



## wwPDB EM Validation Summary Report ⓘ

Dec 2, 2025 – 12:44 pm GMT

PDB ID : 9I1I / pdb\_00009i1i  
EMDB ID : EMD-52570  
Title : Cryo-EM structure of mouse RNF213 (WB3/WB4 + ATP)  
Authors : Grabarczyk, D.B.; Ahel, J.; Clausen, T.  
Deposited on : 2025-01-16  
Resolution : 4.50 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.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

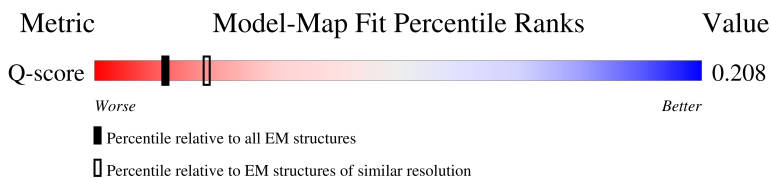
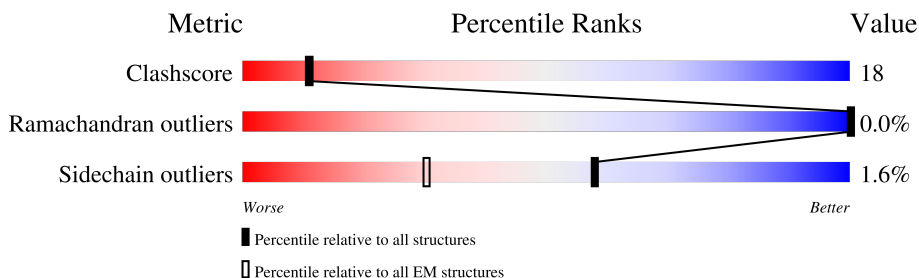
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 4.50 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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	5161	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36852 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.

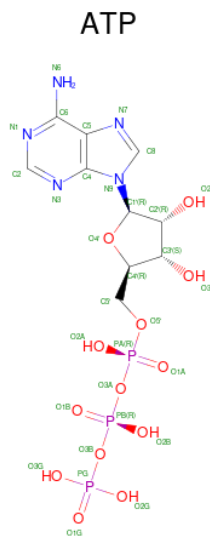
- Molecule 1 is a protein called E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4584	Total	C	N	O	S	0	0
			36787	23443	6326	6799	219		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2449	GLN	GLU	engineered mutation	UNP E9Q555
A	2806	GLN	GLU	engineered mutation	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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

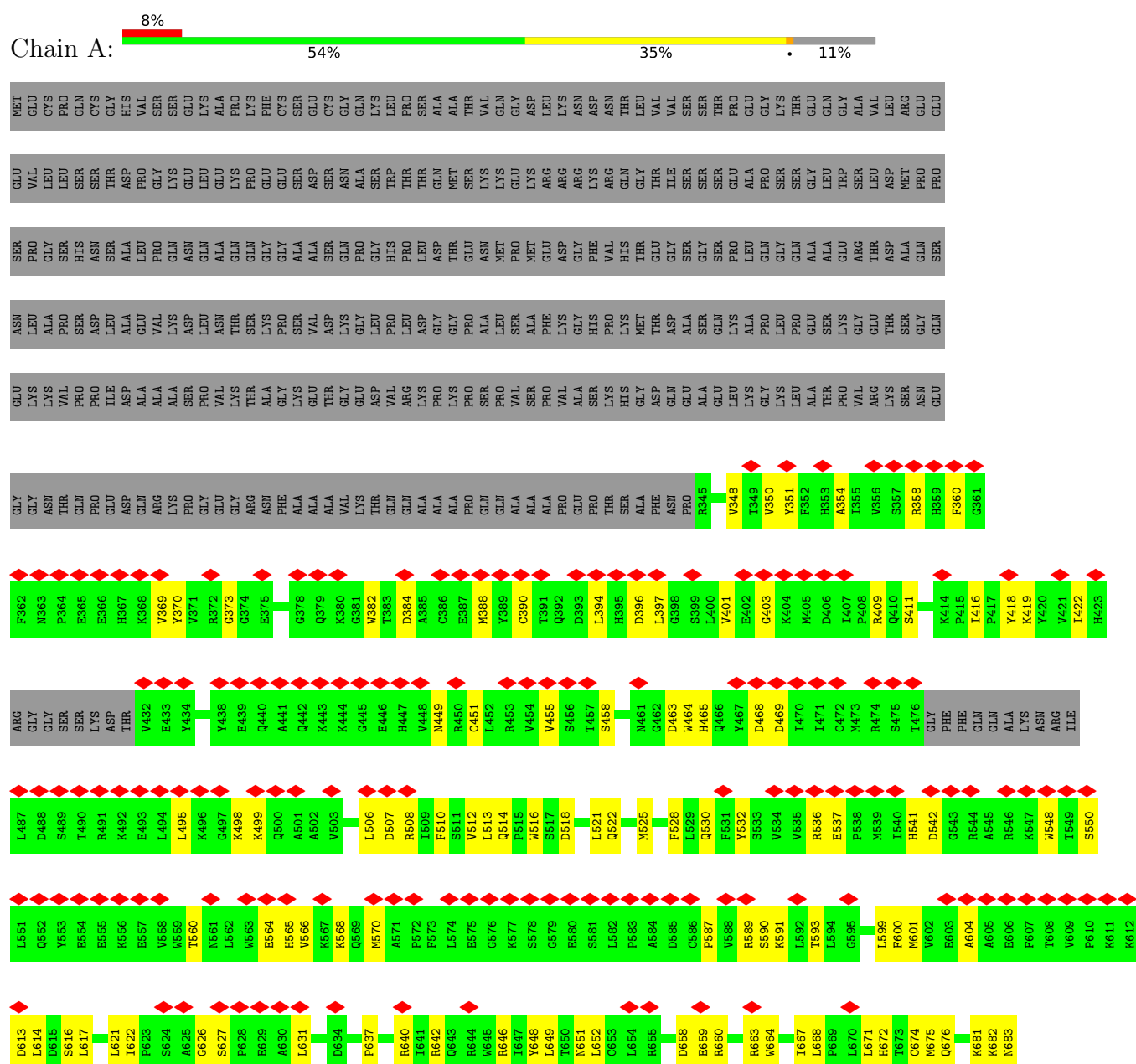
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Zn 2 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: E3 ubiquitin-protein ligase RNF213







