wwPDB EM Validation Summary Report (i)

May 11, 2026 – 06:15 PM JST

PDB ID	:	9UQ0 / pdb_00009uq0
EMDB ID	:	EMD-64408
Title	:	Structure of human MCM2-7 single hexamer with MCM3-WHD attached to MCM2-CTD
Authors	:	Lam, W.H.; Fan, X.; Zhai, Y.
Deposited on	:	2025-04-29
Resolution	:	3.47 Å(reported)
Based on initial model	:	7W1Y

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:

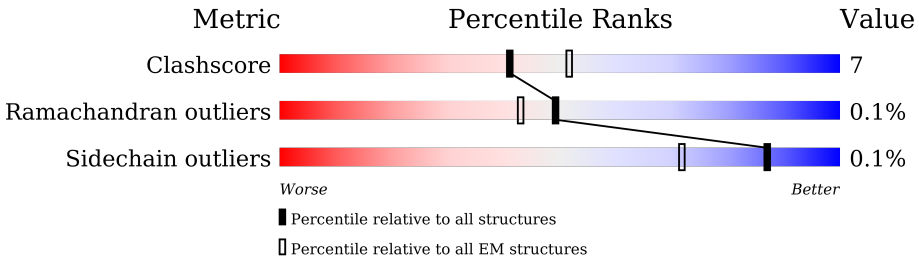
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

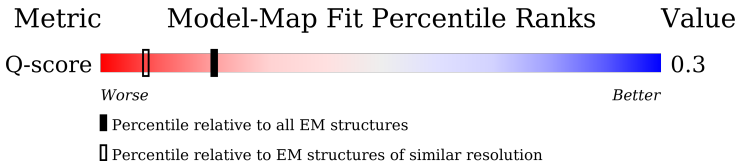
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	2	904	6% 67% 10% 23%
2	3	808	7% 63% 11% 25%
3	4	863	12% 64% 13% 23%
4	5	734	24% 61% 15% 24%

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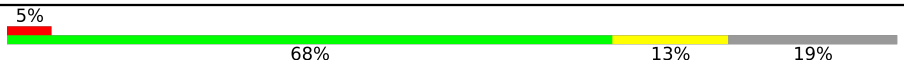
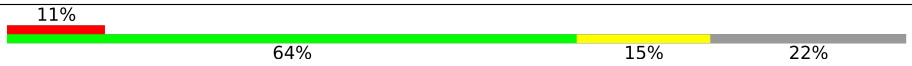
Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 28580 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	697	5342	3365	939	1009	29	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	605	4463	2804	767	870	22	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	663	4919	3091	863	942	23	0	0

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	560	4218	2653	732	811	22	0	0

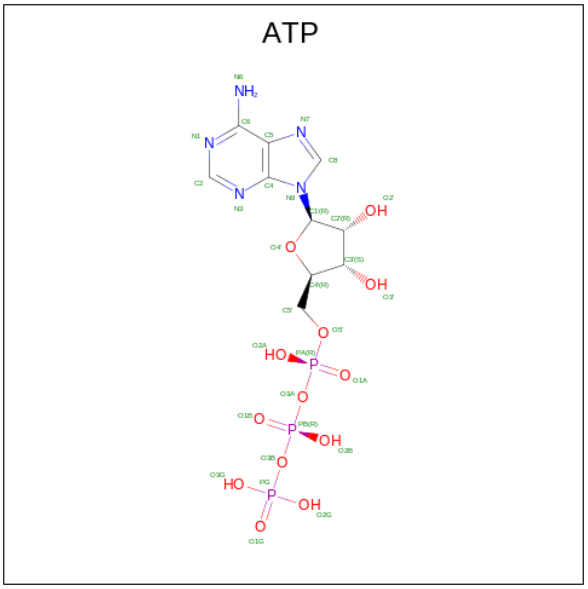
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	667	5250	3299	921	1003	27	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	564	4234	2647	735	828	24	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	4	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	6	1	Total	C	N	O	P	0
			31	10	5	13	3	

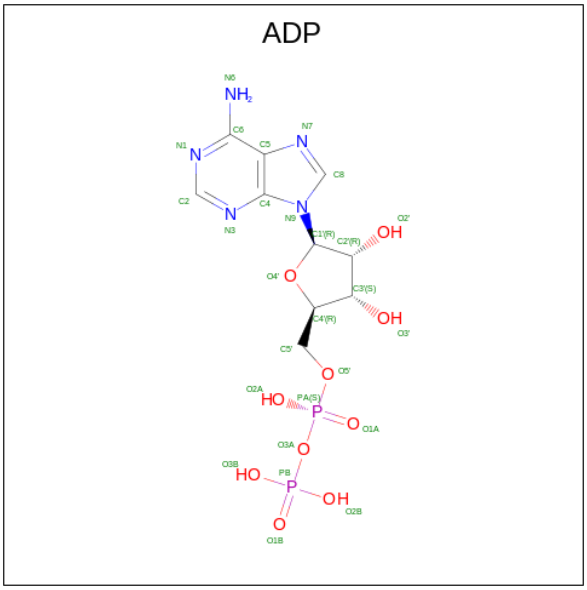
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	2	1	Total	Zn	0
			1	1	
8	4	1	Total	Zn	0
			1	1	
8	6	1	Total	Zn	0
			1	1	
8	7	1	Total	Zn	0
			1	1	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
9	2	1	Total Mg 1 1	0
9	4	1	Total Mg 1 1	0
9	6	1	Total Mg 1 1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



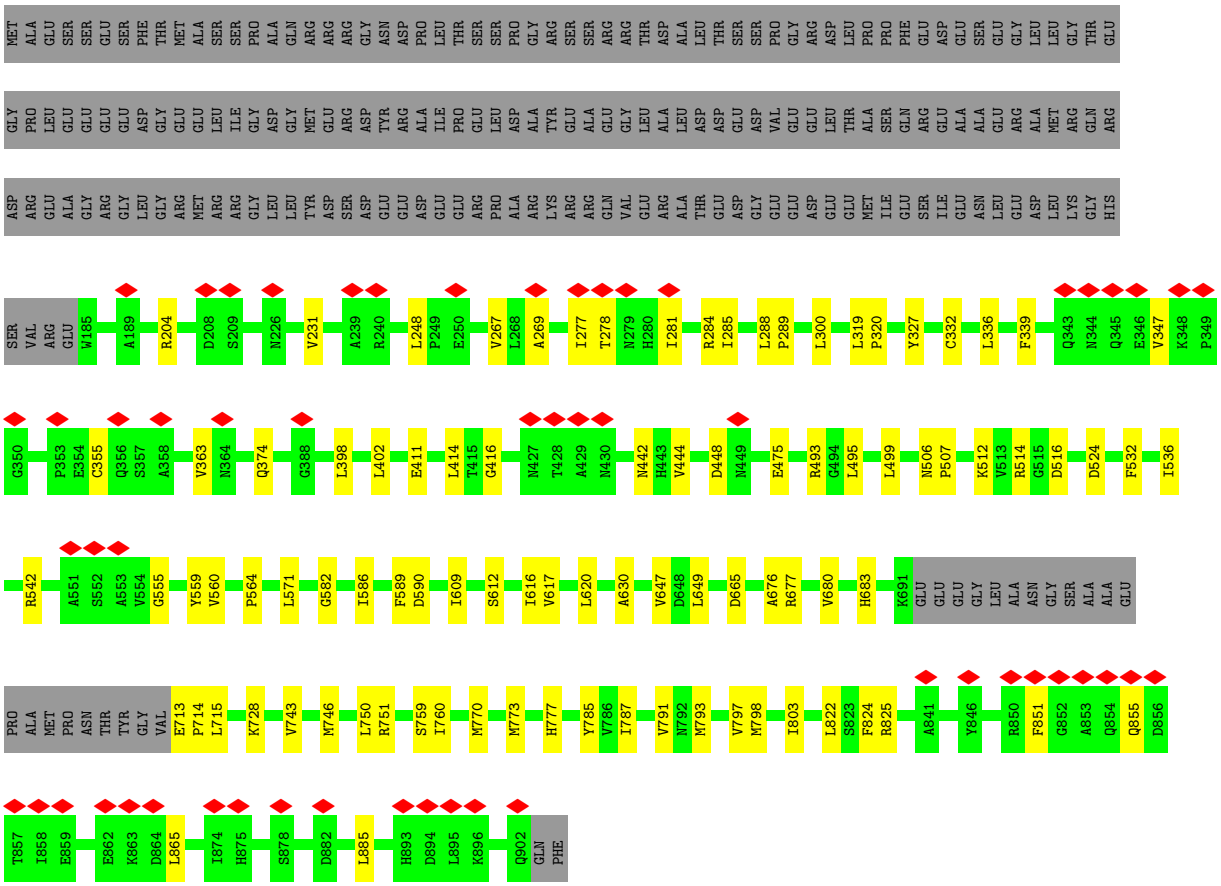
Mol	Chain	Residues	Atoms	AltConf
10	3	1	Total C N O P 27 10 5 10 2	0
10	7	1	Total C N O P 27 10 5 10 2	0

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.

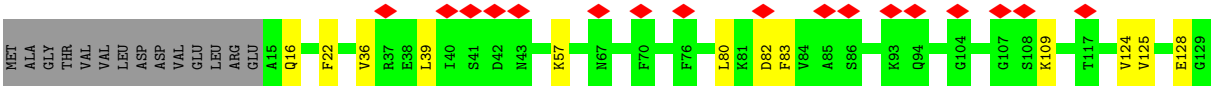
• Molecule 1: DNA replication licensing factor MCM2

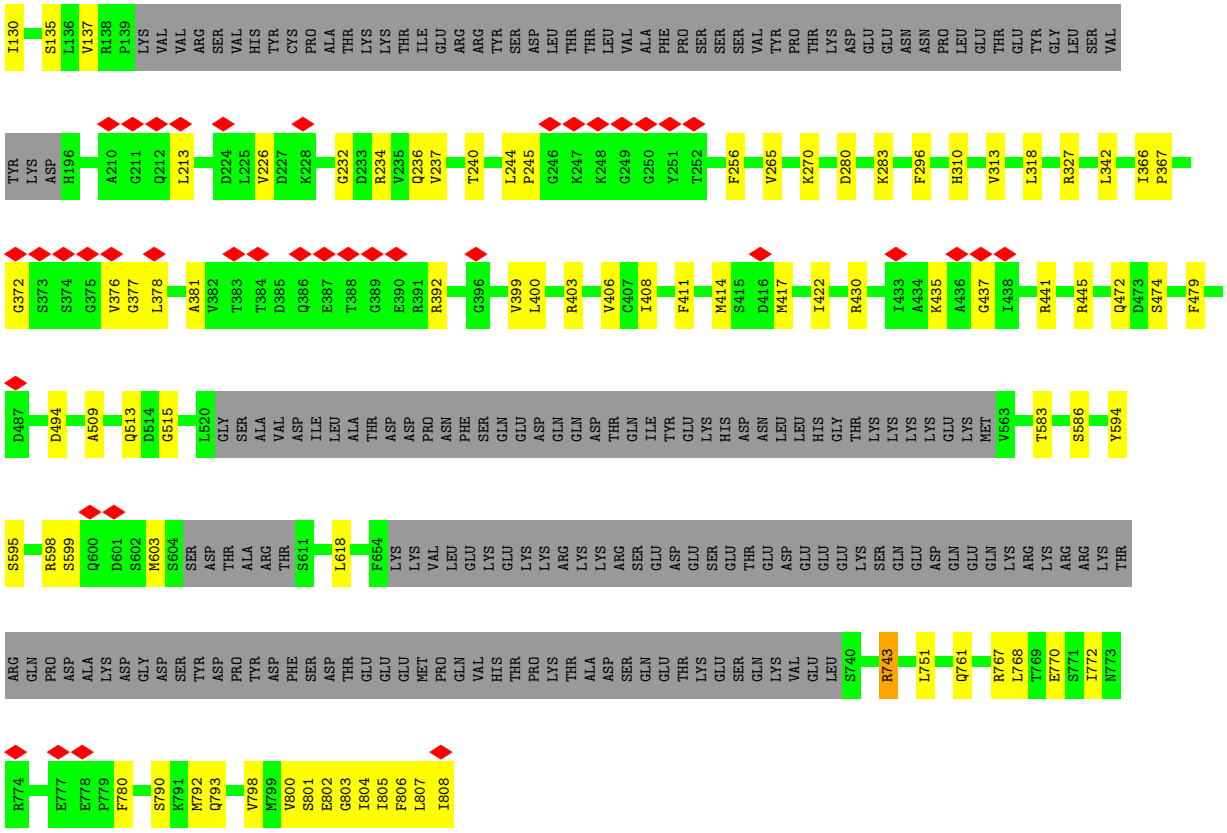
Chain 2:



