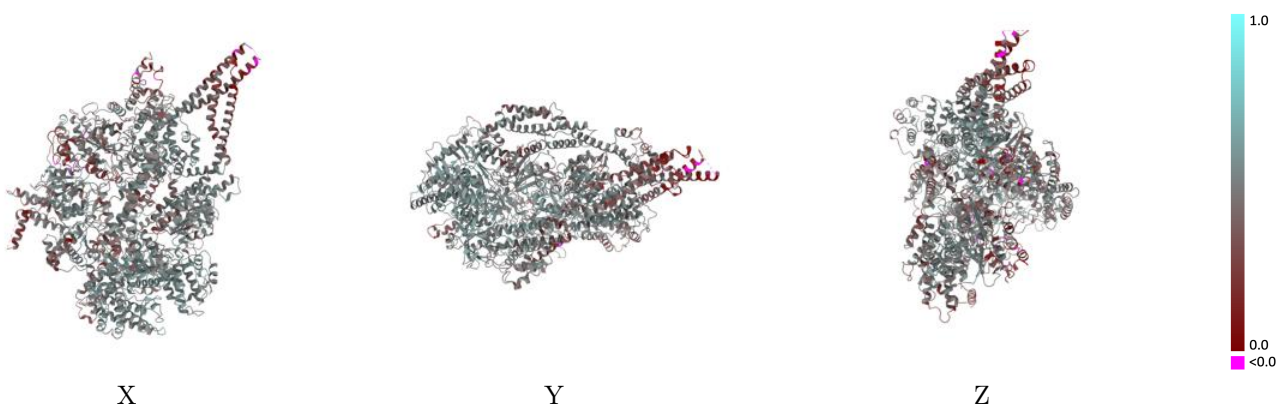
This section contains information regarding the fit between EMDB map EMD-81336 and PDB model 27PZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



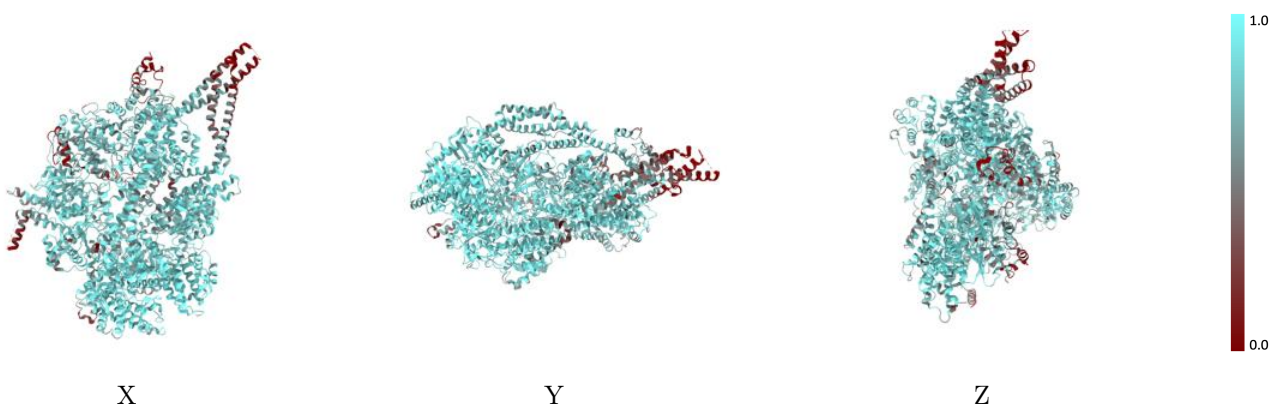
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



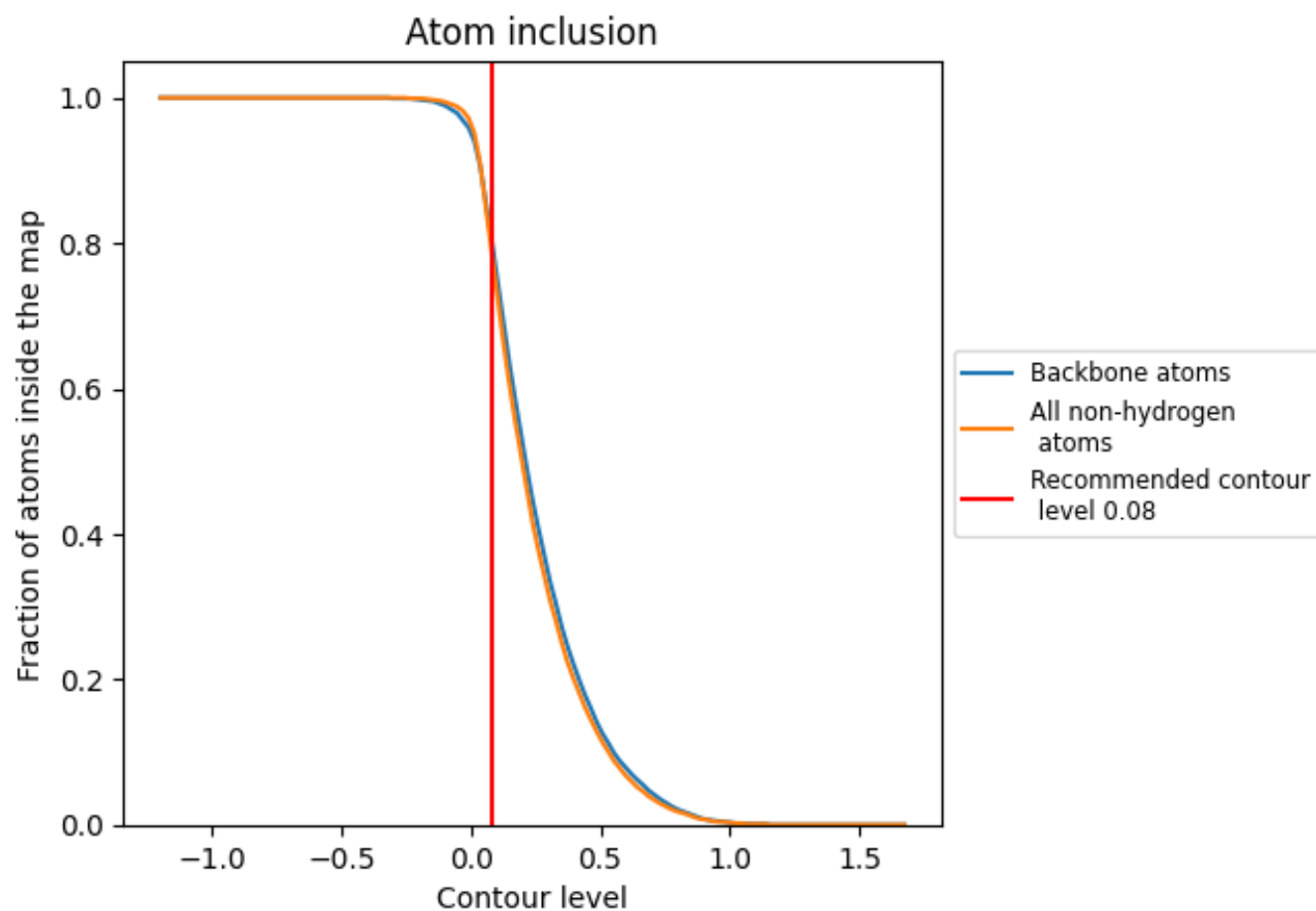
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.4680
A	0.7880	0.4680