V2803	V2910	D2995	Y3087	Q3260	L3349	GLN	R3591	S3682	L3781	V3856
L2804	E2910	G2996	L3092	A3261	V3350	GLU	D3592	F3689	H3785	R3867
Q2805	F2911	A2997	G3093	H5282	A3351	MET	G3593	F3689	A3988	L3869
V2807	L2914	E2998	T3094	M3265	K3354	GLU	M3502	T3692	P3786	Q3786
G2808	R2915	S2999	H3095	T3266	R3504	ILE	R3503	V3696	Q3787	Q3788
L2809	D2916	R3000	R3096	H3267	R3505	GLU	R3504	V3696	V3788	L3789
		Y3001	V3097	H3268	E3360	THR	L3507	V3696	L3792	L3876
D2812	T2921	L3002	K3099	R3271	T3364	SER	T3602	Q3700	L3792	A3877
	K2922	G3004	R3100	R3277	Q3365	GLN	S3603	F3701	A3795	L3878
P2817	M2923	V3003	R3100	T3277	G3366	LYS	P3604	P3702	A3796	V3879
L2818	L3005	T3006	F3105	T3279	T3367	LEU	A3605	A3704	E3797	V3880
K2819	A2926	R3007		F3280	K3368	ALA	D3516	Q3705	K3798	E3881
H2822	K2927			S3281	T3279	GLU	R3519	Q3706	L3801	H3882
				S3282	F3280	ALA	Q3608	Q3707	L3801	V3883
L2825	S2931			S3283	S3281	GLU	R3525	K3708	L3801	L3884
P2836	K2932	L3015	E3111	L2822	V3373	MET	R3529	L3709	E3805	L3885
K2837	R2933	Q3016	E3112	A3293	F3375	VAL	H3532	L3710	L3808	G3886
K2838	G2934	Q3017	K3113	S3294	T3376	GLU	H3532	Q3711	L3809	T3887
K2839	L2935	Q3018	E3114	S3295	T3377	ASP	N3536	L3712	A3810	
V2840	Q2938	F3019	V3115	E3295	K3378	SER	N3536	S3713	F3811	L3891
G2841	D2939		Q3119	S3297	R3379	GLU	E3539	K3715	C3816	L3905
F2842	D2940		F3120	R3297	L3379	GLU	E3540	D3716	L3909	L3909
G2844	H2942		V3122	A3300	M3381	MET	R3544	F3717	C3816	L3911
L2845	P3123	Q3034	P3123	A3300	R3382	LYS	R3544	L3720	K3821	E3910
		Q3035	L3124	P3303	G3383	LYS	R3544	L3720	L3824	E3911
L2850	A2944	Q3035	T3125	P3303	S3384	ALA	R3544	S3726	L3824	E3911
D2851	V2944	Q3041	N3126	Q3310	F3391	SER	K3547	R3727	L3825	D3912
P2852	L2945		R3127	T3311	F3391	ASP	E3548	E3728	L3825	K3926
A2853	G2950	N3045	L3128	D3219	L3395	PRO	M3549	A3736	L3826	R3919
K2854	D2951	I3046	E3129	T3312	L3395	ARG	V3550	E3734	L3832	K3926
K2855	D2952	I3046	K3130	T3312	L3395	SER	E3553	E3744	L3835	K3937
V2856	L2954	K3050	H3131	E3314	L3395	CYS	E3553	E3744	L3835	K3937
K2857			T3132	S3315	L3395	ASP	E3553	E3744	L3835	K3937
				S3316	L3395		E3553	E3744	L3835	K3937
F2860	A2967	R2968	L3133	F3317	H3400	CYS	A3559	D3752	L3840	S3940
V2861	R2968	R2969	D3134	F3317	I3401	CYS	L3560	E3753	L3841	R3941
S2862	K2970		L3135	V3326	D3402	ARG	Q3561	E3753	L3842	F3942
R2863	E2971		M3135	T3327	D3403	SER	E3562	E3753	L3843	F3942
				F3237	L3404	ASP	E3562	E3753	L3844	H3951
S2874	T2975		S3145	K3332	D3413		T3565	P3758	E3844	A3954
L2878	V2976		Q3148	V3333	T3415		F3566	L3759	L3845	Q3955
	E2977		E3149	V3333	T3415		R3567	S3760	V3845	Q3955
D2882	L2978			Q3240	T3415		H3568	P3762	V3846	D3956
R2883	I2979			Q3241	T3415		V3574	W3763	C3947	
L2884				Y3246	T3415		Q3575	V3764	L3851	F3961
V2885	T2983		Q3152	F3340	S3423		V3578	V3765	L3852	C3962
Q2886	P2987		A3154	D3341	K3427		L3582	H3766	S3855	D3963
	N3076		R3155	D3342	F3428		I3586	R3772	T3859	C3967
	Q3077		E3156	G3343	F3428		I3589	T3773	L3860	L3966
	Y3078		A3158	T3344	E3429		I3589	S3778	L3863	R3969
				R3345	ASP				Q3971	T3971
				S3346	LYS				Q3972	
				A3347	PRO				Q3972	
				Q3348	GLU				T3973	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00484	Depositor
Map size (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.17	0/37557	0.40	2/50804 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2051	ARG	CA-C-N	-5.71	105.81	122.38
1	A	2051	ARG	C-N-CA	-5.71	105.81	122.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4165	GLU	Peptide

### 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	36787	0	36880	1338	0
2	A	62	0	24	11	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
All	All	36852	0	36904	1338	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 18.

The worst 5 of 1338 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:1619:LEU:HD21	1:A:1622:LEU:HB3	1.49	0.95
1:A:1216:THR:HG21	1:A:1245:CYS:HB2	1.53	0.90
1:A:3025:PRO:HB3	1:A:3058:MET:HB2	1.57	0.87
1:A:2114:ALA:O	2:A:5201:ATP:N6	2.09	0.86
1:A:3006:THR:HG21	1:A:3011:ALA:HB2	1.58	0.85

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	4552/5161 (88%)	4198 (92%)	353 (8%)	1 (0%)	<b>100</b> <b>100</b>

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4166	PRO

### 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	4111/4604 (89%)	4044 (98%)	67 (2%)	58 74

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4270	MET
1	A	4590	HIS
1	A	5082	LEU
1	A	2211	PHE
1	A	2135	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3502	ASN
1	A	4313	GLN
1	A	3514	ASN
1	A	3890	HIS
1	A	4342	GLN

### 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

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	ATP	A	5201	3	26,33,33	0.64	0	31,52,52	0.85	2 (6%)
2	ATP	A	5205	-	26,33,33	0.62	0	31,52,52	0.81	2 (6%)

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	ATP	A	5201	3	-	5/18/38/38	0/3/3/3
2	ATP	A	5205	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5201	ATP	C5-C6-N6	2.28	123.82	120.35
2	A	5205	ATP	C5-C6-N6	2.26	123.79	120.35
2	A	5201	ATP	C3'-C2'-C1'	2.21	104.31	100.98
2	A	5205	ATP	PB-O3B-PG	2.06	139.91	132.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5205	ATP	PB-O3B-PG-O1G
2	A	5205	ATP	PB-O3B-PG-O2G
2	A	5201	ATP	C5'-O5'-PA-O3A
2	A	5201	ATP	PA-O3A-PB-O2B

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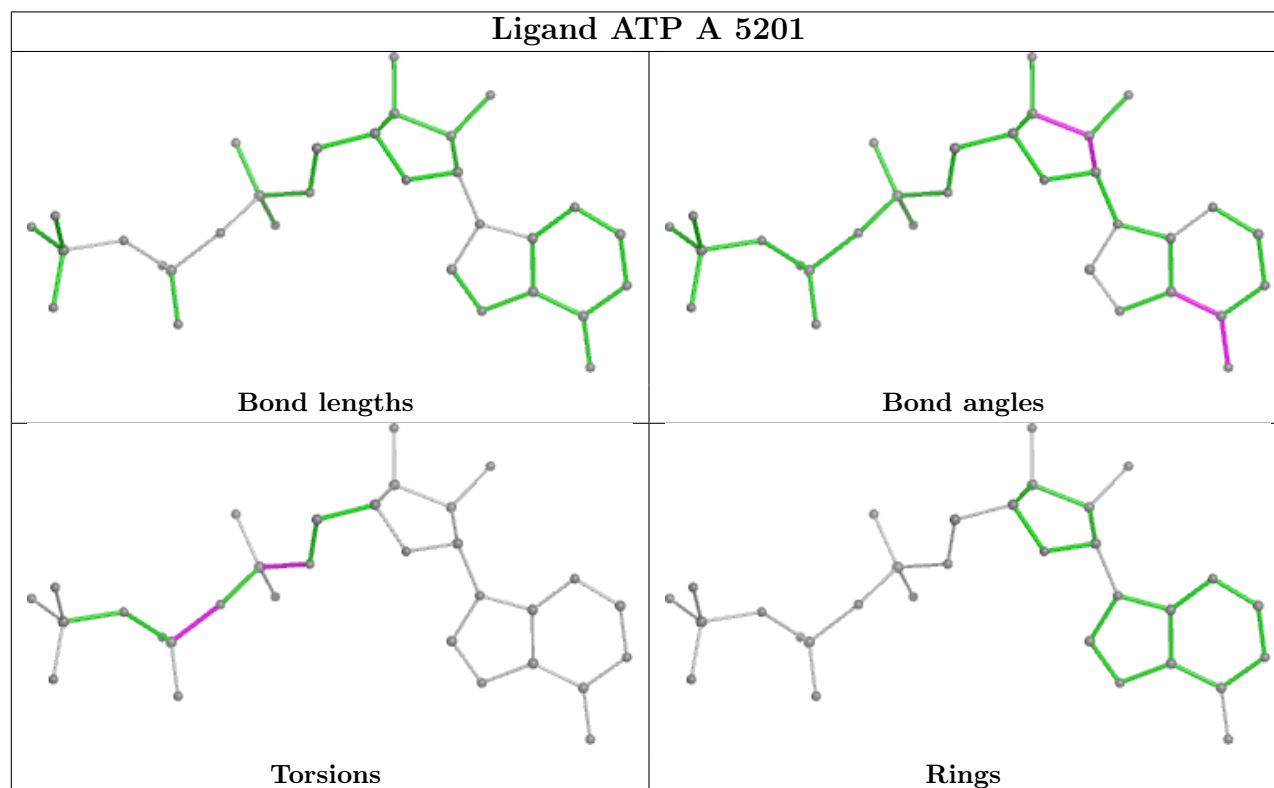
Mol	Chain	Res	Type	Atoms
2	A	5205	ATP	PA-O3A-PB-O1B

