wwPDB EM Validation Summary Report ⓘ

Nov 27, 2023 – 08:51 PM JST

PDB ID	:	8KG9
EMDB ID	:	EMD-37215
Title	:	Yeast replisome in state III
Authors	:	Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on	:	2023-08-17
Resolution	:	4.52 Å(reported)
Based on initial model	:	6SKL

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:

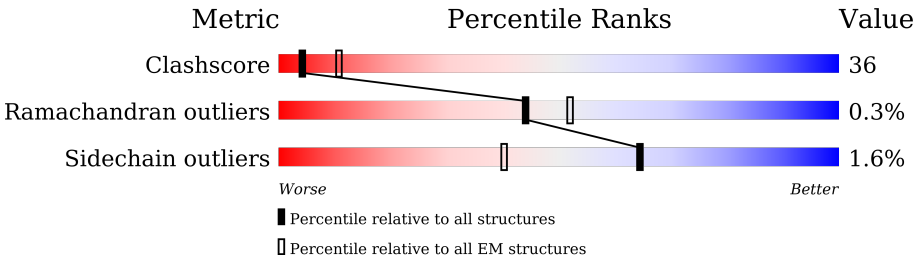
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 4.52 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	2	868	28% 49% 23%
2	3	971	23% 42% 34%
3	4	933	29% 43% 28%
4	5	775	34% 53% 13%
5	6	1017	20% 40% 38%
6	7	845	28% 46% 25%
7	A	208	34% 55% 7%
8	B	213	34% 57% 9%

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Mol	Chain	Length	Quality of chain
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	J	61	
15	M	2222	
16	N	689	

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
18	ADP	2	902	-	-	X	-
18	ADP	3	1001	-	-	X	-
20	AGS	5	803	-	-	X	-
20	AGS	7	903	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 63507 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	668	5270	3310	948	993	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	637	4948	3116	881	938	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	676	5390	3386	937	1036	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	676	5325	3347	919	1035	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	629	4955	3124	868	938	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	636	4945	3125	861	933	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	200	Total	C	N	O	S	0	0
			1633	1024	282	318	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	193	Total	C	N	O	S	0	0
			1617	1039	286	287	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	172	Total	C	N	O	S	0	0
			1387	904	223	253	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4599	2935	778	872	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	424	Total	C	N	O	S	0	0
			3404	2188	564	637	15		
12	G	422	Total	C	N	O	S	0	0
			3380	2172	557	636	15		
12	H	425	Total	C	N	O	S	0	0
			3411	2193	565	638	15		

- Molecule 13 is a DNA chain called DNA (70-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	15	Total	C	N	O	P	0	0
			307	150	42	100	15		

- Molecule 14 is a DNA chain called DNA (61-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	8	Total	C	N	O	P	0	0
			159	76	29	46	8		

- Molecule 15 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	812	Total	C	N	O	S	0	0
			6447	4162	1059	1192	34		

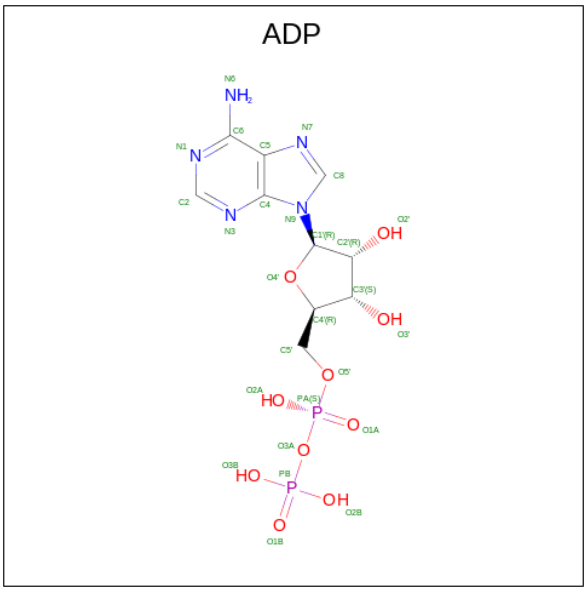
- Molecule 16 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	529	Total	C	N	O	S	0	0
			4199	2684	716	782	17		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	5	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	
17	M	2	Total	Zn	0
			2	2	

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

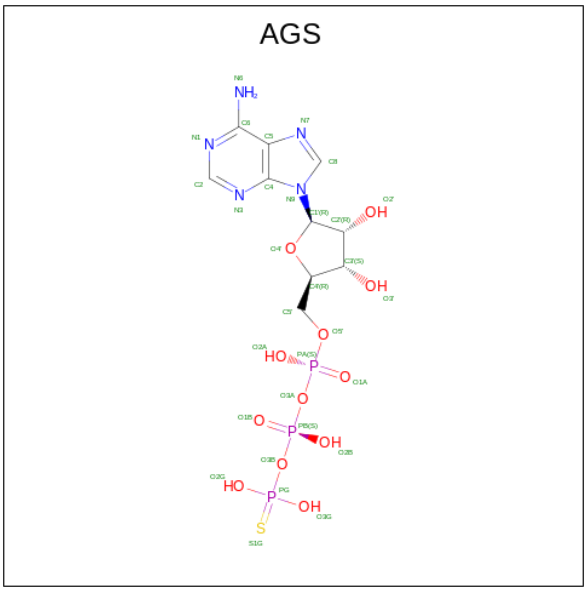


Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	2	1	Total	Mg	0
			1	1	
19	5	2	Total	Mg	0
			2	2	
19	7	1	Total	Mg	0
			1	1	

- Molecule 20 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



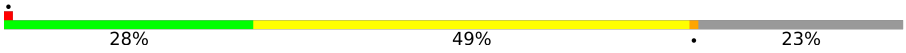
Mol	Chain	Residues	Atoms						AltConf
20	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
20	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

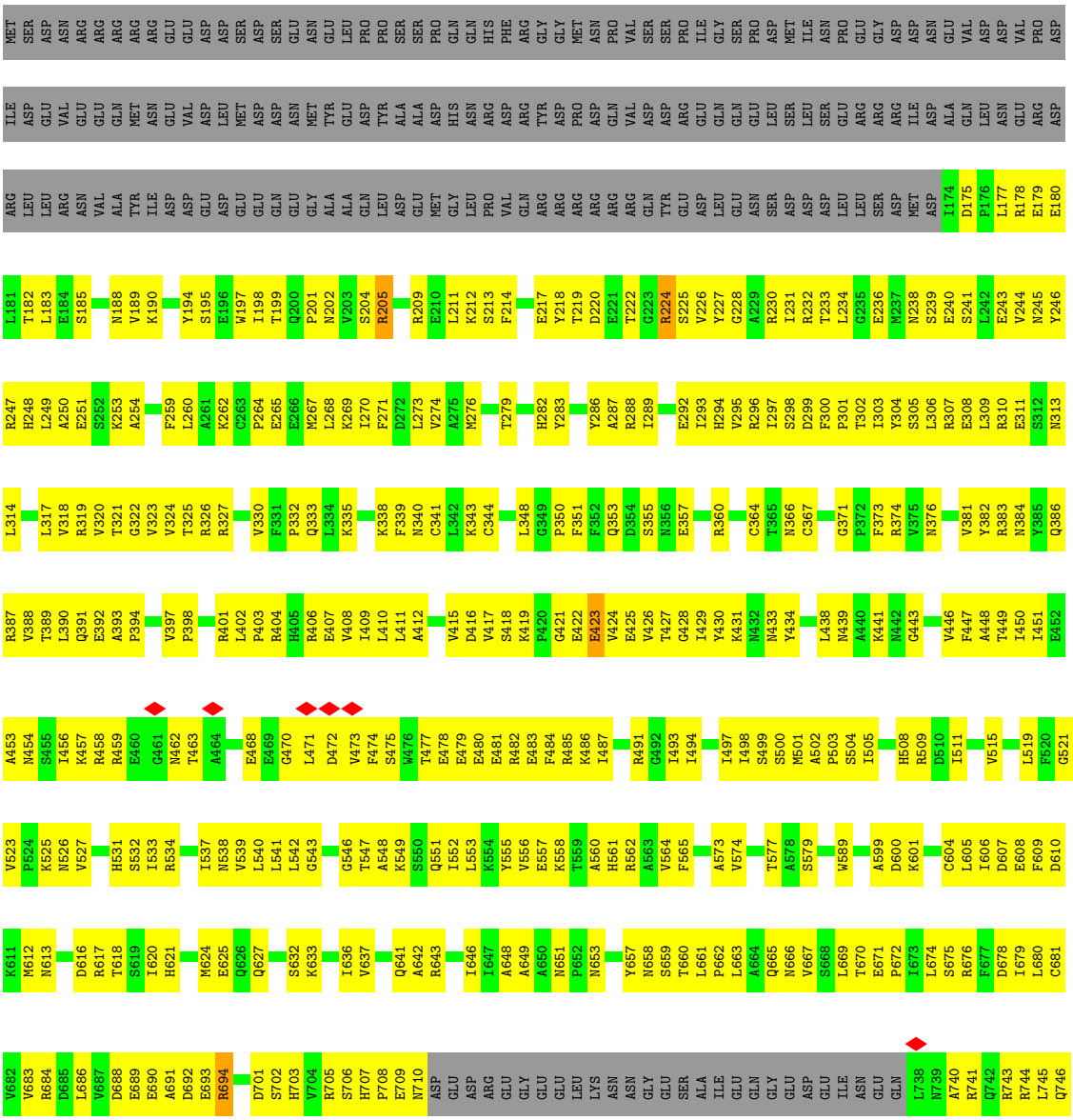
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA replication licensing factor MCM2

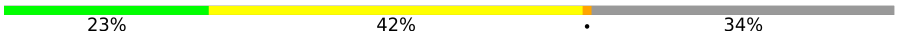
Chain 2:

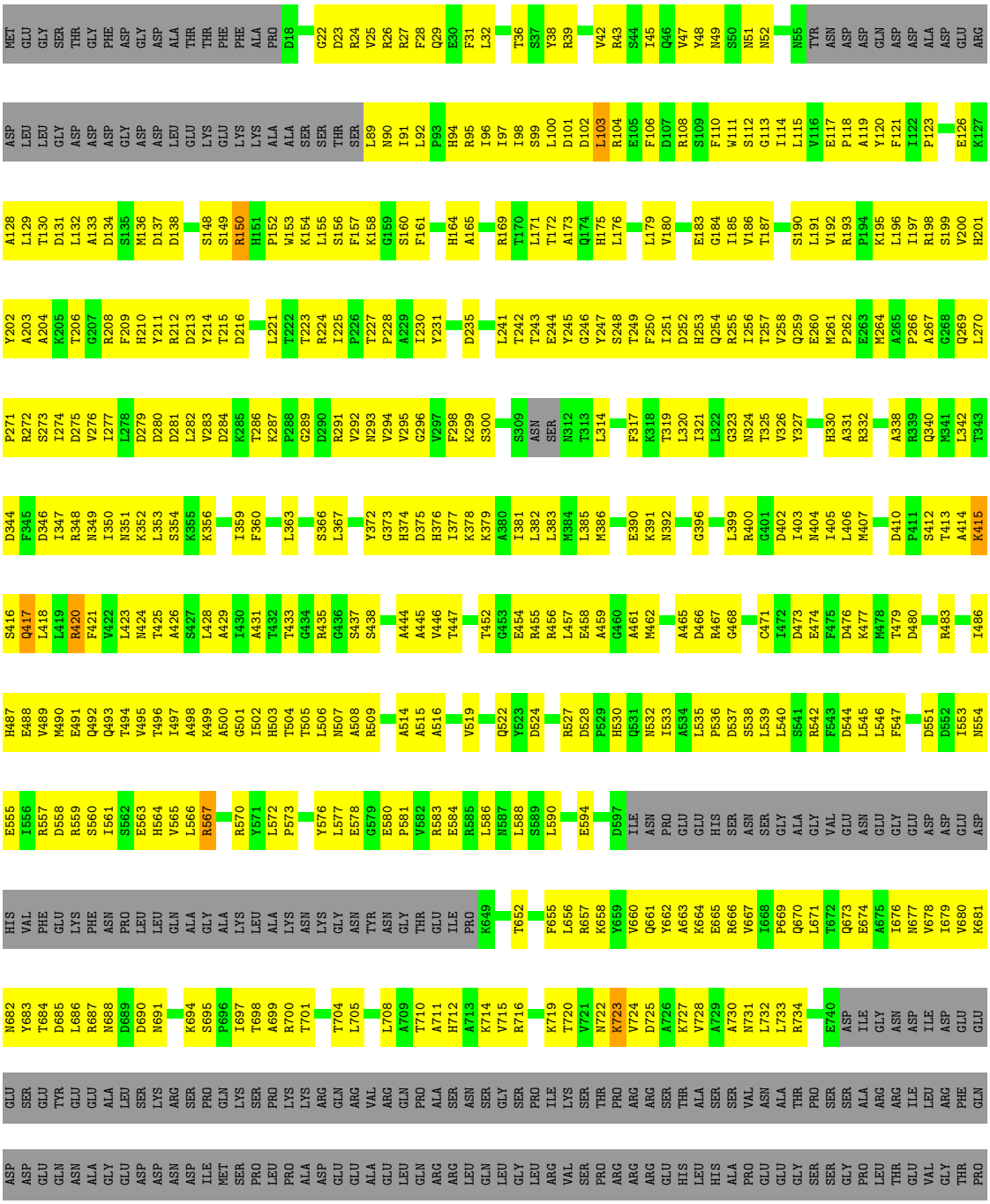


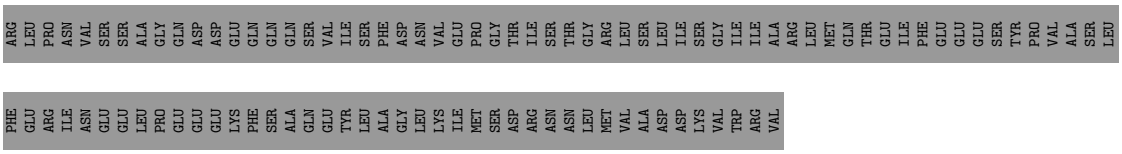


• Molecule 2: DNA replication licensing factor MCM3

Chain 3:

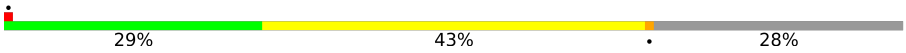


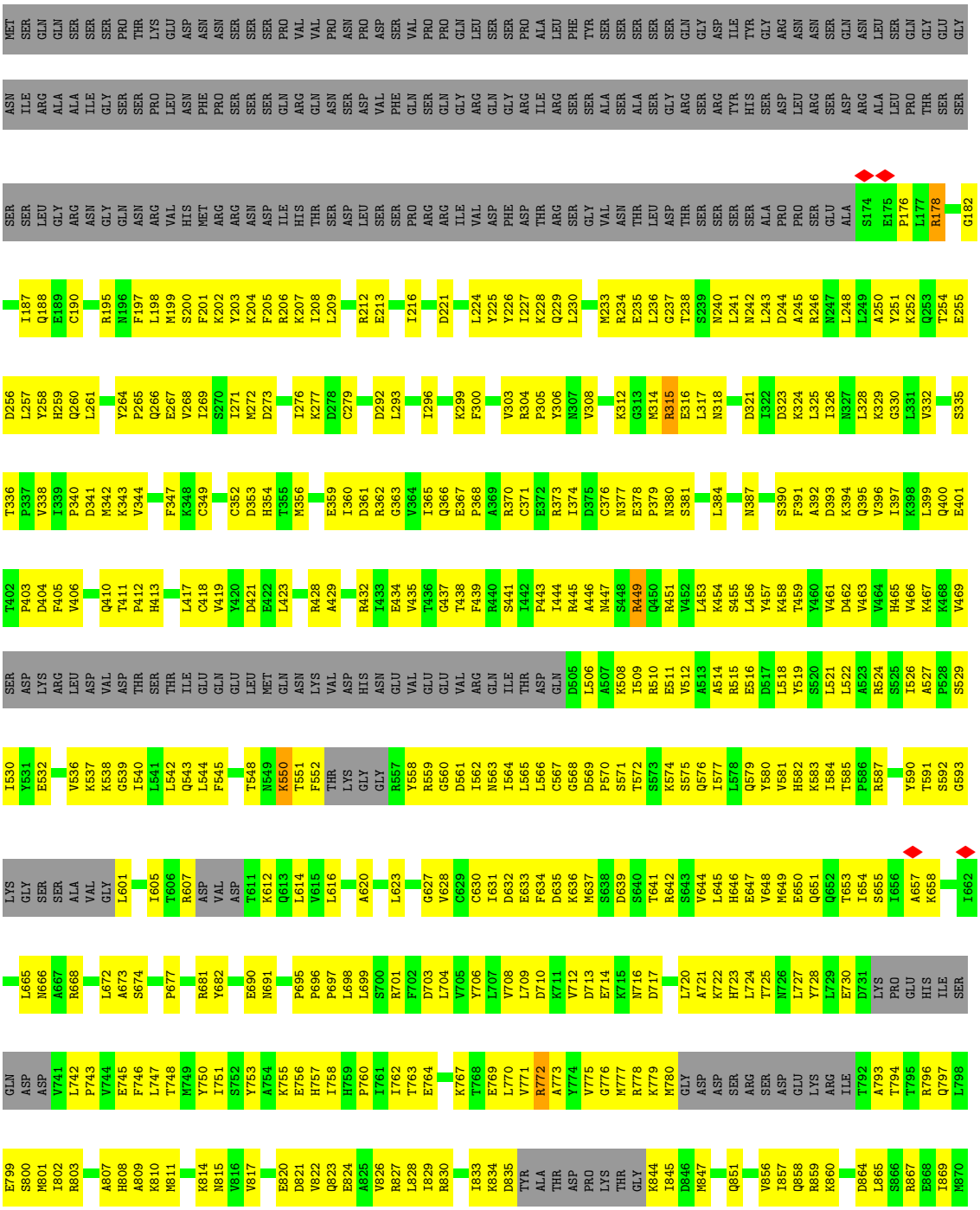




• Molecule 3: DNA replication licensing factor MCM4

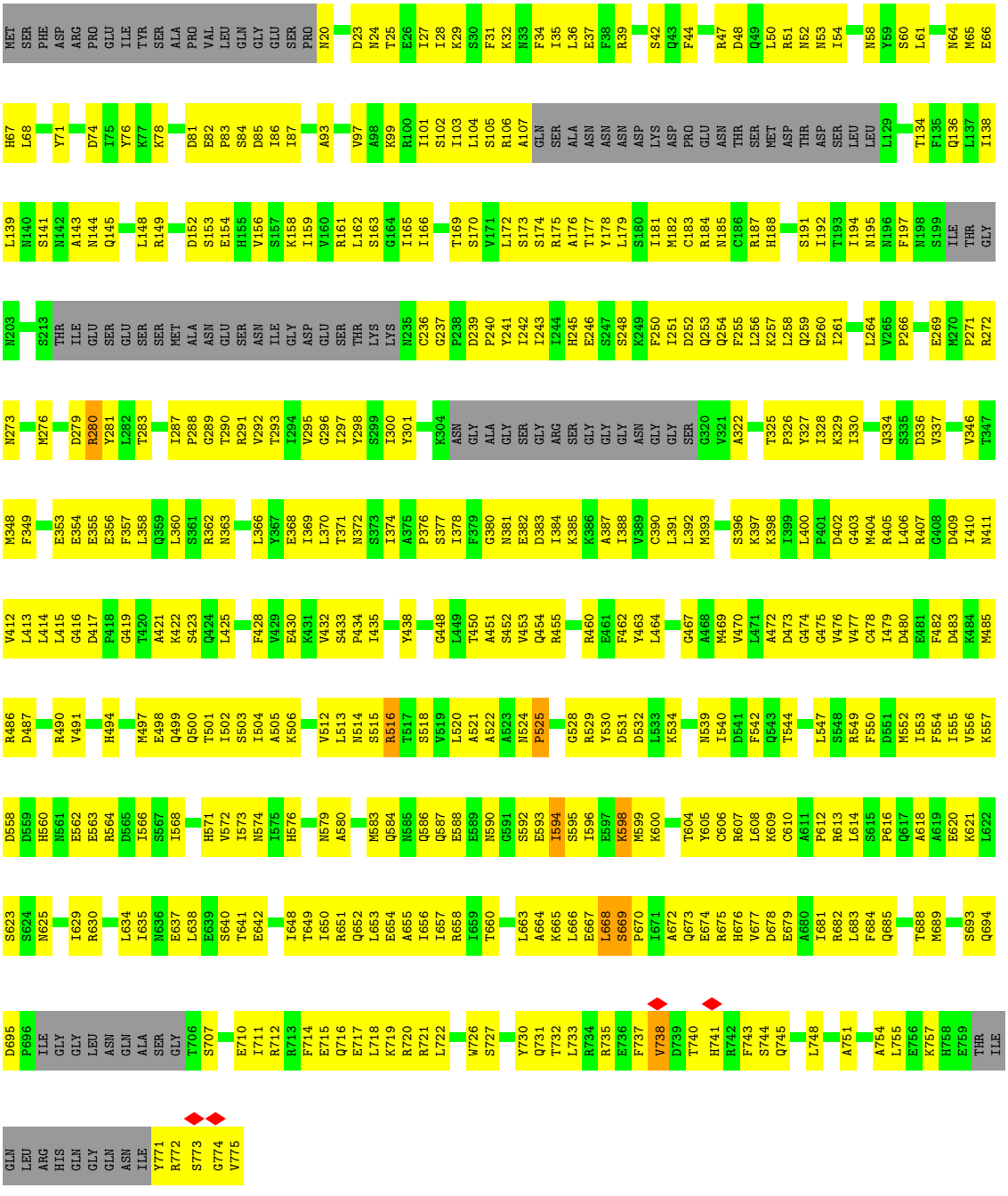
Chain 4:





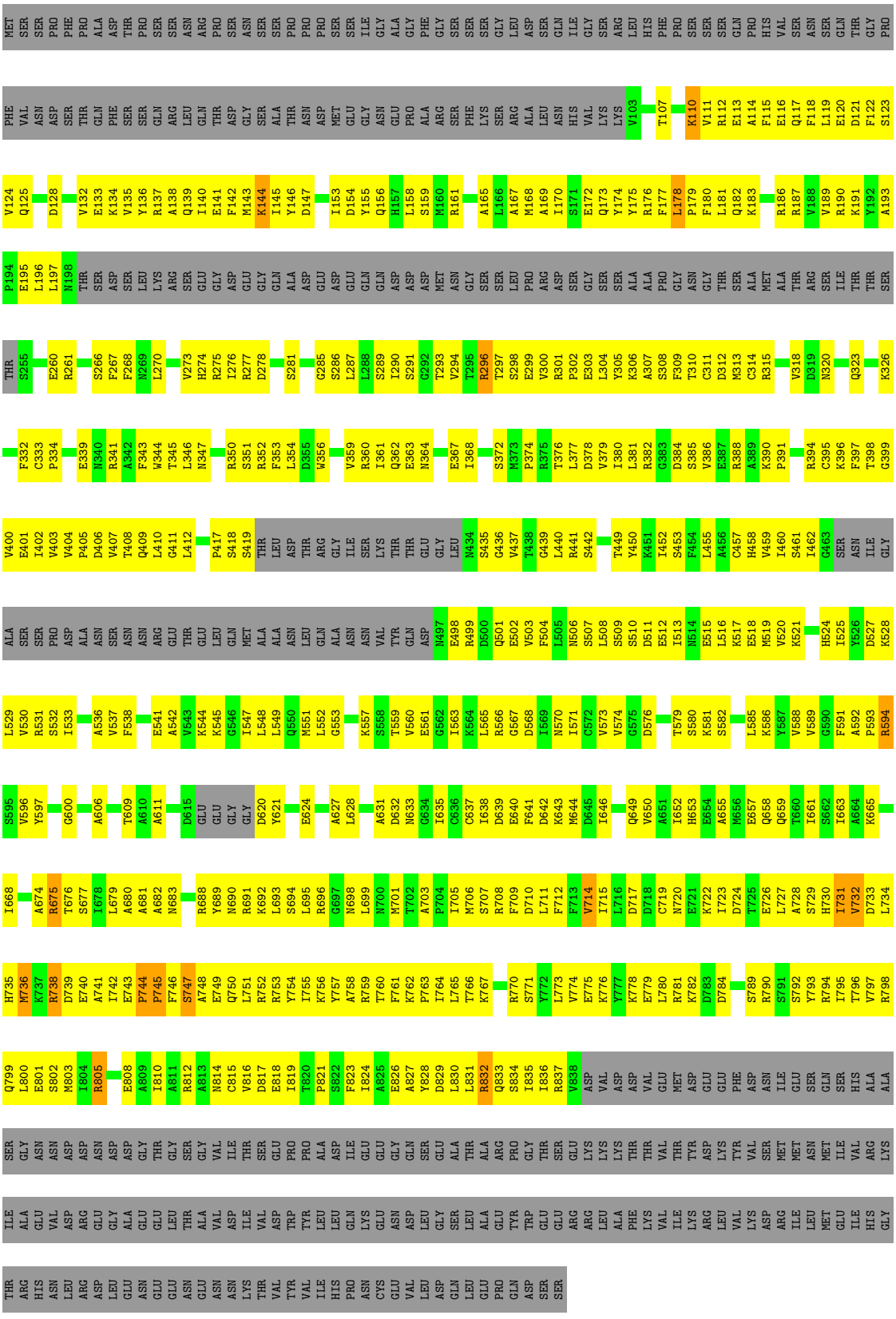
• Molecule 4: Minichromosome maintenance protein 5

Chain 5:



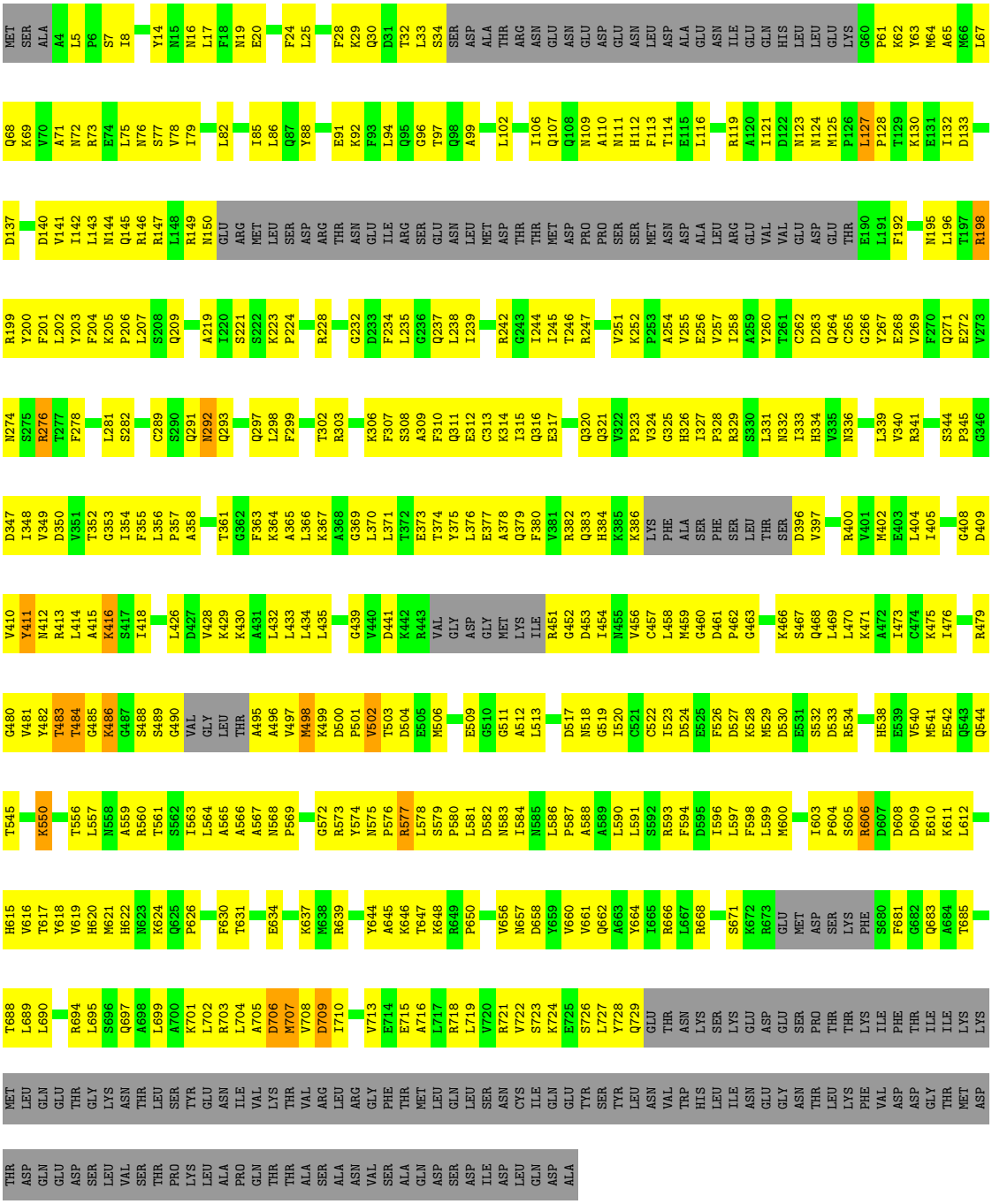
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



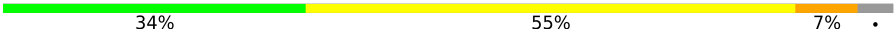
• Molecule 6: DNA replication licensing factor MCM7

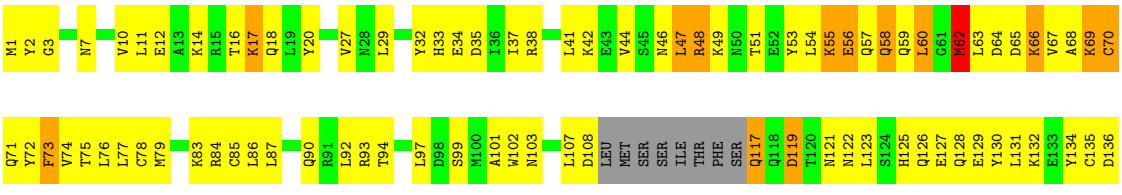
Chain 7: 28% 46% • 25%

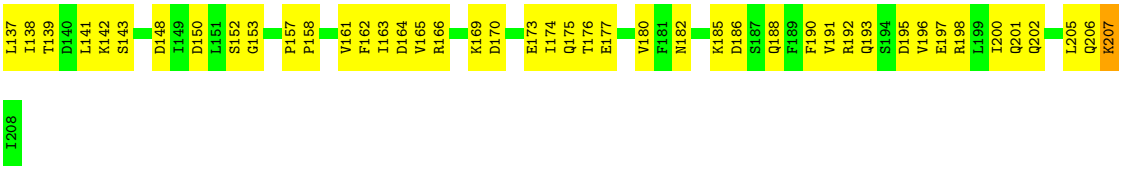


• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:

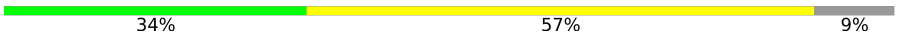


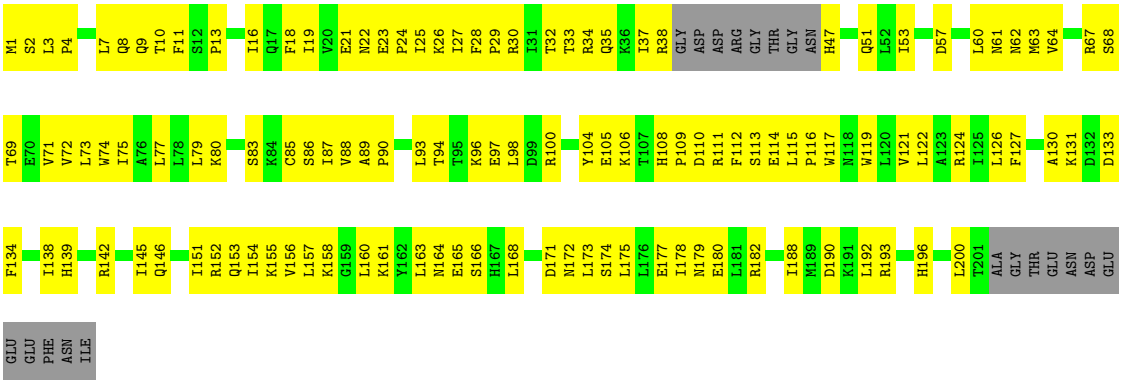




• Molecule 8: DNA replication complex GINS protein PSF2

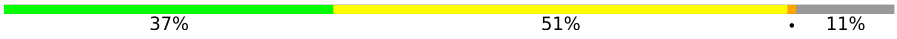
Chain B:

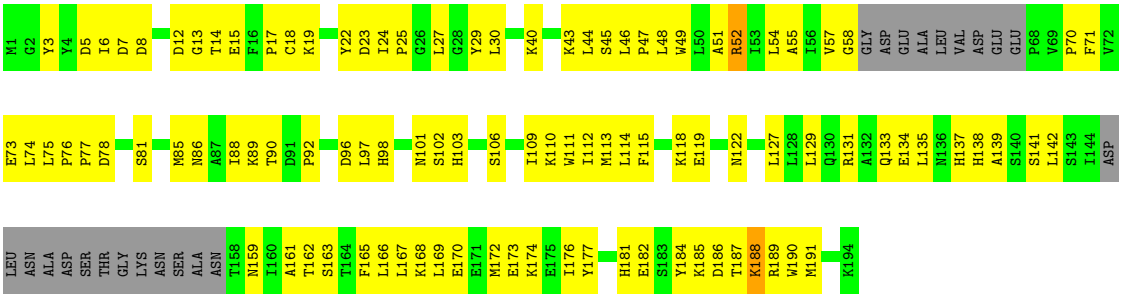




• Molecule 9: DNA replication complex GINS protein PSF3

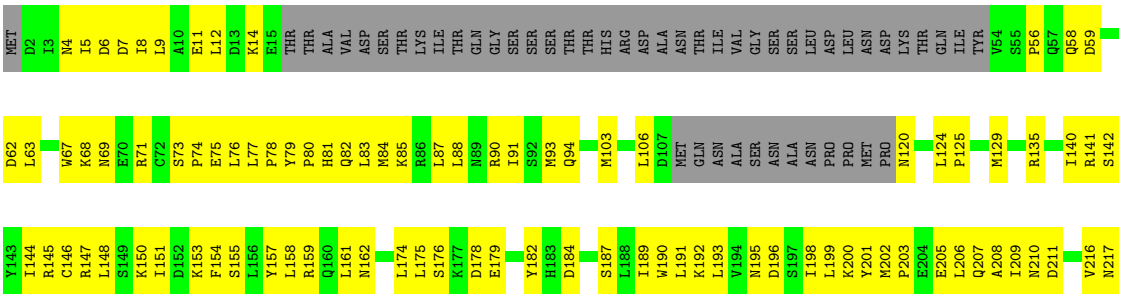
Chain C:

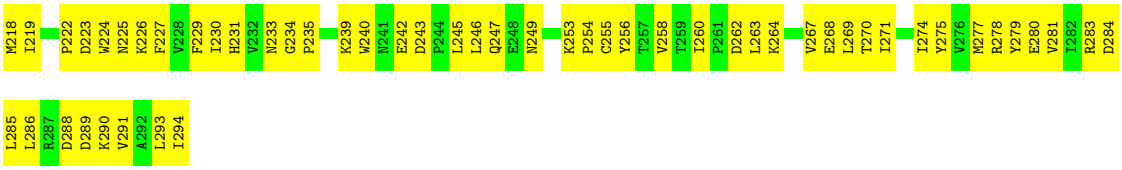




• Molecule 10: DNA replication complex GINS protein SLD5

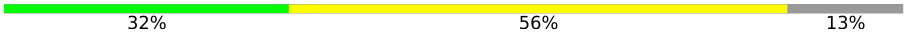
Chain D:

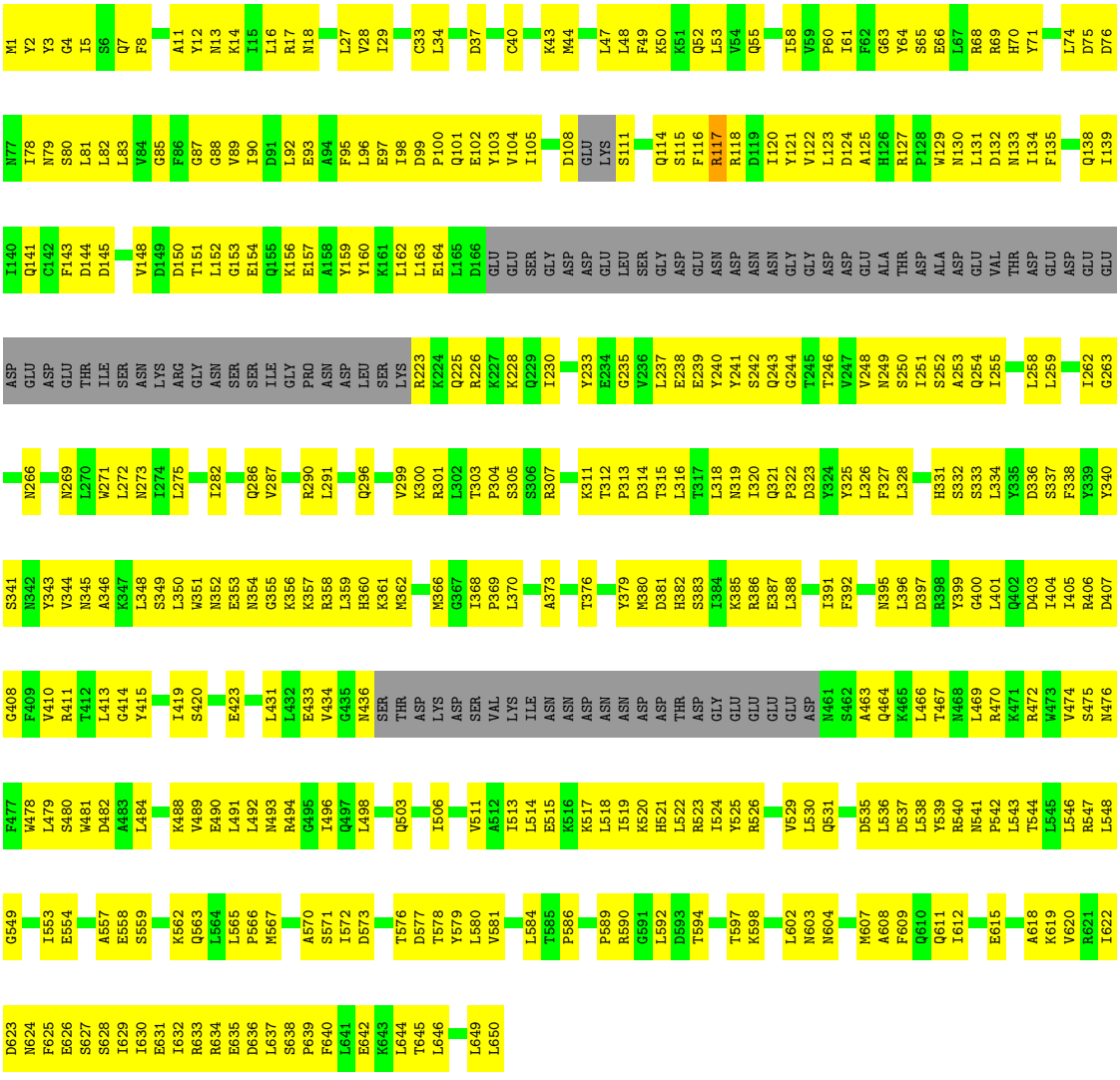




• Molecule 11: Cell division control protein 45

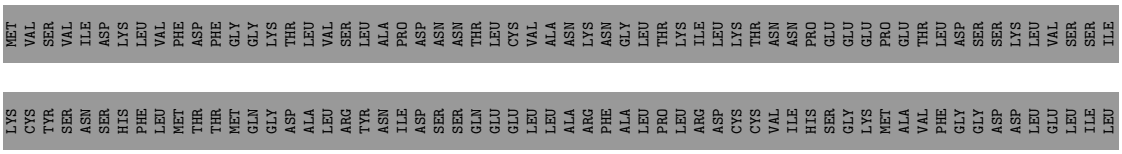
Chain E:

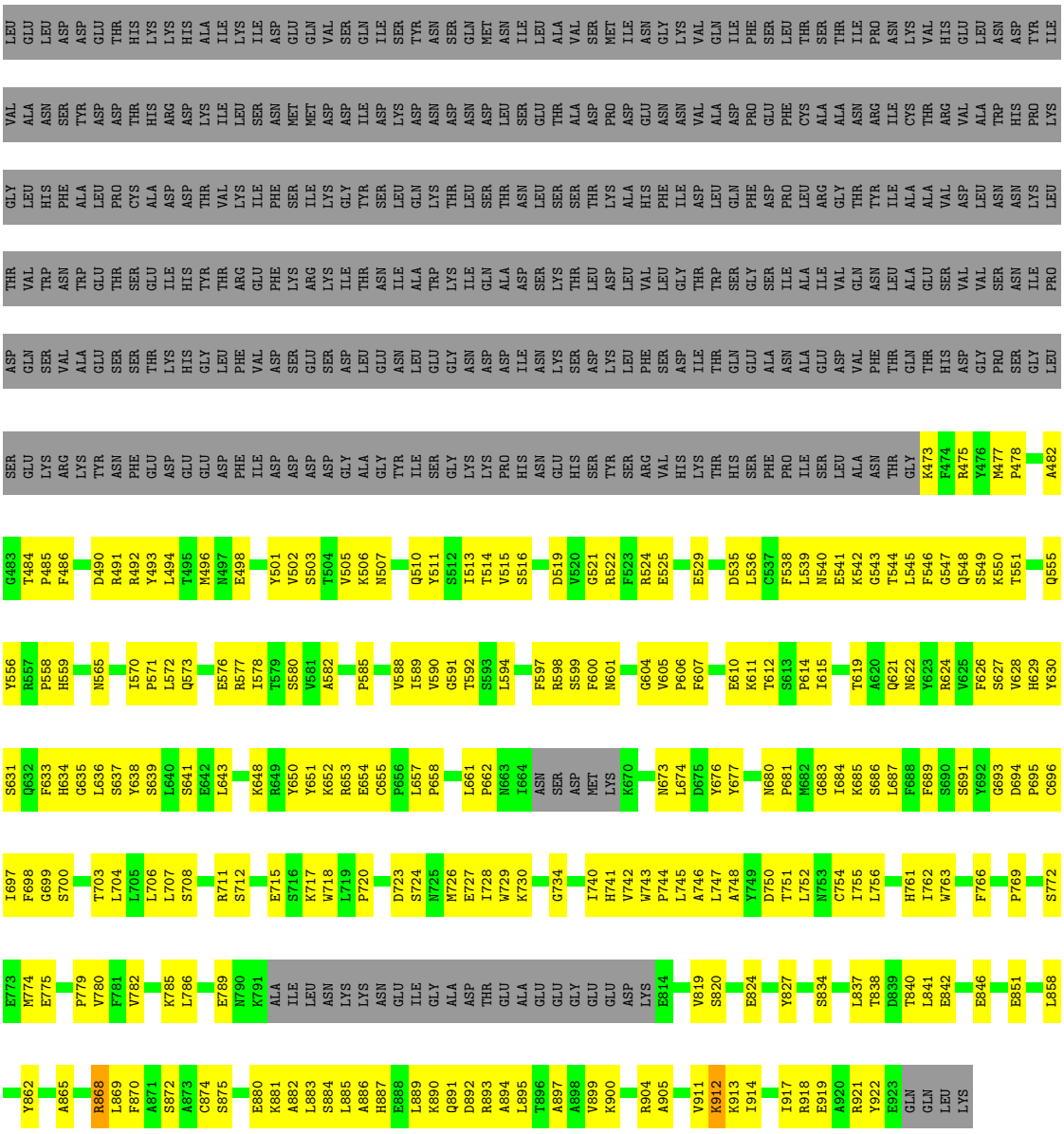




• Molecule 12: DNA polymerase alpha-binding protein

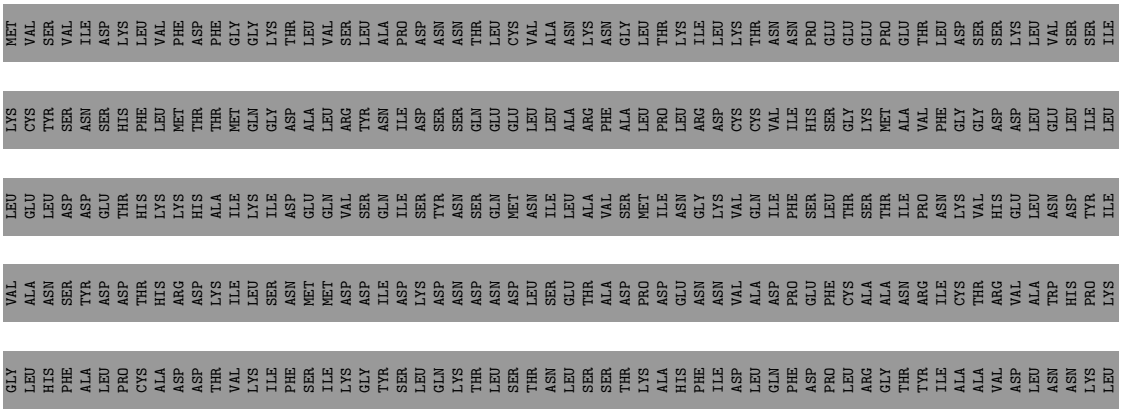
Chain F:

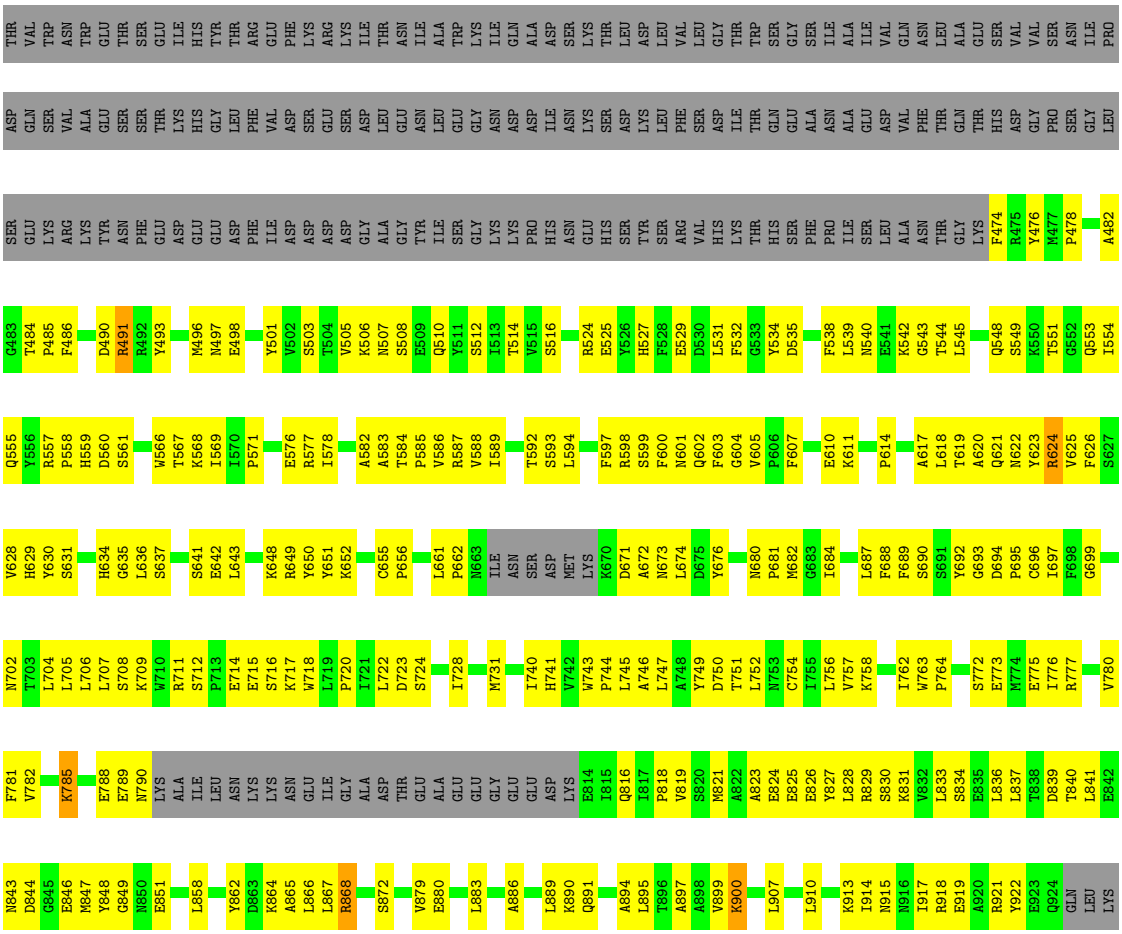




• Molecule 12: DNA polymerase alpha-binding protein

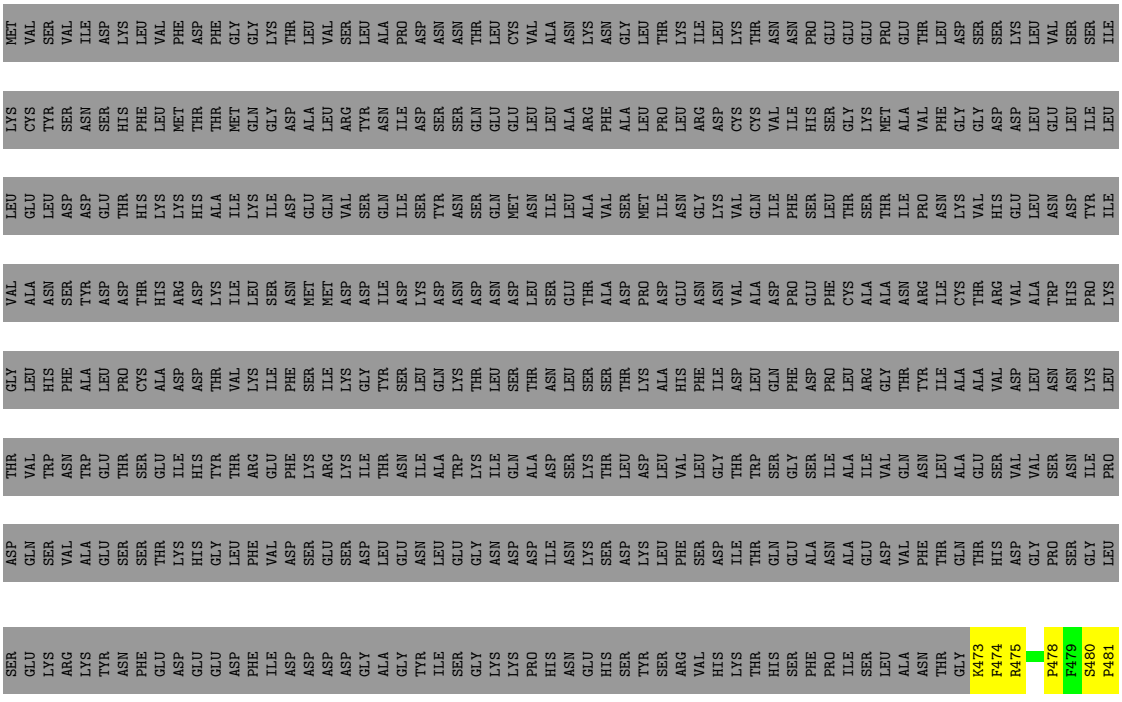
Chain G:

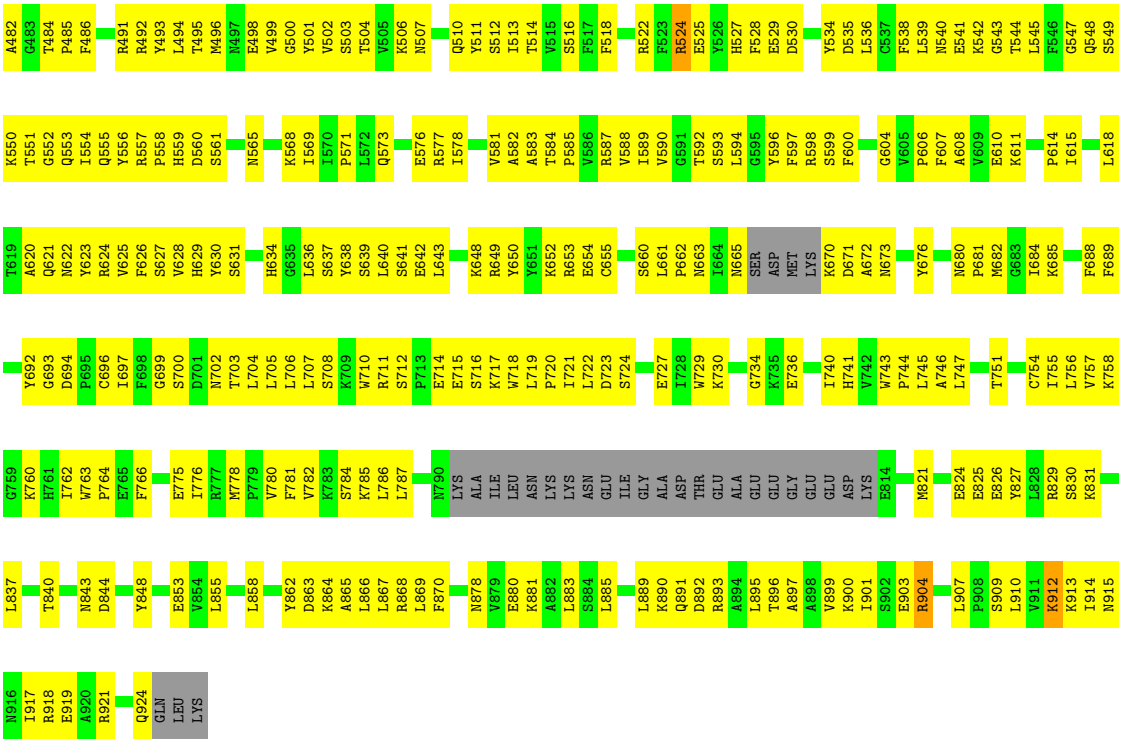




• Molecule 12: DNA polymerase alpha-binding protein

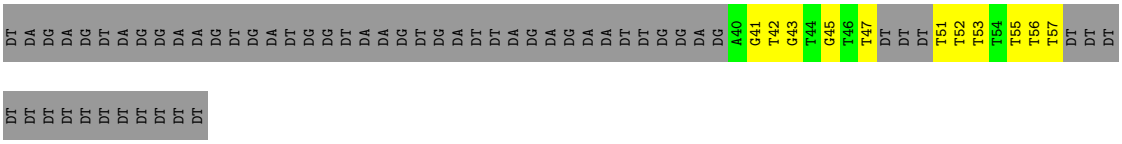
Chain H:





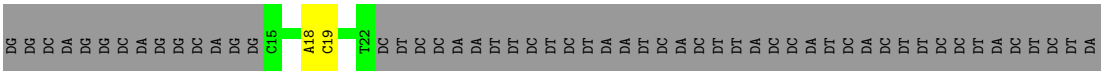
• Molecule 13: DNA (70-mer)

Chain I:



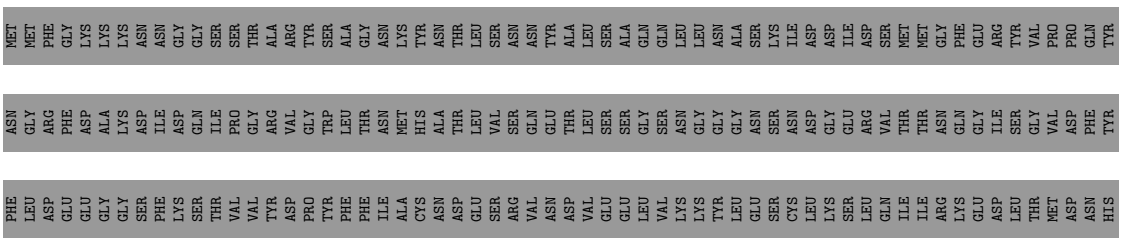
• Molecule 14: DNA (61-mer)

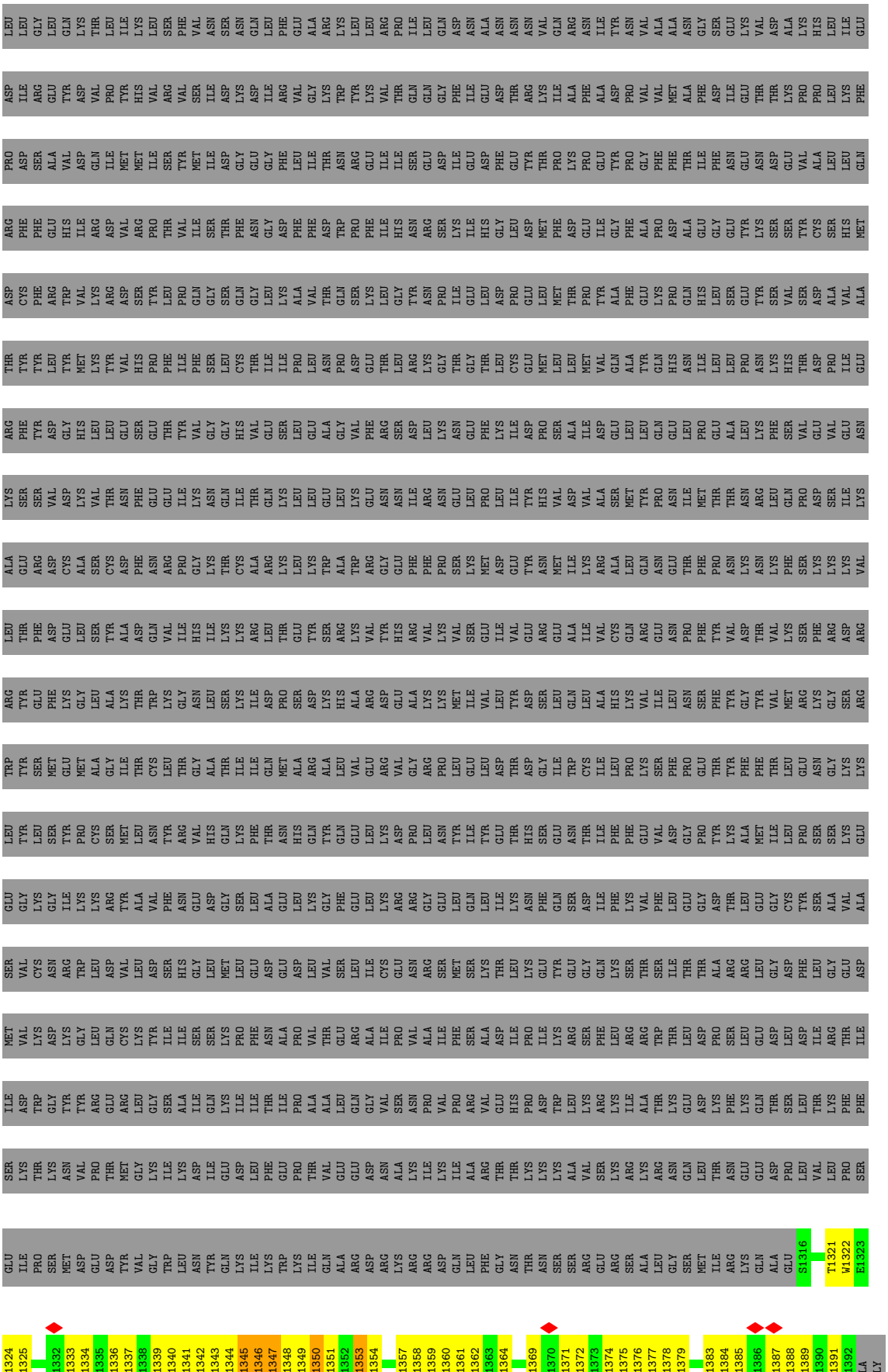
Chain J:

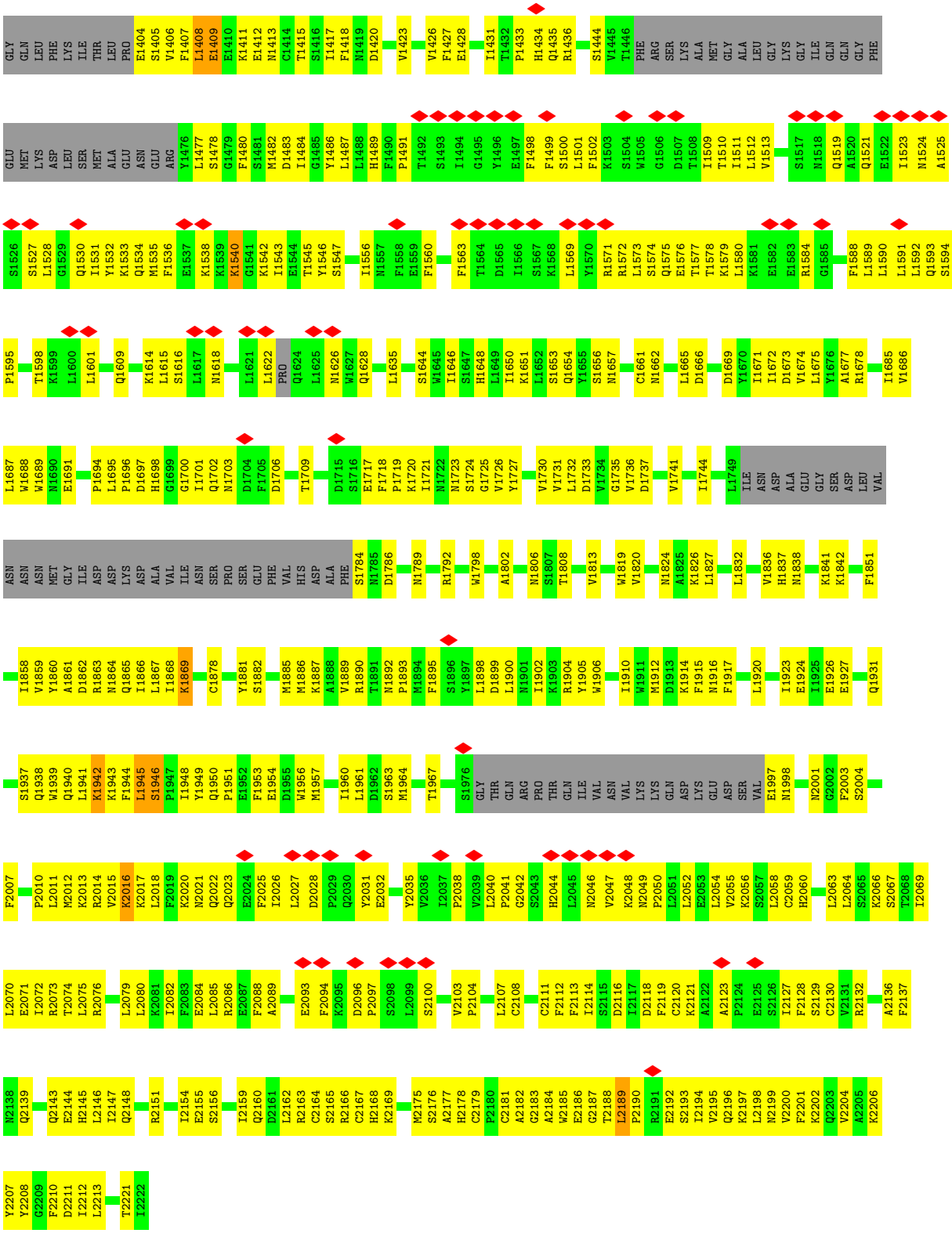


• Molecule 15: DNA polymerase epsilon catalytic subunit A

Chain M:

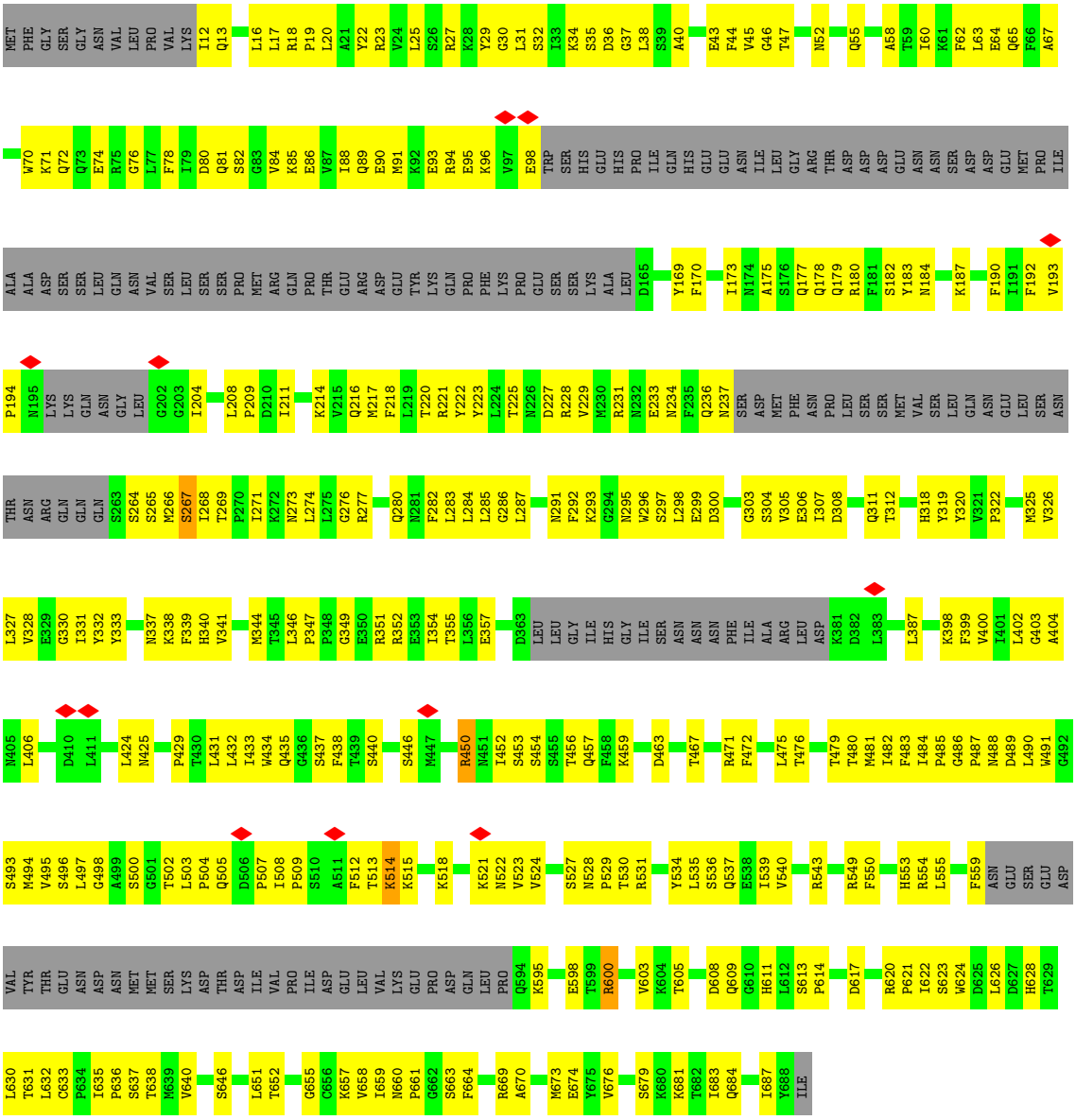






• Molecule 16: DNA polymerase epsilon subunit B

Chain N:


MET PHE GLY SER GLY ASN VAL LEU PRO VAL LYS I12 Q13 L16 L17 R18 P19 L20 A21 Y22 R23 V24 L25 S26 R27 K28 Y29 G30 L31 S32 I33 K34 S35 D36 G37 L38 S39 A40 E43 F44 V45 G46 T47 N52 Q55 A58 T59 I60 K61 F62 L63 E64 Q65 F66 A67
W70 K71 Q72 Q73 E74 R75 G76 L77 F78 I79 D80 Q81 S82 G83 V84 K85 E86 V87 I88 Q89 E90 M91 K92 E93 R94 E95 K96 V97 E98 TRP SER HIS GLU HIS PRO ILE GLN HIS GLU GLU ASN ILE LEU GLY ARG THR ASP ASP GLU ASN ASN SER ASP ASP GLU MET PRO ILE
ALA ALA ASP SER SER LEU GLN ASN VAL SER LEU SER SER PRO MET ARG GLN PRO THR GLU ARG ASP GLU TYR LYS GLN PRO PHE LYS PRO GLU SER SER LYS ALA LEU D165 Y169 F170 I173 N174 A175 S176 Q177 Q178 Q179 R180 F181 S182 Y183 N184 K187 F190 I191 F192 V193
P194 N195 LYS LYS GLN ASN GLY LEU G202 G203 I204 L208 P209 D210 I211 K214 V215 Q216 M217 F218 L219 T220 R221 Y222 Y223 L224 T225 N226 D227 R228 V229 M230 R231 N232 E233 N234 F235 Q236 N237 SER ASP MET PHE ASN PRO LEU SER SER MET VAL SER LEU GLN ASN GLU LEU SER ASN
THR ASN ARG GLN GLN GLN S263 S264 S265 M266 S267 I268 T269 P270 I271 K272 N273 L274 L275 G276 R277 Q280 N281 F282 L283 L284 L285 G286 L287 N291 F292 K293 G294 N295 W296 S297 L298 E299 D300 G303 S304 V305 E306 I307 D308 Q311 T312 H318 Y319 Y320 V321 P322 M325 V326
L327 V328 E329 G330 I331 Y332 Y333 N337 K338 F339 H340 V341 M344 T345 L346 P347 P348 G349 E350 R351 R352 E353 I354 T355 L356 E357 D363 LEU LEU GLY ILE HIS GLY ILE SER ASN ASN ASN PHE ILE ALA ARG LEU ASP K381 D382 L383 L387 K398 F399 V400 I401 L402 G403 A404
N405 L406 D410 L411 L424 M425 P429 T430 L431 L432 I433 W434 Q435 G436 S437 F438 T439 S440 S446 M447 R450 N451 I452 S453 S454 S455 T456 Q457 F458 K459 D463 T467 R471 F472 L475 T476 T479 T480 M481 I482 F483 I484 P485 G486 P487 N488 D489 L490 W491 G492
S493 M494 V495 S496 L497 G498 A499 S500 G501 T502 L503 P504 Q505 D506 P507 I508 P509 S510 A511 F512 T513 K514 K515 K518 K521 N522 V523 V524 S527 N528 P529 T530 R531 Y534 L535 S536 Q537 E538 I539 V540 R543 R549 F550 H553 R554 L555 F559 ASN GLU SER GLU ASP
VAL TYR THR GLU ASN ASP ASN MET MET SER LYS ASP THR ASP ILE VAL PRO ILE ASP GLU LEU VAL LYS GLU PRO ASP GLN LEU PRO Q594 K595 E598 T599 R600 V603 K604 T605 D608 Q609 G610 H611 L612 S613 P614 D617 R620 P621 I622 S623 W624 D625 L626 D627 H628 T629
L630 T631 L632 C633 P634 I635 P636 S637 T638 M639 V640 S646 L651 T652 G655 C656 K657 V658 I659 N660 P661 G662 S663 F664 R669 A670 M673 E674 Y675 V676 S679 K680 K681 I682 I683 Q684 I687 Y688 ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17199	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 ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.030	Depositor
Minimum map value	-0.192	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: MG, ZN, ADP, AGS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.29	0/5360	0.56	0/7241
2	3	0.29	0/5032	0.54	1/6827 (0.0%)
3	4	0.25	0/5459	0.53	0/7363
4	5	0.28	1/5402 (0.0%)	0.55	1/7300 (0.0%)
5	6	0.29	0/5036	0.60	0/6799
6	7	0.30	0/5019	0.53	1/6789 (0.0%)
7	A	0.37	0/1653	0.55	0/2224
8	B	0.27	0/1650	0.48	0/2231
9	C	0.28	0/1420	0.45	0/1918
10	D	0.28	0/2040	0.48	0/2755
11	E	0.27	0/4685	0.48	0/6343
12	F	0.29	0/3489	0.50	0/4724
12	G	0.28	0/3465	0.51	0/4696
12	H	0.28	0/3496	0.49	0/4735
13	I	0.45	0/339	1.12	0/520
14	J	0.46	0/177	0.78	0/269
15	M	0.30	0/6586	0.50	1/8926 (0.0%)
16	N	0.27	0/4290	0.51	0/5811
All	All	0.29	1/64598 (0.0%)	0.53	4/87471 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	525	PRO	N-CD	-5.68	1.40	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	668	LEU	CA-CB-CG	5.73	128.49	115.30
15	M	2189	LEU	CA-CB-CG	5.54	128.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	103	LEU	CA-CB-CG	5.18	127.22	115.30
6	7	127	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5270	0	5304	448	0
2	3	4948	0	4991	425	0
3	4	5390	0	5467	420	0
4	5	5325	0	5351	431	0
5	6	4955	0	4959	508	0
6	7	4945	0	4987	409	0
7	A	1633	0	1631	157	0
8	B	1617	0	1674	129	0
9	C	1387	0	1405	101	0
10	D	2004	0	2001	146	0
11	E	4599	0	4584	333	0
12	F	3404	0	3352	224	0
12	G	3380	0	3310	224	0
12	H	3411	0	3355	236	0
13	I	307	0	178	12	0
14	J	159	0	90	2	0
15	M	6447	0	6368	397	0
16	N	4199	0	4163	253	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
17	M	2	0	0	0	0
18	2	27	0	12	19	0
18	3	27	0	12	16	0
19	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	5	2	0	0	0	0
19	7	1	0	0	0	0
20	5	31	0	12	12	0
20	7	31	0	12	9	0
All	All	63507	0	63218	4549	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 36.

The worst 5 of 4549 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)
3:4:802:ILE:HG13	5:6:736:MET:SD	1.57	1.44
5:6:735:HIS:O	5:6:736:MET:HG2	1.28	1.32
3:4:802:ILE:CG1	5:6:736:MET:SD	2.21	1.28
3:4:802:ILE:CD1	5:6:736:MET:SD	2.27	1.22
2:3:499:LYS:HA	6:7:490:GLY:HA2	1.19	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	664/868 (76%)	621 (94%)	42 (6%)	1 (0%)	47	81
2	3	629/971 (65%)	580 (92%)	49 (8%)	0	100	100
3	4	658/933 (70%)	616 (94%)	40 (6%)	2 (0%)	41	76
4	5	662/775 (85%)	609 (92%)	50 (8%)	3 (0%)	29	68
5	6	619/1017 (61%)	547 (88%)	67 (11%)	5 (1%)	19	60
6	7	622/845 (74%)	570 (92%)	47 (8%)	5 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	A	196/208 (94%)	183 (93%)	12 (6%)	1 (0%)	29 68
8	B	189/213 (89%)	184 (97%)	5 (3%)	0	100 100
9	C	166/194 (86%)	164 (99%)	2 (1%)	0	100 100
10	D	237/294 (81%)	230 (97%)	7 (3%)	0	100 100
11	E	560/650 (86%)	548 (98%)	12 (2%)	0	100 100
12	F	418/927 (45%)	404 (97%)	14 (3%)	0	100 100
12	G	416/927 (45%)	408 (98%)	8 (2%)	0	100 100
12	H	419/927 (45%)	410 (98%)	9 (2%)	0	100 100
15	M	800/2222 (36%)	725 (91%)	72 (9%)	3 (0%)	34 72
16	N	517/689 (75%)	490 (95%)	27 (5%)	0	100 100
All	All	7772/12660 (61%)	7289 (94%)	463 (6%)	20 (0%)	44 76

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	178	LEU
5	6	714	VAL
15	M	1945	LEU
4	5	669	SER
5	6	744	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2	578/770 (75%)	570 (99%)	8 (1%)	67 81
2	3	541/835 (65%)	535 (99%)	6 (1%)	73 85
3	4	614/848 (72%)	607 (99%)	7 (1%)	73 85
4	5	602/688 (88%)	598 (99%)	4 (1%)	84 90
5	6	543/886 (61%)	529 (97%)	14 (3%)	46 67
6	7	544/753 (72%)	530 (97%)	14 (3%)	46 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	A	184/193 (95%)	167 (91%)	17 (9%)	9 31
8	B	183/198 (92%)	183 (100%)	0	100 100
9	C	155/173 (90%)	153 (99%)	2 (1%)	69 82
10	D	234/279 (84%)	234 (100%)	0	100 100
11	E	510/586 (87%)	509 (100%)	1 (0%)	93 96
12	F	375/825 (46%)	373 (100%)	2 (0%)	88 93
12	G	372/825 (45%)	365 (98%)	7 (2%)	57 75
12	H	375/825 (46%)	372 (99%)	3 (1%)	81 89
15	M	713/2014 (35%)	696 (98%)	17 (2%)	49 69
16	N	467/629 (74%)	459 (98%)	8 (2%)	60 78
All	All	6990/11327 (62%)	6880 (98%)	110 (2%)	64 79

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	56	GLU
9	C	188	LYS
16	N	681	LYS
15	M	1946	SER
7	A	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
11	E	52	GLN
12	H	629	HIS
11	E	402	GLN
12	G	629	HIS
15	M	1435	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	AGS	5	803	19	26,33,33	0.80	1 (3%)	26,52,52	0.79	1 (3%)
18	ADP	3	1001	19	24,29,29	0.73	0	29,45,45	0.78	1 (3%)
18	ADP	2	902	19	24,29,29	0.66	0	29,45,45	0.88	1 (3%)
20	AGS	7	903	-	26,33,33	0.81	1 (3%)	26,52,52	0.86	1 (3%)

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
20	AGS	5	803	19	-	6/17/38/38	0/3/3/3
18	ADP	3	1001	19	-	5/12/32/32	0/3/3/3
18	ADP	2	902	19	-	6/12/32/32	0/3/3/3
20	AGS	7	903	-	-	7/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	903	AGS	PG-S1G	2.13	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	803	AGS	PG-S1G	2.07	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	903	AGS	C5-C6-N6	2.29	123.83	120.35
18	2	902	ADP	C5-C6-N6	2.27	123.81	120.35
18	3	1001	ADP	C5-C6-N6	2.27	123.80	120.35
20	5	803	AGS	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	2	902	ADP	PA-O3A-PB-O3B
18	3	1001	ADP	PA-O3A-PB-O2B
18	3	1001	ADP	C5'-O5'-PA-O1A
20	5	803	AGS	C5'-O5'-PA-O3A
20	5	803	AGS	O4'-C4'-C5'-O5'

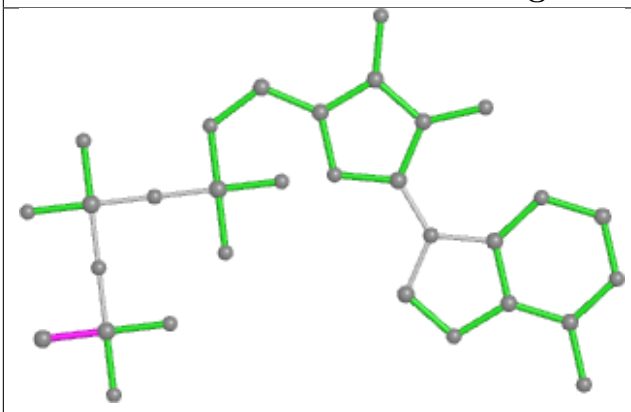
There are no ring outliers.

4 monomers are involved in 56 short contacts:

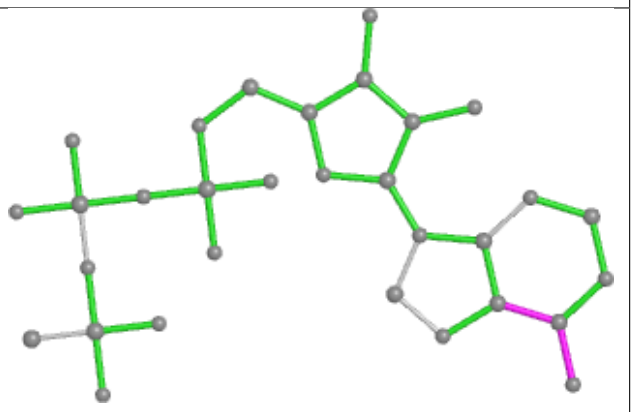
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	5	803	AGS	12	0
18	3	1001	ADP	16	0
18	2	902	ADP	19	0
20	7	903	AGS	9	0

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

Ligand AGS 5 803



Bond lengths



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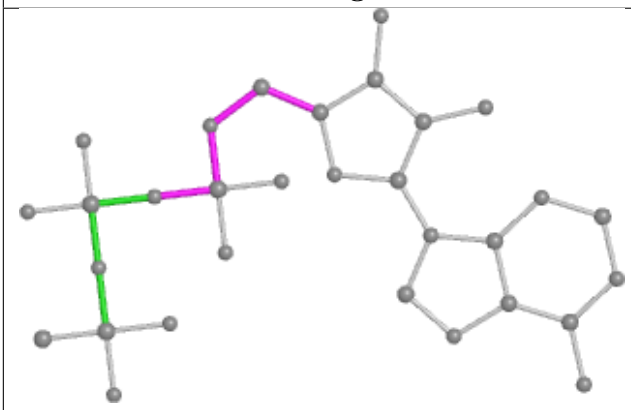
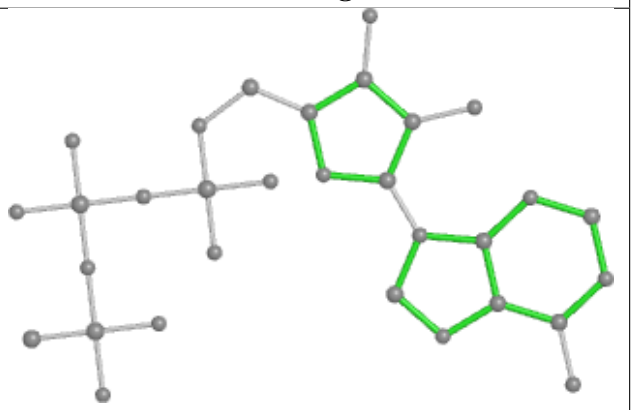
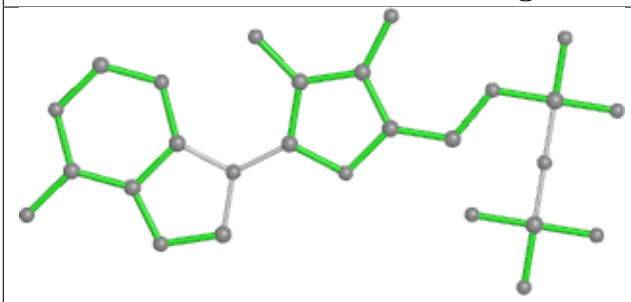


