



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 05:08 PM UTC

PDB ID : 3JBY / pdb_00003jby
EMDB ID : EMD-6488
Title : Cryo-electron microscopy structure of RAG Paired Complex (C2 symmetry)
Authors : Ru, H.; Chambers, M.G.; Fu, T.-M.; Tong, A.B.; Liao, M.; Wu, H.
Deposited on : 2015-10-22
Resolution : 3.70 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.dev132
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) : 2.49

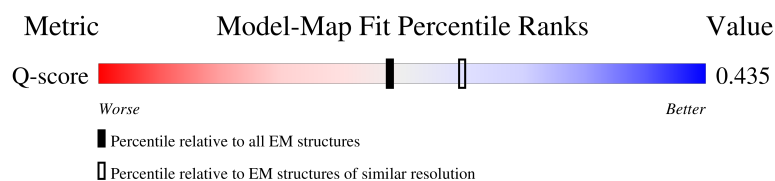
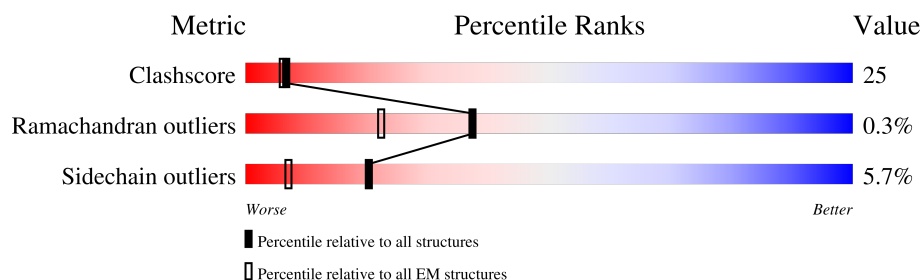
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



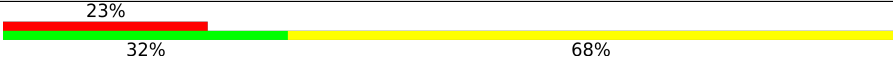
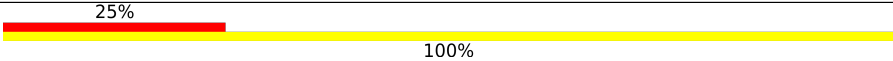
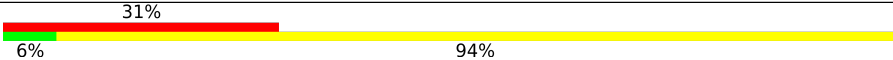
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	764	 7% 40% 30% • 28%
1	C	764	 8% 40% 30% • 28%
2	B	533	 12% 32% 32% • 34%
2	D	533	 13% 32% 33% • 34%

Continued on next page...

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Mol	Chain	Length	Quality of chain
3	E	15	
3	H	15	
4	F	31	
4	G	31	
5	I	16	
5	J	16	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16846 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	550	Total	C	N	O	S	0	0
			4435	2781	786	834	34		
1	C	550	Total	C	N	O	S	0	0
			4435	2781	786	834	34		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	GLY	-	expression tag	UNP O13033
A	269	GLY	-	expression tag	UNP O13033
A	270	SER	-	expression tag	UNP O13033
C	268	GLY	-	expression tag	UNP O13033
C	269	GLY	-	expression tag	UNP O13033
C	270	SER	-	expression tag	UNP O13033

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called 5'-D(P*CP*AP*CP*AP*GP*TP*GP*CP*TP*AP*CP*AP*GP*AP*C)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	15	Total	C	N	O	P	0	0
			306	145	59	87	15		
3	H	15	Total	C	N	O	P	0	0
			306	145	59	87	15		

- Molecule 4 is a DNA chain called RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	31	Total	C	N	O	P	0	0
			639	303	120	185	31		
4	G	31	Total	C	N	O	P	0	0
			639	303	120	185	31		

- Molecule 5 is a DNA chain called 'D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*T
P*CP*TP*TP*A)-3'.

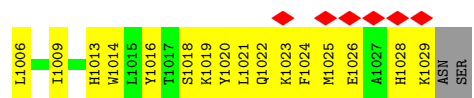
Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	16	Total	C	N	O	P	0	0
			326	156	54	100	16		
5	J	16	Total	C	N	O	P	0	0
			326	156	54	100	16		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

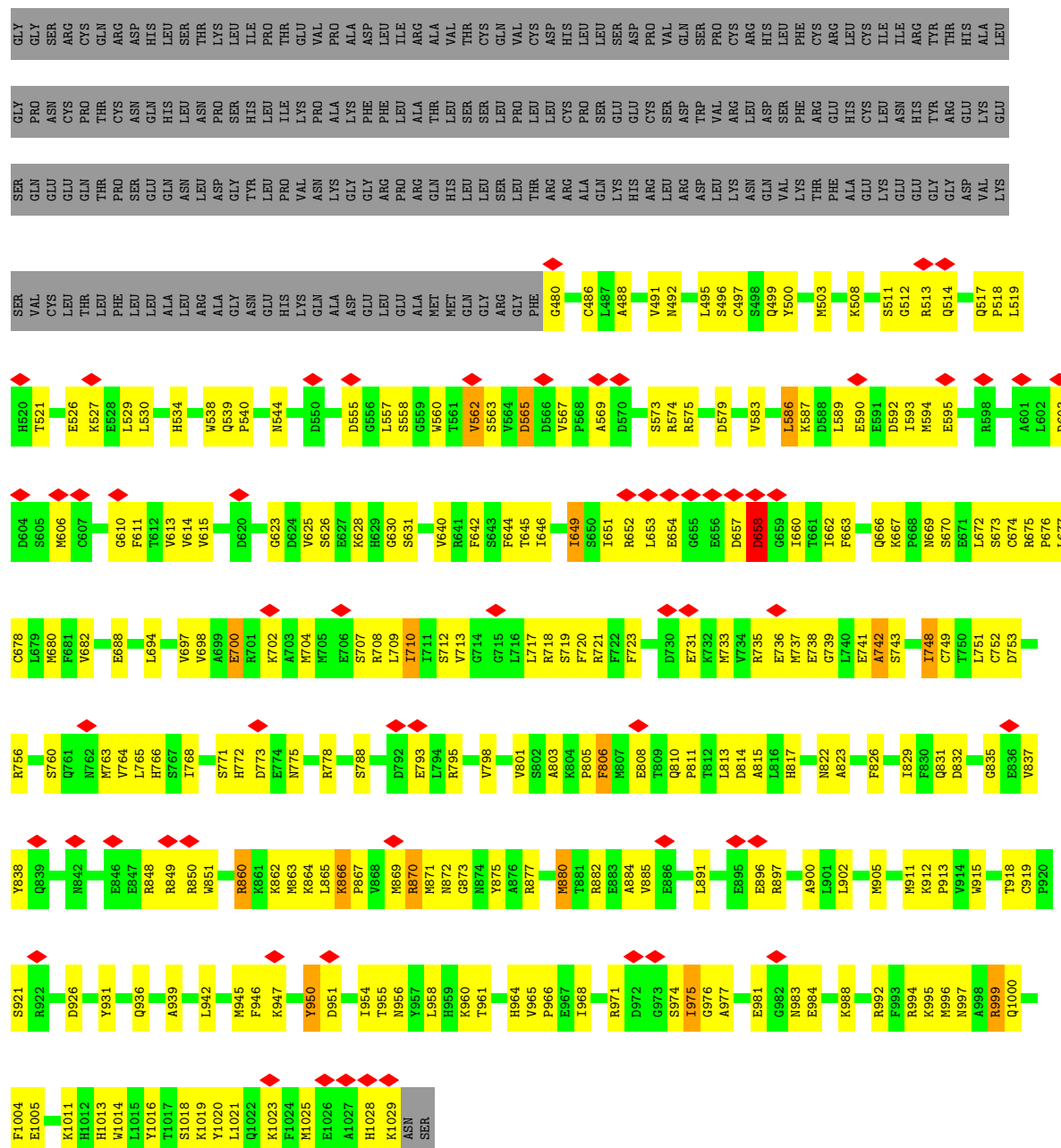
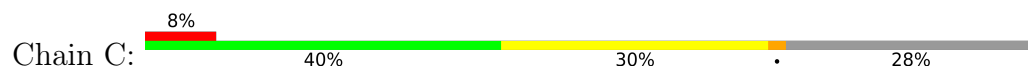
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Ca	0
			2	2	
7	C	2	Total	Ca	0
			2	2	

