



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 11:53 PM UTC

PDB ID : 7OTP / pdb_00007otp
EMDB ID : EMD-13064
Title : DNA-PKcs in complex with ATPgammaS-Mg
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 3.40 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

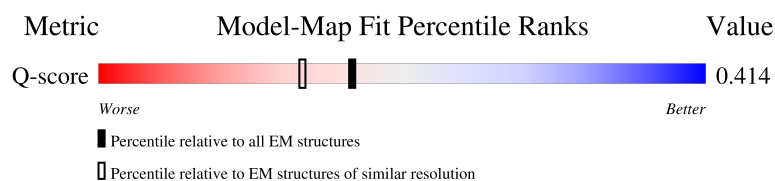
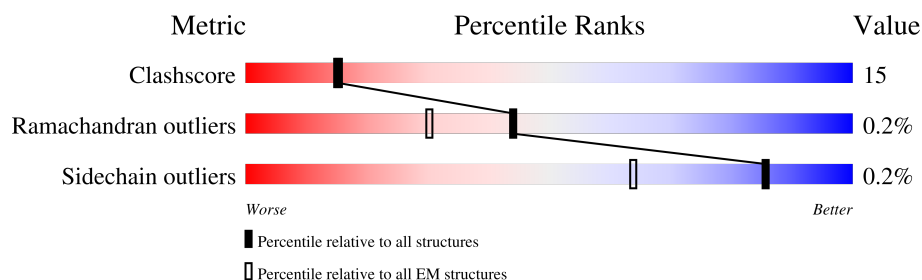
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	4148	

2 Entry composition [i](#)

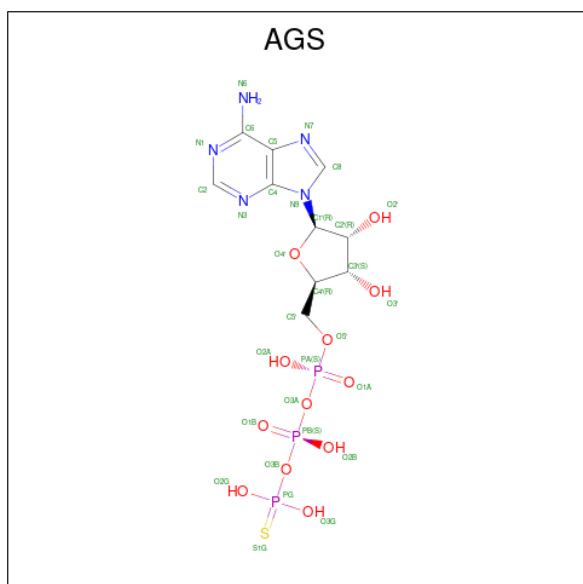
There are 3 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	3656	Total	C	N	O	S	0	0
			29006	18606	4902	5307	191		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



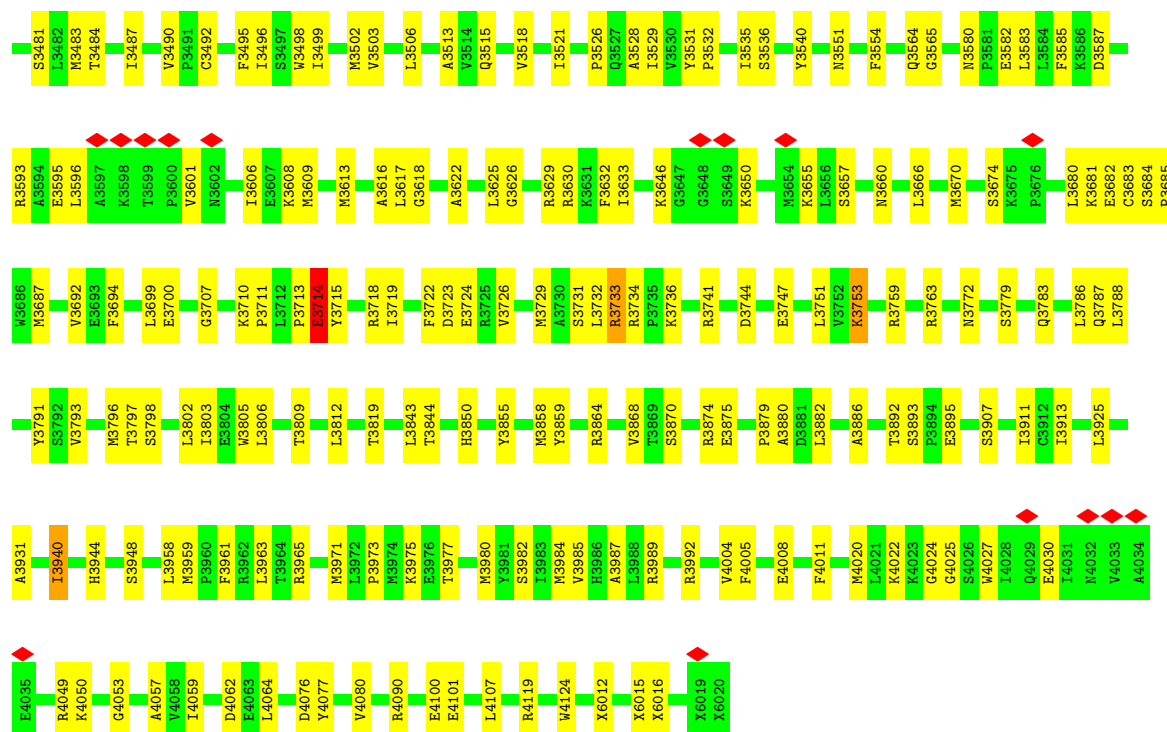
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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

