



## wwPDB EM Validation Summary Report ⓘ

Oct 16, 2022 – 01:22 pm BST

PDB ID : 7PGQ  
EMDB ID : EMD-13392  
Title : GAP-SecPH region of human neurofibromin isoform 2 in closed conformation.  
Authors : Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.  
Deposited on : 2021-08-15  
Resolution : 3.50 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:

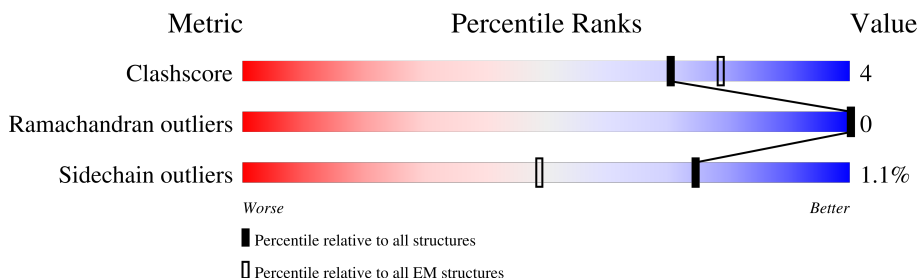
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 3.50 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)
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	F	2839	
1	N	2839	

## 2 Entry composition [i](#)

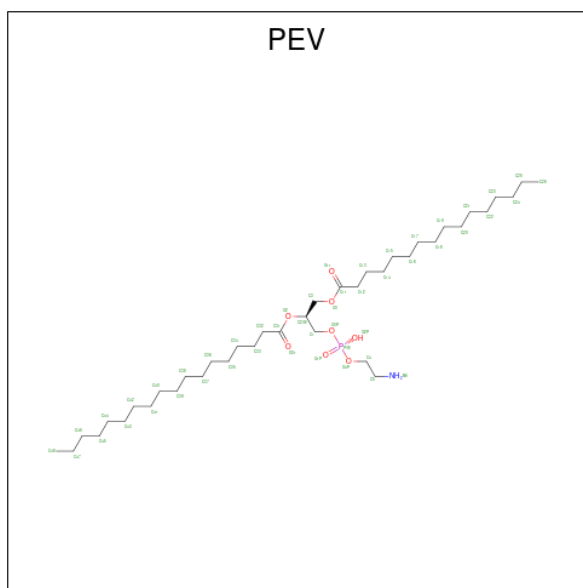
There are 3 unique types of molecules in this entry. The entry contains 31585 atoms, of which 15884 are hydrogens and 0 are deuteriums.

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 Neurofibromin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	F	1320	21053	6700	10550	1778	1950	75	0	0
1	N	650	10405	3317	5257	868	939	24	0	0

- Molecule 2 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).

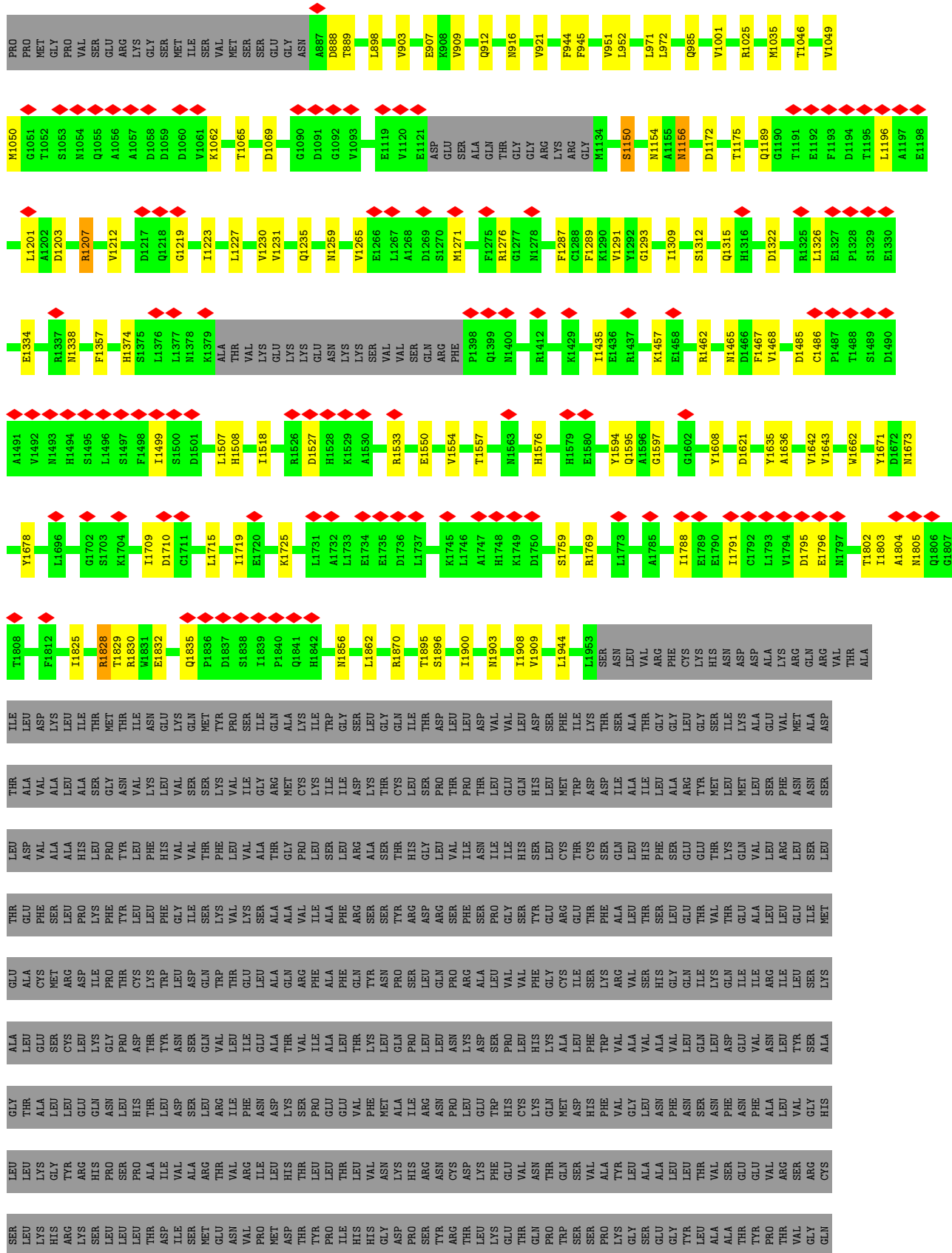


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	F	1	126	39	77	1	8	1	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	F	1	1	1	0









