Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 06:38 pm GMT

PDB ID	:	4CG5
EMDB ID	:	EMD-2511
Title	:	Cryo-EM of the Sec61-complex bound to the 80S ribosome translating a secretory substrate
Authors	:	Gogala, M.; Becker, T.; Beatrix, B.; Barrio-Garcia, C.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2013-11-21
Resolution	:	7.40 Å(reported)
Based on initial model	:	2WWB

This is a Full wwPDB EM Validation 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 (i) 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 (i)) were used in the production of this report:

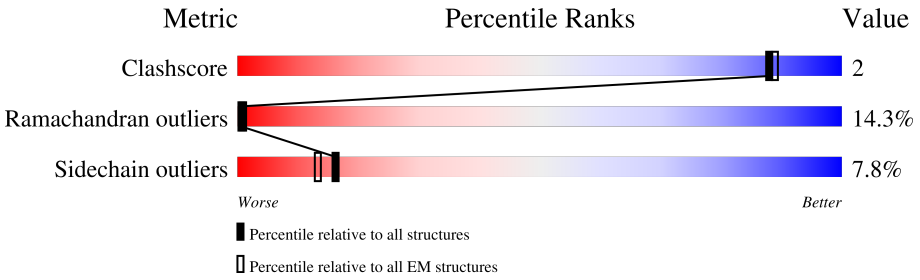
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.40 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 <=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	476	15% 72% 18% • • 5%
2	B	68	• 81% 10% 9%
3	C	36	14% 75% 14% 6% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4252 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 PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	452	3477	2275	560	619	23	0	0

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	62	494	326	86	79	3	0	0

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

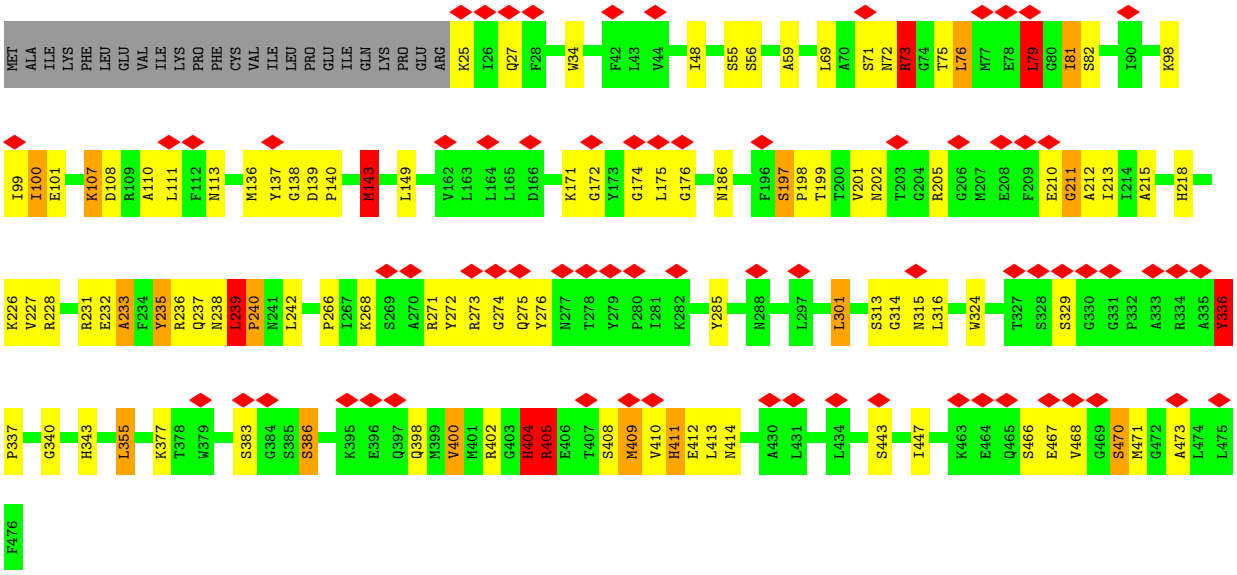
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	36	281	188	44	47	2	0	0

3 Residue-property plots (i)

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.

