



# wwPDB EM Validation Summary Report ⓘ

Jun 29, 2026 – 04:23 PM EDT

PDB ID : 9Y5R / pdb\_00009y5r  
EMDB ID : EMD-72520  
Title : Eukaryotic translation initiation factor 2-B (eIF2B) bound to phosphorylated eIF2alpha (NTD)  
Authors : Dalwadi, U.; Croll, T.; Subramanian, A.; Lee, D.J.; Arthur, C.; Walter, P.; Frost, A.  
Deposited on : 2025-09-05  
Resolution : 3.01 Å (reported)  
Based on initial model : 6o9z

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:

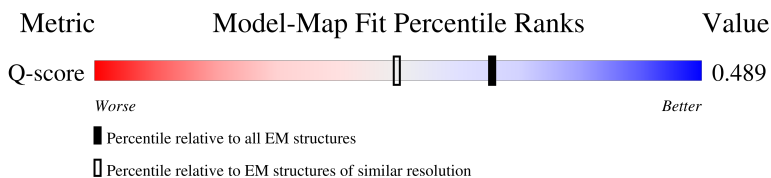
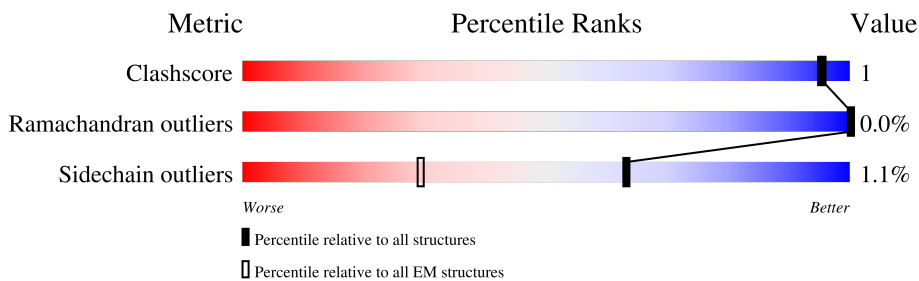
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





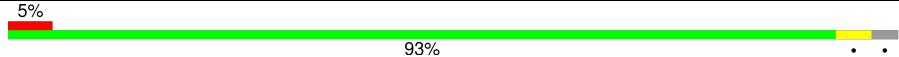
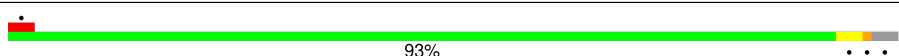
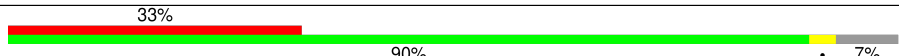
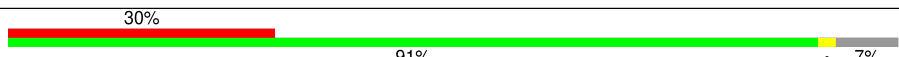
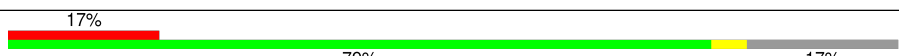

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 ( 2.51 - 3.51 )

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	721	 56% 39%
1	B	721	 57% 39%
2	C	368	 79% 9% 12%
2	D	368	 80% 7% 12%

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Mol	Chain	Length	Quality of chain
3	E	523	
3	F	523	
4	G	305	
4	H	305	
5	I	452	
5	J	452	
6	L	222	
6	M	222	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 31588 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 Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		
1	B	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	587	VAL	ILE	conflict	UNP Q13144
B	587	VAL	ILE	conflict	UNP Q13144

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	322	Total	C	N	O	S	0	0
			2523	1596	442	470	15		
2	D	322	Total	C	N	O	S	0	0
			2523	1596	442	470	15		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P49770
C	-15	HIS	-	expression tag	UNP P49770
C	-14	HIS	-	expression tag	UNP P49770
C	-13	HIS	-	expression tag	UNP P49770
C	-12	HIS	-	expression tag	UNP P49770
C	-11	HIS	-	expression tag	UNP P49770
C	-10	HIS	-	expression tag	UNP P49770
C	-9	GLY	-	expression tag	UNP P49770
C	-8	GLY	-	expression tag	UNP P49770
C	-7	GLY	-	expression tag	UNP P49770
C	-6	SER	-	expression tag	UNP P49770

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLU	-	expression tag	UNP P49770
C	-4	ASN	-	expression tag	UNP P49770
C	-3	LEU	-	expression tag	UNP P49770
C	-2	TYR	-	expression tag	UNP P49770
C	-1	PHE	-	expression tag	UNP P49770
C	0	GLN	-	expression tag	UNP P49770
C	1	SER	-	expression tag	UNP P49770
D	-16	MET	-	initiating methionine	UNP P49770
D	-15	HIS	-	expression tag	UNP P49770
D	-14	HIS	-	expression tag	UNP P49770
D	-13	HIS	-	expression tag	UNP P49770
D	-12	HIS	-	expression tag	UNP P49770
D	-11	HIS	-	expression tag	UNP P49770
D	-10	HIS	-	expression tag	UNP P49770
D	-9	GLY	-	expression tag	UNP P49770
D	-8	GLY	-	expression tag	UNP P49770
D	-7	GLY	-	expression tag	UNP P49770
D	-6	SER	-	expression tag	UNP P49770
D	-5	GLU	-	expression tag	UNP P49770
D	-4	ASN	-	expression tag	UNP P49770
D	-3	LEU	-	expression tag	UNP P49770
D	-2	TYR	-	expression tag	UNP P49770
D	-1	PHE	-	expression tag	UNP P49770
D	0	GLN	-	expression tag	UNP P49770
D	1	SER	-	expression tag	UNP P49770

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	356	2770	1751	493	512	14	0	0
3	F	356	2770	1751	493	512	14	0	0

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	296	2302	1477	381	432	12	0	0
4	H	296	2302	1477	381	432	12	0	0

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	420	Total	C	N	O	S	0	0
			3260	2062	560	612	26		
5	J	420	Total	C	N	O	S	0	0
			3260	2062	560	612	26		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
6	L	184	Total	C	N	O	P	S	0	0
			1514	953	267	287	1	6		
6	M	184	Total	C	N	O	P	S	0	0
			1514	953	267	287	1	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-34	MET	-	initiating methionine	UNP P05198
L	-33	GLY	-	expression tag	UNP P05198
L	-32	SER	-	expression tag	UNP P05198
L	-31	SER	-	expression tag	UNP P05198
L	-30	HIS	-	expression tag	UNP P05198
L	-29	HIS	-	expression tag	UNP P05198
L	-28	HIS	-	expression tag	UNP P05198
L	-27	HIS	-	expression tag	UNP P05198
L	-26	HIS	-	expression tag	UNP P05198
L	-25	HIS	-	expression tag	UNP P05198
L	-24	SER	-	expression tag	UNP P05198
L	-23	SER	-	expression tag	UNP P05198
L	-22	GLY	-	expression tag	UNP P05198
L	-21	LEU	-	expression tag	UNP P05198
L	-20	VAL	-	expression tag	UNP P05198
L	-19	PRO	-	expression tag	UNP P05198
L	-18	ARG	-	expression tag	UNP P05198
L	-17	GLY	-	expression tag	UNP P05198
L	-16	SER	-	expression tag	UNP P05198
L	-15	HIS	-	expression tag	UNP P05198
L	-14	MET	-	expression tag	UNP P05198
L	-13	ALA	-	expression tag	UNP P05198
L	-12	SER	-	expression tag	UNP P05198
L	-11	MET	-	expression tag	UNP P05198
L	-10	THR	-	expression tag	UNP P05198