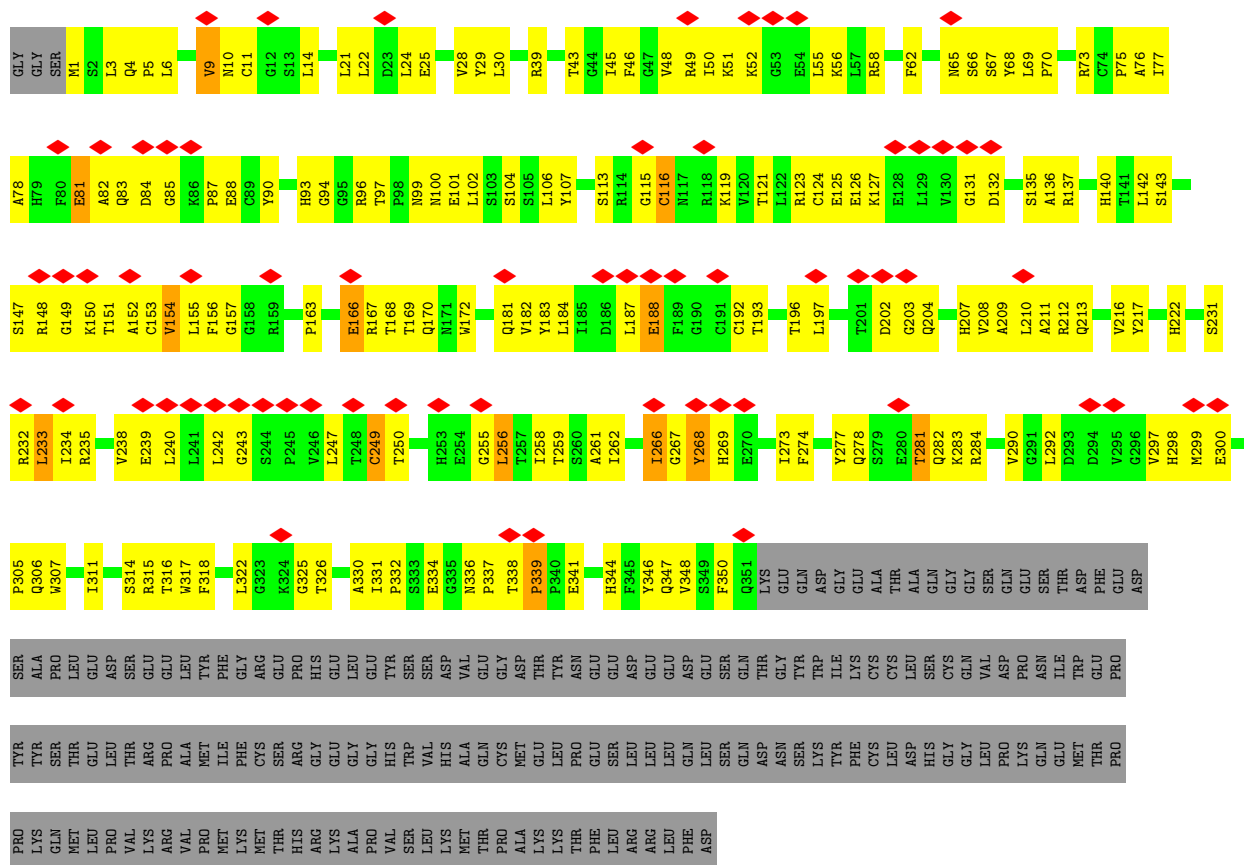


• Molecule 1: V(D)J recombination-activating protein 1

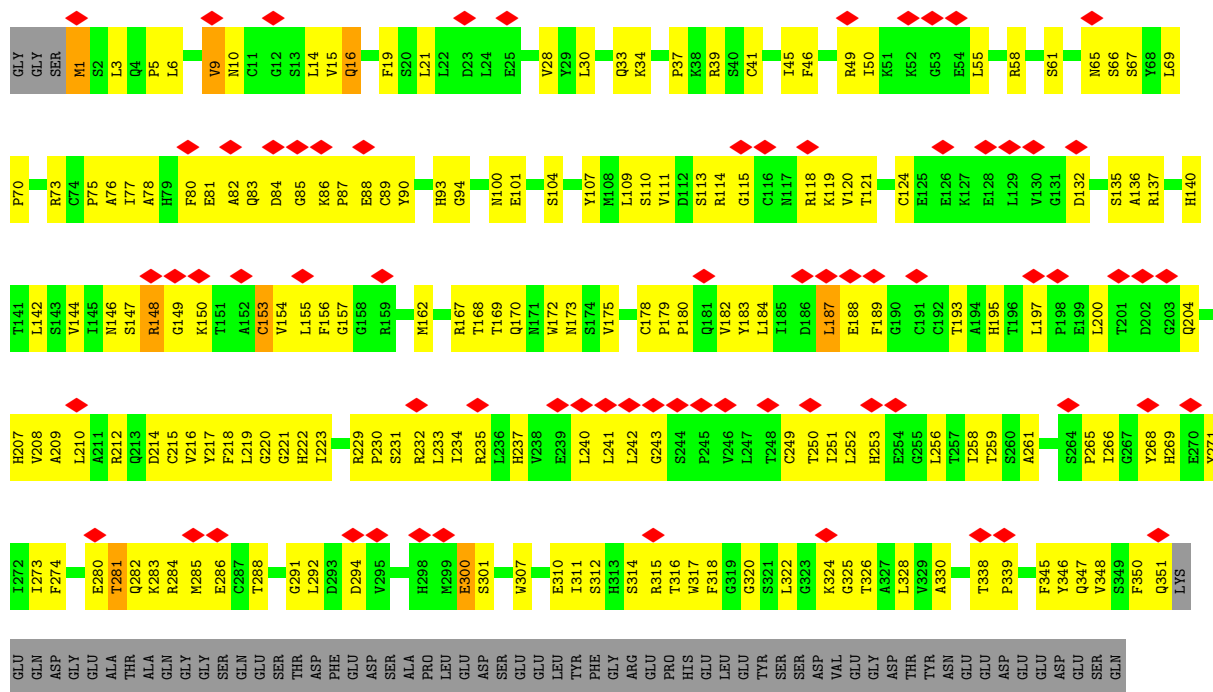


• Molecule 2: V(D)J recombination-activating protein 2



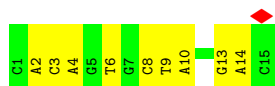


• Molecule 2: V(D)J recombination-activating protein 2

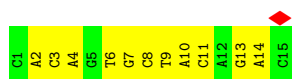


THR	GLY	TYR	TRP	LYS	ILE	LYS	CYS	CYS	LEU	LEU	SER	GLN	VAL	ASP	PRO	ASN	GLN	ILE	TRP	GLU	PRO	TYR	LYS	SER	THR	GLU	LEU	LEU	ARG	PRO	ALA	MET	ILE	PHE	CYS	THR	SER	ARG	GLY	GLU	GLY	GLY	HIS	TRP	VAL	THR	HIS	ALA	GLN	CYS	PRO	MET	GLY	LEU	PRO	THR	PHE	ARG	LEU	LEU	GLN	SER	GLN
ASP	ASN	SER	LYS	TYR	PHE	CYS	CYS	ASP	HIS	LEU	GLY	GLY	LEU	PRO	GLN	GLN	GLU	MET	TRP	THR	PRO	PRO	LYS	LYS	GLN	MET	LEU	PRO	VAL	LYS	ARG	VAL	PRO	MET	LYS	PHE	THR	SER	HIS	ARG	LYS	ALA	PRO	VAL	SER	LEU	LYS	MET	THR	PRO	ALA	GLY	VAL	SER	LEU	LEU	ARG	LEU	ARG	PHE	ASP		

- Molecule 3: 5'-D(P*CP*AP*CP*AP*GP*TP*GP*CP*TP*AP*CP*AP*GP*AP*C)-3'



- Molecule 3: 5'-D(P*CP*AP*CP*AP*GP*TP*GP*CP*TP*AP*CP*AP*GP*AP*C)-3'



- Molecule 4: RSS intermediate reverse strand



- Molecule 4: RSS intermediate reverse strand



- Molecule 5: '-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',



- Molecule 5: '-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	40607	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.086	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	236.16, 236.16, 236.16	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.23, 1.23, 1.23	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.73	1/4526 (0.0%)	0.96	6/6095 (0.1%)
1	C	0.73	0/4526	0.94	3/6095 (0.0%)
2	B	0.65	1/2784 (0.0%)	0.86	3/3784 (0.1%)
2	D	0.63	1/2784 (0.0%)	0.87	4/3784 (0.1%)
3	E	0.84	0/343	0.74	0/526
3	H	0.87	0/343	0.76	0/526
4	F	0.71	1/717 (0.1%)	0.70	0/1105
4	G	0.72	0/717	0.71	0/1105
5	I	0.70	0/363	0.80	0/558
5	J	0.67	0/363	0.91	0/558
All	All	0.70	4/17466 (0.0%)	0.89	16/24136 (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	2
1	C	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	339	PRO	CA-C	6.34	1.58	1.52
4	F	15	DG	C1'-N9	-5.89	1.34	1.46
2	B	339	PRO	CA-C	5.45	1.57	1.52