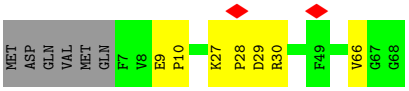
• Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1

Chain A:



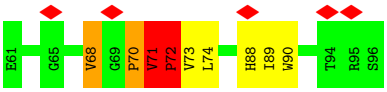
• Molecule 2: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA

Chain B:



• Molecule 3: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53248	Depositor
Resolution determination method	Not provided	
CTF correction method	ON 3D-VOLUME (SPIDER)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	148721	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.649	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	455.36322, 455.36322, 455.36322	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2374, 1.2374, 1.2374	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.96	0/3552	1.23	19/4815 (0.4%)
2	B	0.94	0/504	1.04	0/673
3	C	0.89	0/289	1.34	2/391 (0.5%)
All	All	0.96	0/4345	1.22	21/5879 (0.4%)

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	7

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	ARG	NE-CZ-NH2	-9.19	115.71	120.30
3	C	70	PRO	CA-N-CD	-7.43	101.10	111.50
1	A	235	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	A	235	TYR	CB-CG-CD1	7.04	125.22	121.00
1	A	336	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	386	SER	N-CA-CB	6.45	120.18	110.50
1	A	336	TYR	CB-CG-CD1	6.36	124.82	121.00
1	A	73	ARG	N-CA-CB	6.27	121.89	110.60
1	A	79	LEU	N-CA-CB	6.22	122.83	110.40
3	C	70	PRO	CB-CA-C	6.11	127.27	112.00
1	A	210	GLU	C-N-CA	6.04	134.99	122.30
1	A	408	SER	C-N-CA	5.74	136.05	121.70
1	A	466	SER	C-N-CA	5.72	135.99	121.70
1	A	470	SER	N-CA-CB	5.69	119.03	110.50
1	A	409	MET	N-CA-C	5.60	126.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	GLY	C-N-CA	5.57	135.61	121.70
1	A	405	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	233	ALA	N-CA-CB	5.31	117.54	110.10
1	A	408	SER	N-CA-CB	5.06	118.09	110.50
1	A	239	LEU	CB-CA-C	5.04	119.78	110.20
1	A	231	ARG	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	MET	Peptide
1	A	266	PRO	Peptide
1	A	336	TYR	Peptide
1	A	377	LYS	Peptide
1	A	383	SER	Peptide
1	A	55	SER	Peptide
1	A	56	SER	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	3477	0	3575	12	0
2	B	494	0	527	1	0
3	C	281	0	294	3	0
All	All	4252	0	4396	16	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 2.

All (16) 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:A:404:HIS:CG	1:A:405:ARG:H	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:HIS:CG	3:C:89:ILE:H	2.20	0.60
1:A:197:SER:H	1:A:198:PRO:HD3	1.78	0.48
1:A:236:ARG:HB3	1:A:239:LEU:HD23	1.94	0.48
1:A:239:LEU:HB2	1:A:240:PRO:HD2	1.97	0.47
1:A:268:LYS:H	1:A:276:TYR:HB3	1.80	0.46
1:A:443:SER:H	1:A:447:ILE:HD12	1.81	0.46
1:A:404:HIS:CG	1:A:405:ARG:N	2.83	0.46
1:A:411:HIS:HB2	1:A:414:ASN:HB3	1.98	0.46
1:A:76:LEU:H	1:A:76:LEU:HD13	1.82	0.45
1:A:149:LEU:H	1:A:149:LEU:HD22	1.83	0.43
1:A:215:ALA:HB3	1:A:218:HIS:CD2	2.52	0.43
3:C:88:HIS:CG	3:C:89:ILE:N	2.85	0.43
2:B:9:GLU:HB2	2:B:10:PRO:HD3	2.01	0.43
3:C:71:VAL:HG22	3:C:72:PRO:HD2	2.00	0.43
1:A:239:LEU:HB2	1:A:240:PRO:CD	2.51	0.41

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	450/476 (94%)	333 (74%)	50 (11%)	67 (15%)	0 3
2	B	60/68 (88%)	52 (87%)	3 (5%)	5 (8%)	1 12
3	C	34/36 (94%)	25 (74%)	3 (9%)	6 (18%)	0 2
All	All	544/580 (94%)	410 (75%)	56 (10%)	78 (14%)	1 4

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	59	ALA

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	73	ARG
1	A	79	LEU
1	A	81	ILE
1	A	82	SER
1	A	100	ILE
1	A	107	LYS
1	A	108	ASP
1	A	111	LEU
1	A	113	ASN
1	A	199	THR
1	A	201	VAL
1	A	202	ASN
1	A	211	GLY
1	A	212	ALA
1	A	228	ARG
1	A	232	GLU
1	A	233	ALA
1	A	238	ASN
1	A	239	LEU
1	A	271	ARG
1	A	272	TYR
1	A	273	ARG
1	A	301	LEU
1	A	313	SER
1	A	315	ASN
1	A	336	TYR
1	A	337	PRO
1	A	400	VAL
1	A	409	MET
1	A	410	VAL
1	A	467	GLU
1	A	468	VAL
1	A	470	SER
1	A	473	ALA
2	B	30	ARG
3	C	68	VAL
3	C	70	PRO
3	C	71	VAL
3	C	72	PRO
1	A	75	THR
1	A	98	LYS

