Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:43 PM JST

PDB ID	:	7C0M
EMDB ID	:	EMD-30267
Title	:	Human cGAS-nucleosome complex
Authors	:	Kujirai, T.; Zierhut, C.; Takizawa, Y.; Kim, R.; Negishi, L.; Uruma, N.; Hirai, S.; Funabiki, H.; Kurumizaka, H.
Deposited on	:	2020-05-01
Resolution	:	3.90 Å(reported)

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 ⓘ 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:

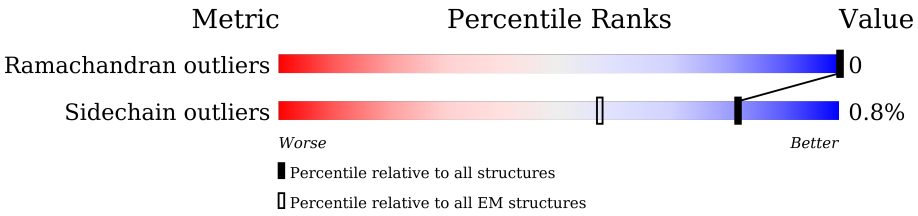
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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)
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	139	69% · 30%
1	E	139	· 70% 30%
1	a	139	· 69% · 30%
1	e	139	· 70% 30%
2	B	106	78% 22%
2	F	106	73% · 26%
2	b	106	· 78% 22%
2	f	106	· 73% · 26%
3	C	133	· 77% · 23%

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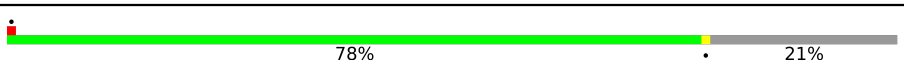
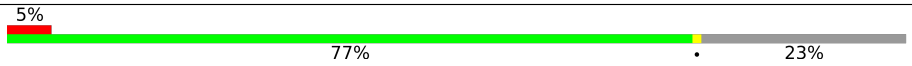
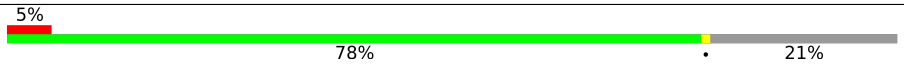
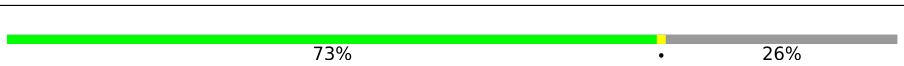
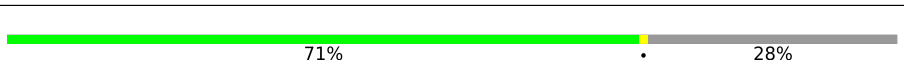
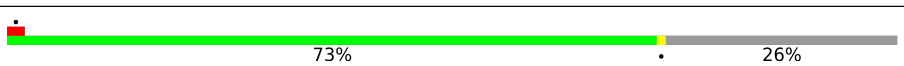
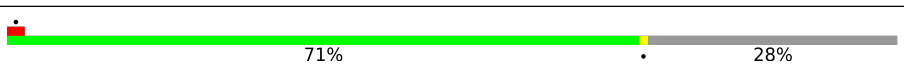
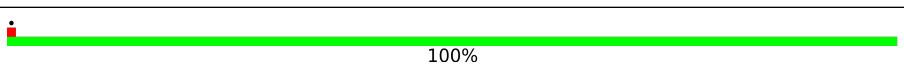
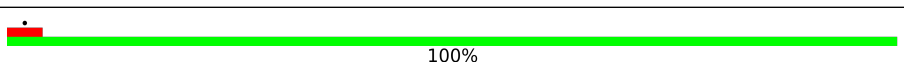
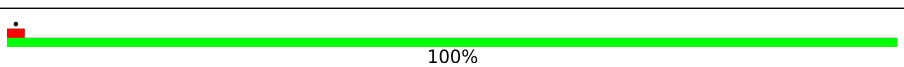
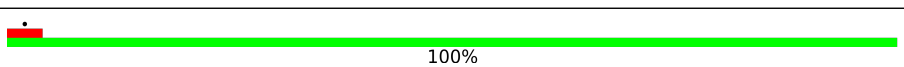
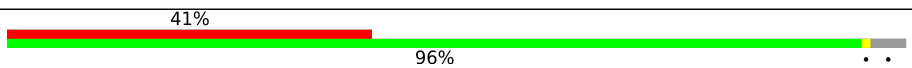
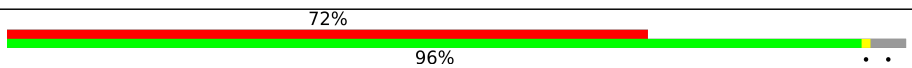
Mol	Chain	Length	Quality of chain
3	G	133	
3	c	133	
3	g	133	
4	D	129	
4	H	129	
4	d	129	
4	h	129	
5	I	145	
5	i	145	
6	J	145	
6	j	145	
7	K	380	
7	k	380	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29816 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
1	E	97	Total	C	N	O	S	0	0
			799	503	155	137	4		
1	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
1	e	97	Total	C	N	O	S	0	0
			799	503	155	137	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
A	0	MET	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431
E	0	MET	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
a	0	MET	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
e	0	MET	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total 661	C 418	N 129	O 113	S 1	0	0
2	F	78	Total 618	C 391	N 120	O 106	S 1	0	0
2	b	83	Total 661	C 418	N 129	O 113	S 1	0	0
2	f	78	Total 618	C 391	N 120	O 106	S 1	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
B	0	MET	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
F	0	MET	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
b	0	MET	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
f	0	MET	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	103	Total 796	C 502	N 155	O 139	0	0
3	G	105	Total 810	C 511	N 158	O 141	0	0
3	c	103	Total 796	C 502	N 155	O 139	0	0
3	g	105	Total 810	C 511	N 158	O 141	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
C	0	MET	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
G	0	MET	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
c	0	MET	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
g	0	MET	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			745	468	136	139	2		
4	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
4	d	95	Total	C	N	O	S	0	0
			745	468	136	139	2		
4	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
D	0	MET	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
H	0	MET	-	expression tag	UNP P06899
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
h	0	MET	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	145	Total	C	N	O	P	0	0
			2952	1404	537	867	144		
5	i	145	Total	C	N	O	P	0	0
			2952	1404	537	867	144		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	P	0	0
			2987	1416	558	869	144		
6	j	145	Total	C	N	O	P	0	0
			2987	1416	558	869	144		

- Molecule 7 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	366	Total	C	N	O	S	3	0
			3013	1924	520	554	15		
7	k	366	Total	C	N	O	S	3	0
			3013	1924	520	554	15		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	149	GLY	-	expression tag	UNP Q8N884
K	150	SER	-	expression tag	UNP Q8N884
K	523	GLU	-	expression tag	UNP Q8N884
K	524	ASN	-	expression tag	UNP Q8N884
K	525	LEU	-	expression tag	UNP Q8N884
K	526	TYR	-	expression tag	UNP Q8N884
K	527	PHE	-	expression tag	UNP Q8N884
K	528	GLN	-	expression tag	UNP Q8N884
k	149	GLY	-	expression tag	UNP Q8N884

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Chain	Residue	Modelled	Actual	Comment	Reference
k	150	SER	-	expression tag	UNP Q8N884
k	523	GLU	-	expression tag	UNP Q8N884
k	524	ASN	-	expression tag	UNP Q8N884
k	525	LEU	-	expression tag	UNP Q8N884
k	526	TYR	-	expression tag	UNP Q8N884
k	527	PHE	-	expression tag	UNP Q8N884
k	528	GLN	-	expression tag	UNP Q8N884

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

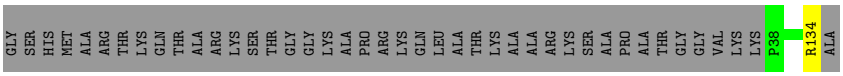
Mol	Chain	Residues	Atoms	AltConf
8	K	1	Total Zn 1 1	0
8	k	1	Total Zn 1 1	0

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.

