



## wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 01:41 AM EST

PDB ID : 8RRV  
EMDB ID : EMD-19466  
Title : Structure of RyR1 in detergent in close state in complex with FKBP and Nb9657.  
Authors : Li, C.; Efremov, R.G.  
Deposited on : 2024-01-23  
Resolution : 3.20 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

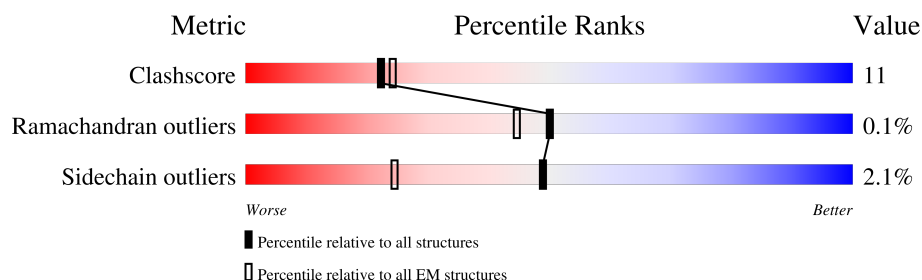
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	5037	
1	E	5037	
1	G	5037	
1	J	5037	
2	A	107	
2	D	107	
2	H	107	
2	I	107	

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Mol	Chain	Length	Quality of chain
3	C	137	<div><div>18%</div><div><div></div><div>61%</div><div>28%</div><div>• 8%</div></div></div>
3	F	137	<div><div>18%</div><div><div></div><div>63%</div><div>27%</div><div>• 8%</div></div></div>
3	K	137	<div><div>18%</div><div><div></div><div>62%</div><div>27%</div><div>• 8%</div></div></div>
3	M	137	<div><div>17%</div><div><div></div><div>62%</div><div>28%</div><div>• 8%</div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142968 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	E	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	G	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	J	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3221	SER	THR	conflict	UNP P11716
E	3221	SER	THR	conflict	UNP P11716
G	3221	SER	THR	conflict	UNP P11716
J	3221	SER	THR	conflict	UNP P11716

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 3 is a protein called nanobody9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total 967	C 597	N 170	O 195	S 5	0	0
3	F	126	Total 967	C 597	N 170	O 195	S 5	0	0
3	K	126	Total 967	C 597	N 170	O 195	S 5	0	0
3	M	126	Total 967	C 597	N 170	O 195	S 5	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	E	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0



- Molecule 1: Ryanodine receptor 1



F2973	I2974	A2975	E2978	S2989	P2990	T2912	A2913	E2992	I2995	P2996	F2997	F2998	L3002	L3003	P3004	L3005	N3006	N3007	Q3008	F3009	F3010	T3011	C3014	L3015	L3016	F3017	L3018	H3030	N3033	K3034	E3035	K3036	E3037	M3038	I3039	T3040	S3041	L3042	F3043	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	D3060			
E2828	G2829	E2830	GLU	GLU	ARG	THR	THR	LYS	LYS	THR	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	L2871	L2876	N2881	Y2882	H2883	N2884	T2885	W2886	K2889	R2890	K2891	L2894	K2897	
N2756	K2757	F2758	A2759	T2762	H2763	E2764	K2765	K2766	A2767	F2768	D2769	K2770	T2771	Q2772	N2773	N2774	K2775	S2776	Y2777	G2778	E2779	N2780	V2781	E2784	L2785	K2786	T2787	H2788	P2789	T2790	L2791	K2792	P2793	Y2794	K2795	T2796	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	R2806	L2813	K2814	A2815	N2816	T2822	L2823	E2824	K2825	A2826	R2827
L2882	L2886	K2689	K2690	Q2693	Y2696	R2697	M2700	P2701	C2702	L2703	K2704	A2705	L2706	L2710	P2711	P2712	D2713	Y2714	V2715	S2720	SER	LYS	ALA	GLU	LYS	ALA	GLU	VAL	ASP	ALA	GLU	N2734	F2735	D2736	P2737	R2738	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755						
F2569	T2572	E2573	H2574	R2575	L2576	M2577	M2578	Y2587	R2588	R2591	Q2599	L2603	L2610	C2611	R2612	Y2613	L2614	R2615	M2618	L2619	L2623	R2624	V2627	L2630	L2633	A2637	K2638	M2639	H2647	K2653	C2656	L2657	P2658	W2661	F2664	E2670	H2673	L2678	F2679															
V2467	G2468	I2469	L2472	L2476	P2477	K2489	A2492	V2495	P2496	D2497	H2498	K2499	A2500	S2501	L2504	R2508	N2514	Q2515	F2517	L2518	L2519	L2522	D2523	V2524	G2525	F2526	A2532	A2533	S2534	L2536	D2537	T2538	F2541	S2542	M2546	L2550	Y2553	L2559	T2563	L2568														
E2381	E2382	A2383	I2384	R2385	E2388	P2389	P2390	P2395	GLY	VAL	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	L2418	G2419	H2420	A2421	I2422	M2423	S2424	F2425	D2431	R2435	K2447	A2450	L2451	R2452	I2453	R2454	A2455	I2456	L2457	R2458	L2463	D2464	D2465	L2466						
M2228	Y2238	I2242	S2243	R2244	Q2247	Y2256	S2261	G2264	L2265	Q2268	T2271	P2272	L2273	D2274	S2279	V2280	N2283	L2286	L2290	D2294	K2297	C2310	L2313	P2325	Q2328	E2329	R2330	R2336	V2352	L2356	L2368	L2376	L2377	I2380																				
L1624	V1628	P1633	L1639	P1642	D1649	E1652	R1656	L1667	R1668	R1671	L1676	G1677	N1678	D1690	Q1693	L1694	E1699	R1708	Y1712	L1715	R1727	L1738	T1739	P1740	Q1559	R1560	I1562	E1565	E1583	L1786	P1787	ALA	ALA	GLY	VAL	ALA	E1793																	
R1421	D1422	D1423	P1424	E1426	I1427	Y1435	S1436	P1445	S1446	C1447	V1448	M1476	G1477	D1478	Y1483	H1484	S1485	S1486	L1487	K1488	C1489	V1501	S1502	P1503	G1504	GLN	GLY	R1508	V1520	M1527	V1554	L1555	Q1559	R1560	I1562	E1565	E1583	N1586	T1617	A1620	R1623													









WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

- Molecule 1: Ryanodine receptor 1

[illegible]








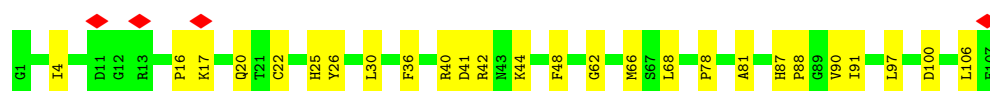








Chain D:  76% 24%



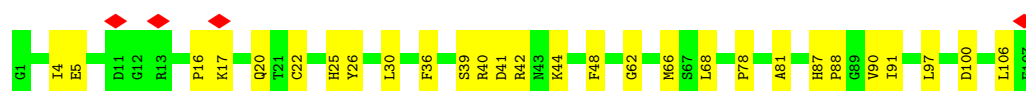
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  74% 26%



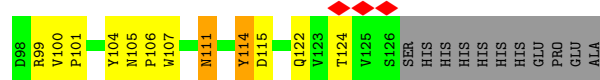
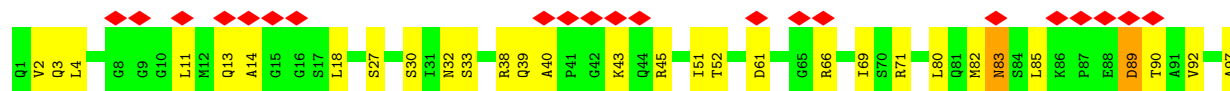
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain I:  74% 26%



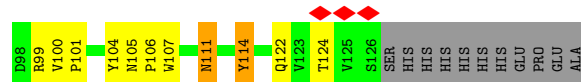
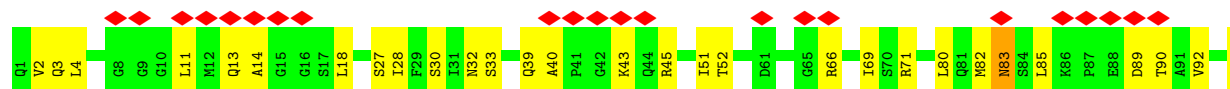
- Molecule 3: nanobody9657

Chain C:  18% 61% 28% 8%



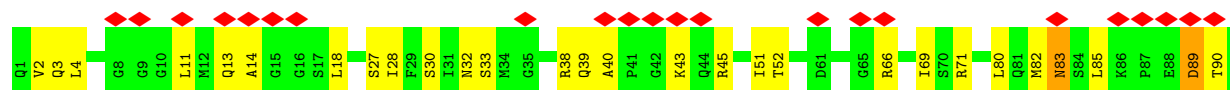
- Molecule 3: nanobody9657

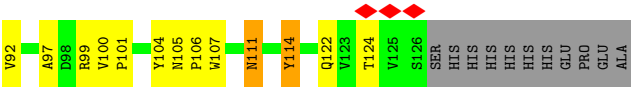
Chain F:  18% 63% 27% 8%



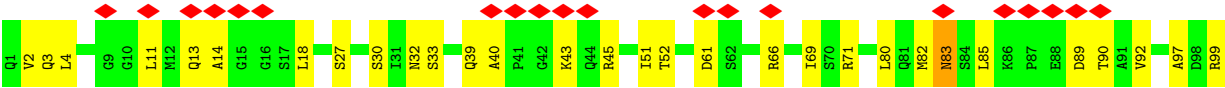
- Molecule 3: nanobody9657

Chain K:  18% 62% 27% 8%





• Molecule 3: nanobody9657



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.350	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.076	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	499.96802, 499.96802, 499.96802	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.488, 1.488, 1.488	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	B	0.25	0/34727	0.50	2/47063 (0.0%)
1	E	0.25	0/34727	0.50	2/47063 (0.0%)
1	G	0.25	0/34727	0.50	2/47063 (0.0%)
1	J	0.25	0/34727	0.50	2/47063 (0.0%)
2	A	0.26	0/834	0.51	0/1123
2	D	0.26	0/834	0.51	0/1123
2	H	0.25	0/834	0.51	0/1123
2	I	0.26	0/834	0.51	0/1123
3	C	0.25	0/987	0.51	0/1340
3	F	0.25	0/987	0.51	0/1340
3	K	0.25	0/987	0.51	0/1340
3	M	0.25	0/987	0.51	0/1340
All	All	0.25	0/146192	0.50	8/198104 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1503	PRO	N-CA-CB	5.74	110.19	103.30
1	E	1503	PRO	N-CA-CB	5.74	110.19	103.30
1	G	1503	PRO	N-CA-CB	5.70	110.14	103.30
1	J	1503	PRO	N-CA-CB	5.70	110.14	103.30
1	E	4097	MET	CB-CG-SD	-5.16	96.94	112.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	B	33956	0	33378	744	0
1	E	33956	0	33378	756	0
1	G	33956	0	33378	749	0
1	J	33956	0	33378	765	0
2	A	818	0	824	17	0
2	D	818	0	824	17	0
2	H	818	0	824	19	0
2	I	818	0	824	19	0
3	C	967	0	916	36	0
3	F	967	0	916	34	0
3	K	967	0	916	36	0
3	M	967	0	916	36	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
All	All	142968	0	140472	3180	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 11.