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Mol	Chain	Res	Type
1	A	140	PRO
1	A	143	MET
1	A	176	GLY
1	A	213	ILE
1	A	274	GLY
1	A	314	GLY
1	A	386	SER
1	A	404	HIS
1	A	411	HIS
1	A	471	MET
2	B	66	VAL
1	A	71	SER
1	A	136	MET
1	A	139	ASP
1	A	171	LYS
1	A	174	GLY
1	A	324	TRP
1	A	340	GLY
1	A	355	LEU
1	A	398	GLN
1	A	412	GLU
2	B	29	ASP
1	A	110	ALA
1	A	137	TYR
1	A	227	VAL
1	A	329	SER
2	B	27	LYS
3	C	90	TRP
1	A	237	GLN
1	A	138	GLY
1	A	172	GLY
2	B	28	PRO
3	C	73	VAL
1	A	197	SER

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	375/398 (94%)	343 (92%)	32 (8%)	10	33
2	B	53/59 (90%)	53 (100%)	0	100	100
3	C	32/32 (100%)	28 (88%)	4 (12%)	4	19
All	All	460/489 (94%)	424 (92%)	36 (8%)	16	36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	34	TRP
1	A	48	ILE
1	A	69	LEU
1	A	73	ARG
1	A	76	LEU
1	A	79	LEU
1	A	81	ILE
1	A	99	ILE
1	A	100	ILE
1	A	101	GLU
1	A	107	LYS
1	A	143	MET
1	A	175	LEU
1	A	186	ASN
1	A	205	ARG
1	A	226	LYS
1	A	235	TYR
1	A	240	PRO
1	A	242	LEU
1	A	275	GLN
1	A	285	TYR
1	A	301	LEU
1	A	316	LEU
1	A	336	TYR
1	A	343	HIS
1	A	355	LEU
1	A	400	VAL
1	A	402	ARG
1	A	404	HIS
1	A	405	ARG
1	A	413	LEU
3	C	68	VAL
3	C	71	VAL

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Mol	Chain	Res	Type
3	C	72	PRO
3	C	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS

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)

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.

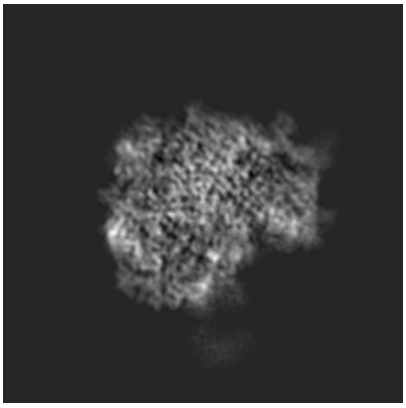
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2511. These allow visual inspection of the internal detail of the map and identification of artifacts.

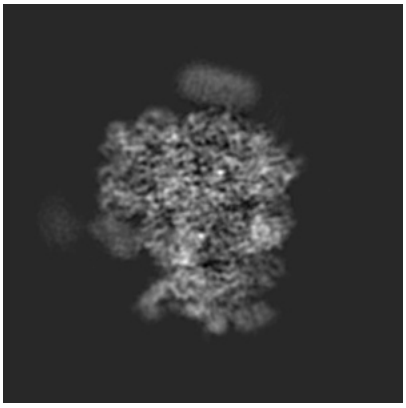
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

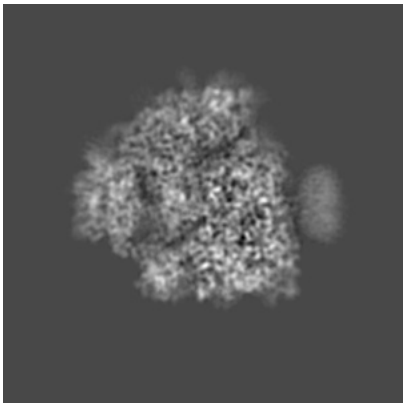
6.1.1 Primary map



X



Y

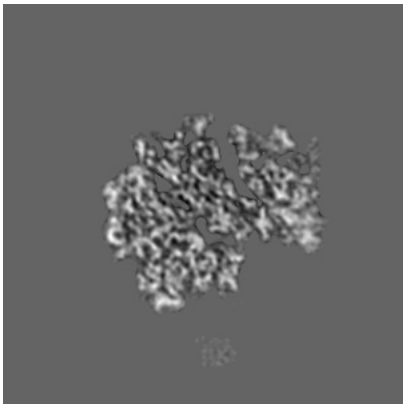


Z

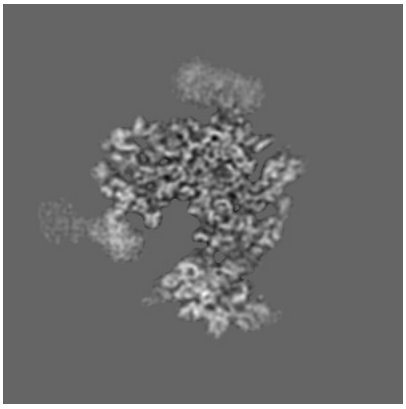
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

