Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 11:52 AM EST

PDB ID	:	6PTN
EMDB ID	:	EMD-20472
Title	:	Structure of Ctf4 trimer in complex with two CMG helicases
Authors	:	Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.
Deposited on	:	2019-07-16
Resolution	:	5.80 Å(reported)

This is a Full wwPDB EM Validation 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 (1)) were used in the production of this report:

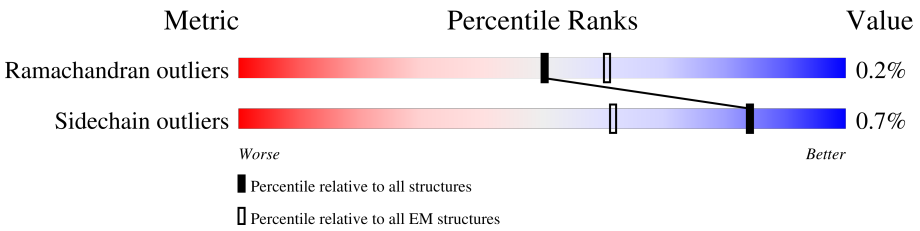
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 5.80 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	E	927	• 46% 54%
1	F	927	5% 46% 54%
1	G	927	• 46% 54%
2	A	208	16% 99% •
2	a	208	12% 99% •
3	B	213	9% 84% • 15%
3	b	213	5% 84% • 15%
4	C	194	16% 80% • 18%
4	c	194	8% 80% • 18%

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Mol	Chain	Length	Quality of chain
5	D	294	11% 80% 20%
5	d	294	9% 80% 20%
6	H	650	16% 83% 15%
6	h	650	17% 83% 15%
7	2	868	54% 72% 27%
7	i	868	47% 72% 27%
8	3	971	39% 61% 39%
8	j	971	28% 61% 39%
9	4	933	61% 72% 27%
9	k	933	52% 72% 27%
10	5	775	45% 76% 23%
10	l	775	39% 76% 23%
11	6	1017	48% 59% 40%
11	m	1017	37% 59% 40%
12	7	845	64% 78% 22%
12	n	845	50% 78% 22%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 91630 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 polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	424	3416	2193	566	642	15	1	0
1	F	431	3472	2227	576	653	16	1	0
1	G	424	3416	2193	566	642	15	1	0

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

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

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

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

- Molecule 4 is a protein called DNA replication complex GINS protein PSF3.

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

- Molecule 5 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	234	1924	1224	315	372	13	0	0
5	D	234	1924	1224	315	372	13	0	0

- Molecule 6 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	h	553	4482	2862	763	844	13	0	0
6	H	553	4482	2862	763	844	13	0	0

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	i	634	4970	3122	897	934	17	0	0
7	2	634	4970	3122	897	934	17	0	0

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	j	594	4659	2936	832	878	13	0	0
8	3	594	4659	2936	832	878	13	0	0

- Molecule 9 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	k	682	5410	3397	946	1039	28	0	0
9	4	682	5410	3397	946	1039	28	0	0

- Molecule 10 is a protein called Minichromosome maintenance protein 5.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	5	597	4688	2946	808	910	24	0	0

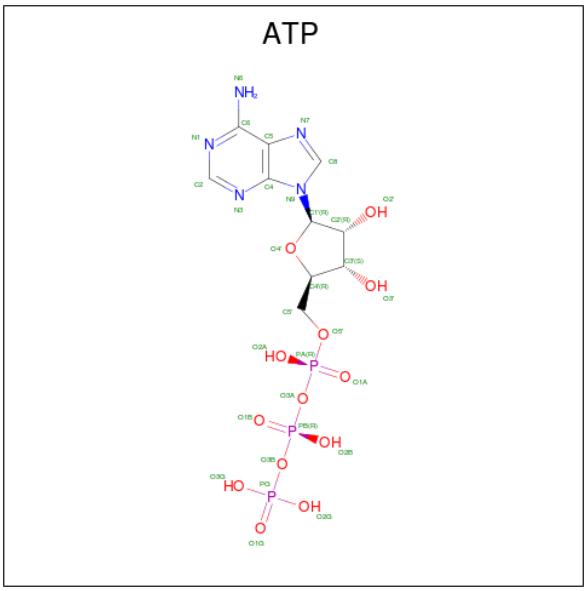
- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	m	614	4720	2971	836	893	20	0	0
11	6	614	4720	2971	836	893	20	0	0

- Molecule 12 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	n	663	5220	3290	904	996	30	0	0
12	7	663	5220	3290	904	996	30	0	0

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



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

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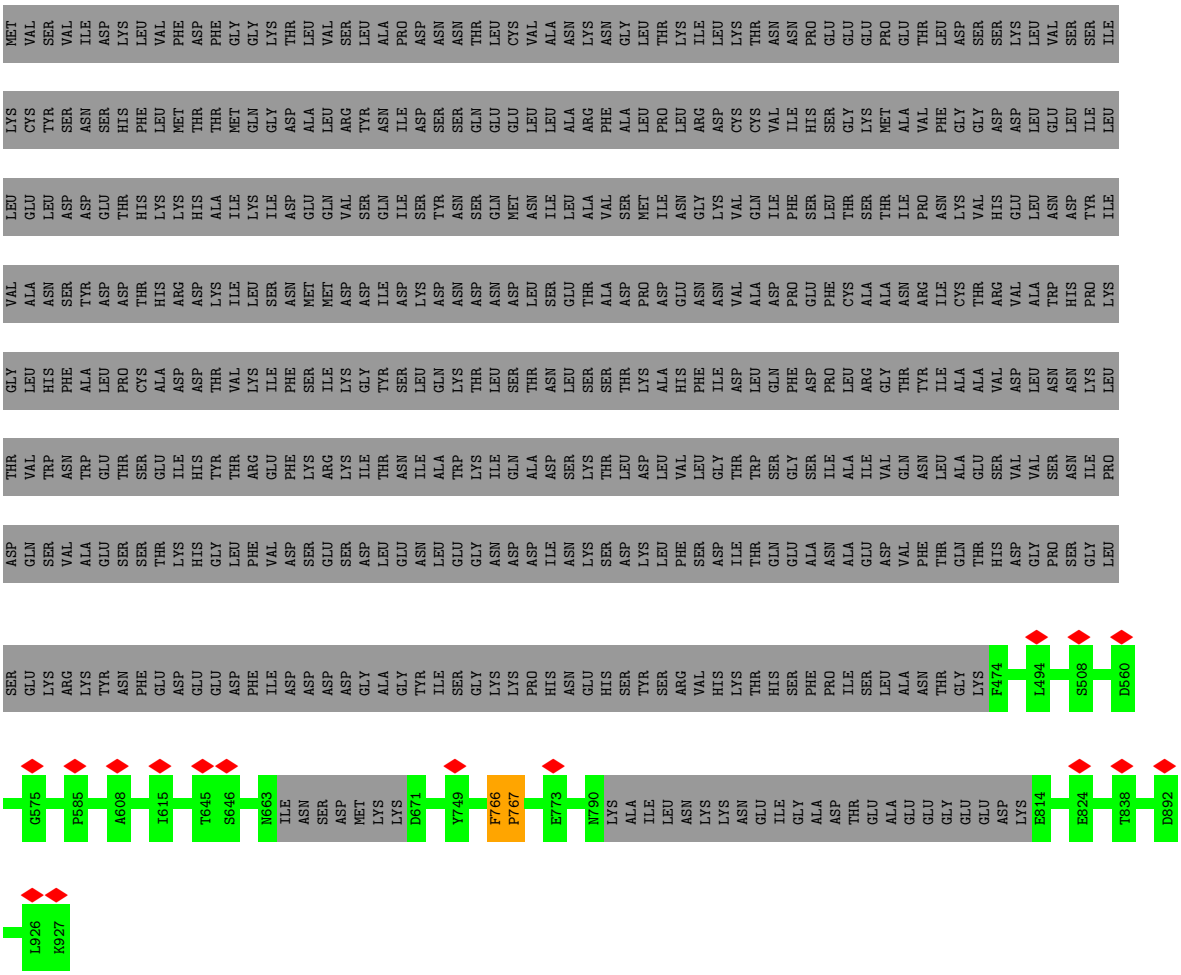
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	j	1	31	10	5	13	3	0
			Total	C	N	O	P	
13	l	1	31	10	5	13	3	0
			Total	C	N	O	P	
13	2	1	31	10	5	13	3	0
			Total	C	N	O	P	
13	3	1	31	10	5	13	3	0
			Total	C	N	O	P	
13	5	1	31	10	5	13	3	0

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.

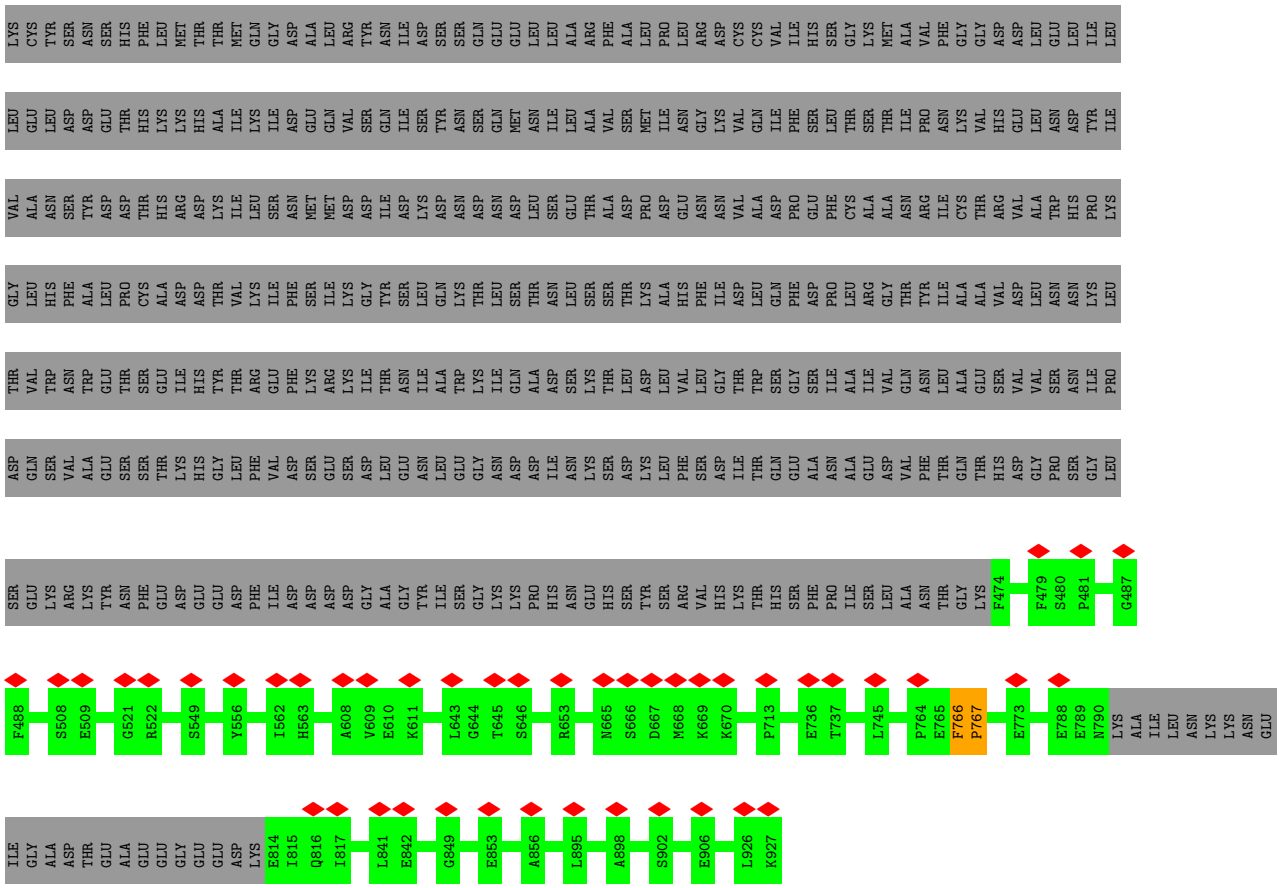
- Molecule 1: DNA polymerase alpha-binding protein

Chain E:



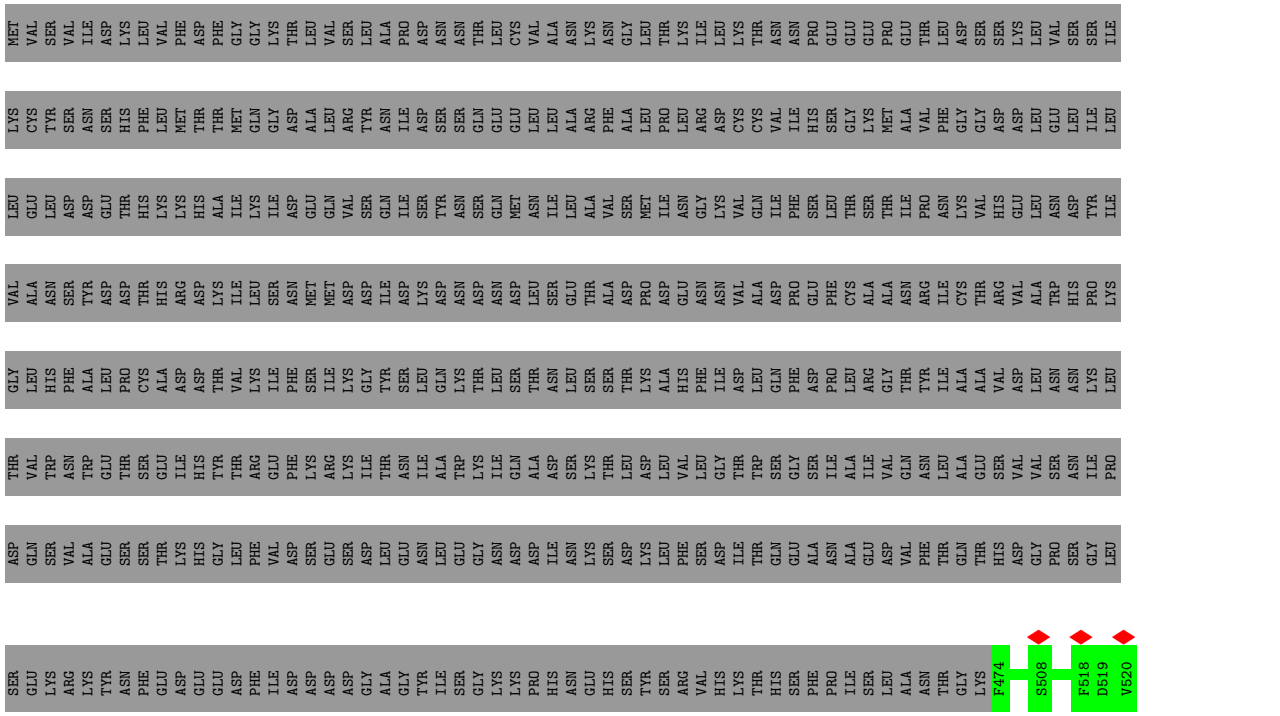
- Molecule 1: DNA polymerase alpha-binding protein

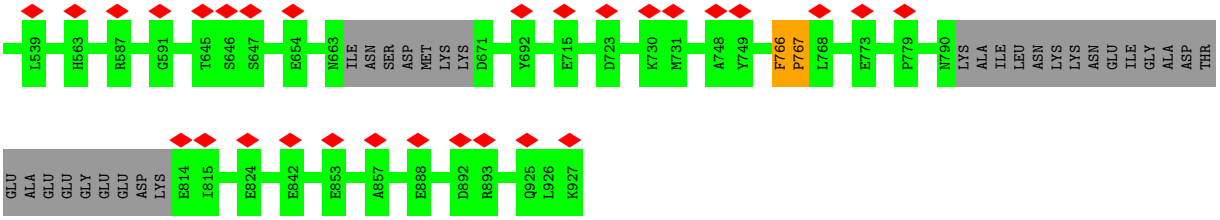
Chain F:



- Molecule 1: DNA polymerase alpha-binding protein

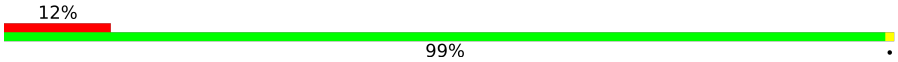
Chain G: 46% 54%





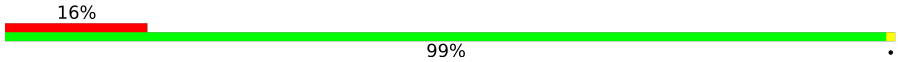
• Molecule 2: DNA replication complex GINS protein PSF1

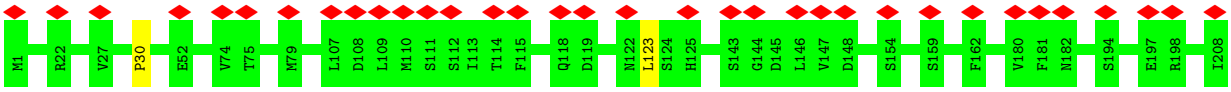
Chain a:



• Molecule 2: DNA replication complex GINS protein PSF1

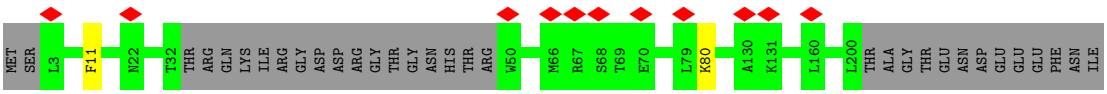
Chain A:





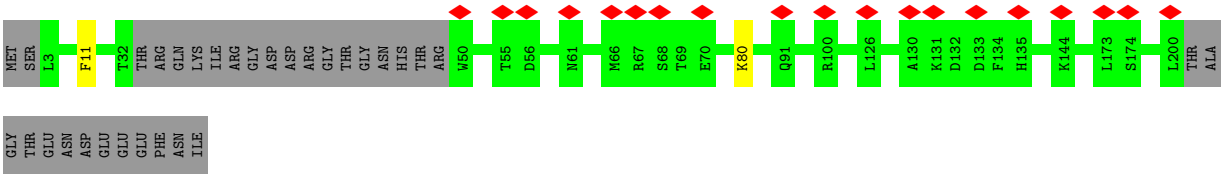
• Molecule 3: DNA replication complex GINS protein PSF2

Chain b:



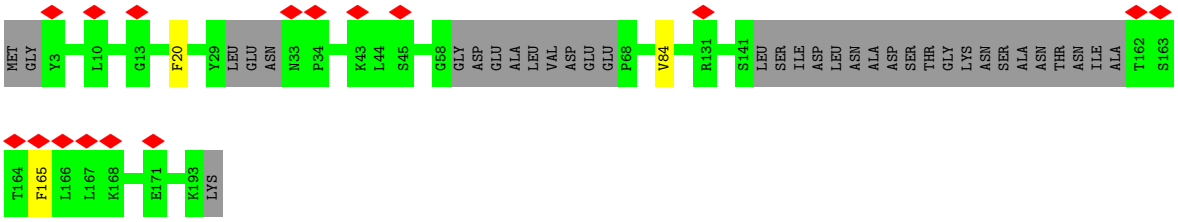
• Molecule 3: DNA replication complex GINS protein PSF2

Chain B:



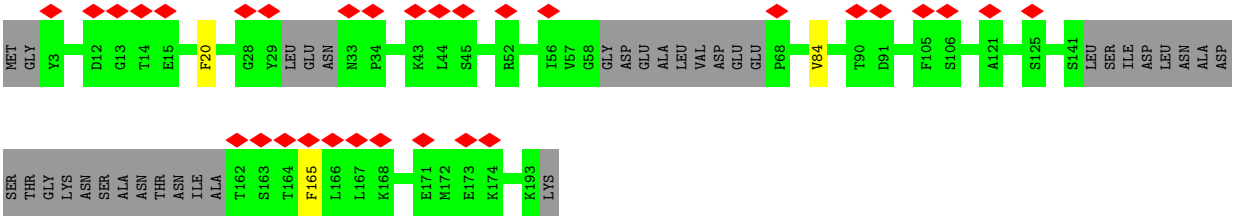
• Molecule 4: DNA replication complex GINS protein PSF3

Chain c:



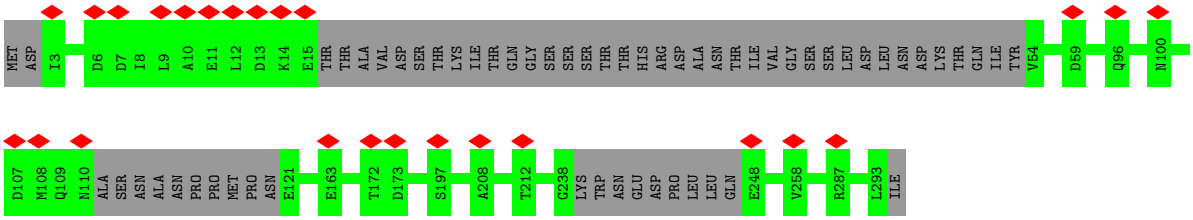
- Molecule 4: DNA replication complex GINS protein PSF3

Chain C:



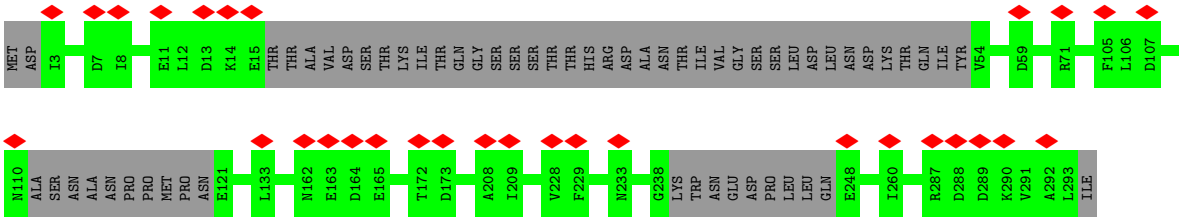
- Molecule 5: DNA replication complex GINS protein SLD5

Chain d:



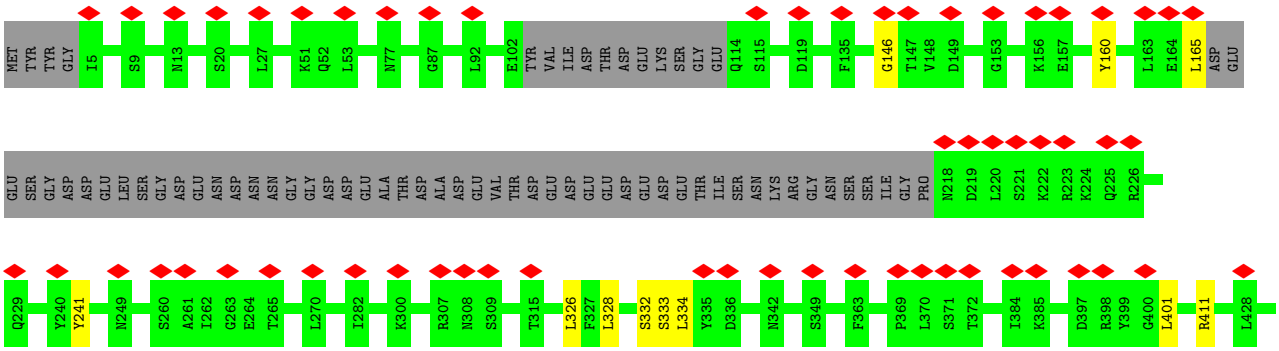
- Molecule 5: DNA replication complex GINS protein SLD5

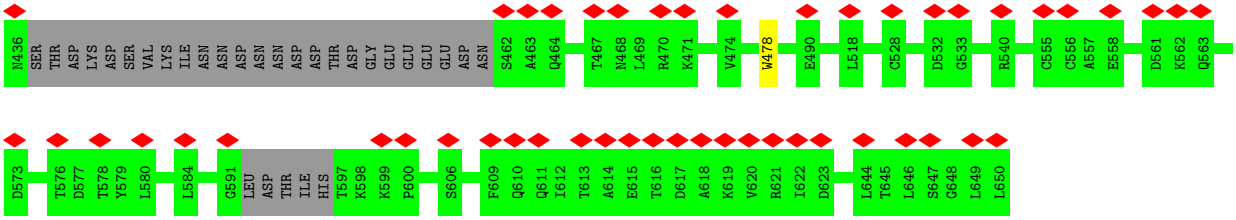
Chain D:



- Molecule 6: Cell division control protein 45

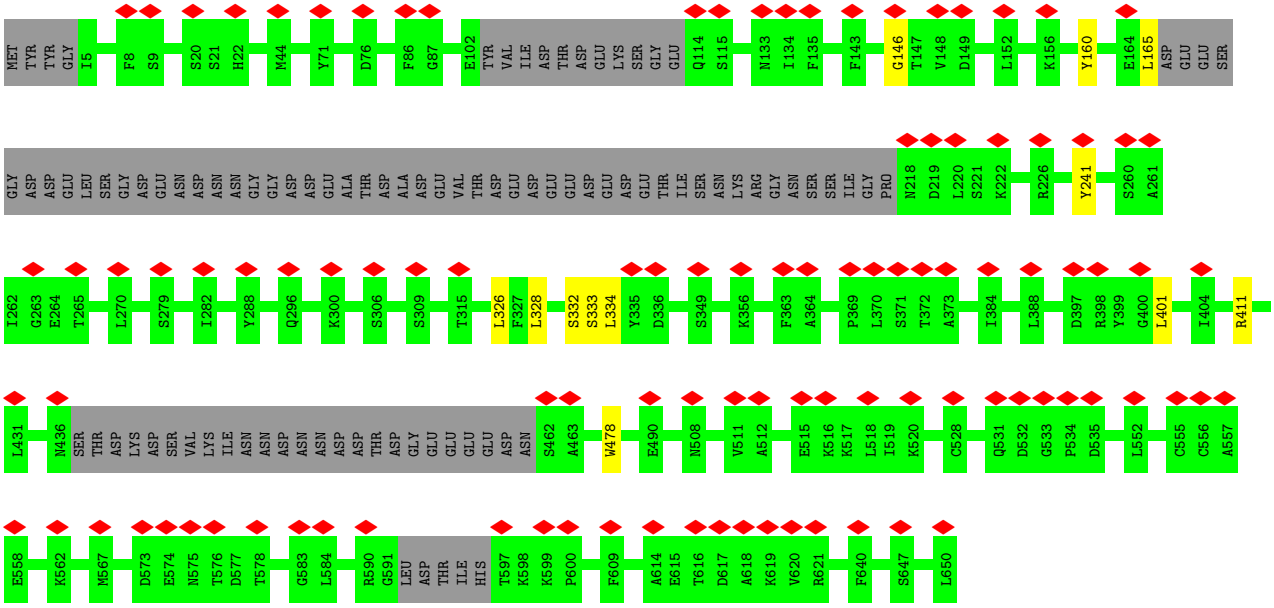
Chain h:





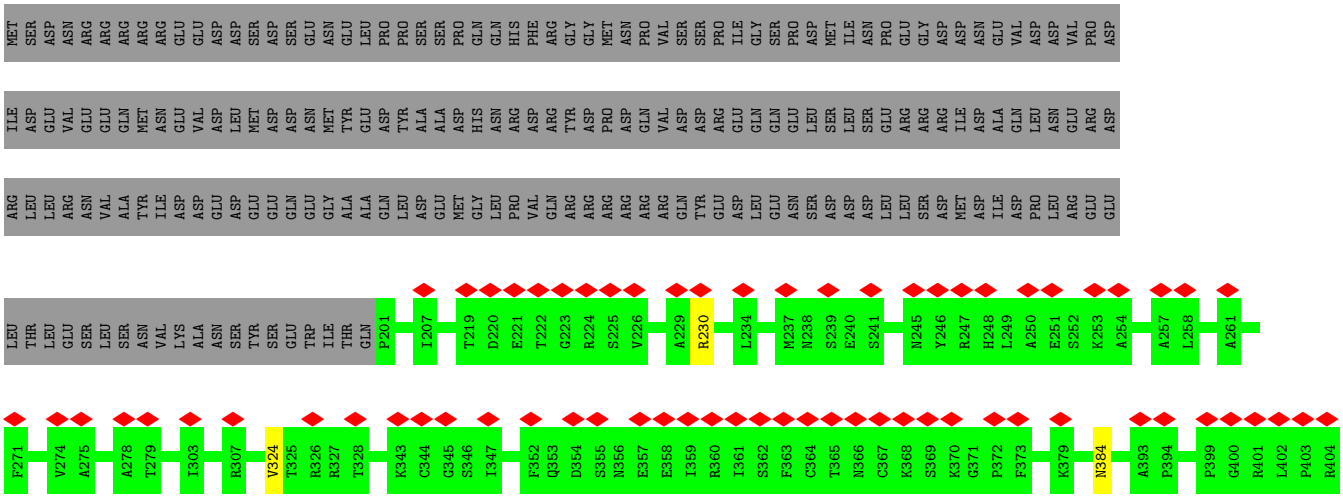
- Molecule 6: Cell division control protein 45

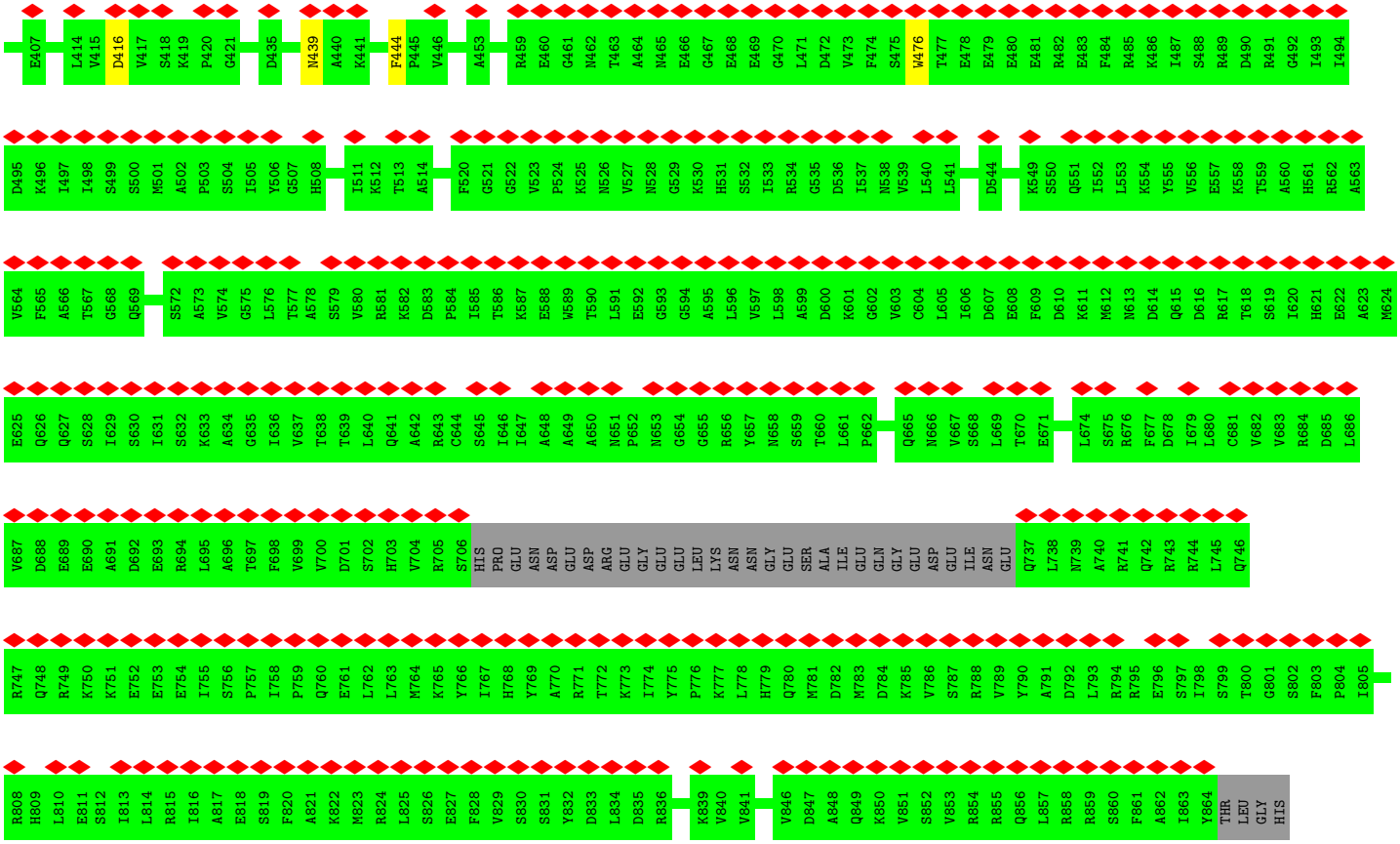
Chain H:



- Molecule 7: DNA replication licensing factor MCM2

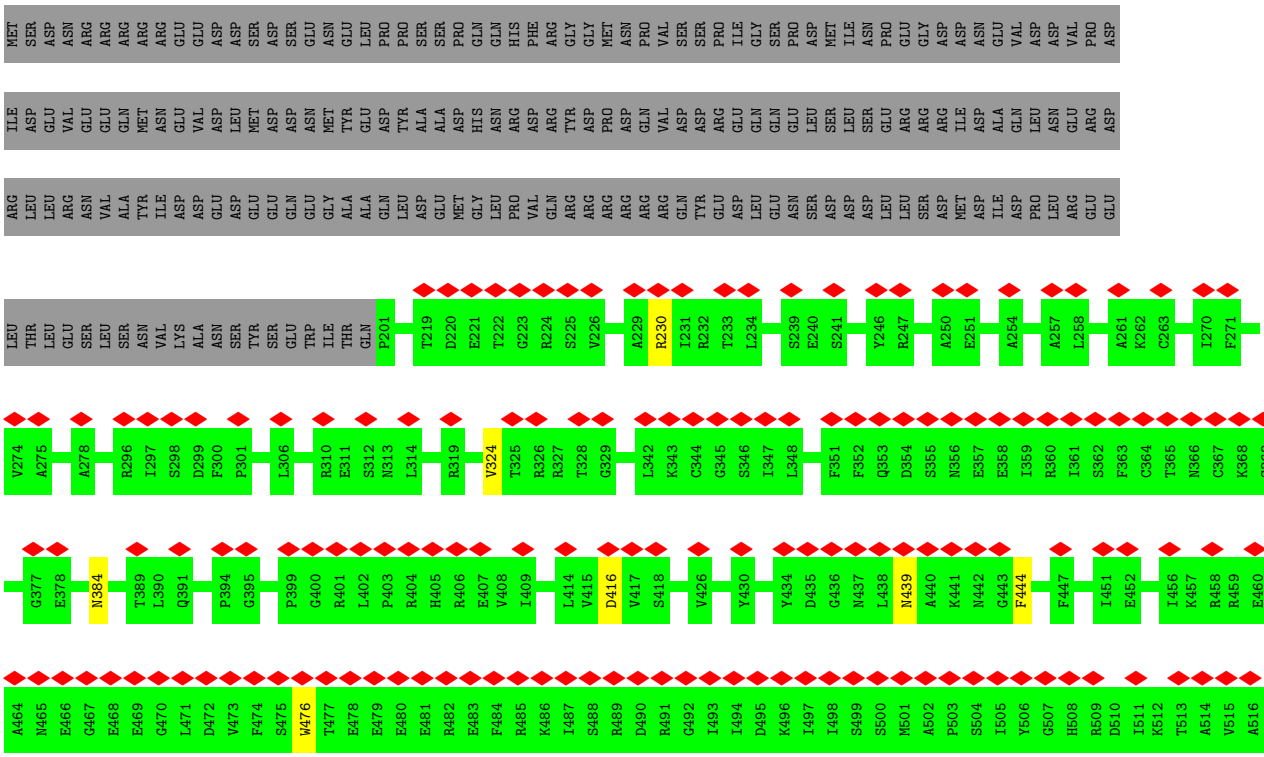
Chain i:

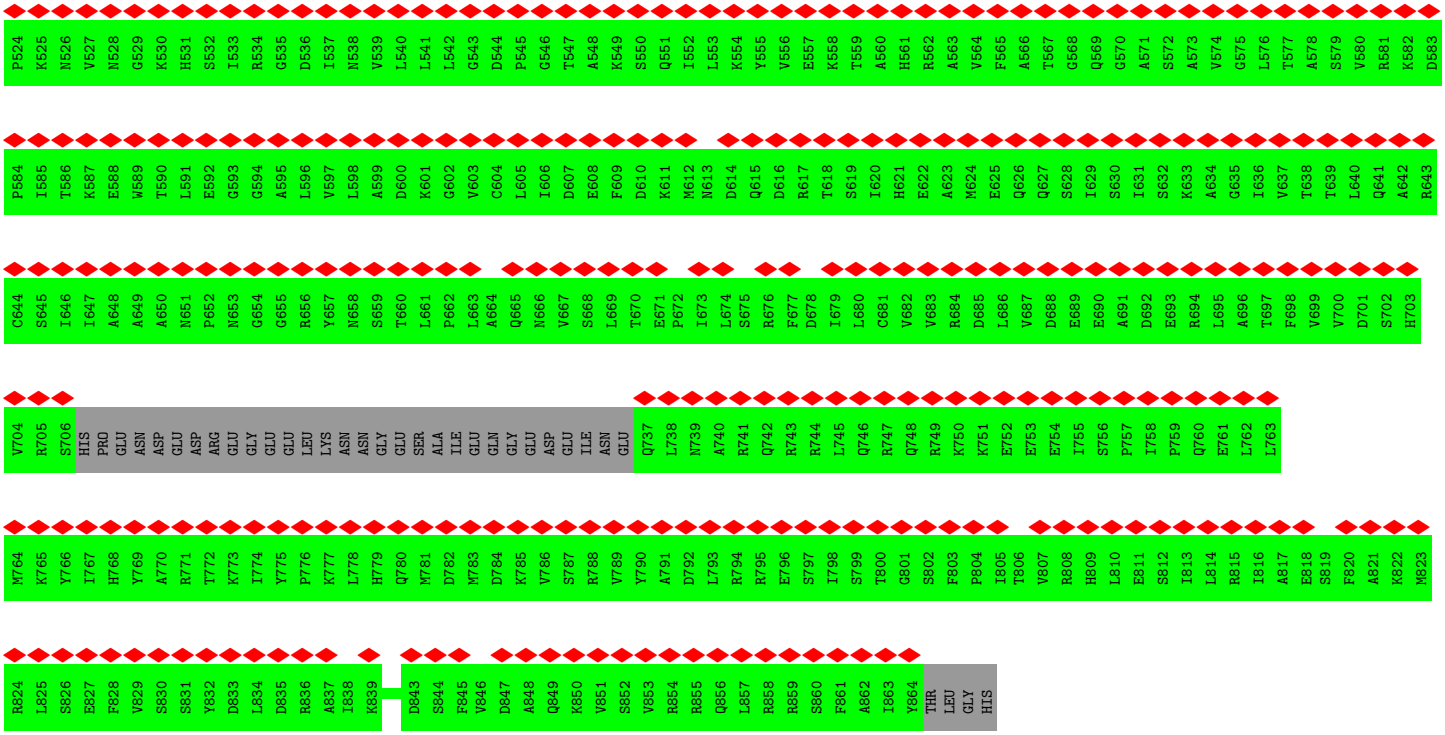




- Molecule 7: DNA replication licensing factor MCM2

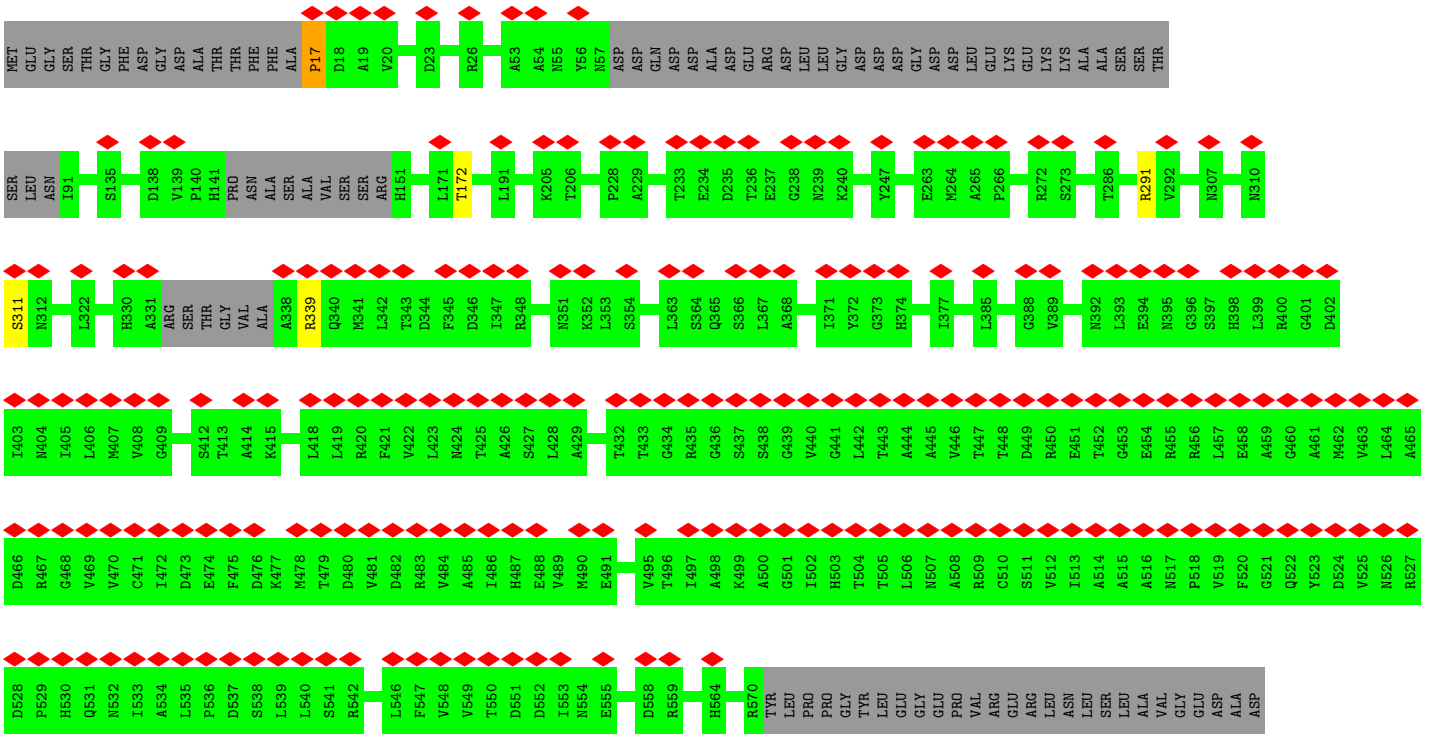
Chain 2:

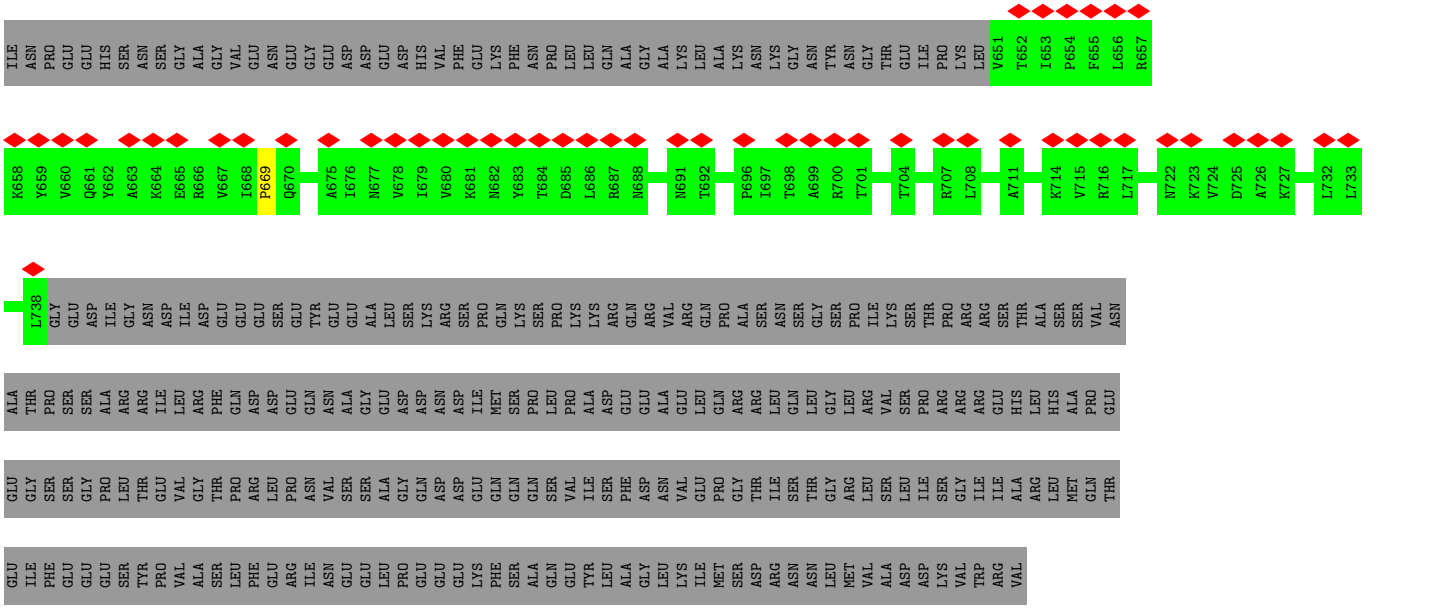




- Molecule 8: DNA replication licensing factor MCM3

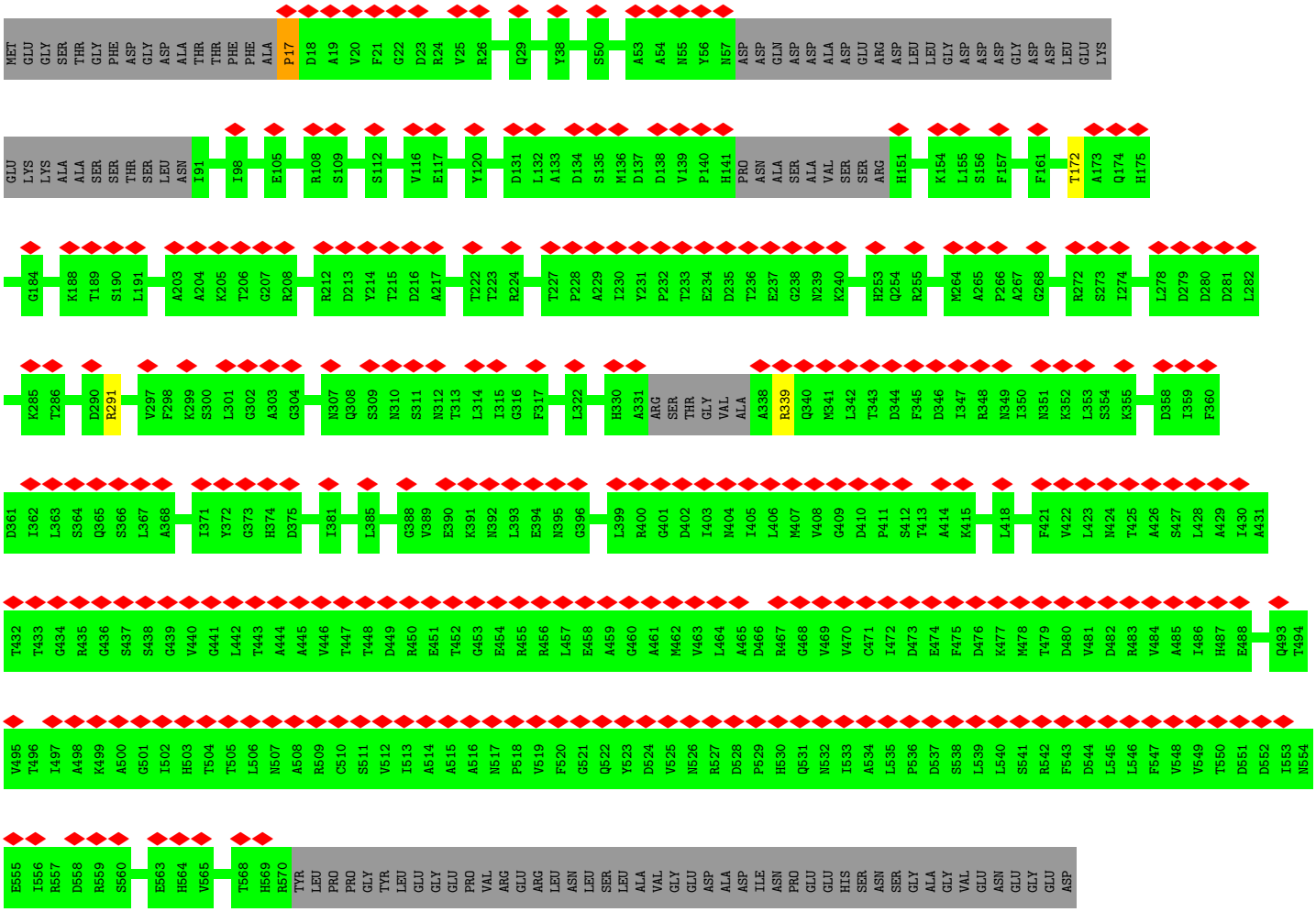
Chain j:

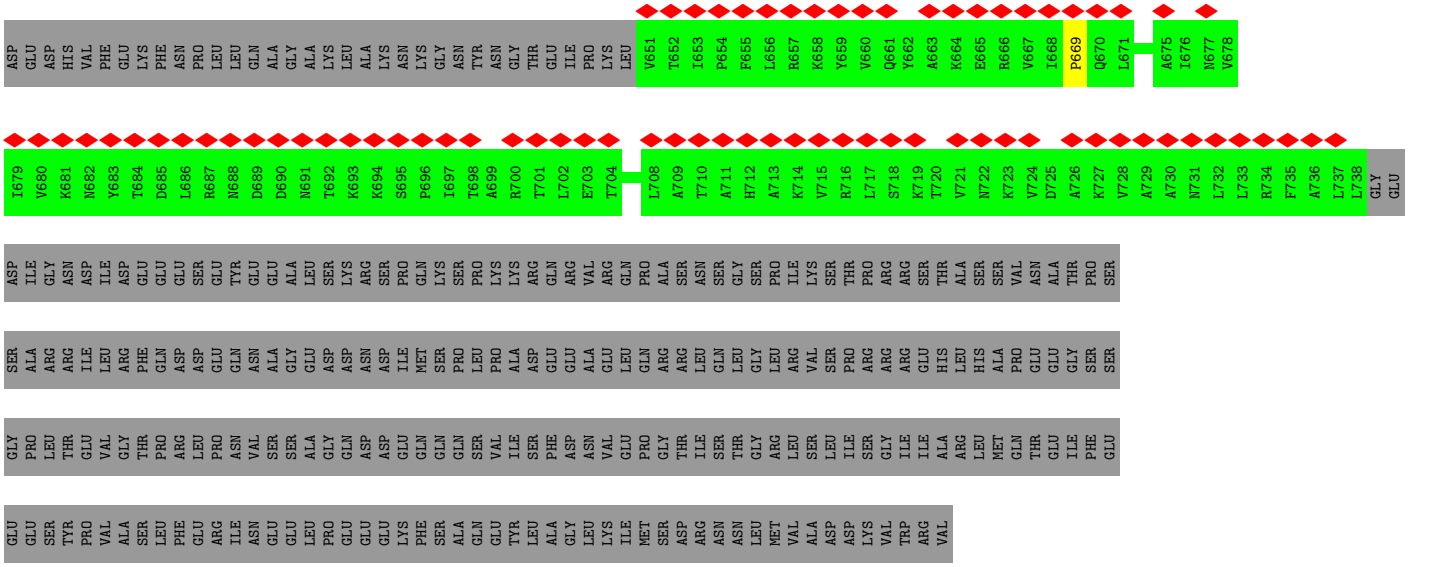




- Molecule 8: DNA replication licensing factor MCM3

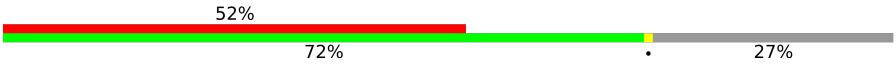
Chain 3:

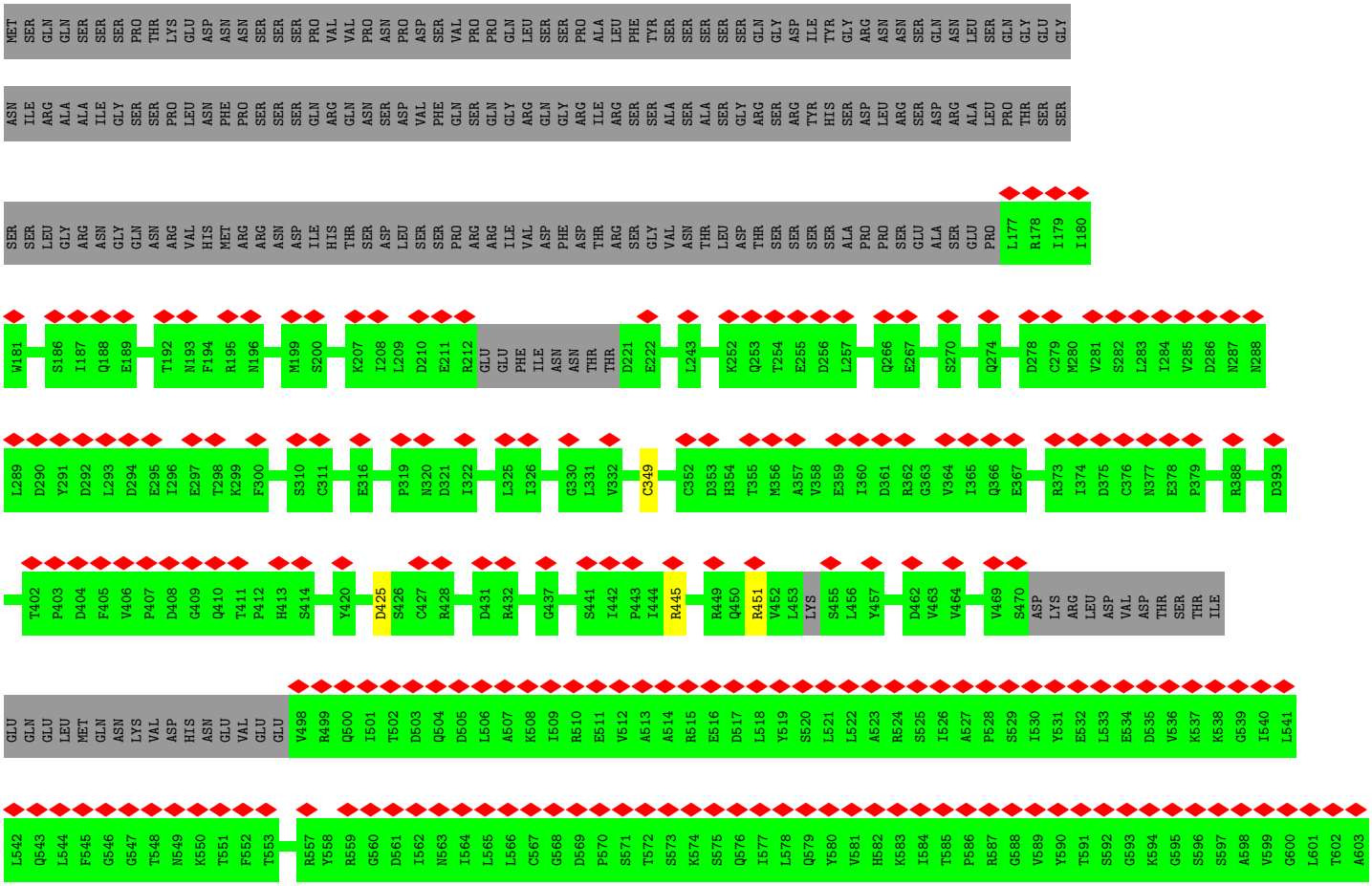




- Molecule 9: DNA replication licensing factor MCM4

Chain k:





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 V682 N683 P684 N685 L686 P687 V688 T689 E690 N691 I692 D693 P697 L698 L699 D703 L704 V705 Y706 L707 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 P743 V744 E745 F746 L747 T748 M749 Y750 I751 S752 Y753 A754 K755 E756 H757 I758 H759 P760 I761 I762 T763 E764 A765 A766 K767 T768 E769 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 M811 K812 L813 K814 N815 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 Q853 K854 S855 V856 I857 Q858 R859 K860 L861 Q862 E863 D864 L865 S866 R867 E868 I869 M870 N871 V872 L873 K874 D875 Q876 A877 S878 D879 S880 M881 S882 F883 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 E921 G922 V923 R924 R925 S926 V927 R928 L929 ASN ASN ARG VAL

- Molecule 9: DNA replication licensing factor MCM4

Chain 4: 61% 72% 27%

MET SER GLN GLN SER SER SER PRO THR LYS GLU ASP ASN ASN SER SER SER PRO VAL VAL PRO ASN PRO ASP SER VAL PRO PRO GLN LEU SER SER PRO ALA LEU PHE TYR SER SER SER SER SER GLN GLY ASP ILE TYR GLY ARG ASN ASN SER GLN ASN LEU SER GLN GLY GLU GLY

ASN ILE ARG ALA ALA ILE GLY SER SER PRO 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 SER ASP ARG ALA LEU PRO THR SER SER

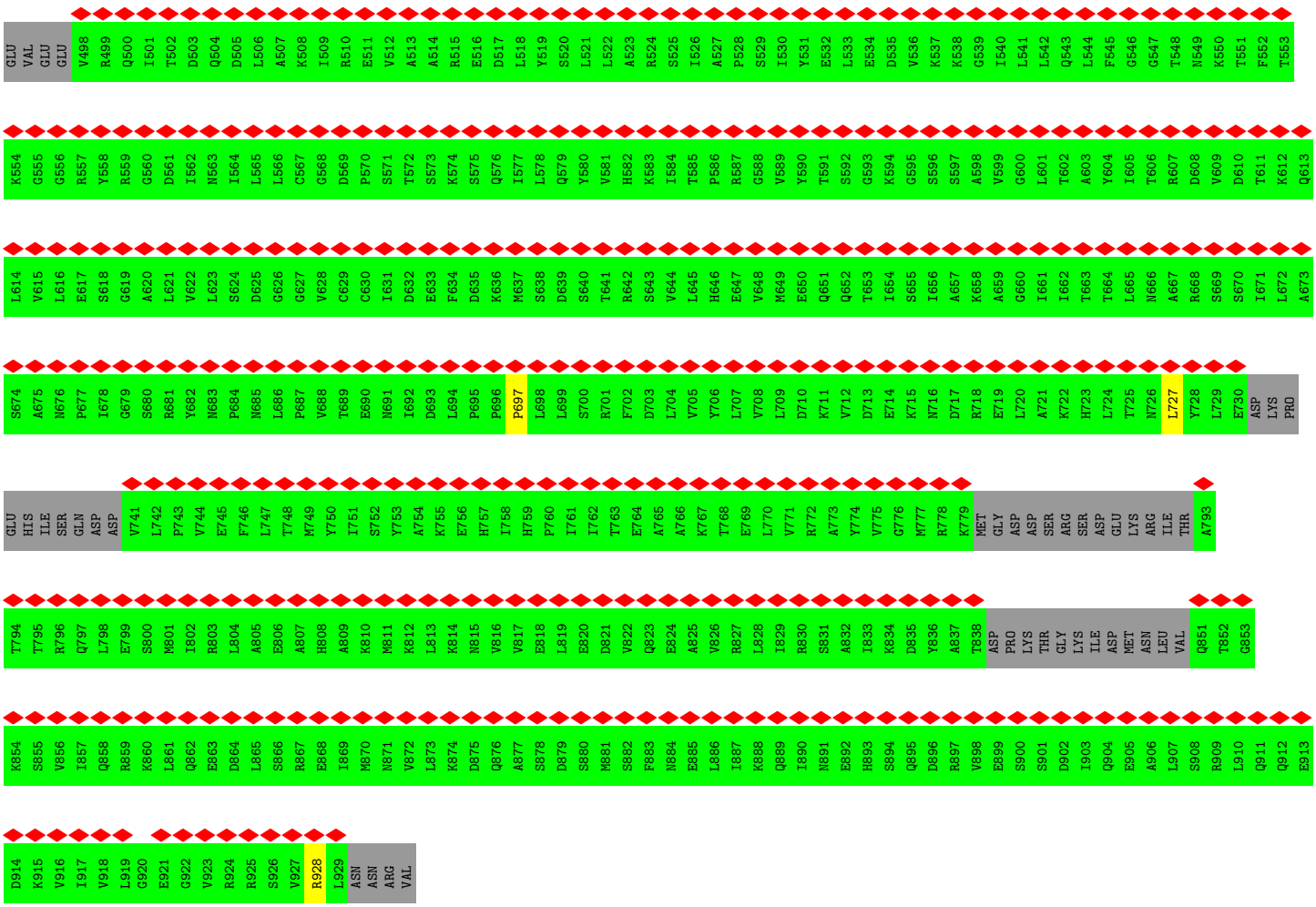
SER SER LEU GLY ARG ASN GLY GLN ASN ARG VAL HIS MET ARG ARG ASN ASP ILE HIS THR SER ASP LEU SER SER PRO ARG ARG ILE VAL ASP PHE ASP THR ARG SER GLY VAL ASN THR LEU ASP THR SER SER SER SER ALA PRO PRO SER GLU ALA SER GLU PRO L177 R178 I179 I180

