



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:22 PM EST

PDB ID : 3JBY
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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

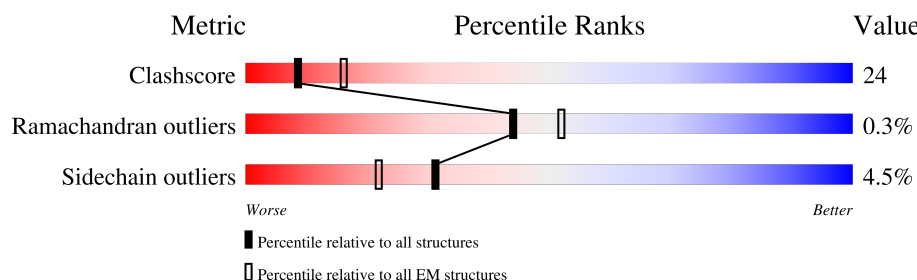
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>7%</div> <div>42%</div> <div>28%</div> <div>•</div> <div>28%</div> </div>
1	C	764	<div> <div>8%</div> <div>42%</div> <div>28%</div> <div>•</div> <div>28%</div> </div>
2	B	533	<div> <div>12%</div> <div>33%</div> <div>32%</div> <div>•</div> <div>34%</div> </div>
2	D	533	<div> <div>13%</div> <div>32%</div> <div>31%</div> <div>•</div> <div>34%</div> </div>
3	E	15	<div> <div>7%</div> <div>27%</div> <div>47%</div> <div>27%</div> </div>
3	H	15	<div> <div>7%</div> <div>13%</div> <div>67%</div> <div>20%</div> </div>
4	F	31	<div> <div>16%</div> <div>42%</div> <div>48%</div> <div>10%</div> </div>
4	G	31	<div> <div>23%</div> <div>29%</div> <div>55%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
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		

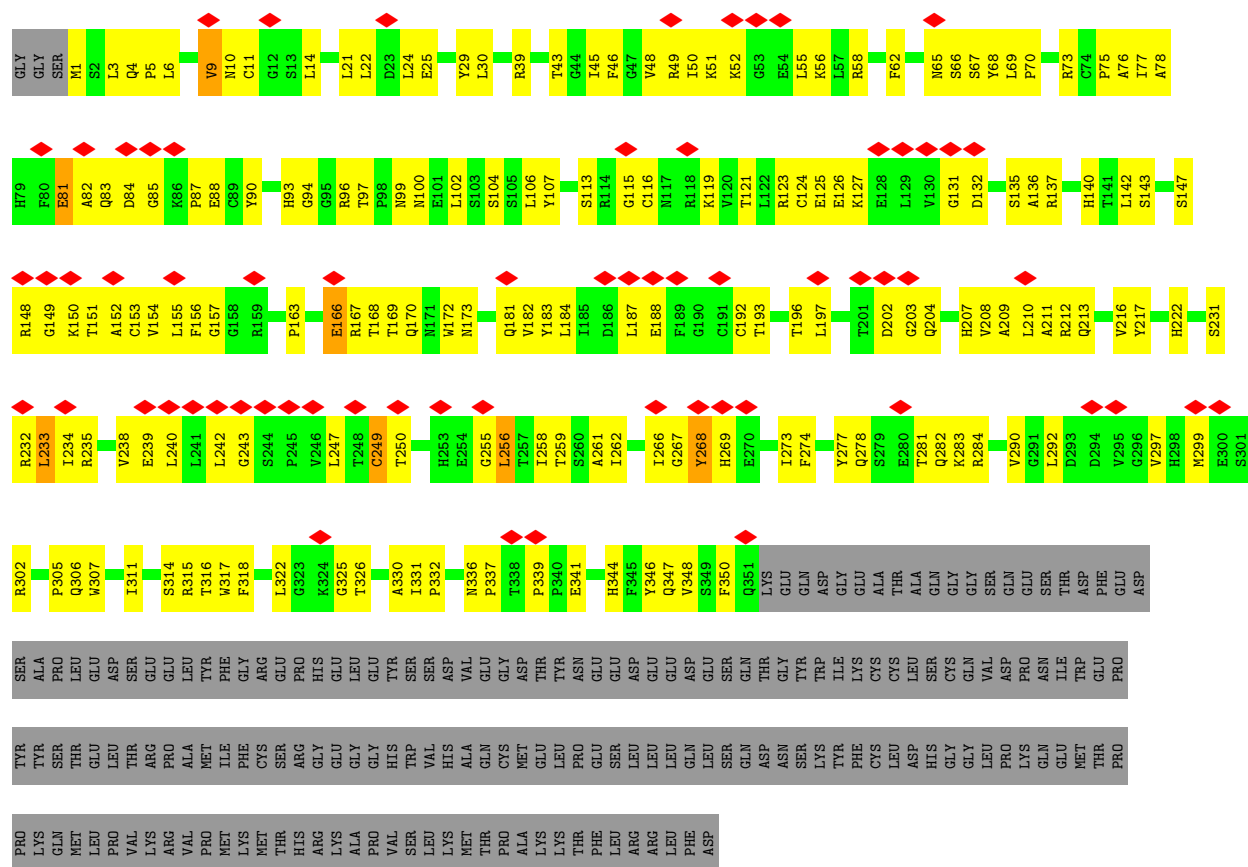
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