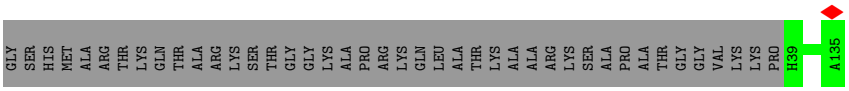
• Molecule 1: Histone H3.1

Chain A:



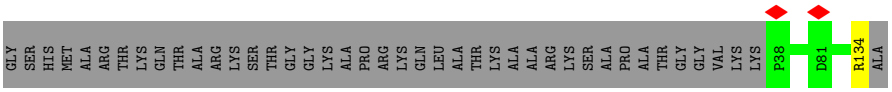
• Molecule 1: Histone H3.1

Chain E:



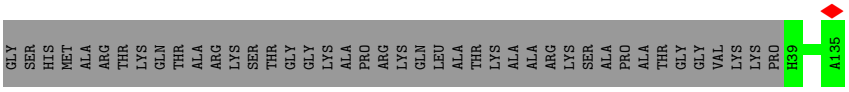
• Molecule 1: Histone H3.1

Chain a:



• Molecule 1: Histone H3.1

Chain e:

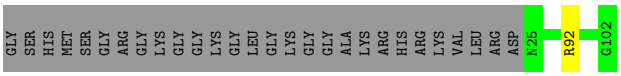


• Molecule 2: Histone H4

Chain B:

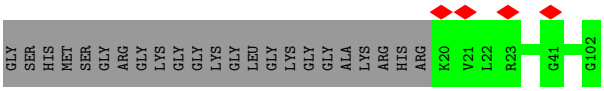
• Molecule 2: Histone H4

Chain F:



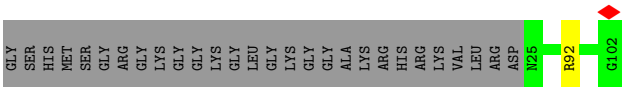
• Molecule 2: Histone H4

Chain b:



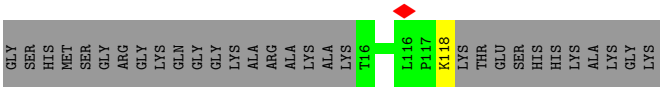
• Molecule 2: Histone H4

Chain f:



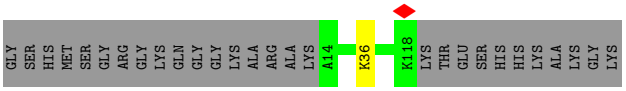
• Molecule 3: Histone H2A type 1-B/E

Chain C:



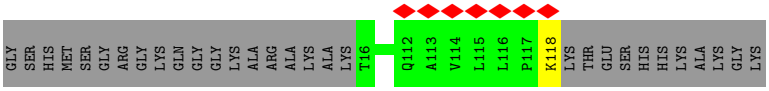
• Molecule 3: Histone H2A type 1-B/E

Chain G:



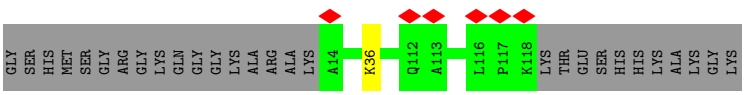
• Molecule 3: Histone H2A type 1-B/E

Chain c:



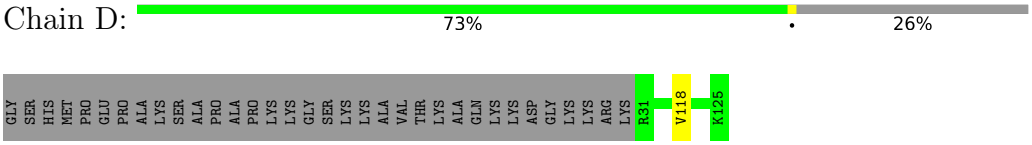
• Molecule 3: Histone H2A type 1-B/E

Chain g:



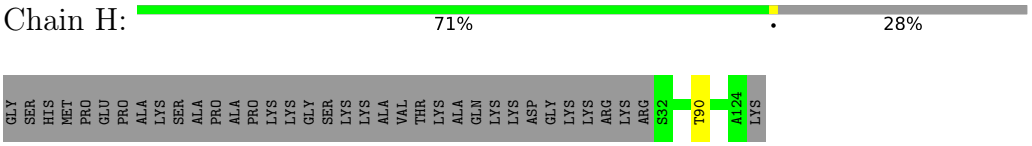
• Molecule 4: Histone H2B type 1-J

Chain D:



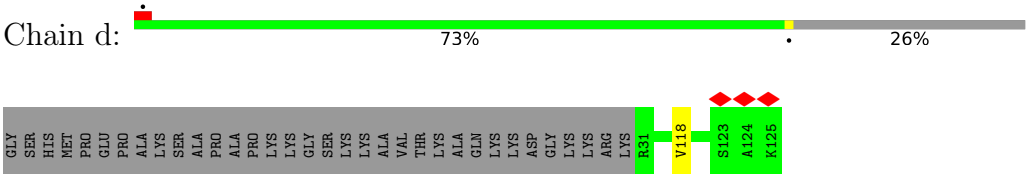
• Molecule 4: Histone H2B type 1-J

Chain H:



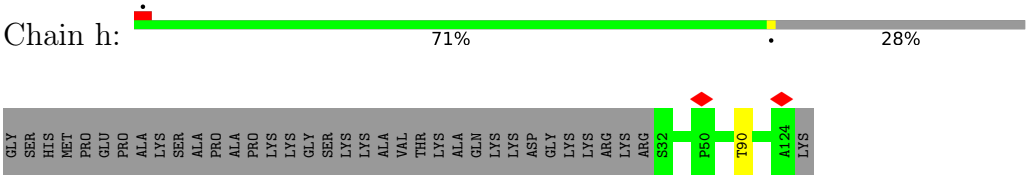
• Molecule 4: Histone H2B type 1-J

Chain d:



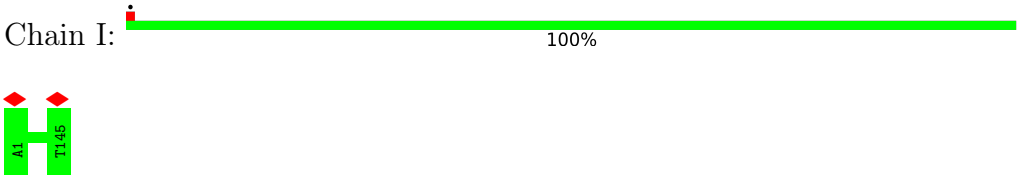
• Molecule 4: Histone H2B type 1-J

Chain h:



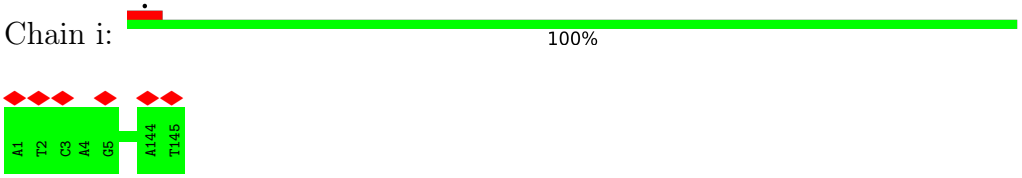
• Molecule 5: DNA (145-MER)

Chain I:



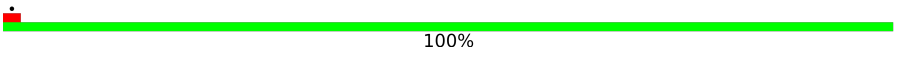
• Molecule 5: DNA (145-MER)

Chain i:



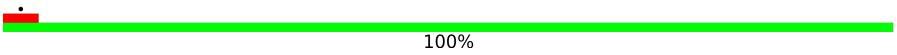
• Molecule 6: DNA (145-MER)

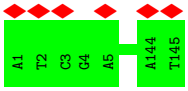
Chain J:



• Molecule 6: DNA (145-MER)

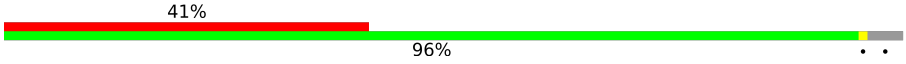
Chain j:

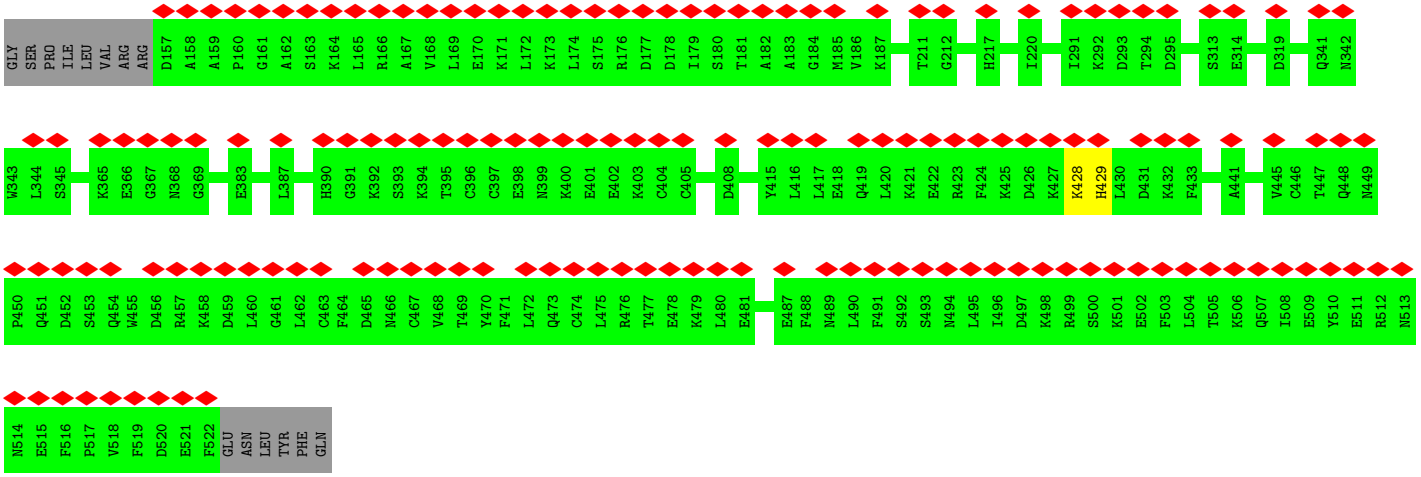




• Molecule 7: Cyclic GMP-AMP synthase

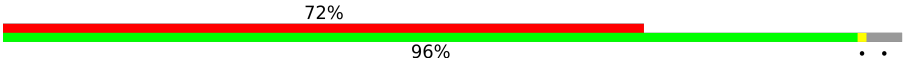
Chain K:

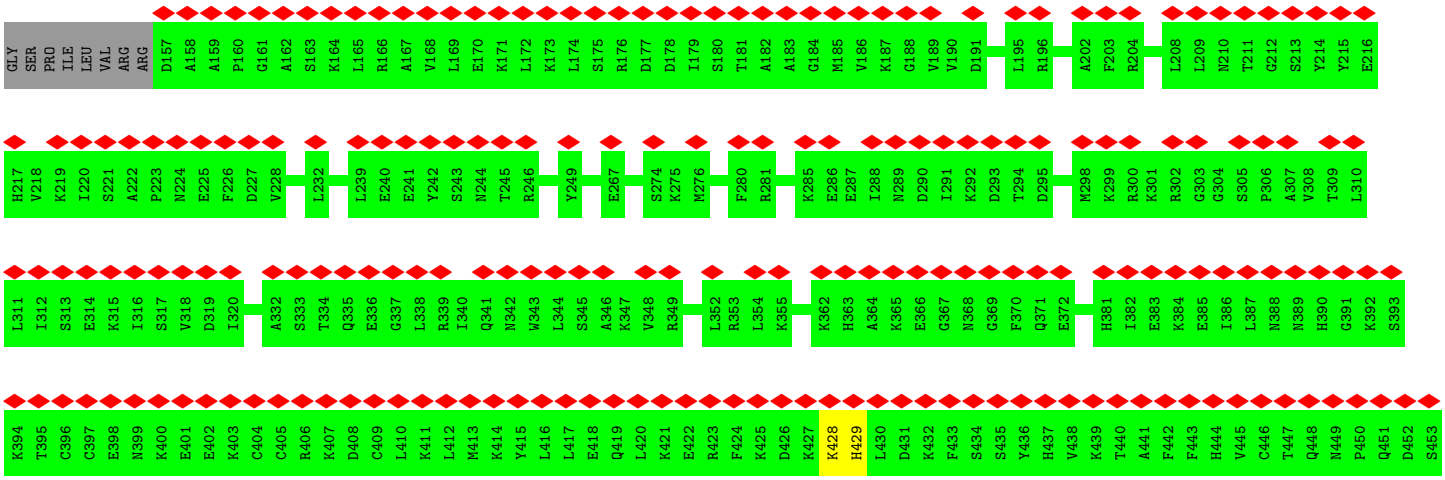




• Molecule 7: Cyclic GMP-AMP synthase

Chain k:





Q454 W455 D456 R457 K458 D459 L460 G461 L462 C463 F464 D465 N466 C467 V468 T469 Y470 F471 L472 Q473 C474 L475 R476 T477 E478 K479 L480 E481 N482 Y483 F484 I485 P486 E487 F488 N489 L490 F491 S492 S493 N494 L495 I496 D497 K498 R499 S500 K501 E502 F503 L504 T505 K506 Q507 I508 E509 Y510 E511 R512 N513
N514 E515 F516 P517 V518 F519 D520 E521 F522 GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0119	Depositor
Map size (Å)	262.5, 262.5, 262.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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

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	0.67	0/813	0.57	0/1090
1	E	0.67	0/810	0.55	0/1086
1	a	0.68	0/813	0.57	0/1090
1	e	0.67	0/810	0.55	0/1086
2	B	0.73	0/668	0.59	0/894
2	F	0.76	0/625	0.58	0/837
2	b	0.73	0/668	0.59	0/894
2	f	0.76	0/625	0.58	0/837
3	C	0.66	0/806	0.58	0/1089
3	G	0.61	0/820	0.54	0/1107
3	c	0.66	0/806	0.58	0/1089
3	g	0.61	0/820	0.54	0/1107
4	D	0.63	0/756	0.52	0/1015
4	H	0.64	0/736	0.56	0/990
4	d	0.63	0/756	0.52	0/1015
4	h	0.64	0/736	0.56	0/990
5	I	1.02	0/3308	0.97	0/5099
5	i	1.02	0/3308	0.98	0/5099
6	J	1.03	0/3354	0.95	0/5180
6	j	1.03	0/3354	0.95	0/5180
7	K	0.30	0/3074	0.49	0/4124
7	k	0.30	0/3074	0.48	0/4124
All	All	0.80	0/31540	0.76	0/45022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
1	E	95/139 (68%)	95 (100%)	0	0	100	100
1	a	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
1	e	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
2	B	81/106 (76%)	74 (91%)	7 (9%)	0	100	100
2	F	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
2	b	81/106 (76%)	74 (91%)	7 (9%)	0	100	100
2	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
3	C	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
3	G	103/133 (77%)	93 (90%)	10 (10%)	0	100	100
3	c	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
3	g	103/133 (77%)	93 (90%)	10 (10%)	0	100	100
4	D	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
4	H	91/129 (70%)	83 (91%)	8 (9%)	0	100	100
4	d	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
4	h	91/129 (70%)	83 (91%)	8 (9%)	0	100	100
7	K	365/380 (96%)	351 (96%)	14 (4%)	0	100	100
7	k	365/380 (96%)	351 (96%)	14 (4%)	0	100	100
All	All	2200/2788 (79%)	2079 (94%)	121 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	85/113 (75%)	84 (99%)	1 (1%)	71	83
1	E	84/113 (74%)	84 (100%)	0	100	100
1	a	85/113 (75%)	84 (99%)	1 (1%)	71	83
1	e	84/113 (74%)	84 (100%)	0	100	100
2	B	68/81 (84%)	68 (100%)	0	100	100
2	F	63/81 (78%)	62 (98%)	1 (2%)	62	79
2	b	68/81 (84%)	68 (100%)	0	100	100
2	f	63/81 (78%)	62 (98%)	1 (2%)	62	79
3	C	82/102 (80%)	81 (99%)	1 (1%)	71	83
3	G	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	c	82/102 (80%)	81 (99%)	1 (1%)	71	83
3	g	83/102 (81%)	82 (99%)	1 (1%)	71	83
4	D	81/107 (76%)	80 (99%)	1 (1%)	71	83
4	H	79/107 (74%)	78 (99%)	1 (1%)	69	82
4	d	81/107 (76%)	80 (99%)	1 (1%)	71	83
4	h	79/107 (74%)	78 (99%)	1 (1%)	69	82
7	K	337/349 (97%)	335 (99%)	2 (1%)	86	91
7	k	337/349 (97%)	335 (99%)	2 (1%)	86	91
All	All	1924/2310 (83%)	1908 (99%)	16 (1%)	82	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
3	C	118	LYS
4	D	118	VAL
2	F	92	ARG
3	G	36	LYS
4	H	90	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	K	428	LYS
7	K	429	HIS
1	a	134	ARG
3	c	118	LYS
4	d	118	VAL
2	f	92	ARG
3	g	36	LYS
4	h	90	THR
7	k	428	LYS
7	k	429	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	ASN
4	D	47	GLN
4	D	63	ASN
3	G	73	ASN
7	K	210	ASN
7	K	264	GLN
7	K	289	ASN
7	K	429	HIS
7	K	437	HIS
7	K	466	ASN
7	K	482	ASN
7	K	514	ASN
3	c	73	ASN
4	d	47	GLN
4	d	63	ASN
3	g	73	ASN
7	k	210	ASN
7	k	264	GLN
7	k	289	ASN
7	k	429	HIS
7	k	437	HIS
7	k	466	ASN
7	k	482	ASN
7	k	514	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

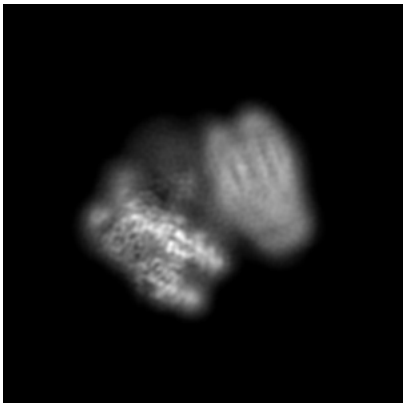
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30267. These allow visual inspection of the internal detail of the map and identification of artifacts.

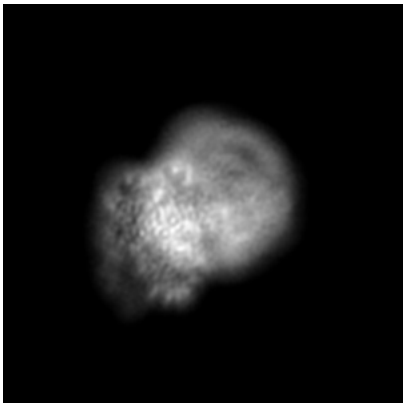
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

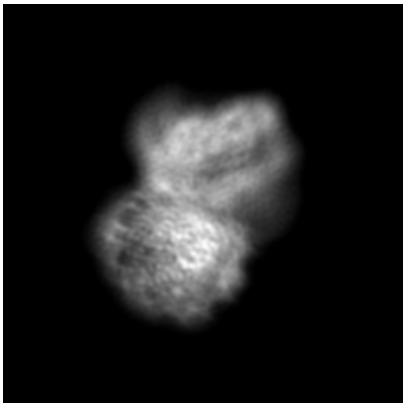
6.1.1 Primary map



X



Y

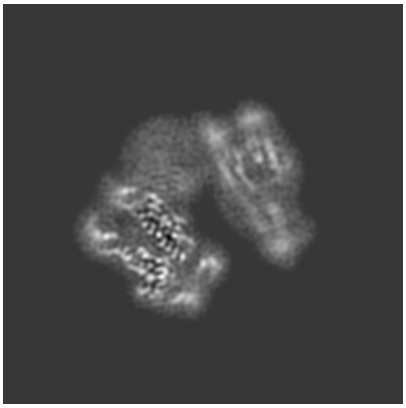


Z

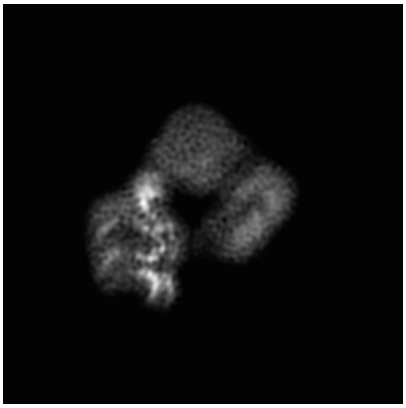
The images above show the map projected in three orthogonal directions.