W181 N184 V185 S186 I187 Q188 E189 C190 T191 T192 N193 F194 R195 N196 F197 L198 M199 S200 F201 K202 Y203 R206 K207 I208 L209 D210 E211 R212 GLU GLU PHE ILE ASN ASN THR THR D221 E222 E223 M233 R234 E235 L236 G237 T238 L241 N242 L243 D244 A245 L248 L249 A250 Y251 K252

Q253 T254 E255 D256 L257 Q266 E267 V268 I269 S270 I271 M272 D273 Q274 T275 I276 K277 D278 C279 M280 V281 S282 L283 I284 V285 D286 N287 N288 L289 D290 Y291 D292 L293 D294 E295 I296 E297 T298 K299 F300 Y301 K302 V303 R304 P305 G309 S310 C311 K312 G313 E316 L317 N318 P319 N320 D321 I322

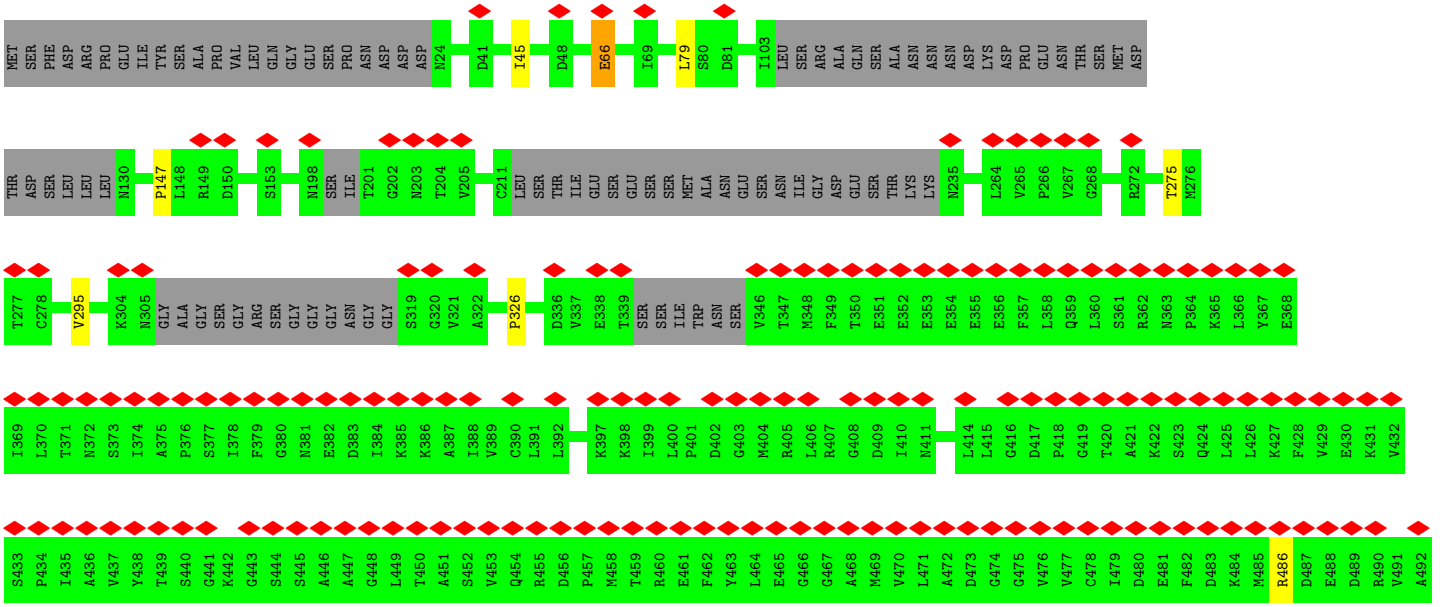
D323 K324 R334 C349 N350 V351 C352 D353 H354 T355 M356 A357 V358 E359 I360 D361 R362 G363 V364 I365 Q366 E367 P368 A369 R370 C371 E372 R373 I374 D375 C376 N377 E378 P379 N387 E401 T402 P403 D404 F405 Y406 P407 D408 G409 Q410 T411 P412 H413 S414 C418 V419 Y420 D421 E422

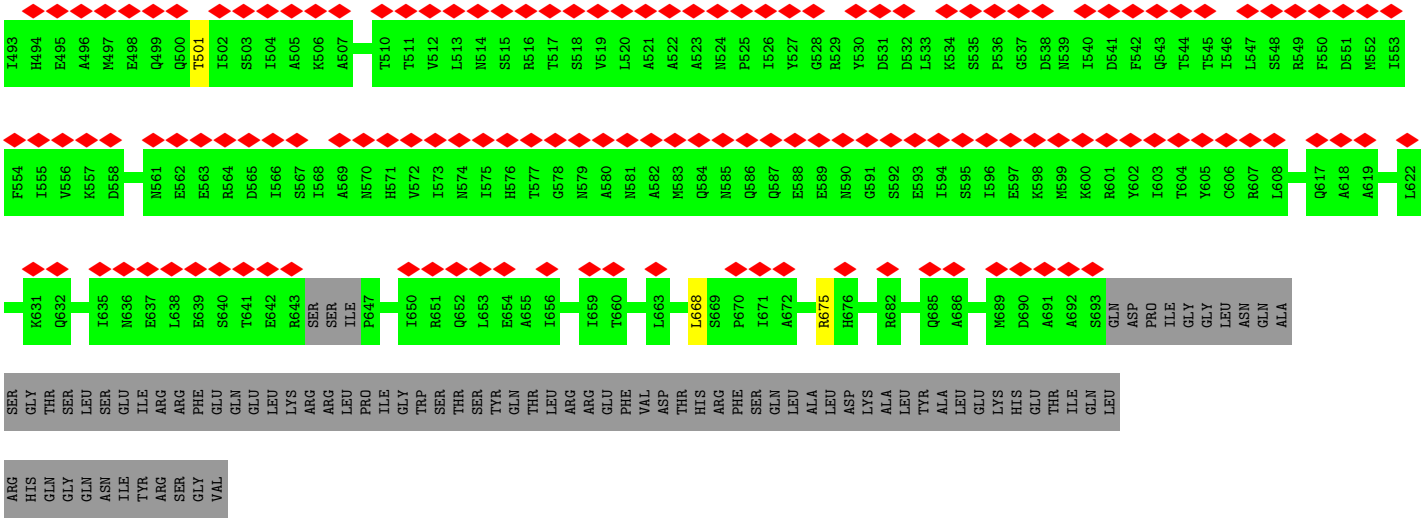
D425 S426 C427 R428 D431 T436 R440 S441 I442 P443 I444 R445 A446 N447 S448 R449 Q450 R451 V452 L453 LYS S455 L456 Y457 Y460 V463 V464 H465 K468 V469 S470 ASP LYS ARG LEU ASP VAL ASP THR SER THR ILE GLU GLN GLU LEU MET GLN ASN LYS VAL ASP HIS ASN



- Molecule 10: Minichromosome maintenance protein 5

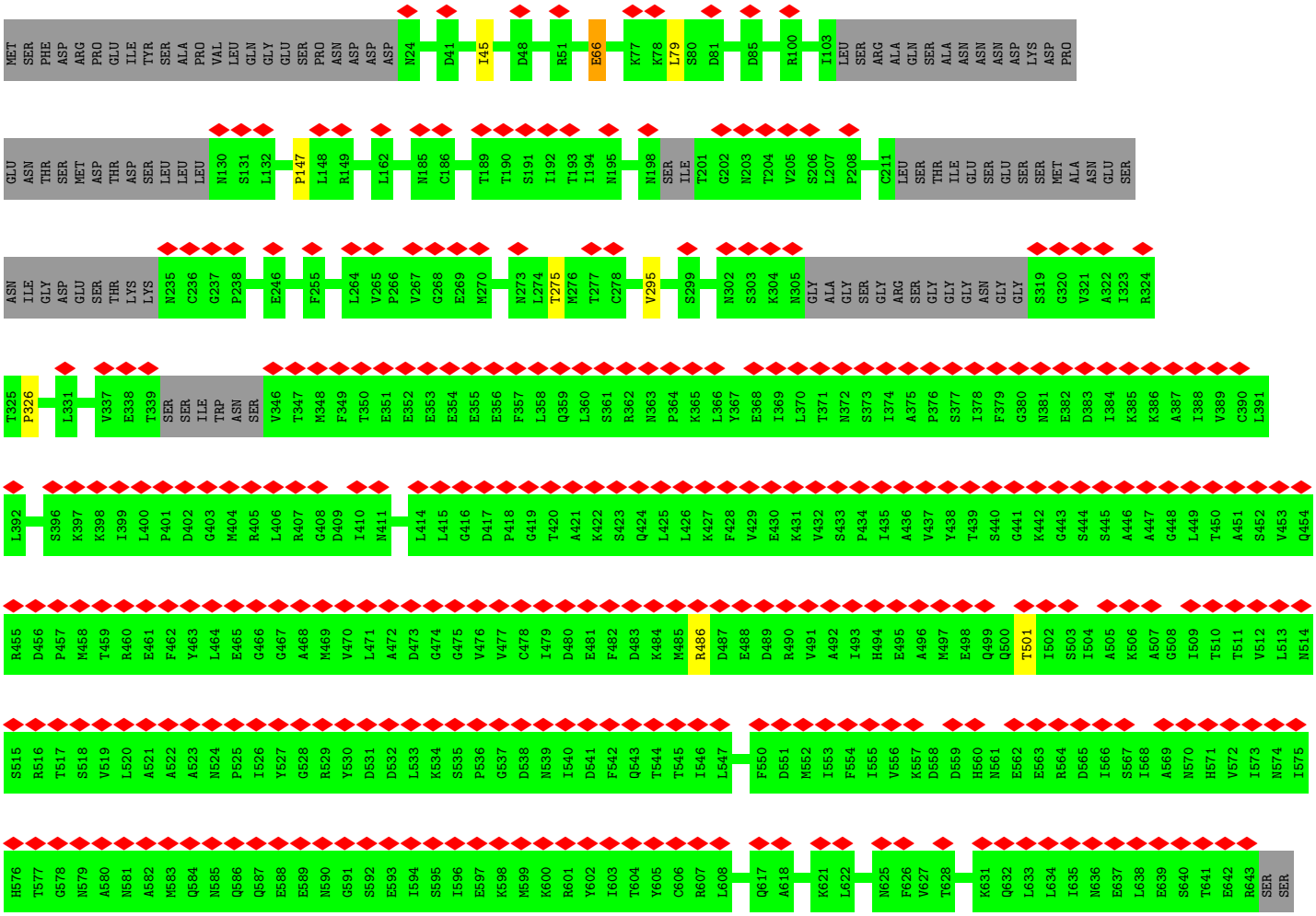
Chain l:

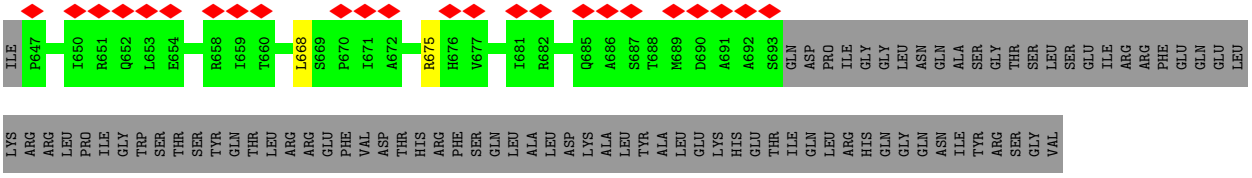




- Molecule 10: Minichromosome maintenance protein 5

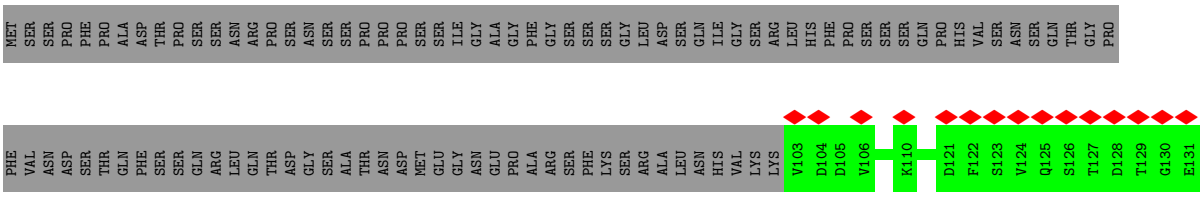
Chain 5:

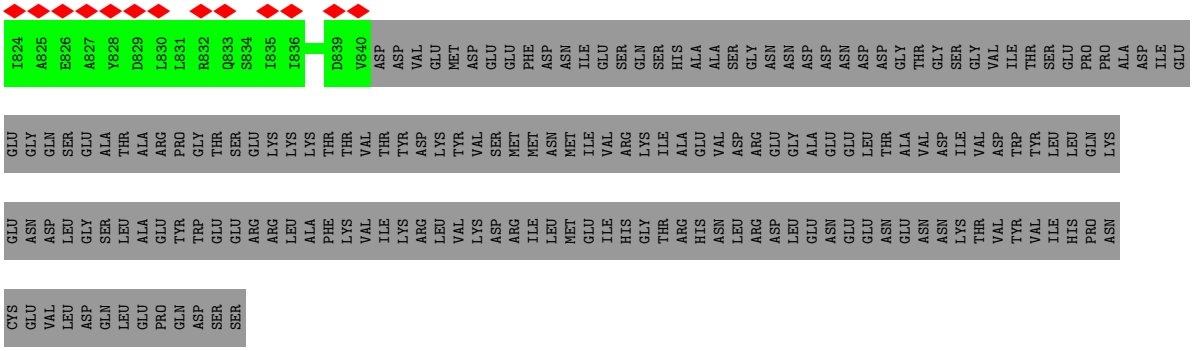




• Molecule 11: DNA replication licensing factor MCM6

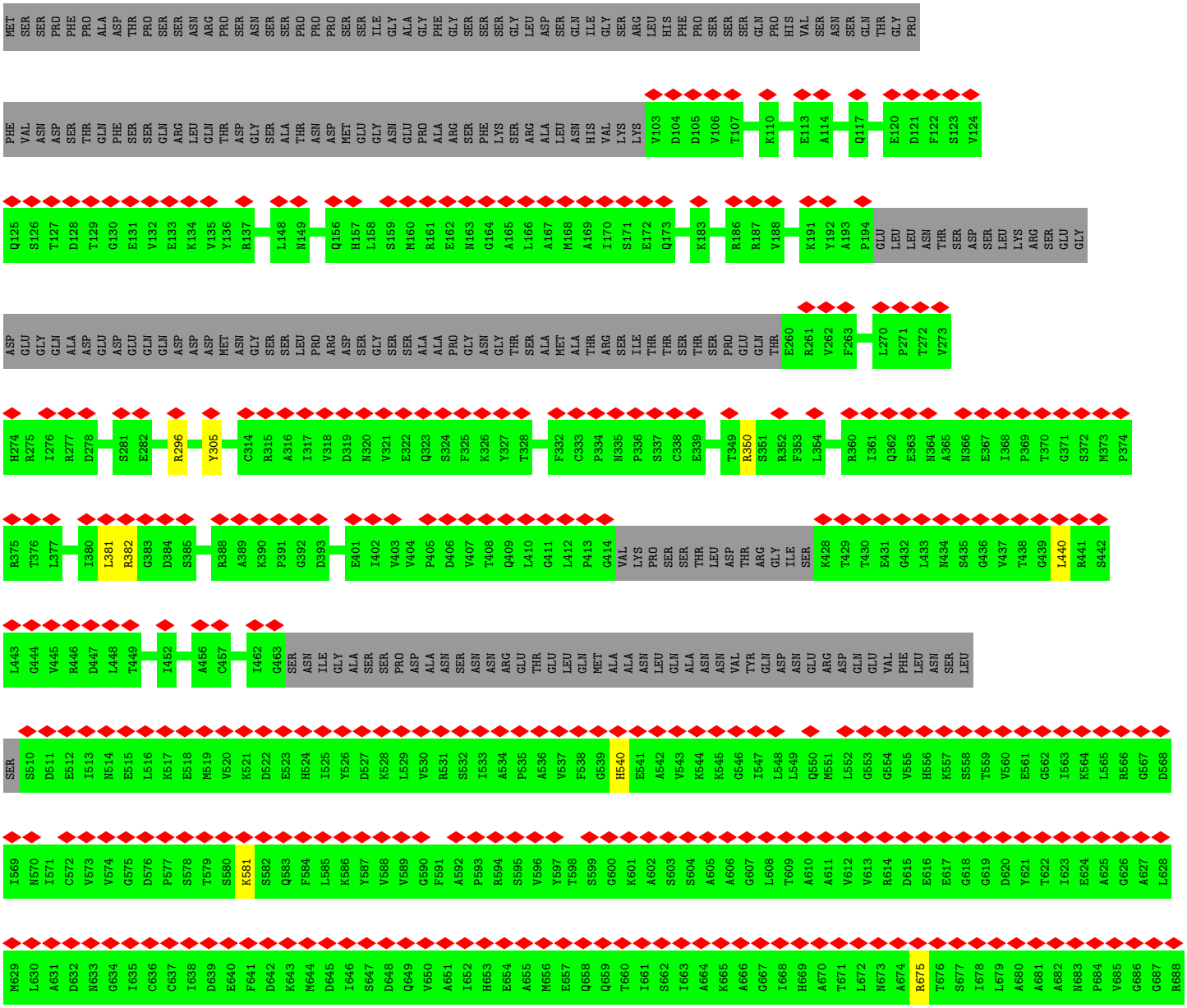
Chain m:

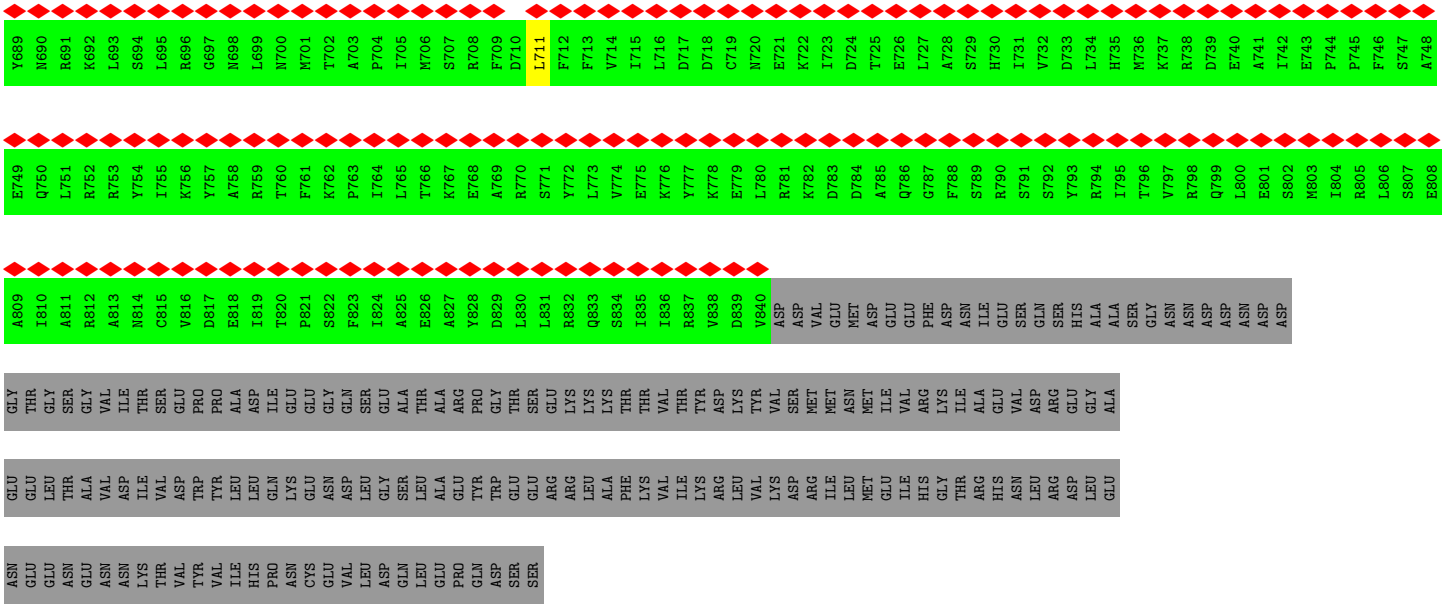




- Molecule 11: DNA replication licensing factor MCM6

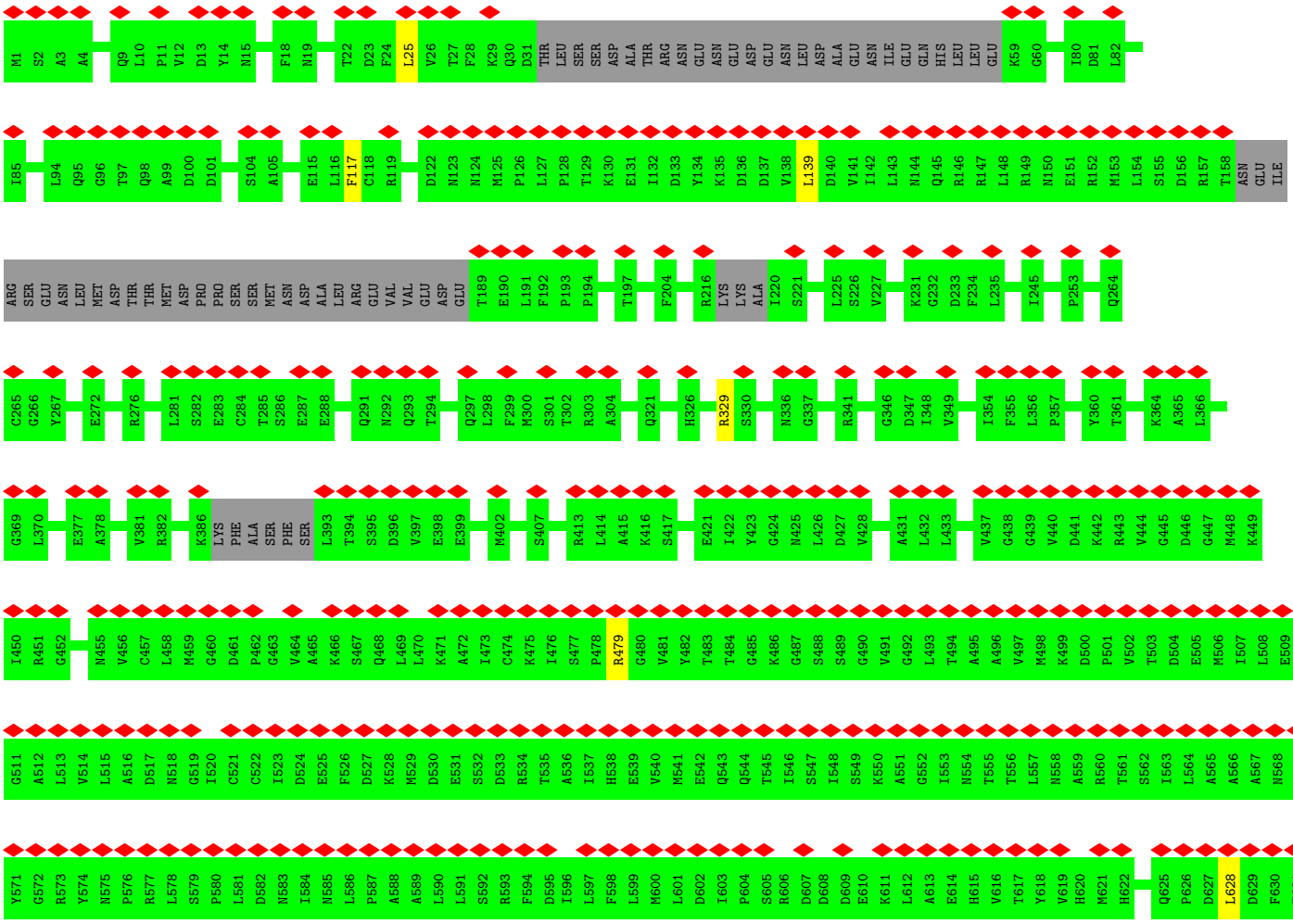
Chain 6:





- Molecule 12: DNA replication licensing factor MCM7

Chain n:



P632 V633 E634 P635 S636 K637 M638 R639 E640 Y641 I642 A643 Y644 A645 K646 T647 K648 R649 P650 V651 M652 S653 E654 A655 V656 N657 D658 Y659 V660 V661 Q662 A663 Y664 I665 R666 L667 R668 Q669 D670 S671 K672 R673 E674 M675 D676 S677 K678 F679 S680 F681 G682 Q683 A684 T685 P686 R687 T688 L689 L690 G691

I692 I693 R694 L695 S696 Q697 A698 L699 A700 K701 D706 M707 V708 D709 I710 D711 D712 V713 E714 E715 A716 L717 R718 K724 E725 S726 L727 Y728 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 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

- Molecule 12: DNA replication licensing factor MCM7

Chain 7: 64% 78% 22%

M1 S2 A3 A4 L5 P6 S7 I8 Q9 L10 P11 V12 D13 Y14 N15 N16 L17 F18 N19 E20 T21 T22 D23 F24 L25 V26 T27 F28 K29 Q30 D31 THR LEU SER SER ASP ALA THR ARG ASN GLU ASN GLU ASP GLU ASN LEU ASP ALA GLU ASN ILE GLU GLN HIS LEU LEU GLU K59 G60

P61 K62 Y63 M64 A65 R73 E74 L75 V78 I79 I80 D81 L82 Q89 N90 E91 K92 F93 L94 Q95 G96 T97 Q98 A99 D100 D101 L102 V103 S104 A105 I106 N111 H112 F113 T114 E115 L116 F117 C118 R119 A120 I121 D122 N123 N124 M125 P126 L127 P128 T129 K130 E131 I132 D133 Y134 K135

D136 D137 V138 L139 D140 V141 I142 L143 N144 Q145 R146 R147 L148 R149 N150 E151 R152 M153 L154 S155 D156 R157 T158 ASN GLU ILE ARG SER GLU ASN LEU MET ASP THR THR MET ASP PRO PRO SER SER MET ASN ASP ALA LEU ARG GLU VAL VAL GLU ASP GLU T189 E190 L191 F192 P193 P194 N195

L196 T197 R198 R199 Y200 F201 L202 Y203 F204 K205 P206 L207 S208 Y215 R216 LYS LYS ALA I220 P224 L225 S226 V227 R228 L235 I244 I245 V257 Y260 D263 Q264 C265 G266 Y267 E268 V269 F270 Q271 E272 V273 N274 S275 R276 T277 F278 T279 P280 L281 S282 E283 C284 T285 S286

E287 E288 C289 S290 Q291 N292 Q293 T294 K295 G296 Q297 L298 F299 R303 A309 F310 I315 Q316 E317 L318 S319 Q320 Q321 V324 G325 H326 I327 P328 R329 H334 V335 N336 G337 V340 R341 S342 L343 S344 P345 G346 D347 P357 A358 P359 Y360 T361 G362 F363 K364 A365 L366 K367 A368

G369 L370 L371 T372 E373 E377 A378 Q379 K386 LYS PHE ALA SER PHE SER L393 T394 S395 D396 V397 E398 E399 R400 V401 M402 E403 L404 I405 T406 S407 G408 D409 V410 Y411 N412 R413 L414 A415 K416 S417 I418 A419 P420 E421 I422 Y423 G424 N425 L426 D427 V428 K429 K430 A431 L432 L433 L434 L435

L436 V437 G438 G439 V440 D441 K442 R443 V444 G445 D446 G447 M448 K449 I450 R451 G452 D453 I454 M455 V456 C457 L458 M459 G460 D461 P462 G463 V464 A465 K466 S467 Q468 L469 L470 K471 A472 I473 C474 K475 I476 S477 P478 R479 G480 V481 Y482 T483 T484 G485 K486 G487 S488 S489 G490 V491 G492 L493 T494 A495

A496 V497 M498 K499 D500 P501 V502 T503 D504 E505 M506 I507 L508 E509 G510 G511 A512 L513 V514 L515 A516 D517 N518 G519 I520 C521 C522 I523 D524 E525 F526 D527 K528 M529 D530 E531 S532 D533 K534 T535 A536 I537 H538 E539 V540 M541 E542 Q543 Q544 T545 I546 S547 I548 S549 K550 A551 G552 I553 N554 T555

N558 A559 R560 T561 S562 I563 L564 A565 A566 A567 N568 P569 L570 Y571 G572 R573 Y574 N575 P576 R577 L578 S579 P580 L581 D582 N583 I584 N585 L586 P587 A588 A589 L590 L591 S592 R593 F594 D595 I596 L597 F598 L599 M600 L601 D602 I603 P604 S605 R606 D607 D608 D609 E610 K611 L612 A613 E614 H615 V616

T617 Y618 V619 H620 M621 H622 N623 K624 Q625 P626 D627 L628 D629 F630 T631 P632 V633 E634 P635 S636 K637 M638 R639 E640 Y641 I642 A643 Y644 A645 K646 T647 K648 R649 P650 V651 M652 S653 E654 A655 V656 N657 D658 Y659 V660 V661 Q662 A663 Y664 I665 R666 L667 R668 Q669 D670 S671 K672 R673 E674 M675 D676

S677 K678 F679 S680 F681 G682 Q683 A684 T685 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 S723 K724 E725 S726 L727 Y728 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 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, Not provided	
Number of particles used	53853	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 ($e^-/Å^2$)	50	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	0.087	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0246	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	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: 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	E	0.41	0/3501	0.60	3/4741 (0.1%)
1	F	0.40	0/3558	0.61	3/4817 (0.1%)
1	G	0.40	0/3500	0.62	3/4738 (0.1%)
2	A	0.42	0/1718	0.66	2/2314 (0.1%)
2	a	0.43	0/1718	0.66	2/2314 (0.1%)
3	B	0.46	1/1545 (0.1%)	0.65	0/2092
3	b	0.46	1/1545 (0.1%)	0.65	0/2092
4	C	0.47	0/1320	0.63	1/1784 (0.1%)
4	c	0.47	0/1320	0.63	1/1784 (0.1%)
5	D	0.43	0/1956	0.58	0/2638
5	d	0.43	0/1956	0.58	0/2638
6	H	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	h	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
7	2	0.45	0/5051	0.64	1/6821 (0.0%)
7	i	0.45	0/5051	0.64	1/6821 (0.0%)
8	3	0.44	0/4739	0.78	3/6425 (0.0%)
8	j	0.44	0/4739	0.78	3/6425 (0.0%)
9	4	0.37	0/5479	0.62	2/7392 (0.0%)
9	k	0.37	0/5479	0.61	2/7392 (0.0%)
10	5	0.47	0/4750	0.69	4/6412 (0.1%)
10	l	0.47	0/4750	0.69	4/6412 (0.1%)
11	6	0.43	0/4789	0.65	3/6466 (0.0%)
11	m	0.43	0/4789	0.65	3/6466 (0.0%)
12	7	0.37	0/5299	0.61	3/7160 (0.0%)
12	n	0.37	0/5299	0.61	3/7160 (0.0%)
All	All	0.43	4/92977 (0.0%)	0.65	57/125650 (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	E	0	1
1	F	0	1
1	G	0	1
8	3	0	1
8	j	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	478	TRP	CB-CG	-6.12	1.39	1.50
6	H	478	TRP	CB-CG	-6.07	1.39	1.50
3	B	11	PHE	C-N	-5.28	1.22	1.34
3	b	11	PHE	C-N	-5.25	1.22	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	17	PRO	CA-C-O	-29.18	50.16	120.20
8	3	17	PRO	CA-C-O	-29.18	50.17	120.20
8	3	17	PRO	CA-C-N	15.27	150.80	117.20
8	j	17	PRO	CA-C-N	15.23	150.72	117.20
1	G	766	PHE	C-N-CD	-13.93	89.95	120.60
8	j	17	PRO	O-C-N	-13.06	101.80	122.70
8	3	17	PRO	O-C-N	-13.01	101.88	122.70
1	F	766	PHE	C-N-CD	-10.80	96.84	120.60
1	E	766	PHE	C-N-CD	-10.31	97.92	120.60
1	G	766	PHE	C-N-CA	8.47	157.59	122.00
1	F	766	PHE	C-N-CA	8.29	156.84	122.00
1	E	766	PHE	C-N-CA	8.09	155.96	122.00
10	5	79	LEU	CA-CB-CG	7.61	132.81	115.30
10	l	79	LEU	CA-CB-CG	7.61	132.80	115.30
12	7	628	LEU	CA-CB-CG	7.45	132.44	115.30
12	7	139	LEU	CA-CB-CG	7.44	132.42	115.30
12	n	139	LEU	CA-CB-CG	7.43	132.40	115.30
12	n	628	LEU	CA-CB-CG	7.42	132.37	115.30
11	m	440	LEU	CA-CB-CG	7.40	132.33	115.30
11	6	440	LEU	CA-CB-CG	7.40	132.31	115.30
10	l	668	LEU	CA-CB-CG	7.28	132.03	115.30
10	5	668	LEU	CA-CB-CG	7.25	131.97	115.30
9	k	727	LEU	CA-CB-CG	6.75	130.83	115.30
9	4	727	LEU	CA-CB-CG	6.74	130.80	115.30
7	i	416	ASP	CB-CG-OD1	6.19	123.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2	416	ASP	CB-CG-OD1	6.15	123.83	118.30
2	a	123	LEU	CB-CG-CD1	-6.05	100.71	111.00
2	A	123	LEU	CB-CG-CD1	-6.05	100.71	111.00
6	h	333	SER	N-CA-C	6.03	127.28	111.00
6	H	333	SER	N-CA-C	6.02	127.26	111.00
10	l	66	GLU	N-CA-C	5.93	127.02	111.00
10	5	66	GLU	N-CA-C	5.92	127.00	111.00
6	H	326	LEU	N-CA-C	-5.87	95.16	111.00
6	h	326	LEU	N-CA-C	-5.86	95.17	111.00
6	h	328	LEU	CA-CB-CG	5.83	128.71	115.30
6	H	328	LEU	CA-CB-CG	5.83	128.71	115.30
6	h	401	LEU	CA-CB-CG	5.65	128.29	115.30
11	6	382	ARG	N-CA-C	5.63	126.21	111.00
11	m	382	ARG	N-CA-C	5.63	126.21	111.00
6	H	401	LEU	CA-CB-CG	5.61	128.20	115.30
2	a	123	LEU	CA-CB-CG	5.60	128.18	115.30
2	A	123	LEU	CA-CB-CG	5.59	128.16	115.30
11	6	711	LEU	CA-CB-CG	-5.53	102.58	115.30
12	7	25	LEU	CA-CB-CG	5.51	127.97	115.30
12	n	25	LEU	CA-CB-CG	5.50	127.95	115.30
11	m	711	LEU	CA-CB-CG	-5.49	102.67	115.30
1	E	767	PRO	CA-N-CD	-5.47	103.84	111.50
6	H	165	LEU	CA-CB-CG	5.41	127.73	115.30
6	h	165	LEU	CA-CB-CG	5.37	127.66	115.30
10	5	45	ILE	N-CA-C	5.14	124.89	111.00
1	F	767	PRO	CA-N-CD	-5.14	104.31	111.50
10	l	45	ILE	N-CA-C	5.13	124.84	111.00
9	4	425	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	767	PRO	CA-N-CD	-5.06	104.42	111.50
9	k	425	ASP	CB-CG-OD2	5.03	122.82	118.30
4	c	165	PHE	N-CA-C	5.02	124.56	111.00
4	C	165	PHE	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	3	17	PRO	Mainchain
1	E	766	PHE	Peptide
1	F	766	PHE	Peptide
1	G	766	PHE	Peptide
8	j	17	PRO	Mainchain

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	E	419/927 (45%)	407 (97%)	11 (3%)	1 (0%)	47	81
1	F	428/927 (46%)	415 (97%)	12 (3%)	1 (0%)	47	81
1	G	417/927 (45%)	407 (98%)	9 (2%)	1 (0%)	47	81
2	A	206/208 (99%)	179 (87%)	26 (13%)	1 (0%)	29	69
2	a	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	69
3	B	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	b	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
4	C	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
4	c	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
5	D	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	d	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
6	H	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	25	66
6	h	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	25	66
7	2	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
7	i	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
8	3	584/971 (60%)	506 (87%)	77 (13%)	1 (0%)	47	81
8	j	584/971 (60%)	506 (87%)	76 (13%)	2 (0%)	41	76
9	4	668/933 (72%)	579 (87%)	89 (13%)	0	100	100
9	k	668/933 (72%)	578 (86%)	90 (14%)	0	100	100
10	5	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	47	81
10	l	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	6	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	47	81
11	m	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	47	81
12	7	653/845 (77%)	556 (85%)	97 (15%)	0	100	100
12	n	653/845 (77%)	554 (85%)	99 (15%)	0	100	100
All	All	11318/16717 (68%)	9873 (87%)	1427 (13%)	18 (0%)	50	81

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	h	334	LEU
6	H	334	LEU
1	G	767	PRO
6	h	332	SER
10	l	147	PRO
11	m	305	TYR
6	H	332	SER
10	5	147	PRO
11	6	305	TYR
1	E	767	PRO
2	a	30	PRO
2	A	30	PRO
8	j	311	SER
8	j	669	PRO
8	3	669	PRO
1	F	767	PRO
6	h	146	GLY
6	H	146	GLY

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	E	377/825 (46%)	377 (100%)	0	100	100
1	F	384/825 (46%)	384 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	377/825 (46%)	377 (100%)	0	100	100
2	A	193/193 (100%)	193 (100%)	0	100	100
2	a	193/193 (100%)	193 (100%)	0	100	100
3	B	171/198 (86%)	170 (99%)	1 (1%)	86	92
3	b	171/198 (86%)	170 (99%)	1 (1%)	86	92
4	C	144/173 (83%)	142 (99%)	2 (1%)	67	80
4	c	144/173 (83%)	142 (99%)	2 (1%)	67	80
5	D	225/279 (81%)	225 (100%)	0	100	100
5	d	225/279 (81%)	225 (100%)	0	100	100
6	H	499/586 (85%)	496 (99%)	3 (1%)	86	92
6	h	499/586 (85%)	496 (99%)	3 (1%)	86	92
7	2	535/770 (70%)	529 (99%)	6 (1%)	73	84
7	i	535/770 (70%)	529 (99%)	6 (1%)	73	84
8	3	515/835 (62%)	512 (99%)	3 (1%)	86	92
8	j	515/835 (62%)	512 (99%)	3 (1%)	86	92
9	4	610/848 (72%)	604 (99%)	6 (1%)	76	86
9	k	610/848 (72%)	605 (99%)	5 (1%)	81	89
10	5	534/688 (78%)	527 (99%)	7 (1%)	69	82
10	l	534/688 (78%)	527 (99%)	7 (1%)	69	82
11	6	493/886 (56%)	487 (99%)	6 (1%)	71	83
11	m	493/886 (56%)	487 (99%)	6 (1%)	71	83
12	7	585/753 (78%)	581 (99%)	4 (1%)	84	90
12	n	585/753 (78%)	581 (99%)	4 (1%)	84	90
All	All	10146/14893 (68%)	10071 (99%)	75 (1%)	84	90

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	80	LYS
4	c	20	PHE
4	c	84	VAL
6	h	160	TYR
6	h	241	TYR
6	h	411	ARG