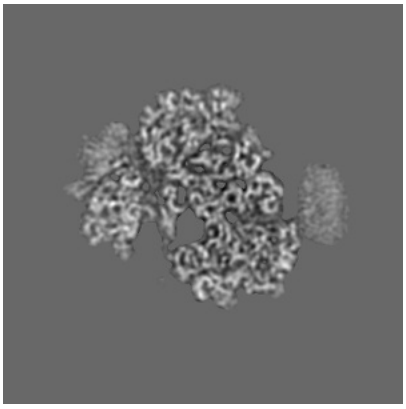
6.2.1 Primary map



X Index: 184



Y Index: 184

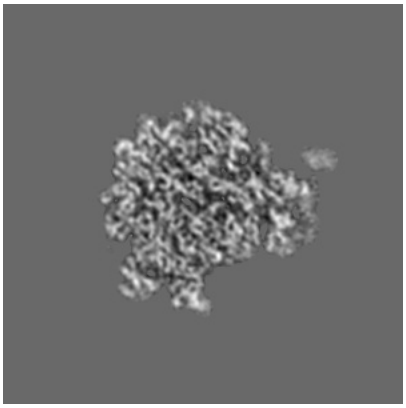


Z Index: 184

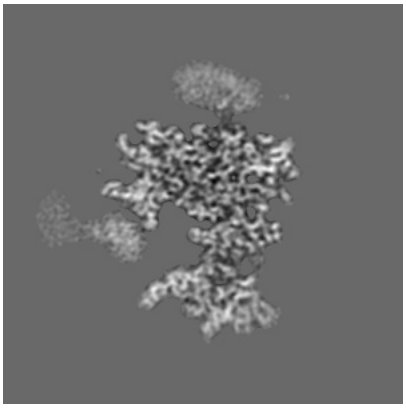
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

