



## wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 07:15 am BST

PDB ID : 7NI4  
EMDB ID : EMD-12350  
Title : Human ATM kinase domain with bound M4076 inhibitor  
Authors : Stakyte, K.; Rotheneder, M.  
Deposited on : 2021-02-11  
Resolution : 3.00 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.dev92
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)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

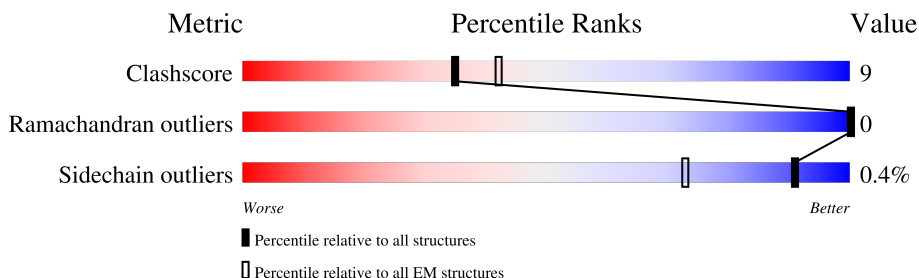
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	3056	 36% 11% 53%
1	B	3056	 38% 9% 53%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23236 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.

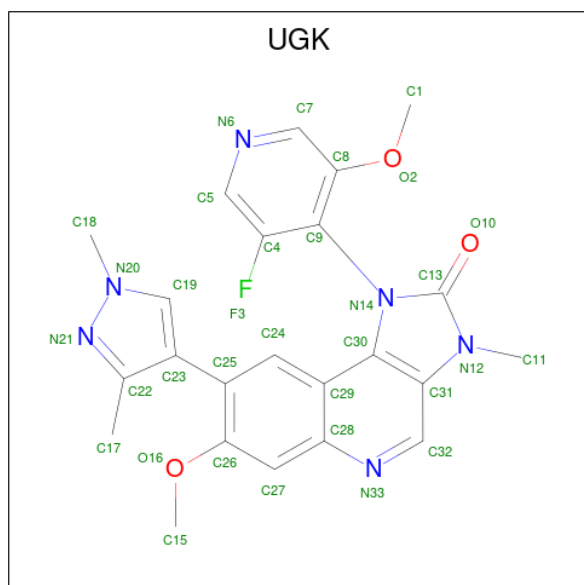
- Molecule 1 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1432	Total	C	N	O	S	0	0
			11584	7374	1982	2148	80		
1	B	1432	Total	C	N	O	S	0	0
			11584	7374	1982	2148	80		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

- Molecule 3 is 8-(1,3-dimethylpyrazol-4-yl)-1-(3-fluoranyl-5-methoxy-pyridin-4-yl)-7-methoxy-3-methyl-imidazo[4,5-c]quinolin-2-one (three-letter code: UGK) (formula: C<sub>23</sub>H<sub>21</sub>FN<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

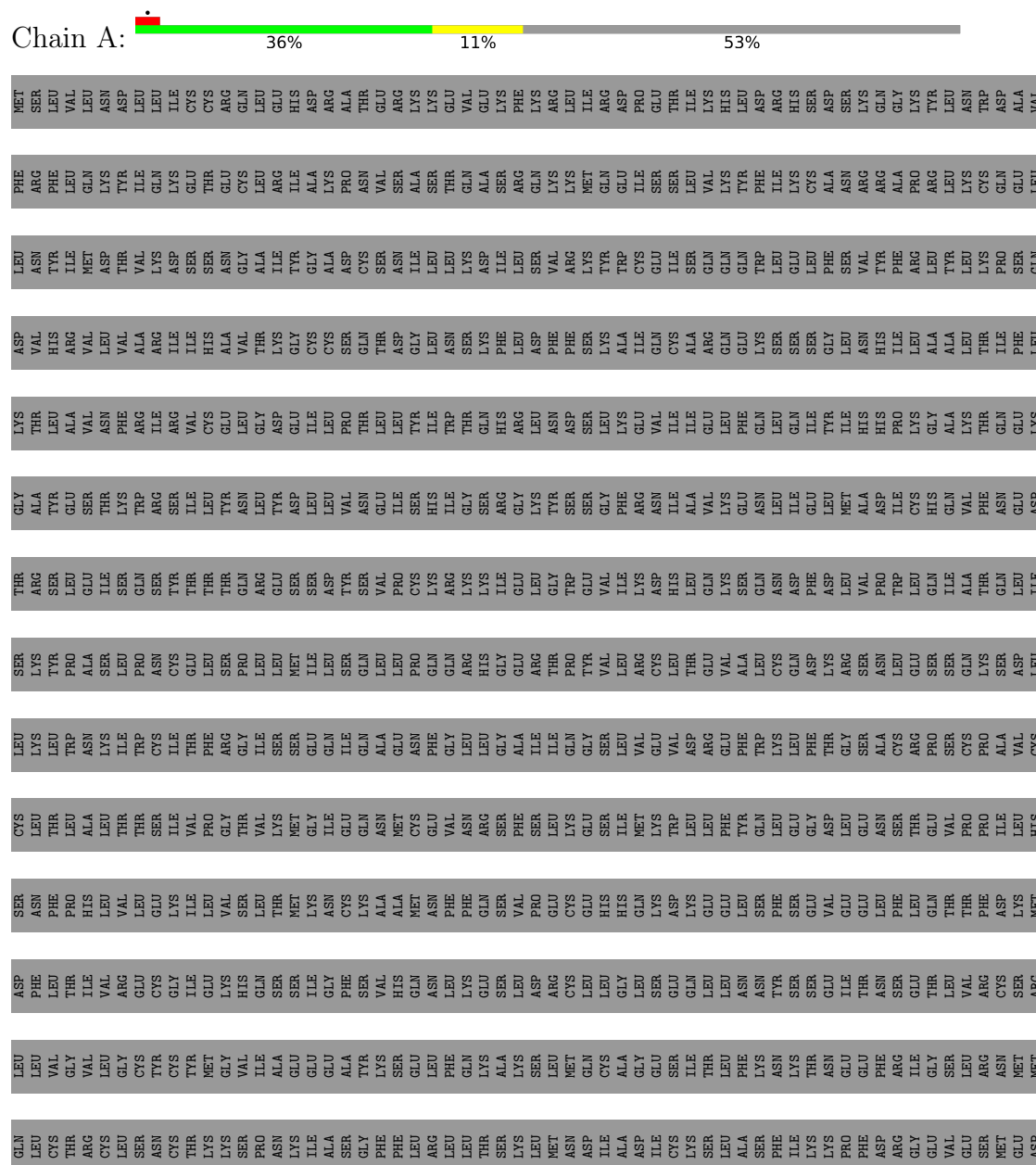


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 33	C 23	F 1	N 6	O 3	0
3	B	1	Total 33	C 23	F 1	N 6	O 3	0

