wwPDB EM Validation Summary Report

Oct 22, 2024 – 05:34 AM JST

PDB ID	:	8XGC
EMDB ID	:	EMD-38317
Title	:	Structure of yeast replisome associated with FACT and histone hexamer, Composite map
Authors	:	Li, N.; Gao, Y.; Yu, D.; Gao, N.; Zhai, Y.
Deposited on	:	2023-12-15
Resolution	:	3.70 Å(reported)

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

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

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

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

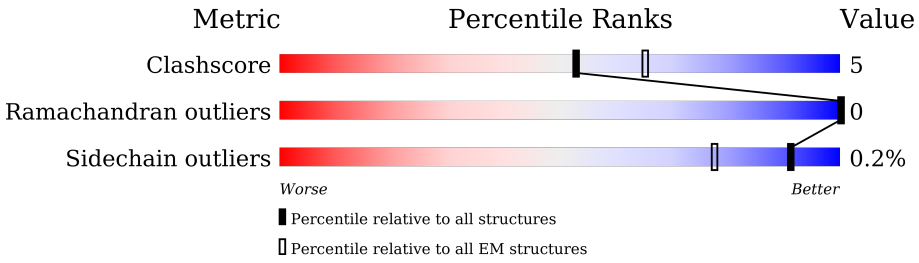
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	16% 75% 14% 10%
2	3	971	10% 54% 9% 37%
3	4	933	24% 61% 12% 27%
4	5	775	13% 75% 13% 13%
5	6	1017	9% 54% 9% 38%
6	7	845	32% 65% 10% 25%
7	8	2222	33% 6% 61%
8	9	689	13% 69% 14% 17%

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Mol	Chain	Length	Quality of chain
9	A	208	16% 79% 16% 5%
10	B	251	61% 15% 24%
11	C	194	9% 78% 10% 12%
12	D	294	13% 71% 11% 18%
13	E	650	14% 75% 11% 14%
14	F	927	40% 6% 54%
14	G	927	40% 5% 54%
14	H	927	41% 5% 54%
15	I	1238	5% 53% 8% 40%
16	J	317	26% 70%
17	K	1096	98%
18	L	1035	13% 41% 7% 52%
19	M	552	50% 68% 31%
20	N	136	7% 48% 9% 43%
20	R	136	52% 14% 34%
21	O	103	5% 53% 17% 29%
21	S	103	10% 64% 18% 17%
22	P	132	60% 9% 31%
23	Q	131	5% 62% 8% 31%
24	X	51	33% 86% 14%
25	Y	39	33% 85% 15%

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 82765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	778	6161	3835	1105	1198	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	613	4795	3026	854	902	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	679	5269	3313	922	1005	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	678	5376	3379	937	1036	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	634	4991	3151	875	940	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	635	4919	3112	860	923	24	0	0

- Molecule 7 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	857	Total	C	N	O	S	0	0
			6945	4496	1137	1274	38		

- Molecule 8 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	573	Total	C	N	O	S	0	0
			4594	2947	788	840	19		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	197	Total	C	N	O	S	0	0
			1611	1012	277	313	9		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	192	Total	C	N	O	S	0	0
			1609	1034	285	286	4		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	171	Total	C	N	O	S	0	0
			1379	899	222	252	6		

- Molecule 12 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1988	1266	325	385	12		

- Molecule 13 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	562	Total	C	N	O	S	0	0
			4550	2906	766	864	14		

- Molecule 14 is a protein called DNA polymerase alpha-binding protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	745	Total	C	N	O	S	0	0
			6057	3897	1027	1114	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	94	Total	C	N	O	S	0	0
			788	507	144	133	4		

- Molecule 17 is a protein called Mediator of replication checkpoint protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	K	20	Total	C	N	O	0	0
			163	102	23	38		

- Molecule 18 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	493	Total	C	N	O	S	0	0
			3474	2177	616	671	10		

- Molecule 19 is a protein called FACT complex subunit POB3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	M	379	Total	C	N	O	0	0
			1876	1118	379	379		

- Molecule 20 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	N	77	Total	C	N	O	0	0
			629	399	118	112		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	90	Total 741	C 469	N 142	O 130	0	0

- Molecule 21 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	O	73	Total 583	C 365	N 114	O 104	0	0
21	S	85	Total 684	C 431	N 135	O 118	0	0

- Molecule 22 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	P	91	Total 703	C 439	N 139	O 125	0	0

- Molecule 23 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	91	Total 706	C 444	N 121	O 140	S 1	0	0

- Molecule 24 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	51	Total 1041	C 507	N 156	O 327	P 51	0	0

- Molecule 25 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	39	Total 796	C 382	N 149	O 226	P 39	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	2	1	Total 1	Zn 1	0

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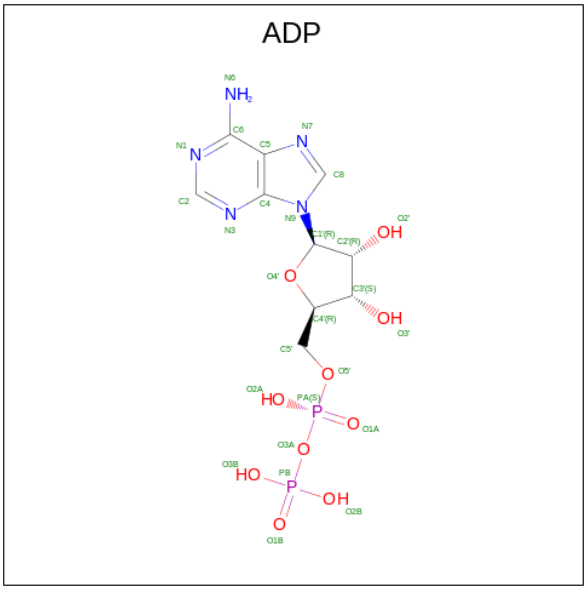
Mol	Chain	Residues	Atoms	AltConf
26	4	1	Total Zn 1 1	0
26	5	1	Total Zn 1 1	0
26	6	1	Total Zn 1 1	0
26	7	1	Total Zn 1 1	0
26	8	2	Total Zn 2 2	0

- Molecule 27 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



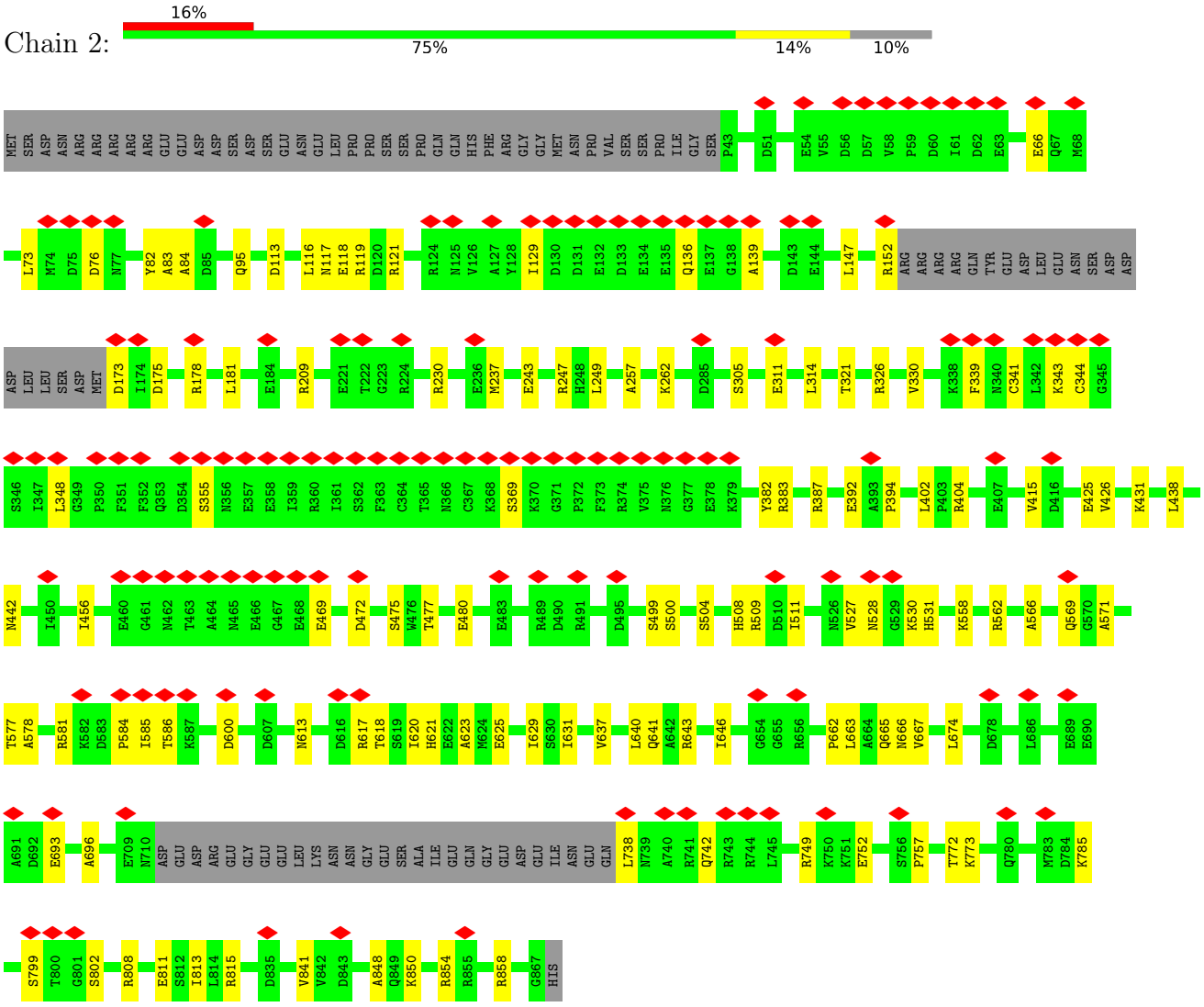
Mol	Chain	Residues	Atoms	AltConf
27	2	1	Total C N O P 27 10 5 10 2	0
27	3	1	Total C N O P 27 10 5 10 2	0
27	5	1	Total C N O P 27 10 5 10 2	0
27	6	1	Total C N O P 27 10 5 10 2	0
27	7	1	Total C N O P 27 10 5 10 2	0

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.

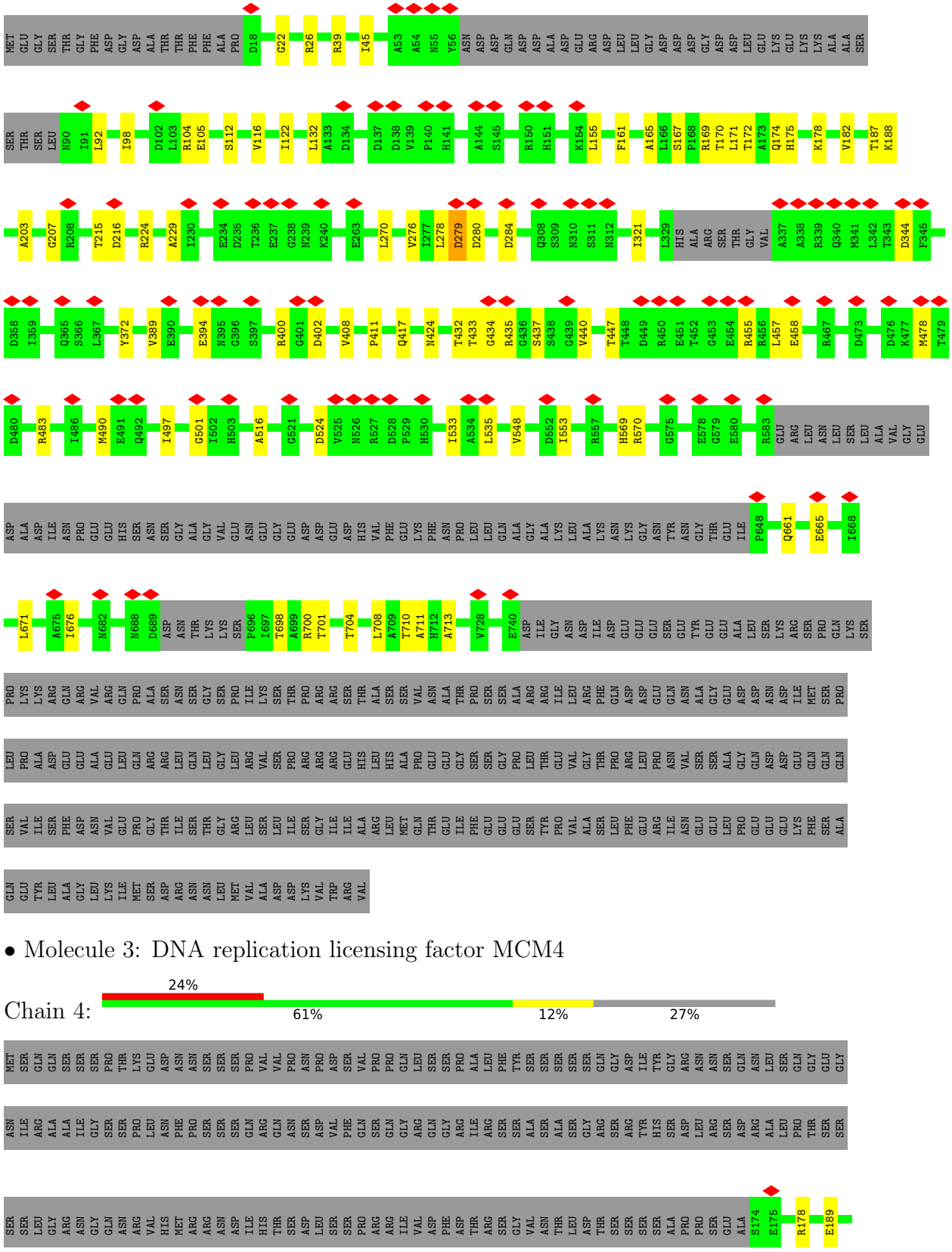
- Molecule 1: DNA replication licensing factor MCM2

Chain 2:



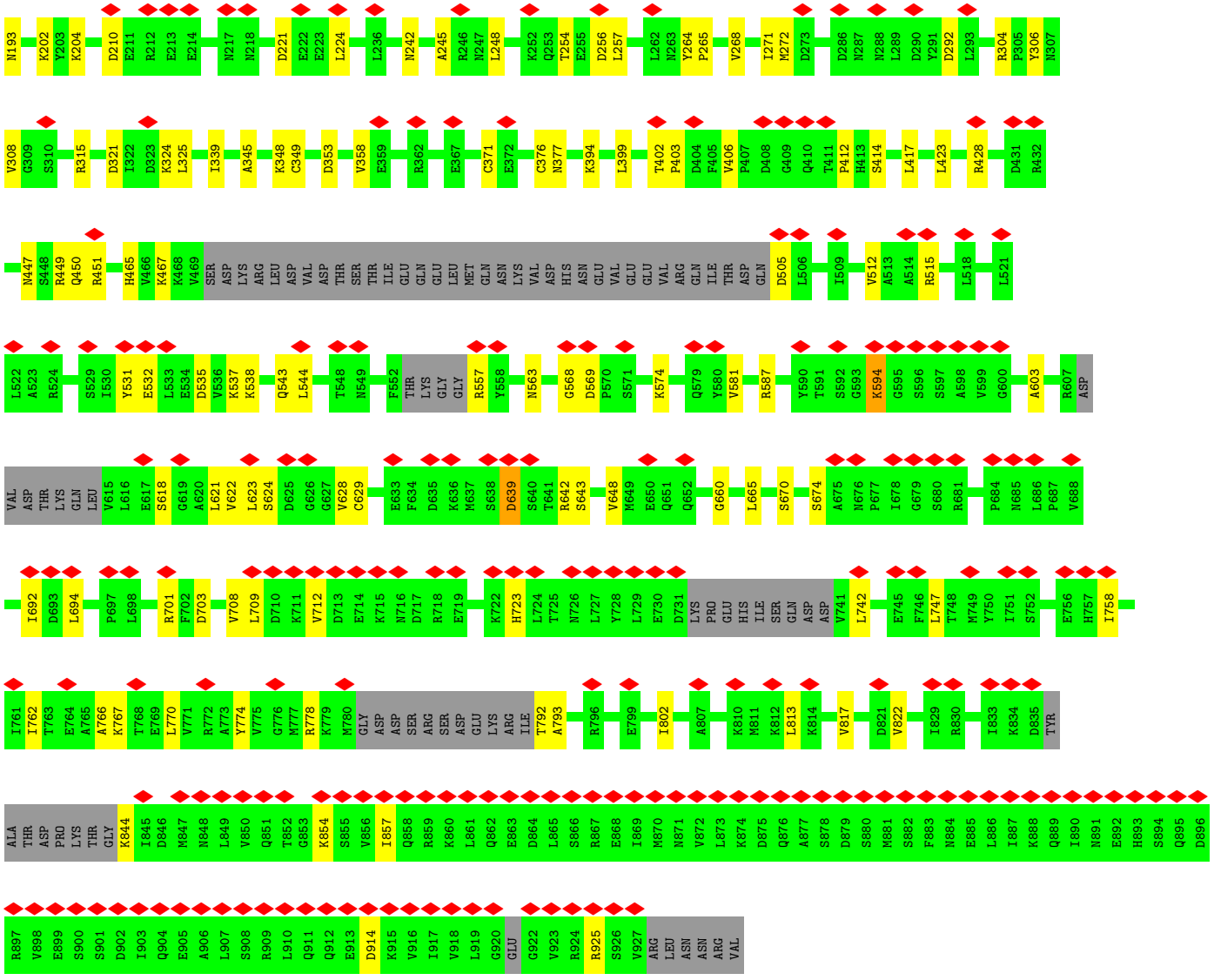
- Molecule 2: DNA replication licensing factor MCM3