The worst 5 of 3180 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:J:4961:CYS:SG	1:J:4983:HIS:CE1	2.58	0.97
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	2.58	0.96
1:E:4961:CYS:SG	1:E:4983:HIS:CE1	2.58	0.96
1:G:4961:CYS:SG	1:G:4983:HIS:CE1	2.58	0.95
1:B:870:ILE:HA	1:B:873:LYS:HE2	1.57	0.86

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	B	4247/5037 (84%)	4148 (98%)	96 (2%)	3 (0%)	48	80
1	E	4247/5037 (84%)	4149 (98%)	96 (2%)	2 (0%)	100	100
1	G	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100	100
1	J	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100	100
2	A	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	D	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	H	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	I	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	C	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	F	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	K	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	M	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
All	All	17904/21124 (85%)	17472 (98%)	423 (2%)	9 (0%)	50	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4117	ALA
1	E	4117	ALA
1	G	4117	ALA
1	J	4117	ALA
1	B	375	LYS

### 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	B	3658/4276 (86%)	3584 (98%)	74 (2%)	50	75
1	E	3658/4276 (86%)	3584 (98%)	74 (2%)	50	75
1	G	3658/4276 (86%)	3584 (98%)	74 (2%)	50	75
1	J	3658/4276 (86%)	3584 (98%)	74 (2%)	50	75
2	A	88/88 (100%)	87 (99%)	1 (1%)	70	86
2	D	88/88 (100%)	87 (99%)	1 (1%)	70	86
2	H	88/88 (100%)	87 (99%)	1 (1%)	70	86
2	I	88/88 (100%)	87 (99%)	1 (1%)	70	86
3	C	104/114 (91%)	99 (95%)	5 (5%)	21	55
3	F	104/114 (91%)	99 (95%)	5 (5%)	21	55
3	K	104/114 (91%)	99 (95%)	5 (5%)	21	55
3	M	104/114 (91%)	99 (95%)	5 (5%)	21	55
All	All	15400/17912 (86%)	15080 (98%)	320 (2%)	49	74

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	436	LEU
1	J	3933	PHE
1	J	1025	ARG
1	J	2738	ARG
3	C	3	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	877	ASN
1	J	4574	ASN
1	G	3150	HIS
1	J	3970	GLN
1	J	3150	HIS

### 5.3.3 RNA ⓘ

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 [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

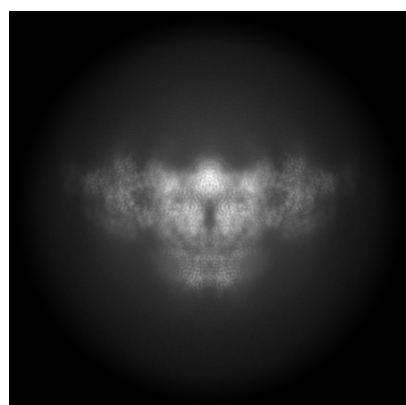
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19466. These allow visual inspection of the internal detail of the map and identification of artifacts.

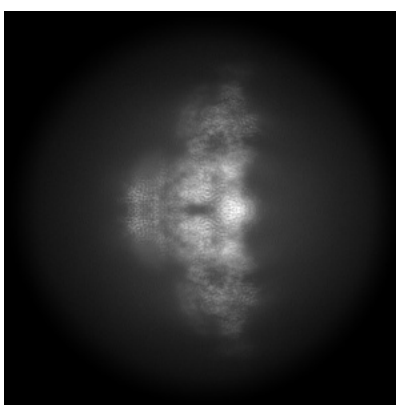
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

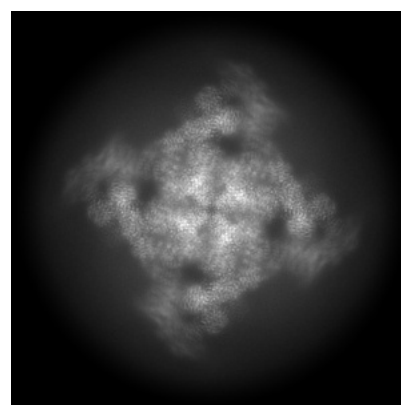
#### 6.1.1 Primary map



X



Y

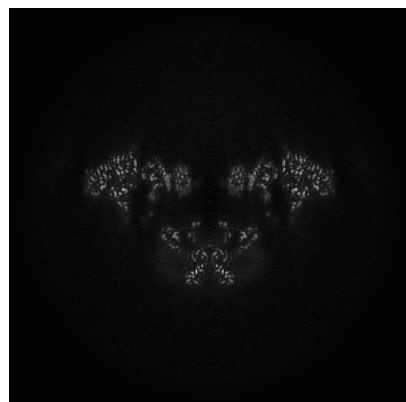


Z

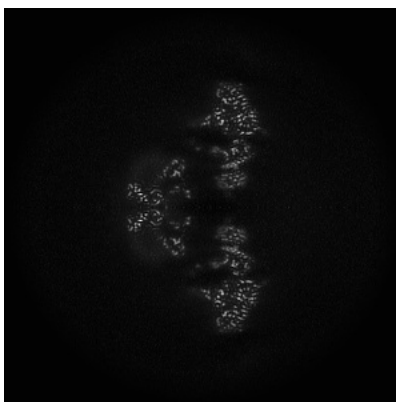
The images above show the map projected in three orthogonal directions.

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

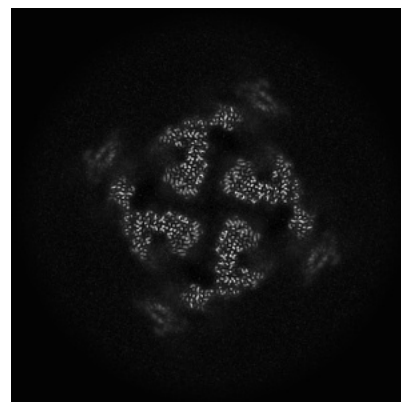
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

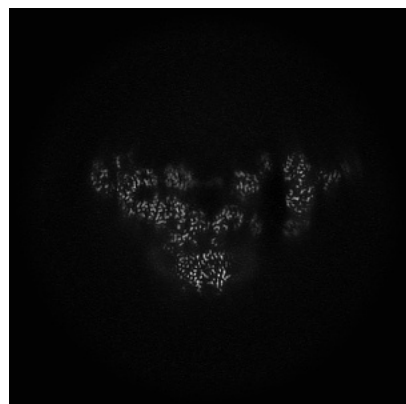


Z Index: 168

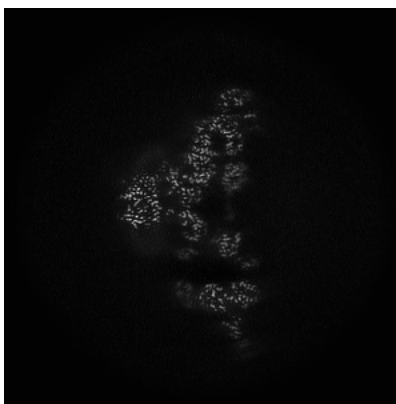
The images above show central slices of the map in three orthogonal directions.