• Molecule 2: DNA replication licensing factor MCM3

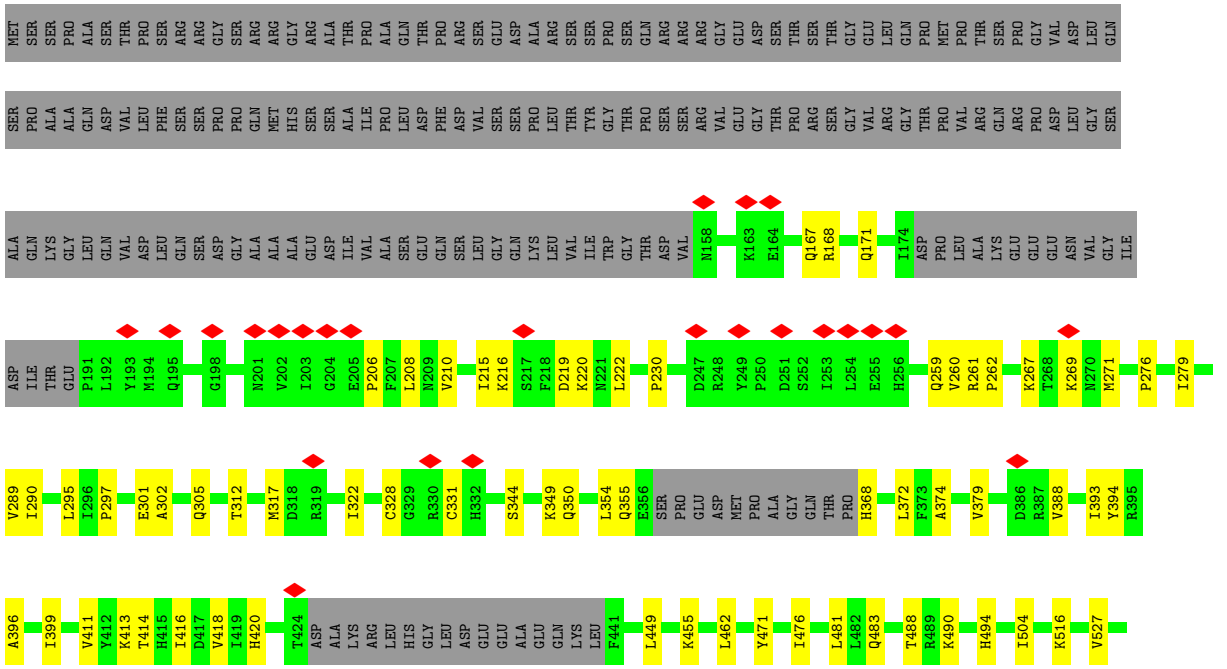
Chain 3:

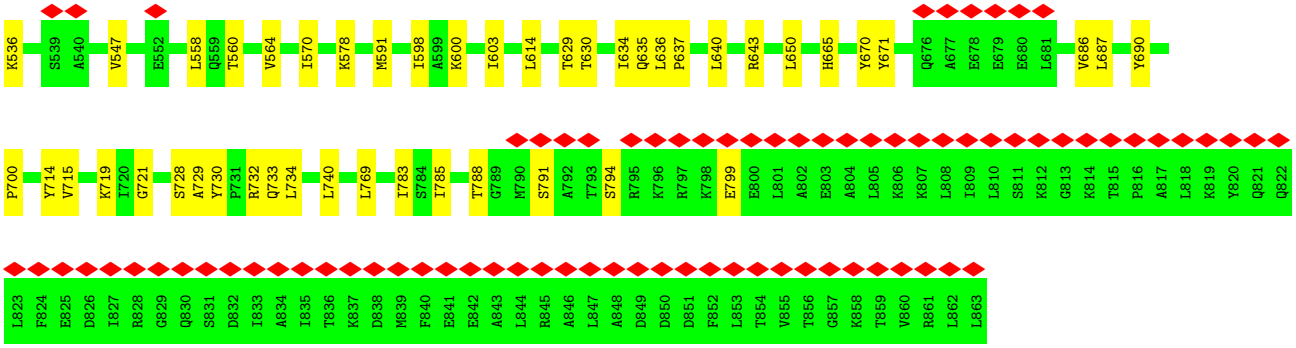




• Molecule 3: DNA replication licensing factor MCM4

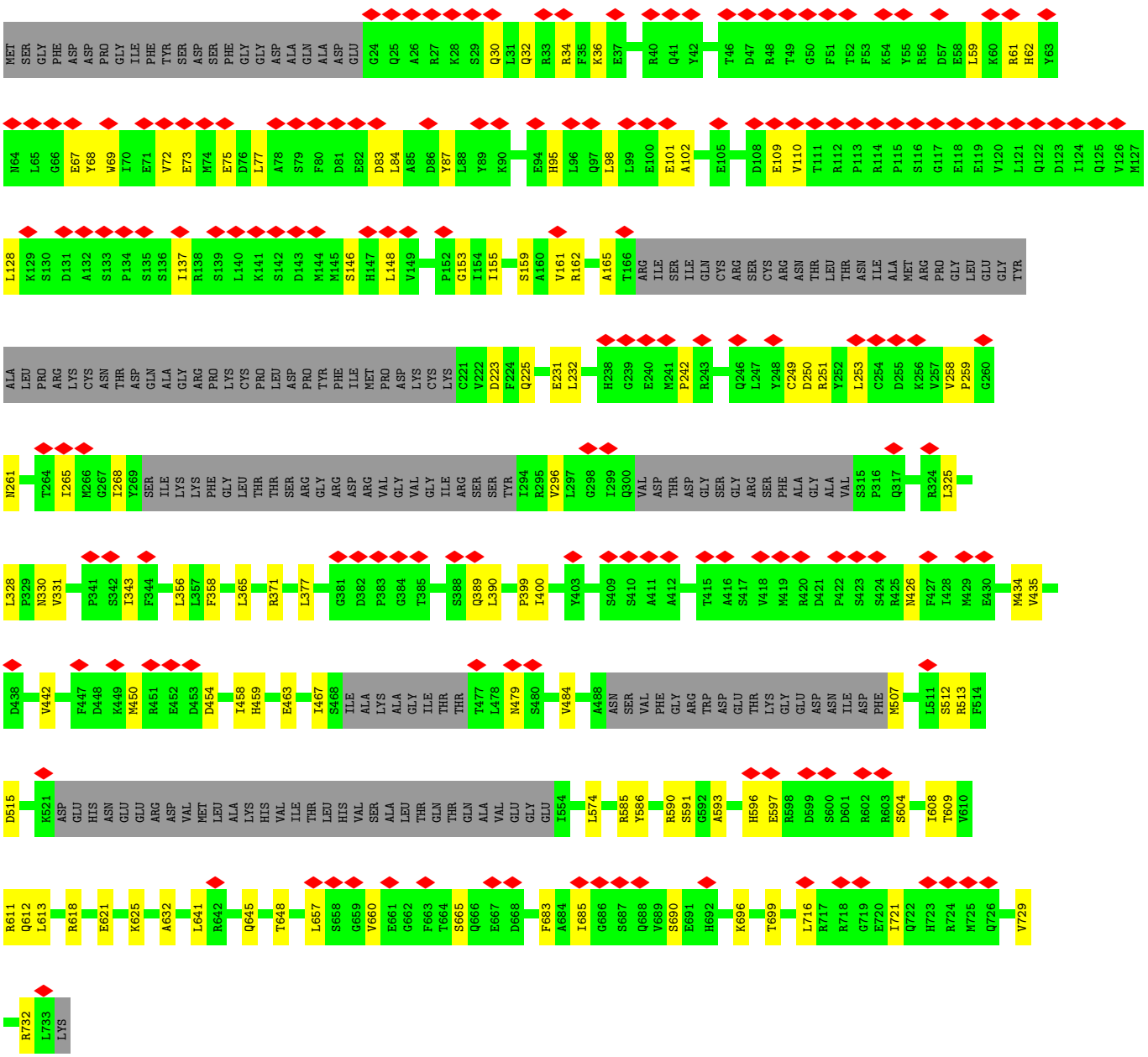
Chain 4:





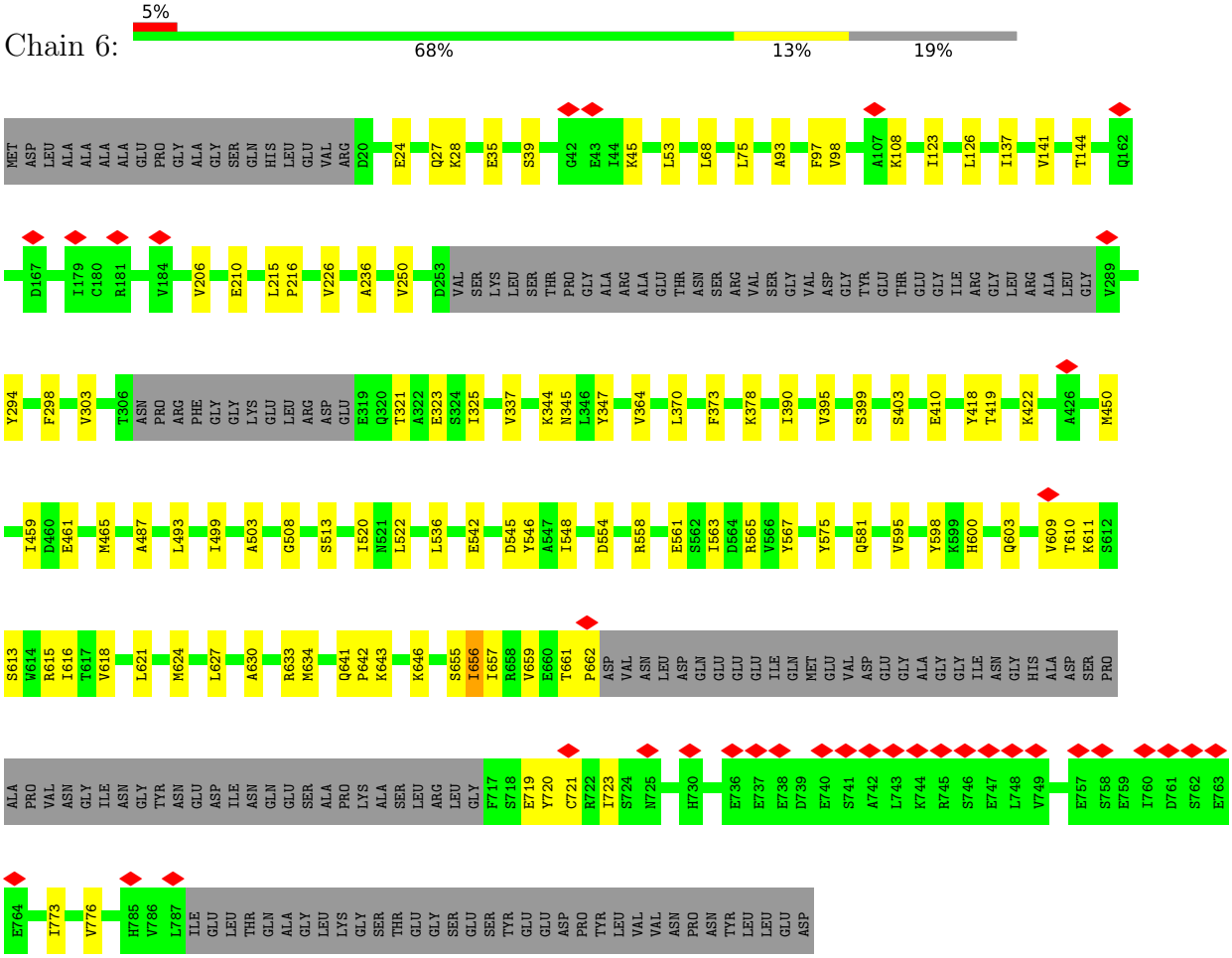
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:



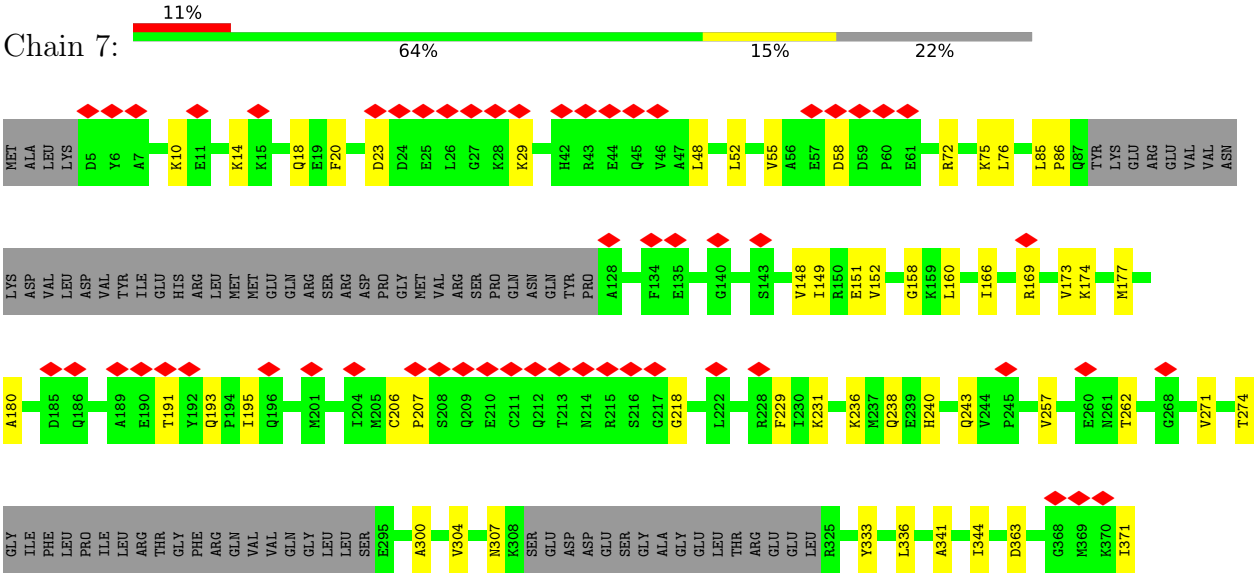
• Molecule 5: DNA replication licensing factor MCM6

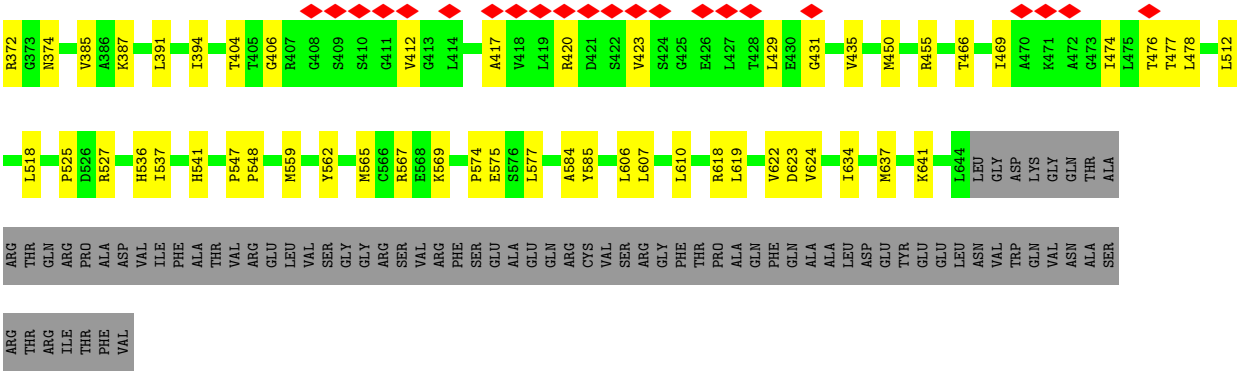
Chain 6:



• Molecule 6: DNA replication licensing factor MCM7

Chain 7:




R372 G373 N374 V385 A386 K387 L391 I394 T404 T405 G406 R407 G408 S409 S410 G411 V412 G413 L414 A417 V418 L419 R420 D421 S422 V423 S424 G425 E426 L427 T428 L429 E430 G431 V435 M450 R455 T466 I469 A470 K471 A472 G473 I474 L475 T476 T477 L478 L512
L518 P525 D526 R527 H536 I537 H541 P547 P548 M559 Y562 M565 C566 R567 E568 K569 P574 E575 S576 L577 A584 Y585 L606 L607 L610 R618 L619 V622 D623 V624 I634 M637 K641 L644 LEU GLY ASP LYS GLY GLN THR ALA
ARG THR GLN ARG PRO ALA ASP VAL ILE PHE ALA THR VAL ARG GLU LEU VAL SER GLY GLY ARG SER VAL ARG PHE SER GLU ALA GLU GLN ARG CYS VAL SER ARG GLY PHE THR PRO ALA GLN PHE GLN ALA ALA LEU ASP GLU TYR GLU GLU LEU ASN VAL TRP GLN VAL ASN ALA SER
ARG THR ARG ILE THR PHE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	331533	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 ($e^-/Å^2$)	51.00	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47170	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.34	0/5441	0.46	0/7383
2	3	0.35	0/4524	0.47	0/6139
3	4	0.11	0/4997	0.24	0/6793
4	5	0.09	0/4276	0.29	0/5775
5	6	0.31	0/5332	0.44	0/7210
6	7	0.10	0/4297	0.25	0/5842
All	All	0.25	0/28867	0.38	0/39142

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	2	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	751	ARG	Sidechain

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	2	5342	0	5182	60	0
2	3	4463	0	4315	78	0
3	4	4919	0	4664	74	0
4	5	4218	0	4121	67	0
5	6	5250	0	5182	73	0
6	7	4234	0	4066	63	0
7	2	31	0	12	1	0
7	4	31	0	12	0	0
7	6	31	0	12	2	0
8	2	1	0	0	0	0
8	4	1	0	0	0	0
8	6	1	0	0	0	0
8	7	1	0	0	0	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	6	1	0	0	0	0
10	3	27	0	12	1	0
10	7	27	0	12	0	0
All	All	28580	0	27590	390	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 7.

The worst 5 of 390 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)
2:3:800:VAL:HG23	2:3:805:ILE:HD13	1.38	1.05
2:3:800:VAL:CG2	2:3:805:ILE:HD13	1.93	0.98
2:3:768:LEU:O	2:3:772:ILE:HD12	1.62	0.98
3:4:328:CYS:HB2	3:4:331:CYS:HB3	1.55	0.89
2:3:768:LEU:CD1	2:3:772:ILE:HD11	2.09	0.83

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	2	693/904 (77%)	652 (94%)	41 (6%)	0	100 100
2	3	595/808 (74%)	578 (97%)	17 (3%)	0	100 100
3	4	655/863 (76%)	628 (96%)	27 (4%)	0	100 100
4	5	546/734 (74%)	521 (95%)	24 (4%)	1 (0%)	43 74
5	6	659/821 (80%)	622 (94%)	36 (6%)	1 (0%)	43 74
6	7	556/719 (77%)	532 (96%)	24 (4%)	0	100 100
All	All	3704/4849 (76%)	3533 (95%)	169 (5%)	2 (0%)	49 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	656	ILE
4	5	660	VAL

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	2	566/781 (72%)	566 (100%)	0	100 100
2	3	458/707 (65%)	456 (100%)	2 (0%)	84 81
3	4	494/753 (66%)	494 (100%)	0	100 100
4	5	435/625 (70%)	435 (100%)	0	100 100
5	6	578/724 (80%)	578 (100%)	0	100 100
6	7	437/619 (71%)	437 (100%)	0	100 100
All	All	2968/4209 (70%)	2966 (100%)	2 (0%)	87 87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	743	ARG
2	3	808	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
5	6	597	GLN
6	7	465	GLN
5	6	603	GLN
6	7	238	GLN
3	4	294	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	3	901	-	27,29,29	1.35	4 (14%)	42,45,45	1.98	10 (23%)
7	ATP	6	902	9	29,33,33	0.31	0	44,52,52	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	ATP	4	902	9	29,33,33	0.31	0	44,52,52	0.49	0
7	ATP	2	1001	9	29,33,33	0.34	0	44,52,52	0.48	1 (2%)
10	ADP	7	801	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	11 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	3	901	-	-	4/16/32/32	0/3/3/3
7	ATP	6	902	9	-	2/22/38/38	0/3/3/3
7	ATP	4	902	9	-	1/22/38/38	0/3/3/3
7	ATP	2	1001	9	-	5/22/38/38	0/3/3/3
10	ADP	7	801	-	-	2/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	901	ADP	C5-C4	4.52	1.47	1.39
10	7	801	ADP	C5-C4	4.35	1.47	1.39
10	7	801	ADP	C5-C6	2.63	1.48	1.41
10	3	901	ADP	C5-C6	2.63	1.48	1.41
10	3	901	ADP	C8-N7	2.41	1.36	1.31

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	901	ADP	C5-C4-N3	-6.30	118.53	126.75
10	7	801	ADP	C5-C4-N3	-6.16	118.72	126.75
10	3	901	ADP	N3-C4-N9	4.91	135.18	127.08
10	7	801	ADP	N3-C4-N9	4.76	134.93	127.08
10	3	901	ADP	C2-N3-C4	3.92	121.02	111.75

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	1001	ATP	C5'-O5'-PA-O3A
7	4	902	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

