wwPDB EM Validation Summary Report (i)

Apr 2, 2024 – 10:44 pm BST

PDB ID	:	8OL1
EMDB ID	:	EMD-16936
Title	:	cGAS-Nucleosome in complex with SPSB3-ELOBC (composite structure)
Authors	:	Xu, P.B.; Ablasser, A.
Deposited on	:	2023-03-29
Resolution	:	3.50 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 (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:

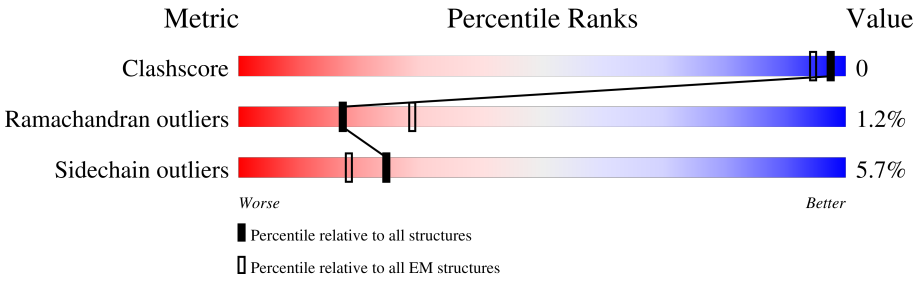
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	98	90% 9%
1	E	98	82% 15%
2	B	81	81% 16%
2	F	81	83% 14%
3	C	108	6% 82% 15%
4	D	95	12% 82% 18%
5	G	107	93% 6%
6	H	94	90% 10%

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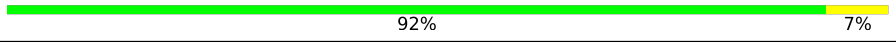
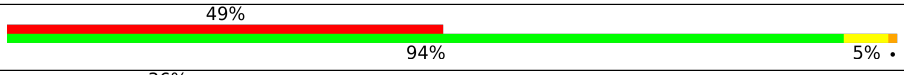
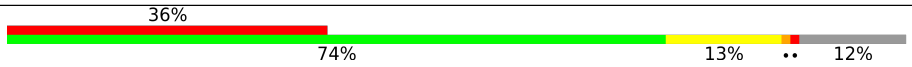
Mol	Chain	Length	Quality of chain
7	I	145	
8	J	145	
9	K	362	
10	L	244	
11	M	112	
12	N	118	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18376 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			810	511	157	140	2		
1	E	98	Total	C	N	O	S	0	0
			810	511	157	140	2		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
2	F	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

- Molecule 3 is a protein called Histone H2A type 1-H.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	108	Total	C	N	O	0	0
			829	523	162	144		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			746	467	136	141	2		

- Molecule 5 is a protein called Histone H2A type 1-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	107	Total	C	N	O	0	0
			822	518	161	143		

- Molecule 6 is a protein called Histone H2B type 1-N.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	94	Total	C	N	O	S	0	0
			737	461	134	140	2		

- Molecule 7 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	145	Total	C	N	O	P	0	0
			2954	1404	537	869	144		

- Molecule 8 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	145	Total	C	N	O	P	0	0
			2985	1414	560	867	144		

- Molecule 9 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	362	Total	C	N	O	S	0	0
			2966	1895	510	546	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	285	ALA	LYS	engineered mutation	UNP Q8N884
K	300	ALA	ARG	engineered mutation	UNP Q8N884
K	428	ALA	LYS	engineered mutation	UNP Q8N884

- Molecule 10 is a protein called SPRY domain-containing SOCS box protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	221	Total	C	N	O	S	0	0
			1737	1093	306	323	15		

- Molecule 11 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	112	Total	C	N	O	S	0	0
			873	553	139	173	8		

- Molecule 12 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	104	Total	C	N	O	S	0	0
			822	520	138	159	5		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

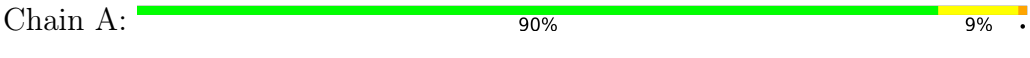
Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Zn	0
			1	1	

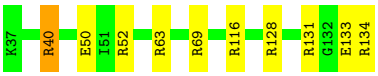
3 Residue-property plots (i)

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 H3.2

Chain A:





• Molecule 1: Histone H3.2

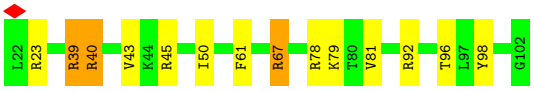
Chain E:

• Molecule 2: Histone H4

Chain B:

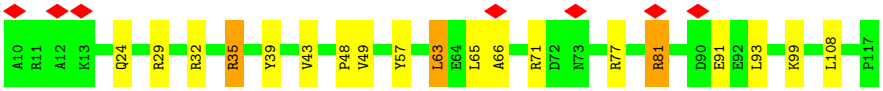
• Molecule 2: Histone H4

Chain F:



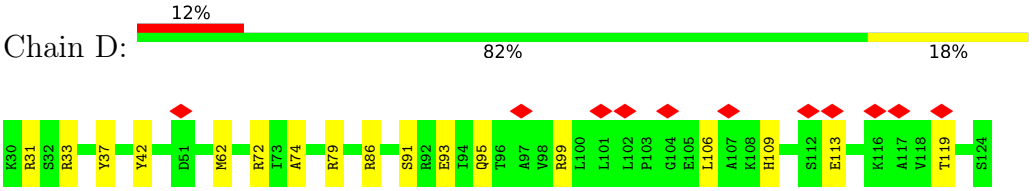
• Molecule 3: Histone H2A type 1-H

Chain C:



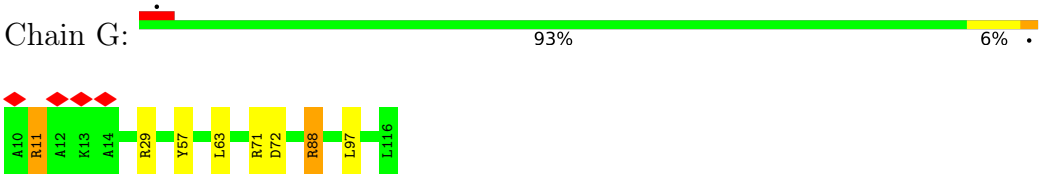
• Molecule 4: Histone H2B type 1-H

Chain D:



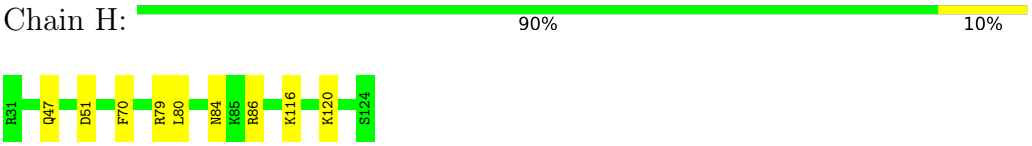
• Molecule 5: Histone H2A type 1-J

Chain G:



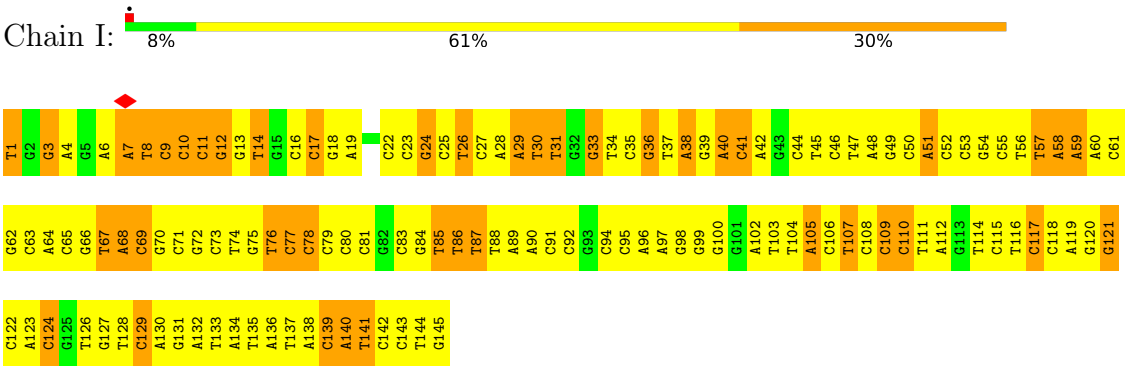
• Molecule 6: Histone H2B type 1-N

Chain H:



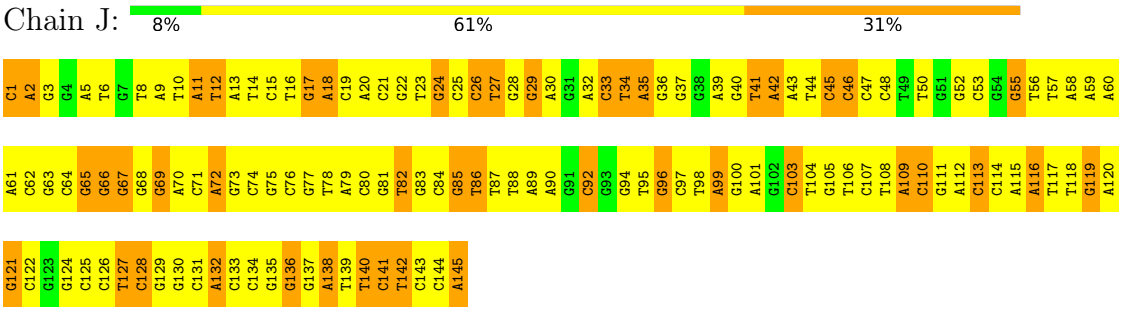
• Molecule 7: DNA (145-MER)

Chain I:



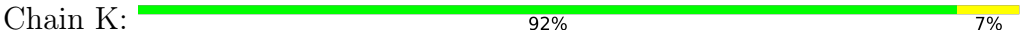
• Molecule 8: DNA (145-MER)

Chain J:

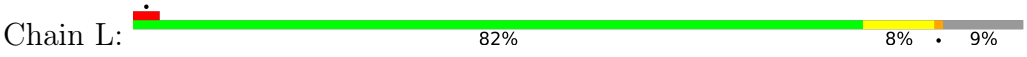


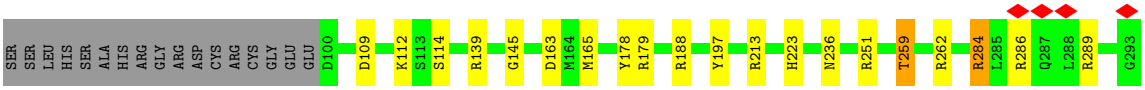
• Molecule 9: Cyclic GMP-AMP synthase

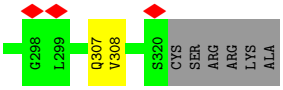
Chain K:



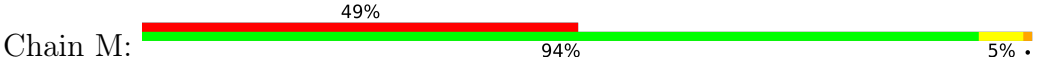
• Molecule 10: SPRY domain-containing SOCS box protein 3