### 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: Serine-protein kinase ATM











Q2972	ARG	L2656	E2814	Q2414	A2262	L2095	THR	L1845	C1726	Q1620
PRO	L2659	L2417	P2271	L2418	P2272	E2096	THR	L1867	A1732	L1621
GLU	E2660	K2418	E2272	K2419	E2273	Q2100	I1986	Q1968	A1733	E1622
ASP	V2664	ALA	R2273	LYS	Y2281	Q2101	S1987	F1969	V1734	D1626
THR	M2667	GLU	Y2284	GLY	S2285	W2104	L1989	L1874	L1737	Q1627
GLU	E2668	VAL	S2286	LEU	G2287	W2109	S1990	R1875	K1738	M1628
HIS	E2670	GLY	G2287	ARG	V2288	H2110	E1991	H1876	N1739	V1629
PRO	F2671	LEU	V2288	THR	THR	C2112	K1992	PHE	I1740	D1630
THR	L2572	ARG	W2287	SER	VAL	THR	S1993	SER	T1743	M1632
LEU	T2573	GLU	V2288	VAL	LYS	SER	K1994	THR	L1743	R1633
ASN	K2574	HIS	K2307	GLY	GLY	THR	E1995	ARG	S1748	D1637
ASP	PRO	GLU	K2308	LEU	VAL	SER	E1996	ARG	F1749	M1638
ASP	GLU	THR	L2309	ARG	LYS	SER	I1999	THR	W1750	D1641
GLN	VAL	THR	L2310	THR	GLY	LYS	D2003	SER	E1751	G1642
GLY	ALA	THR	L2311	GLY	VAL	GLU	E2007	THR	K1754	I1643
CYS	ARG	THR	L2312	LEU	G2121	G2121	R2010	PRO	L1761	L1647
LYS	ARG	ASN	K2313	LEU	H2125	H2125	ASP	ALA	L1764	N1650
ASN	ARG	THR	L2319	ARG	E2126	E2126	LEU	ASN	L1764	L1651
ASN	ILE	THR	L2324	THR	R2136	R2136	SER	ASP	K1772	L1652
SER	THR	THR	A2324	THR	K2148	K2148	GLU	SER	K1773	Q1653
THR	VAL	VAL	A2325	VAL	C2159	C2159	SER	GLU	E1779	S1654
THR	LYS	VAL	N2326	VAL	R2160	R2160	GLU	GLU	F1780	K1656
THR	VAL	VAL	N2327	VAL	K2161	K2161	H1895	H1895	D1781	E1664
THR	VAL	VAL	L2330	VAL	S2162	S2162	F1896	F1896	K1782	K1665
THR	VAL	VAL	T2348	VAL	L2163	L2163	R1897	R1897	E1783	E1669
THR	VAL	VAL	L2350	VAL	R2191	R2191	C1899	C1899	N1784	E1677
THR	VAL	VAL	E2351	VAL	S2192	S2192	T1908	T1908	N1783	H1690
THR	VAL	VAL	N2352	VAL	T2193	T2193	M1909	M1909	P1797	S1691
THR	VAL	VAL	V2355	VAL	H2195	H2195	R1921	R1921	E1800	K1892
THR	VAL	VAL	A2368	VAL	R2196	R2196	S1924	S1924	W1805	D1693
THR	VAL	VAL	GLY	VAL	Q2197	Q2197	D1930	D1930	I1806	Y1696
THR	VAL	VAL	ASN	VAL	E2200	E2200	L1936	L1936	L1814	L1700
THR	VAL	VAL	TYR	VAL	K2213	K2213	K1943	K1943	D1815	Q1709
THR	VAL	VAL	ASP	VAL	V2229	V2229	E1971	E1971	S1816	T1710
THR	VAL	VAL	GLY	VAL	E2232	E2232	K1972	K1972	T1711	T1711
THR	VAL	VAL	GLY	VAL	L2233	L2233	ARG	ARG	K1820	F1712
THR	VAL	VAL	SER	VAL	L2234	L2234	SER	SER	K1821	I1713
THR	VAL	VAL	S2376	VAL	K2237	K2237	LEU	LEU	E1822	L1715
THR	VAL	VAL	GLY	VAL	E2238	E2238	PHE	PHE	I1823	L1715
THR	VAL	VAL	THR	VAL	R2241	R2241	ALA	ALA	Q1824	L1718
THR	VAL	VAL	GLY	VAL	K2243	K2243	GLY	GLY	Q1825	L1718
THR	VAL	VAL	ASP	VAL	E2411	E2411	GLY	GLY	L1826	T1721
THR	VAL	VAL	THR	VAL	S2408	S2408	SER	SER	K1834	E1724
THR	VAL	VAL	GLY	VAL	E2409	E2409	GLN	GLN	D1836	D1725
THR	VAL	VAL	ASP	VAL	F2410	F2410	SER	SER	Q1839	
THR	VAL	VAL	THR	VAL	E2411	E2411	SER	SER		
THR	VAL	VAL	GLY	VAL	D2551	D2551				
THR	VAL	VAL	THR	VAL						
THR	VAL	VAL	ASP	VAL						
THR	VAL	VAL	GLY	VAL						
THR	VAL	VAL	THR	VAL						
THR	VAL	VAL	ASP	VAL						
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THR	VAL	VAL	GLY	VAL						
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THR	VAL	VAL	ASP	VAL						
THR	VAL	VAL	GLY	VAL						
THR	VAL	VAL	THR	VAL					</	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	455866	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0213	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5295, 0.5295, 0.5295	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: ZN, UGK

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	0.27	0/11798	0.49	0/15921
1	B	0.27	0/11798	0.48	0/15921
All	All	0.27	0/23596	0.49	0/31842

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	11584	0	11686	226	0
1	B	11584	0	11686	186	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	0	0	0
3	B	33	0	0	2	0
All	All	23236	0	23372	405	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 9.

The worst 5 of 405 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:B:1591:LEU:HD12	1:B:1591:LEU:O	1.77	0.85
1:B:1590:LEU:HD12	1:B:1590:LEU:O	1.76	0.85
1:B:2722:LEU:HD21	1:B:2767:LEU:HD22	1.61	0.80
1:A:2480:HIS:HB3	1:A:2483:TRP:HD1	1.48	0.77
1:A:1557:ILE:HD13	1:A:1560:LYS:HZ1	1.51	0.76

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	1416/3056 (46%)	1387 (98%)	29 (2%)	0	100	100
1	B	1416/3056 (46%)	1389 (98%)	27 (2%)	0	100	100
All	All	2832/6112 (46%)	2776 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1292/2780 (46%)	1286 (100%)	6 (0%)	88	96
1	B	1292/2780 (46%)	1288 (100%)	4 (0%)	92	97

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2584/5560 (46%)	2574 (100%)	10 (0%)	91	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1591	LEU
1	B	1592	GLU
1	B	2213	LYS
1	A	2070	ASN
1	A	2277	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1549	ASN
1	B	2070	ASN
1	B	3037	GLN
1	A	2002	GLN
1	A	1867	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	UGK	A	3202	-	35,37,37	0.75	1 (2%)	41,56,56	0.74	0
3	UGK	B	3202	-	35,37,37	0.76	1 (2%)	41,56,56	0.74	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
3	UGK	A	3202	-	-	2/12/12/12	0/5/5/5
3	UGK	B	3202	-	-	2/12/12/12	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3202	UGK	C23-C22	3.91	1.42	1.38
3	A	3202	UGK	C23-C22	3.80	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3202	UGK	C22-C23-C25-C26
3	B	3202	UGK	C22-C23-C25-C26
3	A	3202	UGK	C8-C9-N14-C30
3	B	3202	UGK	C8-C9-N14-C30