Chain 3:



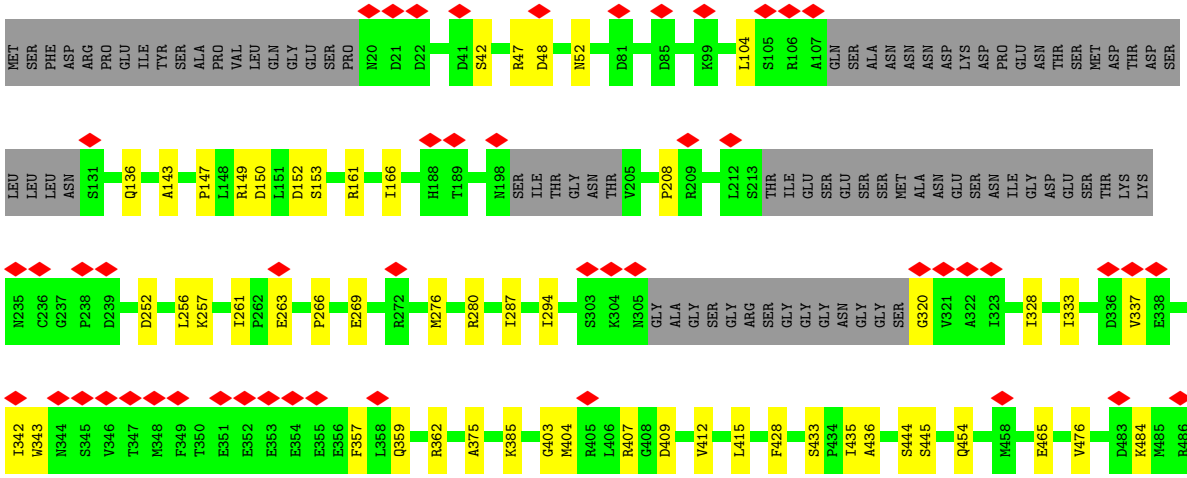
• Molecule 3: DNA replication licensing factor MCM4

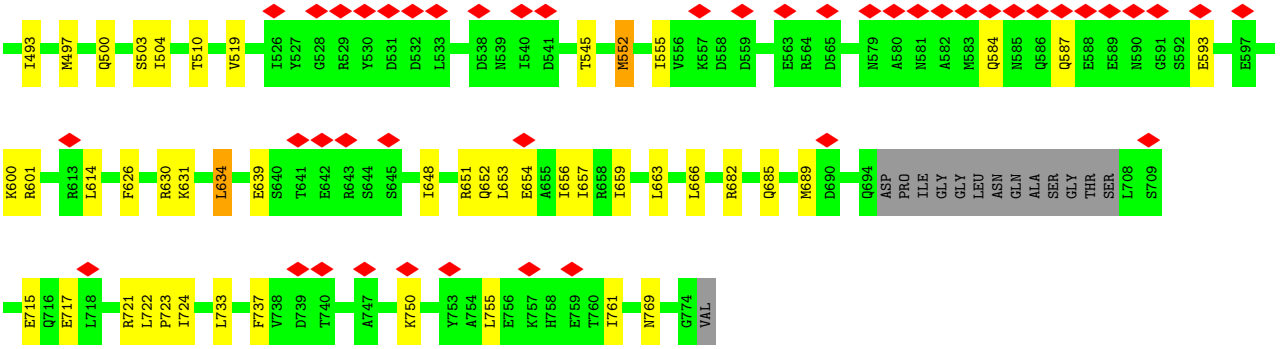
Chain 4:



• Molecule 4: Minichromosome maintenance protein 5

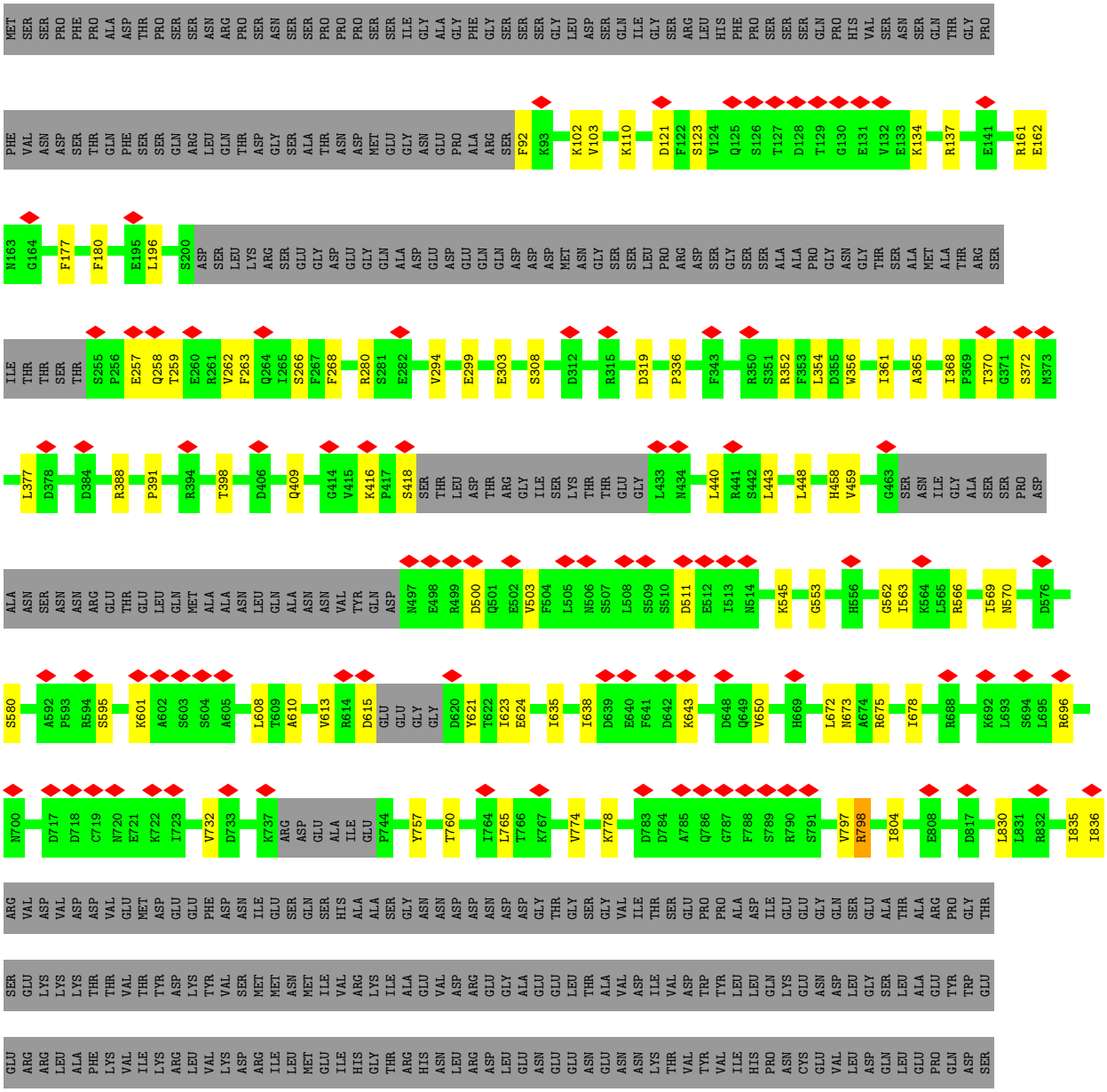
Chain 5:





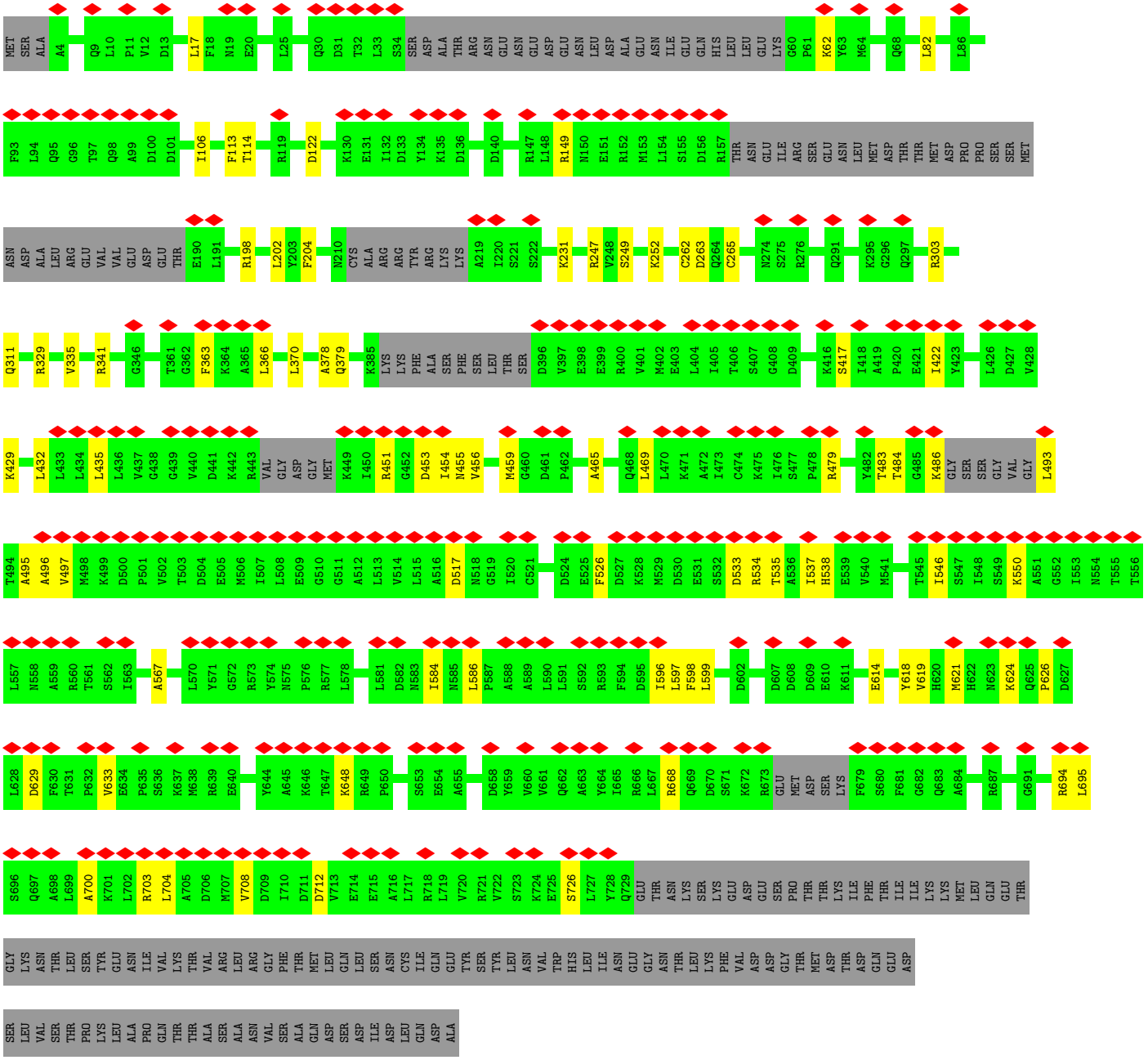
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



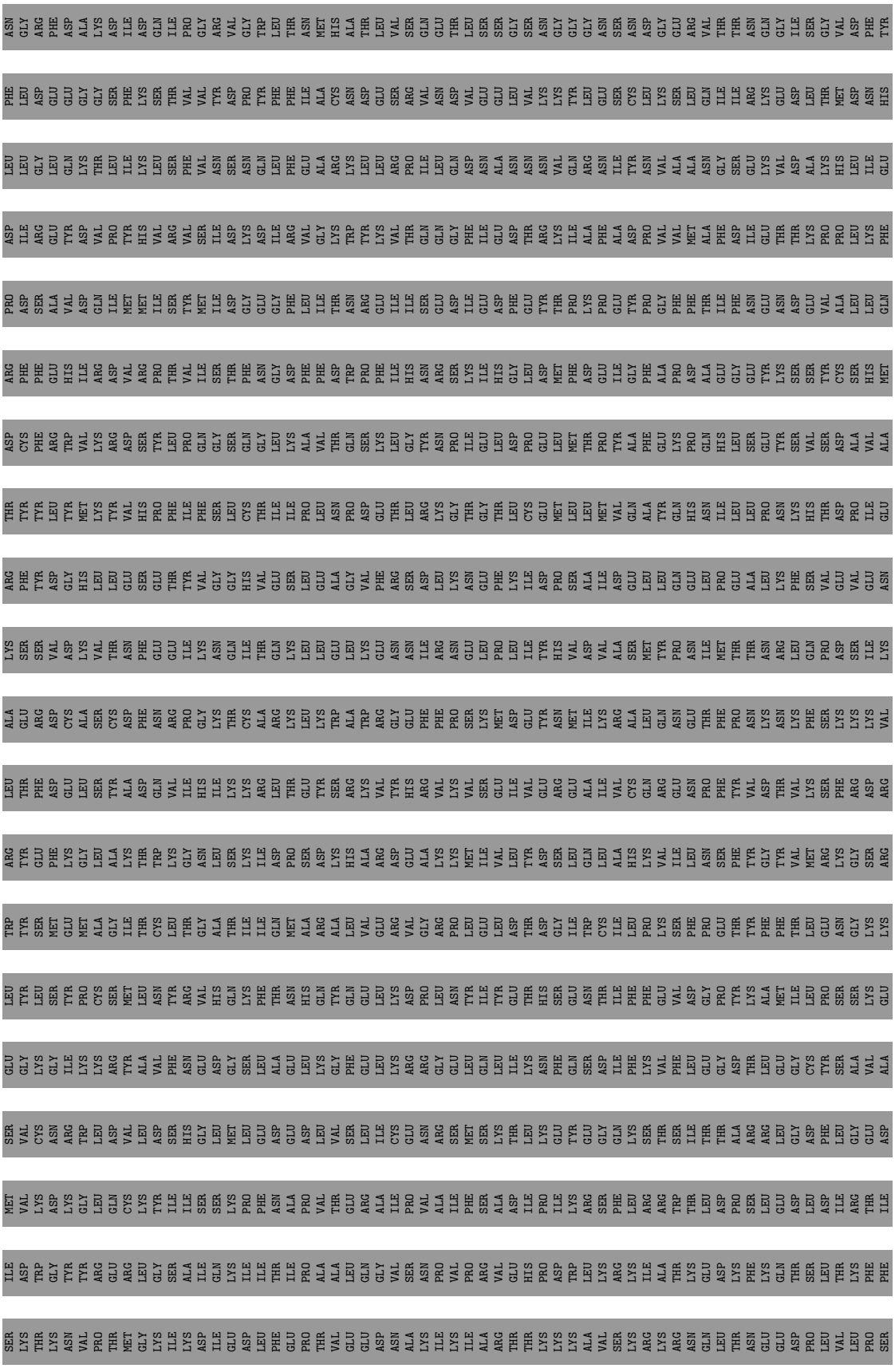
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



• Molecule 7: DNA polymerase epsilon catalytic subunit A

Chain 8:


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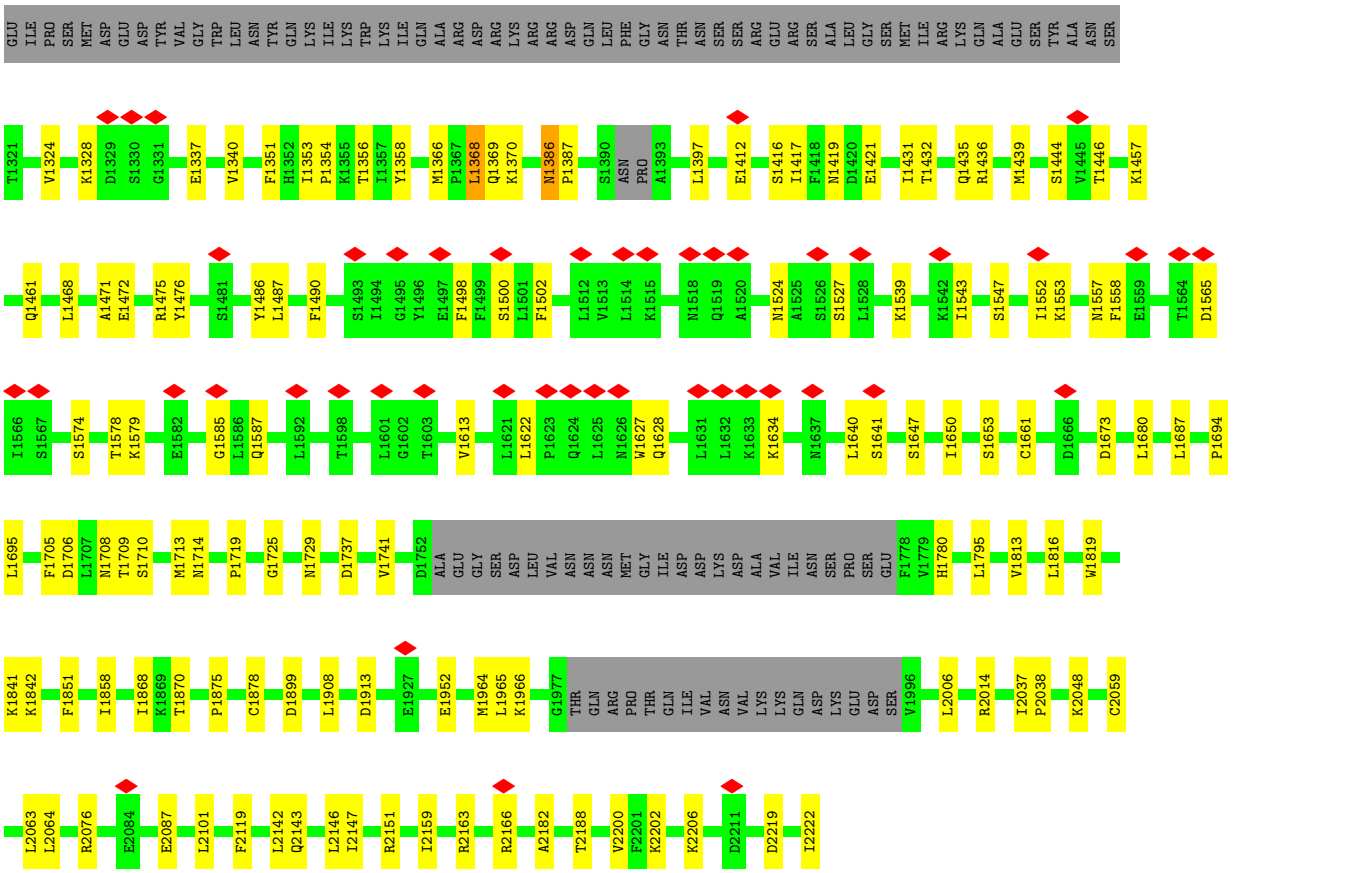
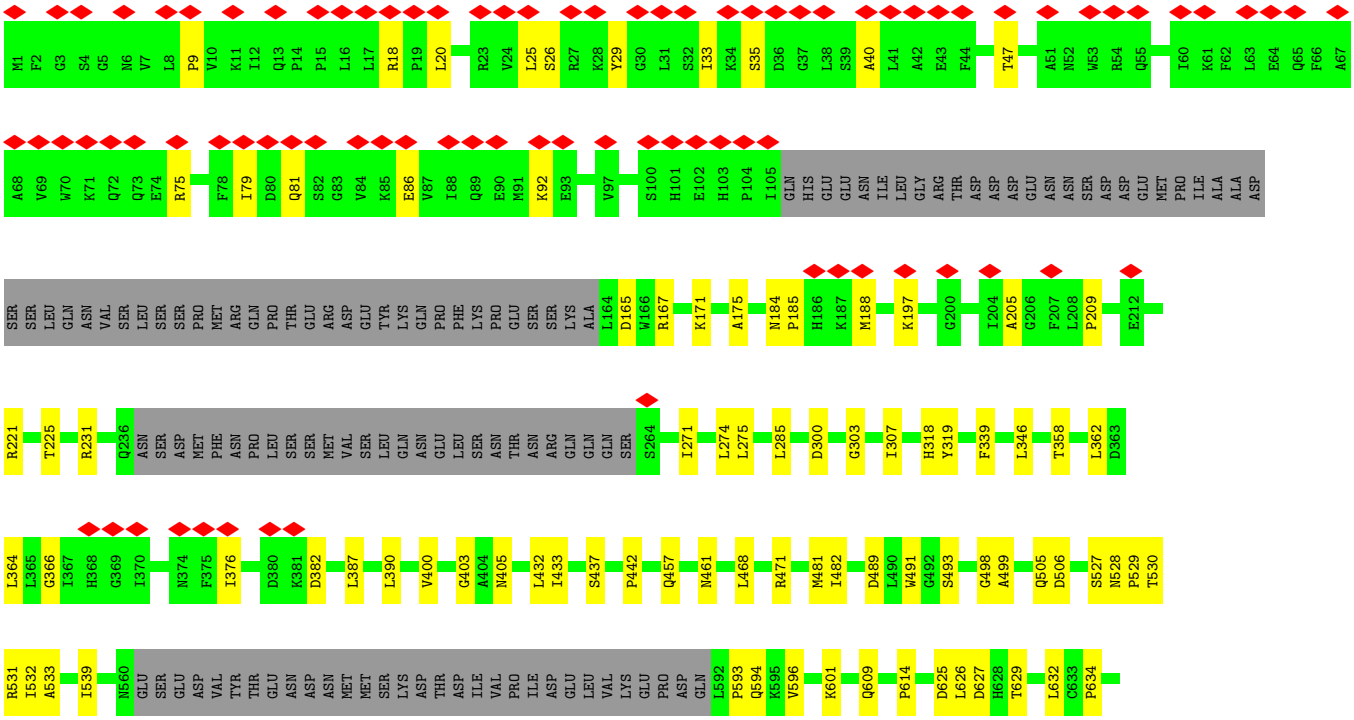
GLU GLY LYS GLY ILE ARG VAL ALA ASP GLY SER LEU ALA GLU LEU LYS GLY PHE GLU LEU LEU LYS ARG GLU LEU ILE LYS ASN PHE GLN SER ASP ILE PHE LYS VAL PHE LEU GLU GLY CYS TYR SER ALA VAL ALA
SER VAL CYS ASN ARG TRP LEU ASP VAL LEU ASP ASN ARG SER MET SER LYS THR LEU LYS GLU TYR GLU GLY GLN LYS SER THR SER ILE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



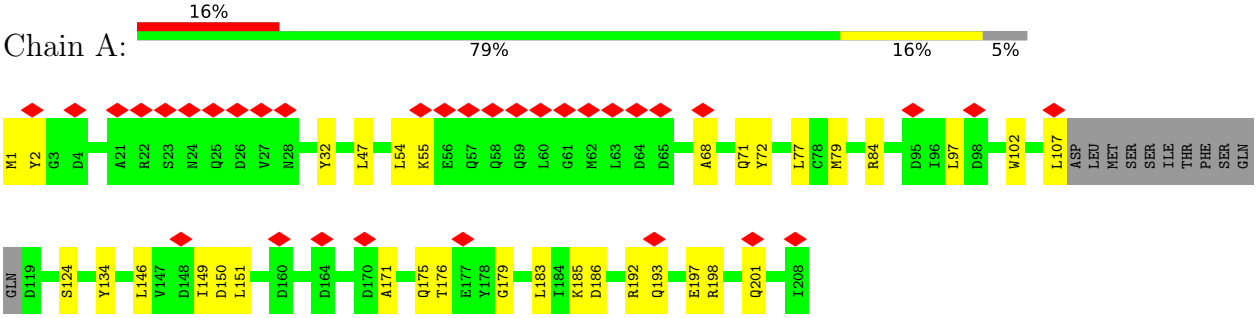
• Molecule 8: DNA polymerase epsilon subunit B

Chain 9:



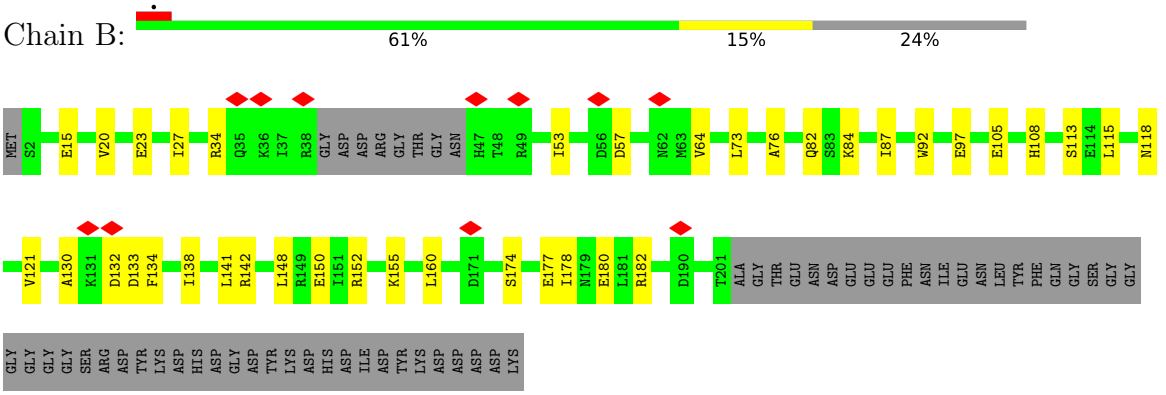
• Molecule 9: DNA replication complex GINS protein PSF1

Chain A:



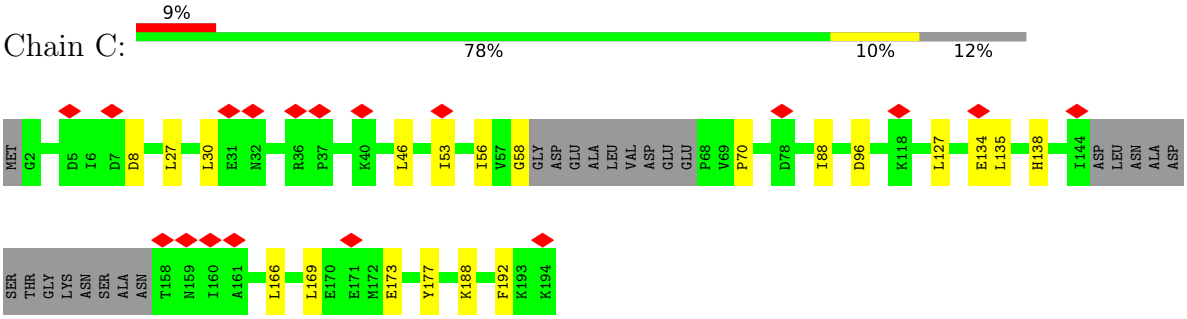
• Molecule 10: DNA replication complex GINS protein PSF2

Chain B:



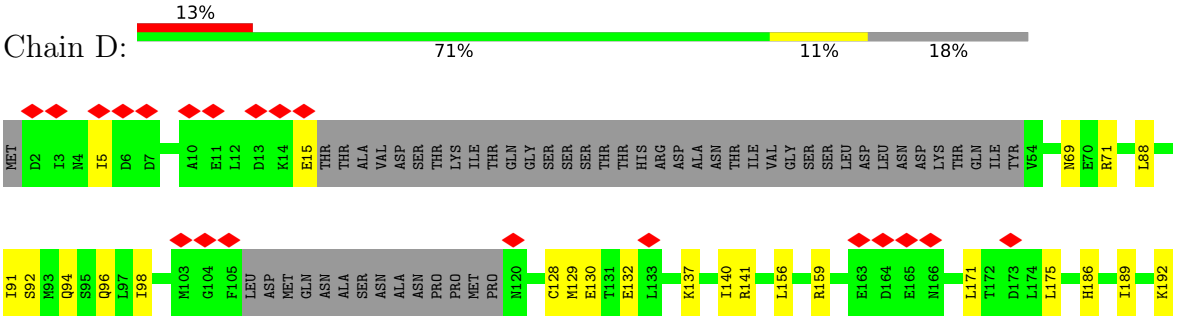
• Molecule 11: DNA replication complex GINS protein PSF3

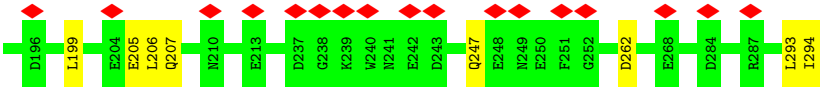
Chain C:



• Molecule 12: DNA replication complex GINS protein SLD5

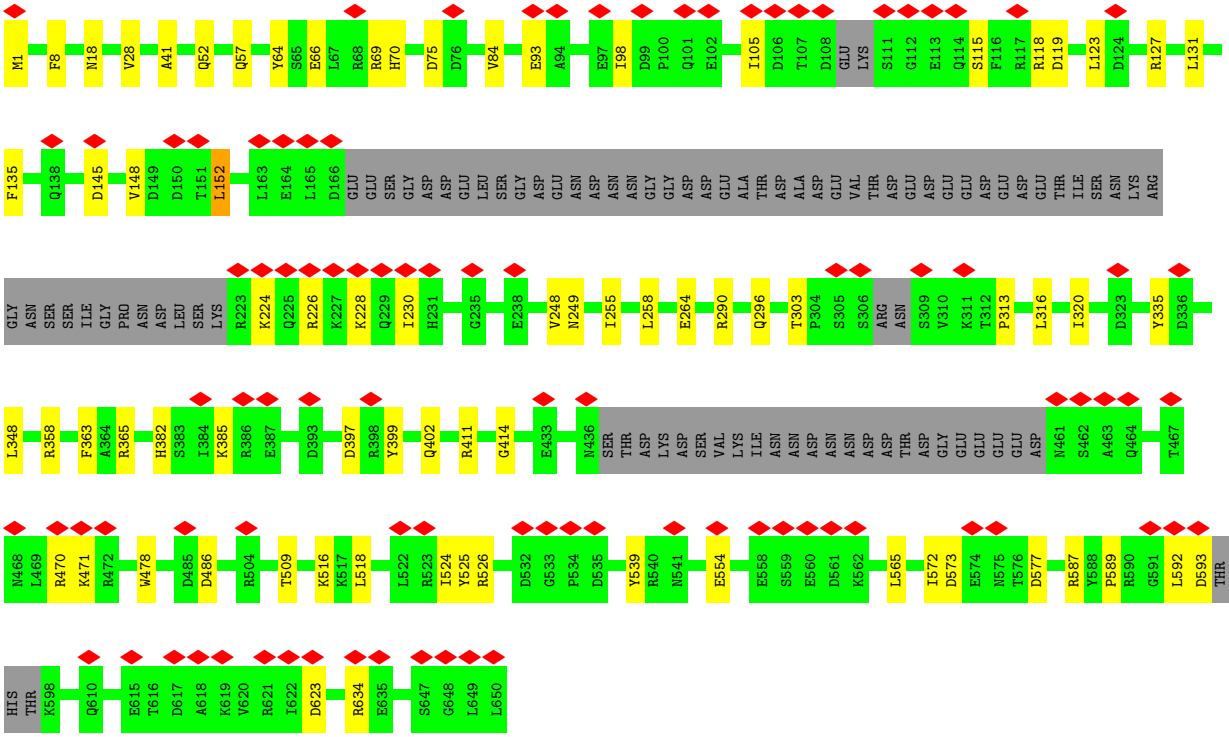
Chain D:





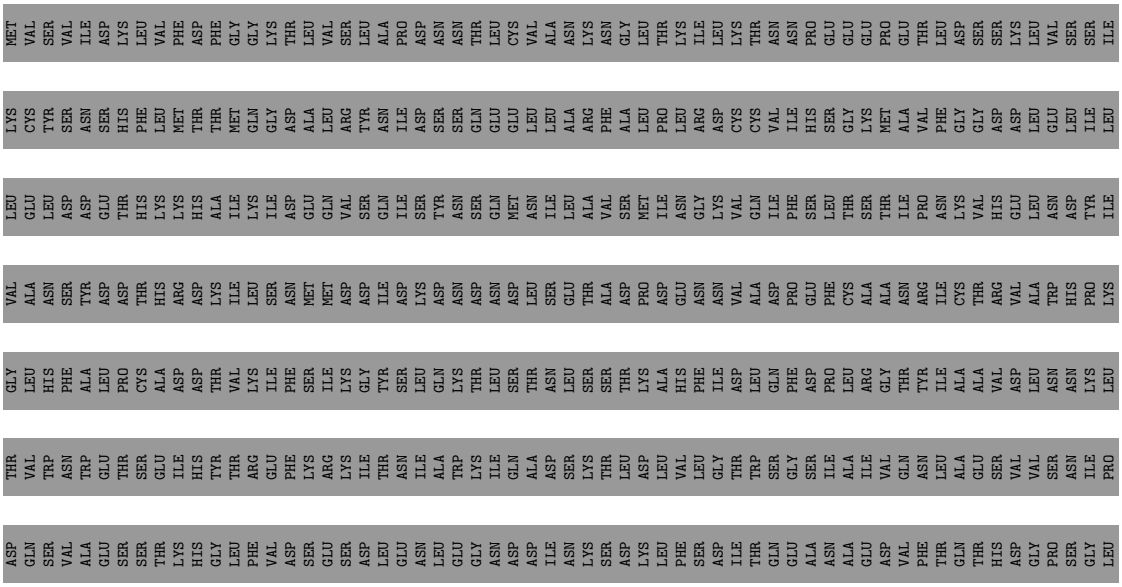
• Molecule 13: Cell division control protein 45