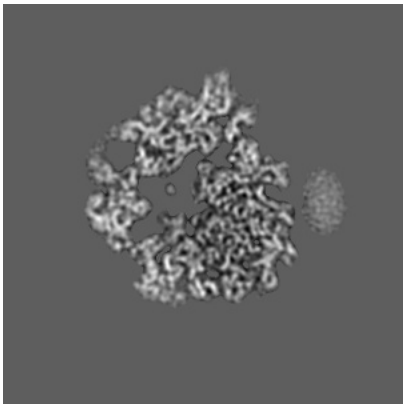
6.3.1 Primary map



X Index: 213



Y Index: 192

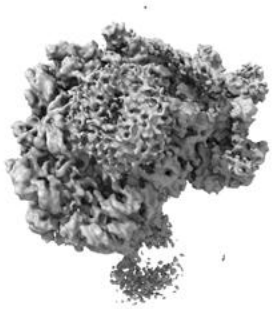


Z Index: 169

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

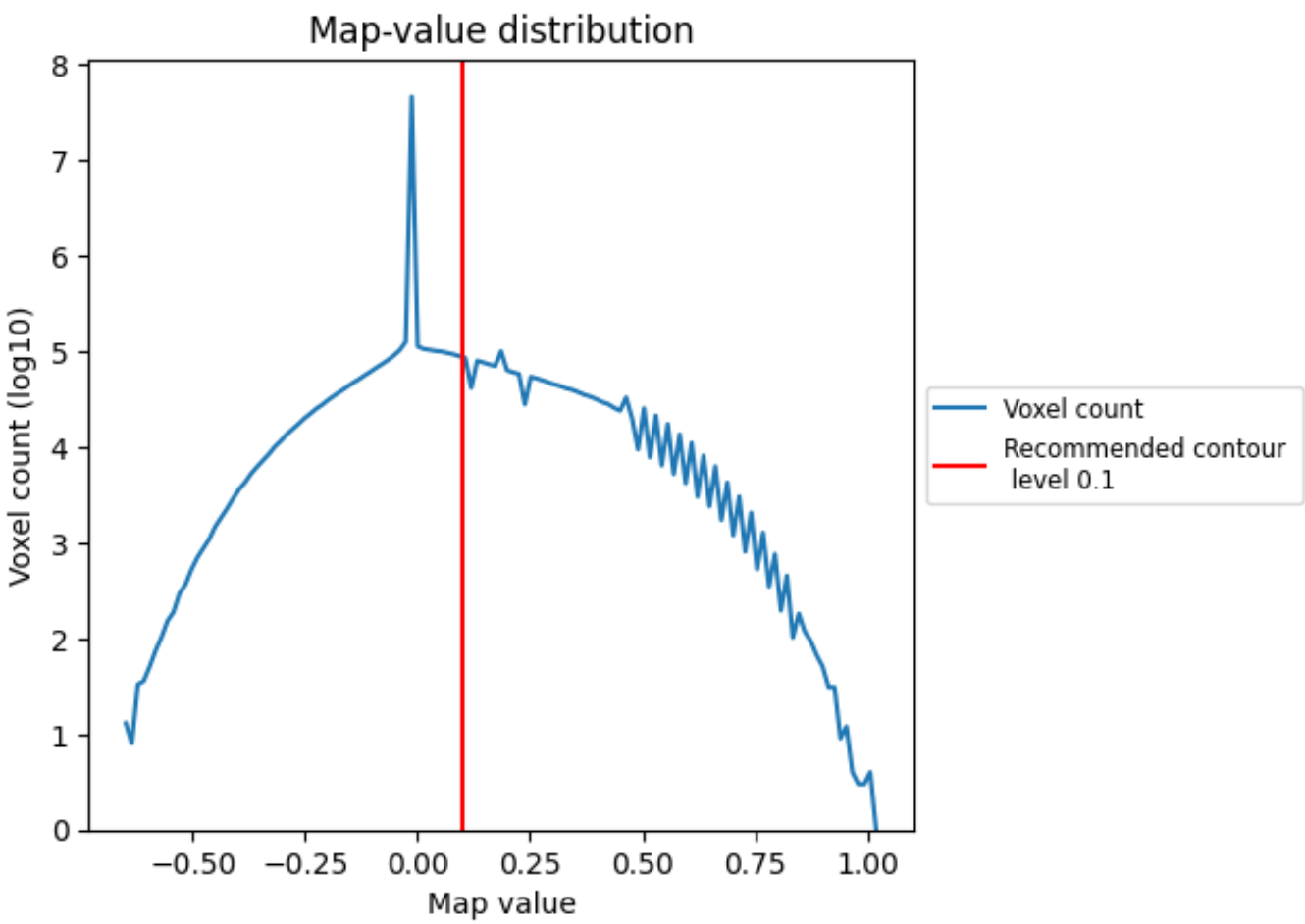
6.5 Mask visualisation (i)

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

7 Map analysis (i)

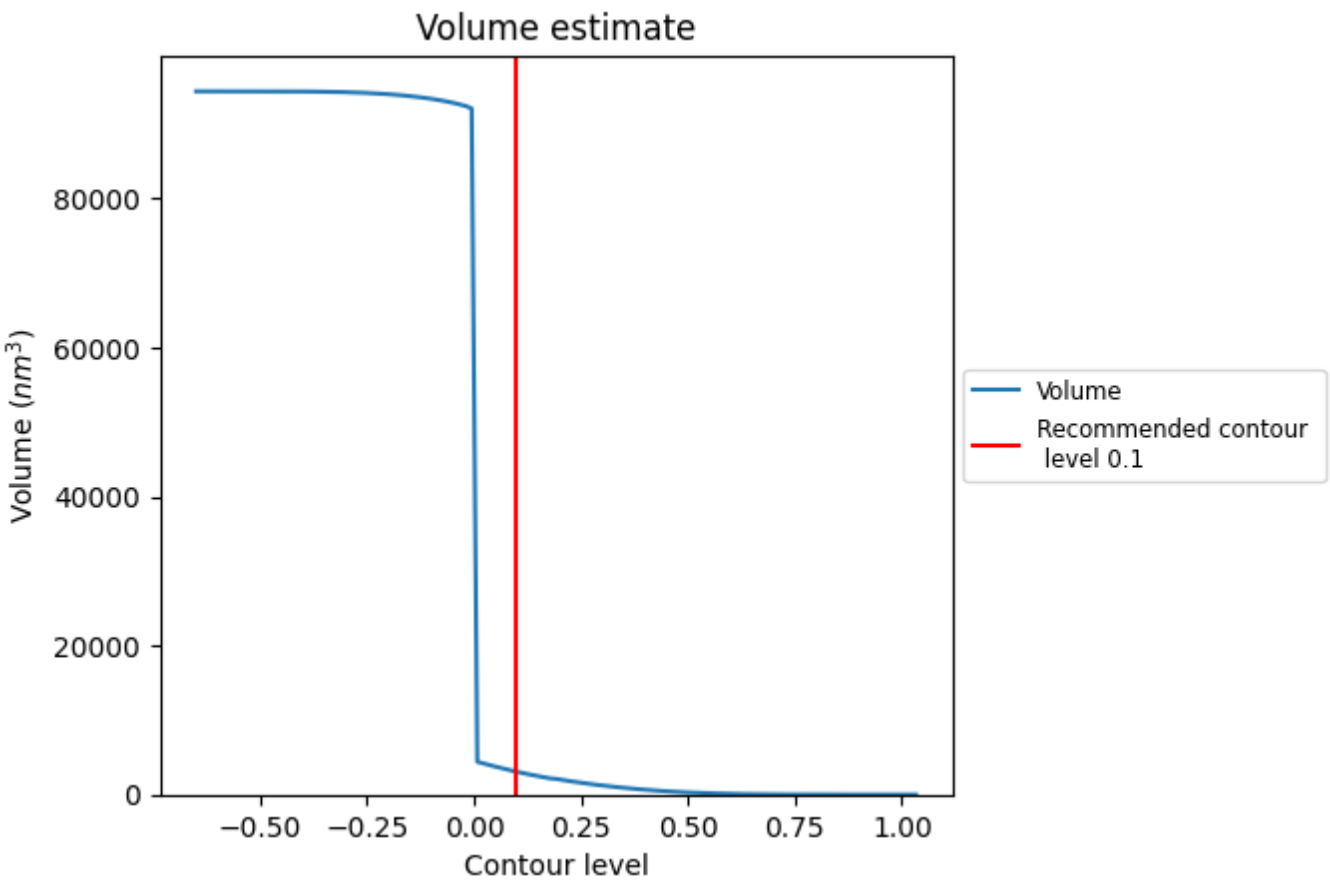
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