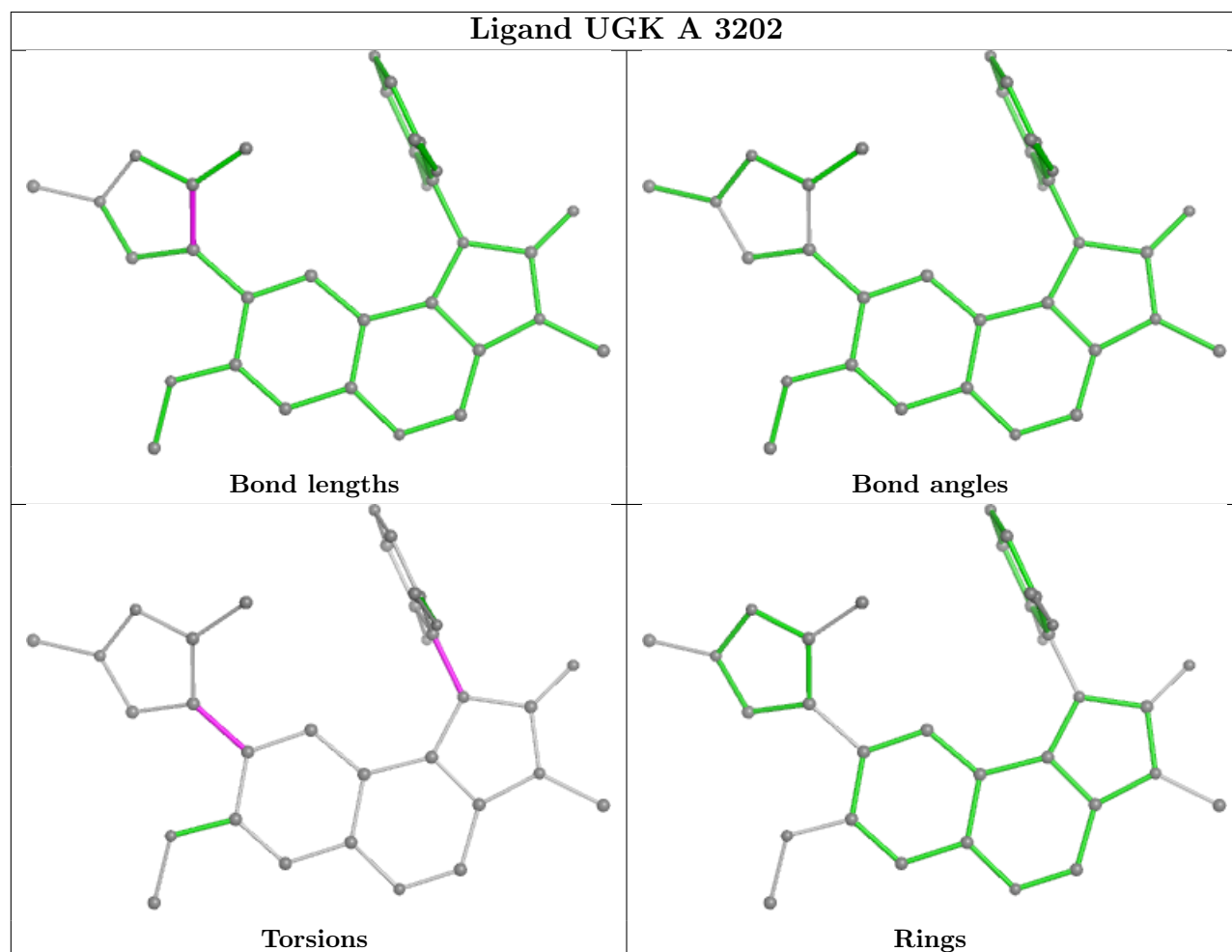
There are no ring outliers.

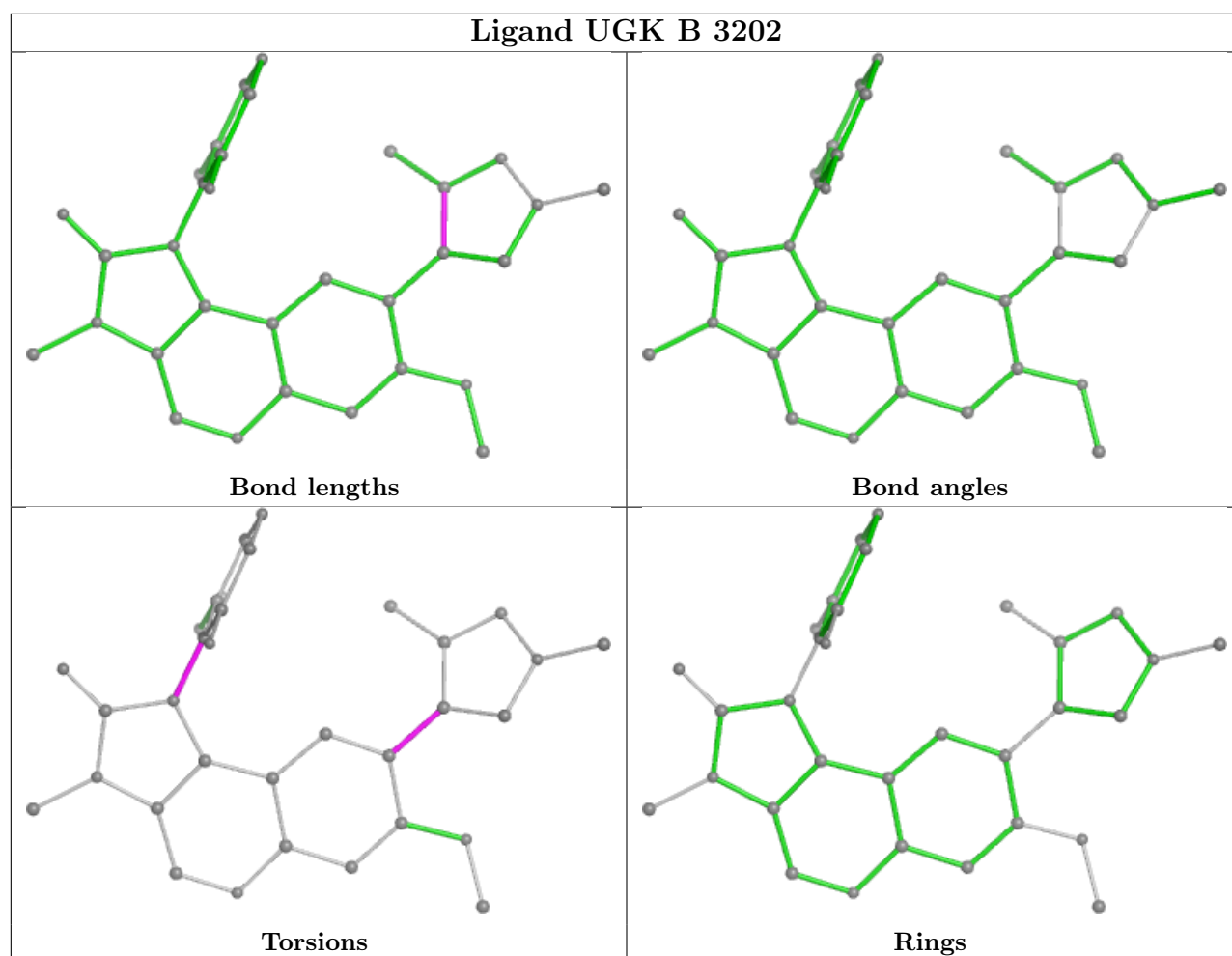
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3202	UGK	2	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.



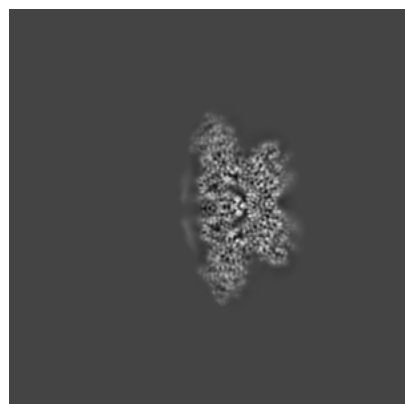
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12350. These allow visual inspection of the internal detail of the map and identification of artifacts.

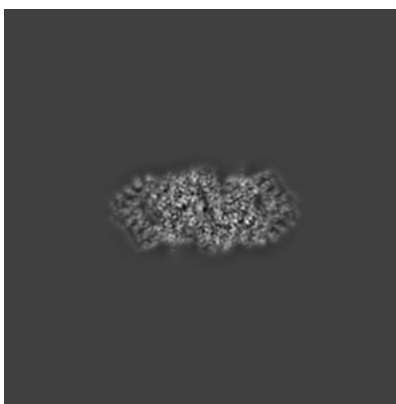
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

