



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 15, 2017 – 01:52 PM EST

PDB ID : 5UDB
EMDB ID: : EMD-8540
Title : Structural basis of MCM2-7 replicative helicase loading by ORC-Cdc6 and Cdt1
Authors : Yuan, Z.; Riera, A.; Bai, L.; Sun, J.; Spanos, C.; Chen, Z.A.; Barbon, M.; Rappsilber, J.; Stillman, B.; Speck, C.; Li, H.
Deposited on : 2016-12-25
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

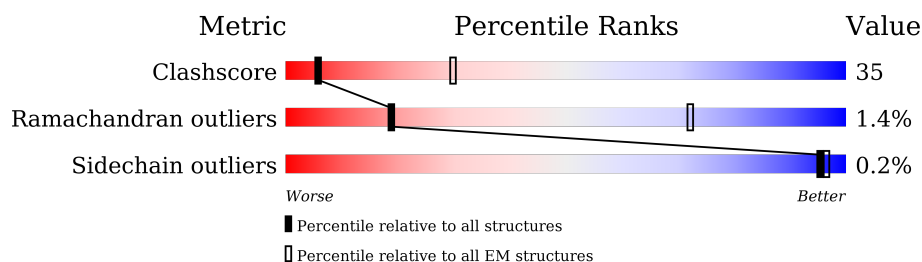
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.







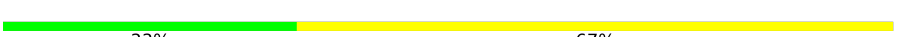
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	868	
2	3	971	
3	4	933	
4	5	775	
5	6	1017	
6	7	845	
7	8	604	
8	9	513	
9	A	914	

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Mol	Chain	Length	Quality of chain
10	B	620	
11	C	616	
12	D	529	
13	E	479	
14	F	435	
15	M	39	
16	N	39	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	AGS	2	2001	-	-	X	-
17	AGS	6	1101	-	-	X	-
17	AGS	7	2001	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 57577 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
1	2	605	Total	C	N	O	S	0	0
			4755	2984	865	891	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	659	Total	C	N	O	S	0	0
			5177	3243	938	982	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	751	Total	C	N	O	S	0	0
			5969	3727	1043	1168	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	580	Total	C	N	O	S	0	0
			4527	2852	781	873	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	693	Total	C	N	O	S	0	0
			5394	3403	946	1021	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	726	Total	C	N	O	S	0	0
			5740	3619	993	1096	32		

- Molecule 7 is a protein called Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	519	Total	C	N	O	S	0	0
			4163	2650	715	779	19		

- Molecule 8 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	376	Total	C	N	O	S	0	0
			3005	1928	503	557	17		

- Molecule 9 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	372	Total	C	N	O	S	0	0
			2963	1893	492	561	17		

- Molecule 10 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	319	Total	C	N	O	S	0	0
			2636	1708	433	481	14		

- Molecule 11 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	510	Total	C	N	O	S	0	0
			4234	2737	697	785	15		

- Molecule 12 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	447	Total	C	N	O	S	0	0
			3615	2311	611	680	13		

- Molecule 13 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	417	Total	C	N	O	S	0	0
			3417	2229	542	633	13		

- Molecule 14 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	15	Total	C	N	O	S	0	0
			135	86	23	25	1		

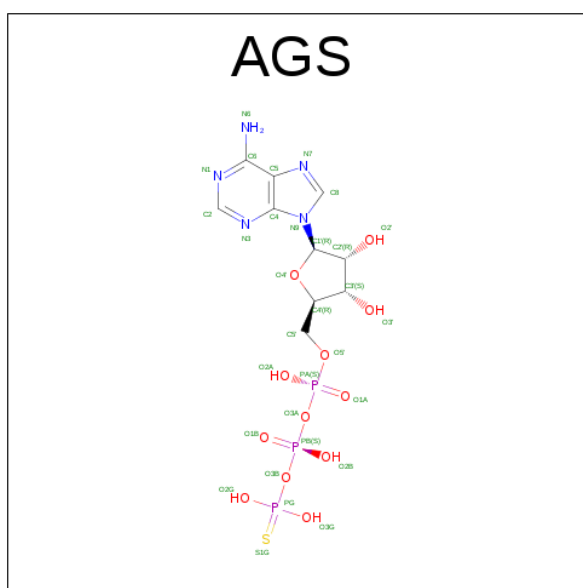
- Molecule 15 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	39	Total	C	N	O	P	0	0
			795	383	127	246	39		

- Molecule 16 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	39	Total	C	N	O	P	0	0
			804	382	161	222	39		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