1	A	985	SER	C-N	5.32	1.40	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	339	PRO	N-CA-C	9.16	121.88	110.70
1	A	999	ARG	N-CA-C	8.52	120.34	111.14
2	D	338	THR	CA-C-N	8.23	128.86	120.38
2	D	338	THR	C-N-CA	8.23	128.86	120.38
2	B	339	PRO	N-CA-C	7.79	120.21	110.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1004	PHE	Peptide
1	A	658	ASP	Peptide
1	C	658	ASP	Peptide
1	C	742	ALA	Peptide

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	A	4435	0	4378	203	0
1	C	4435	0	4378	215	0
2	B	2714	0	2665	155	0
2	D	2714	0	2665	148	0
3	E	306	0	168	13	0
3	H	306	0	168	17	0
4	F	639	0	349	31	0
4	G	639	0	349	33	0
5	I	326	0	182	25	0
5	J	326	0	182	30	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	0	0
7	C	2	0	0	0	0
All	All	16846	0	15484	795	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 25.

The worst 5 of 795 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:B:140:HIS:HD2	2:B:155:LEU:HD11	1.19	1.07
2:D:140:HIS:HD2	2:D:155:LEU:HD11	1.23	1.00
2:B:82:ALA:HA	2:B:87:PRO:HB3	1.48	0.94
1:C:866:LYS:HD2	1:C:867:PRO:HD2	1.47	0.94
1:C:749:CYS:SG	1:C:964:HIS:NE2	2.41	0.93

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	548/764 (72%)	523 (95%)	24 (4%)	1 (0%)	43	72
1	C	548/764 (72%)	520 (95%)	28 (5%)	0	100	100
2	B	349/533 (66%)	335 (96%)	12 (3%)	2 (1%)	21	52
2	D	349/533 (66%)	335 (96%)	12 (3%)	2 (1%)	21	52
All	All	1794/2594 (69%)	1713 (96%)	76 (4%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	268	TYR
2	B	268	TYR
2	D	9	VAL
2	B	9	VAL
1	A	834	ILE

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	489/681 (72%)	462 (94%)	27 (6%)	19	46
1	C	489/681 (72%)	454 (93%)	35 (7%)	13	40
2	B	303/465 (65%)	285 (94%)	18 (6%)	18	44
2	D	303/465 (65%)	292 (96%)	11 (4%)	31	54
All	All	1584/2292 (69%)	1493 (94%)	91 (6%)	20	45

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	658	ASP
1	C	848	ARG
1	C	698	VAL
1	C	748	ILE
1	C	870	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	629	HIS
1	C	810	GLN
2	D	347	GLN
1	C	772	HIS
1	C	822	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](#)

Of 6 ligands modelled in this entry, 6 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.