M1981	T1982	I1983	H1984	E1985	I1992	I1996	S1999	L2000	G2001	Q2002	I2003	T2004	D2005	L2006	L2007	D2008	F2014	I2015	K2016	T2017	S2018	A2019	T2020	G2021	G2022	L2023	K2027	A2028	E2029	M2030	M2031	I2058	T2061	L2073	A2079	R2083	L2088	S2093	L2103	V2107	V2111	S2180	S2181																																		
Y2182	R2183	D2184	R2185	S2186	F2187	S2188	P2189	G2190	S2191	Y2192	E2193	I2268	K2280	G2281	P2282	Q2288	Q2302	P2303	N2306	K2307	D2308	E2327	Q2340	L2367	M2374	V2378	L2395	R2411	F2430	V2431	N2432	R2452	C2453	S2454	L2455	K2456	H2457	R2458	LYS	SER	LEU	LEU	LEU	THR	ASP																																
ILE	SER	MET	GLU	ASN	VAL	PRO	ASP	THR	THR	LYS	PRO	THR	ARG	TYR	PRO	ILE	HIS	HIS	ARG	ASP	THR	GLY	THR	GLN	ALA	PRO	TRP	N2306	LYS	SER	ARG	GLN	PRO	LYS	GLY	GLY	TYR	LEU	ALA	ALA	PRO	THR	LYS	TYR	PRO	THR	VAL	GLY	ALA	GLN	THR	SER	PRO	ASP	TYR	ARG	ALA	ALA	MET	ARG	GLU	THR	THR	ASP	PRO	TYR	GLU	ALA	MET	ARG	GLU	THR	THR	GLN	ILE	SER	ASP
MET	GLY	GLN	PRO	SER	GLN	ALA	ASN	THR	THR	LYS	PRO	THR	LYS	LEU	LEU	GLY	THR	THR	ARG	LYS	ASP	PHE	ASP	HIS	LEU	ILE	LEU	SER	LYS	ASP	THR	THR	THR	ARG	GLN	ASP	THR	THR	THR	LYS	ILE	THR	THR	THR	ALA	PRO	PRO	THR	LYS	MET	ARG	GLU	THR	THR	THR	ASP	PRO	THR	TYR	GLU	MET	ARG	GLU	THR	THR	GLN	ARG	ILE	SER	ILE	SER	SER					
SER	SER	GLN	HIS	PRO	HIS	LEU	ARG	LYS	VAL	SER	VAL	SER	SER	GLU	S2601	N2602	V2603	L2604	L2605	D2606	E2607	E2608	V2609	L2610	T2611	D2612	P2613	K2614	I2615	Q2616	A2617	L2618	L2619	L2620	L2623	L2626	V2627	D2632	E2633	F2634	D2635	Q2636	R2637	I2638	L2639	Y2640	E2641	Y2642	L2643	A2644	E2645	A2646	S2647	V2648	V2649	F2650																					
P2651	K2652	V2653	F2654	P2655	V2656	V2657	H2658	N2659	L2660	L2661	D2662	S2663	K2664	I2665	N2666	T2667	L2668	L2669	S2670	L2671	C2672	Q2673	D2674	P2675	N2676	L2677	L2678	N2679	P2680	I2681	H2682	G2683	I2684	V2685	Q2686	S2687	V2688	V2689	Y2690	H2691	E2692	E2693	S2694	P2695	P2696	Q2697	Y2698	Q2699	T2700	S2701	Y2702	L2703	Q2704	S2705	F2706	L2711	L2738																				
PRO	THR	THR	GLY	HIS	CYS	ASN	SER	GLY	THR	THR	GLU	THR	THR	ALA	ALA	GLN	VAL	GLN	PRO	PRO	PRO	ALA	SER	LEU	GLN	SER	GLY	LEU	LEU	LEU	LEU	LEU	LEU	ALA	THR	SER	SER	GLN	HIS	SER	PRO	GLY	ILE	ASP	LYS	GLU	ASN	VAL	GLU	LEU	GLU	SER	THR	THR	GLY	ILE	VAL																				



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100684	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 ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	0.5	Depositor
Maximum defocus (nm)	2.1	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.062	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	344.0, 344.0, 344.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.72, 1.72, 1.72	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: PEV, 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	F	0.25	0/10719	0.43	0/14518
1	N	0.26	0/5257	0.45	0/7144
All	All	0.25	0/15976	0.44	0/21662

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	F	10503	10550	10556	83	0
1	N	5148	5257	5257	33	0
2	F	49	77	77	0	0
3	F	1	0	0	0	0
All	All	15701	15884	15890	115	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 4.

The worst 5 of 115 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:F:1230:VAL:HG21	1:F:1518:ILE:HG22	1.47	0.94
1:N:2088:LEU:O	1:N:2093:SER:OG	1.91	0.87
1:F:907:GLU:N	1:F:907:GLU:OE1	2.12	0.82
1:F:1219:GLY:O	1:F:1259:ASN:ND2	2.15	0.80
1:F:985:GLN:N	1:F:985:GLN:OE1	2.15	0.78

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	F	1308/2839 (46%)	1291 (99%)	17 (1%)	0	100	100
1	N	646/2839 (23%)	640 (99%)	6 (1%)	0	100	100
All	All	1954/5678 (34%)	1931 (99%)	23 (1%)	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	F	1180/2531 (47%)	1163 (99%)	17 (1%)	67	85
1	N	581/2531 (23%)	579 (100%)	2 (0%)	92	97
All	All	1761/5062 (35%)	1742 (99%)	19 (1%)	74	88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1635	TYR
1	N	2367	LEU
1	N	2432	ASN
1	F	1828	ARG
1	F	1374	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1856	ASN
1	F	1943	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](#)

Of 2 ligands modelled in this entry, 1 is 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	PEV	F	2901	-	48,48,48	0.31	0	51,53,53	0.25	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	PEV	F	2901	-	-	9/52/52/52	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

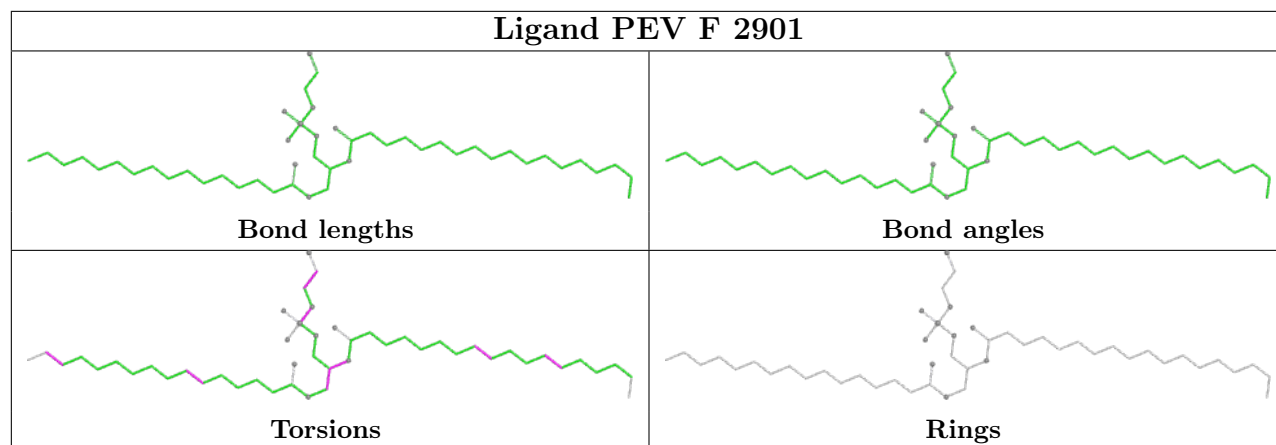
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2901	PEV	O4P-C4-C5-N6
2	F	2901	PEV	C4-O4P-P-O3P
2	F	2901	PEV	C37-C38-C39-C40
2	F	2901	PEV	C41-C42-C43-C44
2	F	2901	PEV	C15-C16-C17-C18

There are no ring outliers.

