wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 07:25 AM EST

PDB ID	:	3JC7
EMDB ID	:	EMD-6536
Title	:	Structure of the eukaryotic replicative CMG helicase and pumpjack motion
Authors	:	Li, H.; Bai, L.; Yuan, Z.; Sun, J.; Georgescu, R.E.; Liu, J.; O'Donnell, M.E.
Deposited on	:	2015-11-24
Resolution	:	4.80 Å(reported)
Based on initial model	:	2Q9Q

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:

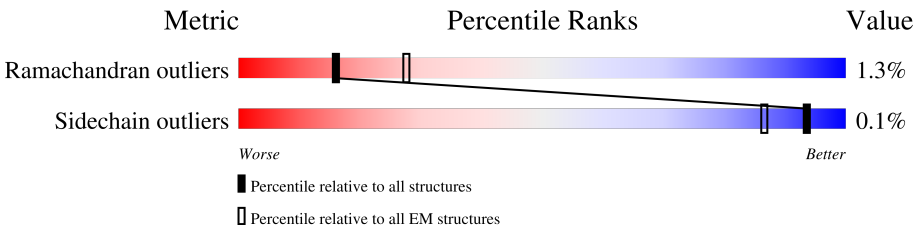
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.80 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	2	868	39% 65% • 34%
2	3	971	21% 58% • 41%
3	4	933	37% 65% • 33%
4	5	775	39% 81% • 16%
5	6	1017	35% 63% • 34%
6	7	845	33% 76% • 22%
7	c	650	33% 84% • 15%
8	D	294	24% 73% • 25%
9	B	213	30% 85% 15%

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Mol	Chain	Length	Quality of chain
10	A	208	45% 97%
11	C	194	31% 81% 18%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 40298 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	576	4531	2859	809	847	16	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	577	4521	2857	800	851	13	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	621	4911	3092	845	947	27	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	654	5172	3250	897	1001	24	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	668	5204	3290	913	978	23	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	657	5176	3266	900	982	28	0	0

- Molecule 7 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	c	553	4470	2852	759	846	13	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	22	ALA	HIS	CONFLICT	UNP Q08032
c	155	GLU	GLN	CONFLICT	UNP Q08032
c	551	THR	TRP	CONFLICT	UNP Q08032

- Molecule 8 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	221	1820	1159	300	348	13	0	0

- Molecule 9 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	181	1513	978	261	270	4	0	0

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	208	1691	1062	287	332	10	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ALA	VAL	CONFLICT	UNP Q12488
A	192	GLN	ARG	CONFLICT	UNP Q12488
A	207	LEU	LYS	CONFLICT	UNP Q12488

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	159	1288	843	207	232	6	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

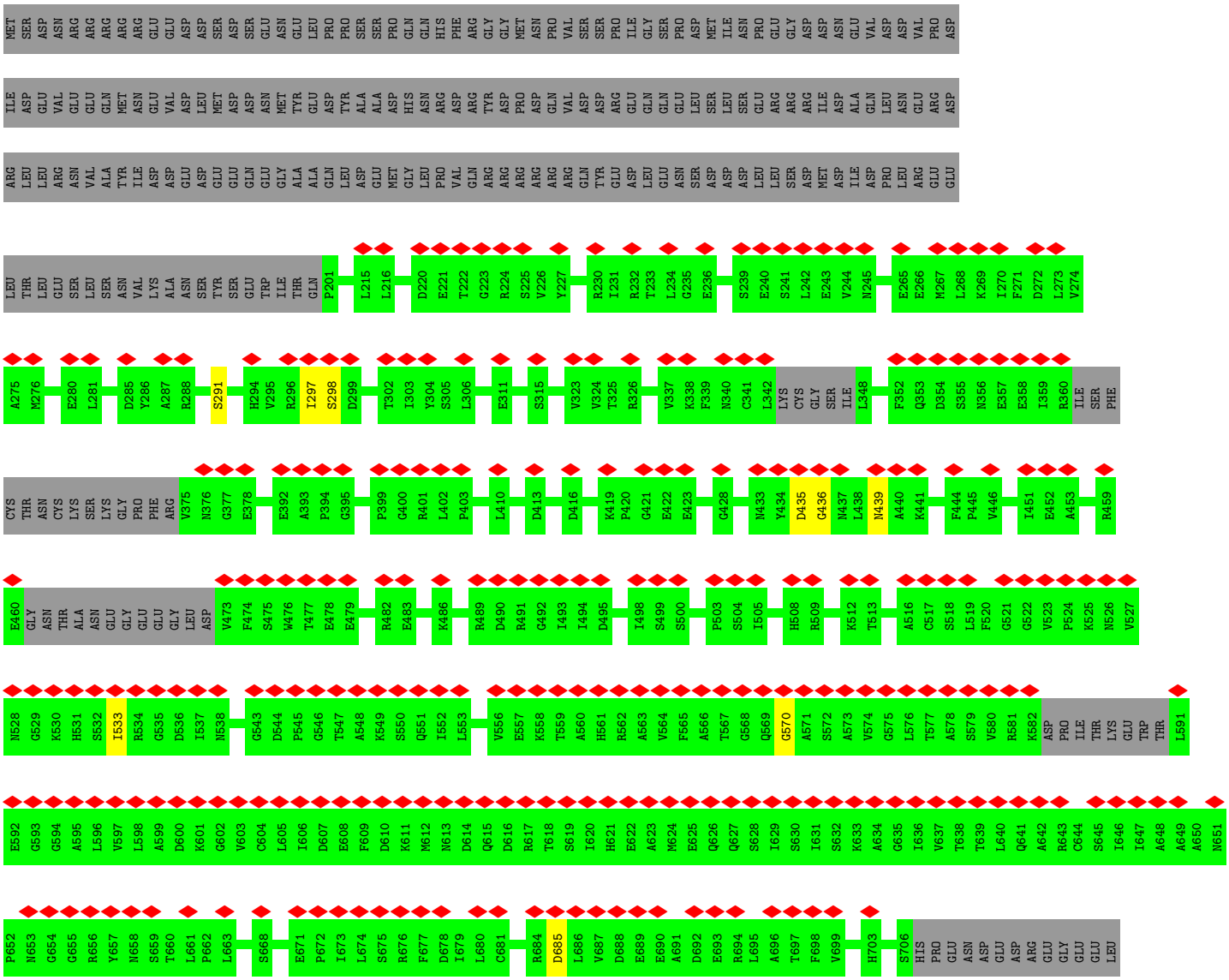
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
12	7	1	1	1	0

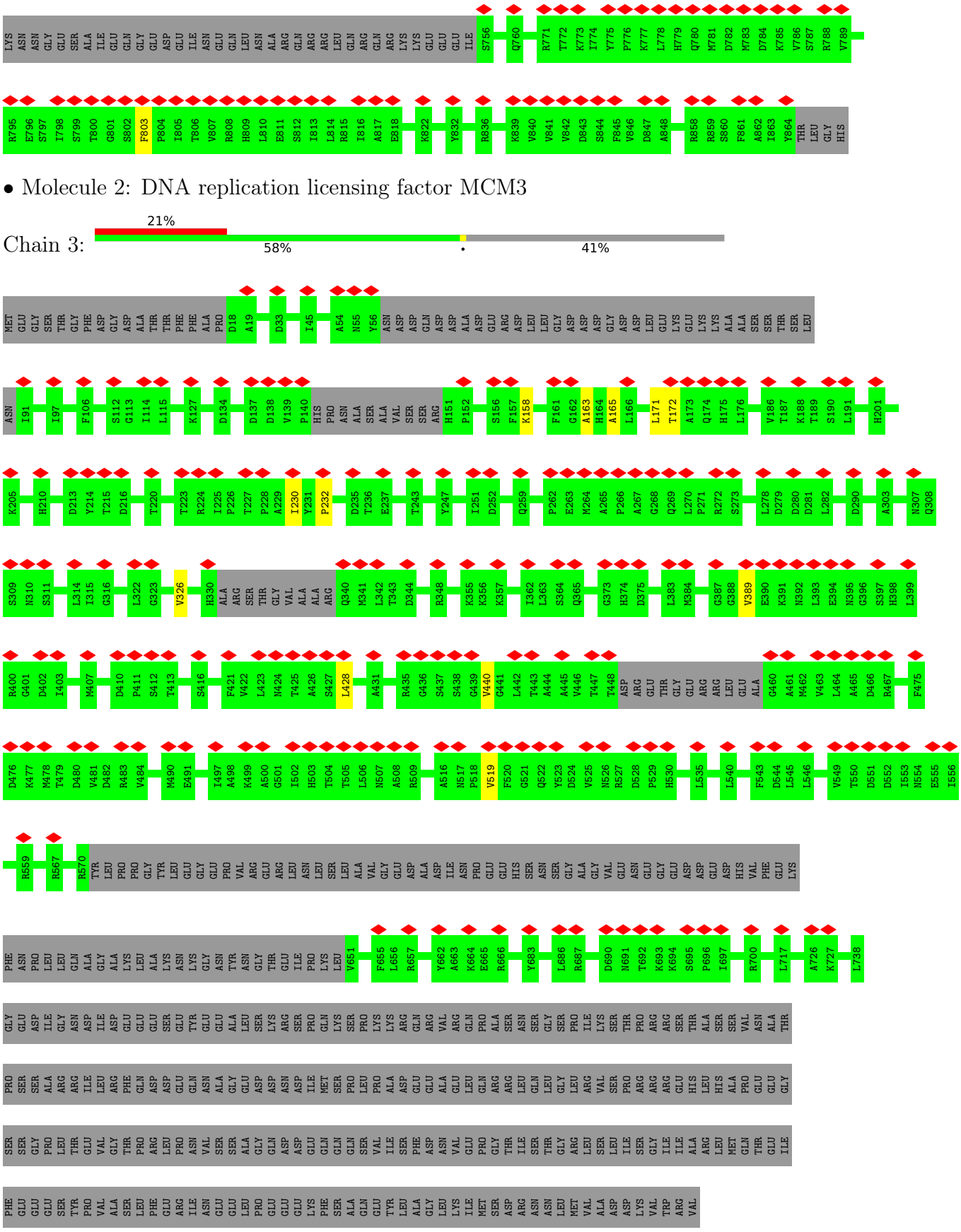
3 Residue-property plots (i)

