



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 03:51 PM EST

PDB ID : 6PTO  
EMDB ID : EMD-20473  
Title : Structure of Ctf4 trimer in complex with three CMG helicases  
Authors : Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.  
Deposited on : 2019-07-16  
Resolution : 7.00 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

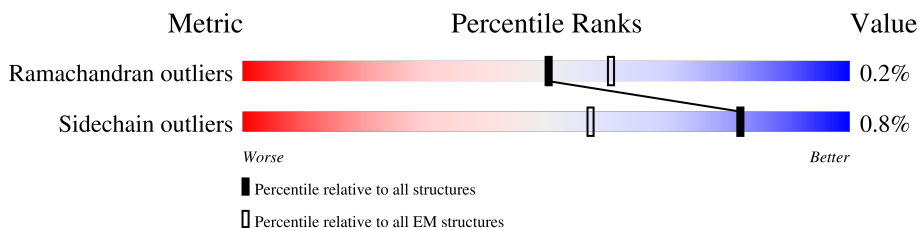
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 7.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	X	927	46% 54%
1	Y	927	46% 54%
1	Z	927	46% 54%
2	A	208	19% 99%
2	a	208	23% 99%
2	n	208	12% 99%
3	B	213	7% 84% 15%
3	b	213	6% 84% 15%
3	o	213	5% 84% 15%



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Mol	Chain	Length	Quality of chain	
4	C	194	17%	80% 18%
4	c	194	19%	81% 18%
4	p	194	10%	80% 18%
5	D	294	9%	80% 20%
5	d	294	6%	80% 20%
5	q	294	5%	80% 20%
6	E	650	16%	83% 15%
6	e	650	12%	83% 15%
6	r	650	14%	83% 15%
7	2	868	56%	72% 27%
7	F	868	51%	72% 27%
7	h	868	45%	72% 27%
8	3	971	40%	61% 39%
8	G	971	39%	61% 39%
8	i	971	24%	61% 39%
9	4	933	63%	72% 27%
9	H	933	59%	72% 27%
9	j	933	51%	72% 27%
10	5	775	46%	76% 23%
10	I	775	43%	76% 23%
10	k	775	36%	76% 23%
11	6	1017	49%	59% 40%
11	J	1017	45%	59% 40%
11	l	1017	36%	59% 40%
12	7	845	65%	78% 22%

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Mol	Chain	Length	Quality of chain
12	K	845	
12	m	845	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 132192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		
1	Y	431	Total	C	N	O	S	0	0
			3464	2223	574	651	16		
1	Z	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

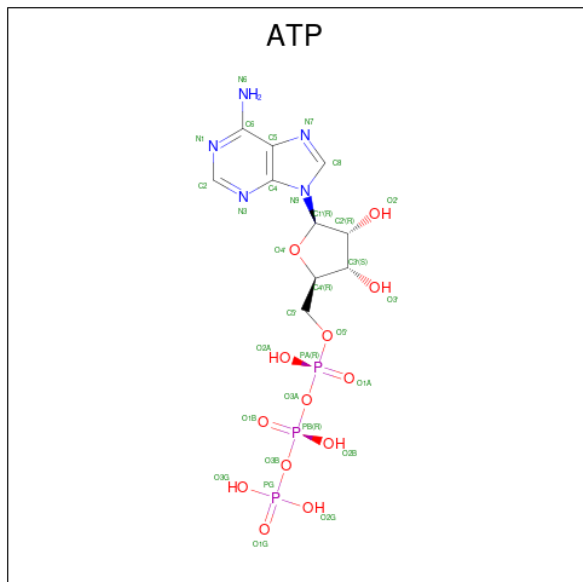
- Molecule 11 is a protein called DNA replication licensing factor MCM6.

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

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

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

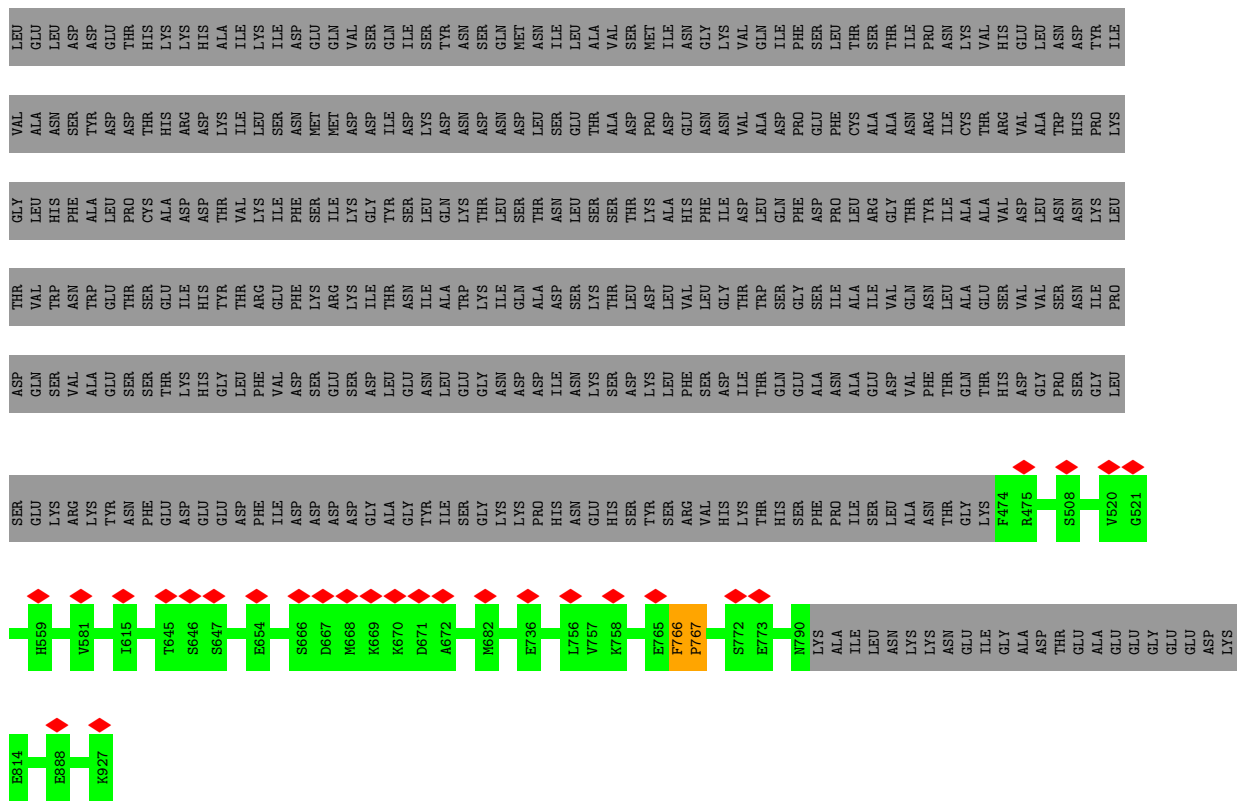
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



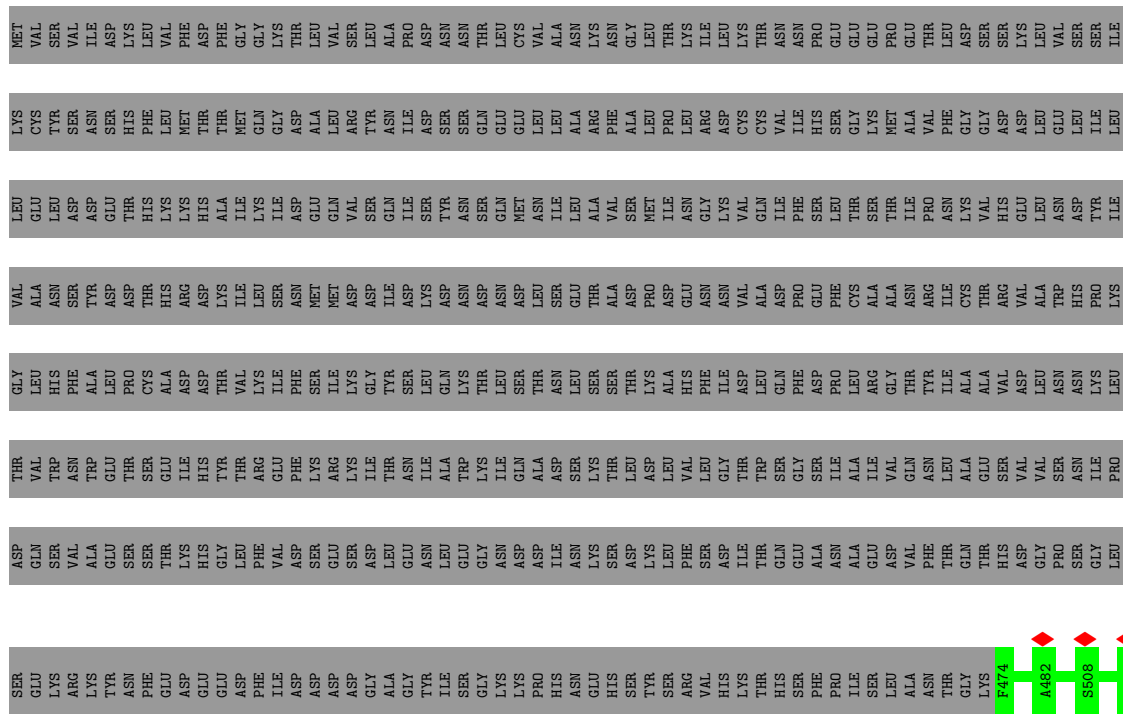
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	h	1	Total 31	C 10	N 5	O 13	P 3	0
13	i	1	Total 31	C 10	N 5	O 13	P 3	0
13	k	1	Total 31	C 10	N 5	O 13	P 3	0
13	2	1	Total 31	C 10	N 5	O 13	P 3	0
13	3	1	Total 31	C 10	N 5	O 13	P 3	0
13	5	1	Total 31	C 10	N 5	O 13	P 3	0

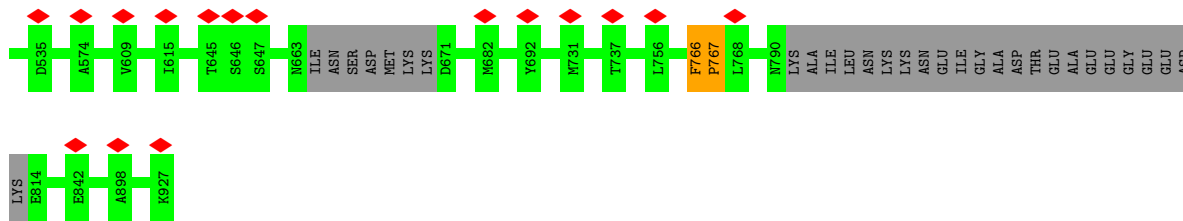




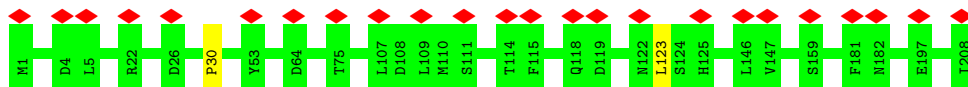


• Molecule 1: DNA polymerase alpha-binding protein

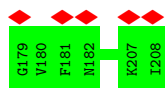
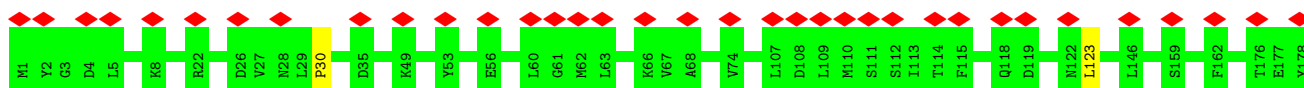




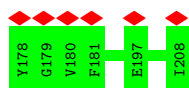
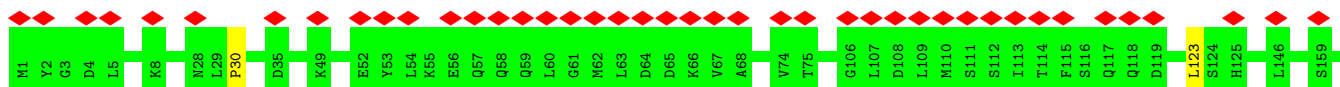
• Molecule 2: DNA replication complex GINS protein PSF1



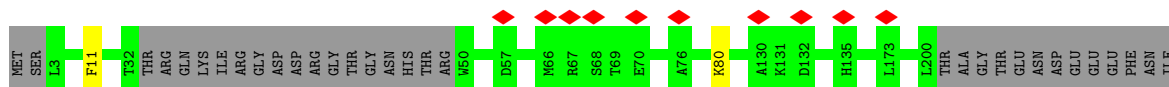
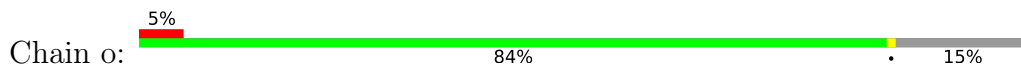
• Molecule 2: DNA replication complex GINS protein PSF1



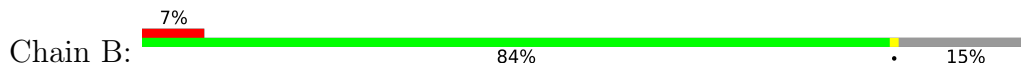
• Molecule 2: DNA replication complex GINS protein PSF1

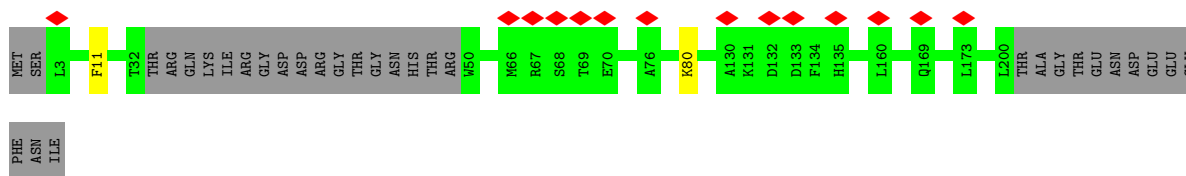


• Molecule 3: DNA replication complex GINS protein PSF2

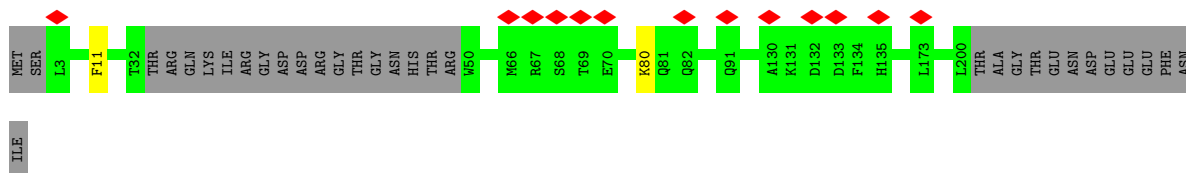
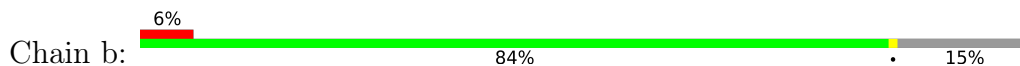


• Molecule 3: DNA replication complex GINS protein PSF2

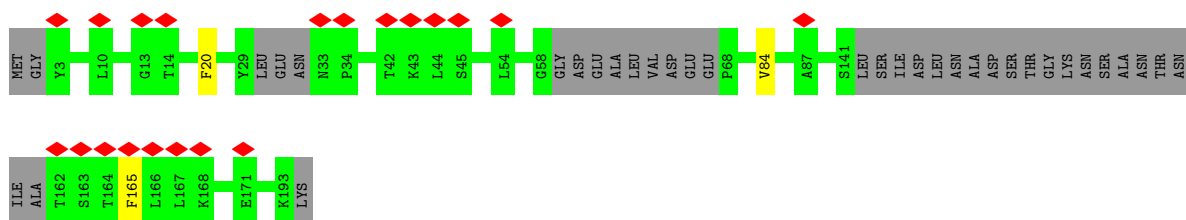
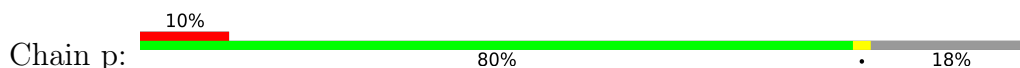




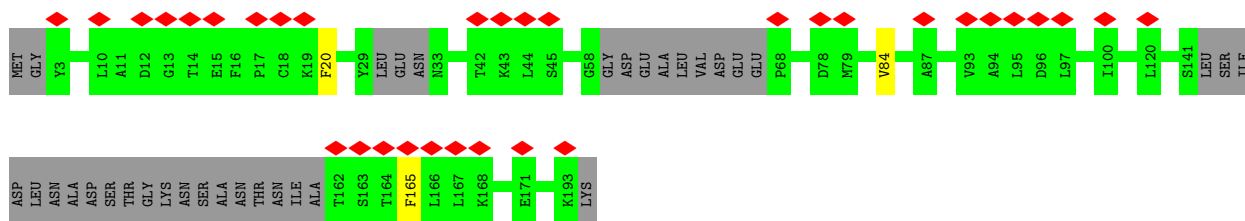
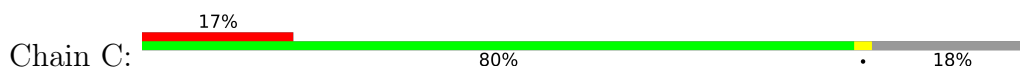
• Molecule 3: DNA replication complex GINS protein PSF2



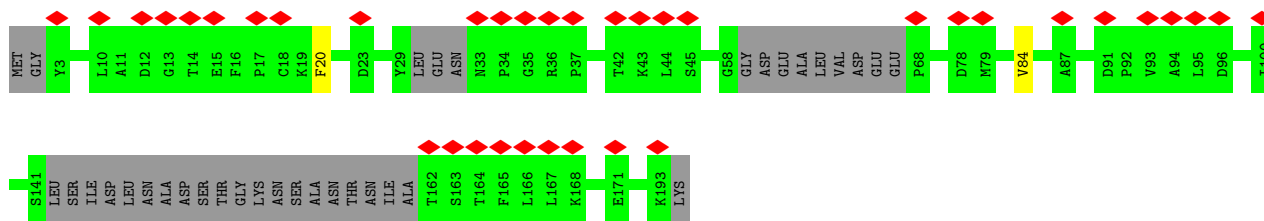
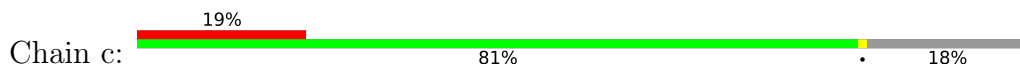
• Molecule 4: DNA replication complex GINS protein PSF3



