



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2025 – 05:32 PM JST

PDB ID : 8YGA
EMDB ID : EMD-39240
Title : The tetramer Structure of DSR2 alone
Authors : Gao, X.; Zhu, H.; Cui, S.
Deposited on : 2024-02-26
Resolution : 4.53 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

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>.

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

EMDB validation analysis : 0.0.1.dev117
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) : 2.41.2

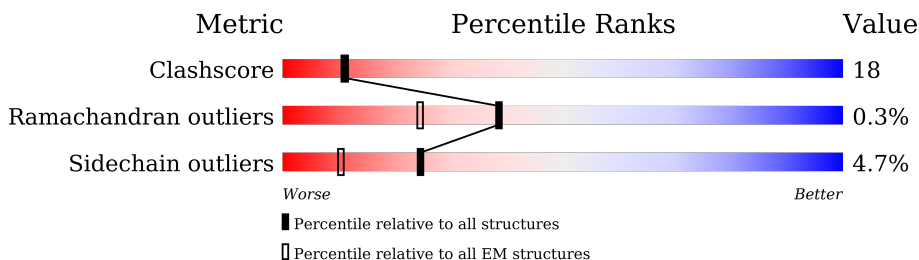
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.53 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 ≥ 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	1005	 5% 61% 35% . .
1	B	1005	 5% 63% 33% . .
1	C	1005	 5% 62% 34% . .
1	D	1005	 5% 58% 37% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33140 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	B	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	C	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	D	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		

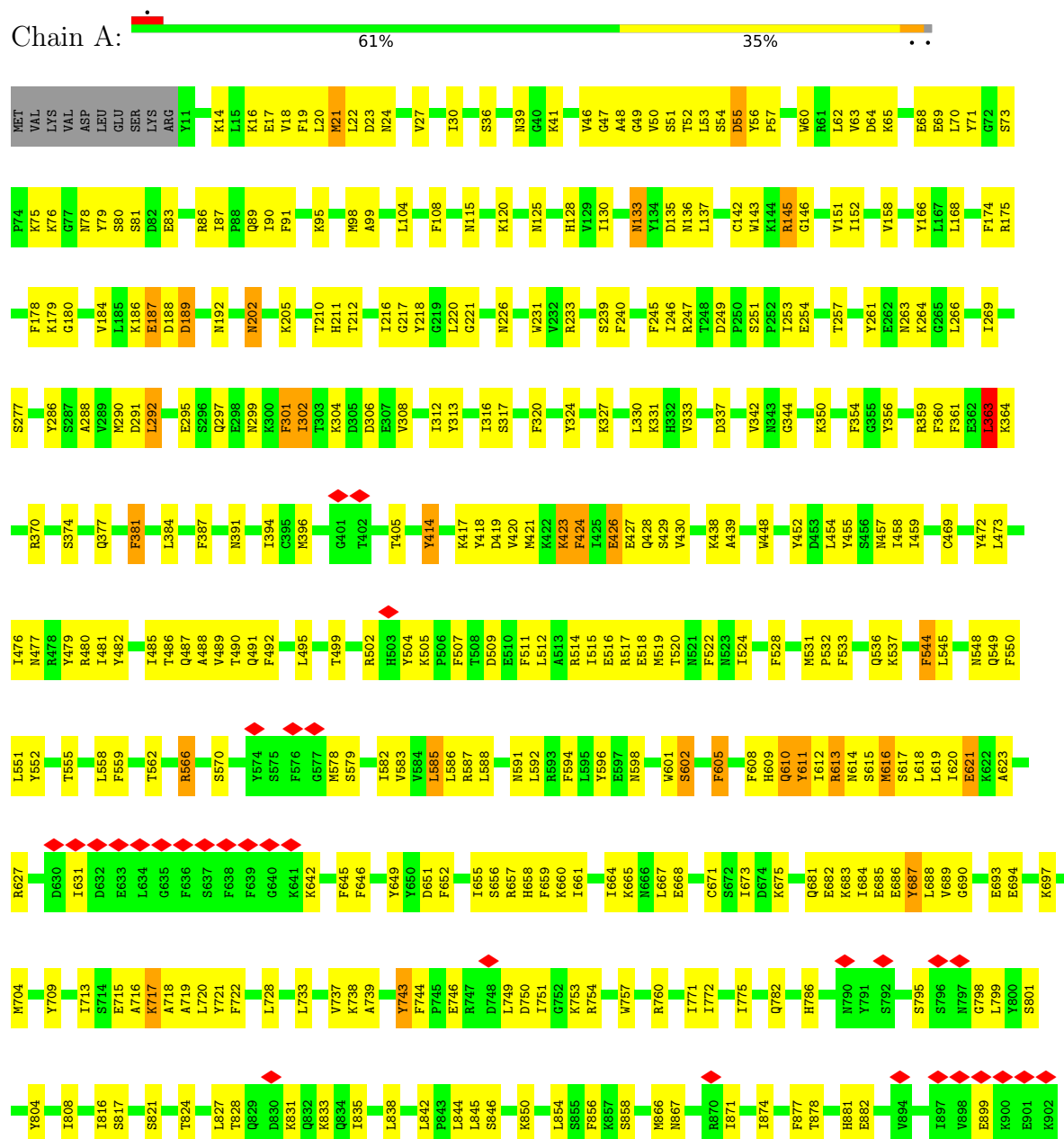
There are 4 discrepancies between the modelled and reference sequences:

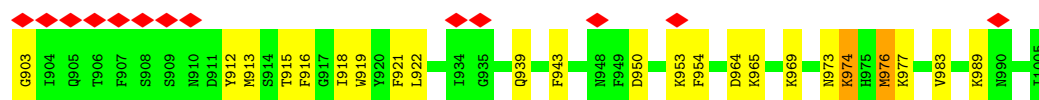
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	HIS	engineered mutation	UNP D4G637
B	171	ALA	HIS	engineered mutation	UNP D4G637
C	171	ALA	HIS	engineered mutation	UNP D4G637
D	171	ALA	HIS	engineered mutation	UNP D4G637