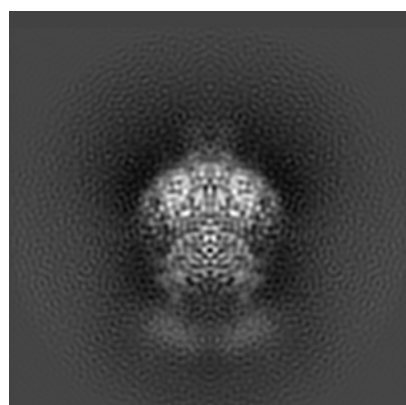
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6488. These allow visual inspection of the internal detail of the map and identification of artifacts.

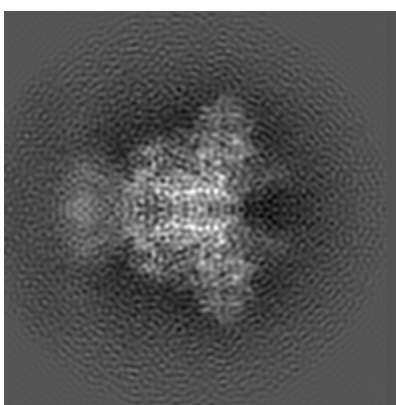
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

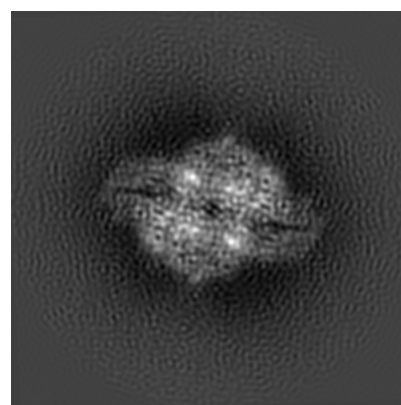
6.1.1 Primary map



X



Y

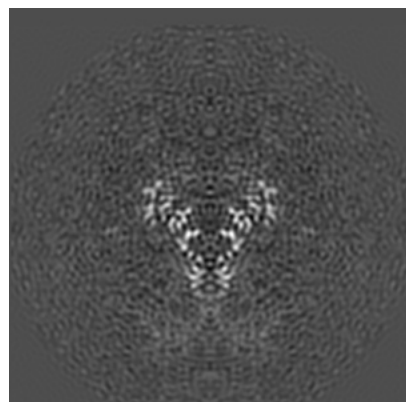


Z

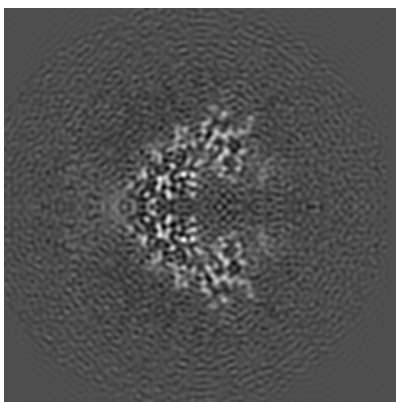
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

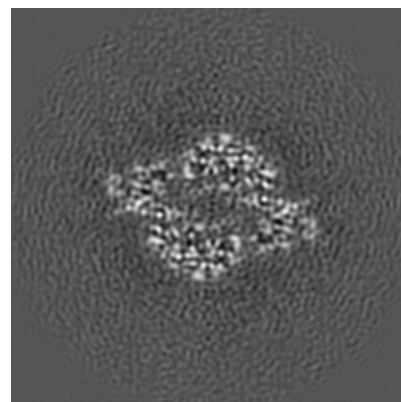
6.2.1 Primary map



X Index: 96



Y Index: 96

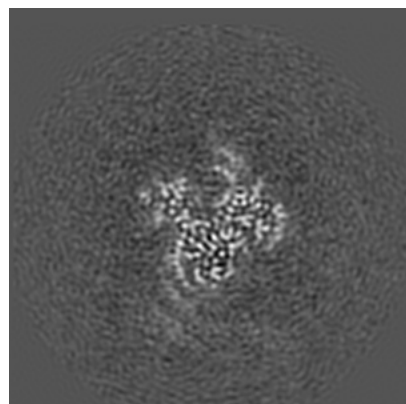


Z Index: 96

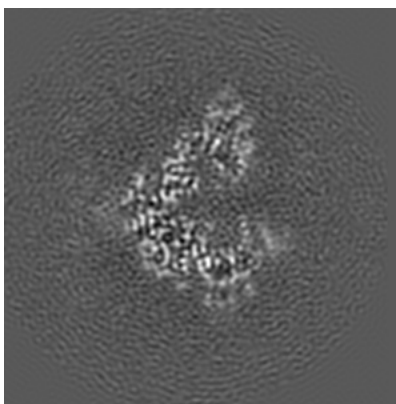
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

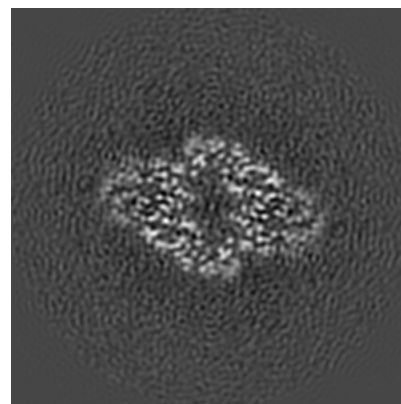
6.3.1 Primary map



X Index: 104



Y Index: 93

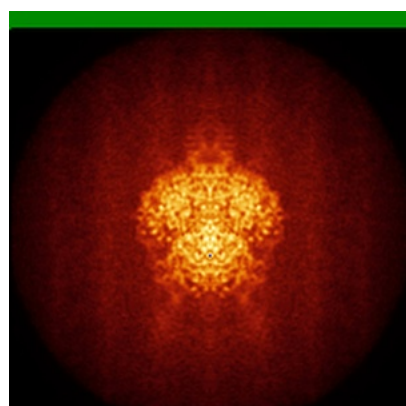


Z Index: 103

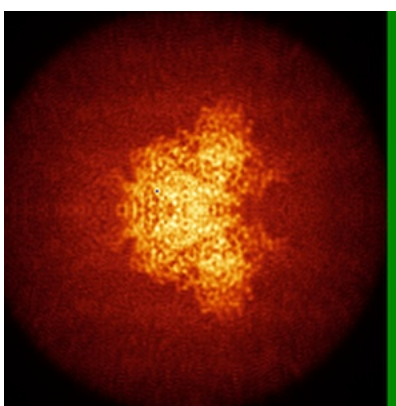
The images above show the largest variance slices of the map in three orthogonal directions.