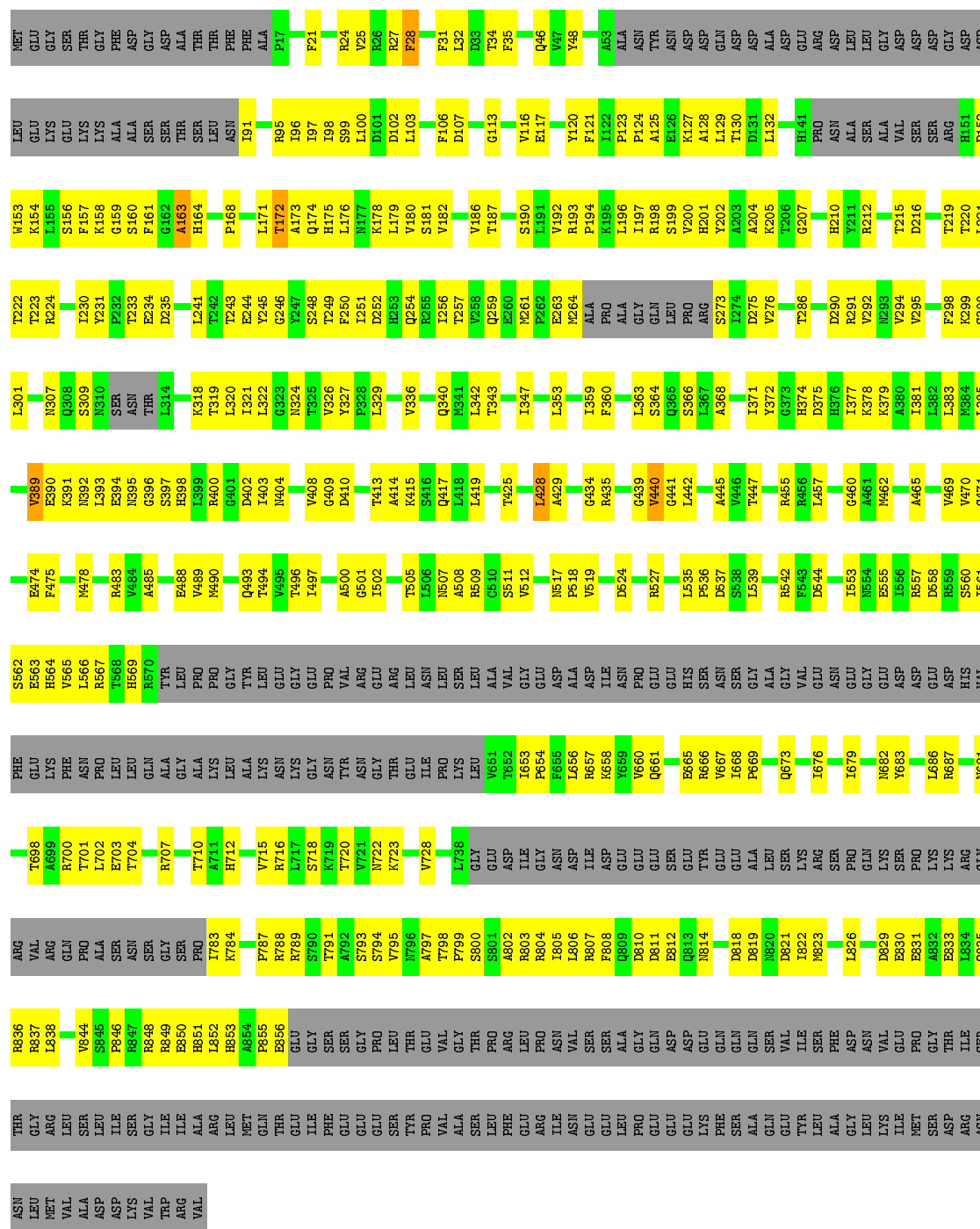
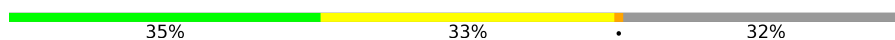
Mol	Chain	Residues	Atoms						AltConf
17	2	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	3	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	6	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	7	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

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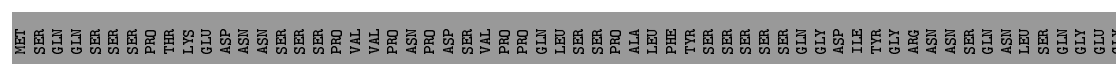
Mol	Chain	Residues	Atoms						AltConf
17	9	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

