



# wwPDB EM Validation Summary Report ⓘ

Jan 29, 2022 – 06:18 am GMT

PDB ID : 7OTW  
EMDB ID : EMD-13068  
Title : DNA-PKcs in complex with AZD7648  
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.  
Deposited on : 2021-06-10  
Resolution : 2.99 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](mailto: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.

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

EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

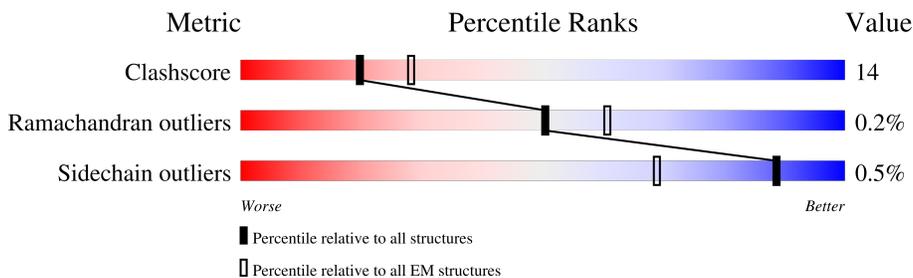
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.99 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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](#)

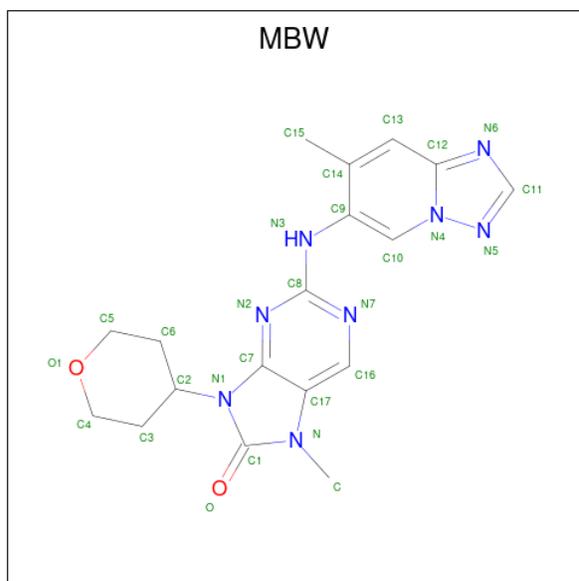
There are 2 unique types of molecules in this entry. The entry contains 29038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	29010	18609	4903	5307	191	0	0

- Molecule 2 is 7-methyl-2-[(7-methyl-[1,2,4]triazolo[1,5-a]pyridin-6-yl)amino]-9-(oxan-4-yl)purin-8-one (three-letter code: MBW) (formula: C<sub>18</sub>H<sub>20</sub>N<sub>8</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