3 Residue-property plots

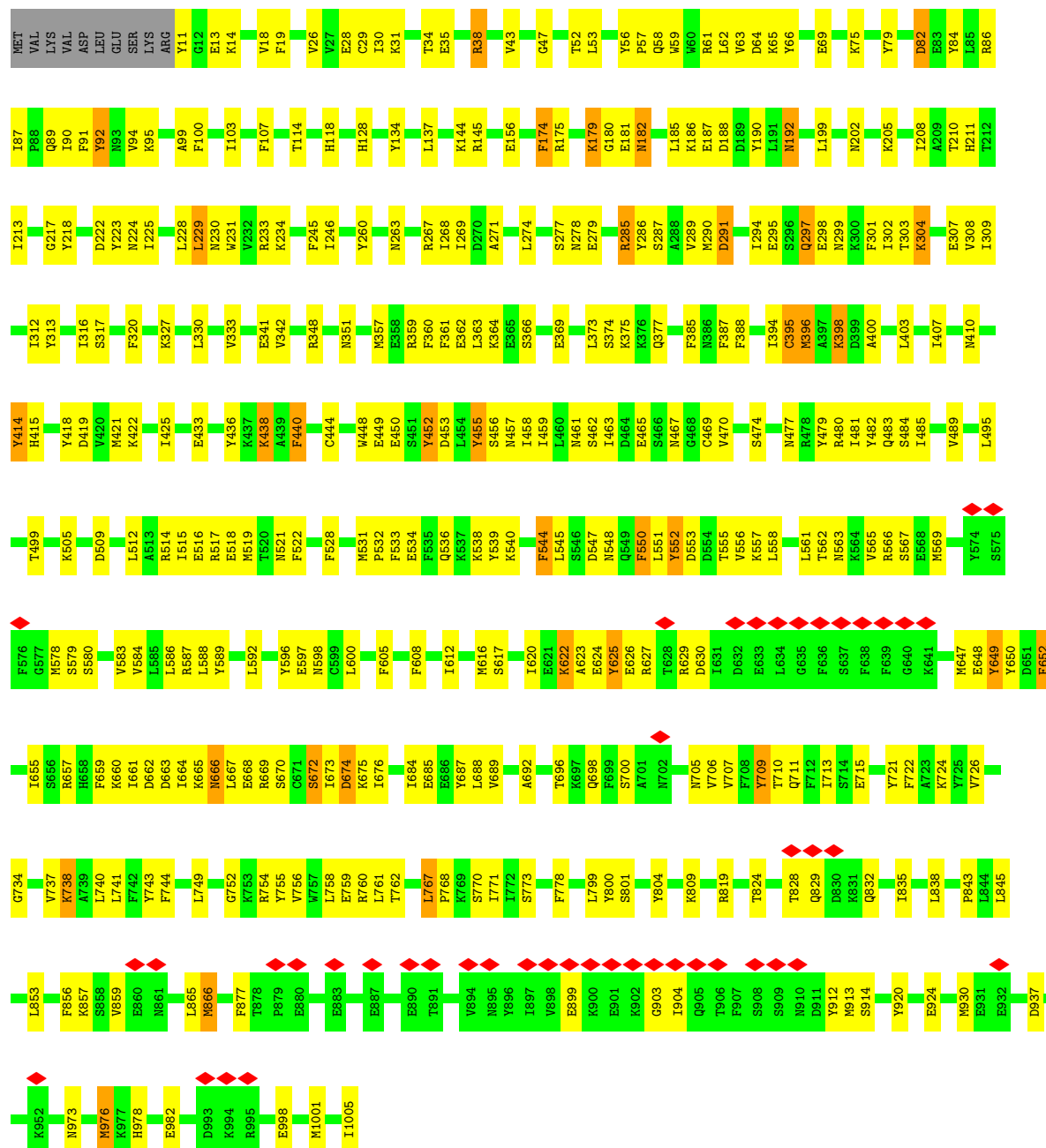
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SIR2-like domain-containing protein





• Molecule 1: SIR2-like domain-containing protein



• Molecule 1: SIR2-like domain-containing protein



K902	G903	I904	S909	M936	D937	Y940	I955	P956	S957	Y958	I961	L967	I970	K977	I981	L984	R987	Y988	S991	L997	L1000	M1001	N1002	Y1003	F1004	I1005																											
S801	R802	D803	Y804	K809	H810	F811	I816	S817	K818	R819	L820	T824	L827	T828	Q829	Q832	I835	D836	F837	L838	K840	L844	L845	S851	H852	L853	L854	S855	F856	K857	N861	I862	R863	D864	L865	M866	N867	R870	L884	I885	R885	Q882	Y896	E899									
A723	K724	Y725	V726	K727	L728	S729	E730	E731	G732	L733	G734	K735	I736	V737	K738	A739	L740	L741	F742	Y743	P745	E746	R747	D748	L749	D750	I751	G752	K753	R754	Y755	V756	W757	L758	E759	R760	L761	T762	L767	P768	K769	S770	I771	I774	D777	V780	L781	Q782	A783	H786	L799	Y800	
F652	V653	N654	R657	H658	F659	K660	I661	D662	D663	I664	K665	N666	L667	E668	R669	L673	D674	I675	L676	R677	F678	G679	E680	K683	I684	E685	E686	R613	N614	L618	L619	I620	Y625	E626	R627	T628	R629	D630	I631	D632	E633	L634	G635	F636	S637	F638	F639	G640	K641	M647	E648	Y649	D651
S575	F576	S579	S580	D581	V584	L585	L586	R587	L588	Y589	R593	F594	L595	Y596	E597	N598	C599	S604	E607	F608	H609	Q610	Y611	I612	R613	N614	L618	L619	I620	Y625	E626	R627	T628	D629	I631	D632	E633	L634	G635	F636	S637	F638	F639	G640	K641	M647	E648	Y649	D651				
L384	F385	N386	F387	F388	E389	K390	N391	I394	C395	K398	E408	Y414	H415	D419	V420	M421	K422	K423	F424	I425	K438	A439	F440	F441	L442	R447	W448	E449	D453	L454	Y455	S456	M457	I458	I459	S462	E465	S466	M467	G468	C469	V470	Y471	Q475	R478	Y479							
T294	E295	S296	Q297	E298	F301	K304	D305	D306	I309	I312	Y313	I316	S317	P318	L322	Q323	Y324	I325	R326	K327	D329	K331	D337	V342	N351	Y356	M357	E358	R359	F361	E362	L363	K364	E365	S366	E369	L373	S374	K375	K376	Q377	Y378	E379	R380									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64553	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.574	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/8478	0.56	5/11418 (0.0%)
1	B	0.29	0/8478	0.55	2/11418 (0.0%)
1	C	0.29	0/8478	0.53	0/11418
1	D	0.31	0/8478	0.59	5/11418 (0.0%)
All	All	0.30	0/33912	0.56	12/45672 (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	B	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CB-CG-OD1	8.24	125.72	118.30
1	B	229	LEU	CA-CB-CG	6.61	130.50	115.30
1	D	532	PRO	CA-N-CD	-5.92	103.22	111.50
1	A	363	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	767	LEU	CA-CB-CG	5.64	128.26	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	GLN	Peptide
1	D	297	GLN	Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
1	D	58	GLN	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	8285	0	8120	298	0
1	B	8285	0	8120	298	0
1	C	8285	0	8120	281	0
1	D	8285	0	8120	335	0
All	All	33140	0	32480	1183	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 1183 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:973:ASN:HB3	1:B:976:MET:HE3	1.55	0.87
1:B:627:ARG:HH12	1:B:675:LYS:HG2	1.43	0.82
1:D:425:ILE:HD11	1:D:442:LEU:HG	1.59	0.82
1:C:588:LEU:HD11	1:C:612:ILE:HD12	1.61	0.82
1:D:45:PHE:HB2	1:D:213:ILE:HD11	1.61	0.82

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	993/1005 (99%)	927 (93%)	65 (6%)	1 (0%)	48	83
1	B	993/1005 (99%)	919 (92%)	73 (7%)	1 (0%)	48	83
1	C	993/1005 (99%)	932 (94%)	56 (6%)	5 (0%)	25	64
1	D	993/1005 (99%)	906 (91%)	81 (8%)	6 (1%)	22	59
All	All	3972/4020 (99%)	3684 (93%)	275 (7%)	13 (0%)	38	72

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	521	ASN
1	C	846	SER
1	C	847	THR
1	D	223	TYR
1	D	521	ASN

5.3.2 Protein sidechains ⓘ

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	912/922 (99%)	874 (96%)	38 (4%)	25	47
1	B	912/922 (99%)	872 (96%)	40 (4%)	24	46
1	C	912/922 (99%)	872 (96%)	40 (4%)	24	46
1	D	912/922 (99%)	860 (94%)	52 (6%)	17	39
All	All	3648/3688 (99%)	3478 (95%)	170 (5%)	24	44

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	936	MET
1	D	415	HIS
1	D	21	MET
1	D	282	TYR
1	D	523	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	118	HIS
1	D	115	ASN
1	C	536	GLN
1	C	939	GLN
1	C	351	ASN

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 [i](#)

There are no ligands in this entry.