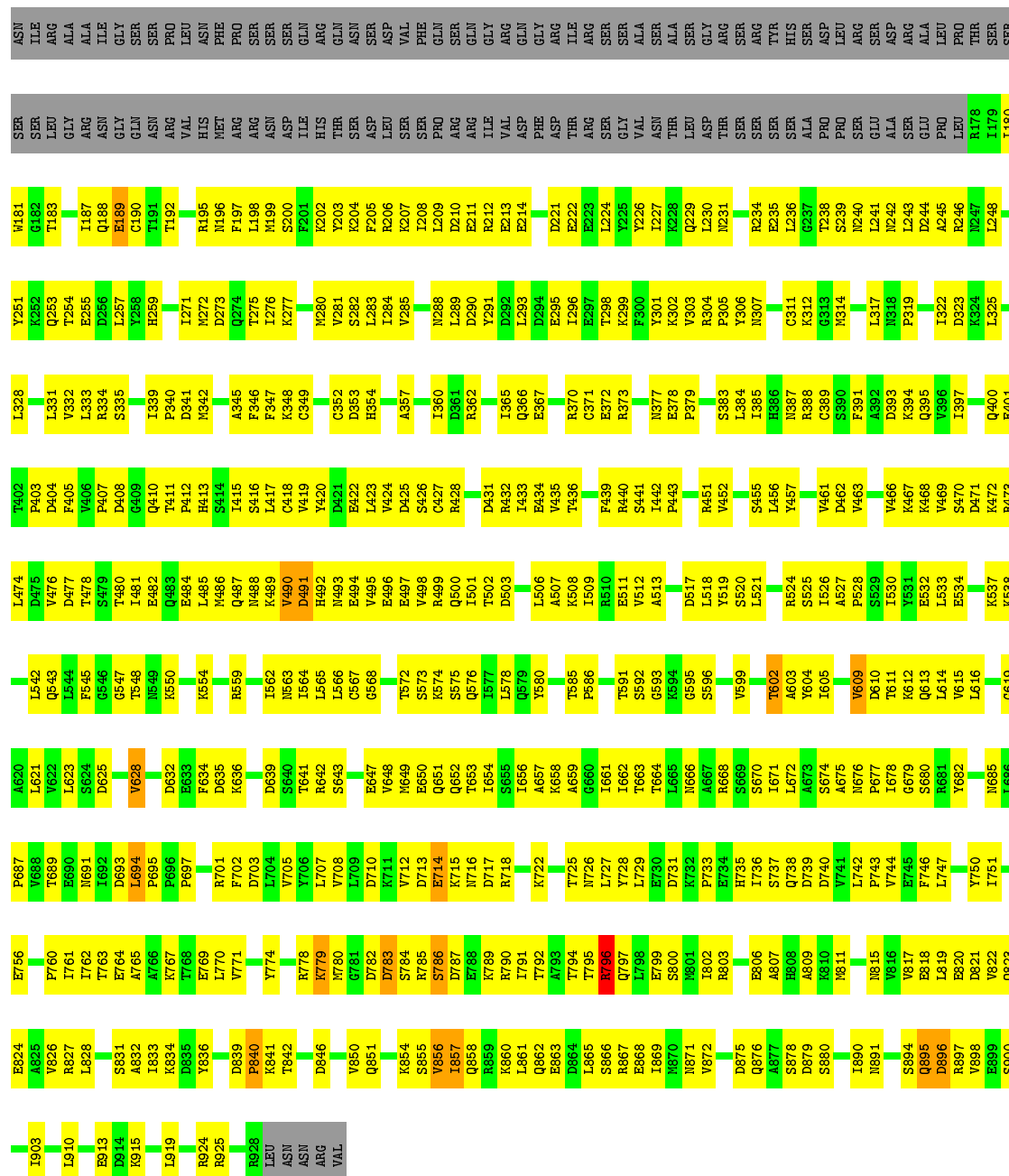
Chain 3:



- Molecule 3: DNA replication licensing factor MCM4

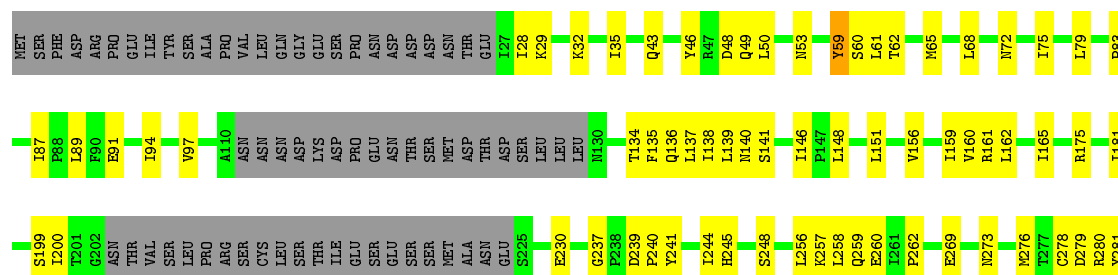
Chain 4:

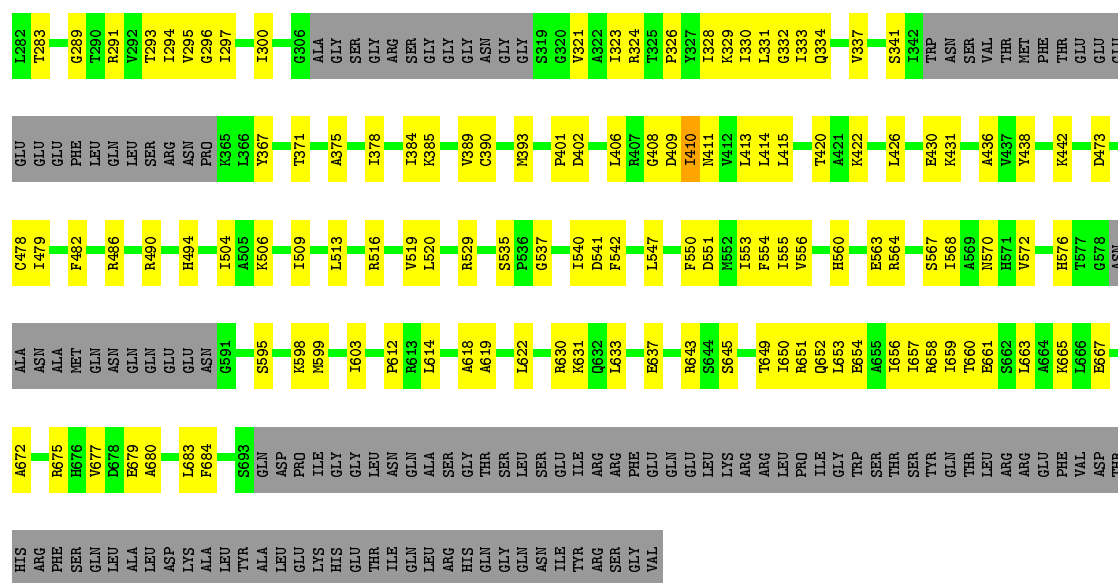




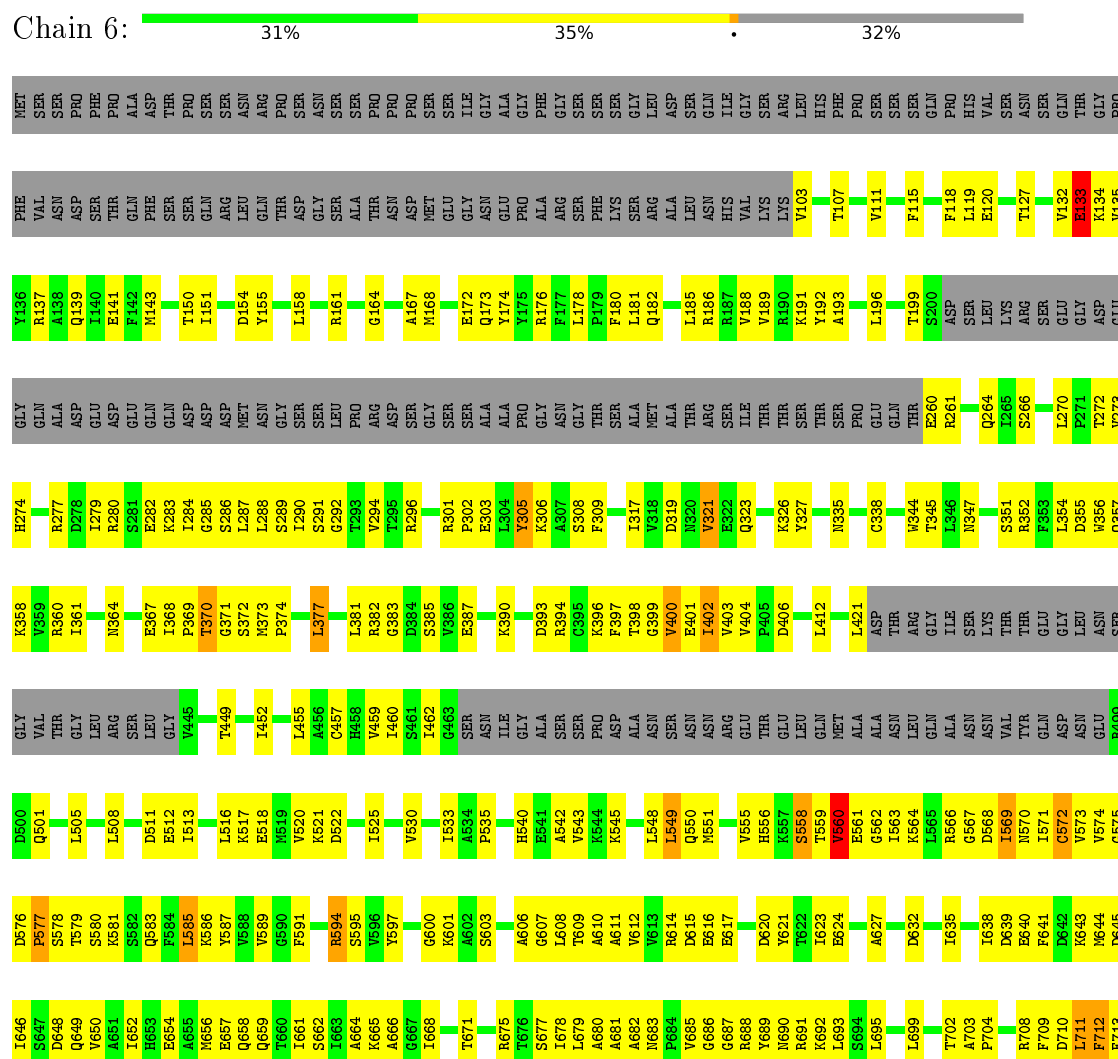
- Molecule 4: Minichromosome maintenance protein 5

