



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:17 AM UTC

PDB ID : 7OTY / pdb_00007oty
EMDB ID : EMD-13069
Title : DNA-PKcs in complex with M3814
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 2.96 Å(reported)

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

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

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

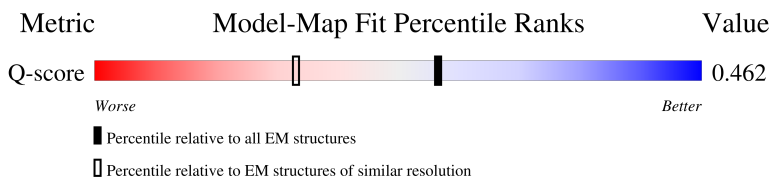
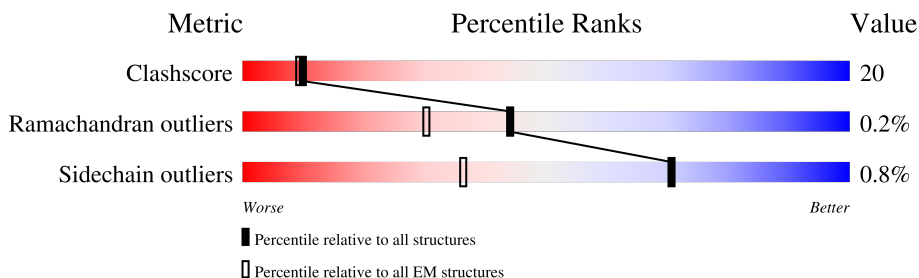
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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	4148	

2 Entry composition [i](#)

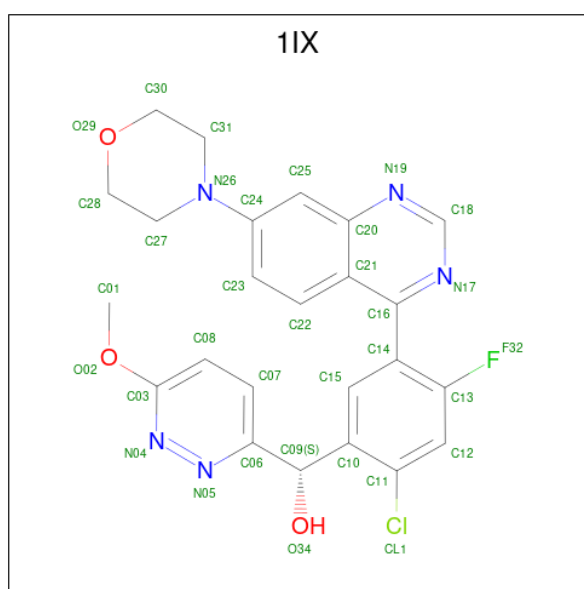
There are 2 unique types of molecules in this entry. The entry contains 29034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3656	29000	18604	4900	5305	191	0	0

- Molecule 2 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (CCD ID: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
2	A	1	34	24	1	1	5	3	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-PKCs







K6020	L3424	L3425	Q3326	N3327	L3328	L3329	T3332	R3335	L3336	R3336	L3254	A3255	K3256	K3257	L3258	L3259	L3262	E3344	L3348	E3265	S3266	K3267	T3268	R3269	D3270	D3271	K3272	L3273	K3276	V3277	Q3278	C3281	E3282	L3283	S3284	H3285	S3288	R3289	C3293	S3294	E3295	Q3296	V3297	L3298	L3301	D3308	E3309	N3310	N3311	L3316	N3319	A3322	D3325
	L3424	R3425	Q3326	N3327	L3328	L3329	T3332	R3335	I3336	R3336	L3254	ALA	SER	VAL	ILE	ASP	SER	ALA	GLU	L3439	Y3442	K3449	K3450	L3451	K3452	A3453	L3454	N3459	R3462	L3463	K3464	F3465	P3466	L3469	R3474	E3478	T3479	L3480	L3482	L3487	V3490	P3491	C3492	W3493	F3495	I3496	S3497	W3498	I3499	S3500	H3501	K3502	L3505
	L3506	V3512	A3513	Q3514	Q3515	V3518	E3519	E3520	I3521	T3522	P3526	Q3527	A3528	I3529	V3530	Y3531	T3535	E3538	F3542	K3543	N3551	K3552	E3553	F3554	V3555	I3558	L3562	V3567	I3568	Q3569	N3573	A3574	L3575	E3582	L3583	L3584	F3585	K3586	D3587	W3588	R3593	A3594	E3595	L3596	A3597	K3598	T3599						
	P3600	V3601	N3602	K3603	K3604	N3605	L3606	E3607	K3608	N3609	Y3610	E3611	Y3614	L3617	G3618	D3619	P3620	K3621	A3622	P3623	R3629	I3633	K3638	E3639	F3640	D3641	K3642	H3643	F3644	G3645	K3646	S3649	K3650	L3651	K3655	L3656	S3657	D3658	F3659	M3660	D3661	I3662	T3663	N3664	H3665	L3666	L3667	L3668	K3669	M3670	N3671	K3672	D3673
	P3676	P3677	K3681	S3684	P3685	W3686	K3687	S3688	K3691	V3692	E3693	F3694	L3695	K3696	N3697	E3698	L3699	E3700	I3701	Q3704	G3707	K3710	P3711	L3712	P3713	E3714	R3718	F3722	D3723	M3729	A3730	S3731	L3732	R3733	R3734	R3737	L3738	I3739	P3749	F3750	L3751	V3752	K3753	G3754	G3755	E3756	R3759						
	Q3760	R3763	A3776	L3786	R3789	T3790	Y3791	S3792	V3793	M3796	T3797	S3798	R3799	L3800	G3801	L3802	I3803	E3804	E3807	V3810	T3811	L3812	K3813	T3819	M3820	Y3855	M3858	Y3859	R3864	T3867	V3868	V3878	D3881	L3882	L3883	K3884	R3885	A3886	F3887	V3888	R3889	M3890	E3895	L3898									
	L3910	L3911	C3912	L3913	L3917	L3925	K3929	K3932	E3933	L3938	G3939	L3940	G3943	F3946	A3949	L3953	P3960	R3961	L3962	L3963	T3964	R3965	Q3966	F3967	K3971	L3972	P3973	E3976	V3985	F3991	R3992	P3995	D3996	G3996	L3997	L3998	T3999	N4000	T4001	N4002	D4003	V4004	F4005	D4012									
	K4013	K4014	N4015	F4016	E4017	Q4018	K4019	M4020	L4021	K4022	K4023	G4024	G4025	Q4029	E4030	I4031	N4032	V4033	A4034	E4035	C4045	K4048	R4049	D4062	Y4077	A4081	S4084	K4085	D4086	R4090	E4101	T4102	Q4103	V4104	M4108	D4109	Q4110	A4111	T4112	R4119	T4120	M4121	E4122	G4123	W4124	E4125	M4128						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.272	Depositor
Minimum map value	-2.388	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.29	Depositor
Map size ($\text{\AA}$)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.304, 1.304, 1.304	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: IIX

