wwPDB EM Validation Summary Report (i)

May 19, 2024 – 01:21 pm BST

PDB ID	:	6SKL
EMDB ID	:	EMD-10227
Title	:	Cryo-EM structure of the CMG Fork Protection Complex at a replication fork - Conformation 1
Authors	:	Yeeles, J.; Baretic, D.; Jenkyn-Bedford, M.
Deposited on	:	2019-08-16
Resolution	:	3.70 Å(reported)
Based on initial models	:	5U8S, 4C8H, 5MQI

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

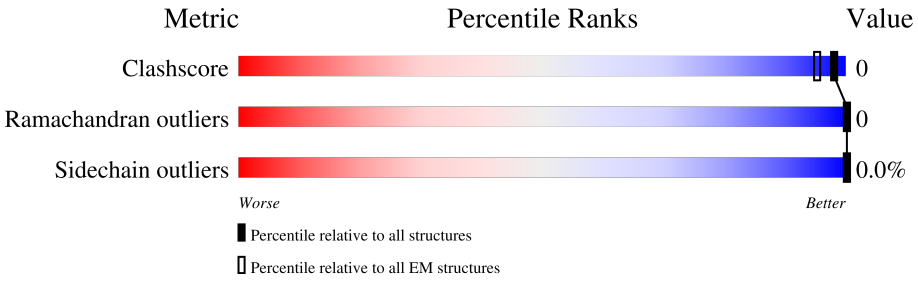
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.70 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	27% 71% 6% 23%
2	3	971	12% 59% · 37%
3	4	933	46% 68% · 27%
4	5	775	16% 75% · 21%
5	6	1017	23% 59% · 37%
6	7	845	33% 71% · 25%
7	A	208	25% 89% 5% 5%
8	B	213	7% 85% · · 9%

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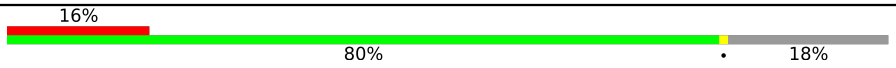
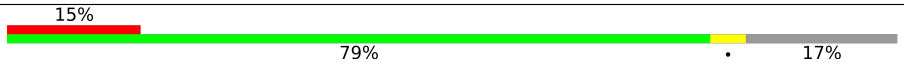
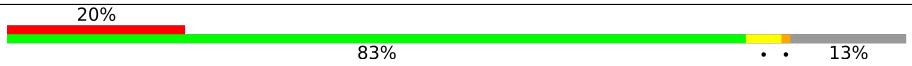
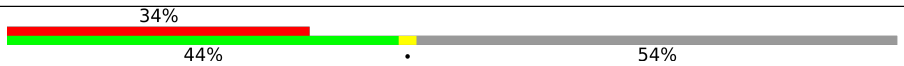
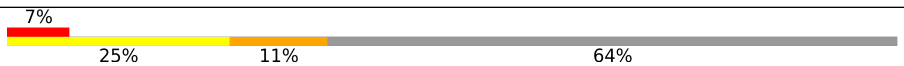
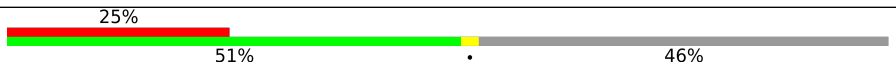
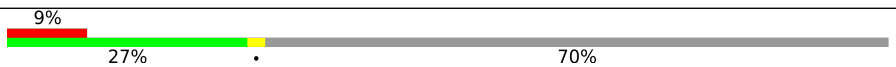
Mol	Chain	Length	Quality of chain
9	C	217	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	85	
14	J	61	
15	X	1238	
16	Y	317	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 118220 atoms, of which 59036 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	H	N	O	S		
1	2	669	10572	3310	5301	948	995	18	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	616	9707	3041	4886	862	905	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	679	10882	3389	5484	939	1039	31	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	611	9676	3018	4874	826	934	24	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	637	10044	3162	5031	881	945	25	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	635	9980	3142	5018	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	197	Total	C	H	N	O	S	0	0
			3227	1012	1616	277	313	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	193	Total	C	H	N	O	S	0	0
			3292	1039	1675	286	287	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	177	Total	C	H	N	O	S	0	0
			2858	924	1436	230	260	8		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	initiating methionine	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	243	Total	C	H	N	O	S	0	0
			4008	1276	2004	327	389	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	564	Total	C	H	N	O	S	0	0
			9129	2916	4560	772	867	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	424	Total	C	H	N	O	S	0	0
			6759	2188	3355	564	637	15		
12	G	422	Total	C	H	N	O	S	0	0
			6693	2172	3313	557	636	15		
12	H	425	Total	C	H	N	O	S	0	0
			6769	2193	3358	565	638	15		

- Molecule 13 is a DNA chain called DNA fork, leading-strand template.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	I	37	Total	C	H	N	O	P	0	0
			1192	370	430	116	239	37		

- Molecule 14 is a DNA chain called DNA fork, lagging-strand template.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	J	22	Total	C	H	N	O	P	0	0
			686	211	248	74	131	22		

- Molecule 15 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	X	665	Total	C	H	N	O	S	0	0
			10990	3505	5580	912	974	19		

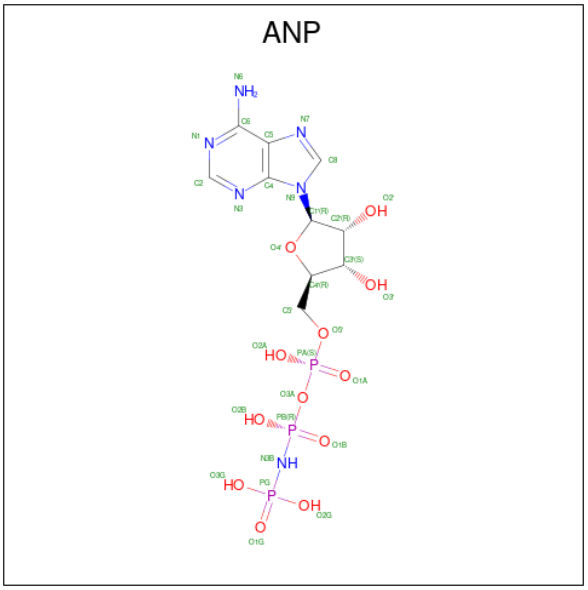
- Molecule 16 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Y	94	Total	C	H	N	O	S	0	0
			1616	507	828	144	133	4		

- 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	

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
18	2	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
18	3	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
18	5	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

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

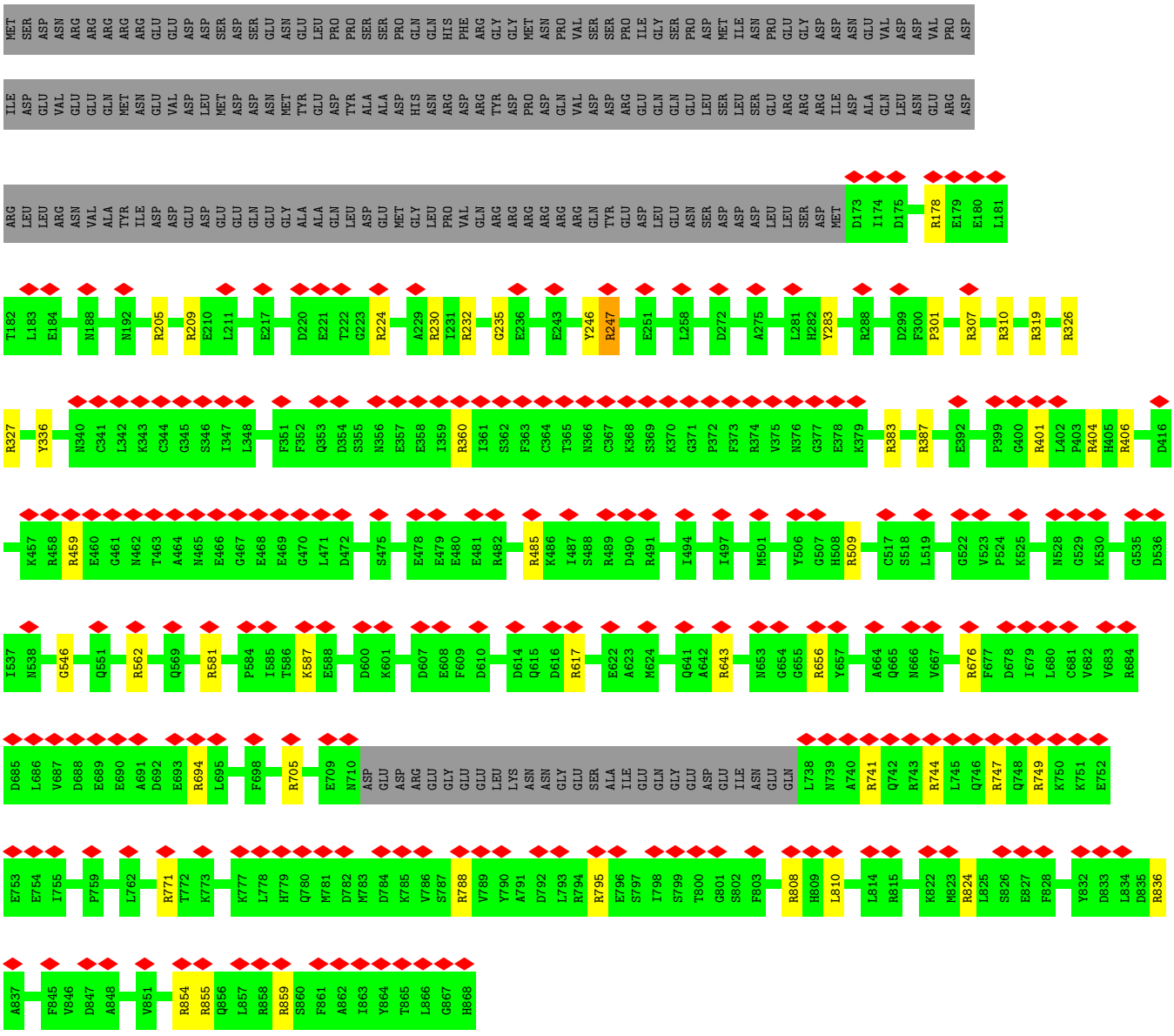
Mol	Chain	Residues	Atoms	AltConf
19	2	1	Total Mg 1 1	0
19	3	1	Total Mg 1 1	0
19	5	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

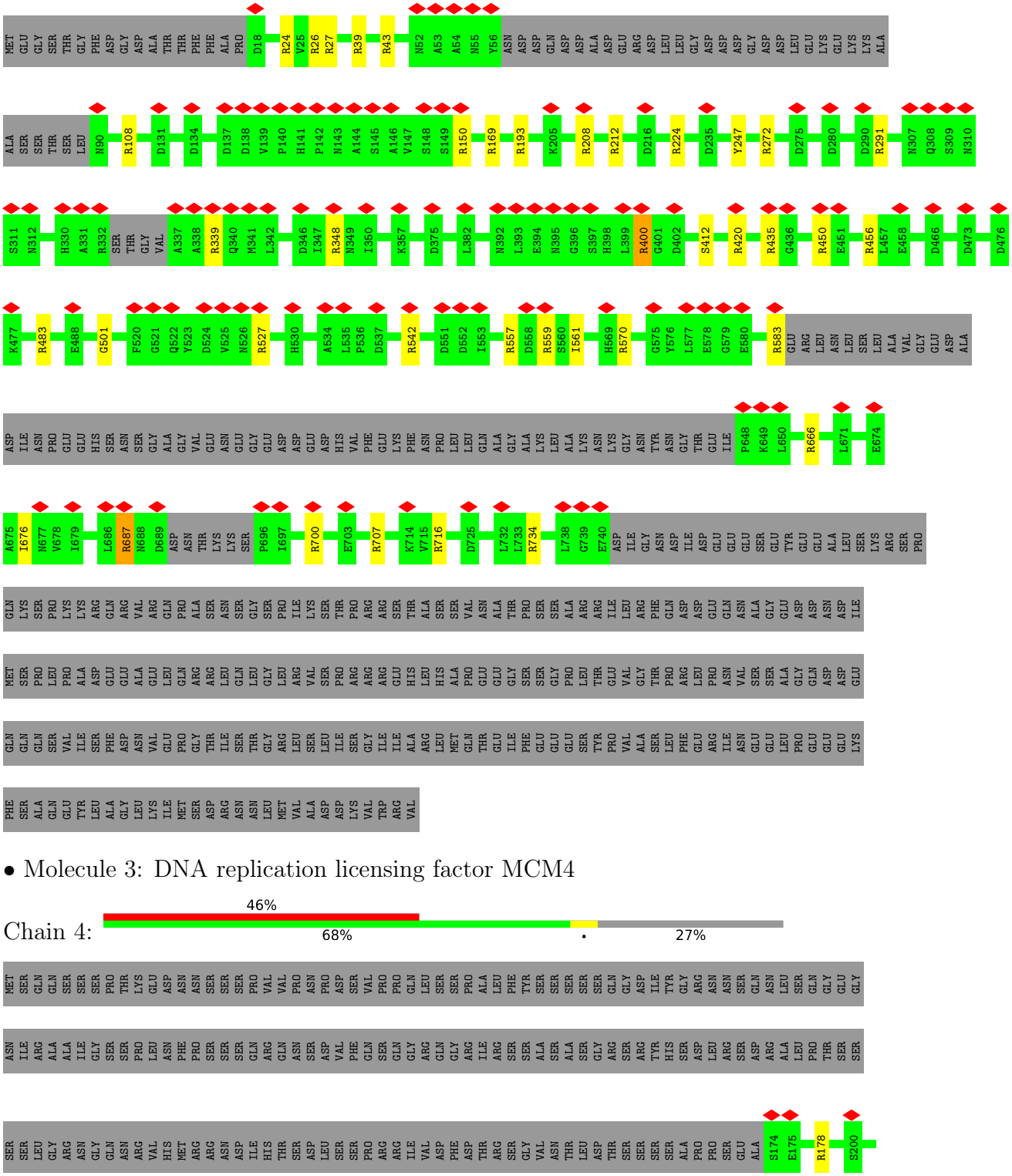
- Molecule 1: DNA replication licensing factor MCM2