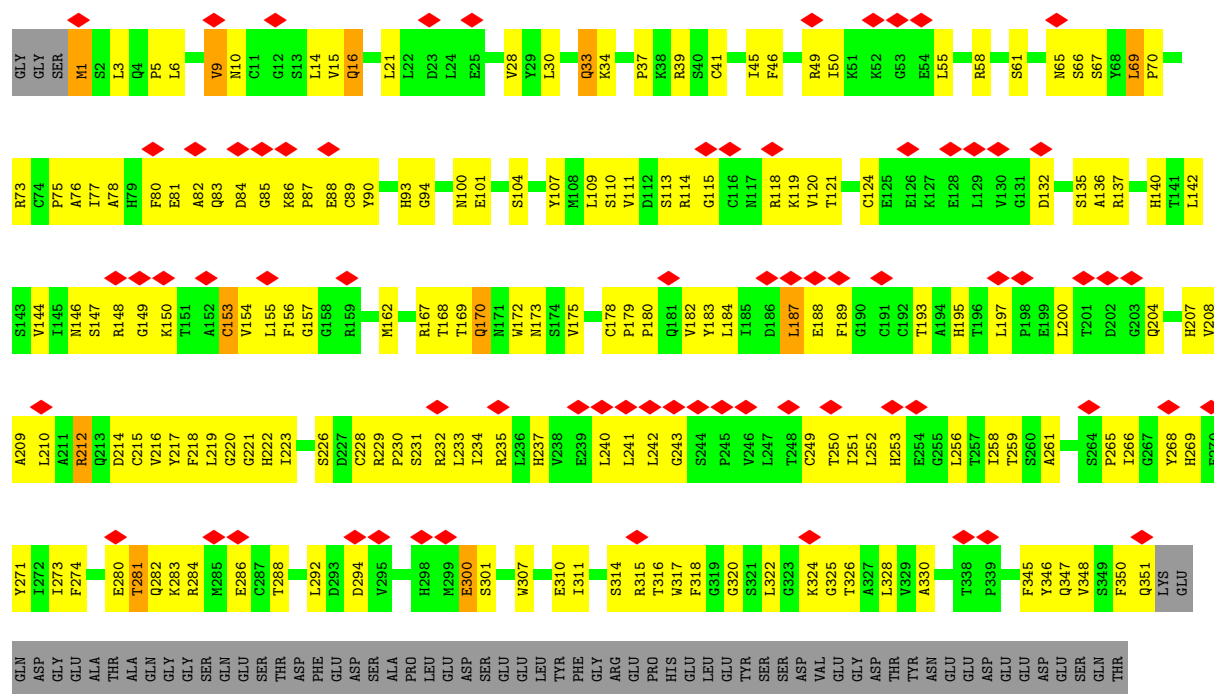
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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





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



ASN	SER	LYS	TYR	PHE	CYS	LEU	ASP	HIS	GLY	GLY	LEU	PRO	LYS	GLN	GLU	GLN	MET	THR	PRO	PRO	PRO	LYS	LYS	GLN	MET	MET	LEU	PRO	VAL	ARG	LYS	ALA	VAL	PRO	PRO	MET	MET	THR	THR	HIS	ARG	LYS	LYS	ALA	VAL	SER	LEU	MET	MET	LYS	THR	THR	PHE	LEU	ARG	ARG	LEU	LEU	PHE
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|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|
| C1 | A2 | C3 | A4 | G5 | T6 | G7 | C8 | T9 | A10 | C11 | A12 | G13 | A14 | C15 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|

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|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|
| C1 | A2 | C3 | A4 | G5 | T6 | G7 | C8 | T9 | A10 | C11 | A12 | G13 | A14 | C15 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|

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- | Category | Count |
|----------|-------|
| G1 | 1 |
| T2 | 1 |
| C3 | 1 |
| T4 | 1 |
| G5 | 1 |
| T6 | 1 |
| A7 | 1 |
| G8 | 1 |
| C9 | 1 |
| A10 | 1 |
| C11 | 1 |
| T12 | 1 |
| G13 | 1 |
| T14 | 1 |
| G15 | 1 |
| G19 | 1 |
| C25 | 3 |
| C26 | 1 |
| A27 | 1 |
| G28 | 1 |
| A29 | 1 |
| T30 | 1 |
| C31 | 1 |

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- | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|
| G1 | A2 | T3 | C4 | T5 | G6 | G7 | C8 | C9 | T10 | G11 | T12 | C13 | T14 | T15 | A16 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|
| G1 | A2 | T3 | C4 | T5 | G6 | G7 | C8 | C9 | T10 | G11 | T12 | C13 | T14 | T15 | A16 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|

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 (\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 (\AA)	1.23, 1.23, 1.23	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, 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	2/4526 (0.0%)	0.90	9/6095 (0.1%)
1	C	0.72	3/4526 (0.1%)	0.88	12/6095 (0.2%)
2	B	0.65	0/2784	0.84	0/3784
2	D	0.63	0/2784	0.83	1/3784 (0.0%)
3	E	1.78	6/343 (1.7%)	1.21	1/526 (0.2%)
3	H	1.82	6/343 (1.7%)	1.23	2/526 (0.4%)
4	F	1.51	8/717 (1.1%)	1.23	4/1105 (0.4%)
4	G	1.53	13/717 (1.8%)	1.25	3/1105 (0.3%)
5	I	1.45	6/363 (1.7%)	1.36	2/558 (0.4%)
5	J	1.41	0/363	1.54	6/558 (1.1%)
All	All	0.90	44/17466 (0.3%)	0.96	40/24136 (0.2%)

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

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	15	DG	C1'-N9	-8.98	1.34	1.47
4	G	11	DC	C3'-O3'	-8.59	1.32	1.44
3	H	7	DG	C3'-O3'	-8.37	1.33	1.44
3	E	6	DT	C3'-O3'	-8.12	1.33	1.44
3	H	6	DT	C1'-N1	-7.61	1.36	1.47

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	6	DG	O5'-P-OP2	-11.57	95.29	105.70
4	F	15	DG	C8-N9-C4	8.80	109.92	106.40
1	A	530	LEU	CB-CG-CD2	-7.83	97.70	111.00
1	A	1006	LEU	CB-CG-CD2	-7.61	98.07	111.00
4	G	15	DG	O4'-C1'-N9	-7.00	103.10	108.00

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	190	0
1	C	4435	0	4378	195	0
2	B	2714	0	2665	154	0
2	D	2714	0	2665	146	0
3	E	306	0	168	13	0
3	H	306	0	168	17	0
4	F	639	0	349	30	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	760	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 24.