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: DNA replication licensing factor MCM2

Chain 2:

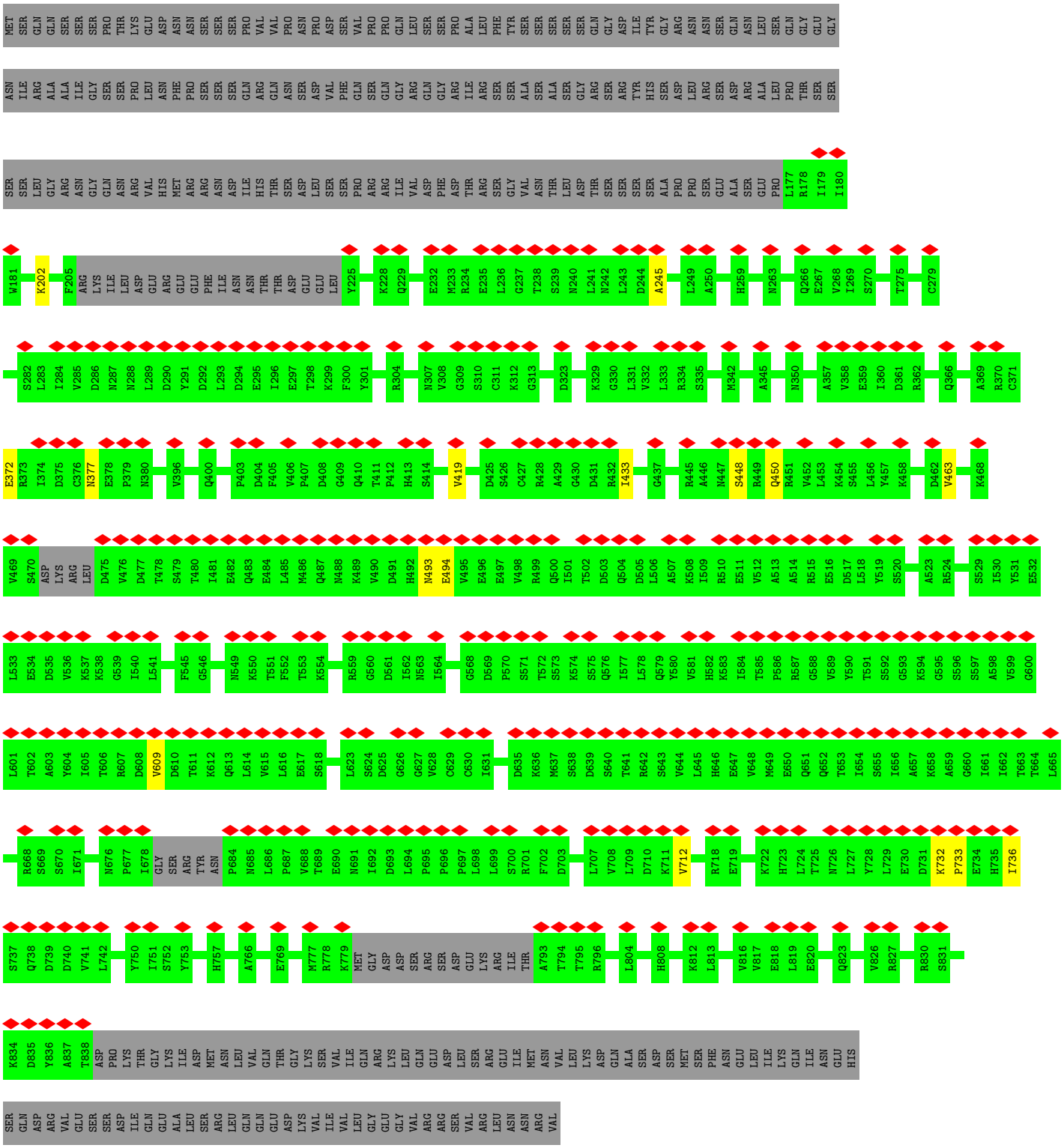




- Molecule 2: DNA replication licensing factor MCM3

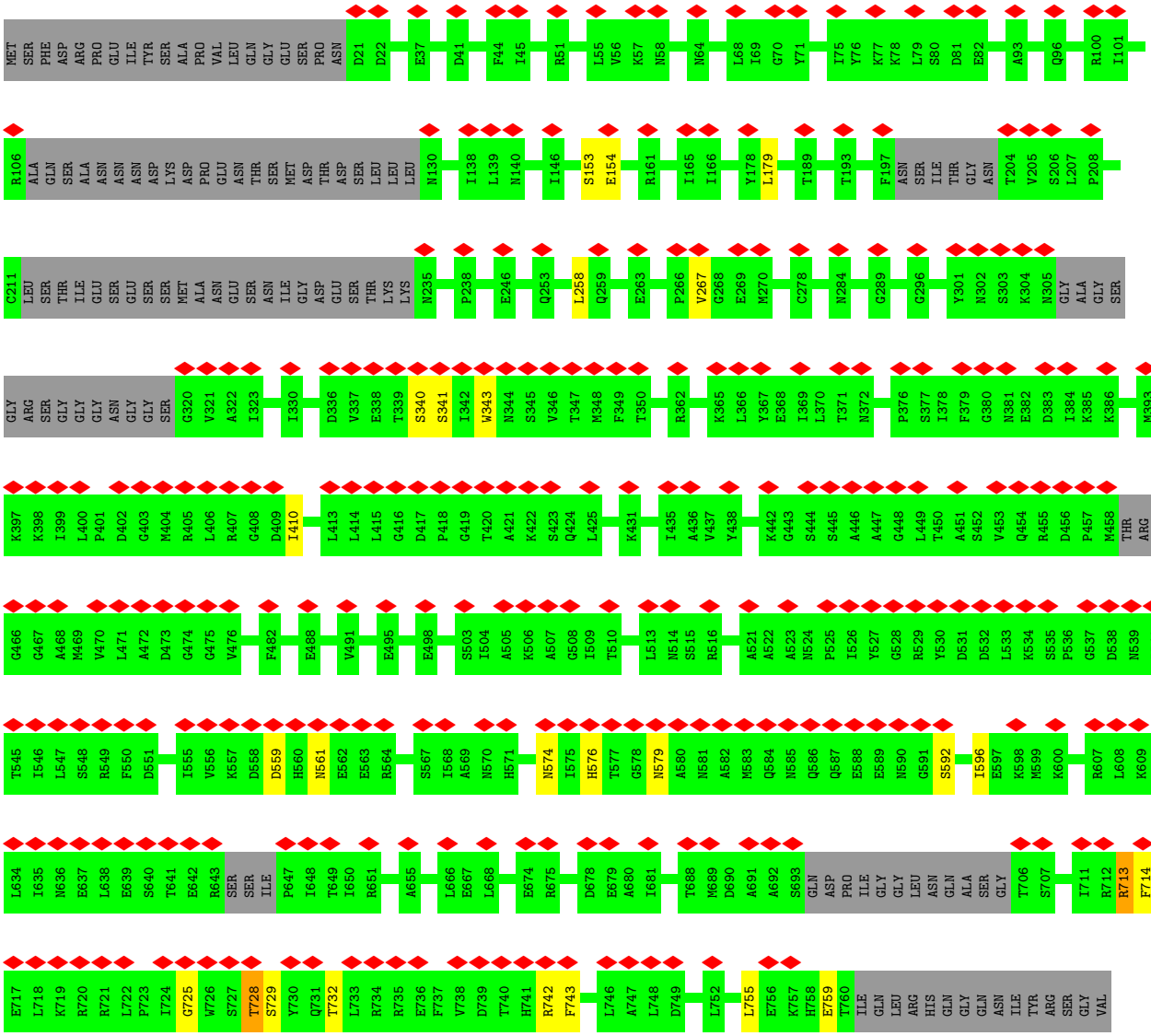
• Molecule 3: DNA replication licensing factor MCM4