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	0.52	0/29492	0.61	8/39881 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3494	GLN	N-CA-C	-7.43	102.87	110.97
1	A	3492	CYS	N-CA-C	6.71	119.81	107.73
1	A	3753	LYS	N-CA-C	-6.64	100.00	109.96
1	A	1884	LEU	CA-C-N	-6.37	113.97	120.85
1	A	1884	LEU	C-N-CA	-6.37	113.97	120.85

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	29000	0	29178	1076	0
2	A	34	0	0	1	0
All	All	29034	0	29178	1076	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 20.

The worst 5 of 1076 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:1019:ASP:H	1:A:1020:PRO:CD	1.54	1.21
1:A:3575:LEU:CD1	1:A:3802:LEU:HD11	1.71	1.19
1:A:3752:VAL:HG22	1:A:3802:LEU:CD2	1.75	1.17
1:A:3075:LYS:O	1:A:3079:GLU:HG2	1.49	1.13
1:A:1019:ASP:H	1:A:1020:PRO:HD2	1.10	1.08

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	3602/4148 (87%)	3230 (90%)	365 (10%)	7 (0%)	43	66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1019	ASP
1	A	3692	VAL
1	A	3495	PHE
1	A	2787	HIS
1	A	3406	ALA

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	3194/3671 (87%)	3170 (99%)	24 (1%)	73 85

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3695	LEU
1	A	3751	LEU
1	A	3729	MET
1	A	3803	ILE
1	A	2460	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3390	GLN
1	A	3494	GLN
1	A	1771	GLN
1	A	1614	GLN
1	A	3501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1IX	A	6101	-	38,38,38	2.96	15 (39%)	53,54,54	2.65	23 (43%)

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	1IX	A	6101	-	-	4/18/26/26	0/5/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	1IX	O29-C30	-10.87	1.00	1.42
2	A	6101	1IX	C12-C13	5.36	1.46	1.37
2	A	6101	1IX	C21-C20	-5.35	1.34	1.42
2	A	6101	1IX	C14-C16	5.18	1.55	1.49
2	A	6101	1IX	C16-N17	-4.23	1.28	1.32

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	1IX	C30-O29-C28	7.98	135.69	109.88
2	A	6101	1IX	C10-C09-C06	-6.43	105.09	111.20
2	A	6101	1IX	C18-N19-C20	5.55	121.74	115.43
2	A	6101	1IX	C21-C20-N19	-4.75	117.78	122.82
2	A	6101	1IX	C21-C16-N17	-4.69	119.95	123.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