The worst 5 of 760 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%)	47	78
1	C	548/764 (72%)	520 (95%)	28 (5%)	0	100	100
2	B	349/533 (66%)	335 (96%)	12 (3%)	2 (1%)	25	62
2	D	349/533 (66%)	335 (96%)	12 (3%)	2 (1%)	25	62
All	All	1794/2594 (69%)	1713 (96%)	76 (4%)	5 (0%)	44	74

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%)	469 (96%)	20 (4%)	30	59
1	C	489/681 (72%)	463 (95%)	26 (5%)	22	54
2	B	303/465 (65%)	291 (96%)	12 (4%)	31	60
2	D	303/465 (65%)	289 (95%)	14 (5%)	27	57
All	All	1584/2292 (69%)	1512 (96%)	72 (4%)	31	57

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	992	ARG
2	D	300	GLU
2	D	16	GLN
2	D	175	VAL
2	B	116	CYS

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

Mol	Chain	Res	Type
2	D	213	GLN
2	D	170	GLN
1	C	629	HIS
1	C	997	ASN
2	B	347	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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.

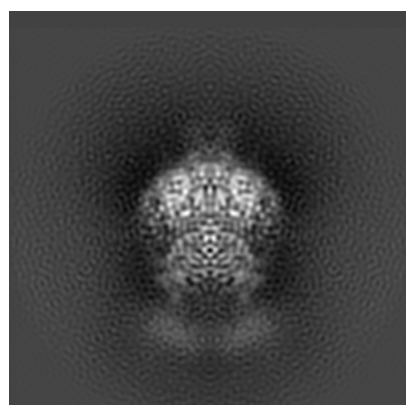
6 Map visualisation [i](#)

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.

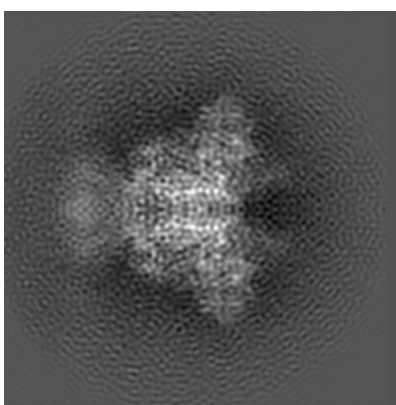
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

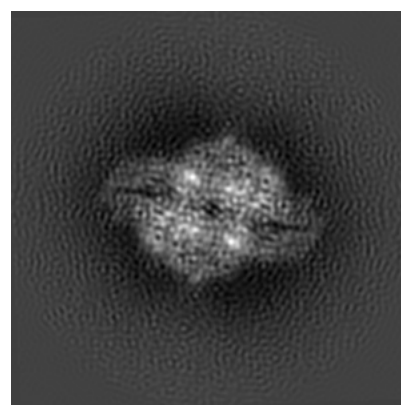
6.1.1 Primary map



X



Y

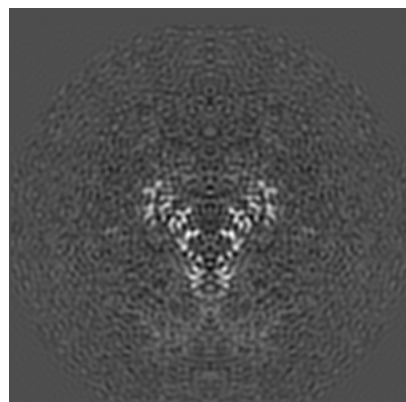


Z

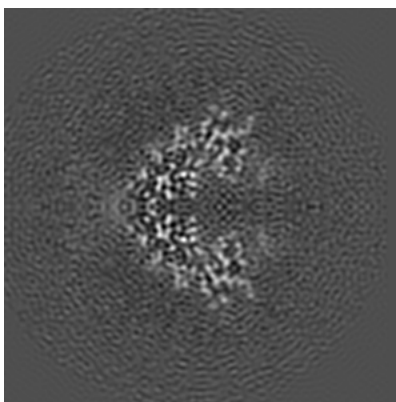
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

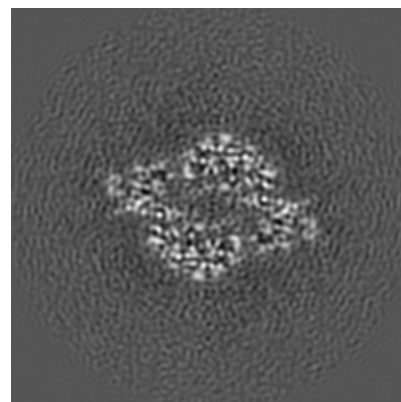
6.2.1 Primary map



X Index: 96



Y Index: 96

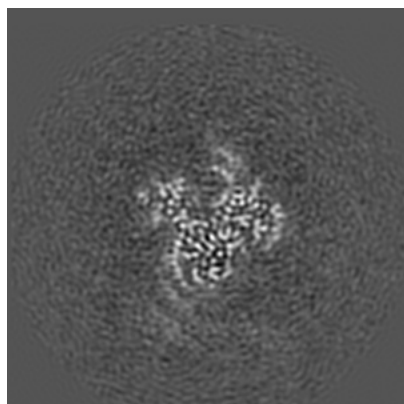


Z Index: 96

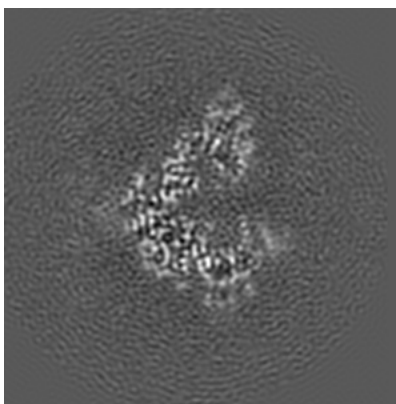
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