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-9	GLY	-	expression tag	UNP P05198
L	-8	GLY	-	expression tag	UNP P05198
L	-7	GLN	-	expression tag	UNP P05198
L	-6	GLN	-	expression tag	UNP P05198
L	-5	MET	-	expression tag	UNP P05198
L	-4	GLY	-	expression tag	UNP P05198
L	-3	ARG	-	expression tag	UNP P05198
L	-2	GLY	-	expression tag	UNP P05198
L	-1	SER	-	expression tag	UNP P05198
L	0	GLU	-	expression tag	UNP P05198
L	1	PHE	-	expression tag	UNP P05198
M	-34	MET	-	initiating methionine	UNP P05198
M	-33	GLY	-	expression tag	UNP P05198
M	-32	SER	-	expression tag	UNP P05198
M	-31	SER	-	expression tag	UNP P05198
M	-30	HIS	-	expression tag	UNP P05198
M	-29	HIS	-	expression tag	UNP P05198
M	-28	HIS	-	expression tag	UNP P05198
M	-27	HIS	-	expression tag	UNP P05198
M	-26	HIS	-	expression tag	UNP P05198
M	-25	HIS	-	expression tag	UNP P05198
M	-24	SER	-	expression tag	UNP P05198
M	-23	SER	-	expression tag	UNP P05198
M	-22	GLY	-	expression tag	UNP P05198
M	-21	LEU	-	expression tag	UNP P05198
M	-20	VAL	-	expression tag	UNP P05198
M	-19	PRO	-	expression tag	UNP P05198
M	-18	ARG	-	expression tag	UNP P05198
M	-17	GLY	-	expression tag	UNP P05198
M	-16	SER	-	expression tag	UNP P05198
M	-15	HIS	-	expression tag	UNP P05198
M	-14	MET	-	expression tag	UNP P05198
M	-13	ALA	-	expression tag	UNP P05198
M	-12	SER	-	expression tag	UNP P05198
M	-11	MET	-	expression tag	UNP P05198
M	-10	THR	-	expression tag	UNP P05198
M	-9	GLY	-	expression tag	UNP P05198
M	-8	GLY	-	expression tag	UNP P05198
M	-7	GLN	-	expression tag	UNP P05198
M	-6	GLN	-	expression tag	UNP P05198
M	-5	MET	-	expression tag	UNP P05198
M	-4	GLY	-	expression tag	UNP P05198

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	ARG	-	expression tag	UNP P05198
M	-2	GLY	-	expression tag	UNP P05198
M	-1	SER	-	expression tag	UNP P05198
M	0	GLU	-	expression tag	UNP P05198
M	1	PHE	-	expression tag	UNP P05198

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Cl 1 1	0
7	F	1	Total Cl 1 1	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
8	E	1	Total Zn 1 1	0
8	F	1	Total Zn 1 1	0







MET	ALA	ALA	VAL	VAL	VAL	VAL	ARG	GLU	GLY	SER	GLY	SER	GLY	SER	GLY	MET	LYS	ALA	GLU	LEU	PRO	PRO	GLY	GLY	ALA	VAL	VAL	ARG	GLN	LEU	ARG	LYS	GLU	GLU	LYS	LYS	LYS	GLN	GLN	GLN	LYS	LYS	ARG	LYS	LYS	ARG	GLU	GLU	GLY	GLY	ALA	GLU	PRO	GLU	THR
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GLY	SER	ALA	ALA	VAL	SER	ALA	ALA	ALA	CYS	GLN	ASP	VAL	VAL	GLY	THR	THR	ARG	GLU	PRO	PRO	PRO	GLU	GLY	SER	GLY	VAL	VAL	LYS	ILE	PRO	GLY	LEU	LEU	LEU	LEU	THR	THR	PRO	PRO	GLY	ARG	GLN	LYS	VAL	VAL	ASP	ASP	LEU	LEU	LEU	LEU	ARG	ARG	LEU	VAL	LYS	LYS	LYS	PRO	GLU	GLU	ARG	ARG	GLN	GLN	V167	M196	N245	R250	C266	R355	L403
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T420	A421	Q422	K466	R467	V471	R483	D490	L499	M506	I507	P508	S511	V512	L516	R517	W518	K519	S520	S521	D522	GLN
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- Molecule 4: Translation initiation factor eIF-2B subunit alpha



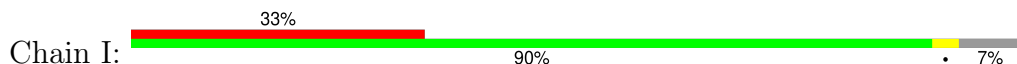
M1	D2	D3	E16	D19	V24	R28	R28	E40	E82	K110	I111	R132	V133	E139	I186	M203	V229	F239	D255	T256	LYS	VAL	ALA	GLN	THR	GLY	GLN	ASP	L266	K267	E268	E268	D274	L305
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- Molecule 4: Translation initiation factor eIF-2B subunit alpha



M1	D2	D19	V24	R28	D37	L71	K90	I111	V178	I186	V229	D245	A254	D255	T256	LYS	VAL	ALA	GLN	THR	GLY	GLN	ASP	L266	K267	E268	D274	S279	L305
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- Molecule 5: Translation initiation factor eIF-2B subunit gamma



M1	G11	G12	G13	S14	R15	M16	T17	D18	L19	T20	S21	S22	A65	E66	F67	K68	K72	P73	D74	D80	D81	A82	D83	M84	K98	D111	D119	Q136	D137	S138	I139	E140	P141	V142	P143	G144	Q145	K146	G147	K148	K149	K150	A151	V152	E153	D156	F157	S185
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R192	T197	R225	P230	S238	ALA	ALA	SER	SER	GLN	GLN	GLY	GLN	GLU	GLU	LYS	GLU	GLU	GLU	ASP	LEU	LYS	LYS	GLU	GLU	LEU	SER	D262	E269	A270	N271	T272	L273	N274	L275	A276	P277	Y278	D279	A284	C285	R286	C287	D288	R289	W290	E291	T292	D292	L293	S294	R295	S296
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C334	P335	E336	E337	S342	S343	A344	Q345	I346	V347	S348	K349	H350	L351	V352	G353	V354	D355	S356	L357	I358	G359	P360	E361	T362	Q363	I364	G365	E366	K367	S368	S369	I370	K371	R372	G376	S377	S378	C379	L380	I381	K382	D383	R384	V385	T386	I387	T388	N389	C390	R391	N394	S395	V396	T397	V398	E399
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E400	G401	S402	N403	I404	V408	I409	C410	N411	N412	A413	V414	I415	E416	K417	G418	A419	D420	I421	K422	D423	C424	L425	I426	G427	S428	G429	Q430	R431	I432	E433	A434	K435	A436	K437	R438	V439	N440	E441	V442	I443	VAL	GLY	ASN	ASP	GLN	LEU	MET	GLU	ILE
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- Molecule 5: Translation initiation factor eIF-2B subunit gamma



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.564	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	357.44, 357.44, 357.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8936, 0.8936, 0.8936	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, SEP, CL

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	0.65	0/3497	1.07	3/4758 (0.1%)
1	B	0.65	0/3497	1.10	4/4758 (0.1%)
2	C	0.71	0/2572	1.21	11/3477 (0.3%)
2	D	0.71	0/2572	1.18	10/3477 (0.3%)
3	E	0.70	0/2822	1.13	7/3835 (0.2%)
3	F	0.72	0/2822	1.13	2/3835 (0.1%)
4	G	0.66	0/2338	1.11	4/3155 (0.1%)
4	H	0.67	0/2338	1.12	2/3155 (0.1%)
5	I	0.59	0/3310	1.00	5/4470 (0.1%)
5	J	0.58	0/3310	1.00	2/4470 (0.0%)
6	L	0.54	0/1527	1.10	4/2053 (0.2%)
6	M	0.53	0/1527	1.08	2/2053 (0.1%)
All	All	0.65	0/32132	1.10	56/43496 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	3
2	C	0	4
2	D	0	3
3	E	0	5
3	F	0	5
4	G	0	1
5	I	0	2
5	J	0	4
All	All	0	35

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	317	PRO	CB-CA-C	-8.20	103.68	111.39
4	G	274	ASP	CA-CB-CG	7.02	119.62	112.60
4	G	110	LYS	CB-CA-C	-6.42	100.14	110.79
3	E	490	ASP	CA-CB-CG	6.41	119.01	112.60
3	F	490	ASP	CA-CB-CG	6.37	118.97	112.60

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	175	GLU	Peptide
1	A	211	ARG	Sidechain
1	A	65	ARG	Sidechain

## 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	3423	0	3419	11	0
1	B	3423	0	3419	11	0
2	C	2523	0	2527	9	0
2	D	2523	0	2527	9	0
3	E	2770	0	2829	12	0
3	F	2770	0	2830	5	0
4	G	2302	0	2378	5	0
4	H	2302	0	2378	4	0
5	I	3260	0	3357	4	0
5	J	3260	0	3357	2	0
6	L	1514	0	1526	1	0
6	M	1514	0	1526	1	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1	0	0	0	0
All	All	31588	0	32073	66	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 1.