Torsions

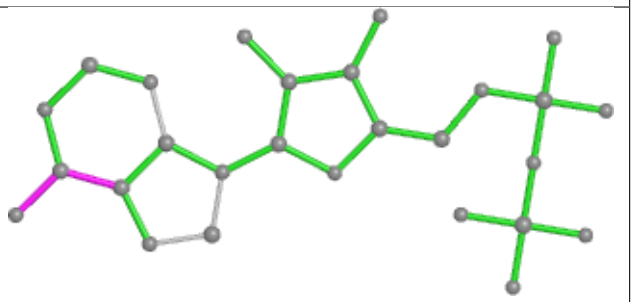


Rings

Ligand ADP 3 1001



Bond lengths



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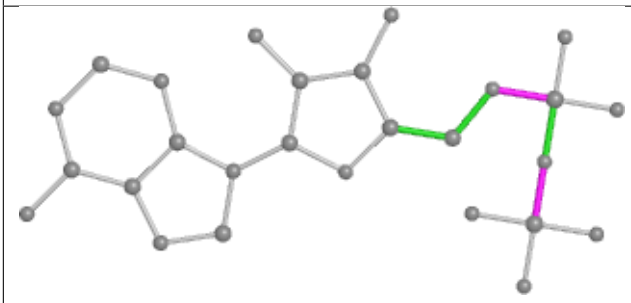
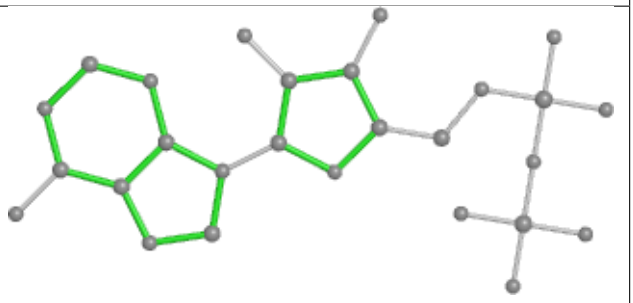
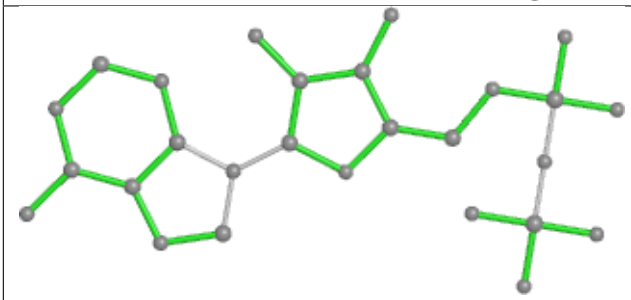


Torsions

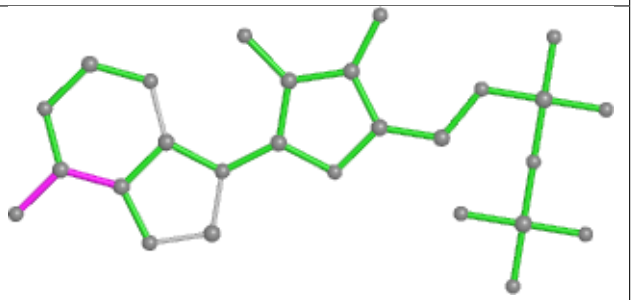


Rings

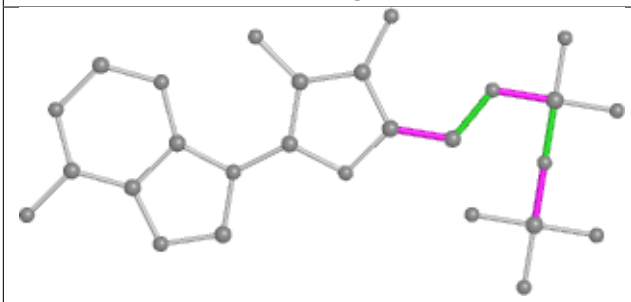
Ligand ADP 2 902



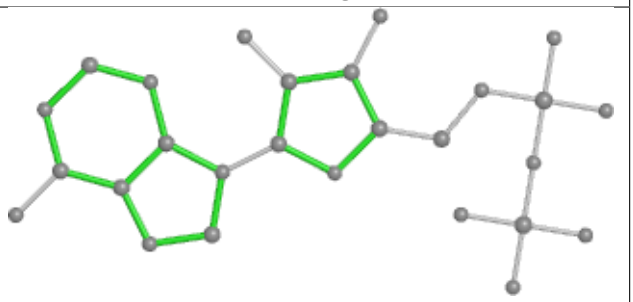
Bond lengths



Bond angles

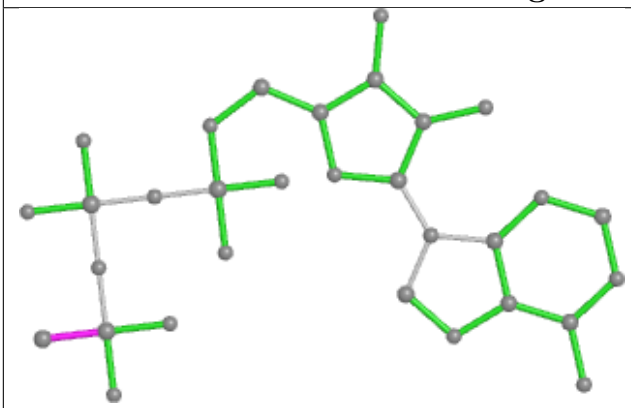


Torsions

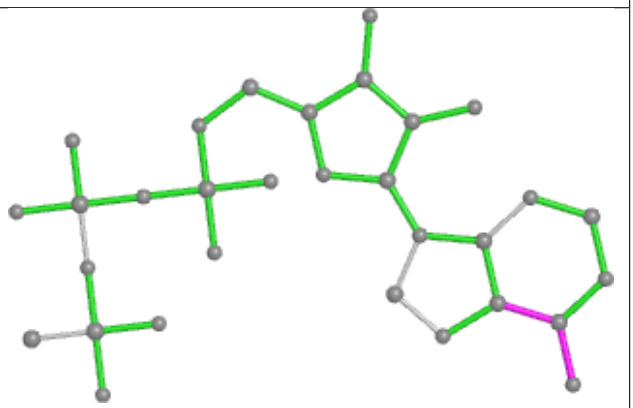


Rings

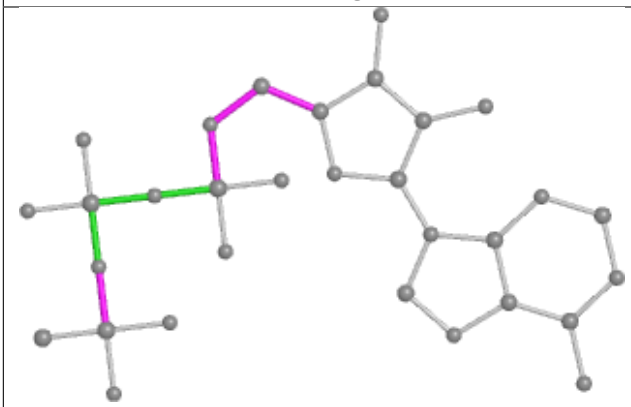
Ligand AGS 7 903



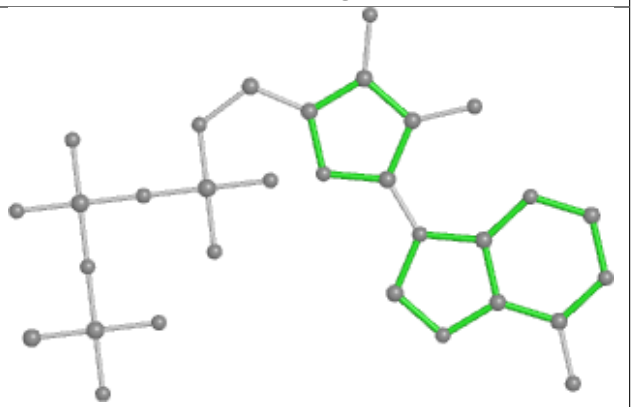
Bond lengths



Bond angles



Torsions



Rings

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.

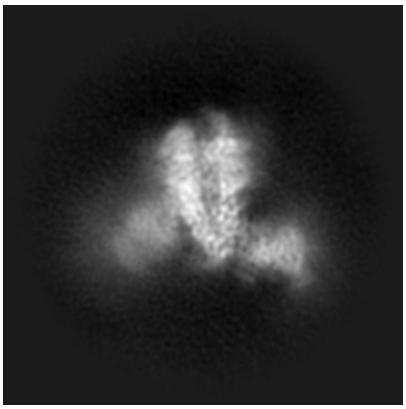
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37215. These allow visual inspection of the internal detail of the map and identification of artifacts.

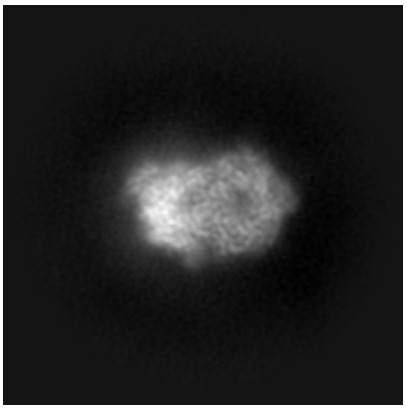
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

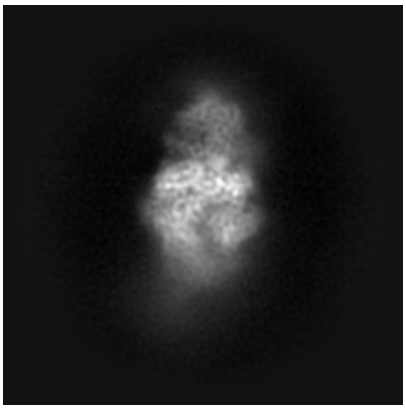
6.1.1 Primary map



X

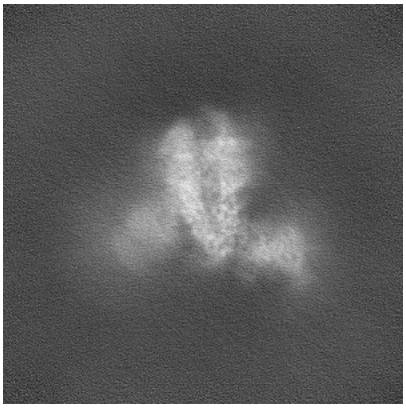


Y

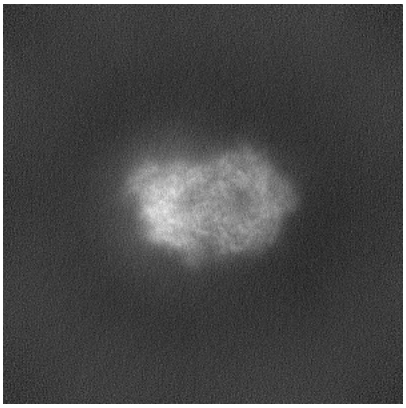


Z

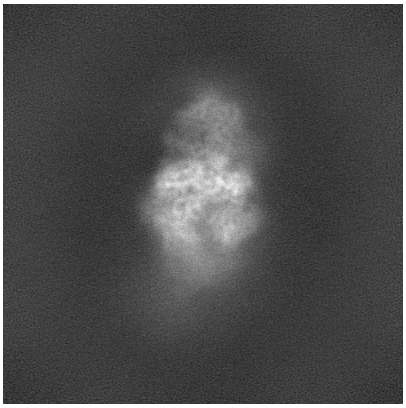
6.1.2 Raw map



X



Y

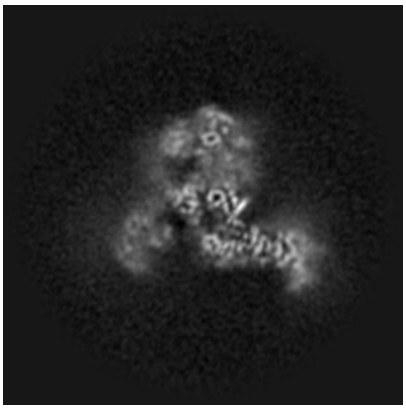


Z

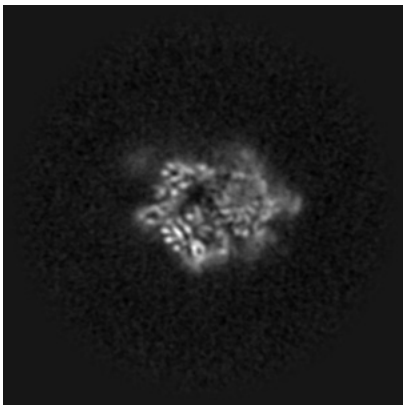
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

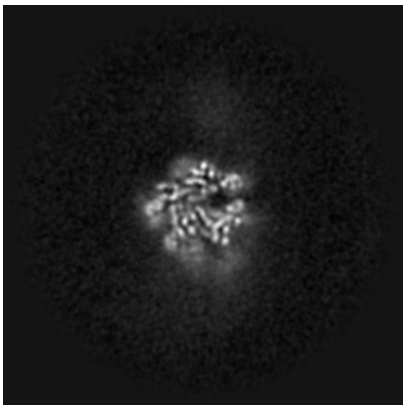
6.2.1 Primary map



X Index: 220

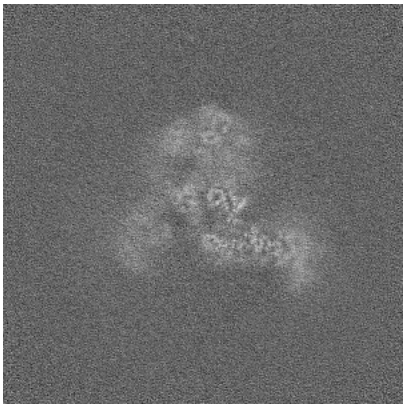


Y Index: 220

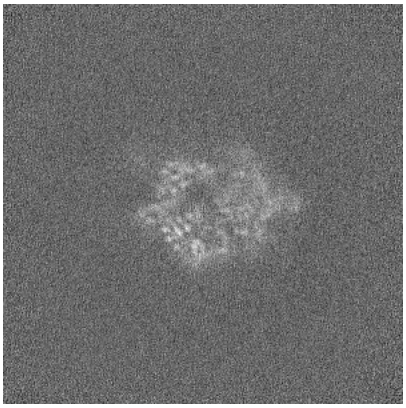


Z Index: 220

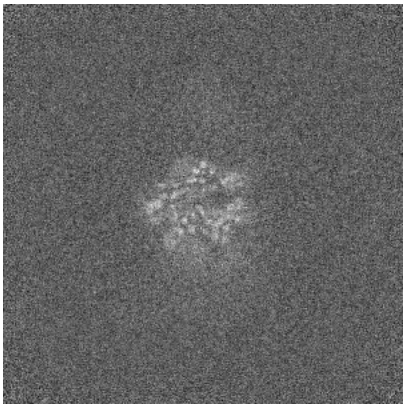
6.2.2 Raw map



X Index: 220



Y Index: 220

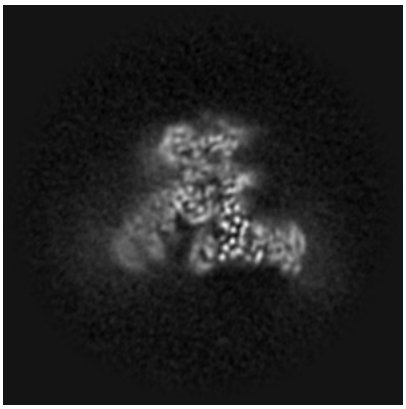


Z Index: 220

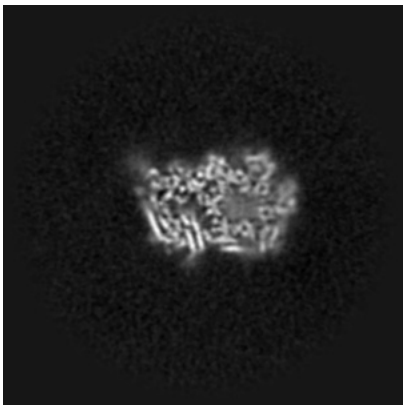
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