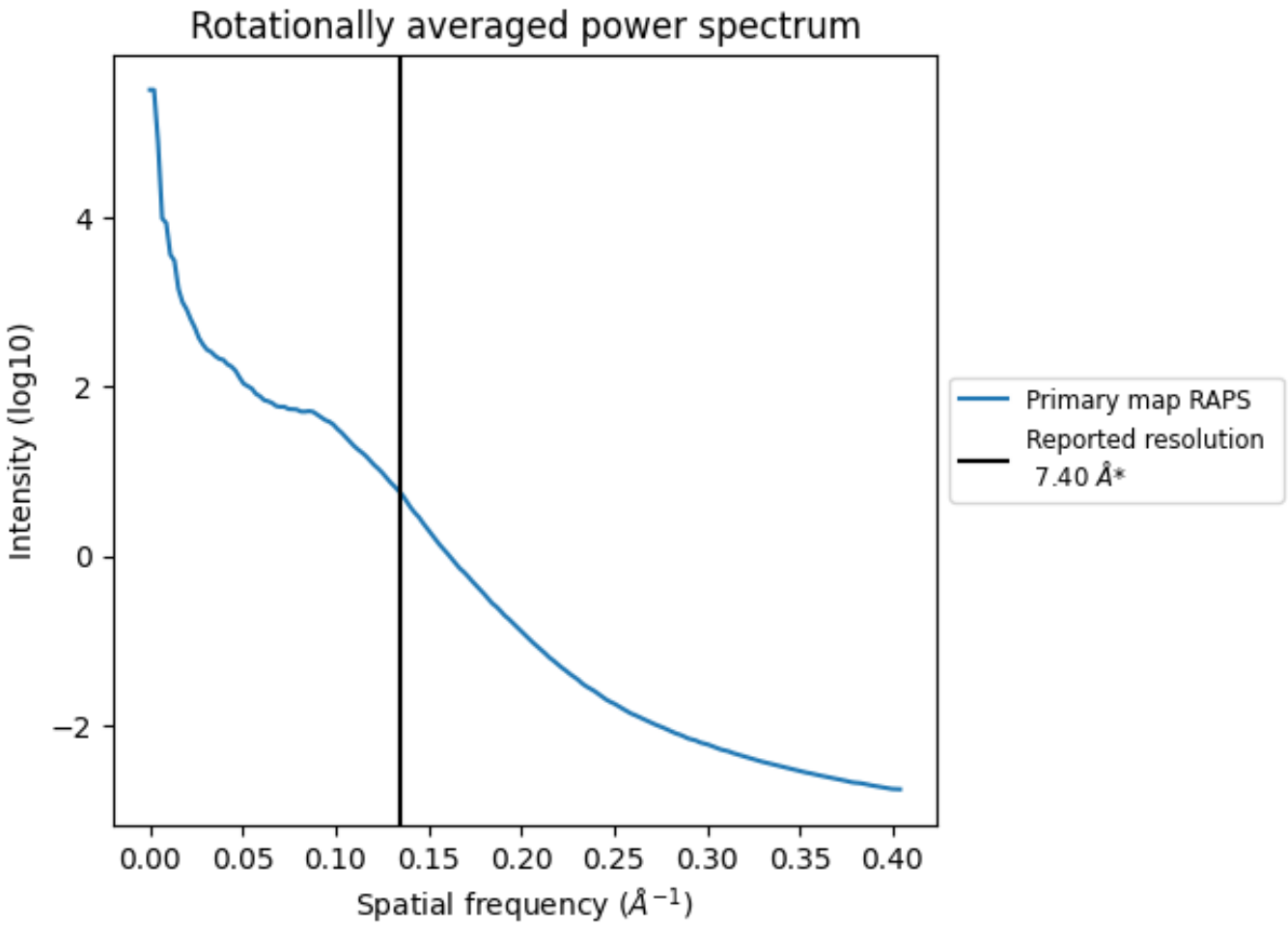
7.2 Volume estimate (i)