The worst 5 of 66 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)
2:C:274:LEU:HB3	2:C:340:MET:HE1	1.68	0.74
1:A:66:VAL:HG13	1:A:76:ILE:HB	1.71	0.71
2:D:236:THR:HG21	2:D:245:LEU:HD22	1.71	0.71
1:B:66:VAL:HG13	1:B:76:ILE:HB	1.73	0.70
2:C:236:THR:HG21	2:C:245:LEU:HD22	1.77	0.67

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	433/721 (60%)	418 (96%)	15 (4%)	0	100	100
1	B	433/721 (60%)	417 (96%)	16 (4%)	0	100	100
2	C	318/368 (86%)	310 (98%)	7 (2%)	1 (0%)	36	68
2	D	318/368 (86%)	312 (98%)	6 (2%)	0	100	100
3	E	354/523 (68%)	347 (98%)	7 (2%)	0	100	100
3	F	354/523 (68%)	350 (99%)	4 (1%)	0	100	100
4	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
4	H	292/305 (96%)	286 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	416/452 (92%)	386 (93%)	30 (7%)	0	100	100
5	J	416/452 (92%)	394 (95%)	22 (5%)	0	100	100
6	L	181/222 (82%)	175 (97%)	6 (3%)	0	100	100
6	M	181/222 (82%)	175 (97%)	6 (3%)	0	100	100
All	All	3988/5182 (77%)	3856 (97%)	131 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	194	CYS

### 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	384/626 (61%)	378 (98%)	6 (2%)	55	78
1	B	384/626 (61%)	379 (99%)	5 (1%)	61	80
2	C	274/312 (88%)	269 (98%)	5 (2%)	51	76
2	D	274/312 (88%)	273 (100%)	1 (0%)	84	89
3	E	312/444 (70%)	305 (98%)	7 (2%)	45	73
3	F	312/444 (70%)	307 (98%)	5 (2%)	55	78
4	G	253/260 (97%)	251 (99%)	2 (1%)	73	85
4	H	253/260 (97%)	249 (98%)	4 (2%)	55	78
5	I	369/398 (93%)	366 (99%)	3 (1%)	73	85
5	J	369/398 (93%)	369 (100%)	0	100	100
6	L	168/198 (85%)	166 (99%)	2 (1%)	63	81
6	M	168/198 (85%)	168 (100%)	0	100	100
All	All	3520/4476 (79%)	3480 (99%)	40 (1%)	63	82

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	29	ARG
4	H	71	LEU
3	F	196	MET
3	F	507	ILE
4	H	279	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	208	ASN
5	J	363	GLN
6	M	23	ASN
6	L	23	ASN
5	J	297	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
6	SEP	M	52	6	8,9,10	0.61	0	7,12,14	0.80	0
6	SEP	L	52	6	8,9,10	0.58	0	7,12,14	0.84	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
6	SEP	M	52	6	-	1/6/8/10	-
6	SEP	L	52	6	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	52	SEP	CB-OG-P-O1P
6	M	52	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

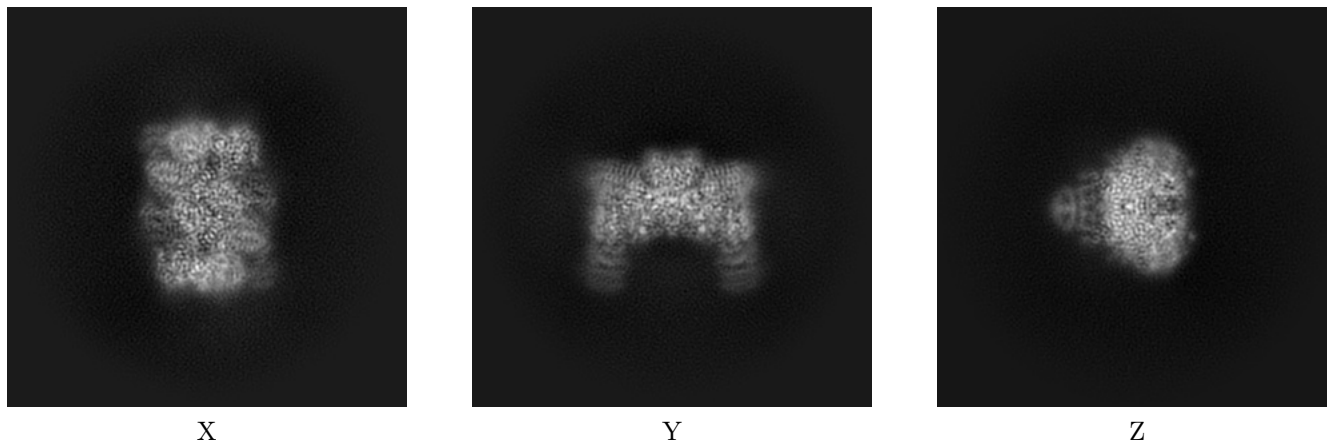
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72520. These allow visual inspection of the internal detail of the map and identification of artifacts.

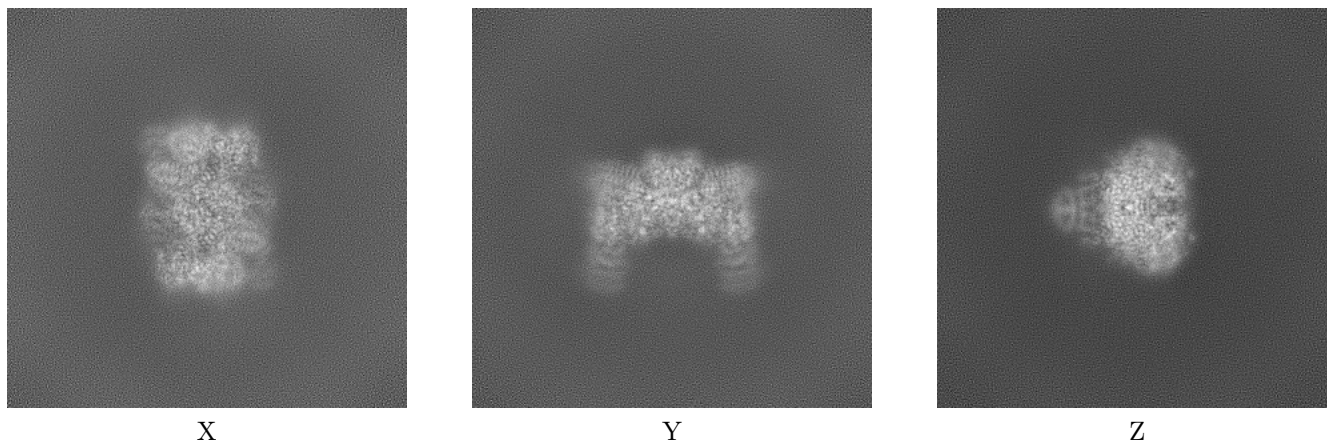
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