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



A3356	E3033	L3160	P2887	LYS	PHE	CYS	T2395	K2320	L2235	V2150	PRO
R3357	P3034	L3161	E2894	GLN	THR	GLU	L2396	E2321	E2236	I2151	THR
E3361	M3044	R3162	E2894	ALA	LEU	PHE	C2397	V2322	L2237	I2152	VAL
A3381	S3047	N3166	L2898	VAL	THR	GLN	L2398	L2323	L2241	T2153	HIS
R3382	K3048	P3169	L2899	GLY	THR	GLU	L2399	G2324	L2242	F2157	ASP
Q3383	L3051	D3170	L2900	VAL	ALA	THR	V2400	L2326	L2245	Y2160	ASP
L3384	D3058	M3173	P2902	LEU	ASP	ILE	W2408	L2327	W2245	Y2160	VAL
S3386	Q3059	K3176	ALA	THR	ASP	THR	L2415	L2328	L2249	W2164	LEU
E3387	D3066	I3182	ALA	ARG	ASP	ASP	L2411	L2329	S2250	L2164	GLU
E3395	M3069	I3183	LYS	HIS	ASP	PHE	Y2412	V2330	L2251	L2168	GLU
A3396	L3072	R3186	GLY	ASP	THR	ARG	L2415	K2334	P2252	S2167	M2085
PRO	E3072	I3187	LEU	ASP	THR	THR	M2424	W2335	Y2253	L2088	
PRO	L3073	C3187	ARG	THR	THR	THR	R2431	L2337	L2254	W2089	
TRP	Q3074	I3193	LYS	THR	THR	VAL	C2435	E2338	L2256	R2090	
TRP	I3077	E3194	ALA	THR	THR	LEU	L2439	S2340	F2257	S2174	
CYS	L3078	E3197	ARG	THR	THR	THR	M2442	W2341	F2260	M2094	
GLY	L3197	THR	P2917	ASP	THR	PRO	P2443	L2344	S2261	A2095	
A3406	PRO	LEU	ALA	THR	THR	PHE	M2445	L2344	L2261	P2096	
PRO	PRO	PRO	LYS	THR	THR	THR	P2445	L2344	D2269	L2097	
TRP	E3072	I3197	GLY	THR	THR	VAL	L2451	L2344	N2270	T2098	
TRP	L3073	C3187	ARG	THR	THR	VAL	P2445	L2344	L2100	A2099	
TRP	Q3074	I3193	LYS	THR	THR	GLN	L2451	L2344	Y2184	V2101	
TRP	I3077	E3194	ALA	THR	THR	GLN	L2451	L2344	M2185	K2102	
CYS	L3078	E3197	ARG	THR	THR	GLN	L2451	L2344	V2187	S2107	
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344	E2188	L2108	
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344	V2190	GLY	
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344	L2193	PRO	
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344	L2194	PRO	
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344	S2185	GLN	
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344	W2196	GLY	
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344	P2206	GLU	
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344	K2207	ASP	
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344	Y2285	VAL	
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344	D2289	P2119	
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344	P2290	R2120	
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344	C2292	D2121	
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344	G2293	L2122	
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344	L2214	L2121	
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344	L2215	L2122	
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344	L2216	W2126	
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344	L2219	G2134	
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344	M2220	W2135	
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344	G2221	P2136	
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344	H2222	I2137	
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344	V2223	N2141	
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344	K2227	I2142	
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344	V2230	F2145	
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344	G2231	L2146	
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344	R2232	K2147	
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344	A2318	N2148	
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344	A2319	L2149	
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344			
TRP	I3077	E3194	ALA	THR	THR	THR	L2451	L2344			
CYS	L3078	E3197	ARG	THR	THR	THR	L2451	L2344			
GLY	L3197	THR	P2917	ASP	THR	THR	L2451	L2344			
A3406	PRO	LEU	ALA	THR	THR	THR	L2451	L2344			
PRO	PRO	PRO	LYS	THR	THR	THR	L2451	L2344			
TRP	E3072	I3197	GLY	THR	THR	THR	L2451	L2344			
TRP	L3073	C3187	ARG	THR	THR	THR	L2451	L2344			
TRP	Q3074	I3193	LYS	THR	THR	THR	L2451	L2344</			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63313	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 ($e^-/\text{\AA}^2$)	46.8	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	2.339	Depositor
Minimum map value	-1.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, AGS

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	0.30	0/29498	0.49	4/39889 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3715	TYR	N-CA-C	-9.09	101.15	112.88
1	A	722	LYS	N-CA-C	7.54	117.91	108.19
1	A	1239	PRO	CA-N-CD	-5.26	104.64	112.00
1	A	721	TYR	O-C-N	5.25	129.14	123.10

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	29006	0	29184	810	0
2	A	31	0	11	3	0
3	A	2	0	0	0	0
All	All	29039	0	29195	813	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 15.