Chain 2:



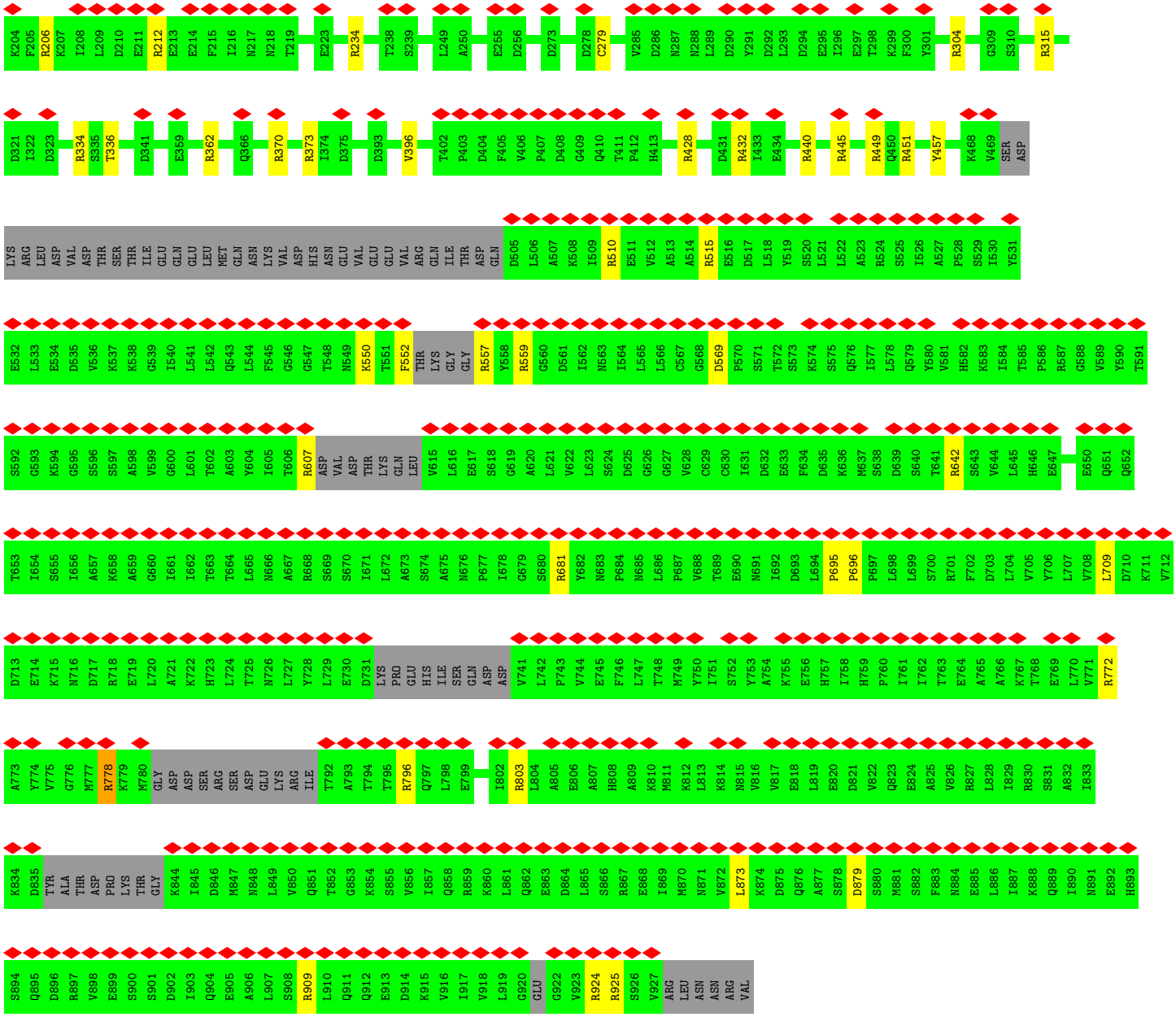
• Molecule 2: DNA replication licensing factor MCM3

Chain 3:



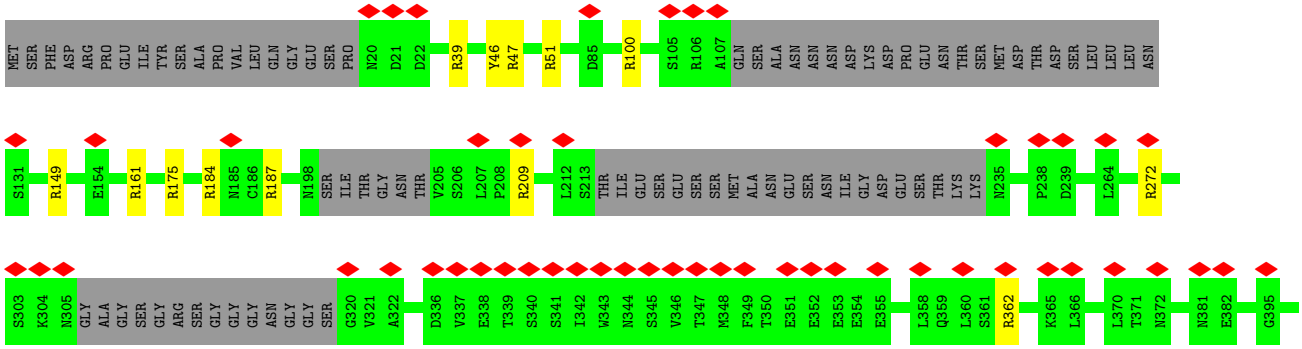
• Molecule 3: DNA replication licensing factor MCM4

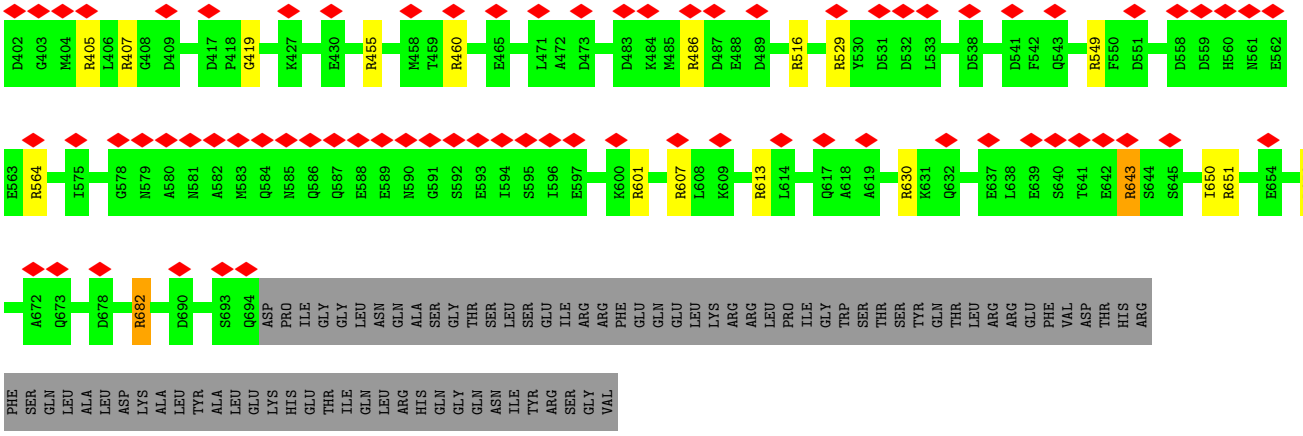
Chain 4:

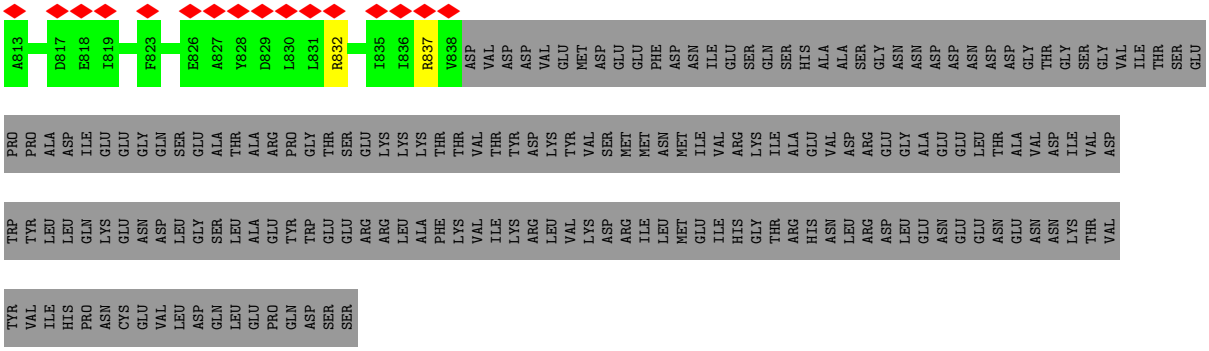


• Molecule 4: Minichromosome maintenance protein 5

Chain 5:

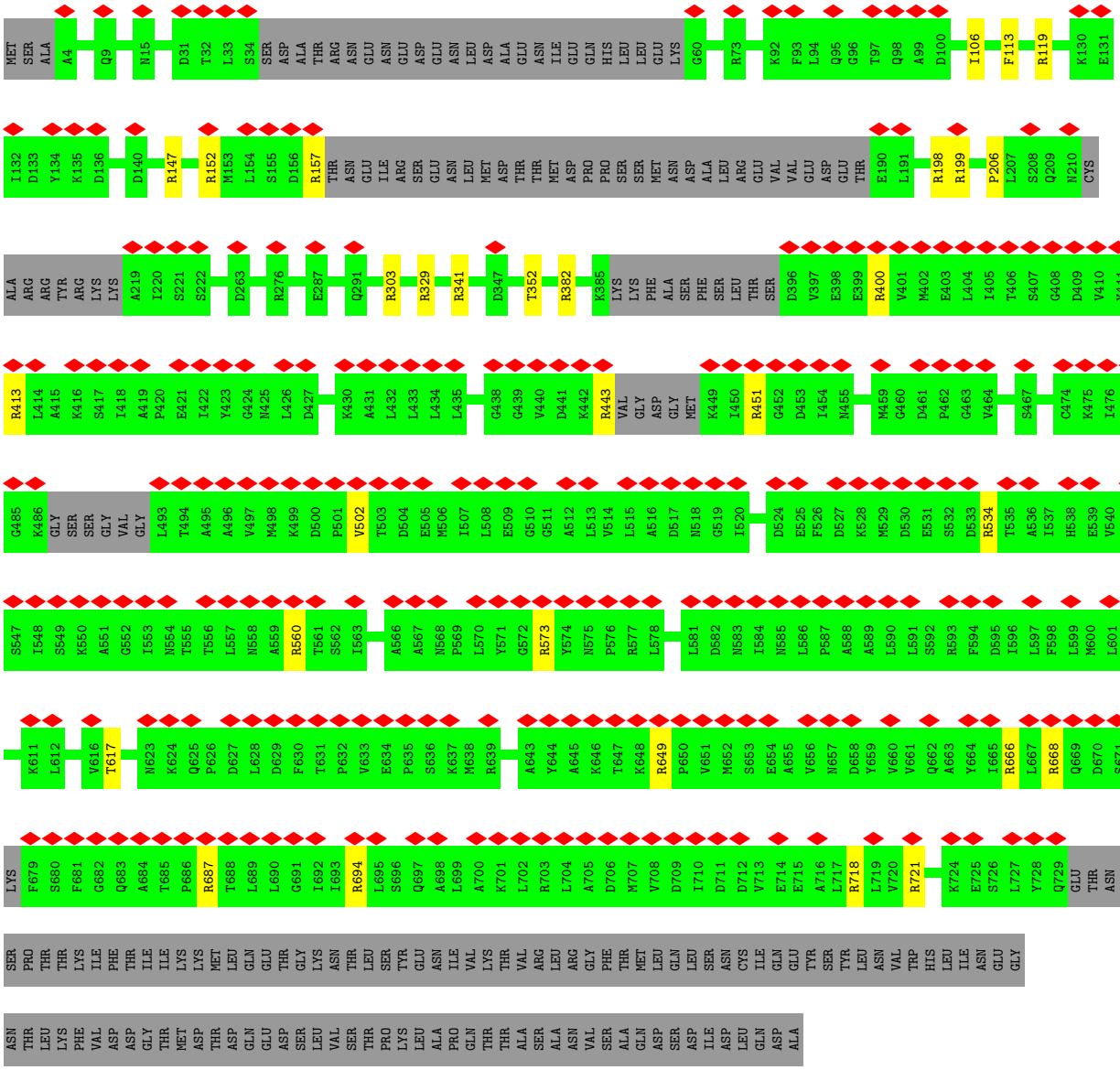






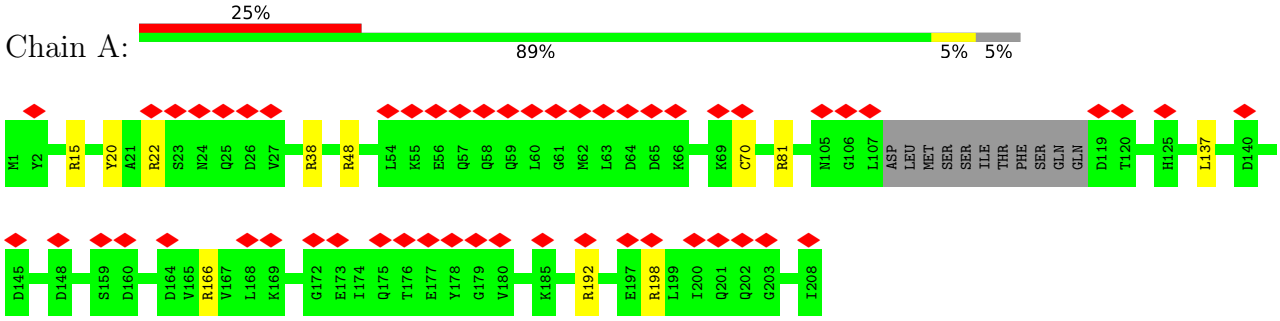
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