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.

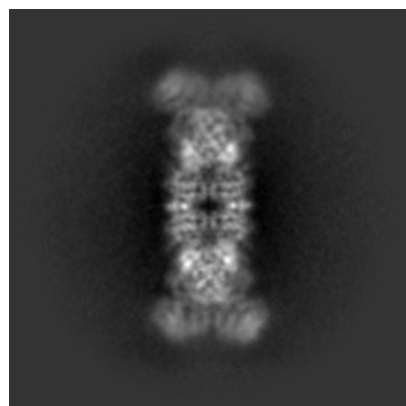
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39240. These allow visual inspection of the internal detail of the map and identification of artifacts.

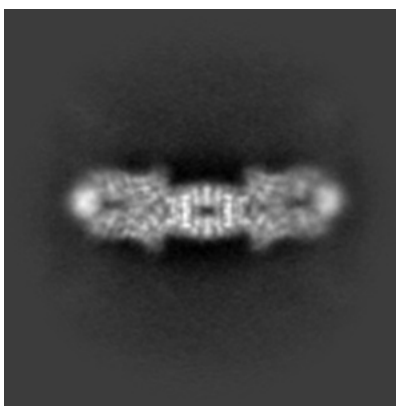
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

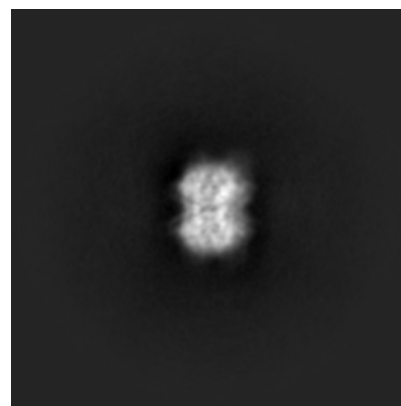
6.1.1 Primary map



X

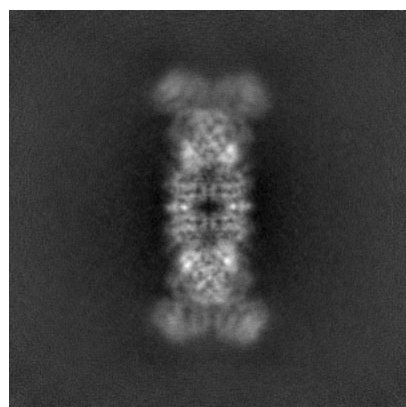


Y

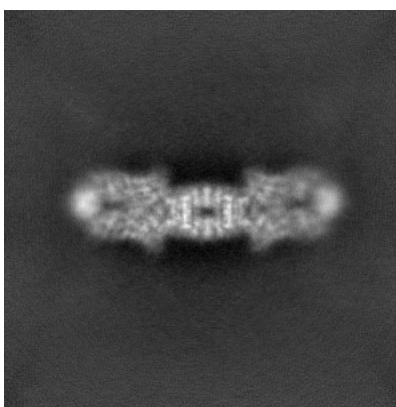


Z

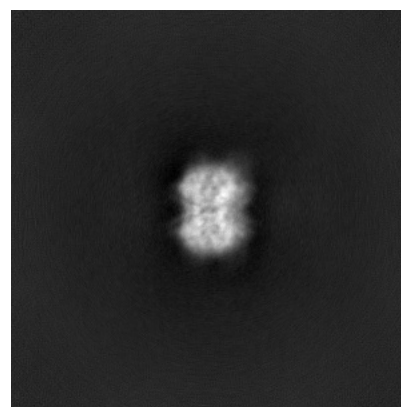
6.1.2 Raw map



X



Y

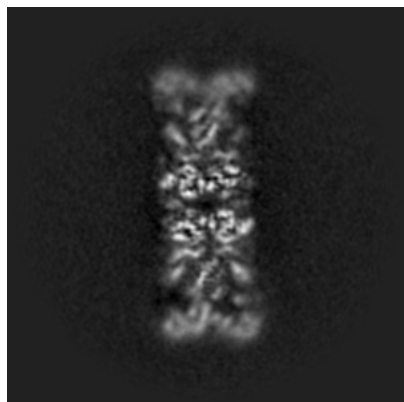


Z

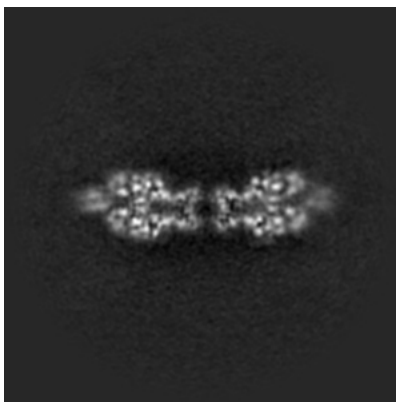
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