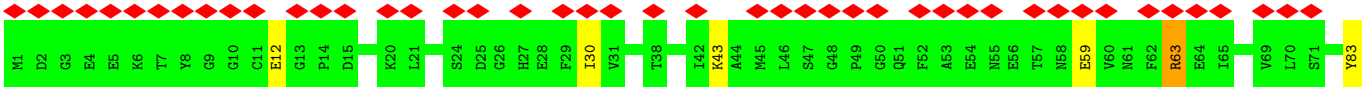


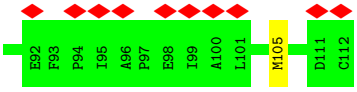




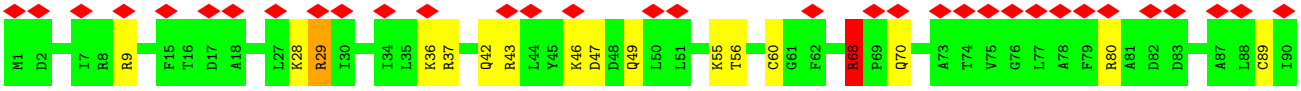
• Molecule 11: Elongin-C

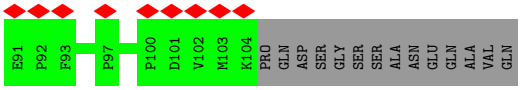






• Molecule 12: Elongin-B





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	592494	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	37.819	Depositor
Minimum map value	-13.291	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.929	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	365.184, 365.184, 365.184	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	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	0.71	0/822	1.25	9/1101 (0.8%)
1	E	0.72	0/822	1.27	9/1101 (0.8%)
2	B	0.75	0/645	1.32	5/862 (0.6%)
2	F	0.75	0/653	1.28	8/873 (0.9%)
3	C	0.71	0/839	1.22	5/1131 (0.4%)
4	D	0.70	0/757	1.20	6/1015 (0.6%)
5	G	0.67	0/831	1.18	4/1119 (0.4%)
6	H	0.65	0/748	1.07	2/1004 (0.2%)
7	I	1.62	1/3310 (0.0%)	2.42	288/5103 (5.6%)
8	J	1.63	0/3352	2.39	281/5176 (5.4%)
9	K	0.64	0/3026	1.02	12/4060 (0.3%)
10	L	0.65	0/1779	1.07	8/2401 (0.3%)
11	M	0.69	0/892	0.97	1/1204 (0.1%)
12	N	0.68	0/838	1.06	5/1132 (0.4%)
All	All	1.10	1/19314 (0.0%)	1.72	643/27282 (2.4%)

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	1
1	E	0	2
2	F	0	1
3	C	0	3
4	D	0	2
5	G	0	2
7	I	0	49
8	J	0	52
9	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	L	0	3
11	M	0	1
12	N	0	3
All	All	0	121

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	83	DC	C4-N4	-5.03	1.29	1.33

The worst 5 of 643 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	138	DA	N1-C6-N6	-10.68	112.19	118.60
7	I	4	DA	N1-C6-N6	-10.19	112.49	118.60
7	I	9	DC	O4'-C1'-N1	9.89	114.92	108.00
8	J	145	DA	N1-C6-N6	-9.76	112.75	118.60
9	K	236	ARG	NE-CZ-NH2	9.32	124.96	120.30

There are no chirality outliers.

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ARG	Sidechain
3	C	32	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	57	TYR	Sidechain
4	D	37	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	810	0	848	0	0
1	E	810	0	848	4	0
2	B	638	0	676	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	646	0	687	4	0
3	C	829	0	889	6	0
4	D	746	0	769	3	0
5	G	822	0	882	0	0
6	H	737	0	756	0	0
7	I	2954	0	1627	0	0
8	J	2985	0	1628	1	0
9	K	2966	0	2994	0	0
10	L	1737	0	1697	1	0
11	M	873	0	845	0	0
12	N	822	0	824	2	0
13	K	1	0	0	0	0
All	All	18376	0	15970	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 0.

The worst 5 of 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)
3:C:39:TYR:CG	4:D:74:ALA:HB1	2.32	0.64
3:C:63:LEU:O	3:C:66:ALA:HB3	2.11	0.51
3:C:108:LEU:H	3:C:108:LEU:HD23	1.75	0.51
1:E:99:TYR:CD2	2:F:61:PHE:CE2	3.00	0.49
3:C:65:LEU:HD13	3:C:93:LEU:HD21	1.94	0.49

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	96/98 (98%)	90 (94%)	6 (6%)	0	100 100
1	E	96/98 (98%)	87 (91%)	9 (9%)	0	100 100
2	B	78/81 (96%)	71 (91%)	5 (6%)	2 (3%)	5 33
2	F	79/81 (98%)	77 (98%)	2 (2%)	0	100 100
3	C	106/108 (98%)	93 (88%)	11 (10%)	2 (2%)	8 40
4	D	93/95 (98%)	86 (92%)	4 (4%)	3 (3%)	4 29
5	G	105/107 (98%)	101 (96%)	4 (4%)	0	100 100
6	H	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14 52
9	K	360/362 (99%)	331 (92%)	24 (7%)	5 (1%)	11 46
10	L	219/244 (90%)	204 (93%)	12 (6%)	3 (1%)	11 46
11	M	110/112 (98%)	102 (93%)	8 (7%)	0	100 100
12	N	102/118 (86%)	90 (88%)	9 (9%)	3 (3%)	4 31
All	All	1536/1598 (96%)	1416 (92%)	101 (7%)	19 (1%)	17 50

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	ASP
4	D	91	SER
9	K	261	PRO
2	B	25	ASN
9	K	235	PRO

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	85/86 (99%)	83 (98%)	2 (2%)	49 76
1	E	85/86 (99%)	77 (91%)	8 (9%)	8 35
2	B	65/66 (98%)	59 (91%)	6 (9%)	9 36
2	F	66/66 (100%)	59 (89%)	7 (11%)	6 30

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	83/83 (100%)	79 (95%)	4 (5%)	25 60
4	D	82/82 (100%)	79 (96%)	3 (4%)	34 65
5	G	82/82 (100%)	78 (95%)	4 (5%)	25 59
6	H	81/81 (100%)	75 (93%)	6 (7%)	13 44
9	K	331/331 (100%)	315 (95%)	16 (5%)	25 60
10	L	192/211 (91%)	183 (95%)	9 (5%)	26 60
11	M	96/96 (100%)	90 (94%)	6 (6%)	18 51
12	N	92/103 (89%)	87 (95%)	5 (5%)	22 55
All	All	1340/1373 (98%)	1264 (94%)	76 (6%)	24 53

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	L	112	LYS
12	N	46	LYS
10	L	223	HIS
11	M	12	GLU
12	N	70	GLN

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

Mol	Chain	Res	Type
9	K	419	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 1 ligands modelled in this entry, 1 is 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.