Chain 4:



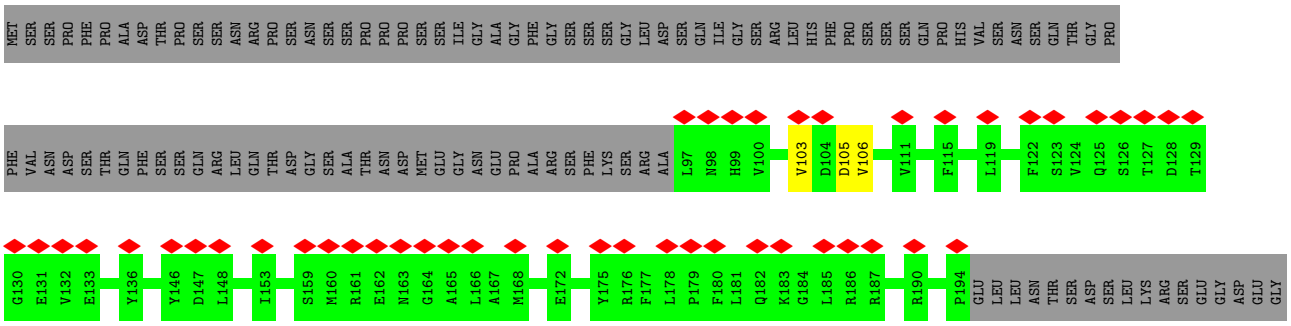
• Molecule 4: Minichromosome maintenance protein 5

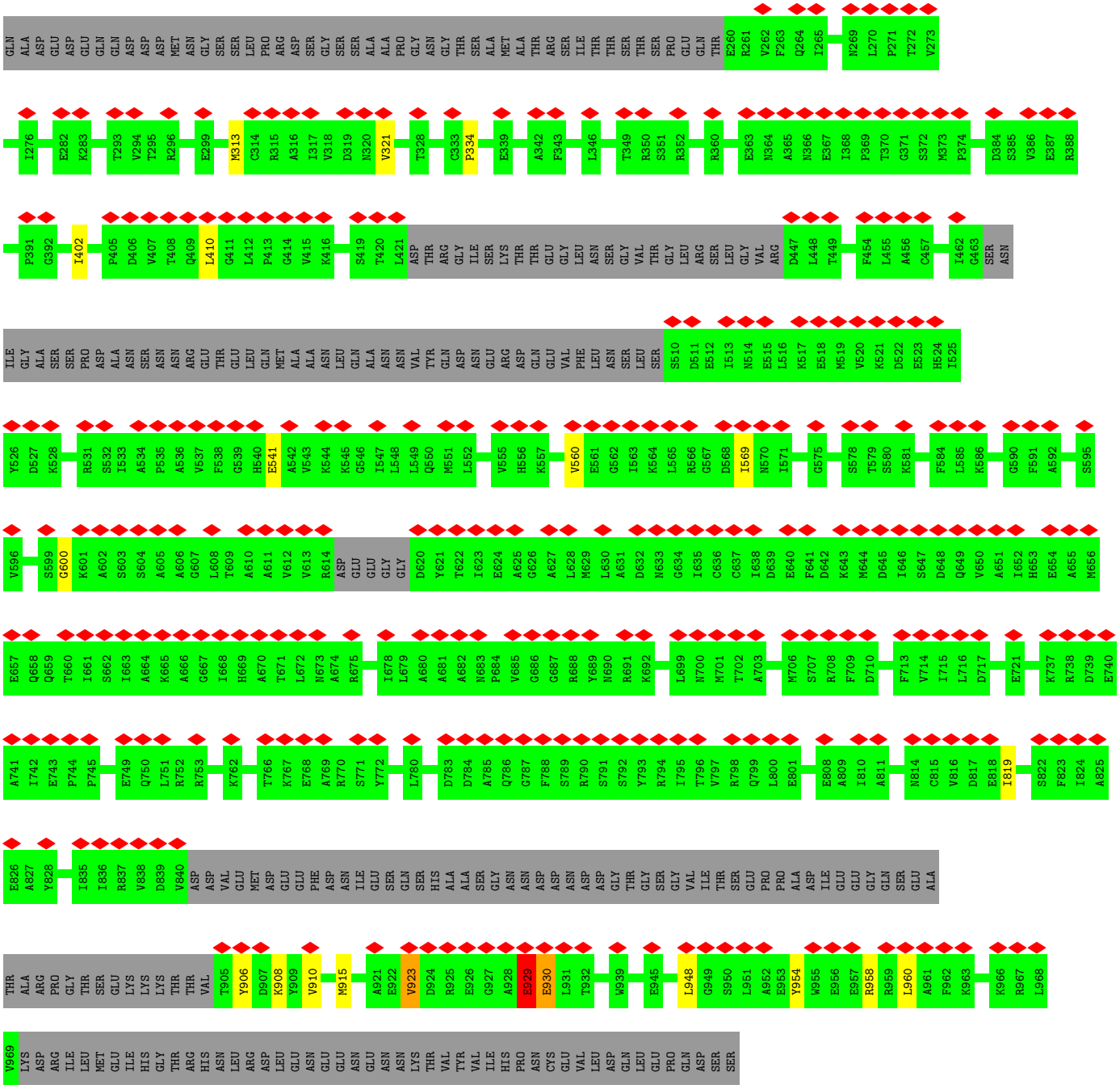
Chain 5:



- Molecule 5: DNA replication licensing factor MCM6

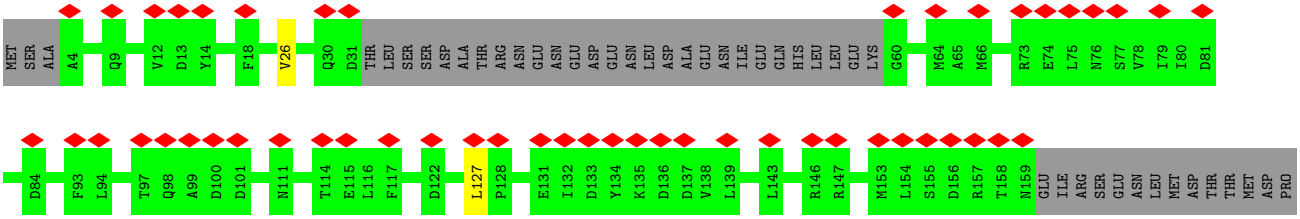
Chain 6:

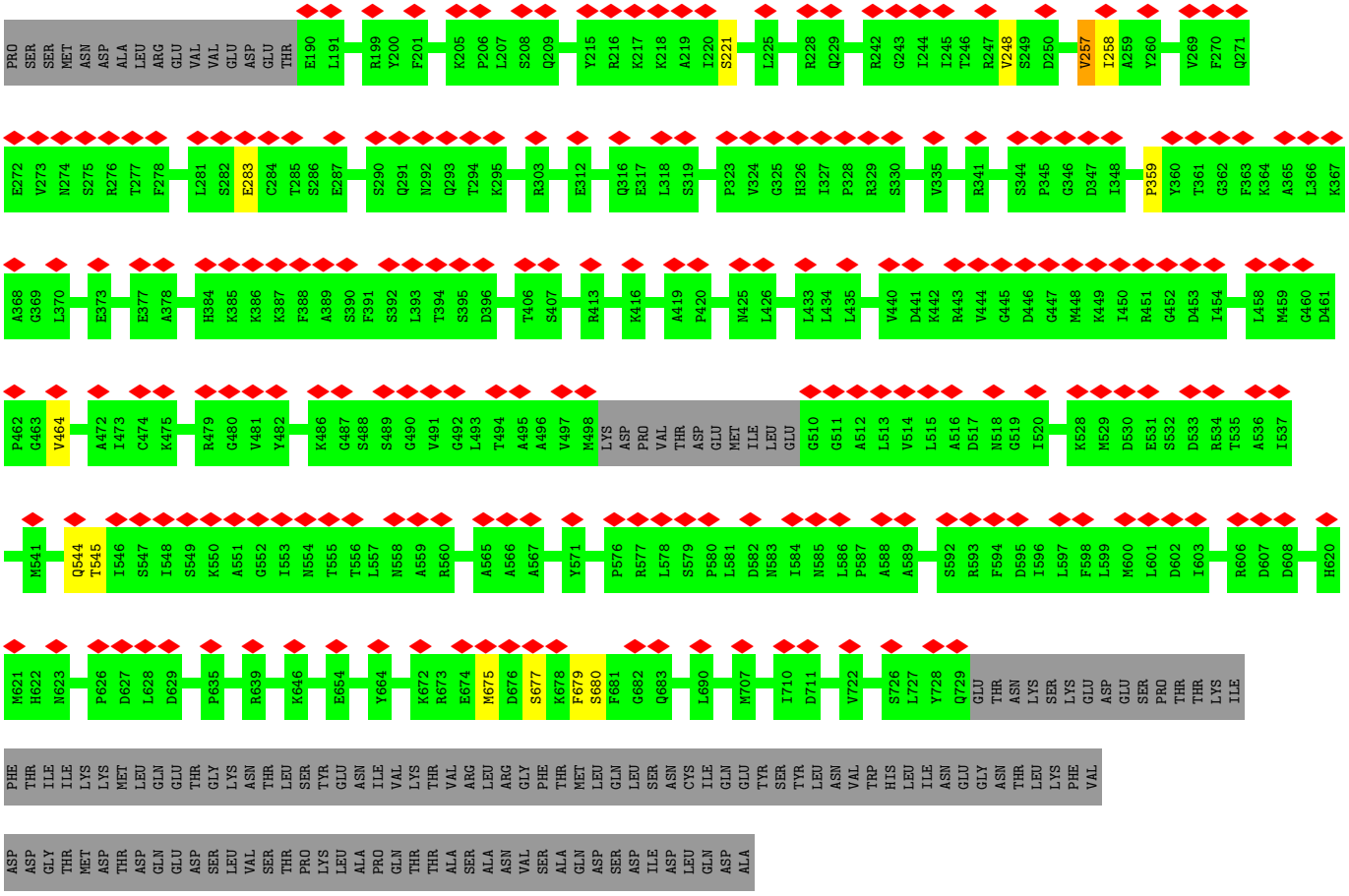




- Molecule 6: DNA replication licensing factor MCM7

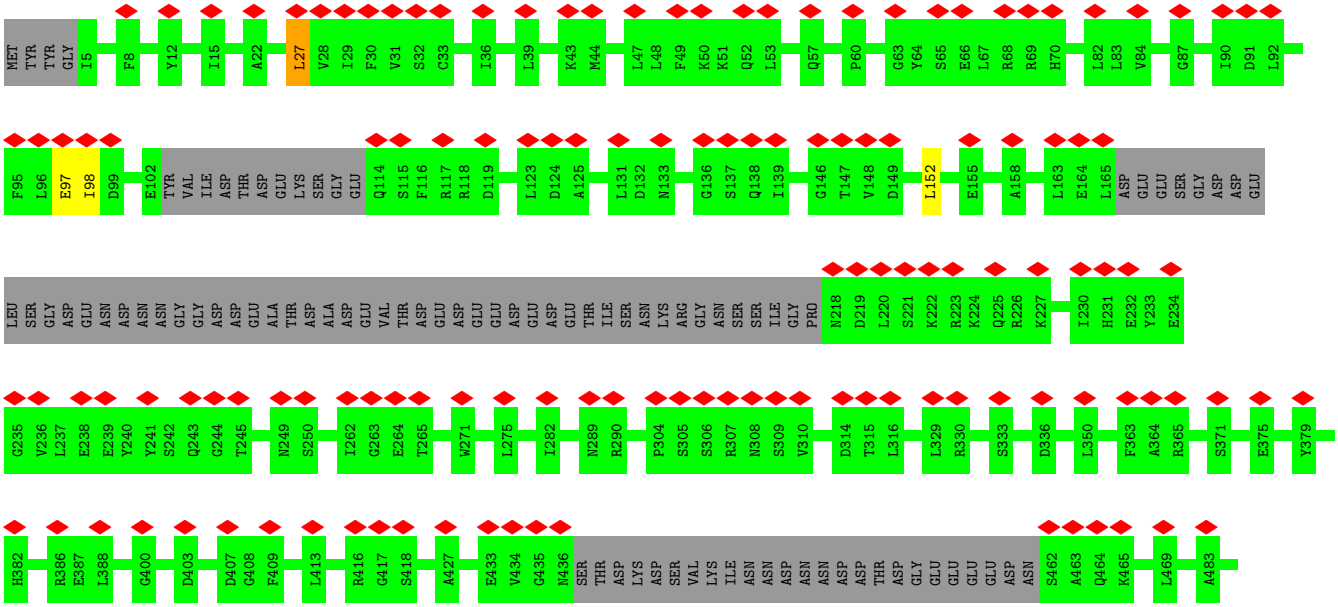
Chain 7:

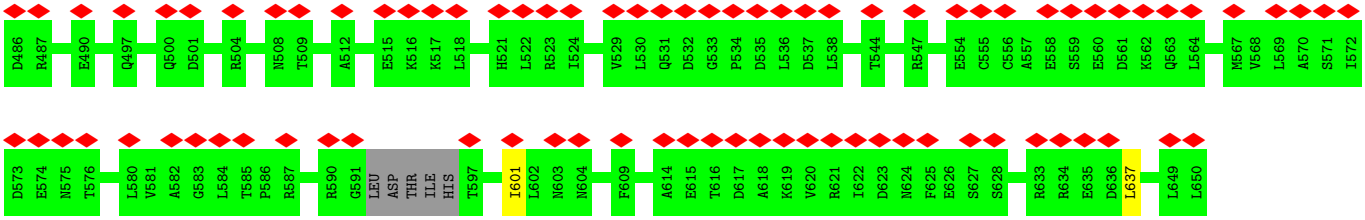




- Molecule 7: Cell division control protein 45

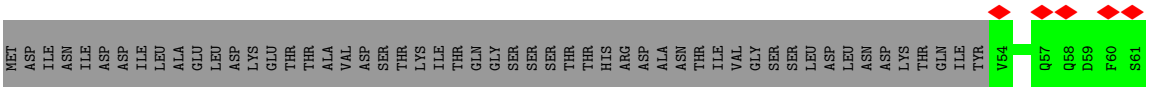
Chain c:

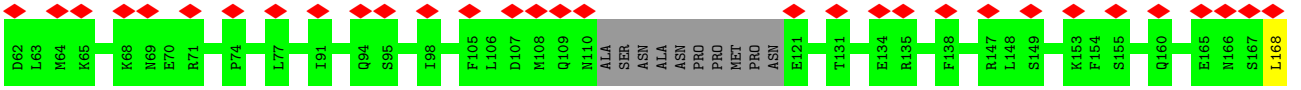


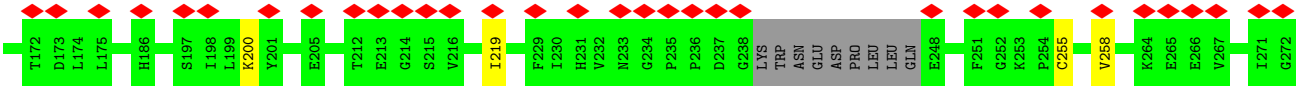


- Molecule 8: DNA replication complex GINS protein SLD5

Chain D:

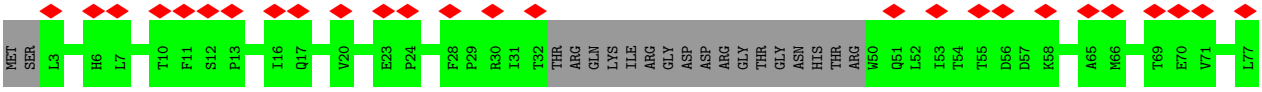


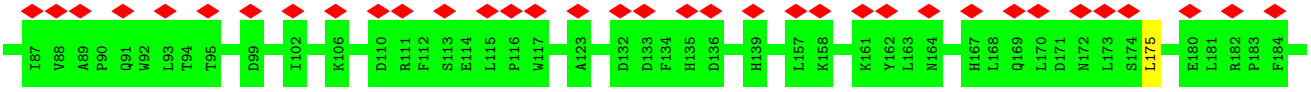


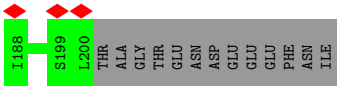


- Molecule 9: DNA replication complex GINS protein PSF2

Chain B:

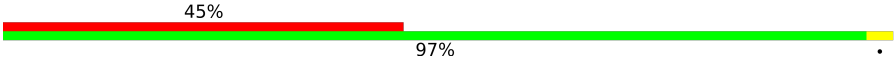


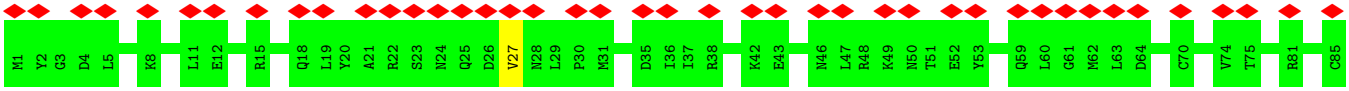


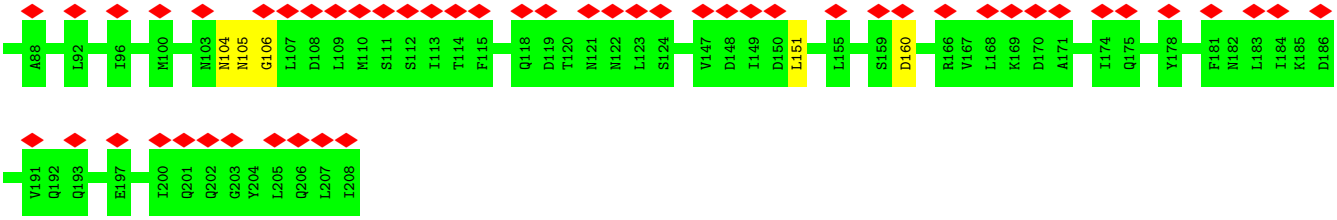


- Molecule 10: DNA replication complex GINS protein PSF1

Chain A:

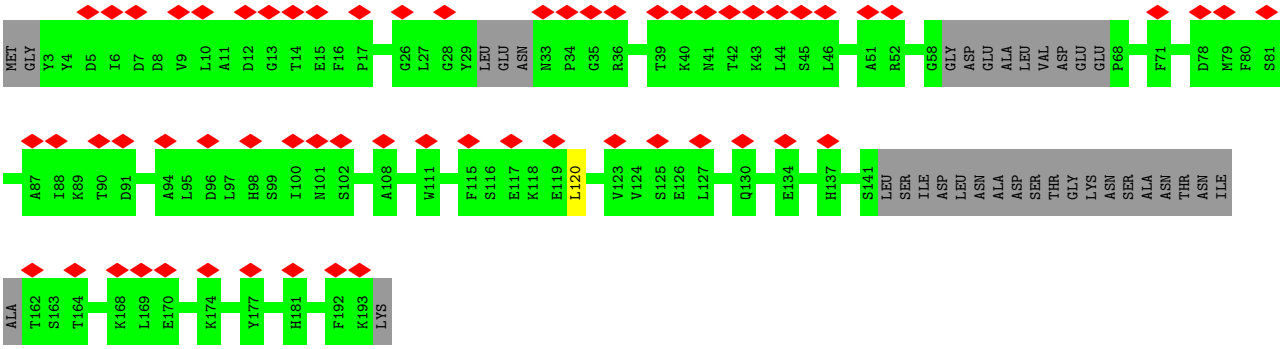






• Molecule 11: DNA replication complex GINS protein PSF3

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	49505	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	2	0.41	0/4604	0.63	2/6215 (0.0%)
2	3	0.50	1/4597 (0.0%)	0.67	1/6232 (0.0%)
3	4	0.41	0/4981	0.65	1/6734 (0.0%)
4	5	0.51	0/5243	0.83	12/7075 (0.2%)
5	6	0.48	1/5282 (0.0%)	0.79	13/7129 (0.2%)
6	7	0.42	0/5256	0.65	1/7099 (0.0%)
7	c	0.39	0/4548	0.63	2/6152 (0.0%)
8	D	0.43	0/1853	0.64	0/2500
9	B	0.44	0/1545	0.69	0/2092
10	A	0.39	0/1713	0.66	0/2309
11	C	0.46	0/1320	0.64	1/1784 (0.1%)
All	All	0.44	2/40942 (0.0%)	0.69	33/55321 (0.1%)

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
2	3	0	3
3	4	0	5
4	5	0	2
5	6	0	6
6	7	0	6
7	c	0	1
8	D	0	2
10	A	0	4
All	All	0	30

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	232	PRO	N-CD	16.15	1.70	1.47
5	6	929	GLU	C-O	7.77	1.38	1.23

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	954	TYR	CB-CG-CD2	-16.47	111.12	121.00
4	5	732	THR	CA-CB-CG2	-14.07	92.70	112.40
4	5	732	THR	OG1-CB-CG2	13.49	141.04	110.00
4	5	742	ARG	CA-CB-CG	10.90	137.38	113.40
5	6	954	TYR	CB-CG-CD1	9.46	126.68	121.00

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	803	PHE	Peptide
2	3	163	ALA	Peptide
2	3	165	ALA	Peptide
2	3	428	LEU	Peptide
3	4	202	LYS	Peptide

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	2	564/868 (65%)	512 (91%)	45 (8%)	7 (1%)	13 50
2	3	563/971 (58%)	515 (92%)	41 (7%)	7 (1%)	13 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4	609/933 (65%)	534 (88%)	65 (11%)	10 (2%)	9	44
4	5	638/775 (82%)	571 (90%)	49 (8%)	18 (3%)	5	32
5	6	656/1017 (64%)	594 (90%)	52 (8%)	10 (2%)	10	46
6	7	647/845 (77%)	572 (88%)	66 (10%)	9 (1%)	11	46
7	c	543/650 (84%)	496 (91%)	45 (8%)	2 (0%)	34	72
8	D	215/294 (73%)	197 (92%)	16 (7%)	2 (1%)	17	56
9	B	177/213 (83%)	163 (92%)	14 (8%)	0	100	100
10	A	206/208 (99%)	181 (88%)	24 (12%)	1 (0%)	29	68
11	C	151/194 (78%)	144 (95%)	7 (5%)	0	100	100
All	All	4969/6968 (71%)	4479 (90%)	424 (8%)	66 (1%)	16	48

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	291	SER
3	4	450	GLN
3	4	609	VAL
3	4	736	ILE
4	5	340	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	495/770 (64%)	495 (100%)	0	100	100
2	3	502/835 (60%)	502 (100%)	0	100	100
3	4	554/848 (65%)	554 (100%)	0	100	100
4	5	589/688 (86%)	589 (100%)	0	100	100
5	6	548/886 (62%)	548 (100%)	0	100	100
6	7	578/753 (77%)	578 (100%)	0	100	100
7	c	498/585 (85%)	496 (100%)	2 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	213/279 (76%)	212 (100%)	1 (0%)	88	93
9	B	171/198 (86%)	170 (99%)	1 (1%)	86	92
10	A	192/192 (100%)	191 (100%)	1 (0%)	88	93
11	C	144/173 (83%)	144 (100%)	0	100	100
All	All	4484/6207 (72%)	4479 (100%)	5 (0%)	93	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	c	27	LEU
7	c	152	LEU
8	D	168	LEU
9	B	175	LEU
10	A	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
9	B	146	GLN
9	B	179	ASN
4	5	49	GLN
3	4	797	GLN
10	A	104	ASN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	7	1
2	3	1
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	386:LYS	C	387:LYS	N	6.57
1	3	310:ASN	C	311:SER	N	5.65
1	4	467:LYS	C	468:LYS	N	3.57

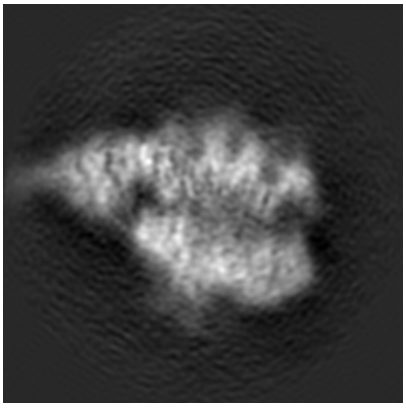
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6536. These allow visual inspection of the internal detail of the map and identification of artifacts.