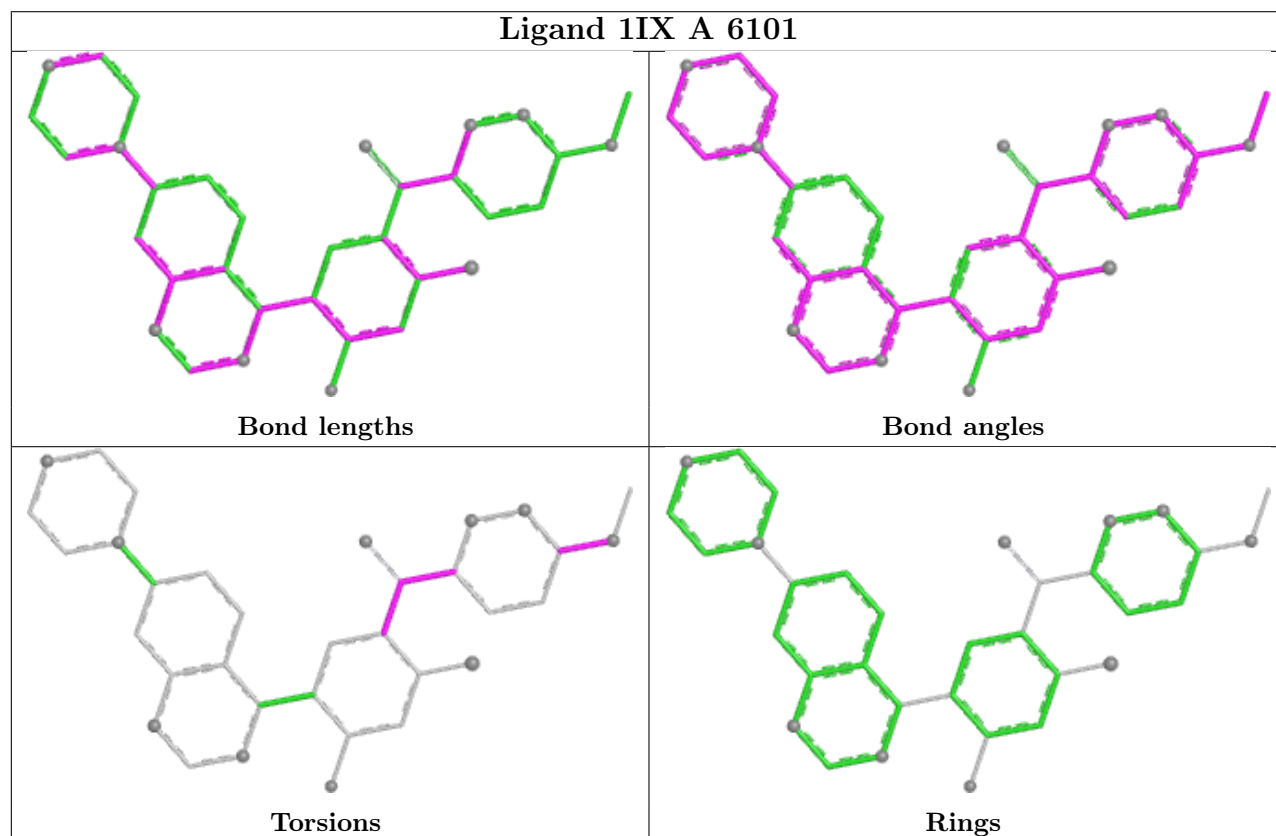
Mol	Chain	Res	Type	Atoms
2	A	6101	1IX	N04-C03-O02-C01
2	A	6101	1IX	C08-C03-O02-C01
2	A	6101	1IX	C06-C09-C10-C11
2	A	6101	1IX	N05-C06-C09-O34

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	1IX	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	82.32

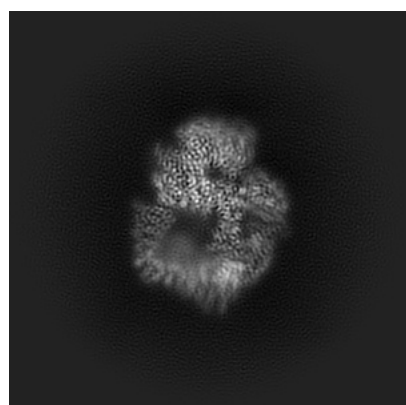
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13069. These allow visual inspection of the internal detail of the map and identification of artifacts.

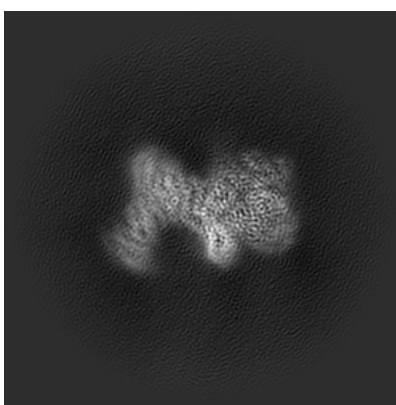
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

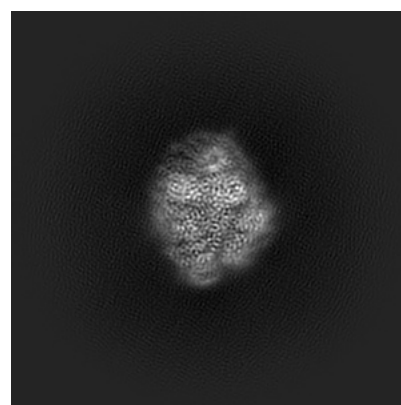
6.1.1 Primary map



X



Y

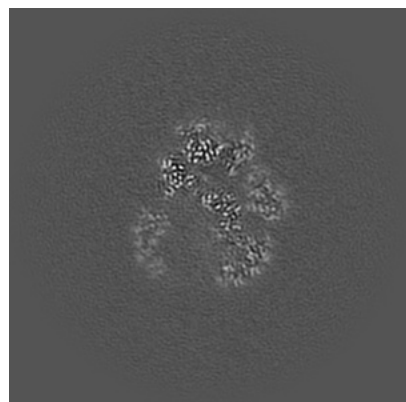


Z

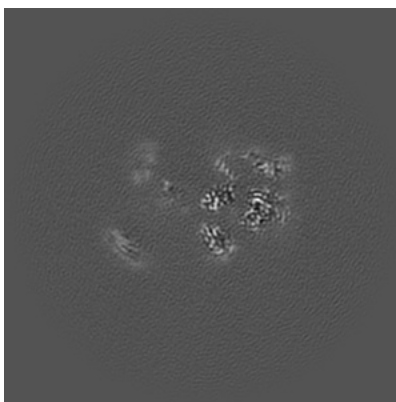
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