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

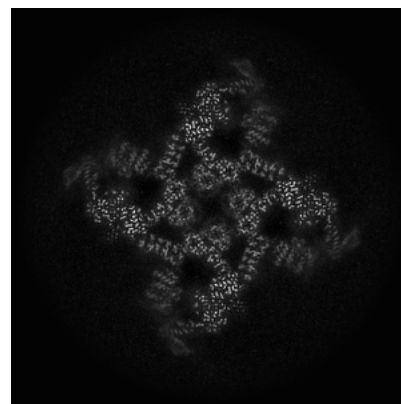
### 6.3.1 Primary map



X Index: 178



Y Index: 178

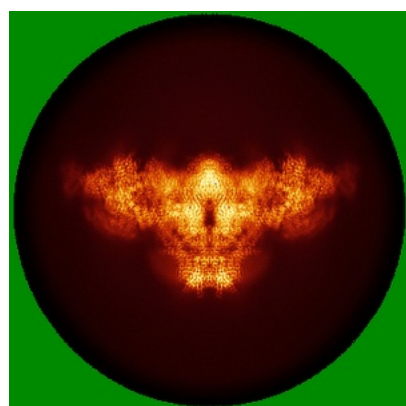


Z Index: 187

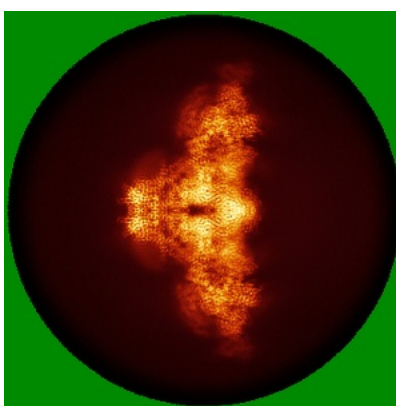
The images above show the largest variance slices of the map in three orthogonal directions.