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

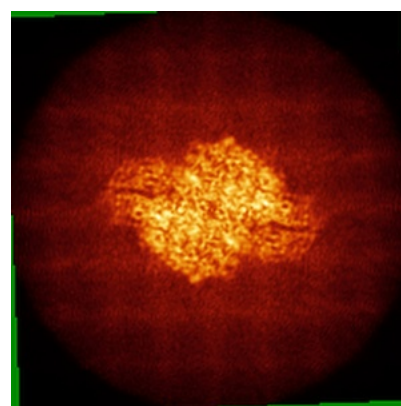
6.4.1 Primary map



X



Y

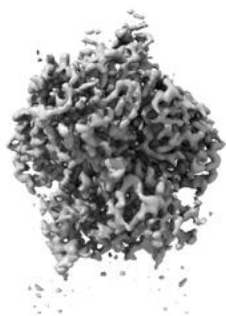


Z

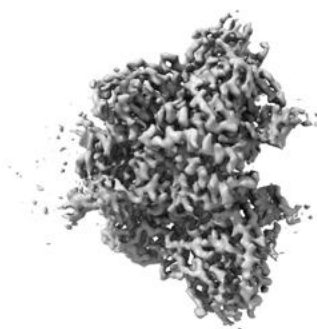
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

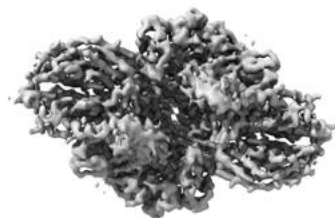
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

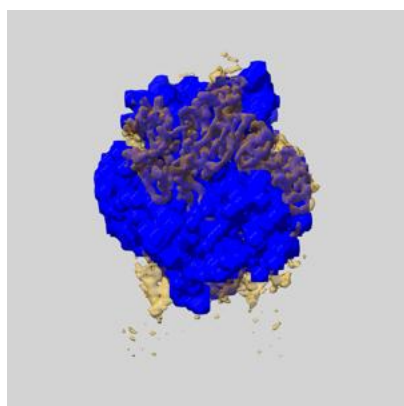
6.6 Mask visualisation [i](#)

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

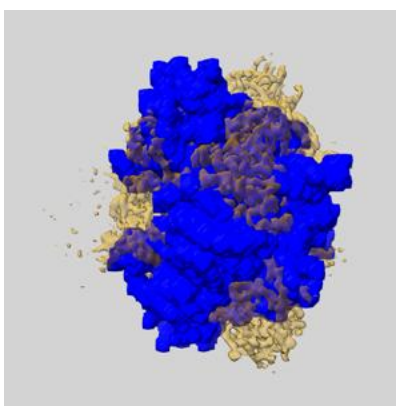
A mask typically either:

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

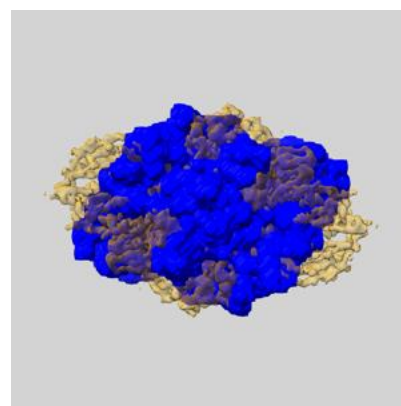
6.6.1 emd_6488_msk_1.map [i](#)