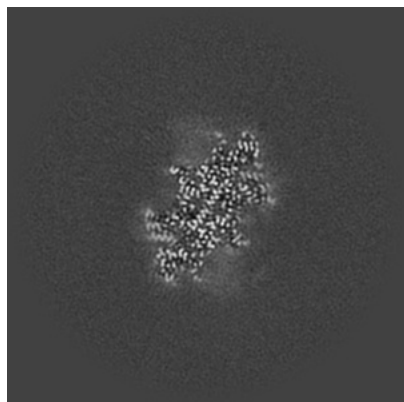
#### 6.1.2 Raw map



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

## 6.2 Central slices [i](#)

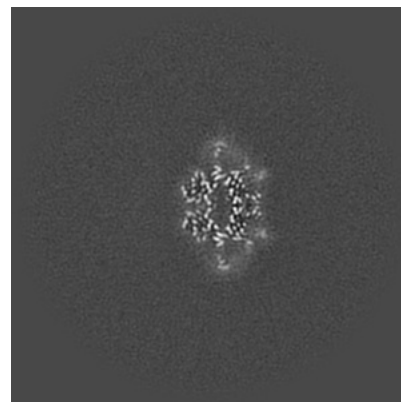
### 6.2.1 Primary map



X Index: 200

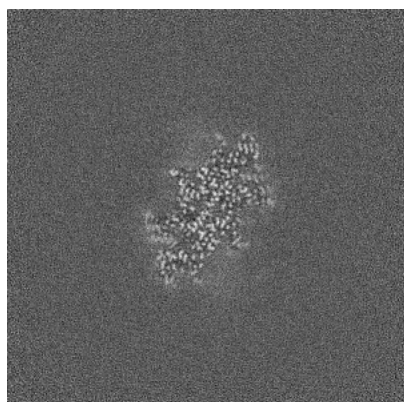


Y Index: 200

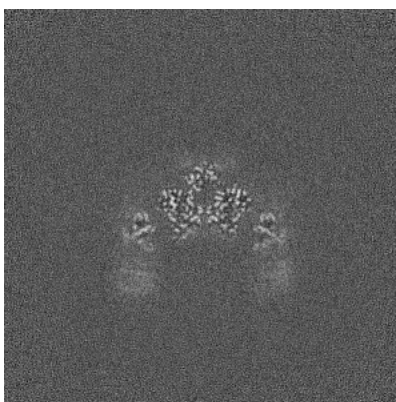


Z Index: 200

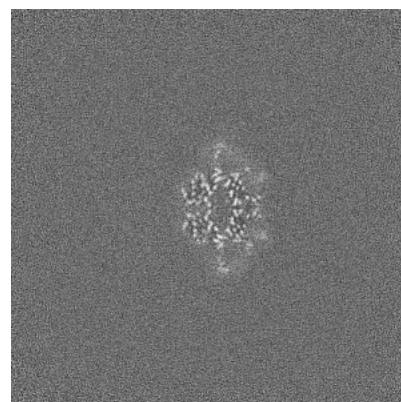
### 6.2.2 Raw map



X Index: 200



Y Index: 200

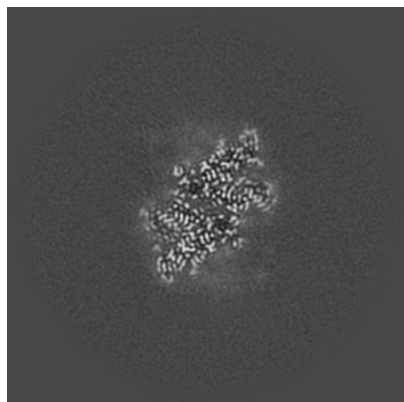


Z Index: 200

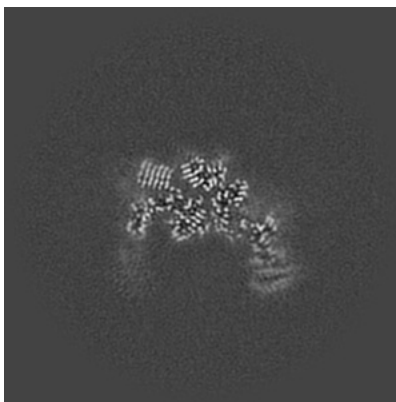
The images above show central slices of the map in three orthogonal directions.