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

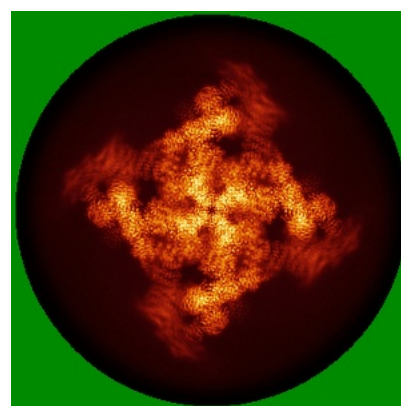
### 6.4.1 Primary map



X



Y

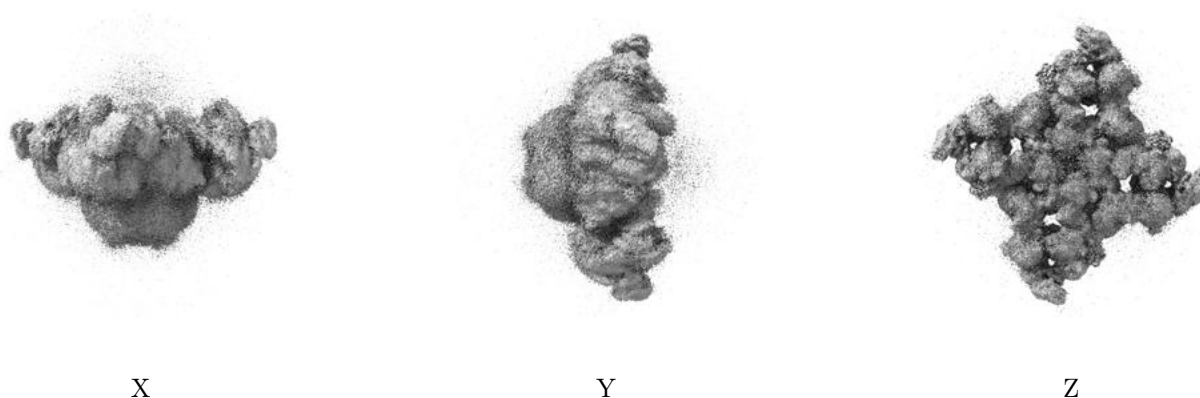


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

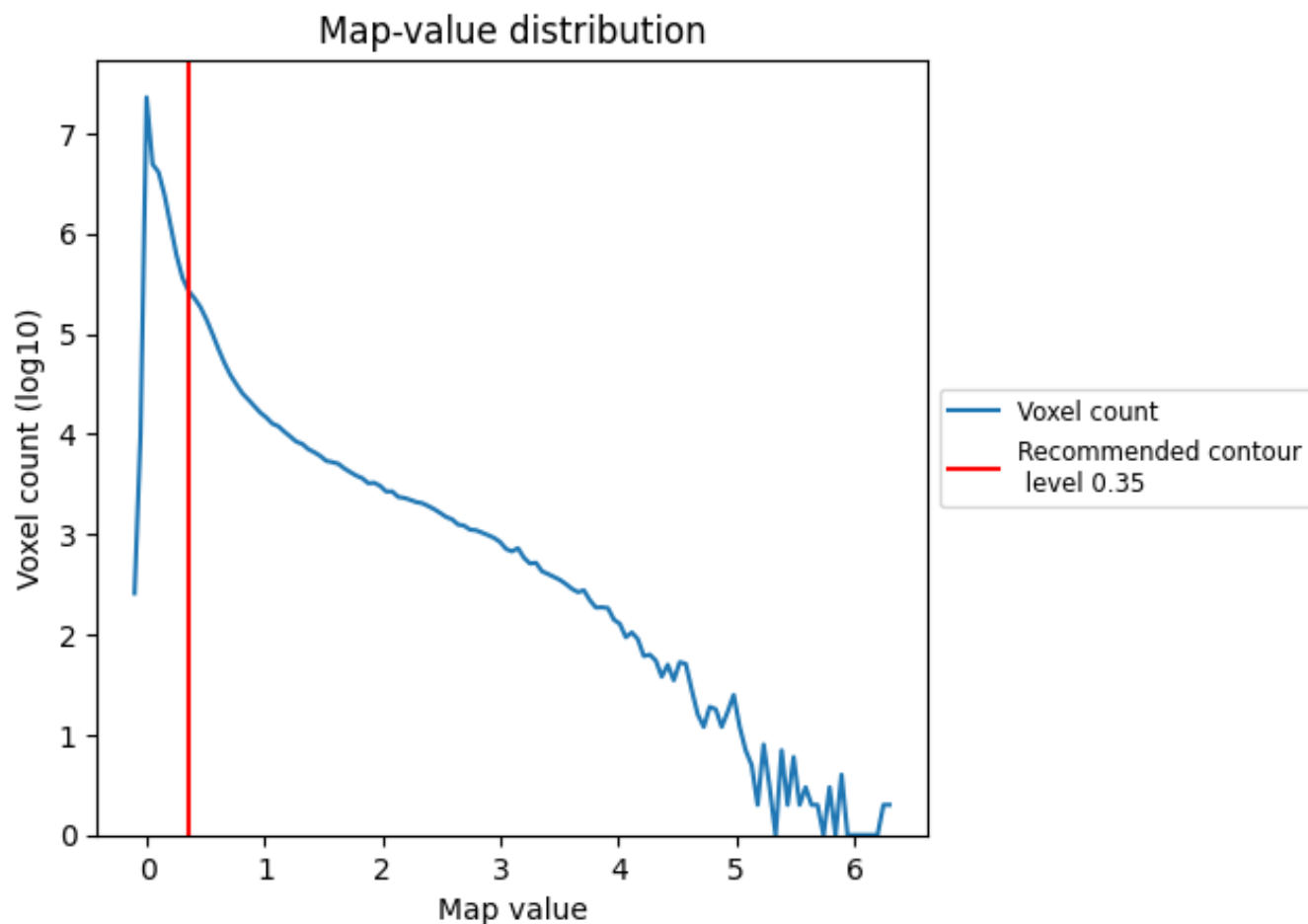
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

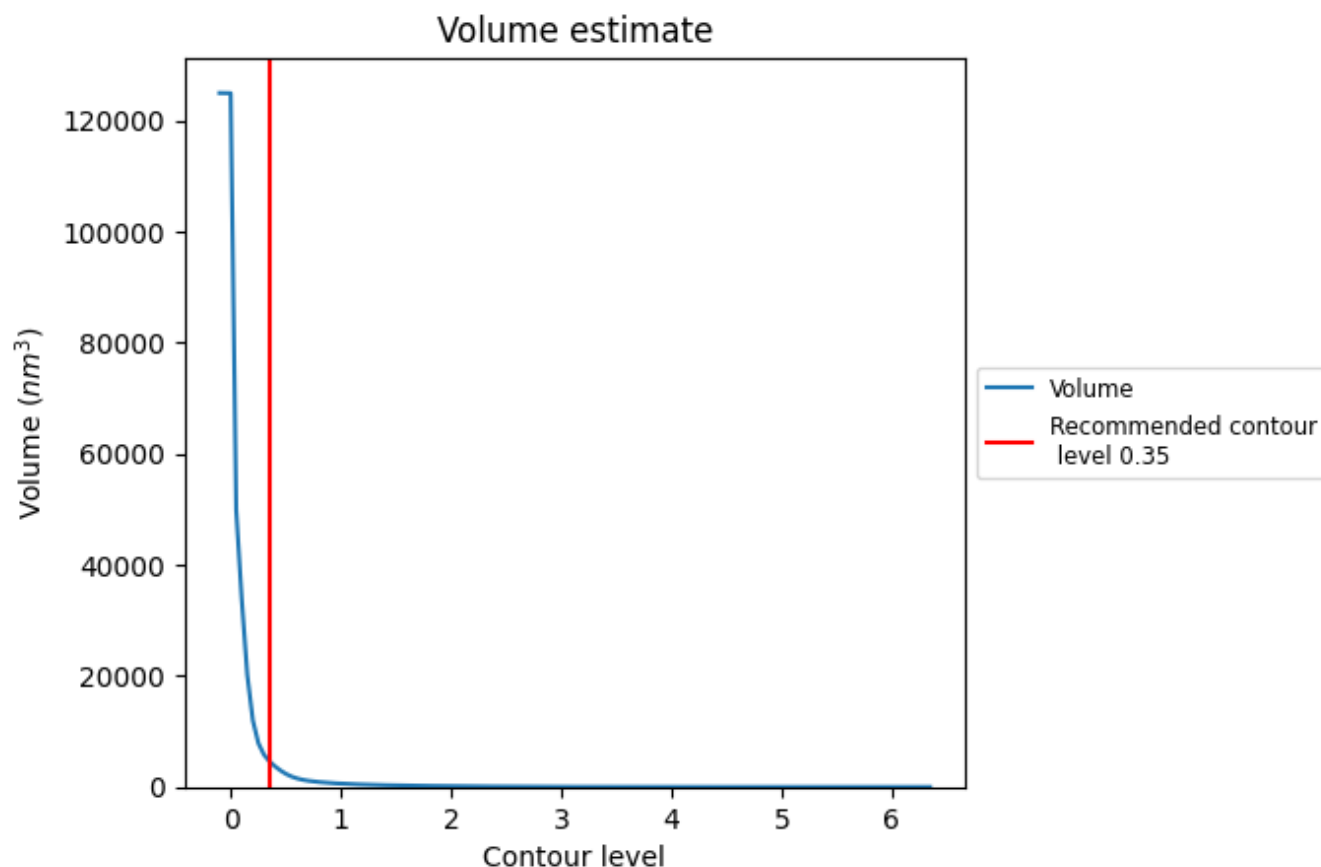
This section contains the results of statistical analysis of the map.