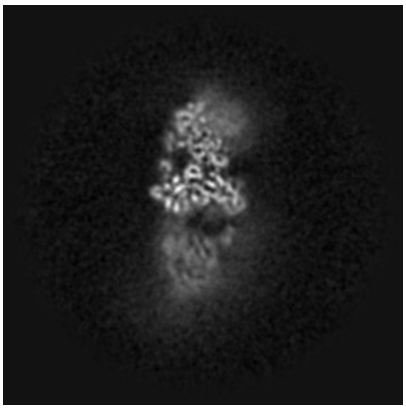
6.3.1 Primary map



X Index: 207

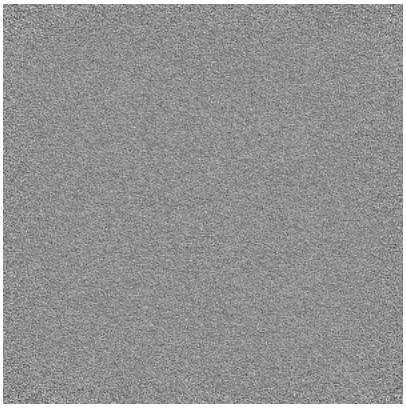


Y Index: 241

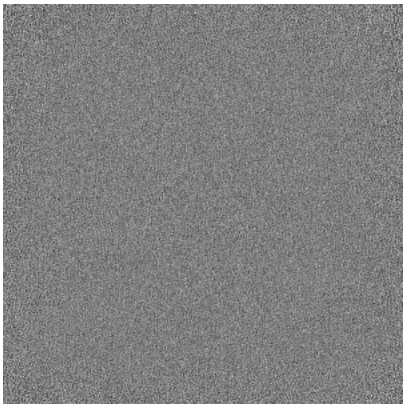


Z Index: 181

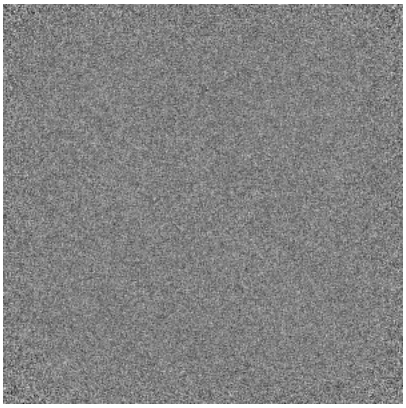
6.3.2 Raw map



X Index: 0



Y Index: 0

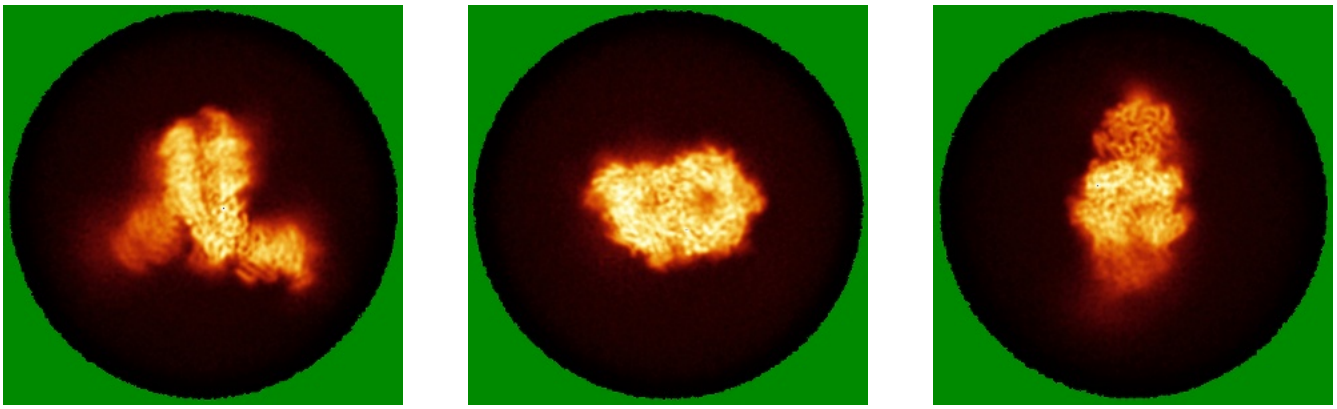


Z Index: 0

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

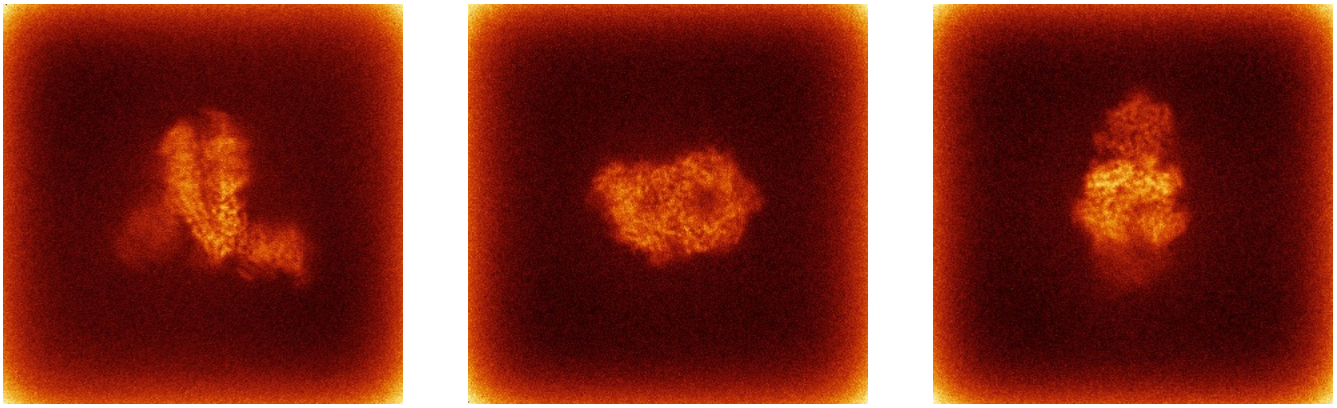
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

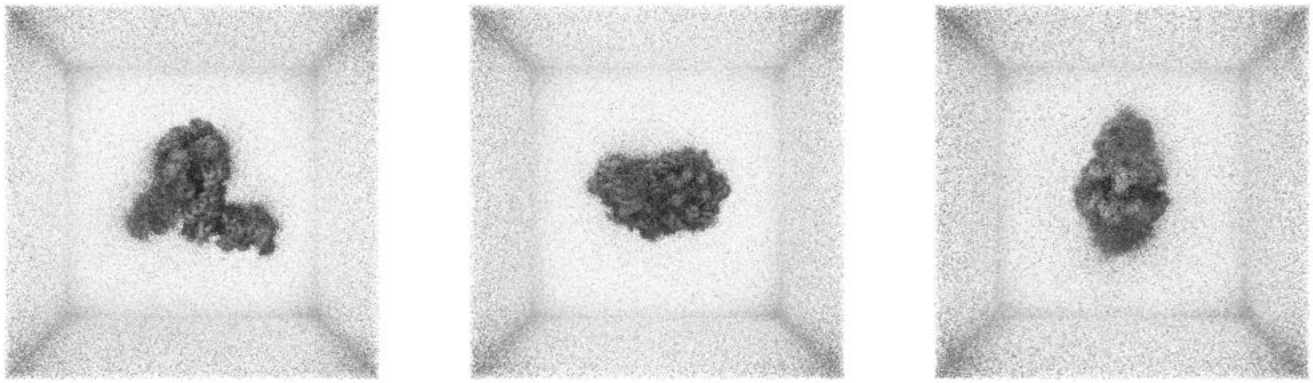
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

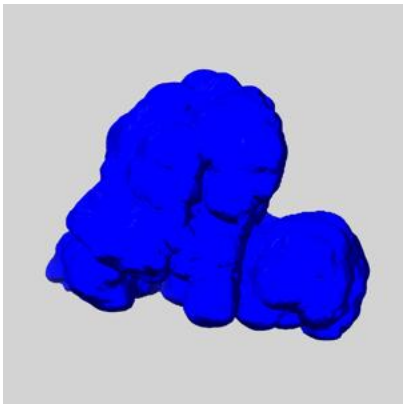
6.6 Mask visualisation (i)

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

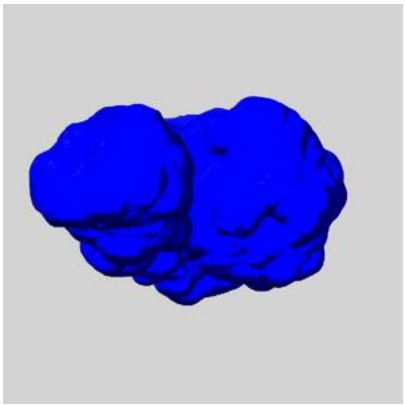
A mask typically either:

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

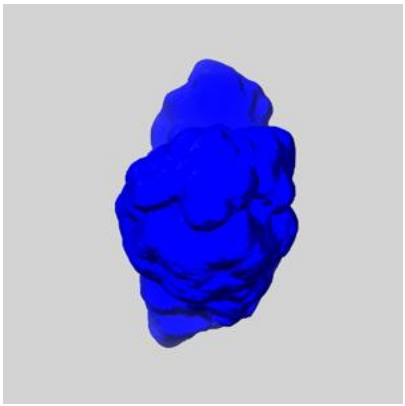
6.6.1 emd_37215_msk_1.map (i)



X



Y

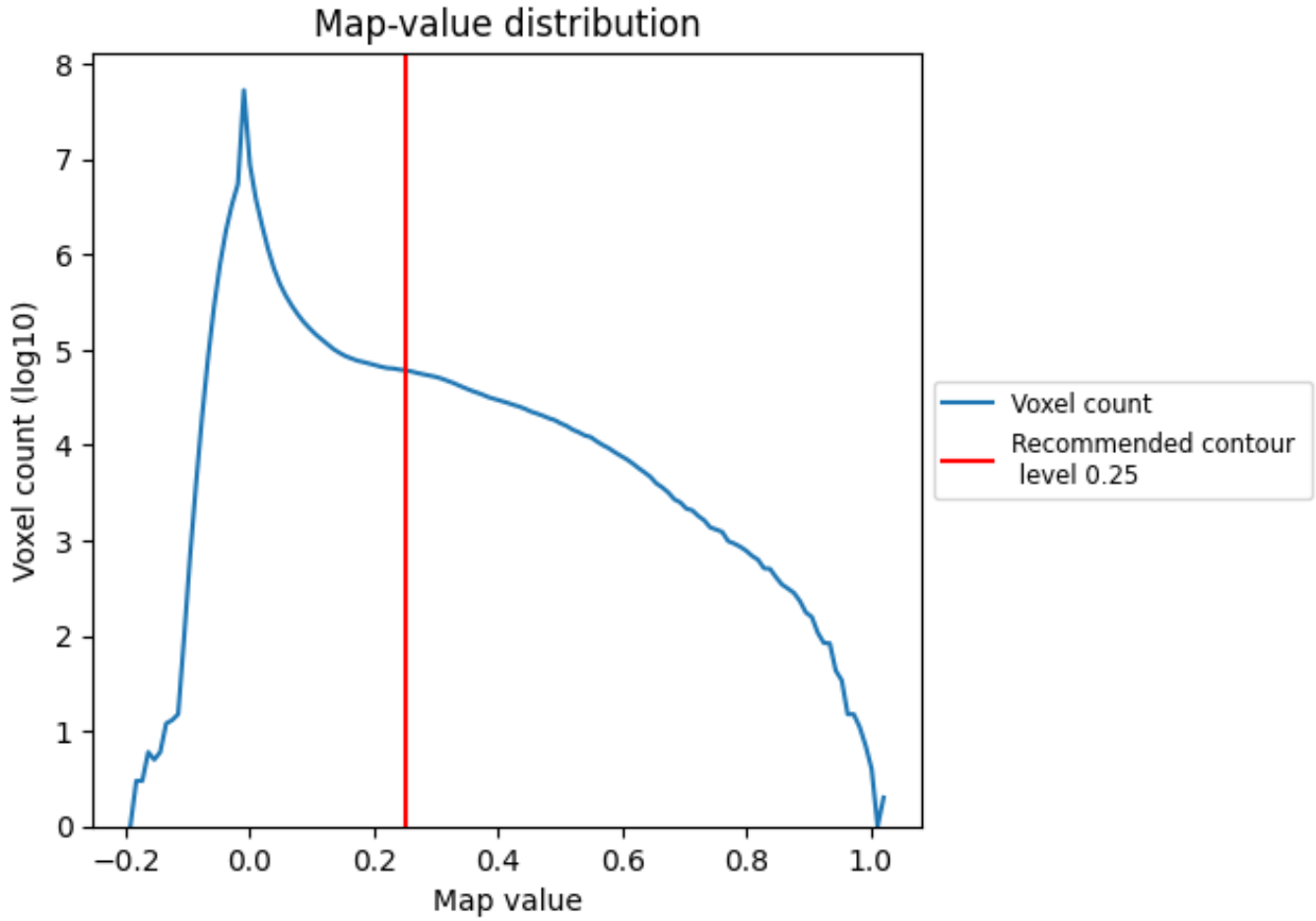


Z

7 Map analysis

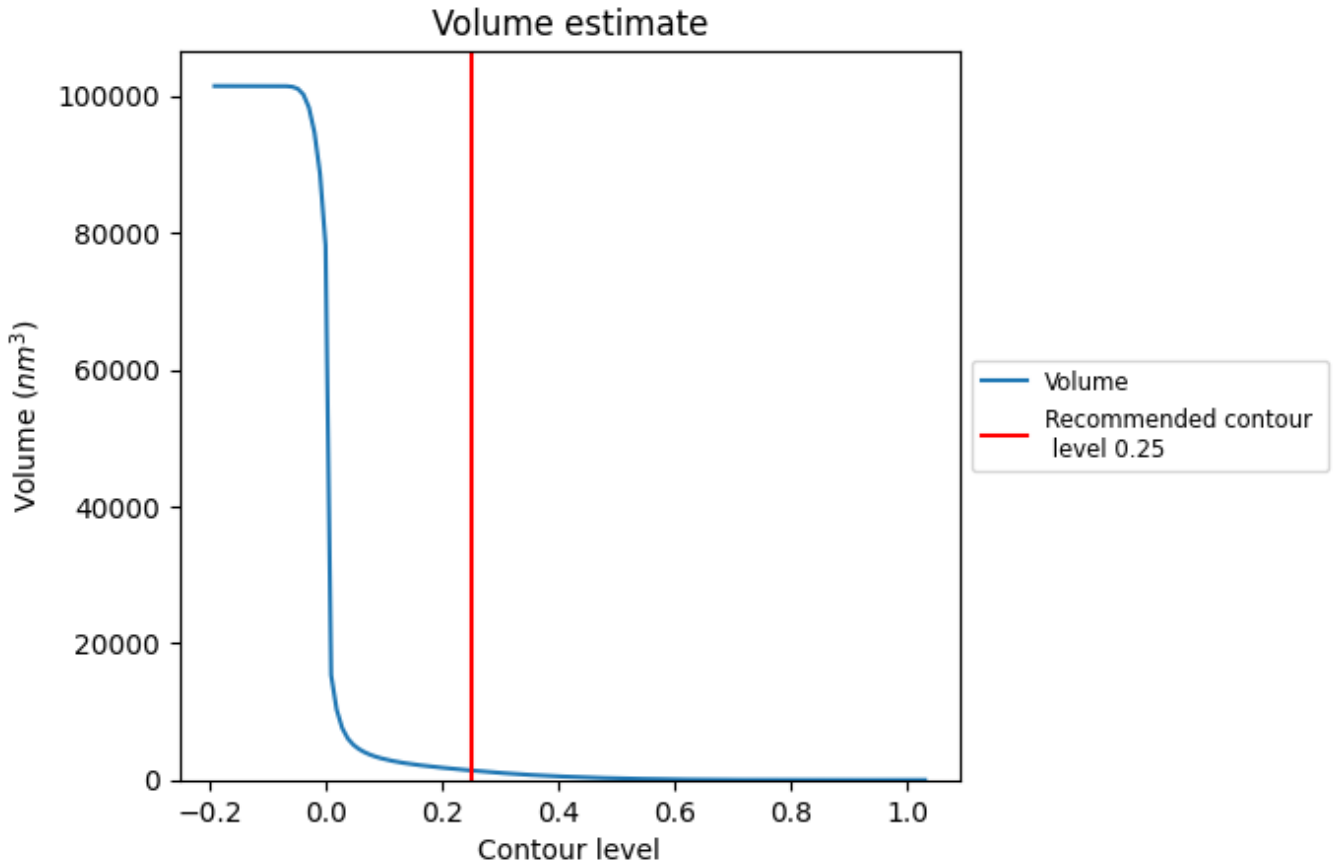
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