6.2 Central slices

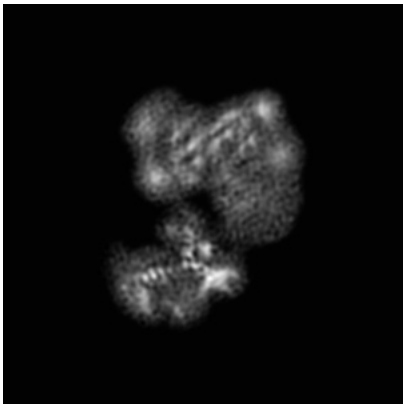
6.2.1 Primary map



X Index: 125



Y Index: 125

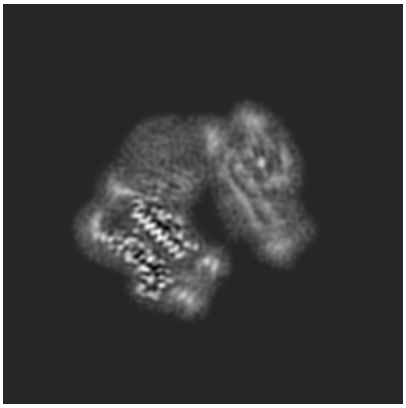


Z Index: 125

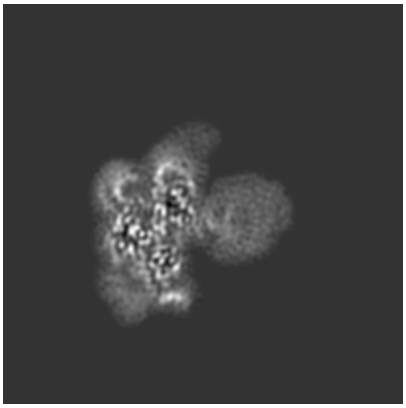
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

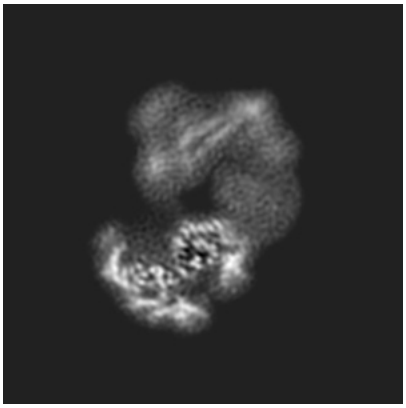
6.3.1 Primary map



X Index: 121



Y Index: 104



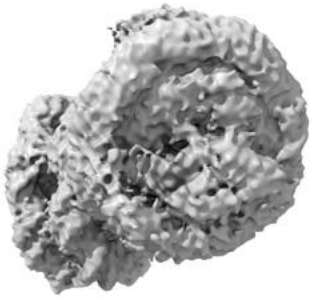
Z Index: 115

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 0.0119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

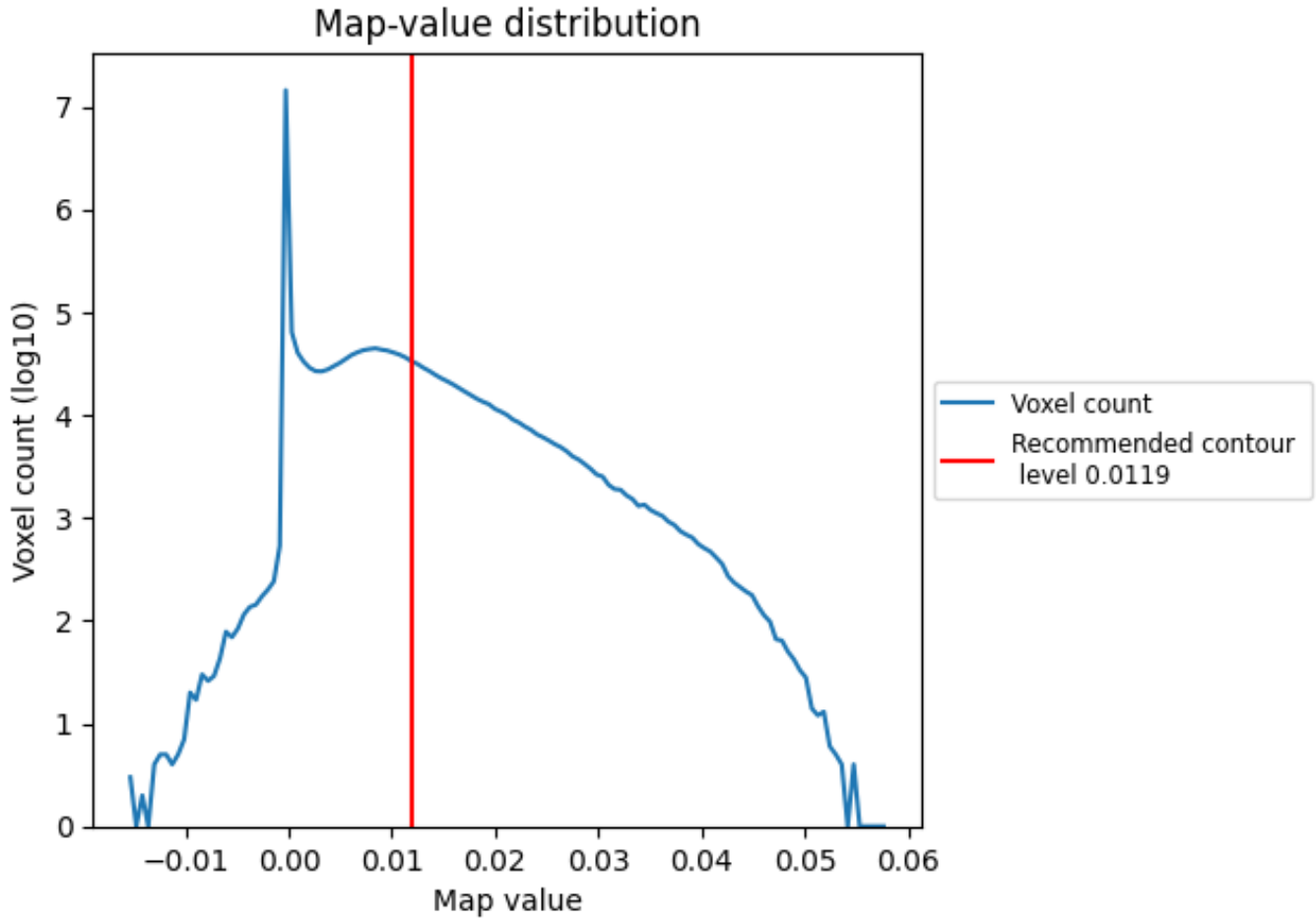
6.5 Mask visualisation (i)