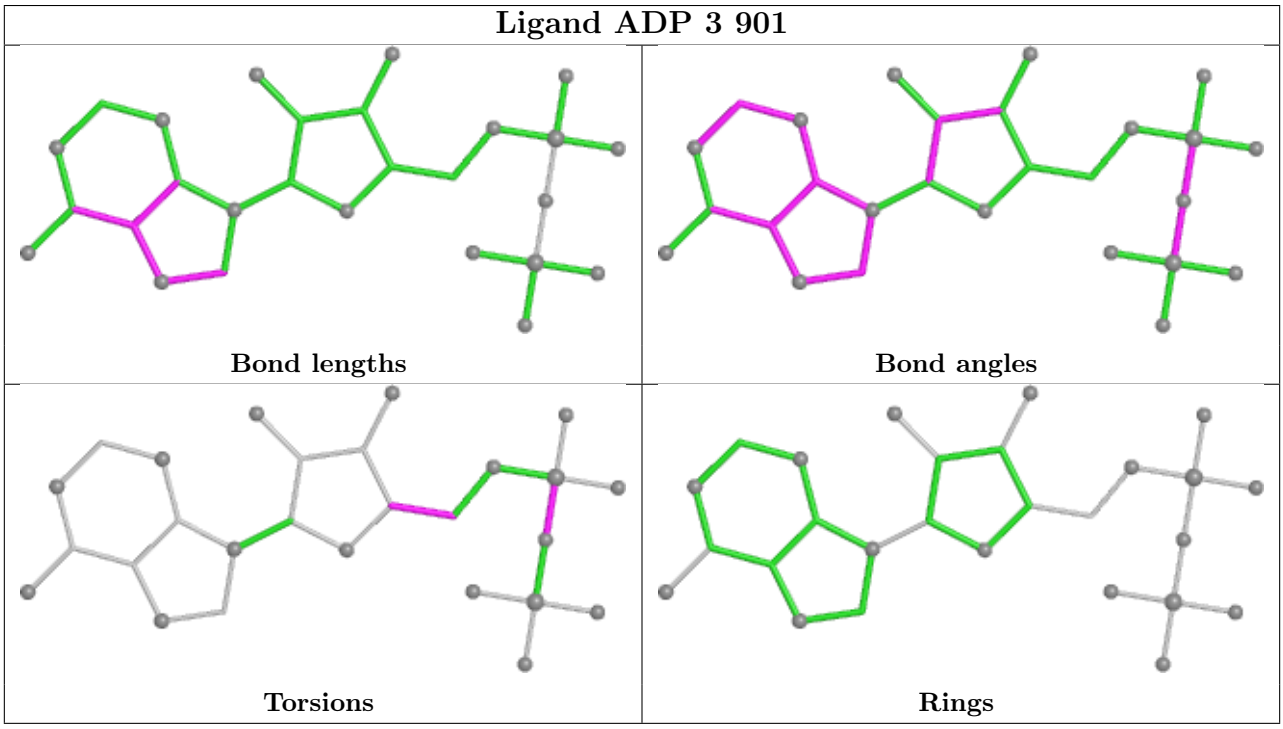
Mol	Chain	Res	Type	Atoms
10	7	801	ADP	O4'-C4'-C5'-O5'
10	7	801	ADP	C3'-C4'-C5'-O5'
10	3	901	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

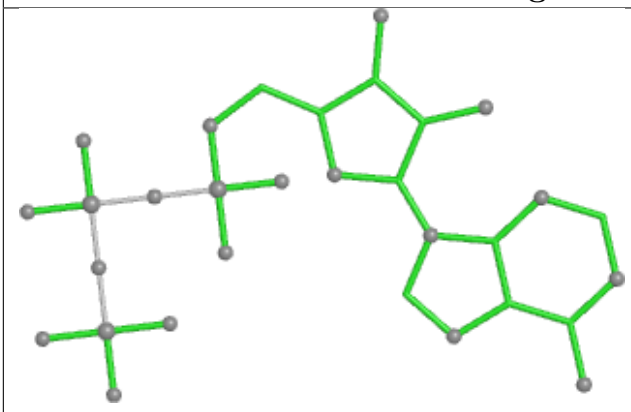
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	3	901	ADP	1	0
7	6	902	ATP	2	0
7	2	1001	ATP	1	0

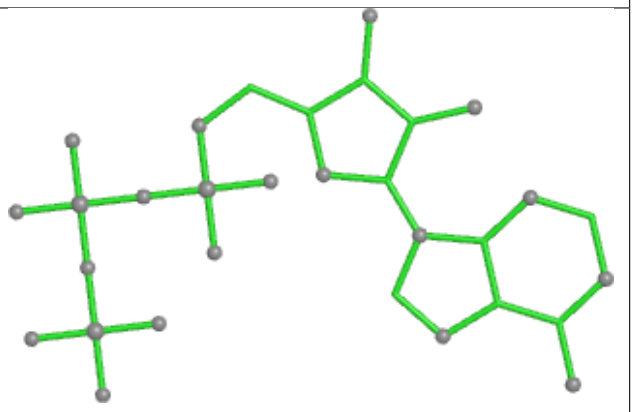
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