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



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

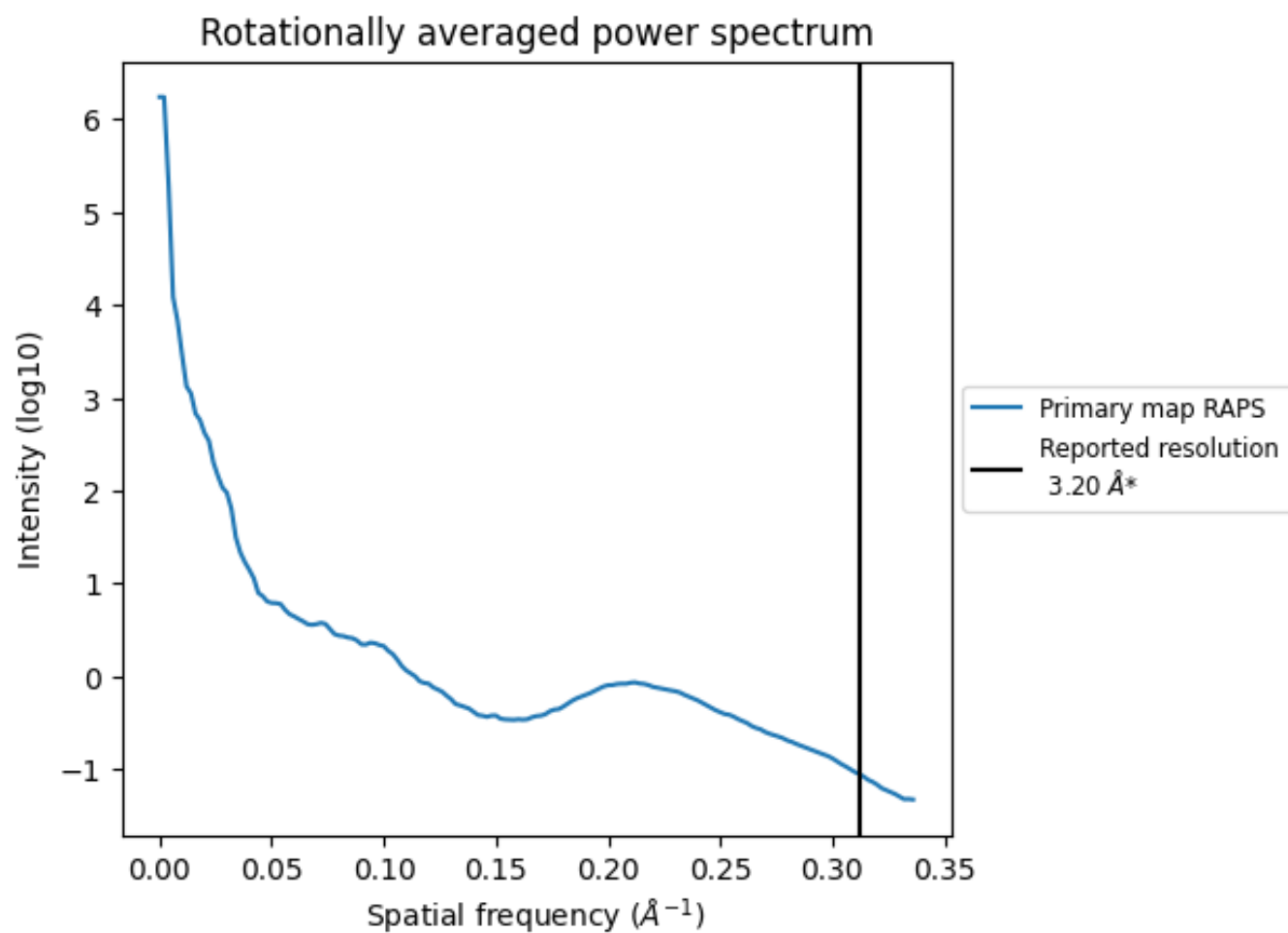
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4570  $\text{nm}^3$ ; this corresponds to an approximate mass of 4129 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 ⓘ