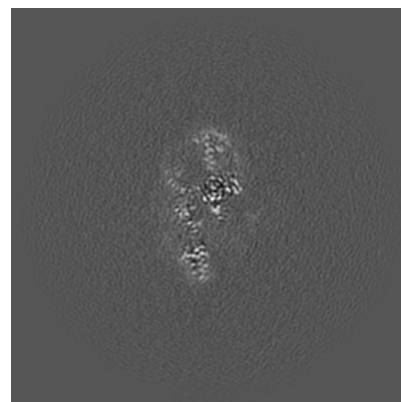
6.2.1 Primary map



X Index: 130



Y Index: 130

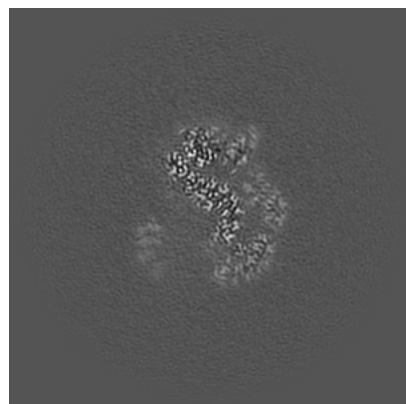


Z Index: 130

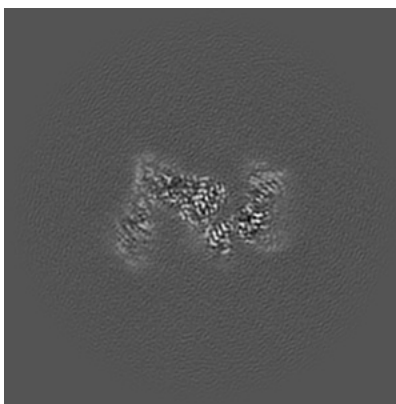
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

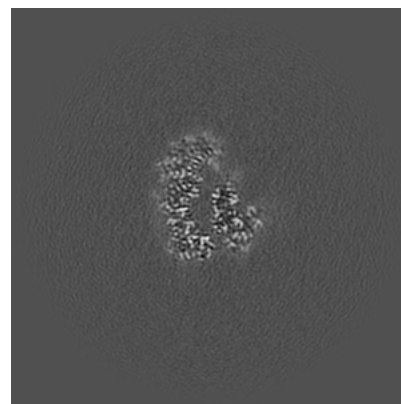
6.3.1 Primary map



X Index: 134



Y Index: 142

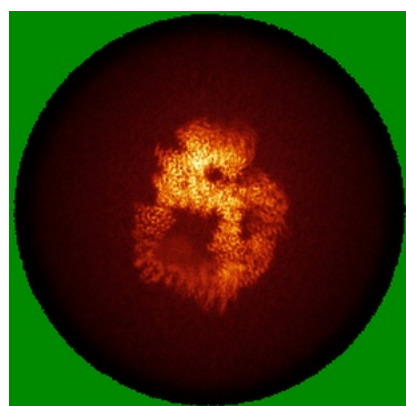


Z Index: 141

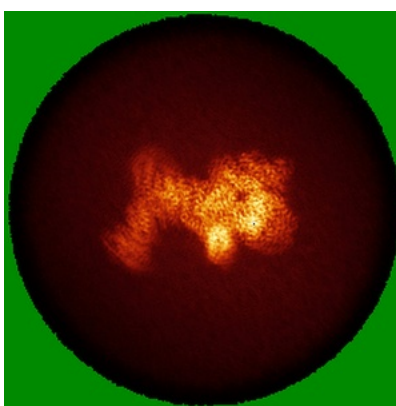
The images above show the largest variance slices of the map in three orthogonal directions.

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

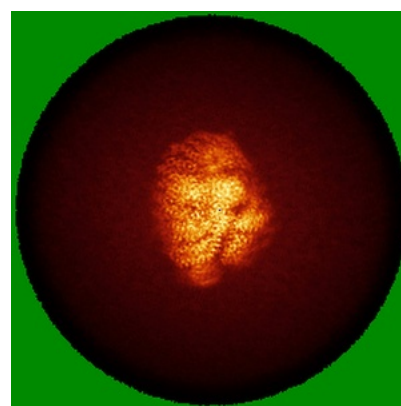
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