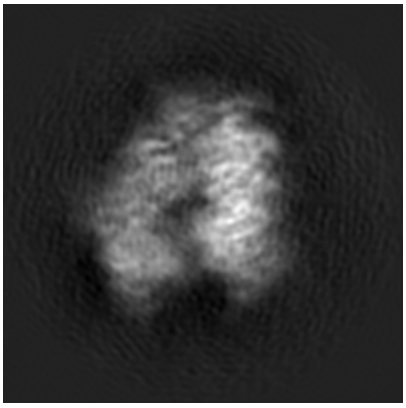
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

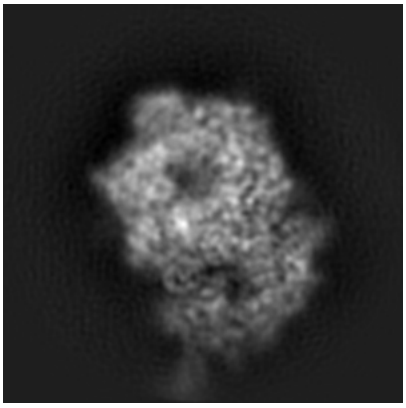
6.1.1 Primary map



X



Y

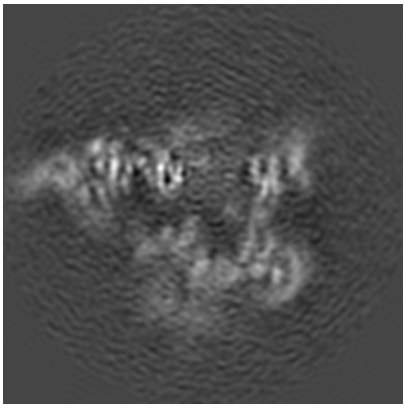


Z

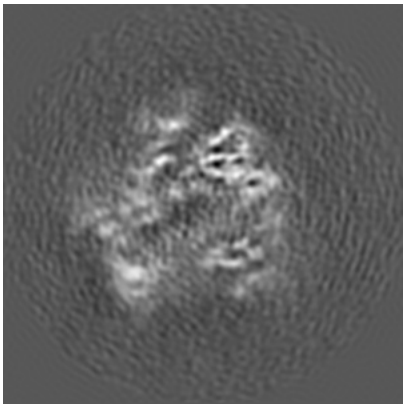
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

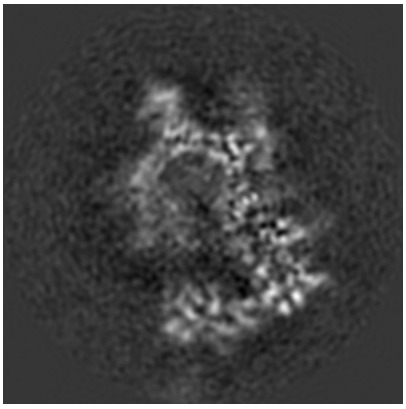
6.2.1 Primary map



X Index: 128



Y Index: 128

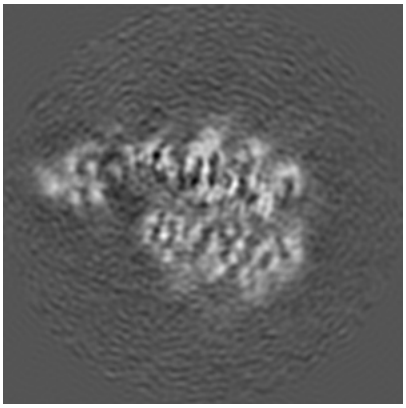


Z Index: 128

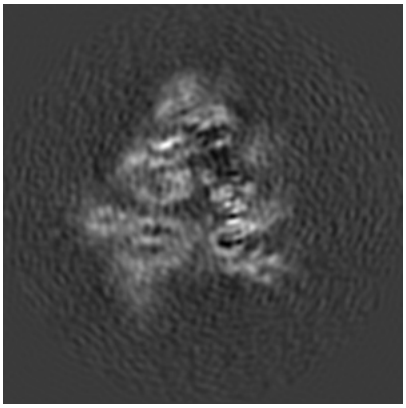
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

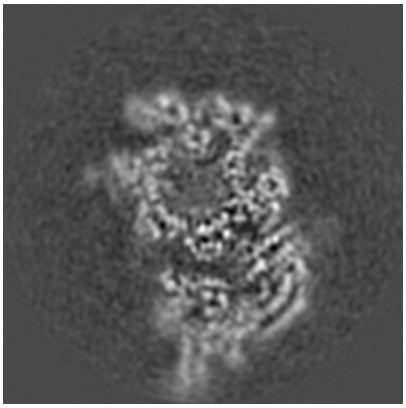
6.3.1 Primary map



X Index: 146



Y Index: 113

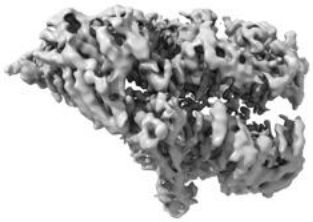


Z Index: 143

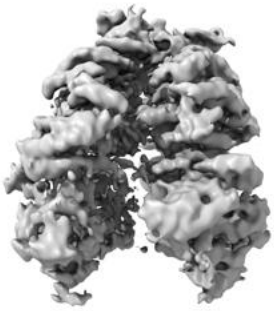
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

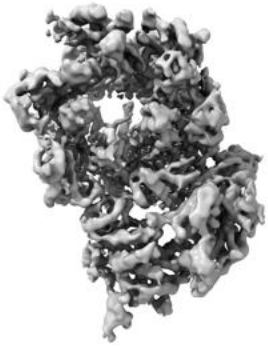
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

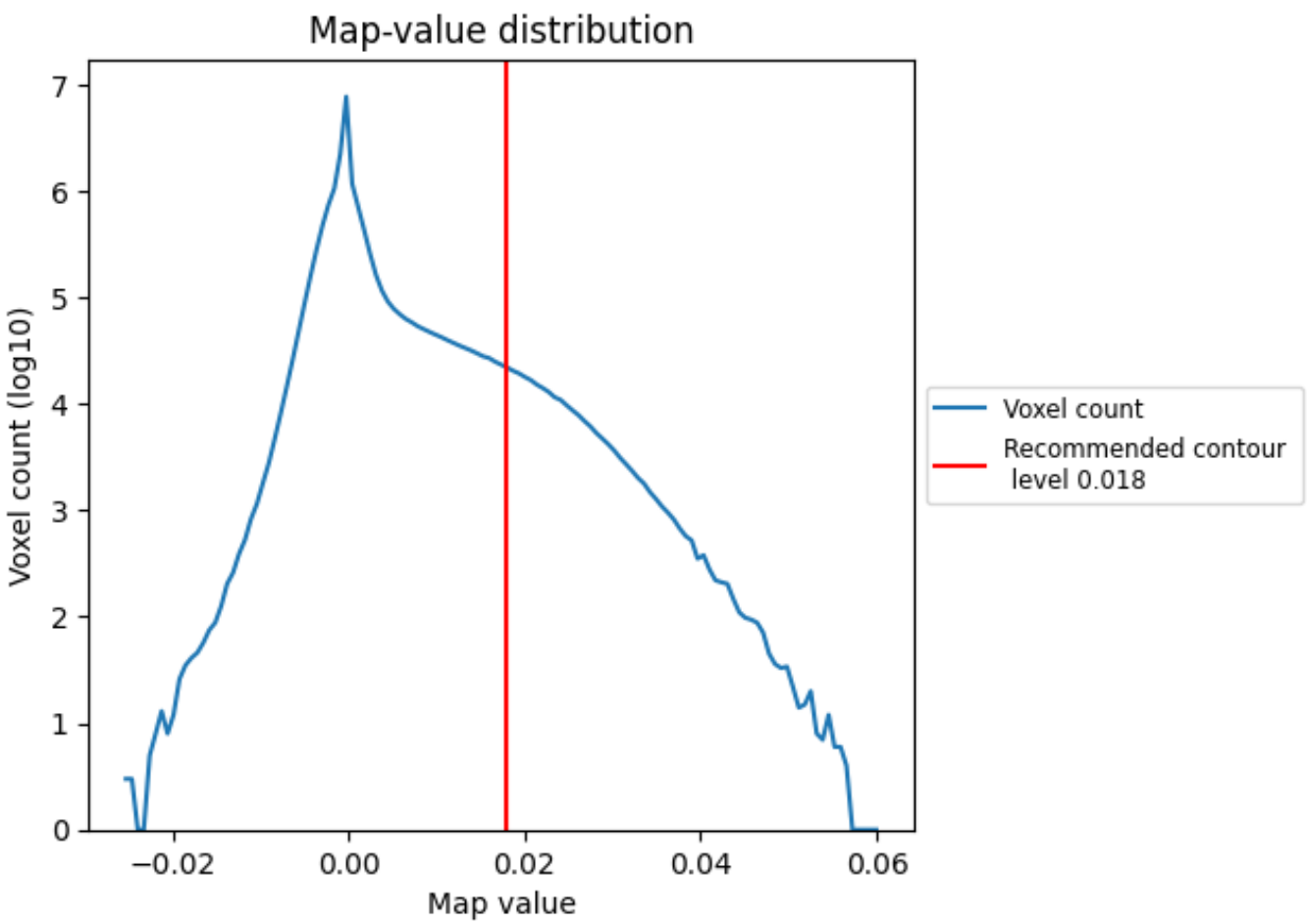
6.5 Mask visualisation (i)