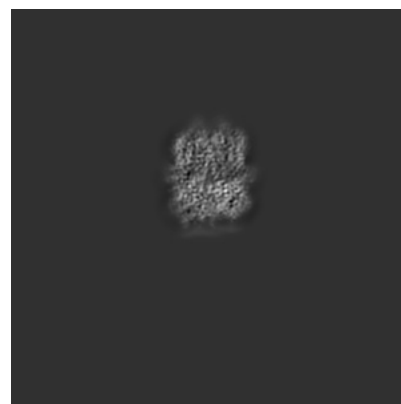
#### 6.1.1 Primary map



X

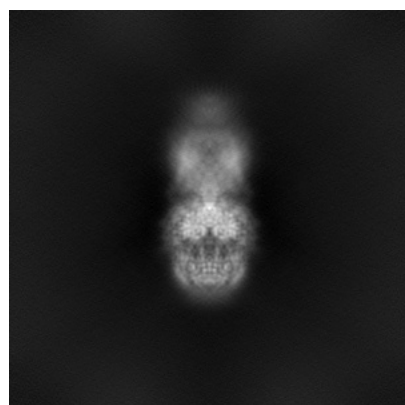


Y

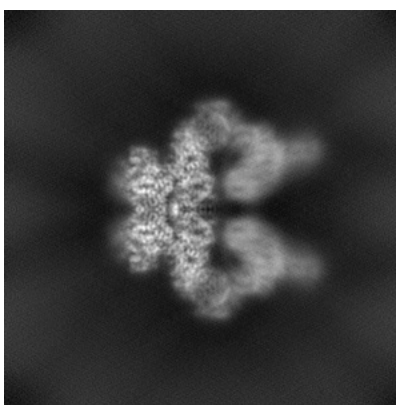


Z

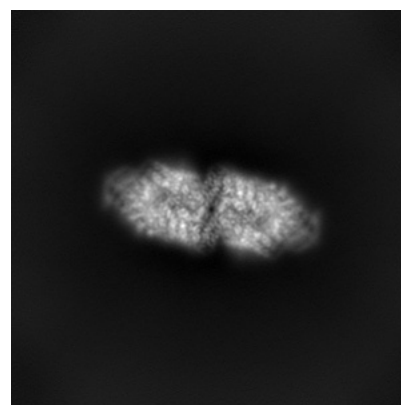
#### 6.1.2 Raw map



X



Y

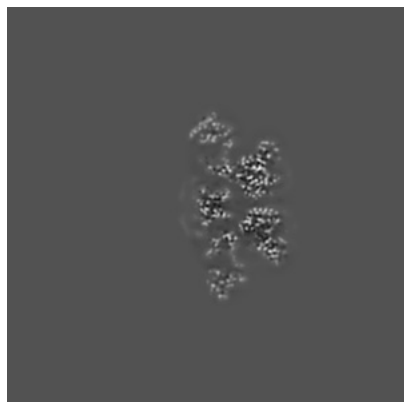


Z

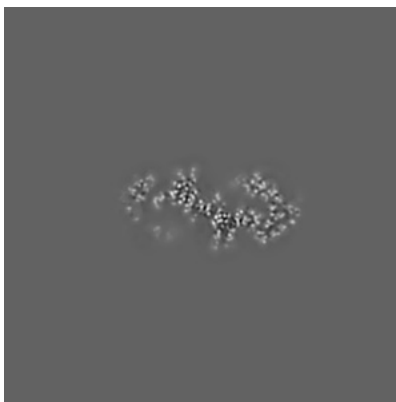
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

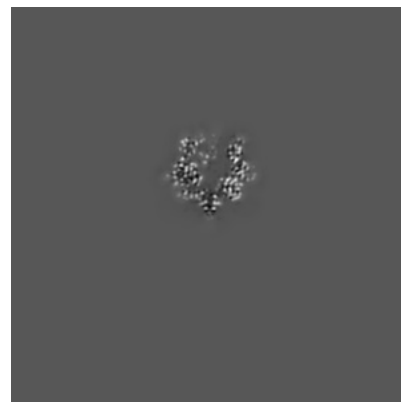
### 6.2.1 Primary map



X Index: 360

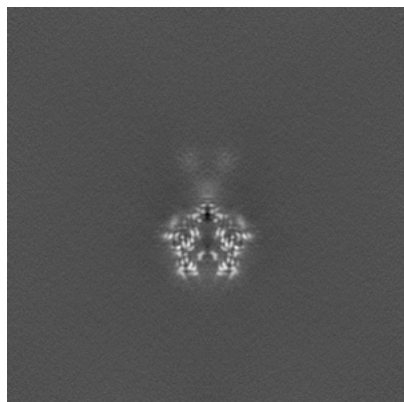


Y Index: 360

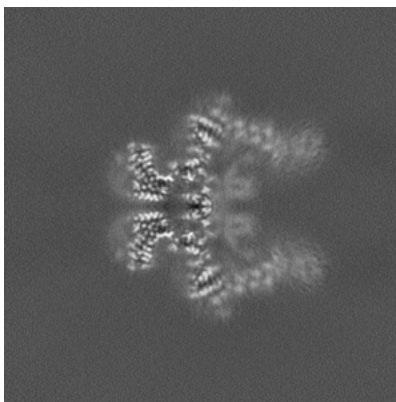


Z Index: 360

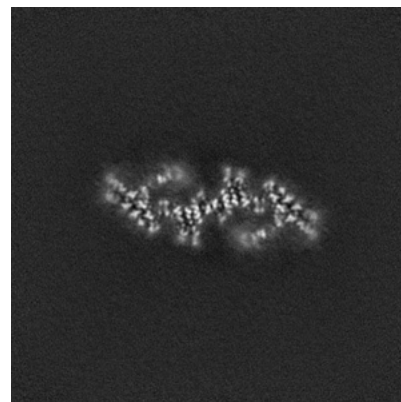
### 6.2.2 Raw map



X Index: 180



Y Index: 180

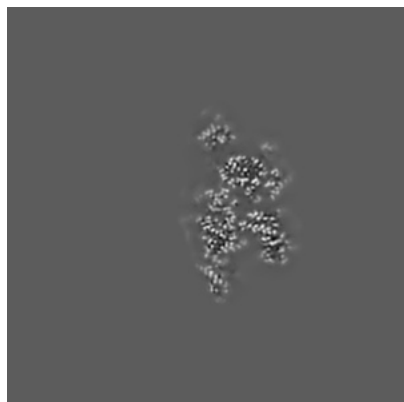


Z Index: 180

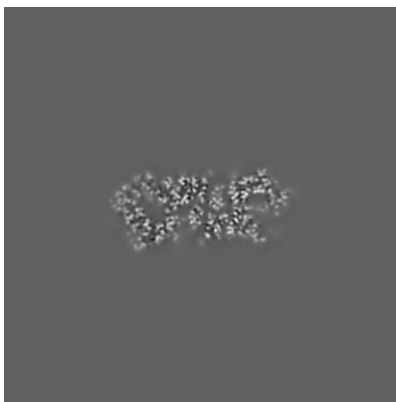
The images above show central slices of the map in three orthogonal directions.