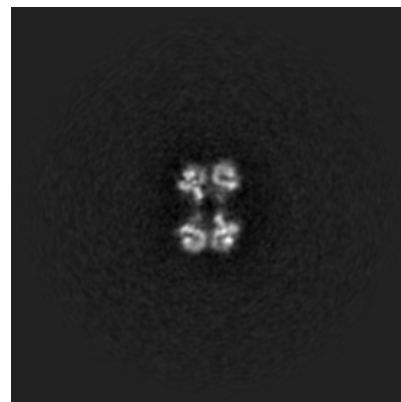
6.2.1 Primary map



X Index: 230

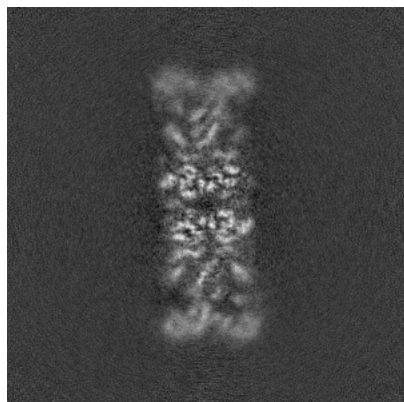


Y Index: 230

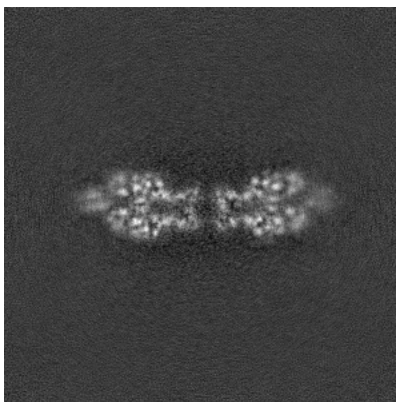


Z Index: 230

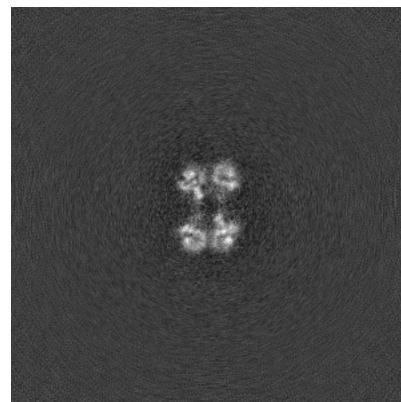
6.2.2 Raw map



X Index: 230



Y Index: 230

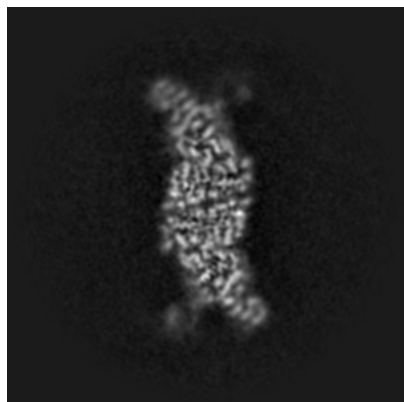


Z Index: 230

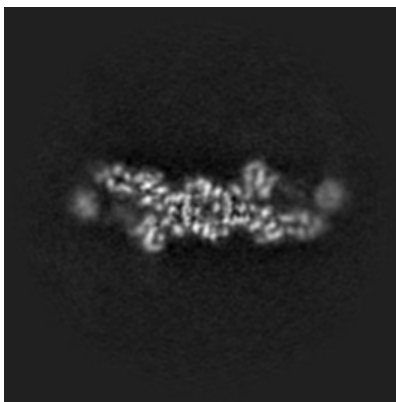
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

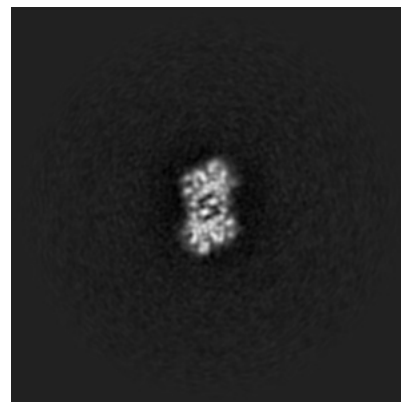
6.3.1 Primary map



X Index: 214

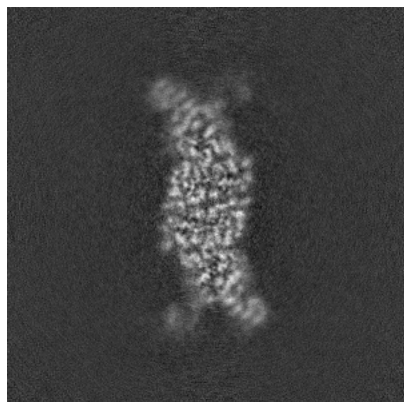


Y Index: 205

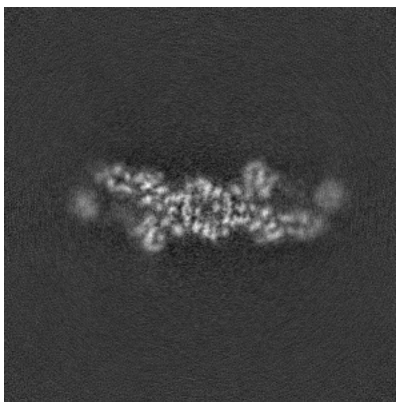


Z Index: 208

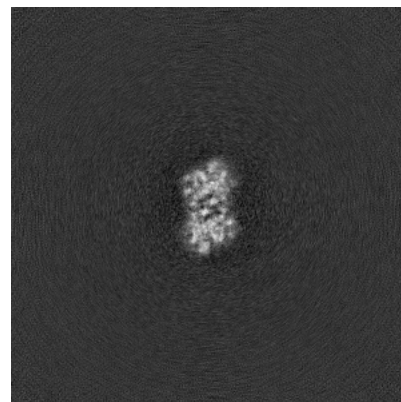
6.3.2 Raw map



X Index: 215



Y Index: 205

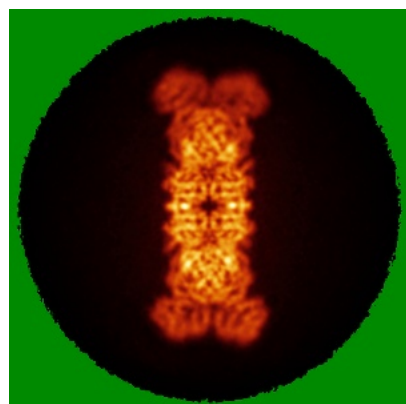


Z Index: 208

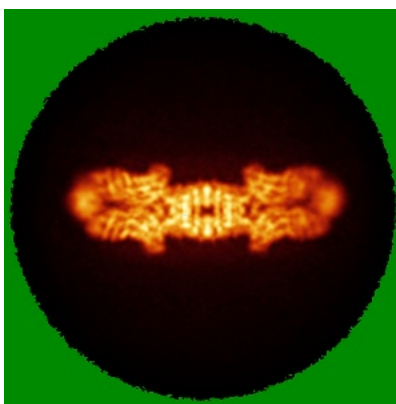
The images above show the largest variance slices of the map in three orthogonal directions.

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

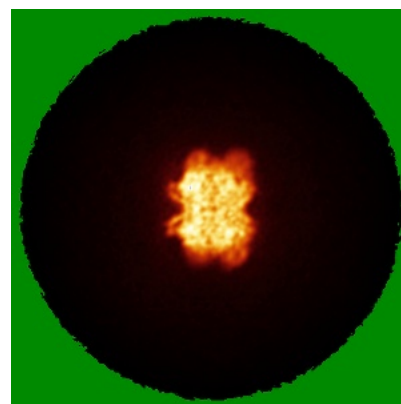
6.4.1 Primary map



X

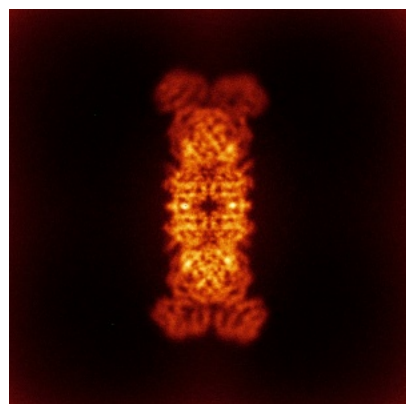


Y

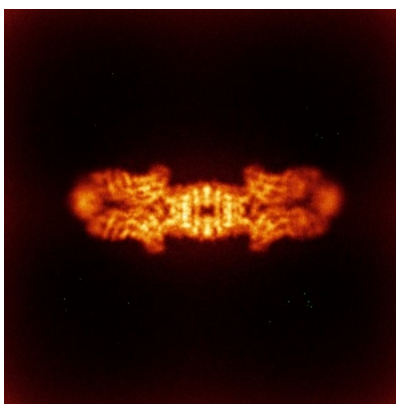


Z

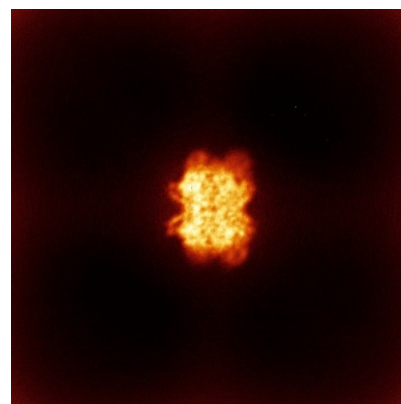
6.4.2 Raw map



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.