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](#)

There are no chain breaks in this entry.

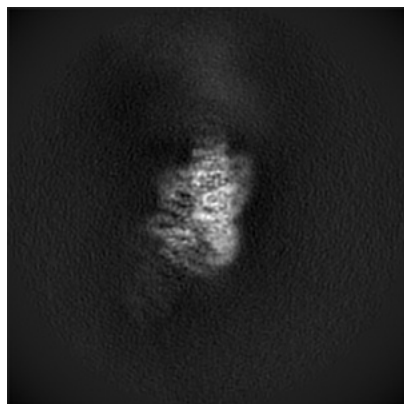
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13392. These allow visual inspection of the internal detail of the map and identification of artifacts.

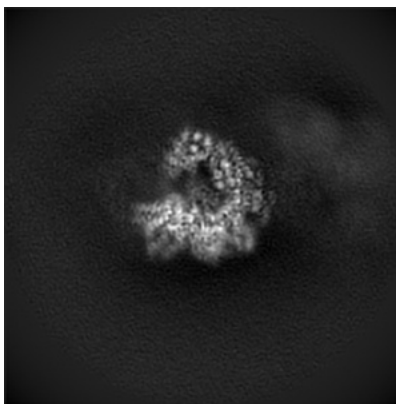
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

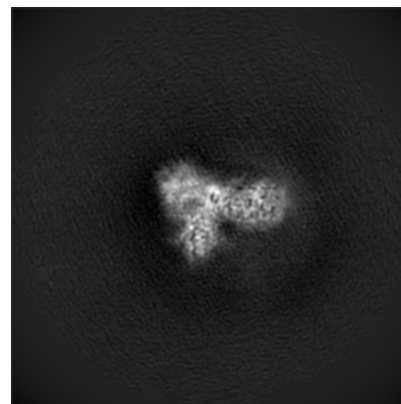
#### 6.1.1 Primary map



X

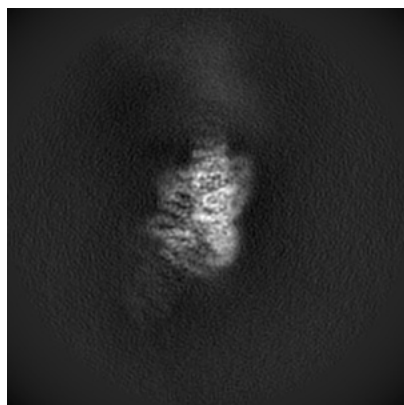


Y

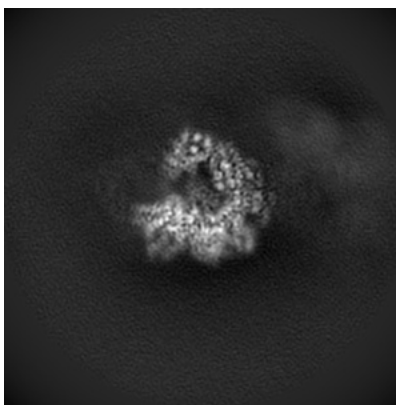


Z

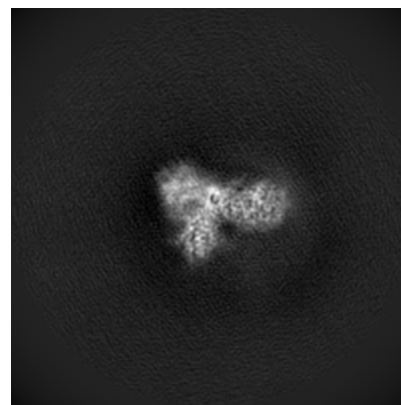
#### 6.1.2 Raw map



X



Y

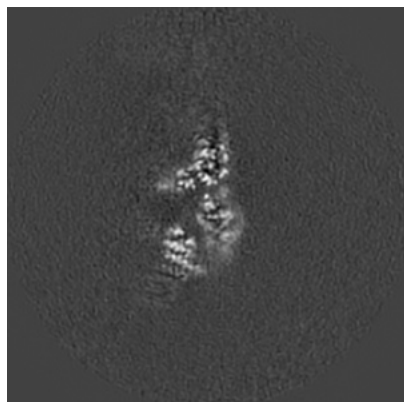


Z

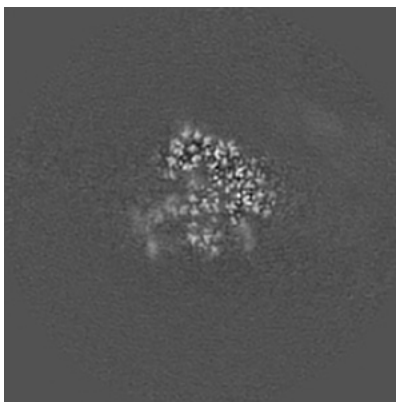
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