The worst 5 of 813 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)
2:A:6101:AGS:C4'	2:A:6101:AGS:O4'	1.63	1.23
1:A:774:GLU:HG2	1:A:858:MET:HE3	1.53	0.90
1:A:189:MET:HG3	1:A:193:ALA:HB2	1.53	0.90
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.41	0.85
1:A:3670:MET:O	1:A:3674:SER:HB3	1.76	0.84

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%)	3284 (91%)	311 (9%)	7 (0%)	43 71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3714	GLU
1	A	3354	ASP
1	A	3406	ALA
1	A	723	ASP
1	A	2787	HIS

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	3195/3671 (87%)	3190 (100%)	5 (0%)	87 85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722	LYS
1	A	3714	GLU
1	A	3733	ARG
1	A	3753	LYS
1	A	3940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3070	HIS
1	A	3166	ASN
1	A	3162	ASN
1	A	3250	ASN
1	A	1331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	AGS	A	6101	3	32,33,33	3.61	11 (34%)	45,52,52	2.02	11 (24%)

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	AGS	A	6101	3	-	4/21/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	AGS	PG-S1G	10.32	2.13	1.90
2	A	6101	AGS	O4'-C4'	8.52	1.63	1.45
2	A	6101	AGS	C3'-C4'	-7.55	1.33	1.53
2	A	6101	AGS	PB-O3A	5.91	1.65	1.59
2	A	6101	AGS	C6-N6	5.26	1.47	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	AGS	C5-C4-N3	-6.26	118.10	126.72
2	A	6101	AGS	N3-C4-N9	4.86	135.43	127.17
2	A	6101	AGS	N3-C2-N1	-4.51	121.75	128.58
2	A	6101	AGS	C2-N3-C4	3.93	121.44	111.83
2	A	6101	AGS	N9-C8-N7	-3.57	108.88	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

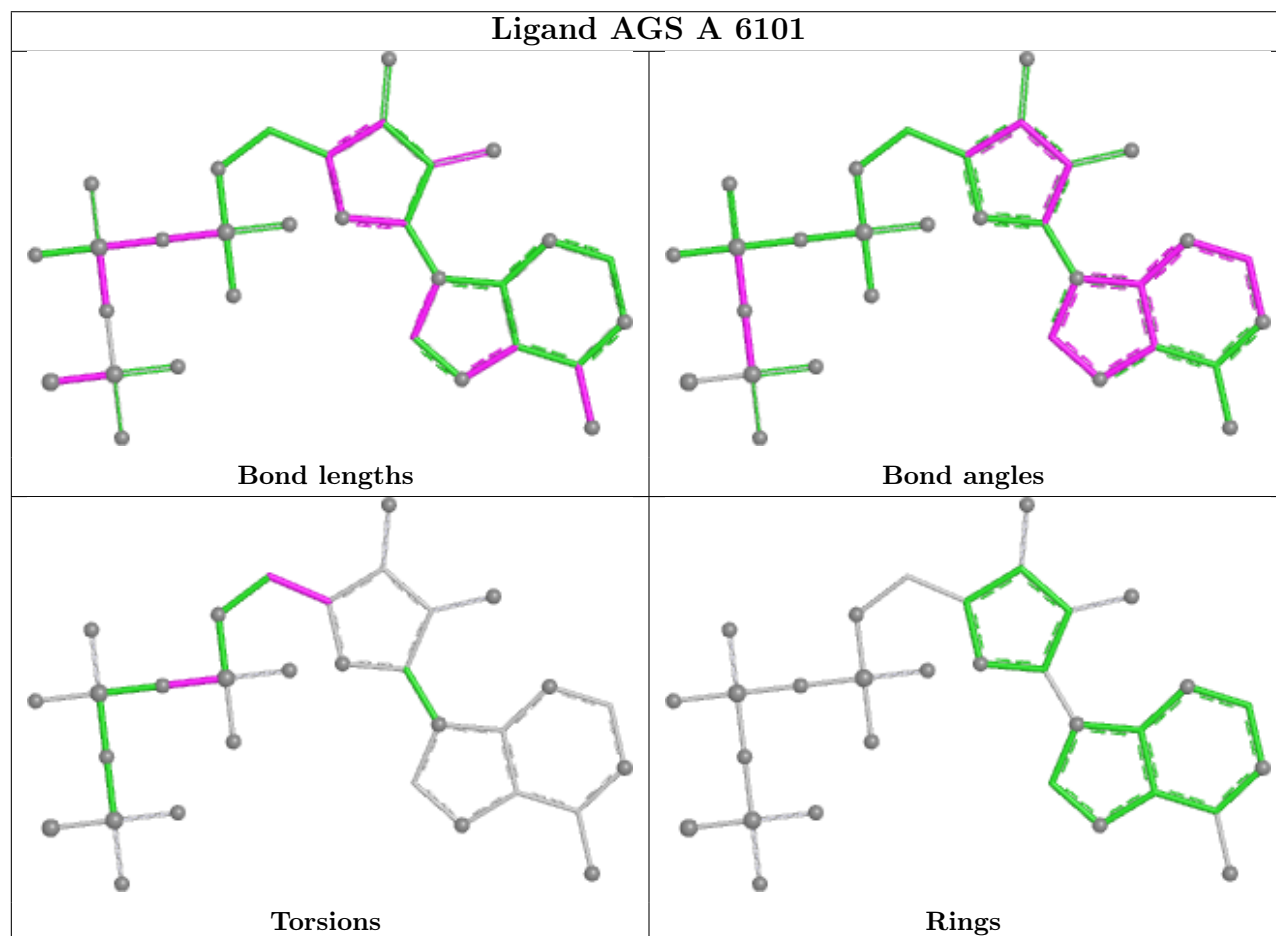
Mol	Chain	Res	Type	Atoms
2	A	6101	AGS	O4'-C4'-C5'-O5'
2	A	6101	AGS	C3'-C4'-C5'-O5'
2	A	6101	AGS	PB-O3A-PA-O1A
2	A	6101	AGS	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	AGS	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	81.75

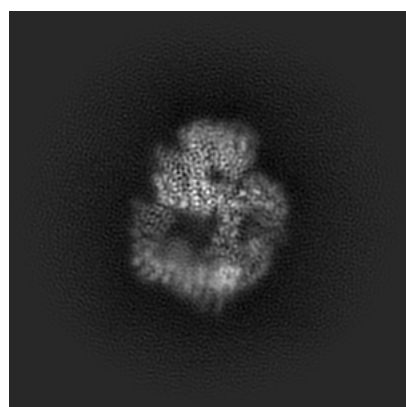
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13064. These allow visual inspection of the internal detail of the map and identification of artifacts.