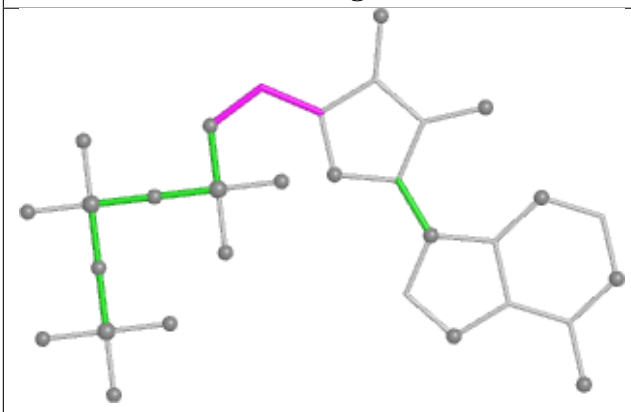
Ligand ATP 6 902



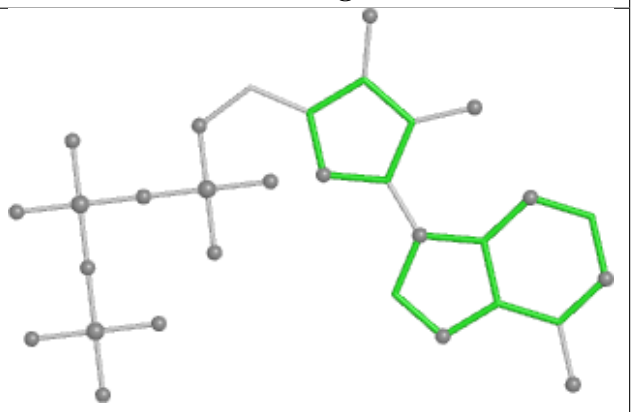
Bond lengths



Bond angles

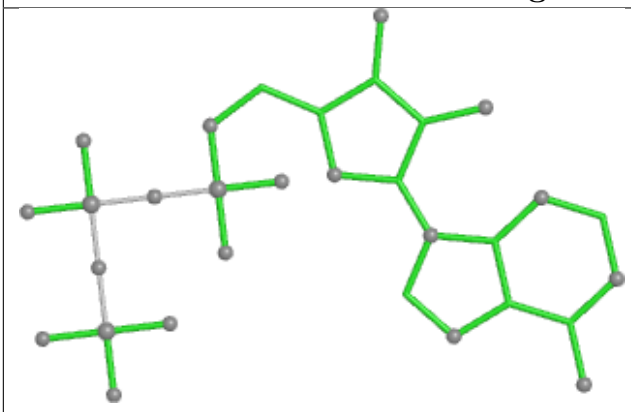


Torsions

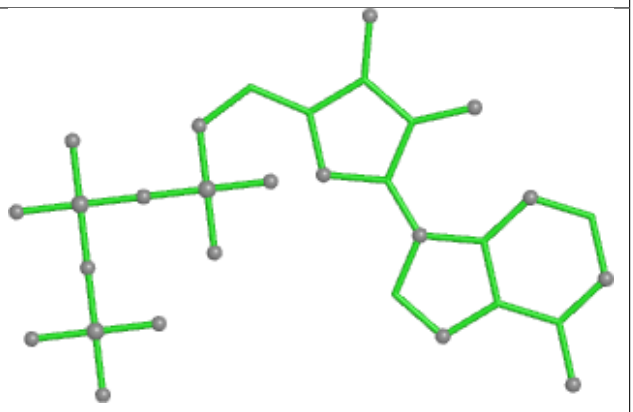


Rings

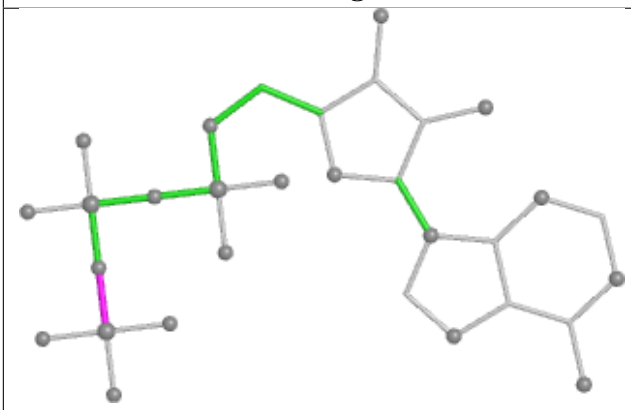
Ligand ATP 4 902



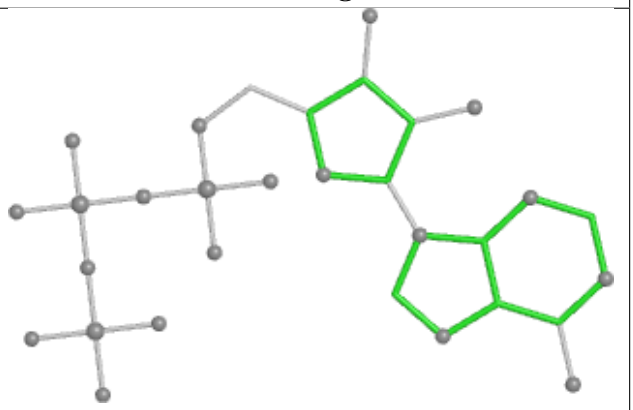
Bond lengths



Bond angles

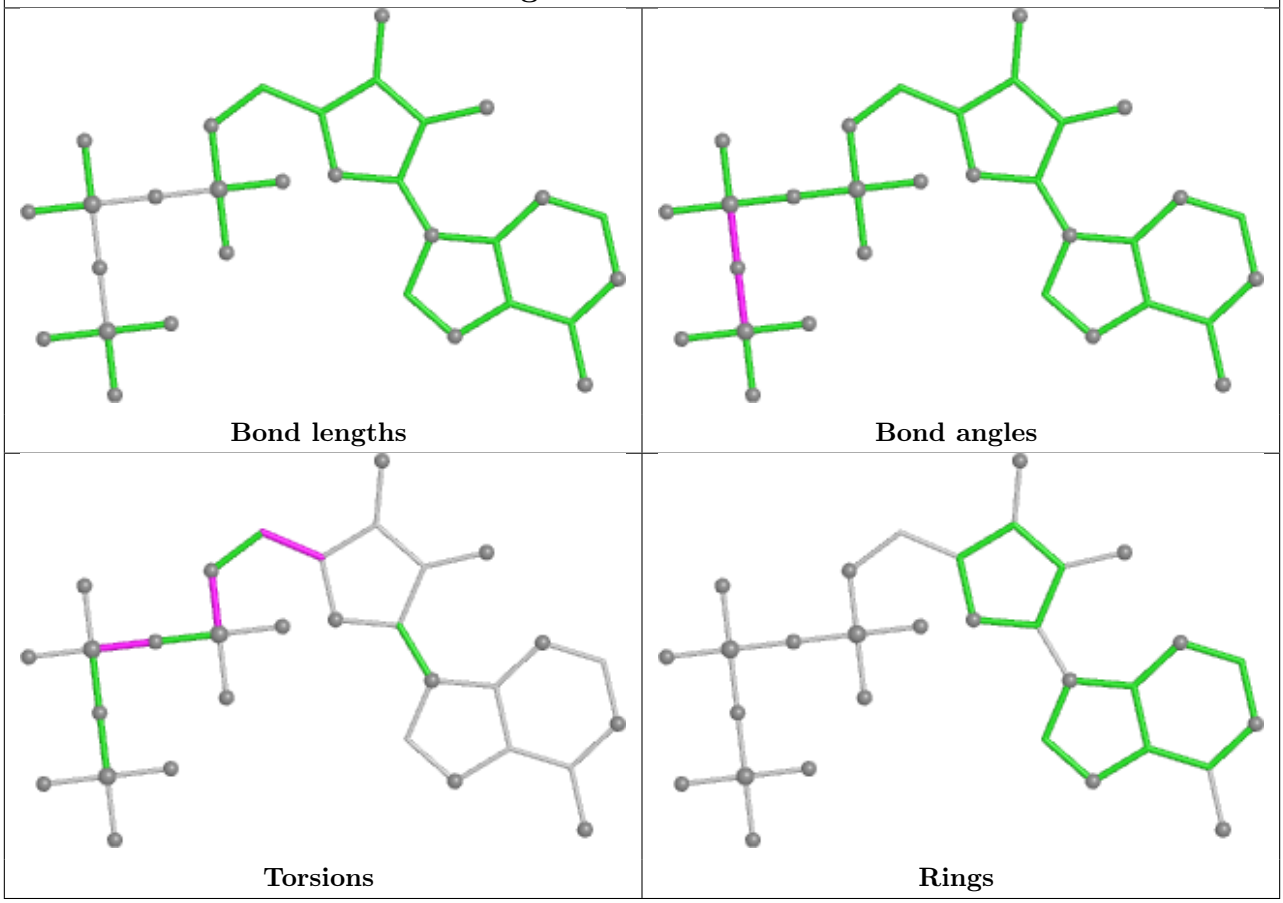


Torsions

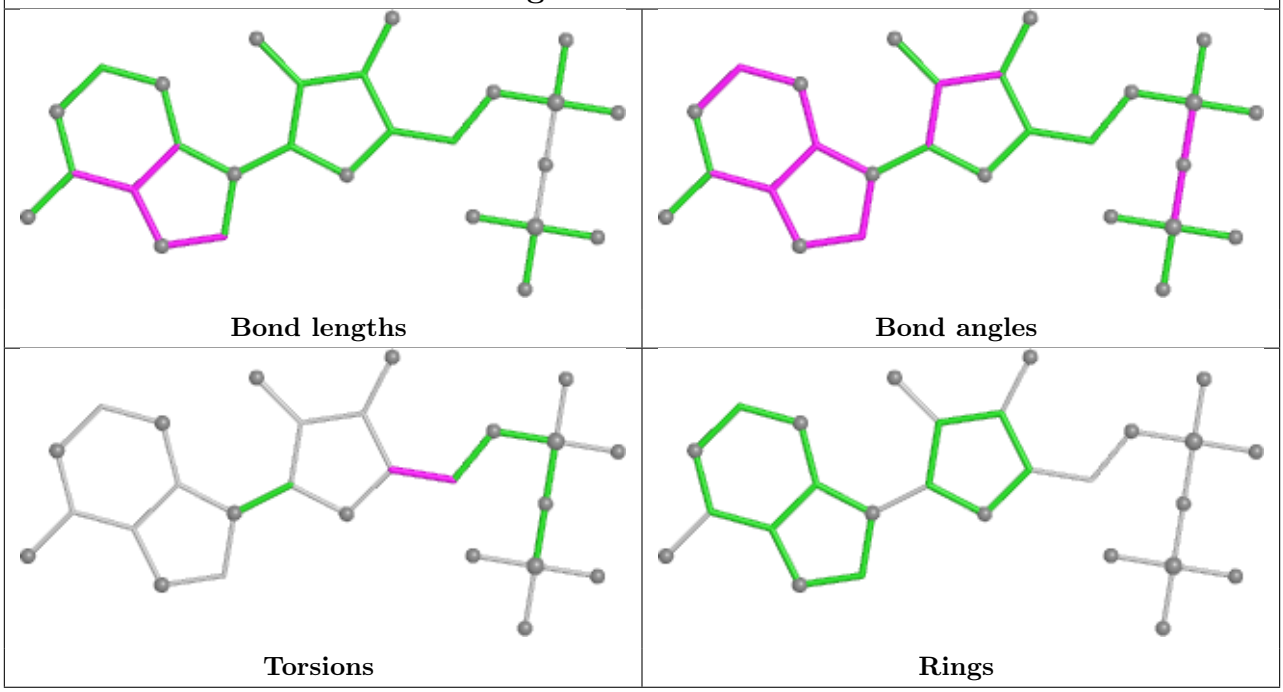


Rings

Ligand ATP 2 1001



Ligand ADP 7 801



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.

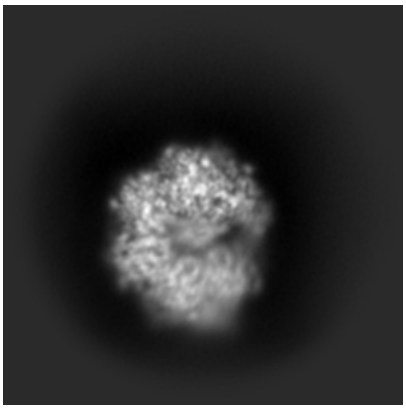
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64408. These allow visual inspection of the internal detail of the map and identification of artifacts.

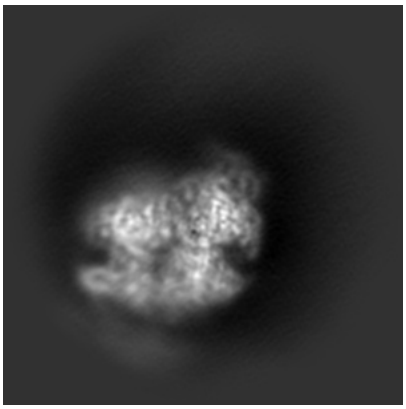
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

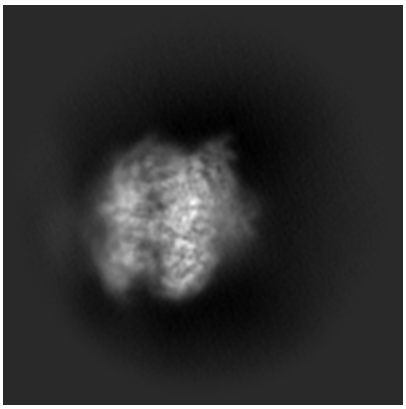
6.1.1 Primary map



X

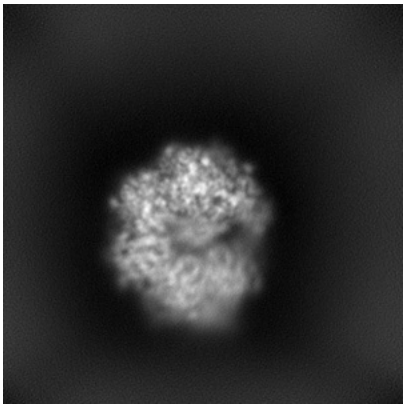


Y

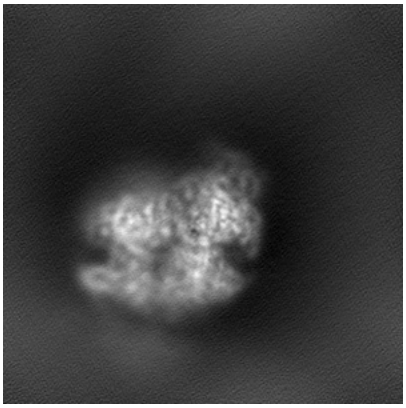


Z

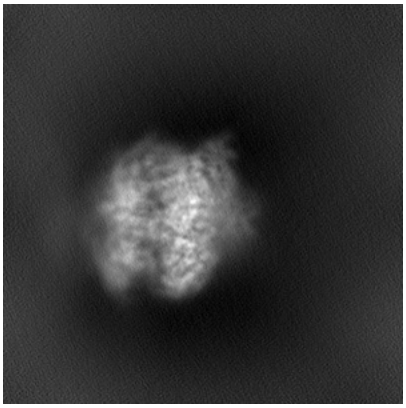
6.1.2 Raw map



X



Y

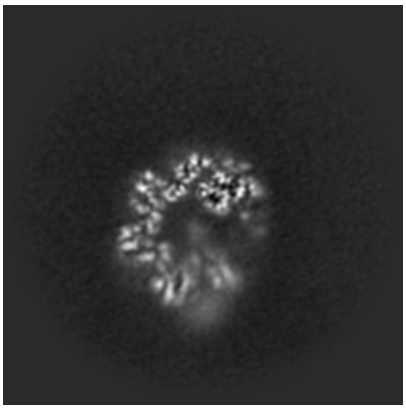


Z

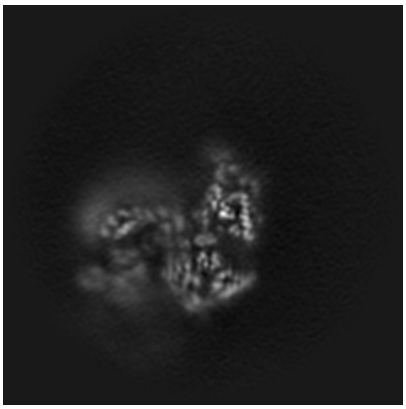
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