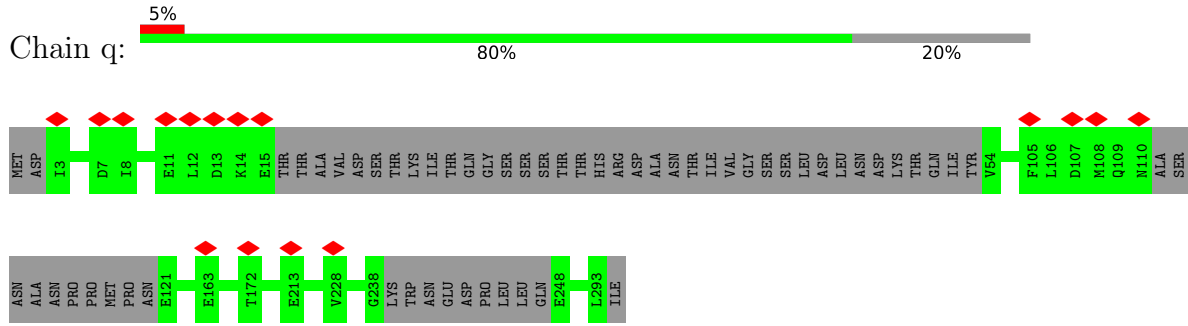
• Molecule 4: DNA replication complex GINS protein PSF3



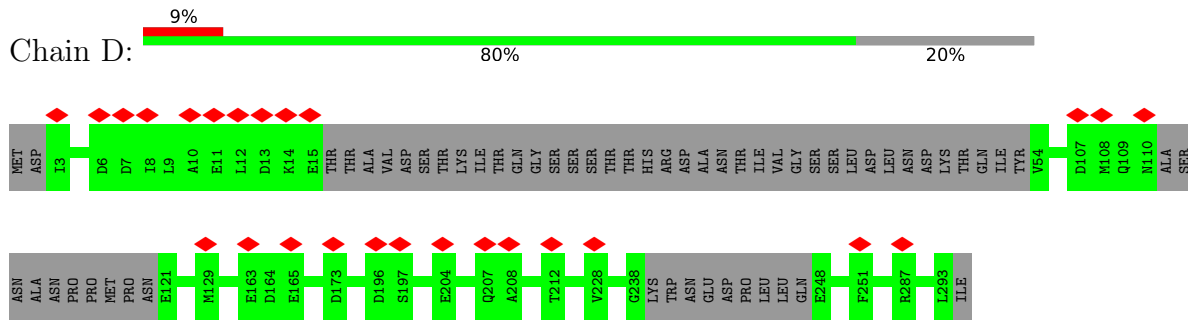
• Molecule 4: DNA replication complex GINS protein PSF3



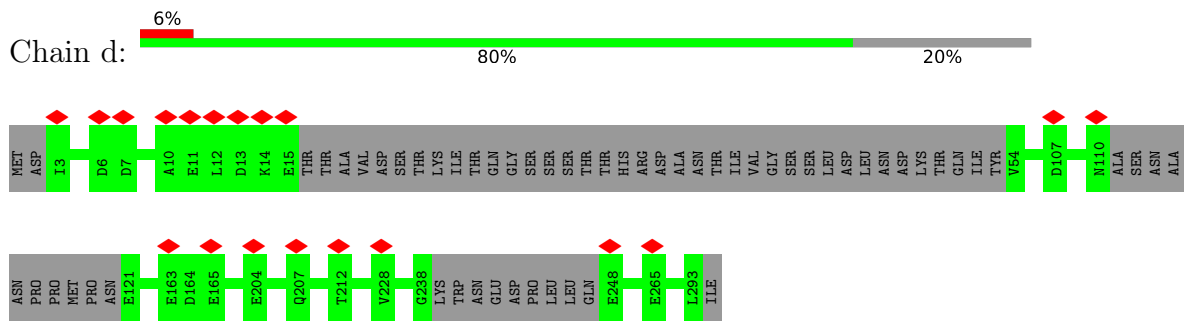
● Molecule 5: DNA replication complex GINS protein SLD5



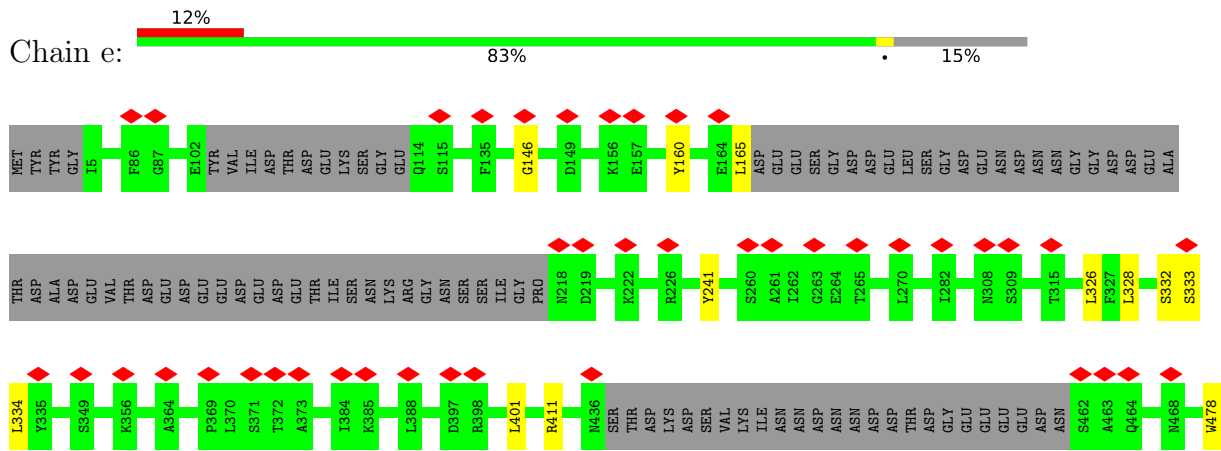
● Molecule 5: DNA replication complex GINS protein SLD5

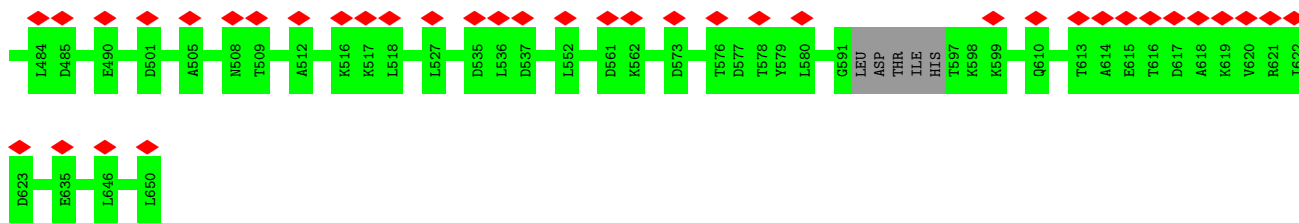


● Molecule 5: DNA replication complex GINS protein SLD5

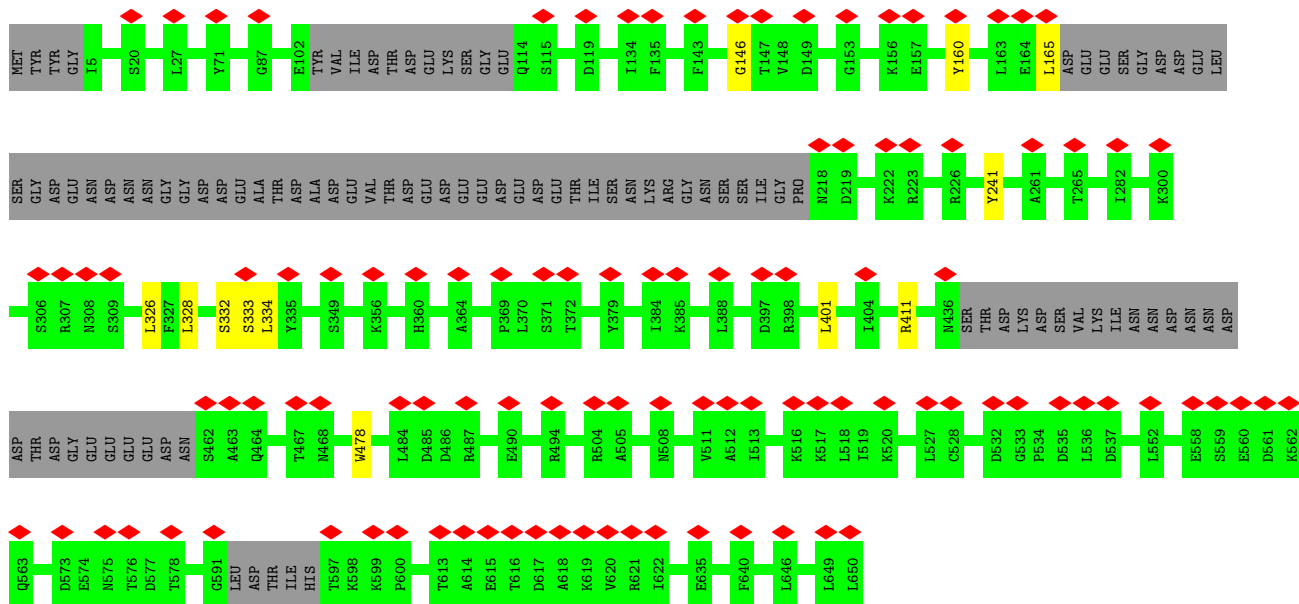
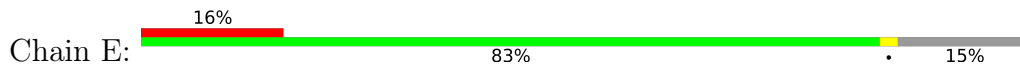


● Molecule 6: Cell division control protein 45

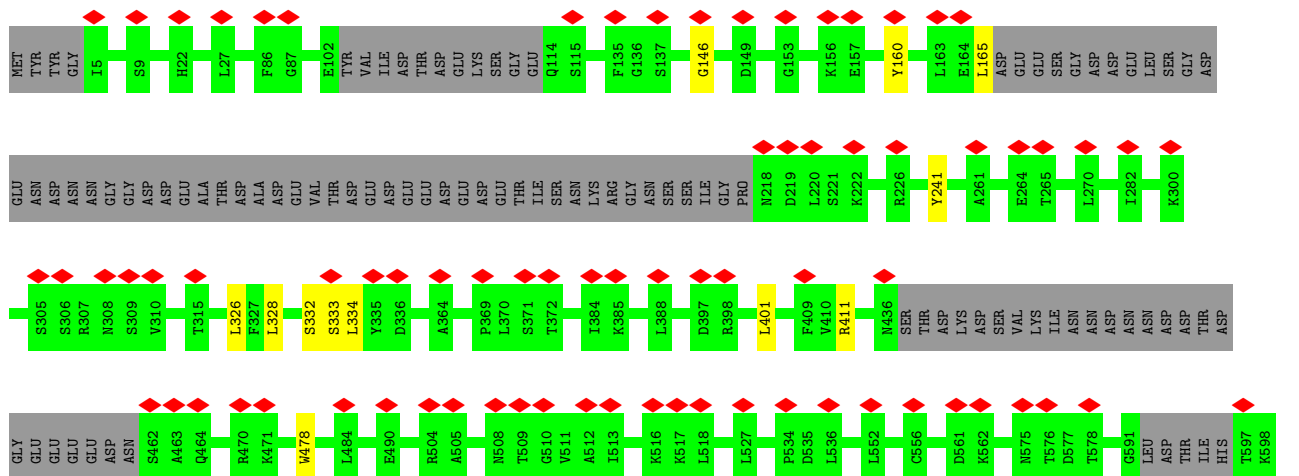
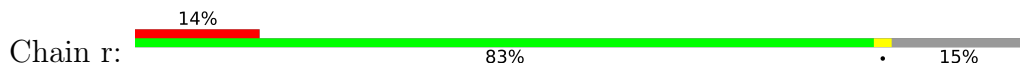




• Molecule 6: Cell division control protein 45



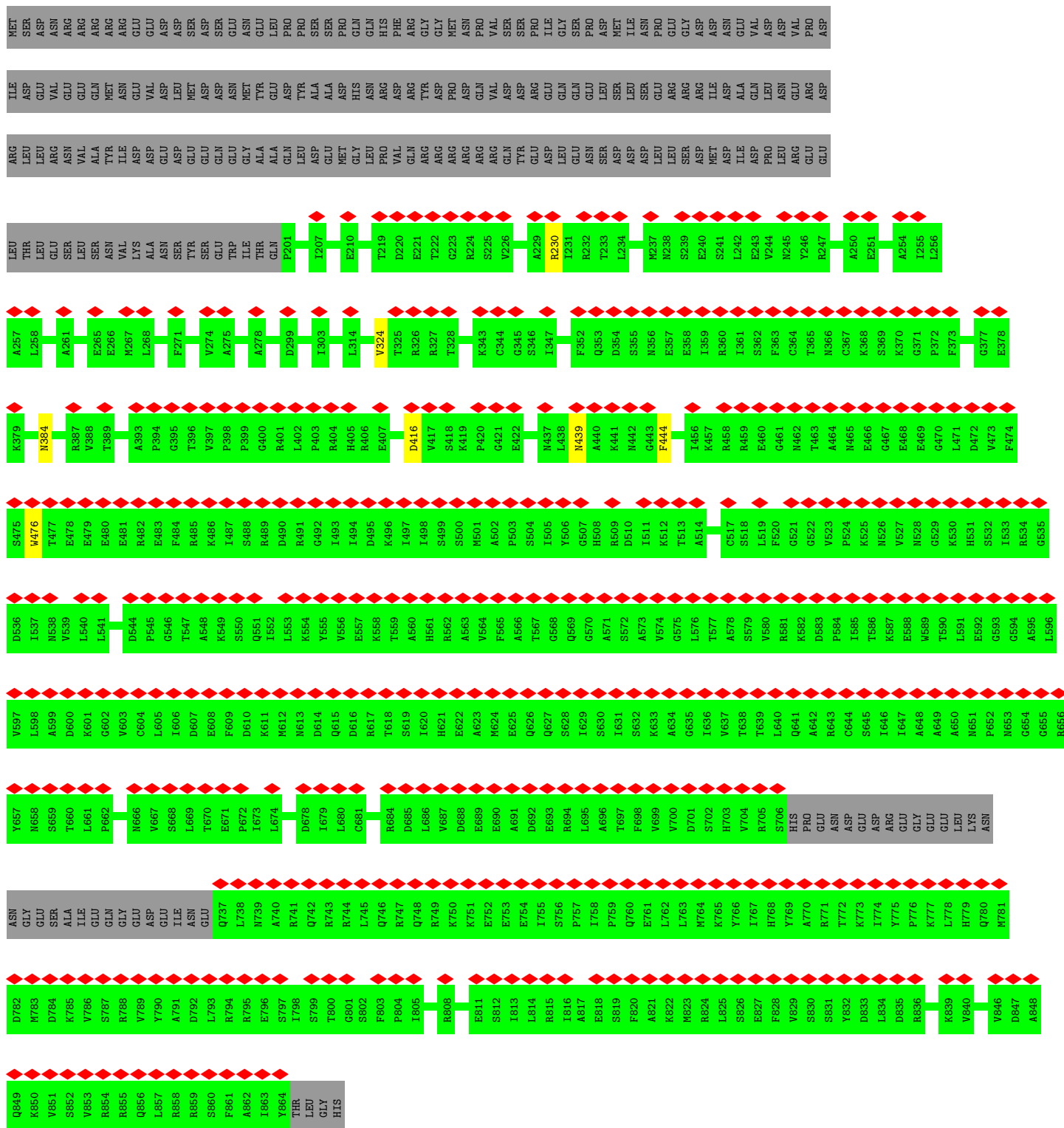
• Molecule 6: Cell division control protein 45



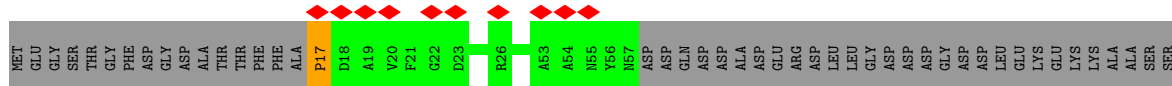


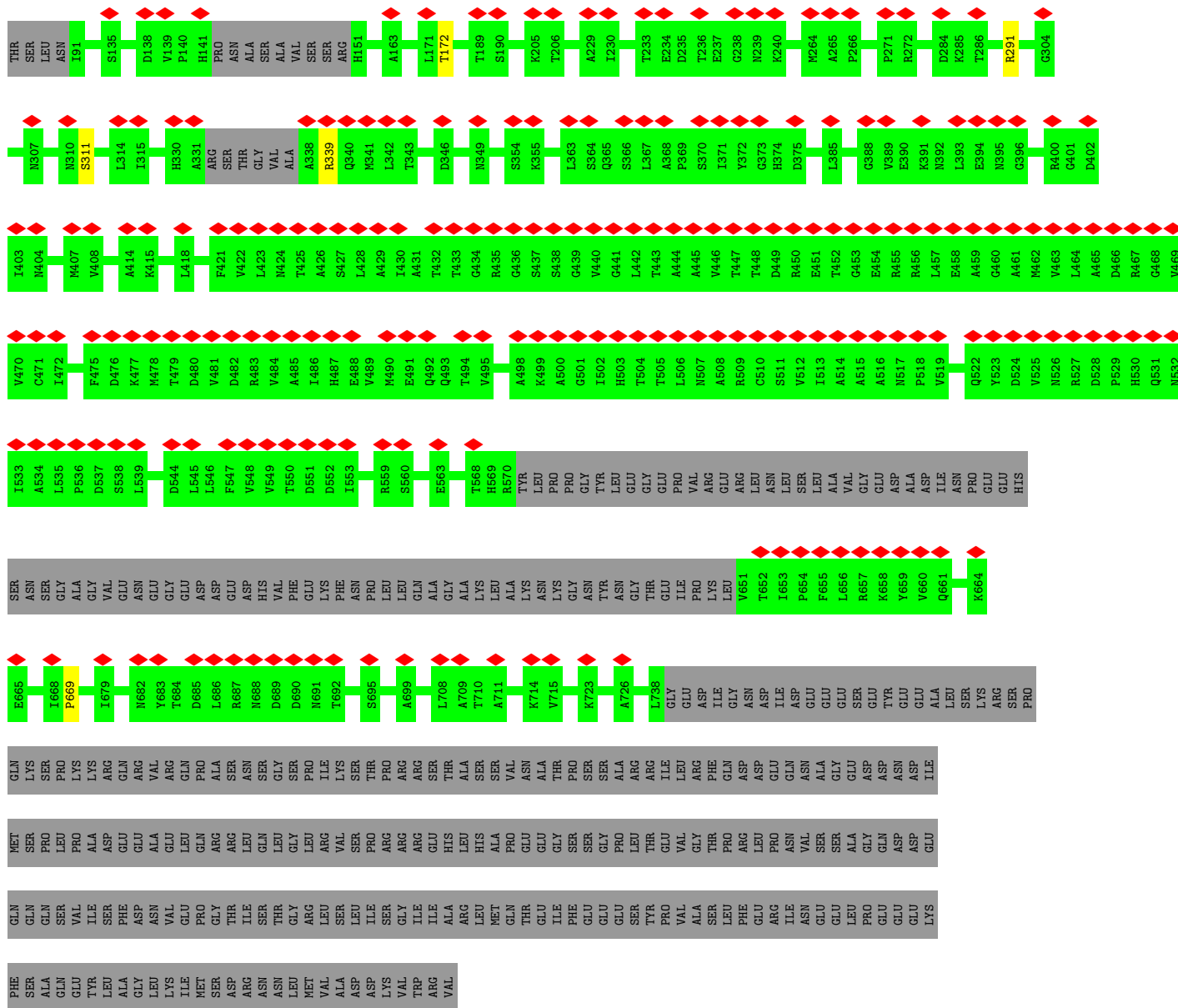




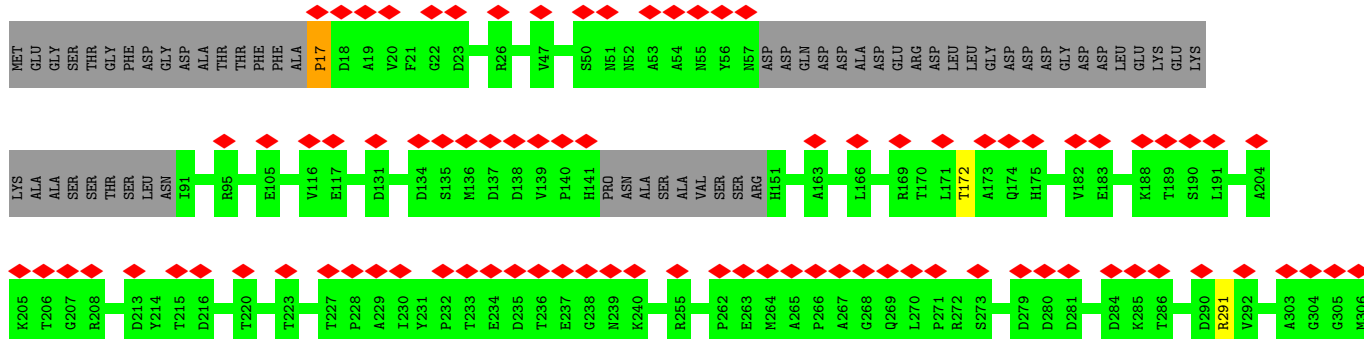
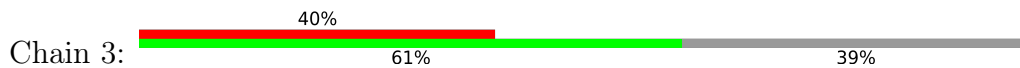