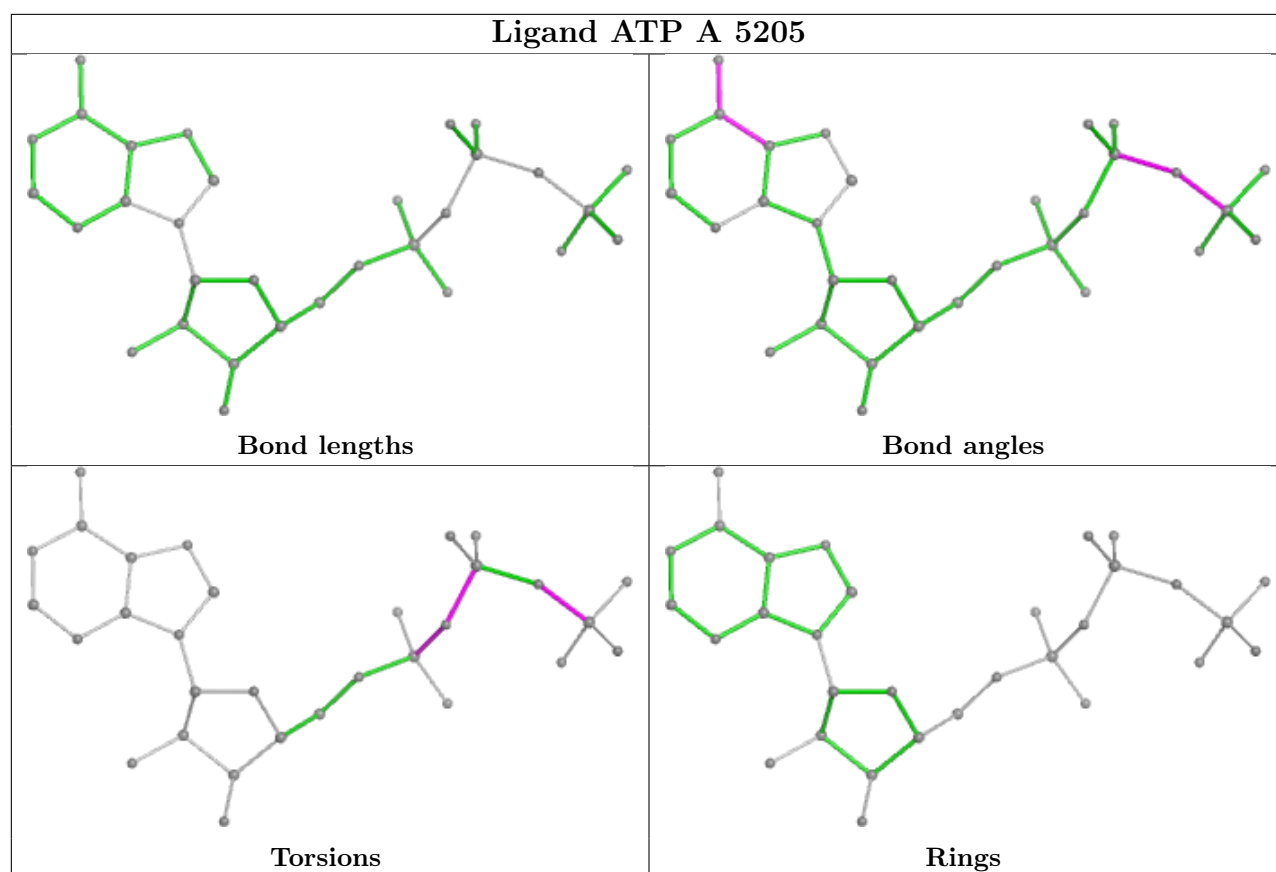
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5201	ATP	4	0
2	A	5205	ATP	7	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.



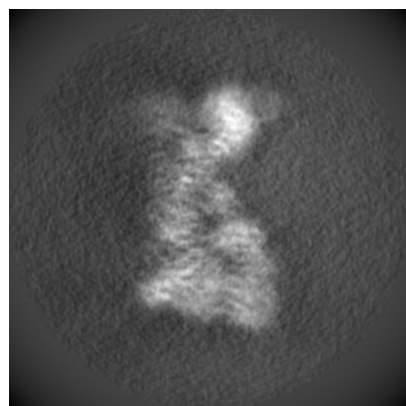
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52570. These allow visual inspection of the internal detail of the map and identification of artifacts.

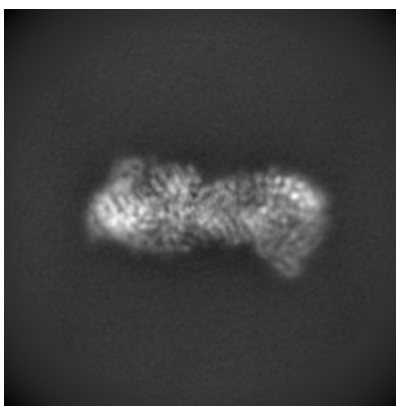
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