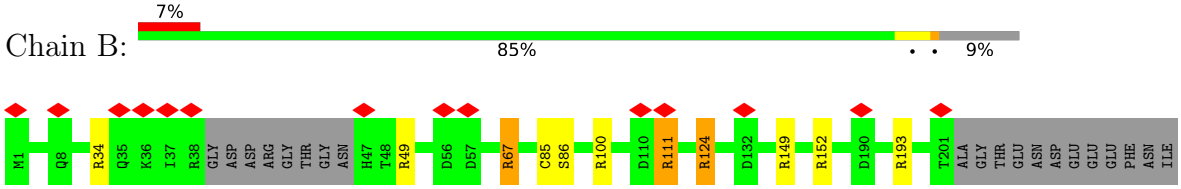
• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:



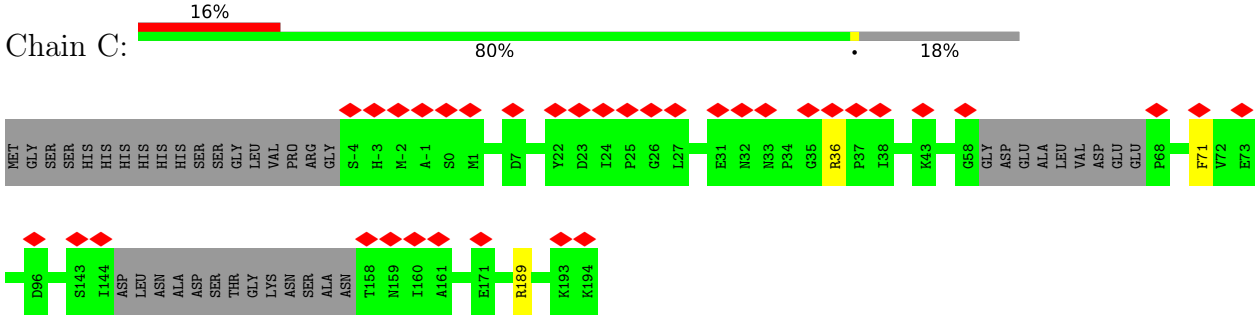
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B:



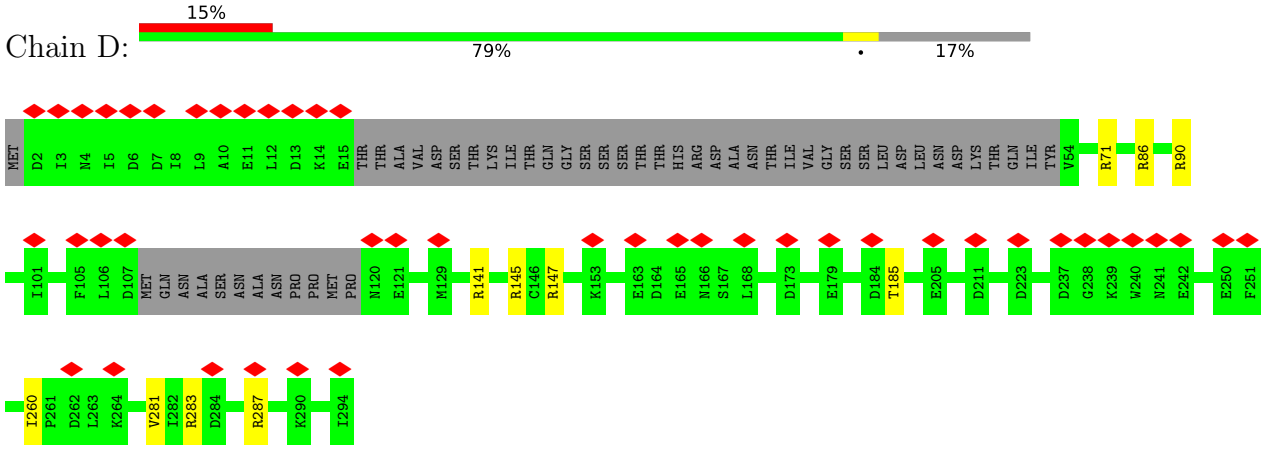
• Molecule 9: DNA replication complex GINS protein PSF3

Chain C:



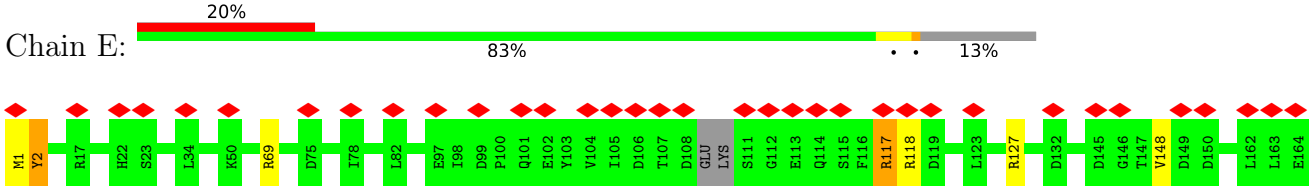
• Molecule 10: DNA replication complex GINS protein SLD5

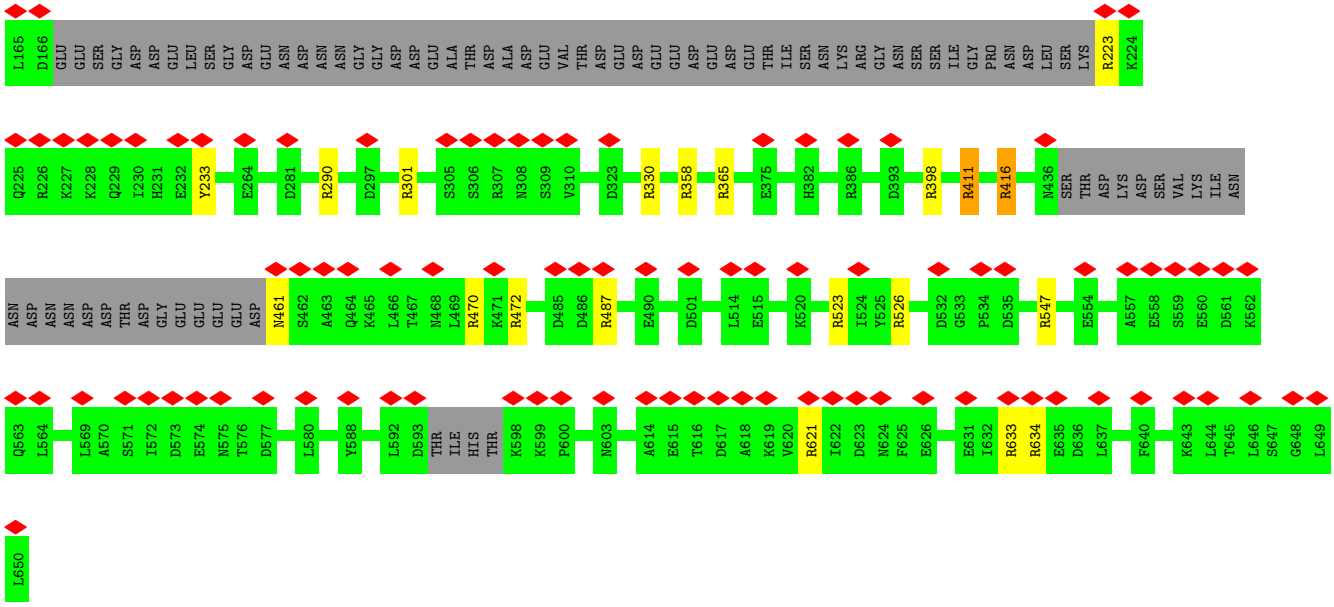
Chain D:



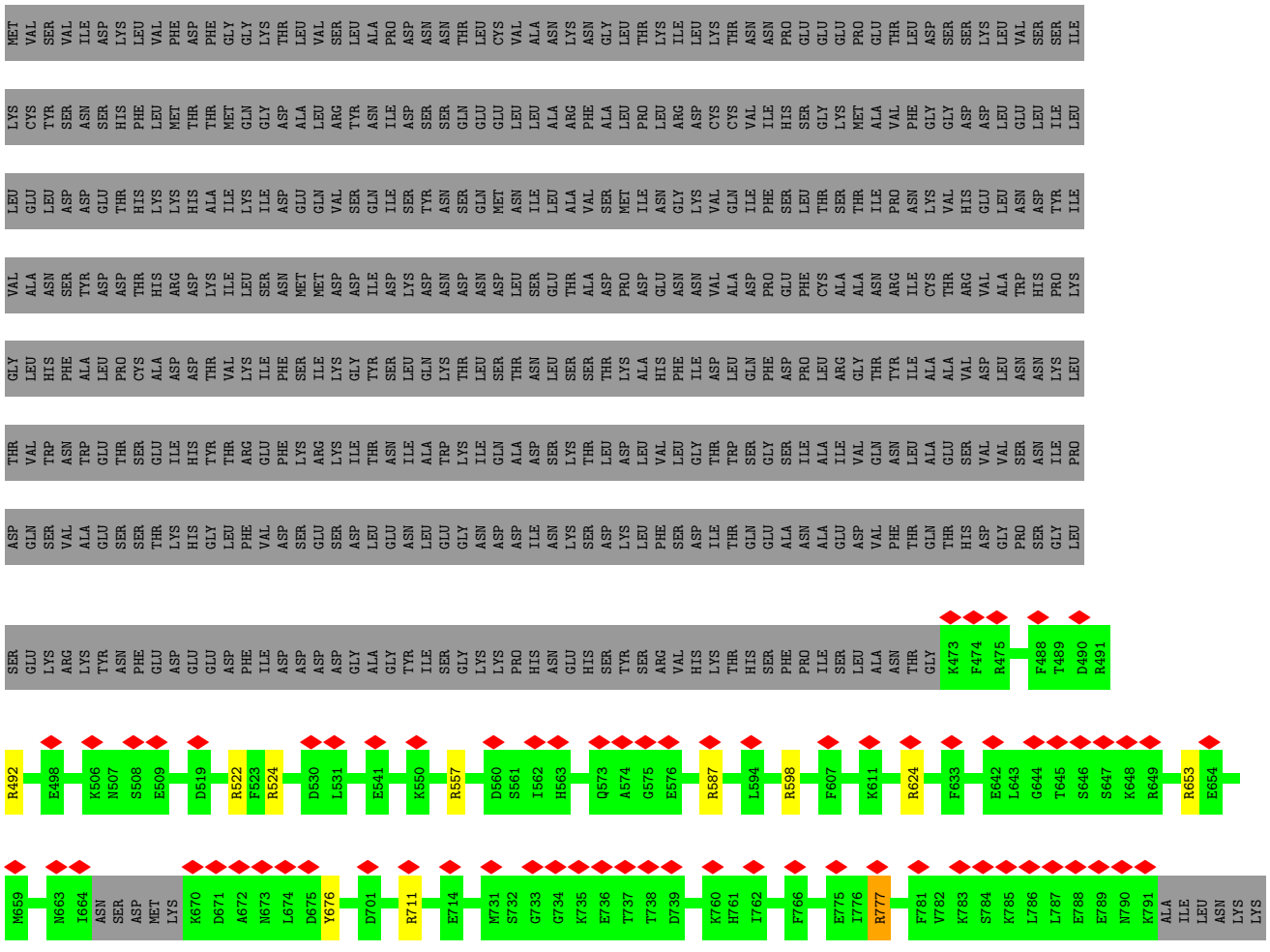
• Molecule 11: Cell division control protein 45

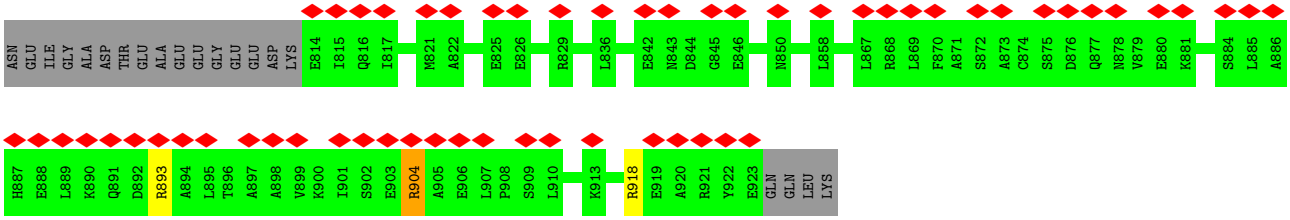
Chain E:



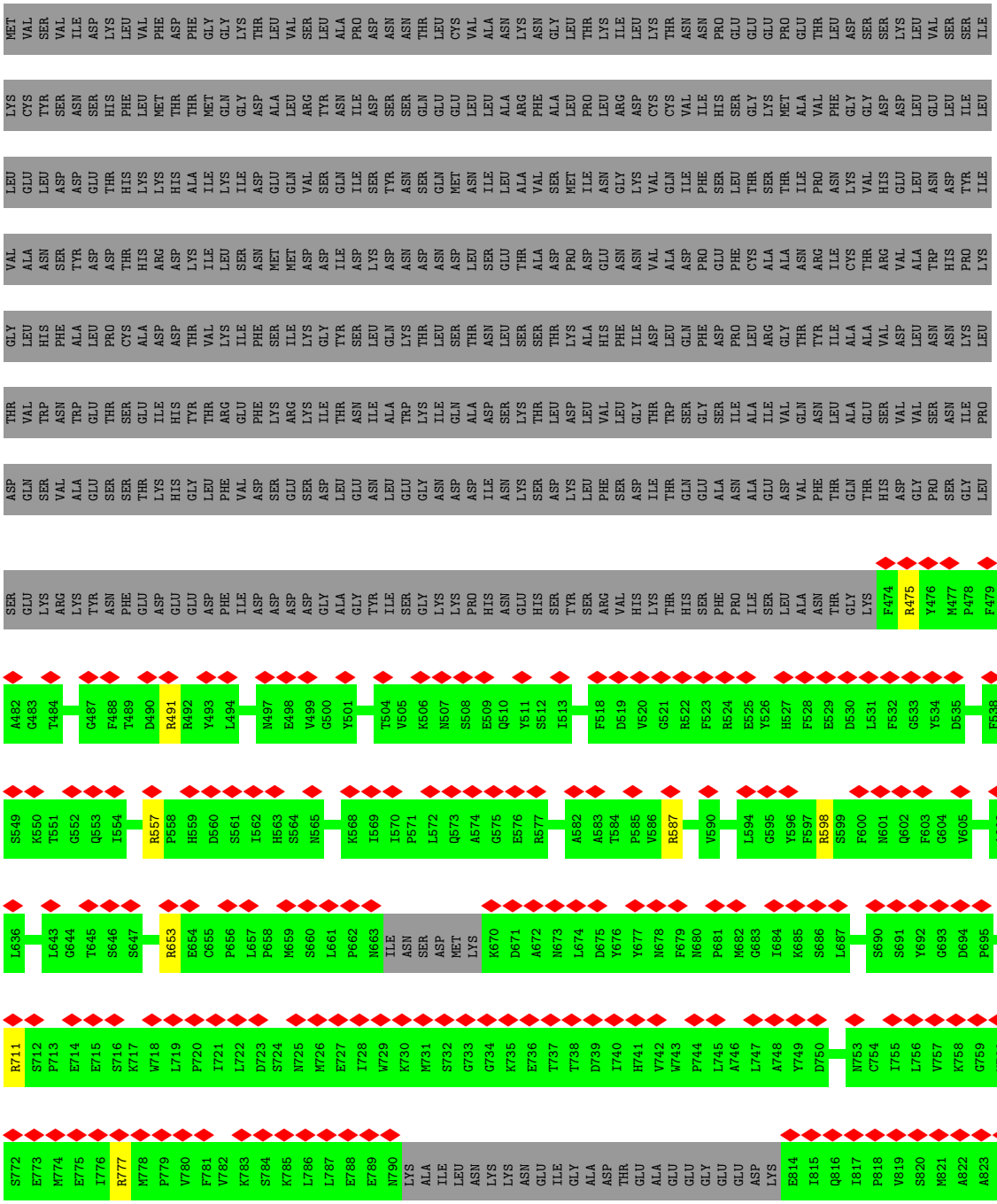


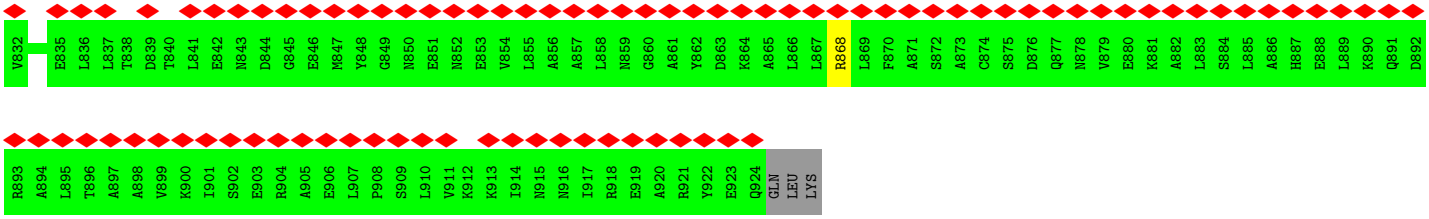
• Molecule 12: DNA polymerase alpha-binding protein



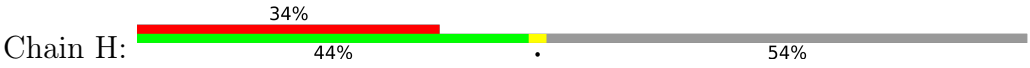


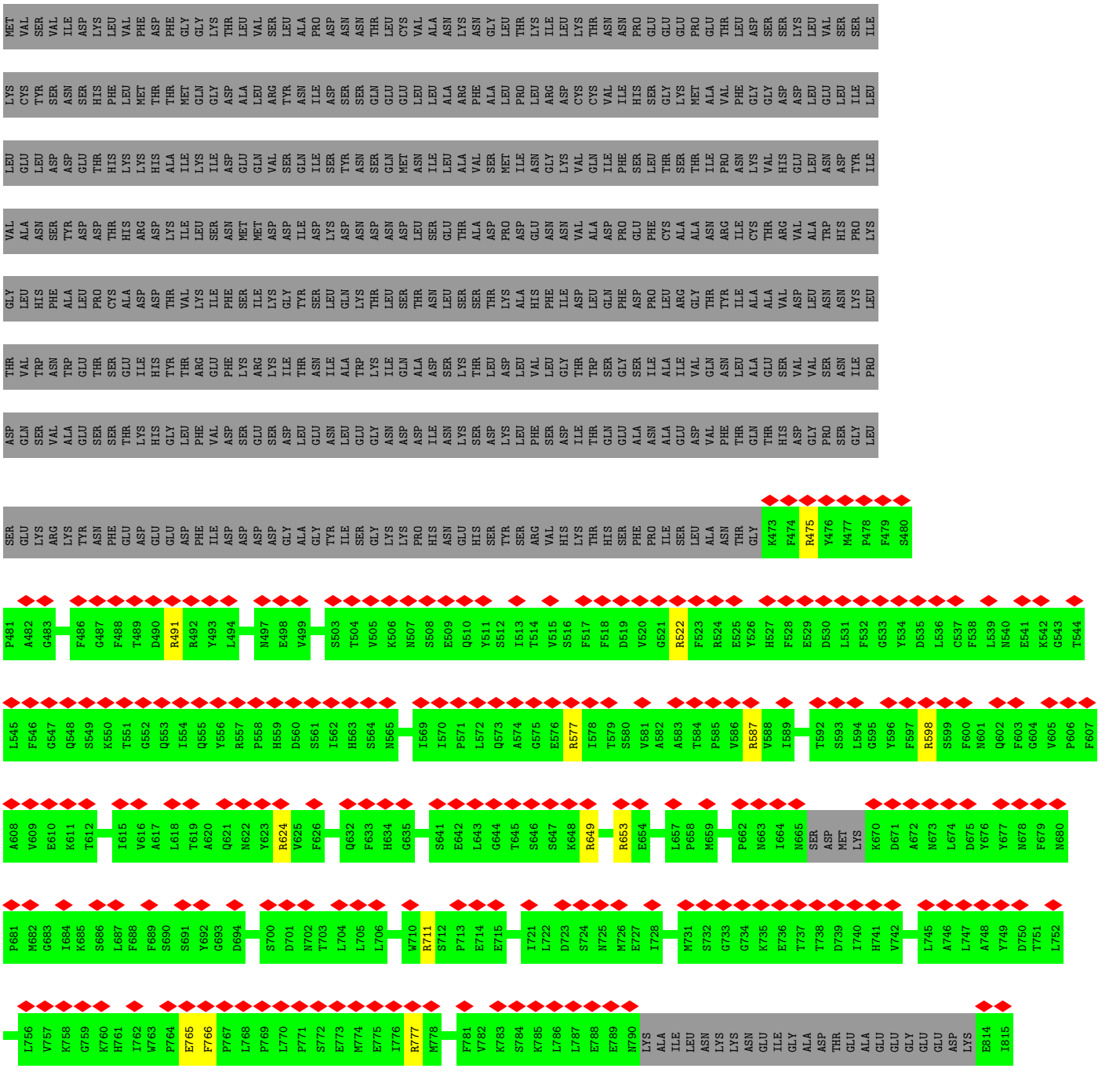
• Molecule 12: DNA polymerase alpha-binding protein

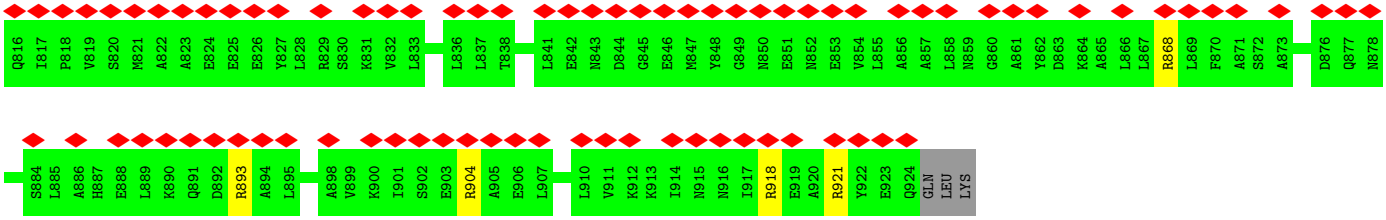




• Molecule 12: DNA polymerase alpha-binding protein

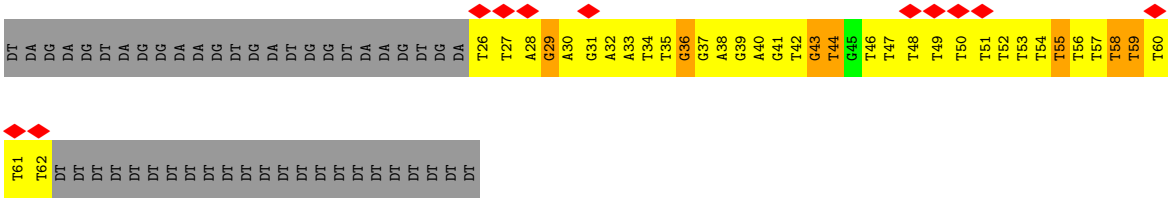






• Molecule 13: DNA fork, leading-strand template

Chain I:

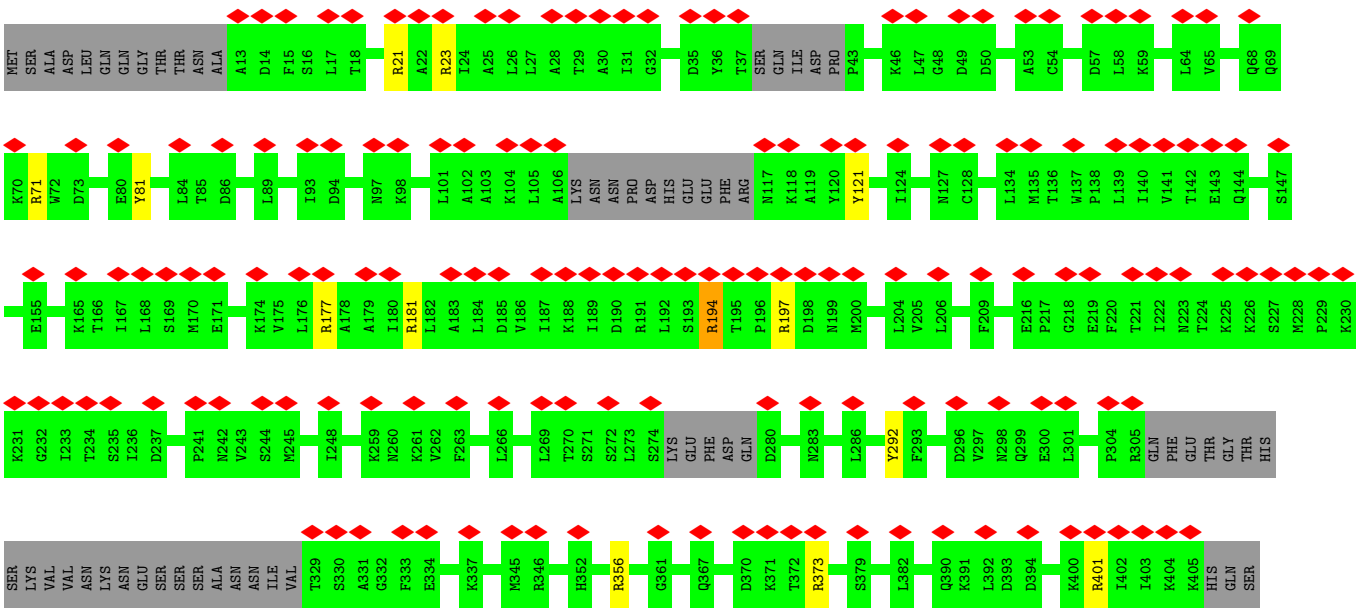


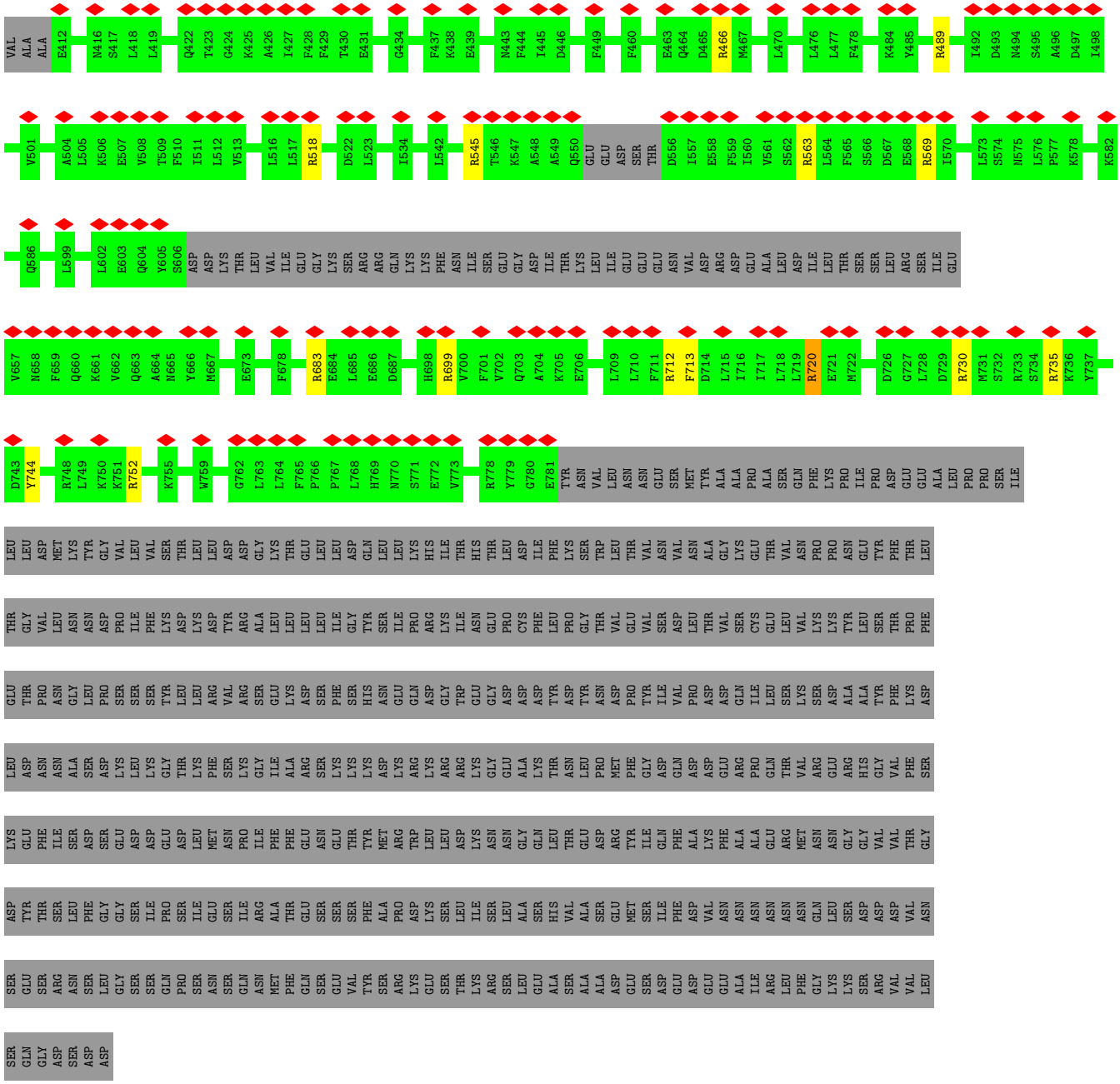
• Molecule 14: DNA fork, lagging-strand template

Chain J:

• Molecule 15: Topoisomerase 1-associated factor 1

Chain X:





• Molecule 16: Chromosome segregation in meiosis protein 3

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

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

THR HIS TYR ASP LEU LEU PRO GLY GLY ASP GLU PHE GLY VAL ASP GLN ASP GLU LEU ASP ALA MET LYS GLU MET GLY PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35000	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 ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.69	0/5361	1.13	43/7244 (0.6%)
2	3	0.65	0/4907	1.07	36/6655 (0.5%)
3	4	0.65	0/5468	1.08	32/7376 (0.4%)
4	5	0.64	0/4869	1.08	30/6581 (0.5%)
5	6	0.67	0/5095	1.10	33/6875 (0.5%)
6	7	0.65	0/5037	1.04	27/6814 (0.4%)
7	A	0.67	0/1631	1.10	9/2194 (0.4%)
8	B	0.69	0/1650	1.09	10/2231 (0.4%)
9	C	0.63	0/1456	0.99	2/1966 (0.1%)
10	D	0.67	0/2040	1.03	8/2755 (0.3%)
11	E	0.68	1/4653 (0.0%)	1.08	21/6297 (0.3%)
12	F	0.70	0/3489	1.04	13/4724 (0.3%)
12	G	0.68	0/3465	1.06	10/4696 (0.2%)
12	H	0.68	0/3496	1.05	16/4735 (0.3%)
13	I	1.59	2/849 (0.2%)	2.52	81/1312 (6.2%)
14	J	1.66	0/488	2.51	50/747 (6.7%)
15	X	0.64	0/5512	1.05	24/7426 (0.3%)
16	Y	0.68	0/804	1.06	7/1074 (0.7%)
All	All	0.70	3/60270 (0.0%)	1.13	452/81702 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	3
2	3	0	3
3	4	0	1
4	5	0	3
5	6	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	1
8	B	0	3
11	E	0	6
12	F	0	3
13	I	0	8
14	J	0	5
15	X	0	5
16	Y	0	1
All	All	0	45

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	461	ASN	N-CA	-5.74	1.34	1.46
13	I	43	DG	C2-N2	-5.23	1.29	1.34
13	I	39	DG	C2-N2	-5.08	1.29	1.34

The worst 5 of 452 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	50	DT	O4'-C1'-N1	12.73	116.91	108.00
7	A	20	TYR	CB-CG-CD1	-12.13	113.72	121.00
12	G	653	ARG	NE-CZ-NH1	10.69	125.64	120.30
5	6	176	ARG	NE-CZ-NH2	10.41	125.51	120.30
8	B	152	ARG	NE-CZ-NH1	10.15	125.37	120.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	247	ARG	Sidechain
1	2	327	ARG	Sidechain
1	2	336	TYR	Sidechain
2	3	247	TYR	Sidechain
2	3	400	ARG	Sidechain

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	5271	5301	5294	5	0
2	3	4821	4886	4882	6	0
3	4	5398	5484	5472	5	0
4	5	4802	4874	4865	3	0
5	6	5013	5031	5022	2	0
6	7	4962	5018	5006	6	0
7	A	1611	1616	1615	2	0
8	B	1617	1675	1674	1	0
9	C	1422	1436	1436	1	0
10	D	2004	2004	2001	2	0
11	E	4569	4560	4556	1	0
12	F	3404	3355	3352	0	0
12	G	3380	3313	3310	0	0
12	H	3411	3358	3355	1	0
13	I	762	430	427	0	0
14	J	438	248	248	1	0
15	X	5410	5580	5573	0	0
16	Y	788	828	827	0	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
18	2	31	13	13	3	0
18	3	31	13	13	2	0
18	5	31	13	13	2	0
19	2	1	0	0	0	0
19	3	1	0	0	0	0
19	5	1	0	0	0	0
All	All	59184	59036	58954	30	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 0.

The worst 5 of 30 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)
2:3:412:SER:H	18:3:1500:ANP:HNB1	1.15	0.92
1:2:546:GLY:H	18:2:902:ANP:HNB1	1.20	0.84
2:3:412:SER:N	18:3:1500:ANP:HNB1	1.90	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:206:PRO:HD3	6:7:352:THR:HG21	1.76	0.66
4:5:419:GLY:H	18:5:801:ANP:HNB1	1.42	0.66

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	665/868 (77%)	642 (96%)	23 (4%)	0	100	100
2	3	606/971 (62%)	591 (98%)	15 (2%)	0	100	100
3	4	663/933 (71%)	631 (95%)	32 (5%)	0	100	100
4	5	601/775 (78%)	580 (96%)	21 (4%)	0	100	100
5	6	625/1017 (62%)	601 (96%)	24 (4%)	0	100	100
6	7	619/845 (73%)	593 (96%)	26 (4%)	0	100	100
7	A	193/208 (93%)	189 (98%)	4 (2%)	0	100	100
8	B	189/213 (89%)	185 (98%)	4 (2%)	0	100	100
9	C	171/217 (79%)	170 (99%)	1 (1%)	0	100	100
10	D	237/294 (81%)	231 (98%)	6 (2%)	0	100	100
11	E	554/650 (85%)	544 (98%)	10 (2%)	0	100	100
12	F	418/927 (45%)	395 (94%)	23 (6%)	0	100	100
12	G	416/927 (45%)	406 (98%)	10 (2%)	0	100	100
12	H	419/927 (45%)	403 (96%)	16 (4%)	0	100	100
15	X	649/1238 (52%)	630 (97%)	19 (3%)	0	100	100
16	Y	92/317 (29%)	92 (100%)	0	0	100	100
All	All	7117/11327 (63%)	6883 (97%)	234 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	577/770 (75%)	577 (100%)	0	100	100
2	3	530/835 (64%)	530 (100%)	0	100	100
3	4	614/848 (72%)	614 (100%)	0	100	100
4	5	548/688 (80%)	548 (100%)	0	100	100
5	6	550/886 (62%)	550 (100%)	0	100	100
6	7	547/753 (73%)	547 (100%)	0	100	100
7	A	182/193 (94%)	182 (100%)	0	100	100
8	B	183/198 (92%)	183 (100%)	0	100	100
9	C	159/192 (83%)	159 (100%)	0	100	100
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	507/586 (86%)	506 (100%)	1 (0%)	93	97
12	F	375/825 (46%)	375 (100%)	0	100	100
12	G	372/825 (45%)	372 (100%)	0	100	100
12	H	375/825 (46%)	375 (100%)	0	100	100
15	X	607/1125 (54%)	606 (100%)	1 (0%)	93	97
16	Y	87/285 (30%)	87 (100%)	0	100	100
All	All	6447/10113 (64%)	6445 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	E	2	TYR
15	X	713	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	400	GLN
6	7	124	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
18	ANP	3	1500	19	29,33,33	1.64	9 (31%)	31,52,52	1.75	4 (12%)
18	ANP	5	801	19	29,33,33	1.53	8 (27%)	31,52,52	1.67	6 (19%)
18	ANP	2	902	19	29,33,33	1.62	8 (27%)	31,52,52	1.70	9 (29%)

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
18	ANP	3	1500	19	-	2/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ANP	5	801	19	-	4/14/38/38	0/3/3/3
18	ANP	2	902	19	-	4/14/38/38	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	1500	ANP	PB-O3A	-4.13	1.53	1.59
18	5	801	ANP	PB-O1B	3.60	1.51	1.46
18	2	902	ANP	PB-O3A	-3.51	1.54	1.59
18	2	902	ANP	PG-O1G	3.36	1.51	1.46
18	3	1500	ANP	PG-O1G	3.28	1.51	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	1500	ANP	O3A-PB-N3B	-4.76	93.38	106.59
18	5	801	ANP	C4-C5-N7	4.68	114.28	109.40
18	3	1500	ANP	PB-O3A-PA	-4.30	117.46	132.62
18	3	1500	ANP	C4-C5-N7	4.29	113.87	109.40
18	2	902	ANP	C4-C5-N7	4.07	113.64	109.40

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	2	902	ANP	PB-N3B-PG-O1G
18	3	1500	ANP	PB-N3B-PG-O1G
18	5	801	ANP	PB-N3B-PG-O1G
18	5	801	ANP	PA-O3A-PB-O1B
18	5	801	ANP	PA-O3A-PB-O2B

There are no ring outliers.