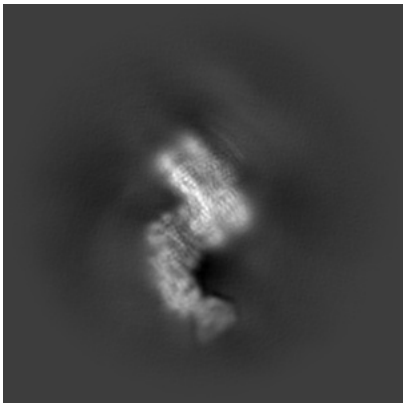
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16936. These allow visual inspection of the internal detail of the map and identification of artifacts.

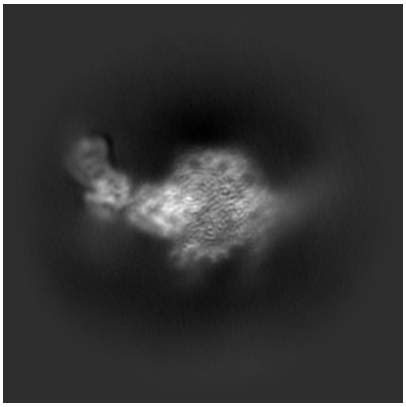
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

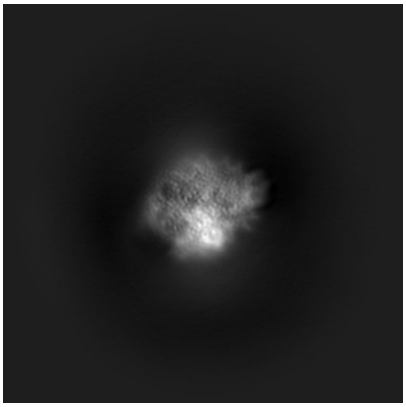
6.1.1 Primary map



X



Y

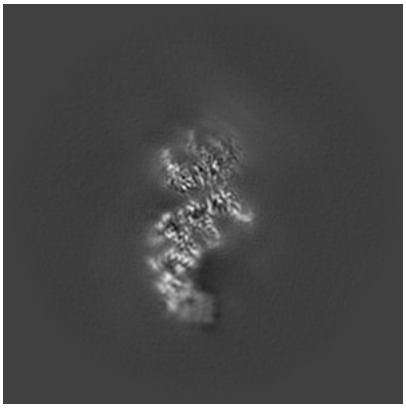


Z

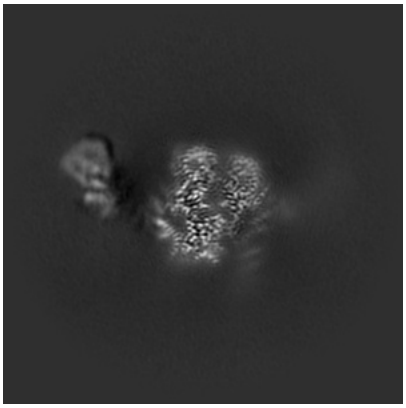
The images above show the map projected in three orthogonal directions.

6.2 Central slices

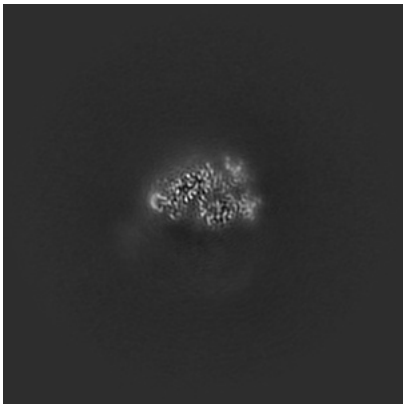
6.2.1 Primary map



X Index: 144



Y Index: 144

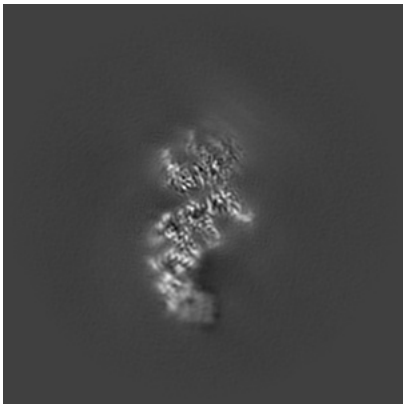


Z Index: 144

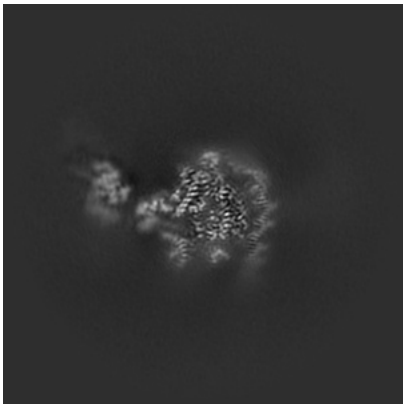
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