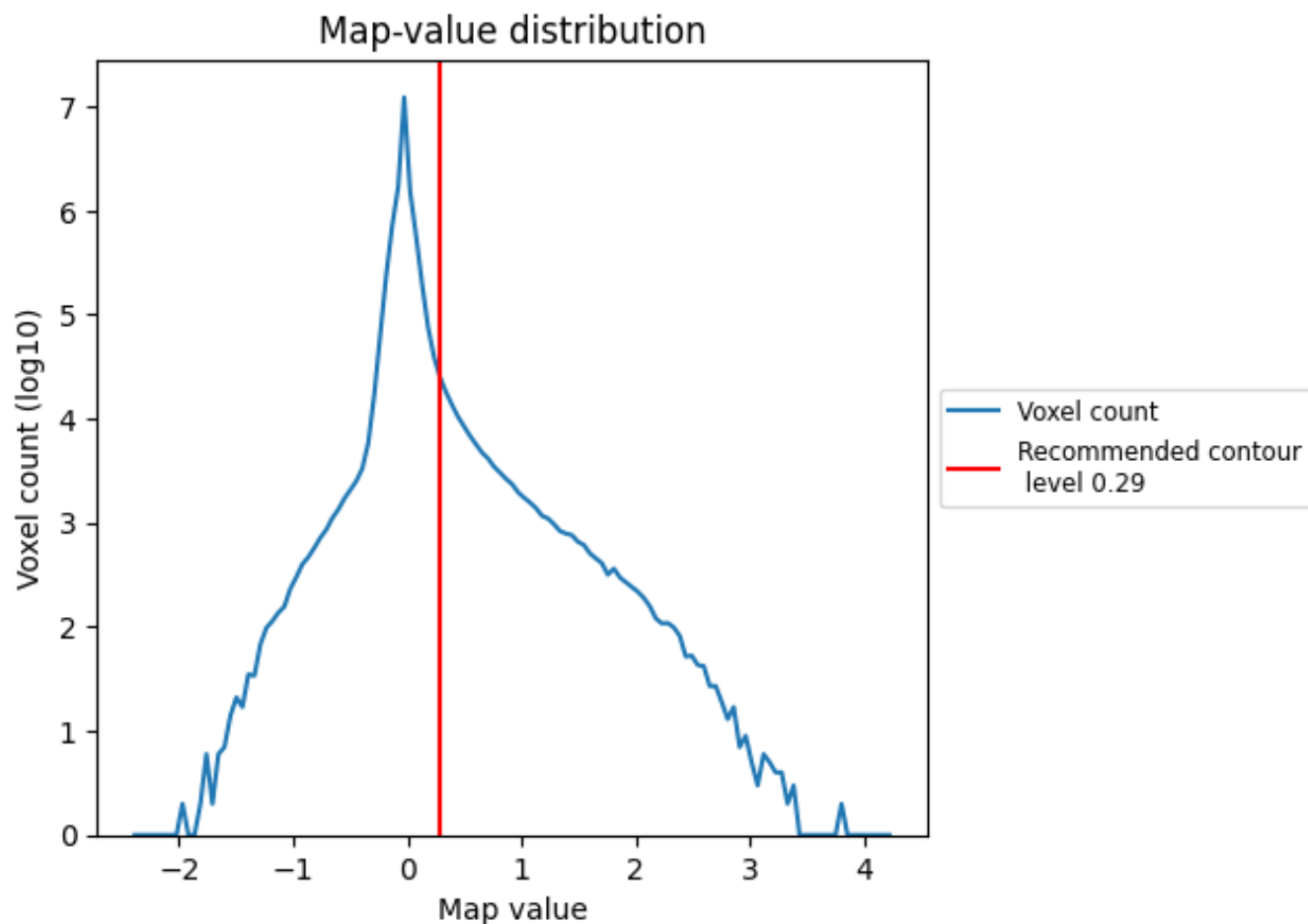
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