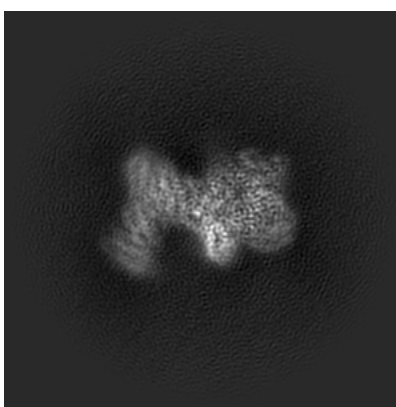
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

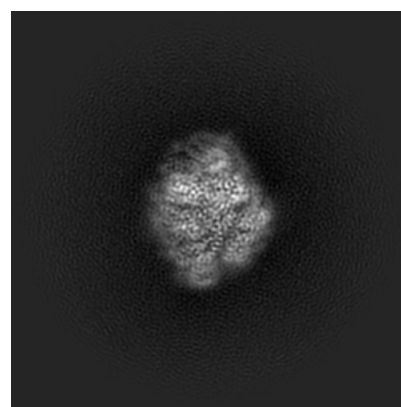
6.1.1 Primary map



X



Y

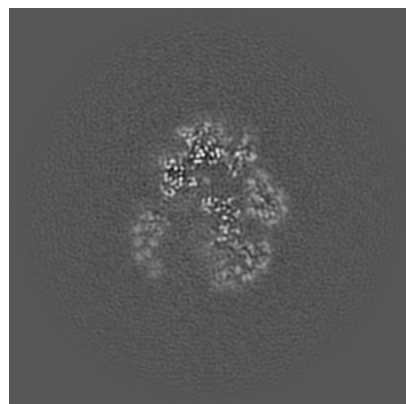


Z

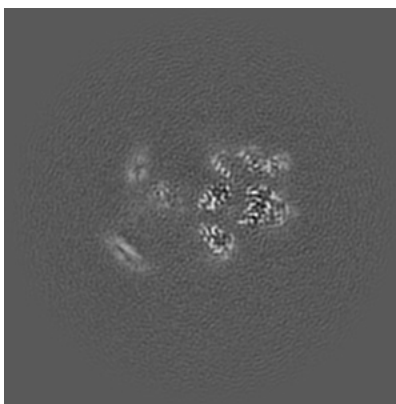
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

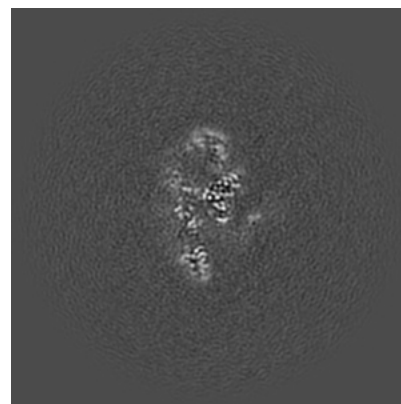
6.2.1 Primary map



X Index: 130



Y Index: 130

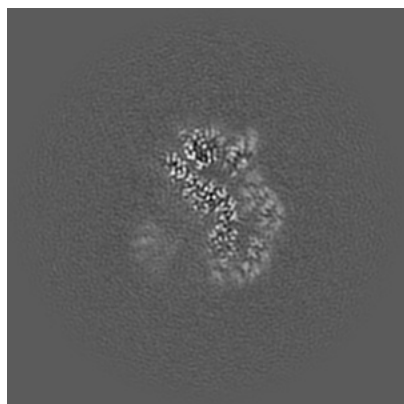


Z Index: 130

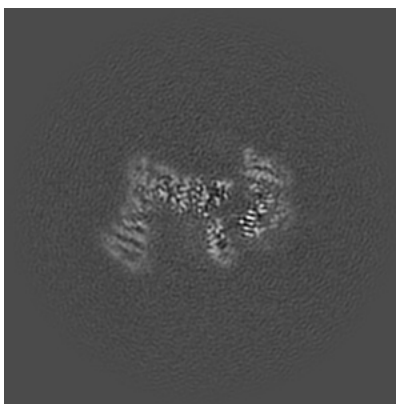
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

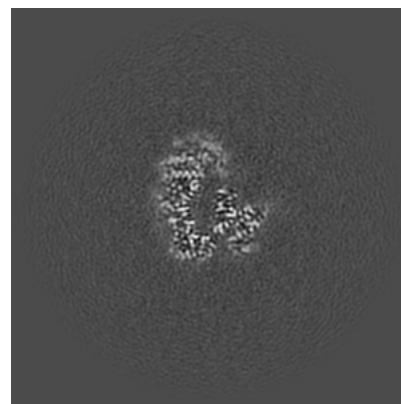
6.3.1 Primary map



X Index: 135



Y Index: 138

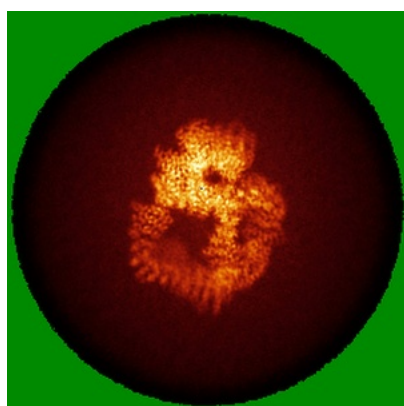


Z Index: 141

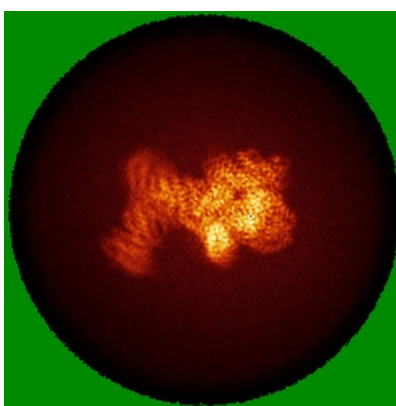
The images above show the largest variance slices of the map in three orthogonal directions.