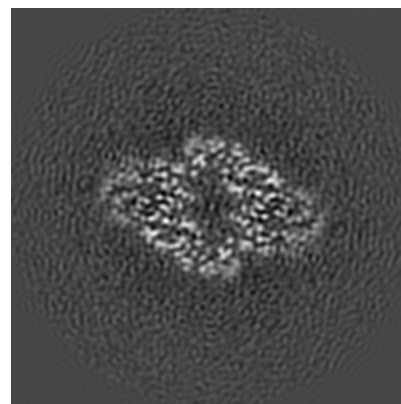
6.3.1 Primary map



X Index: 104



Y Index: 93

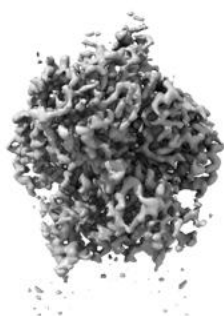


Z Index: 103

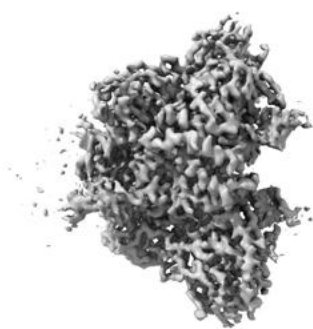
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

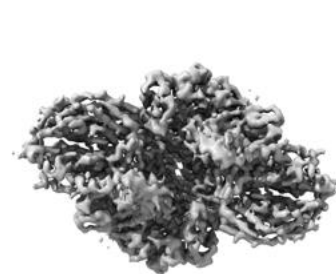
6.4.1 Primary map



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.

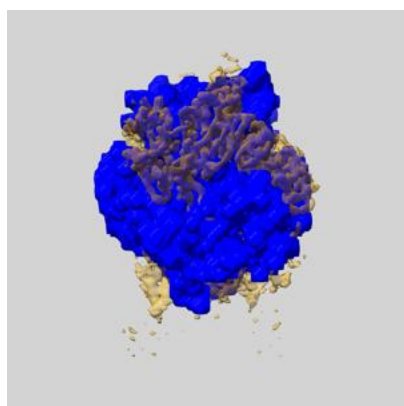
6.5 Mask visualisation [i](#)

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

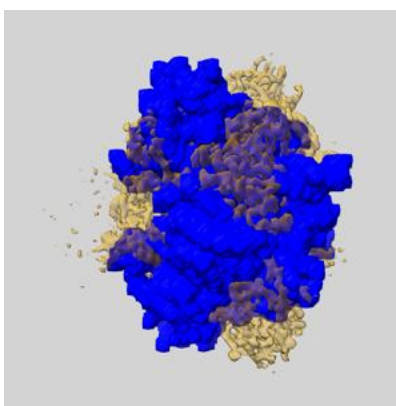
A mask typically either:

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

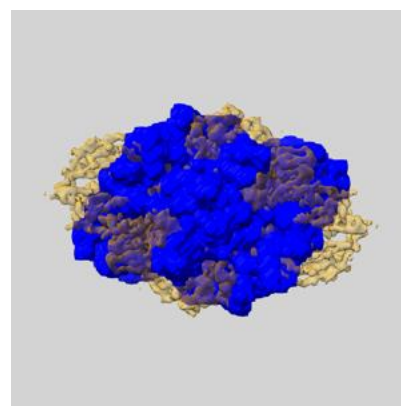
6.5.1 emd_6488_msk.map [i](#)