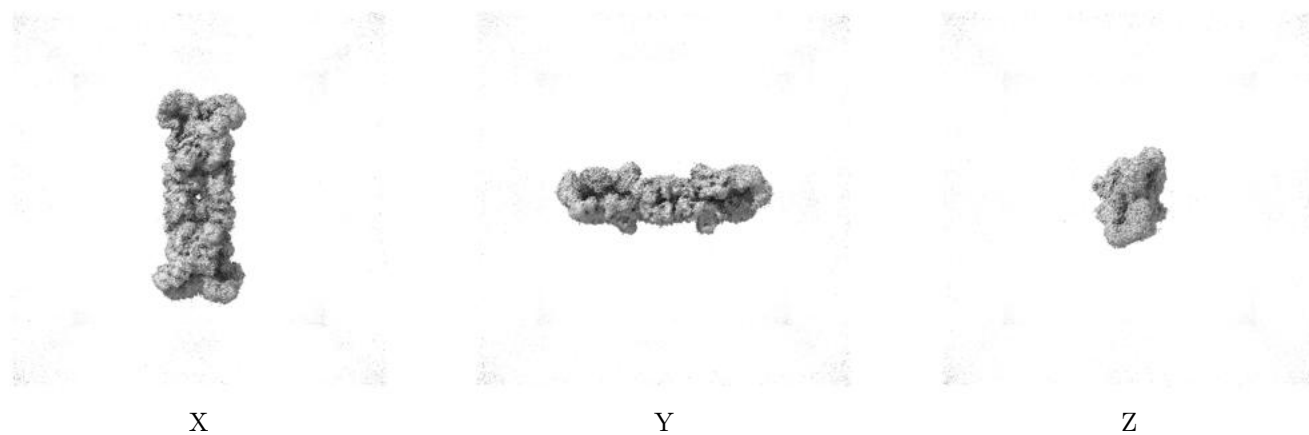
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

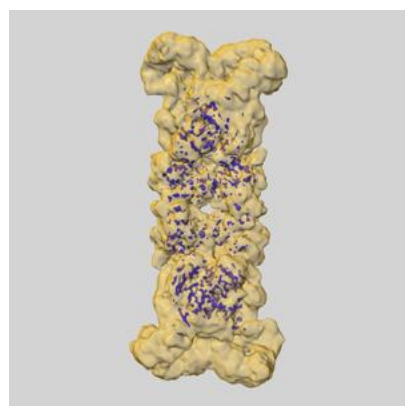
6.6 Mask visualisation [i](#)

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

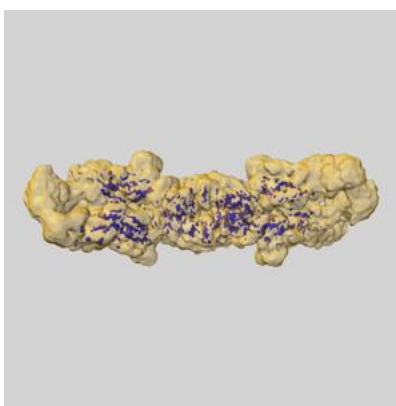
A mask typically either:

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

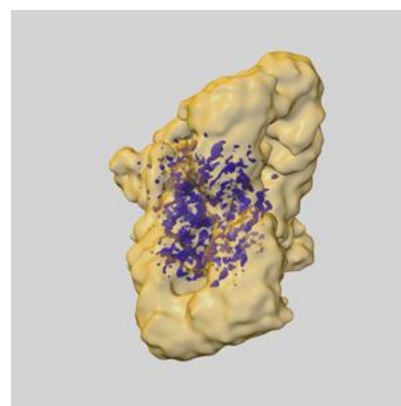
6.6.1 emd_39240_msk_1.map [i](#)