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

7 Map analysis (i)

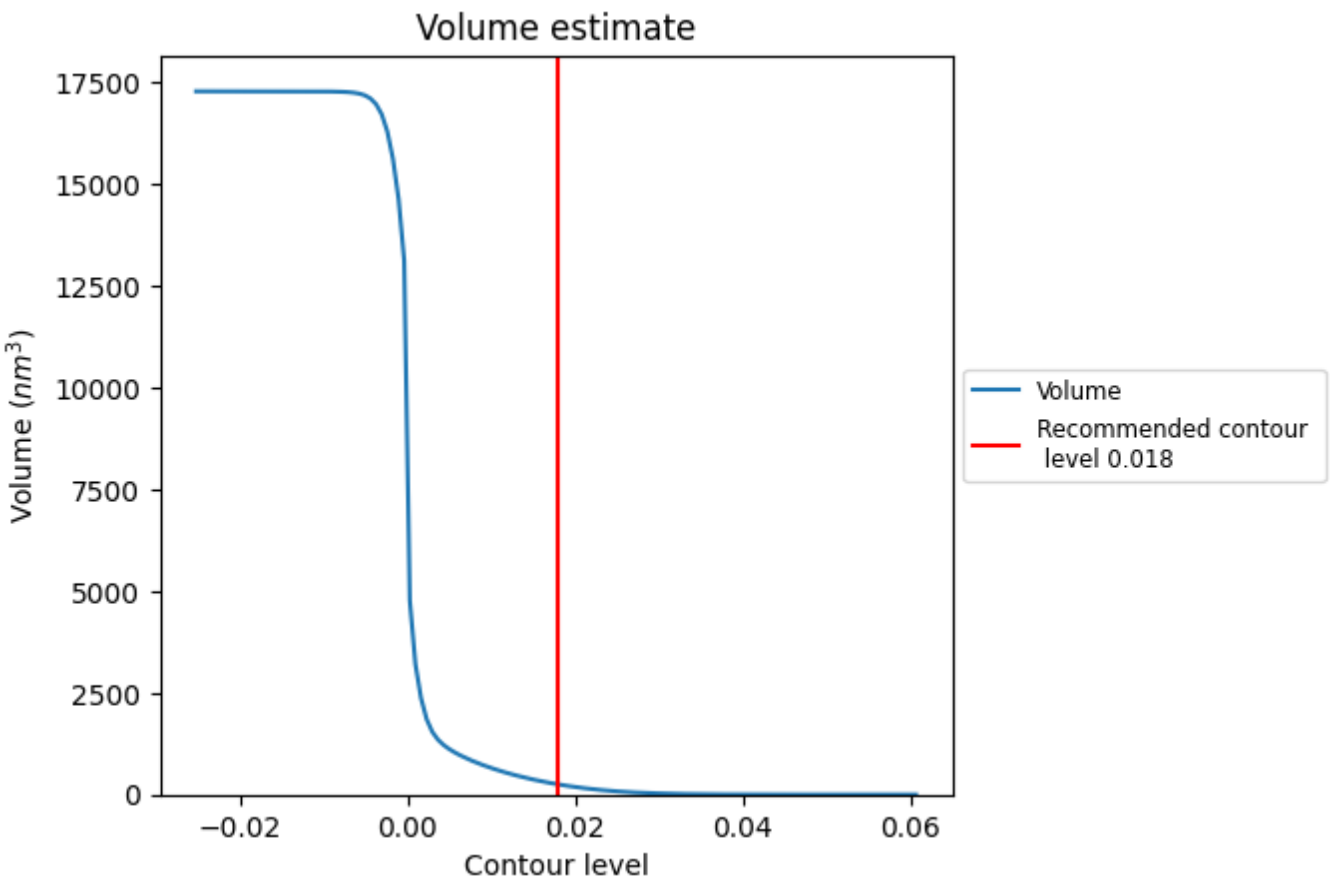
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

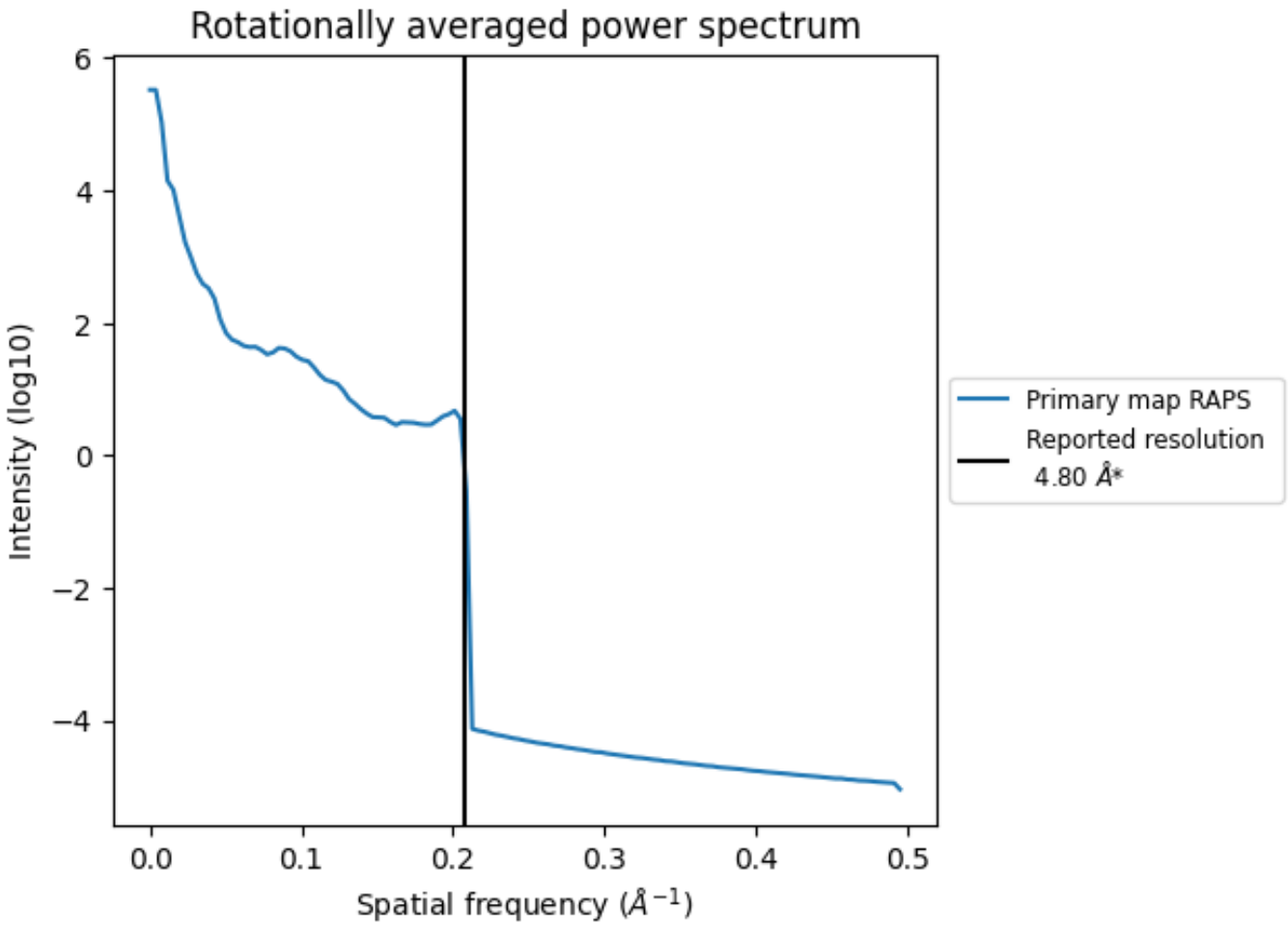
7.2 Volume estimate (i)



The volume at the recommended contour level is 248 nm^3; this corresponds to an approximate mass of 224 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 0.208 Å^{-1}

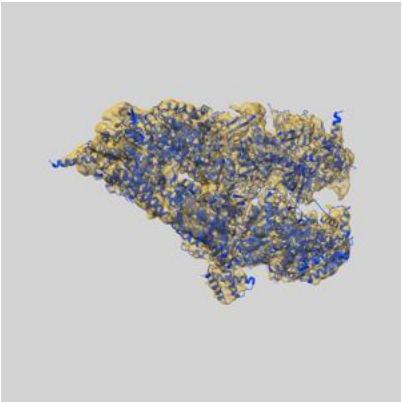
8 Fourier-Shell correlation (i)

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

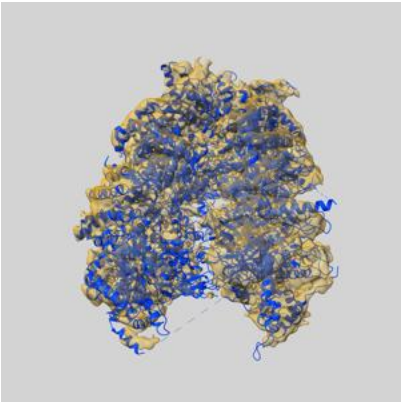
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6536 and PDB model 3JC7. Per-residue inclusion information can be found in section 3 on page 7.