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

7 Map analysis

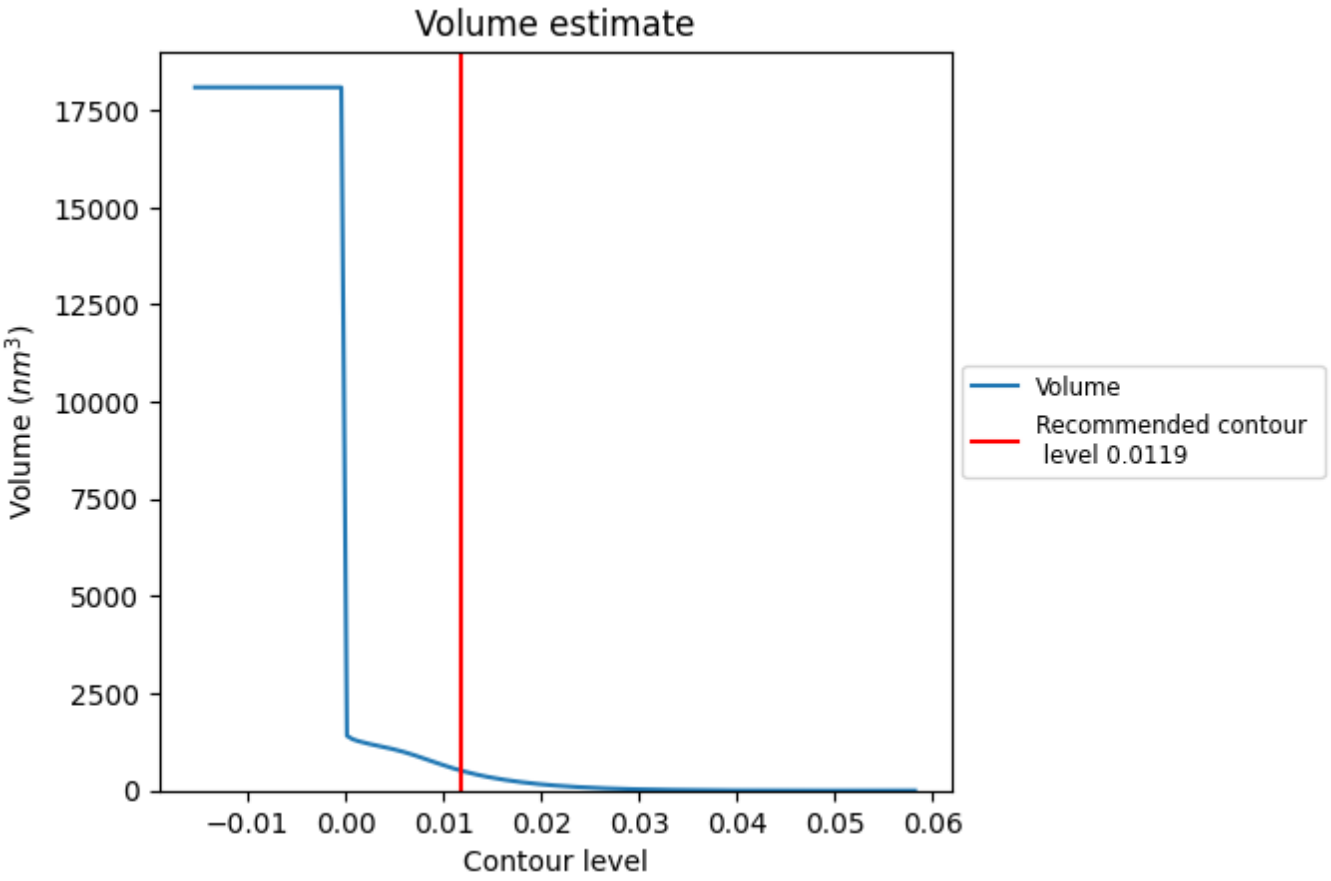
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

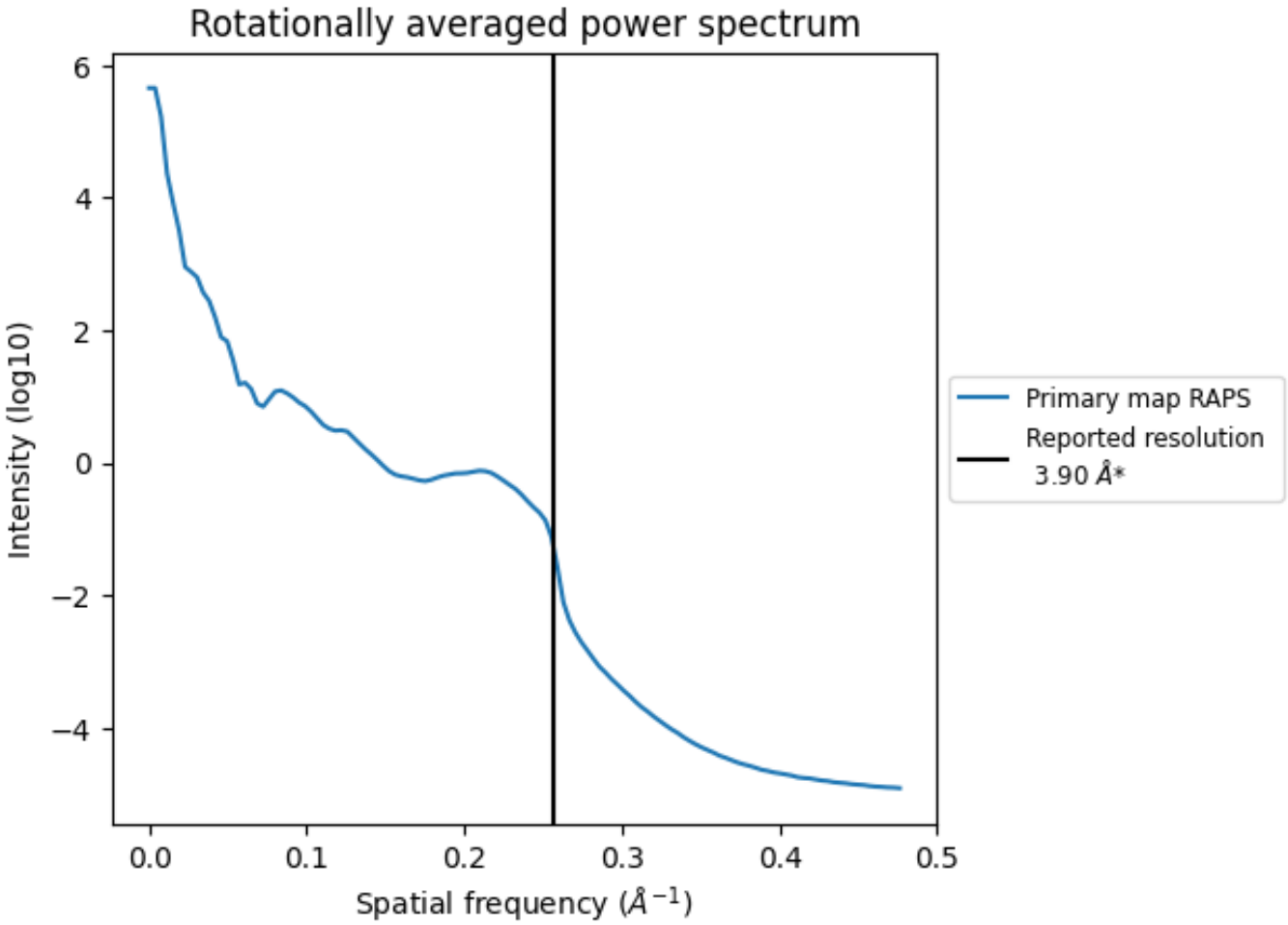
7.2 Volume estimate (i)