X



Y

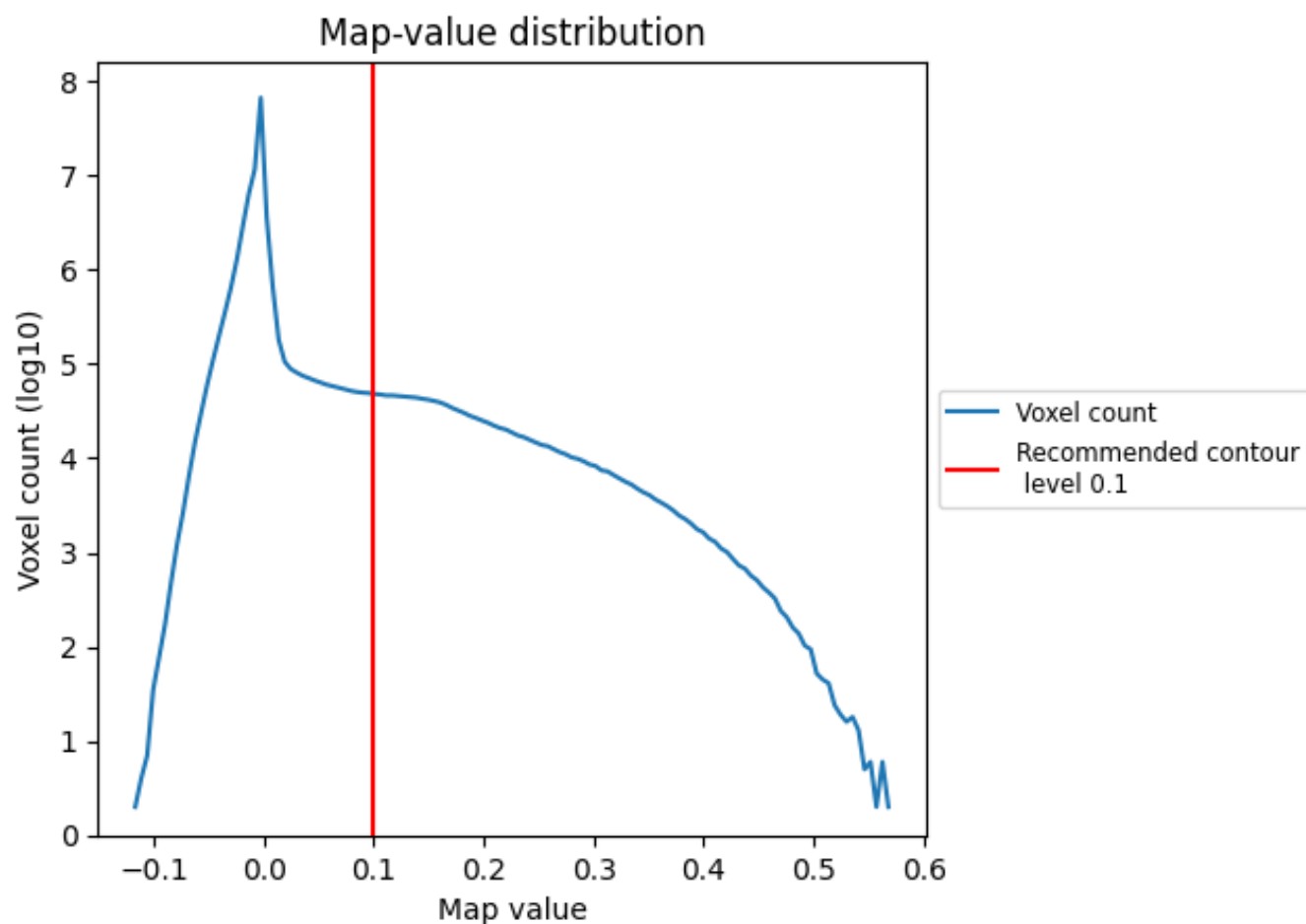


Z

7 Map analysis [i](#)

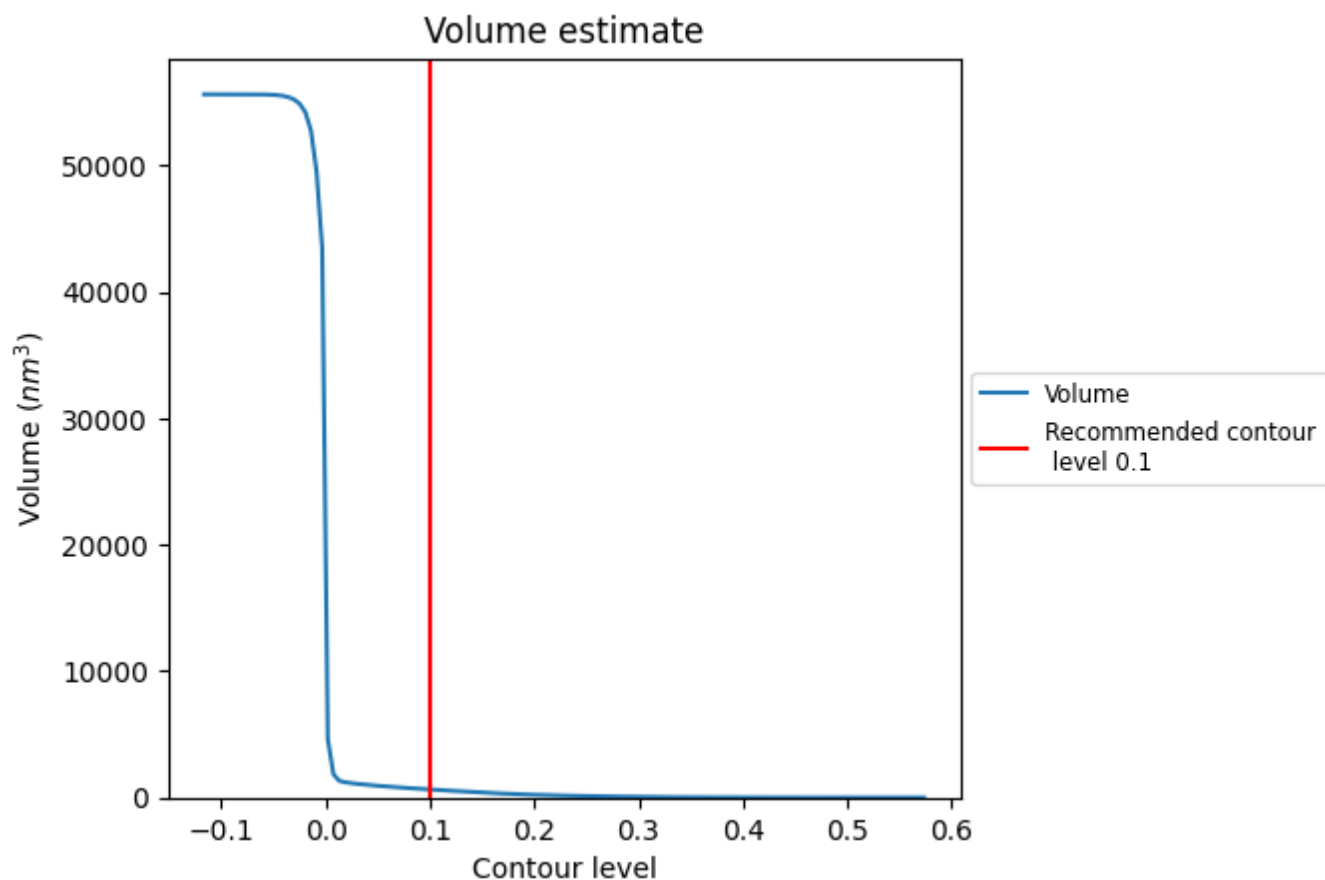
This section contains the results of statistical analysis of the map.

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.

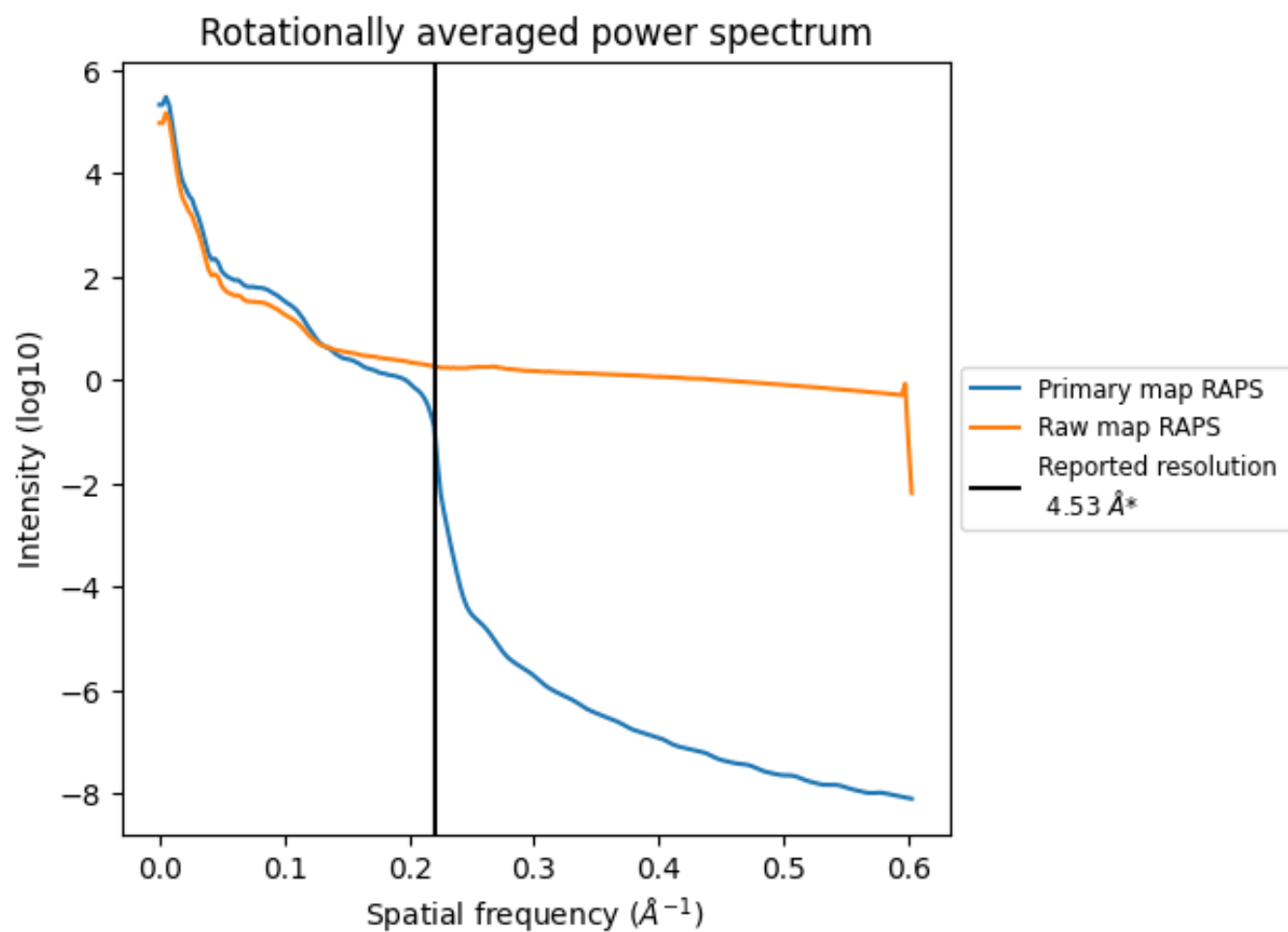
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 640 nm³; this corresponds to an approximate mass of 578 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 ⓘ