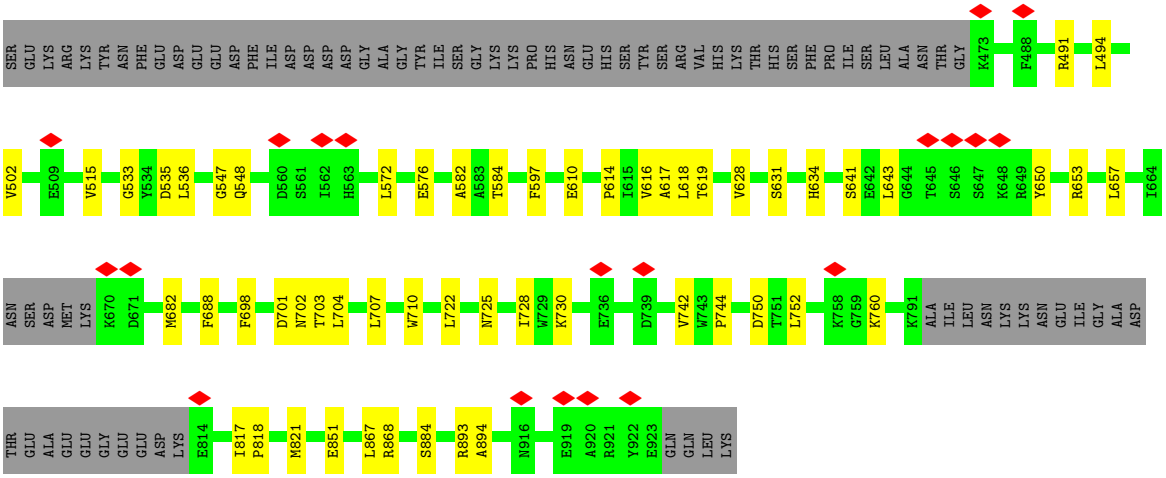
Chain E:



• Molecule 14: DNA polymerase alpha-binding protein

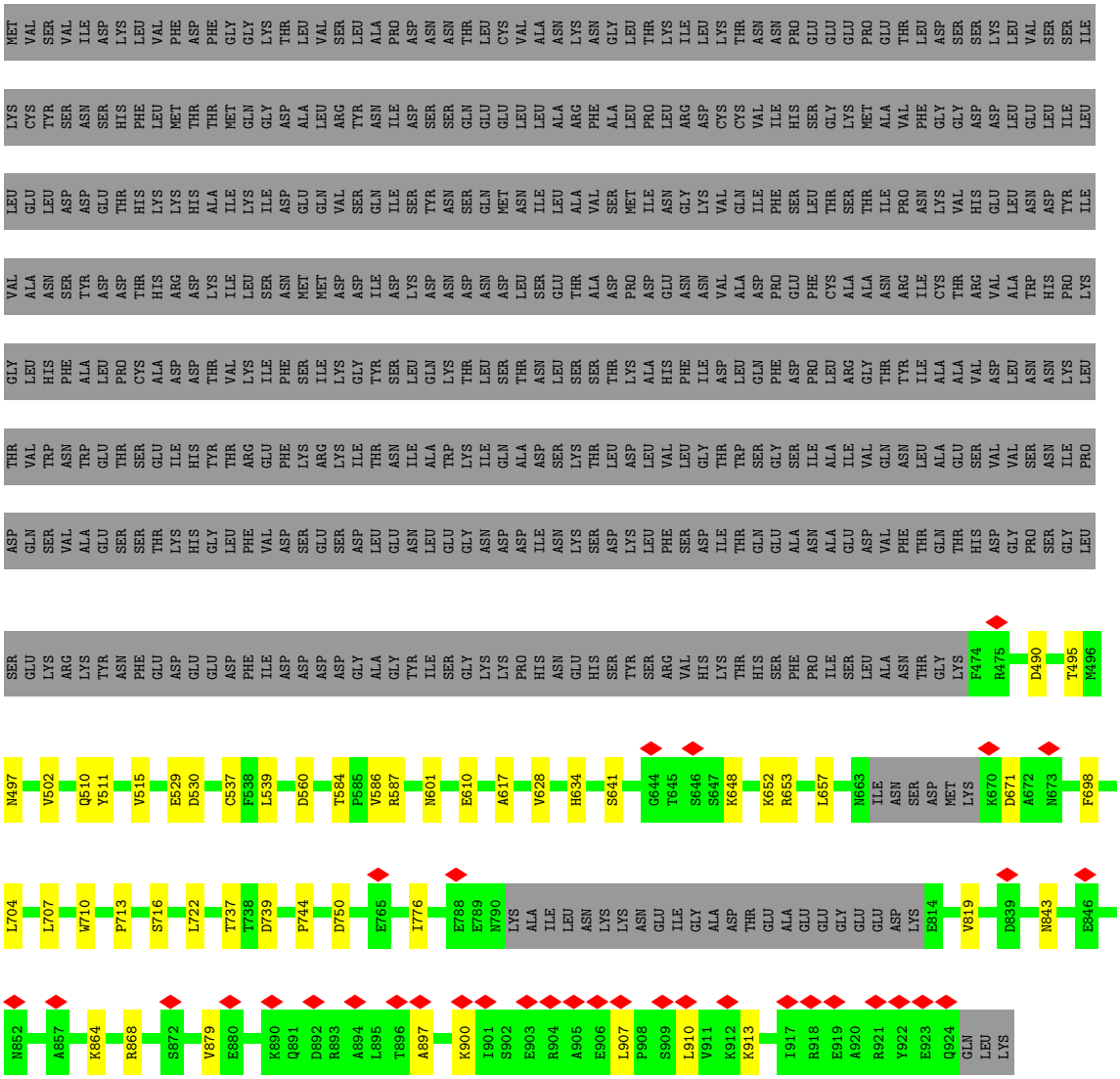
Chain F:





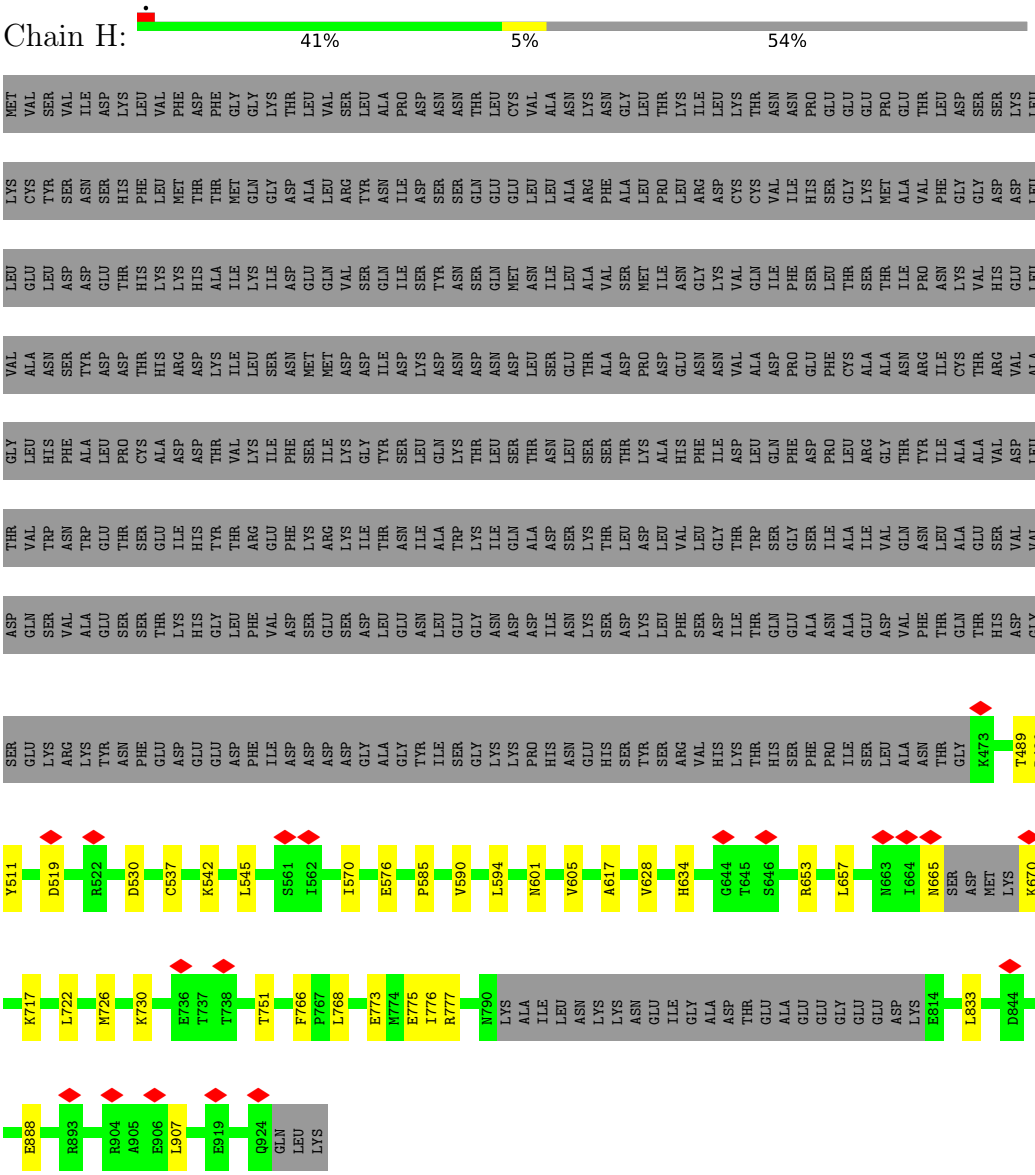
• Molecule 14: DNA polymerase alpha-binding protein

Chain G:



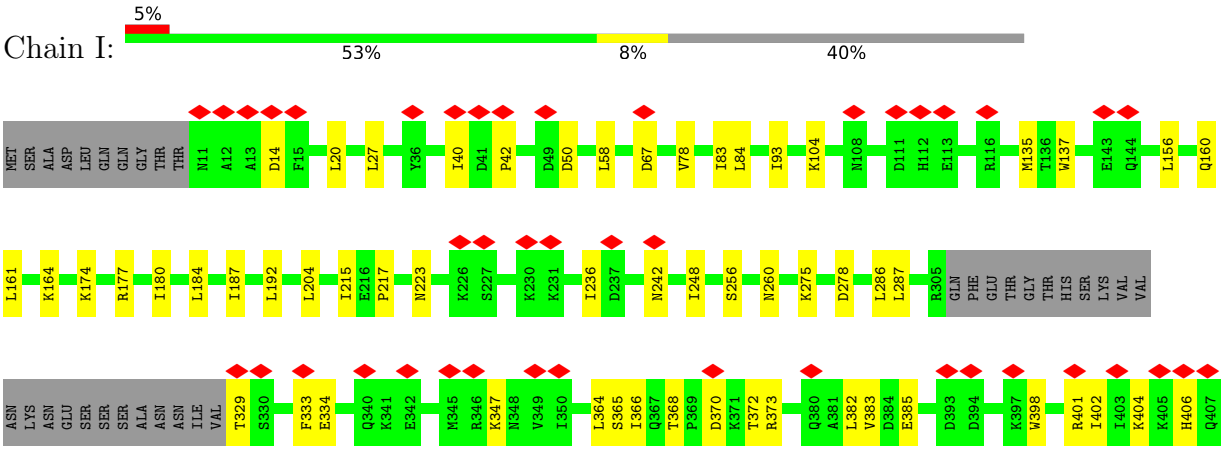
• Molecule 14: DNA polymerase alpha-binding protein

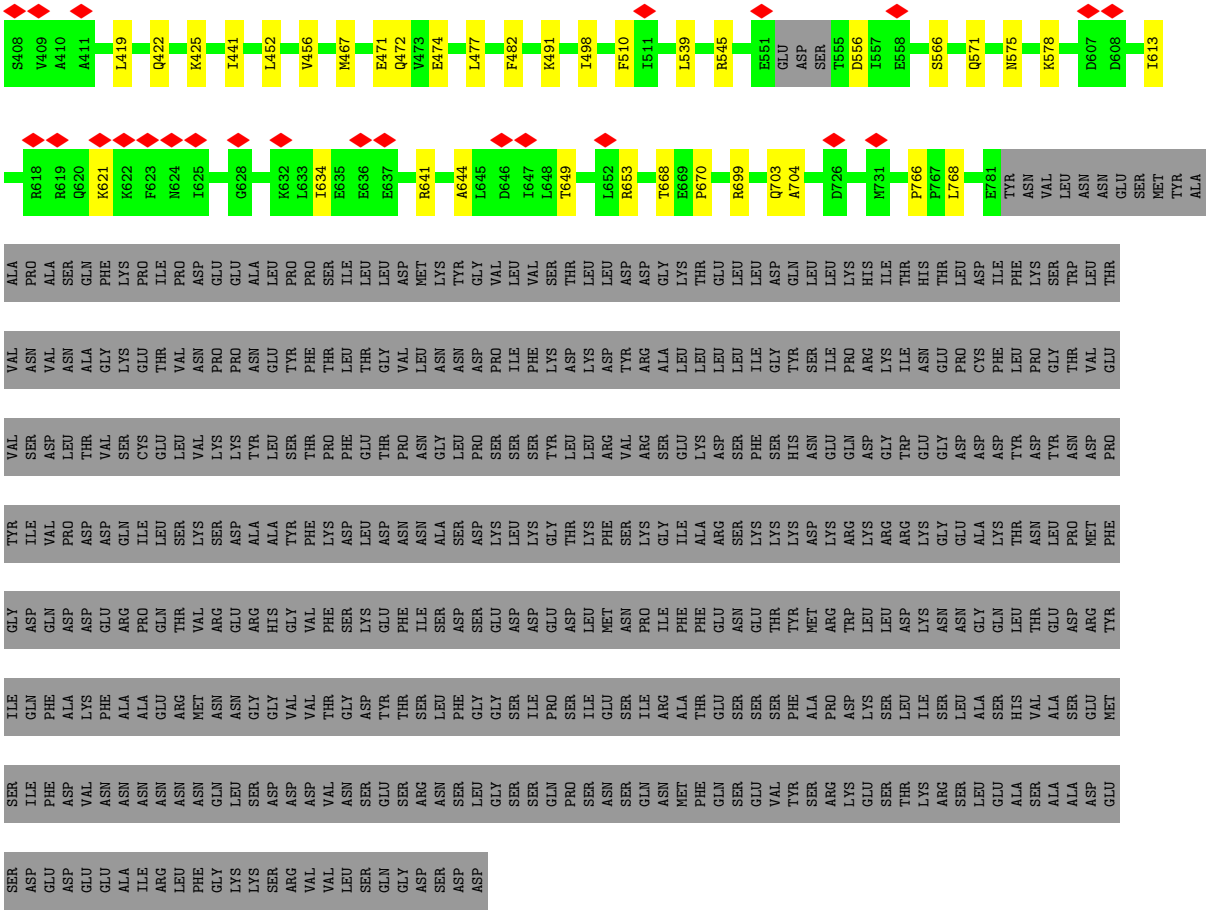
Chain H:



• Molecule 15: Topoisomerase 1-associated factor 1

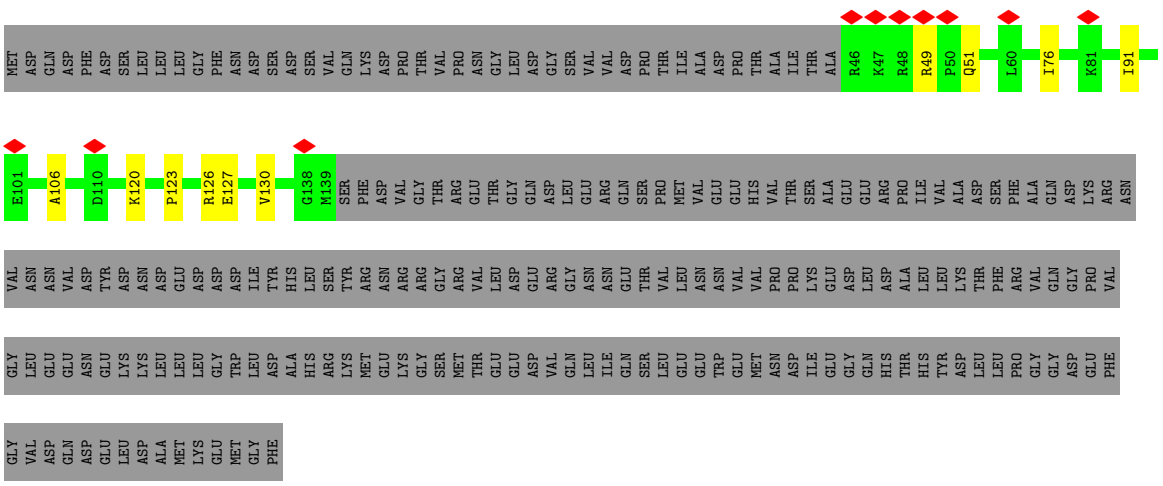
Chain I:





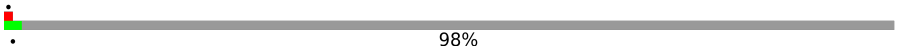
• Molecule 16: Chromosome segregation in meiosis protein 3