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

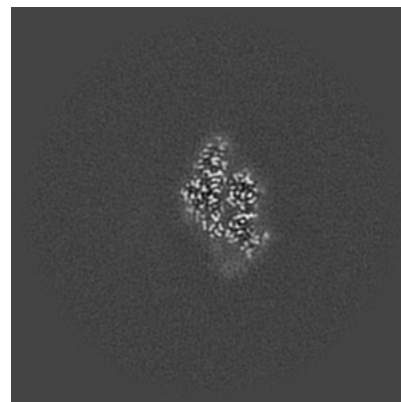
### 6.3.1 Primary map



X Index: 204

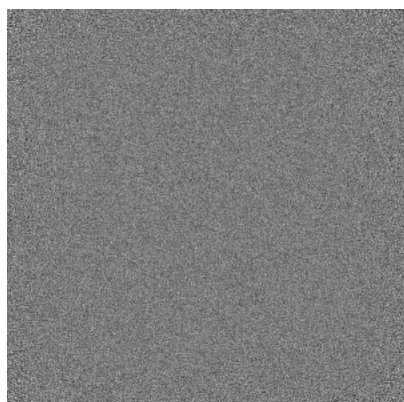


Y Index: 189

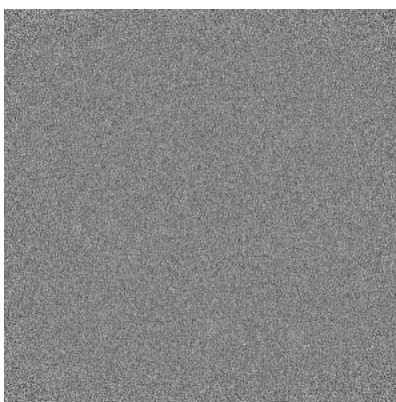


Z Index: 210

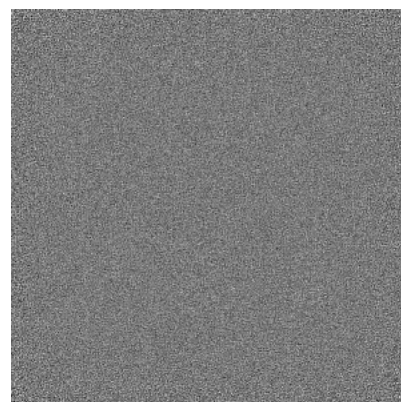
### 6.3.2 Raw map



X Index: 0



Y Index: 0

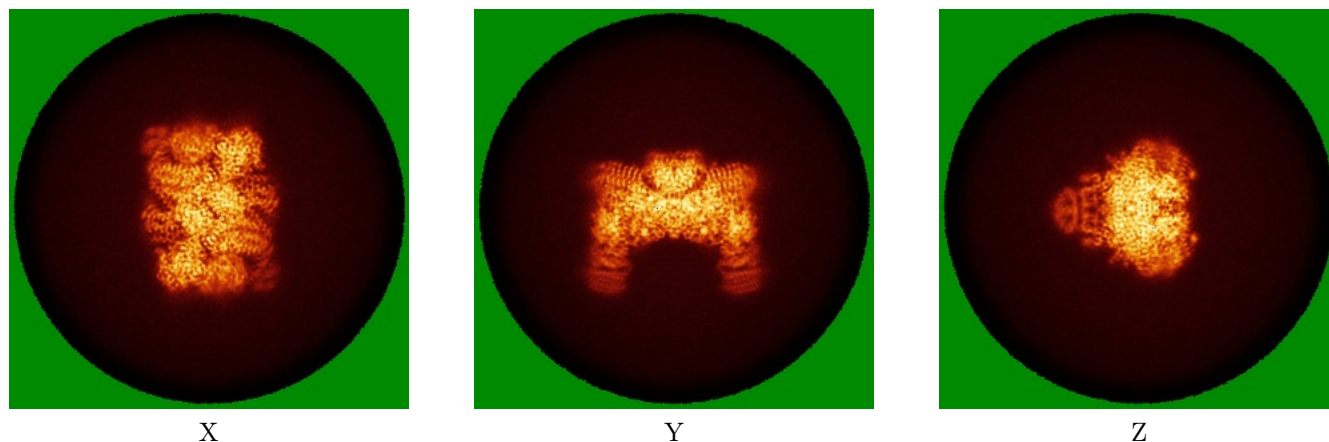


Z Index: 0

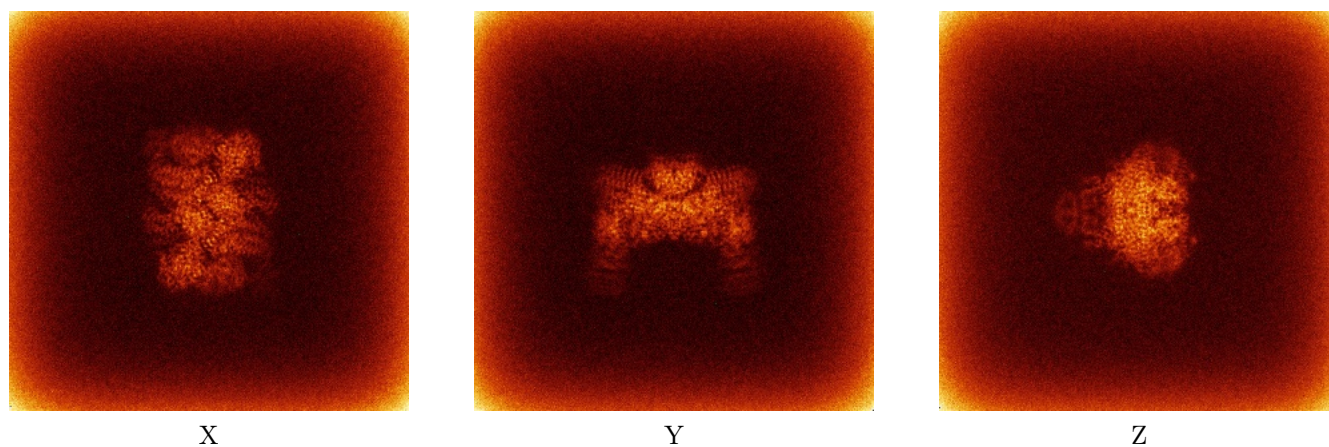
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



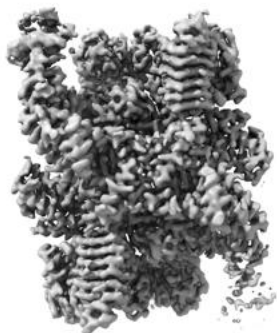
### 6.4.2 Raw map



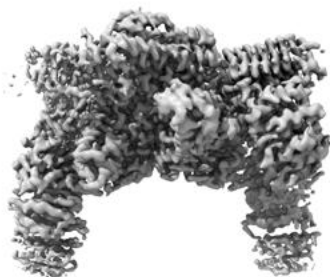
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

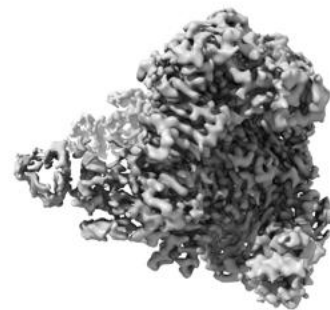
### 6.5.1 Primary map



X



Y



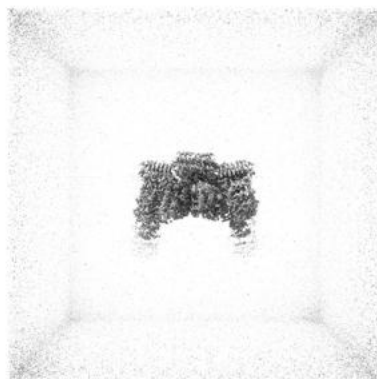
Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

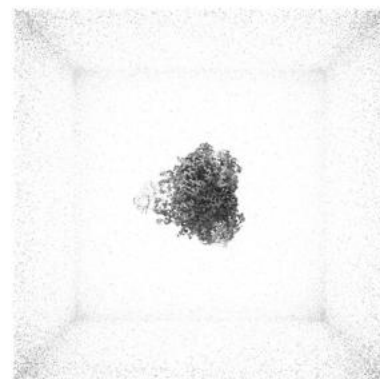
### 6.5.2 Raw map



X



Y



Z

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

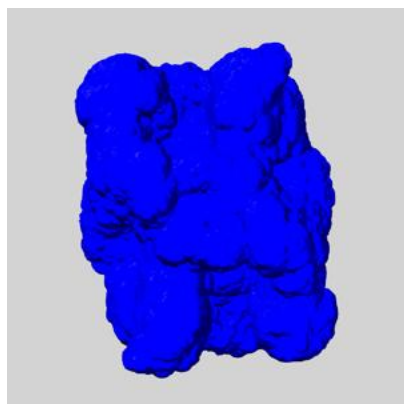
## 6.6 Mask visualisation [i](#)

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

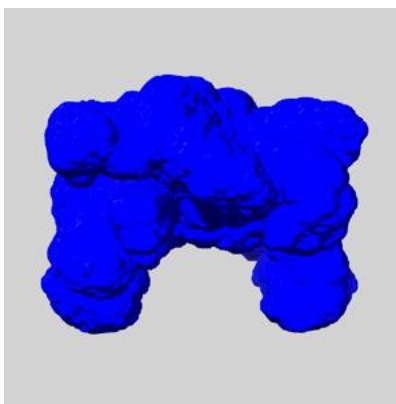
A mask typically either:

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

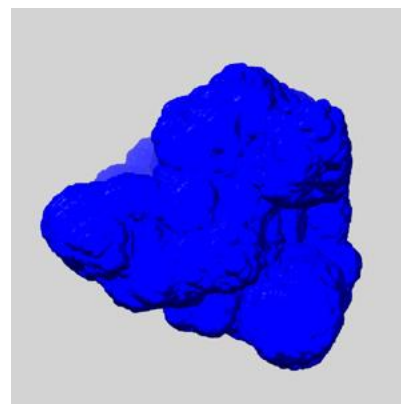
### 6.6.1 emd\_72520\_msk\_1.map [i](#)