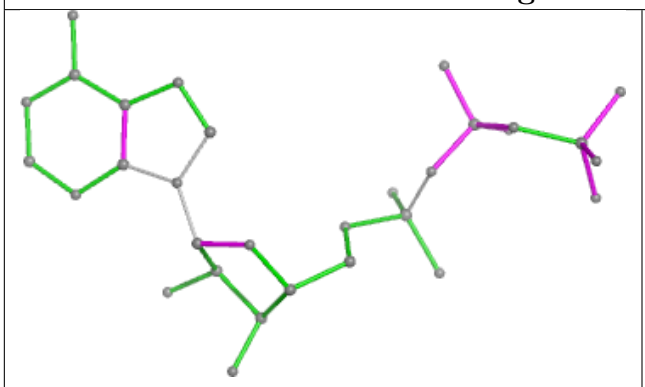
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	1500	ANP	2	0
18	5	801	ANP	2	0
18	2	902	ANP	3	0

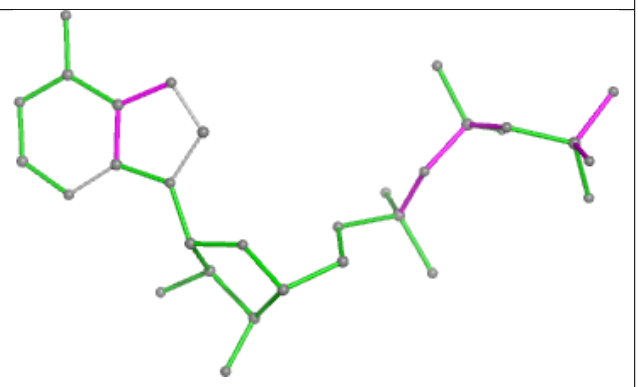
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

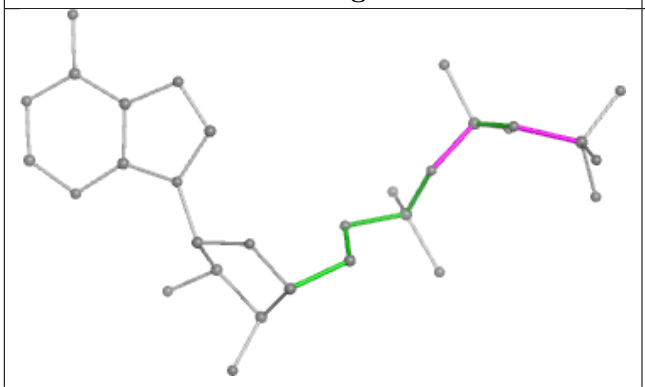
Ligand ANP 3 1500



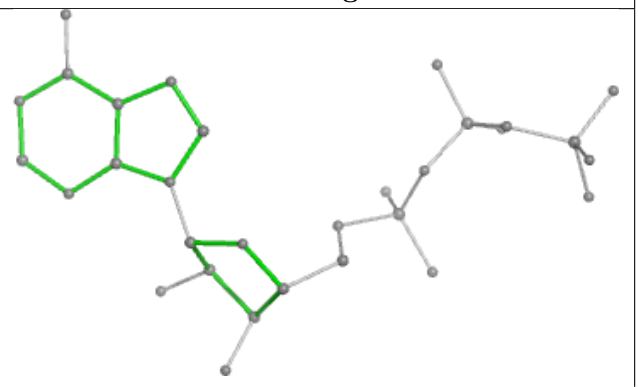
Bond lengths



Bond angles

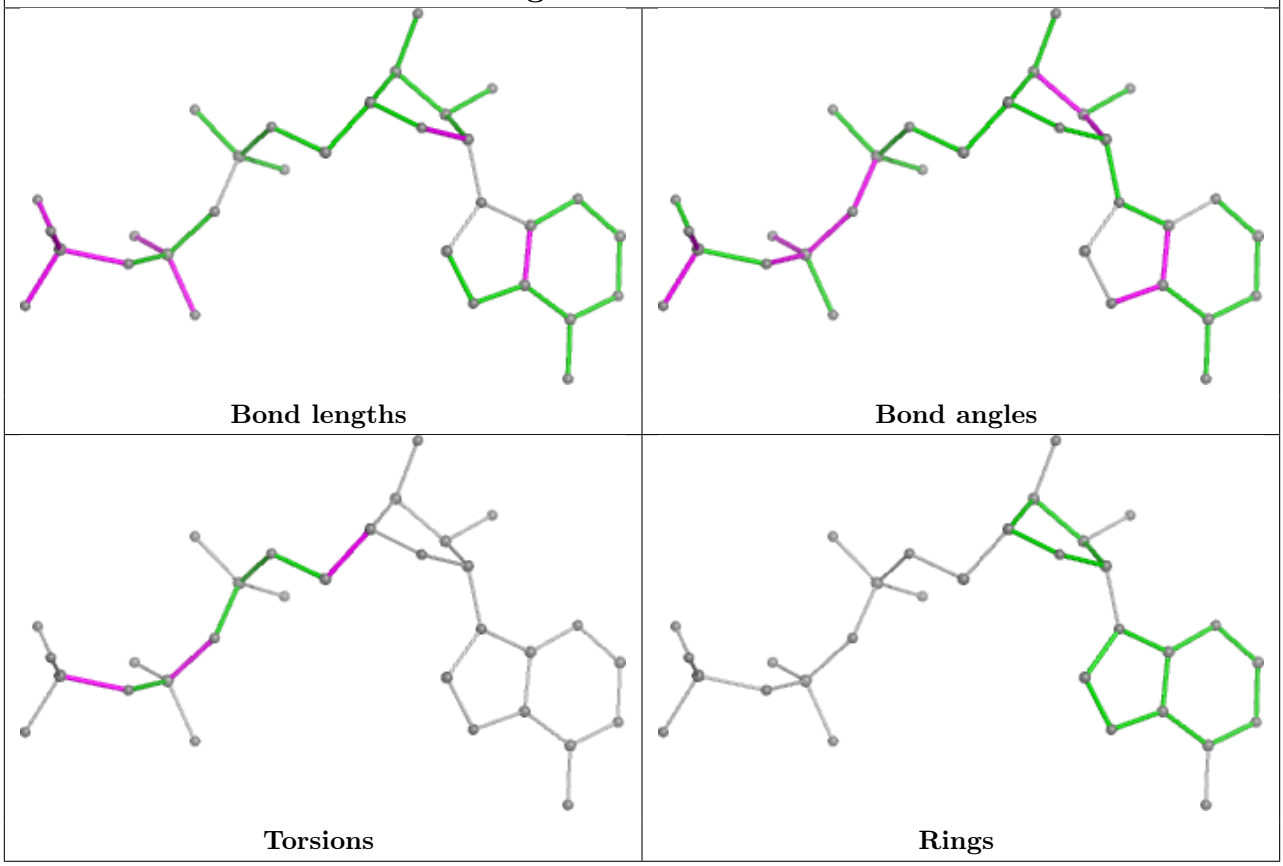


Torsions

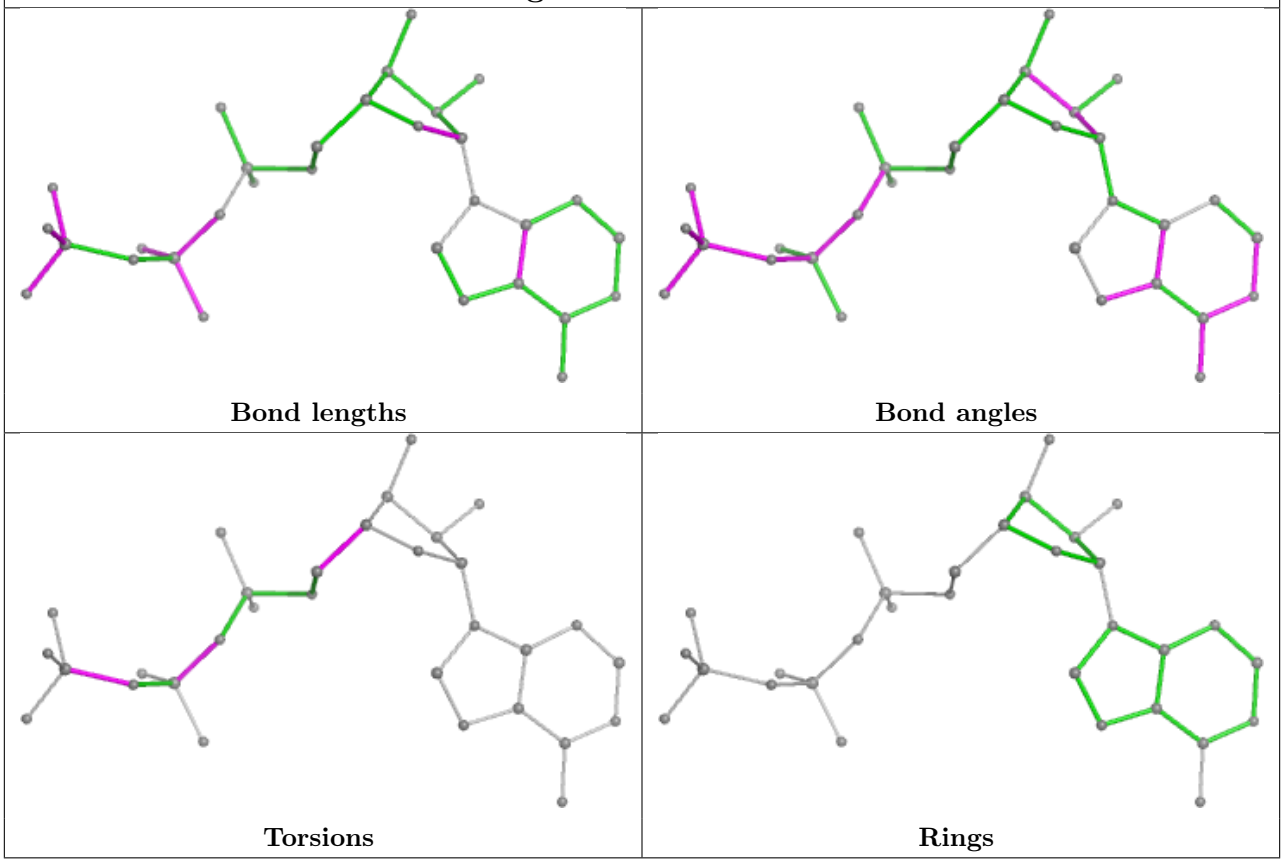


Rings

Ligand ANP 5 801



Ligand ANP 2 902



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.

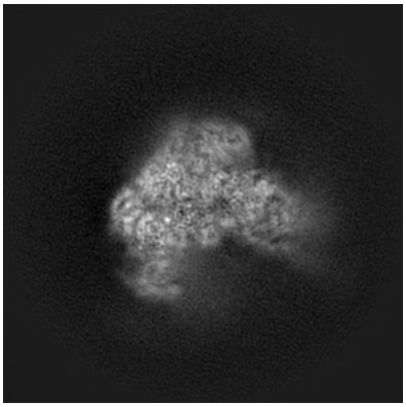
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10227. These allow visual inspection of the internal detail of the map and identification of artifacts.

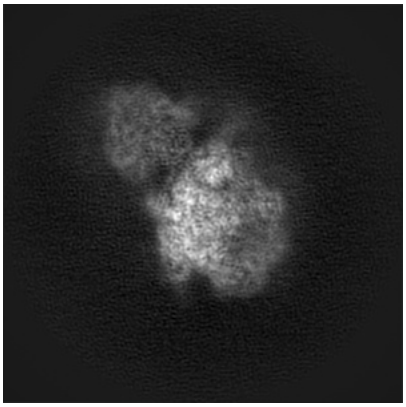
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

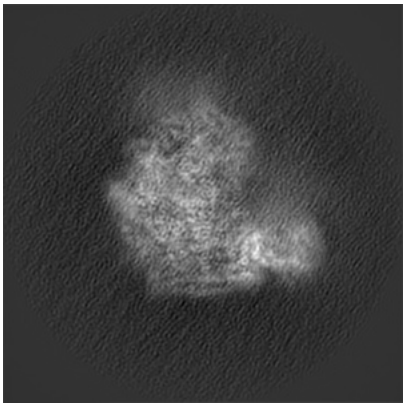
6.1.1 Primary map



X



Y

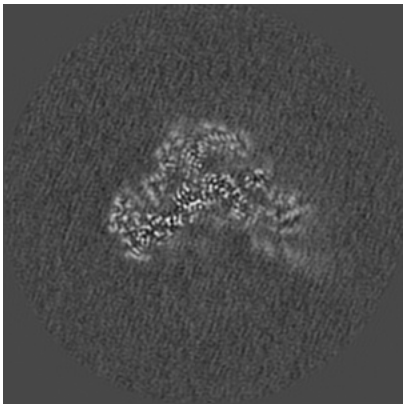


Z

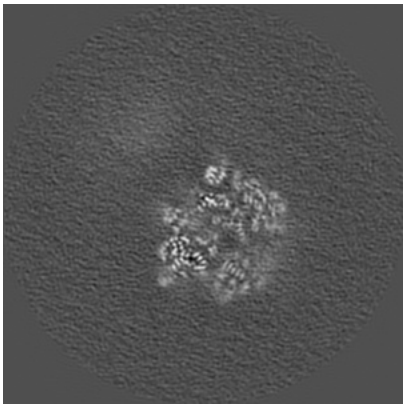
The images above show the map projected in three orthogonal directions.

