wwPDB EM Validation Summary Report

Nov 9, 2024 – 10:57 AM EST

PDB ID	:	5U8T
EMDB ID	:	EMD-8519
Title	:	Structure of Eukaryotic CMG Helicase at a Replication Fork and Implications
Authors	:	Li, B.; Georgescu, R.; Yuan, Z.; Santos, R.; Sun, J.; Zhang, D.; Yurieva, O.; Li, H.; O'Donnell, M.E.
Deposited on	:	2016-12-15
Resolution	:	4.90 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

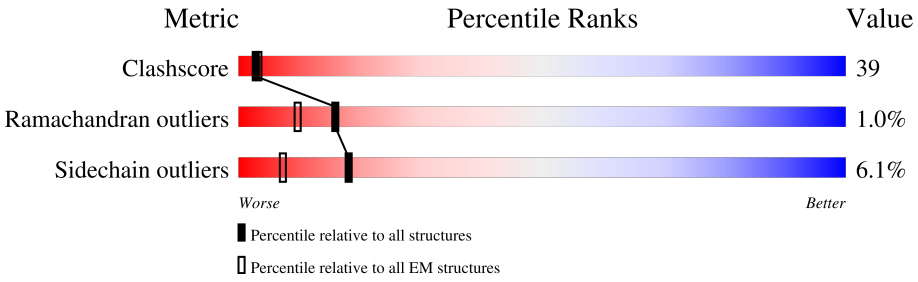
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5% 23% 39% • 33%
2	3	971	5% 23% 34% • 39%
3	4	933	12% 27% 41% • 28%
4	5	775	9% 27% 47% • • 22%
5	6	1017	9% 21% 40% • 35%
6	7	845	18% 31% 44% • 22%
7	A	208	11% 39% 56% 5%
8	B	213	30% 52% • 15%

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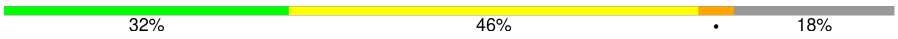
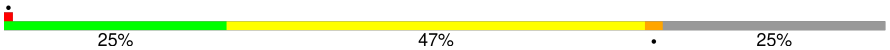
Mol	Chain	Length	Quality of chain
9	C	194	
10	D	294	
11	E	650	
12	F	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ANP	2	901	-	-	X	-
13	ANP	3	1001	-	-	X	-
13	ANP	5	801	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 40788 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	583	4591	2899	818	858	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	589	4624	2915	824	872	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	672	5318	3340	929	1021	28	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	602	4740	2980	815	921	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	661	5142	3247	905	967	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	660	5201	3278	903	991	29	0	0

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

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

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

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

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

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

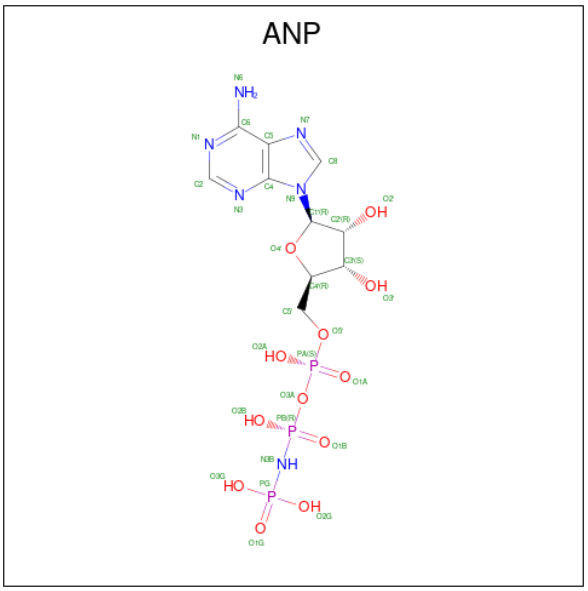
- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 12 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T P*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	14	Total	C	N	O	P	0	0
			280	140	28	98	14		

- Molecule 13 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



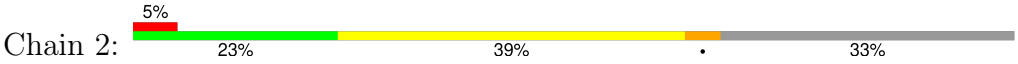
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
13	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
13	5	1	Total	C	N	O	P	0
			31	10	6	12	3	

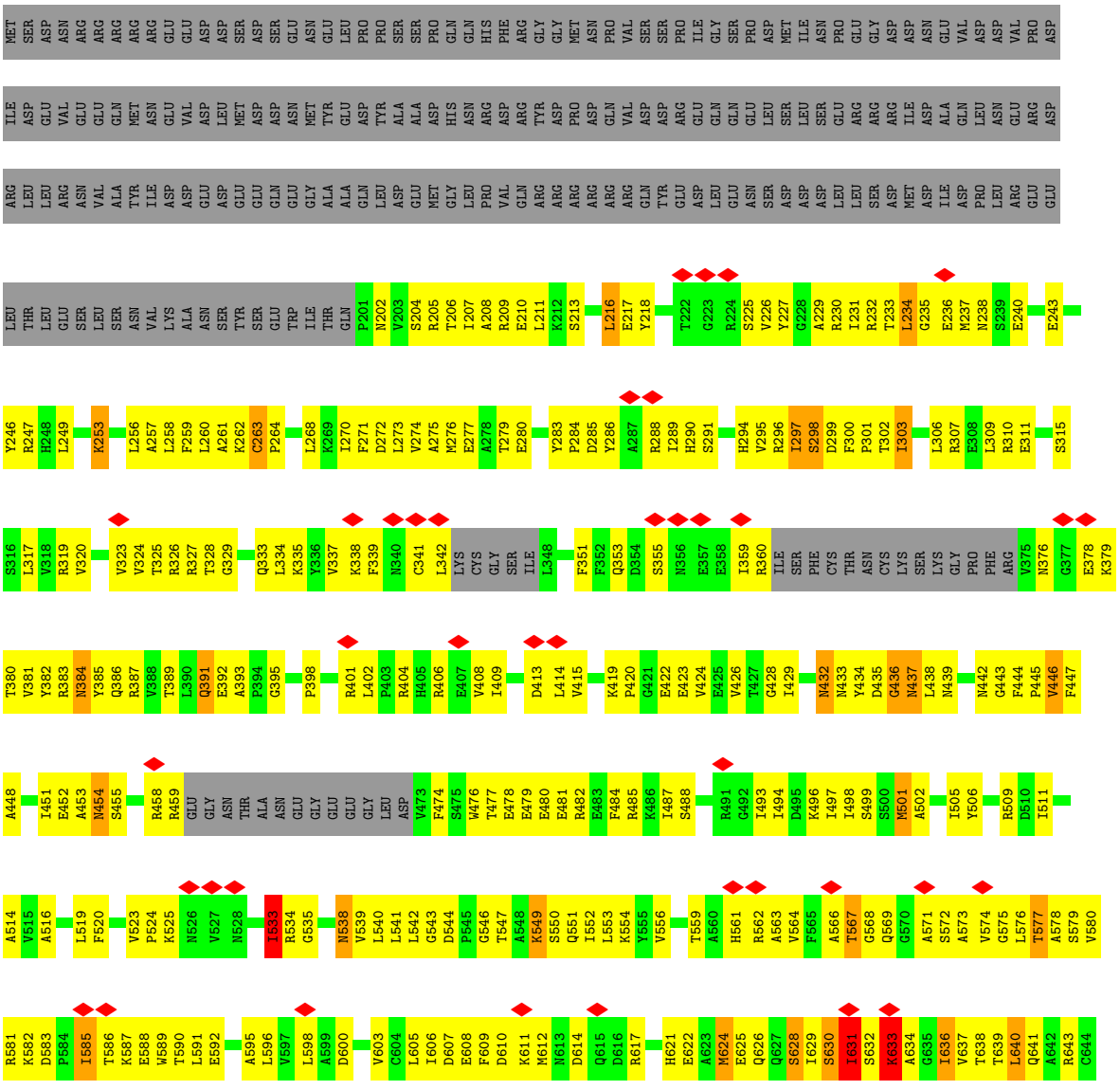
3 Residue-property plots (i)

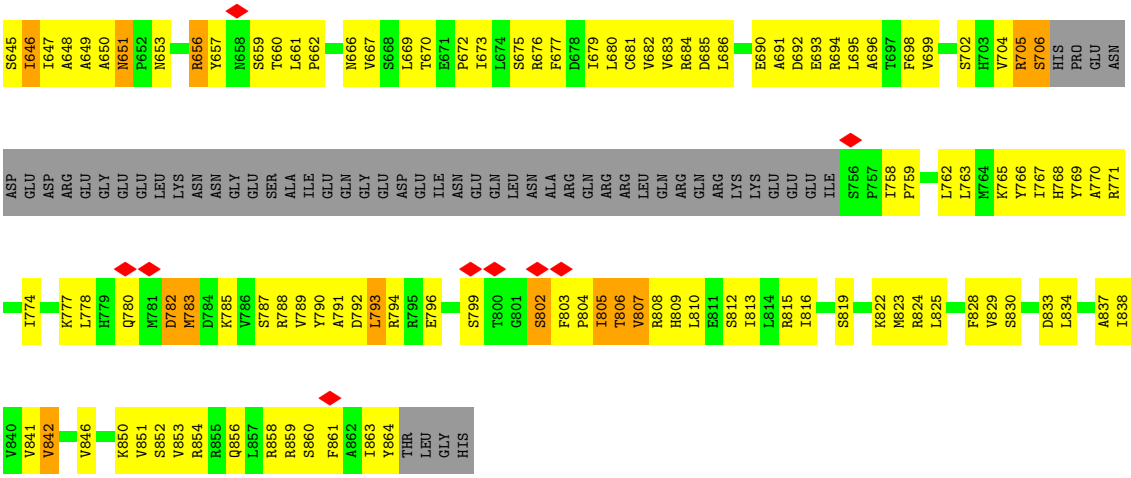
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:

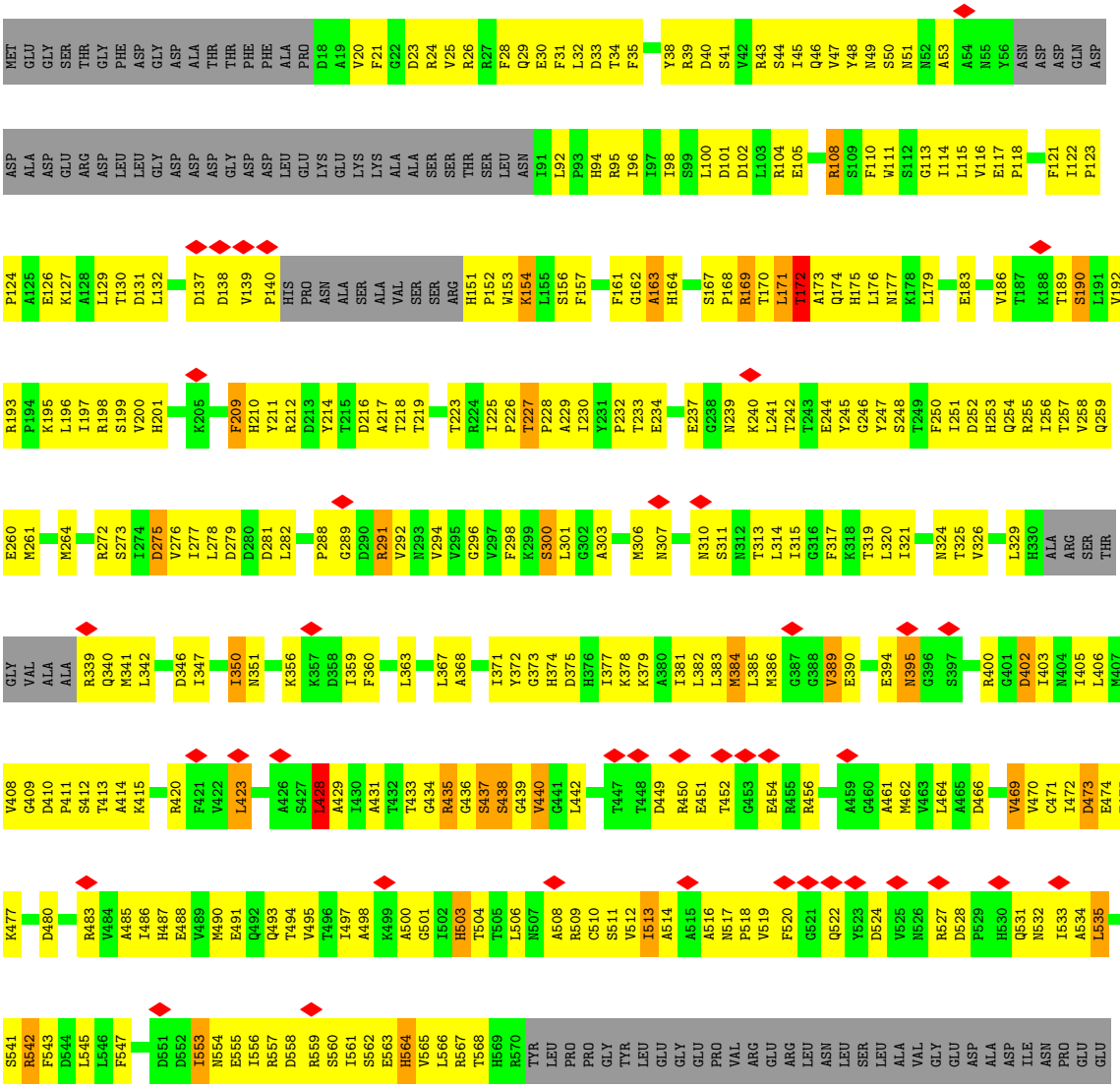


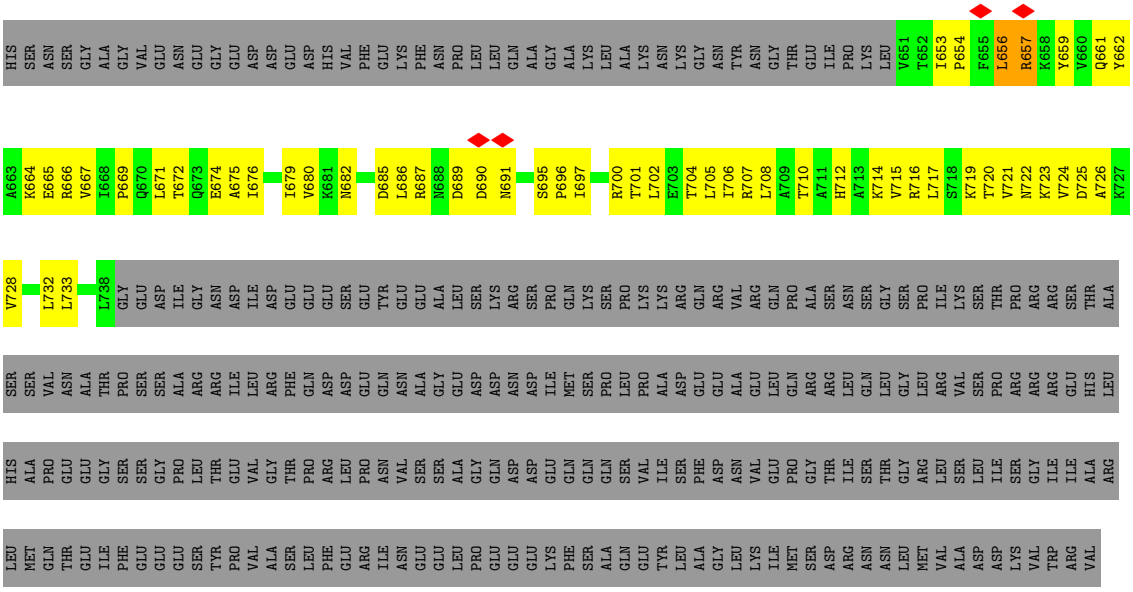




• Molecule 2: DNA replication licensing factor MCM3

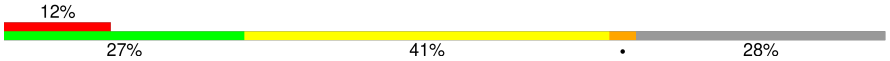
Chain 3:

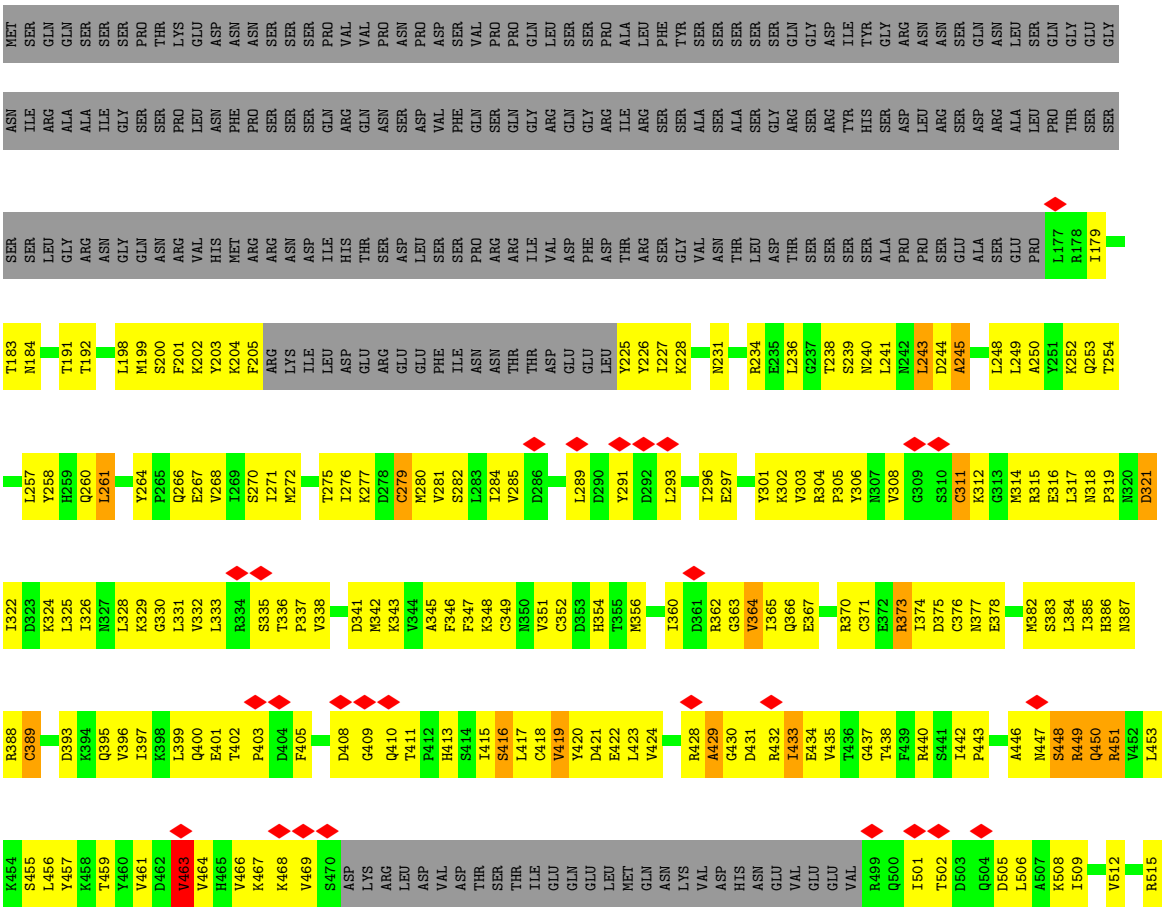


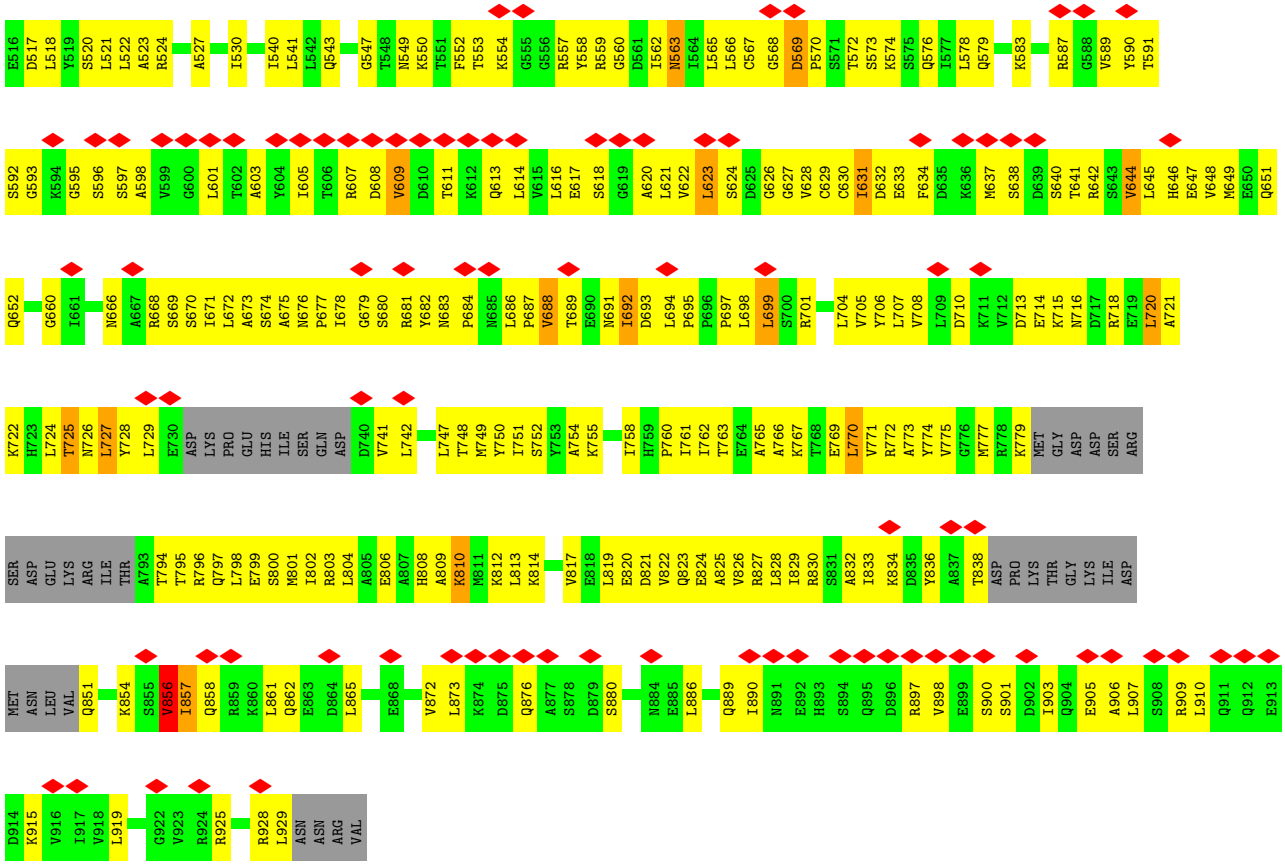


• Molecule 3: DNA replication licensing factor MCM4

Chain 4:

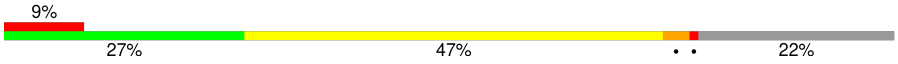


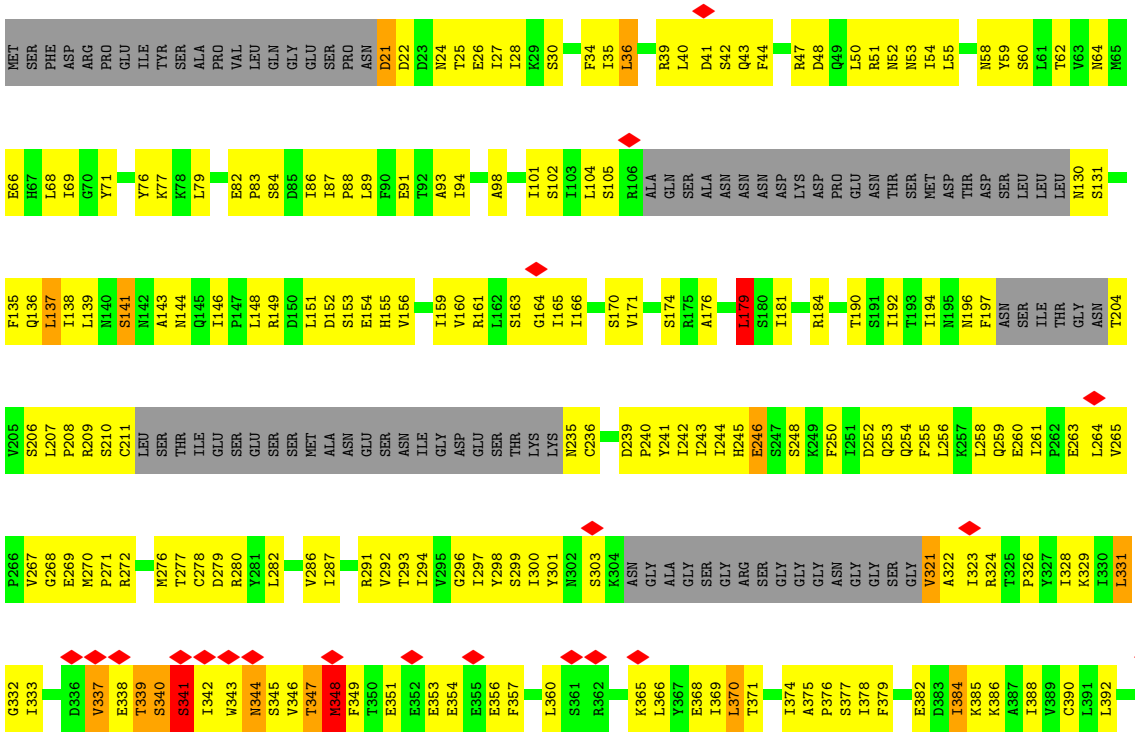


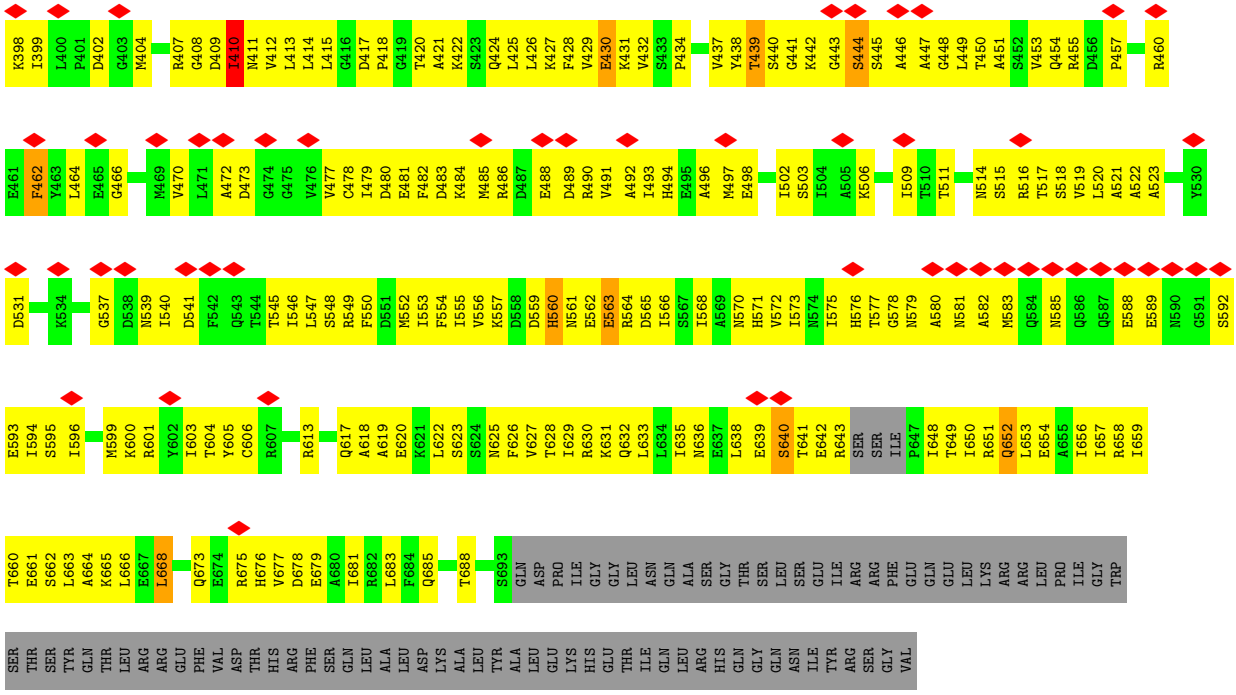


• Molecule 4: Minichromosome maintenance protein 5

Chain 5:

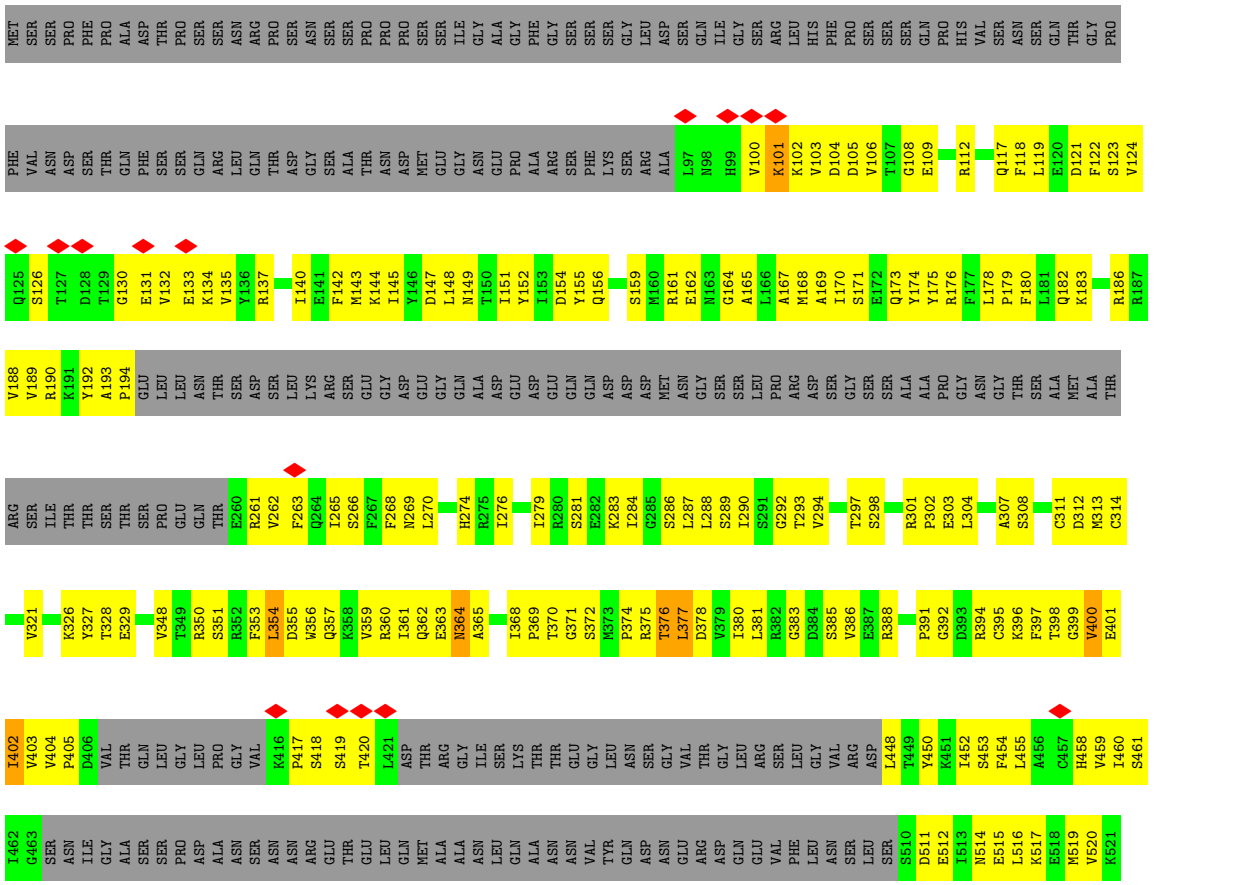


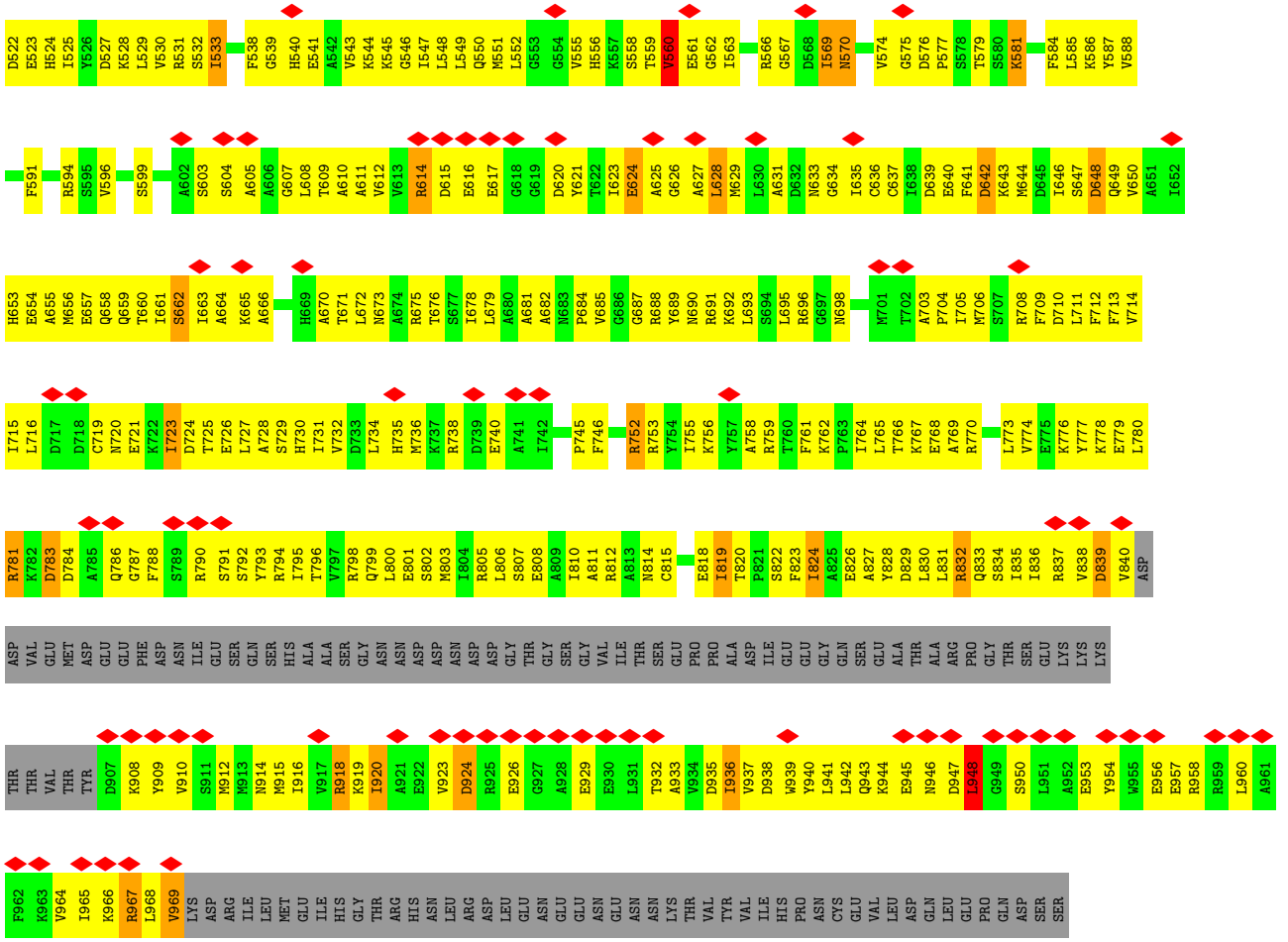




• Molecule 5: DNA replication licensing factor MCM6

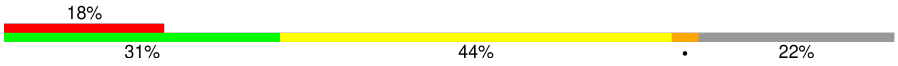
Chain 6:

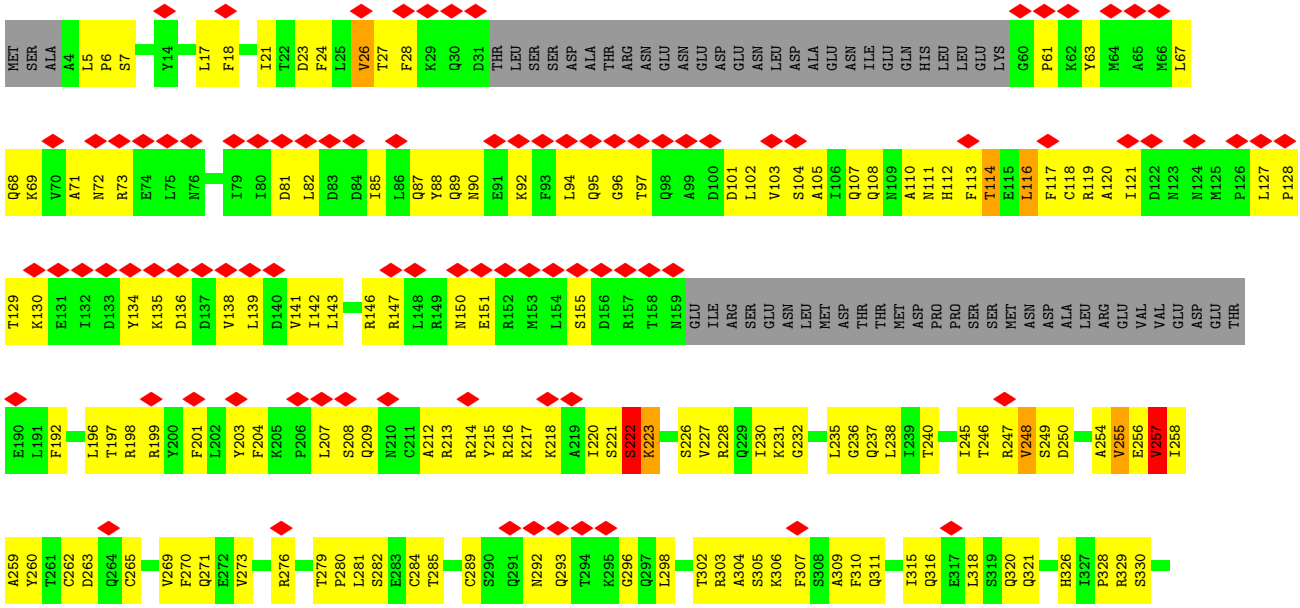


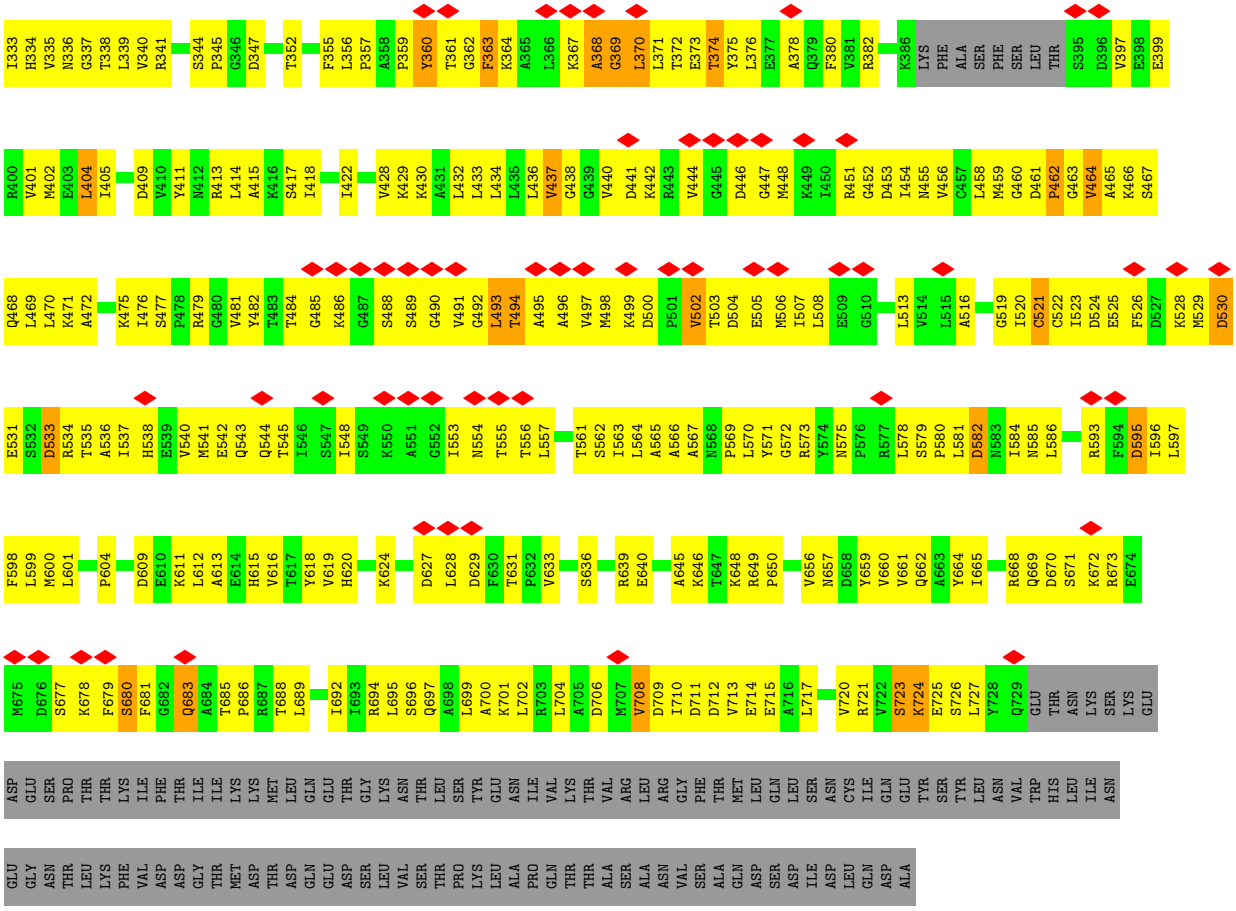


• Molecule 6: DNA replication licensing factor MCM7

Chain 7:

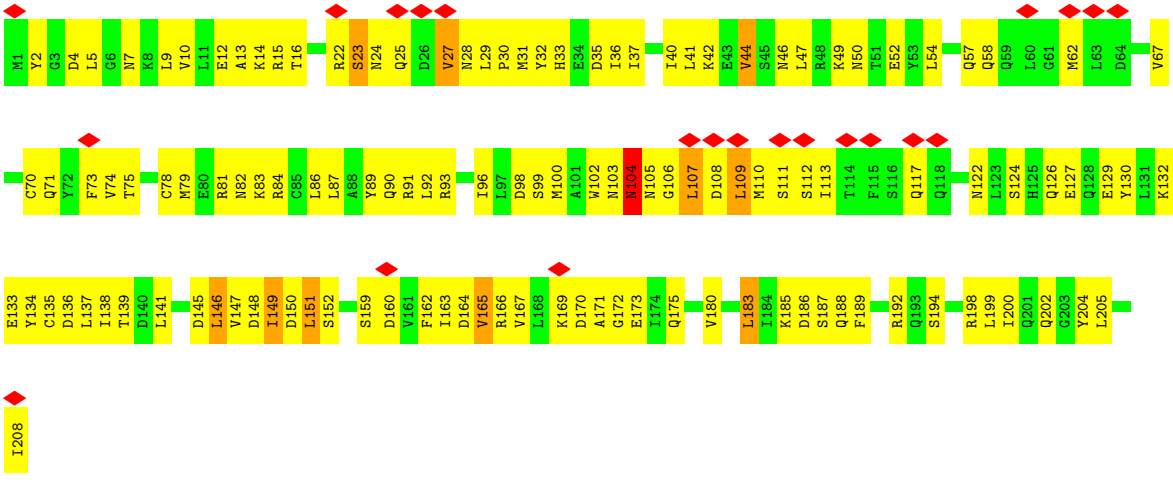






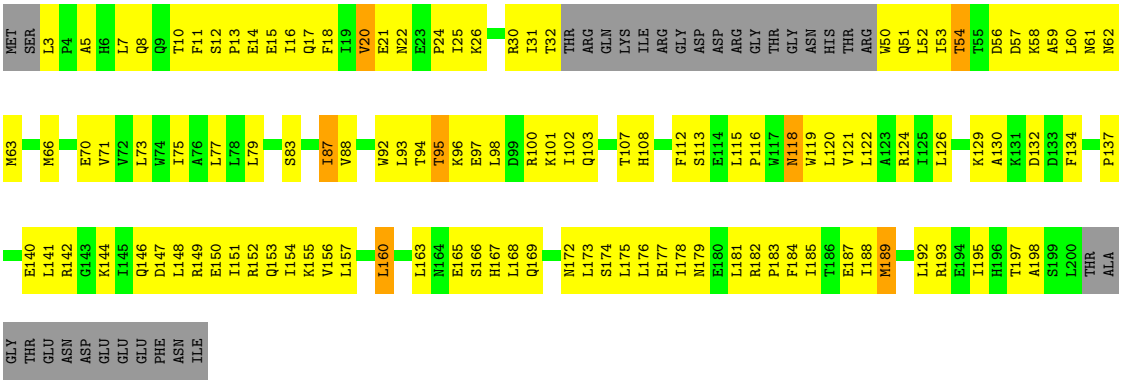
• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:



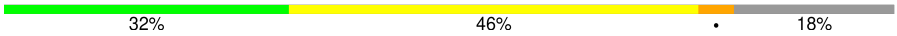
• Molecule 8: DNA replication complex GINS protein PSF2

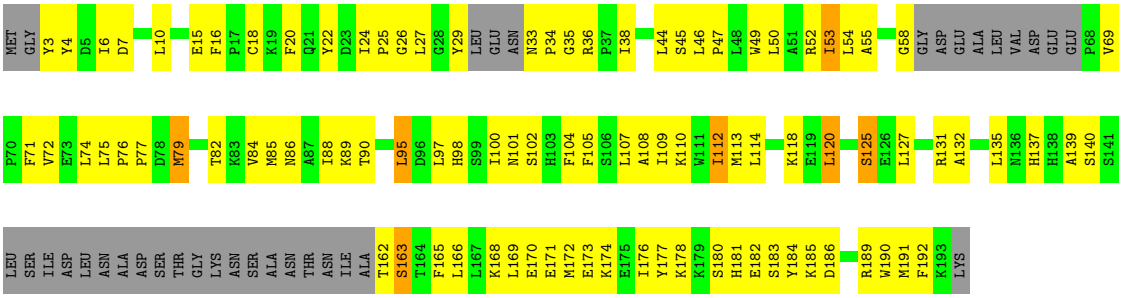
Chain B:



• Molecule 9: DNA replication complex GINS protein PSF3

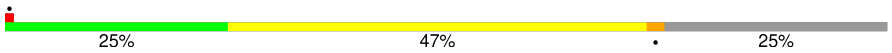
Chain C:

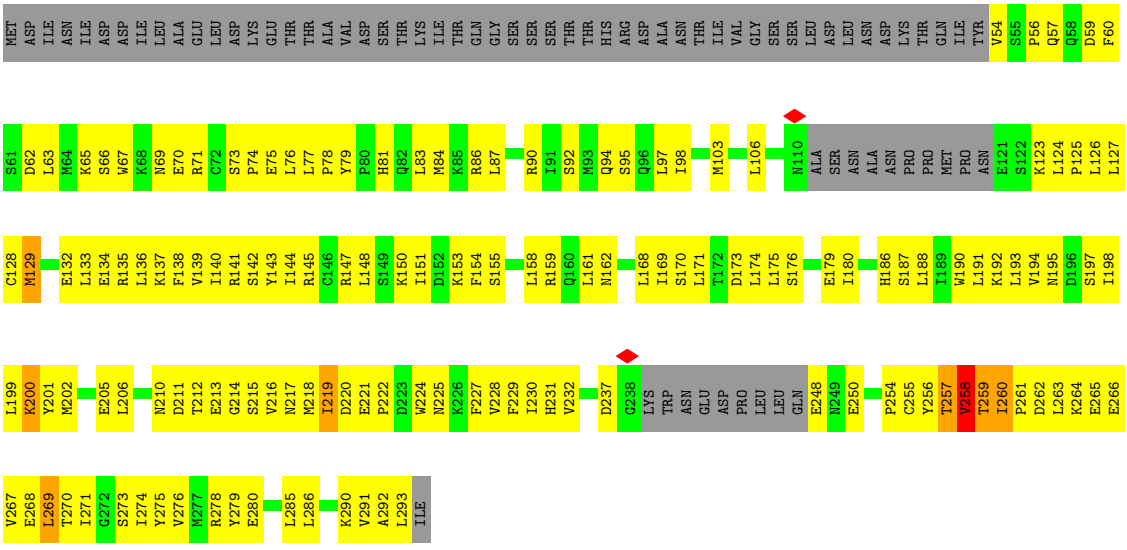




• Molecule 10: DNA replication complex GINS protein SLD5

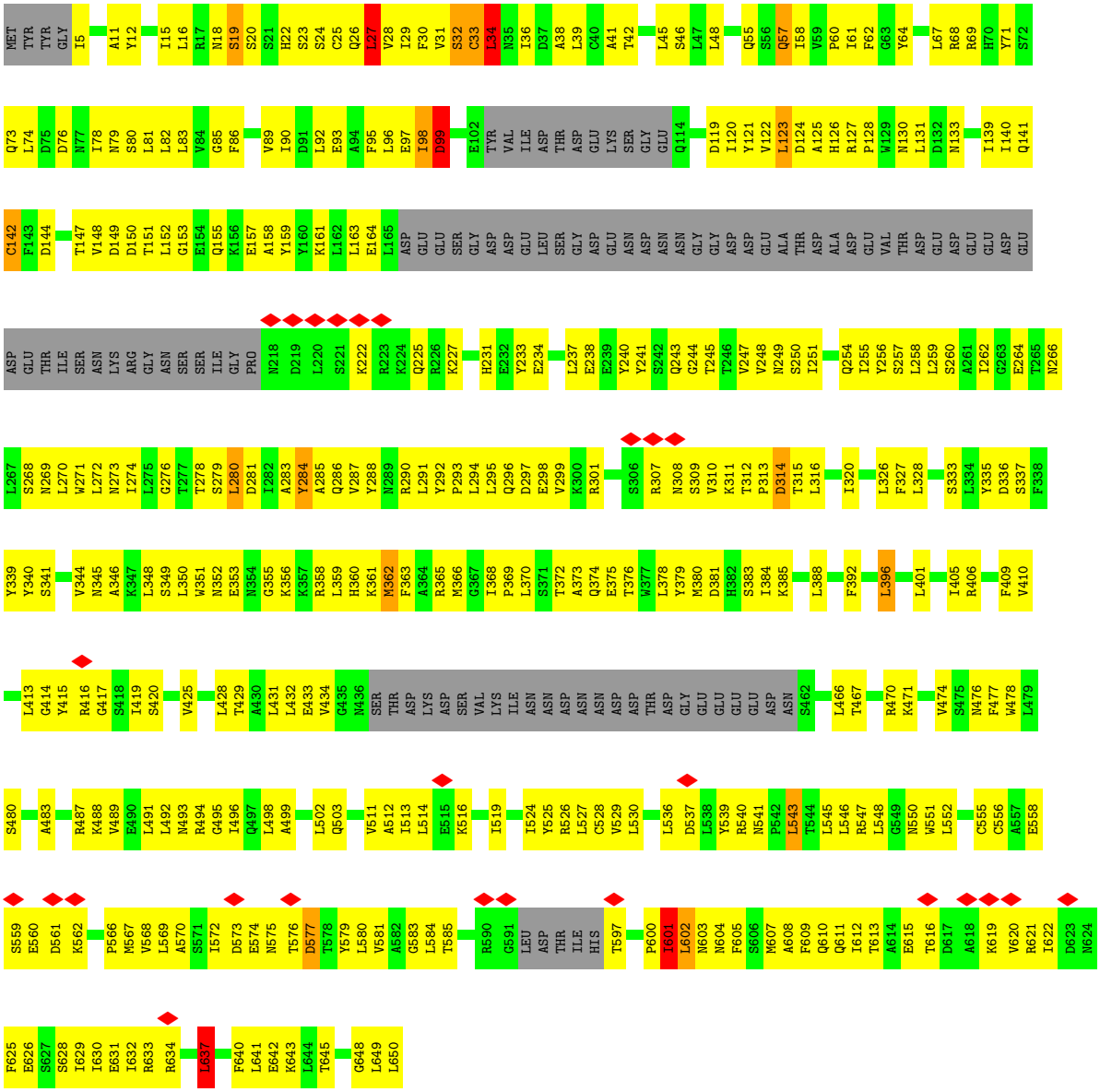
Chain D:





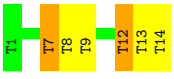
• Molecule 11: Cell division control protein 45

Chain E:



• Molecule 12: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	395443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

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	0.37	1/4668 (0.0%)	0.65	2/6306 (0.0%)
2	3	0.32	0/4702	0.63	1/6374 (0.0%)
3	4	0.31	0/5388	0.63	0/7273
4	5	0.34	0/4805	0.65	1/6489 (0.0%)
5	6	0.36	0/5218	0.69	3/7039 (0.0%)
6	7	0.33	0/5281	0.65	2/7136 (0.0%)
7	A	0.36	0/1718	0.70	1/2314 (0.0%)
8	B	0.33	0/1545	0.62	0/2092
9	C	0.32	0/1320	0.60	1/1784 (0.1%)
10	D	0.34	0/1853	0.69	2/2500 (0.1%)
11	E	0.33	0/4563	0.63	5/6173 (0.1%)
12	F	0.88	1/307 (0.3%)	1.42	3/472 (0.6%)
All	All	0.34	2/41368 (0.0%)	0.66	21/55952 (0.0%)

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	2
2	3	0	5
3	4	0	3
4	5	0	1
5	6	0	1
6	7	0	5
7	A	0	2
10	D	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	633	LYS	CE-NZ	6.70	1.65	1.49
12	F	12	DT	O5'-C5'	-5.01	1.29	1.42

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	369	GLY	N-CA-C	8.34	133.96	113.10
12	F	7	DT	O4'-C4'-C3'	-7.76	101.35	106.00
12	F	12	DT	OP1-P-OP2	7.47	130.81	119.60
10	D	269	LEU	CA-CB-CG	7.46	132.46	115.30
5	6	948	LEU	CA-CB-CG	7.37	132.25	115.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	355	SER	Peptide
1	2	633	LYS	Peptide
2	3	163	ALA	Peptide
2	3	172	THR	Peptide
2	3	428	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4591	0	4639	428	0
2	3	4624	0	4689	376	0
3	4	5318	0	5390	424	0
4	5	4740	0	4798	439	0
5	6	5142	0	5093	499	0
6	7	5201	0	5276	422	0
7	A	1696	0	1698	141	0
8	B	1513	0	1558	124	0
9	C	1288	0	1298	92	0
10	D	1820	0	1824	201	0
11	E	4482	0	4499	367	0
12	F	280	0	169	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	2	31	0	13	9	0
13	3	31	0	13	10	0
13	5	31	0	13	9	0
All	All	40788	0	40970	3219	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 39.

The worst 5 of 3219 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)
10:D:260:ILE:HG13	10:D:266:GLU:CG	1.46	1.45
6:7:221:SER:CA	6:7:222:SER:HB2	1.40	1.44
10:D:260:ILE:CG1	10:D:266:GLU:CD	1.87	1.42
10:D:260:ILE:HG12	10:D:266:GLU:CD	1.38	1.38
10:D:260:ILE:CG1	10:D:266:GLU:OE2	1.74	1.35

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	573/868 (66%)	502 (88%)	63 (11%)	8 (1%)	9 40
2	3	579/971 (60%)	525 (91%)	52 (9%)	2 (0%)	37 72
3	4	660/933 (71%)	577 (87%)	72 (11%)	11 (2%)	7 36
4	5	590/775 (76%)	537 (91%)	48 (8%)	5 (1%)	16 54
5	6	649/1017 (64%)	571 (88%)	72 (11%)	6 (1%)	14 50
6	7	652/845 (77%)	566 (87%)	76 (12%)	10 (2%)	8 39
7	A	206/208 (99%)	185 (90%)	20 (10%)	1 (0%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B	177/213 (83%)	156 (88%)	21 (12%)	0	100	100
9	C	151/194 (78%)	140 (93%)	11 (7%)	0	100	100
10	D	215/294 (73%)	193 (90%)	19 (9%)	3 (1%)	9	40
11	E	543/650 (84%)	488 (90%)	50 (9%)	5 (1%)	14	50
All	All	4995/6968 (72%)	4440 (89%)	504 (10%)	51 (1%)	16	48

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	429	ALA
4	5	596	ILE
6	7	26	VAL
6	7	222	SER
6	7	464	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	502/770 (65%)	460 (92%)	42 (8%)	9	28
2	3	512/835 (61%)	475 (93%)	37 (7%)	12	32
3	4	599/848 (71%)	570 (95%)	29 (5%)	21	43
4	5	542/688 (79%)	500 (92%)	42 (8%)	10	30
5	6	539/886 (61%)	497 (92%)	42 (8%)	10	29
6	7	582/753 (77%)	553 (95%)	29 (5%)	20	42
7	A	193/193 (100%)	182 (94%)	11 (6%)	17	39
8	B	171/198 (86%)	162 (95%)	9 (5%)	19	41
9	C	144/173 (83%)	136 (94%)	8 (6%)	17	39
10	D	213/279 (76%)	207 (97%)	6 (3%)	38	58
11	E	499/586 (85%)	479 (96%)	20 (4%)	27	48
All	All	4496/6209 (72%)	4221 (94%)	275 (6%)	18	37

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	183	LEU
8	B	160	LEU
11	E	99	ASP
3	4	688	VAL
3	4	623	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
4	5	454	GLN
11	E	286	GLN
4	5	676	HIS
9	C	101	ASN
4	5	581	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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	$\#\|Z\|>2$
13	ANP	5	801	-	29,33,33	1.69	5 (17%)	31,52,52	1.05	2 (6%)
13	ANP	3	1001	-	29,33,33	2.27	6 (20%)	31,52,52	1.12	3 (9%)
13	ANP	2	901	-	29,33,33	2.20	6 (20%)	31,52,52	1.12	4 (12%)

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
13	ANP	5	801	-	-	5/14/38/38	0/3/3/3
13	ANP	3	1001	-	-	10/14/38/38	0/3/3/3
13	ANP	2	901	-	-	6/14/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	901	ANP	PG-O1G	7.88	1.58	1.46
13	3	1001	ANP	PG-O1G	7.81	1.58	1.46
13	3	1001	ANP	PB-O1B	6.82	1.56	1.46
13	5	801	ANP	PB-O1B	6.61	1.56	1.46
13	2	901	ANP	PB-O1B	6.10	1.55	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	901	ANP	O1B-PB-N3B	-3.13	107.17	111.77
13	3	1001	ANP	O3G-PG-O1G	-2.63	106.85	113.45
13	3	1001	ANP	O1G-PG-N3B	-2.62	107.92	111.77
13	5	801	ANP	O3A-PA-O1A	-2.45	103.34	110.70
13	5	801	ANP	C5-C6-N6	2.44	124.02	120.31

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	2	901	ANP	PB-N3B-PG-O1G
13	2	901	ANP	C5'-O5'-PA-O1A
13	2	901	ANP	C5'-O5'-PA-O2A
13	2	901	ANP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
13	3	1001	ANP	PB-N3B-PG-O1G

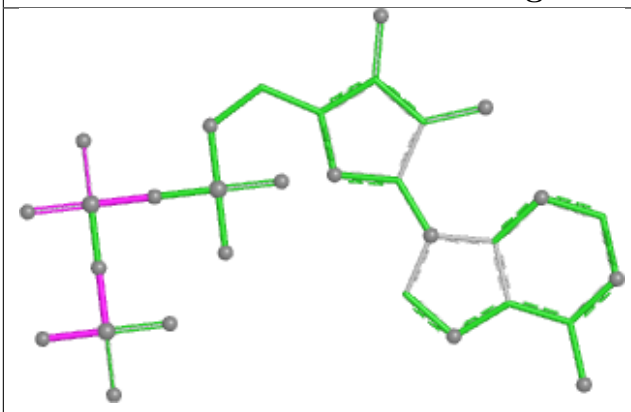
There are no ring outliers.

3 monomers are involved in 28 short contacts:

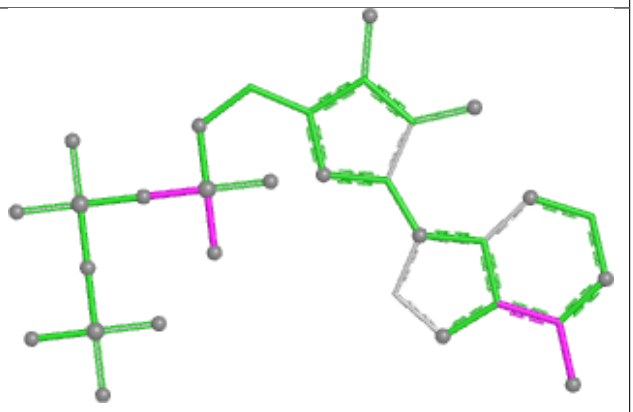
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	801	ANP	9	0
13	3	1001	ANP	10	0
13	2	901	ANP	9	0

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.