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

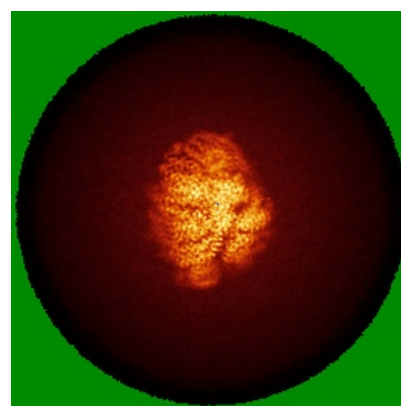
6.4.1 Primary map



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](#)

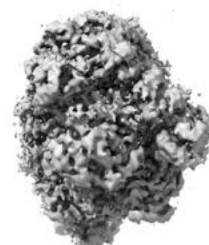
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

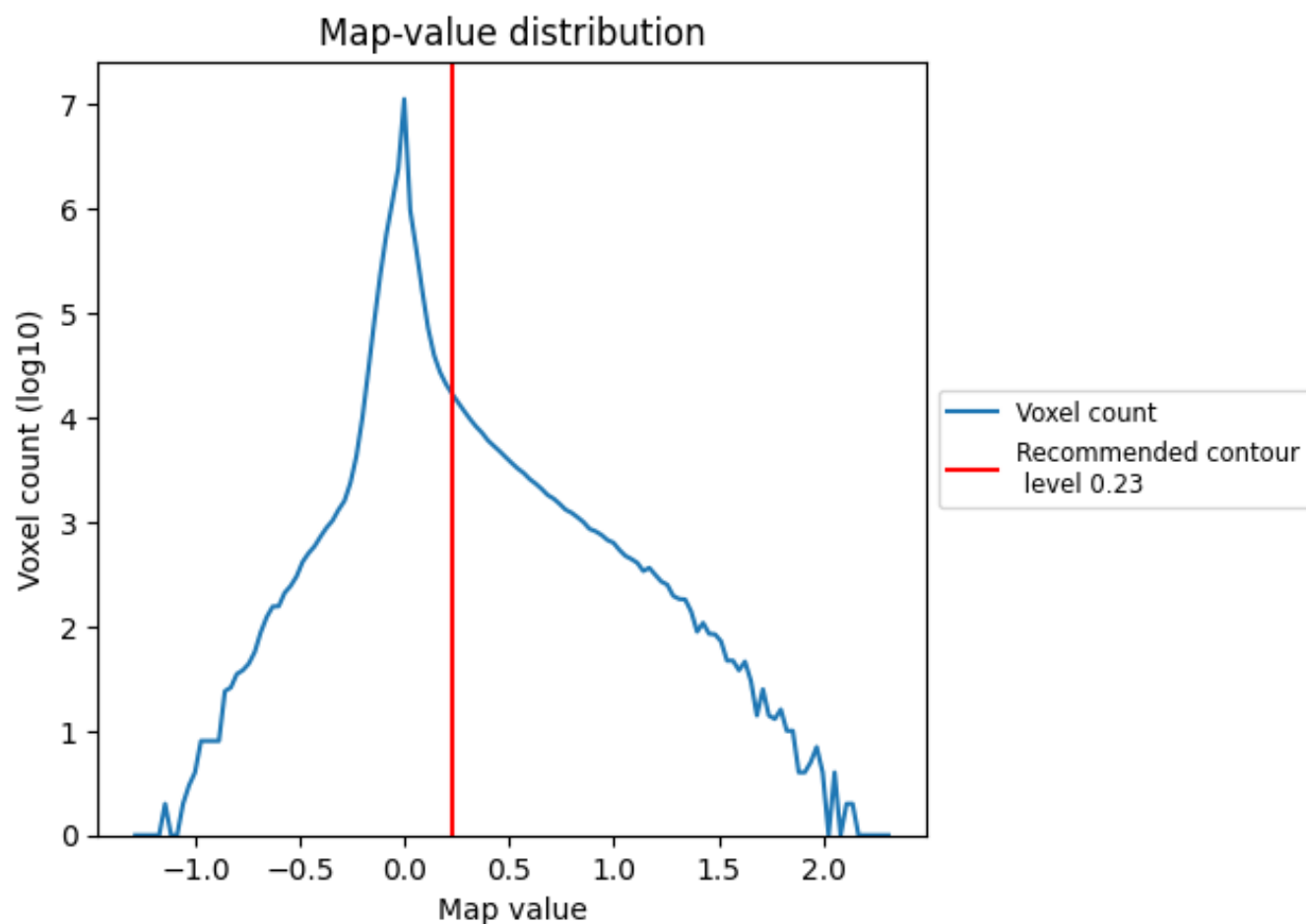
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