X



Y

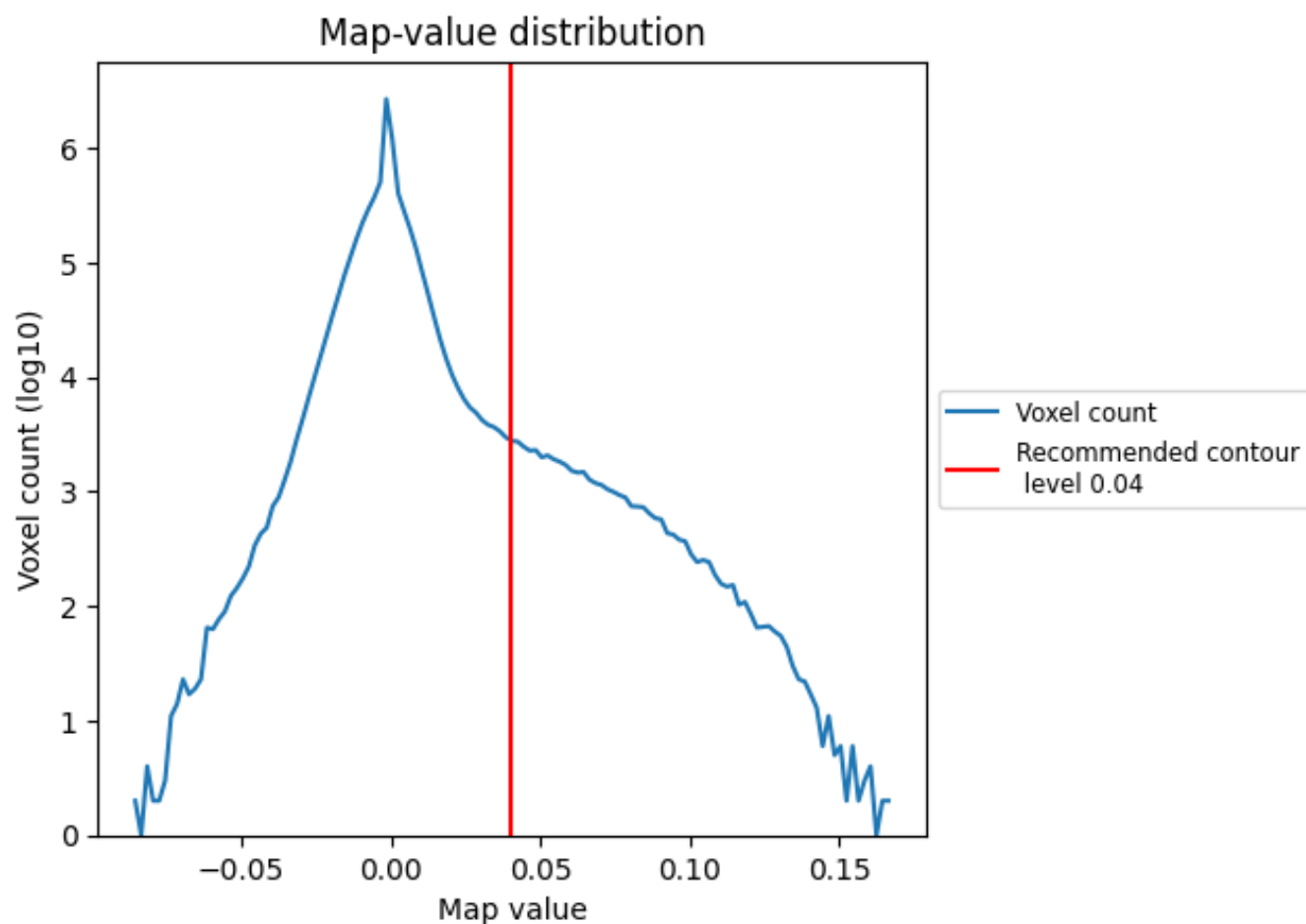


Z

7 Map analysis [i](#)

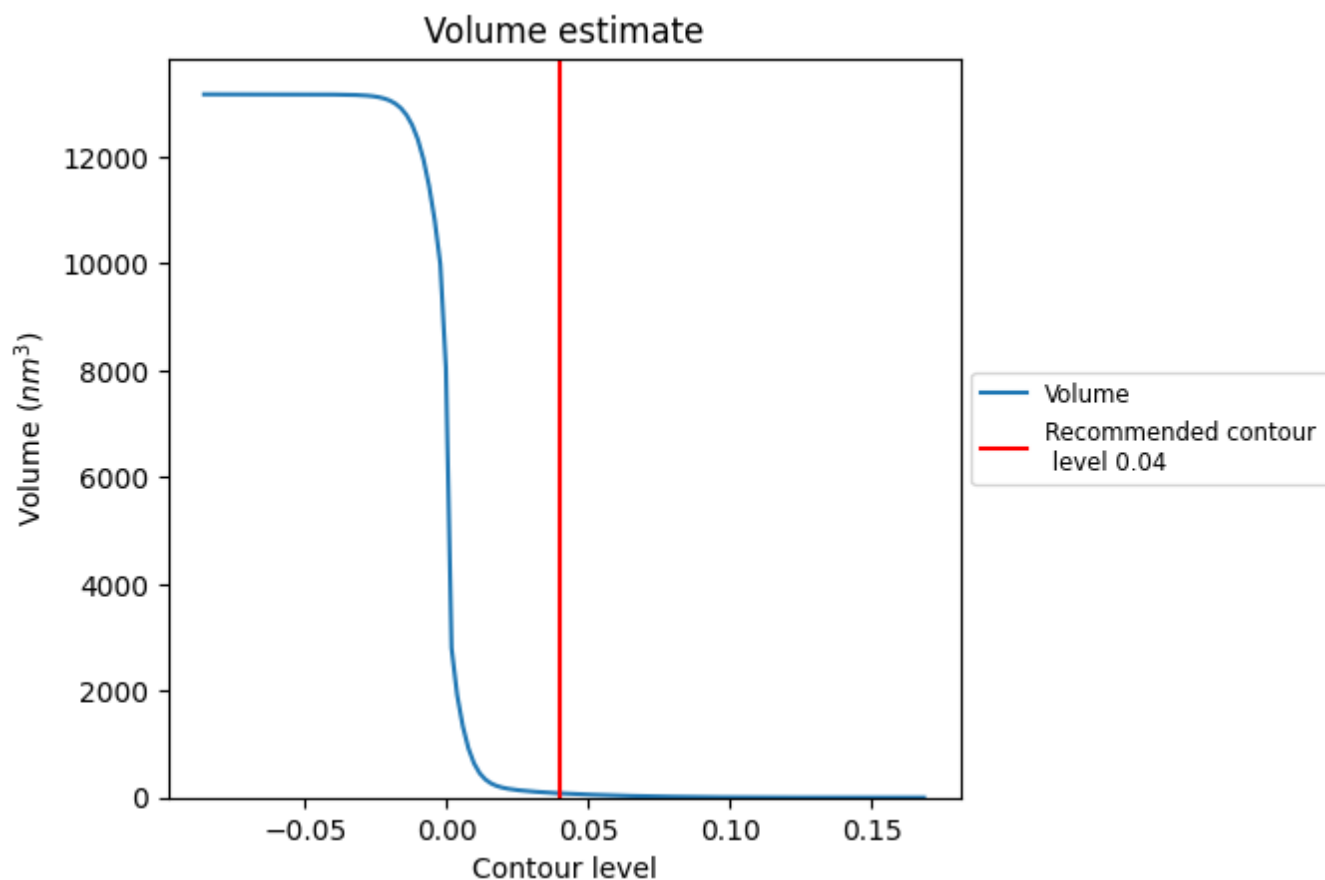
This section contains the results of statistical analysis of the map.

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.

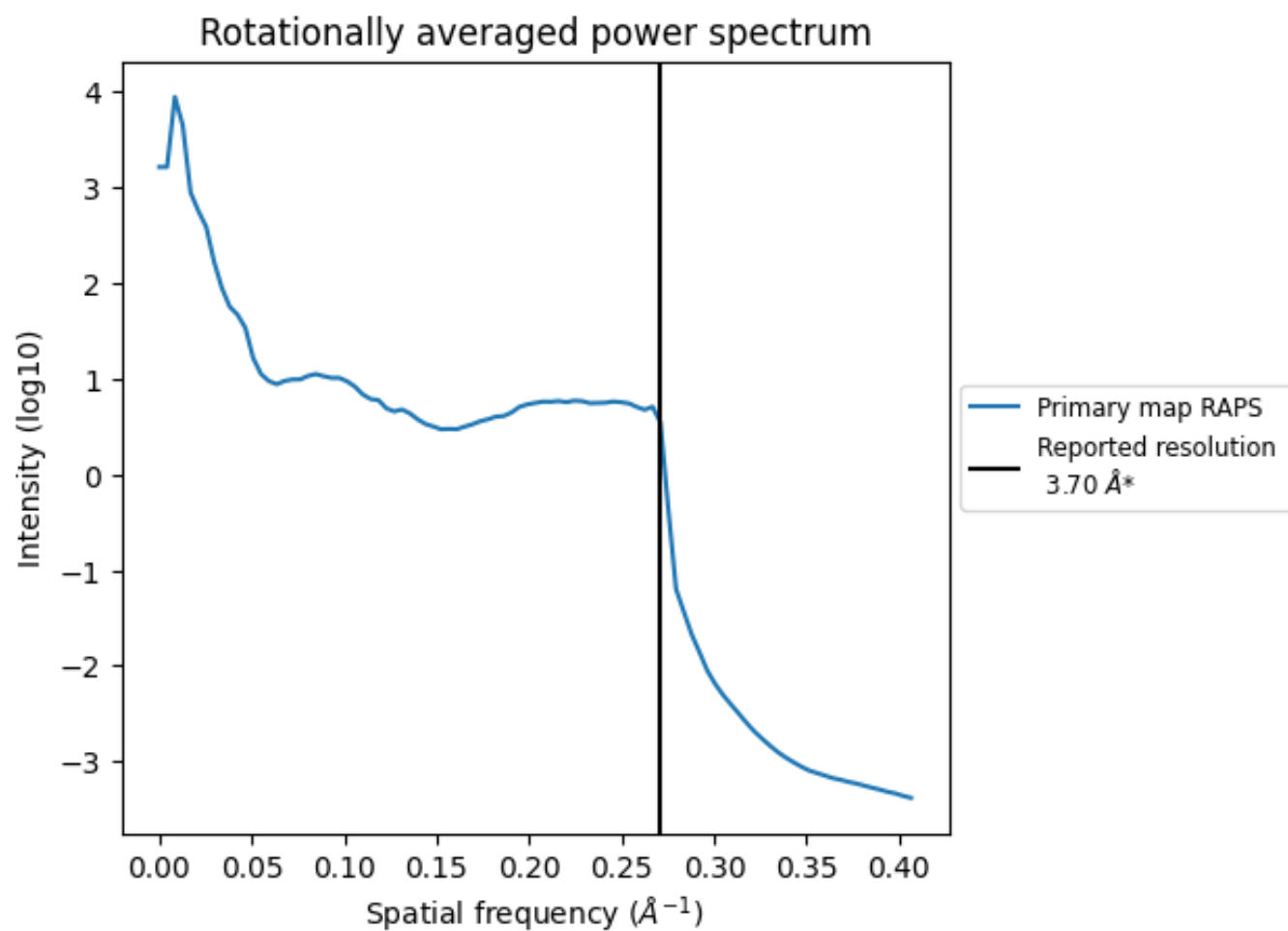
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 72 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 ⓘ