X



Y

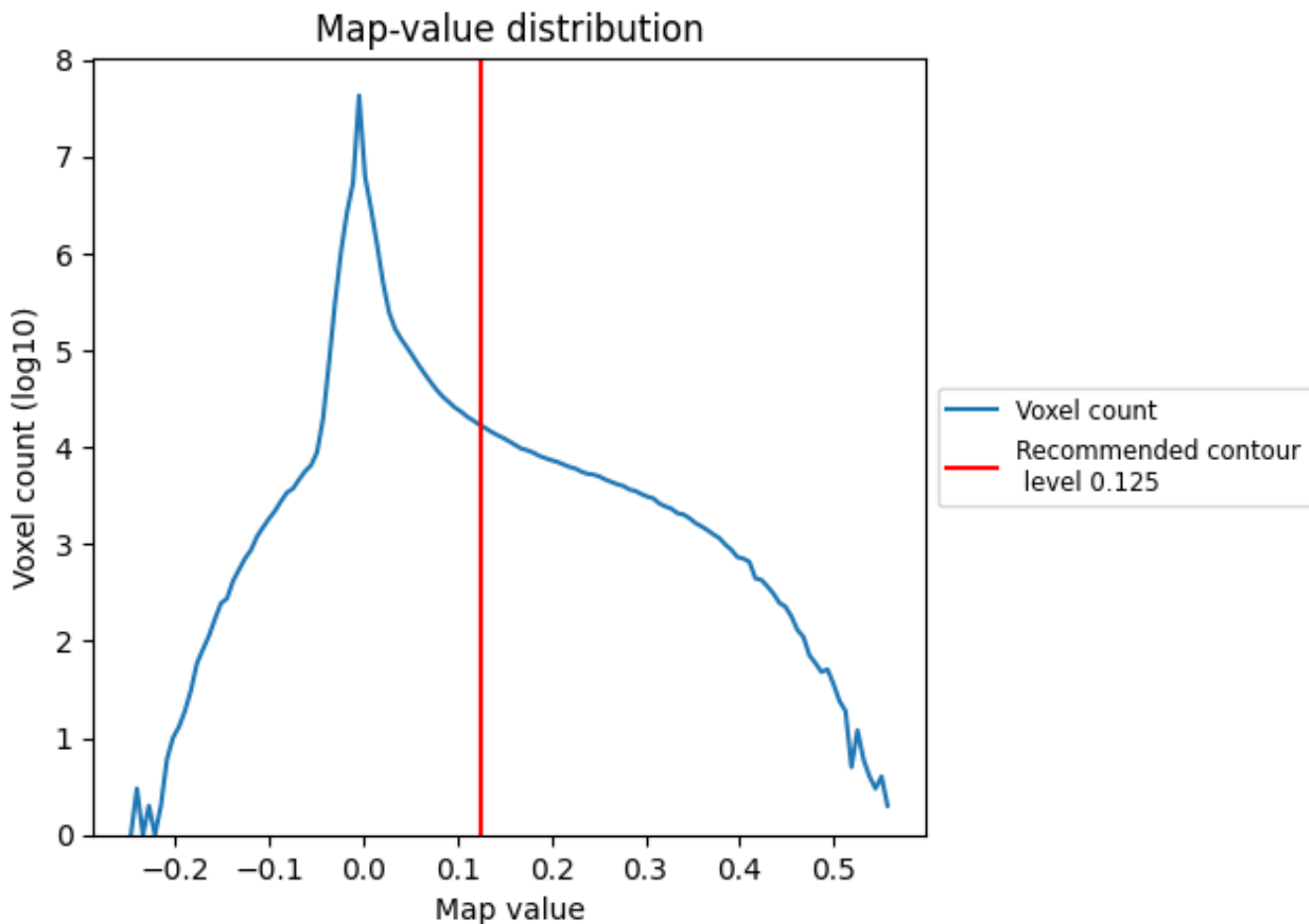


Z

## 7 Map analysis [i](#)

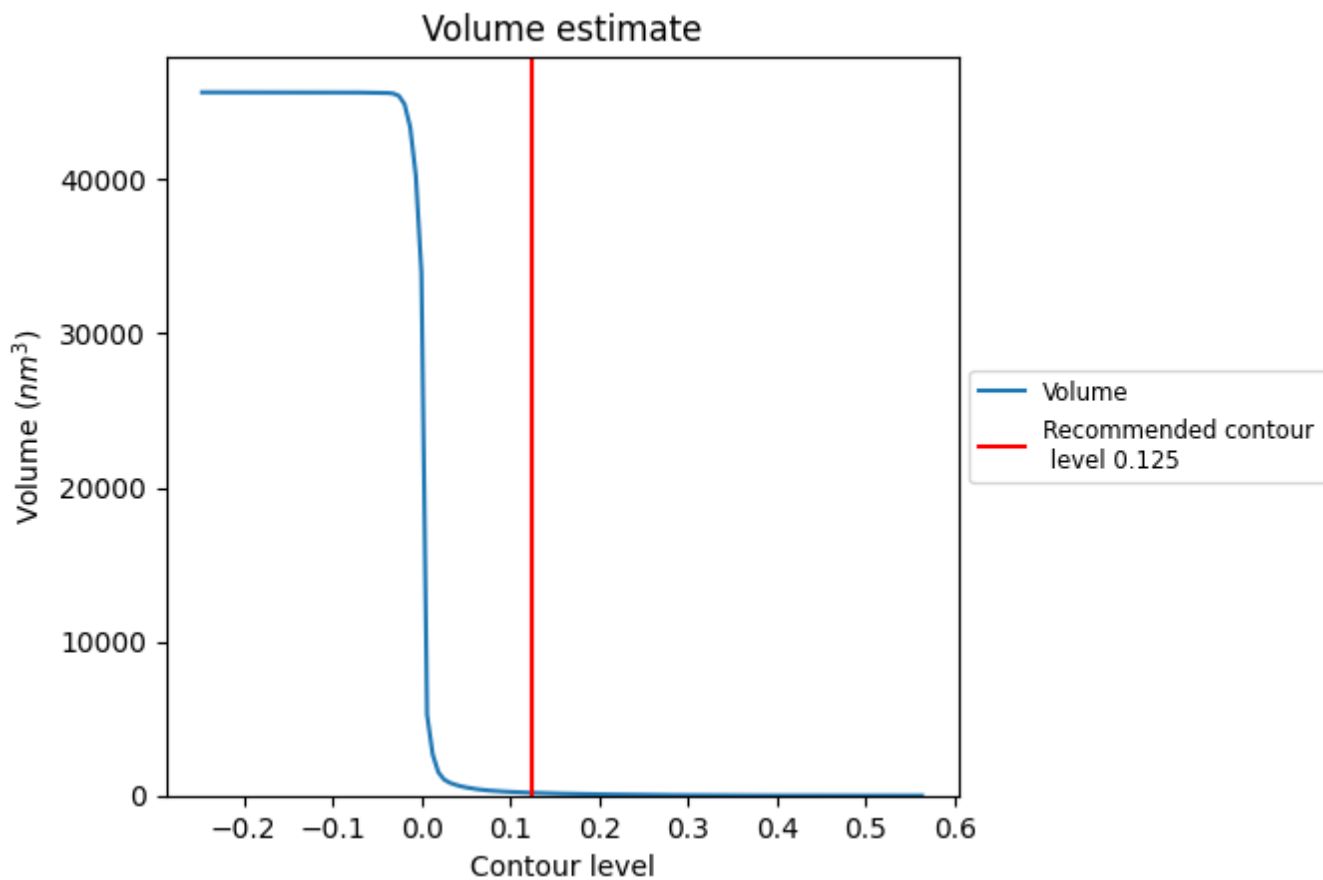
This section contains the results of statistical analysis of the map.