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Mol	Chain	Res	Type
7	i	230	ARG
7	i	324	VAL
7	i	384	ASN
7	i	439	ASN
7	i	444	PHE
7	i	476	TRP
8	j	172	THR
8	j	291	ARG
8	j	339	ARG
9	k	349	CYS
9	k	445	ARG
9	k	451	ARG
9	k	697	PRO
9	k	928	ARG
10	l	66	GLU
10	l	275	THR
10	l	295	VAL
10	l	326	PRO
10	l	486	ARG
10	l	501	THR
10	l	675	ARG
11	m	296	ARG
11	m	350	ARG
11	m	381	LEU
11	m	540	HIS
11	m	581	LYS
11	m	675	ARG
12	n	117	PHE
12	n	329	ARG
12	n	479	ARG
12	n	718	ARG
3	B	80	LYS
4	C	20	PHE
4	C	84	VAL
6	H	160	TYR
6	H	241	TYR
6	H	411	ARG
7	2	230	ARG
7	2	324	VAL
7	2	384	ASN
7	2	439	ASN
7	2	444	PHE

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Mol	Chain	Res	Type
7	2	476	TRP
8	3	172	THR
8	3	291	ARG
8	3	339	ARG
9	4	349	CYS
9	4	445	ARG
9	4	451	ARG
9	4	468	LYS
9	4	697	PRO
9	4	928	ARG
10	5	66	GLU
10	5	275	THR
10	5	295	VAL
10	5	326	PRO
10	5	486	ARG
10	5	501	THR
10	5	675	ARG
11	6	296	ARG
11	6	350	ARG
11	6	381	LEU
11	6	540	HIS
11	6	581	LYS
11	6	675	ARG
12	7	117	PHE
12	7	329	ARG
12	7	479	ARG
12	7	718	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	527	HIS
1	E	573	GLN
1	F	548	GLN
1	F	678	ASN
1	F	790	ASN
1	G	622	ASN
1	G	790	ASN
2	a	28	ASN
2	a	39	ASN
2	a	90	GLN
2	a	182	ASN

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Mol	Chain	Res	Type
3	b	103	GLN
4	c	21	GLN
4	c	41	ASN
4	c	130	GLN
4	c	133	GLN
4	c	181	HIS
6	h	18	ASN
6	h	22	HIS
6	h	26	GLN
6	h	52	GLN
6	h	55	GLN
6	h	70	HIS
6	h	155	GLN
6	h	289	ASN
6	h	331	HIS
6	h	374	GLN
6	h	395	ASN
6	h	468	ASN
6	h	497	GLN
6	h	563	GLN
6	h	604	ASN
7	i	202	ASN
7	i	238	ASN
7	i	245	ASN
7	i	333	GLN
7	i	340	ASN
7	i	433	ASN
7	i	526	ASN
7	i	551	GLN
7	i	779	HIS
7	i	780	GLN
7	i	809	HIS
8	j	51	ASN
8	j	52	ASN
8	j	57	ASN
8	j	210	HIS
8	j	312	ASN
8	j	330	HIS
8	j	351	ASN
8	j	503	HIS
8	j	554	ASN
8	j	677	ASN

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Mol	Chain	Res	Type
9	k	184	ASN
9	k	196	ASN
9	k	274	GLN
9	k	413	HIS
9	k	858	GLN
9	k	876	GLN
10	l	53	ASN
10	l	67	HIS
10	l	185	ASN
10	l	203	ASN
10	l	254	GLN
10	l	539	ASN
10	l	561	ASN
10	l	574	ASN
10	l	617	GLN
10	l	652	GLN
11	m	182	GLN
11	m	514	ASN
11	m	570	ASN
11	m	750	GLN
11	m	814	ASN
11	m	833	GLN
12	n	87	GLN
12	n	150	ASN
12	n	292	ASN
12	n	293	GLN
12	n	316	GLN
12	n	326	HIS
12	n	379	GLN
12	n	383	GLN
12	n	468	GLN
12	n	657	ASN
12	n	683	GLN
2	A	28	ASN
2	A	39	ASN
2	A	90	GLN
2	A	182	ASN
3	B	103	GLN
4	C	21	GLN
4	C	41	ASN
4	C	133	GLN
4	C	181	HIS

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Mol	Chain	Res	Type
6	H	13	ASN
6	H	18	ASN
6	H	22	HIS
6	H	26	GLN
6	H	52	GLN
6	H	55	GLN
6	H	70	HIS
6	H	155	GLN
6	H	289	ASN
6	H	331	HIS
6	H	374	GLN
6	H	395	ASN
6	H	402	GLN
6	H	468	ASN
6	H	497	GLN
6	H	563	GLN
6	H	604	ASN
7	2	202	ASN
7	2	238	ASN
7	2	245	ASN
7	2	333	GLN
7	2	340	ASN
7	2	433	ASN
7	2	526	ASN
7	2	551	GLN
7	2	779	HIS
7	2	780	GLN
7	2	809	HIS
8	3	51	ASN
8	3	52	ASN
8	3	57	ASN
8	3	210	HIS
8	3	312	ASN
8	3	330	HIS
8	3	351	ASN
8	3	554	ASN
8	3	677	ASN
9	4	184	ASN
9	4	196	ASN
9	4	274	GLN
9	4	413	HIS
9	4	858	GLN

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Mol	Chain	Res	Type
9	4	876	GLN
10	5	53	ASN
10	5	67	HIS
10	5	203	ASN
10	5	254	GLN
10	5	539	ASN
10	5	561	ASN
10	5	574	ASN
10	5	617	GLN
10	5	652	GLN
11	6	182	GLN
11	6	514	ASN
11	6	570	ASN
11	6	750	GLN
11	6	814	ASN
11	6	833	GLN
12	7	87	GLN
12	7	292	ASN
12	7	293	GLN
12	7	316	GLN
12	7	326	HIS
12	7	379	GLN
12	7	383	GLN
12	7	468	GLN
12	7	657	ASN
12	7	683	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)

6 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	ATP	5	801	-	26,33,33	0.87	1 (3%)	31,52,52	1.93	7 (22%)
13	ATP	j	1001	-	26,33,33	0.92	1 (3%)	31,52,52	1.90	6 (19%)
13	ATP	2	901	-	26,33,33	0.91	1 (3%)	31,52,52	1.64	5 (16%)
13	ATP	l	801	-	26,33,33	0.86	1 (3%)	31,52,52	1.93	7 (22%)
13	ATP	i	901	-	26,33,33	0.92	1 (3%)	31,52,52	1.64	5 (16%)
13	ATP	3	1001	-	26,33,33	0.91	1 (3%)	31,52,52	1.90	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
13	ATP	5	801	-	-	4/18/38/38	0/3/3/3
13	ATP	j	1001	-	-	4/18/38/38	0/3/3/3
13	ATP	2	901	-	-	6/18/38/38	0/3/3/3
13	ATP	l	801	-	-	4/18/38/38	0/3/3/3
13	ATP	i	901	-	-	6/18/38/38	0/3/3/3
13	ATP	3	1001	-	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	i	901	ATP	C5-C4	2.17	1.46	1.40
13	2	901	ATP	C5-C4	2.12	1.46	1.40
13	j	1001	ATP	C5-C4	2.12	1.46	1.40
13	3	1001	ATP	C5-C4	2.06	1.46	1.40
13	l	801	ATP	C5-C4	2.01	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	801	ATP	C5-C4	2.01	1.46	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	j	1001	ATP	PA-O3A-PB	-6.31	111.18	132.83
13	3	1001	ATP	PA-O3A-PB	-6.30	111.19	132.83
13	5	801	ATP	PA-O3A-PB	-5.28	114.70	132.83
13	l	801	ATP	PA-O3A-PB	-5.28	114.71	132.83
13	5	801	ATP	PB-O3B-PG	-5.04	115.55	132.83
13	l	801	ATP	PB-O3B-PG	-5.03	115.57	132.83
13	i	901	ATP	PA-O3A-PB	-4.66	116.85	132.83
13	2	901	ATP	PA-O3A-PB	-4.63	116.94	132.83
13	3	1001	ATP	PB-O3B-PG	-4.42	117.67	132.83
13	j	1001	ATP	PB-O3B-PG	-4.41	117.70	132.83
13	5	801	ATP	N3-C2-N1	-3.70	122.89	128.68
13	l	801	ATP	N3-C2-N1	-3.68	122.92	128.68
13	i	901	ATP	C3'-C2'-C1'	3.25	105.86	100.98
13	2	901	ATP	C3'-C2'-C1'	3.22	105.83	100.98
13	2	901	ATP	PB-O3B-PG	-3.15	122.03	132.83
13	i	901	ATP	PB-O3B-PG	-3.12	122.12	132.83
13	3	1001	ATP	N3-C2-N1	-3.12	123.80	128.68
13	j	1001	ATP	N3-C2-N1	-3.09	123.84	128.68
13	l	801	ATP	C4-C5-N7	-2.99	106.28	109.40
13	3	1001	ATP	C3'-C2'-C1'	2.96	105.43	100.98
13	j	1001	ATP	C3'-C2'-C1'	2.95	105.42	100.98
13	2	901	ATP	N3-C2-N1	-2.93	124.10	128.68
13	5	801	ATP	C4-C5-N7	-2.93	106.35	109.40
13	i	901	ATP	N3-C2-N1	-2.86	124.20	128.68
13	i	901	ATP	C4-C5-N7	-2.76	106.52	109.40
13	2	901	ATP	C4-C5-N7	-2.70	106.58	109.40
13	l	801	ATP	O3G-PG-O2G	2.27	116.29	107.64
13	5	801	ATP	O3G-PG-O2G	2.26	116.26	107.64
13	l	801	ATP	C3'-C2'-C1'	2.23	104.33	100.98
13	5	801	ATP	C3'-C2'-C1'	2.22	104.32	100.98
13	5	801	ATP	C2-N1-C6	2.21	122.54	118.75
13	l	801	ATP	C2-N1-C6	2.19	122.51	118.75
13	3	1001	ATP	C4-C5-N7	-2.18	107.12	109.40
13	j	1001	ATP	C4-C5-N7	-2.17	107.14	109.40
13	j	1001	ATP	C2'-C3'-C4'	2.14	106.79	102.64
13	3	1001	ATP	C2'-C3'-C4'	2.09	106.70	102.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	i	901	ATP	C5'-O5'-PA-O1A
13	i	901	ATP	C5'-O5'-PA-O2A
13	j	1001	ATP	C5'-O5'-PA-O2A
13	j	1001	ATP	C5'-O5'-PA-O3A
13	2	901	ATP	C5'-O5'-PA-O1A
13	2	901	ATP	C5'-O5'-PA-O2A
13	3	1001	ATP	C5'-O5'-PA-O2A
13	3	1001	ATP	C5'-O5'-PA-O3A
13	i	901	ATP	C3'-C4'-C5'-O5'
13	2	901	ATP	C3'-C4'-C5'-O5'
13	i	901	ATP	O4'-C4'-C5'-O5'
13	2	901	ATP	O4'-C4'-C5'-O5'
13	j	1001	ATP	C3'-C4'-C5'-O5'
13	3	1001	ATP	C3'-C4'-C5'-O5'
13	j	1001	ATP	O4'-C4'-C5'-O5'
13	3	1001	ATP	O4'-C4'-C5'-O5'
13	l	801	ATP	O4'-C4'-C5'-O5'
13	5	801	ATP	O4'-C4'-C5'-O5'
13	i	901	ATP	C4'-C5'-O5'-PA
13	2	901	ATP	C4'-C5'-O5'-PA
13	l	801	ATP	C5'-O5'-PA-O2A
13	5	801	ATP	C5'-O5'-PA-O2A
13	l	801	ATP	C3'-C4'-C5'-O5'
13	5	801	ATP	C3'-C4'-C5'-O5'
13	i	901	ATP	C5'-O5'-PA-O3A
13	l	801	ATP	C5'-O5'-PA-O3A
13	2	901	ATP	C5'-O5'-PA-O3A
13	5	801	ATP	C5'-O5'-PA-O3A

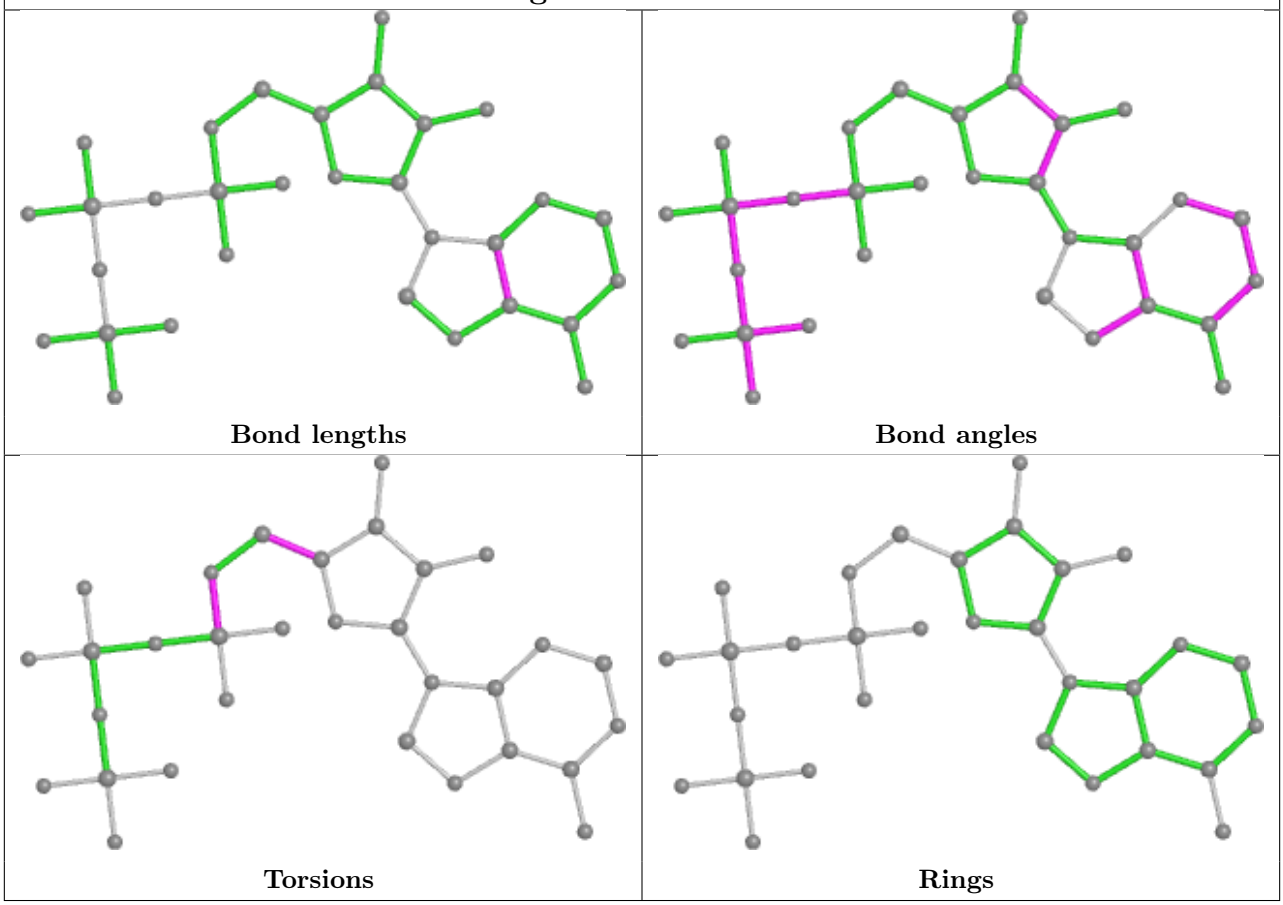
There are no ring outliers.

No monomer is involved in short contacts.

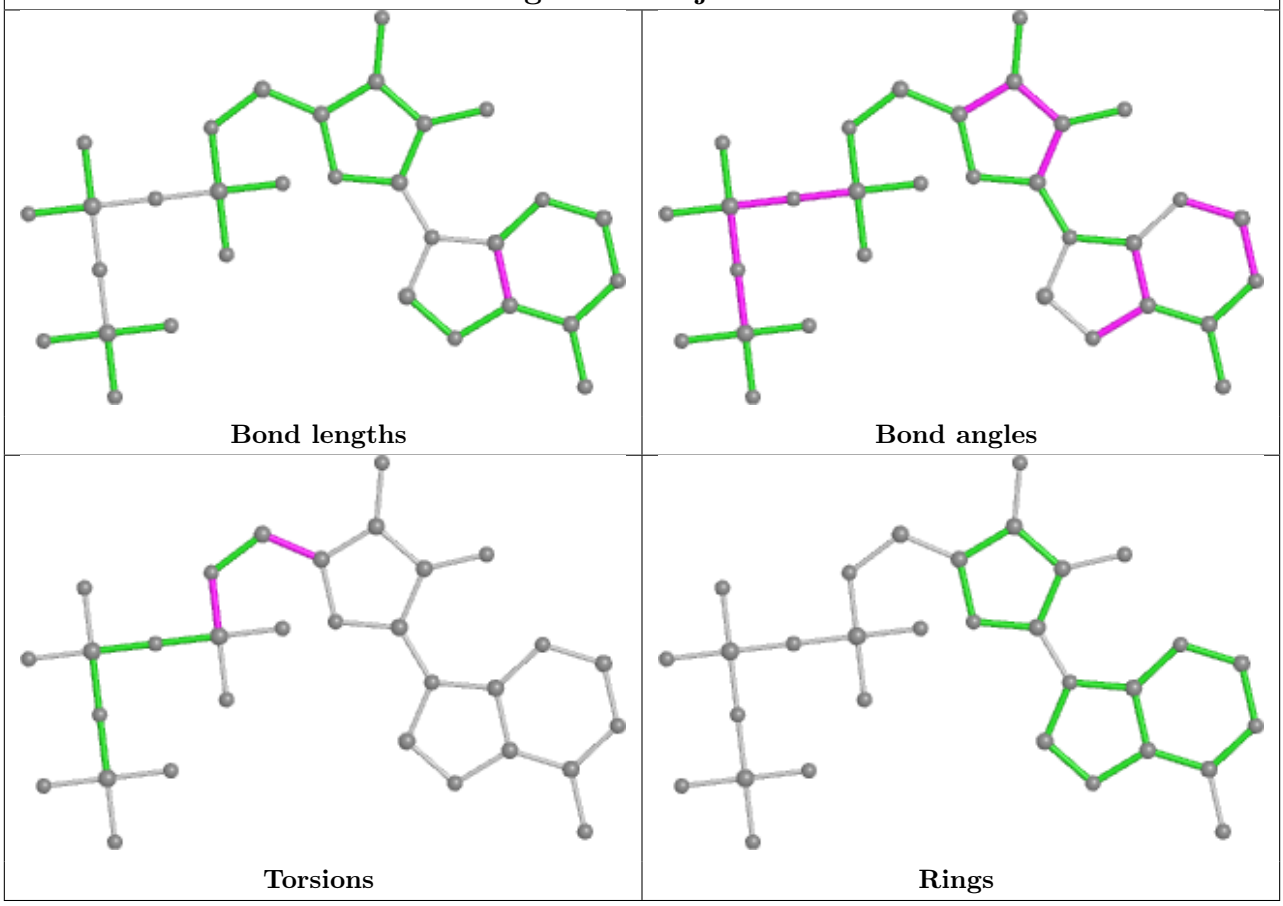
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