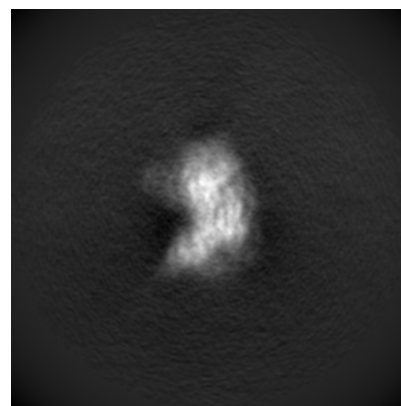
#### 6.1.1 Primary map



X

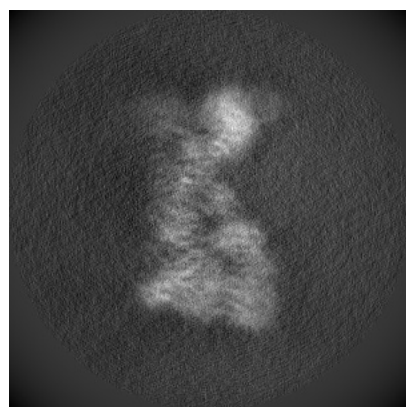


Y

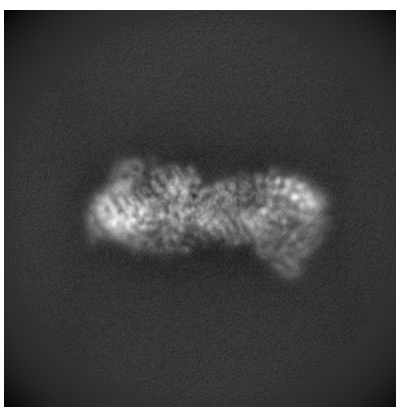


Z

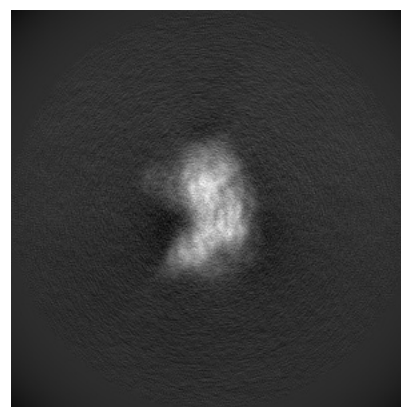
#### 6.1.2 Raw map



X



Y

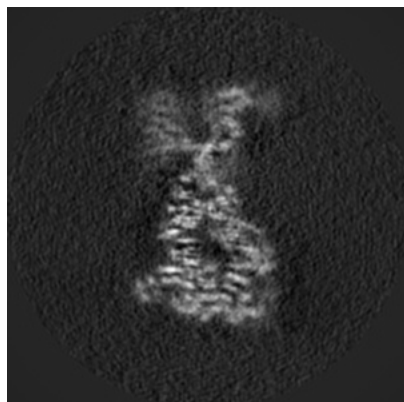


Z

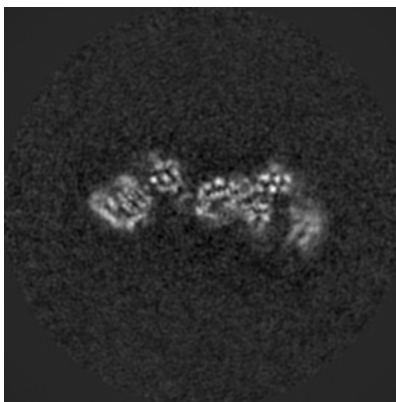
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

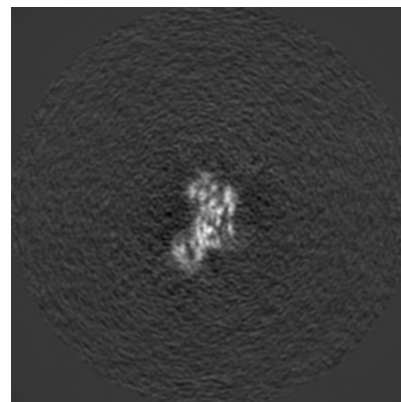
### 6.2.1 Primary map



X Index: 176

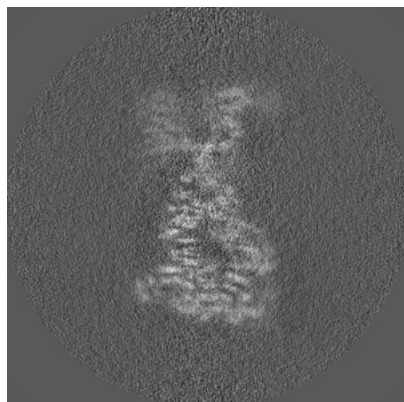


Y Index: 176

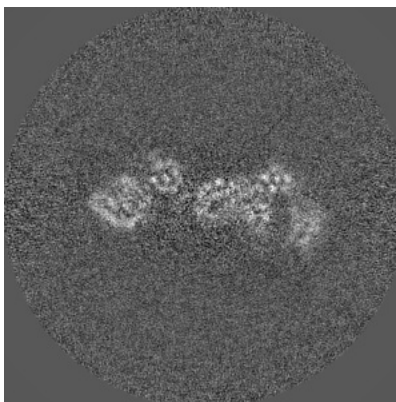


Z Index: 176

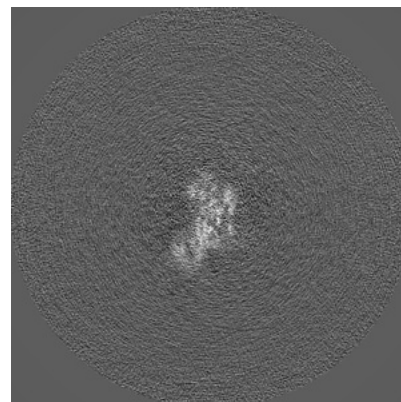
### 6.2.2 Raw map



X Index: 176



Y Index: 176

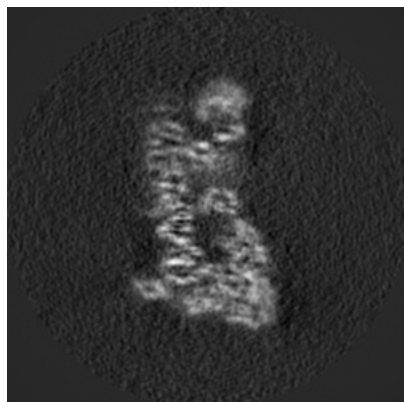


Z Index: 176

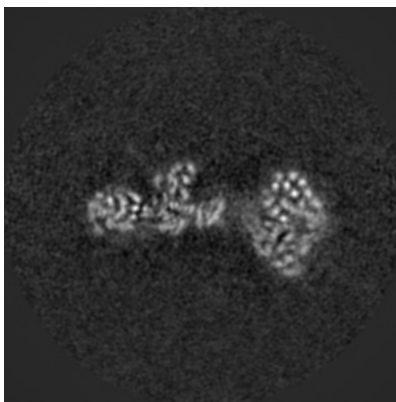
The images above show central slices of the map in three orthogonal directions.