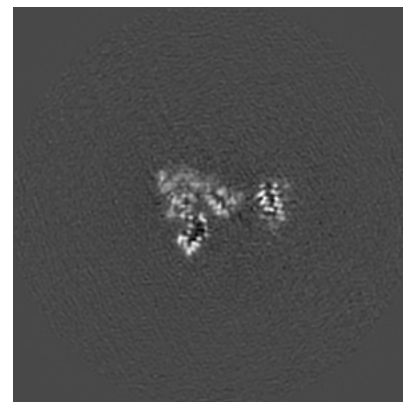
### 6.2.1 Primary map



X Index: 100

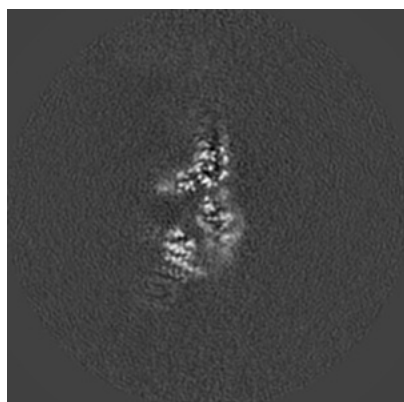


Y Index: 100

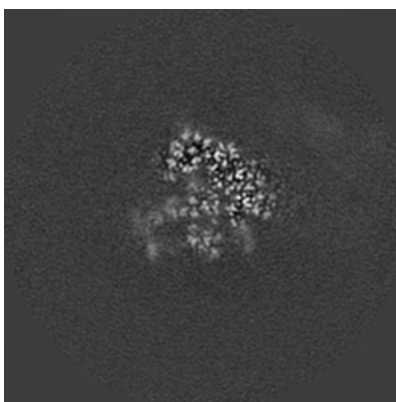


Z Index: 100

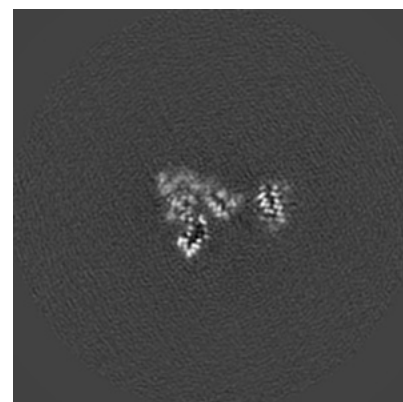
### 6.2.2 Raw map



X Index: 100



Y Index: 100



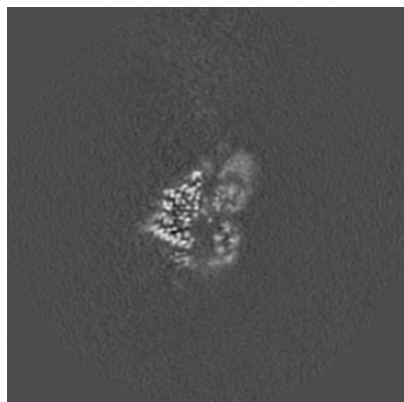
Z Index: 100

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

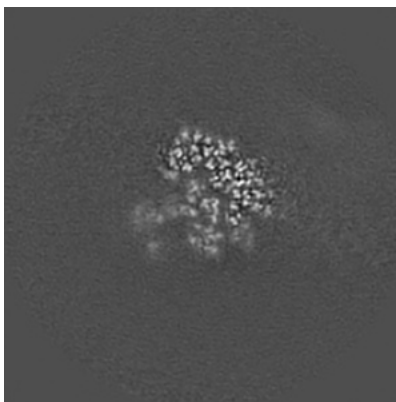


## 6.3 Largest variance slices [i](#)

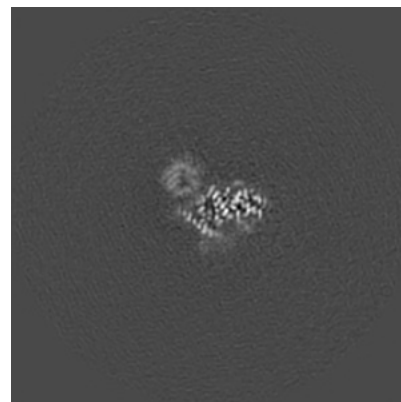
### 6.3.1 Primary map



X Index: 89

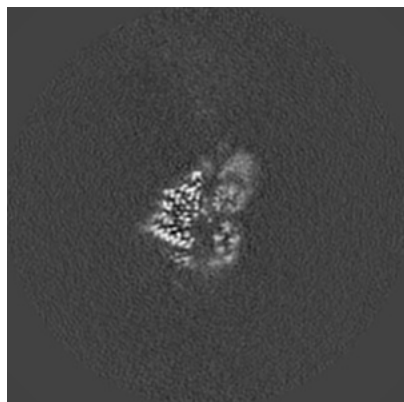


Y Index: 99

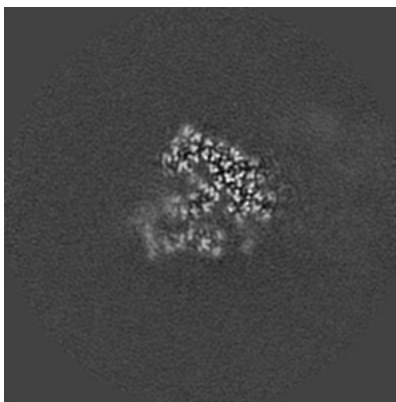


Z Index: 117

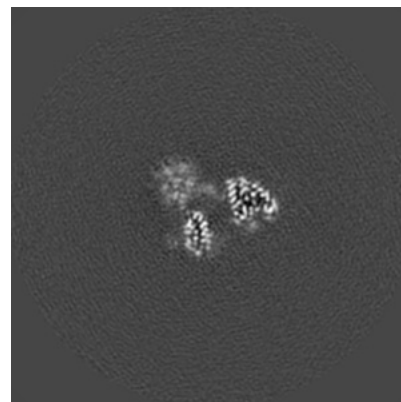
### 6.3.2 Raw map



X Index: 89



Y Index: 102

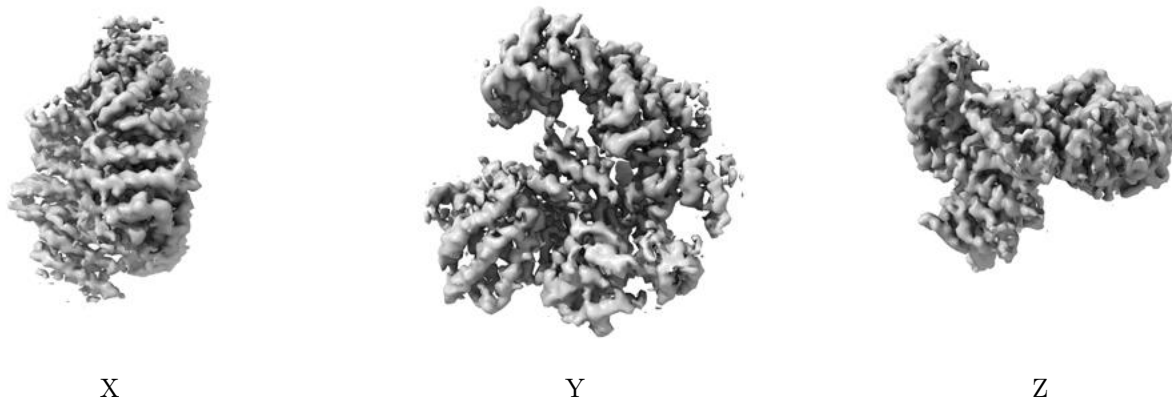


Z Index: 108

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

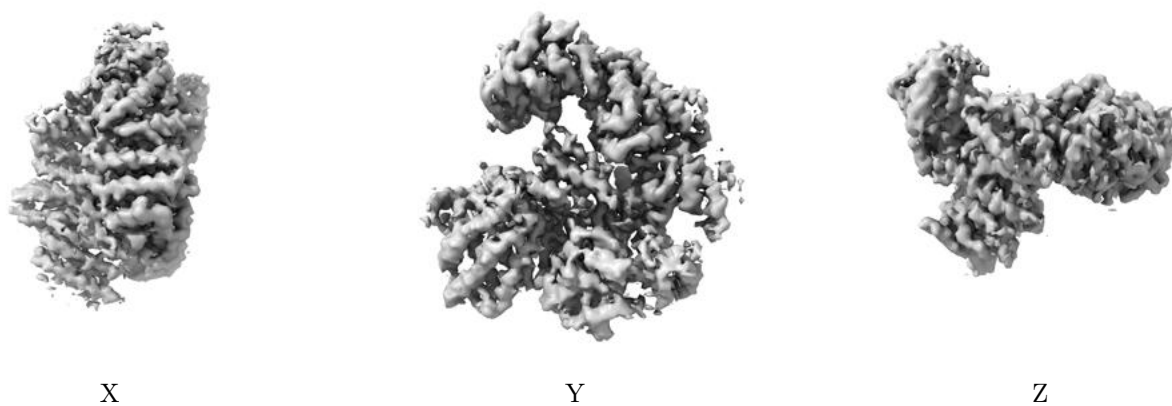
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