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

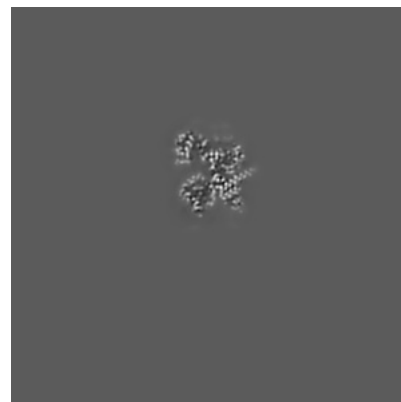
### 6.3.1 Primary map



X Index: 374

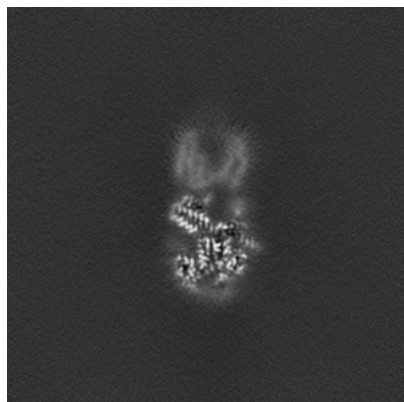


Y Index: 393

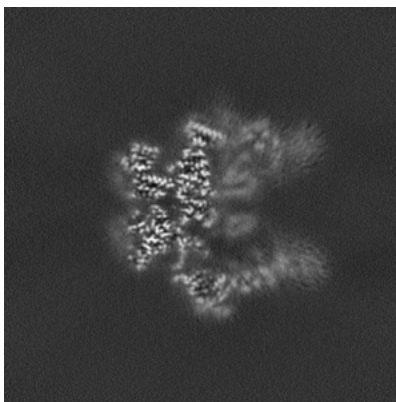


Z Index: 431

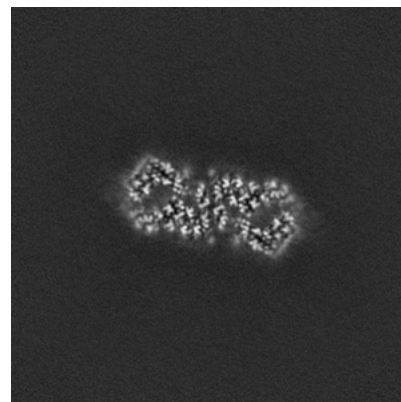
### 6.3.2 Raw map



X Index: 155



Y Index: 186

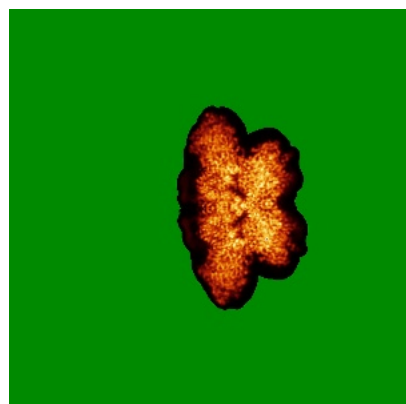


Z Index: 165

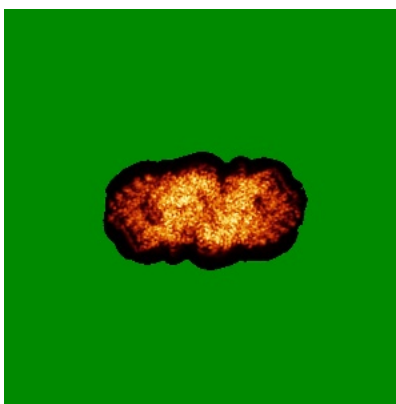
The images above show the largest variance slices of the map in three orthogonal directions.

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

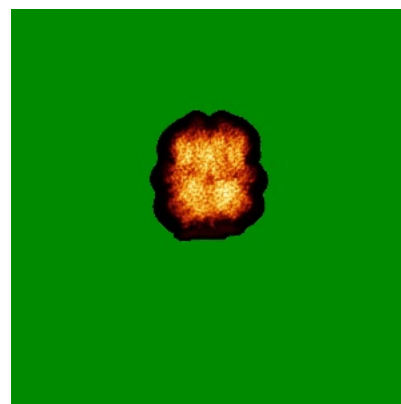
### 6.4.1 Primary map



X

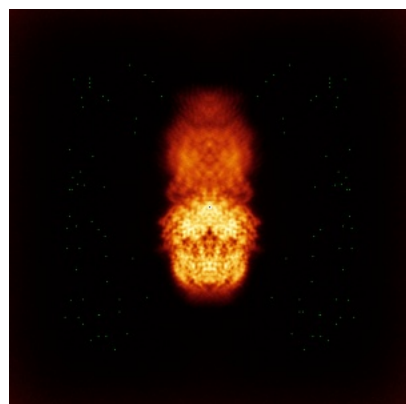


Y

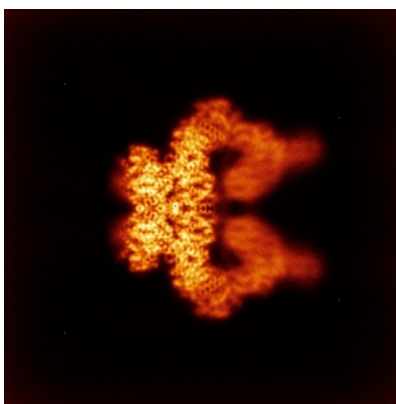


Z

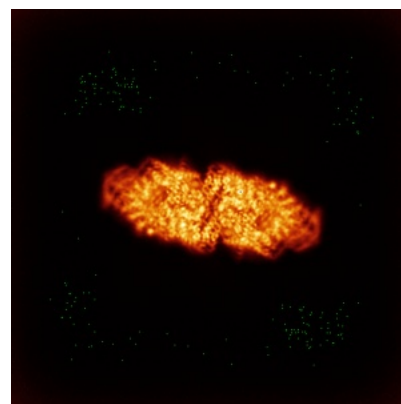
### 6.4.2 Raw map



X



Y

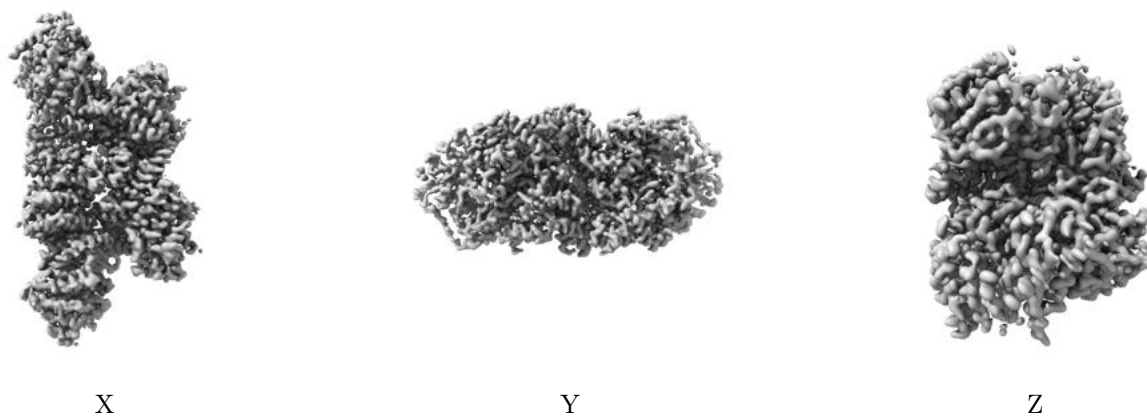


Z

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

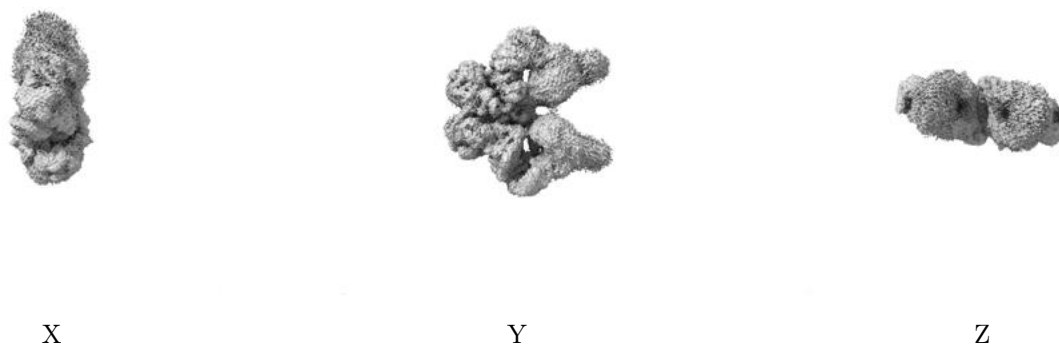
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0213. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