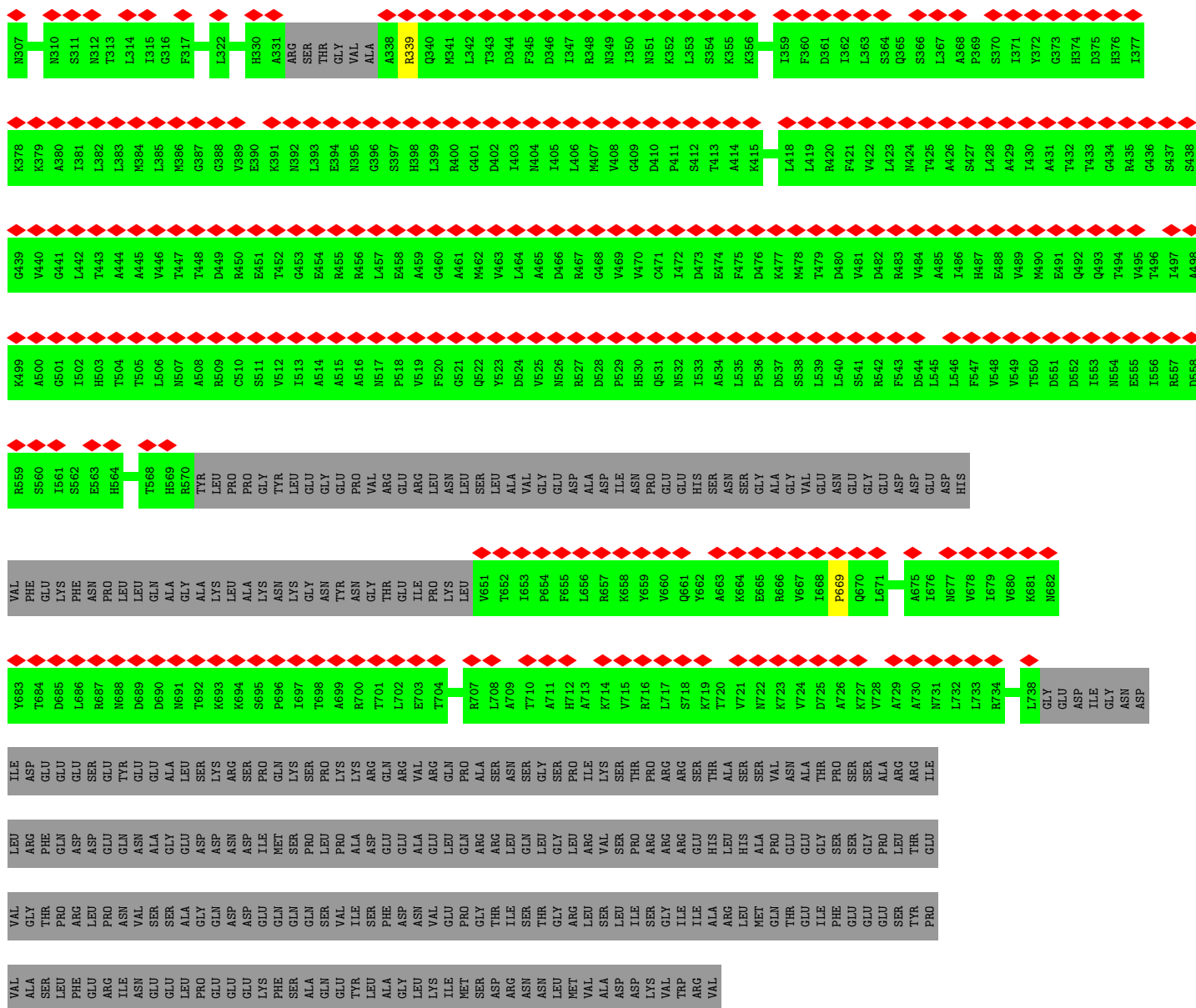
● Molecule 8: DNA replication licensing factor MCM3



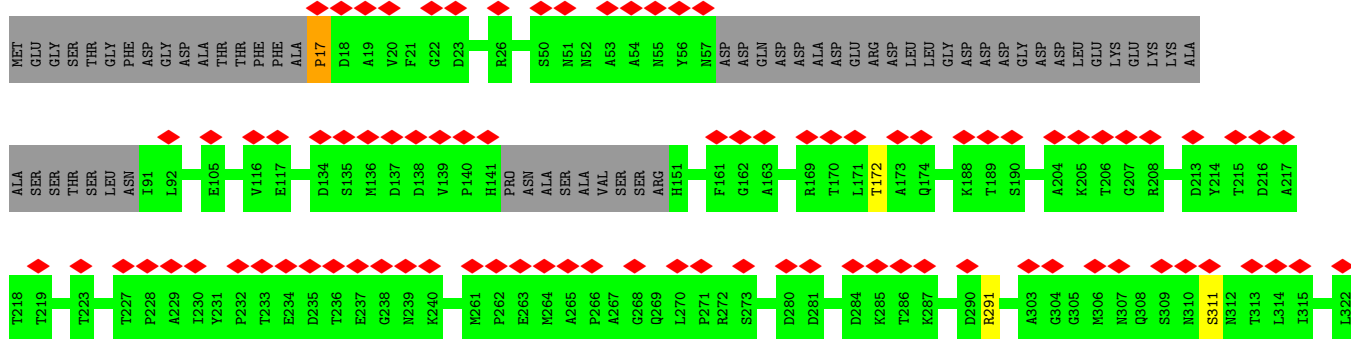
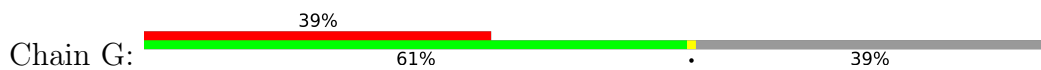


● Molecule 8: DNA replication licensing factor MCM3

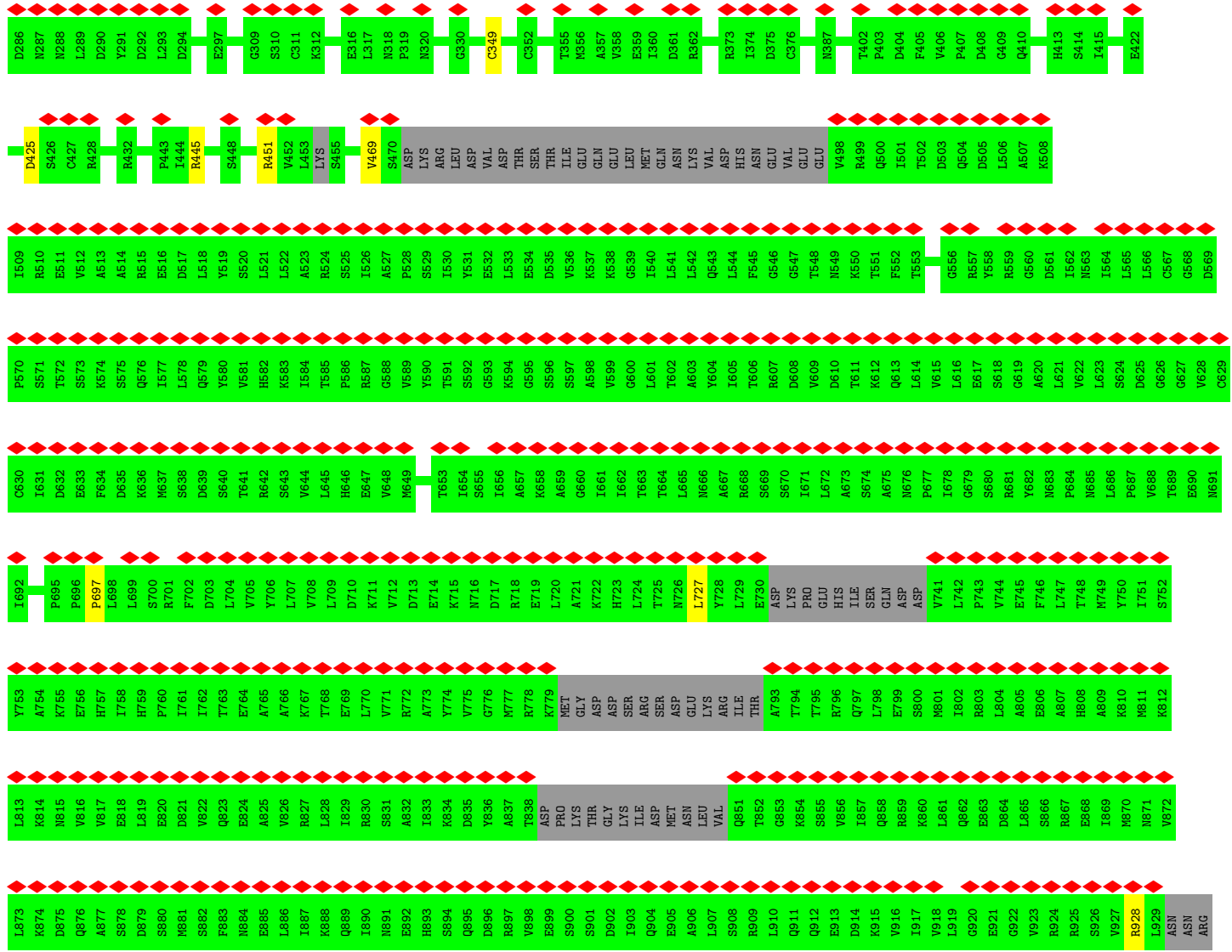




• Molecule 8: DNA replication licensing factor MCM3

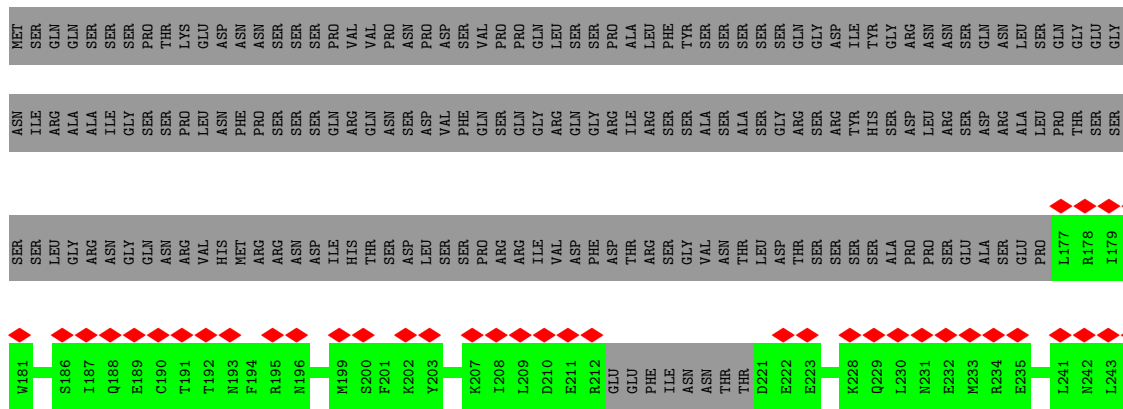




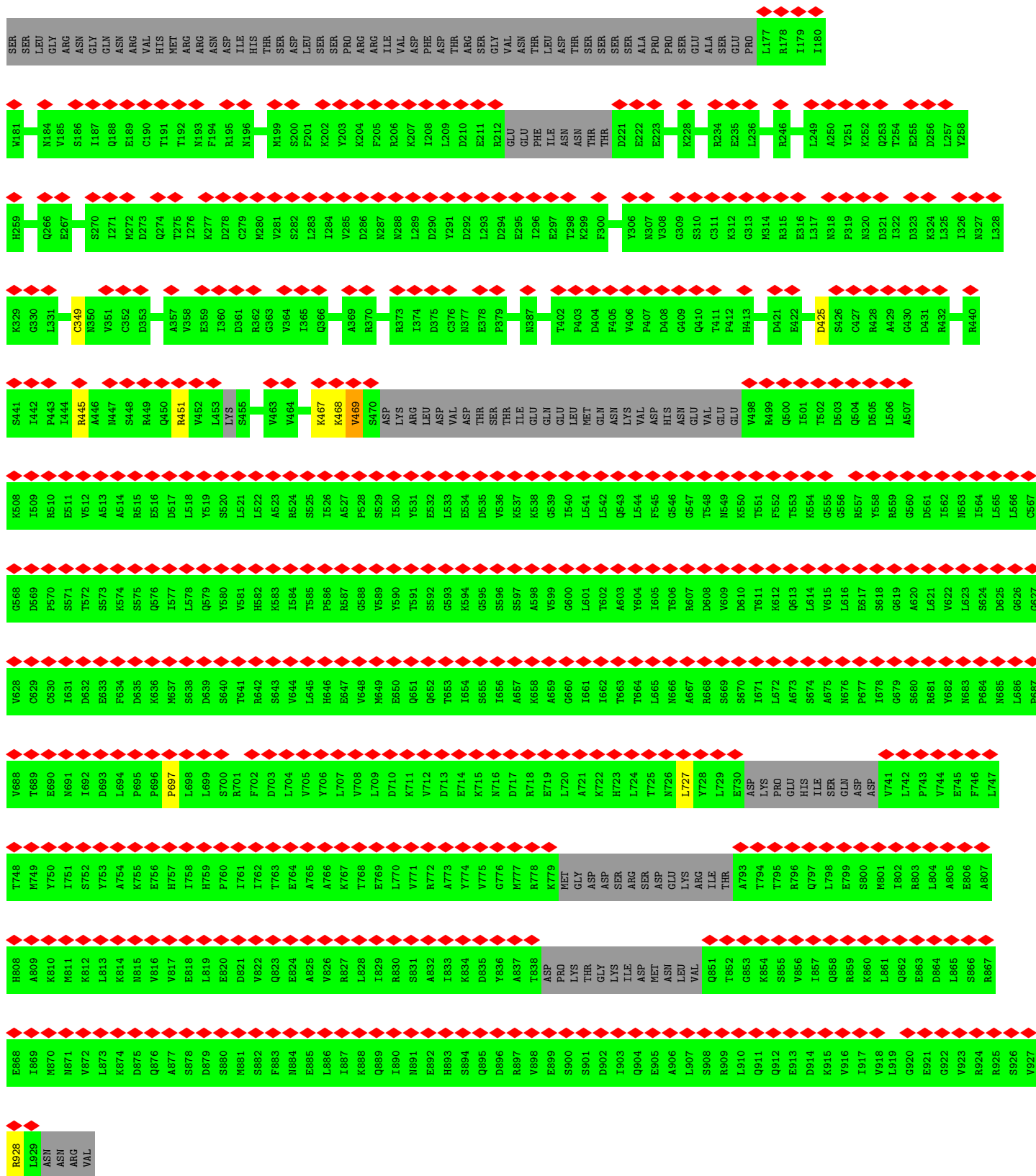


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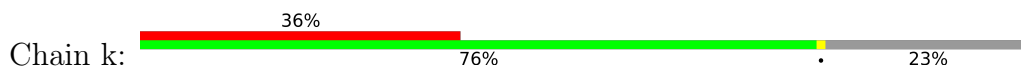
• Molecule 9: DNA replication licensing factor MCM4