X



Y

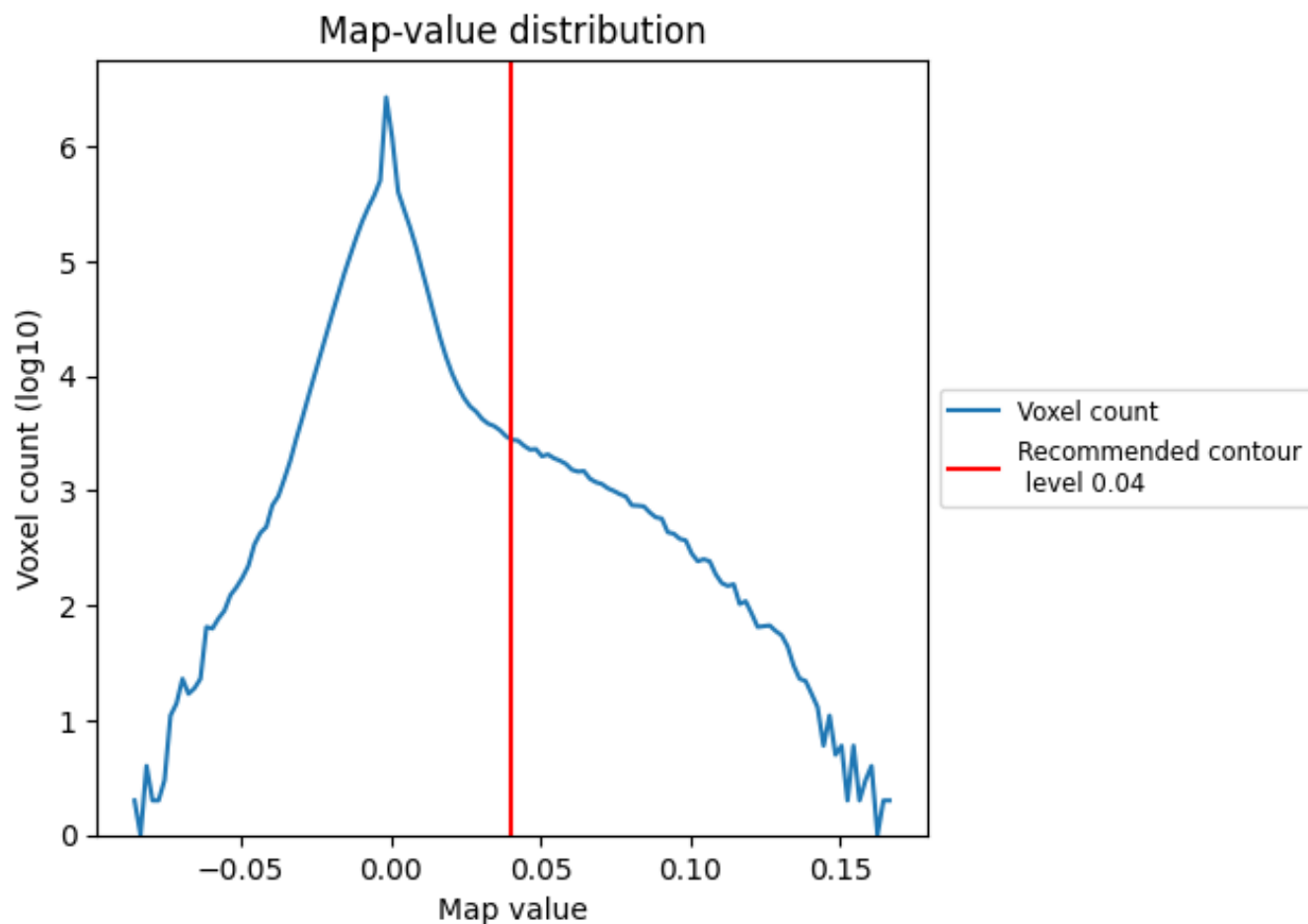


Z

7 Map analysis [i](#)

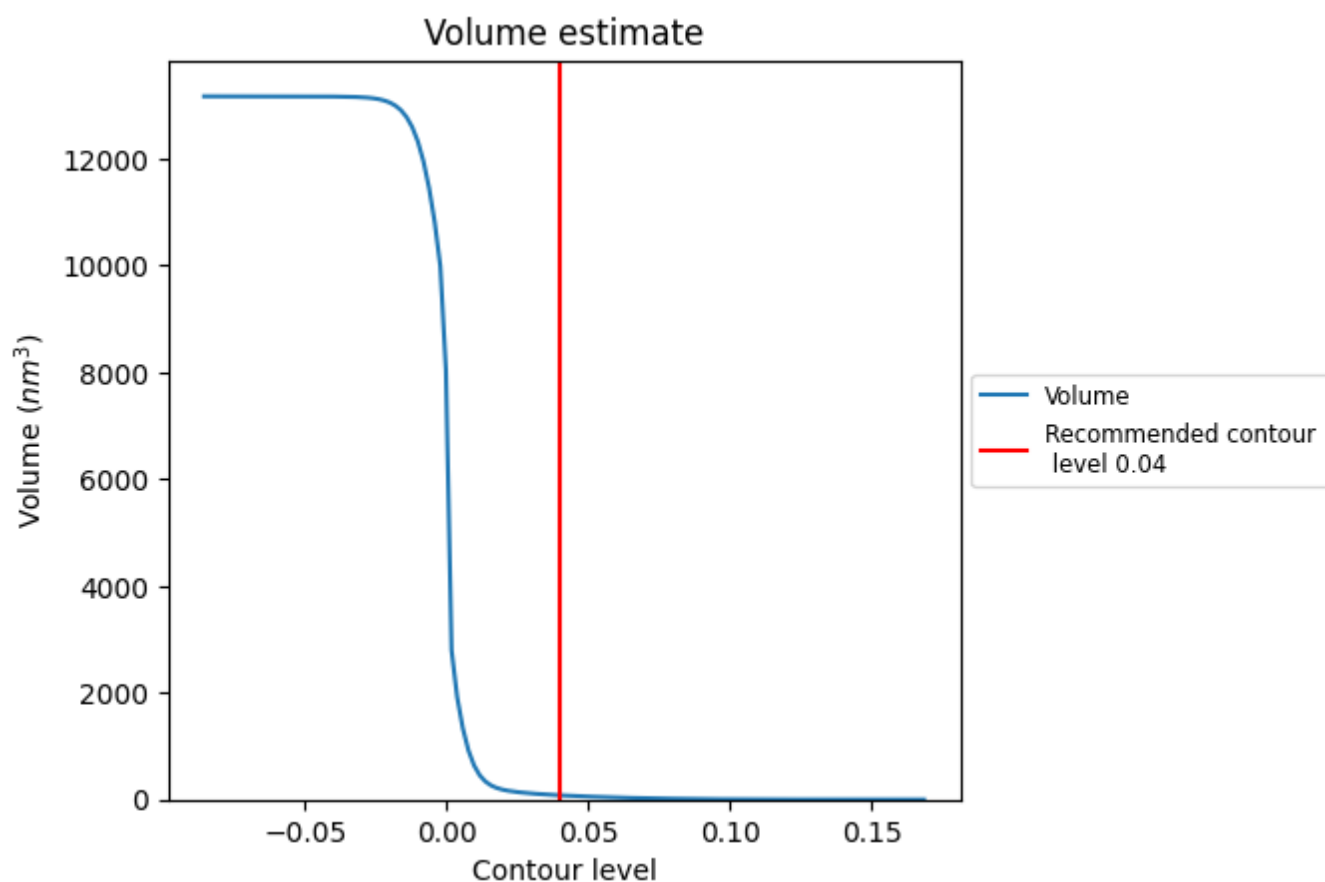
This section contains the results of statistical analysis of the map.

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.