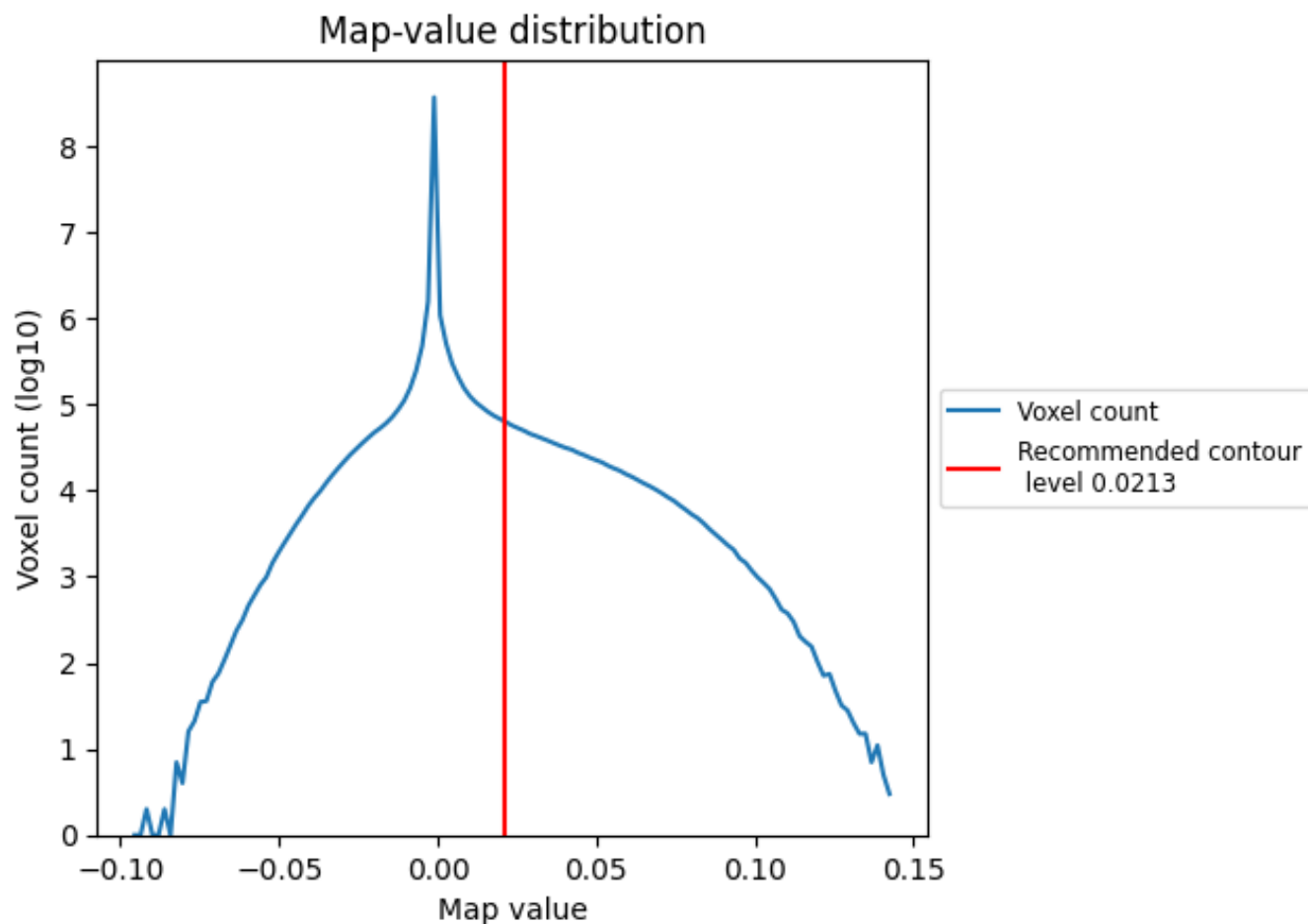
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

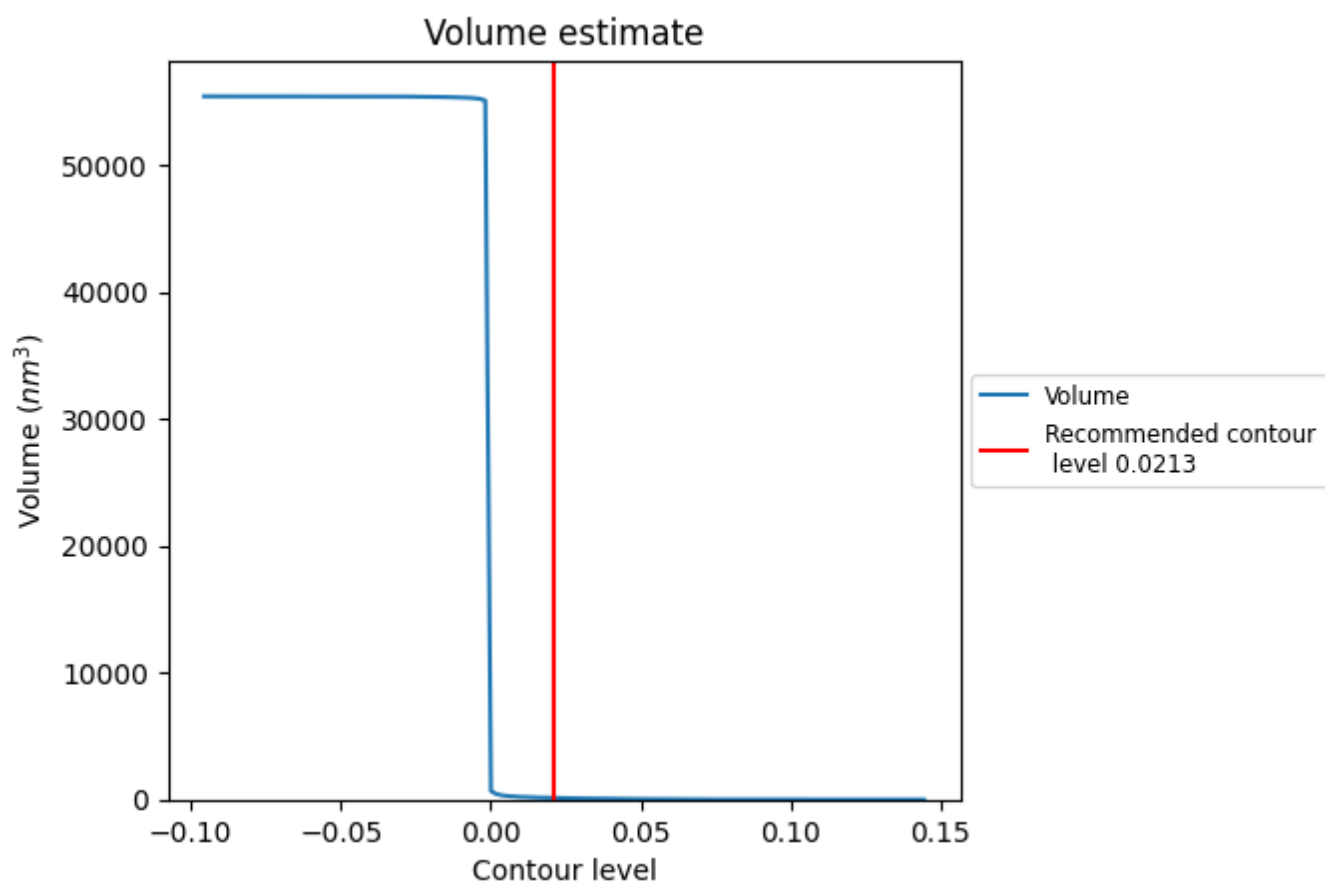
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