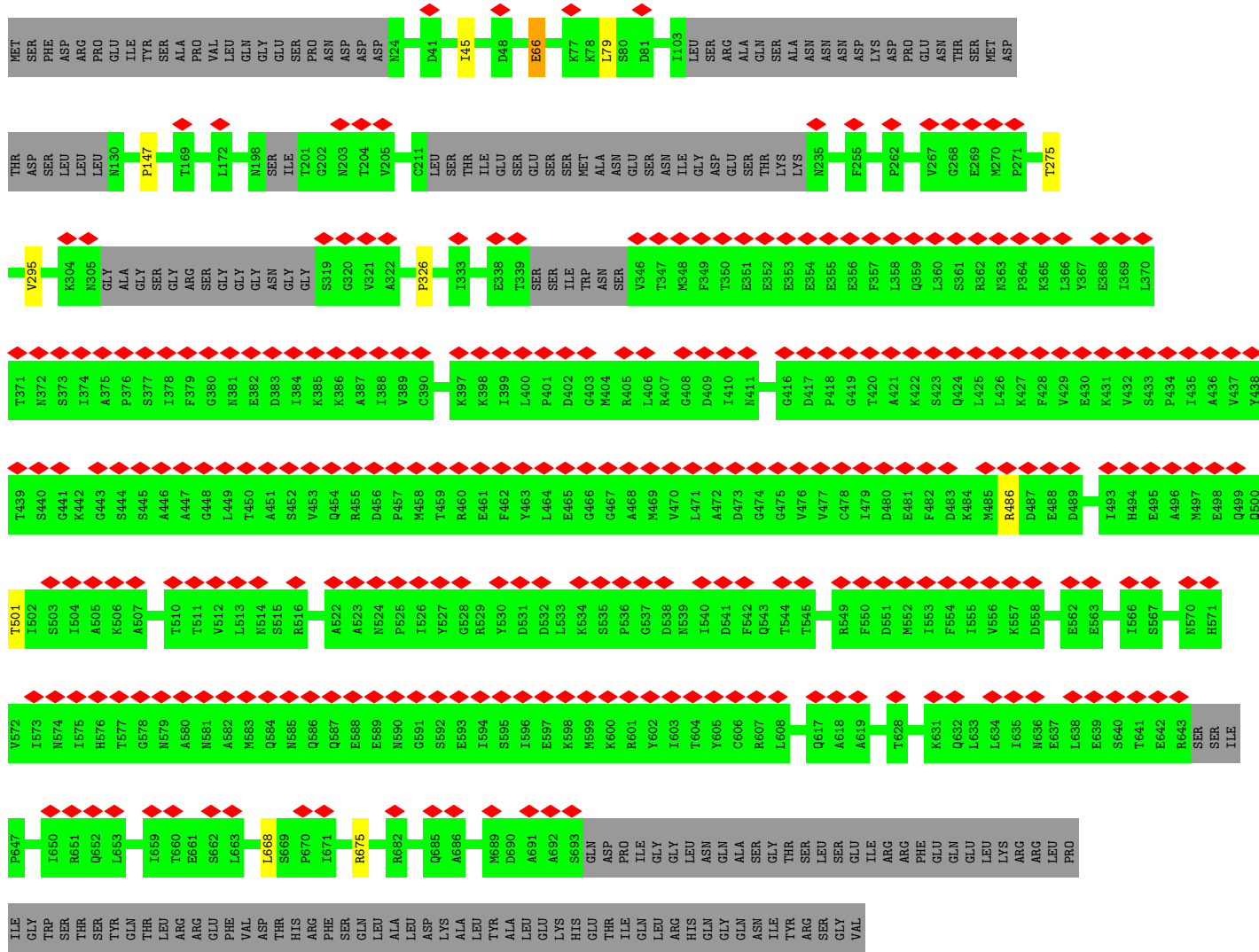




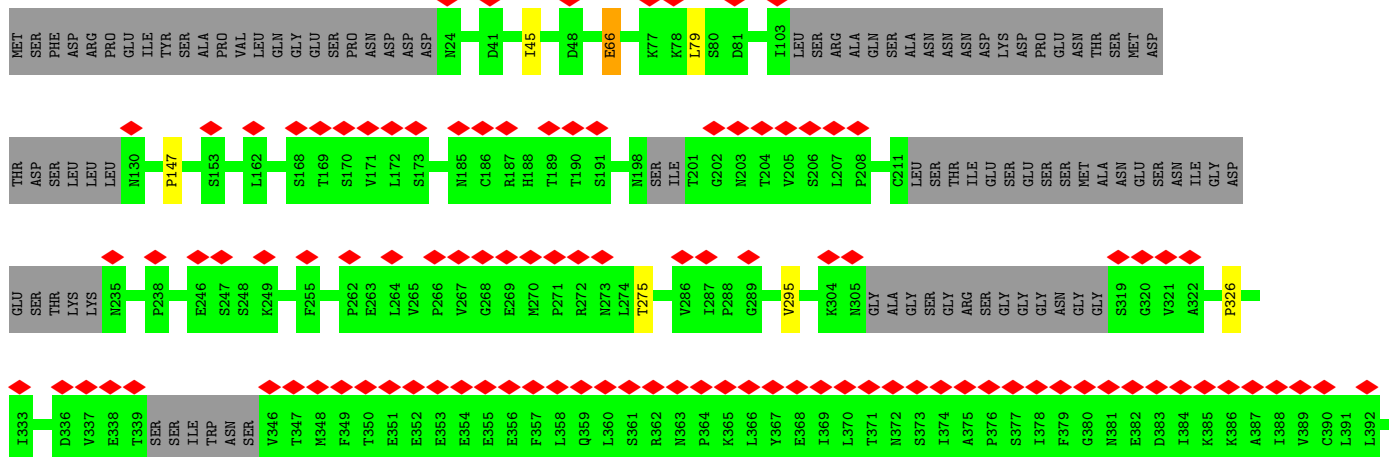
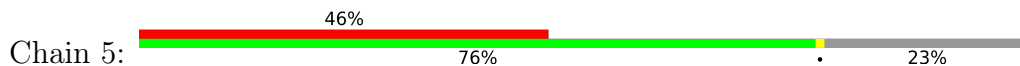


• Molecule 10: Minichromosome maintenance protein 5



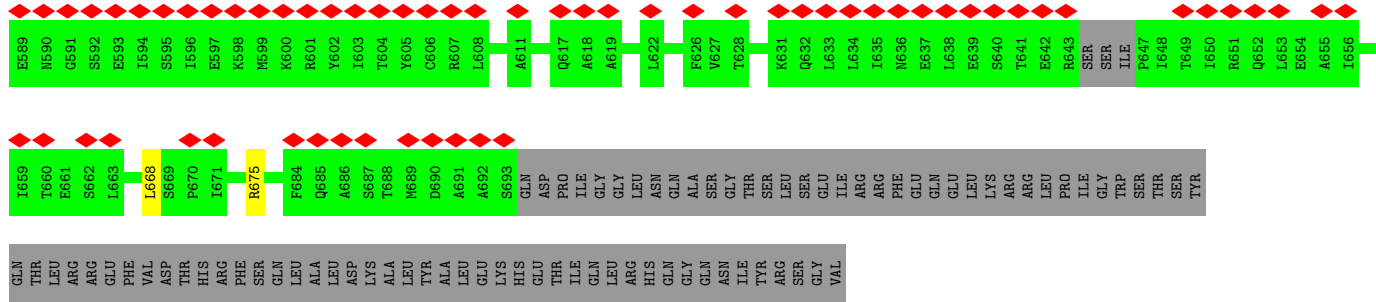


• Molecule 10: Minichromosome maintenance protein 5

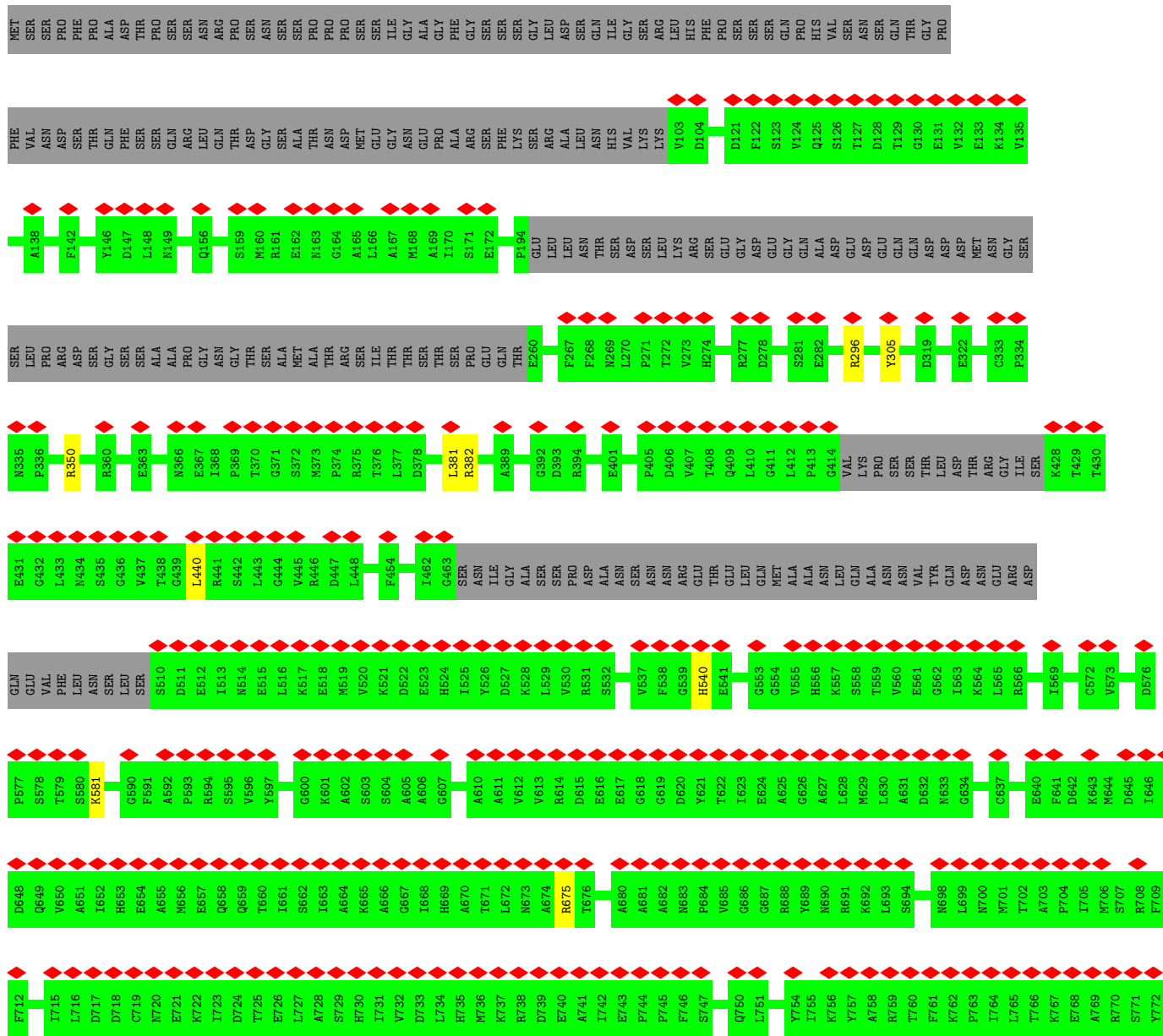






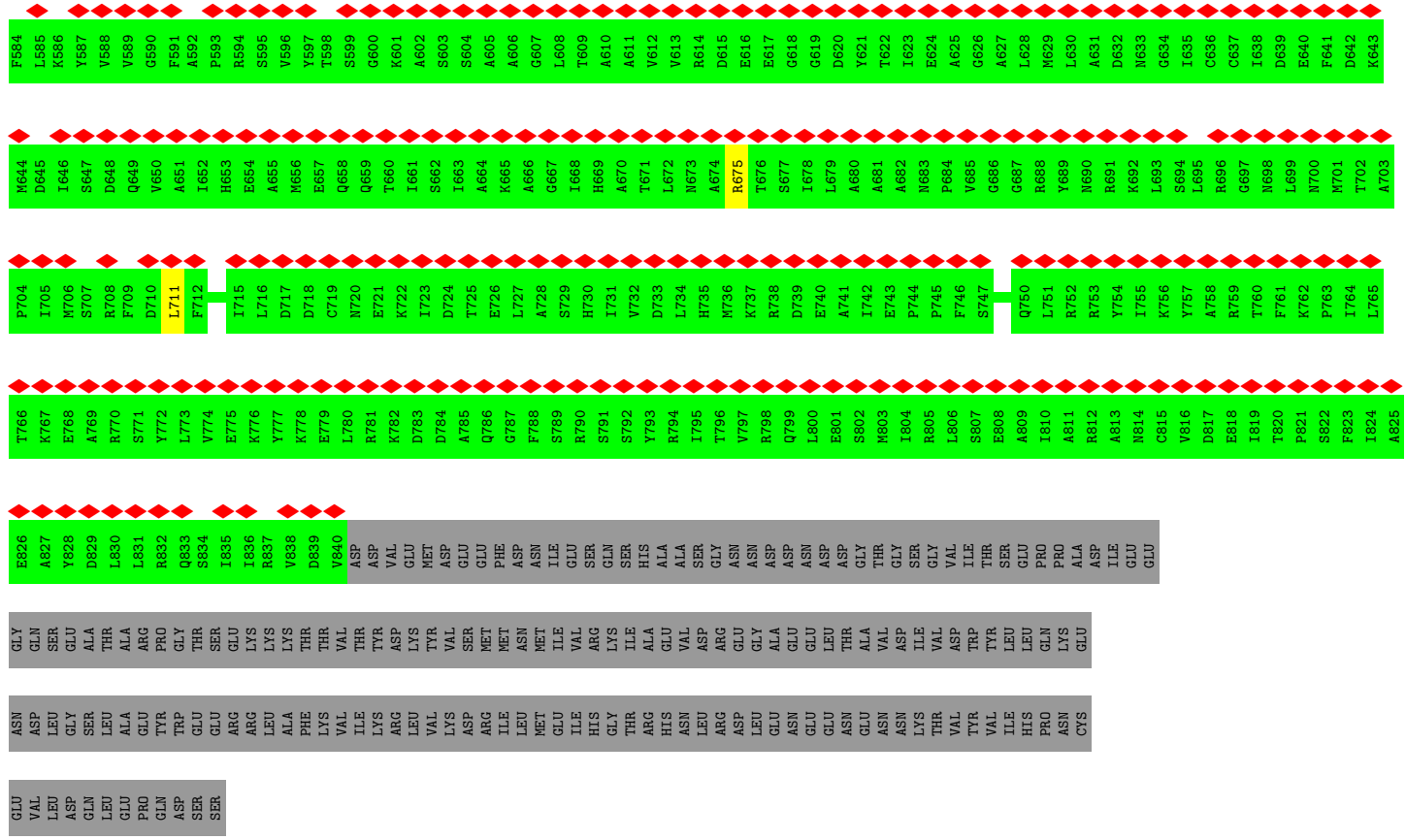


● Molecule 11: DNA replication licensing factor MCM6

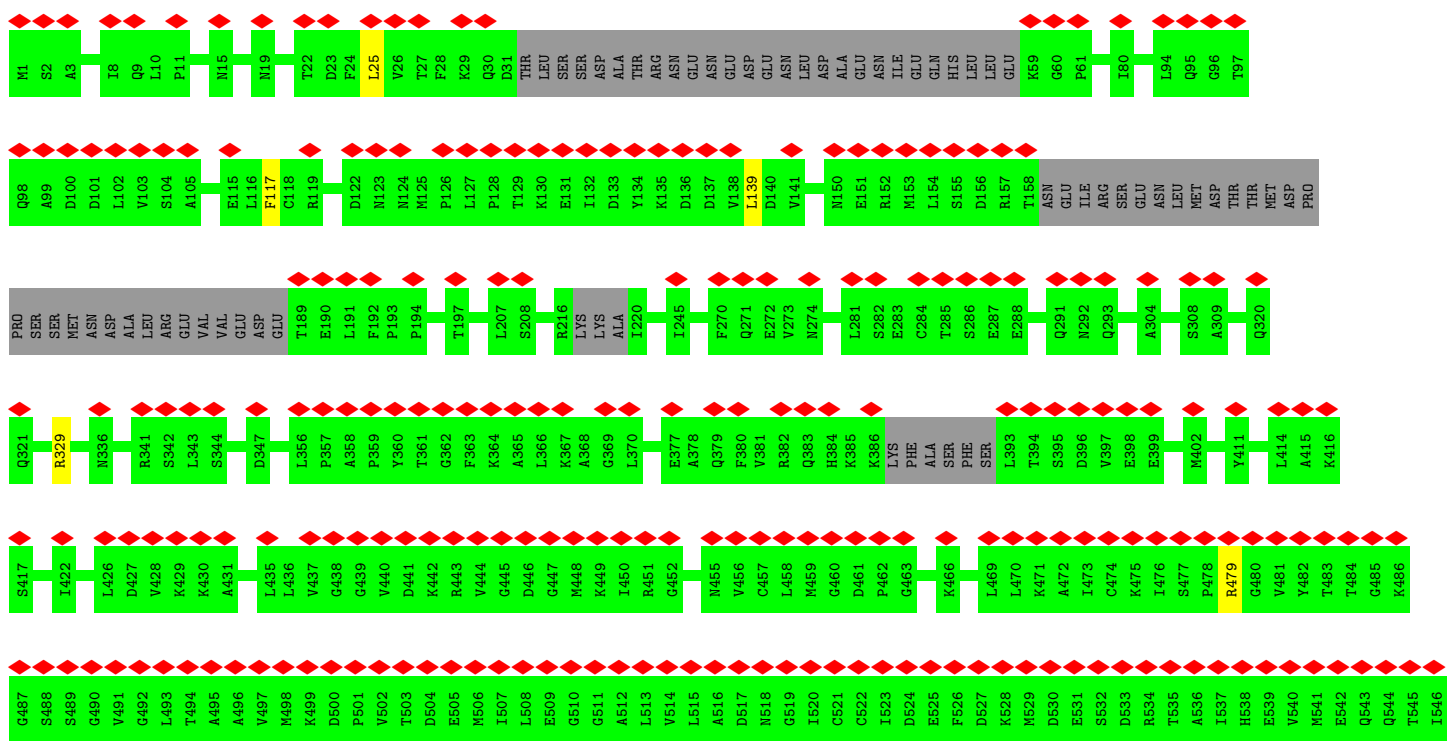
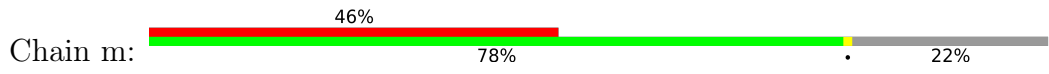








- Molecule 12: DNA replication licensing factor MCM7











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53117	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0234	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	X	0.41	0/3501	0.60	3/4741 (0.1%)
1	Y	0.40	0/3550	0.61	3/4806 (0.1%)
1	Z	0.41	0/3500	0.62	3/4738 (0.1%)
2	A	0.42	0/1718	0.66	2/2314 (0.1%)
2	a	0.42	0/1718	0.66	2/2314 (0.1%)
2	n	0.43	0/1718	0.66	2/2314 (0.1%)
3	B	0.46	1/1545 (0.1%)	0.65	0/2092
3	b	0.46	1/1545 (0.1%)	0.65	0/2092
3	o	0.46	1/1545 (0.1%)	0.65	0/2092
4	C	0.47	0/1320	0.63	1/1784 (0.1%)
4	c	0.47	0/1320	0.63	0/1784
4	p	0.47	0/1320	0.63	1/1784 (0.1%)
5	D	0.43	0/1956	0.58	0/2638
5	d	0.43	0/1956	0.58	0/2638
5	q	0.43	0/1956	0.58	0/2638
6	E	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	e	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	r	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
7	2	0.45	0/5051	0.64	1/6821 (0.0%)
7	F	0.45	0/5051	0.64	1/6821 (0.0%)
7	h	0.45	0/5051	0.64	1/6821 (0.0%)
8	3	0.44	0/4739	0.78	3/6425 (0.0%)
8	G	0.44	0/4739	0.78	3/6425 (0.0%)
8	i	0.44	0/4739	0.78	3/6425 (0.0%)
9	4	0.37	0/5479	0.61	2/7392 (0.0%)
9	H	0.38	1/5479 (0.0%)	0.65	5/7392 (0.1%)
9	j	0.37	0/5479	0.61	2/7392 (0.0%)
10	5	0.47	0/4750	0.69	4/6412 (0.1%)
10	I	0.47	0/4750	0.69	4/6412 (0.1%)
10	k	0.47	0/4750	0.69	4/6412 (0.1%)
11	6	0.43	0/4789	0.65	3/6466 (0.0%)
11	J	0.43	0/4789	0.65	3/6466 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	l	0.43	0/4789	0.65	3/6466 (0.0%)
12	7	0.37	0/5299	0.61	3/7160 (0.0%)
12	K	0.37	0/5299	0.61	3/7160 (0.0%)
12	m	0.37	0/5299	0.61	3/7160 (0.0%)
All	All	0.43	7/134178 (0.0%)	0.66	83/181316 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1
1	Y	0	1
1	Z	0	1
8	3	0	1
8	G	0	1
8	i	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	478	TRP	CB-CG	-6.10	1.39	1.50
6	e	478	TRP	CB-CG	-6.08	1.39	1.50
6	r	478	TRP	CB-CG	-6.07	1.39	1.50
3	o	11	PHE	C-N	-5.28	1.22	1.34
3	B	11	PHE	C-N	-5.27	1.22	1.34
3	b	11	PHE	C-N	-5.25	1.22	1.34
9	H	467	LYS	C-N	5.08	1.45	1.34