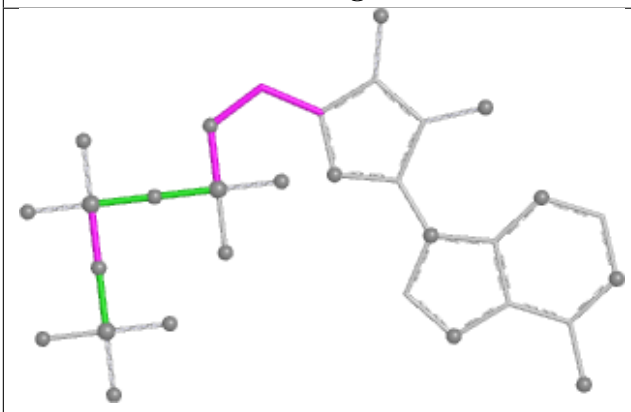
Ligand ANP 5 801



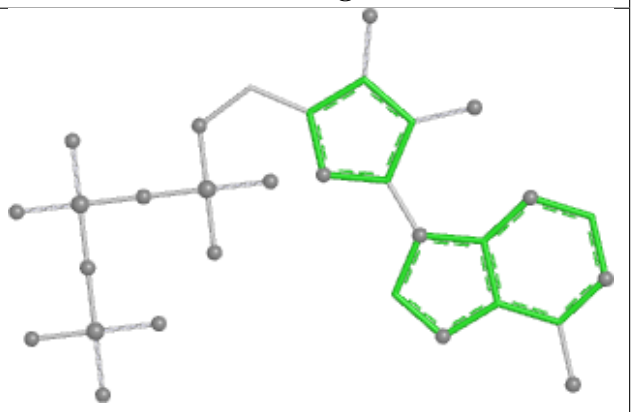
Bond lengths



Bond angles

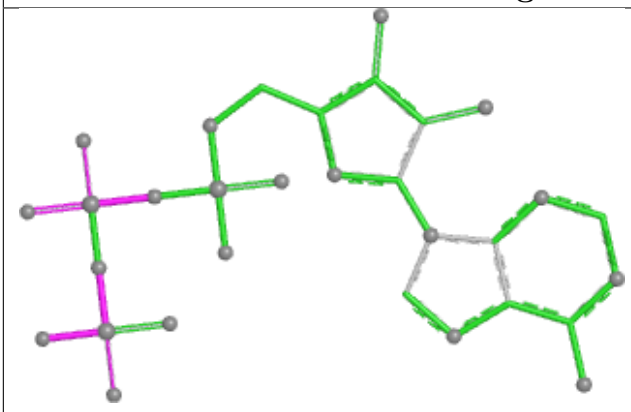


Torsions

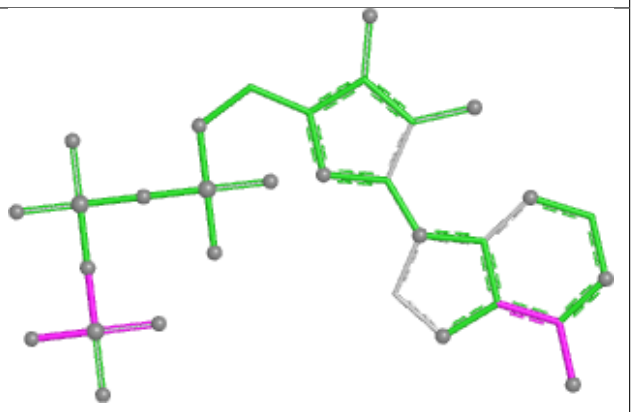


Rings

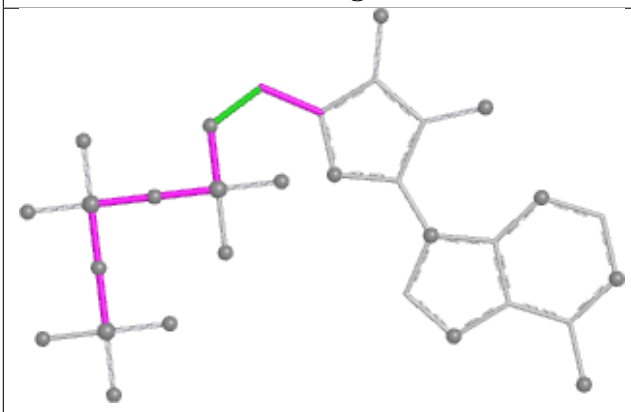
Ligand ANP 3 1001



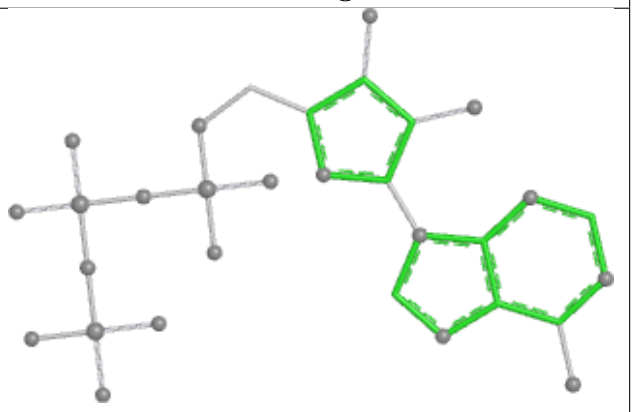
Bond lengths



Bond angles

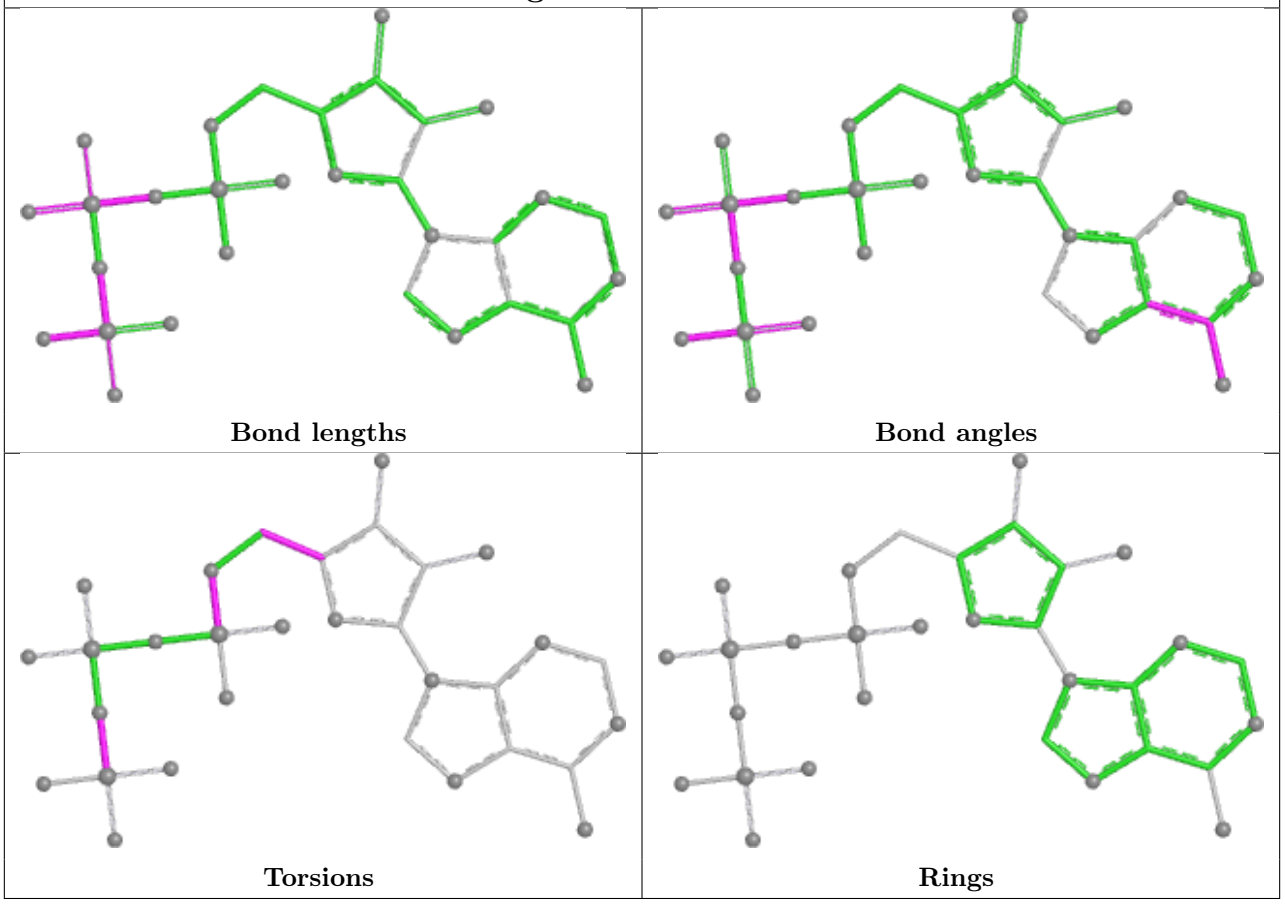


Torsions



Rings

Ligand ANP 2 901



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.

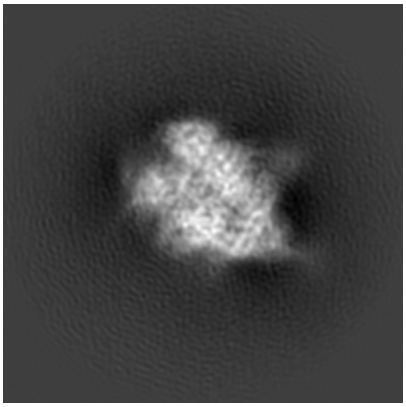
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8519. These allow visual inspection of the internal detail of the map and identification of artifacts.

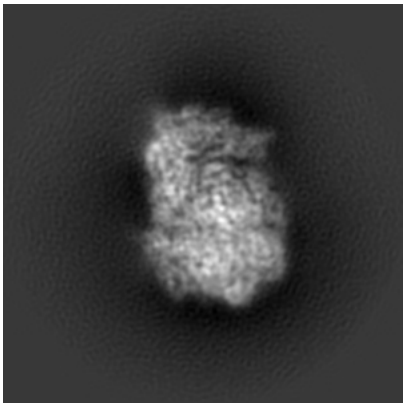
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

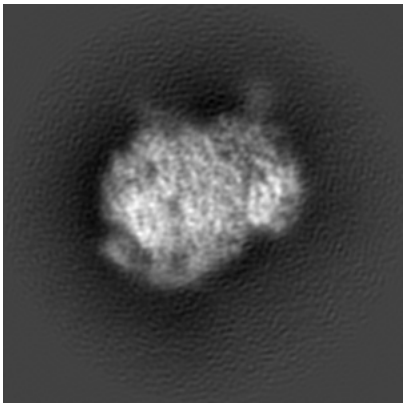
6.1.1 Primary map



X



Y

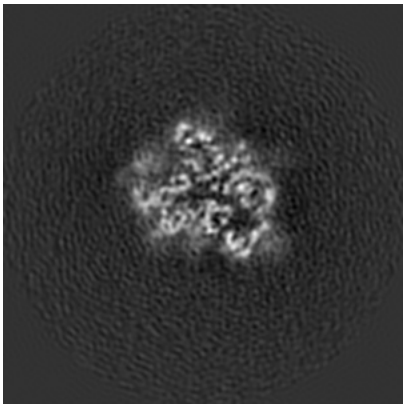


Z

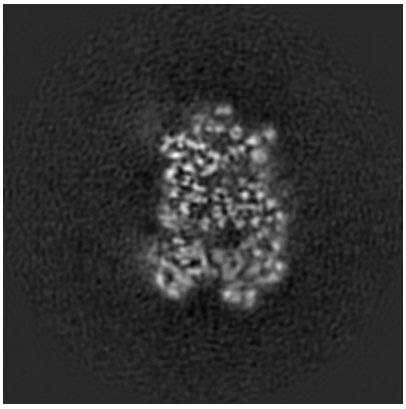
The images above show the map projected in three orthogonal directions.