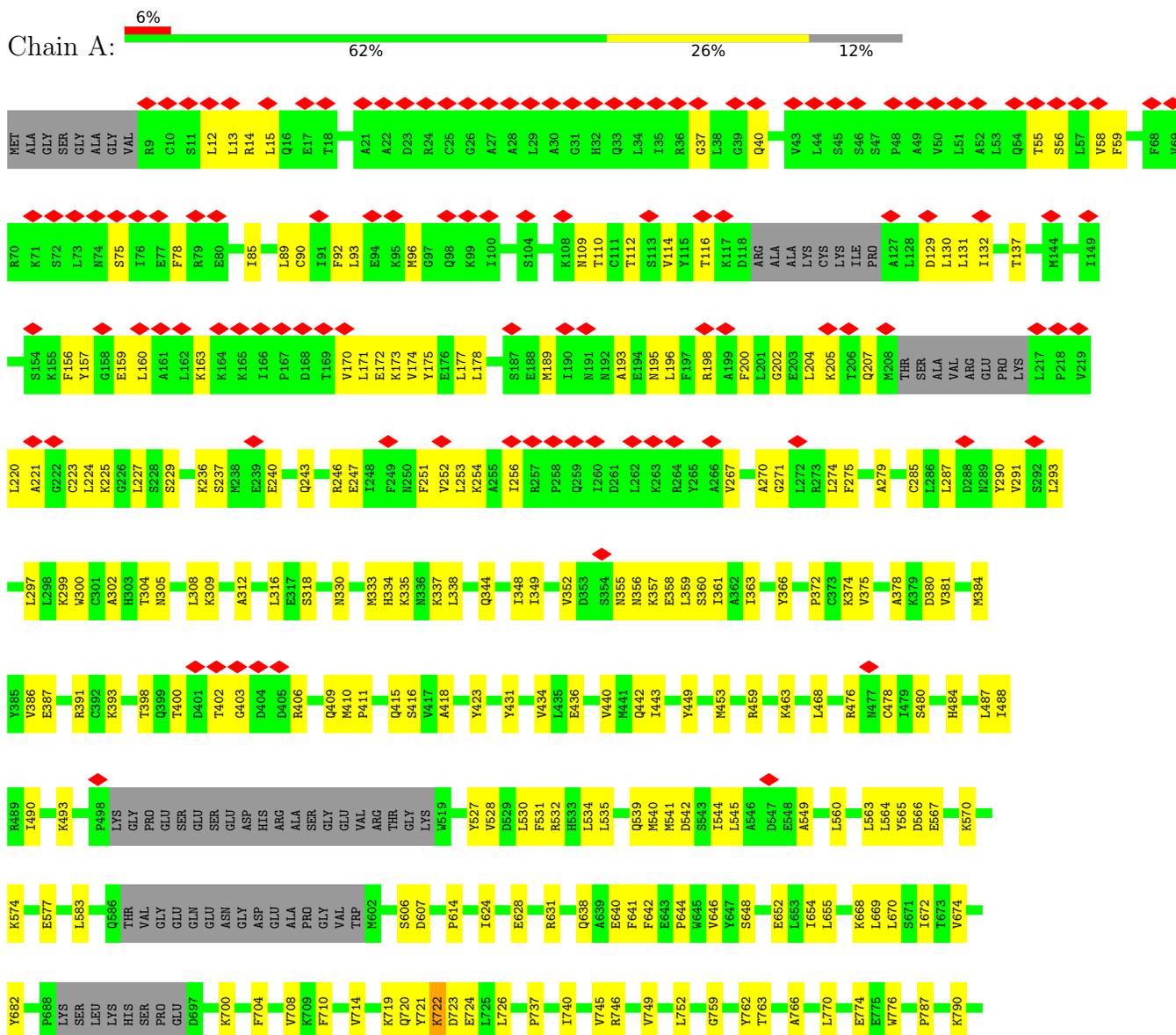


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	28	18	8	2	0

### 3 Residue-property plots

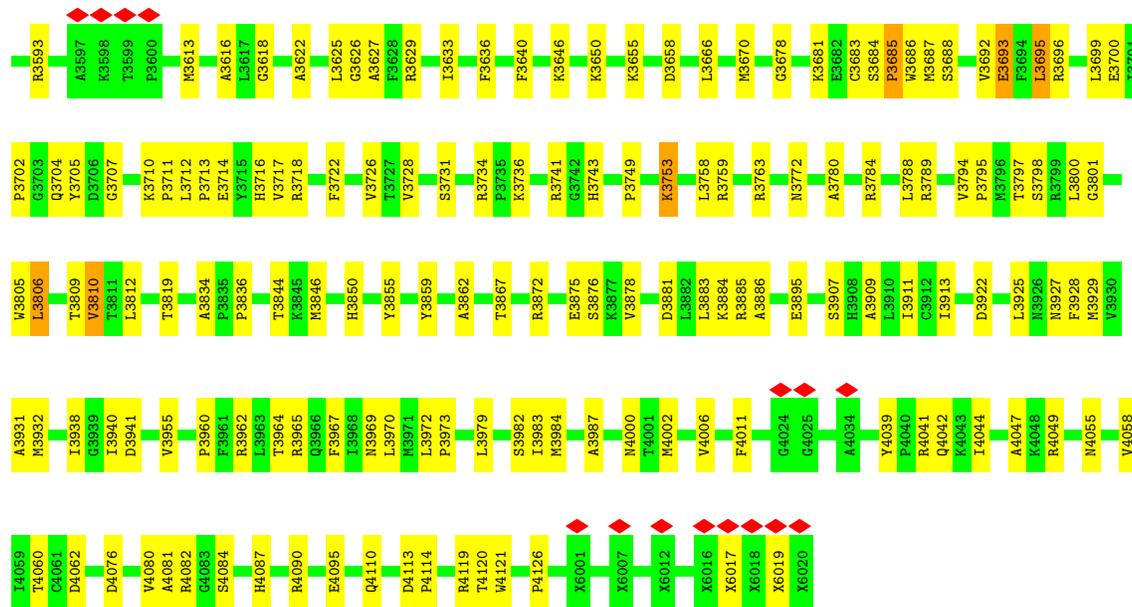
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