The volume at the recommended contour level is 3066 nm^3; this corresponds to an approximate mass of 2769 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 0.135 Å^{-1}

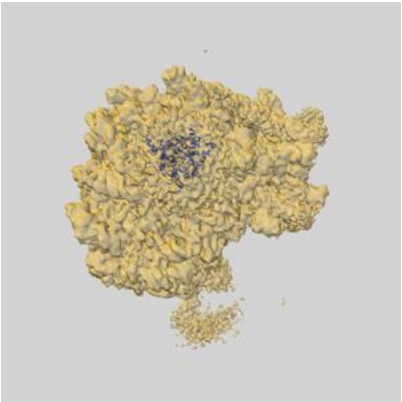
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

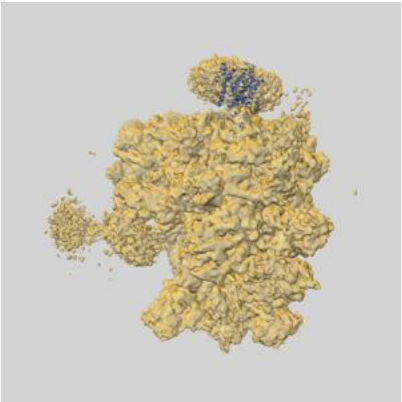
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2511 and PDB model 4CG5. Per-residue inclusion information can be found in section 3 on page 4.

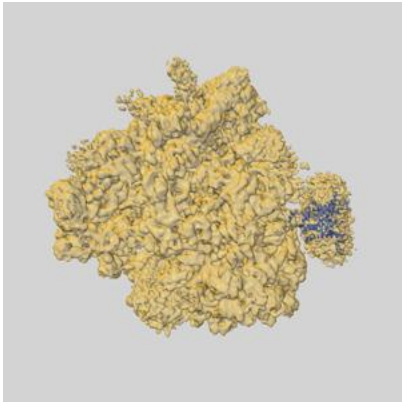
9.1 Map-model overlay (i)



X



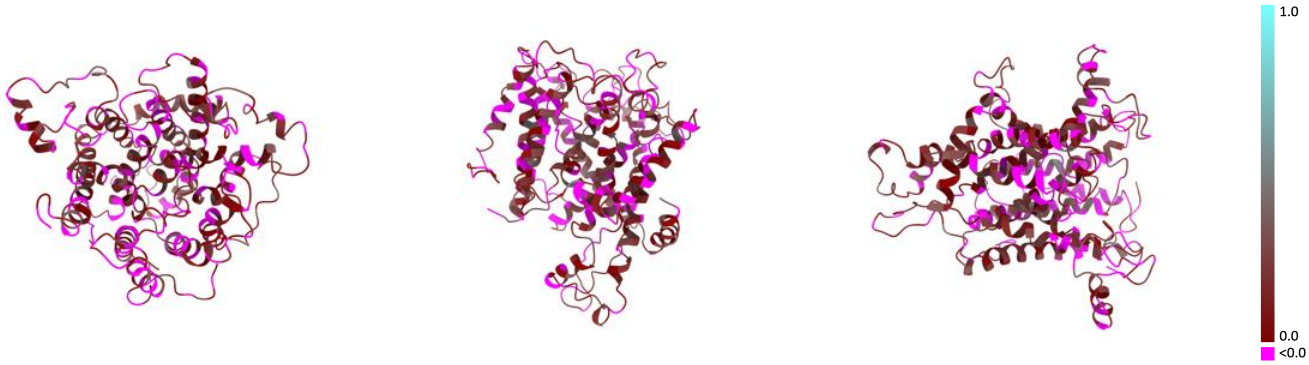
Y



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.

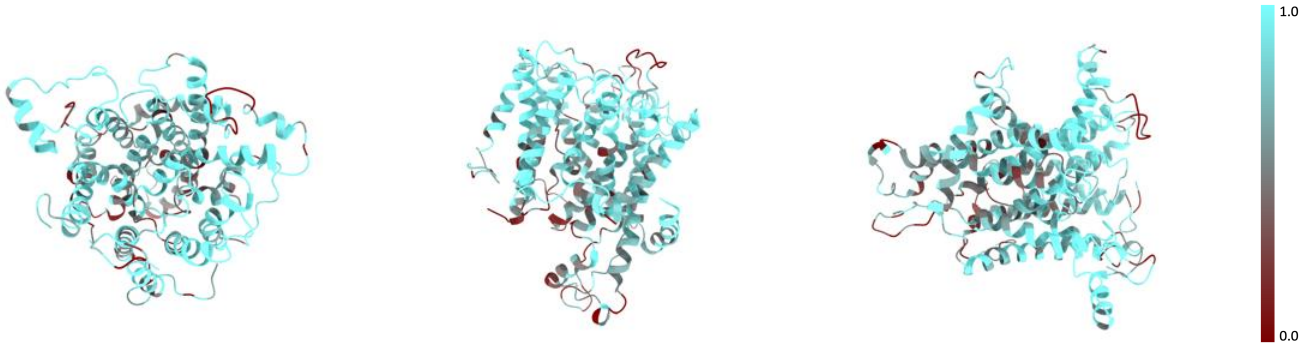
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