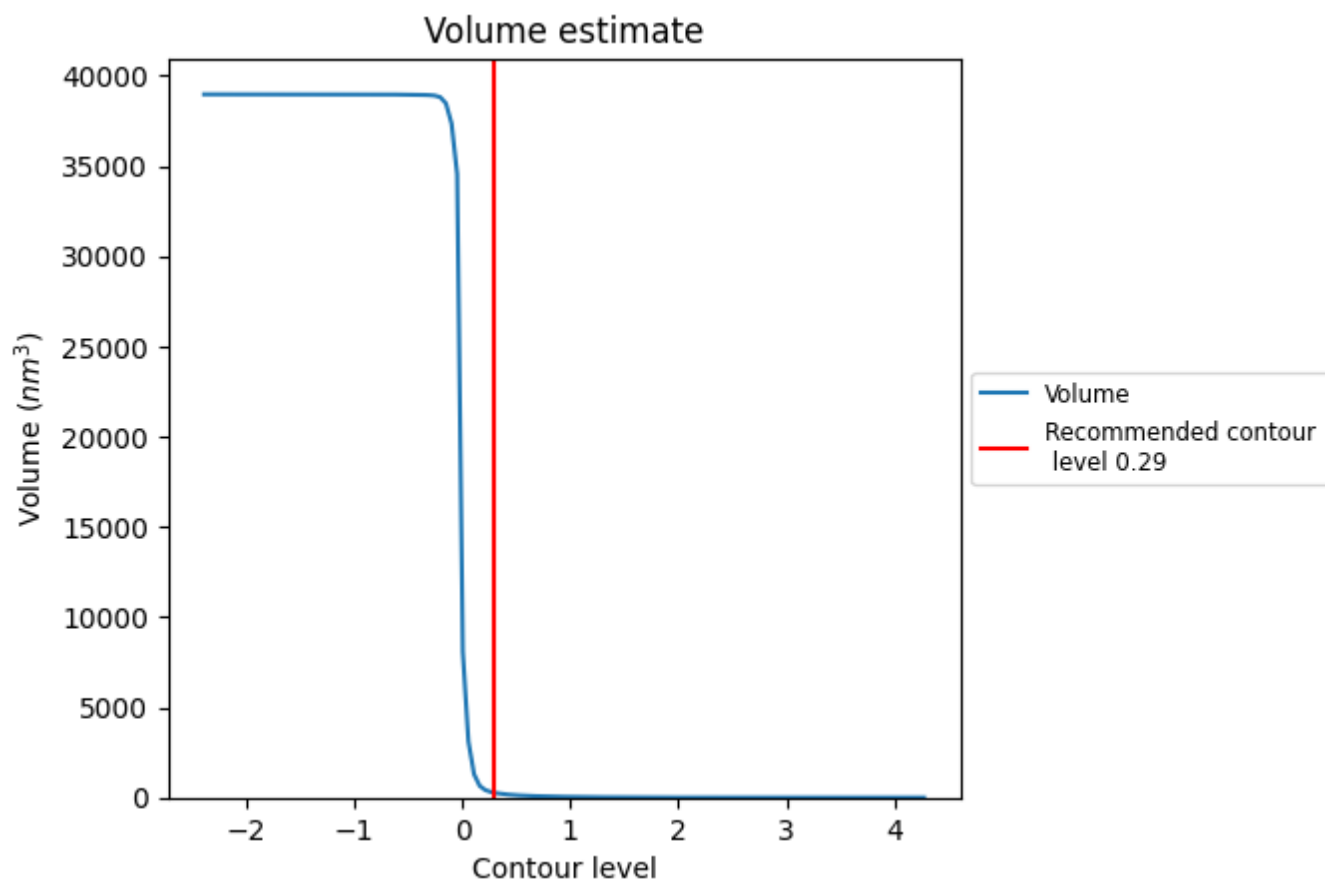
This section contains the results of statistical analysis of the map.

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.

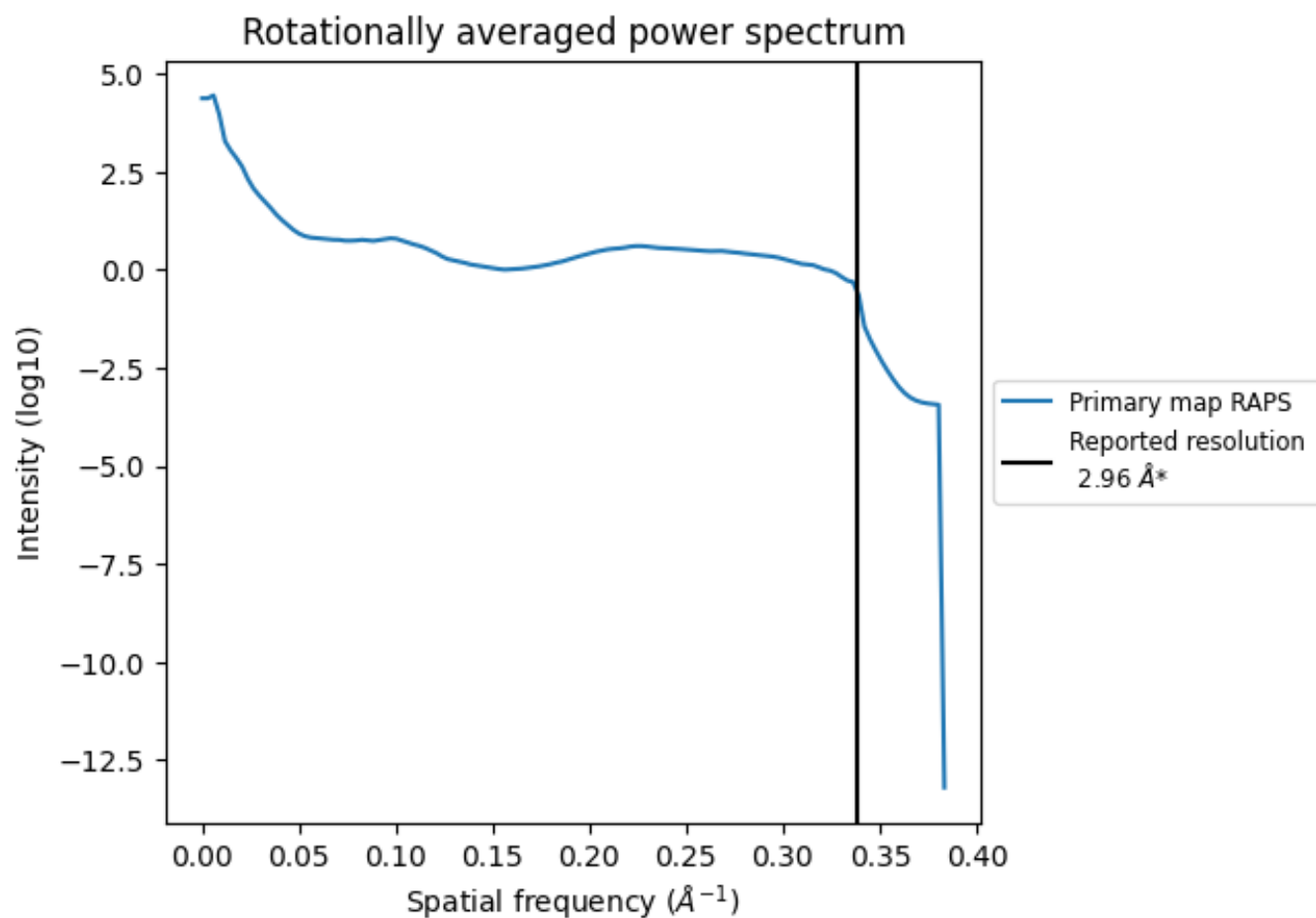
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 0.338 Å⁻¹