6.2 Central slices

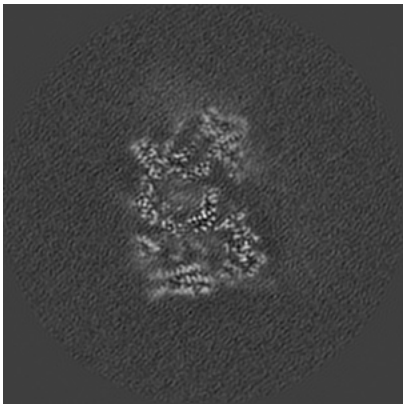
6.2.1 Primary map



X Index: 180



Y Index: 180

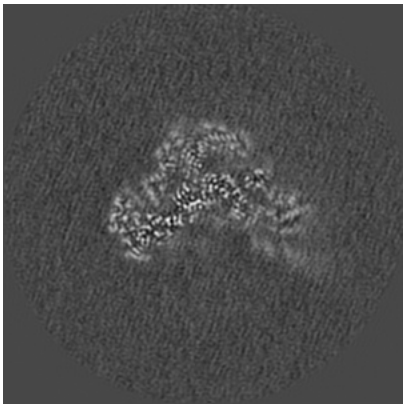


Z Index: 180

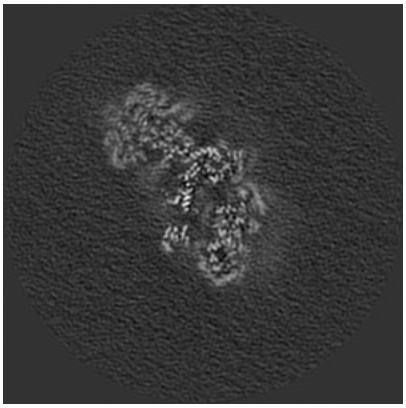
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

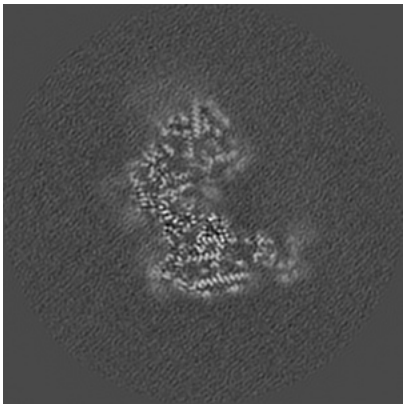
6.3.1 Primary map



X Index: 180



Y Index: 148

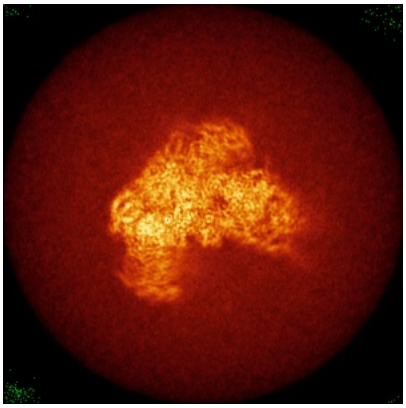


Z Index: 166

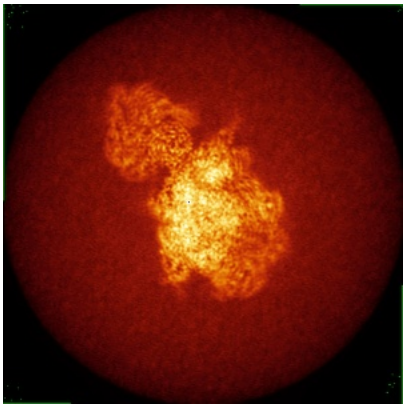
The images above show the largest variance slices of the map in three orthogonal directions.

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

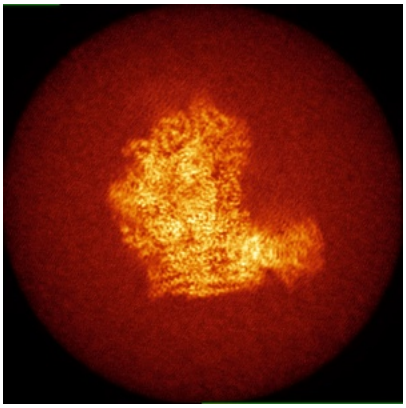
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

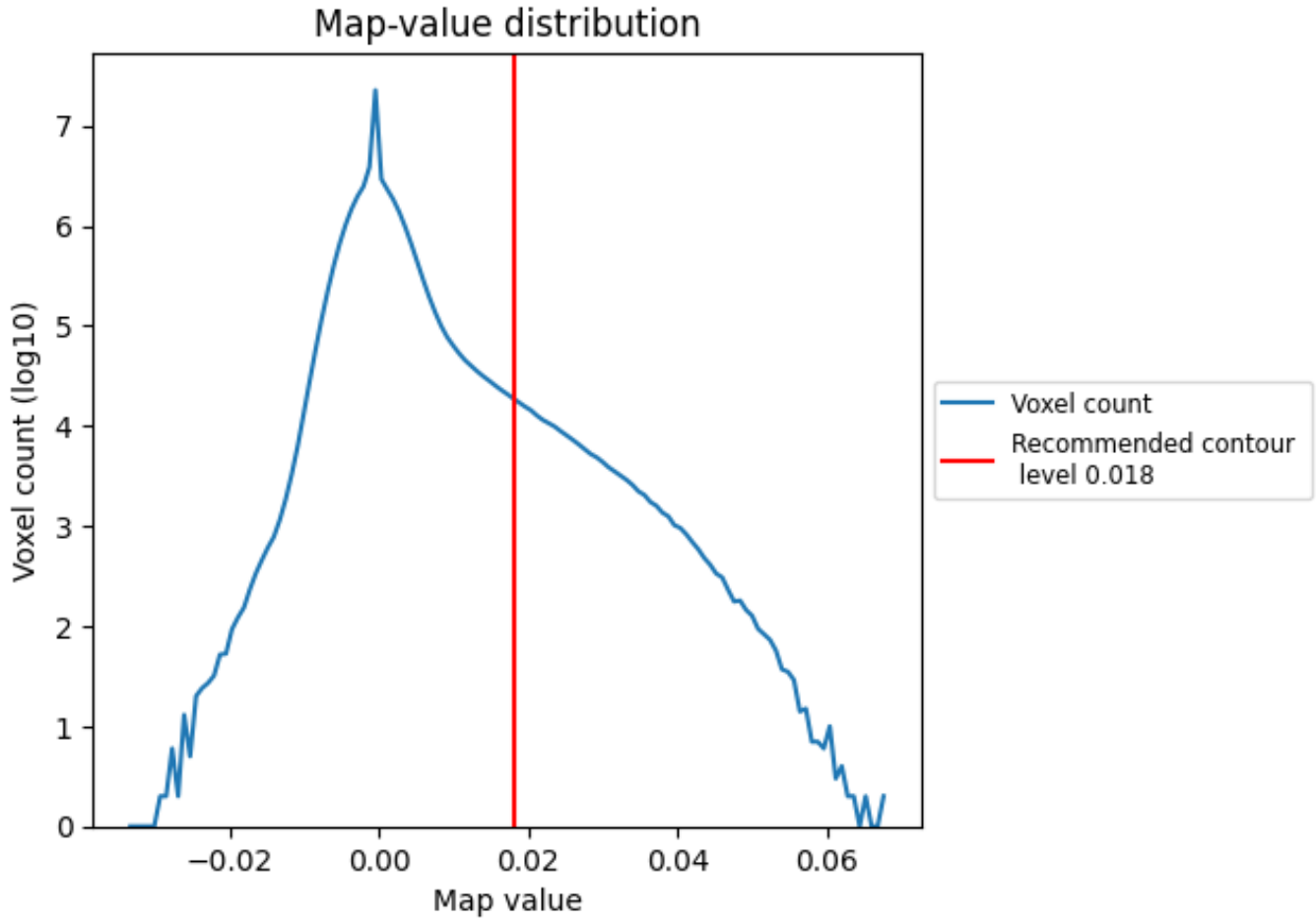
6.6 Mask visualisation (i)

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

7 Map analysis

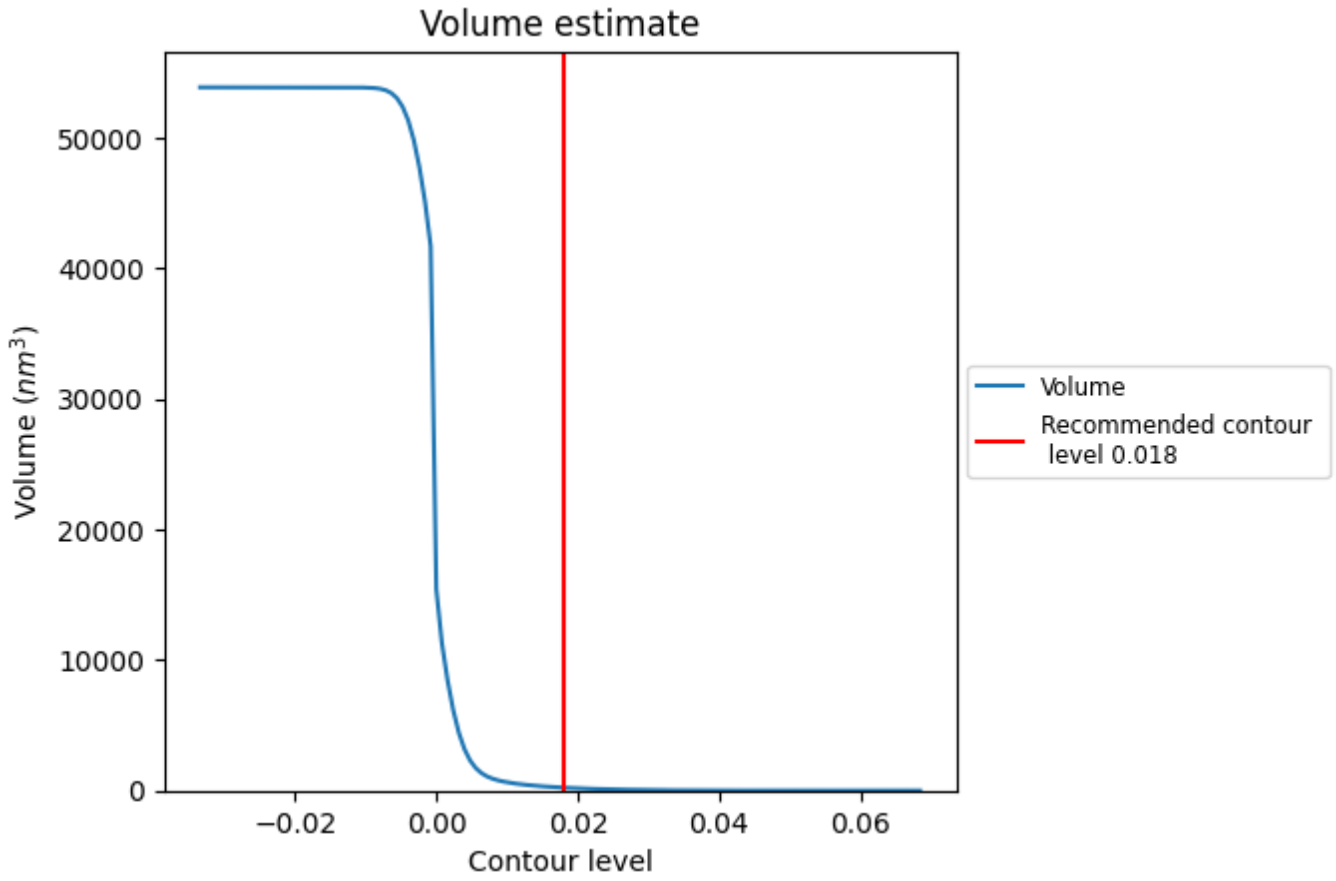
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

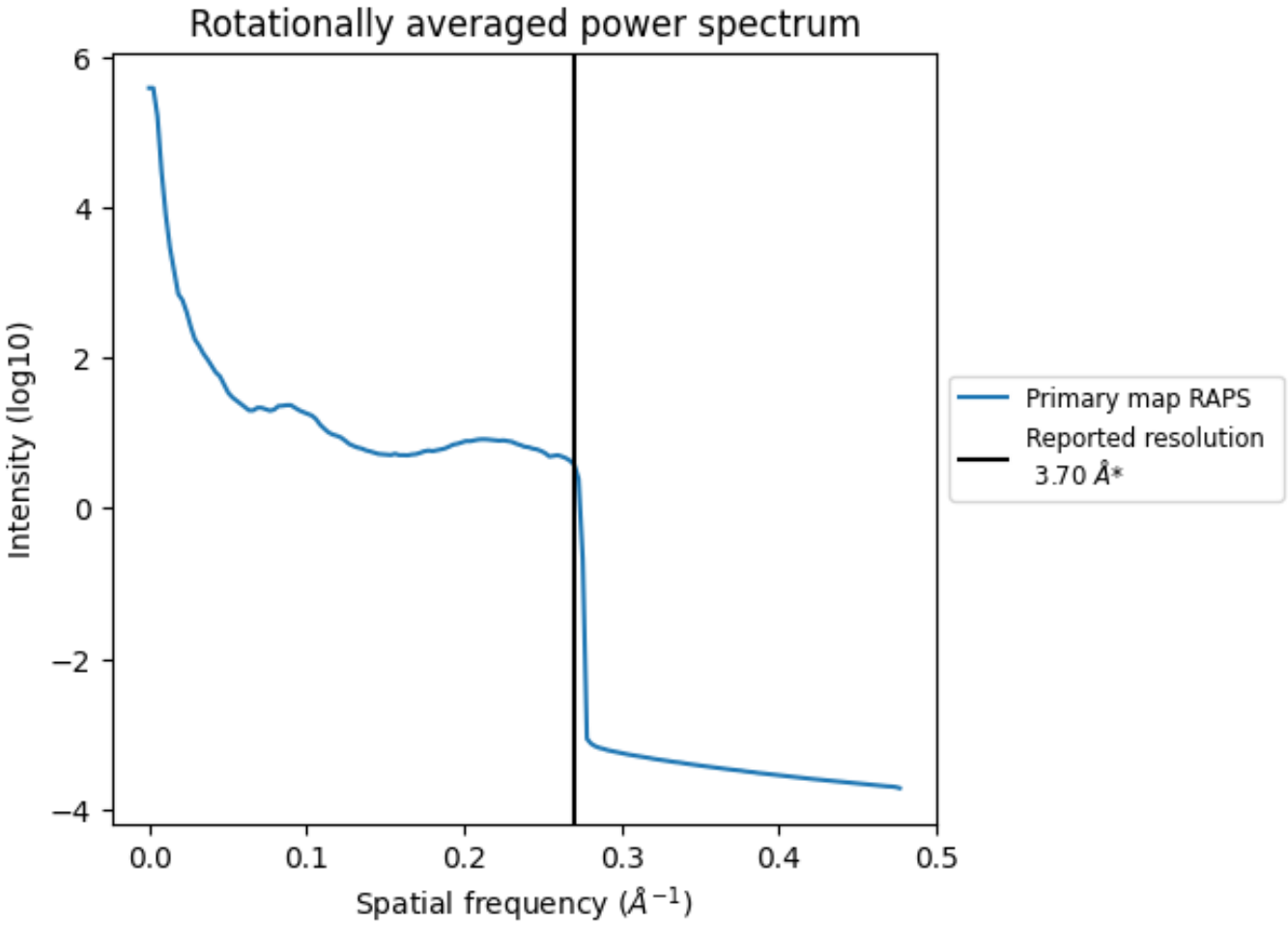
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 201 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)