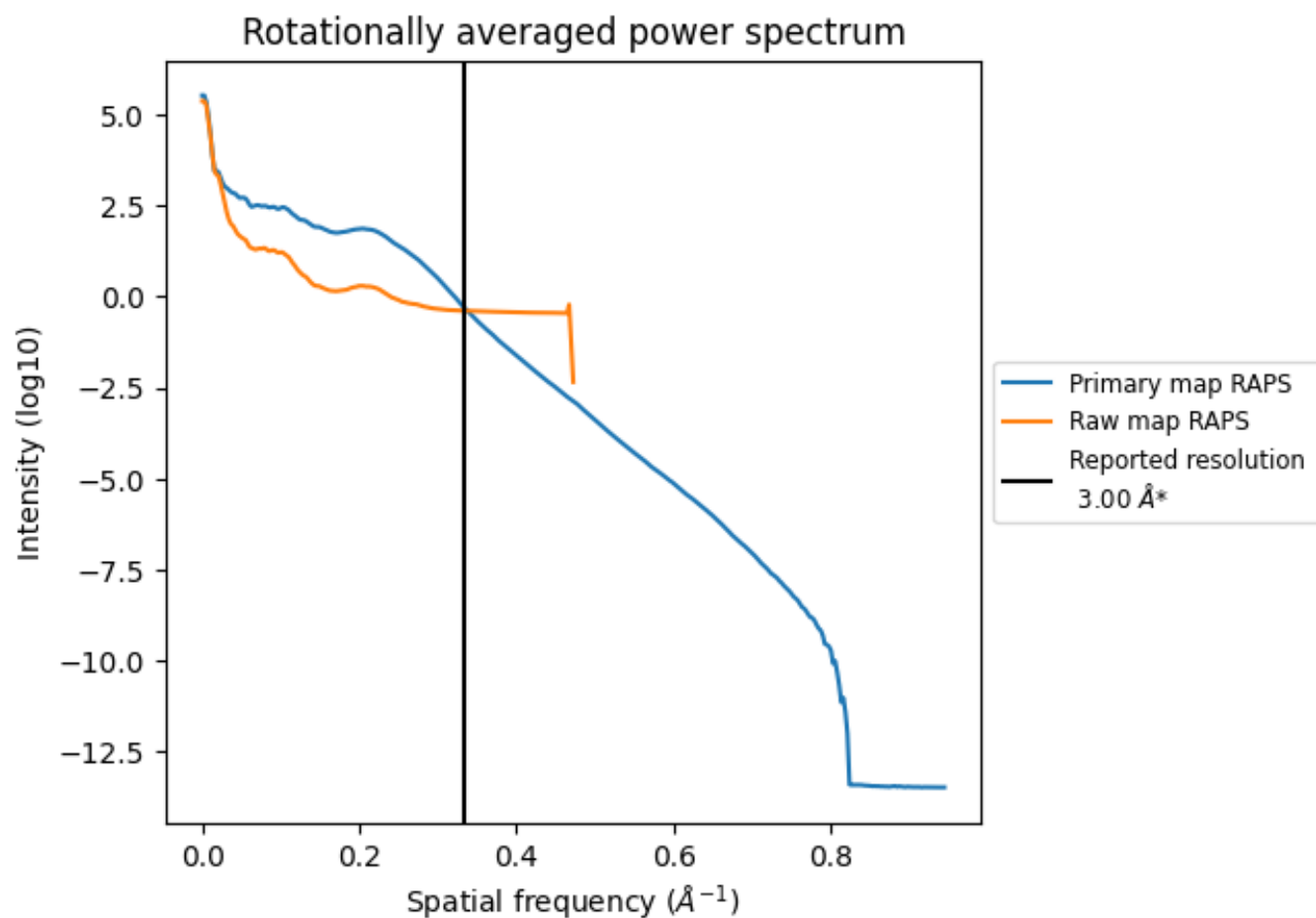
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm<sup>3</sup>; this corresponds to an approximate mass of 115 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 ⓘ



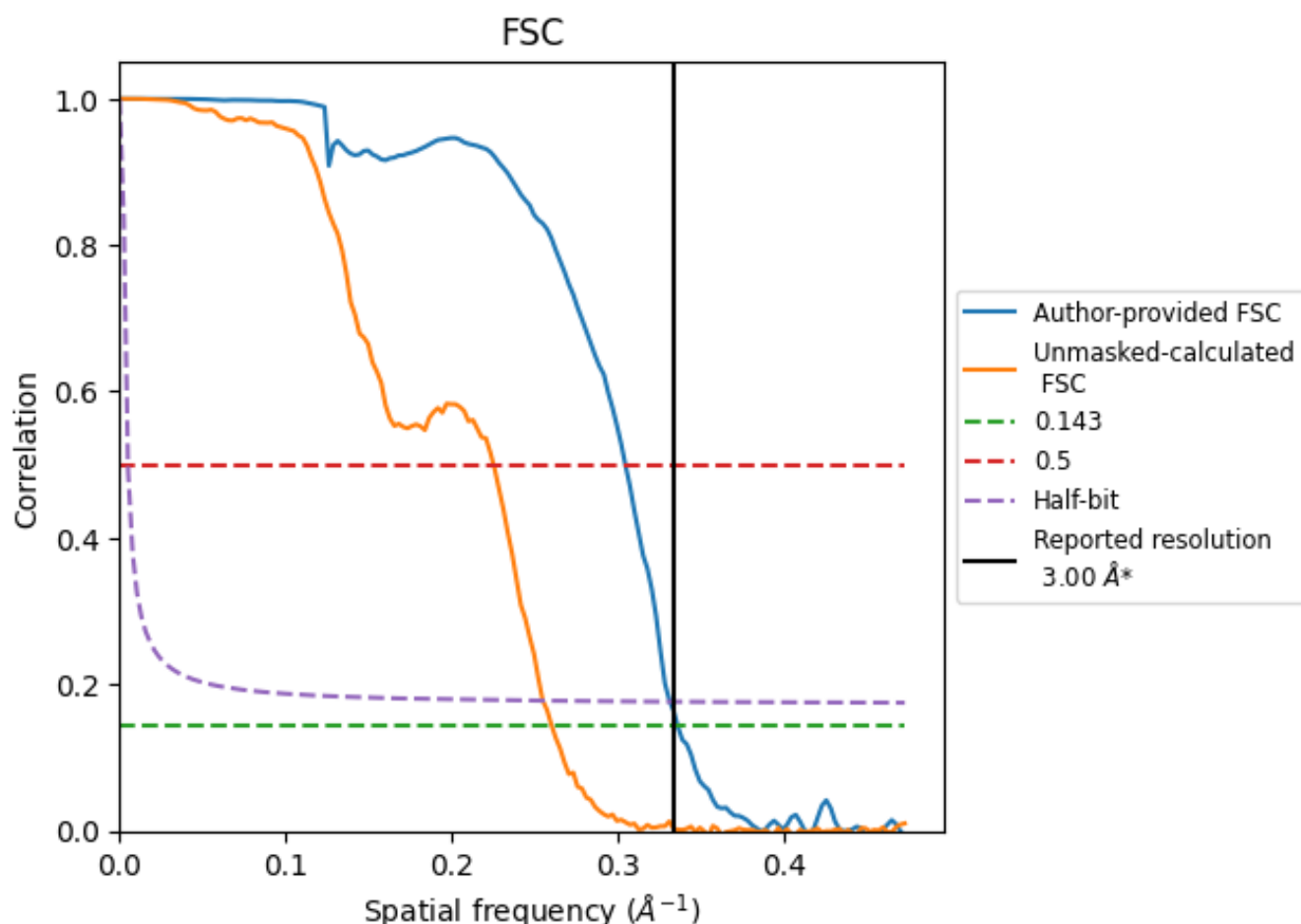
\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>



## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

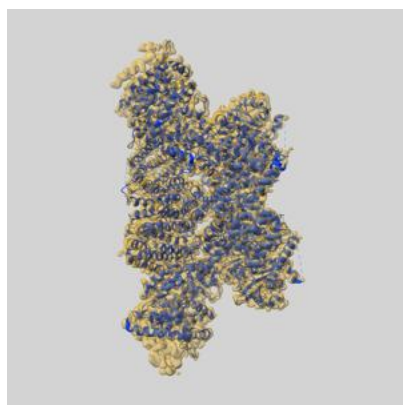
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.29	3.02
Unmasked-calculated*	3.85	4.45	3.93

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.0 by more than 10 %

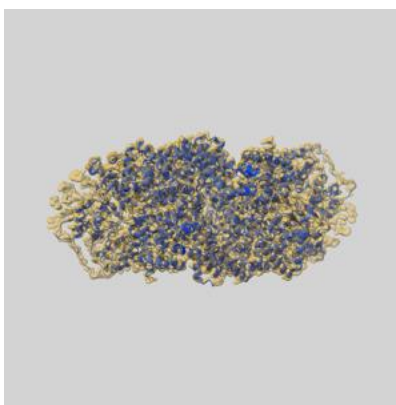
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12350 and PDB model 7NI4. Per-residue inclusion information can be found in section 3 on page 5.