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	17	PRO	CA-C-O	-29.20	50.11	120.20
8	i	17	PRO	CA-C-O	-29.18	50.16	120.20
8	G	17	PRO	CA-C-O	-29.18	50.17	120.20
8	G	17	PRO	CA-C-N	15.27	150.79	117.20
8	3	17	PRO	CA-C-N	15.26	150.76	117.20
8	i	17	PRO	CA-C-N	15.21	150.66	117.20
1	Z	766	PHE	C-N-CD	-13.96	89.89	120.60
8	i	17	PRO	O-C-N	-13.09	101.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	17	PRO	O-C-N	-13.01	101.88	122.70
8	3	17	PRO	O-C-N	-12.99	101.92	122.70
9	H	467	LYS	O-C-N	11.84	141.64	122.70
9	H	467	LYS	C-N-CA	-11.70	92.46	121.70
1	Y	766	PHE	C-N-CD	-10.78	96.89	120.60
1	X	766	PHE	C-N-CD	-10.29	97.95	120.60
9	H	467	LYS	CA-C-N	-8.91	97.60	117.20
1	Z	766	PHE	C-N-CA	8.50	157.70	122.00
1	Y	766	PHE	C-N-CA	8.30	156.86	122.00
1	X	766	PHE	C-N-CA	8.10	156.01	122.00
10	I	79	LEU	CA-CB-CG	7.64	132.88	115.30
10	5	79	LEU	CA-CB-CG	7.61	132.79	115.30
10	k	79	LEU	CA-CB-CG	7.59	132.77	115.30
12	m	628	LEU	CA-CB-CG	7.45	132.44	115.30
12	7	139	LEU	CA-CB-CG	7.44	132.42	115.30
12	K	628	LEU	CA-CB-CG	7.44	132.42	115.30
12	K	139	LEU	CA-CB-CG	7.44	132.40	115.30
12	7	628	LEU	CA-CB-CG	7.43	132.39	115.30
12	m	139	LEU	CA-CB-CG	7.43	132.39	115.30
11	6	440	LEU	CA-CB-CG	7.42	132.36	115.30
11	l	440	LEU	CA-CB-CG	7.41	132.34	115.30
11	J	440	LEU	CA-CB-CG	7.41	132.34	115.30
10	k	668	LEU	CA-CB-CG	7.26	131.99	115.30
10	5	668	LEU	CA-CB-CG	7.26	131.99	115.30
10	I	668	LEU	CA-CB-CG	7.25	131.97	115.30
9	4	727	LEU	CA-CB-CG	6.74	130.81	115.30
9	j	727	LEU	CA-CB-CG	6.74	130.79	115.30
9	H	727	LEU	CA-CB-CG	6.73	130.79	115.30
7	F	416	ASP	CB-CG-OD1	6.28	123.95	118.30
7	2	416	ASP	CB-CG-OD1	6.19	123.87	118.30
7	h	416	ASP	CB-CG-OD1	6.15	123.83	118.30
2	n	123	LEU	CB-CG-CD1	-6.08	100.67	111.00
2	a	123	LEU	CB-CG-CD1	-6.06	100.70	111.00
2	A	123	LEU	CB-CG-CD1	-6.04	100.73	111.00
6	r	333	SER	N-CA-C	6.04	127.30	111.00
6	e	333	SER	N-CA-C	6.03	127.27	111.00
6	E	333	SER	N-CA-C	6.02	127.25	111.00
10	I	66	GLU	N-CA-C	5.95	127.06	111.00
10	k	66	GLU	N-CA-C	5.93	127.02	111.00
10	5	66	GLU	N-CA-C	5.92	127.00	111.00
6	e	326	LEU	N-CA-C	-5.87	95.15	111.00
6	E	326	LEU	N-CA-C	-5.87	95.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	r	326	LEU	N-CA-C	-5.87	95.16	111.00
6	E	328	LEU	CA-CB-CG	5.83	128.72	115.30
6	e	328	LEU	CA-CB-CG	5.81	128.66	115.30
6	r	328	LEU	CA-CB-CG	5.81	128.66	115.30
11	6	382	ARG	N-CA-C	5.65	126.25	111.00
11	J	382	ARG	N-CA-C	5.65	126.25	111.00
11	l	382	ARG	N-CA-C	5.64	126.24	111.00
6	r	401	LEU	CA-CB-CG	5.64	128.27	115.30
6	e	401	LEU	CA-CB-CG	5.63	128.24	115.30
6	E	401	LEU	CA-CB-CG	5.62	128.22	115.30
2	a	123	LEU	CA-CB-CG	5.60	128.18	115.30
2	n	123	LEU	CA-CB-CG	5.58	128.14	115.30
2	A	123	LEU	CA-CB-CG	5.57	128.12	115.30
11	6	711	LEU	CA-CB-CG	-5.53	102.58	115.30
11	J	711	LEU	CA-CB-CG	-5.52	102.59	115.30
12	7	25	LEU	CA-CB-CG	5.52	127.99	115.30
1	X	767	PRO	CA-N-CD	-5.51	103.79	111.50
12	m	25	LEU	CA-CB-CG	5.50	127.96	115.30
12	K	25	LEU	CA-CB-CG	5.50	127.96	115.30
11	l	711	LEU	CA-CB-CG	-5.50	102.64	115.30
6	e	165	LEU	CA-CB-CG	5.40	127.73	115.30
6	E	165	LEU	CA-CB-CG	5.38	127.68	115.30
6	r	165	LEU	CA-CB-CG	5.37	127.65	115.30
1	Y	767	PRO	CA-N-CD	-5.17	104.25	111.50
10	I	45	ILE	N-CA-C	5.14	124.88	111.00
10	5	45	ILE	N-CA-C	5.14	124.87	111.00
10	k	45	ILE	N-CA-C	5.11	124.80	111.00
9	4	425	ASP	CB-CG-OD2	5.09	122.89	118.30
1	Z	767	PRO	CA-N-CD	-5.08	104.39	111.50
9	H	425	ASP	CB-CG-OD2	5.06	122.85	118.30
9	j	425	ASP	CB-CG-OD2	5.04	122.84	118.30
4	p	165	PHE	N-CA-C	5.03	124.57	111.00
4	C	165	PHE	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	3	17	PRO	Mainchain
8	G	17	PRO	Mainchain
1	X	766	PHE	Peptide
1	Y	766	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	Z	766	PHE	Peptide
8	i	17	PRO	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	419/927 (45%)	408 (97%)	10 (2%)	1 (0%)	47	81
1	Y	427/927 (46%)	414 (97%)	12 (3%)	1 (0%)	47	81
1	Z	417/927 (45%)	407 (98%)	9 (2%)	1 (0%)	47	81
2	A	206/208 (99%)	179 (87%)	26 (13%)	1 (0%)	29	69
2	a	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	69
2	n	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	69
3	B	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	b	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	o	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
4	C	151/194 (78%)	140 (93%)	11 (7%)	0	100	100
4	c	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
4	p	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
5	D	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	d	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	q	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
6	E	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	25	66
6	e	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	25	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	r	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	25	66
7	2	630/868 (73%)	538 (85%)	92 (15%)	0	100	100
7	F	630/868 (73%)	538 (85%)	92 (15%)	0	100	100
7	h	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
8	3	584/971 (60%)	506 (87%)	77 (13%)	1 (0%)	47	81
8	G	584/971 (60%)	506 (87%)	76 (13%)	2 (0%)	41	77
8	i	584/971 (60%)	505 (86%)	77 (13%)	2 (0%)	41	77
9	4	668/933 (72%)	579 (87%)	88 (13%)	1 (0%)	51	86
9	H	668/933 (72%)	578 (86%)	88 (13%)	2 (0%)	41	77
9	j	668/933 (72%)	579 (87%)	88 (13%)	1 (0%)	51	86
10	5	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	47	81
10	I	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	47	81
10	k	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	47	81
11	6	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	47	81
11	J	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	47	81
11	l	606/1017 (60%)	507 (84%)	98 (16%)	1 (0%)	47	81
12	7	653/845 (77%)	556 (85%)	97 (15%)	0	100	100
12	K	653/845 (77%)	555 (85%)	98 (15%)	0	100	100
12	m	653/845 (77%)	555 (85%)	98 (15%)	0	100	100
All	All	16344/23685 (69%)	14200 (87%)	2114 (13%)	30 (0%)	50	81

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	j	469	VAL
9	H	469	VAL
6	e	334	LEU
6	E	334	LEU
6	r	334	LEU
9	H	468	LYS
1	Z	767	PRO
6	e	332	SER
10	k	147	PRO
11	l	305	TYR
6	E	332	SER

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Mol	Chain	Res	Type
10	5	147	PRO
11	6	305	TYR
6	r	332	SER
10	I	147	PRO
11	J	305	TYR
1	X	767	PRO
2	n	30	PRO
2	A	30	PRO
2	a	30	PRO
8	i	311	SER
8	i	669	PRO
8	3	669	PRO
8	G	311	SER
8	G	669	PRO
1	Y	767	PRO
6	e	146	GLY
6	E	146	GLY
9	4	469	VAL
6	r	146	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	377/825 (46%)	377 (100%)	0	100	100
1	Y	383/825 (46%)	383 (100%)	0	100	100
1	Z	377/825 (46%)	377 (100%)	0	100	100
2	A	193/193 (100%)	193 (100%)	0	100	100
2	a	193/193 (100%)	193 (100%)	0	100	100
2	n	193/193 (100%)	193 (100%)	0	100	100
3	B	171/198 (86%)	170 (99%)	1 (1%)	86	92
3	b	171/198 (86%)	170 (99%)	1 (1%)	86	92
3	o	171/198 (86%)	170 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	144/173 (83%)	142 (99%)	2 (1%)	67	80
4	c	144/173 (83%)	142 (99%)	2 (1%)	67	80
4	p	144/173 (83%)	142 (99%)	2 (1%)	67	80
5	D	225/279 (81%)	225 (100%)	0	100	100
5	d	225/279 (81%)	225 (100%)	0	100	100
5	q	225/279 (81%)	225 (100%)	0	100	100
6	E	499/586 (85%)	496 (99%)	3 (1%)	86	92
6	e	499/586 (85%)	496 (99%)	3 (1%)	86	92
6	r	499/586 (85%)	496 (99%)	3 (1%)	86	92
7	2	535/770 (70%)	529 (99%)	6 (1%)	73	84
7	F	535/770 (70%)	529 (99%)	6 (1%)	73	84
7	h	535/770 (70%)	529 (99%)	6 (1%)	73	84
8	3	515/835 (62%)	512 (99%)	3 (1%)	86	92
8	G	515/835 (62%)	512 (99%)	3 (1%)	86	92
8	i	515/835 (62%)	512 (99%)	3 (1%)	86	92
9	4	610/848 (72%)	605 (99%)	5 (1%)	81	89
9	H	610/848 (72%)	604 (99%)	6 (1%)	76	86
9	j	610/848 (72%)	605 (99%)	5 (1%)	81	89
10	5	534/688 (78%)	527 (99%)	7 (1%)	69	81
10	I	534/688 (78%)	527 (99%)	7 (1%)	69	81
10	k	534/688 (78%)	527 (99%)	7 (1%)	69	81
11	6	493/886 (56%)	487 (99%)	6 (1%)	71	83
11	J	493/886 (56%)	487 (99%)	6 (1%)	71	83
11	l	493/886 (56%)	487 (99%)	6 (1%)	71	83
12	7	585/753 (78%)	581 (99%)	4 (1%)	84	90
12	K	585/753 (78%)	581 (99%)	4 (1%)	84	90
12	m	585/753 (78%)	581 (99%)	4 (1%)	84	90
All	All	14649/21102 (69%)	14537 (99%)	112 (1%)	82	89

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	o	80	LYS

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	2	230	ARG
7	2	324	VAL
7	2	384	ASN
7	2	439	ASN
7	2	444	PHE
7	2	476	TRP
8	3	172	THR
8	3	291	ARG
8	3	339	ARG
9	4	349	CYS
9	4	445	ARG
9	4	451	ARG
9	4	697	PRO
9	4	928	ARG
10	5	66	GLU
10	5	275	THR
10	5	295	VAL
10	5	326	PRO
10	5	486	ARG
10	5	501	THR
10	5	675	ARG
11	6	296	ARG
11	6	350	ARG
11	6	381	LEU
11	6	540	HIS
11	6	581	LYS
11	6	675	ARG
12	7	117	PHE
12	7	329	ARG
12	7	479	ARG
12	7	718	ARG
3	b	80	LYS
4	c	20	PHE
4	c	84	VAL
6	r	160	TYR
6	r	241	TYR
6	r	411	ARG
7	F	230	ARG
7	F	324	VAL
7	F	384	ASN
7	F	439	ASN
7	F	444	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	F	476	TRP
8	G	172	THR
8	G	291	ARG
8	G	339	ARG
9	H	349	CYS
9	H	445	ARG
9	H	451	ARG
9	H	469	VAL
9	H	697	PRO
9	H	928	ARG
10	I	66	GLU
10	I	275	THR
10	I	295	VAL
10	I	326	PRO
10	I	486	ARG
10	I	501	THR
10	I	675	ARG
11	J	296	ARG
11	J	350	ARG
11	J	381	LEU
11	J	540	HIS
11	J	581	LYS
11	J	675	ARG
12	K	117	PHE
12	K	329	ARG
12	K	479	ARG
12	K	718	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (241) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	527	HIS
1	X	573	GLN
1	Y	507	ASN
1	Y	510	GLN
1	Y	548	GLN
1	Y	678	ASN
1	Y	753	ASN
1	Y	790	ASN
1	Z	622	ASN
1	Z	790	ASN
2	n	28	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	n	39	ASN
2	n	90	GLN
2	n	182	ASN
3	o	103	GLN
4	p	21	GLN
4	p	41	ASN
4	p	130	GLN
4	p	133	GLN
4	p	181	HIS
6	e	7	GLN
6	e	18	ASN
6	e	22	HIS
6	e	26	GLN
6	e	52	GLN
6	e	55	GLN
6	e	70	HIS
6	e	155	GLN
6	e	289	ASN
6	e	331	HIS
6	e	374	GLN
6	e	395	ASN
6	e	402	GLN
6	e	468	ASN
6	e	497	GLN
6	e	563	GLN
6	e	604	ASN
7	h	202	ASN
7	h	238	ASN
7	h	245	ASN
7	h	333	GLN
7	h	340	ASN
7	h	433	ASN
7	h	526	ASN
7	h	551	GLN
7	h	779	HIS
7	h	780	GLN
7	h	809	HIS
8	i	51	ASN
8	i	52	ASN
8	i	57	ASN
8	i	210	HIS
8	i	312	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	i	330	HIS
8	i	351	ASN
8	i	503	HIS
8	i	554	ASN
8	i	677	ASN
9	j	184	ASN
9	j	196	ASN
9	j	274	GLN
9	j	413	HIS
9	j	858	GLN
9	j	876	GLN
10	k	53	ASN
10	k	67	HIS
10	k	203	ASN
10	k	254	GLN
10	k	302	ASN
10	k	539	ASN
10	k	561	ASN
10	k	574	ASN
10	k	617	GLN
10	k	652	GLN
11	l	182	GLN
11	l	514	ASN
11	l	570	ASN
11	l	750	GLN
11	l	814	ASN
11	l	833	GLN
12	m	87	GLN
12	m	292	ASN
12	m	293	GLN
12	m	316	GLN
12	m	326	HIS
12	m	379	GLN
12	m	468	GLN
12	m	657	ASN
12	m	683	GLN
2	A	28	ASN
2	A	39	ASN
2	A	90	GLN
2	A	182	ASN
3	B	103	GLN
4	C	21	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	C	41	ASN
4	C	133	GLN
4	C	181	HIS
6	E	13	ASN
6	E	18	ASN
6	E	22	HIS
6	E	26	GLN
6	E	52	GLN
6	E	55	GLN
6	E	70	HIS
6	E	155	GLN
6	E	289	ASN
6	E	331	HIS
6	E	374	GLN
6	E	395	ASN
6	E	402	GLN
6	E	497	GLN
6	E	563	GLN
6	E	604	ASN
7	2	202	ASN
7	2	238	ASN
7	2	245	ASN
7	2	333	GLN
7	2	340	ASN
7	2	433	ASN
7	2	526	ASN
7	2	551	GLN
7	2	779	HIS
7	2	780	GLN
7	2	809	HIS
8	3	51	ASN
8	3	52	ASN
8	3	57	ASN
8	3	210	HIS
8	3	312	ASN
8	3	330	HIS
8	3	351	ASN
8	3	554	ASN
8	3	677	ASN
9	4	184	ASN
9	4	196	ASN
9	4	274	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	4	413	HIS
9	4	858	GLN
9	4	876	GLN
10	5	53	ASN
10	5	67	HIS
10	5	203	ASN
10	5	254	GLN
10	5	539	ASN
10	5	561	ASN
10	5	574	ASN
10	5	617	GLN
10	5	652	GLN
11	6	182	GLN
11	6	514	ASN
11	6	570	ASN
11	6	750	GLN
11	6	814	ASN
11	6	833	GLN
12	7	87	GLN
12	7	292	ASN
12	7	293	GLN
12	7	316	GLN
12	7	326	HIS
12	7	379	GLN
12	7	468	GLN
12	7	657	ASN
12	7	683	GLN
2	a	28	ASN
2	a	39	ASN
2	a	90	GLN
2	a	182	ASN
3	b	103	GLN
3	b	135	HIS
4	c	21	GLN
4	c	41	ASN
4	c	133	GLN
4	c	181	HIS
6	r	18	ASN
6	r	22	HIS
6	r	26	GLN
6	r	52	GLN
6	r	55	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	r	70	HIS
6	r	155	GLN
6	r	289	ASN
6	r	331	HIS
6	r	374	GLN
6	r	395	ASN
6	r	468	ASN
6	r	497	GLN
6	r	563	GLN
6	r	604	ASN
7	F	202	ASN
7	F	238	ASN
7	F	245	ASN
7	F	333	GLN
7	F	340	ASN
7	F	433	ASN
7	F	526	ASN
7	F	551	GLN
7	F	779	HIS
7	F	780	GLN
7	F	809	HIS
8	G	51	ASN
8	G	52	ASN
8	G	57	ASN
8	G	210	HIS
8	G	312	ASN
8	G	330	HIS
8	G	351	ASN
8	G	503	HIS
8	G	554	ASN
8	G	677	ASN
9	H	184	ASN
9	H	196	ASN
9	H	274	GLN
9	H	413	HIS
9	H	858	GLN
9	H	876	GLN
10	I	53	ASN
10	I	67	HIS
10	I	203	ASN
10	I	254	GLN
10	I	539	ASN