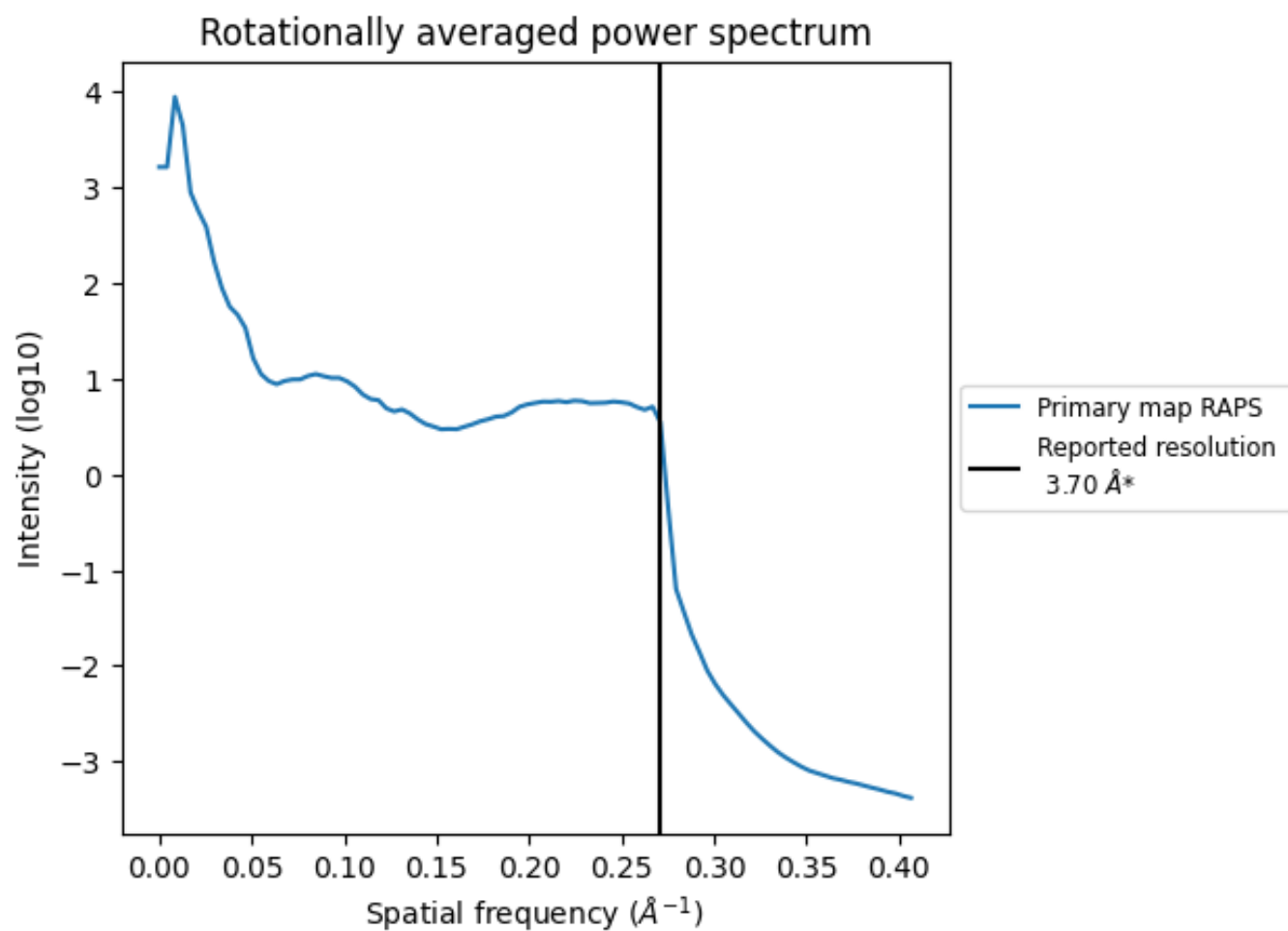
7.2 Volume estimate [i](#)