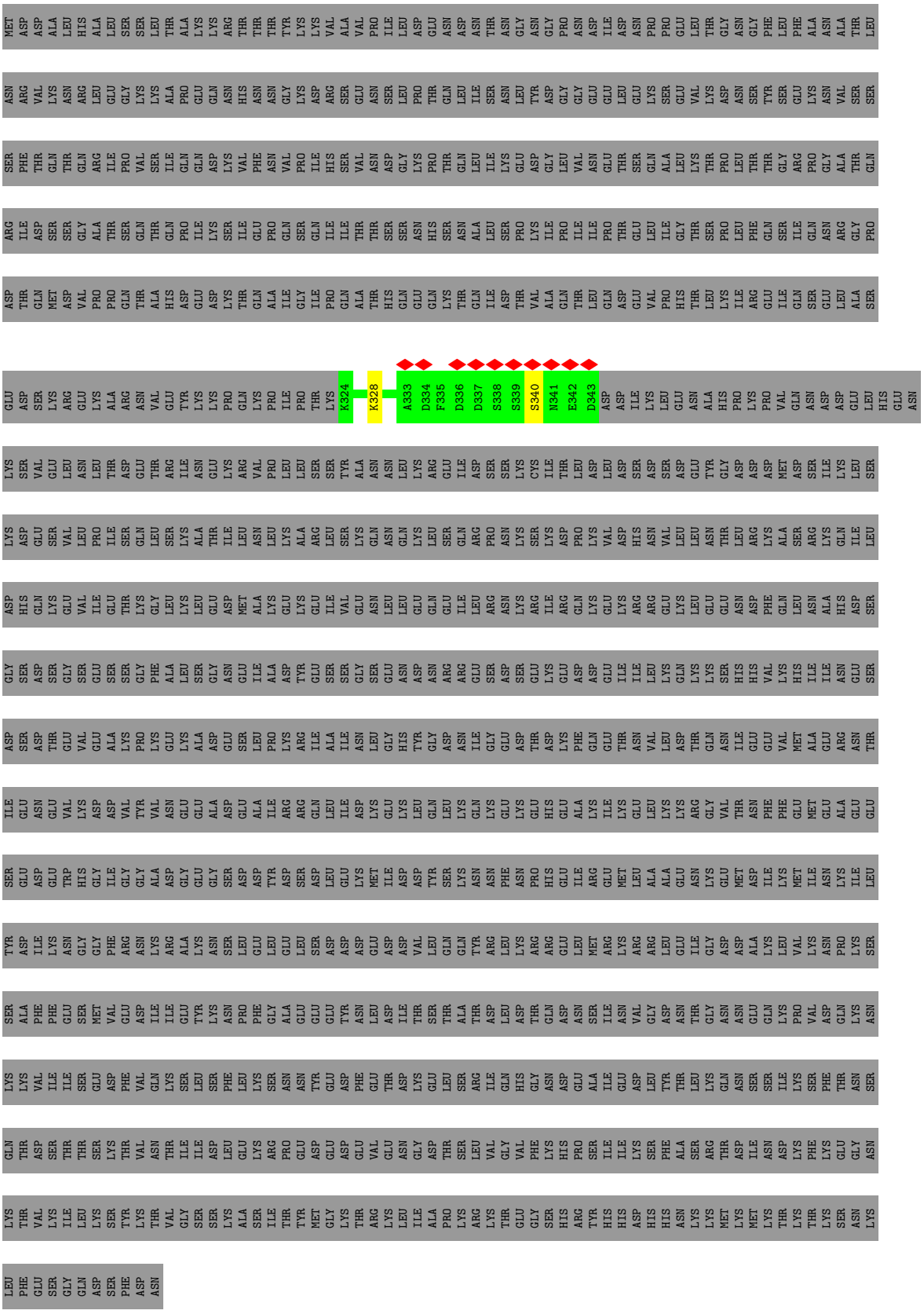
Chain J:



• Molecule 17: Mediator of replication checkpoint protein 1

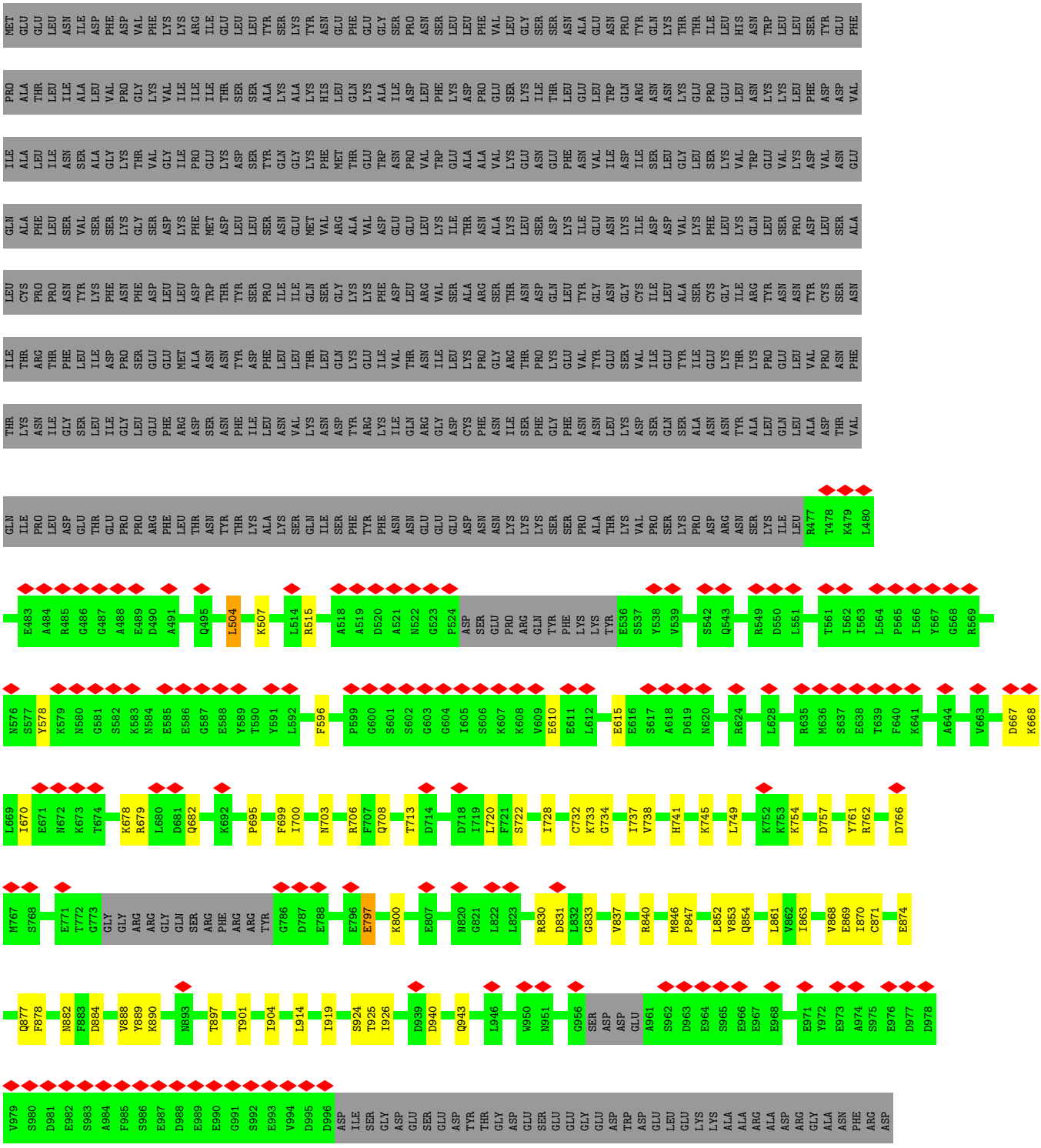
Chain K:





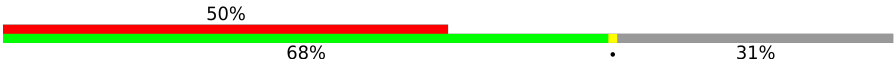
• Molecule 18: FACT complex subunit SPT16

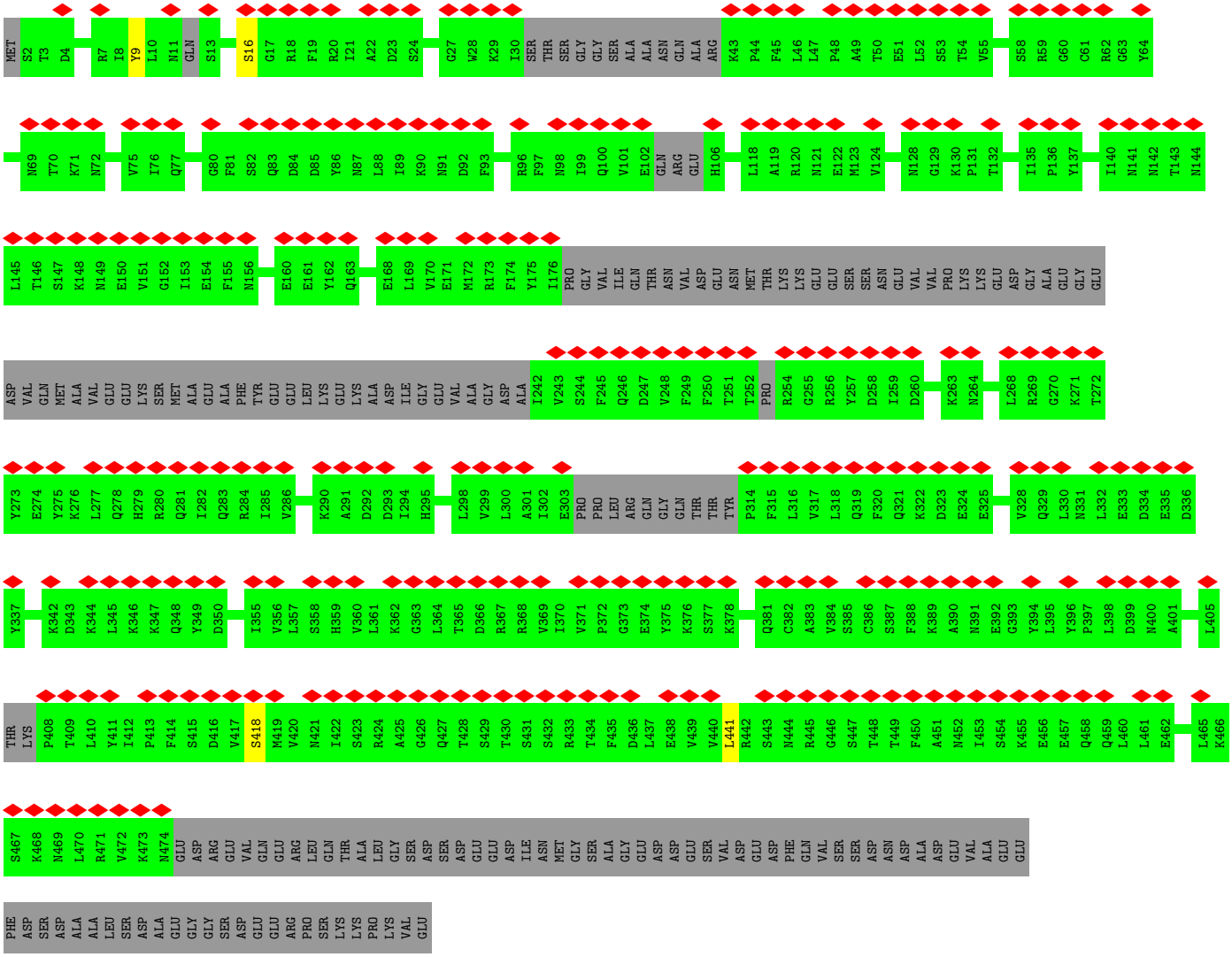
Chain L:



• Molecule 19: FACT complex subunit POB3

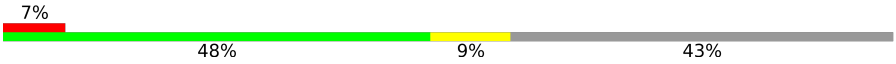
Chain M:

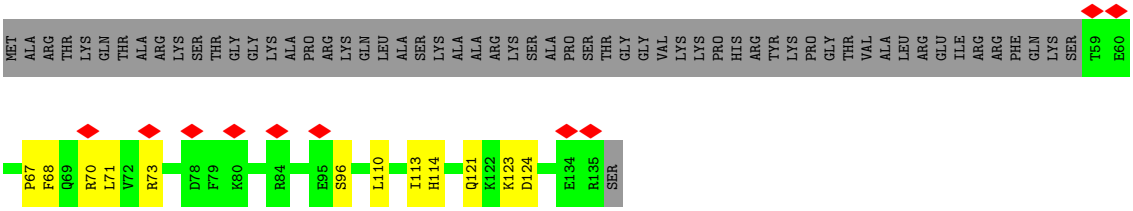




• Molecule 20: Histone H3

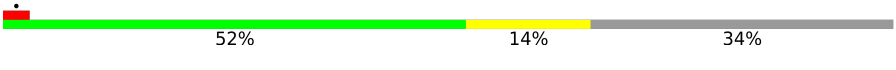
Chain N:





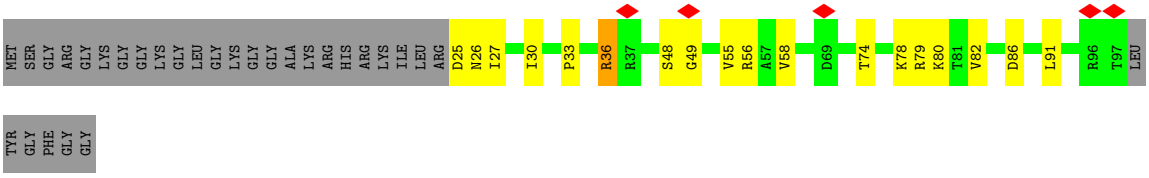
• Molecule 20: Histone H3

Chain R:



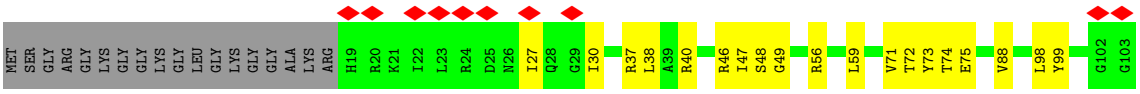
• Molecule 21: Histone H4

Chain O:



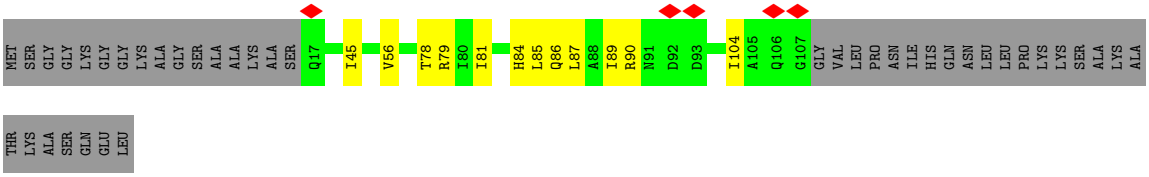
• Molecule 21: Histone H4

Chain S:



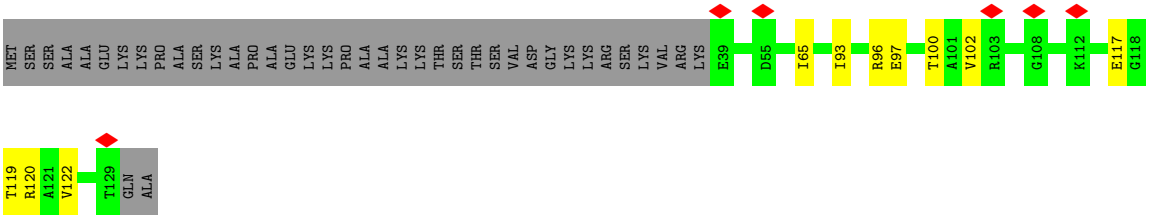
• Molecule 22: Histone H2A.1

Chain P:



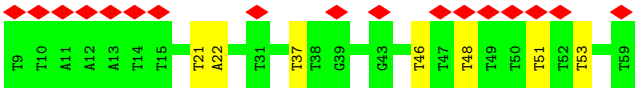
• Molecule 23: Histone H2B.2

Chain Q:



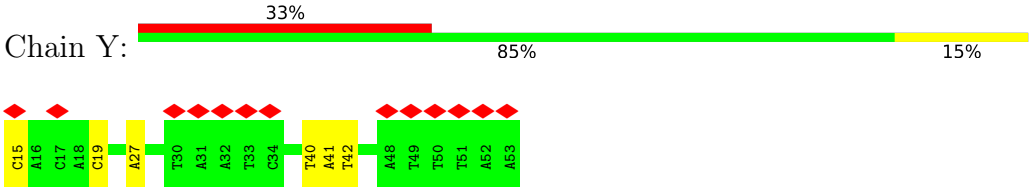
• Molecule 24: DNA (51-MER)

Chain X:



• Molecule 25: DNA (39-MER)

Chain Y:


33%
85%
15%
C15
A16
C17
A18
C19
A27
T30
A31
A32
T33
C34
T40
A41
T42
A48
T49
T50
T51
A52
A53

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	524000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	84.549	Depositor
Minimum map value	-59.011	Depositor
Average map value	0.090	Depositor
Map value standard deviation	1.797	Depositor
Recommended contour level	10	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.28	0/6259	0.61	0/8458
2	3	0.27	0/4880	0.60	1/6619 (0.0%)
3	4	0.28	0/5337	0.65	3/7213 (0.0%)
4	5	0.31	1/5454 (0.0%)	0.61	4/7365 (0.1%)
5	6	0.28	0/5073	0.62	2/6846 (0.0%)
6	7	0.28	0/4993	0.62	2/6757 (0.0%)
7	8	0.30	0/7097	0.60	2/9594 (0.0%)
8	9	0.29	0/4699	0.64	5/6360 (0.1%)
9	A	0.29	0/1631	0.61	0/2194
10	B	0.28	0/1642	0.58	0/2221
11	C	0.28	0/1412	0.57	1/1908 (0.1%)
12	D	0.29	0/2024	0.63	2/2733 (0.1%)
13	E	0.27	0/4633	0.58	2/6269 (0.0%)
14	F	0.29	0/3489	0.58	1/4724 (0.0%)
14	G	0.29	0/3465	0.59	1/4696 (0.0%)
14	H	0.28	0/3496	0.56	1/4735 (0.0%)
15	I	0.29	0/6171	0.59	3/8321 (0.0%)
16	J	0.31	0/804	0.61	0/1074
17	K	0.33	0/166	0.52	0/220
18	L	0.29	0/3522	0.62	3/4786 (0.1%)
19	M	0.24	0/1868	0.47	0/2591
20	N	0.30	0/635	0.78	0/850
20	R	0.37	0/748	0.81	0/1000
21	O	0.36	0/588	0.83	0/788
21	S	0.31	0/692	0.69	0/924
22	P	0.35	0/711	0.68	0/959
23	Q	0.33	0/716	0.68	0/966
24	X	0.62	1/1159 (0.1%)	1.19	2/1789 (0.1%)
25	Y	0.56	0/894	0.96	0/1375
All	All	0.30	2/84258 (0.0%)	0.63	35/114335 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	208	PRO	CG-CD	-7.15	1.27	1.50
24	X	37	DT	C3'-O3'	5.43	1.51	1.44

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	750	ASP	CB-CG-OD2	9.38	126.75	118.30
4	5	208	PRO	N-CD-CG	-9.33	89.21	103.20
7	8	1680	LEU	CA-CB-CG	7.60	132.78	115.30
8	9	632	LEU	CA-CB-CG	7.50	132.55	115.30
8	9	650	ASP	CB-CG-OD2	7.41	124.97	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	6161	0	6082	85	0
2	3	4795	0	4858	61	0
3	4	5269	0	5238	75	0
4	5	5376	0	5440	65	0
5	6	4991	0	5001	59	0
6	7	4919	0	4913	54	0
7	8	6945	0	7025	82	0
8	9	4594	0	4631	55	0
9	A	1611	0	1615	26	0
10	B	1609	0	1662	25	0
11	C	1379	0	1393	13	0
12	D	1988	0	1986	19	0
13	E	4550	0	4536	48	0
14	F	3404	0	3352	34	0
14	G	3380	0	3310	30	0
14	H	3411	0	3355	28	0
15	I	6057	0	6200	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	J	788	0	827	7	0
17	K	163	0	136	1	0
18	L	3474	0	3005	46	0
19	M	1876	0	802	2	0
20	N	629	0	668	12	0
20	R	741	0	791	20	0
21	O	583	0	626	14	0
21	S	684	0	732	16	0
22	P	703	0	737	10	0
23	Q	706	0	722	7	0
24	X	1041	0	593	4	0
25	Y	796	0	440	6	0
26	2	1	0	0	0	0
26	4	1	0	0	0	0
26	5	1	0	0	0	0
26	6	1	0	0	0	0
26	7	1	0	0	0	0
26	8	2	0	0	0	0
27	2	27	0	12	1	0
27	3	27	0	12	3	0
27	5	27	0	12	0	0
27	6	27	0	12	2	0
27	7	27	0	12	2	0
All	All	82765	0	80736	838	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 5.

The worst 5 of 838 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)
18:L:874:GLU:HB3	18:L:884:ASP:O	1.83	0.78
7:8:2059:CYS:O	7:8:2063:LEU:HB2	1.89	0.71
7:8:1490:PHE:HB2	7:8:1498:PHE:HB2	1.73	0.68
3:4:563:ASN:H	3:4:703:ASP:HB2	1.60	0.67
6:7:614:GLU:O	6:7:618:TYR:HB2	1.93	0.67

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	772/868 (89%)	753 (98%)	19 (2%)	0	100	100
2	3	603/971 (62%)	592 (98%)	11 (2%)	0	100	100
3	4	663/933 (71%)	646 (97%)	17 (3%)	0	100	100
4	5	666/775 (86%)	650 (98%)	16 (2%)	0	100	100
5	6	622/1017 (61%)	598 (96%)	24 (4%)	0	100	100
6	7	619/845 (73%)	596 (96%)	23 (4%)	0	100	100
7	8	849/2222 (38%)	829 (98%)	20 (2%)	0	100	100
8	9	565/689 (82%)	549 (97%)	16 (3%)	0	100	100
9	A	193/208 (93%)	187 (97%)	6 (3%)	0	100	100
10	B	188/251 (75%)	177 (94%)	11 (6%)	0	100	100
11	C	165/194 (85%)	160 (97%)	5 (3%)	0	100	100
12	D	235/294 (80%)	226 (96%)	9 (4%)	0	100	100
13	E	550/650 (85%)	532 (97%)	18 (3%)	0	100	100
14	F	418/927 (45%)	406 (97%)	12 (3%)	0	100	100
14	G	416/927 (45%)	402 (97%)	14 (3%)	0	100	100
14	H	419/927 (45%)	412 (98%)	7 (2%)	0	100	100
15	I	739/1238 (60%)	720 (97%)	19 (3%)	0	100	100
16	J	92/317 (29%)	89 (97%)	3 (3%)	0	100	100
17	K	18/1096 (2%)	16 (89%)	2 (11%)	0	100	100
18	L	485/1035 (47%)	464 (96%)	21 (4%)	0	100	100
19	M	363/552 (66%)	350 (96%)	13 (4%)	0	100	100
20	N	75/136 (55%)	75 (100%)	0	0	100	100
20	R	88/136 (65%)	84 (96%)	4 (4%)	0	100	100
21	O	71/103 (69%)	69 (97%)	2 (3%)	0	100	100
21	S	83/103 (81%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	P	89/132 (67%)	88 (99%)	1 (1%)	0	100	100
23	Q	89/131 (68%)	87 (98%)	2 (2%)	0	100	100
All	All	10135/17677 (57%)	9837 (97%)	298 (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	674/770 (88%)	674 (100%)	0	100	100
2	3	528/835 (63%)	528 (100%)	0	100	100
3	4	573/848 (68%)	571 (100%)	2 (0%)	91	94
4	5	609/688 (88%)	609 (100%)	0	100	100
5	6	547/886 (62%)	546 (100%)	1 (0%)	92	96
6	7	532/753 (71%)	531 (100%)	1 (0%)	92	96
7	8	786/2014 (39%)	783 (100%)	3 (0%)	89	93
8	9	517/629 (82%)	517 (100%)	0	100	100
9	A	182/193 (94%)	182 (100%)	0	100	100
10	B	182/228 (80%)	182 (100%)	0	100	100
11	C	154/173 (89%)	154 (100%)	0	100	100
12	D	232/279 (83%)	231 (100%)	1 (0%)	89	93
13	E	505/586 (86%)	505 (100%)	0	100	100
14	F	375/825 (46%)	375 (100%)	0	100	100
14	G	372/825 (45%)	371 (100%)	1 (0%)	91	94
14	H	375/825 (46%)	375 (100%)	0	100	100
15	I	681/1125 (60%)	681 (100%)	0	100	100
16	J	87/285 (30%)	86 (99%)	1 (1%)	70	80
17	K	19/1003 (2%)	18 (95%)	1 (5%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	L	297/935 (32%)	295 (99%)	2 (1%)	81 88
20	N	67/113 (59%)	67 (100%)	0	100 100
20	R	79/113 (70%)	79 (100%)	0	100 100
21	O	63/81 (78%)	62 (98%)	1 (2%)	58 74
21	S	72/81 (89%)	72 (100%)	0	100 100
22	P	71/99 (72%)	71 (100%)	0	100 100
23	Q	79/110 (72%)	79 (100%)	0	100 100
All	All	8658/15302 (57%)	8644 (100%)	14 (0%)	91 96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	D	247	GLN
14	G	843	ASN
21	O	36	ARG
18	L	668	LYS
18	L	679	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	114	HIS
18	L	741	HIS
7	8	2060	HIS
7	8	1708	ASN
14	G	510	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
27	ADP	6	1102	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
27	ADP	5	802	-	24,29,29	0.95	1 (4%)	29,45,45	1.54	4 (13%)
27	ADP	3	1001	-	24,29,29	0.94	1 (4%)	29,45,45	1.38	2 (6%)
27	ADP	7	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.38	4 (13%)
27	ADP	2	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.41	4 (13%)

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
27	ADP	6	1102	-	-	3/12/32/32	0/3/3/3
27	ADP	5	802	-	-	3/12/32/32	0/3/3/3
27	ADP	3	1001	-	-	4/12/32/32	0/3/3/3
27	ADP	7	902	-	-	2/12/32/32	0/3/3/3
27	ADP	2	902	-	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	1102	ADP	C5-C4	2.52	1.47	1.40
27	5	802	ADP	C5-C4	2.49	1.47	1.40
27	7	902	ADP	C5-C4	2.44	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	902	ADP	C5-C4	2.34	1.47	1.40
27	3	1001	ADP	C5-C4	2.22	1.46	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	802	ADP	PA-O3A-PB	-3.98	119.16	132.83
27	6	1102	ADP	C3'-C2'-C1'	3.86	106.78	100.98
27	5	802	ADP	C3'-C2'-C1'	3.66	106.48	100.98
27	2	902	ADP	PA-O3A-PB	-3.62	120.40	132.83
27	2	902	ADP	N3-C2-N1	-3.47	123.25	128.68

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	902	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O2A
27	5	802	ADP	C5'-O5'-PA-O3A
27	6	1102	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

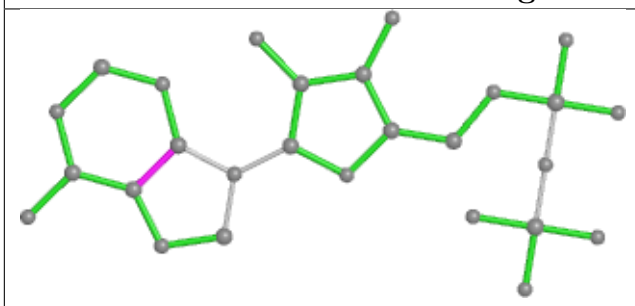
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	1102	ADP	2	0
27	3	1001	ADP	3	0
27	7	902	ADP	2	0
27	2	902	ADP	1	0

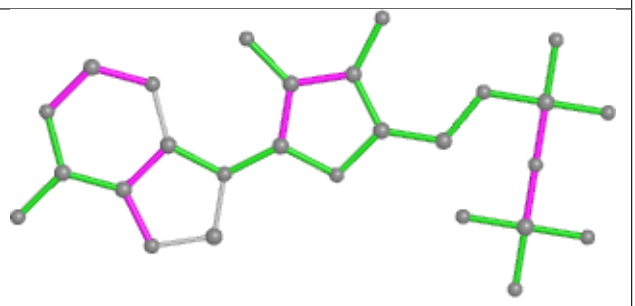
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