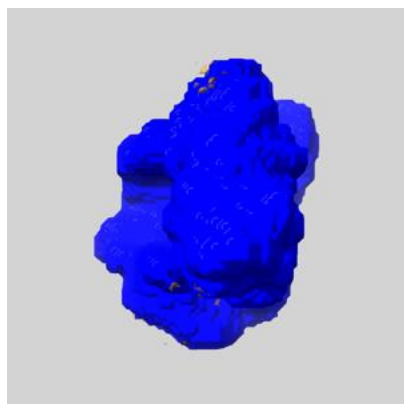
## 6.5 Mask visualisation [i](#)

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

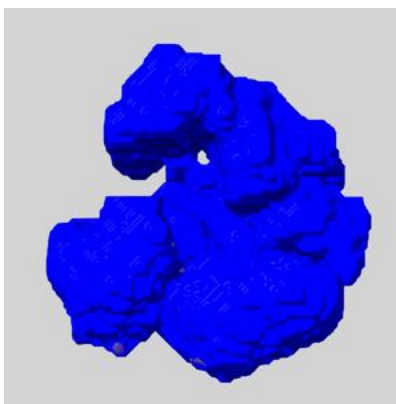
A mask typically either:

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

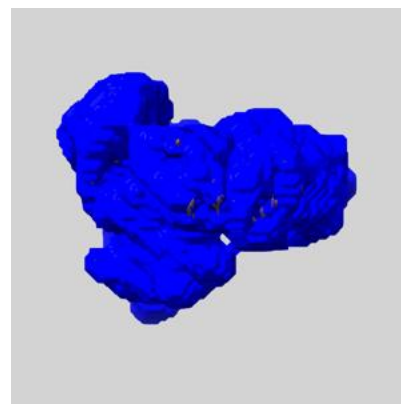
### 6.5.1 emd\_13392\_msk\_1.map [i](#)