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 ⓘ

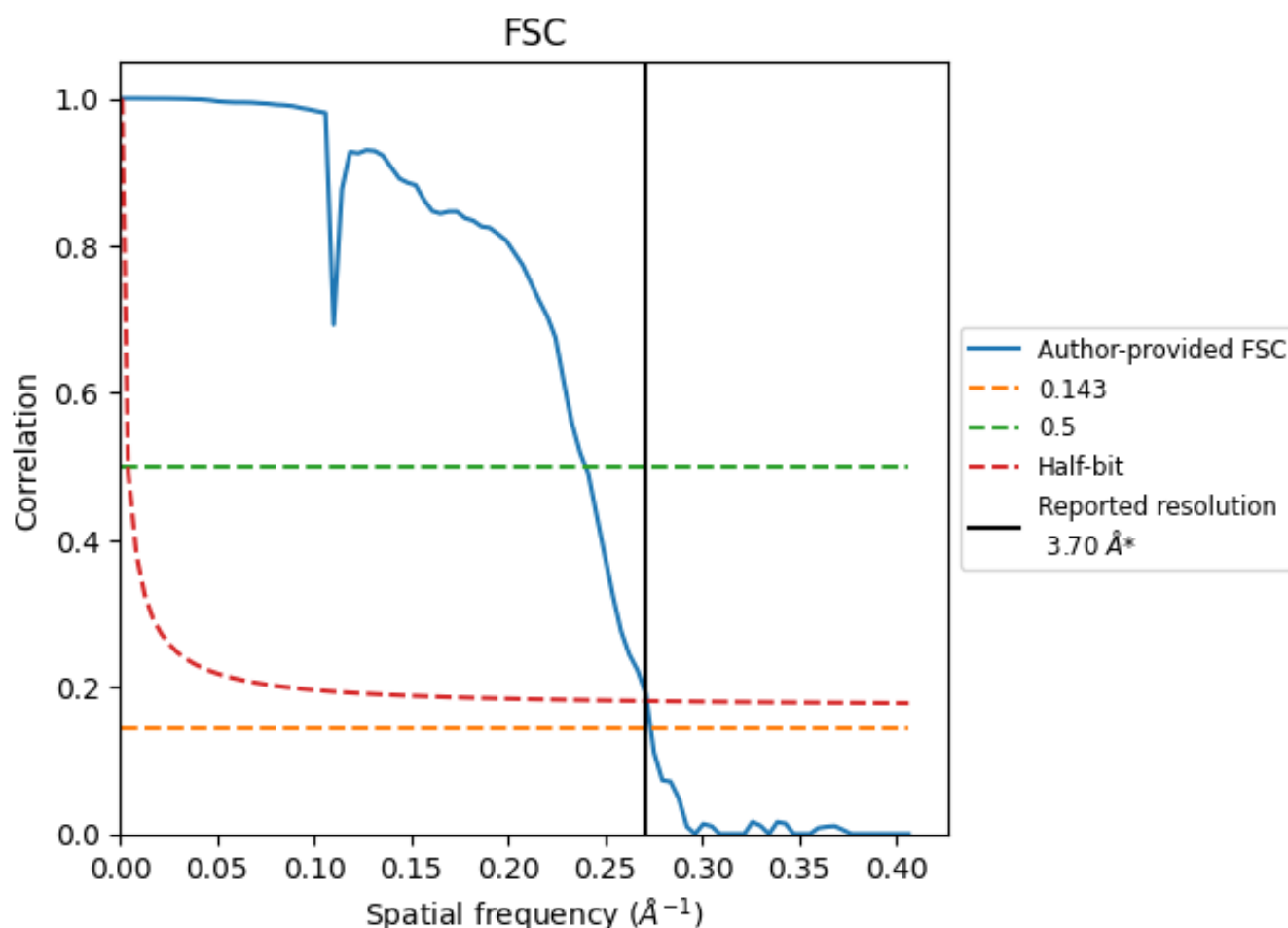


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

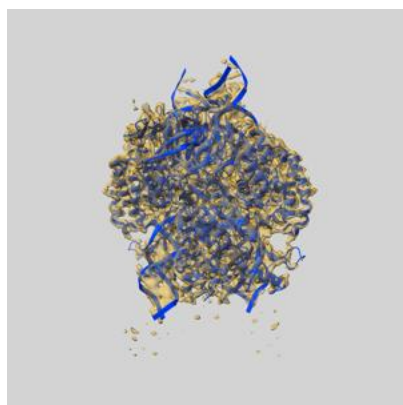
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.66	4.17	3.68
Unmasked-calculated*	-	-	-

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

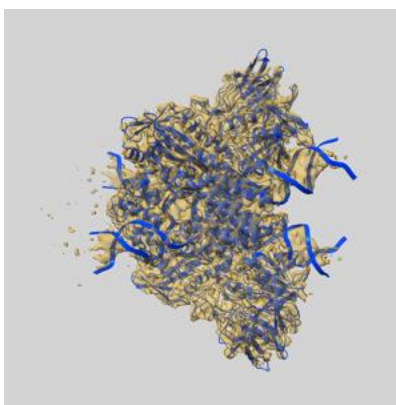
9 Map-model fit [i](#)

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](#).

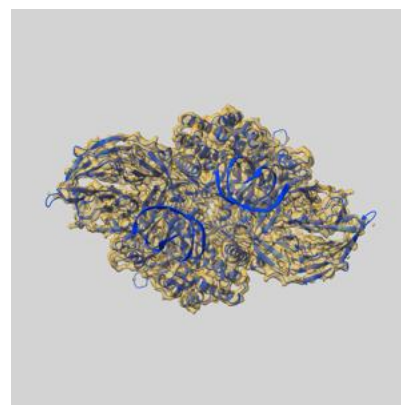
9.1 Map-model overlay [i](#)