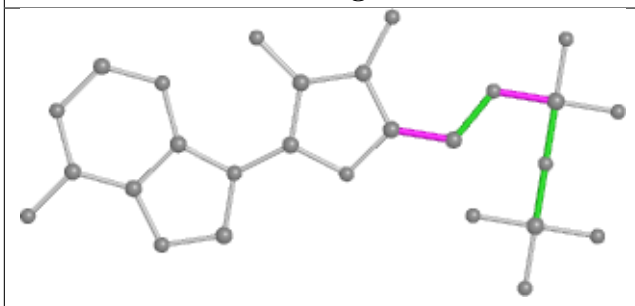
Ligand ADP 6 1102



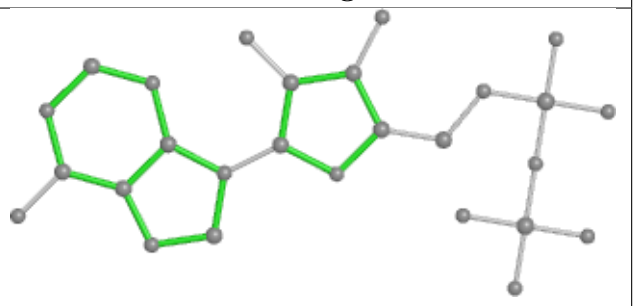
Bond lengths



Bond angles

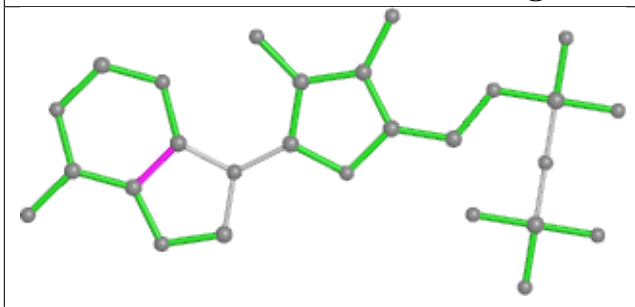


Torsions

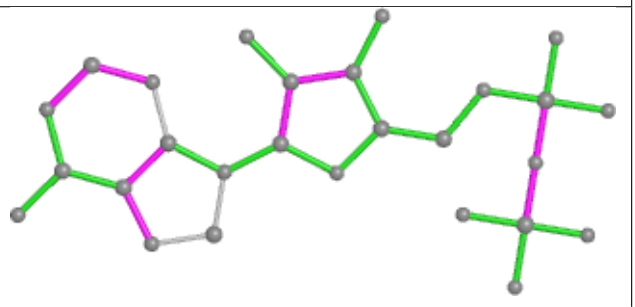


Rings

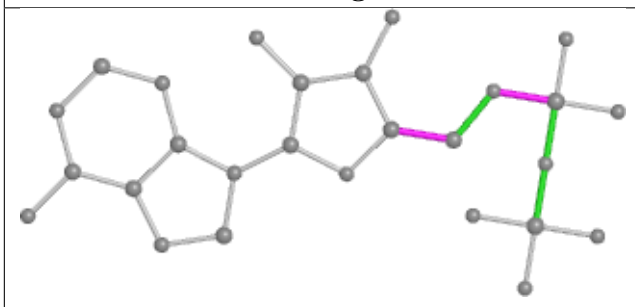
Ligand ADP 5 802



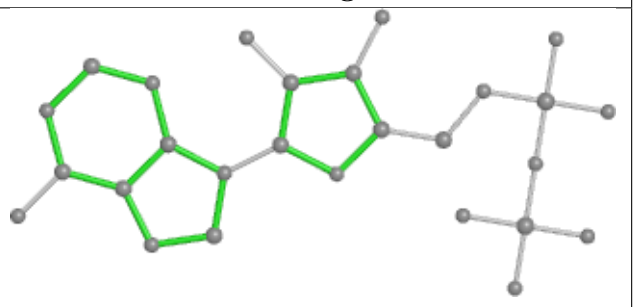
Bond lengths



Bond angles

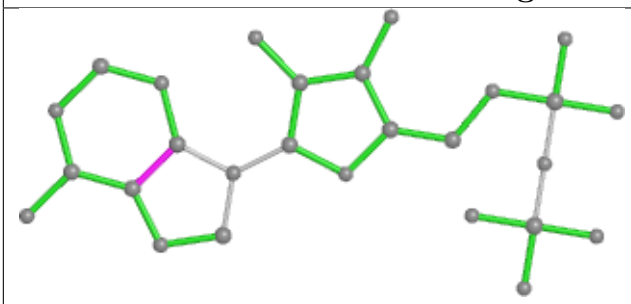


Torsions

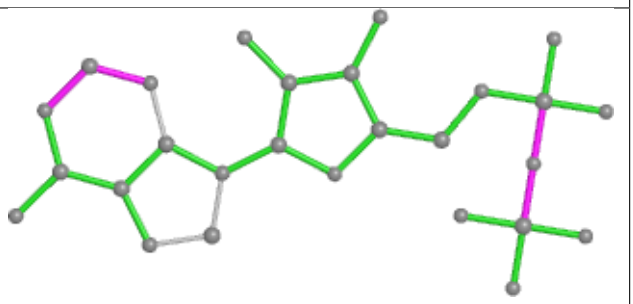


Rings

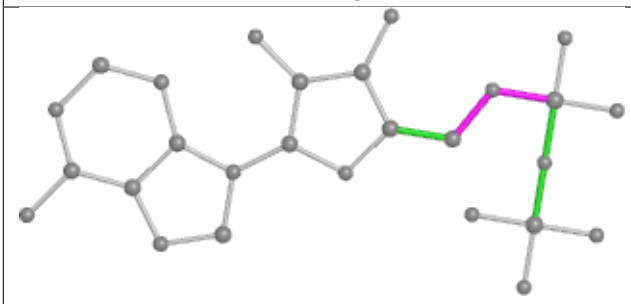
Ligand ADP 3 1001



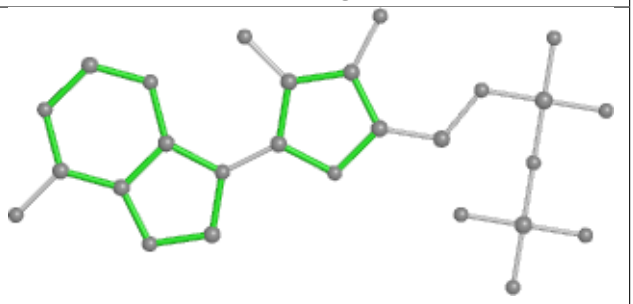
Bond lengths



Bond angles

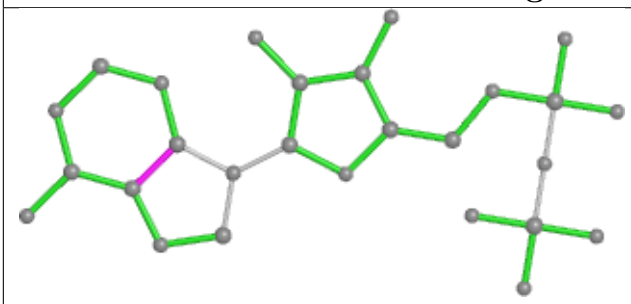


Torsions

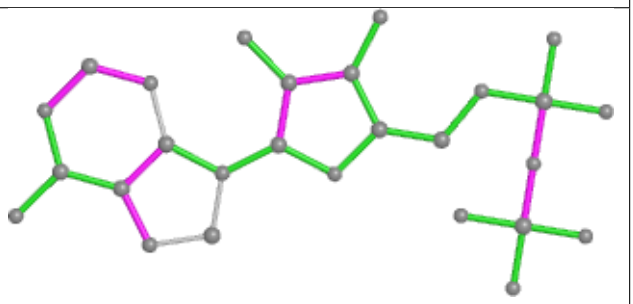


Rings

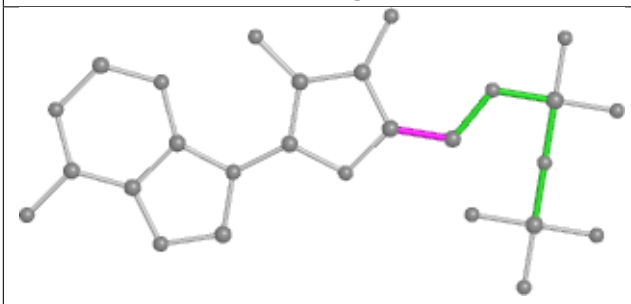
Ligand ADP 7 902



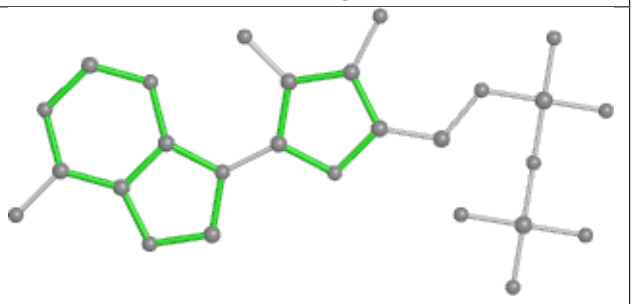
Bond lengths



Bond angles

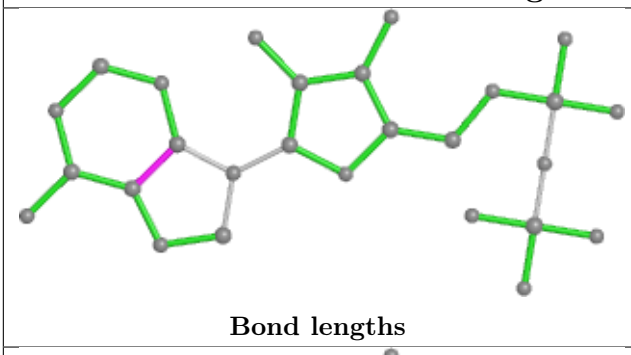


Torsions

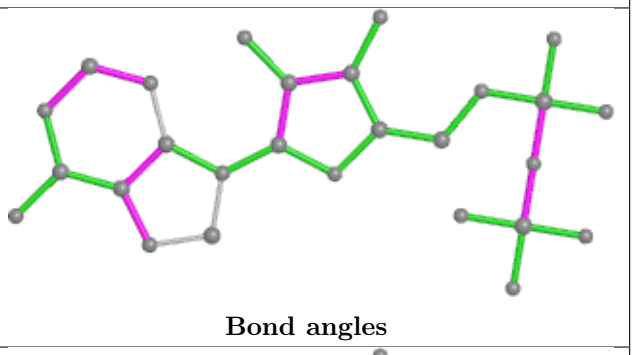


Rings

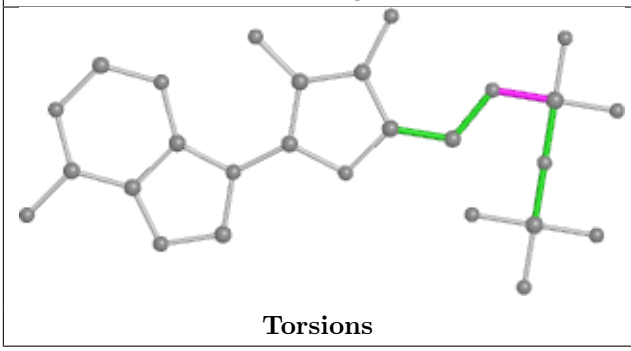
Ligand ADP 2 902



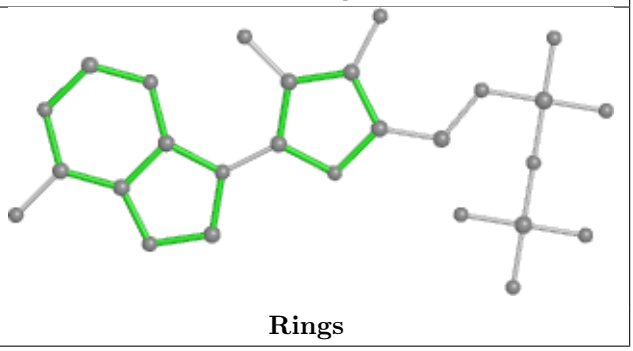
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

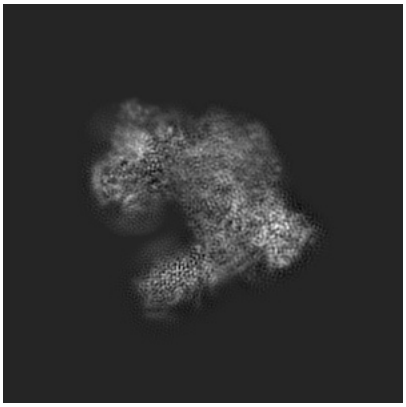
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38317. These allow visual inspection of the internal detail of the map and identification of artifacts.

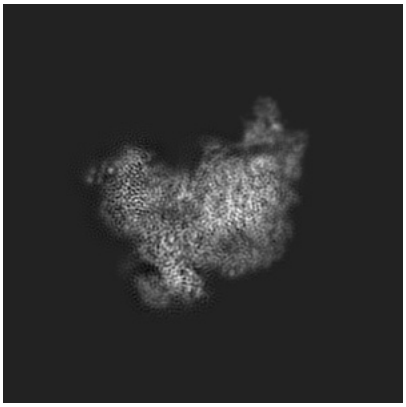
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

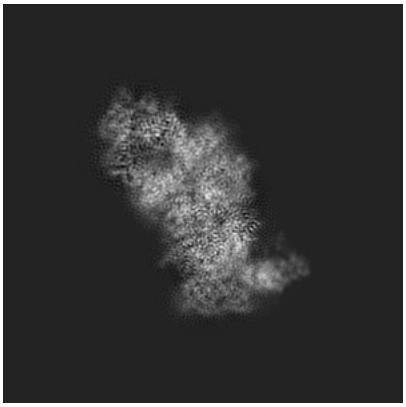
6.1.1 Primary map



X



Y

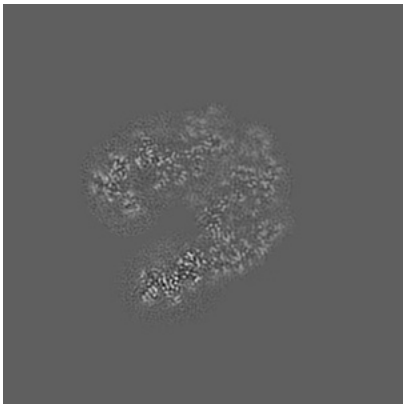


Z

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

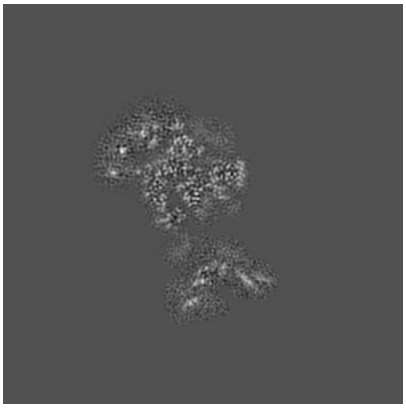
6.2 Central slices

6.2.1 Primary map



X Index: 200

Y Index: 200

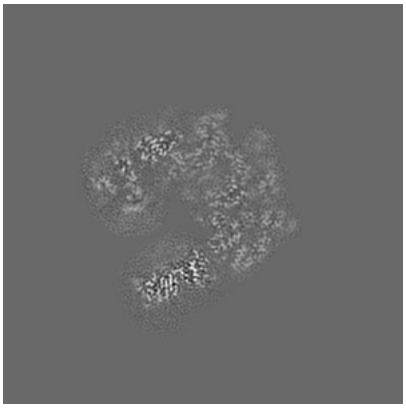


Z Index: 200

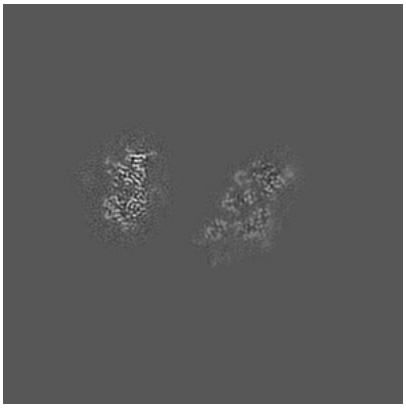
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

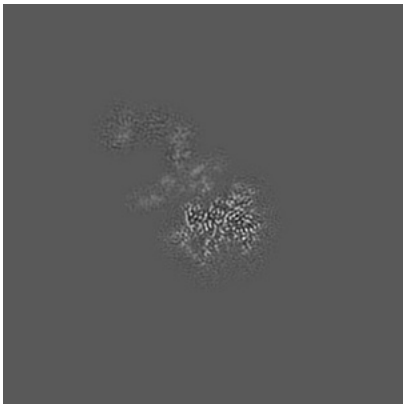
6.3.1 Primary map



X Index: 211



Y Index: 174

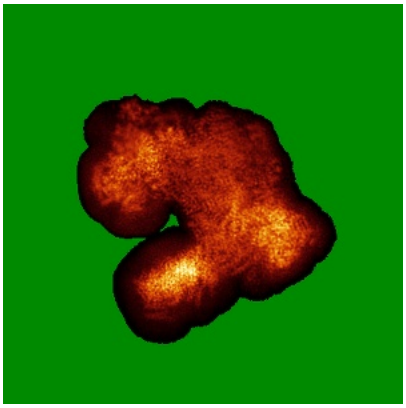


Z Index: 132

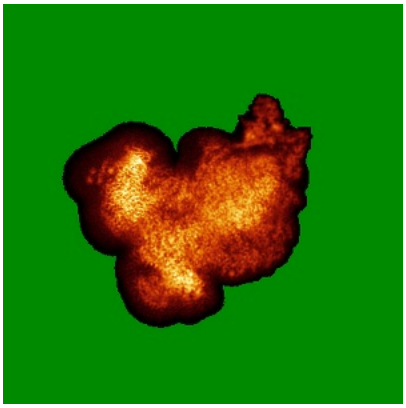
The images above show the largest variance slices of the map in three orthogonal directions.

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

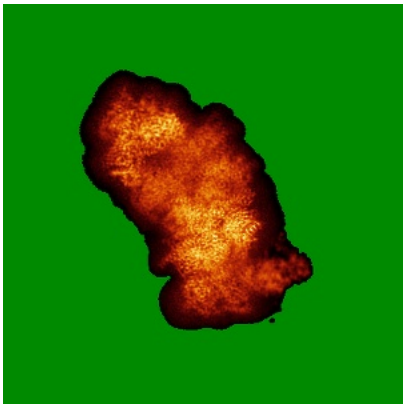
6.4.1 Primary map



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

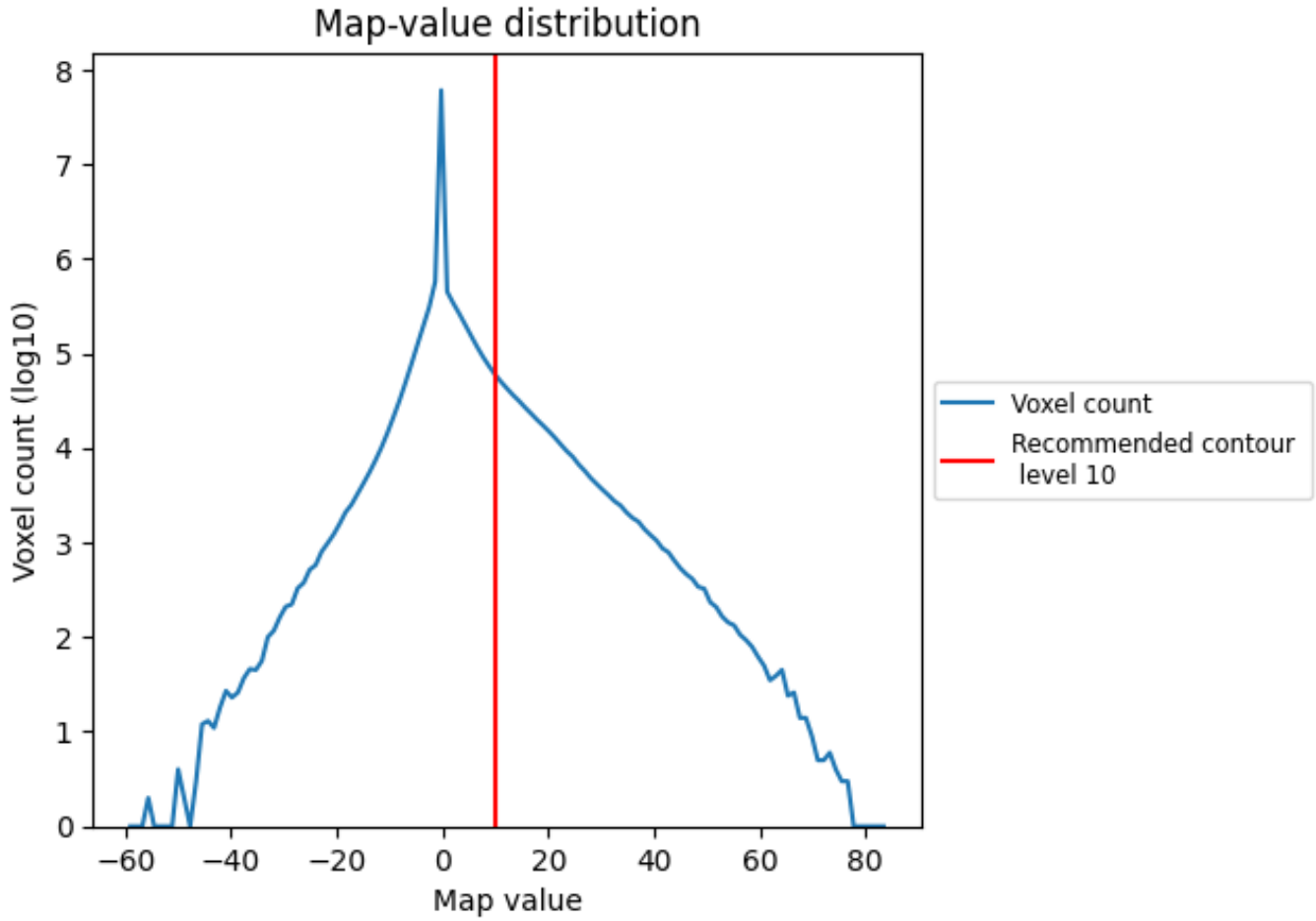
6.6 Mask visualisation (i)