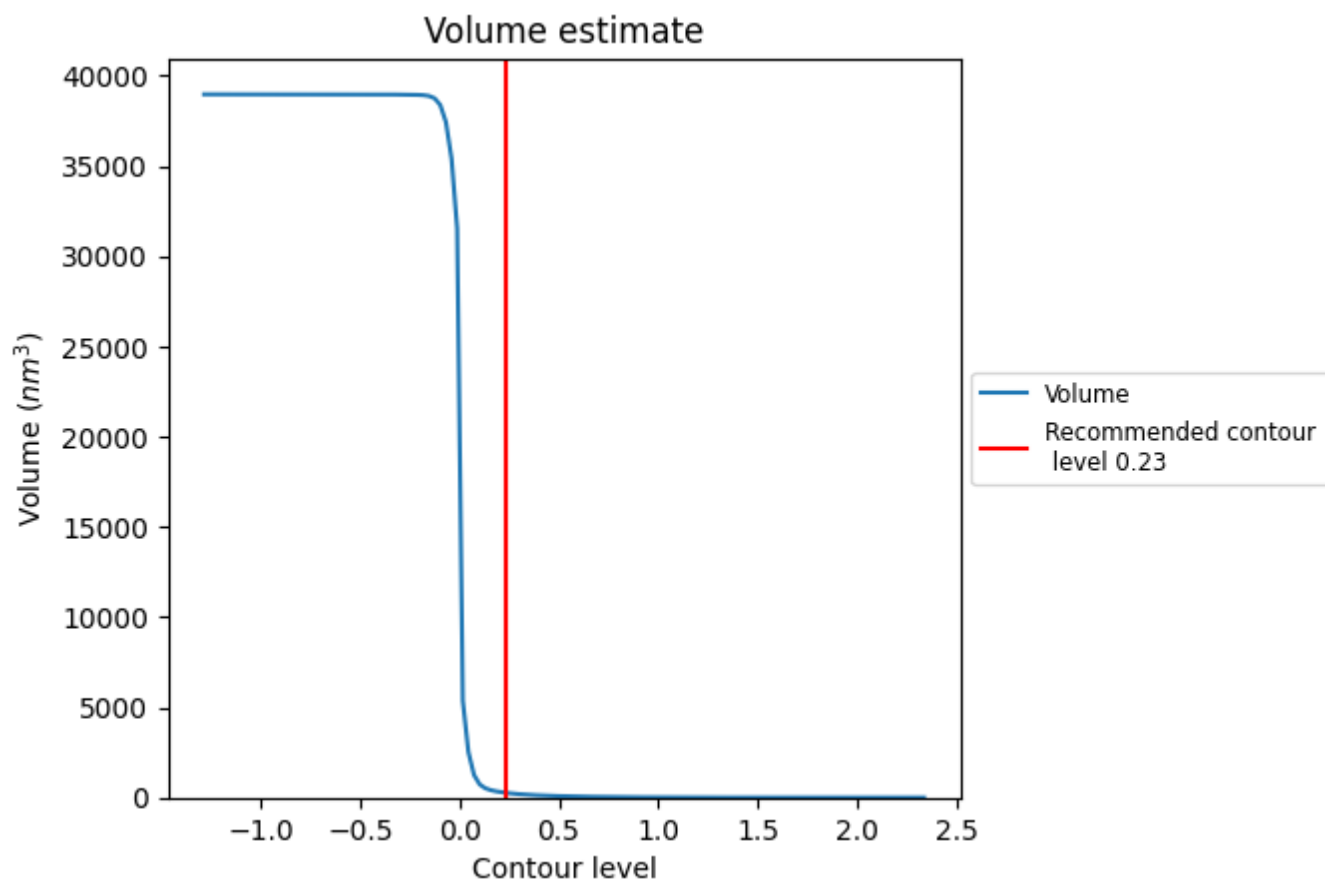
This section contains the results of statistical analysis of the map.

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.