The volume at the recommended contour level is 509 nm^3; this corresponds to an approximate mass of 460 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)

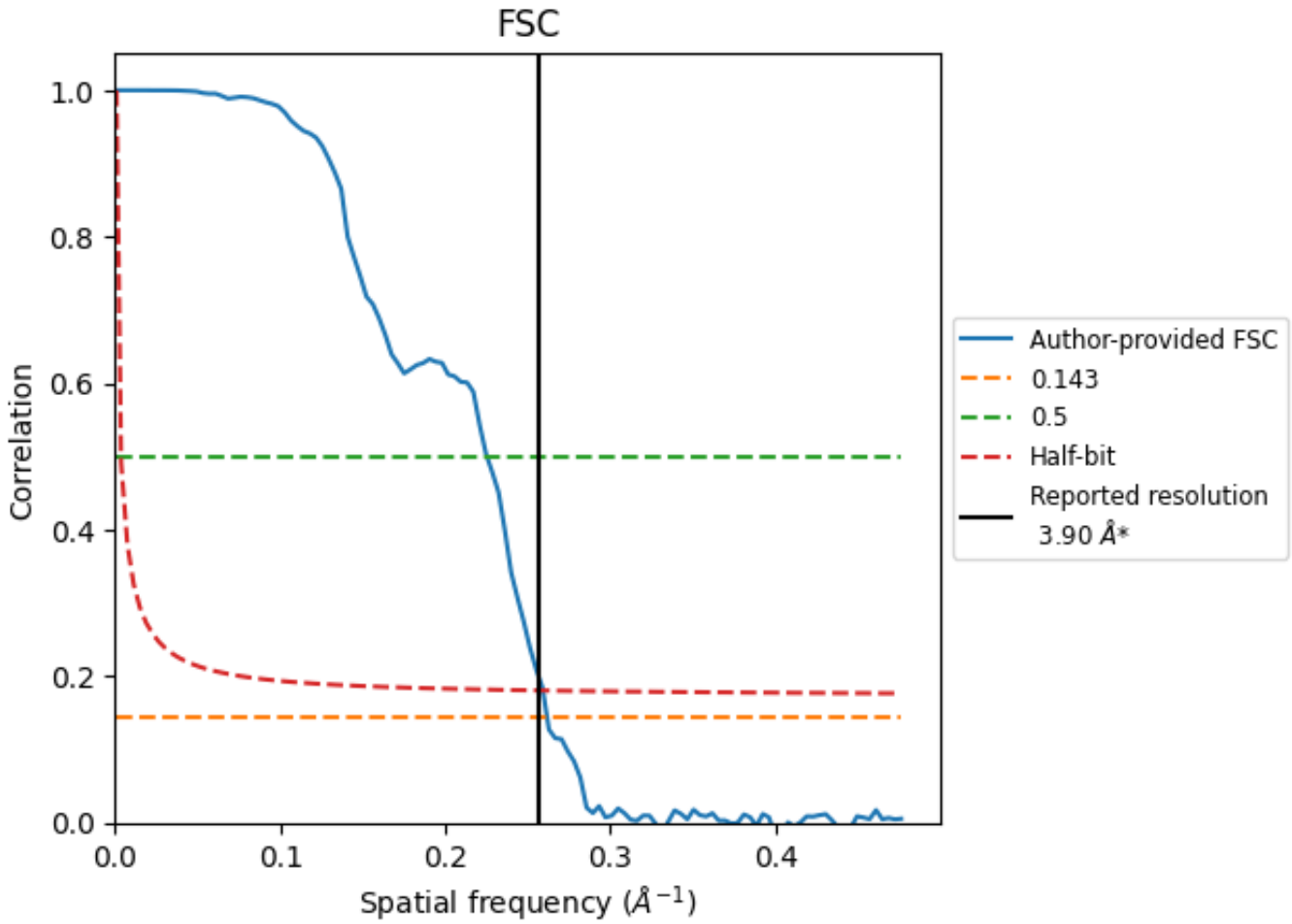


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

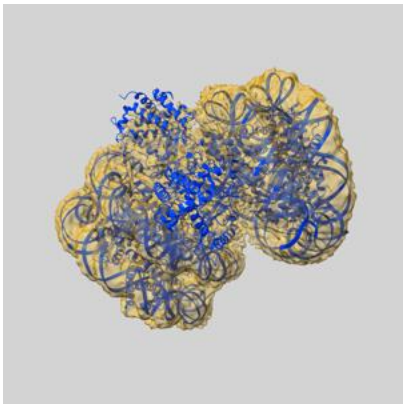
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.82	4.44	3.86
Unmasked-calculated*	-	-	-

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

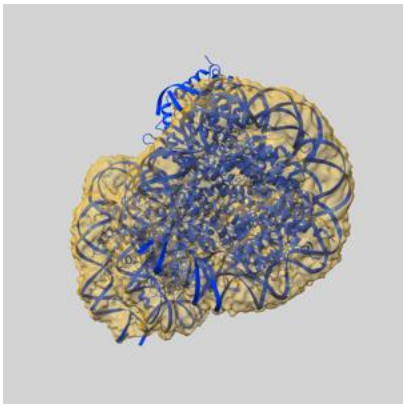
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30267 and PDB model 7C0M. Per-residue inclusion information can be found in section 3 on page 9.

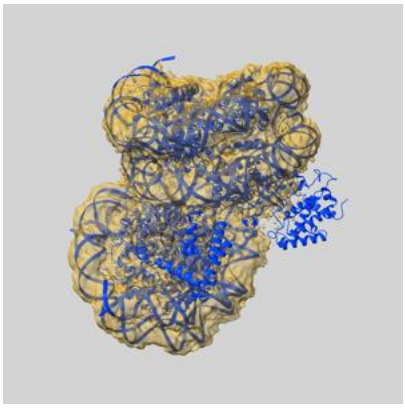
9.1 Map-model overlay



X



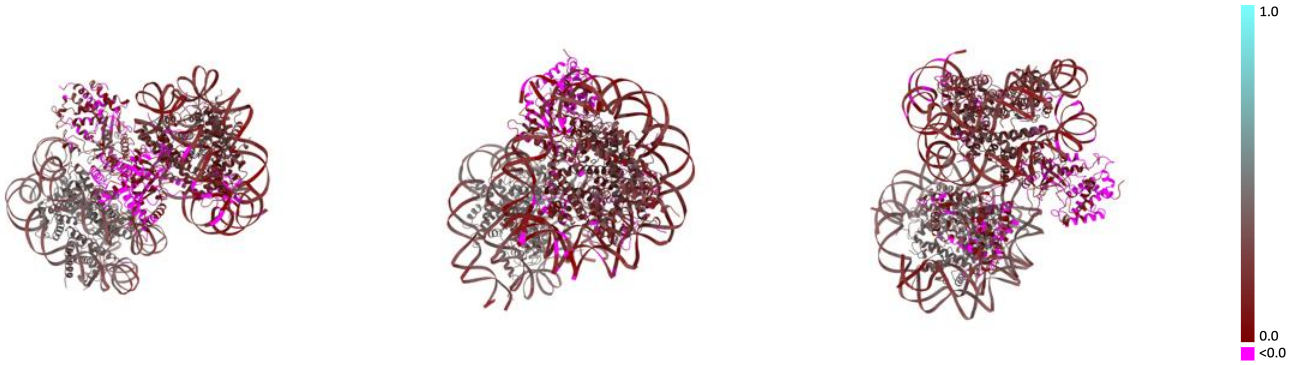
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0119 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.