Q3494	F8495	I3496	S3497	W3498	I3499	S3500	H3501	M3502	V3518	E3519	E3520	I3521	D3522	D3523	P3526	Q3527	A3528	A3529	V3530	V3531	I3535	S3540	S3541	V3542	K3543	D3544	G3548	K3552	E3553	F3554	V3555	K3561	Q3564	V3567	I3568	A3574	L3578	K3579	M3580	L3583	W3588	S3589										
CYS	GLY	PRO	PRO	PRO	PRO	GLU	ASP	ASN	ASN	SER	MET	VAL	ASP	SER	VAL	ILE	ASP	SER	ALA	GLU	LEU	Y3442	L3445	V3446	F3447	E3448	K3449	M3450	L3451	L3454	F3465	F3466	K3467	L3468	L3469	E3478	S3481	M3483	T3484	K3485	S3486	I3487	PRO	PRO	SER	TRP	SER					
L3283	S3284	H3285	S3288	R3289	S3294	L3298	T3299	V3300	L3301	K3302	T3303	D3308	E3309	V3312	Y3315	K3318	L3329	T3332	T3333	Y3334	I3336	E3344	L3348	A3349	E3350	I3351	E3352	D3354	K3355	A3356	I3359	L3360	E3361	S3367	E3394	E3395	K3396	A3396	GLN	PRO	PRO	TRP	SER									
L3197	THR	PRO	LEU	PRO	GLU	ASP	ASN	ASN	SER	MET	VAL	ASP	SER	GLN	ARG	MET	GLU	VAL	GLN	GLN	GLN	D3226	I3231	K3235	K3239	D3244	R3247	M3256	K3257	L3258	L3259	K3260	S3266	K3267	T3268	R3269	D3270	D3271	Q3278	S3279	Y3280	C3281	R3282									
E3033	F3034	L3041	R3046	S3047	T3065	D3066	K3067	A3068	M3069	E3072	L3073	Q3074	L3078	Y3082	L3086	K3100	I3103	I3107	M3111	S3116	L3129	V3132	Q3133	A3134	E3137	I3138	I3142	S3153	Q3154	L3161	P3169	I3182	R3186	C3187	S3191	E3194																
GLU	LEU	ALA	LYS	ARG	VAL	ARG	GLY	LYS	ALA	ARG	P2917	P2918	P2919	V2920	E2925	R2931	D2937	V2938	L2939	K2950	L2976	W2981	T2987	E2988	A2989	E2995	L2999	N3003	A3006	K3009	E3012	Y3013	C3014	T3016	D3020	L3027	N3028	K3029	I3030	W3031	S3032											
GLY	ASP	LEU	PRO	ASP	G2784	I2785	K2786	H2787	S2788	R2800	D2801	K2806	L2812	F2813	L2817	M2820	V2838	F2823	I2832	L2837	R2842	F2843	T2846	T2847	C2857	L2868	L2869	S2877	A2878	G2879	S2883	L2884	P2887	I2890	E2894	L2898	R2899	L2900	L2901	P2902	ALA											
TRP	LEU	THR	GLY	SER	THR	PRO	ASP	THR	ALA	GLN	THR	SER	PRO	GLN	THR	PHE	THR	ALA	GLN	LYS	ARG	TRP	PRO	VAL	ALA	GLY	THR	PRO	ASP	PHE	GLN	LYS	THR	LEU	PRO	GLY	VAL	VAL	LEU	TYR	ASP	VAL	LYS	THR	ASP							
Q2518	L2519	I2520	L2521	R2522	N2523	F2524	W2525	S2526	H2527	E2528	S2533	L2536	L2540	A2541	L2542	H2553	F2554	L2555	S2556	L2557	A2558	T2559	V2563	E2564	S2567	M2568	D2571	Y2572	P2573	N2574	P2575	E2578	PRO	LEU	SER	GLU	CYS	GLY	PHE	GLN	GLU	THR	TYR	THR	ILE	ASP	SER	ASP	TRP	ARG	PHE	
E2389	V2400	C2403	R2404	V2405	E2406	E2410	L2411	Y2412	F2413	Q2414	L2415	D2419	F2420	V2421	Q2422	I2438	M2442	N2443	L2446	V2449	E2450	L2453	L2454	L2455	V2459	E2460	F2461	H2464	P2465	S2466	T2467	T2468	M2473	Y2474	N2475	M2478	E2490	L2498	V2505	L2506	L2510	L2517										
V2304	R2311	Y2312	K2313	Y2316	L2323	I2326	L2327	R2328	Y2329	V2330	R2333	K2334	M2335	I2336	E2339	S2340	K2347	K2350	Q2351	M2354	T2355	M2356	K2357	K2359	F2360	I2361	L2364	M2365	F2371	P2372	P2373	L2374	A2375	D2376	M2380	A2381	V2382	F2383	L2386	P2387	L2393	K2394	Q2395	Y2399	F2400	Q2301						
V2230	F2231	R2232	H2233	M2234	E2235	E2236	I2237	L2238	K2239	C2244	W2245	K2246	D2247	T2251	P2252	Y2253	R2254	L2255	I2256	F2257	E2258	K2259	F2260	S2261	G2262	D2269	N2270	S2271	G2272	I2273	L2274	Q2275	L2276	L2277	G2278	I2279	V2280	M2281	A2282	N2283	P2286	Y2287	Y2288	D2289	P2290	Q2291	C2292	I2294	Q2295	Y2299	F2300	Q2301
M2141	I2142	F2145	L2146	A2147	N2152	T2153	E2154	E2155	V2156	W2164	L2165	S2166	F2167	L2168	E2175	G2178	E2180	G2181	I2182	H2183	V2184	K2185	W2186	I2189	V2190	L2194	S2195	W2196	T2197	G2198	L2199	A2200	T2201	P2202	T2203	G2204	V2205	F2206	K2207	D2208	L2211	M2220	V2223	F2224	K2227	R2228	A2229					



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	164192	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	1.623	Depositor
Minimum map value	-0.529	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.2	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: MBW

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	0.44	0/29502	0.54	0/39893

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29010	0	29194	766	0
2	A	28	0	0	0	0
All	All	29038	0	29194	766	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 14.

The worst 5 of 766 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:3810:VAL:CG2	1:A:3932:MET:SD	2.45	1.05
1:A:3810:VAL:HG21	1:A:3932:MET:SD	2.02	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3812:LEU:HB3	1:A:3925:LEU:O	1.73	0.88
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.06	0.87
1:A:3451:LEU:HD23	1:A:3454:LEU:HD12	1.56	0.87

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%)	3237 (90%)	359 (10%)	6 (0%)	47 82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3693	GLU
1	A	3695	LEU
1	A	2787	HIS
1	A	3495	PHE
1	A	723	ASP

### 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	3196/3671 (87%)	3181 (100%)	15 (0%)	88 96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3355	LYS
1	A	3806	LEU
1	A	3693	GLU
1	A	3810	VAL
1	A	3714	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2305	ASN
1	A	2351	GLN
1	A	3564	GLN
1	A	2365	ASN
1	A	2105	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	MBW	A	6101	-	23,32,32	1.11	1 (4%)	19,47,47	0.57	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	MBW	A	6101	-	-	3/4/16/16	1/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	MBW	C9-C14	3.78	1.48	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6101	MBW	N7-C8-N3-C9
2	A	6101	MBW	N2-C8-N3-C9
2	A	6101	MBW	C10-C9-N3-C8