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

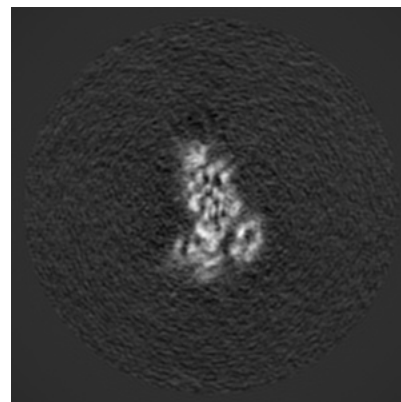
### 6.3.1 Primary map



X Index: 168

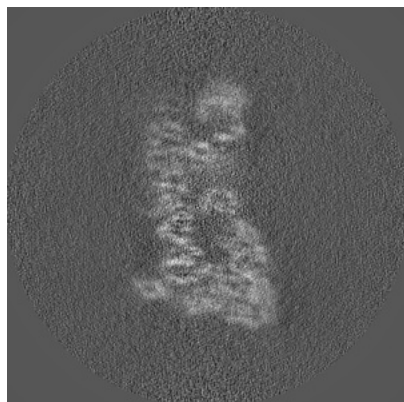


Y Index: 197

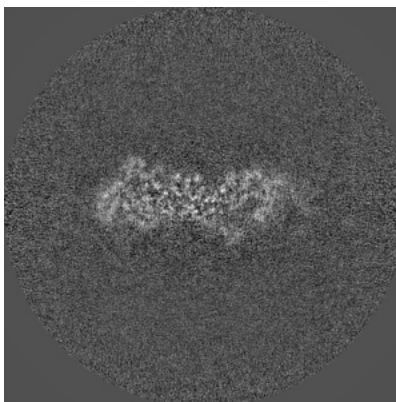


Z Index: 110

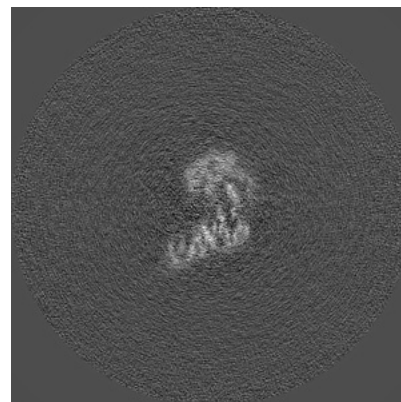
### 6.3.2 Raw map



X Index: 168



Y Index: 160



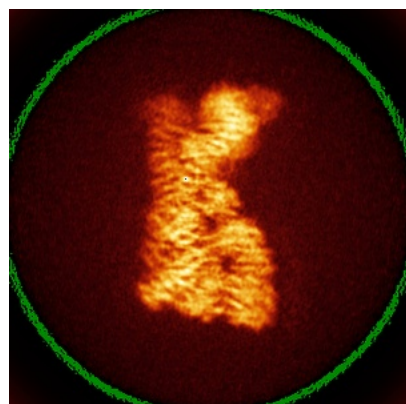
Z Index: 155

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

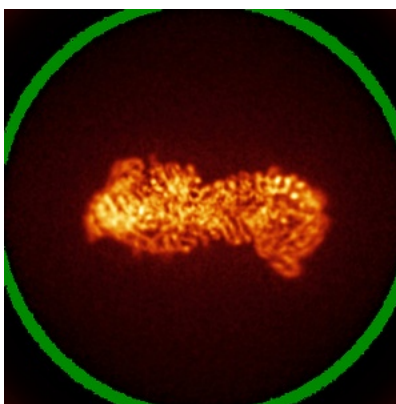


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

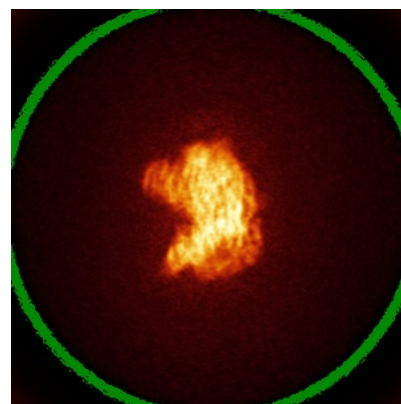
### 6.4.1 Primary map



X

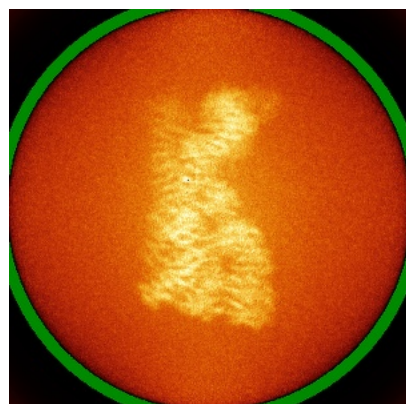


Y

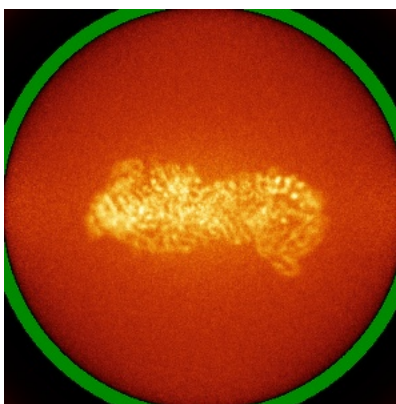


Z

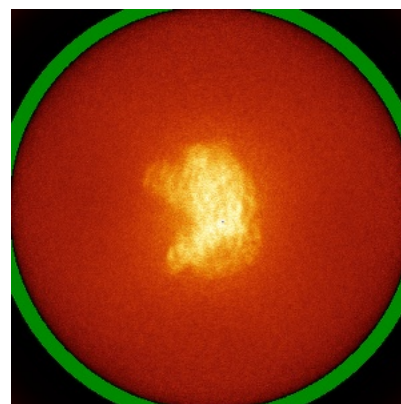
### 6.4.2 Raw map



X



Y



Z

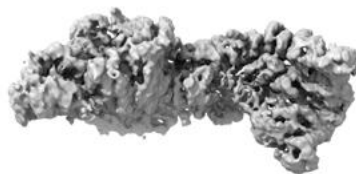
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



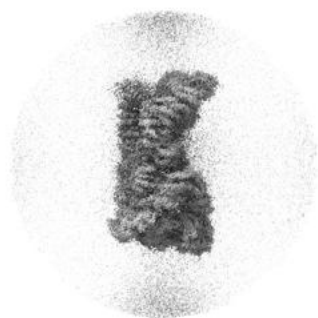
Y



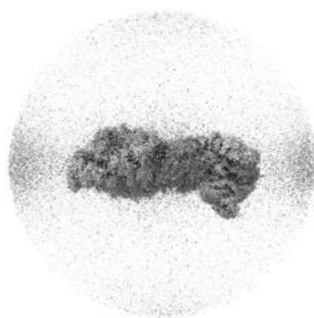
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00484. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

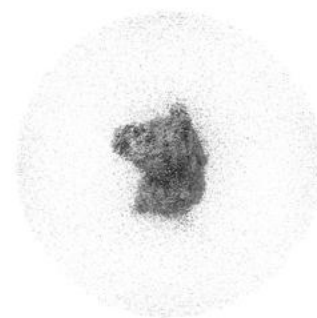
### 6.5.2 Raw map



X



Y



Z

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.

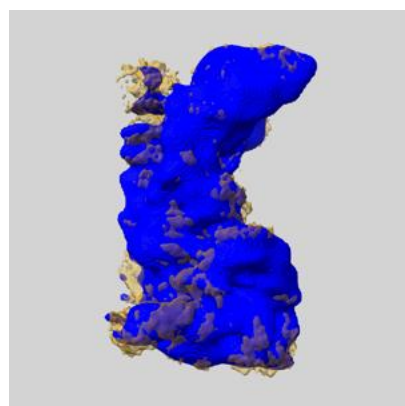
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

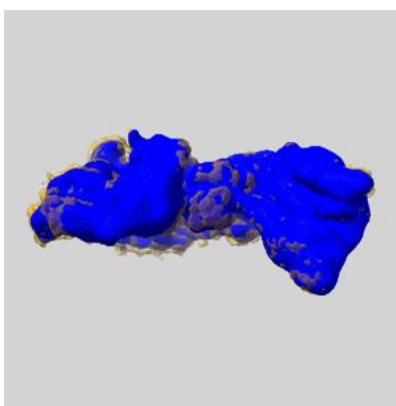
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

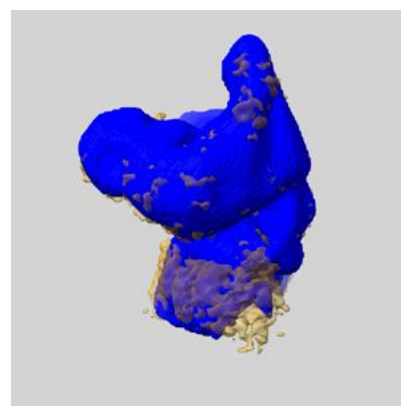
### 6.6.1 emd\_52570\_msk\_1.map [i](#)