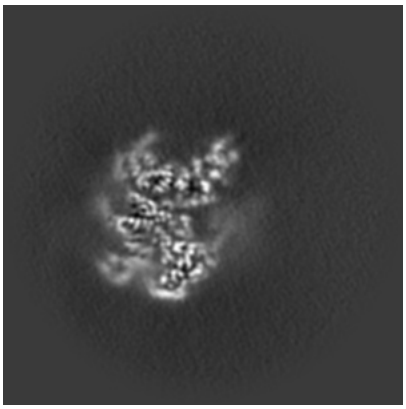
6.2.1 Primary map



X Index: 144

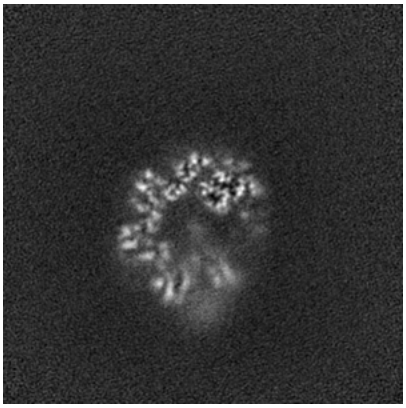


Y Index: 144

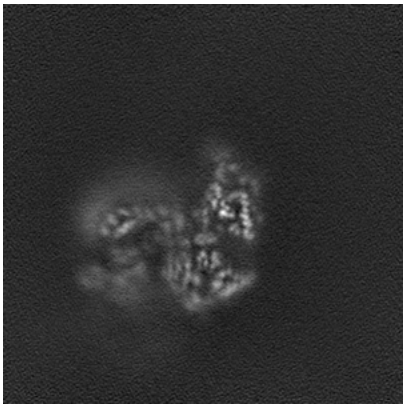


Z Index: 144

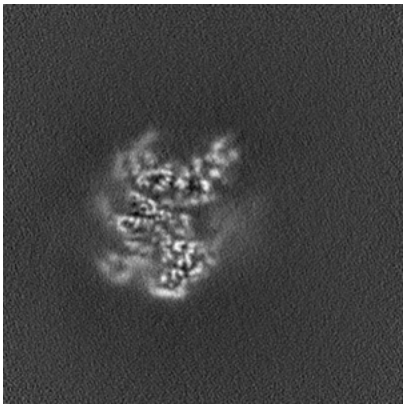
6.2.2 Raw map



X Index: 144



Y Index: 144

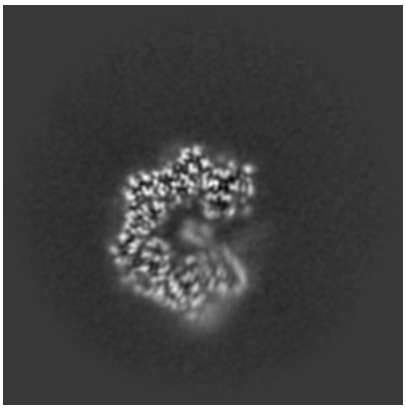


Z Index: 144

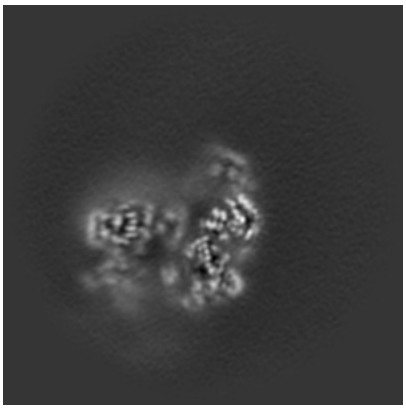
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

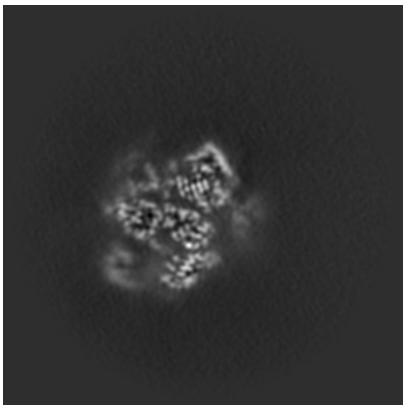
6.3.1 Primary map



X Index: 135

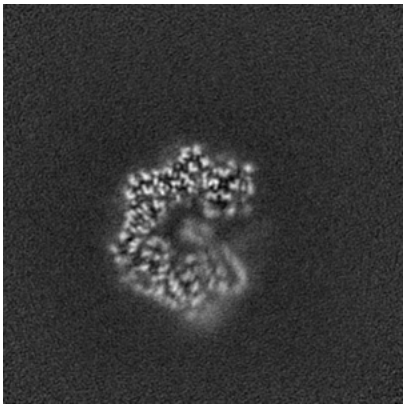


Y Index: 136

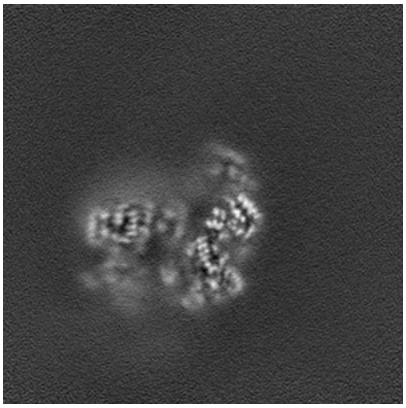


Z Index: 152

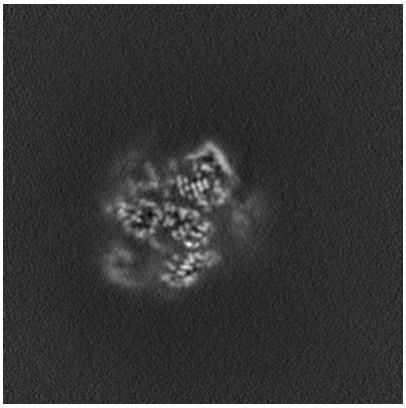
6.3.2 Raw map



X Index: 135



Y Index: 137

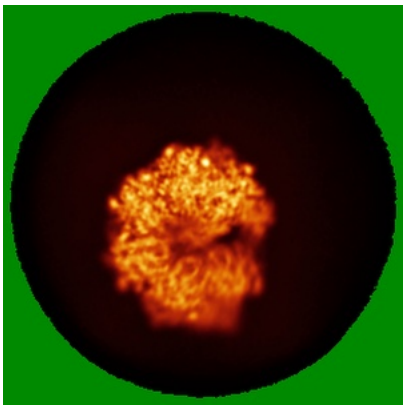


Z Index: 152

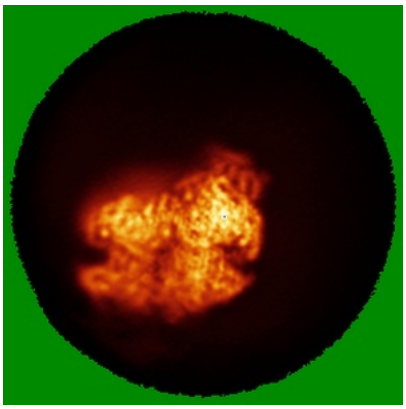
The images above show the largest variance slices of the map in three orthogonal directions.

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

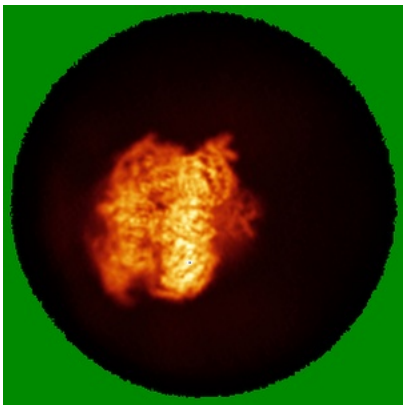
6.4.1 Primary map



X

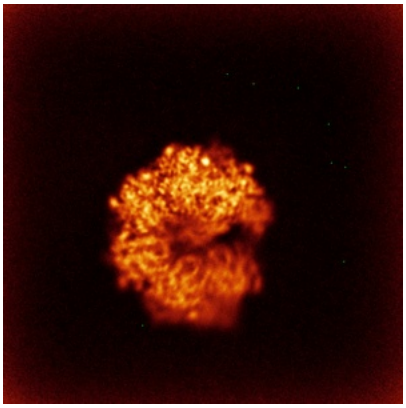


Y

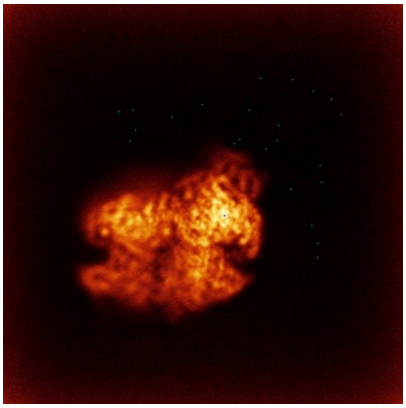


Z

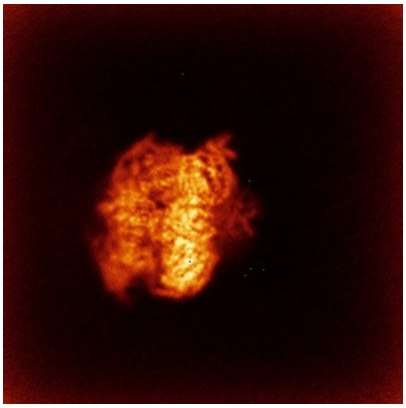
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

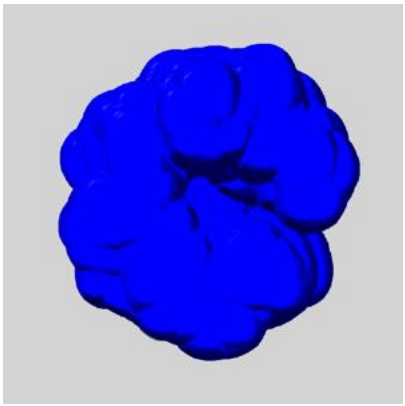
6.6 Mask visualisation (i)

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

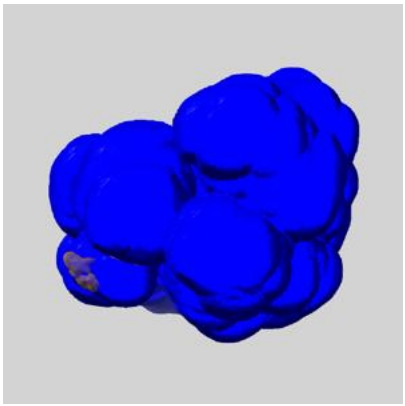
A mask typically either:

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

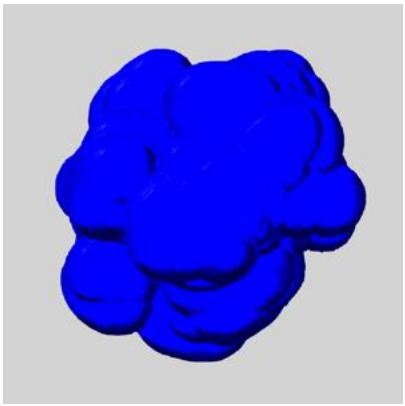
6.6.1 emd_64408_msk_1.map (i)