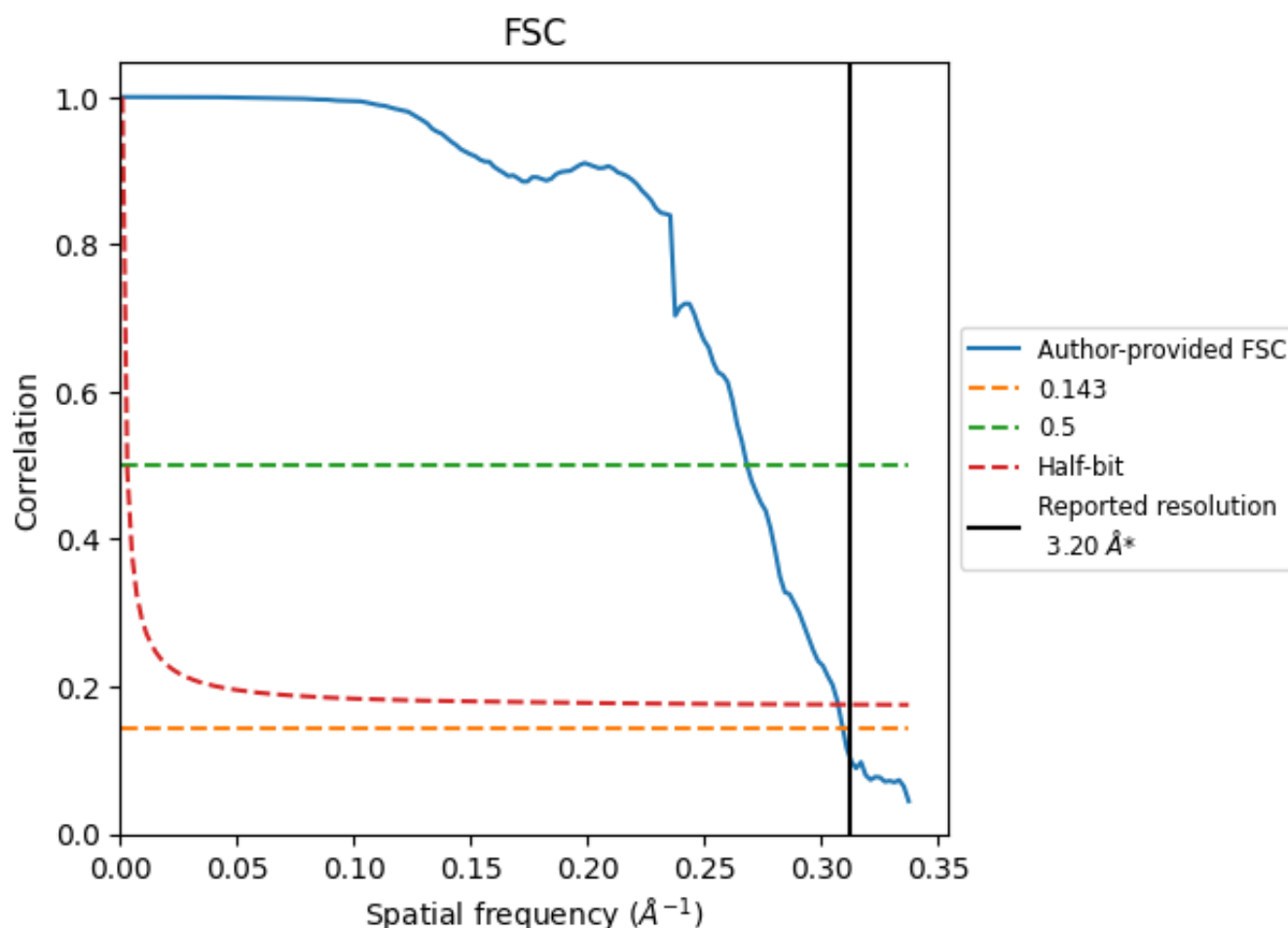
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

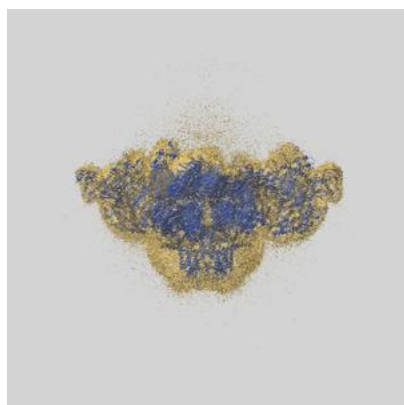
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.73	3.26
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

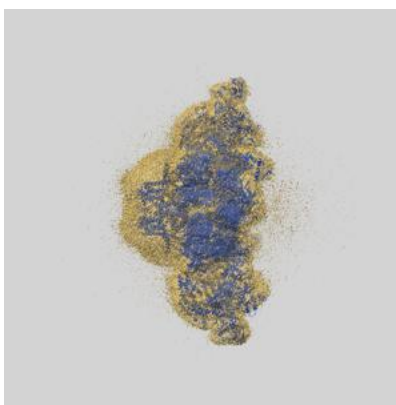
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19466 and PDB model 8RRV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

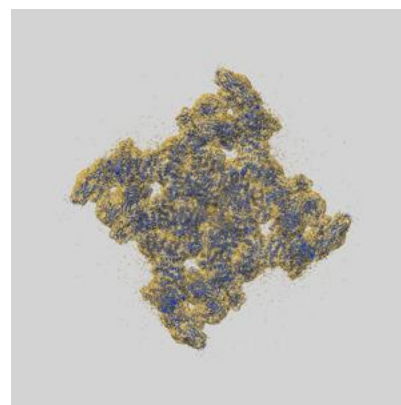
### 9.1 Map-model overlay [i](#)