X



Y

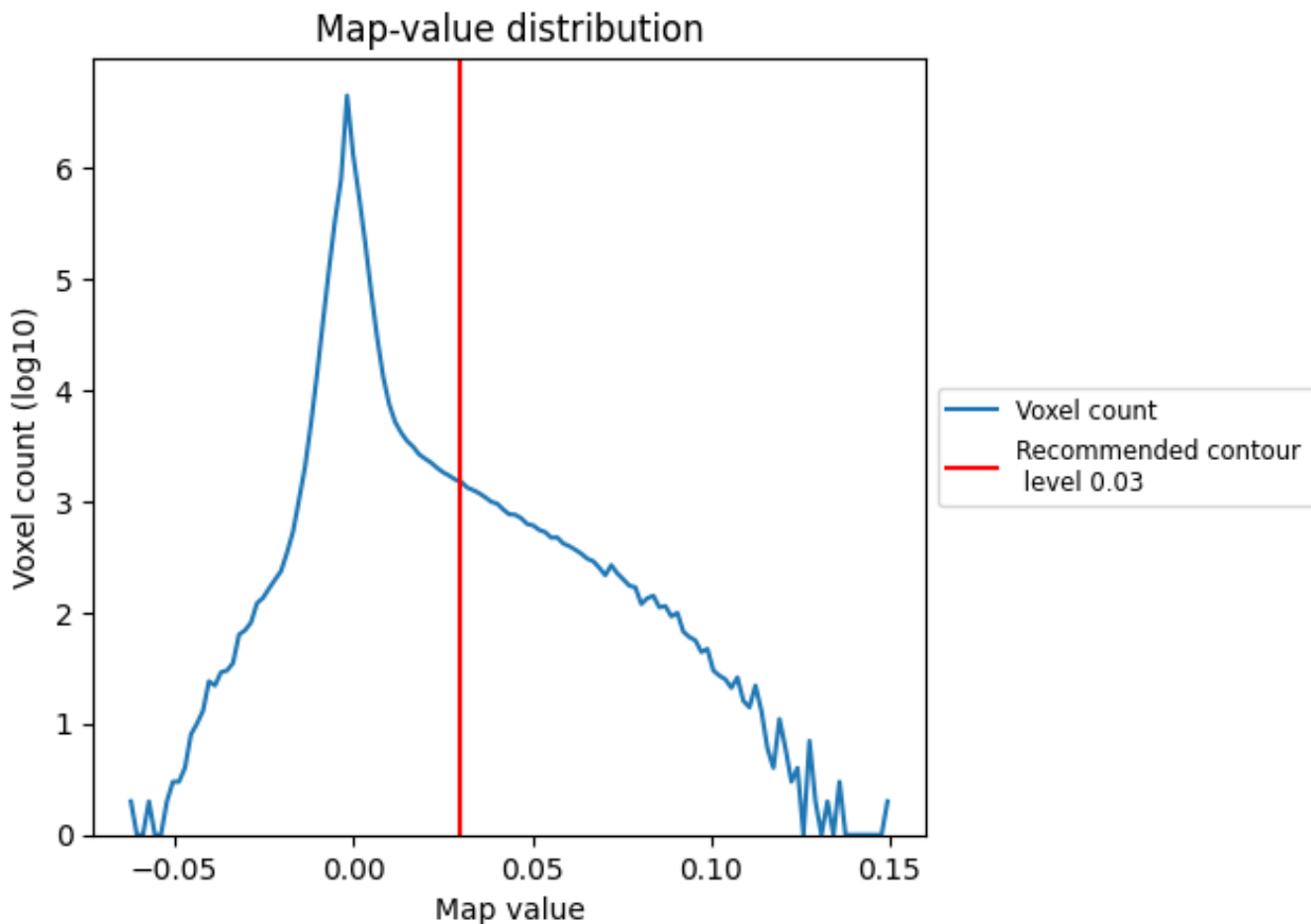


Z

## 7 Map analysis [i](#)

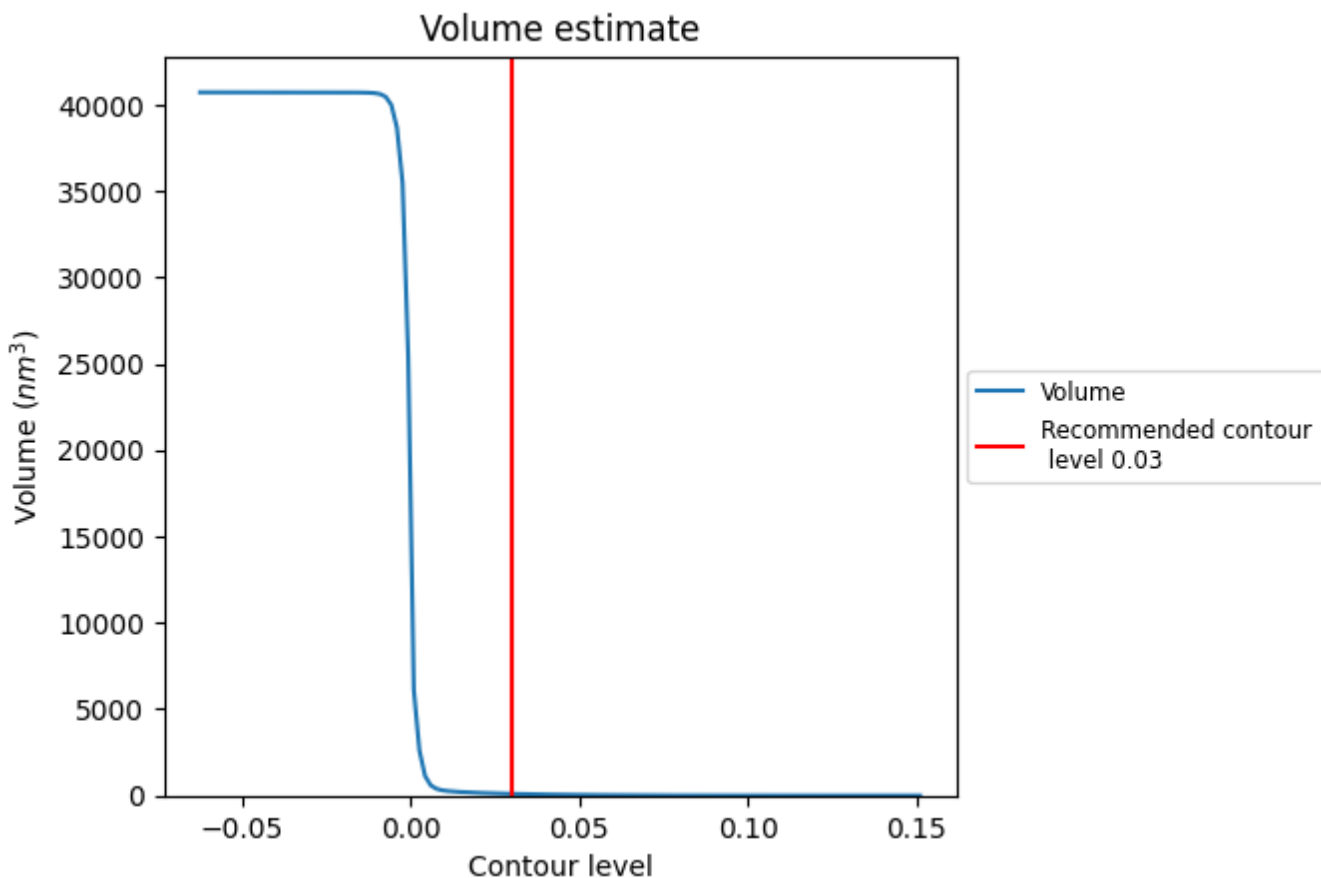
This section contains the results of statistical analysis of the map.

### 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.

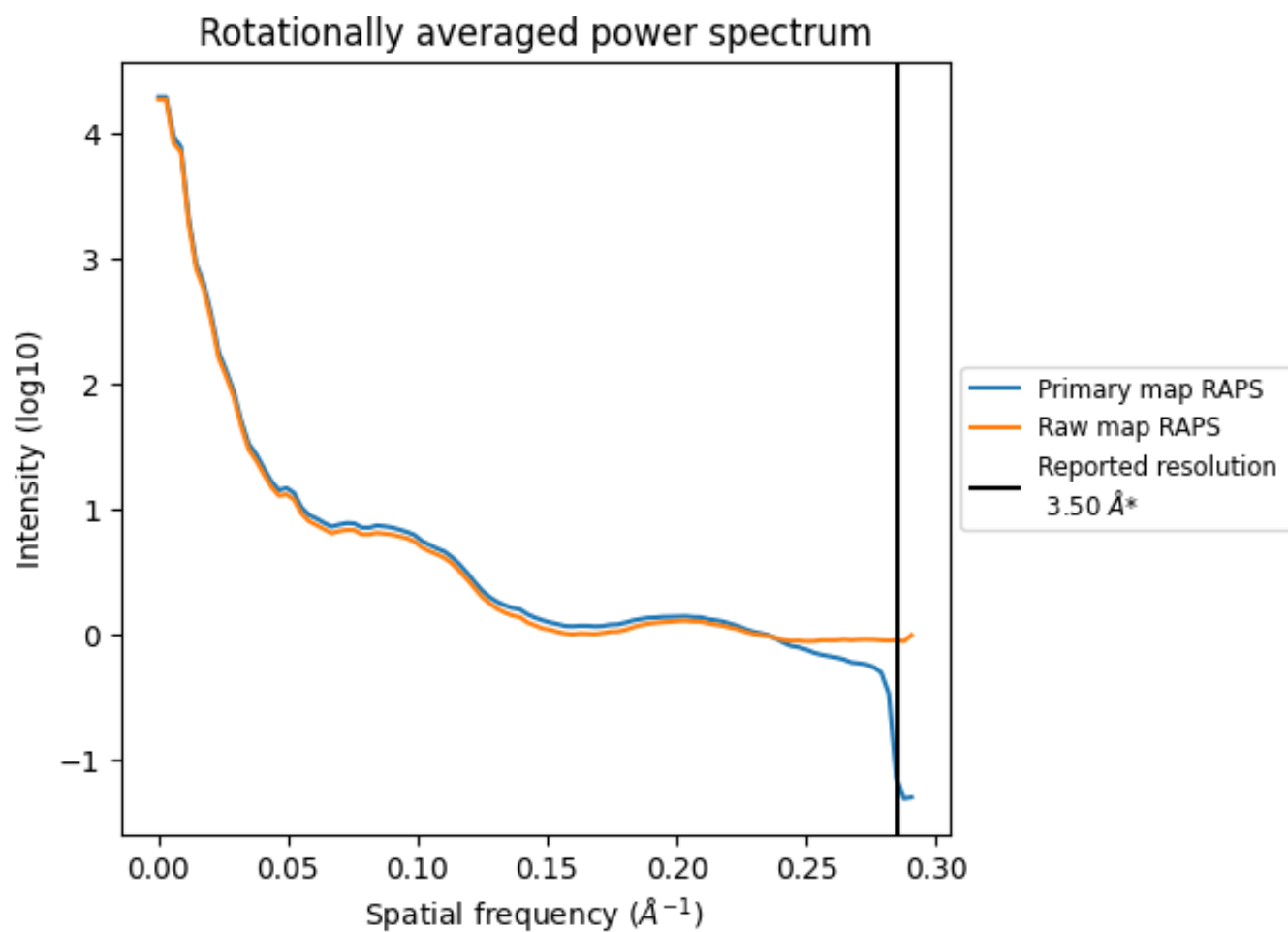
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 100  $\text{nm}^3$ ; this corresponds to an approximate mass of 90 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