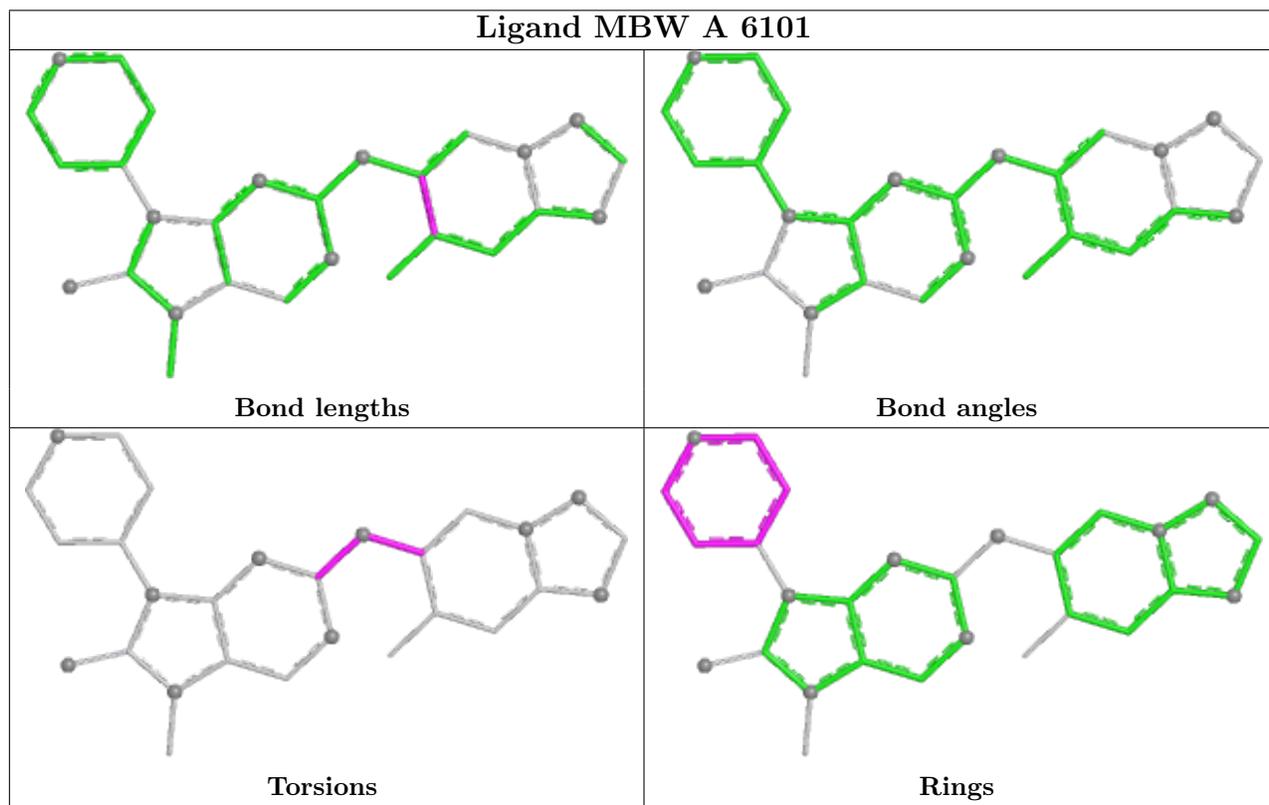
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6101	MBW	C2-C3-C4-C5-C6-O1

No monomer is involved in short contacts.

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	82.11

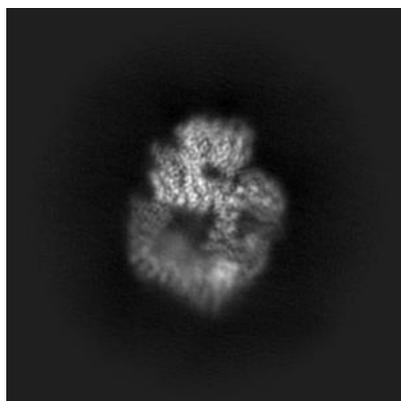
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13068. These allow visual inspection of the internal detail of the map and identification of artifacts.

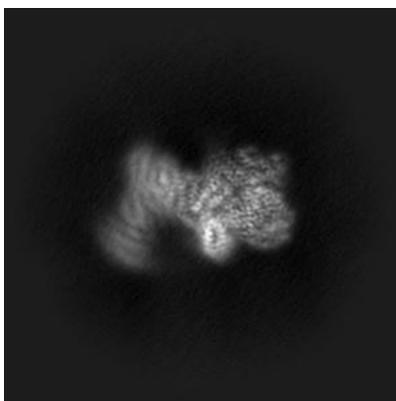
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