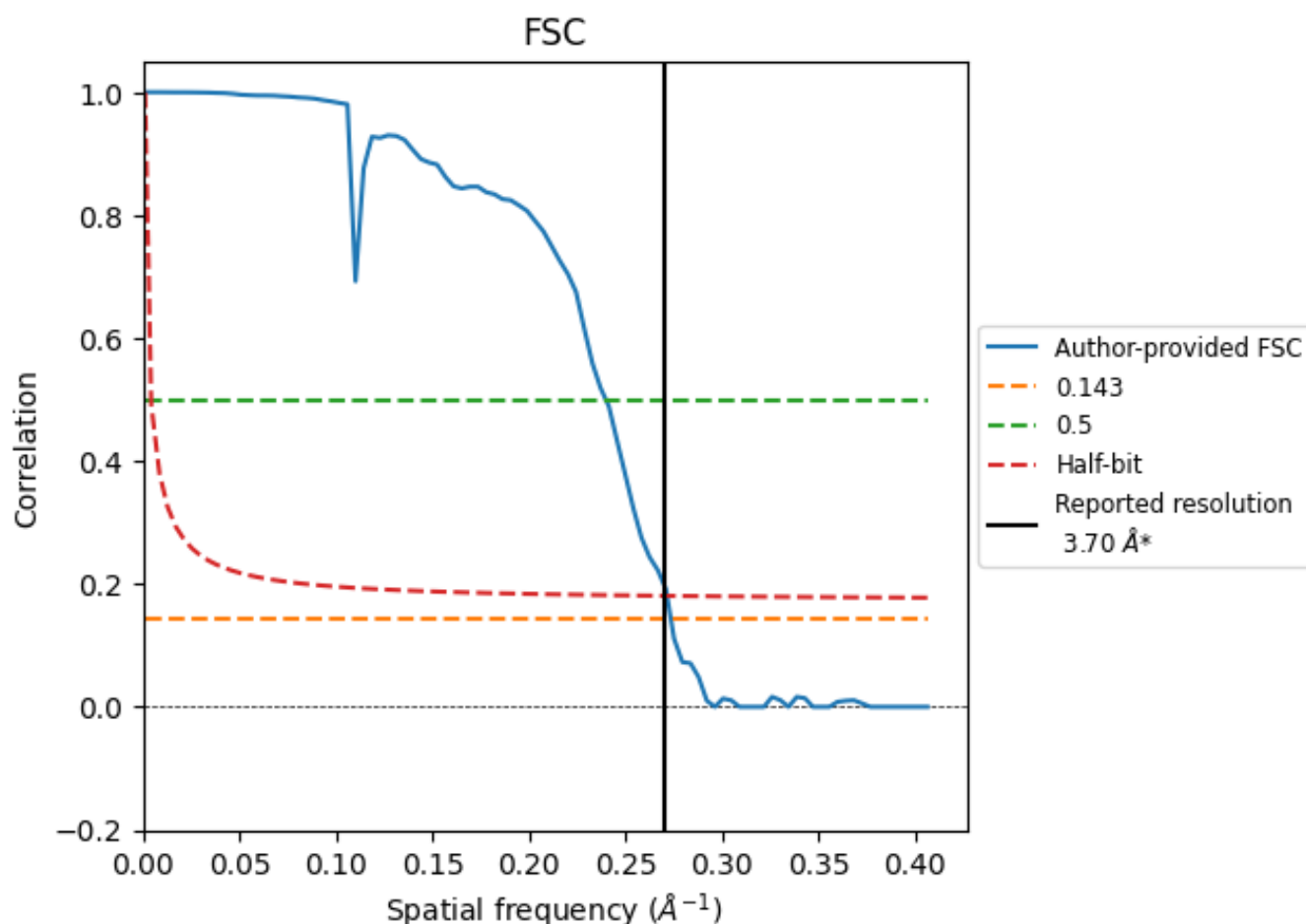


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

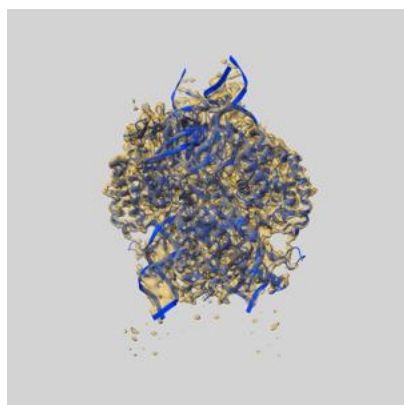
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.66	4.17	3.68
Unmasked-calculated*	-	-	-

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

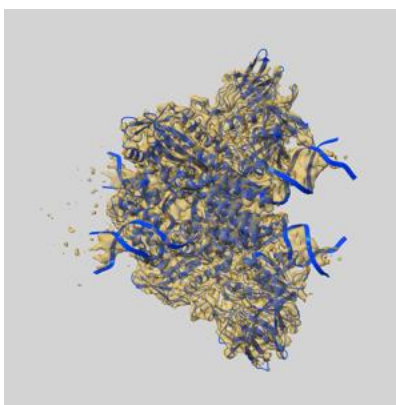
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6488 and PDB model 3JBY. Per-residue inclusion information can be found in section [3](#) on page [6](#).

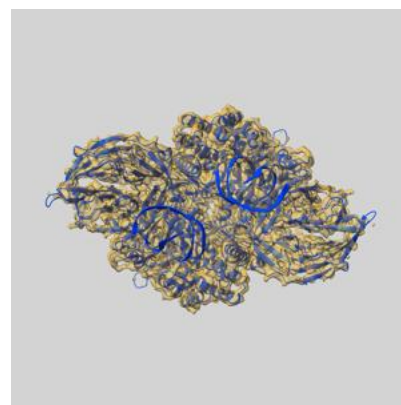
9.1 Map-model overlay [i](#)



