wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 09:55 PM EDT

PDB ID	:	5U8S
EMDB ID	:	EMD-8518
Title	:	Structure of eukaryotic CMG helicase at a replication fork
Authors	:	Li, H.; Li, B.; Georgescu, R.; Yuan, Z.; Santos, R.; Sun, J.; Zhang, D.; Yurieva, O.; O'Donnell, M.E.
Deposited on	:	2016-12-14
Resolution	:	6.10 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:

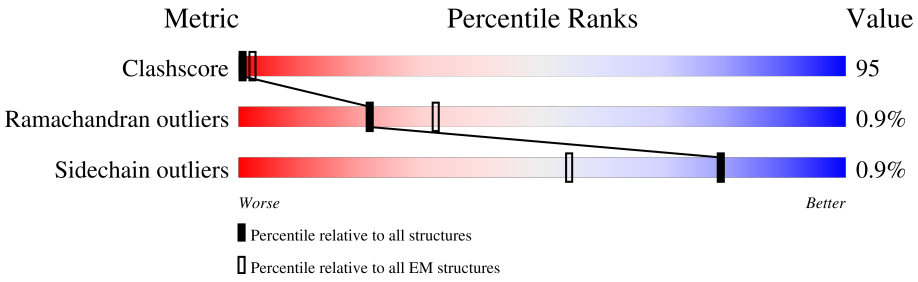
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.10 Å.

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



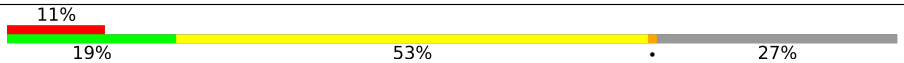
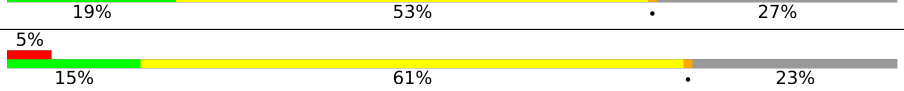
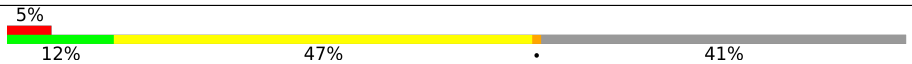
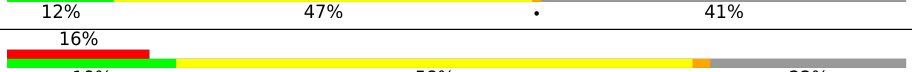
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	7% 15% 82% ·
2	B	213	10% 74% 15%
3	C	194	12% 70% 18%
4	D	294	13% 60% · 25%
5	E	650	· 16% 68% 15%
6	F	26	31% 27% 73%
7	G	14	36% 7% 93%
8	2	868	5% 12% 56% · 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	3	971	
10	4	933	
11	5	775	
12	6	1017	
13	7	845	

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
14	ATP	2	901	-	-	X	-
14	ATP	5	801	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 41018 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 complex GINS protein PSF1.

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

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

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

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

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

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

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

- Molecule 5 is a protein called Cell division control protein 45.

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

- Molecule 6 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	26	527	257	76	168	26	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	14	Total	C	N	O	P	0	0
			287	137	52	84	14		

- Molecule 8 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	602	Total	C	N	O	S	0	0
			4707	2969	841	880	17		

- Molecule 9 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	591	Total	C	N	O	S	0	0
			4638	2925	828	872	13		

- Molecule 10 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	469	VAL	LYS	conflict	UNP P30665
4	470	SER	VAL	conflict	UNP P30665

- Molecule 11 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

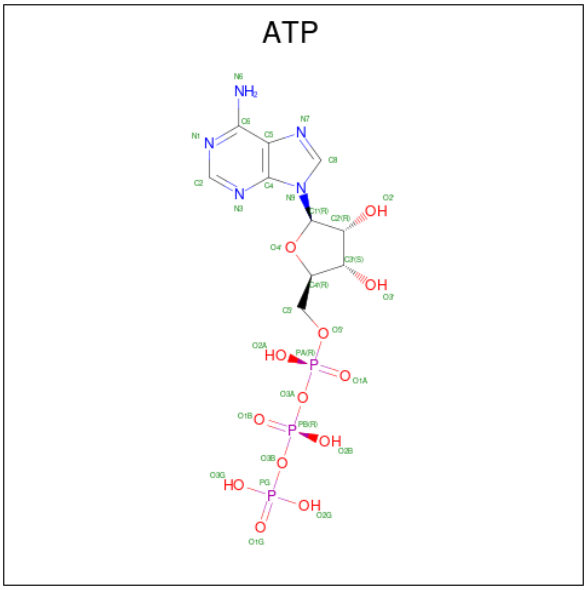
- Molecule 12 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6	604	Total	C	N	O	S	0	0
			4649	2929	822	878	20		

- Molecule 13 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



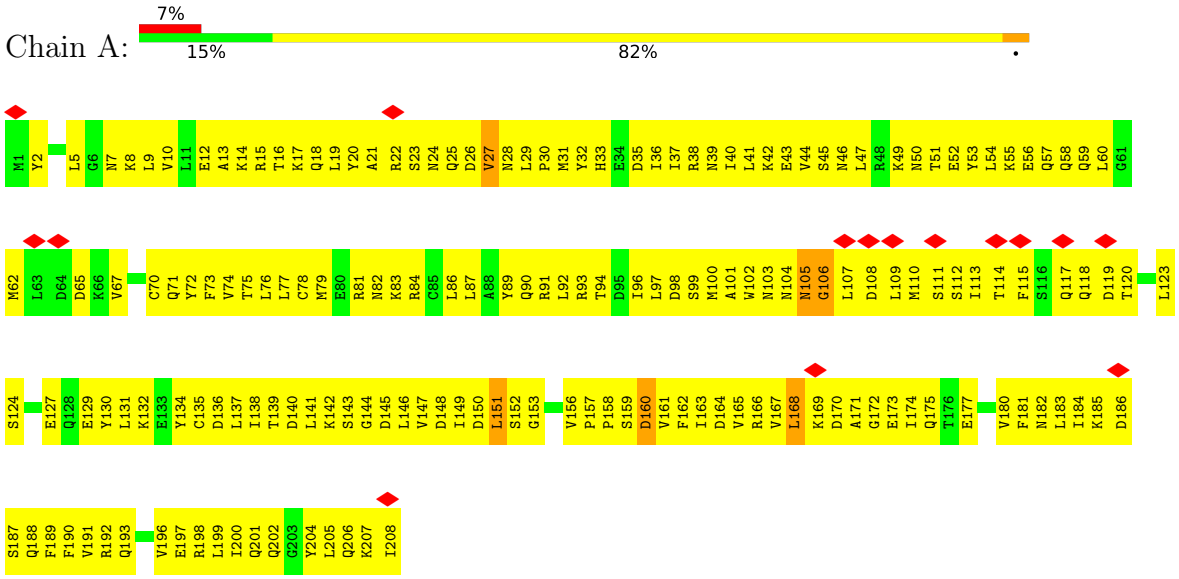
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

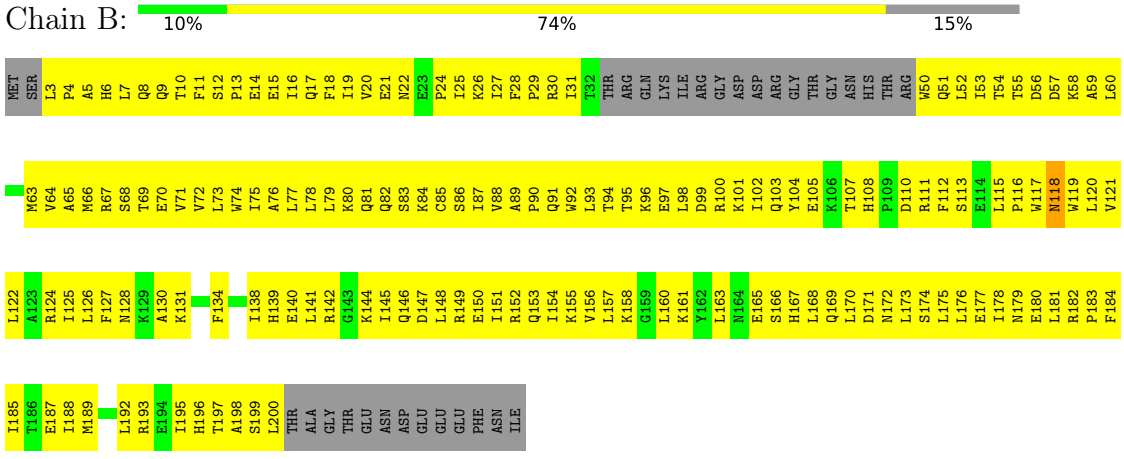
• Molecule 1: DNA replication complex GINS protein PSF1

Chain A:



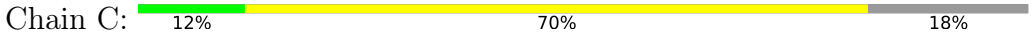
• Molecule 2: DNA replication complex GINS protein PSF2

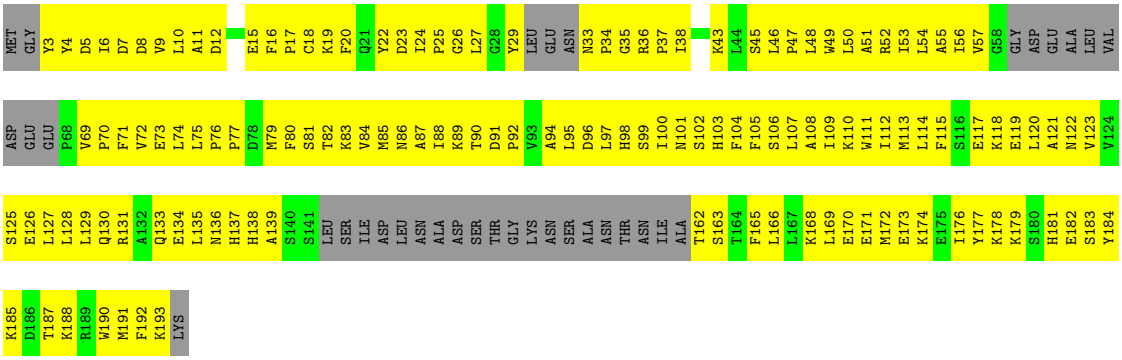
Chain B:



• Molecule 3: DNA replication complex GINS protein PSF3

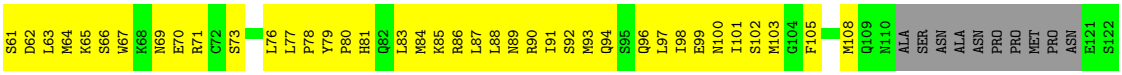
Chain C:

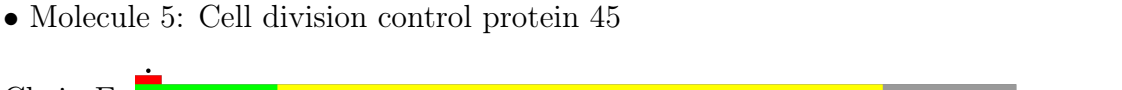


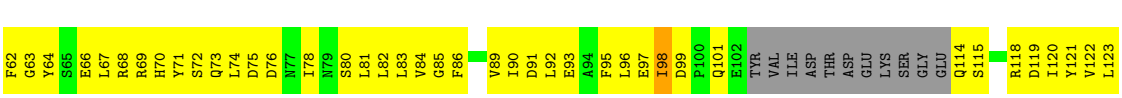


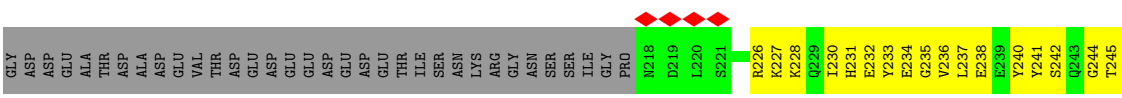
• Molecule 4: DNA replication complex GINS protein SLD5