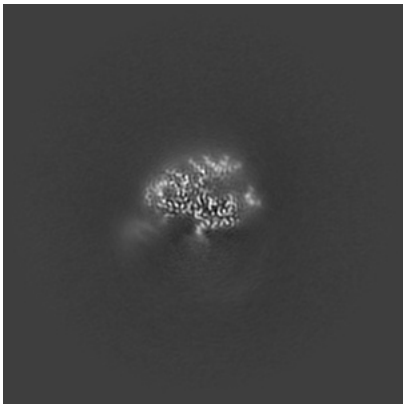
6.3.1 Primary map



X Index: 144



Y Index: 137

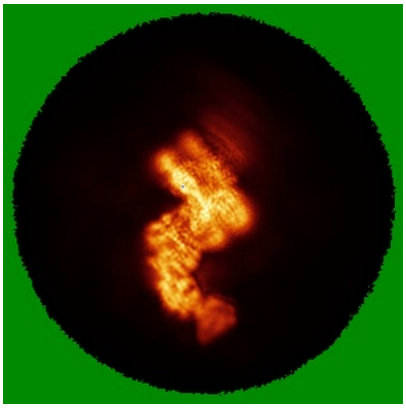


Z Index: 138

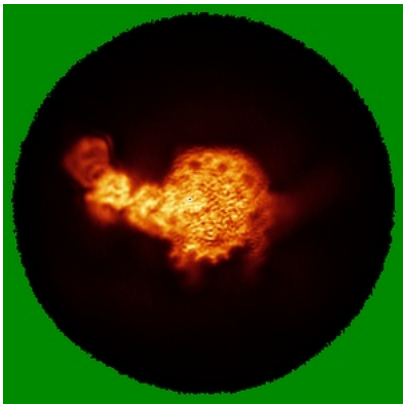
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

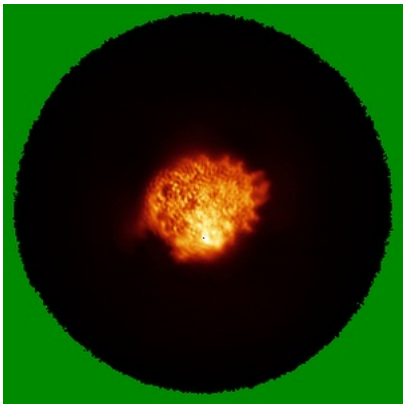
6.4.1 Primary map



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

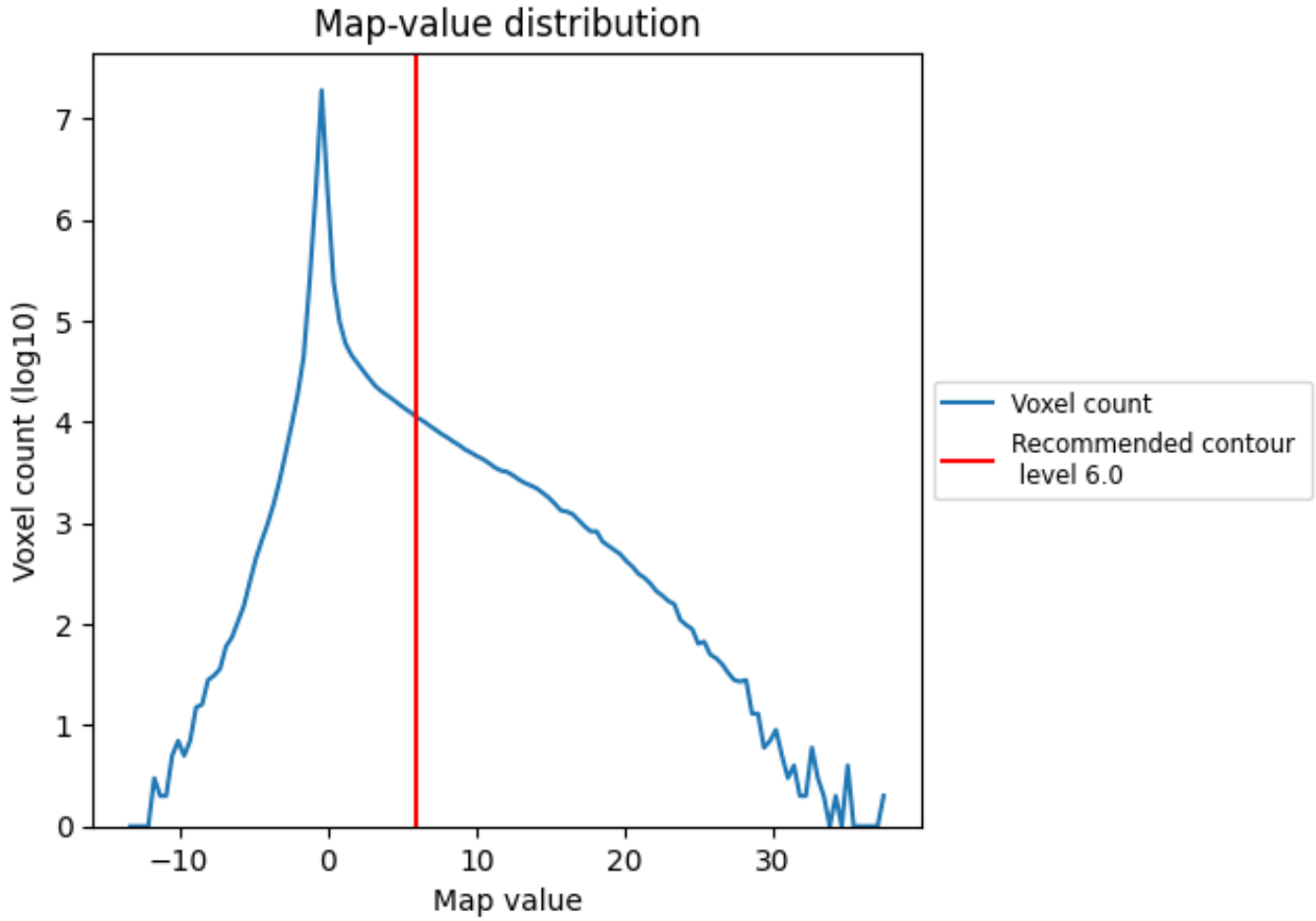
6.6 Mask visualisation (i)