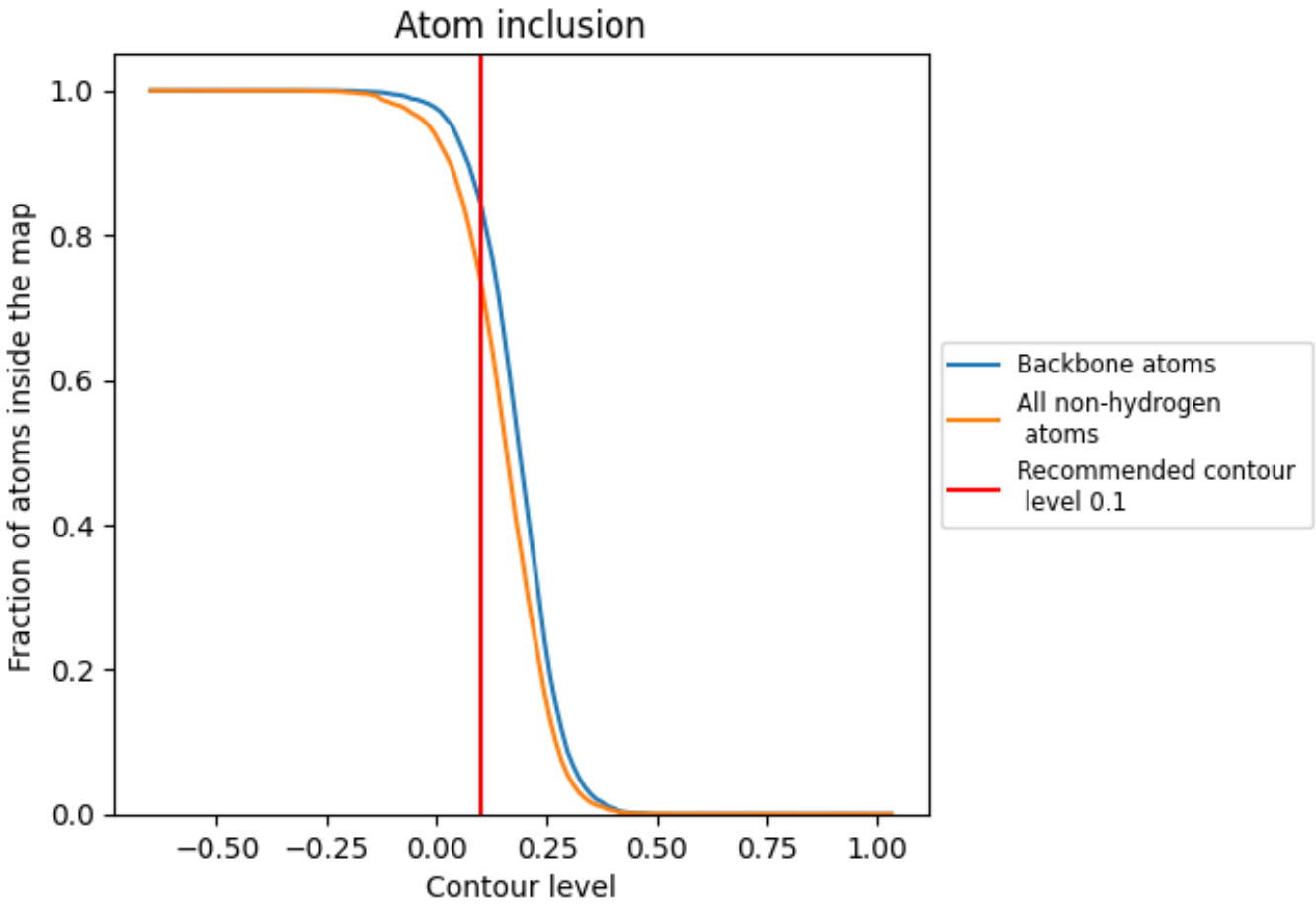
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 84% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7384	0.0860
A	0.7289	0.0850
B	0.8025	0.1320
C	0.7437	0.0180