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Mol	Chain	Res	Type
10	I	561	ASN
10	I	574	ASN
10	I	617	GLN
10	I	652	GLN
11	J	182	GLN
11	J	514	ASN
11	J	570	ASN
11	J	750	GLN
11	J	814	ASN
11	J	833	GLN
12	K	87	GLN
12	K	150	ASN
12	K	292	ASN
12	K	293	GLN
12	K	316	GLN
12	K	326	HIS
12	K	379	GLN
12	K	468	GLN
12	K	657	ASN
12	K	683	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	ATP	i	1001	-	26,33,33	0.92	1 (3%)	31,52,52	1.90	6 (19%)
13	ATP	2	901	-	26,33,33	0.92	1 (3%)	31,52,52	1.64	5 (16%)
13	ATP	5	801	-	26,33,33	0.86	0	31,52,52	1.93	7 (22%)
13	ATP	3	1001	-	26,33,33	0.92	1 (3%)	31,52,52	1.91	6 (19%)
13	ATP	h	901	-	26,33,33	0.92	1 (3%)	31,52,52	1.64	5 (16%)
13	ATP	k	801	-	26,33,33	0.86	0	31,52,52	1.93	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	i	1001	-	-	4/18/38/38	0/3/3/3
13	ATP	2	901	-	-	6/18/38/38	0/3/3/3
13	ATP	5	801	-	-	4/18/38/38	0/3/3/3
13	ATP	3	1001	-	-	4/18/38/38	0/3/3/3
13	ATP	h	901	-	-	6/18/38/38	0/3/3/3
13	ATP	k	801	-	-	4/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	h	901	ATP	C5-C4	2.17	1.46	1.40
13	2	901	ATP	C5-C4	2.15	1.46	1.40
13	i	1001	ATP	C5-C4	2.12	1.46	1.40
13	3	1001	ATP	C5-C4	2.11	1.46	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	1001	ATP	PA-O3A-PB	-6.31	111.16	132.83
13	i	1001	ATP	PA-O3A-PB	-6.31	111.18	132.83
13	k	801	ATP	PA-O3A-PB	-5.28	114.69	132.83
13	5	801	ATP	PA-O3A-PB	-5.26	114.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	k	801	ATP	PB-O3B-PG	-5.03	115.56	132.83
13	5	801	ATP	PB-O3B-PG	-5.03	115.58	132.83
13	h	901	ATP	PA-O3A-PB	-4.64	116.89	132.83
13	2	901	ATP	PA-O3A-PB	-4.63	116.94	132.83
13	3	1001	ATP	PB-O3B-PG	-4.41	117.69	132.83
13	i	1001	ATP	PB-O3B-PG	-4.40	117.72	132.83
13	k	801	ATP	N3-C2-N1	-3.73	122.85	128.68
13	5	801	ATP	N3-C2-N1	-3.72	122.87	128.68
13	h	901	ATP	C3'-C2'-C1'	3.23	105.84	100.98
13	2	901	ATP	C3'-C2'-C1'	3.22	105.83	100.98
13	2	901	ATP	PB-O3B-PG	-3.14	122.06	132.83
13	3	1001	ATP	N3-C2-N1	-3.14	123.78	128.68
13	h	901	ATP	PB-O3B-PG	-3.12	122.12	132.83
13	i	1001	ATP	N3-C2-N1	-3.10	123.83	128.68
13	i	1001	ATP	C3'-C2'-C1'	2.96	105.43	100.98
13	k	801	ATP	C4-C5-N7	-2.96	106.32	109.40
13	3	1001	ATP	C3'-C2'-C1'	2.95	105.41	100.98
13	5	801	ATP	C4-C5-N7	-2.93	106.34	109.40
13	2	901	ATP	N3-C2-N1	-2.90	124.14	128.68
13	h	901	ATP	N3-C2-N1	-2.87	124.19	128.68
13	h	901	ATP	C4-C5-N7	-2.76	106.52	109.40
13	2	901	ATP	C4-C5-N7	-2.73	106.55	109.40
13	k	801	ATP	O3G-PG-O2G	2.28	116.35	107.64
13	5	801	ATP	O3G-PG-O2G	2.26	116.29	107.64
13	k	801	ATP	C3'-C2'-C1'	2.25	104.36	100.98
13	5	801	ATP	C3'-C2'-C1'	2.22	104.32	100.98
13	3	1001	ATP	C4-C5-N7	-2.22	107.08	109.40
13	k	801	ATP	C2-N1-C6	2.21	122.54	118.75
13	5	801	ATP	C2-N1-C6	2.21	122.54	118.75
13	i	1001	ATP	C4-C5-N7	-2.18	107.12	109.40
13	i	1001	ATP	C2'-C3'-C4'	2.12	106.76	102.64
13	3	1001	ATP	C2'-C3'-C4'	2.12	106.76	102.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	h	901	ATP	C5'-O5'-PA-O1A
13	h	901	ATP	C5'-O5'-PA-O2A
13	i	1001	ATP	C5'-O5'-PA-O2A
13	i	1001	ATP	C5'-O5'-PA-O3A
13	2	901	ATP	C5'-O5'-PA-O1A

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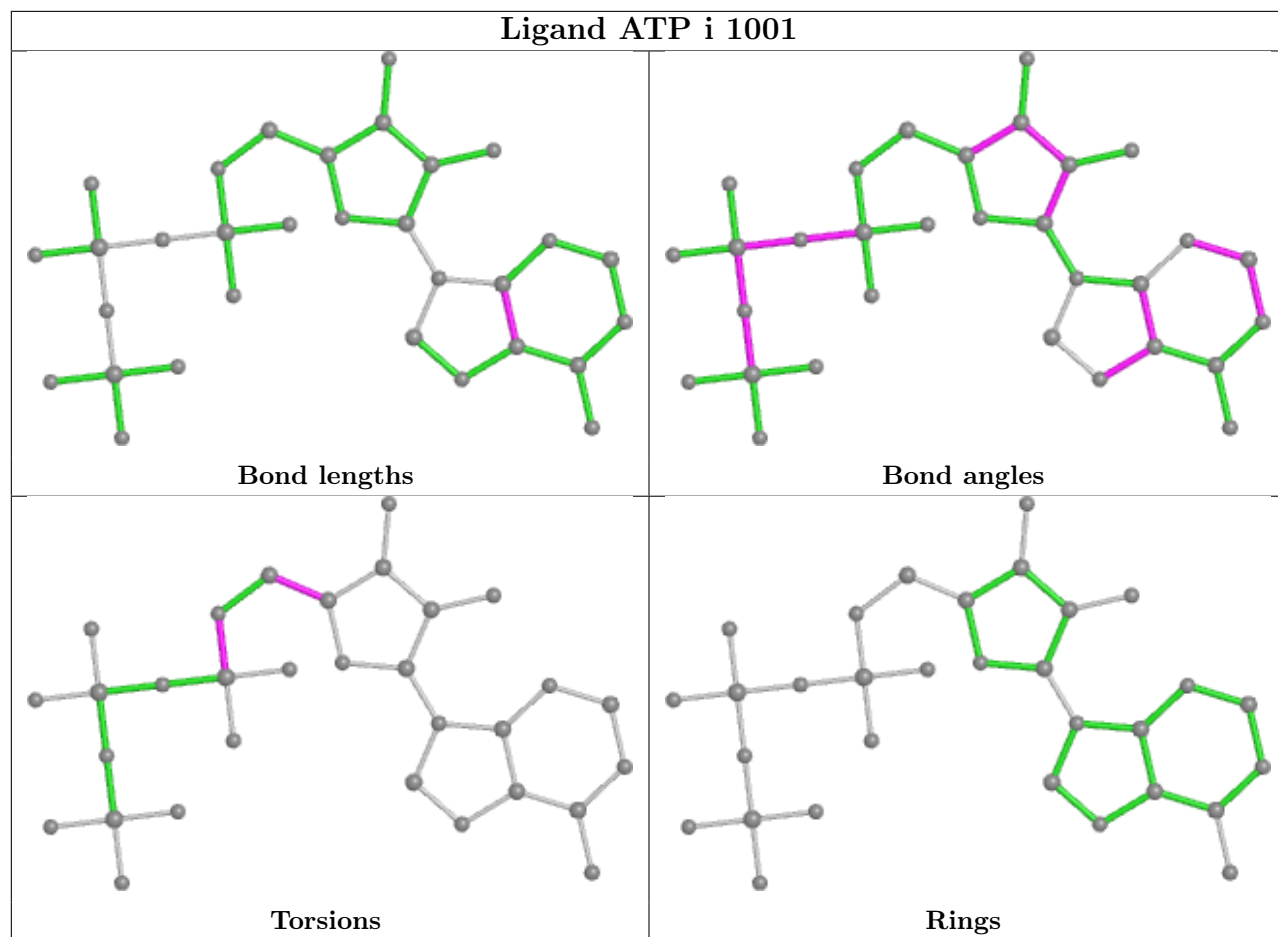
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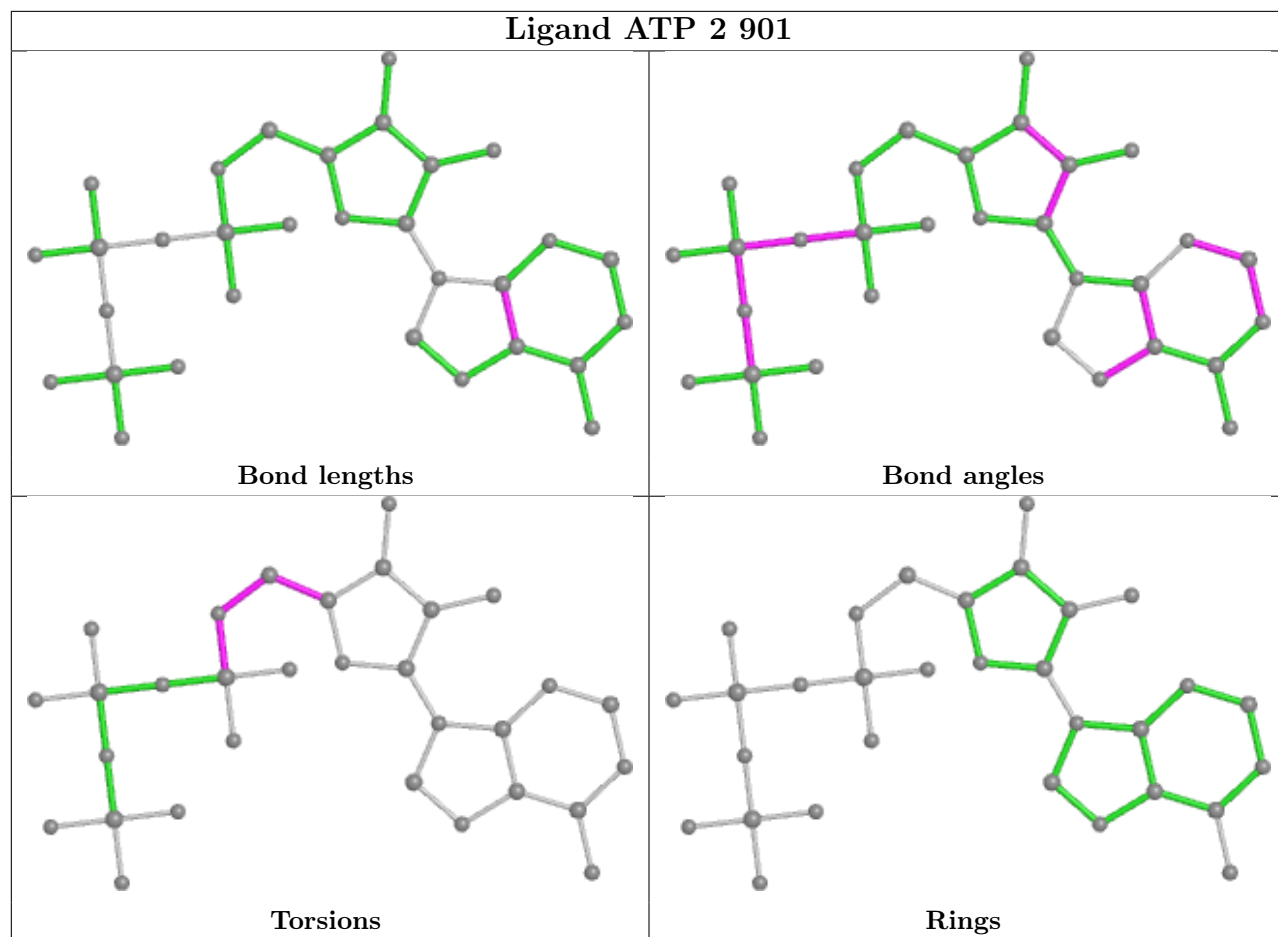
Mol	Chain	Res	Type	Atoms
13	2	901	ATP	C5'-O5'-PA-O2A
13	3	1001	ATP	C5'-O5'-PA-O2A
13	3	1001	ATP	C5'-O5'-PA-O3A
13	h	901	ATP	C3'-C4'-C5'-O5'
13	2	901	ATP	C3'-C4'-C5'-O5'
13	h	901	ATP	O4'-C4'-C5'-O5'
13	2	901	ATP	O4'-C4'-C5'-O5'
13	i	1001	ATP	C3'-C4'-C5'-O5'
13	3	1001	ATP	C3'-C4'-C5'-O5'
13	i	1001	ATP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

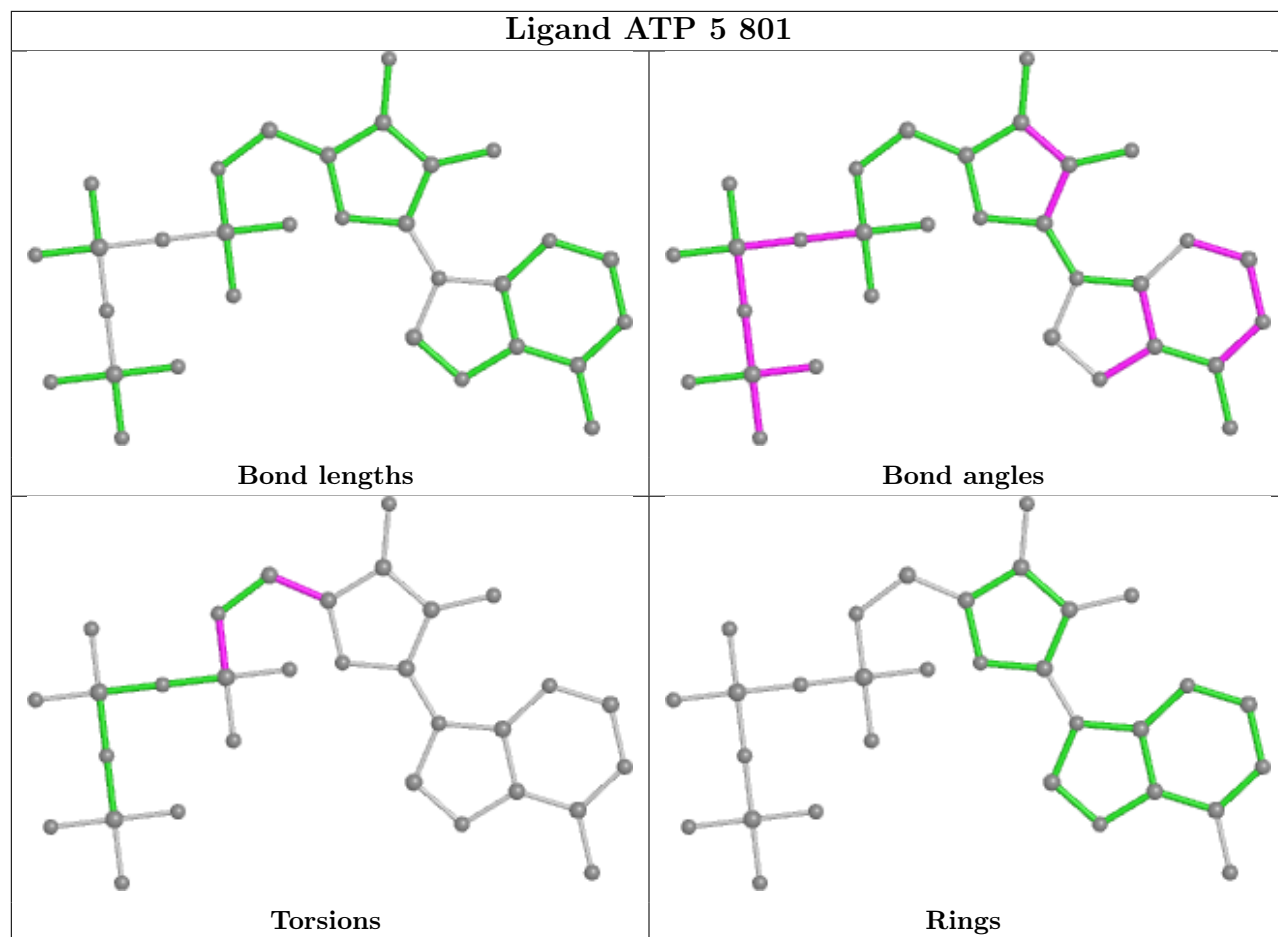
There are no ring outliers.

No monomer is involved in short contacts.