X



Y

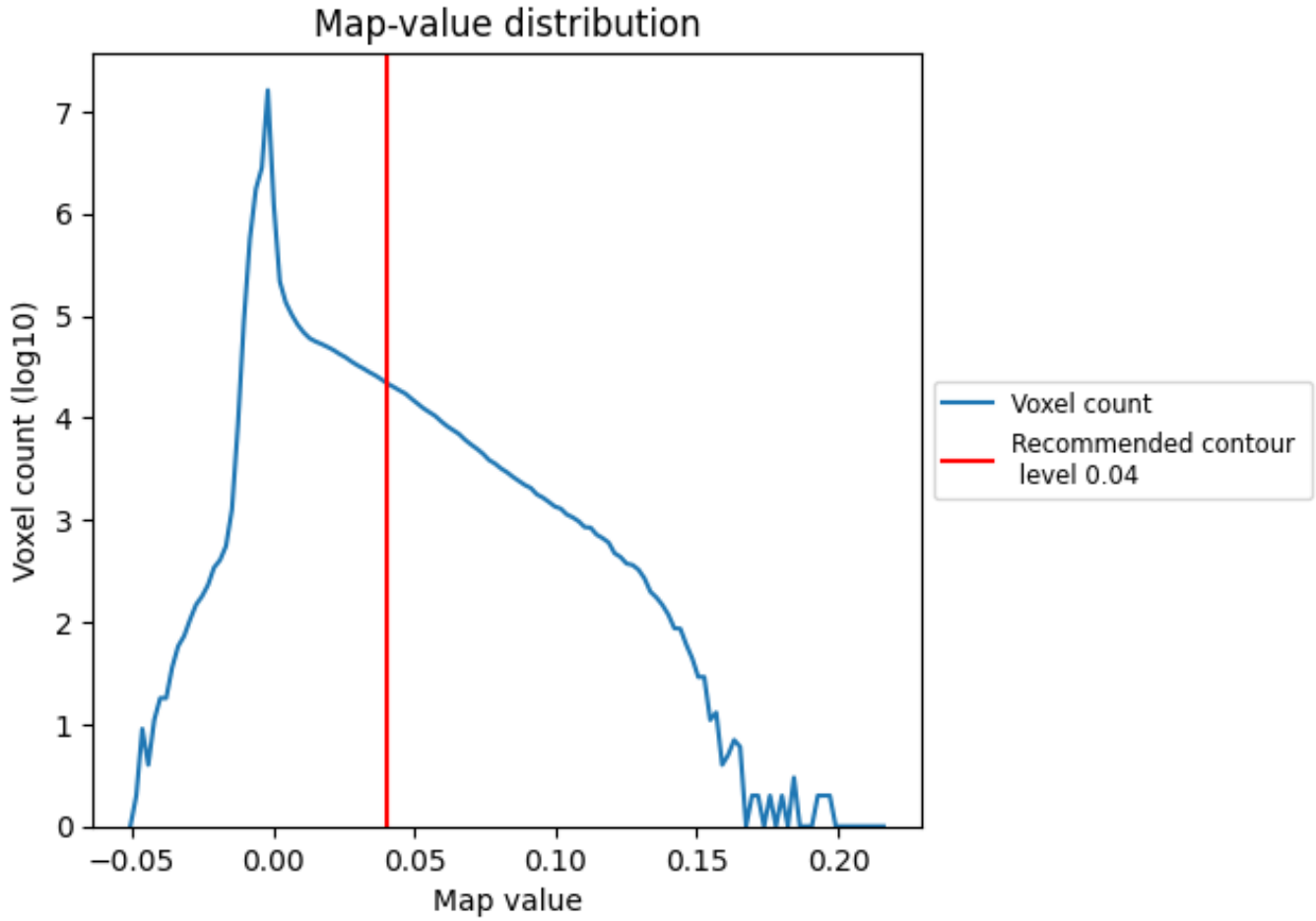


Z

7 Map analysis

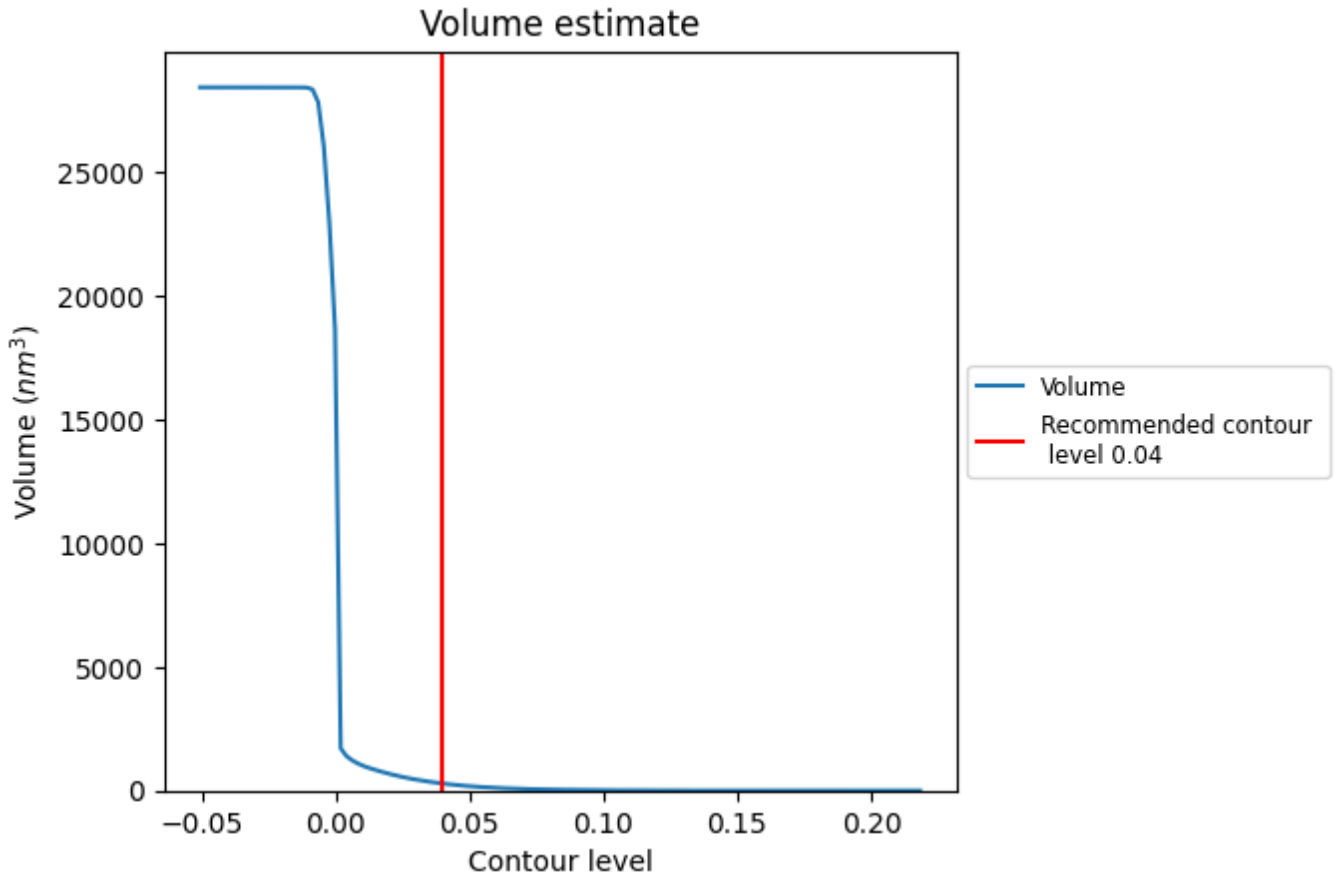
This section contains the results of statistical analysis of the map.

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.

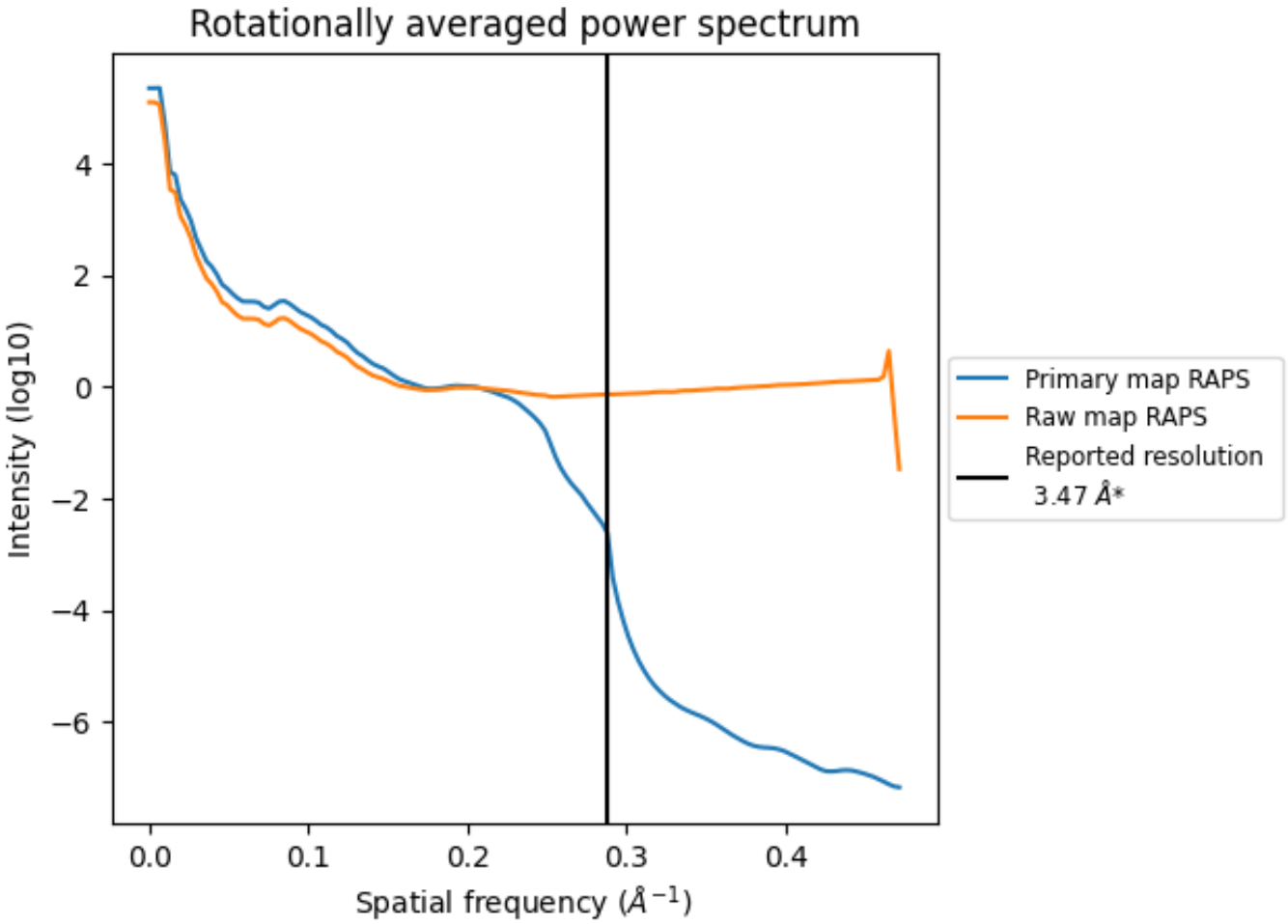
7.2 Volume estimate (i)



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 257 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)