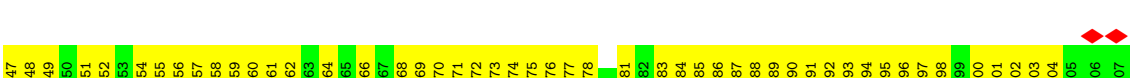
Chain D:





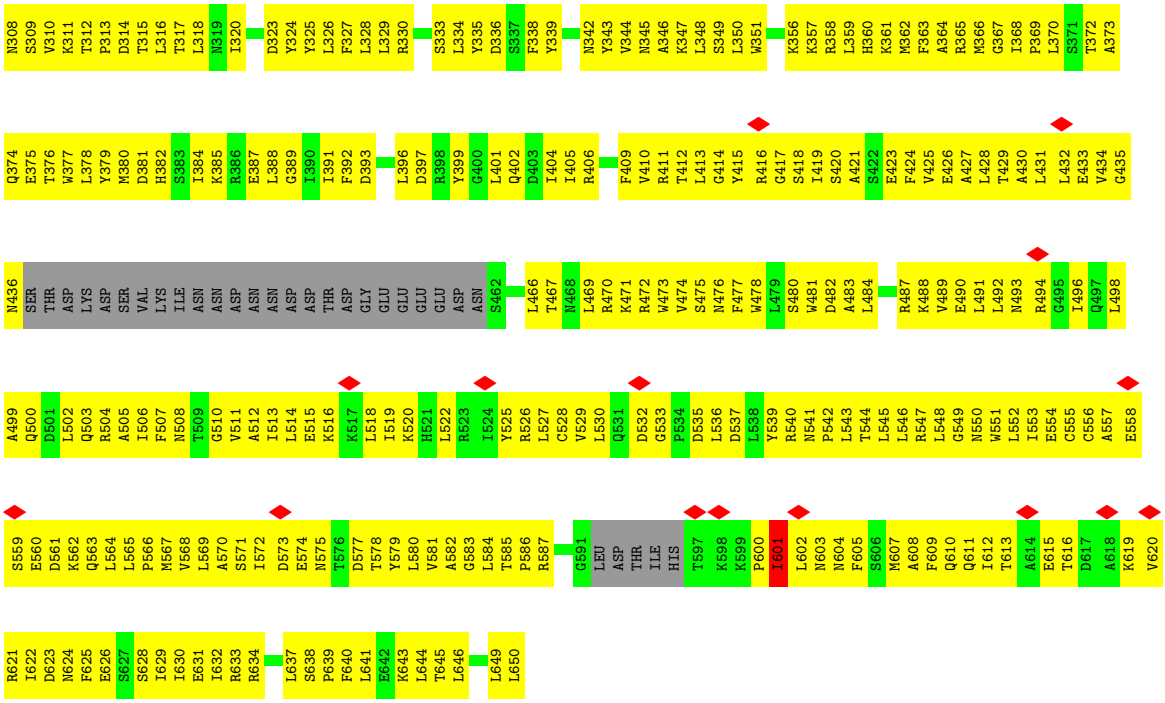






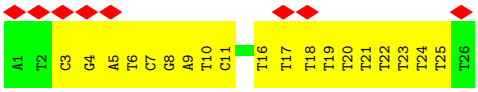
• Molecule 5: Cell division control protein 45

Chain E:



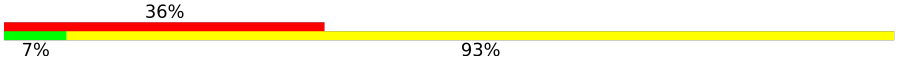
• Molecule 6: DNA (26-MER)

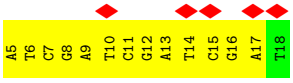
Chain F:



• Molecule 7: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3')

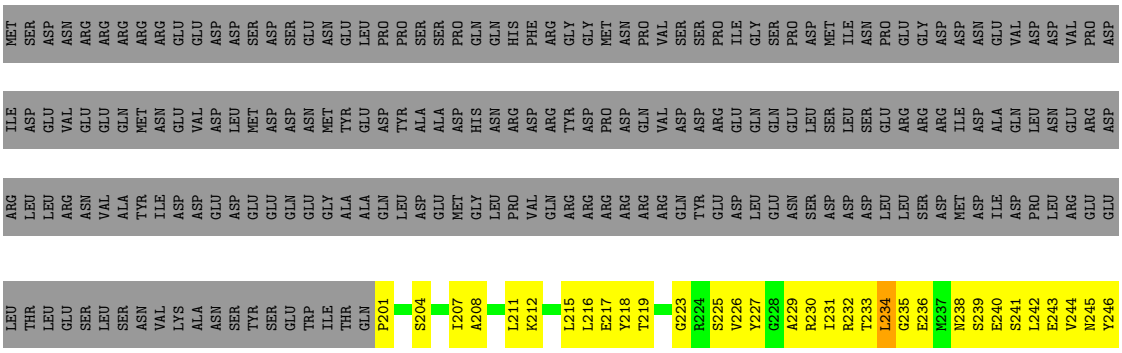
Chain G:

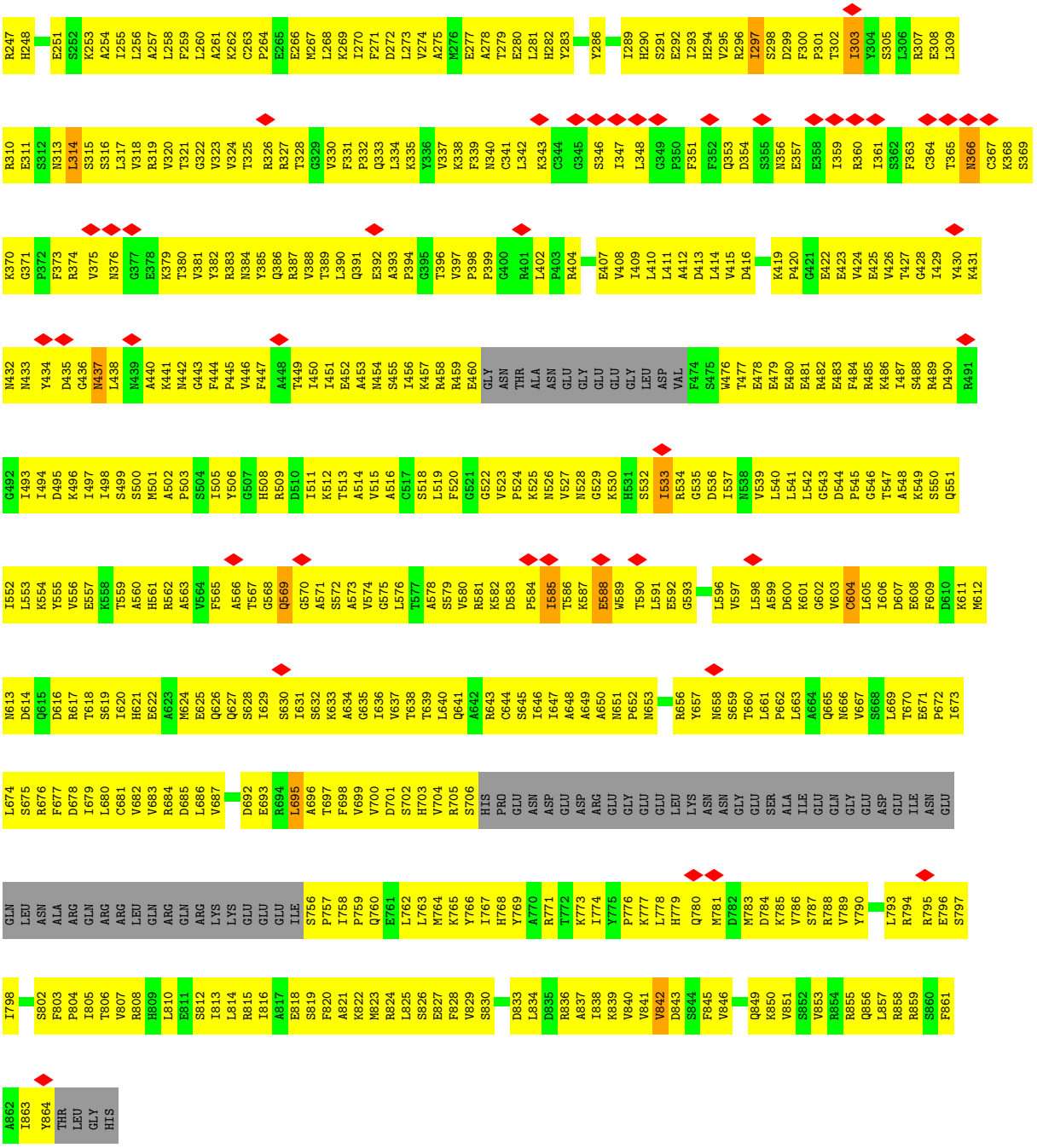




• Molecule 8: DNA replication licensing factor MCM2

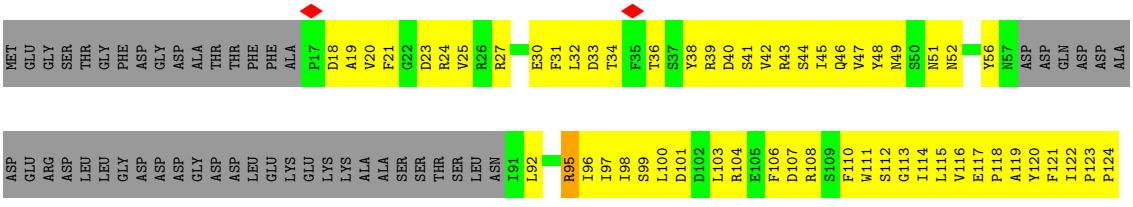
Chain 2:

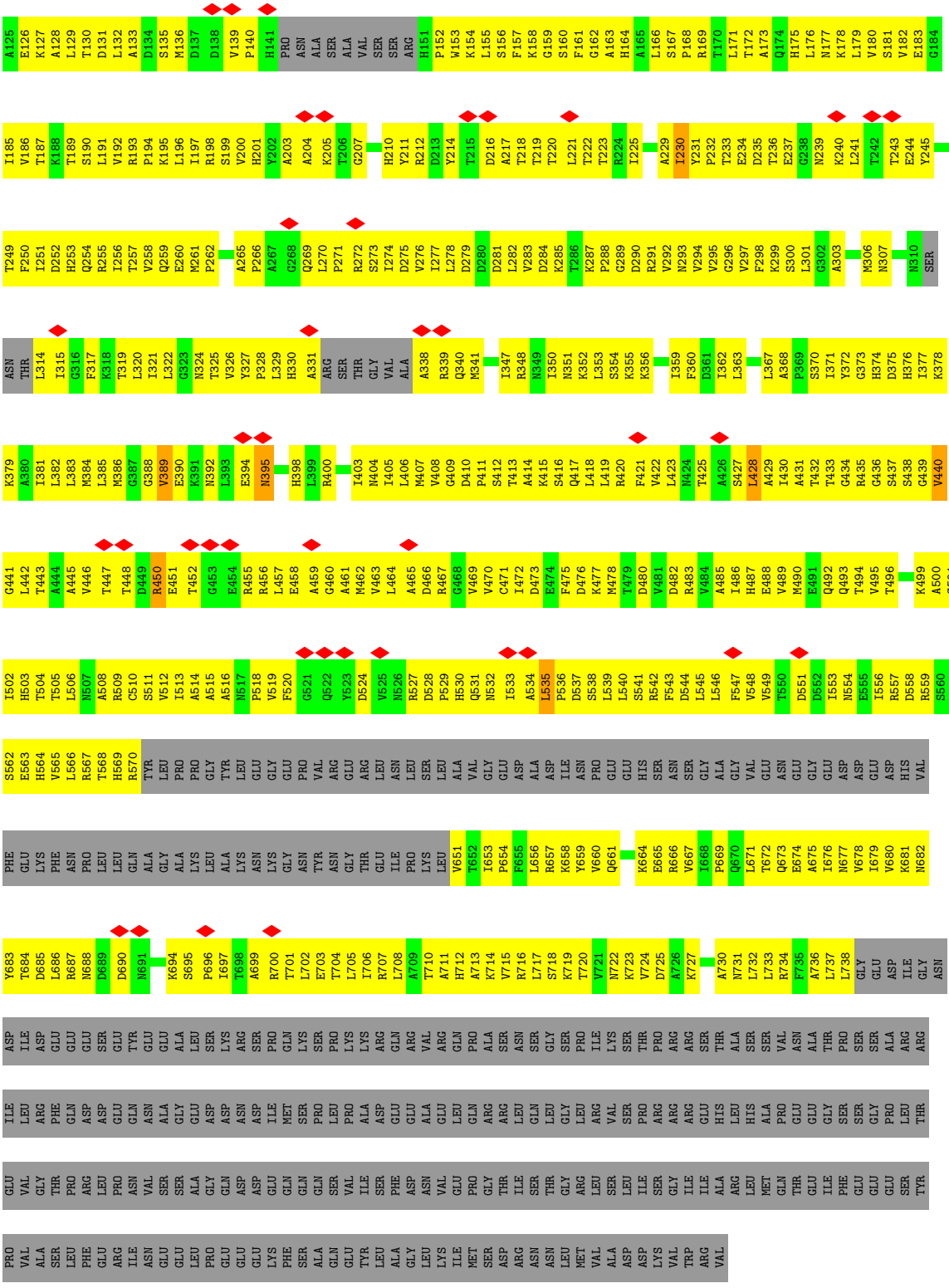




• Molecule 9: DNA replication licensing factor MCM3

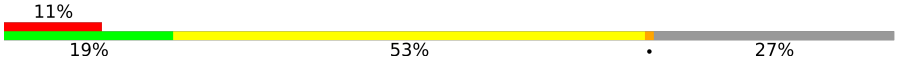
Chain 3:

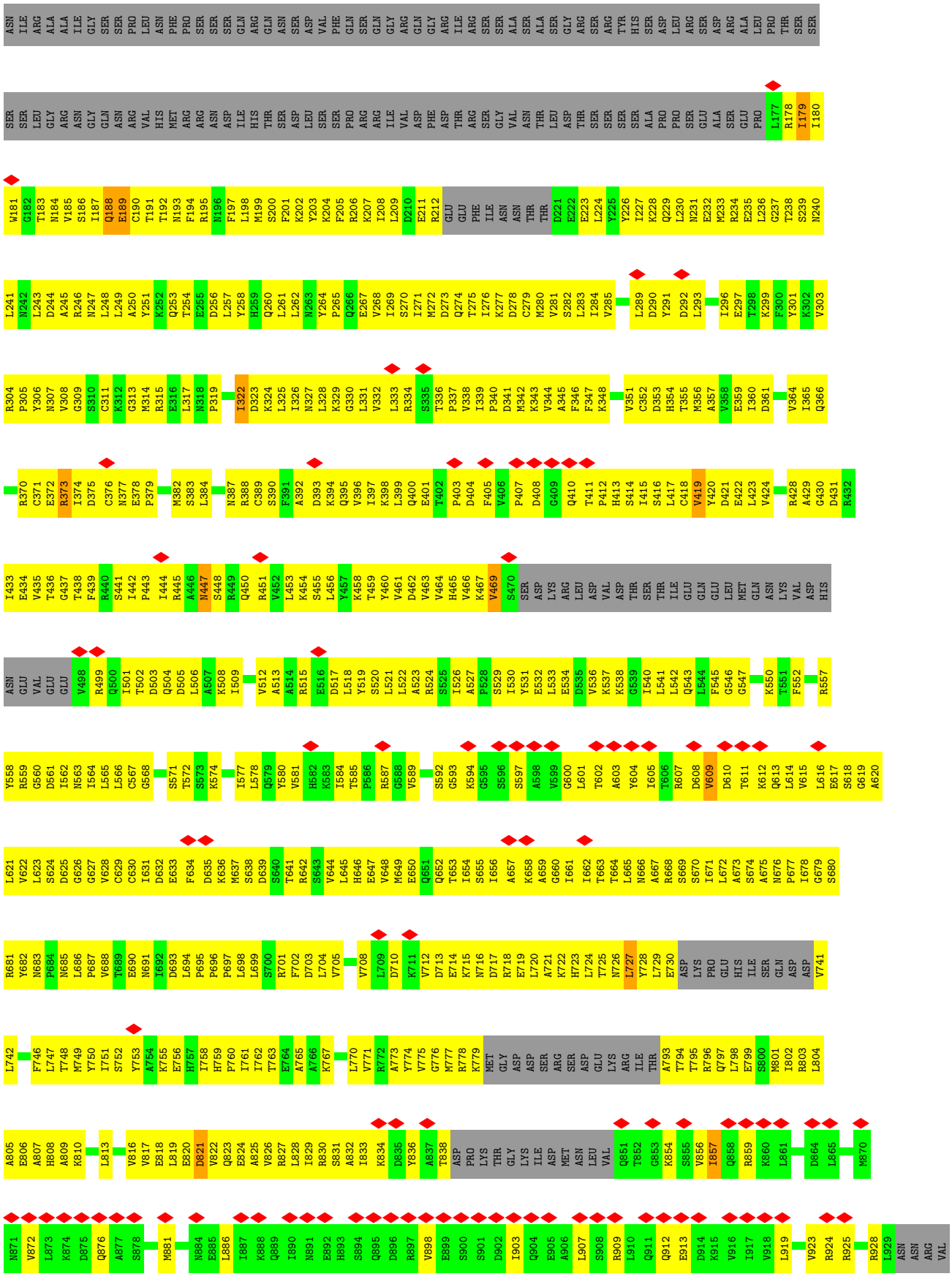




• Molecule 10: DNA replication licensing factor MCM4

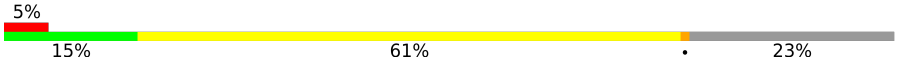
Chain 4:

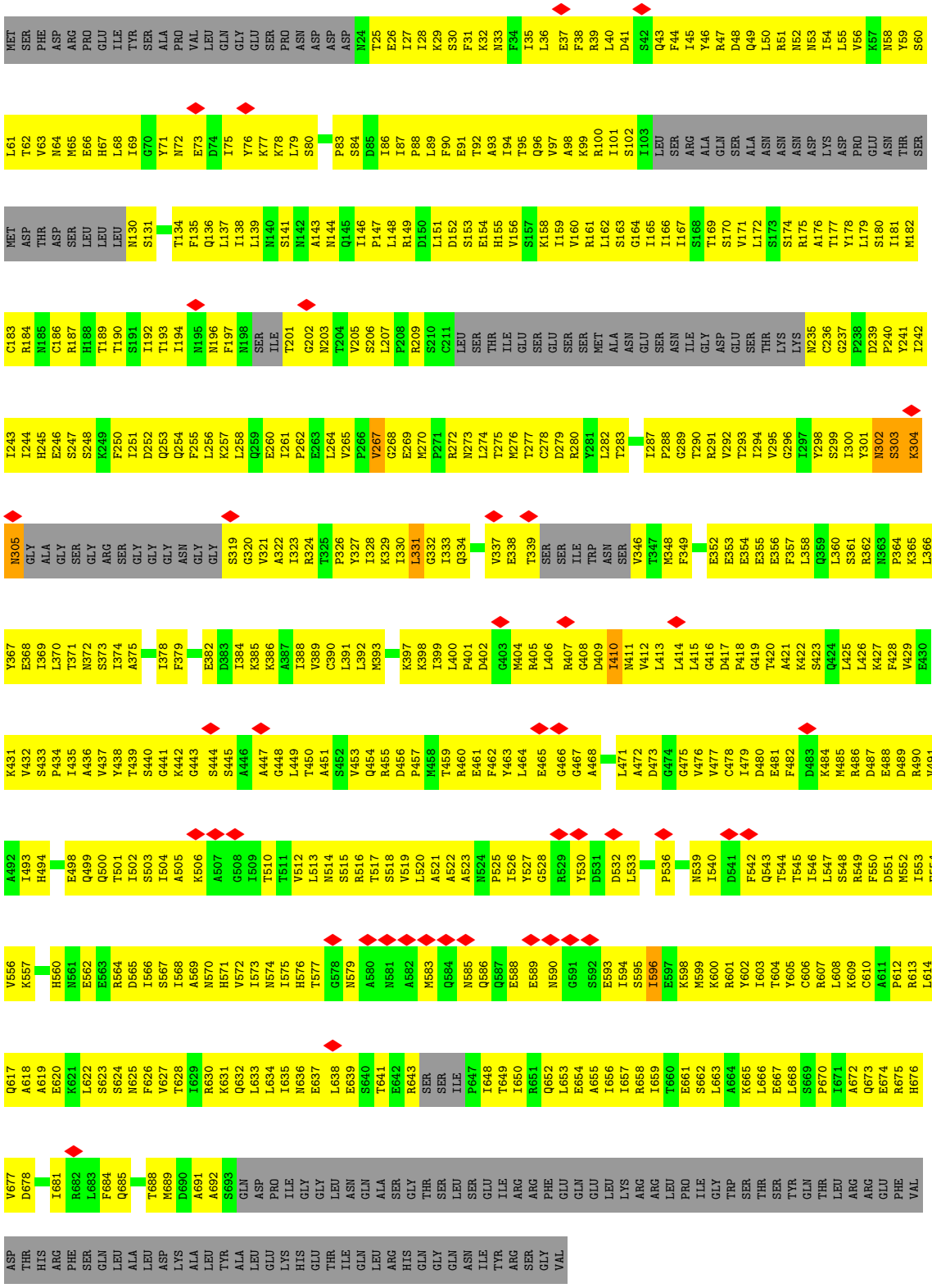



ASN ILE ARG ALA ALA ILE GLY SER SER PRO LEU LEU ASN PHE PRO SER SER SER GLN ARG GLN ASN SER ASP VAL PHE GLN SER GLN GLY ARG GLN GLY ARG ILE ARG SER SER ALA SER ALA SER GLY ARG SER ARG TYR HIS SER ASP LEU ARG LEU ARG SER ASP ARG ALA LEU PRO THR SER SER
SER SER LEU GLY ARG ASN GLY GLN ASN ARG VAL HIS MET ARG ARG ASN ASP ILE HIS THR SER ASP LEU SER SER PRO ARG ARG ILE VAL ASP PHE ASP THR ARG SER GLY VAL ASN THR LEU ASP THR SER SER SER SER ALA PRO PRO SER GLU ALA SER GLU PRO L177 R178 I179 I180
W181 G182 T183 N184 V185 S186 I187 Q188 E189 C190 T191 T192 N193 F194 R195 N196 F197 L198 M199 S200 F201 K202 Y203 K204 F205 R206 K207 I208 L209 D210 E211 R212 GLU GLU PHE ILE ASN ASN THR THR D221 E222 E223 L224 Y225 Y226 I227 K228 Q229 L230 N231 E232 M233 R234 E235 L236 G237 T238 S239 N240
L241 N242 L243 D244 A245 R246 N247 L248 L249 A250 Y251 K252 Q253 T254 E255 D256 L257 Y258 H259 Q260 L261 L262 N263 Y264 P265 Q266 E267 V268 I269 S270 I271 M272 D273 Q274 T275 I276 K277 D278 C279 M280 V281 S282 L283 I284 V285 L289 D290 Y291 D292 L293 I296 E297 T298 K299 P300 Y301 K302 V303
R304 P305 Y306 N307 V308 G309 S310 C311 K312 G313 M314 R315 E316 L317 N318 P319 I322 D323 K324 L325 I326 N327 L328 K329 G330 L331 V332 L333 R334 S335 T336 P337 V338 I339 P340 D341 M342 K343 V344 A345 F346 F347 K348 V351 C352 D353 H354 T355 M356 A357 V358 E359 I360 D361 V364 I365 Q366
R370 C371 E372 R373 I374 D375 C376 N377 E378 P379 M382 S383 L384 N387 R388 C389 S390 F391 A392 D393 K394 Q395 V396 I397 K398 L399 Q400 E401 T402 P403 D404 F405 V406 P407 D408 G409 Q410 T411 P412 H413 S414 I415 S416 L417 C418 V419 Y420 D421 E422 L423 V424 R428 A429 G430 D431 R432
I433 E434 V435 T436 G437 T438 F439 R440 S441 I442 P443 I444 R445 A446 N447 S448 R449 Q450 R451 V452 L453 K454 S455 L456 Y457 K458 T459 Y460 V461 D462 V463 V464 H465 V466 K467 V469 S470 SER ASP LYS ARG LEU ASP VAL ASP THR SER THR ILE GLU GLN GLU LEU MET GLN ASN LYS VAL ASP HIS
ASN GLU VAL GLU GLU V498 R499 Q500 I501 T502 D503 Q504 D505 L506 A507 K508 I509 V512 A513 A514 R515 E516 D517 L518 Y519 S520 L521 L522 A523 R524 S525 I526 A527 P528 S529 I530 Y531 E532 L533 E534 D535 V536 K537 K538 G539 I540 L541 L542 Q543 L544 F545 G546 G547 K550 T551 F552 R557
Y558 R559 G560 D561 I562 N563 I564 L565 L566 C567 G568 S571 T572 S573 K574 I577 L578 Q579 Y580 V581 H582 K583 I584 T585 P586 R587 G588 V589 S592 G593 K594 G595 S596 S597 A598 V599 G600 L601 T602 A603 Y604 I605 T606 R607 D608 V609 D610 T611 K612 Q613 L614 V615 L616 E617 S618 G619 A620
L621 V622 L623 S624 D625 G626 G627 V628 C629 C630 I631 D632 E633 F634 D635 K636 M637 S638 D639 S640 T641 R642 S643 V644 L645 H646 E647 V648 M649 E650 Q651 Q652 T653 I654 S655 I656 A657 K658 A659 G660 I661 I662 T663 T664 L665 N666 A667 R668 S669 S670 I671 L672 A673 S674 A675 N676 P677 I678 G679 S680
R681 Y682 N683 P684 N685 L686 P687 V688 T689 E690 N691 I692 D693 L694 P695 P696 P697 L698 L699 S700 R701 F702 D703 L704 V705 V708 L709 D710 K711 V712 D713 E714 K715 N716 D717 R718 E719 L720 A721 K722 H723 L724 T725 N726 L727 Y728 L729 E730 ASP LYS PRO GLU HIS ILE SER GLN ASP ASP V741
L742 F746 L747 T748 M749 Y750 I751 S752 Y753 A754 K755 E756 H757 I758 H759 P760 I761 I762 T763 E764 A765 A766 K767 L770 V771 R772 A773 Y774 V775 G776 M777 R778 K779 MET GLY ASP ASP SER ARG SER ASP GLU LYS ARG ILE THR A793 T794 T795 R796 Q797 L798 E799 S800 M801 I802 R803 L804
A805 E806 A807 H808 A809 K810 L813 V816 V817 E818 L819 E820 D821 V822 Q823 E824 A825 V826 R827 L828 I829 R830 S831 A832 I833 K834 D835 Y836 A837 T838 ASP PRO LYS THR GLY LYS ILE ASP MET ASN LEU VAL Q851 T852 G853 K854 S855 V856 I857 Q858 R859 K860 L861 D864 L865 M870
N871 V872 L873 K874 D875 Q876 A877 S878 M881 N884 E885 L886 I887 K888 Q889 I890 N891 E892 H893 S894 Q895 D896 R897 V898 E899 S900 S901 D902 I903 Q904 E905 A906 L907 S908 R909 L910 Q911 Q912 E913 D914 K915 V916 I917 V918 L919 V923 R924 R925 R928 L929 ASN ASN ARG VAL

• Molecule 11: Minichromosome maintenance protein 5

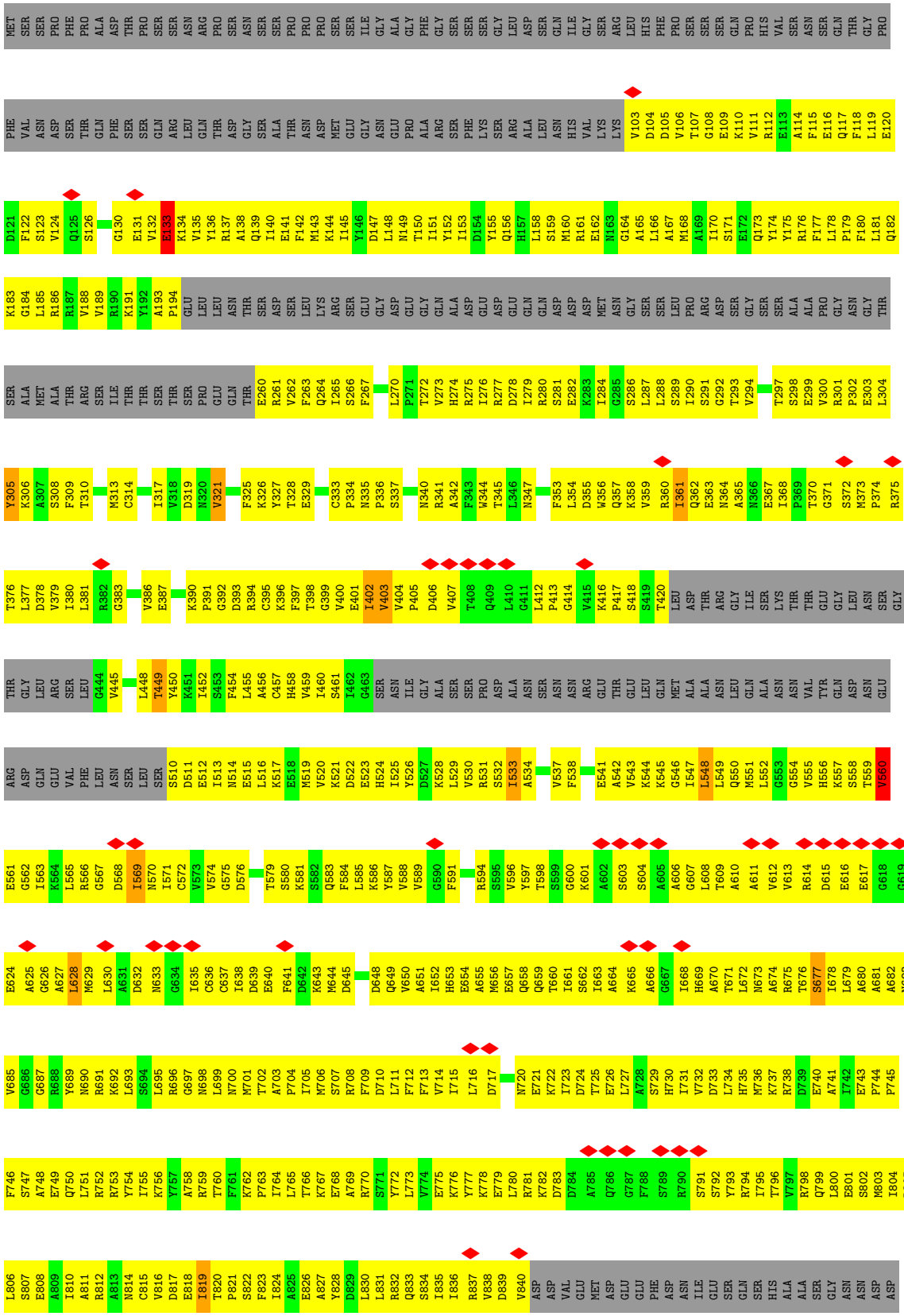
Chain 5:

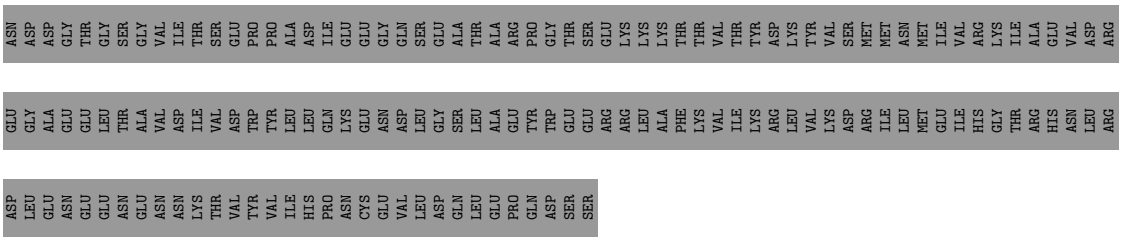




• Molecule 12: DNA replication licensing factor MCM6

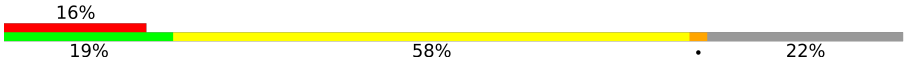
Chain 6:

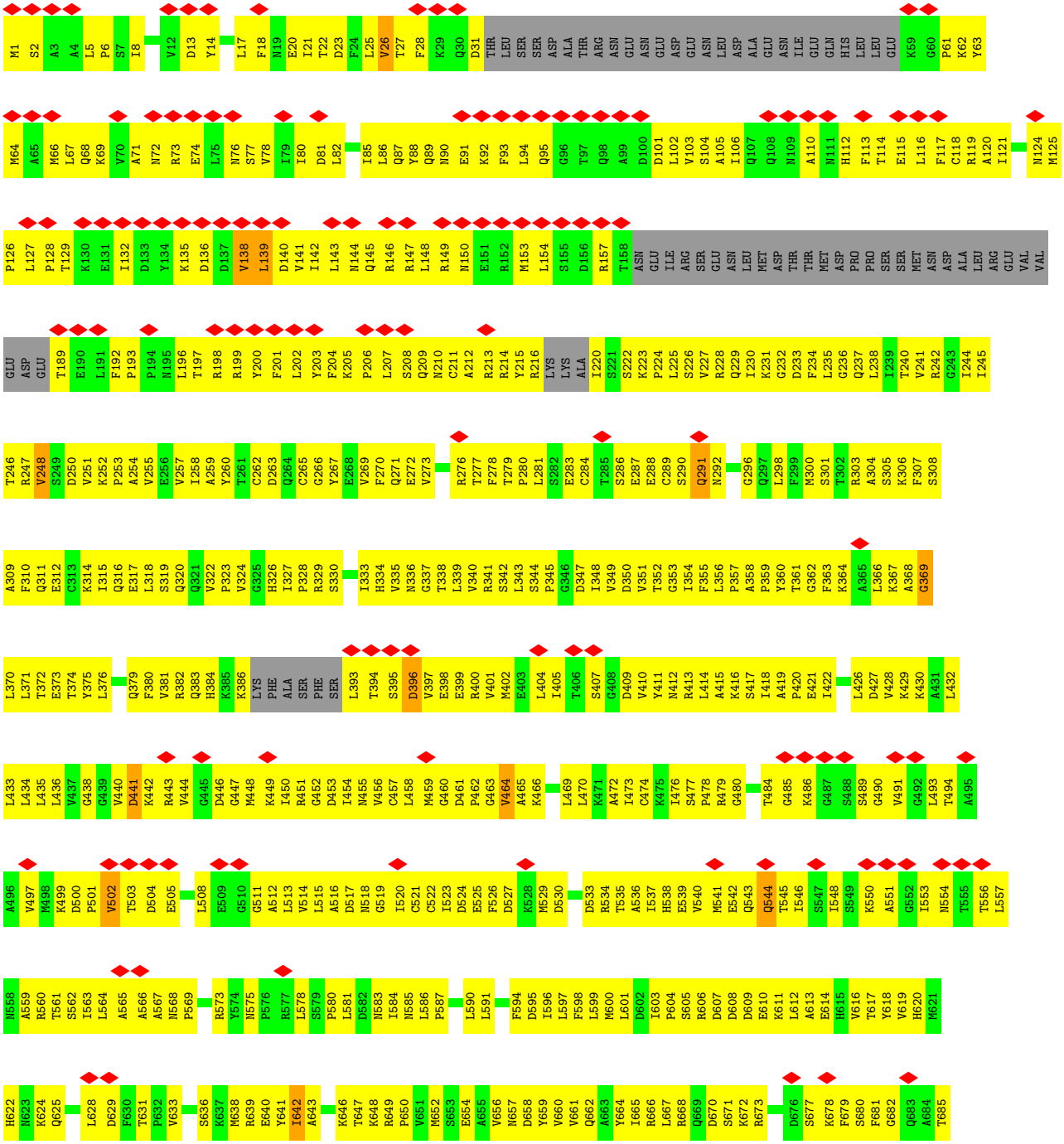


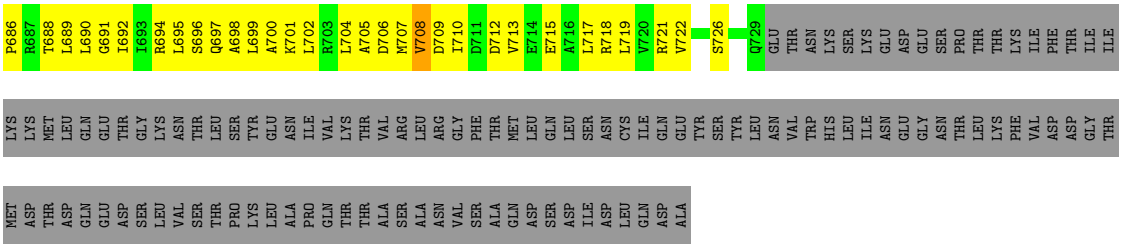


• Molecule 13: DNA replication licensing factor MCM7

Chain 7:






P686 R687 T688 L689 L690 G691 I692 I693 R694 L695 S696 Q697 A698 L699 A700 K701 L702 R703 L704 A705 D706 M707 V708 D709 I710 D711 D712 V713 E714 E715 A716 L717 R718 L719 V720 R721 V722 S726 Q729 GLU THR ASN LYS SER LYS GLU ASP GLU SER PRO THR THR LYS ILE PHE THR ILE ILE
LYS LYS MET LEU GLN GLU THR GLY LYS ASN THR LEU SER TYR GLU ASN ILE VAL LYS THR VAL ARG LEU ARG GLY PHE THR MET LEU GLN LEU SER ASN CYS ILE GLN GLU TYR SER TYR LEU ASN VAL TRP HIS LEU ILE ASN GLU GLY ASN THR LEU LYS PHE VAL ASP ASP GLY THR
MET ASP THR ASP GLN GLU ASP SER LEU VAL SER THR PRO LYS LEU ALA PRO GLN THR THR ALA SER ALA ASN VAL SER ALA GLN ASP SER ASP ILE ASP LEU GLN ASP ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	243796	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	0.079	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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: 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	A	0.24	0/1718	0.51	1/2314 (0.0%)
2	B	0.23	0/1545	0.47	0/2092
3	C	0.23	0/1320	0.41	0/1784
4	D	0.24	0/1853	0.48	0/2500
5	E	0.23	0/4563	0.45	0/6173
6	F	0.48	0/585	0.99	0/901
7	G	0.51	0/321	0.90	0/493
8	2	0.24	0/4787	0.52	1/6469 (0.0%)
9	3	0.23	0/4717	0.49	0/6393
10	4	0.25	0/5480	0.52	0/7395
11	5	0.24	0/4750	0.48	0/6412
12	6	0.24	0/4719	0.51	1/6373 (0.0%)
13	7	0.24	0/5299	0.51	1/7160 (0.0%)
All	All	0.25	0/41657	0.51	4/56459 (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	A	0	1
4	D	0	1
9	3	0	1
10	4	0	2
12	6	0	3
13	7	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	7	369	GLY	N-CA-C	7.97	133.04	113.10
1	A	106	GLY	N-CA-C	7.29	131.32	113.10
8	2	366	ASN	C-N-CA	6.50	137.94	121.70
12	6	628	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	3	428	LEU	Peptide
10	4	373	ARG	Peptide
10	4	408	ASP	Peptide
1	A	160	ASP	Peptide
4	D	258	VAL	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	A	1696	0	1698	437	0
2	B	1513	0	1558	354	0
3	C	1288	0	1298	283	0
4	D	1820	0	1824	452	0
5	E	4482	0	4499	910	0
6	F	527	0	303	50	0
7	G	287	0	159	16	0
8	2	4707	0	4721	1026	0
9	3	4638	0	4701	925	0
10	4	5410	0	5491	980	0
11	5	4688	0	4748	992	0
12	6	4649	0	4589	1048	0
13	7	5220	0	5296	901	0
14	2	31	0	12	12	0
14	3	31	0	12	5	0
14	5	31	0	12	12	0
All	All	41018	0	40921	7794	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 95.

The worst 5 of 7794 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)
11:5:302:ASN:OD1	11:5:324:ARG:CZ	1.64	1.46
5:E:5:ILE:N	5:E:142:CYS:HG	1.30	1.26
13:7:94:LEU:HB2	13:7:95:GLN:HB2	1.21	1.19
13:7:680:SER:HB2	13:7:681:PHE:HA	1.22	1.19
11:5:303:SER:O	11:5:304:LYS:HG3	1.41	1.17

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	206/208 (99%)	182 (88%)	23 (11%)	1 (0%)	29 69
2	B	177/213 (83%)	160 (90%)	17 (10%)	0	100 100
3	C	151/194 (78%)	142 (94%)	9 (6%)	0	100 100
4	D	215/294 (73%)	193 (90%)	20 (9%)	2 (1%)	17 56
5	E	543/650 (84%)	490 (90%)	51 (9%)	2 (0%)	34 72
8	2	596/868 (69%)	535 (90%)	54 (9%)	7 (1%)	13 50
9	3	579/971 (60%)	528 (91%)	48 (8%)	3 (0%)	29 69
10	4	670/933 (72%)	594 (89%)	69 (10%)	7 (1%)	15 54
11	5	583/775 (75%)	549 (94%)	30 (5%)	4 (1%)	22 62
12	6	596/1017 (59%)	528 (89%)	58 (10%)	10 (2%)	9 42
13	7	653/845 (77%)	583 (89%)	60 (9%)	10 (2%)	10 45
All	All	4969/6968 (71%)	4484 (90%)	439 (9%)	46 (1%)	21 56

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	601	ILE
10	4	189	GLU
10	4	419	VAL
10	4	609	VAL
11	5	596	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	190 (98%)	3 (2%)	62	79
2	B	171/198 (86%)	170 (99%)	1 (1%)	86	92
3	C	144/173 (83%)	144 (100%)	0	100	100
4	D	213/279 (76%)	211 (99%)	2 (1%)	78	88
5	E	499/586 (85%)	496 (99%)	3 (1%)	86	92
8	2	508/770 (66%)	502 (99%)	6 (1%)	71	84
9	3	512/835 (61%)	506 (99%)	6 (1%)	71	84
10	4	610/848 (72%)	606 (99%)	4 (1%)	84	90
11	5	534/688 (78%)	528 (99%)	6 (1%)	73	84
12	6	486/886 (55%)	482 (99%)	4 (1%)	81	89
13	7	585/753 (78%)	581 (99%)	4 (1%)	84	90
All	All	4455/6209 (72%)	4416 (99%)	39 (1%)	79	88

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	5	305	ASN
13	7	139	LEU
11	5	331	LEU
12	6	449	THR
13	7	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
10	4	410	GLN
11	5	625	ASN
13	7	620	HIS
10	4	646	HIS
11	5	254	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
14	ATP	3	1001	-	26,33,33	0.93	1 (3%)	31,52,52	1.53	5 (16%)
14	ATP	2	901	-	26,33,33	0.93	1 (3%)	31,52,52	1.70	6 (19%)
14	ATP	5	801	-	26,33,33	0.91	1 (3%)	31,52,52	1.51	6 (19%)

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
14	ATP	3	1001	-	-	3/18/38/38	0/3/3/3
14	ATP	2	901	-	-	4/18/38/38	0/3/3/3
14	ATP	5	801	-	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	901	ATP	C5-C4	2.48	1.47	1.40
14	3	1001	ATP	C5-C4	2.38	1.47	1.40
14	5	801	ATP	C5-C4	2.37	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	901	ATP	PA-O3A-PB	-3.80	119.79	132.83
14	5	801	ATP	N3-C2-N1	-3.75	122.82	128.68
14	2	901	ATP	N3-C2-N1	-3.74	122.83	128.68
14	2	901	ATP	PB-O3B-PG	-3.70	120.12	132.83
14	3	1001	ATP	N3-C2-N1	-3.62	123.02	128.68

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	2	901	ATP	C5'-O5'-PA-O1A
14	2	901	ATP	C5'-O5'-PA-O2A
14	2	901	ATP	C5'-O5'-PA-O3A
14	3	1001	ATP	PG-O3B-PB-O1B
14	5	801	ATP	PA-O3A-PB-O1B

There are no ring outliers.

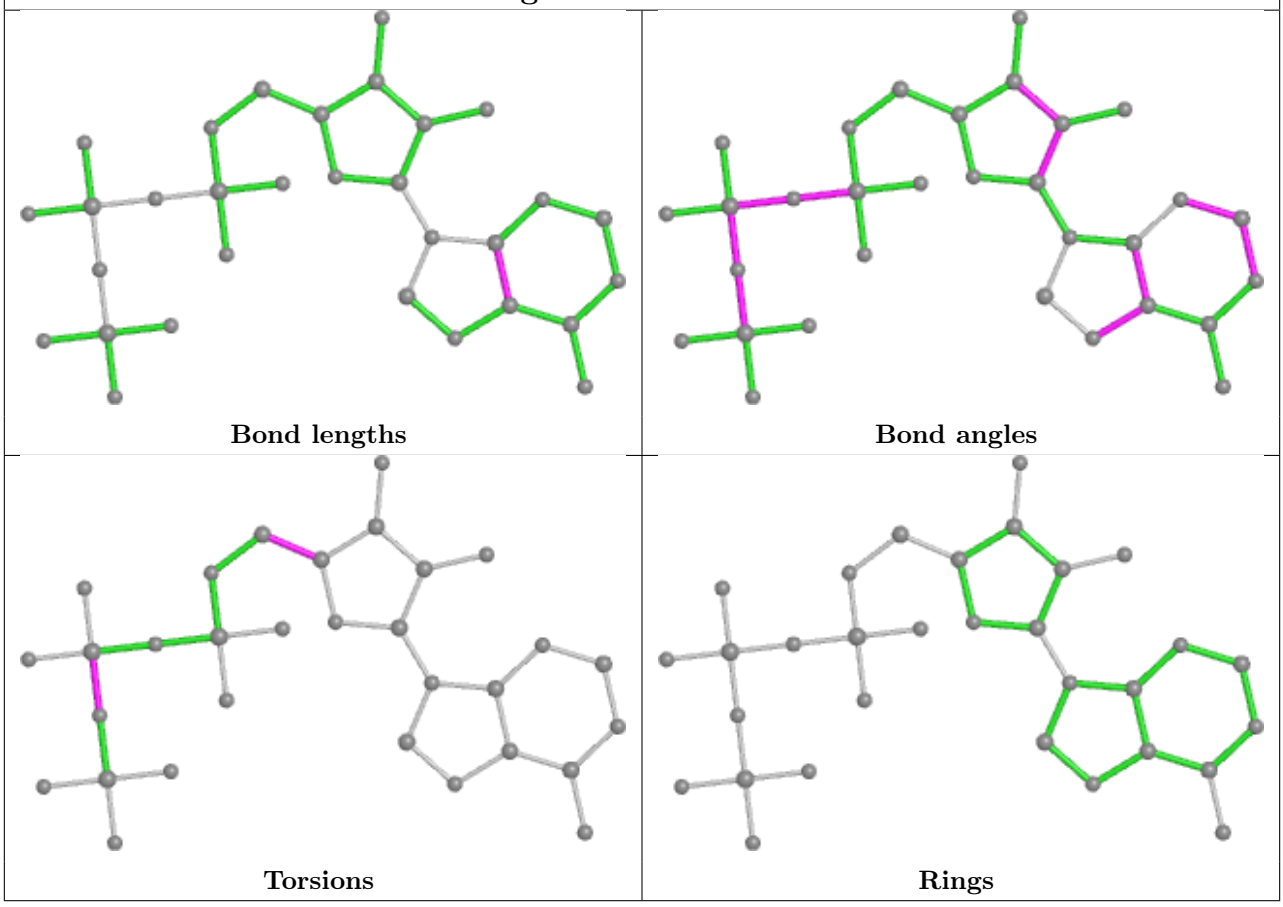
3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	3	1001	ATP	5	0
14	2	901	ATP	12	0
14	5	801	ATP	12	0