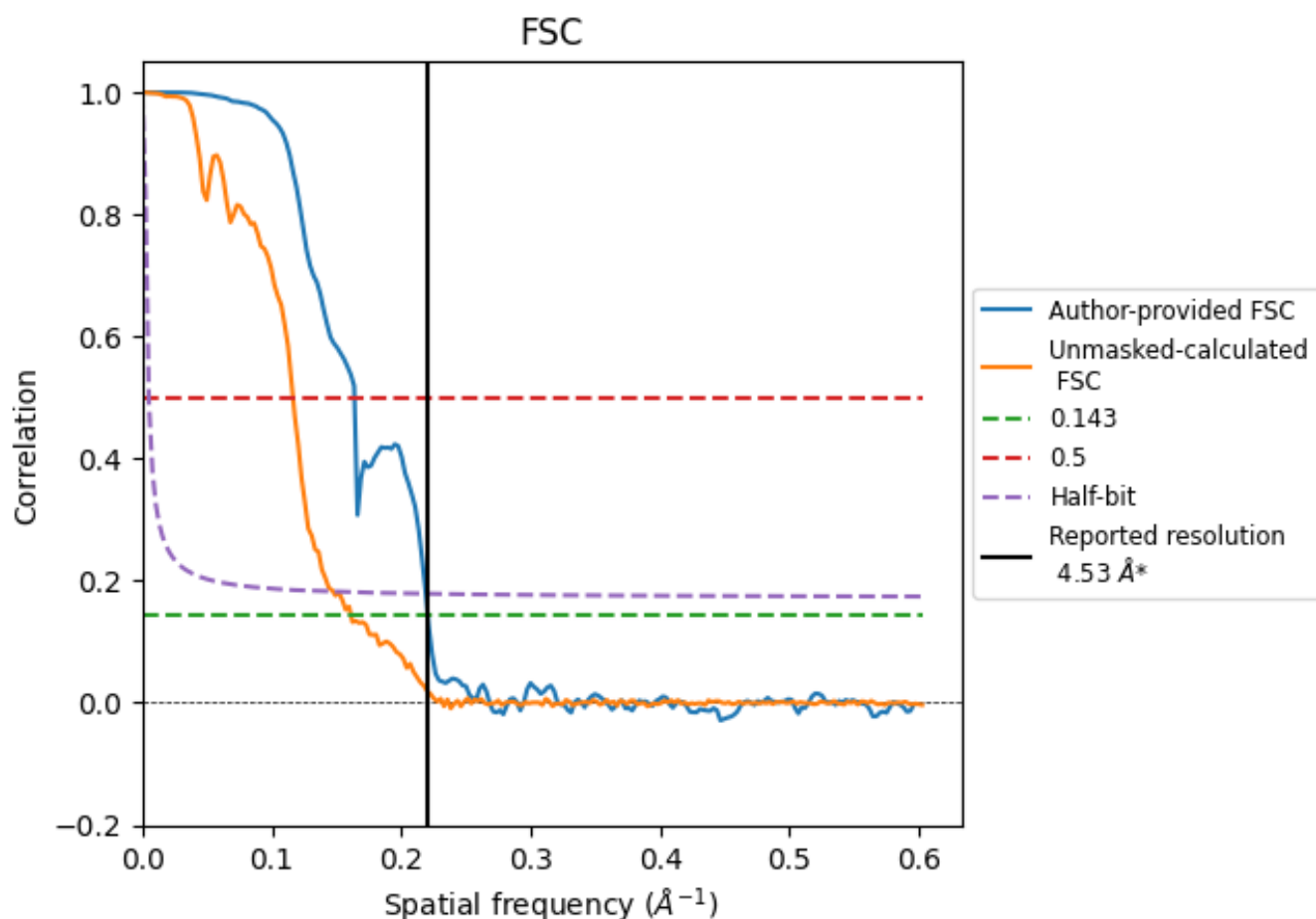


*Reported resolution corresponds to spatial frequency of 0.221 \AA^{-1}

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 0.221 \AA^{-1}

8.2 Resolution estimates [i](#)

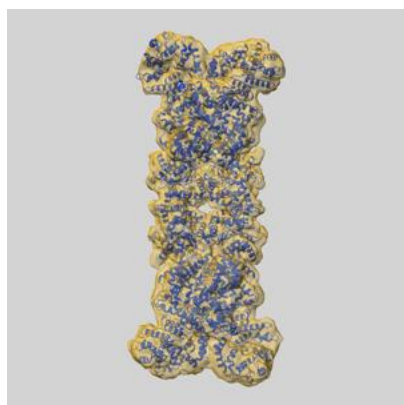
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.53	-	-
Author-provided FSC curve	4.53	6.10	4.57
Unmasked-calculated*	6.20	8.59	6.78

*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 6.20 differs from the reported value 4.53 by more than 10 %

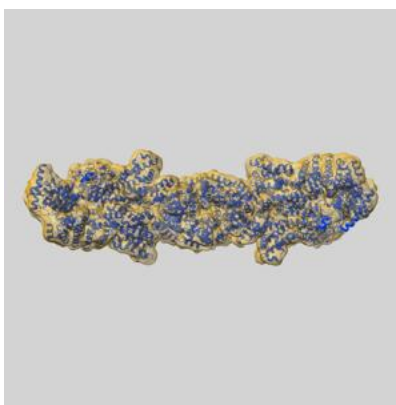
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39240 and PDB model 8YGA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

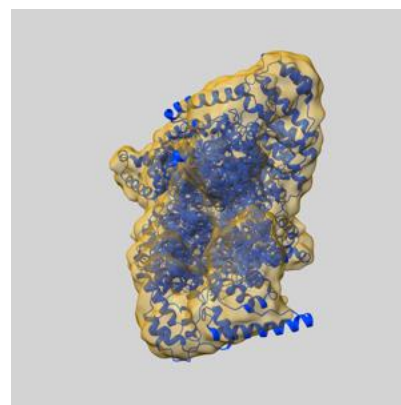
9.1 Map-model overlay [i](#)