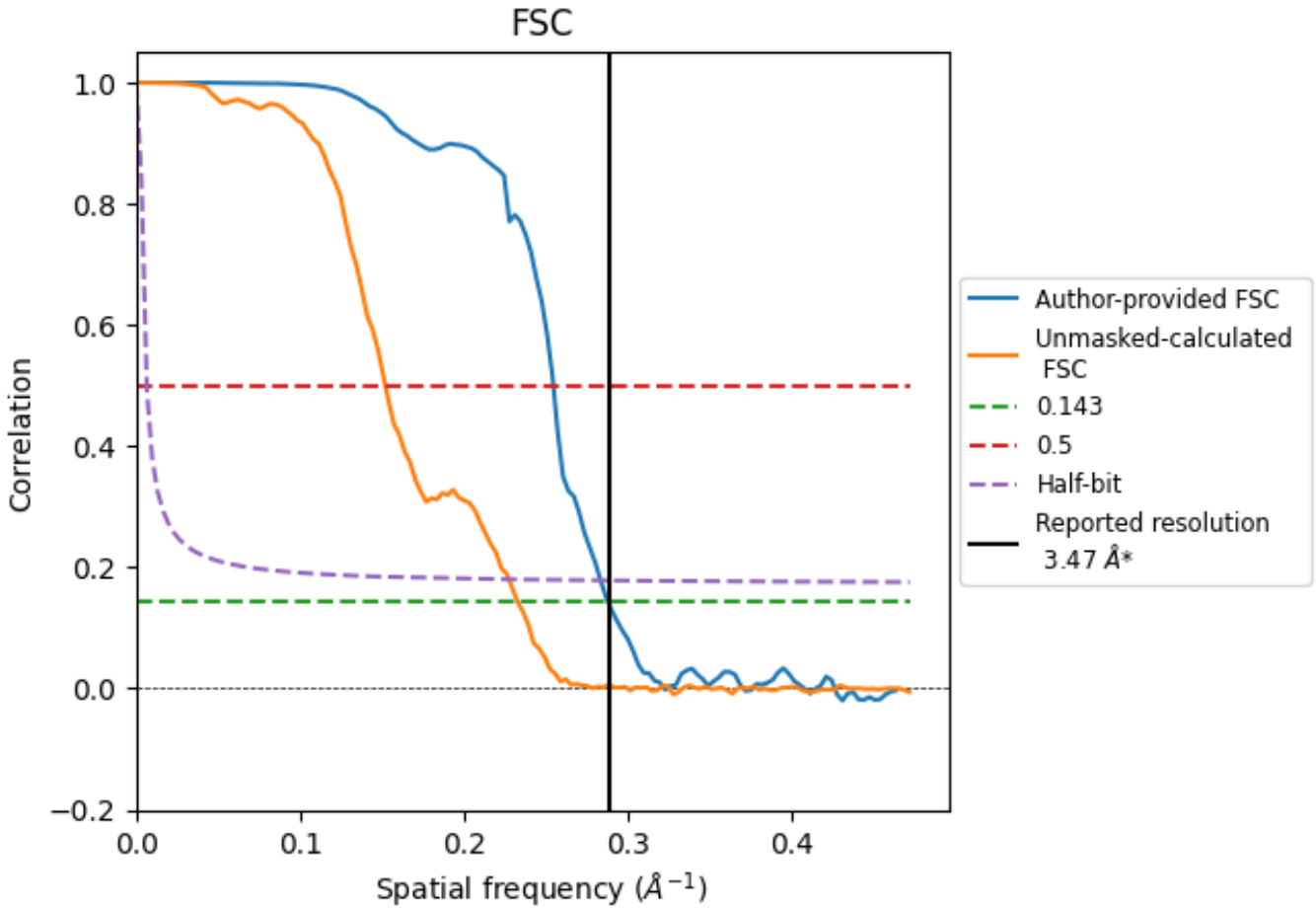


*Reported resolution corresponds to spatial frequency of 0.288 Å^{-1}

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 0.288 Å^{-1}

8.2 Resolution estimates (i)

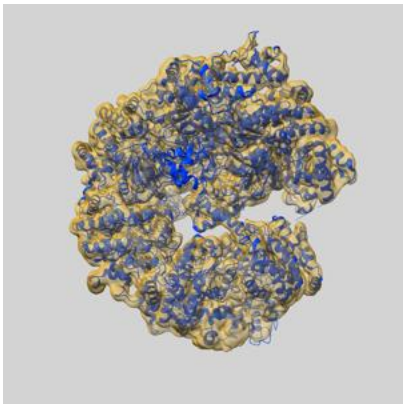
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.93	3.53
Unmasked-calculated*	4.30	6.58	4.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.47 by more than 10 %

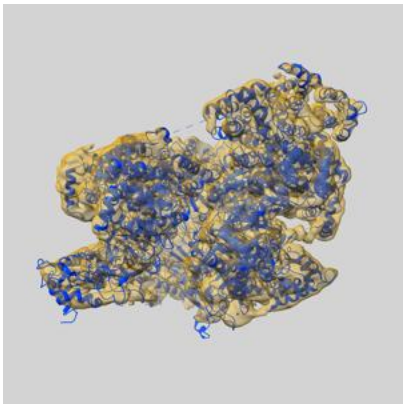
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64408 and PDB model 9UQ0. Per-residue inclusion information can be found in section 3 on page 7.

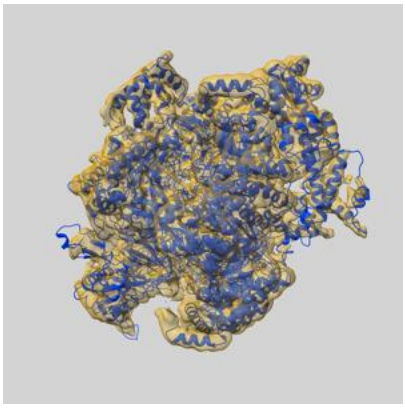
9.1 Map-model overlay



X



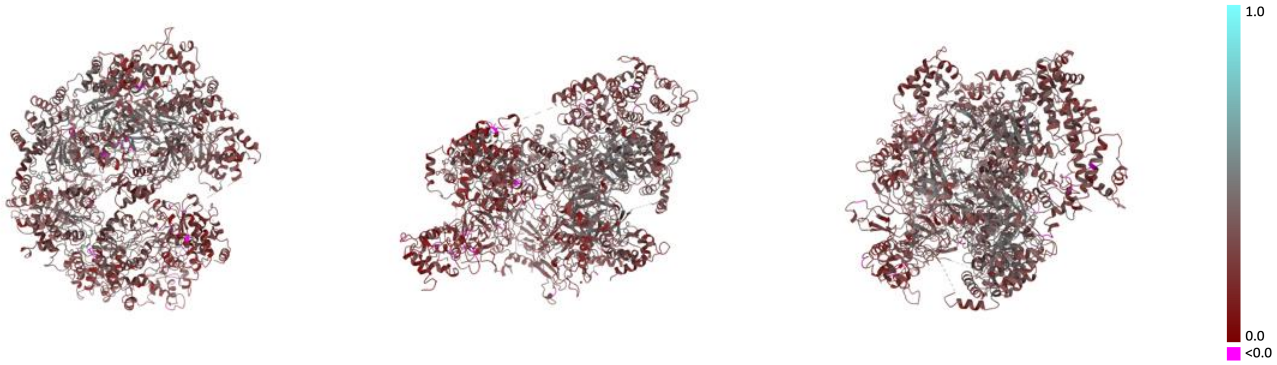
Y



Z

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

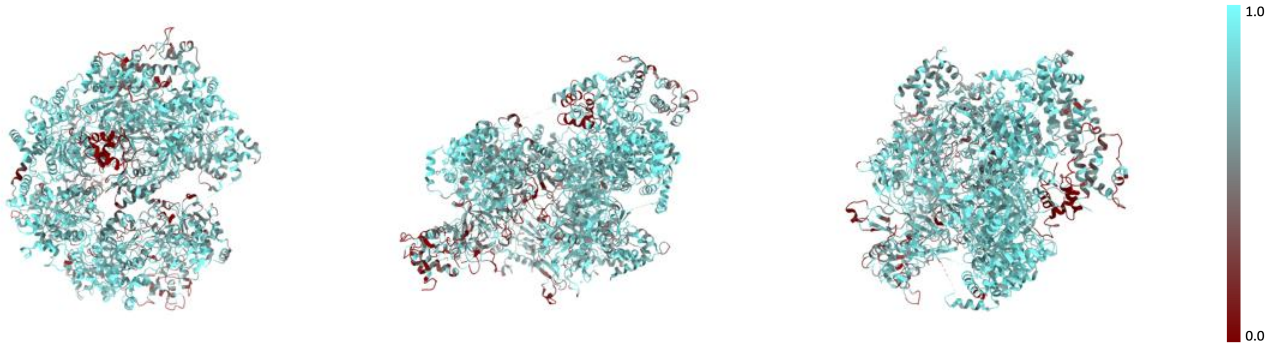
9.2 Q-score mapped to coordinate model (i)



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.

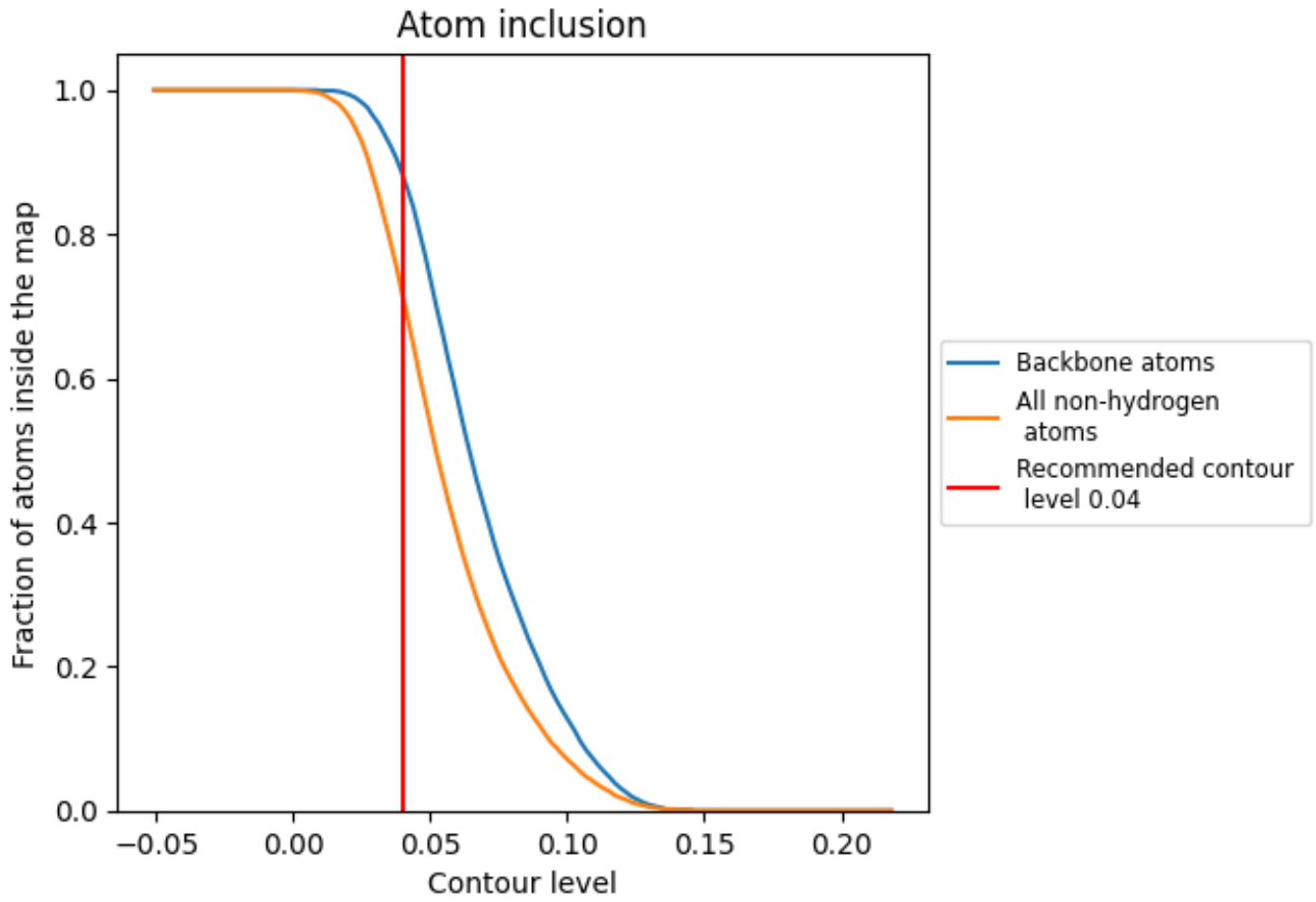
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.3000
2	0.7500	0.3300
3	0.7320	0.2690
4	0.7170	0.3200
5	0.5530	0.2140
6	0.7790	0.3530
7	0.7180	0.2890