X



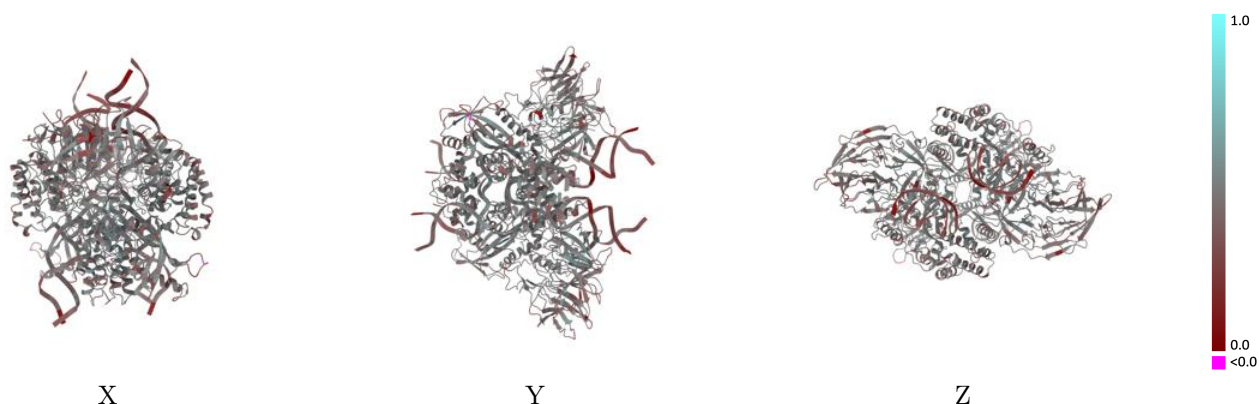
Y



Z

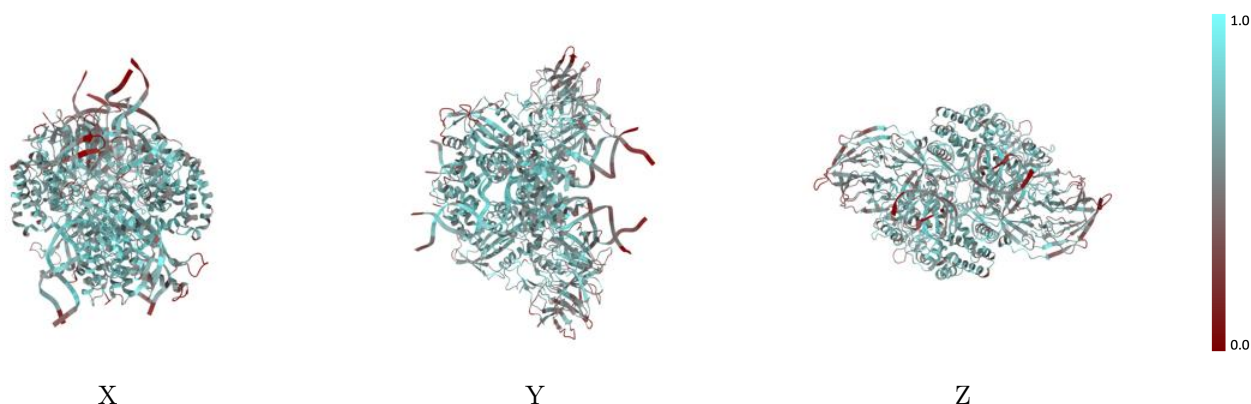
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



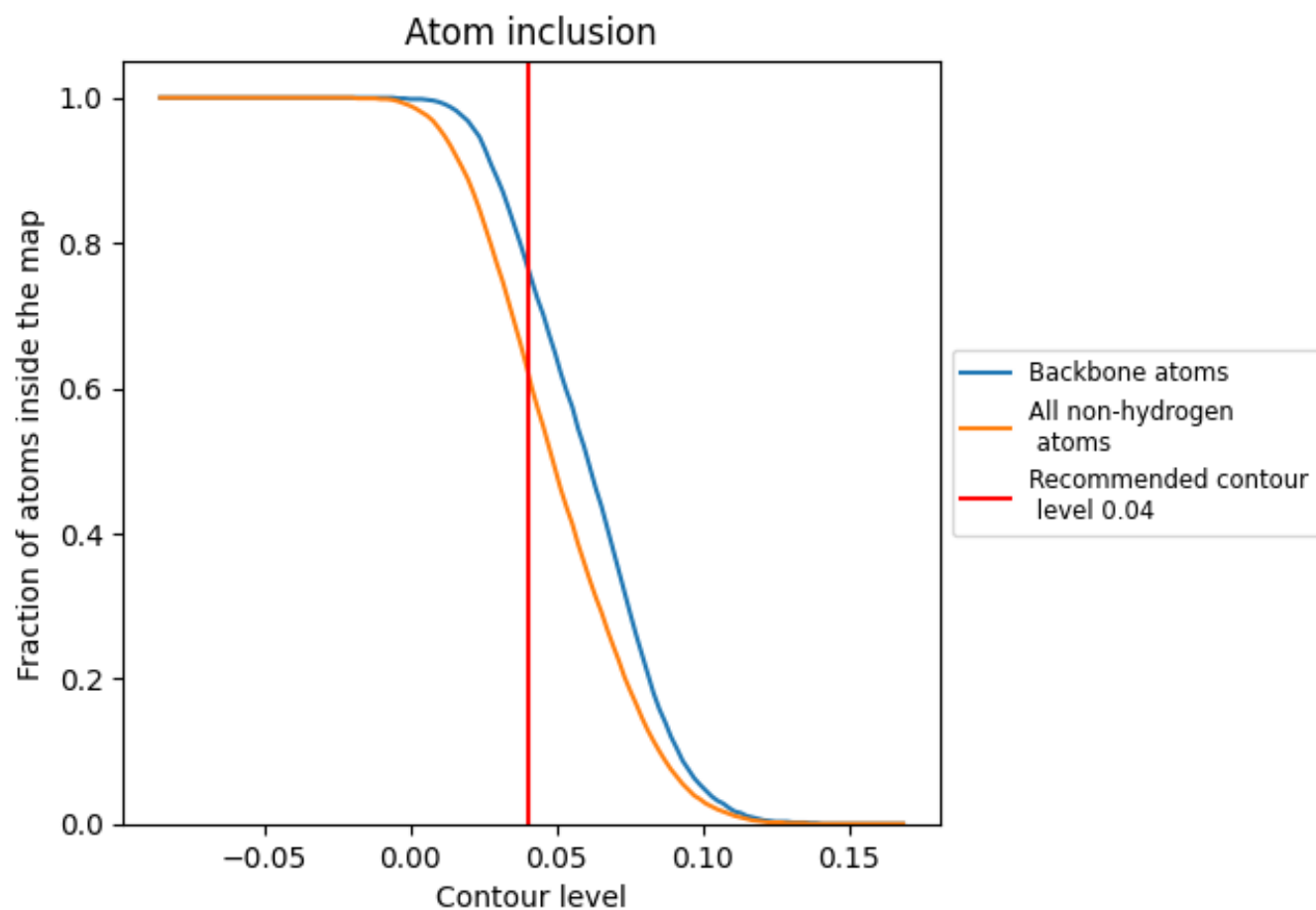
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.4350
A	0.6550	0.4520
B	0.5690	0.4330
C	0.6560	0.4550
D	0.5680	0.4320
E	0.7190	0.4190
F	0.6480	0.3860
G	0.6510	0.3840
H	0.7290	0.4260
I	0.5400	0.3320
J	0.5490	0.3180

1.0

0.0

<0.0