X



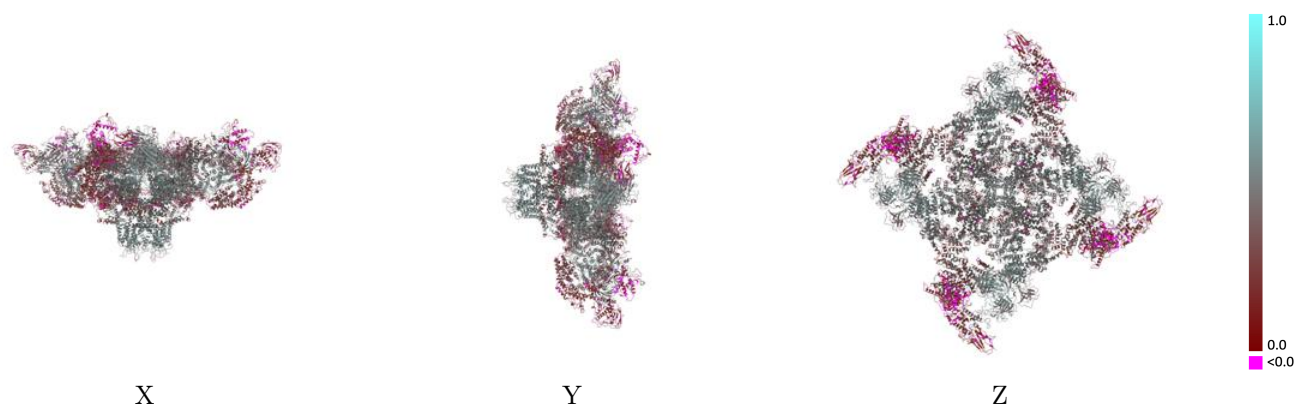
Y



Z

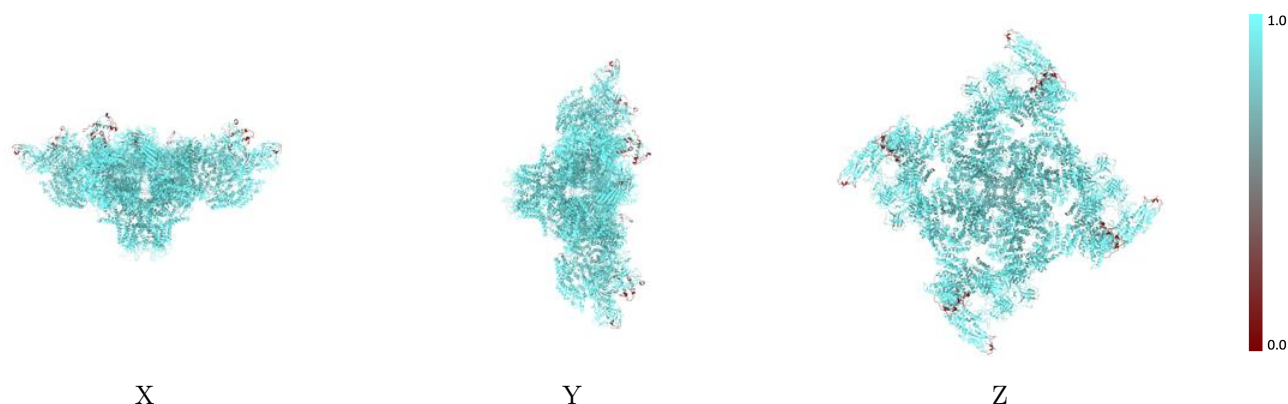
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



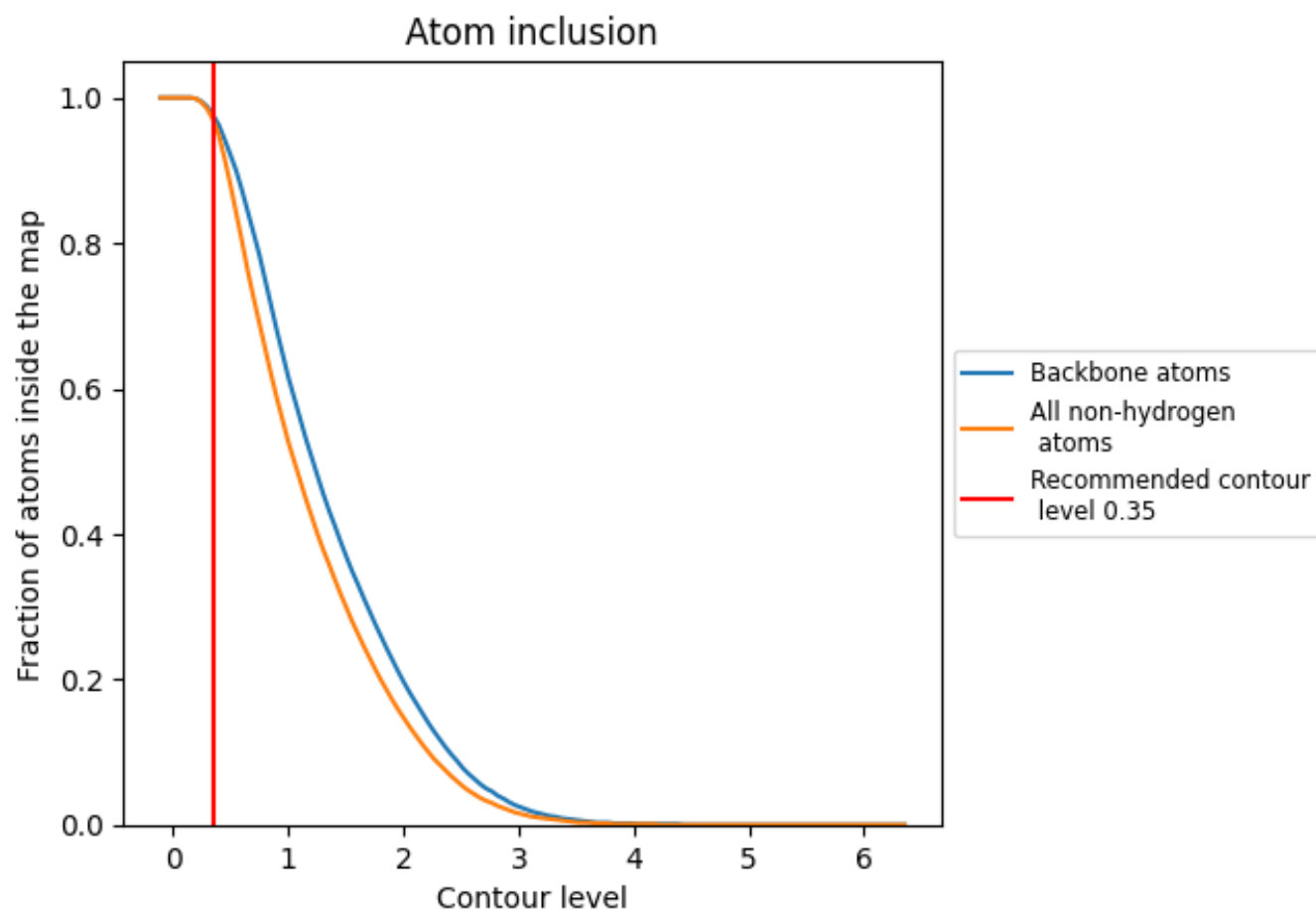
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9700	<div></div> 0.3800
A	<div></div> 0.8810	<div></div> 0.4120
B	<div></div> 0.9770	<div></div> 0.3850
C	<div></div> 0.7720	<div></div> 0.1480
D	<div></div> 0.8780	<div></div> 0.4170
E	<div></div> 0.9780	<div></div> 0.3850
F	<div></div> 0.7760	<div></div> 0.1480
G	<div></div> 0.9770	<div></div> 0.3850
H	<div></div> 0.8860	<div></div> 0.4150
I	<div></div> 0.8810	<div></div> 0.4170
J	<div></div> 0.9770	<div></div> 0.3860
K	<div></div> 0.7770	<div></div> 0.1480
M	<div></div> 0.7720	<div></div> 0.1500