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

7 Map analysis

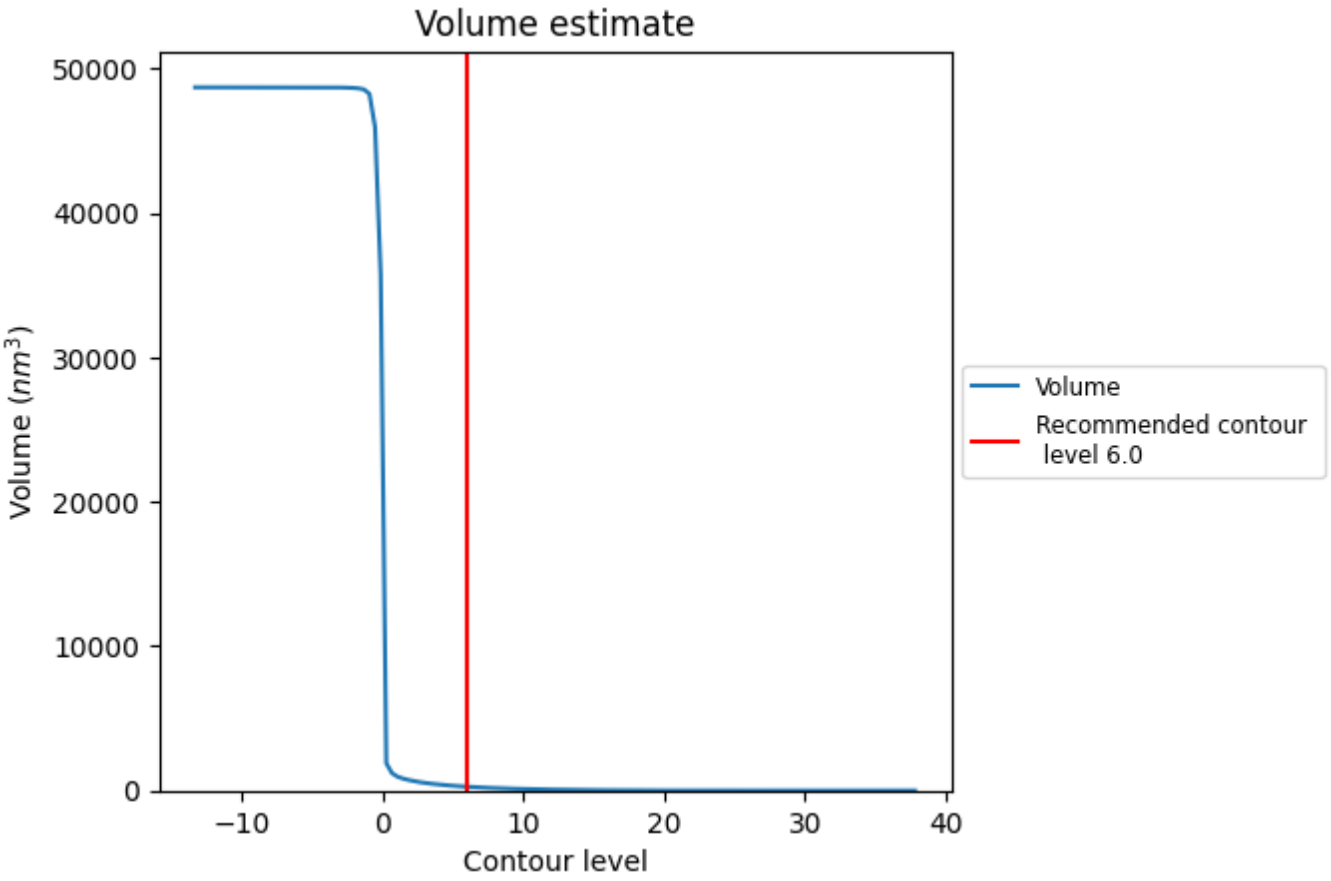
This section contains the results of statistical analysis of the map.

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.