Chain 5: 51% 24% 25%

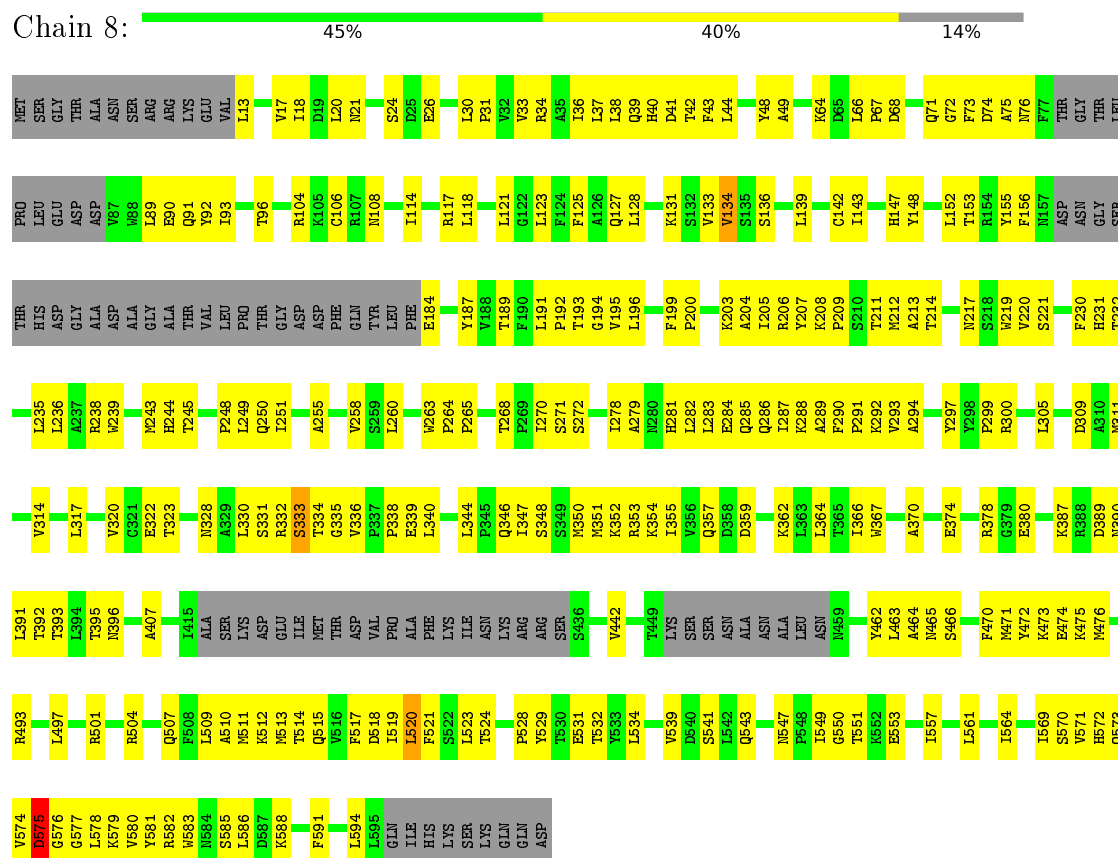




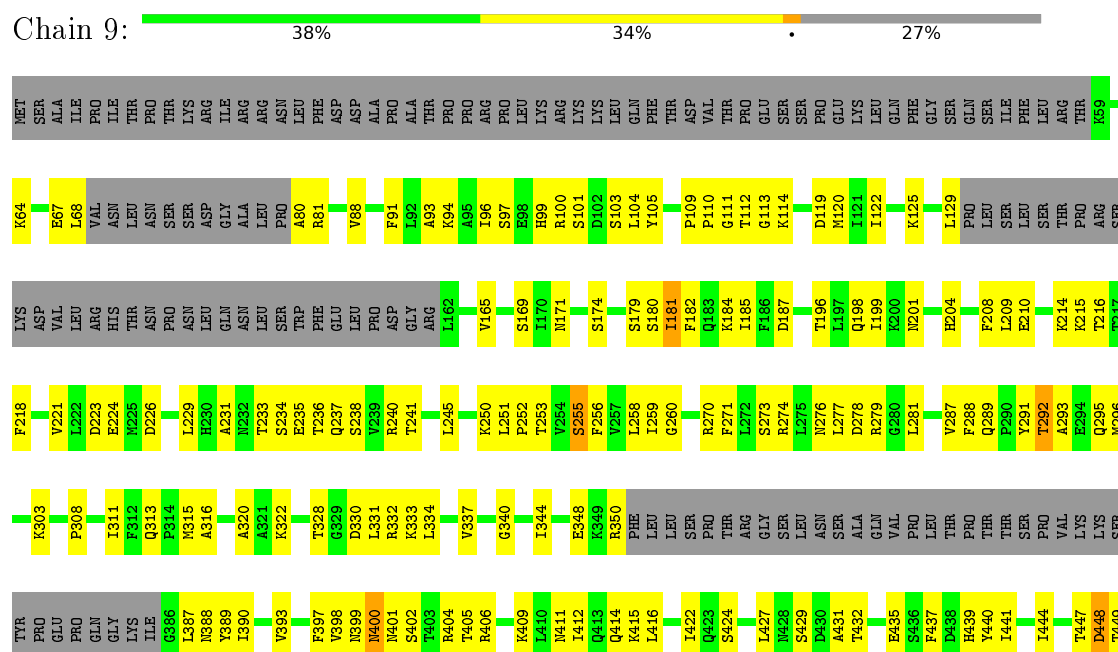
- Molecule 5: DNA replication licensing factor MCM6