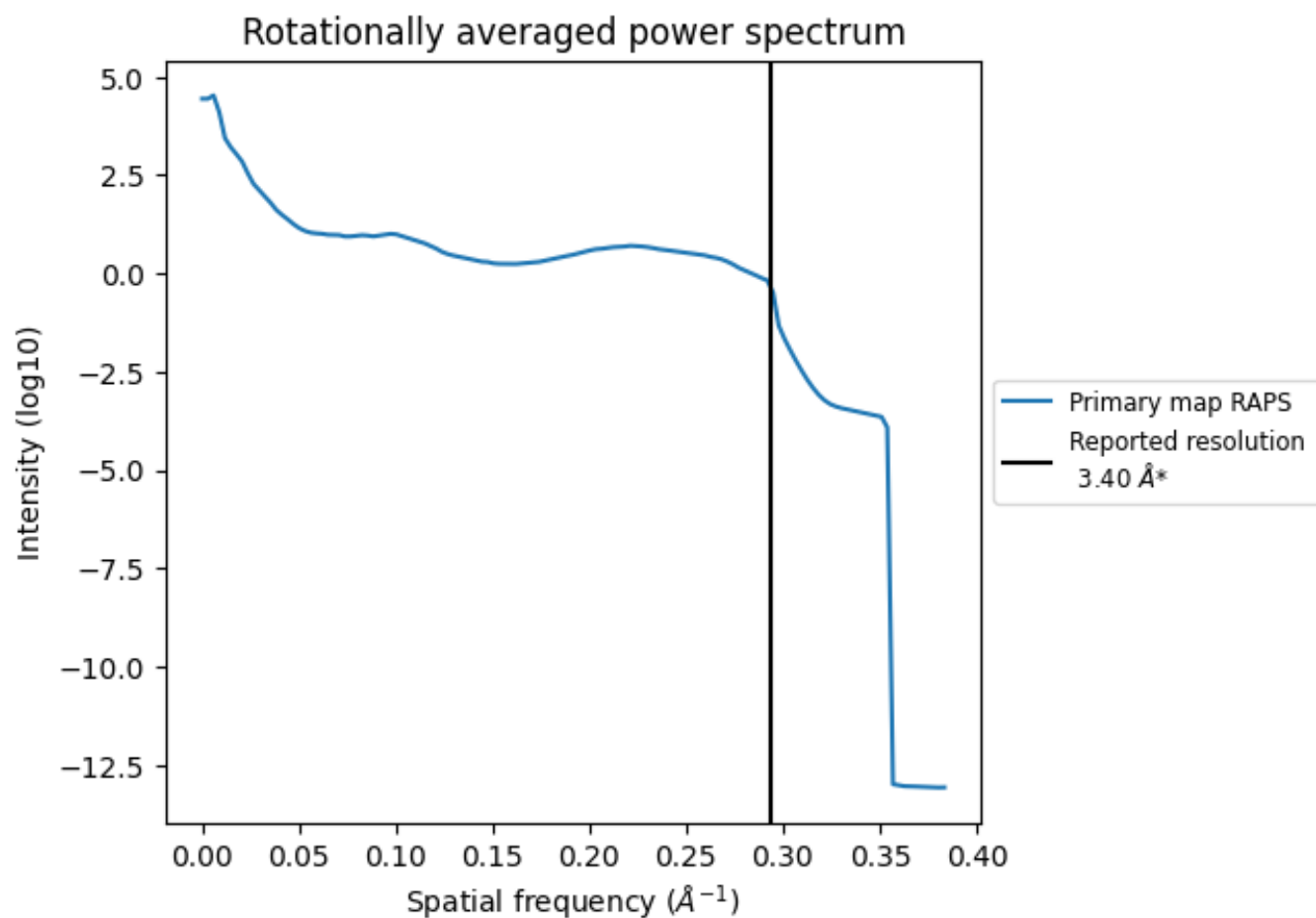
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

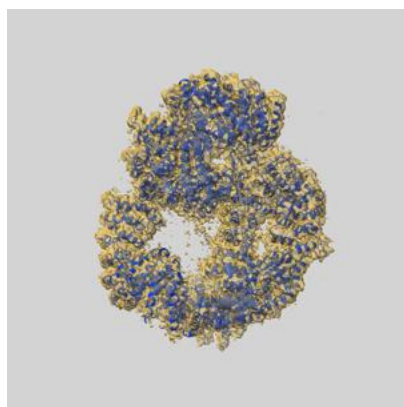
8 Fourier-Shell correlation

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

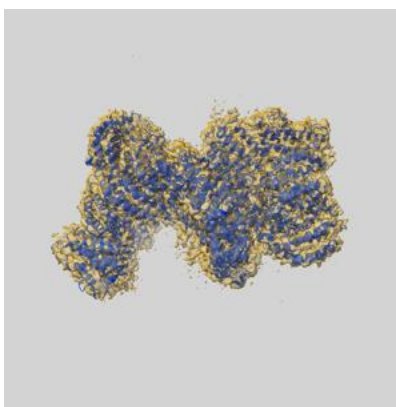
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13064 and PDB model 7OTP. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

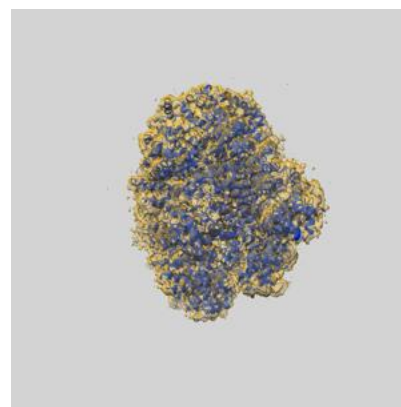
9.1 Map-model overlay [i](#)