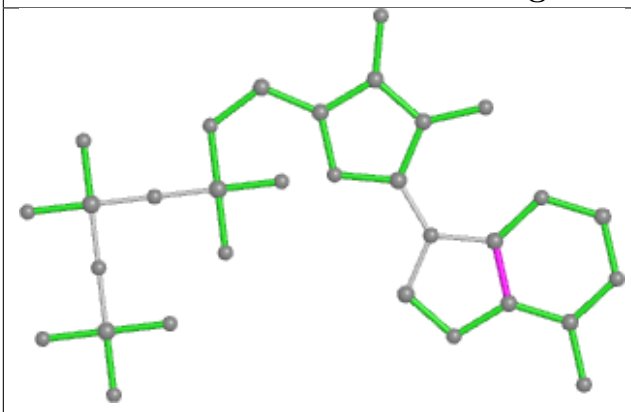
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

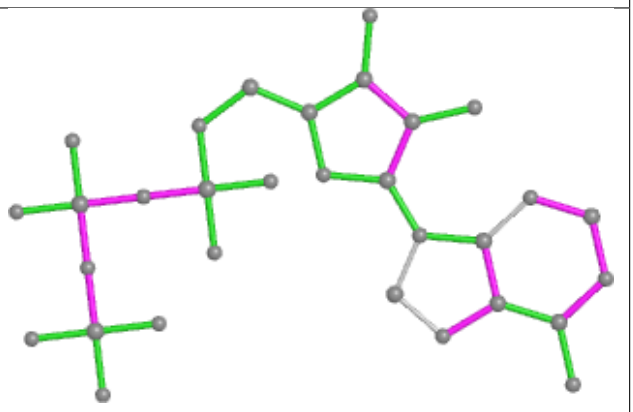
Ligand ATP 3 1001



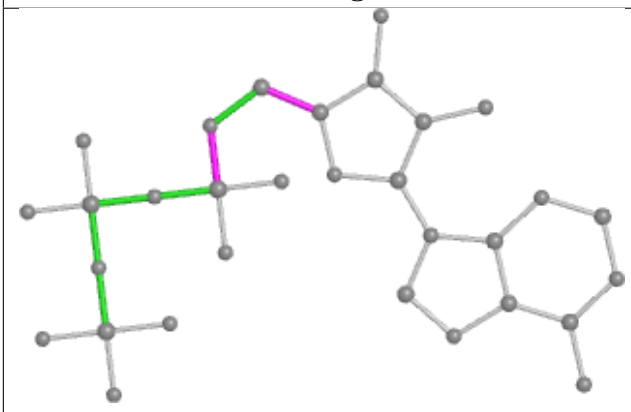
Ligand ATP 2 901



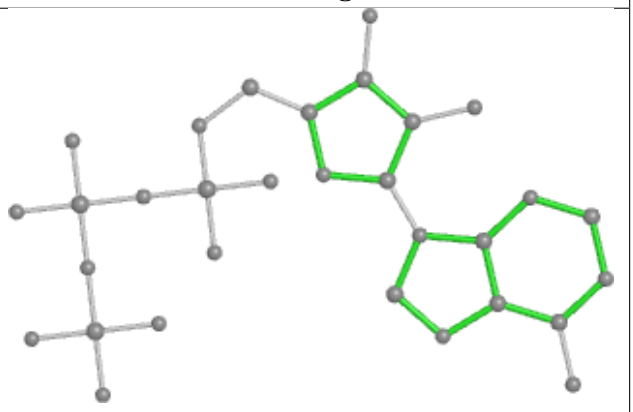
Bond lengths



Bond angles

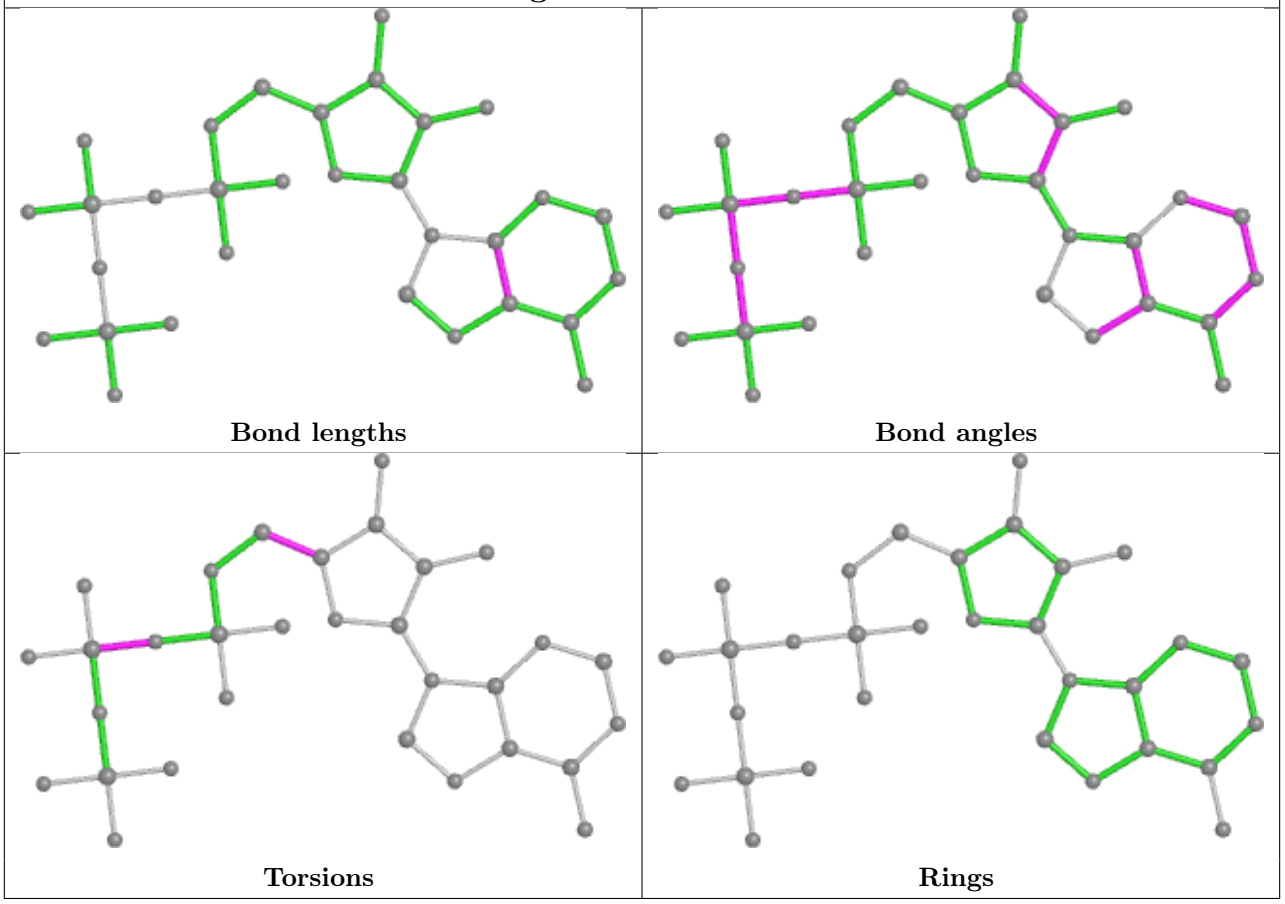


Torsions



Rings

Ligand ATP 5 801



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.

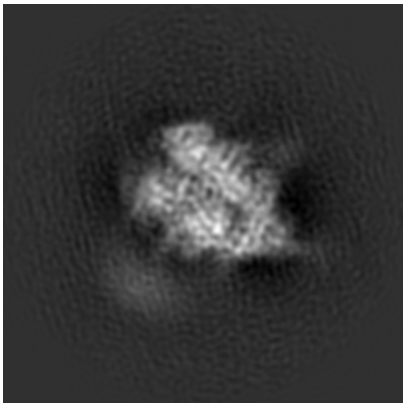
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8518. These allow visual inspection of the internal detail of the map and identification of artifacts.

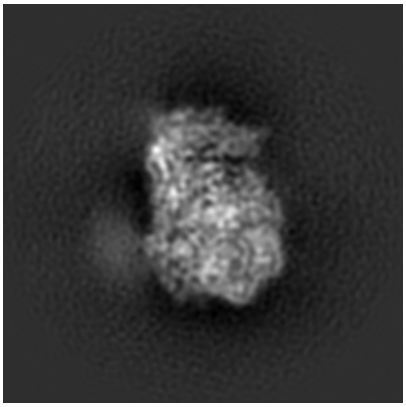
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

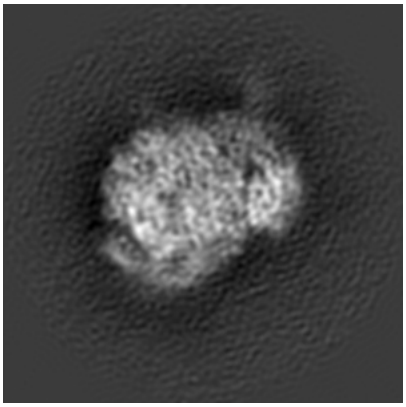
6.1.1 Primary map



X



Y

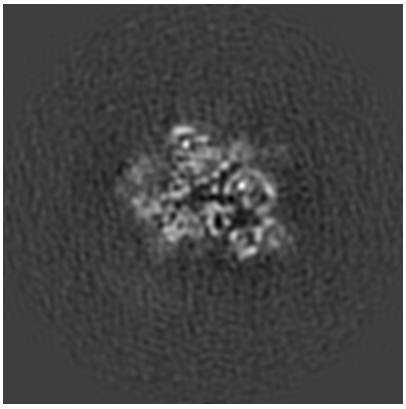


Z

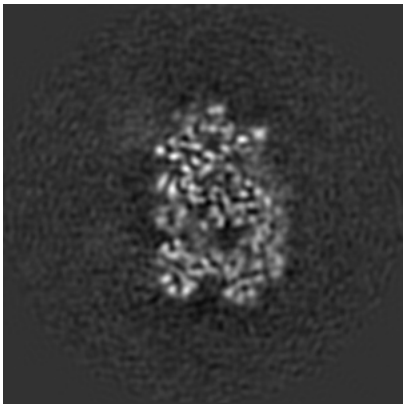
The images above show the map projected in three orthogonal directions.