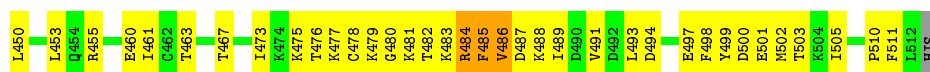


• Molecule 7: Cell division cycle protein CDT1



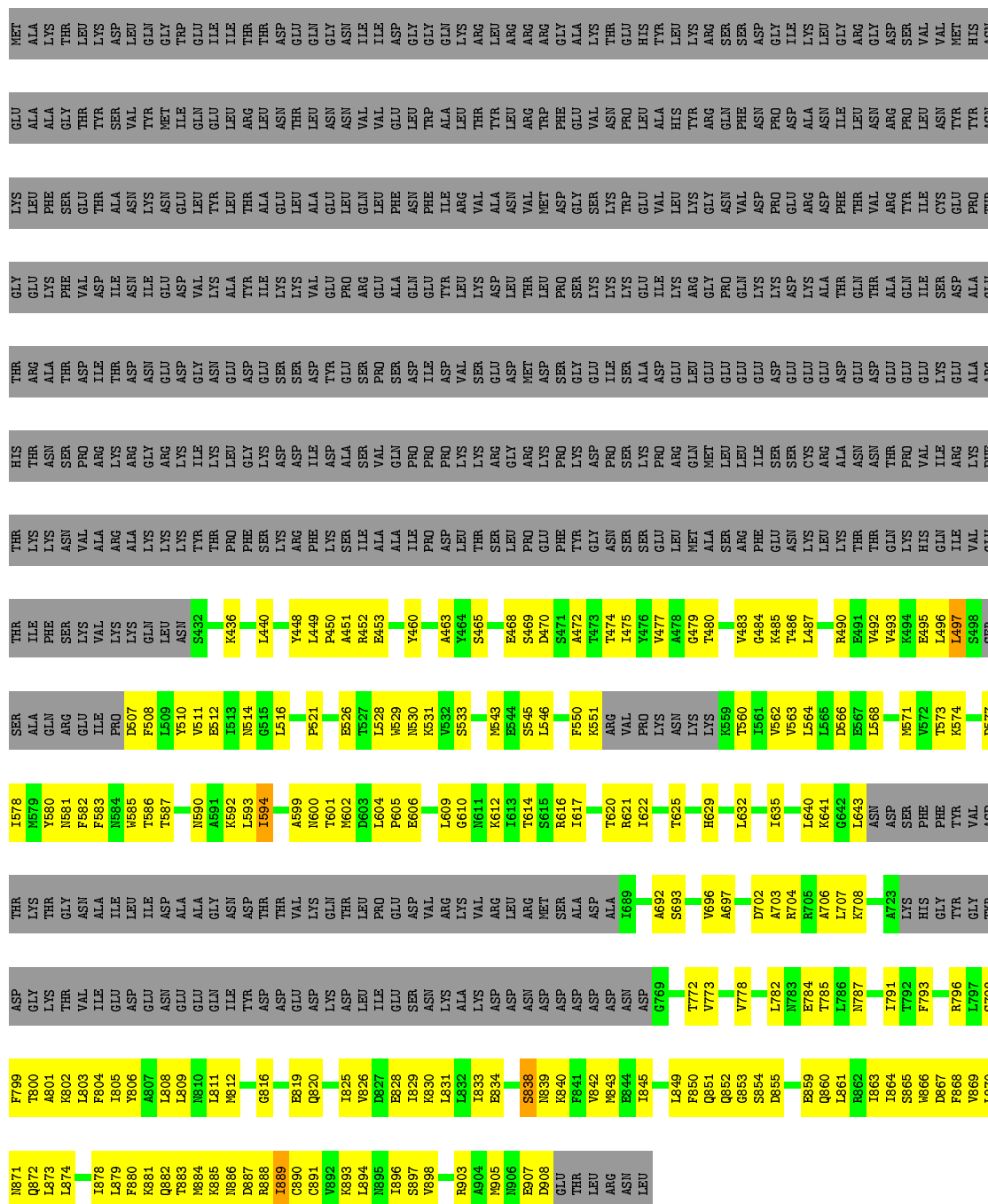
• Molecule 8: Cell division control protein 6





- Molecule 9: Origin recognition complex subunit 1

Chain A:



- Molecule 10: Origin recognition complex subunit 2

Chain B:

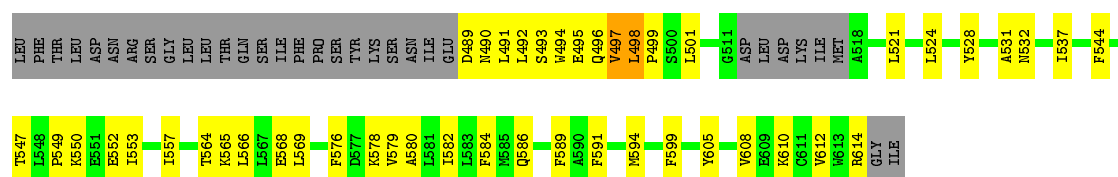


GLY	M520	S455	I379	F312	ASP	THR	THR	LVS	SER	MET
MET	S521	T456	L383	S313	THR	THR	THR	THR	PRO	LEU
ES98	K522	D457	L383	L314	PHE	ASN	ASN	SER	ASP	ASN
IS99	K523	H458	L386	L315	GLU	HIS	HIS	ASN	PRO	GLY
IC00	M524	I459	E387	F316	GLY	ASP	ASP	ASN	ALA	GLU
M601	I525	Y460	E387	I317	TTR	PHE	PHE	LVS	LEU	ASP
P602	A461	A461	L388	G318	PHE	THR	THR	GLN	LVS	PHE
P603	A462	A462	T389	F319	ASP	SER	SER	VAL	PRO	VAL
Y604	L463	L463	T393	G320	GLN	PRO	PRO	MET	GLU	GLU
T605	L464	L464	T393	S321	ARG	LEU	LEU	THR	THR	HIS
Y606	L465	L465	K394	K322	LVS	LVS	LVS	LVS	PRO	ASN
A607	D466	D466	K396	K323	ILE	GLN	GLN	THR	SER	ASP
E608	M467	M467	G397	N324	VAL	ILE	ILE	GLY	ILE	ILE
L609	M468	M468	G397	F325	ARG	ILE	ILE	ILE	ALA	ALA
L610	ASN	K469	K398	L326	THR	MET	MET	LVS	PRO	SER
L612	LEU	A470	K399	L326	ASN	ASN	ASN	GLU	ARG	LEU
L617	SER	Q471	V400	D332	ALA	ALA	ASN	LVS	LVS	PRO
ASN	ALA		I401	I333	LVS	LVS	LEU	ARG	ARG	ALA
THR	THR	M474	I402	L334	SER	GLY	GLY	GLU	GLY	LVS
THR	THR	F475	Q403	S335	ARG	GLU	GLU	ARG	ARG	SER
GLY	GLY	V476	I404	P336	HIS	TTR	LVS	GLU	PRO	SER
PRO	PRO	F477	I405	LVS	THR	LVS	LVS	GLU	ARG	ASN
LVS	LVS	H478	Q405	ILE	MET	ASP	ASP	ILE	LVS	VAL
ARG	ARG	D479	Q414	ALA	THR	SER	SER	GLN	ILE	THR
GLY	GLY	I480	P415	TTR	MET	THR	THR	VAL	GLN	PRO
THR	THR	S481	I416	SER	ALA	SER	SER	ALA	GLU	ARG
Q550	Q550		D417	GLN	PRO	PRO	THR	THR	GLU	LEU
R551	R551	E484	I418	LEU	D268	GLY	GLY	THR	LEU	ASP
T552	T552		K419	ALA		LVS	LVS	THR	THR	ASP
Q553	Q553	E486		Y345	R271	LEU	LEU	TTR	ASP	PRO