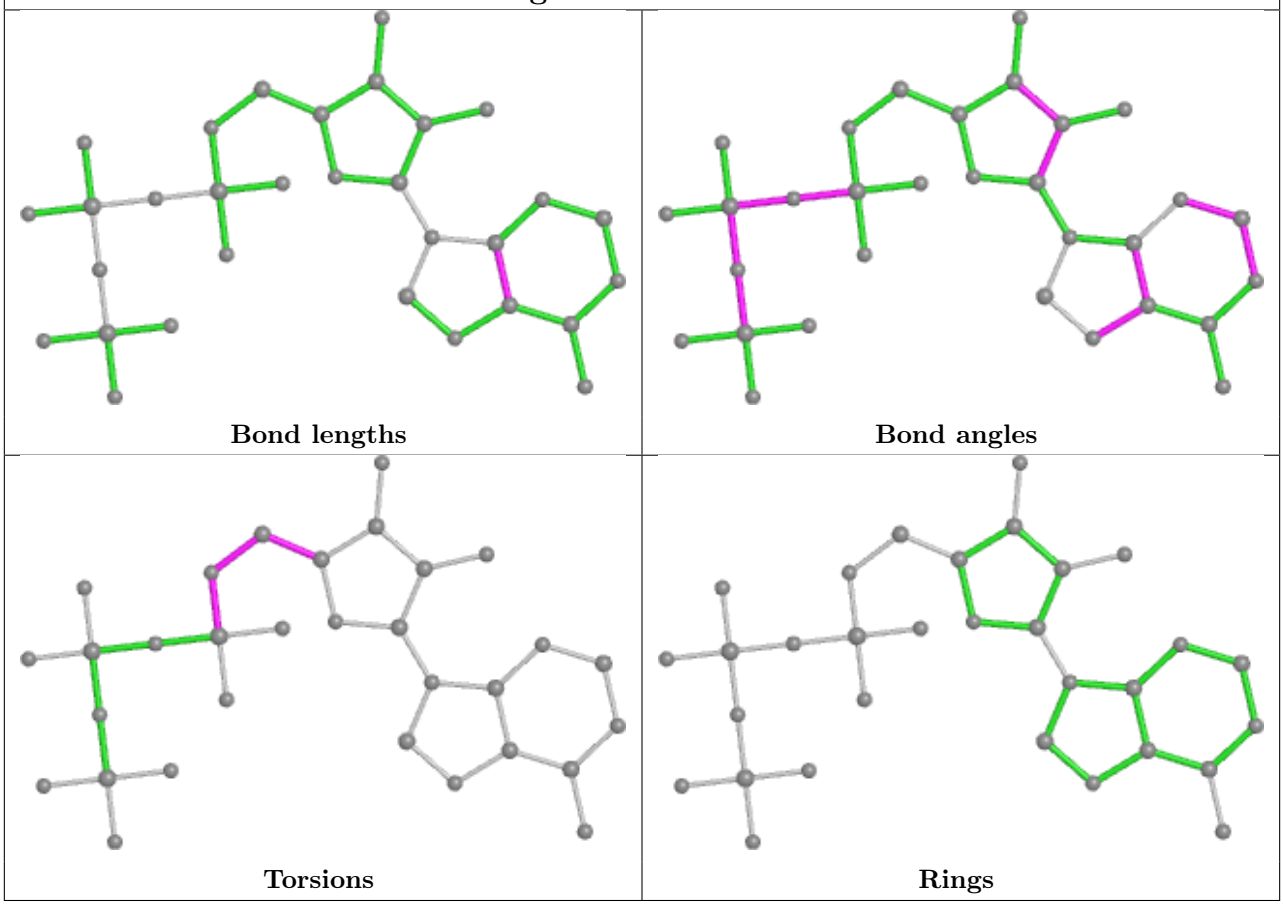
Ligand ATP 5 801



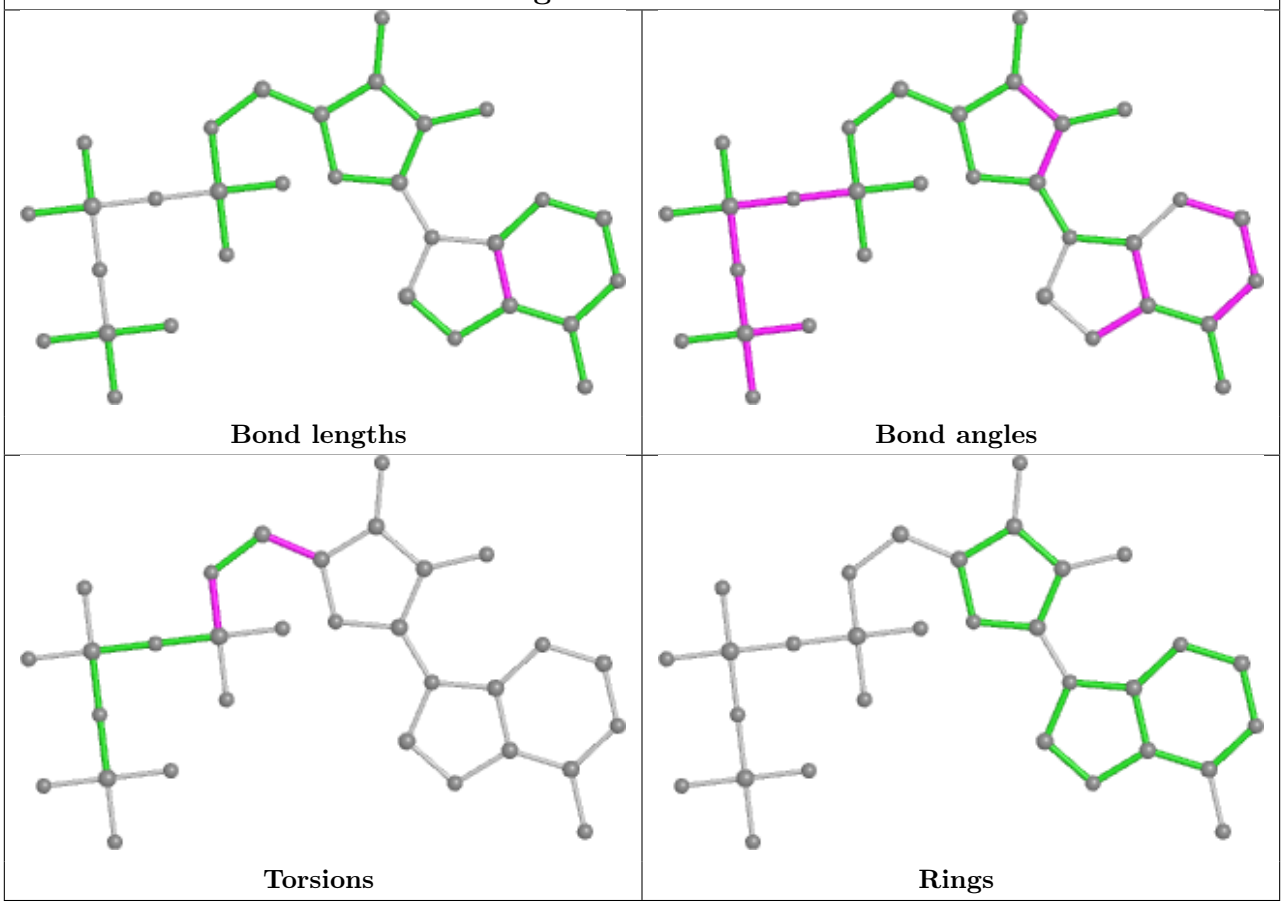
Ligand ATP j 1001



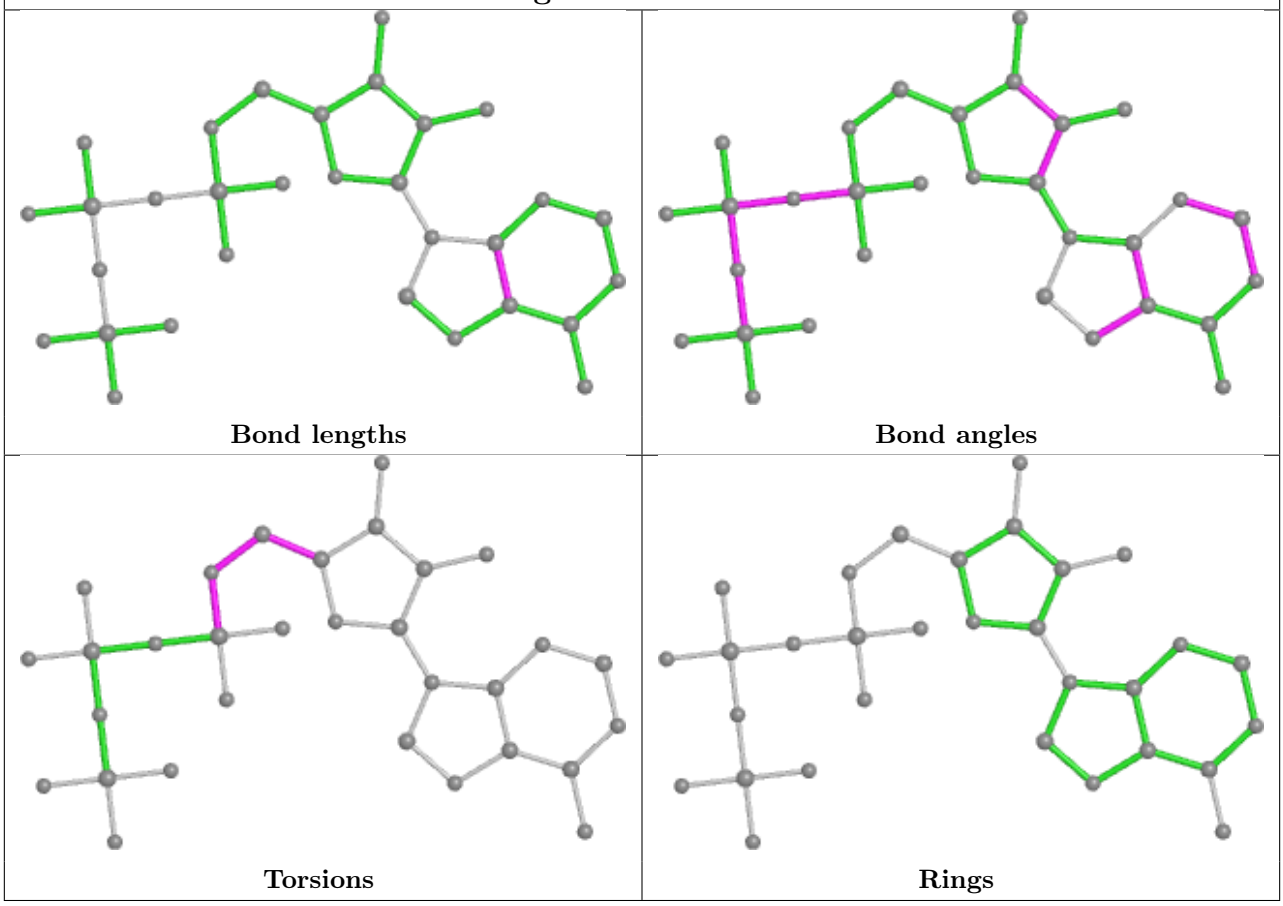
Ligand ATP 2 901

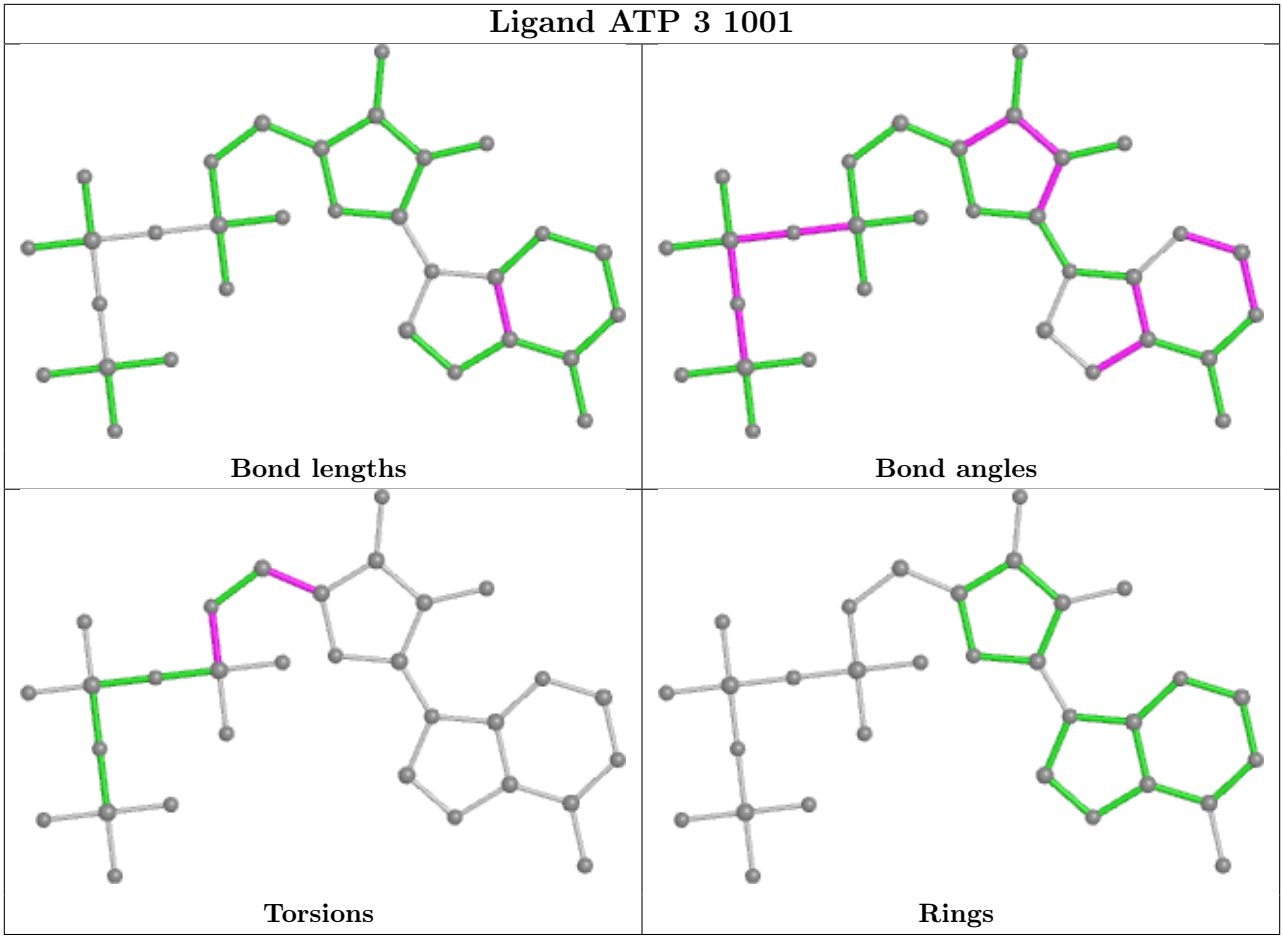


Ligand ATP l 801



Ligand ATP i 901





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
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	776:ILE	C	777:ARG	N	2.04

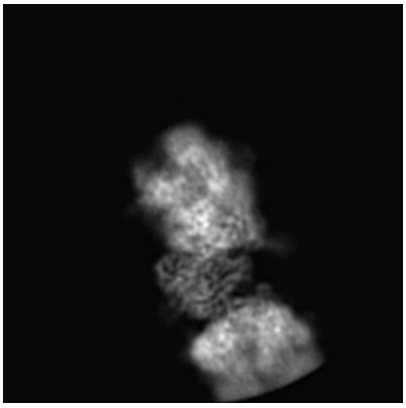
6 Map visualisation (i)

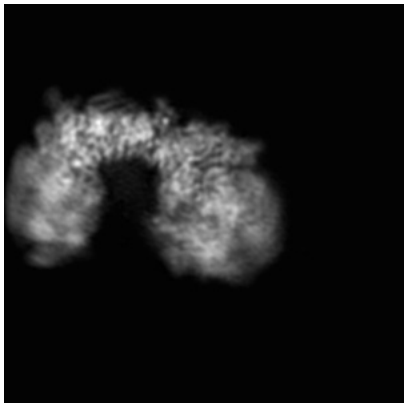
This section contains visualisations of the EMDB entry EMD-20472. These allow visual inspection of the internal detail of the map and identification of artifacts.

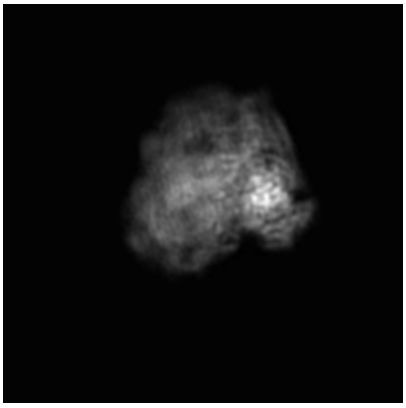
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

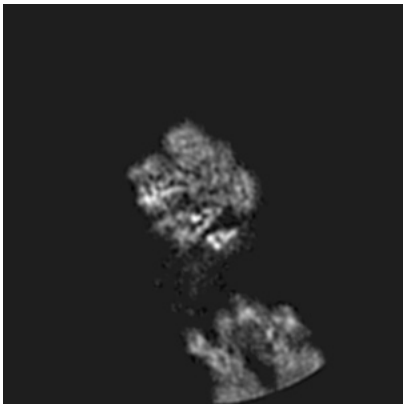

Y

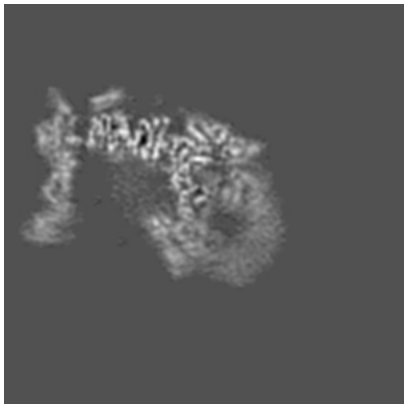

Z

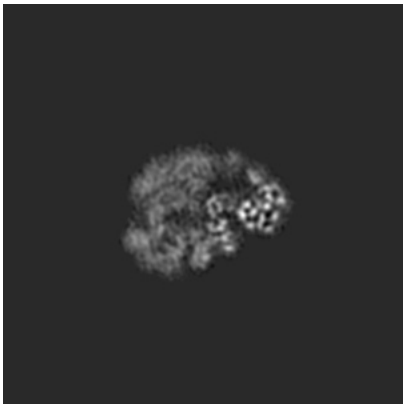
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 200

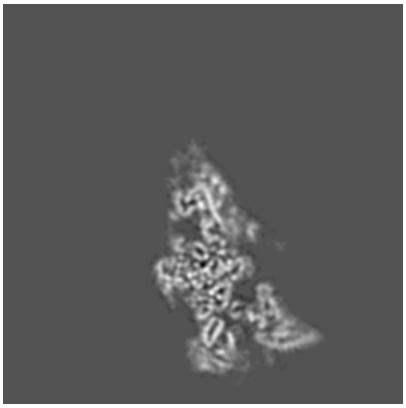

Y Index: 200


Z Index: 200

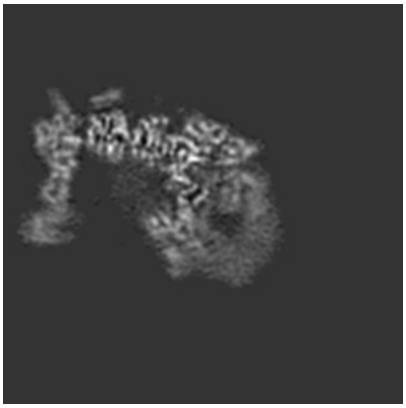
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

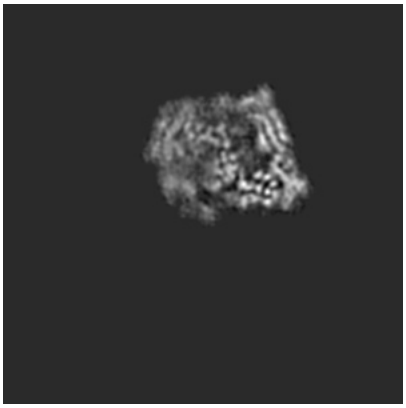
6.3.1 Primary map



X Index: 264



Y Index: 202



Z Index: 68

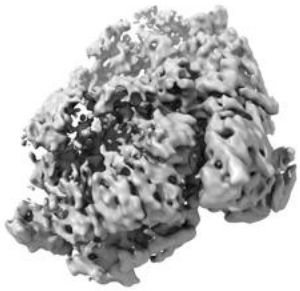
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0246. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