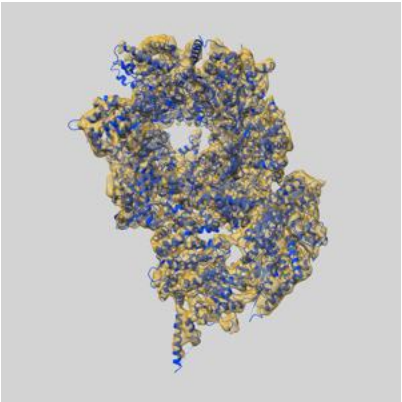
9.1 Map-model overlay (i)



X



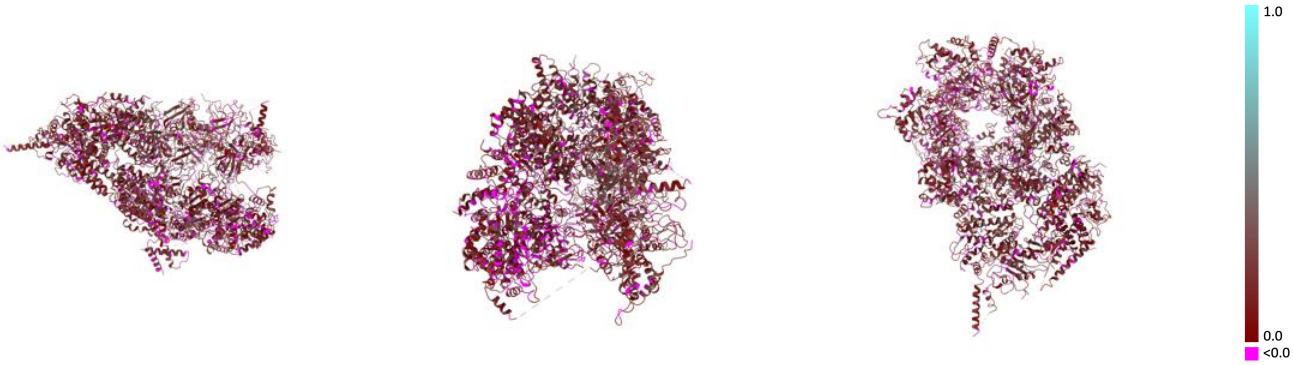
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

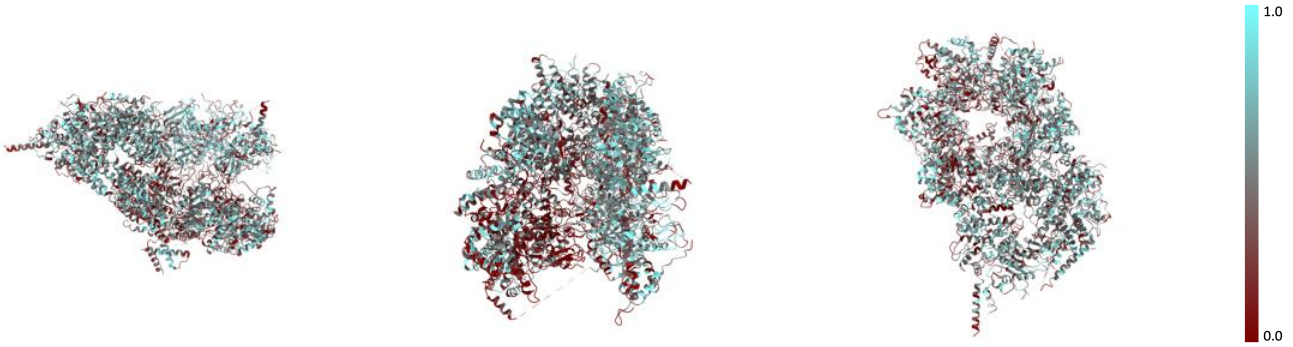
9.2 Q-score mapped to coordinate model (i)



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.

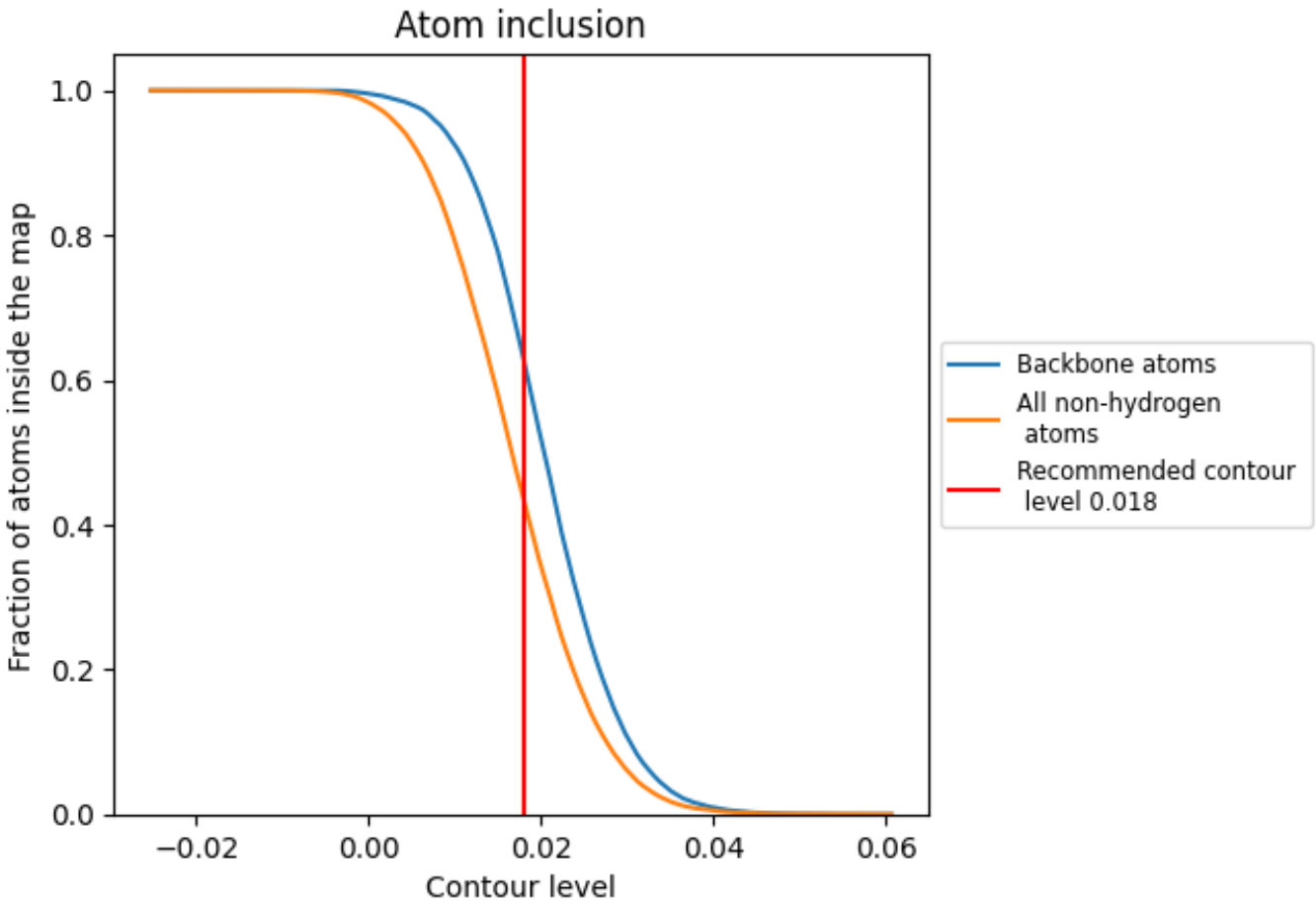
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 43% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4336	0.1510
2	0.3591	0.1370
3	0.5001	0.1760
4	0.3657	0.1200
5	0.4164	0.1670
6	0.4068	0.1290
7	0.4538	0.1510
A	0.4434	0.1580
B	0.4913	0.1370
C	0.4886	0.1930
D	0.5271	0.1530
c	0.4665	0.1730