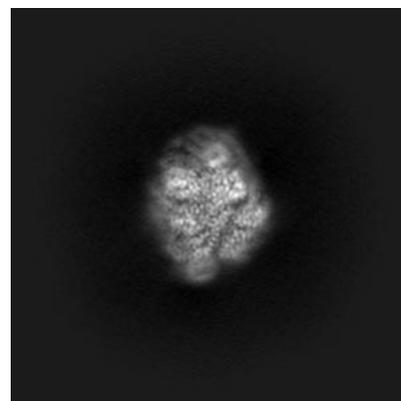
#### 6.1.1 Primary map



X



Y

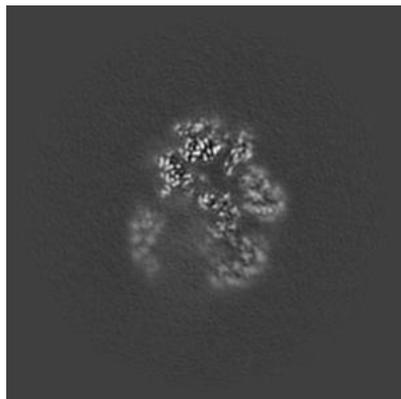


Z

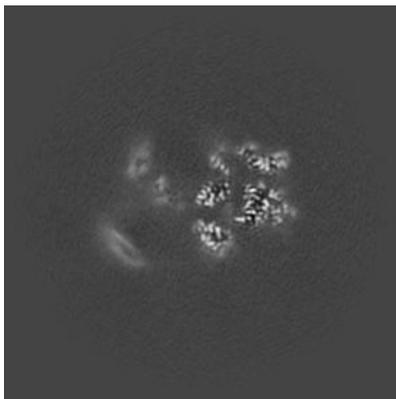
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

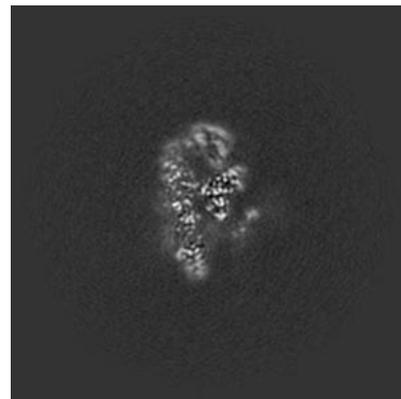
#### 6.2.1 Primary map



X Index: 130



Y Index: 130

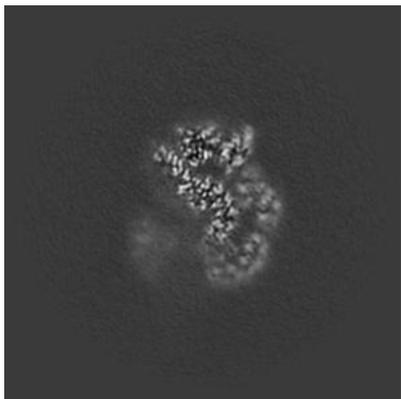


Z Index: 130

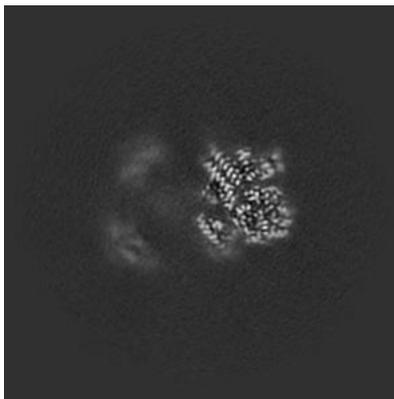
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

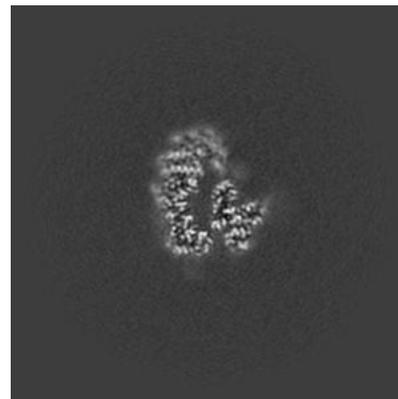
### 6.3.1 Primary map



X Index: 135



Y Index: 120

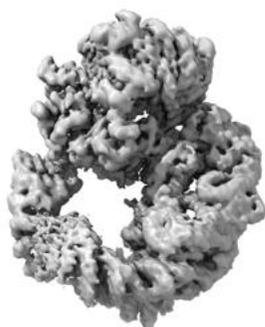


Z Index: 140

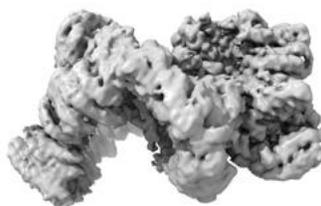
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