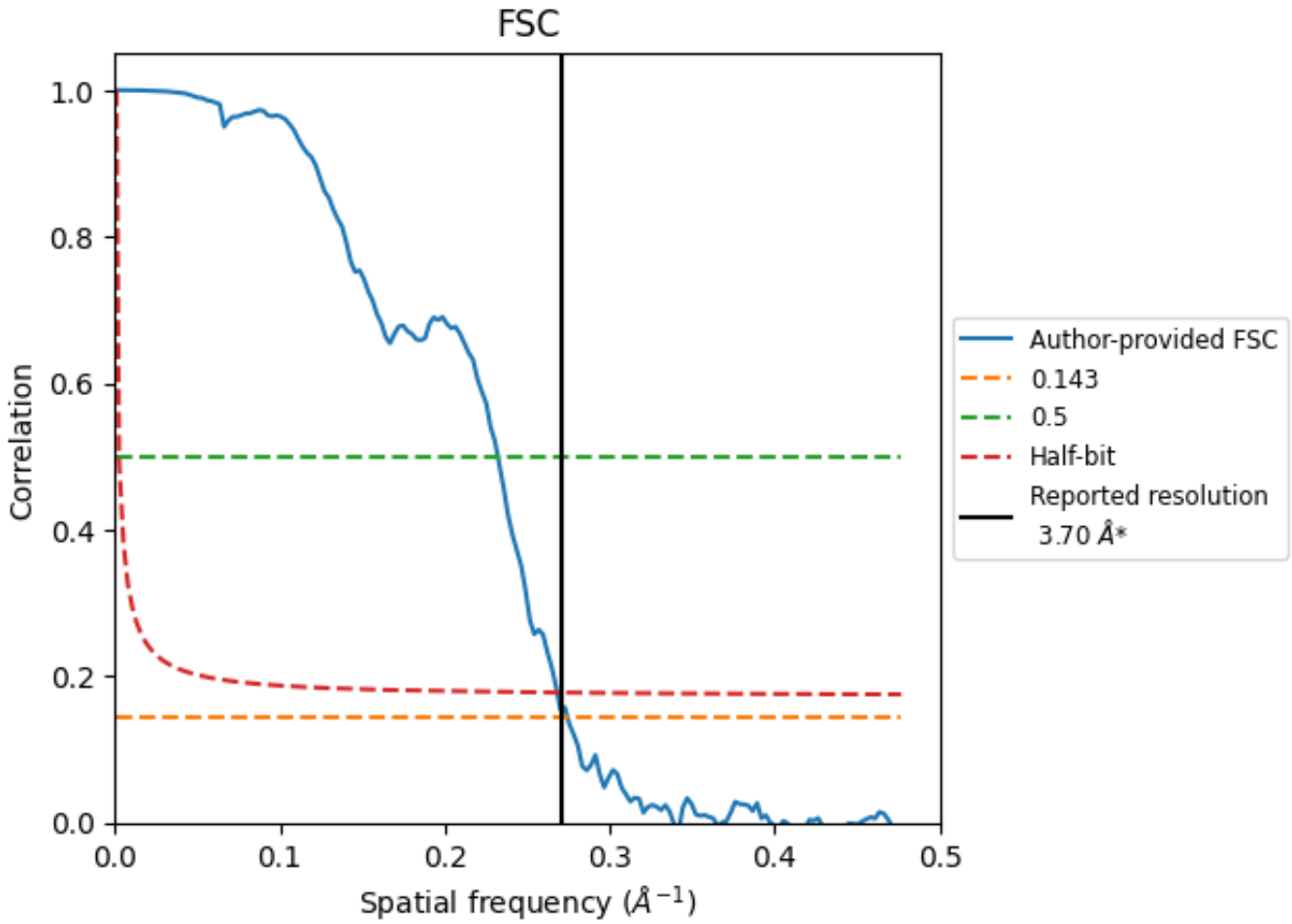


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

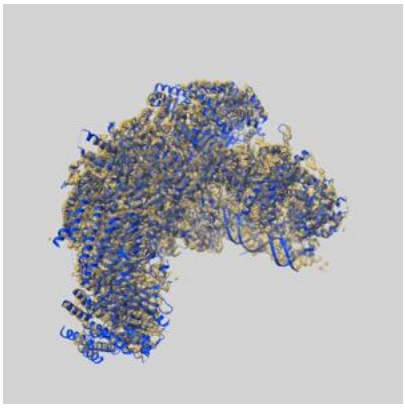
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.31	3.73
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

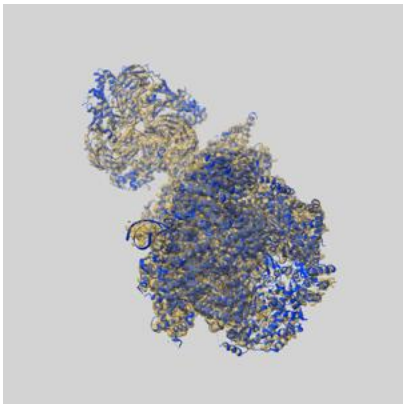
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10227 and PDB model 6SKL. Per-residue inclusion information can be found in section 3 on page 9.

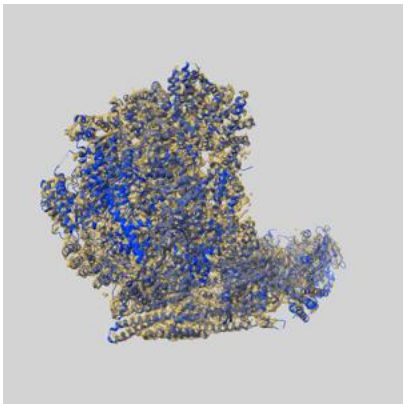
9.1 Map-model overlay



X



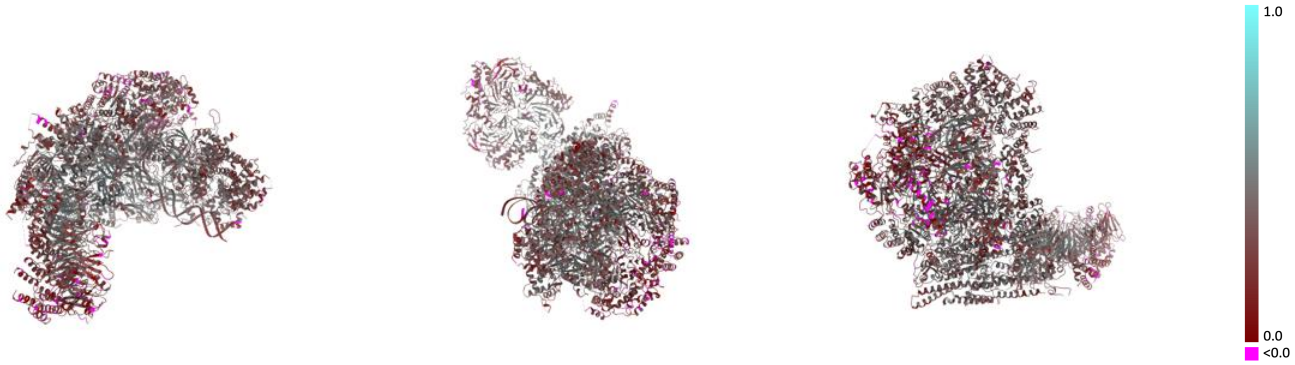
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

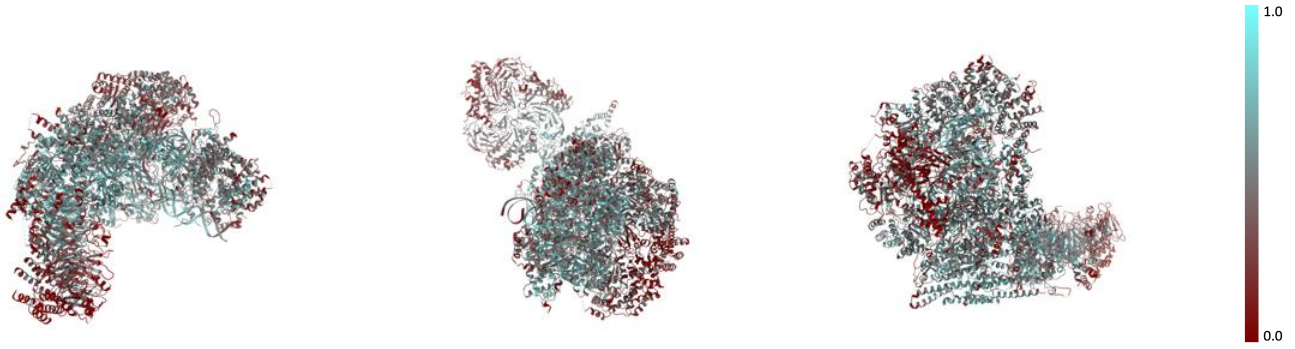
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

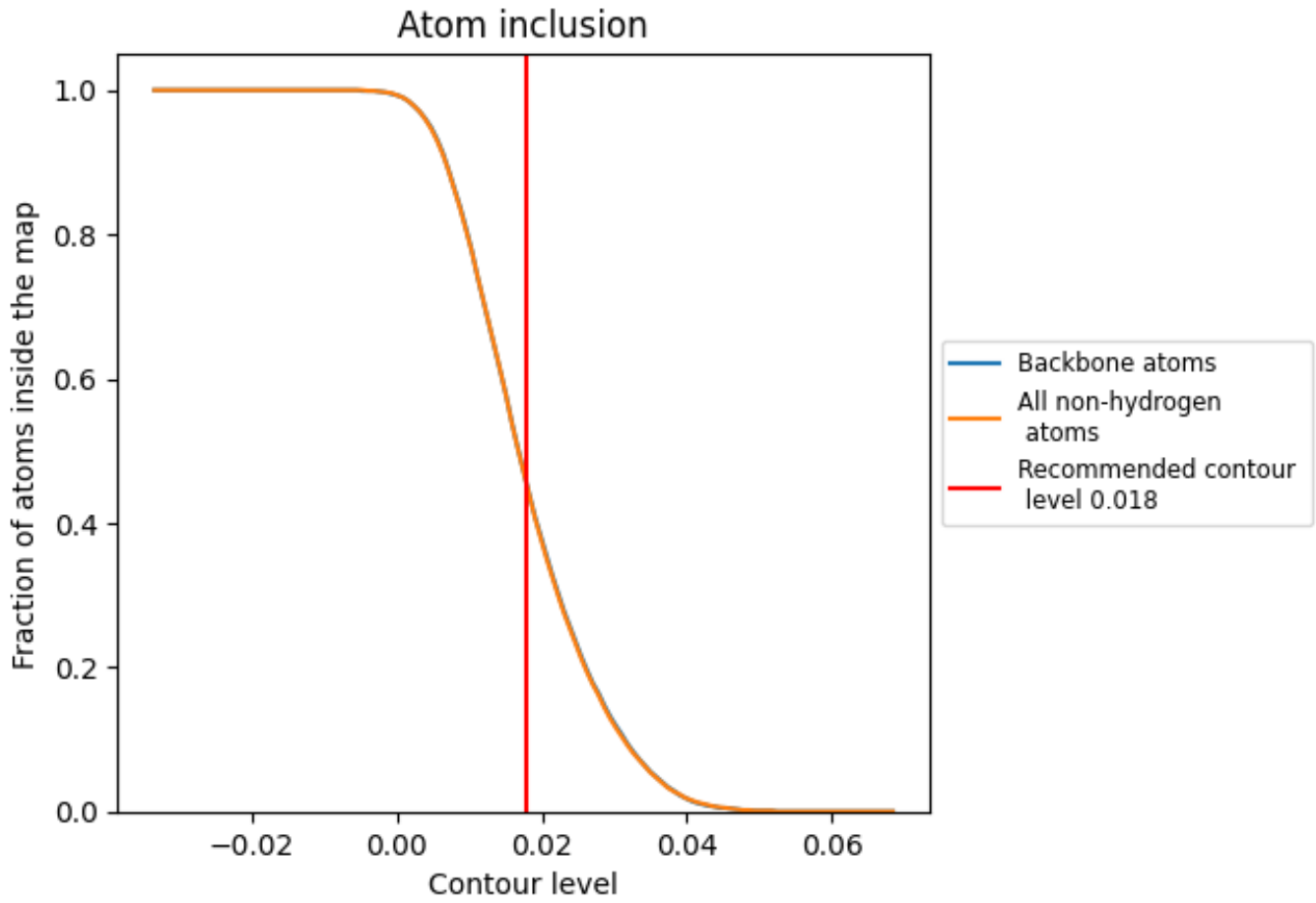
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 45% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4500	0.3520
2	0.4770	0.3730
3	0.5650	0.4100
4	0.2950	0.2520
5	0.5550	0.4200
6	0.4760	0.3570
7	0.4340	0.3250
A	0.5090	0.3620
B	0.6430	0.4560
C	0.5790	0.4180
D	0.5830	0.3980
E	0.5380	0.3970
F	0.4960	0.3800
G	0.2430	0.2560
H	0.2690	0.2680
I	0.5510	0.3190
J	0.6370	0.3460
X	0.4200	0.3340
Y	0.4650	0.3070