X



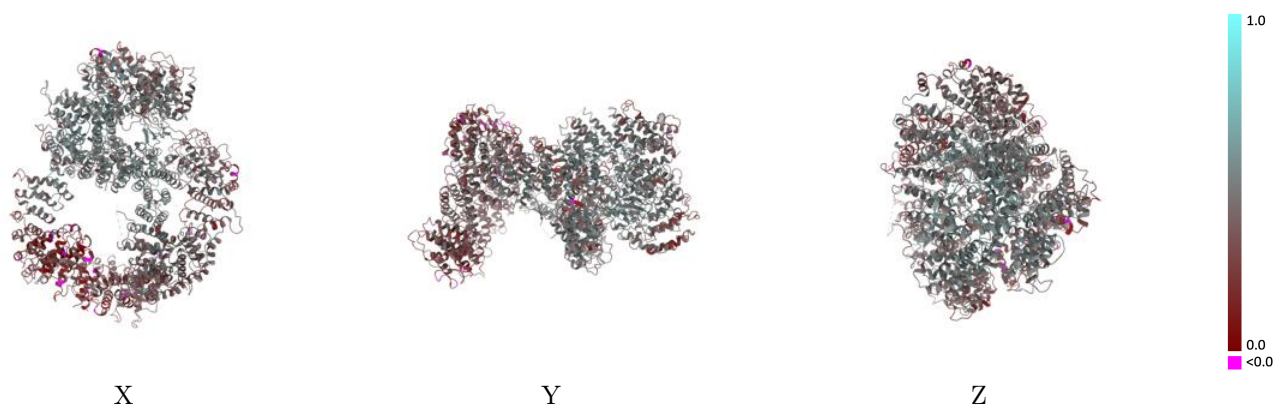
Y



Z

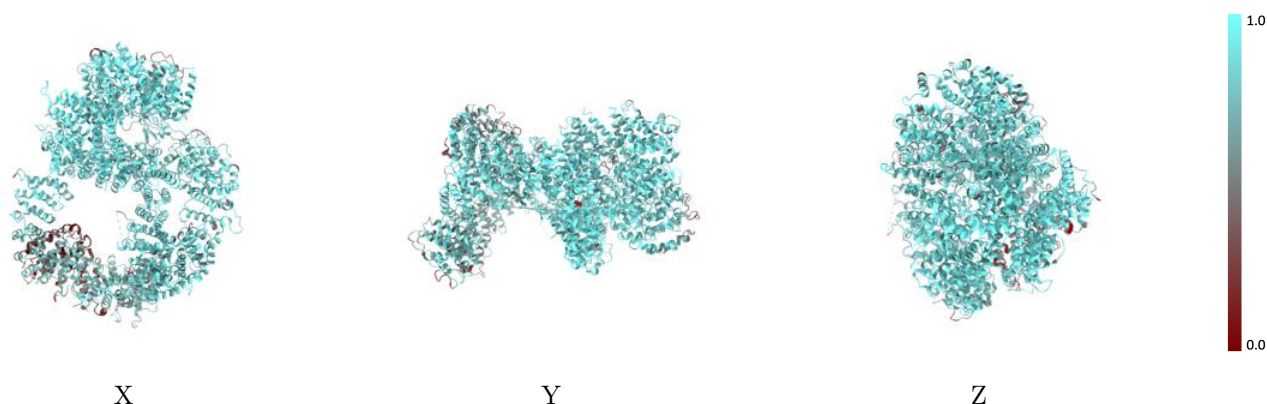
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



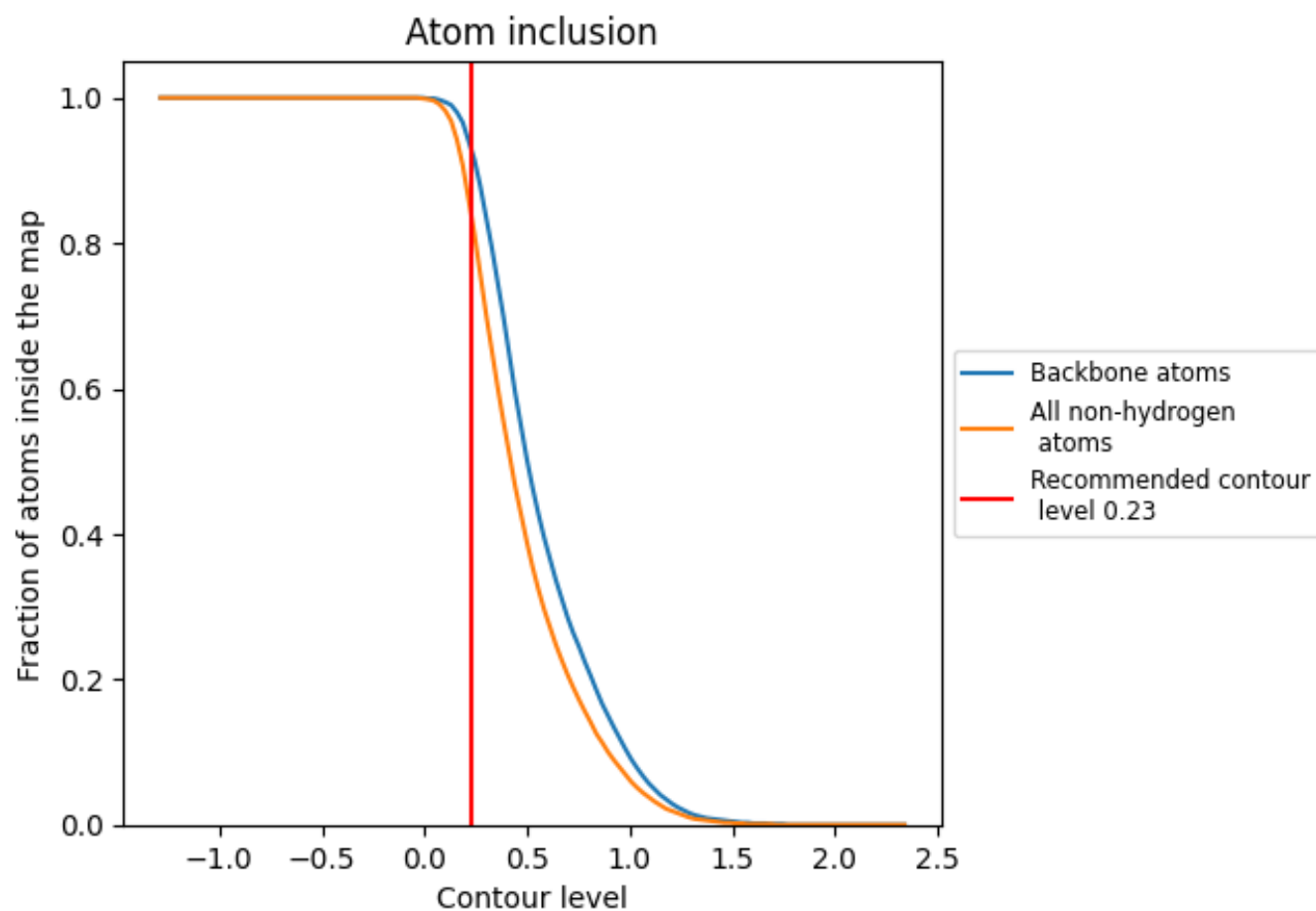
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 84% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.4140
A	0.8360	0.4140