X



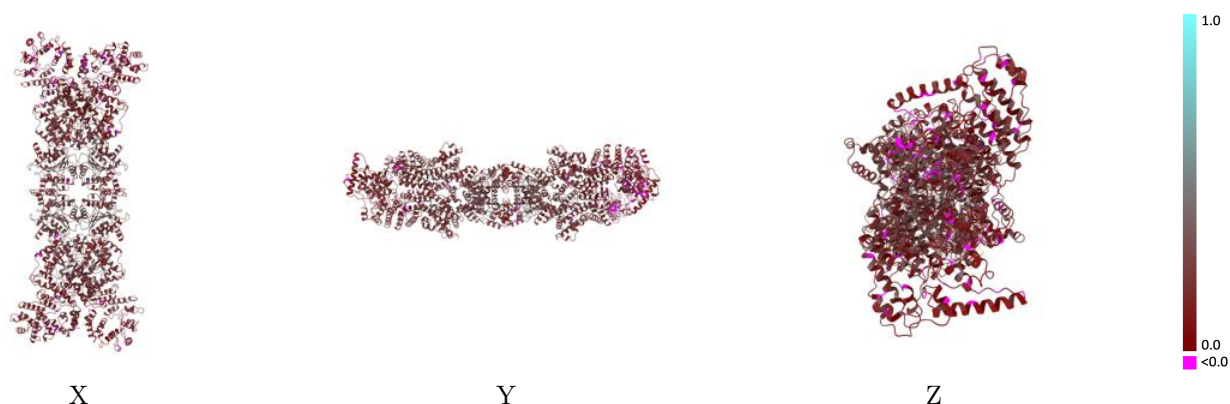
Y



Z

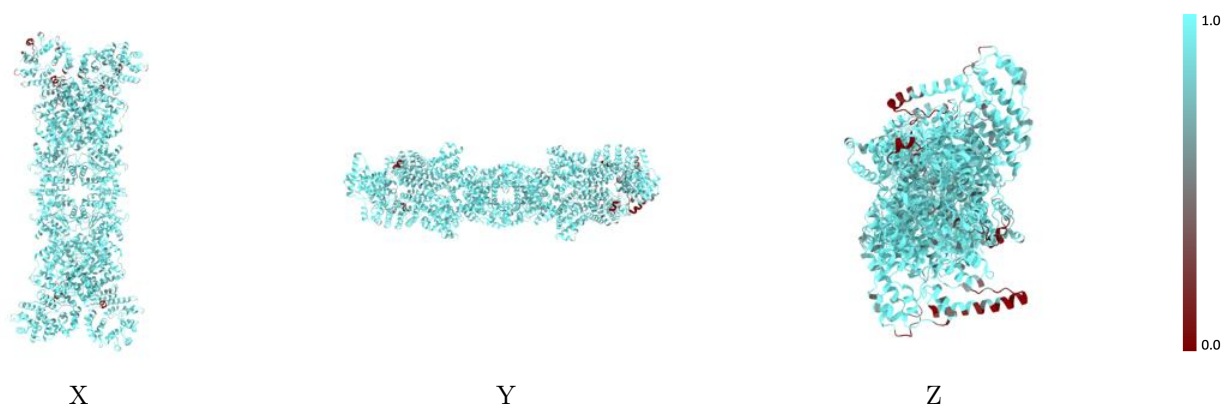
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



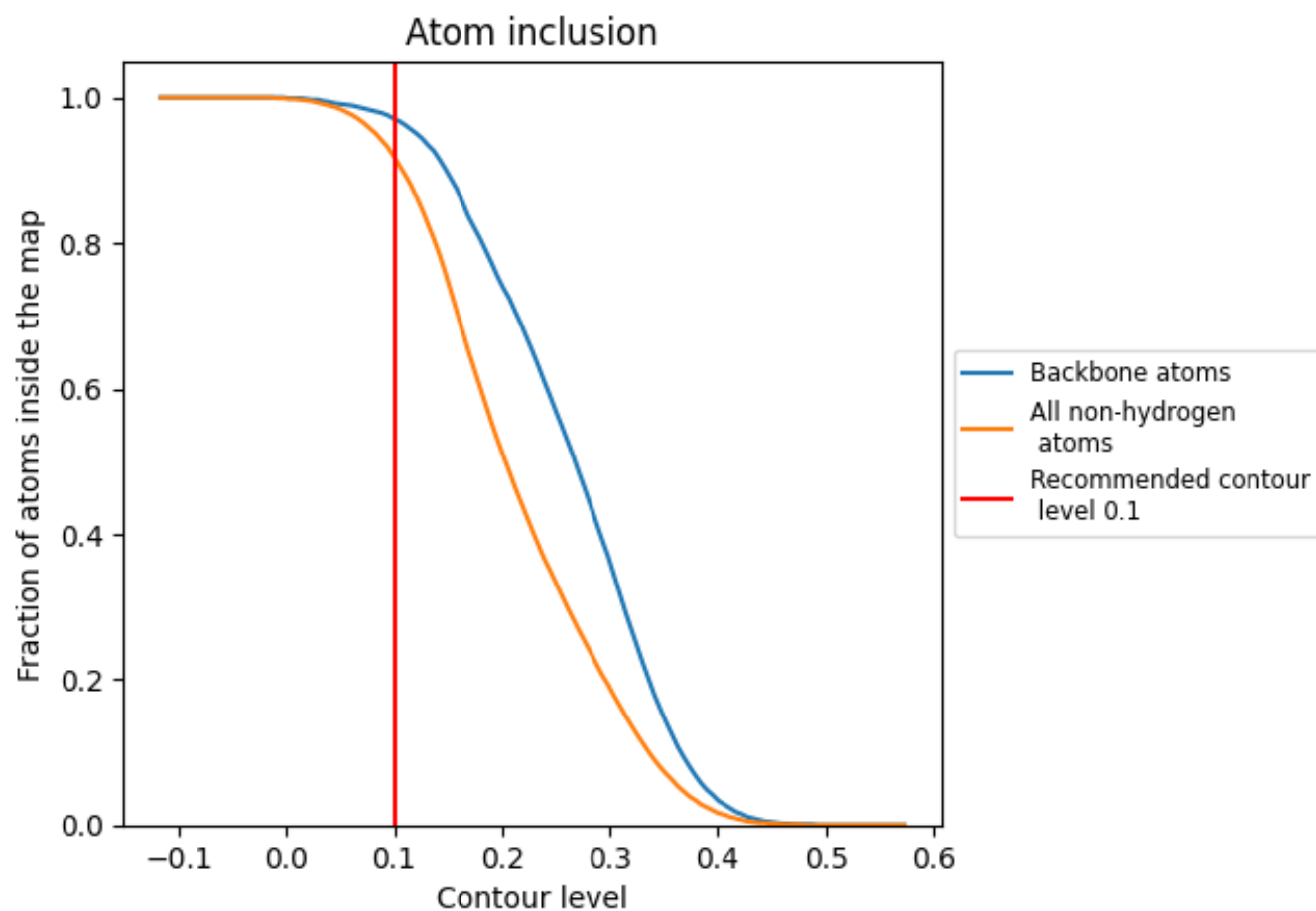
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9190	<div></div> 0.2230
A	<div></div> 0.8950	<div></div> 0.2110
B	<div></div> 0.8950	<div></div> 0.2120
C	<div></div> 0.9410	<div></div> 0.2310
D	<div></div> 0.9450	<div></div> 0.2370