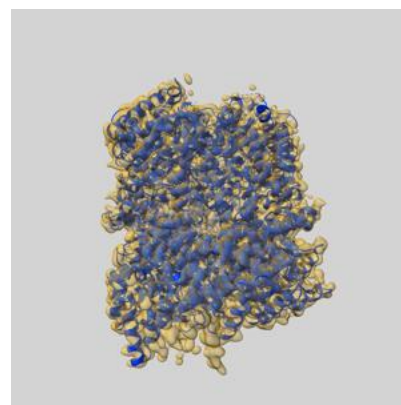
### 9.1 Map-model overlay [i](#)



X



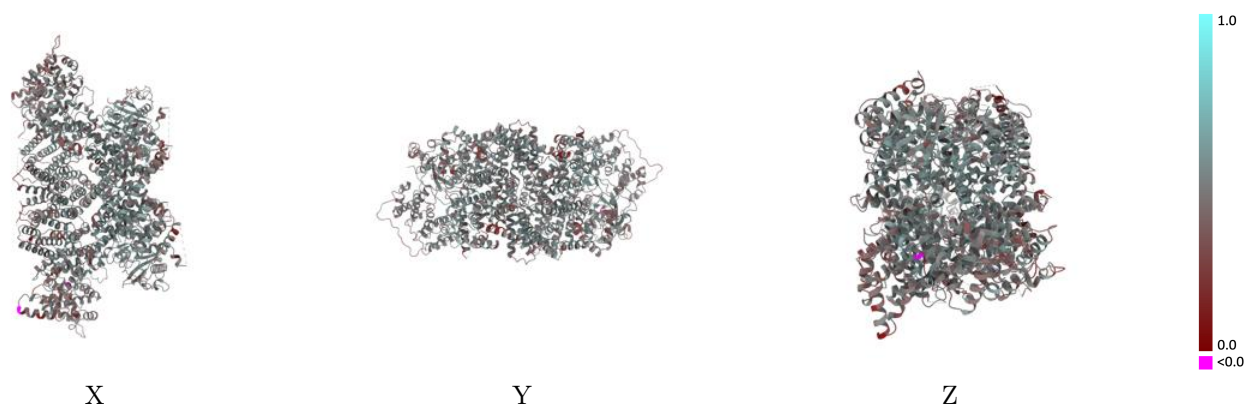
Y



Z

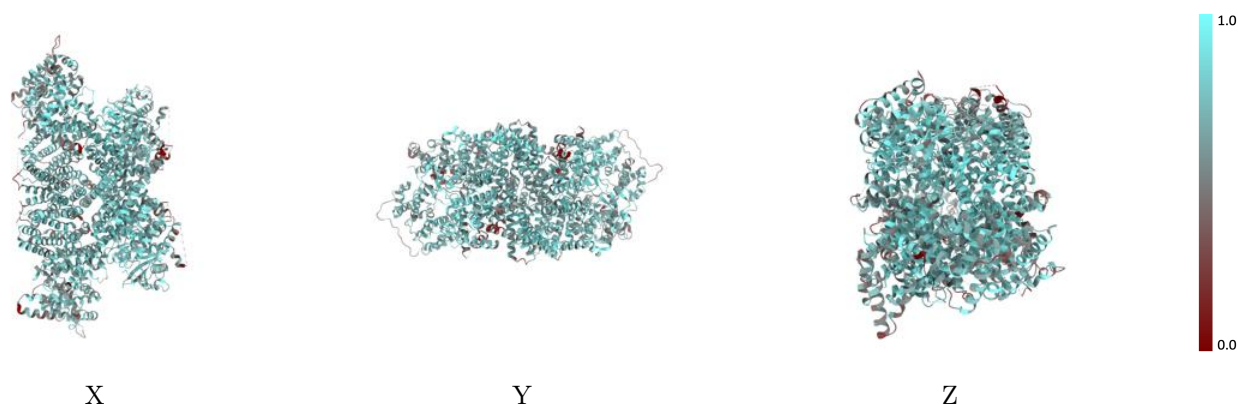
The images above show the 3D surface view of the map at the recommended contour level 0.0213 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



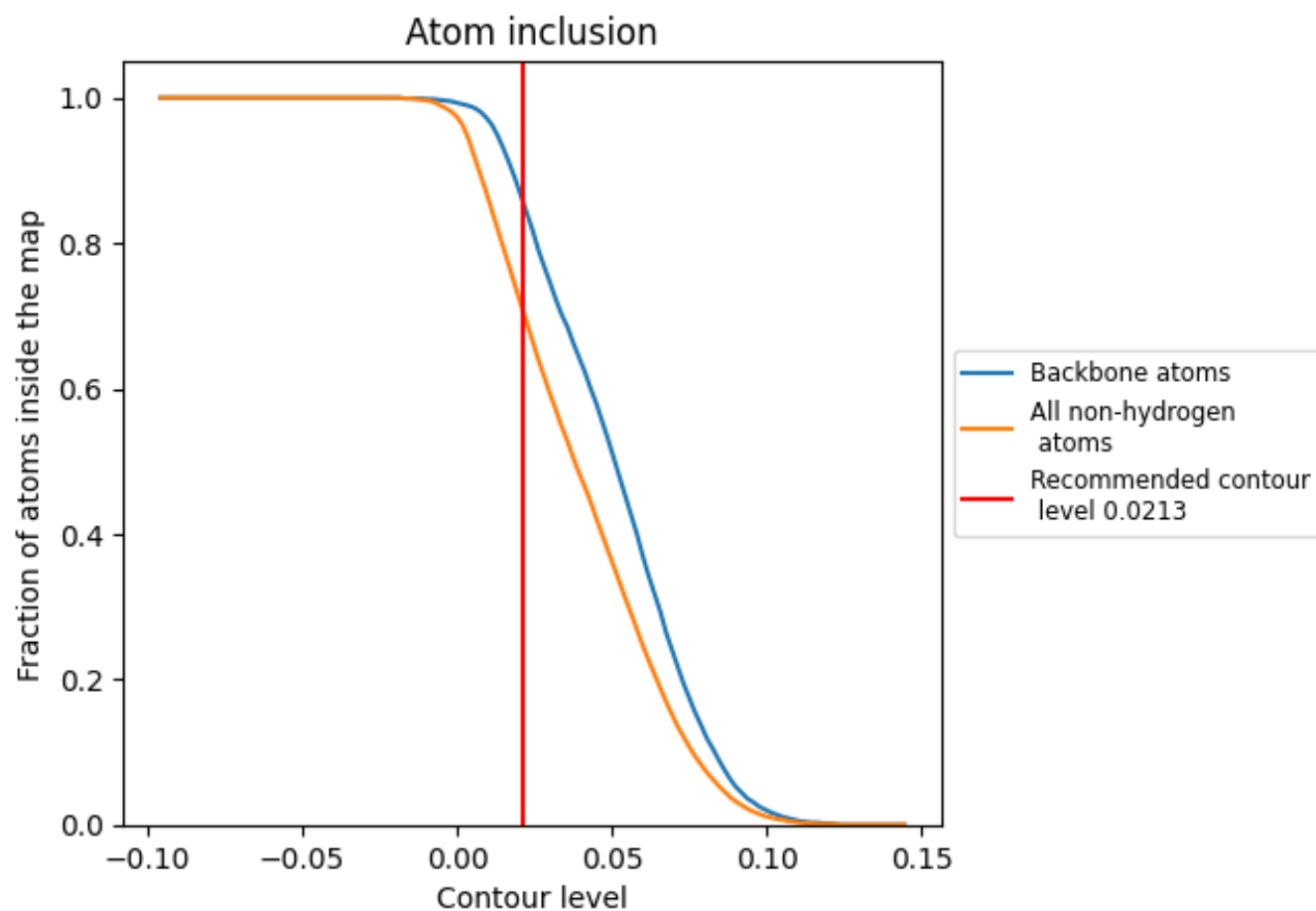
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0213).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.0213) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7070	<div></div> 0.4690
A	<div></div> 0.7080	<div></div> 0.4700
B	<div></div> 0.7070	<div></div> 0.4680