### 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.

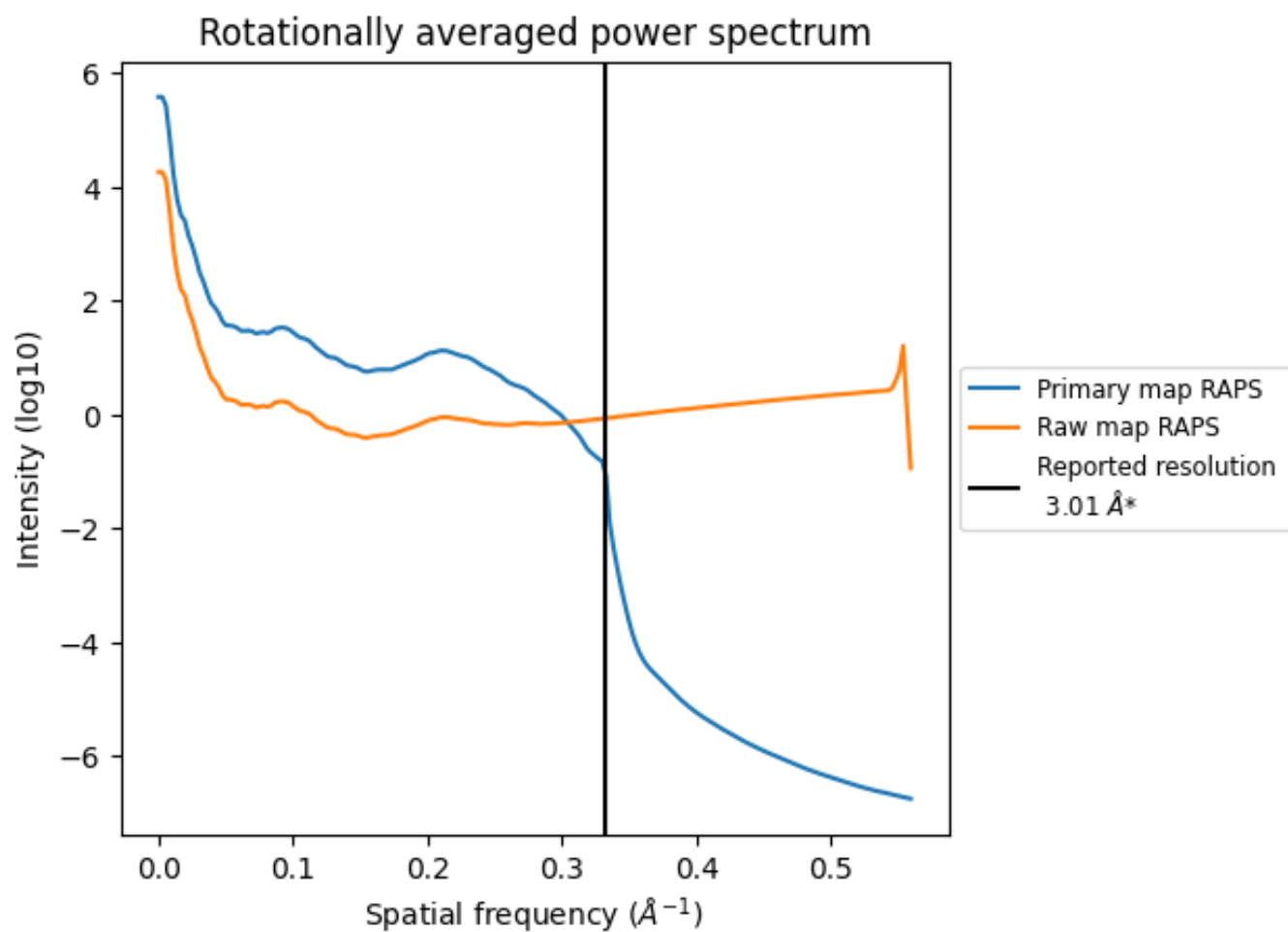
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 177 nm<sup>3</sup>; this corresponds to an approximate mass of 160 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

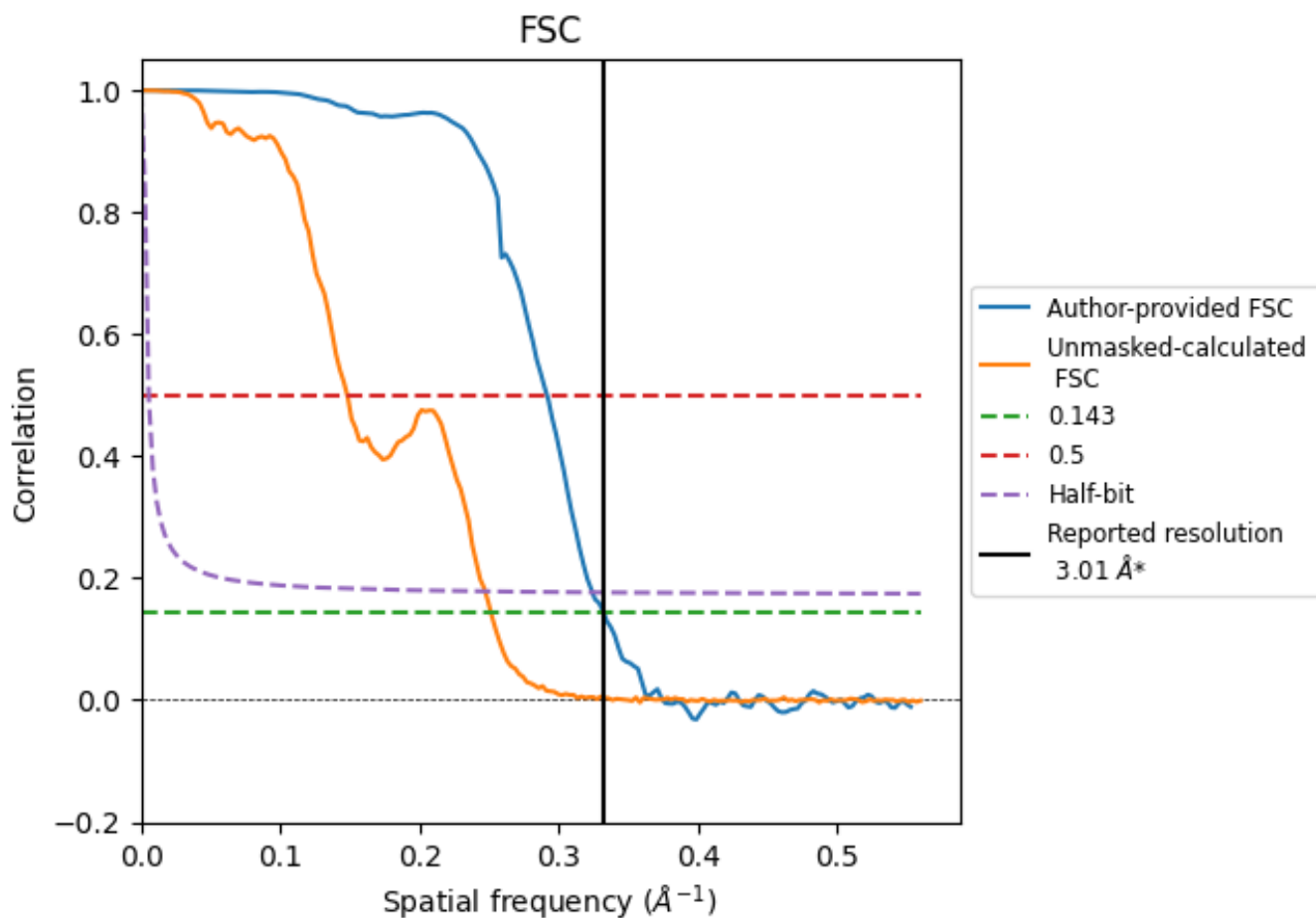


\*Reported resolution corresponds to spatial frequency of 0.332 Å<sup>-1</sup>

## 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 0.332 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

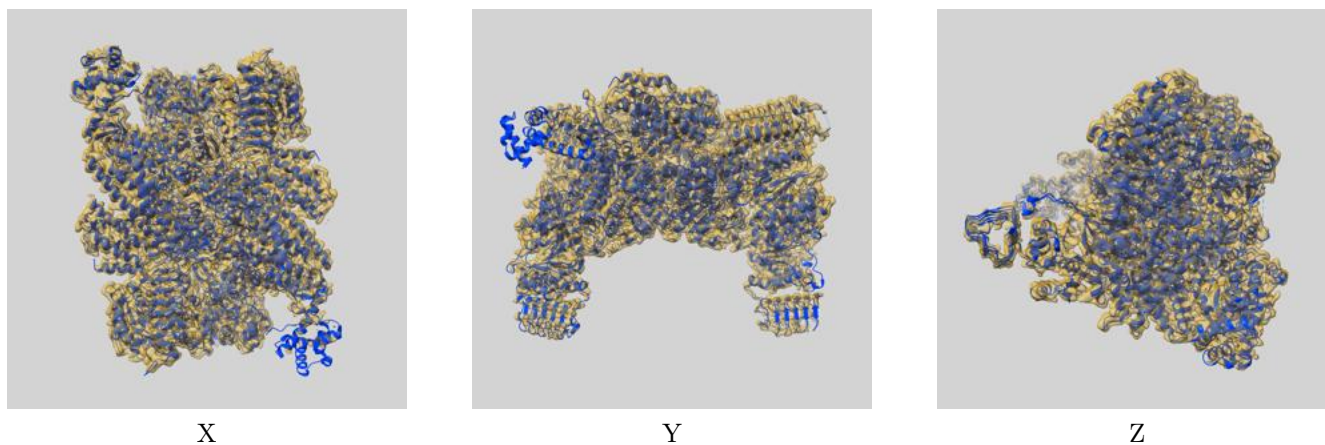
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.43	3.09
Unmasked-calculated*	3.98	6.76	4.05