6.2 Central slices

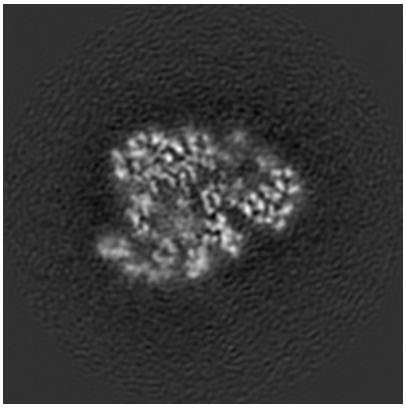
6.2.1 Primary map



X Index: 128



Y Index: 128

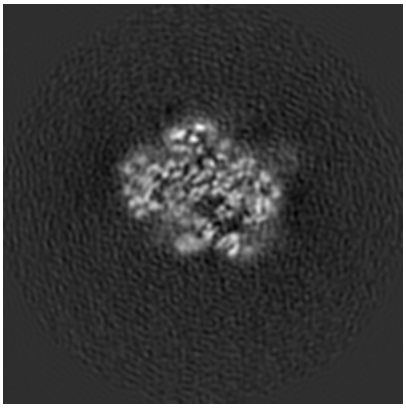


Z Index: 128

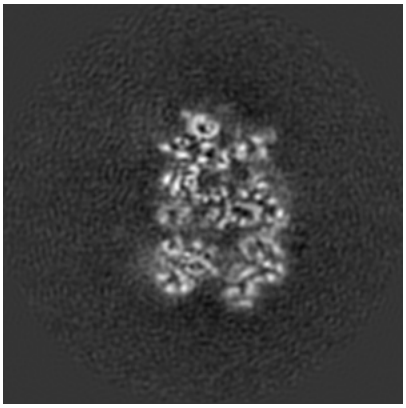
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

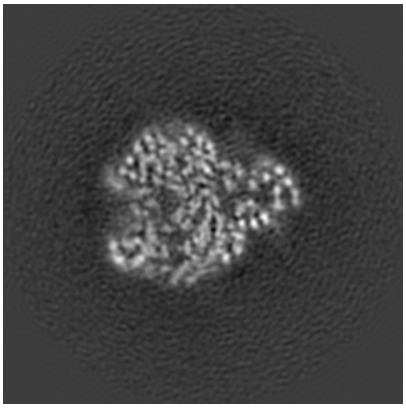
6.3.1 Primary map



X Index: 121



Y Index: 125

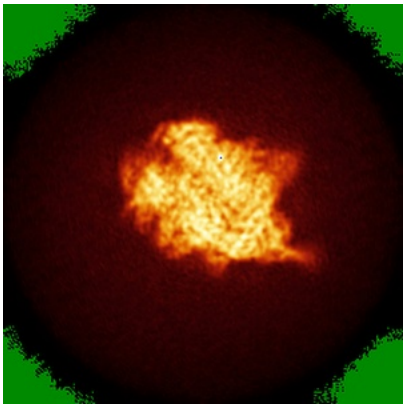


Z Index: 137

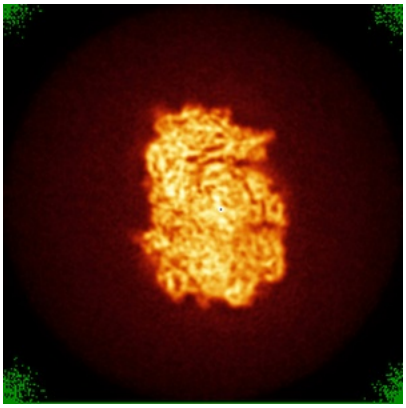
The images above show the largest variance slices of the map in three orthogonal directions.

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

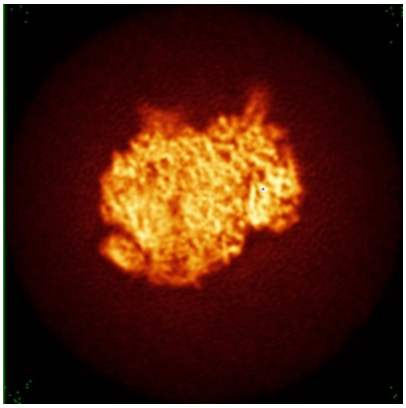
6.4.1 Primary map



X



Y

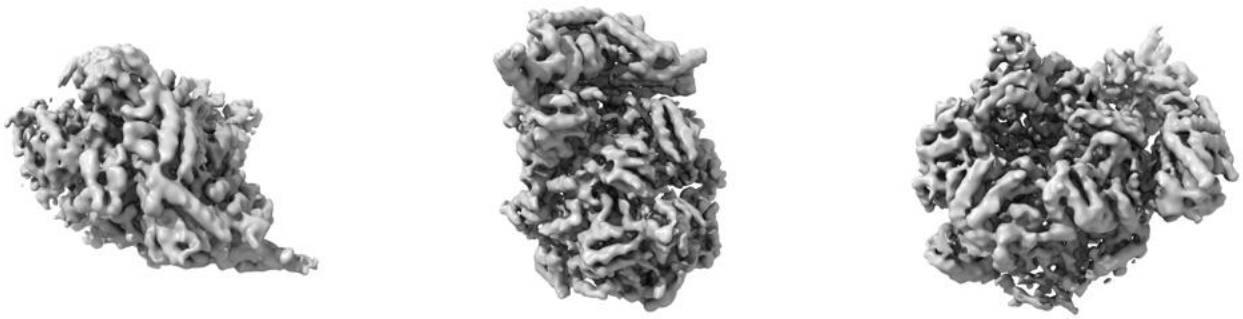


Z

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

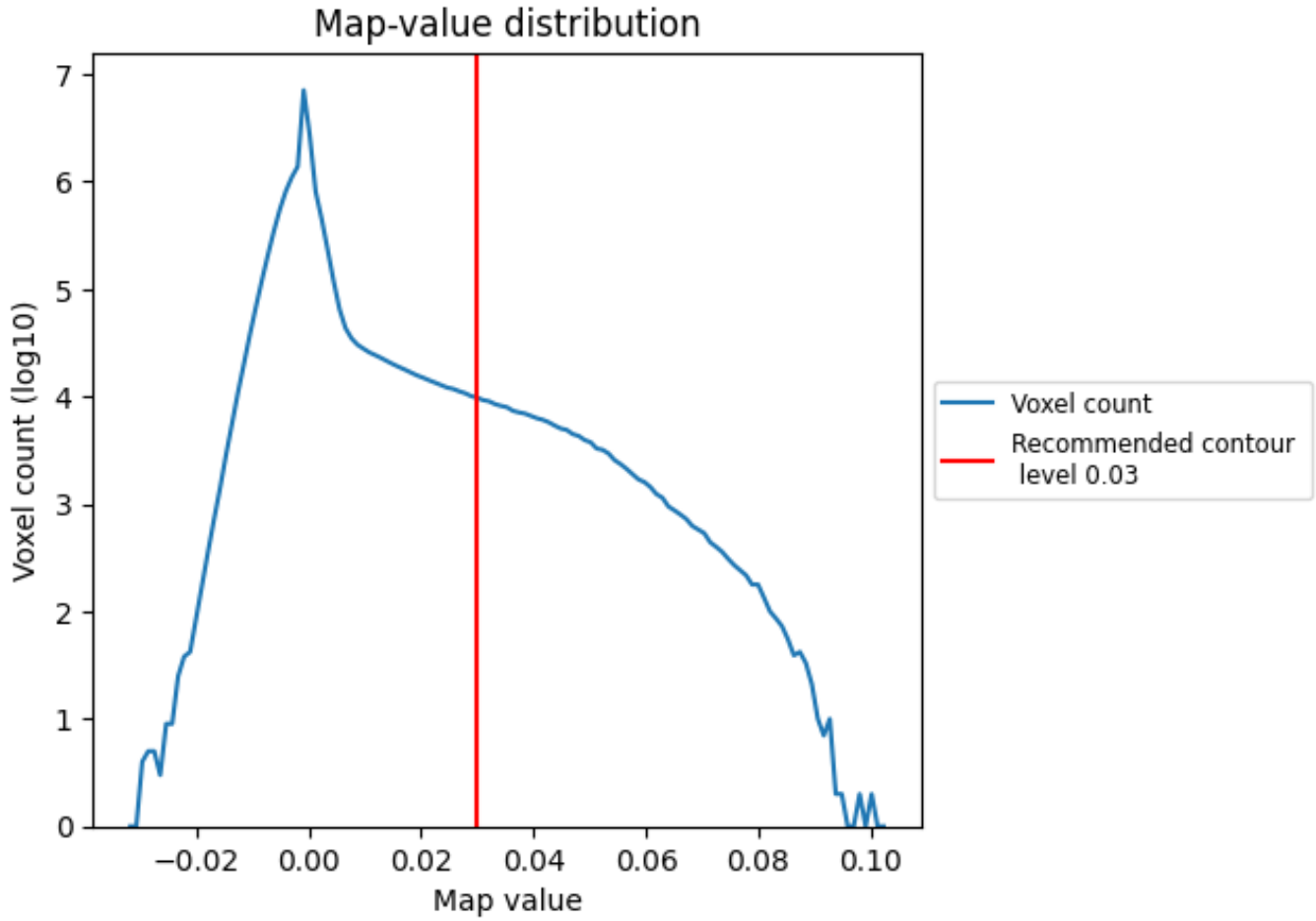
6.6 Mask visualisation (i)

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

7 Map analysis

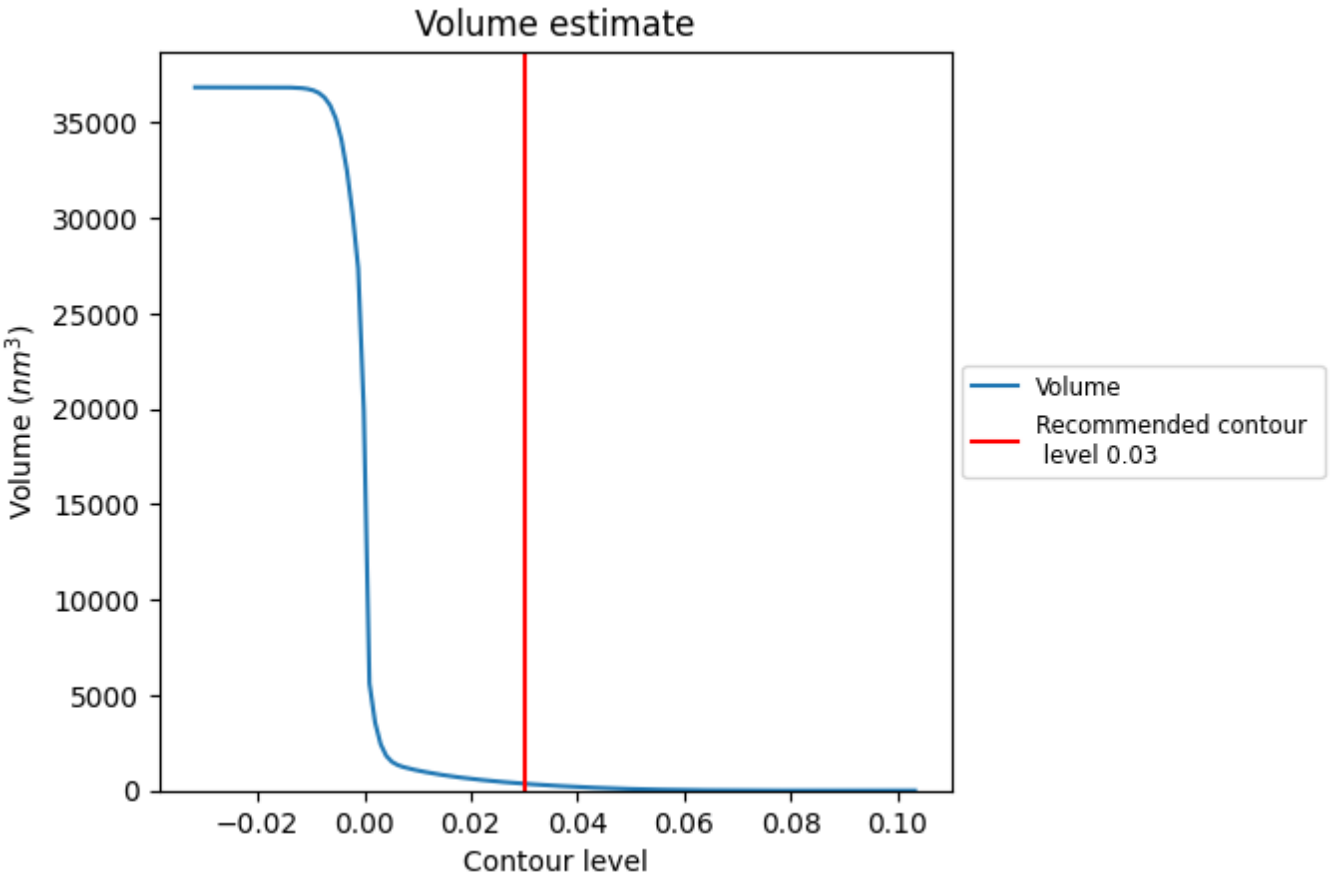
This section contains the results of statistical analysis of the map.

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.