X



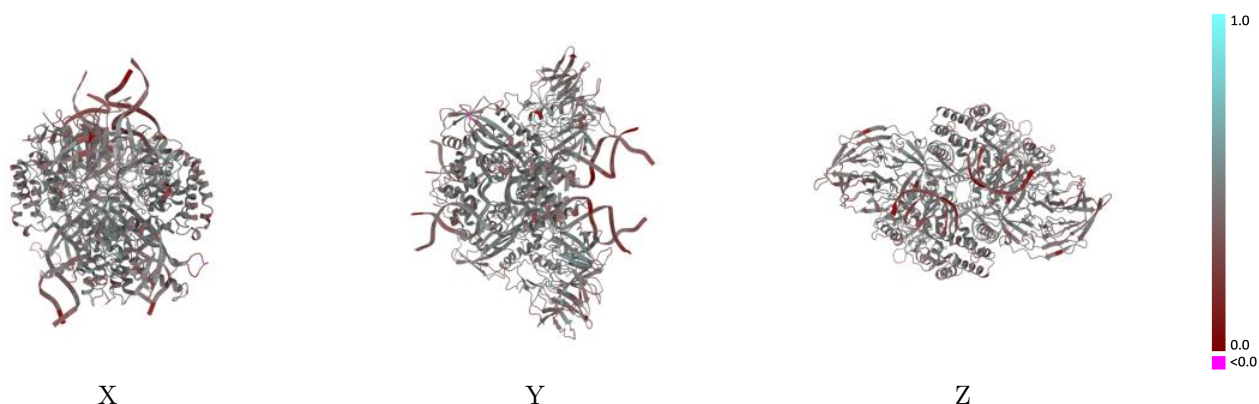
Y



Z

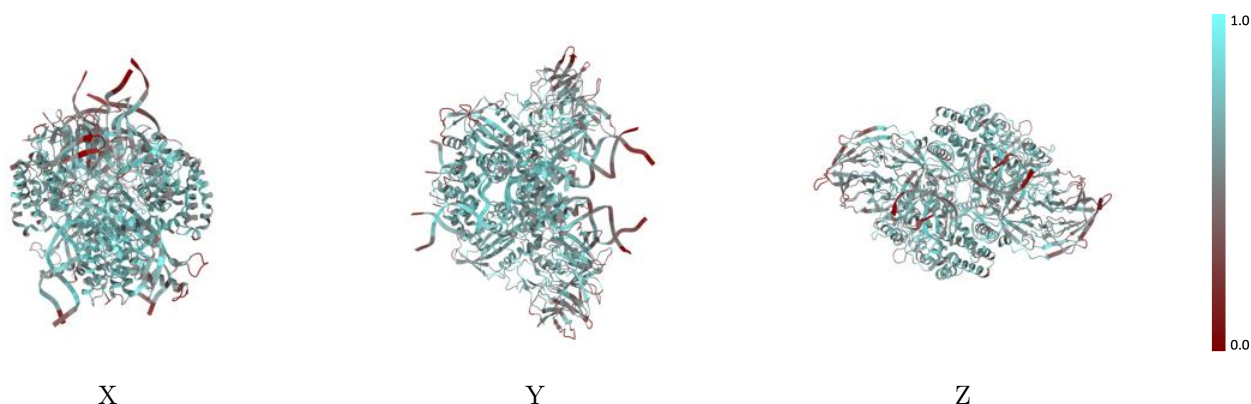
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



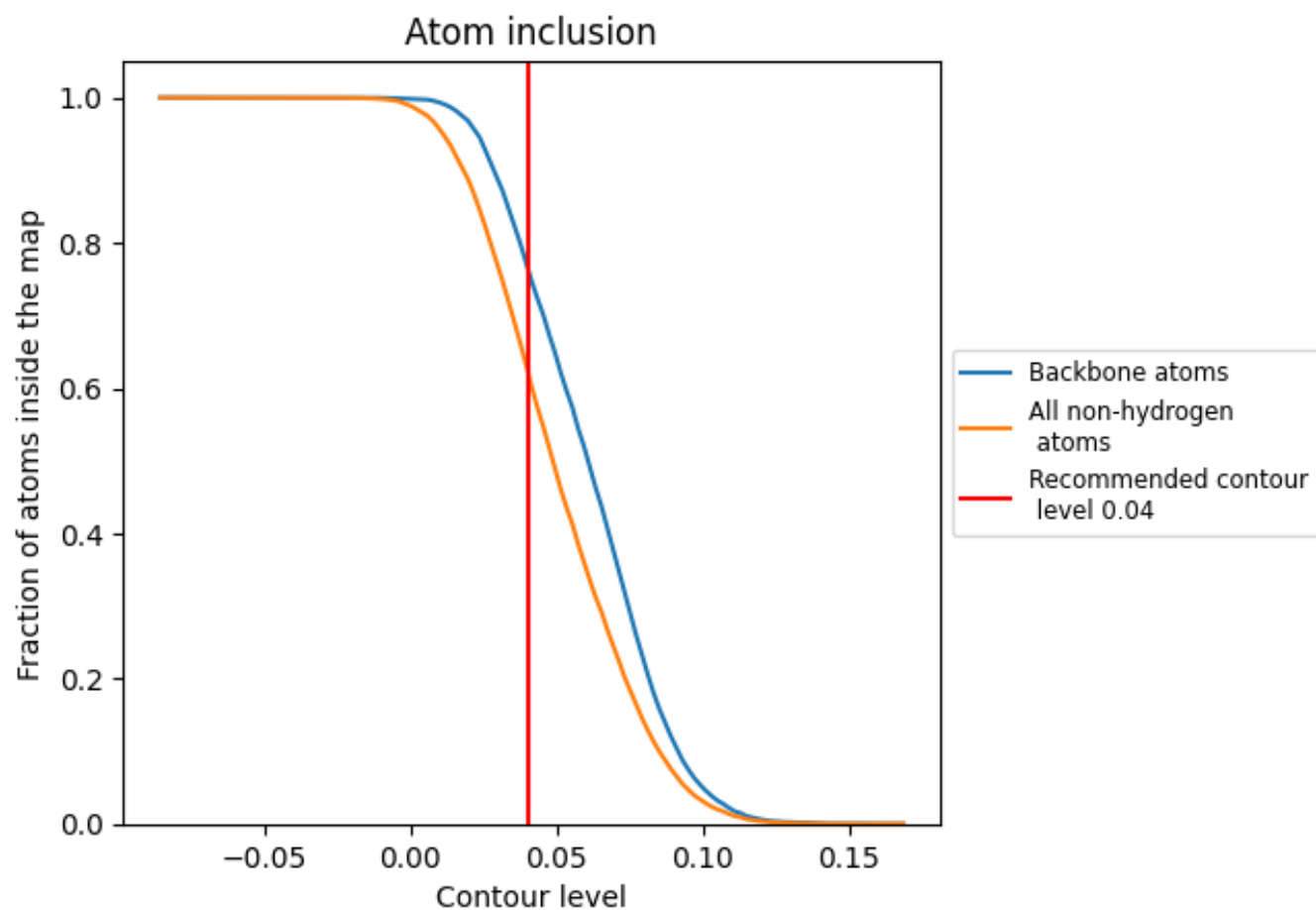
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 63% 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	<div></div> 0.6251	<div></div> 0.4350
A	<div></div> 0.6550	<div></div> 0.4520
B	<div></div> 0.5688	<div></div> 0.4330
C	<div></div> 0.6560	<div></div> 0.4550
D	<div></div> 0.5677	<div></div> 0.4320
E	<div></div> 0.7190	<div></div> 0.4190
F	<div></div> 0.6479	<div></div> 0.3860
G	<div></div> 0.6510	<div></div> 0.3840
H	<div></div> 0.7288	<div></div> 0.4260
I	<div></div> 0.5399	<div></div> 0.3320
J	<div></div> 0.5491	<div></div> 0.3180

1.0

0.0

<0.0