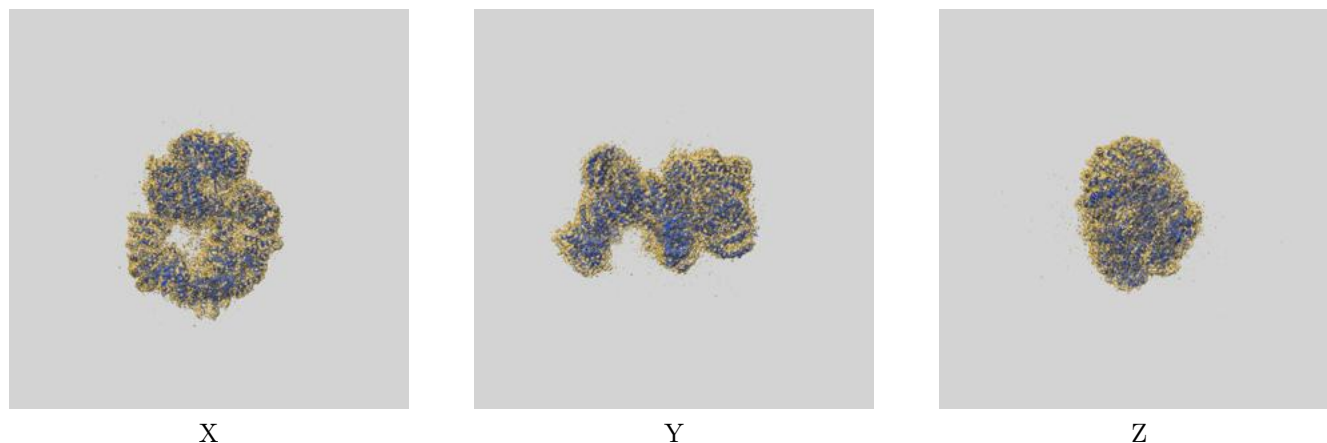
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

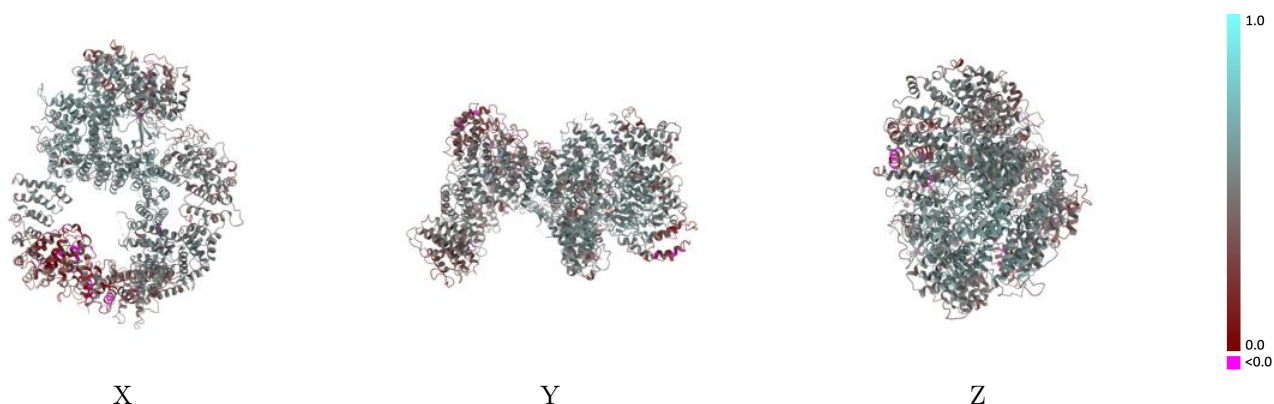
This section contains information regarding the fit between EMDB map EMD-13069 and PDB model 7OTY. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