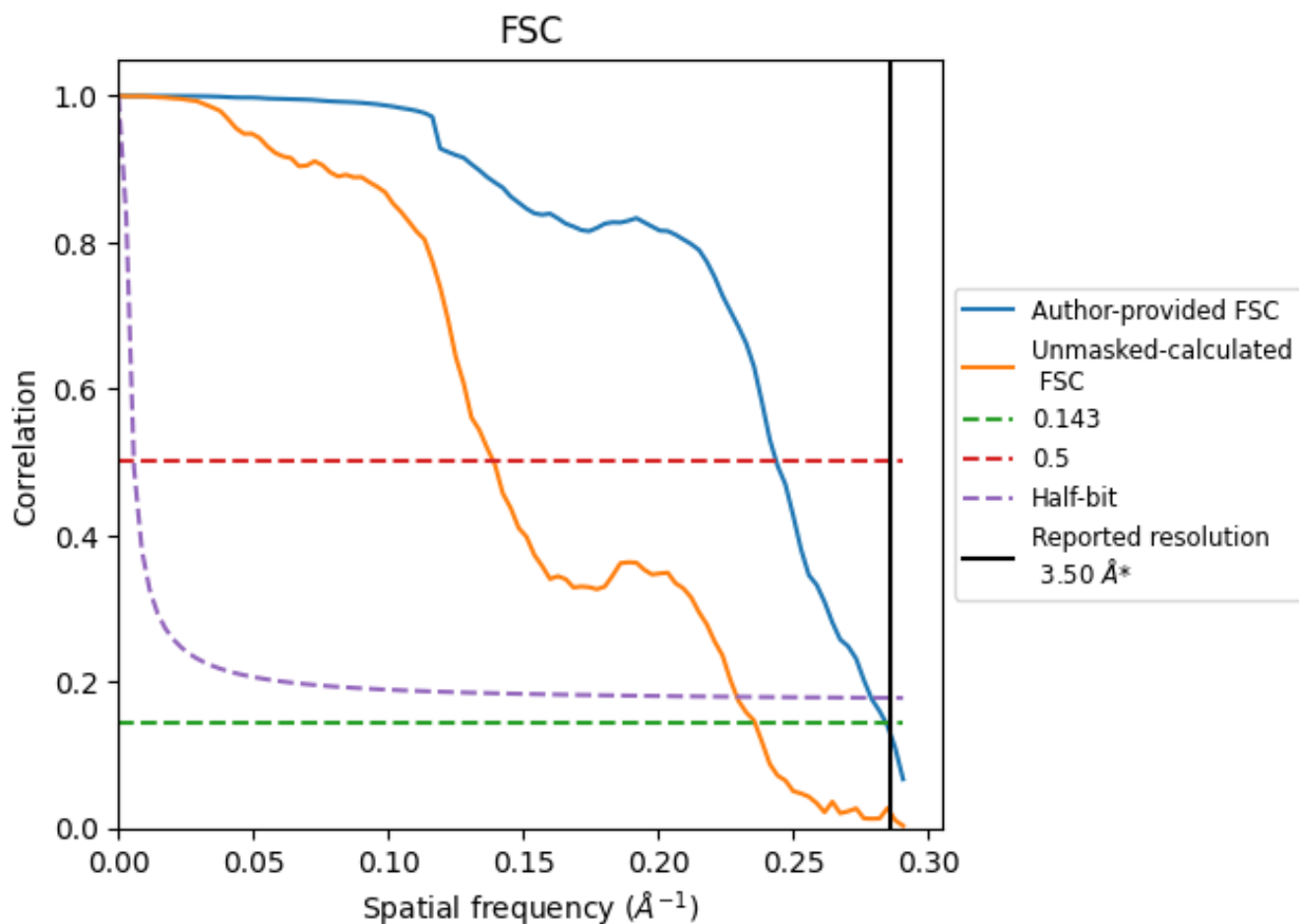


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286 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	3.50	-	-
Author-provided FSC curve	3.52	4.10	3.59
Unmasked-calculated*	4.24	7.19	4.36

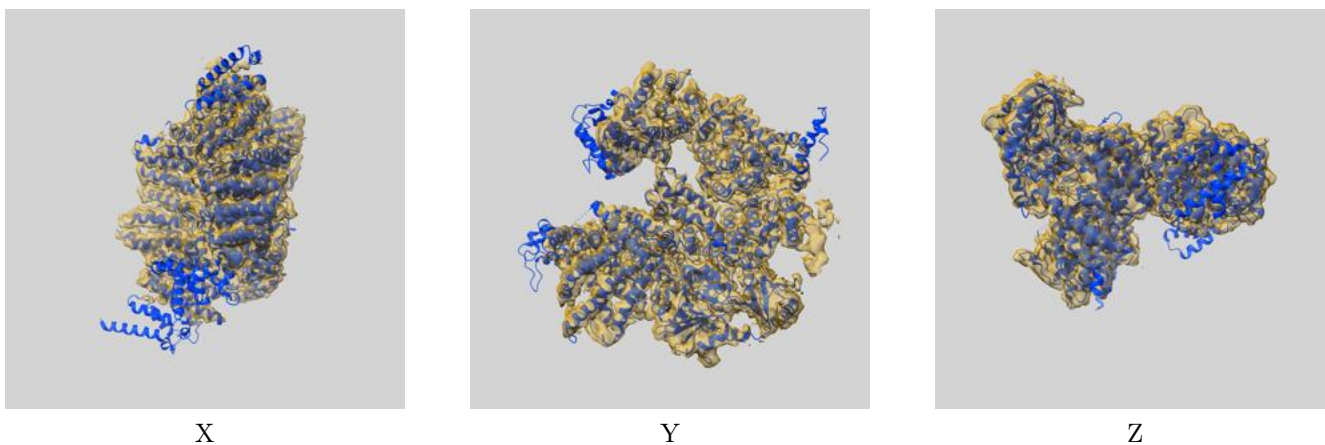
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.5 by more than 10 %