X



Y

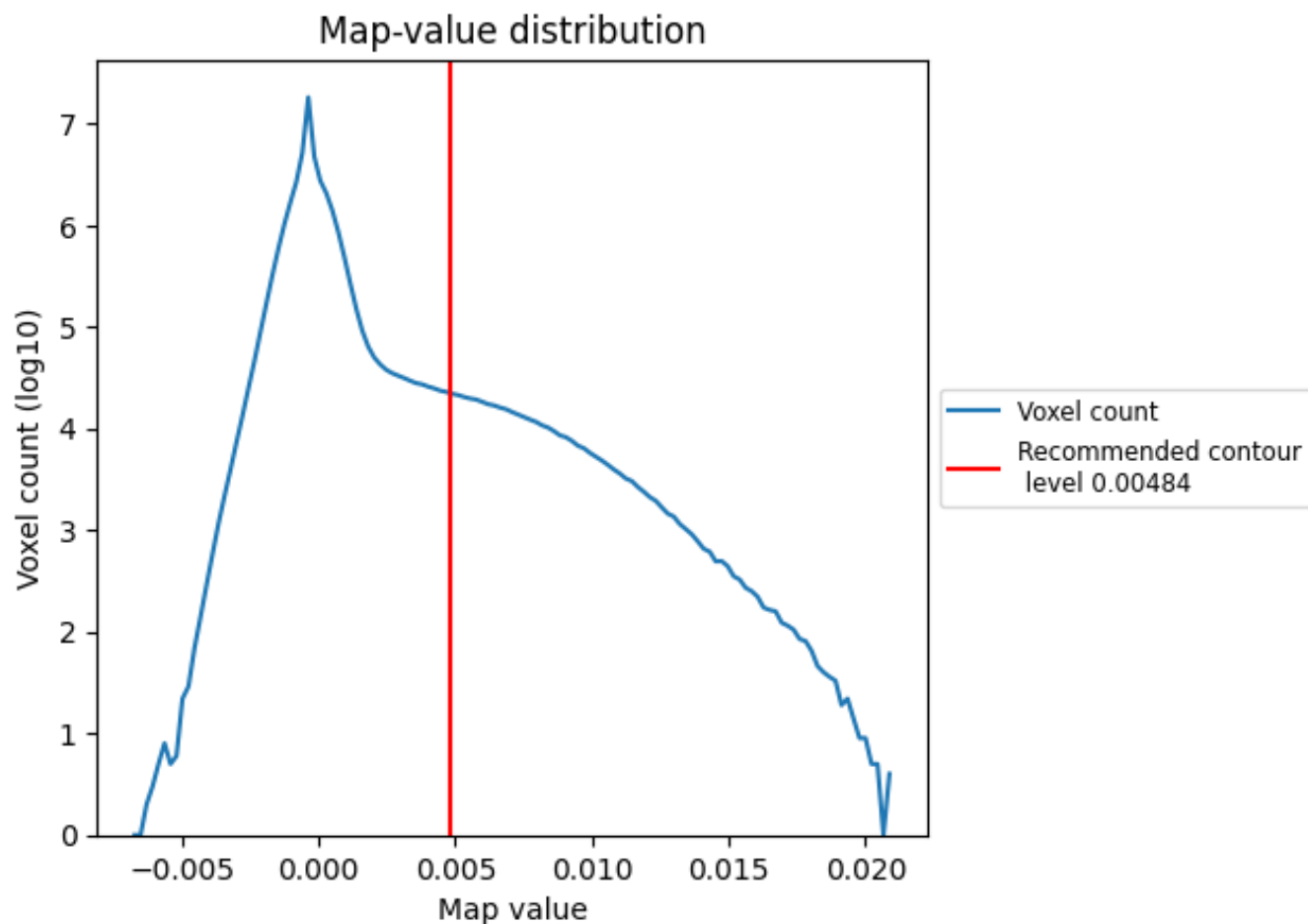


Z

## 7 Map analysis [i](#)

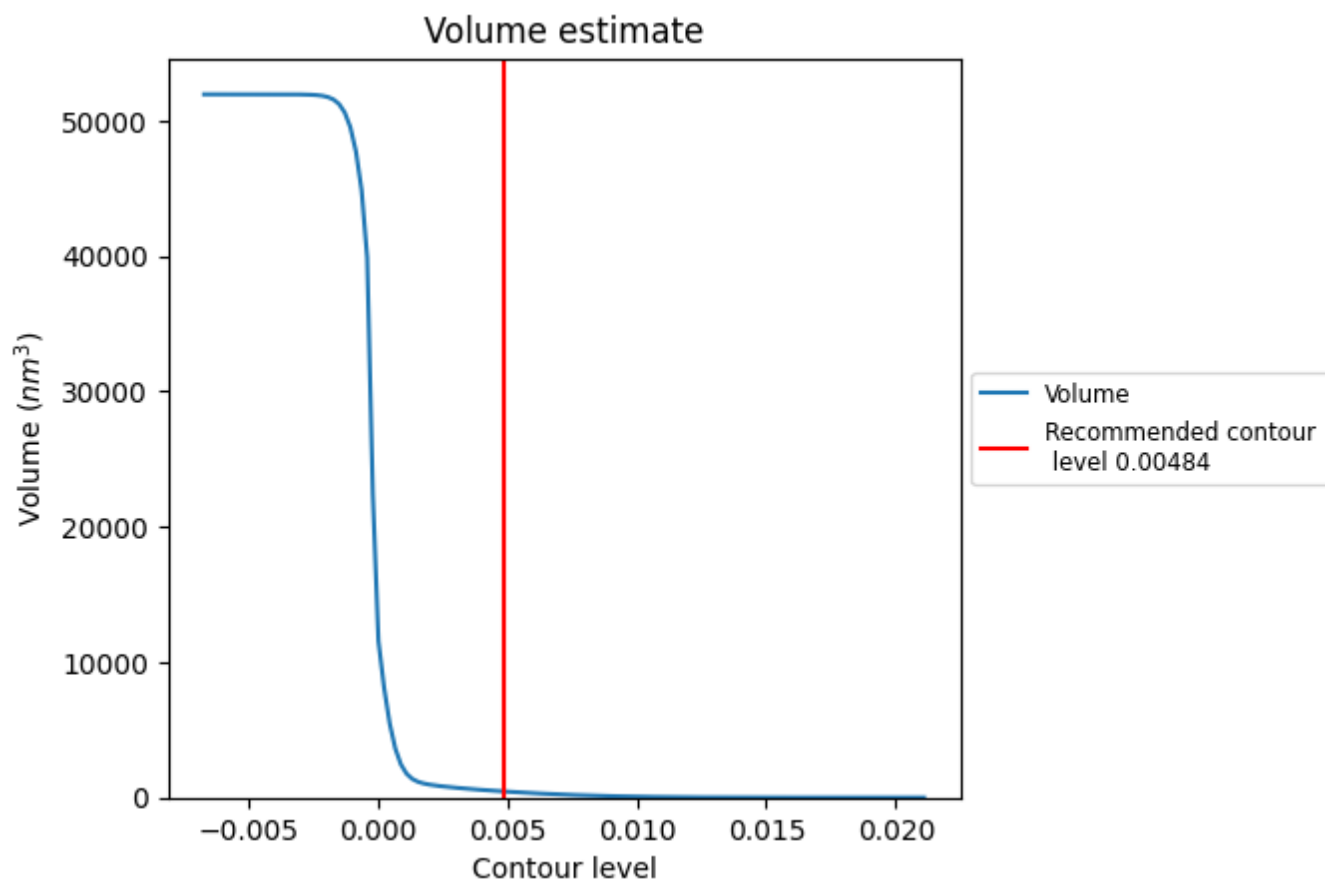
This section contains the results of statistical analysis of the map.