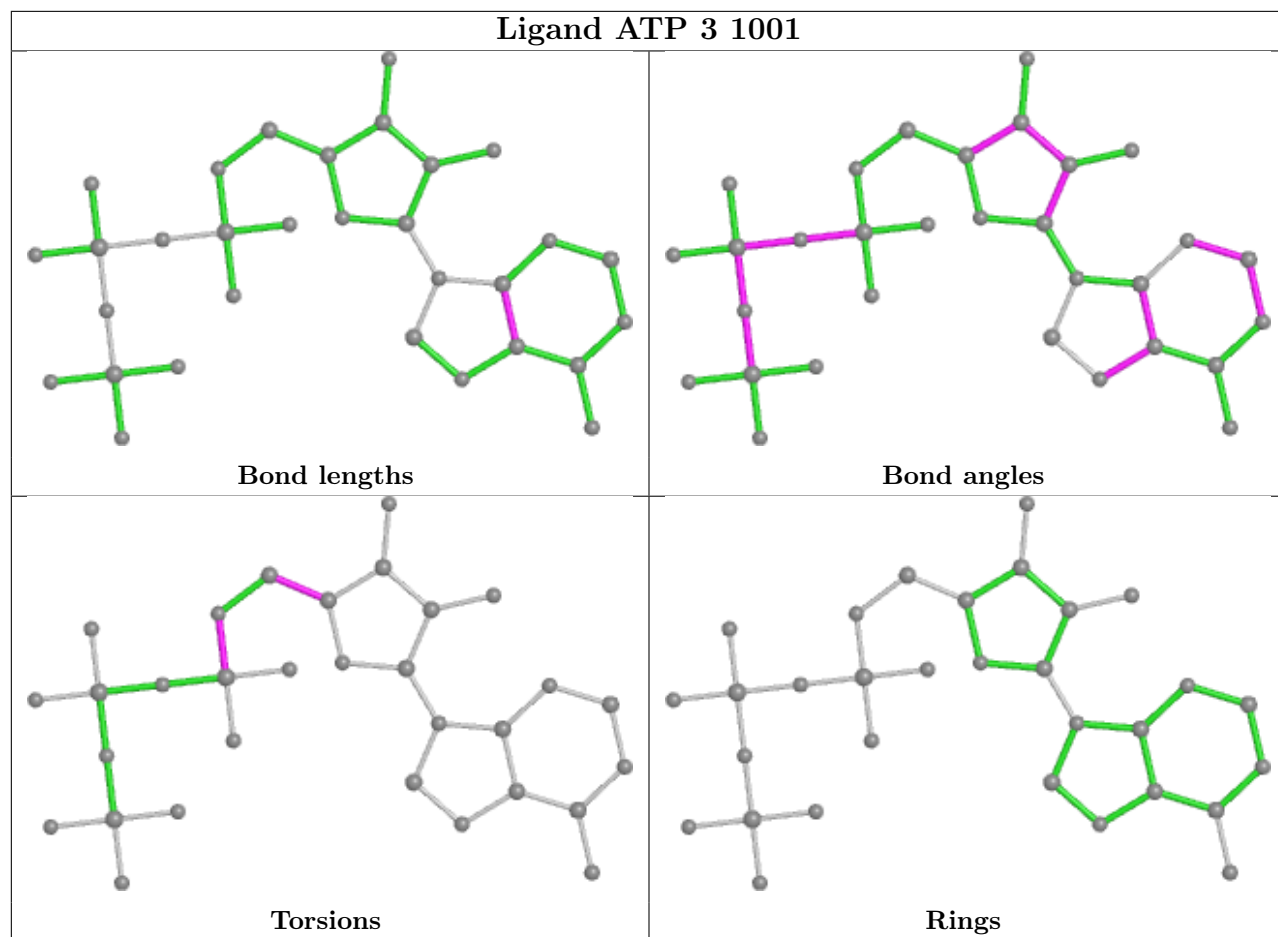
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

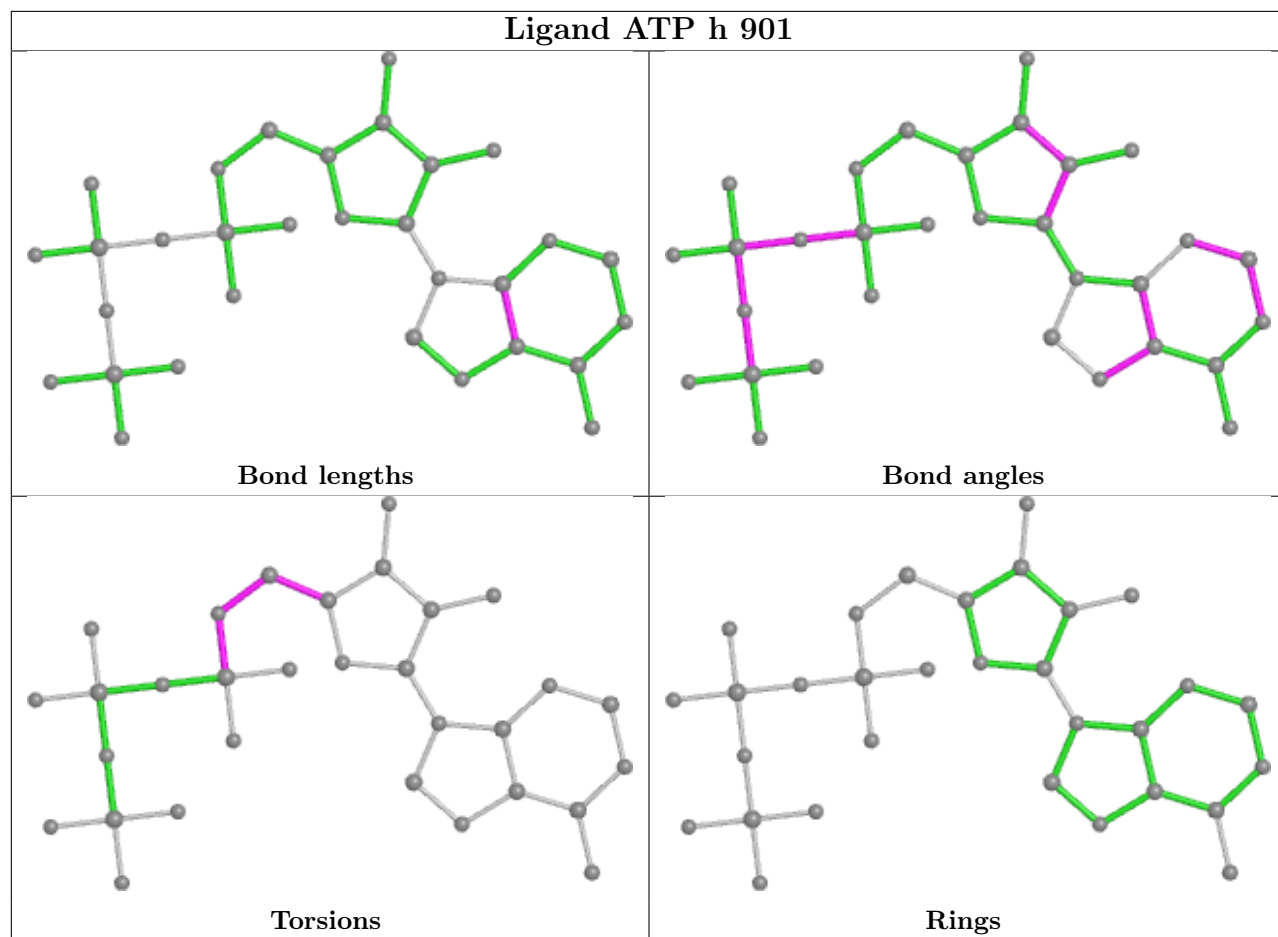


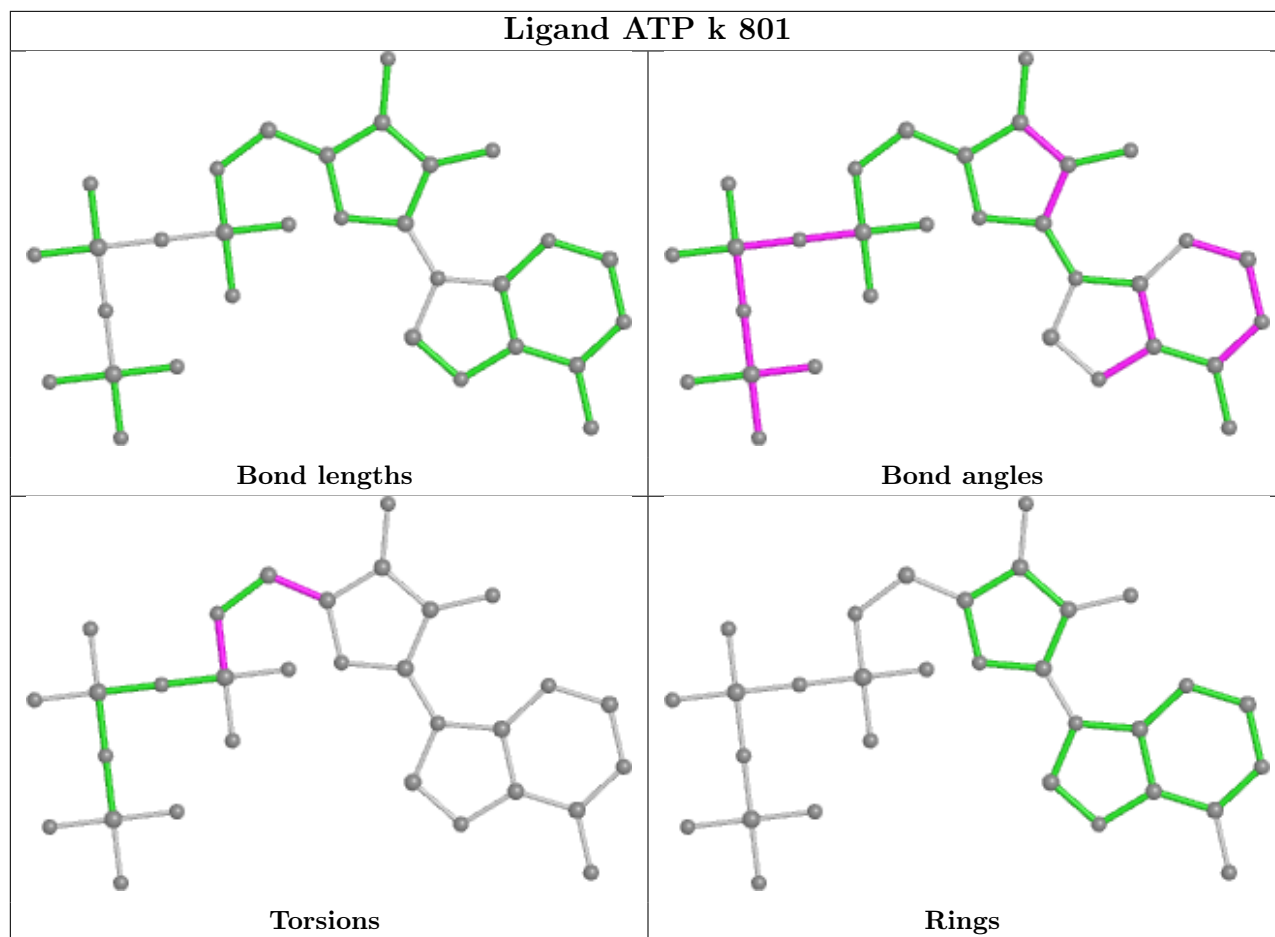












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Z	1

All chain breaks are listed below:

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

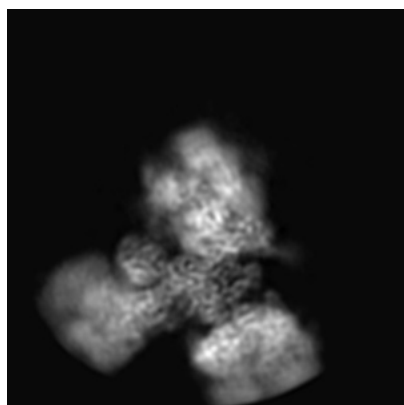
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20473. These allow visual inspection of the internal detail of the map and identification of artifacts.

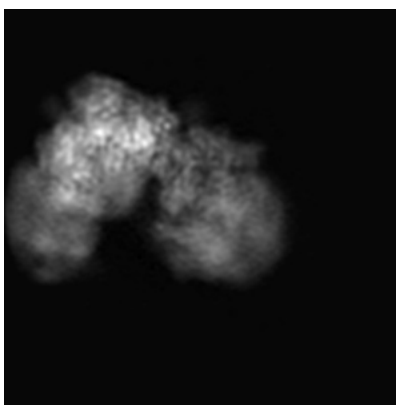
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

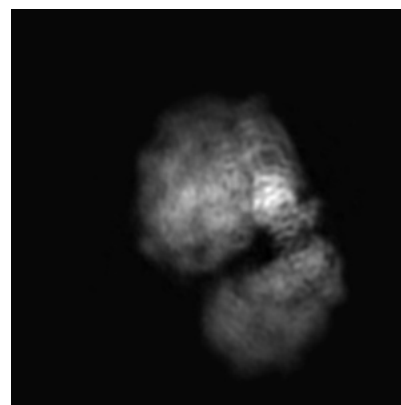
#### 6.1.1 Primary map



X



Y

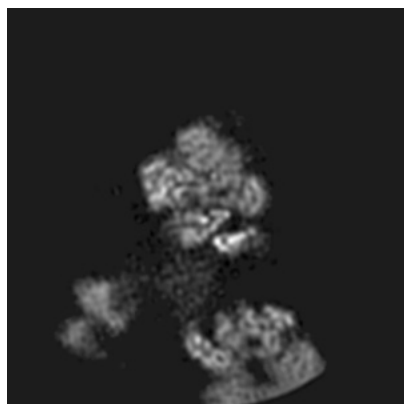


Z

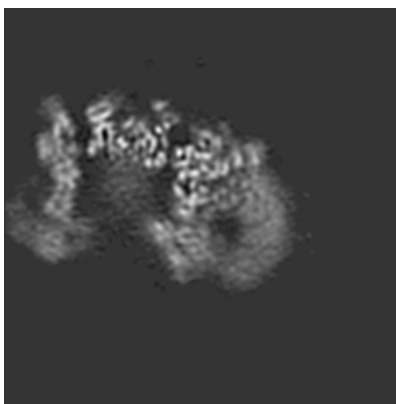
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

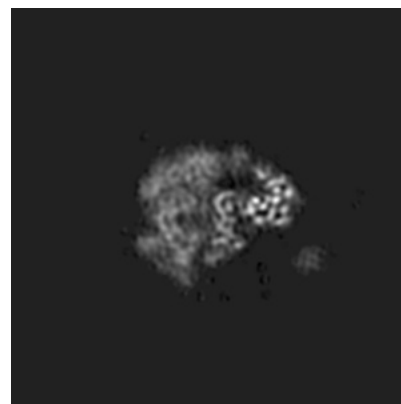
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

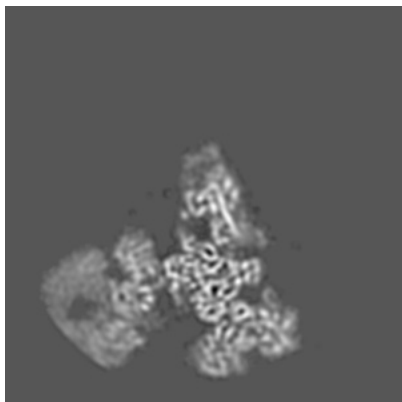


Z Index: 200

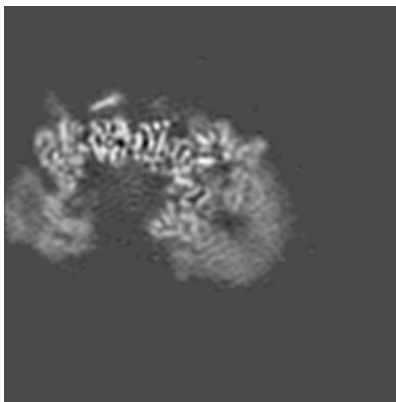
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

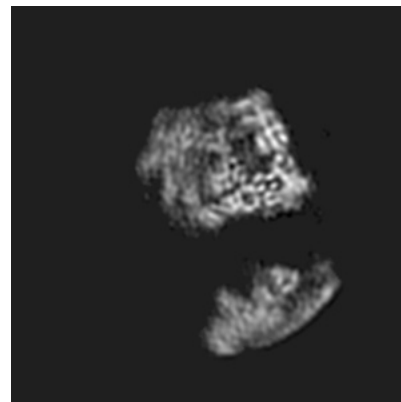
### 6.3.1 Primary map



X Index: 265



Y Index: 207



Z Index: 66

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

## 6.4 Orthogonal surface views [i](#)

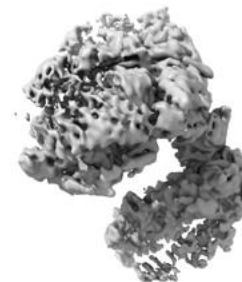
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0234. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

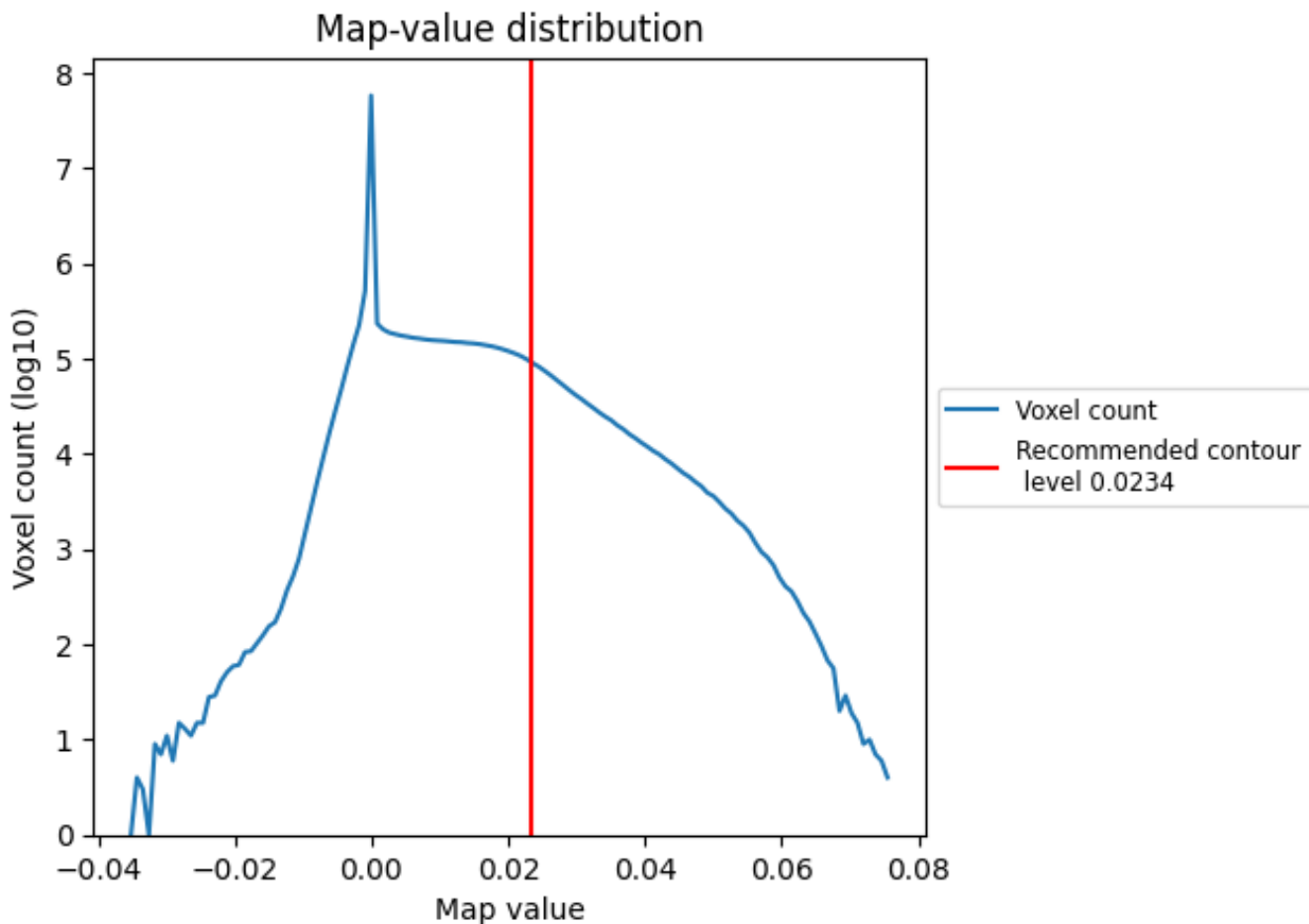
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