\*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 3.98 differs from the reported value 3.01 by more than 10 %

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

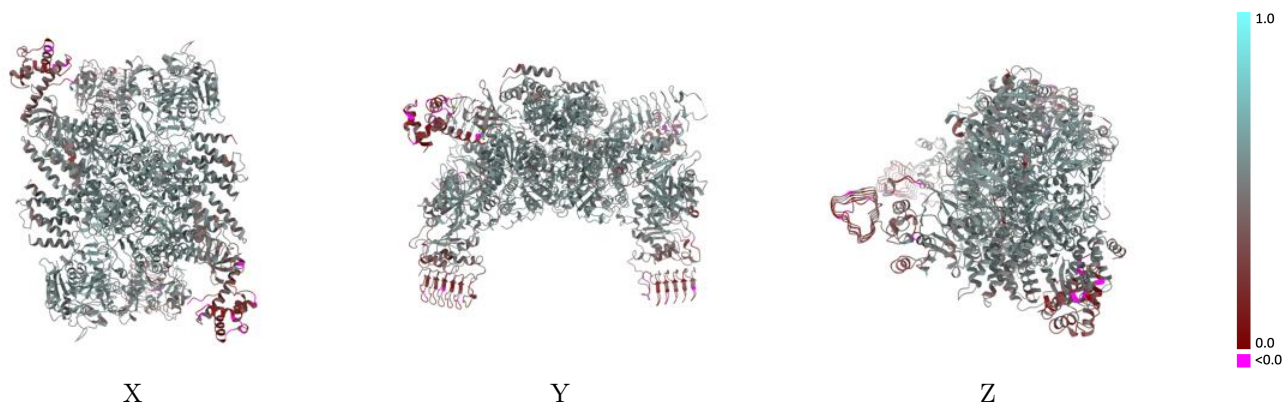
This section contains information regarding the fit between EMDB map EMD-72520 and PDB model 9Y5R. Per-residue inclusion information can be found in section 3 on page 9.

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



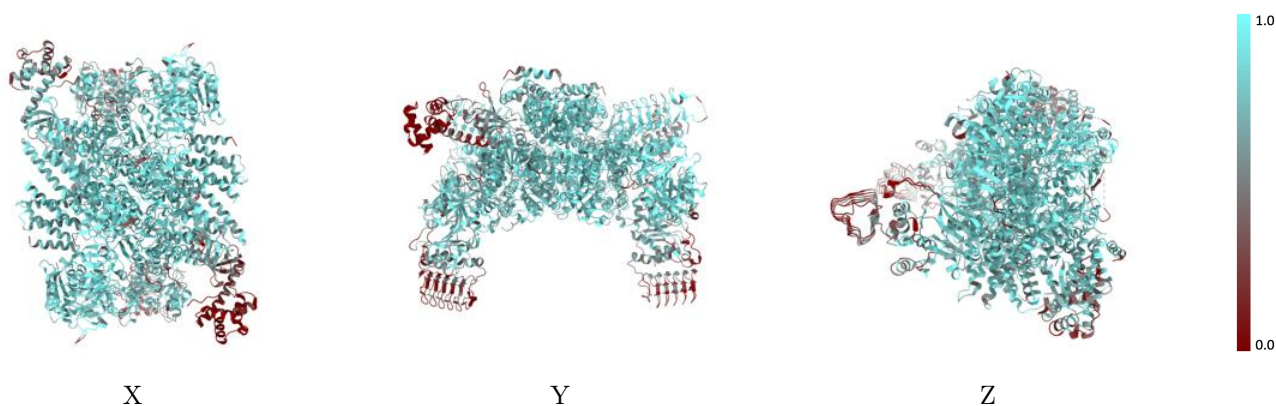
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



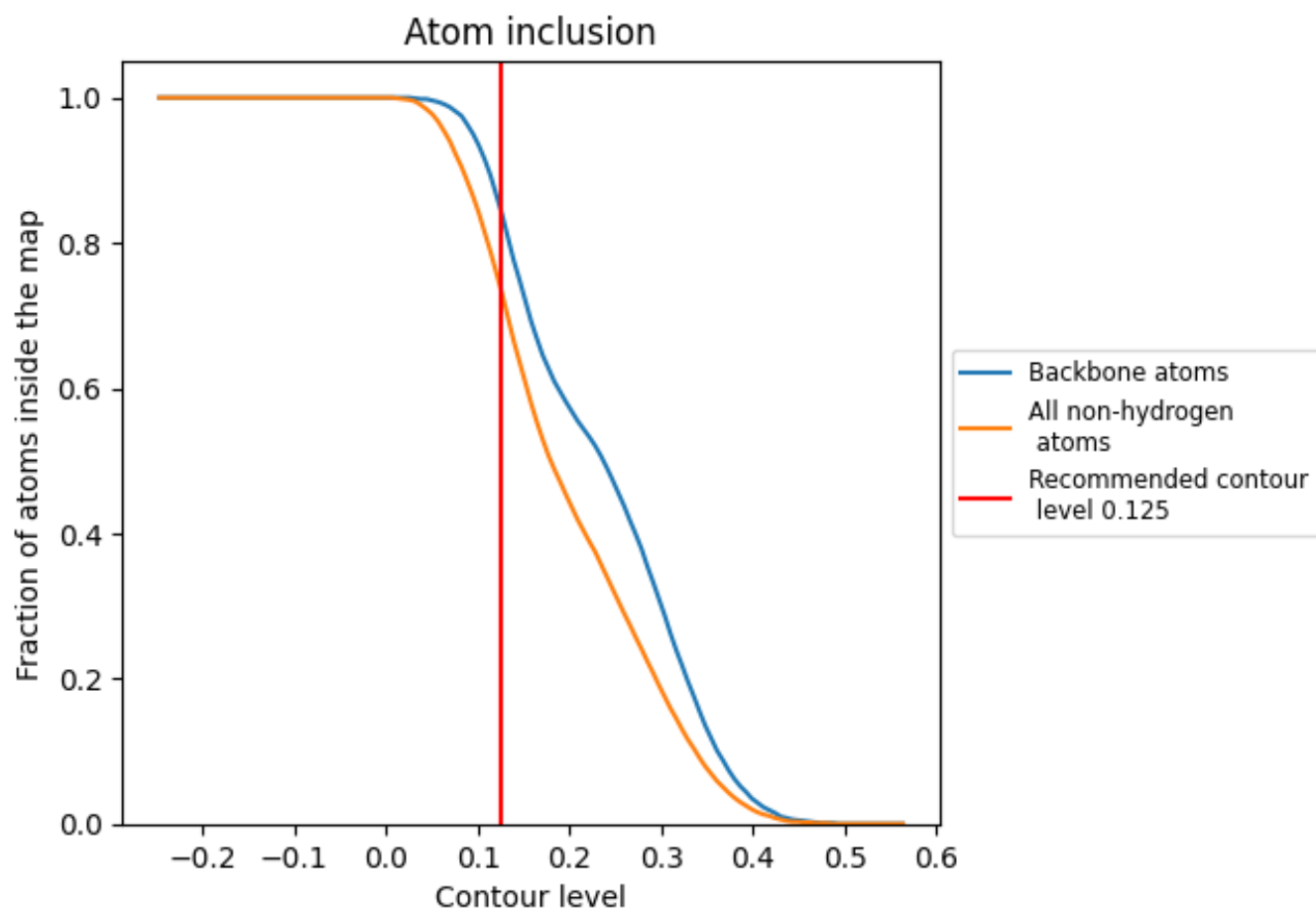
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.4890
A	 0.8330	 0.5340
B	 0.8430	 0.5330
C	 0.8490	 0.5310
D	 0.8420	 0.5290
E	 0.8450	 0.5450
F	 0.8440	 0.5440
G	 0.8050	 0.5240
H	 0.8260	 0.5280
I	 0.5340	 0.4030
J	 0.5580	 0.4080
L	 0.5950	 0.3700
M	 0.2460	 0.3060