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

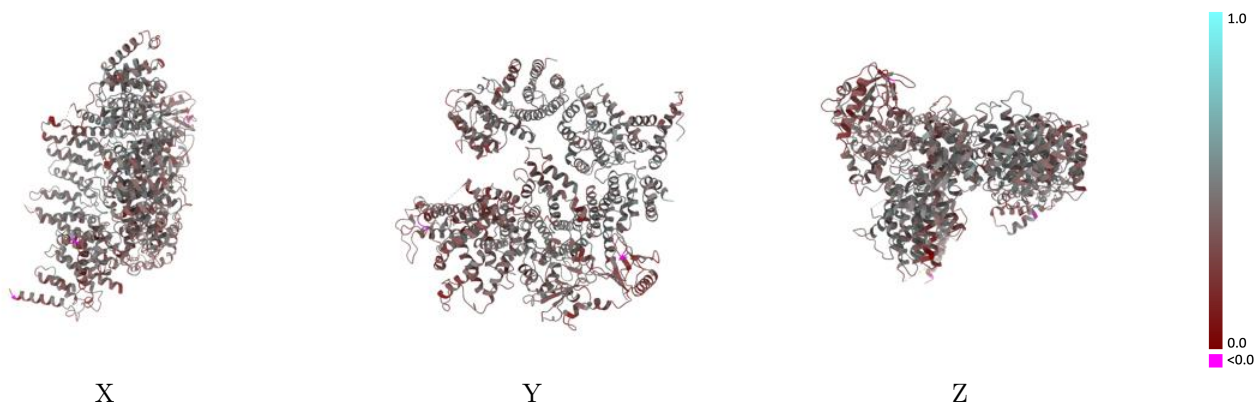
This section contains information regarding the fit between EMDB map EMD-13392 and PDB model 7PGQ. Per-residue inclusion information can be found in section [3](#) on page [4](#).

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



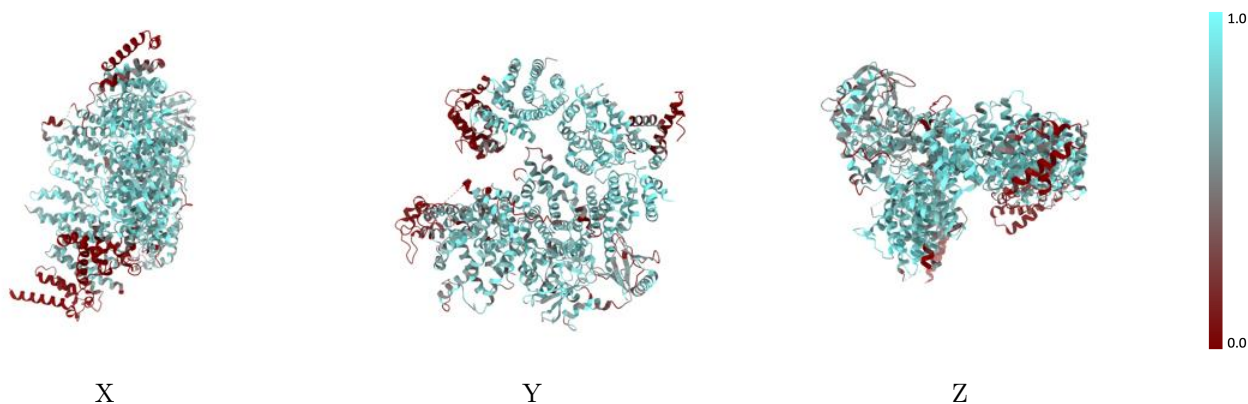
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



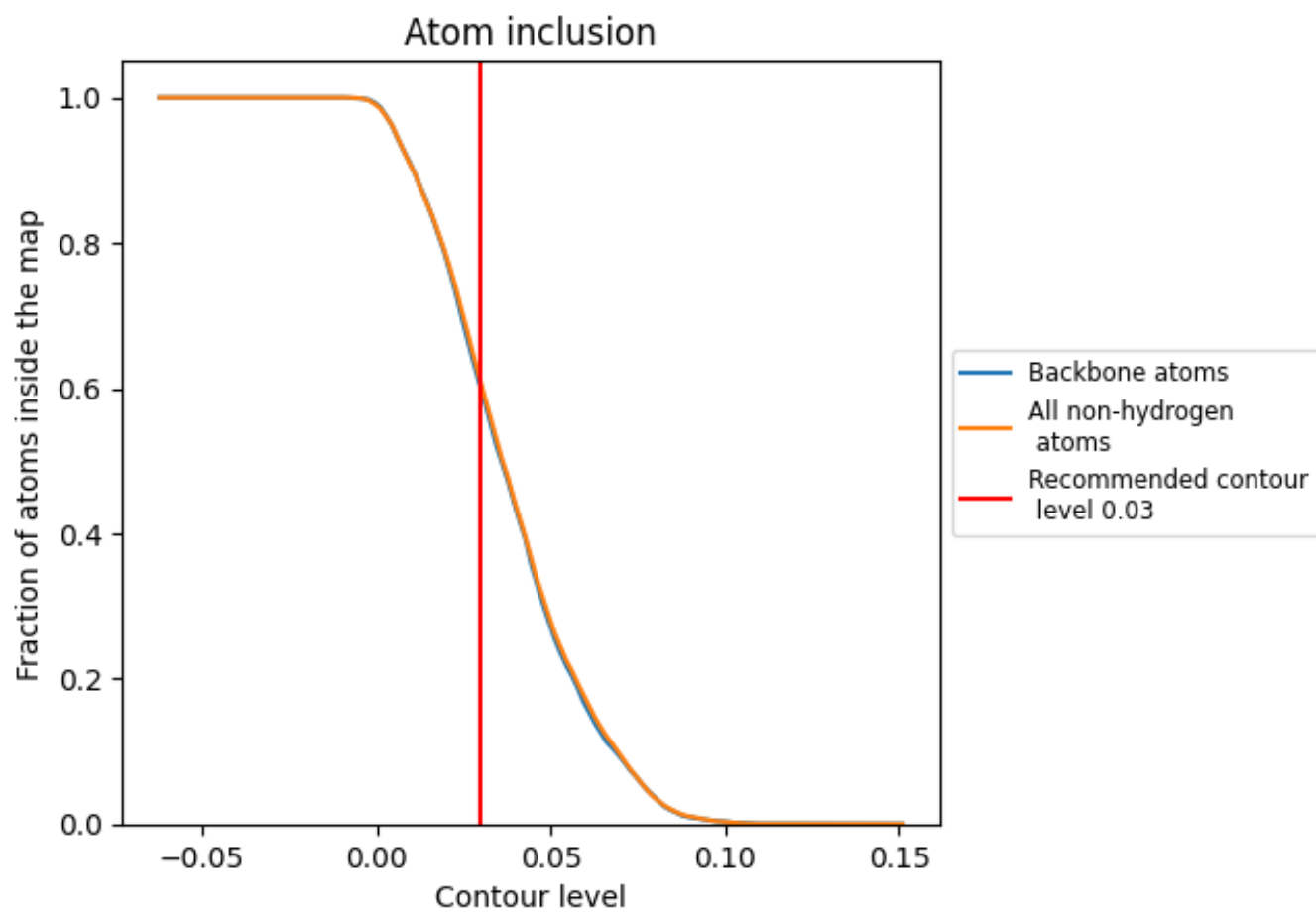
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6067	 0.3950
F	 0.6333	 0.3830
N	 0.5902	 0.4190