6.2 Central slices

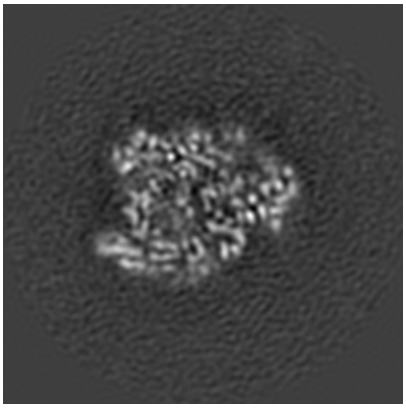
6.2.1 Primary map



X Index: 128



Y Index: 128

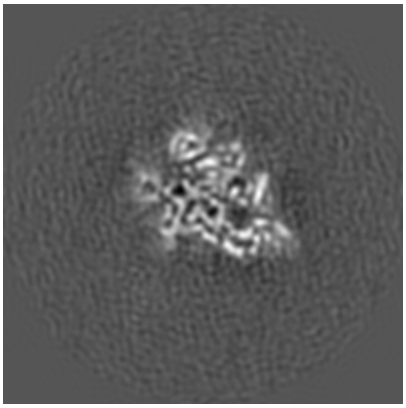


Z Index: 128

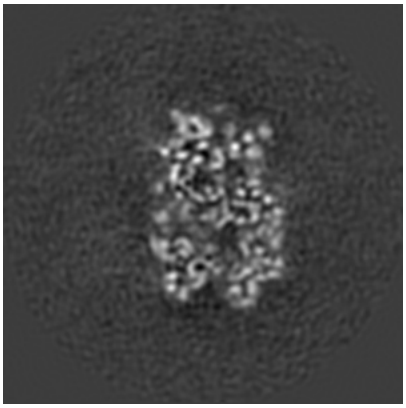
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

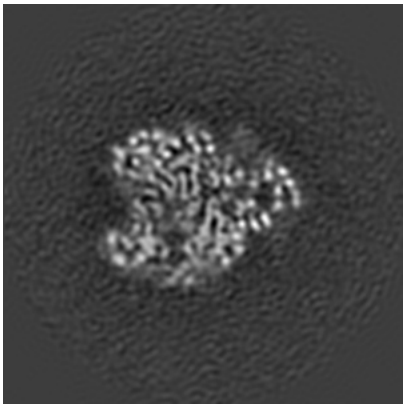
6.3.1 Primary map



X Index: 133



Y Index: 124

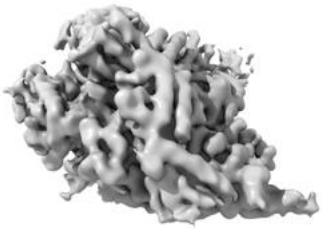


Z Index: 133

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

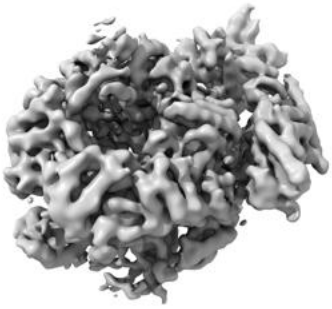
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

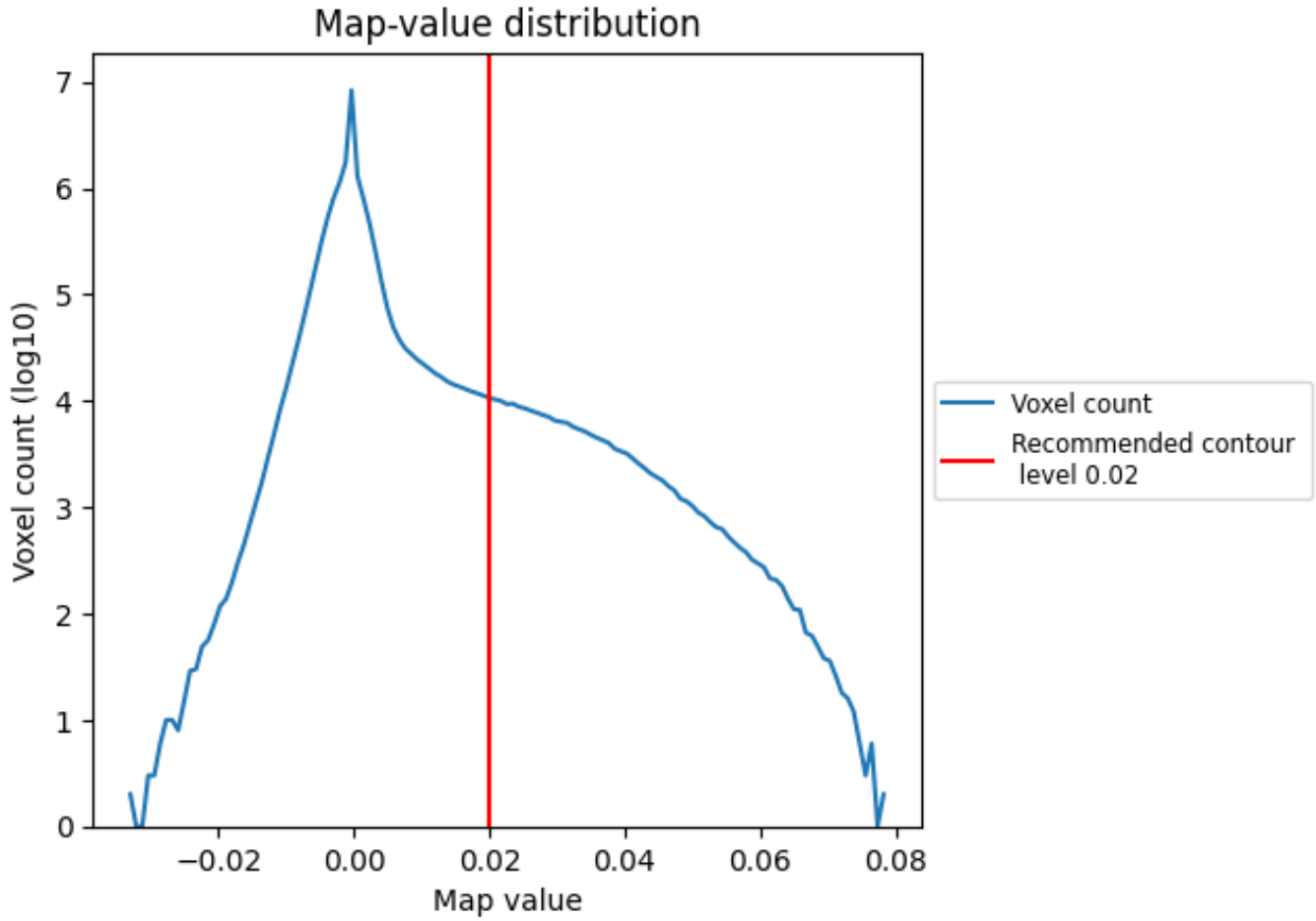
6.5 Mask visualisation (i)

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

7 Map analysis

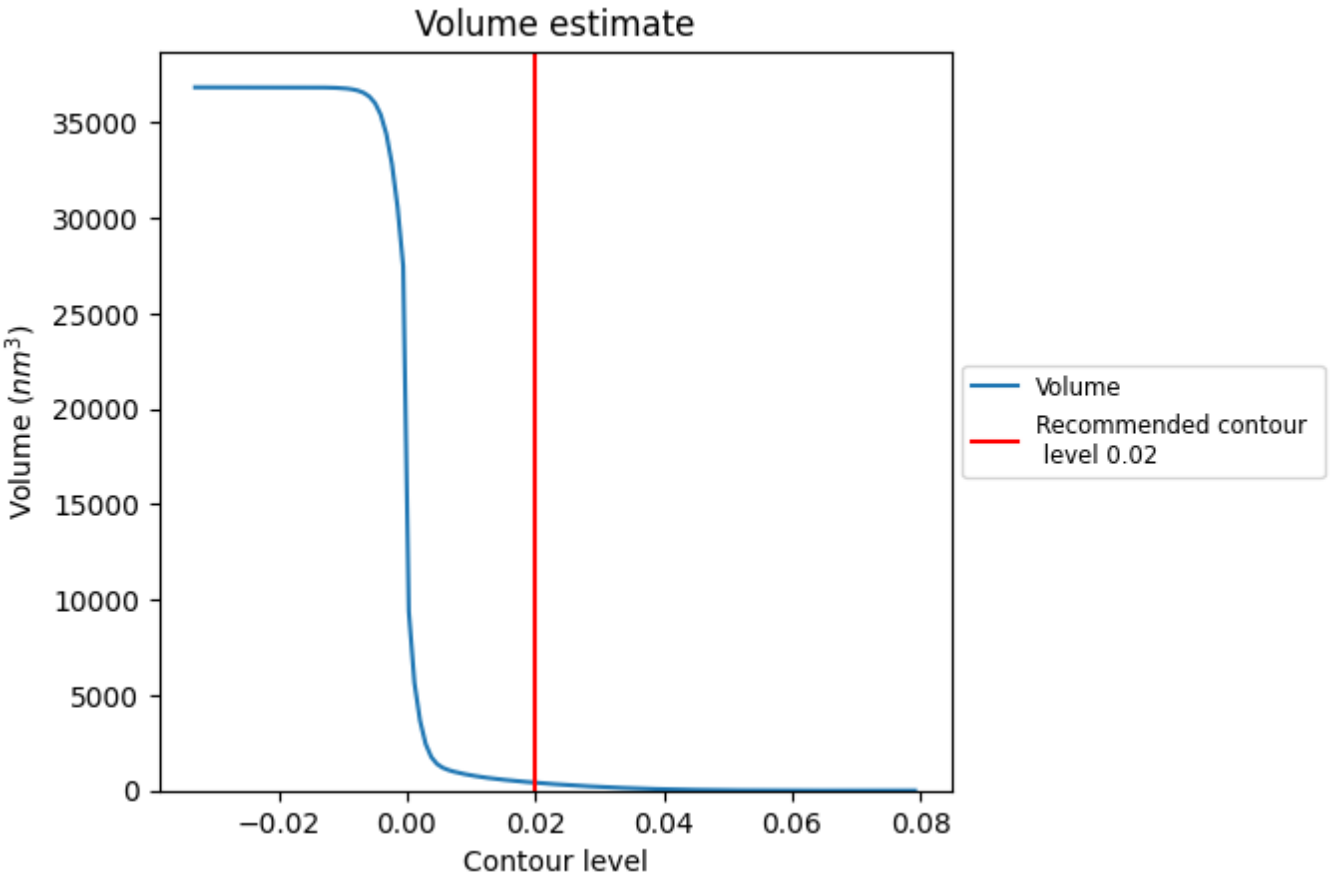
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