### 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](#)

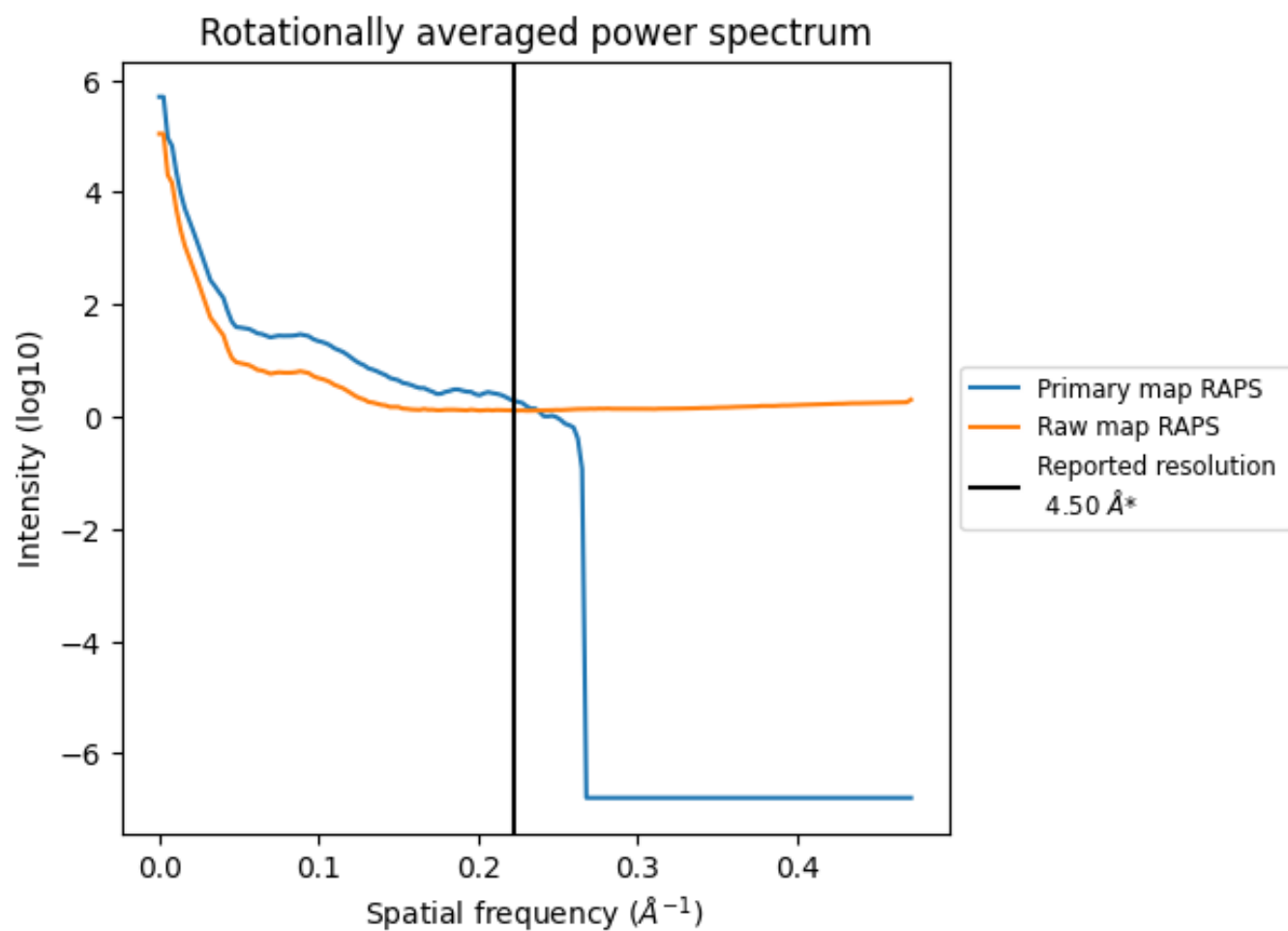


The volume at the recommended contour level is 455 nm<sup>3</sup>; this corresponds to an approximate mass of 411 kDa.

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 ⓘ

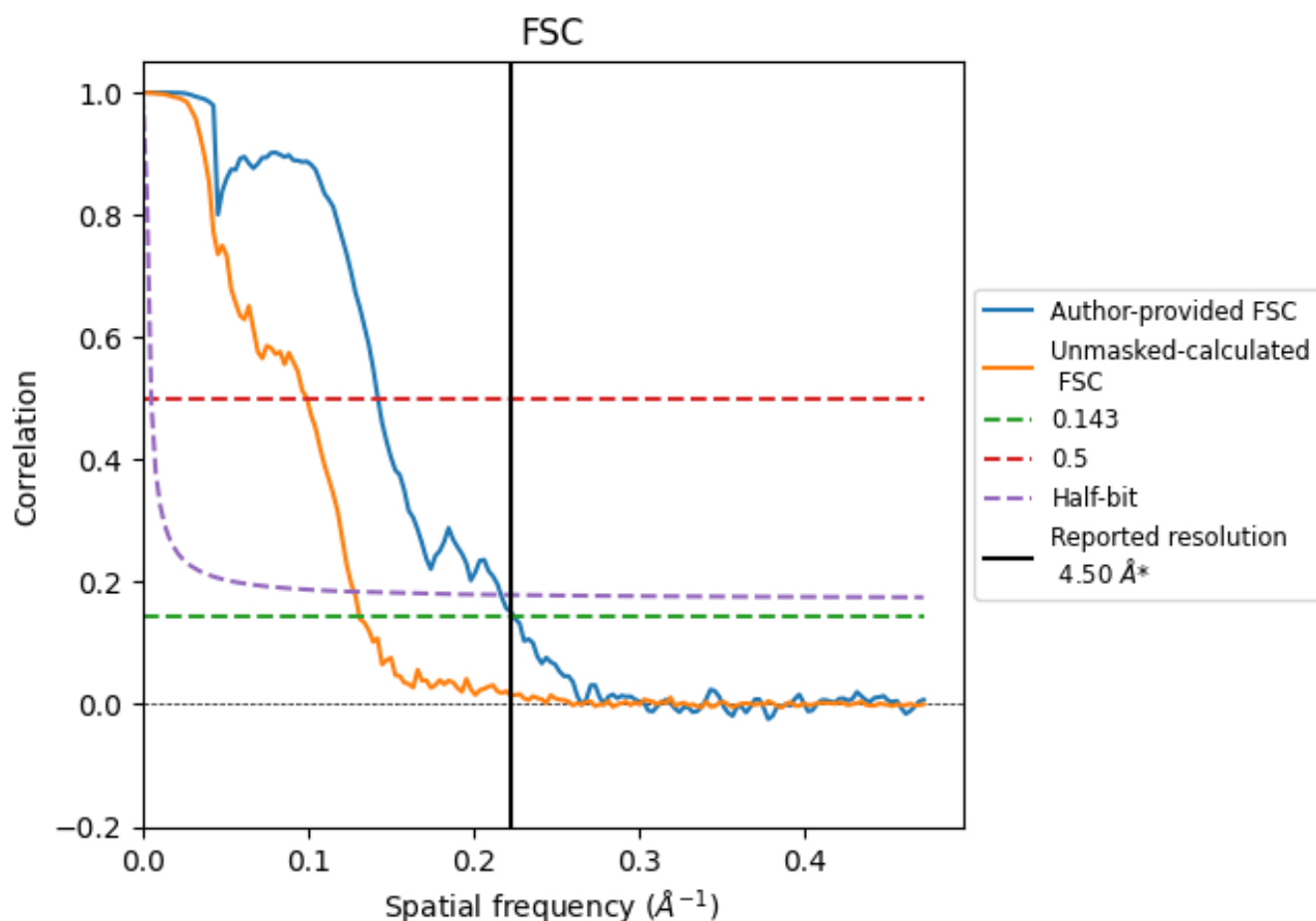


\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

## 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  $0.222 \text{ \AA}^{-1}$

## 8.2 Resolution estimates

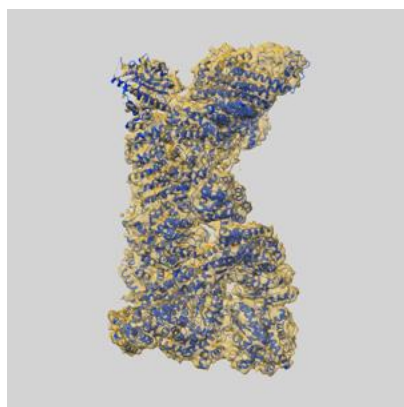
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	7.03	4.62
Unmasked-calculated*	7.63	10.07	7.82

\*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 7.63 differs from the reported value 4.5 by more than 10 %

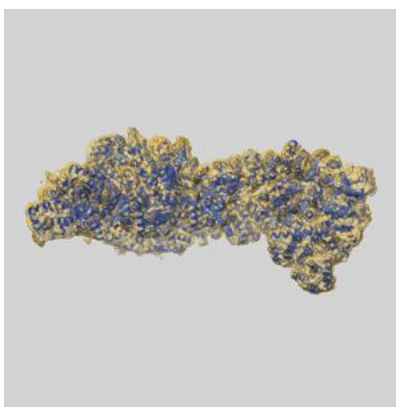
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52570 and PDB model 9I1I. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