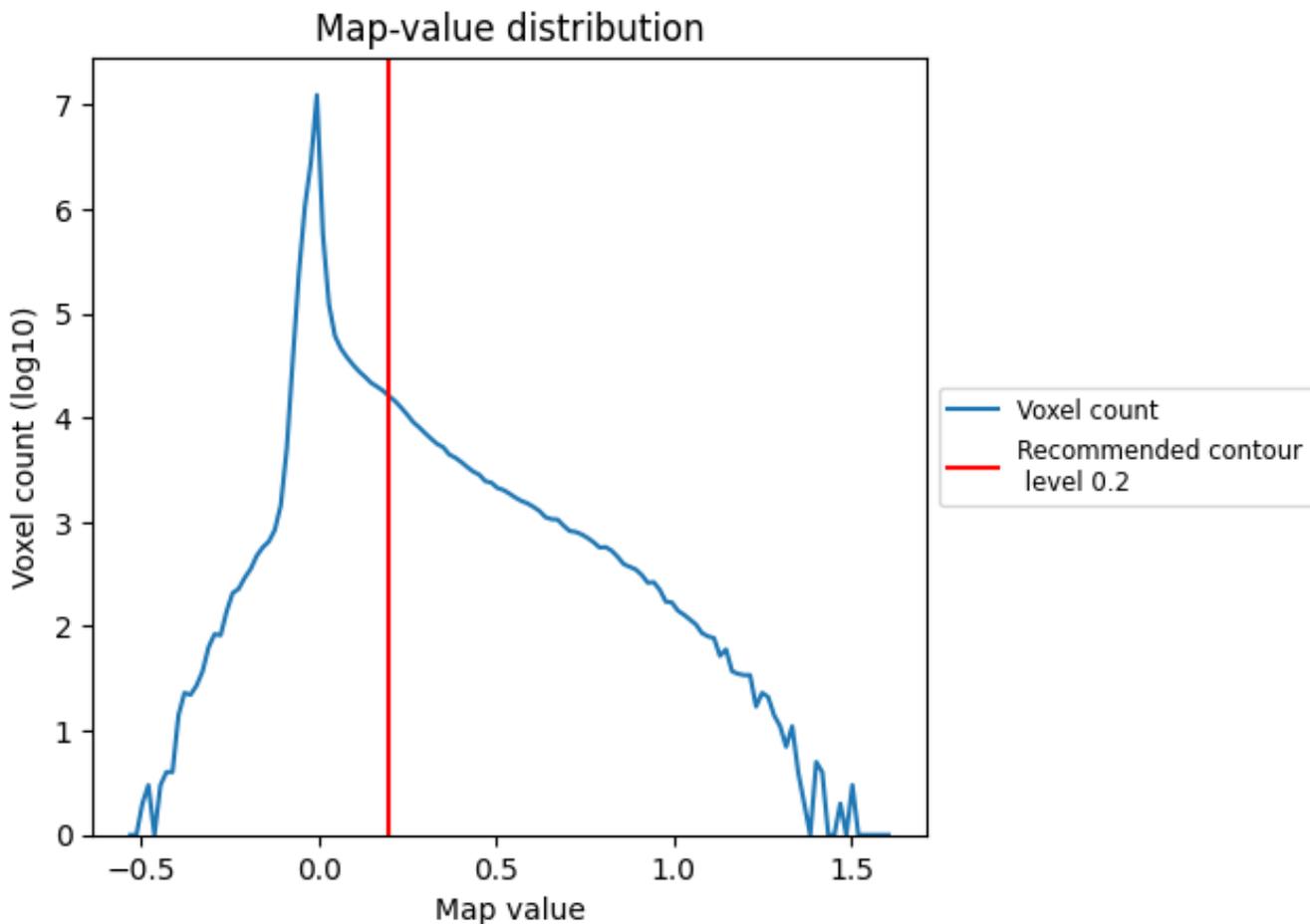
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

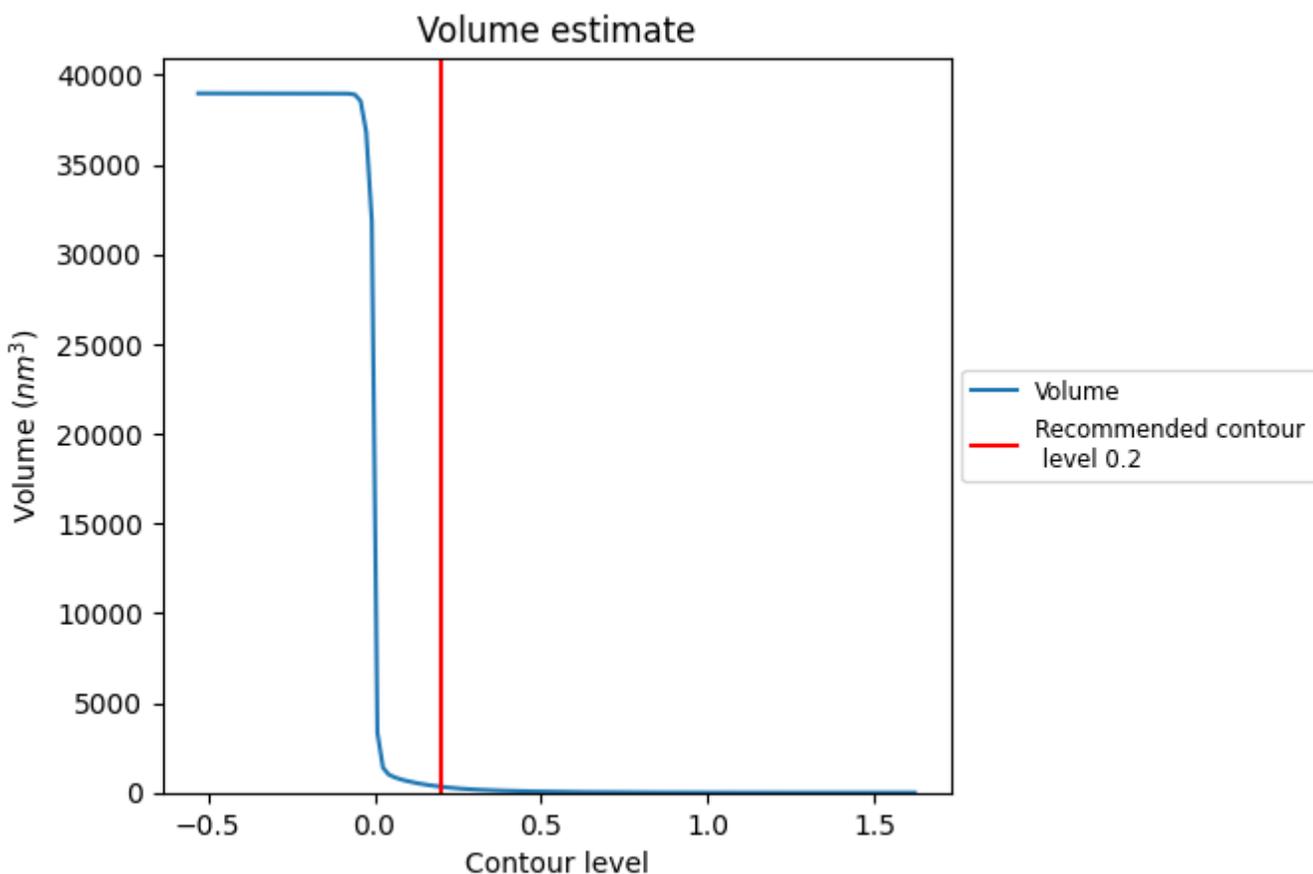
This section contains the results of statistical analysis of the map.