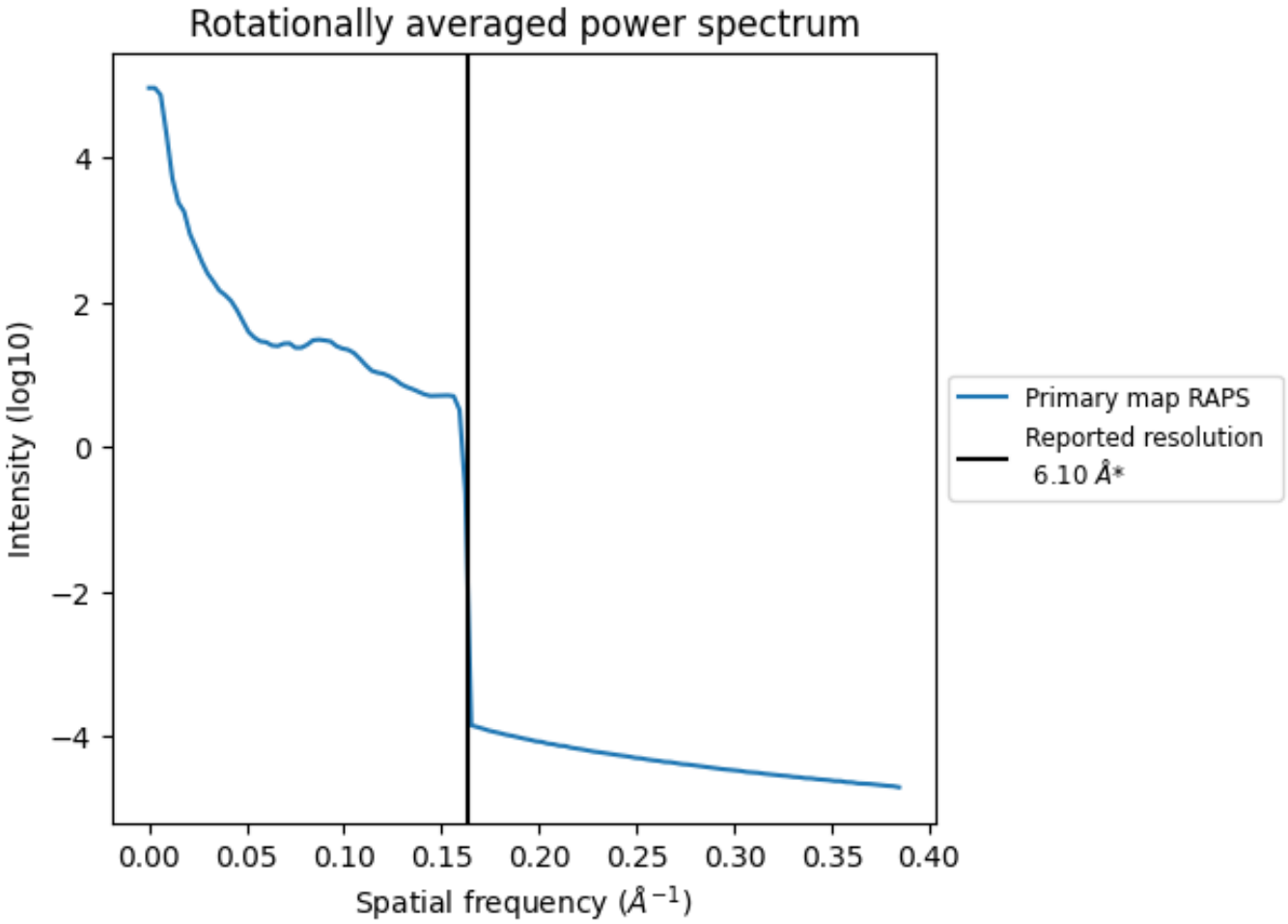
7.2 Volume estimate (i)



The volume at the recommended contour level is 413 nm^3; this corresponds to an approximate mass of 373 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 0.164 Å^{-1}

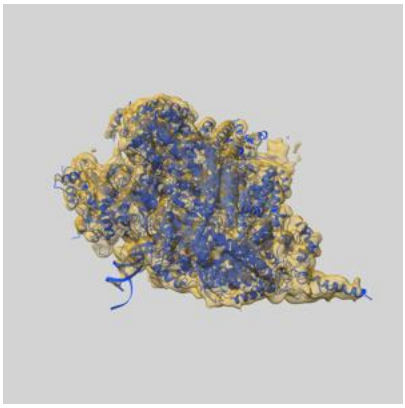
8 Fourier-Shell correlation (i)

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

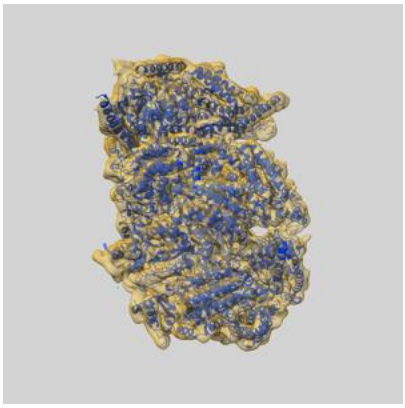
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8518 and PDB model 5U8S. Per-residue inclusion information can be found in section 3 on page 7.

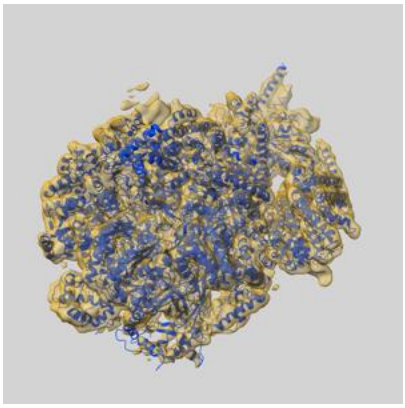
9.1 Map-model overlay



X



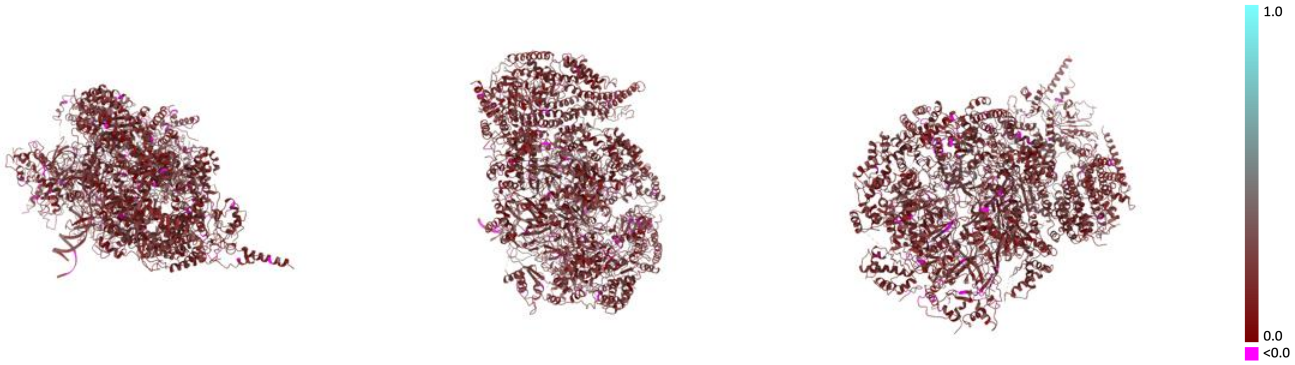
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

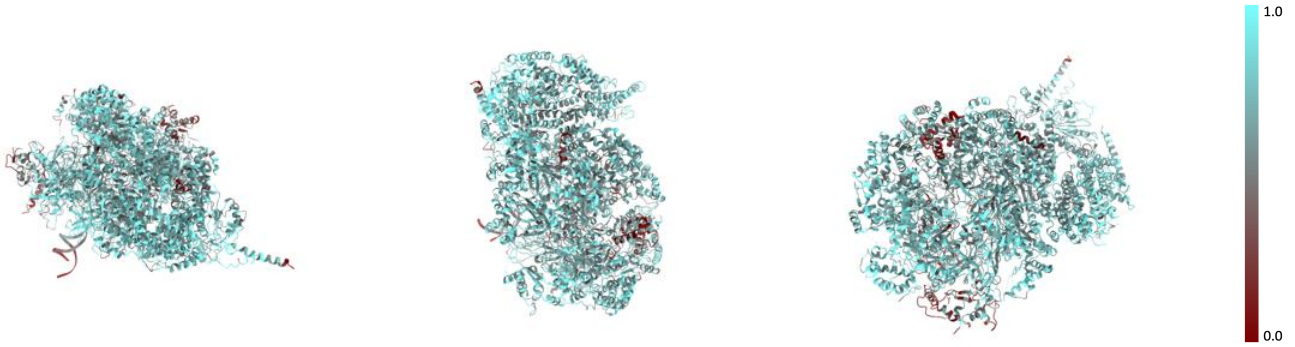
9.2 Q-score mapped to coordinate model (i)



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.

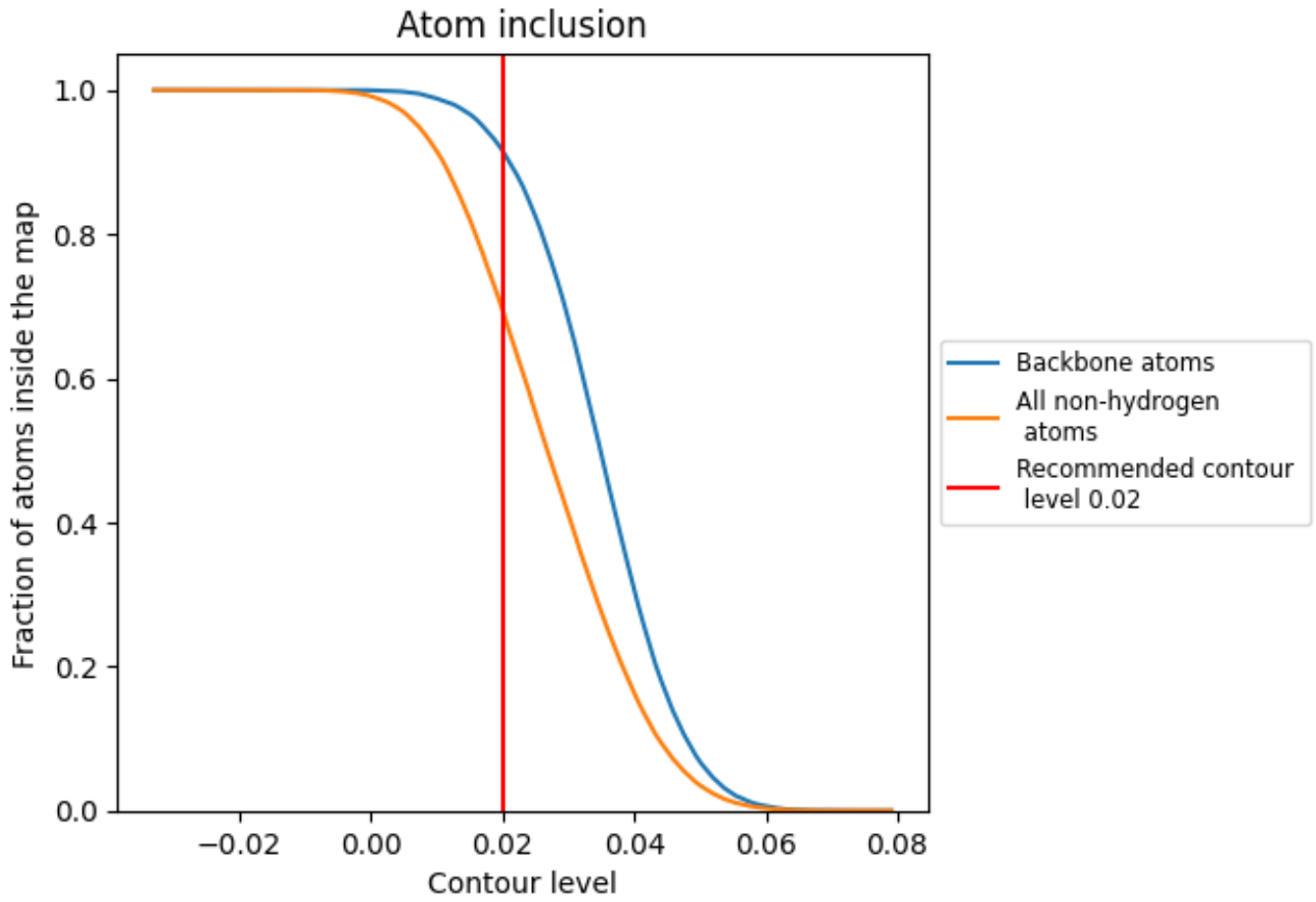
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 69% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6946	0.1990
2	0.7041	0.1990
3	0.7183	0.2070
4	0.6655	0.1880
5	0.6780	0.2030
6	0.7039	0.2020
7	0.6114	0.1920
A	0.6945	0.1880
B	0.7564	0.2070
C	0.7592	0.2000
D	0.7846	0.1990
E	0.7560	0.2010
F	0.5389	0.2370
G	0.4843	0.2260