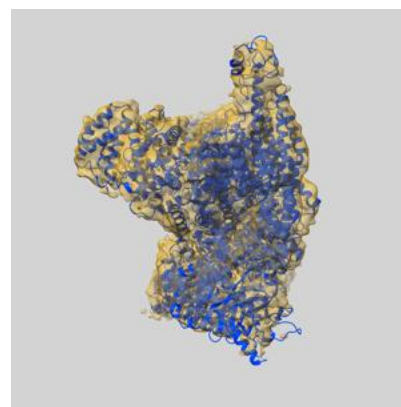
### 9.1 Map-model overlay [i](#)



X



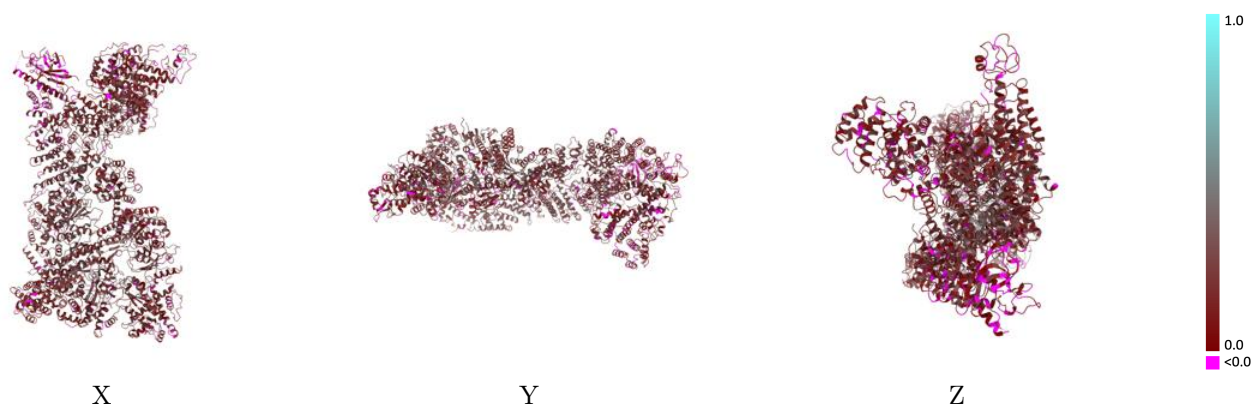
Y



Z

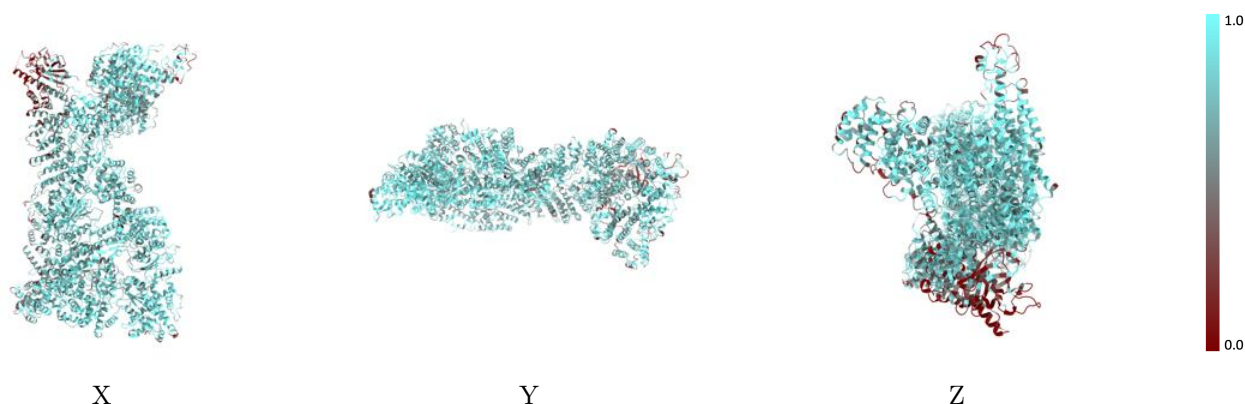
The images above show the 3D surface view of the map at the recommended contour level 0.00484 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



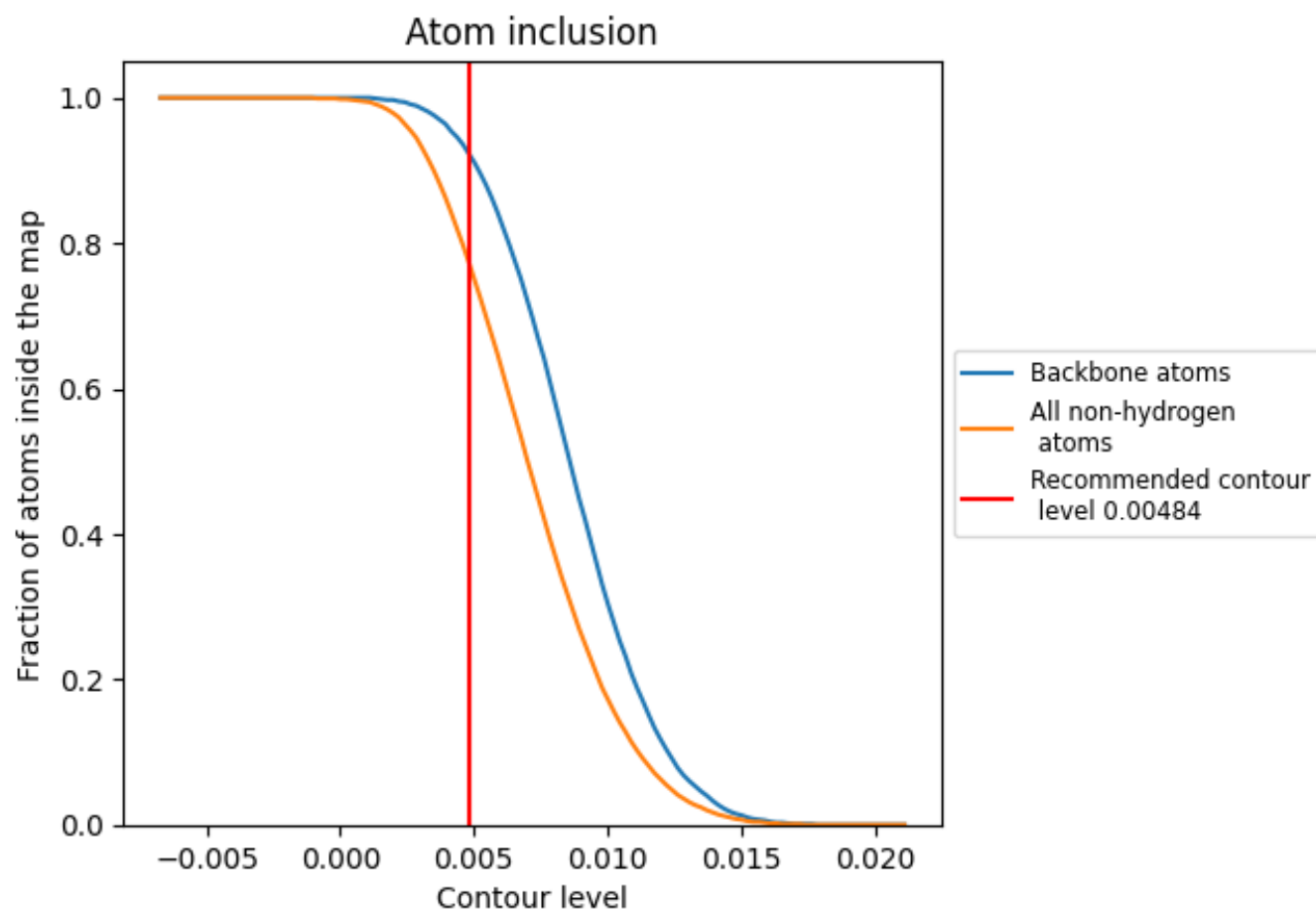
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00484).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 77% 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 (0.00484) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7700	<div></div> 0.2080
A	<div></div> 0.7700	<div></div> 0.2080