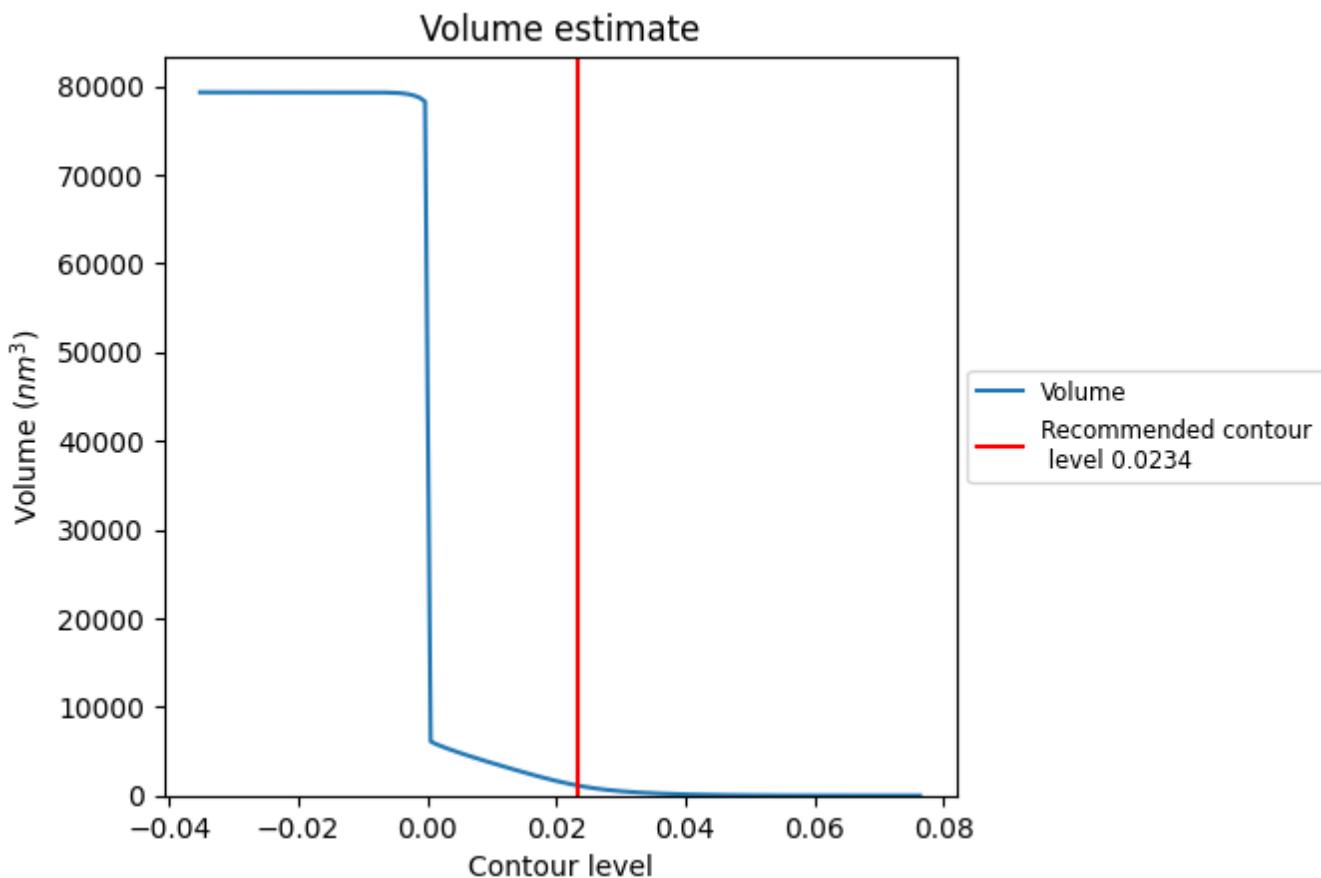
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [\(i\)](#)

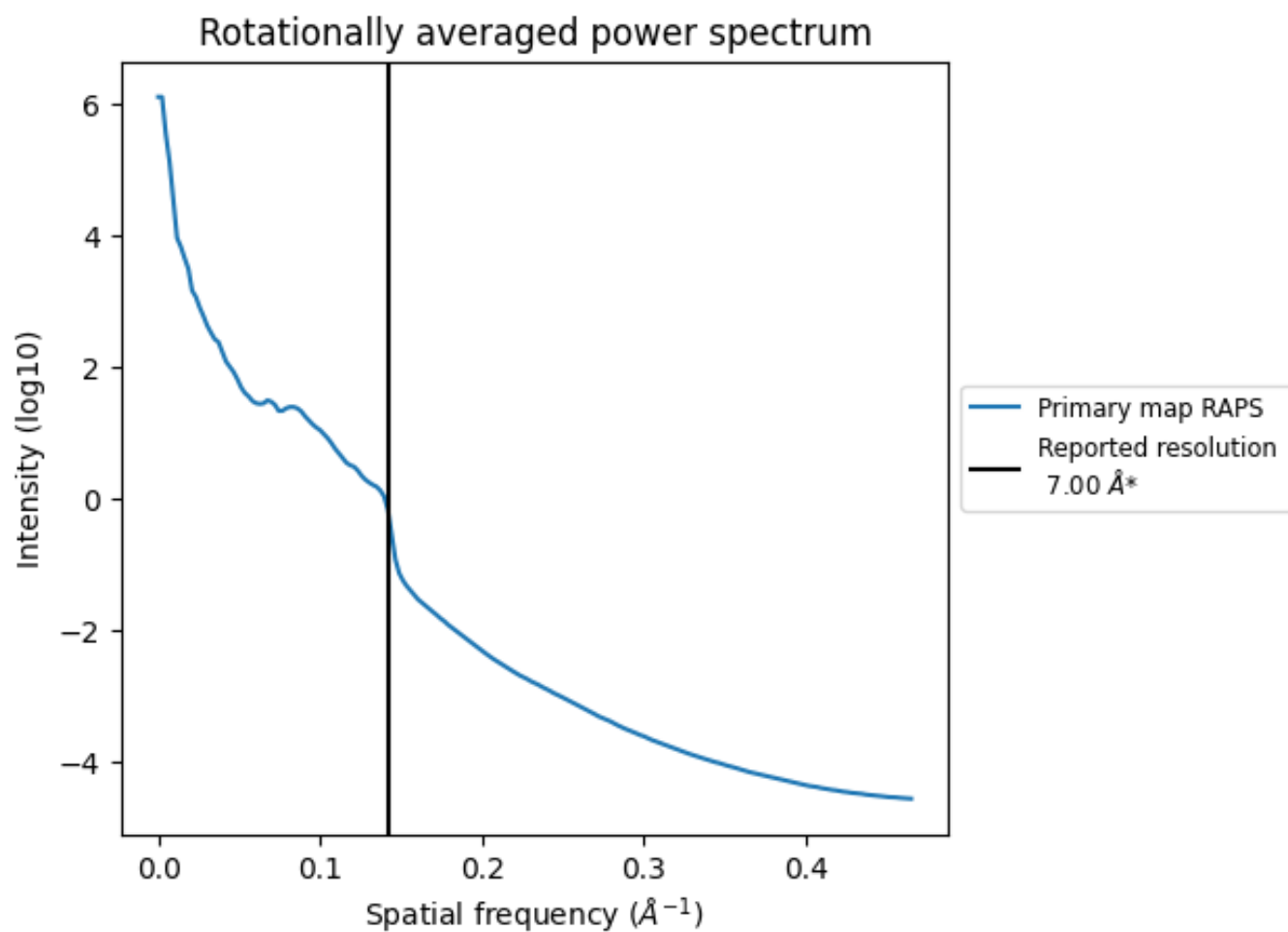


The volume at the recommended contour level is 1122 nm<sup>3</sup>; this corresponds to an approximate mass of 1014 kDa.

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  $0.143 \text{\AA}^{-1}$

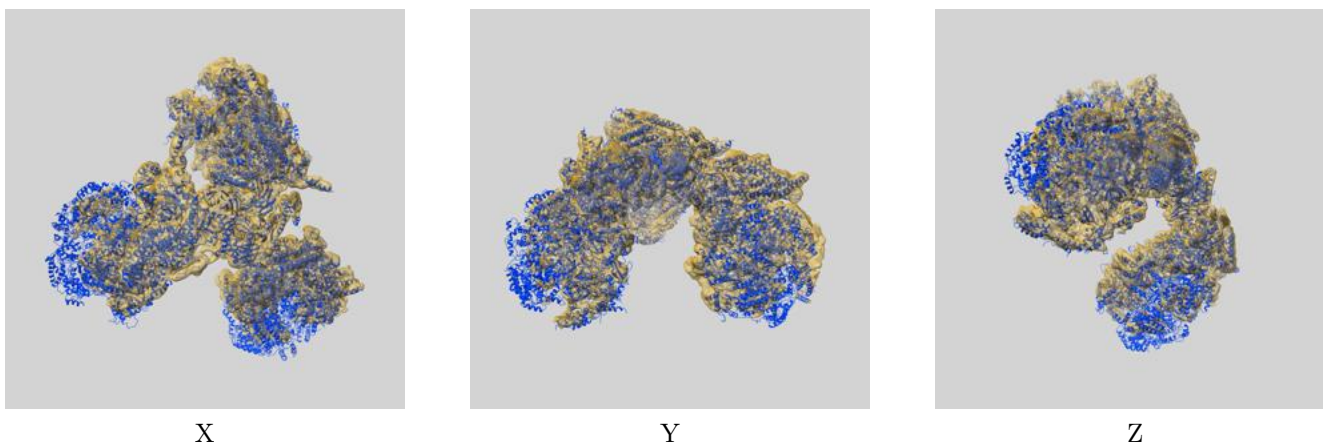
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

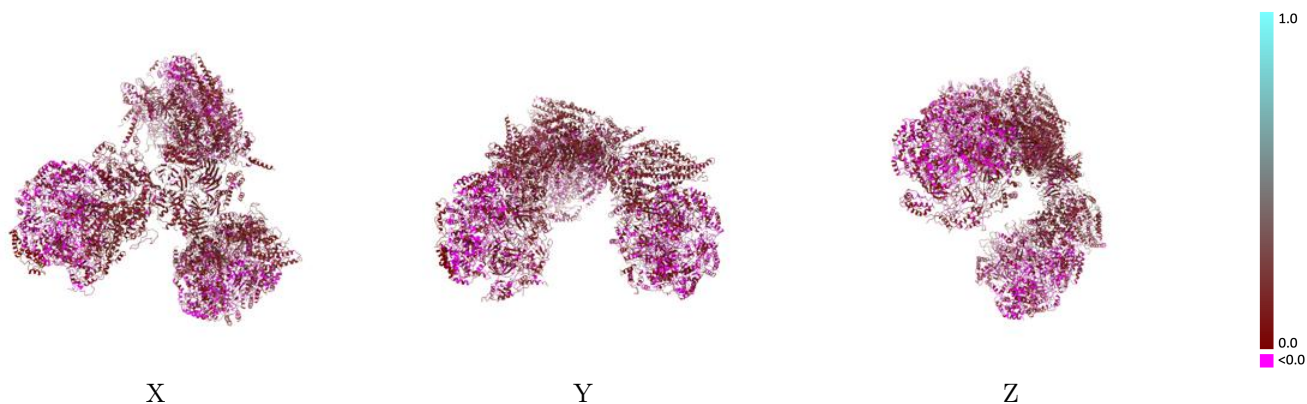
This section contains information regarding the fit between EMDB map EMD-20473 and PDB model 6PTO. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



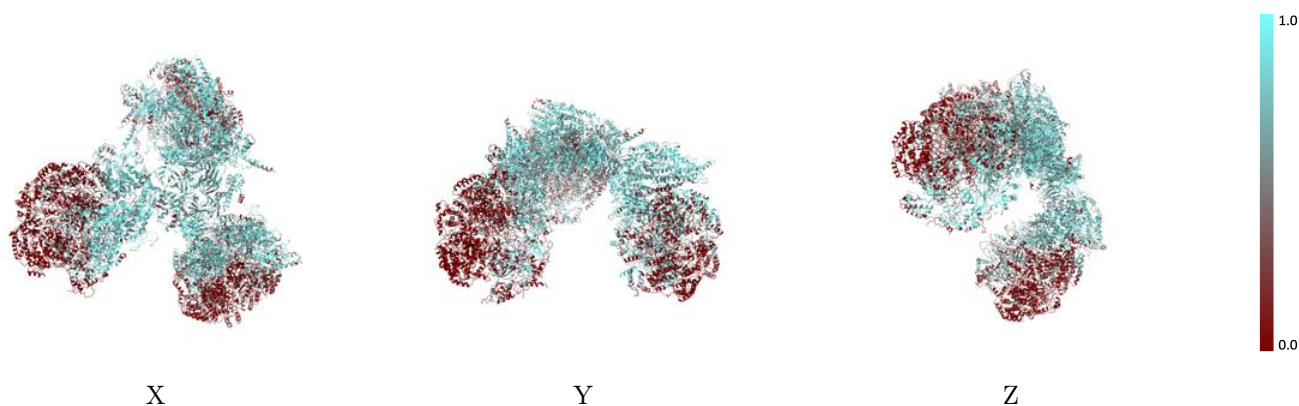
The images above show the 3D surface view of the map at the recommended contour level 0.0234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



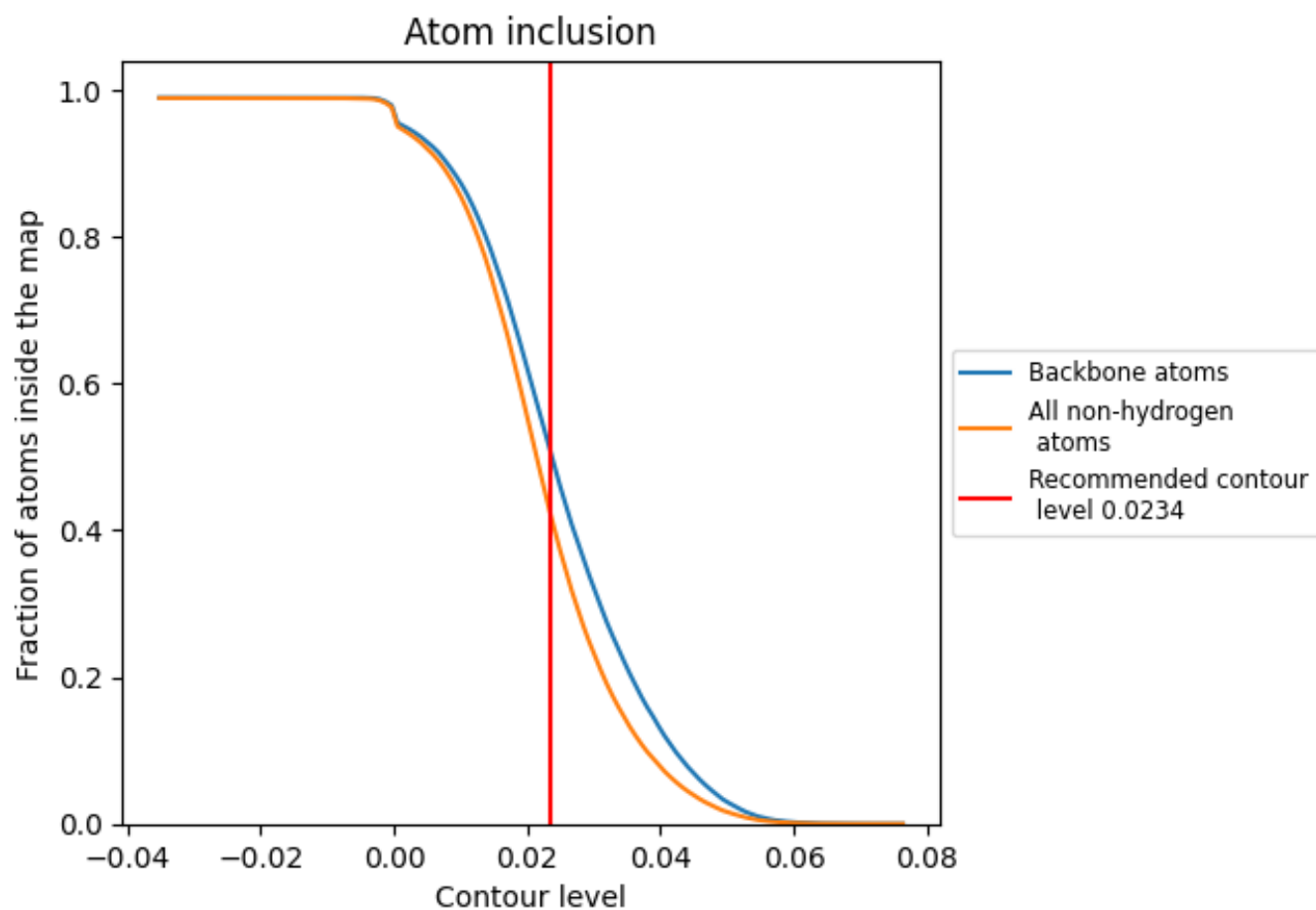
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0234).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 43% 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 (0.0234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4255	 0.0870
2	 0.2186	 0.0410
3	 0.2967	 0.0790
4	 0.1307	 0.0410
5	 0.3338	 0.0720
6	 0.1702	 0.0510
7	 0.1564	 0.0520
A	 0.6578	 0.1510
B	 0.7133	 0.1650
C	 0.6751	 0.1510
D	 0.7319	 0.1650
E	 0.6714	 0.1370
F	 0.2623	 0.0490
G	 0.3148	 0.0730
H	 0.1726	 0.0370
I	 0.3689	 0.0780
J	 0.2409	 0.0570
K	 0.1669	 0.0350
X	 0.7231	 0.1610
Y	 0.7177	 0.1510
Z	 0.7204	 0.1520
a	 0.6518	 0.1330
b	 0.7174	 0.1590
c	 0.6719	 0.1470
d	 0.7663	 0.1680
e	 0.7239	 0.1340
h	 0.3569	 0.0330
i	 0.5375	 0.0840
j	 0.2779	 0.0500
k	 0.4547	 0.0760
l	 0.3826	 0.0590
m	 0.3765	 0.0560
n	 0.7414	 0.1570
o	 0.7402	 0.1680
p	 0.7608	 0.1550



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Chain	Atom inclusion	Q-score
q	 0.7805	 0.1700
r	 0.6997	 0.1360