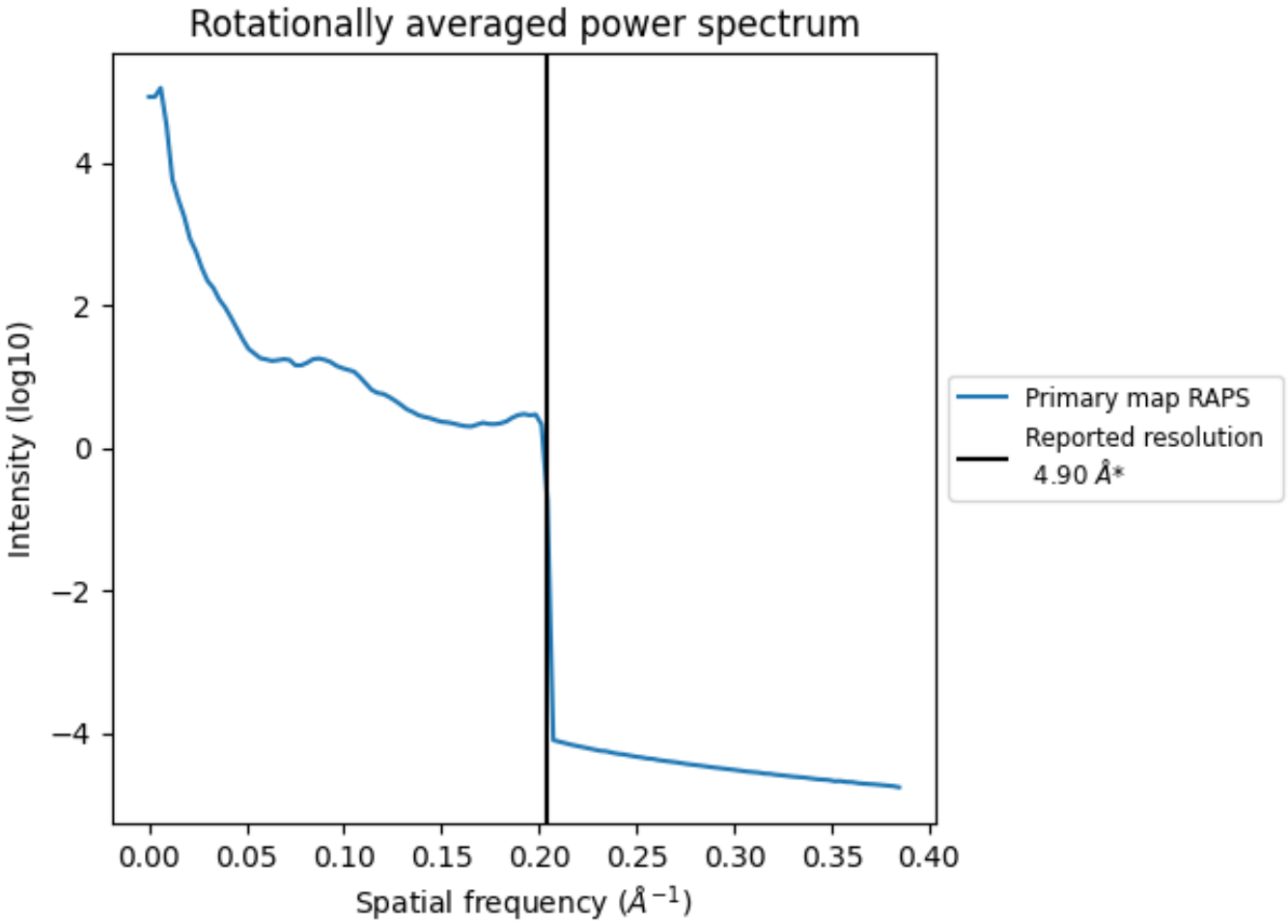
7.2 Volume estimate (i)



The volume at the recommended contour level is 361 nm^3; this corresponds to an approximate mass of 326 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 0.204 Å^{-1}

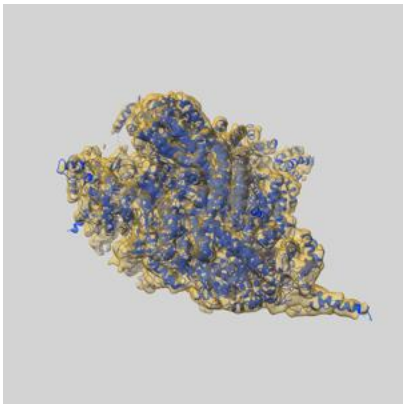
8 Fourier-Shell correlation (i)

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

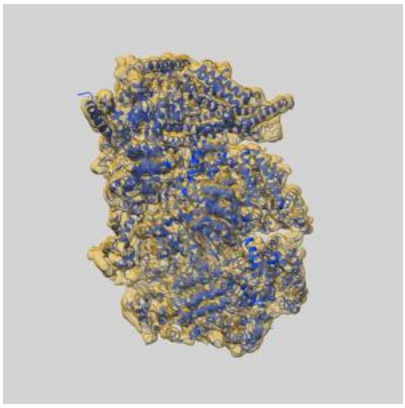
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8519 and PDB model 5U8T. Per-residue inclusion information can be found in section 3 on page 7.

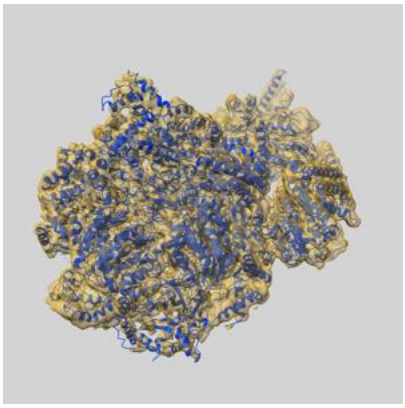
9.1 Map-model overlay



X



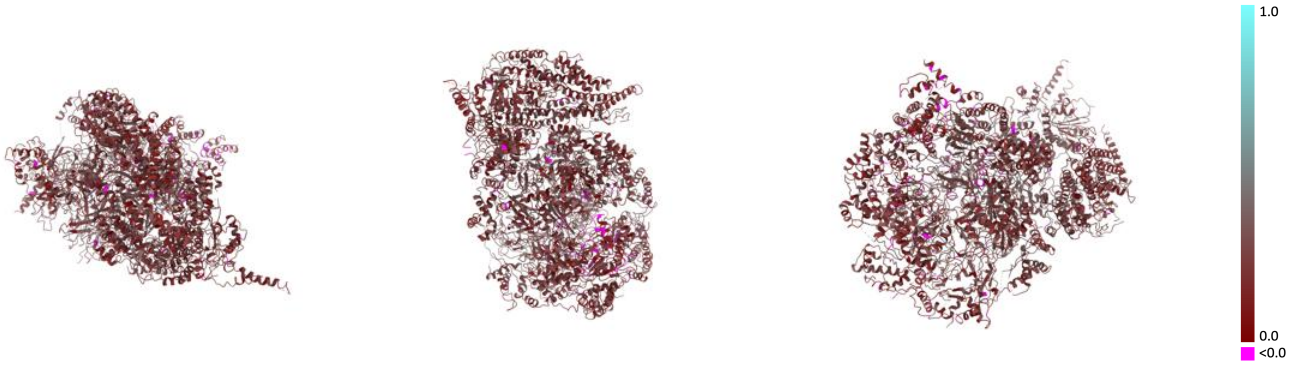
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

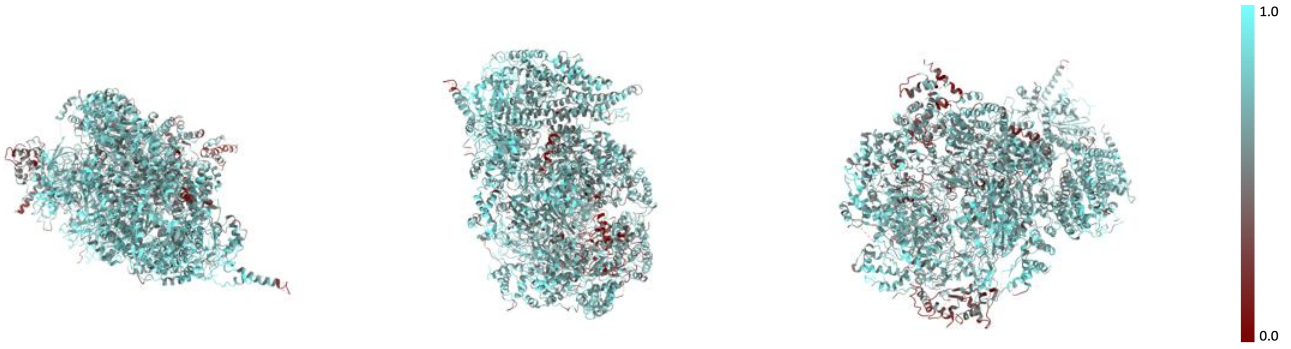
9.2 Q-score mapped to coordinate model (i)



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.

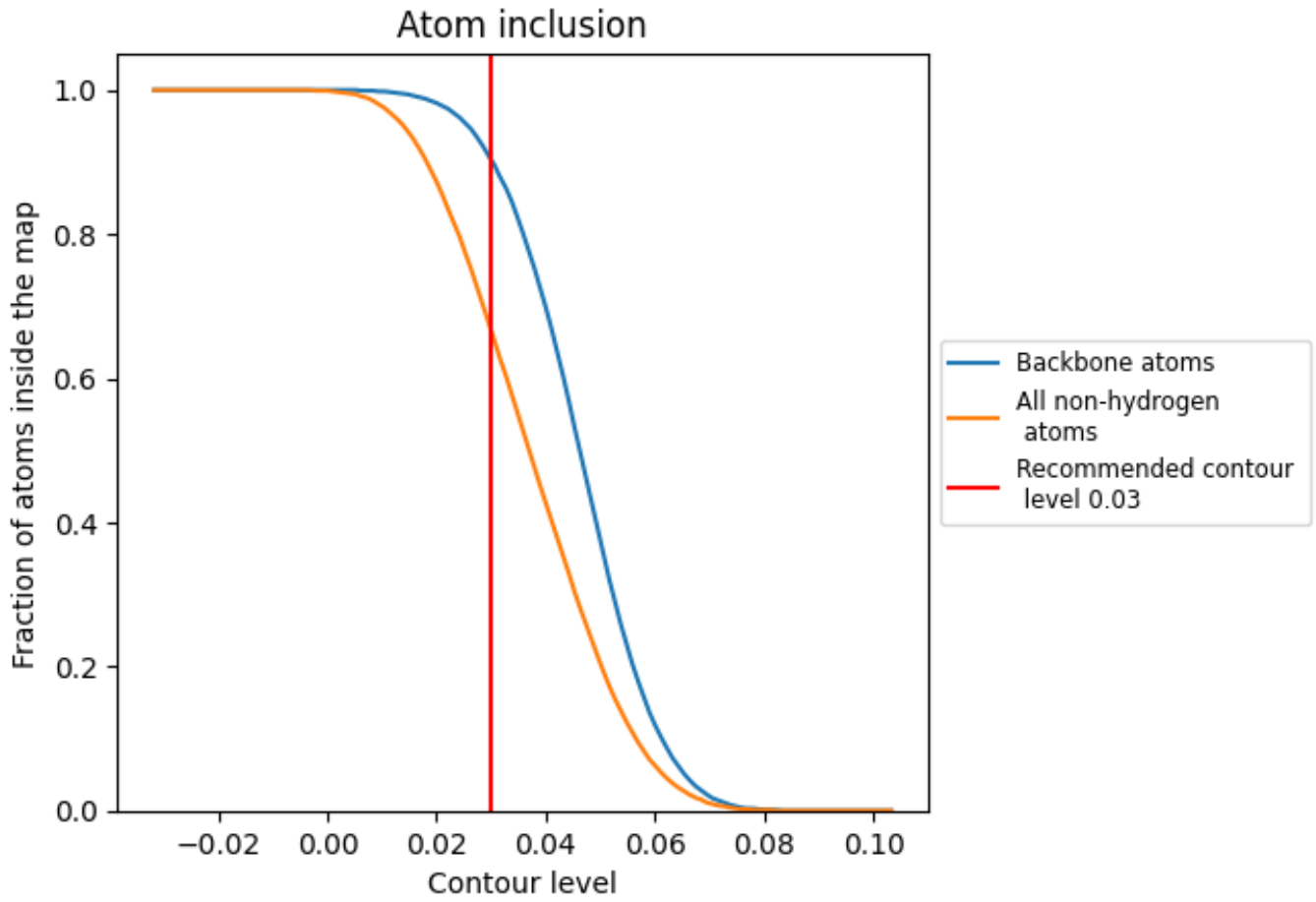
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.2390
2	0.6860	0.2540
3	0.6920	0.2550
4	0.6430	0.2080
5	0.6430	0.2580
6	0.6510	0.2250
7	0.5680	0.2290
A	0.6480	0.2140
B	0.7350	0.2550
C	0.7400	0.2550
D	0.7520	0.2420
E	0.7310	0.2430
F	0.7610	0.3030