### 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.

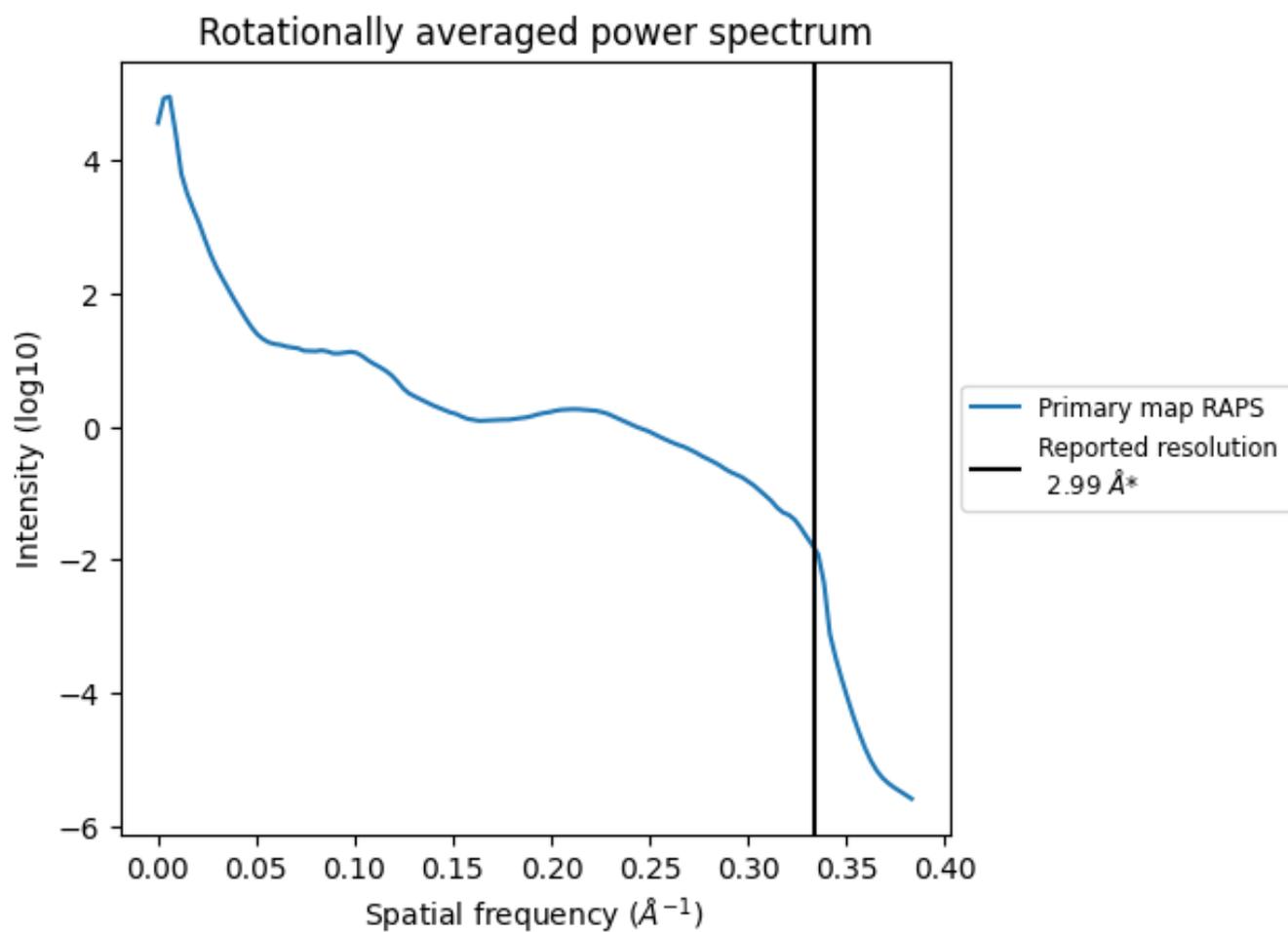
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 328 nm<sup>3</sup>; this corresponds to an approximate mass of 296 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 i