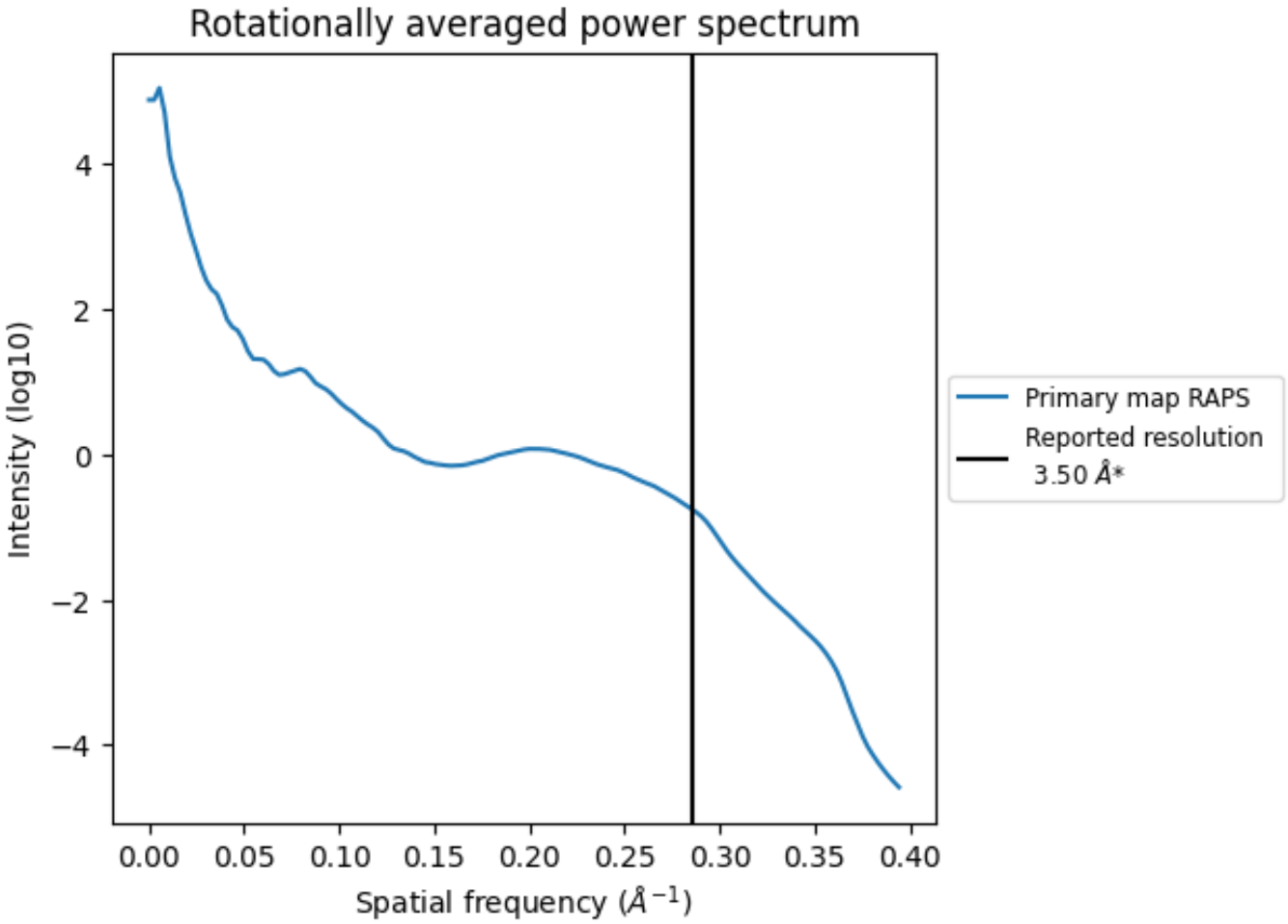
7.2 Volume estimate (i)



The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 241 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 0.286 Å^{-1}

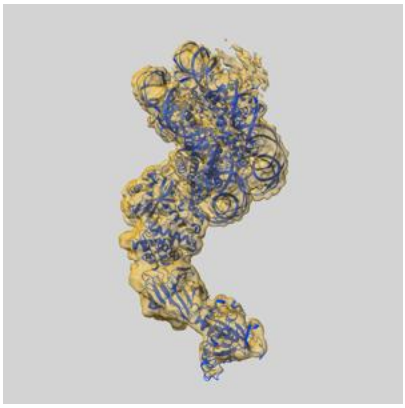
8 Fourier-Shell correlation (i)

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

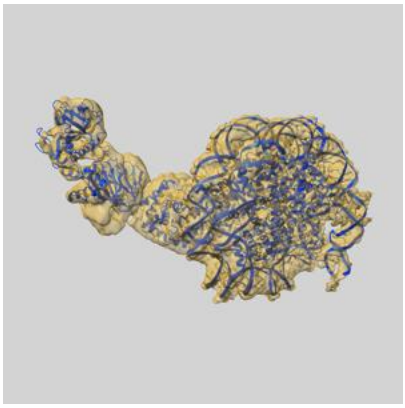
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16936 and PDB model 8OL1. Per-residue inclusion information can be found in section 3 on page 7.

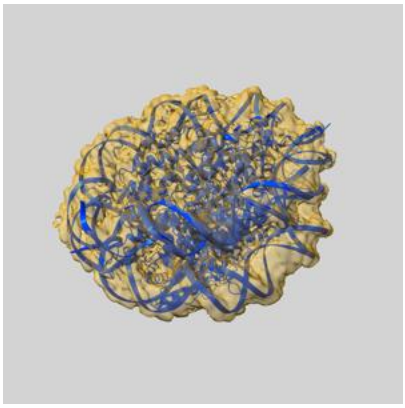
9.1 Map-model overlay



X



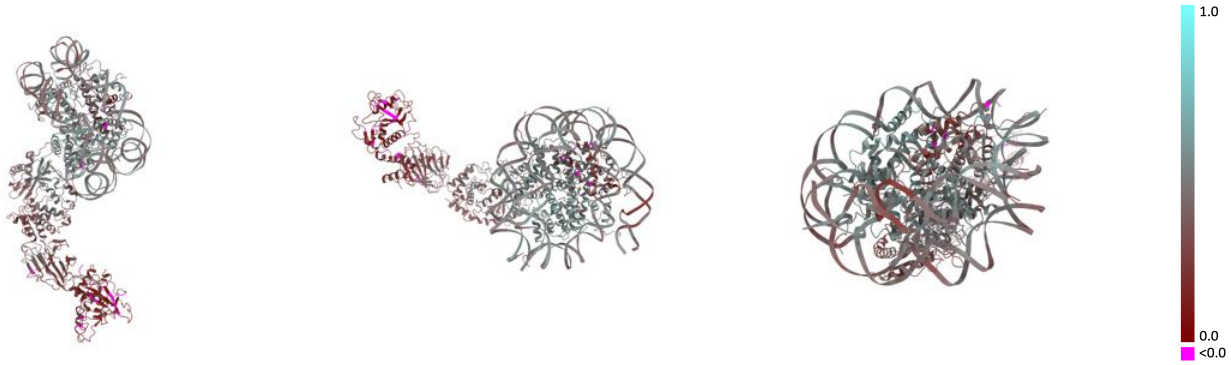
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