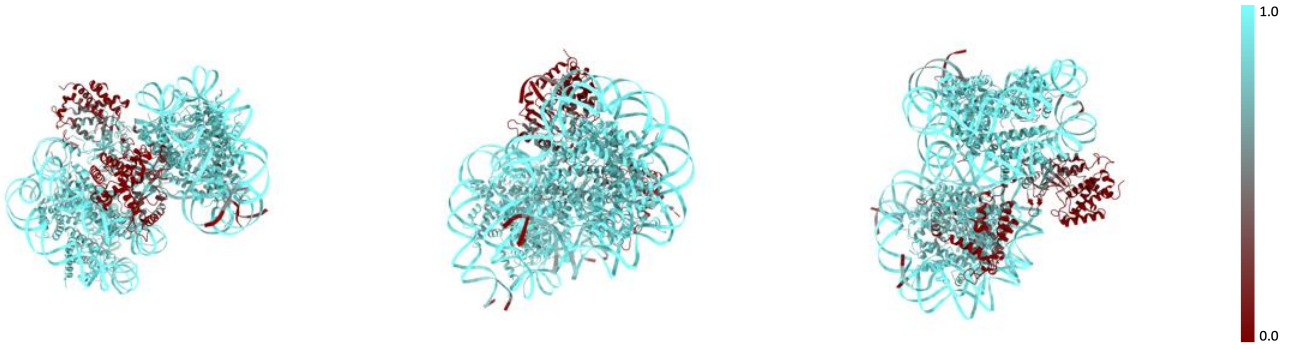
9.2 Q-score mapped to coordinate model (i)



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.

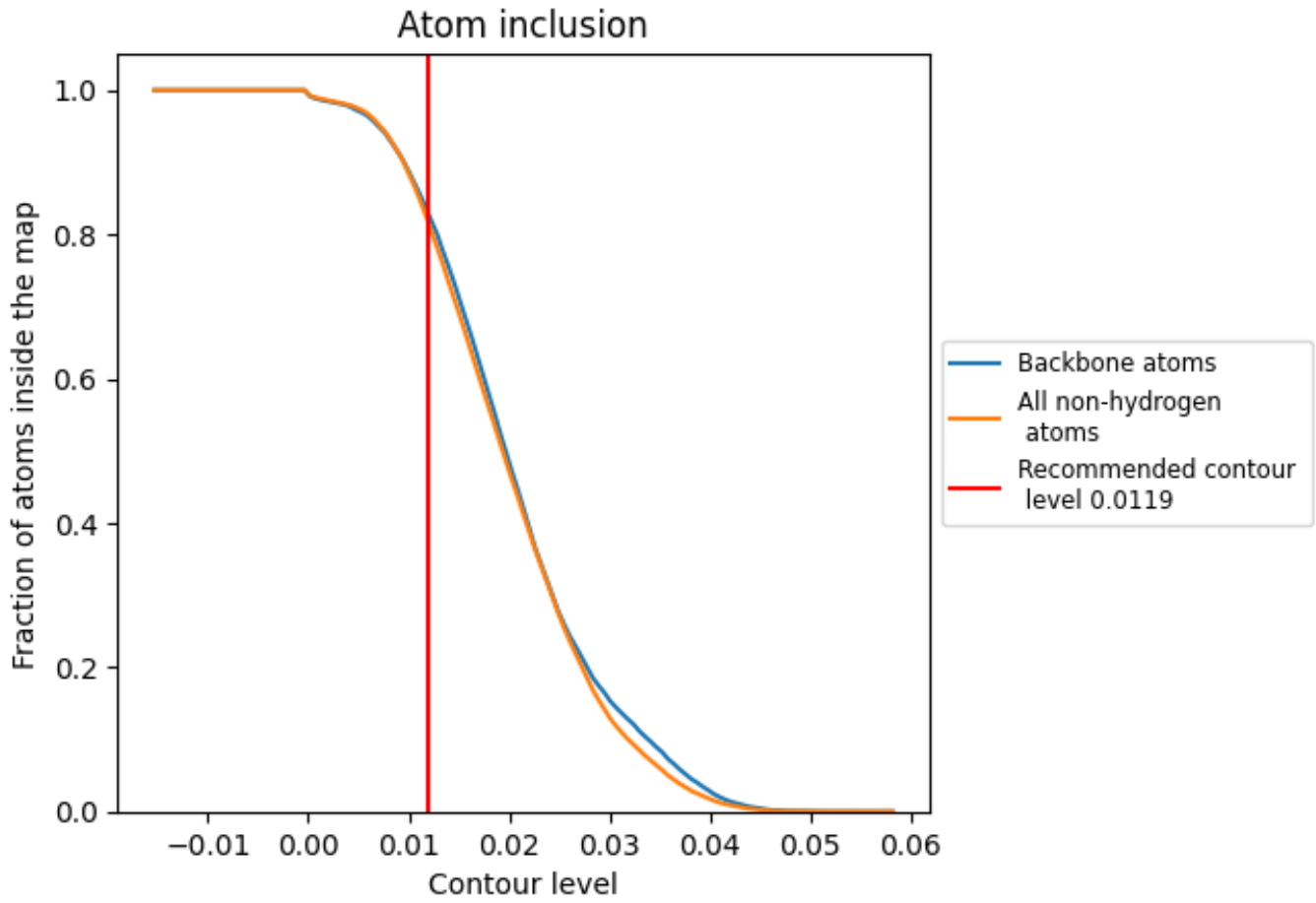
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0119).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8189	0.2250
A	0.9519	0.3820
B	0.9339	0.3980
C	0.9468	0.4110
D	0.9628	0.3930
E	0.9557	0.4010
F	0.9815	0.4290
G	0.9439	0.3940
H	0.9689	0.3920
I	0.9641	0.3010
J	0.9608	0.3050
K	0.4986	0.1440
a	0.9338	0.1330
b	0.9039	0.1540
c	0.9105	0.2140
d	0.9284	0.2120
e	0.9349	0.1980
f	0.9529	0.2350
g	0.9006	0.1850
h	0.9407	0.2230
i	0.9001	0.1440
j	0.8972	0.1380
k	0.2166	0.0310