\*Reported resolution corresponds to spatial frequency of 0.334 Å<sup>-1</sup>

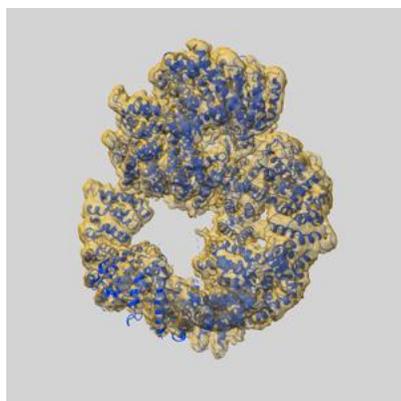
## 8 Fourier-Shell correlation

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

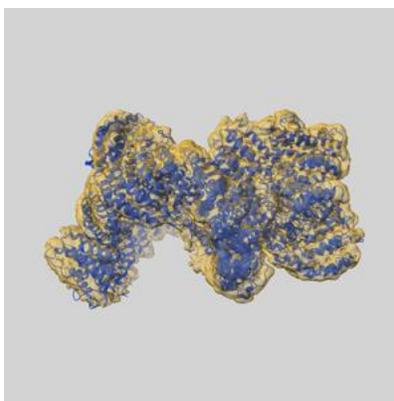
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13068 and PDB model 7OTW. Per-residue inclusion information can be found in section 3 on page 4.

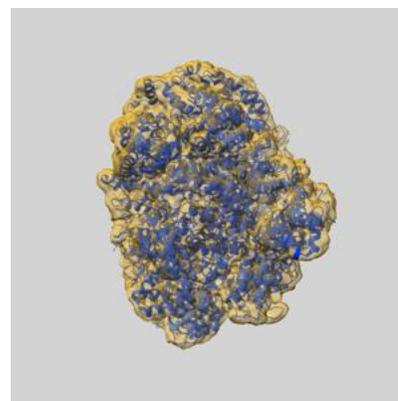
### 9.1 Map-model overlay [i](#)



X



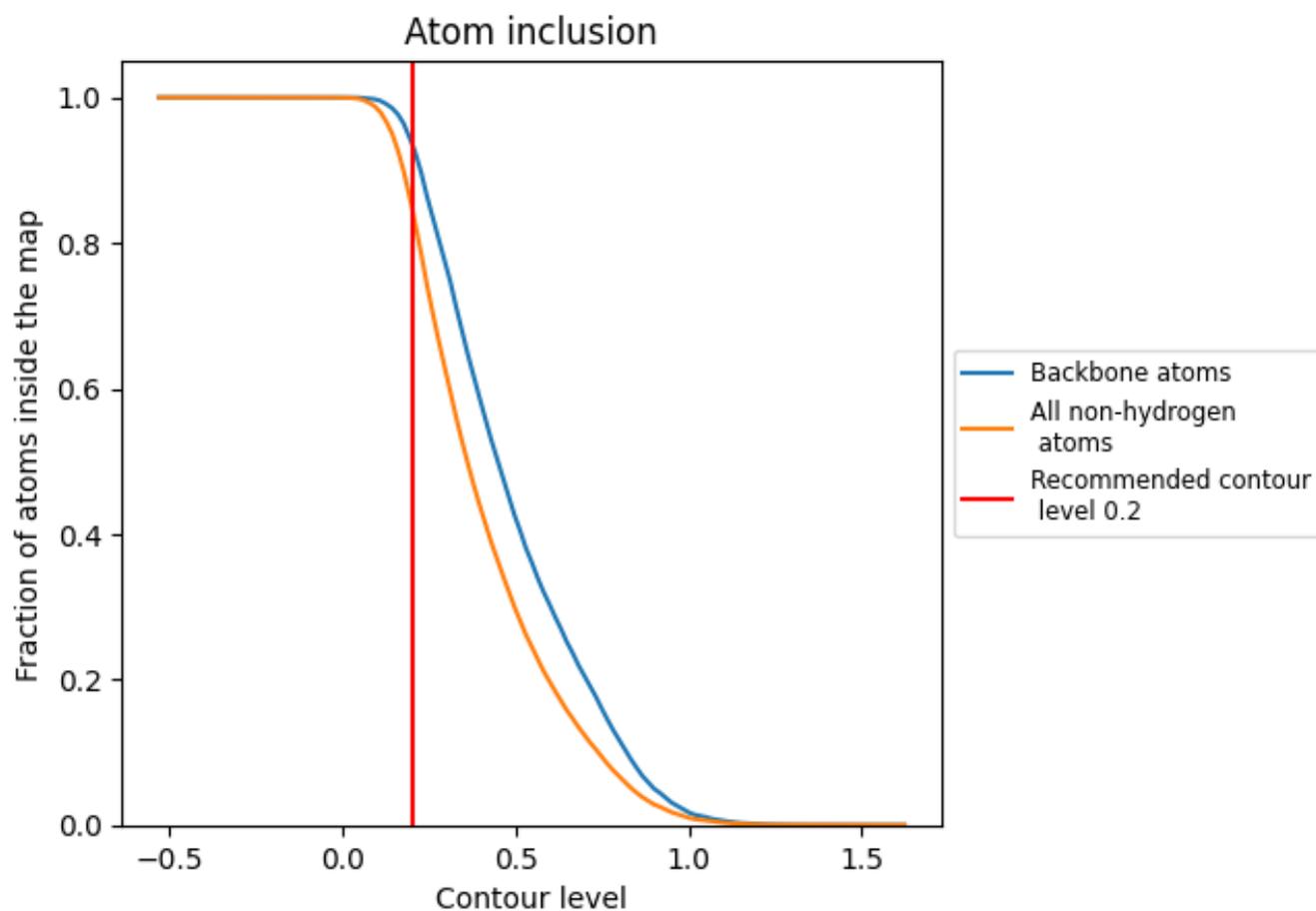
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.