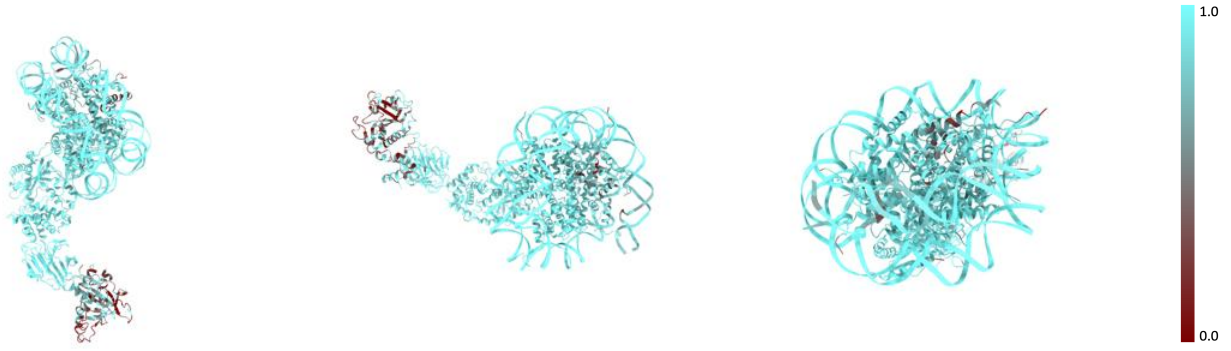
9.2 Q-score mapped to coordinate model



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.

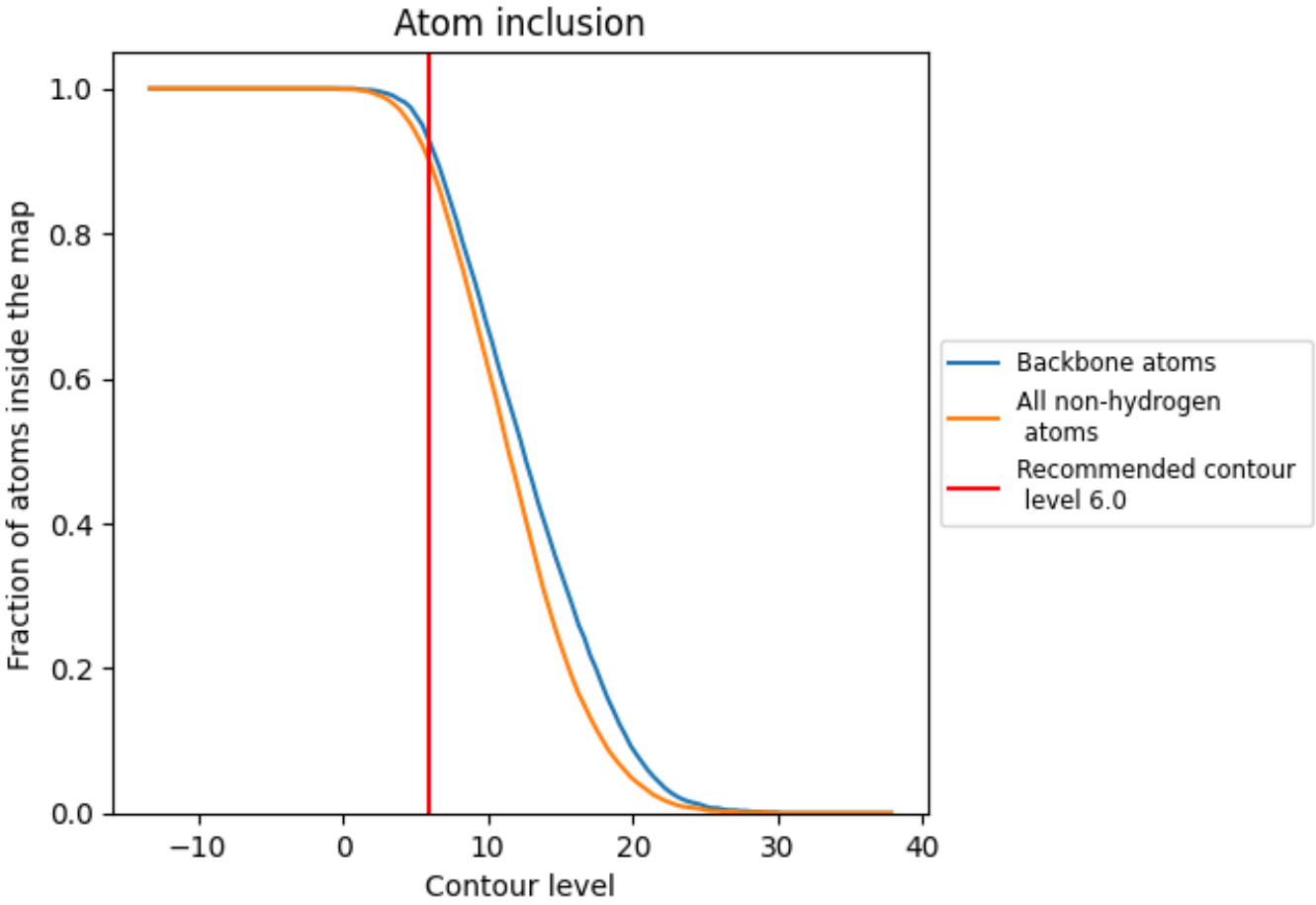
9.3 Atom inclusion mapped to coordinate model



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 (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4000
A	0.9730	0.5200
B	0.9770	0.5110
C	0.7960	0.3770
D	0.7670	0.3400
E	0.9140	0.4890
F	0.9400	0.4990
G	0.9360	0.5040
H	0.9570	0.4970
I	0.9620	0.4490
J	0.9750	0.4500
K	0.9710	0.3650
L	0.9280	0.2880
M	0.4370	0.1750
N	0.4880	0.1610