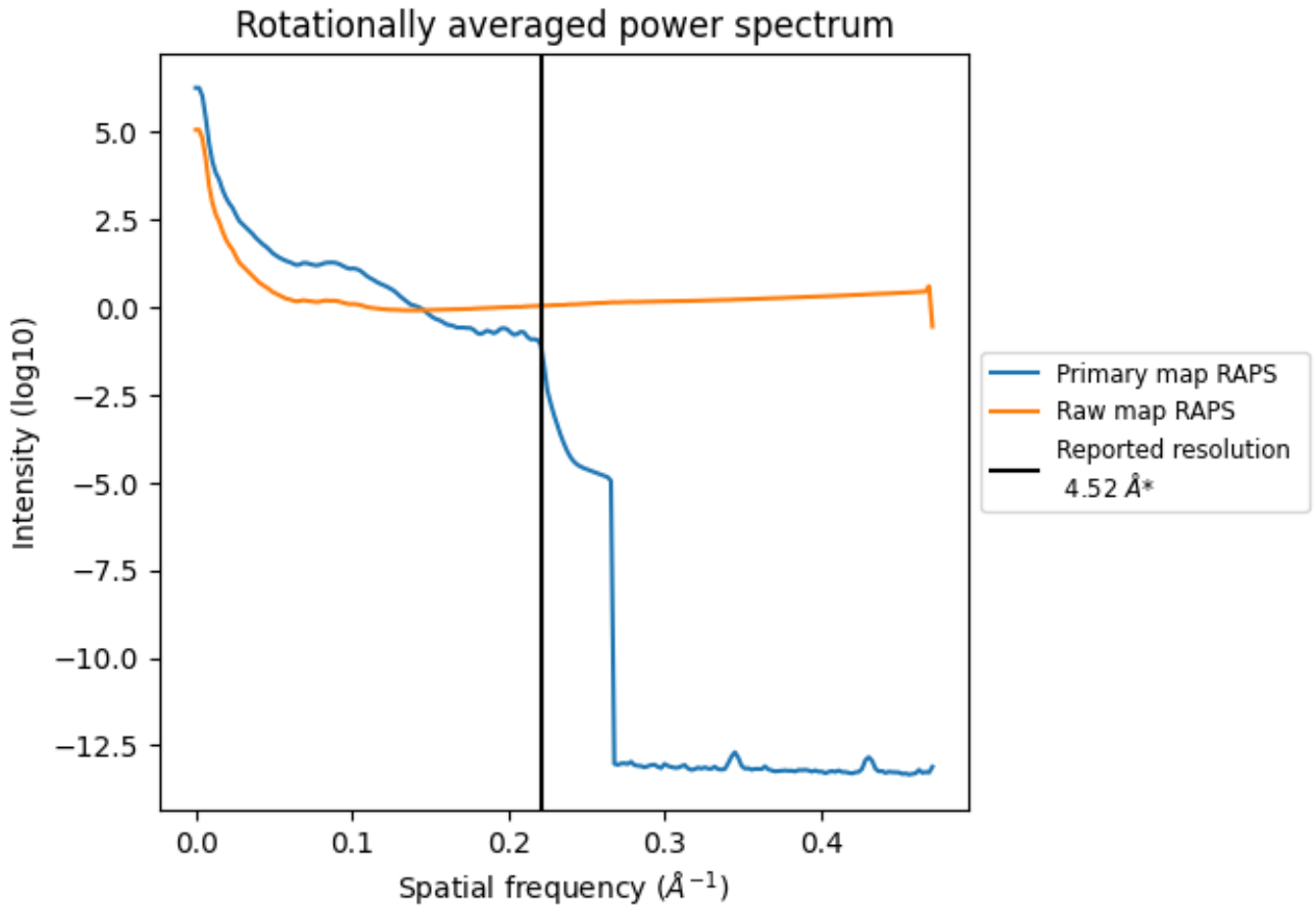
7.2 Volume estimate



The volume at the recommended contour level is 1385 nm^3; this corresponds to an approximate mass of 1251 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)

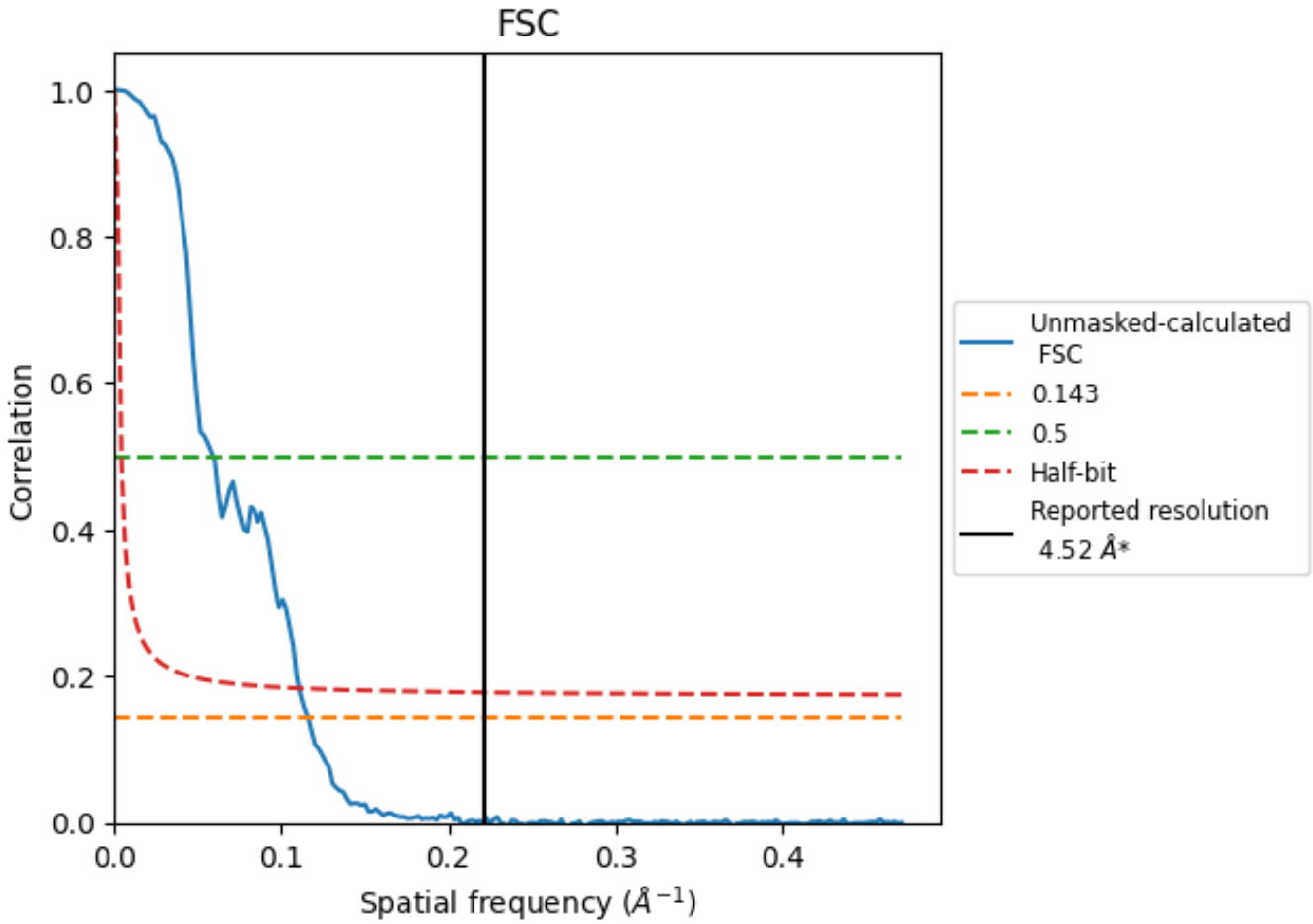


*Reported resolution corresponds to spatial frequency of 0.221 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.221 Å^{-1}

8.2 Resolution estimates (i)

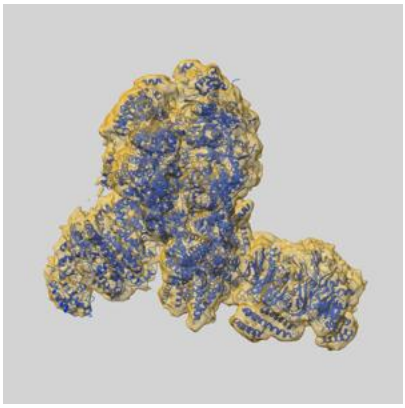
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.62	16.92	9.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.62 differs from the reported value 4.52 by more than 10 %

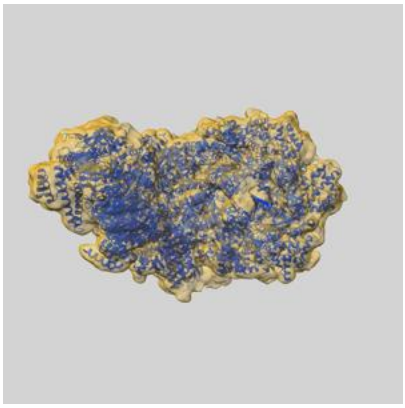
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37215 and PDB model 8KG9. Per-residue inclusion information can be found in section 3 on page 9.

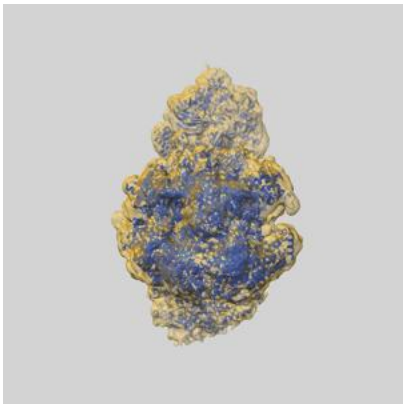
9.1 Map-model overlay



X



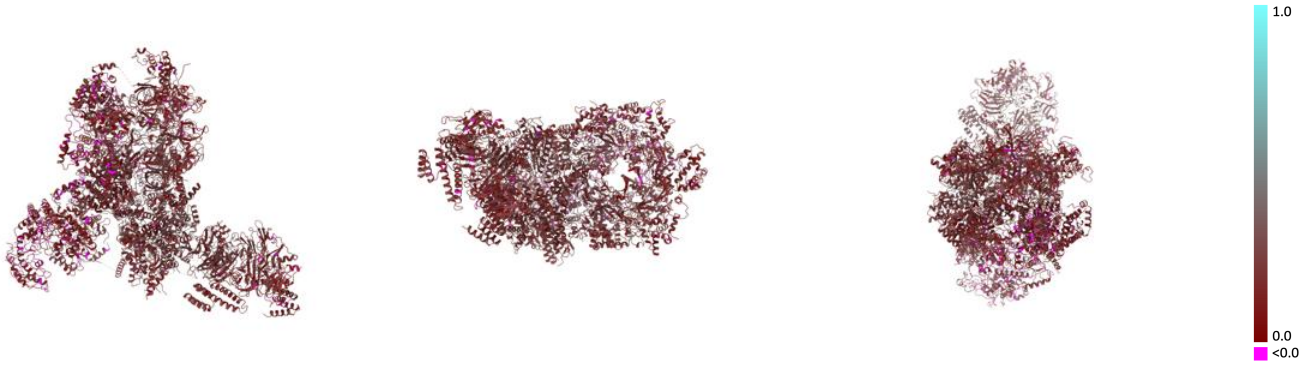
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

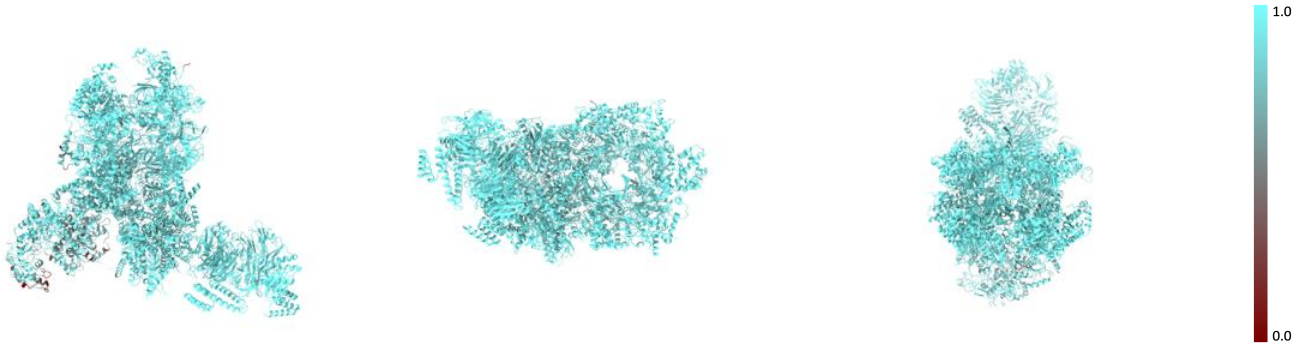
9.2 Q-score mapped to coordinate model (i)



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.

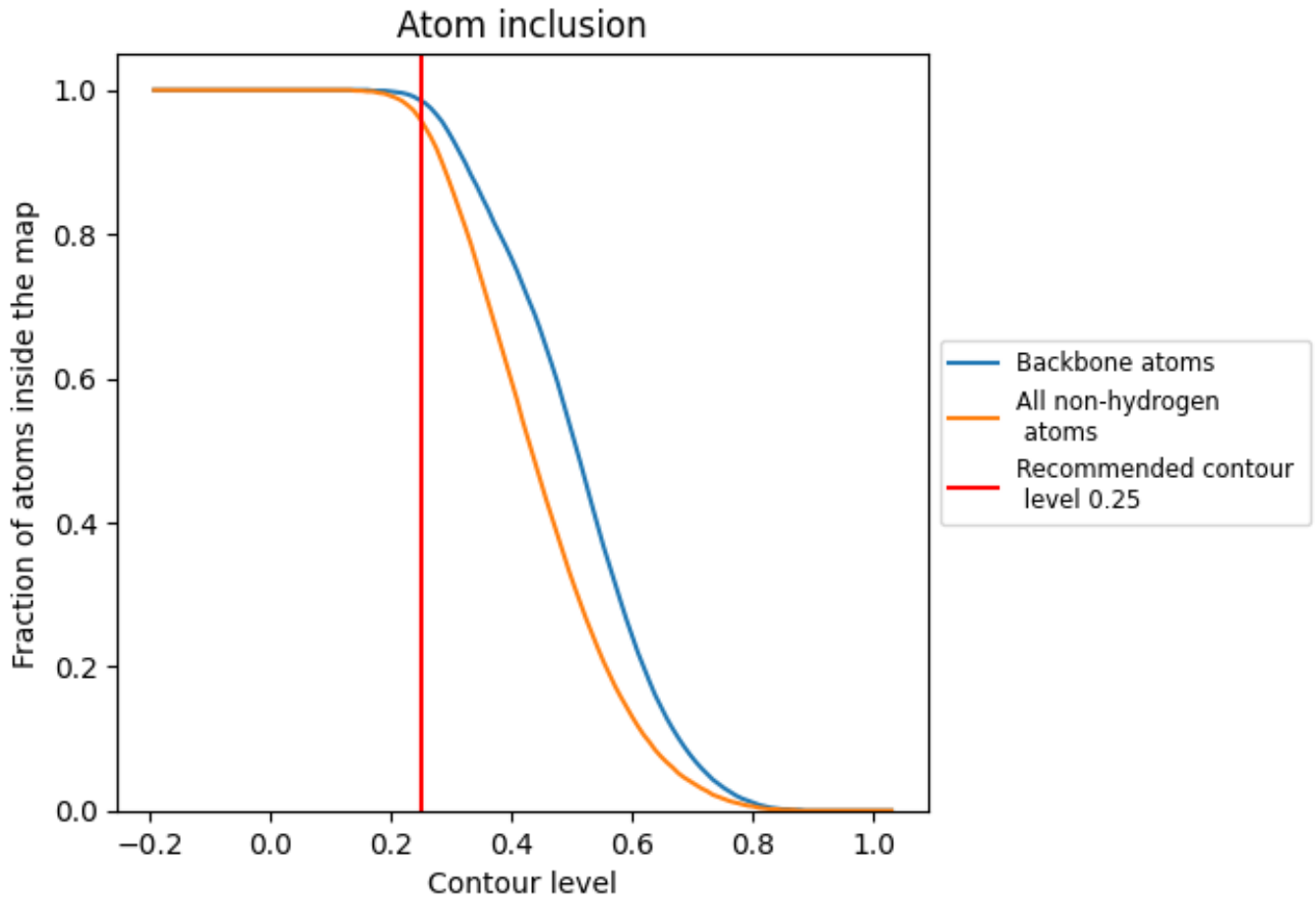
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.1900
2	0.9700	0.1940
3	0.9880	0.2150
4	0.9710	0.1590
5	0.9620	0.1950
6	0.9880	0.1660
7	0.9900	0.1930
A	0.9760	0.2100
B	0.9740	0.2370
C	0.9800	0.2200
D	0.9800	0.2310
E	0.9740	0.2230
F	0.9820	0.2270
G	0.9940	0.1930
H	0.9910	0.2000
I	0.9380	0.1820
J	0.8110	0.1360
M	0.8210	0.1410
N	0.9070	0.1640