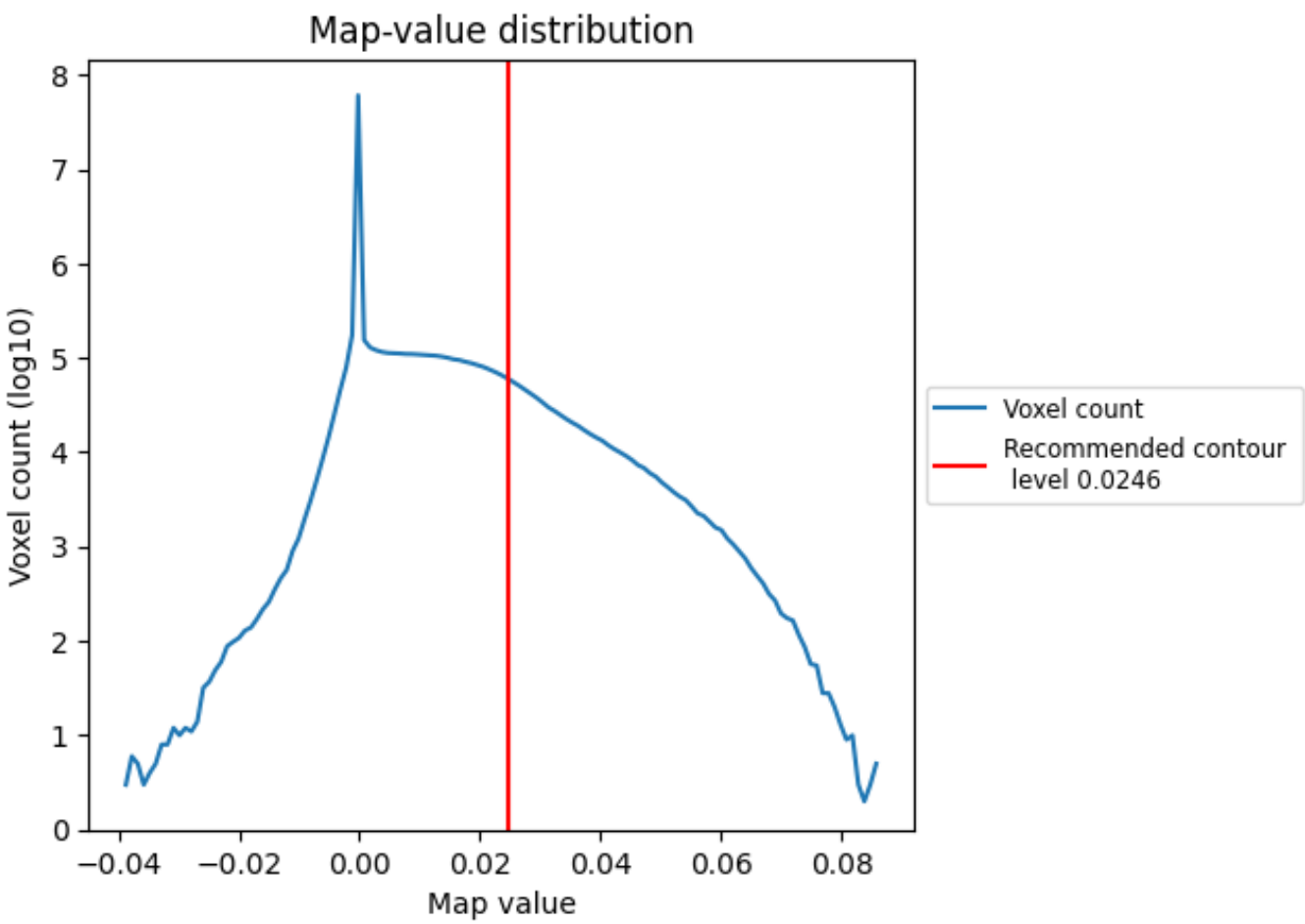
6.5 Mask visualisation (i)

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

7 Map analysis (i)

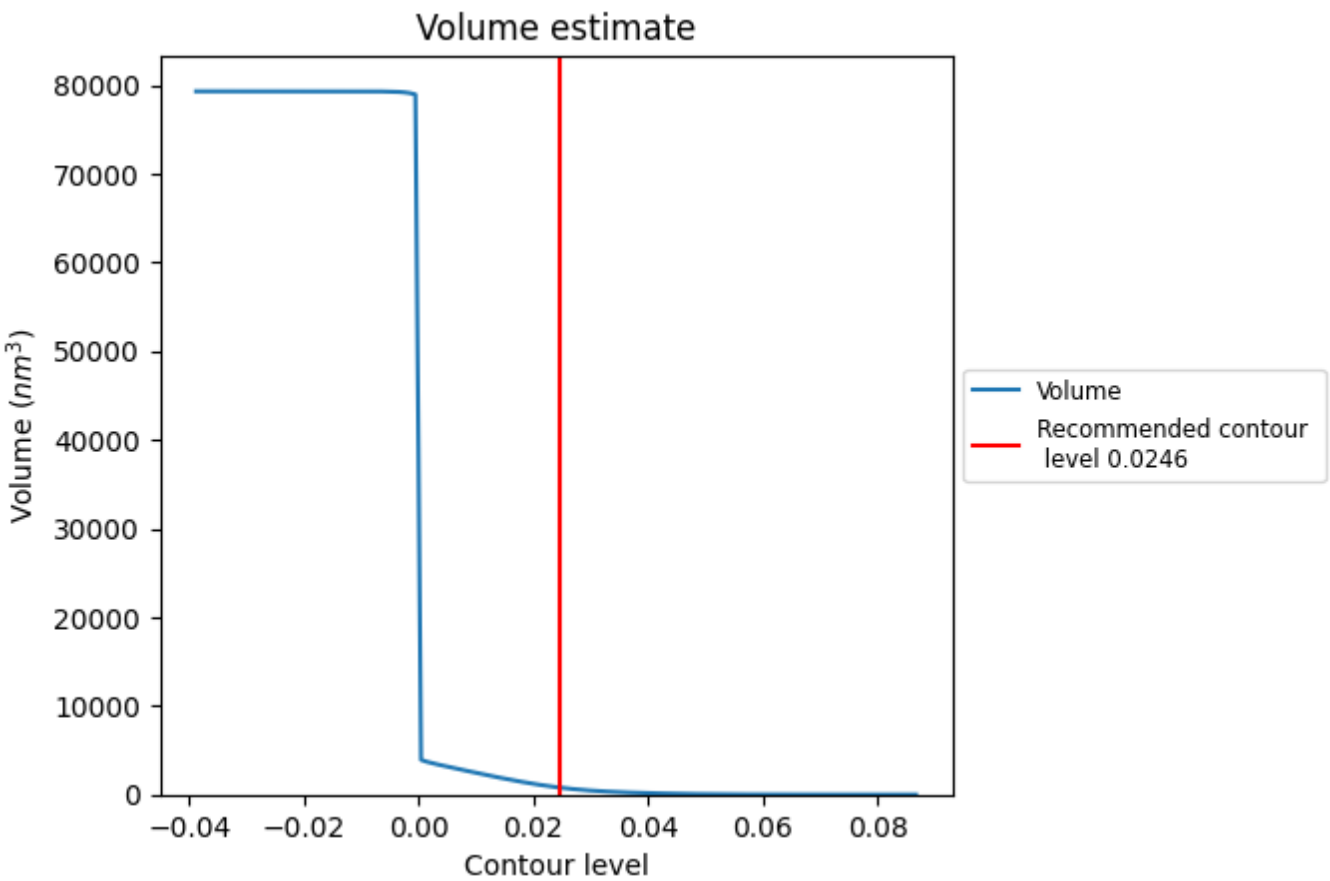
This section contains the results of statistical analysis of the map.

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.

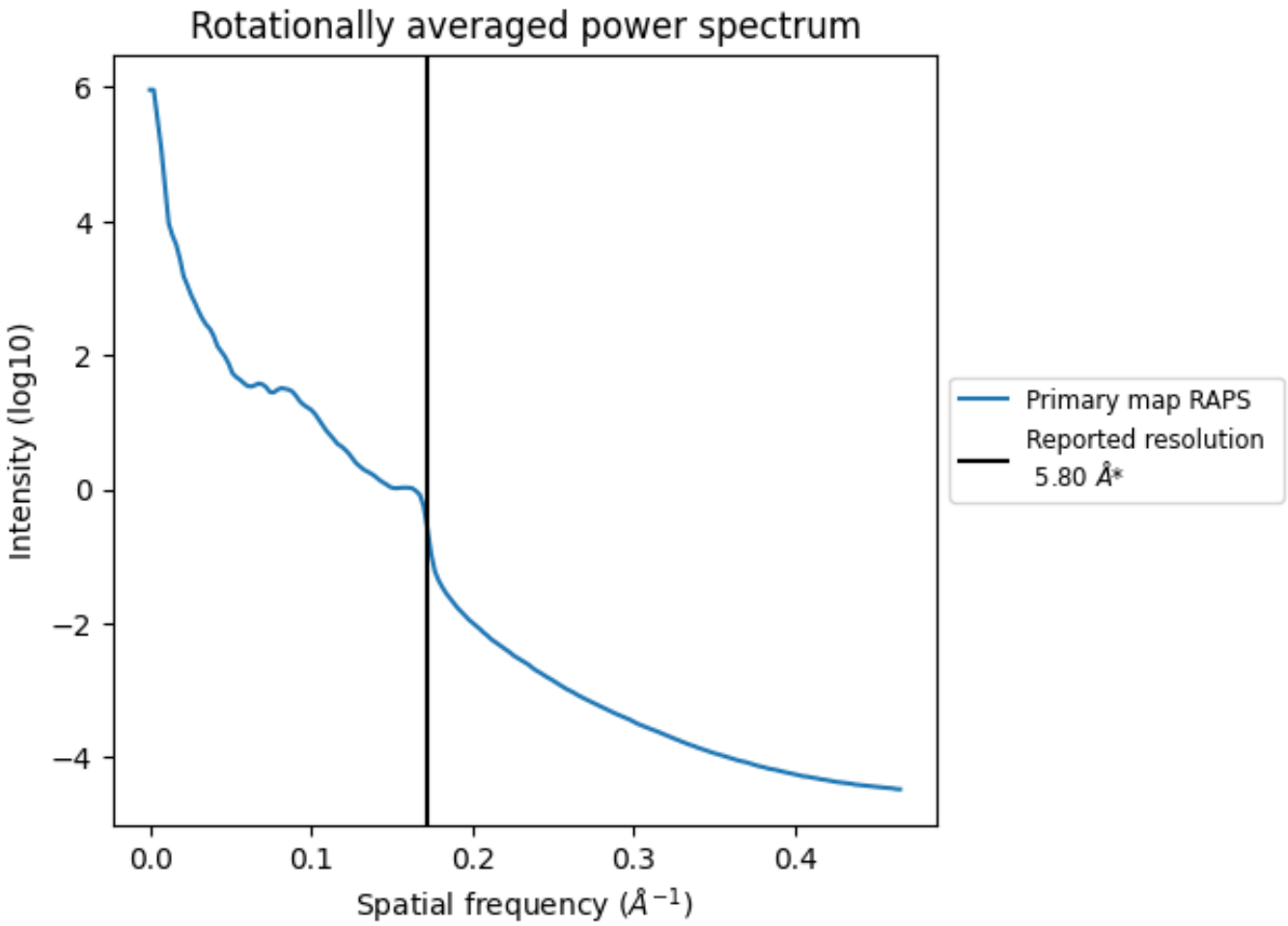
7.2 Volume estimate (i)



The volume at the recommended contour level is 790 nm^3; this corresponds to an approximate mass of 713 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 0.172 Å^{-1}

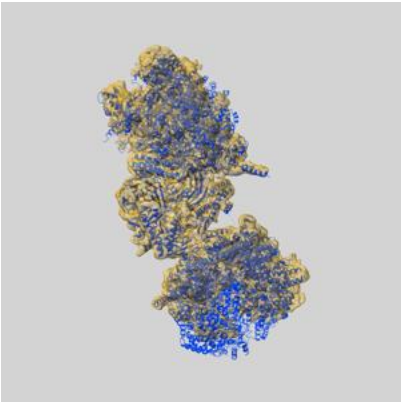
8 Fourier-Shell correlation (i)

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

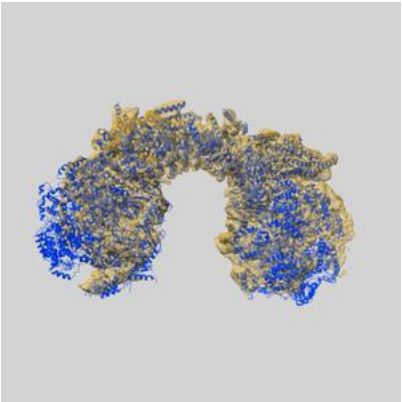
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20472 and PDB model 6PTN. Per-residue inclusion information can be found in section 3 on page 8.

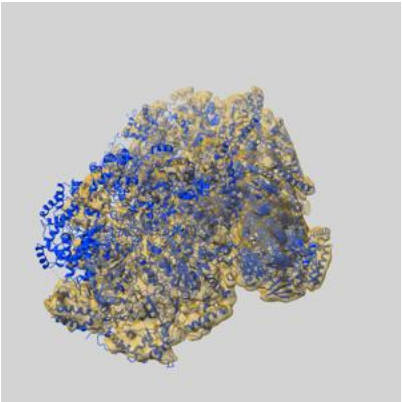
9.1 Map-model overlay (i)



X



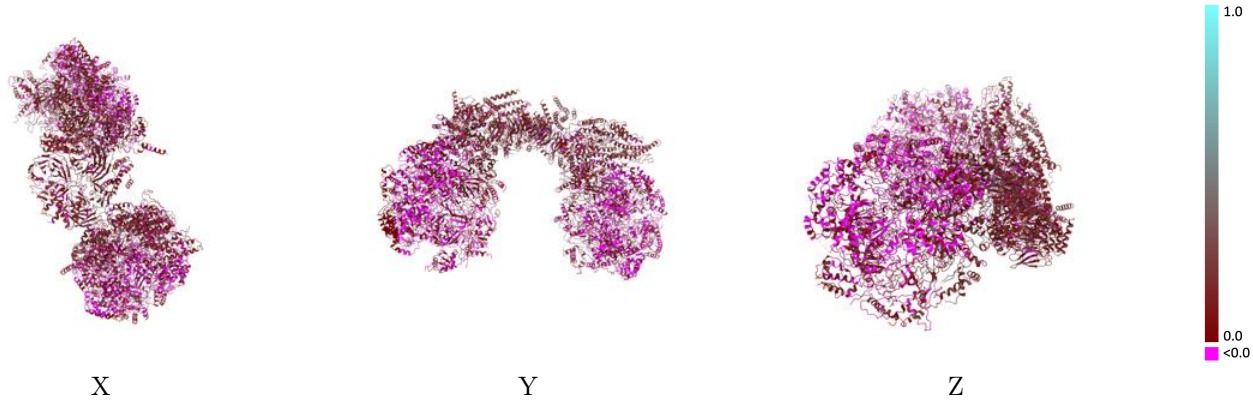
Y



Z

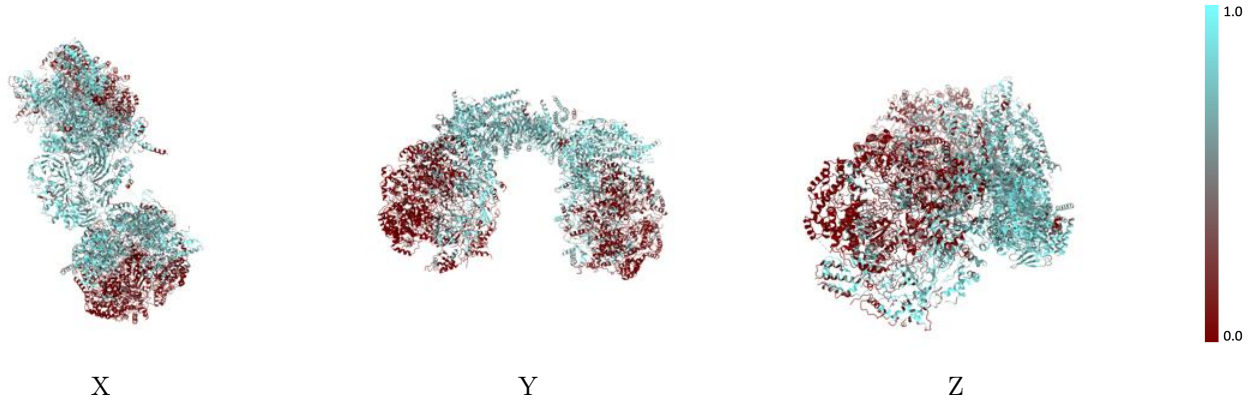
The images above show the 3D surface view of the map at the recommended contour level 0.0246 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



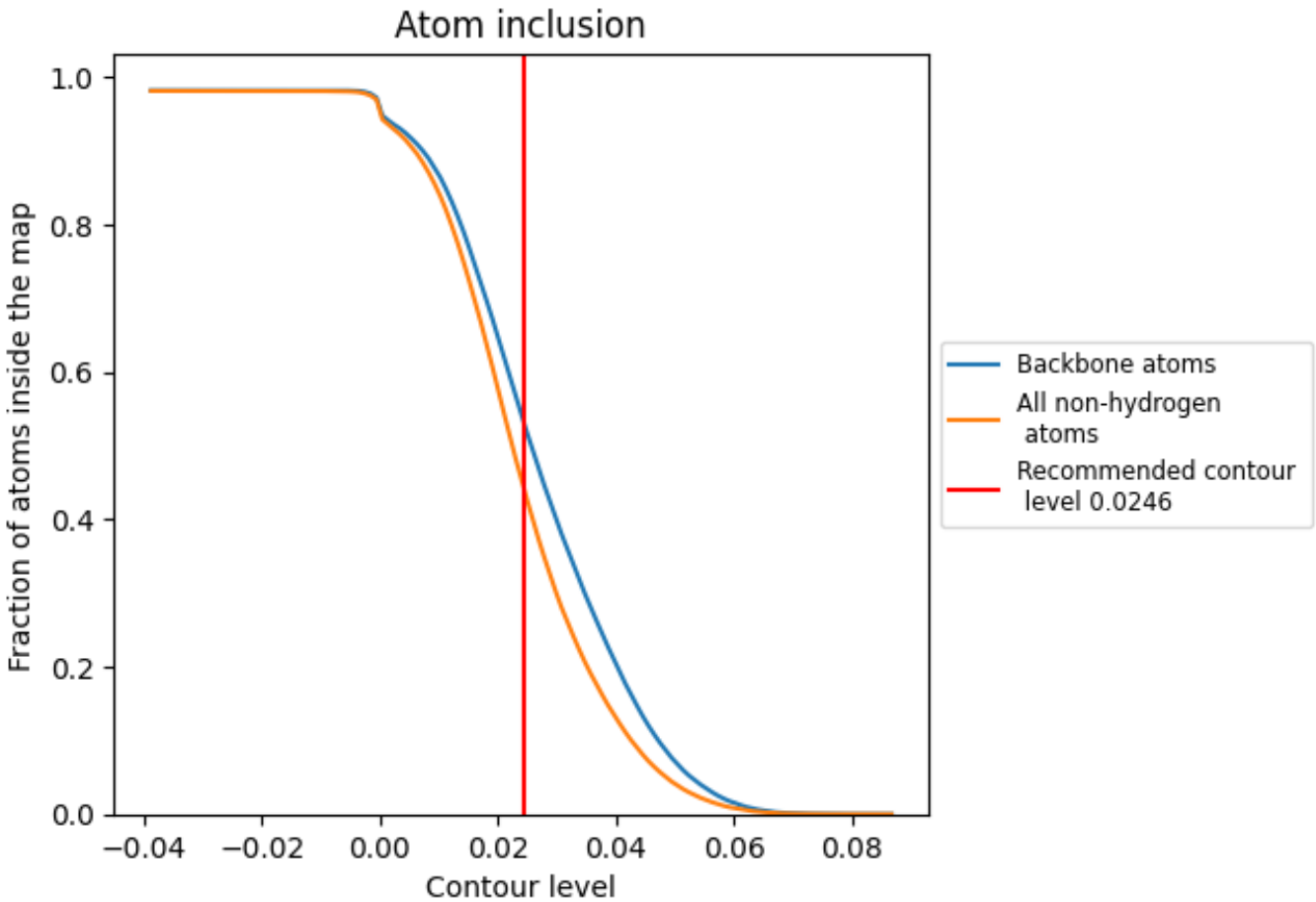
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.0246).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 44% 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 (0.0246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4365	0.0870
2	0.2415	0.0390
3	0.3322	0.0510
4	0.1458	0.0290
5	0.3517	0.0660
6	0.1943	0.0320
7	0.1583	0.0290
A	0.6825	0.1640
B	0.6729	0.1620
C	0.6837	0.1410
D	0.7086	0.1630
E	0.7115	0.1720
F	0.7071	0.1510
G	0.7166	0.1680
H	0.6803	0.1390
a	0.7450	0.1660
b	0.7483	0.1750
c	0.7364	0.1610
d	0.7483	0.1740
h	0.6771	0.1390
i	0.3084	0.0380
j	0.4638	0.0880
k	0.2588	0.0460
l	0.4063	0.0750
m	0.3485	0.0570
n	0.3288	0.0540