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

7 Map analysis

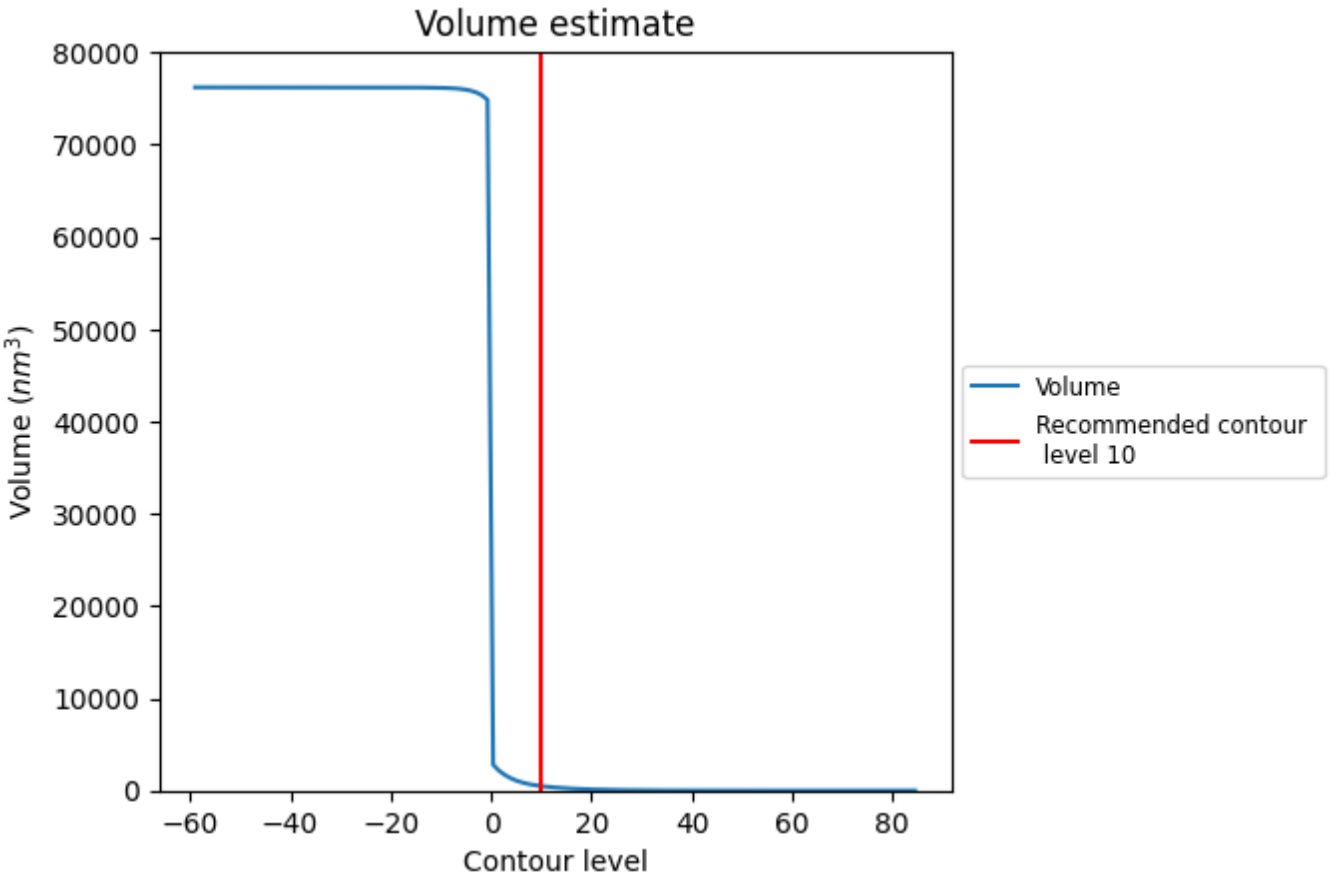
This section contains the results of statistical analysis of the map.

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.

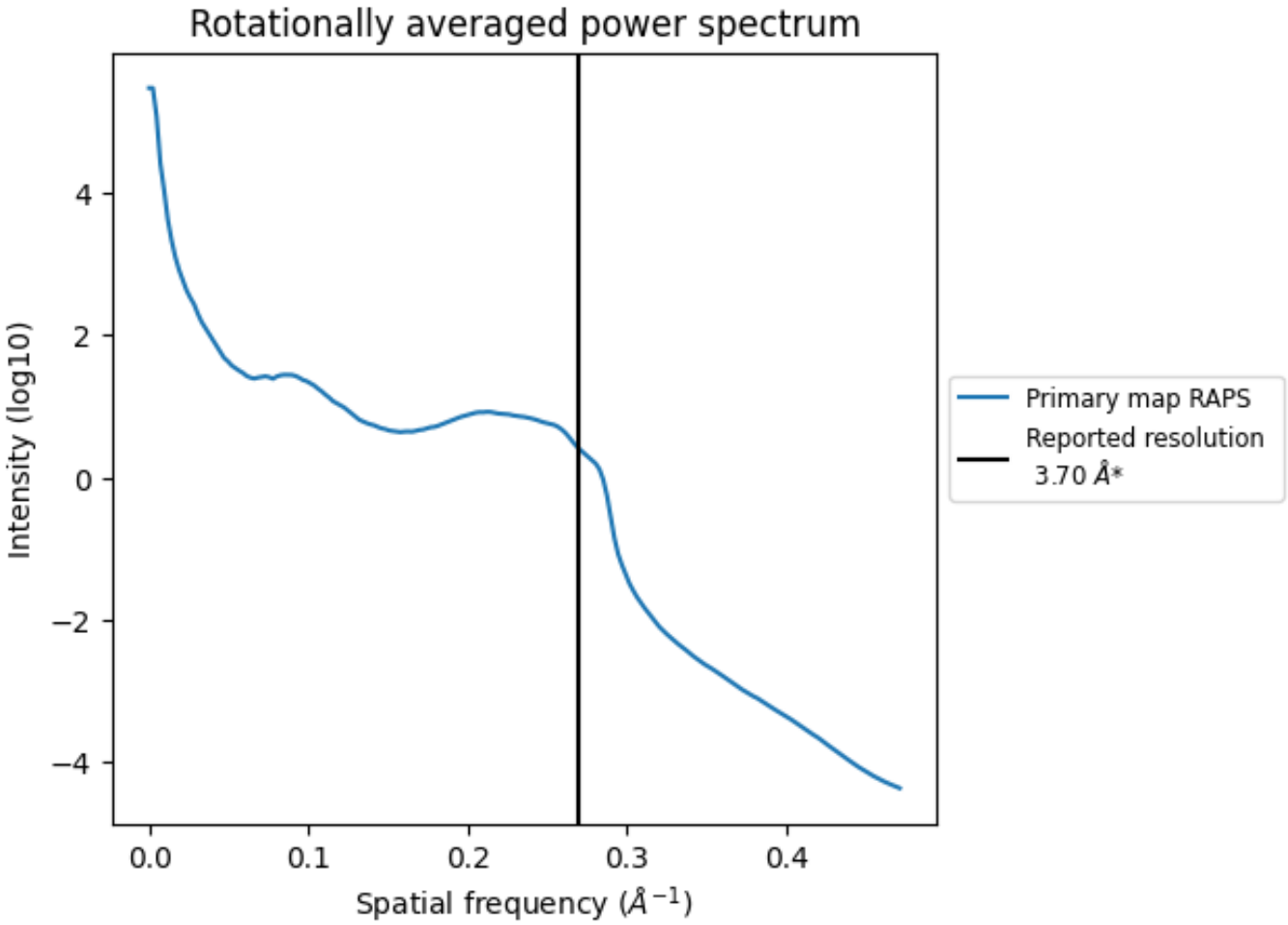
7.2 Volume estimate (i)



The volume at the recommended contour level is 489 nm^3; this corresponds to an approximate mass of 441 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 $Å^{-1}$

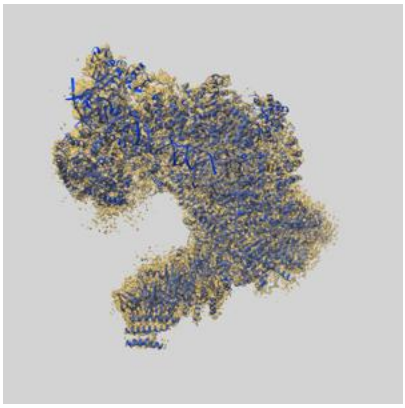
8 Fourier-Shell correlation (i)

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

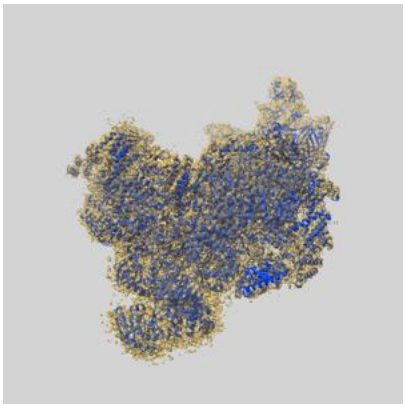
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38317 and PDB model 8XGC. Per-residue inclusion information can be found in section 3 on page 9.

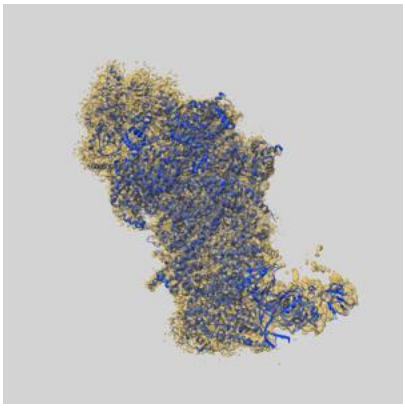
9.1 Map-model overlay



X



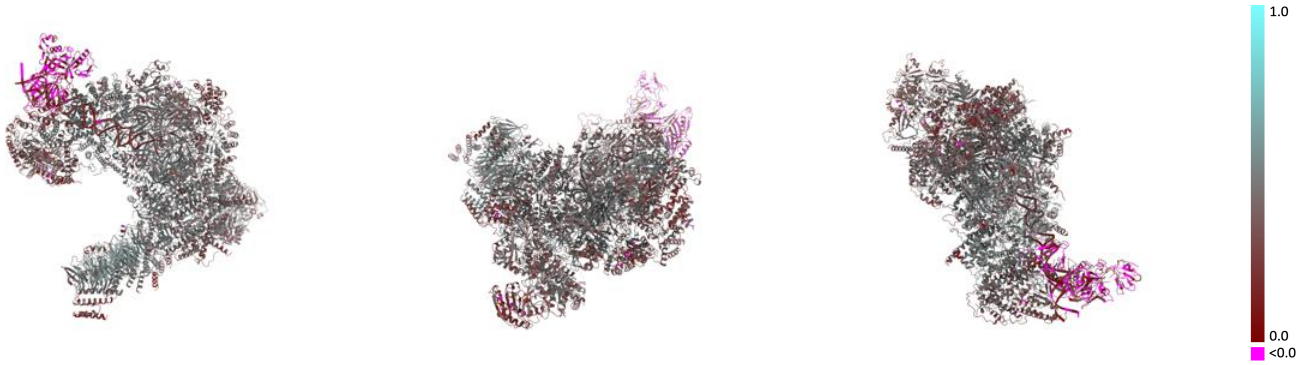
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

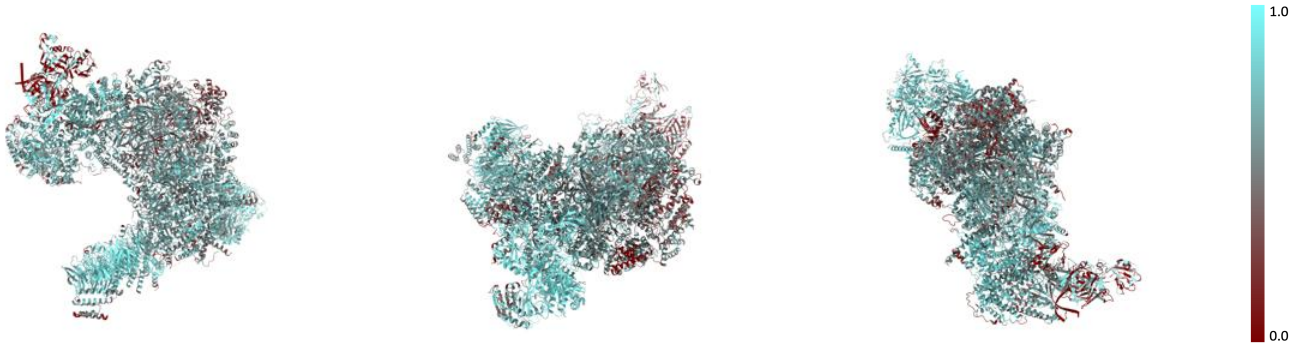
9.2 Q-score mapped to coordinate model (i)



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.

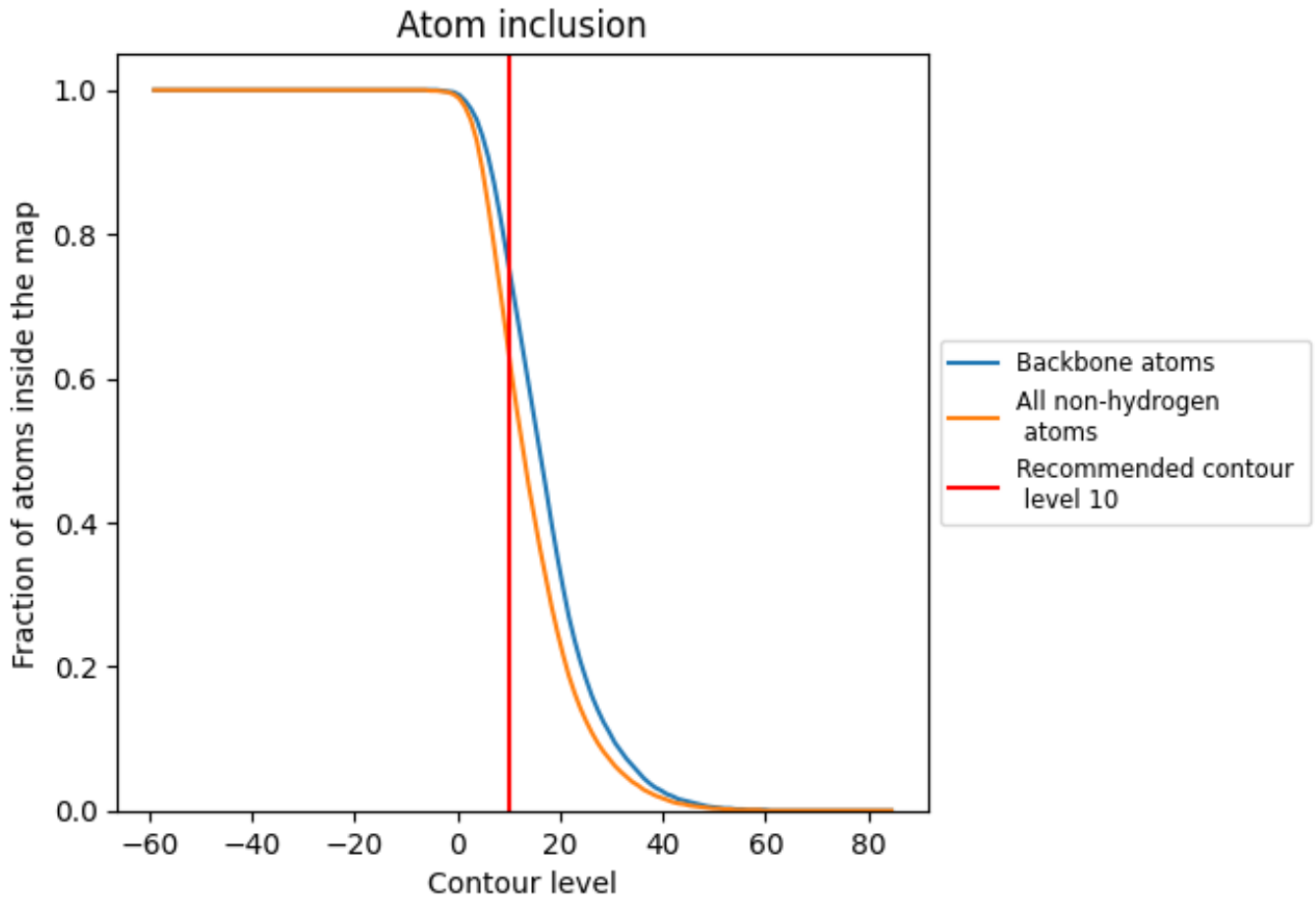
9.3 Atom inclusion mapped to coordinate model (i)



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 (10).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.4070
2	0.6040	0.4400
3	0.6070	0.4410
4	0.4860	0.3860
5	0.6120	0.4410
6	0.6120	0.4360
7	0.4530	0.3750
8	0.7690	0.3780
9	0.7160	0.3940
A	0.5960	0.4030
B	0.6810	0.4620
C	0.6510	0.4430
D	0.6210	0.4240
E	0.6110	0.4400
F	0.7750	0.4910
G	0.7560	0.4550
H	0.7960	0.4740
I	0.7150	0.4640
J	0.6910	0.4390
K	0.4660	0.3630
L	0.5920	0.2970
M	0.2960	0.0490
N	0.6430	0.3600
O	0.6640	0.3510
P	0.7190	0.4000
Q	0.7140	0.3890
R	0.7400	0.4220
S	0.7320	0.4500
X	0.4680	0.1960
Y	0.4420	0.1650