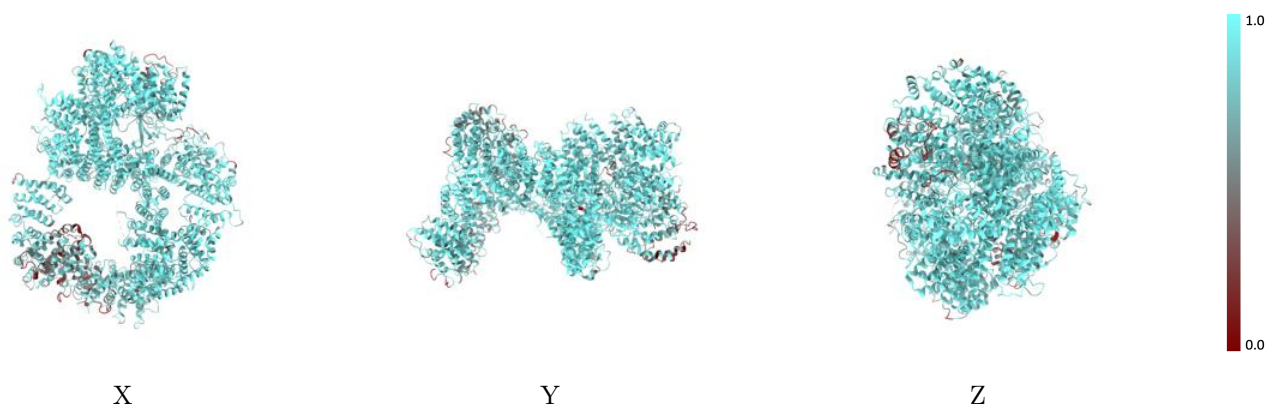
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



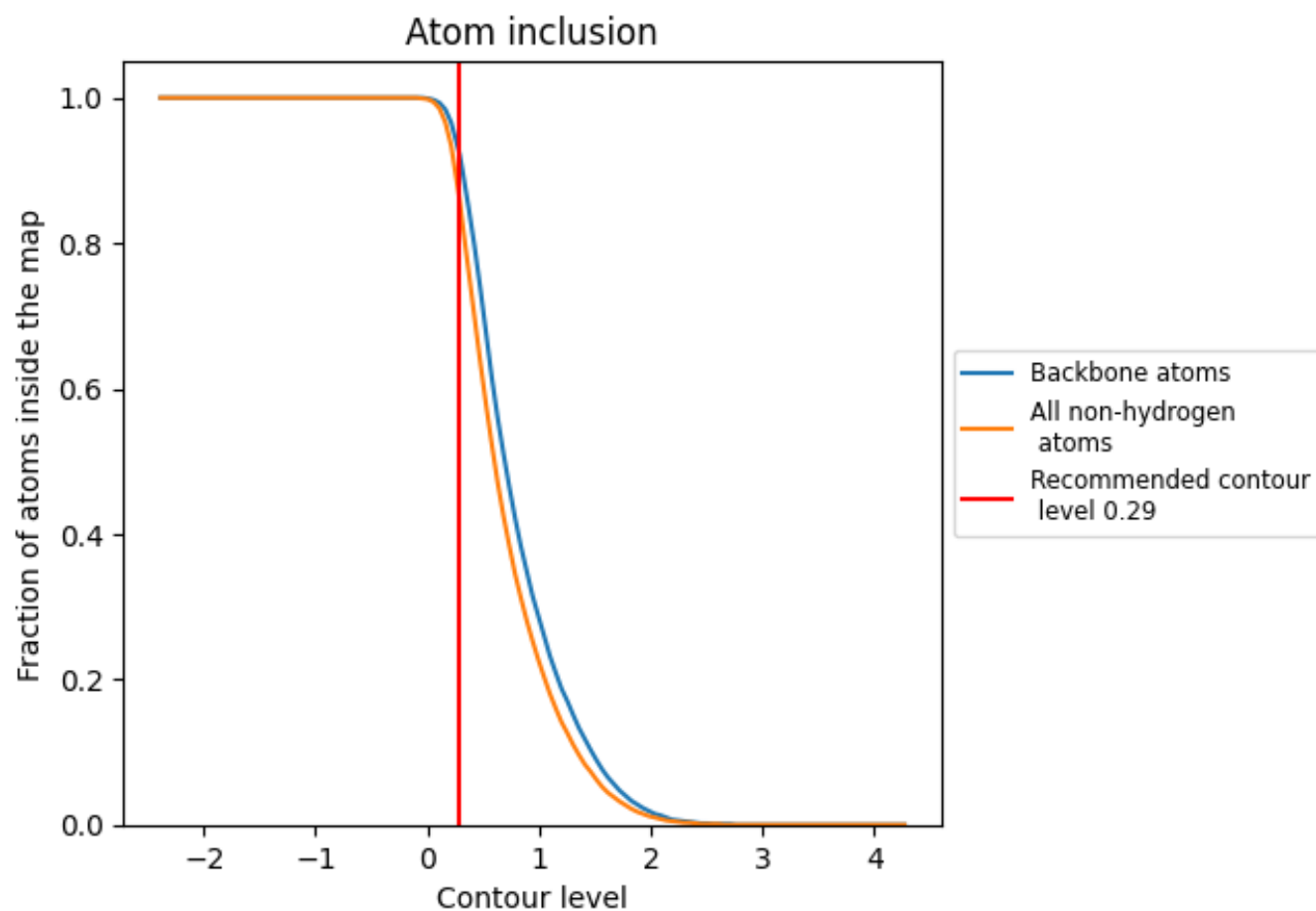
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.4620
A	0.8590	0.4620