V554	V554	T487	I422	E346		THR	THR	GLU	ILE	HIS
E555	E555	V488	V423	L349	S275	LEU	LEU	ASP	ARG	GLY
L556	L556	E489	V424	L349	L276	SER	SER	ASN	LVS	GLU
K557	K557	S490	H425	Q350	M279	ARG	VAL	VAL	LVS	ARG
L558	L558		I426	Q351		ASN	THR	THR	ASP	GLN
F559	F559	Q493	I427	R352	F280	PHE	PRO	PRO	GLU	LEU
M560	M560	D494	D428	K353	F281	THR	THR	GLN	LVS	ARG
H561	H561	V495	Q429	P354	M282	PRO	PRO	ARG	GLY	LEU
A565	A565	M496	P430	V355	E283	THR	THR	ASP	THR	ILE
A566	A566	K497	S431		H284	PRO	PRO	ASP	ILE	HIS
A566	A566	M498	I432	L358	F285	VAL	VAL	ASN	SER	SER
F567	F567	GLY	R433	P359	Q286	PRO	PHE	SER	SER	SER
L573	L573	LVS	R434	C360	R287	LVS	VAL	LVS	LVS	LVS
A574	A574	SER	M435	L361		ASN	ASN	LVS	ASN	ASN
L575	L575	THR	T436	I362	R290	LVS	LVS	ASN	LVS	ASN
		SER	F437	L363	Q291	LVS	SER	ARG	LEU	LEU
		S605	Q438	N364	K292	LEU	LEU	PRO	LVS	LEU
		G506	T439	G365	L293	TTR	GLU	GLU	LEU	LEU
			M440	Y366		GLN	PRO	ASP	ASP	ARG
				Y367	I296	THR	THR	ILE	ILE	ARG
H585	H585	G509	F443	P368		SER	GLU	ASP	THR	SER
M587	M587	A510		S369	R288	GLU	GLU	PRO	THR	VAL
A588	A588		I447	C370	K299	THR	THR	ALA	SER	VAL
M589	M589	V513	R446	N371	M300	LVS	LVS	THR	GLY	GLY
L590	L590	L514	Q449	R372		SER	PRO	ASN	VAL	ASN
T591	T591	Q515	I450	Y373		ALA	ALA	VAL	GLU	GLU
K592	K592	A516	A451	D374	Q303	SER	LVS	LVS	ARG	ARG
M593	M593	L517	I452	V375	F306	SER	SER	LVS	GLU	LVS
ASN	ASN	T518	V453	F376	E307	PHE	THR	SER	GLU	ASN
ASN	ASN	V519	V453			LEU	LEU	THR	SER	SER

- Molecule 11: Origin recognition complex subunit 3

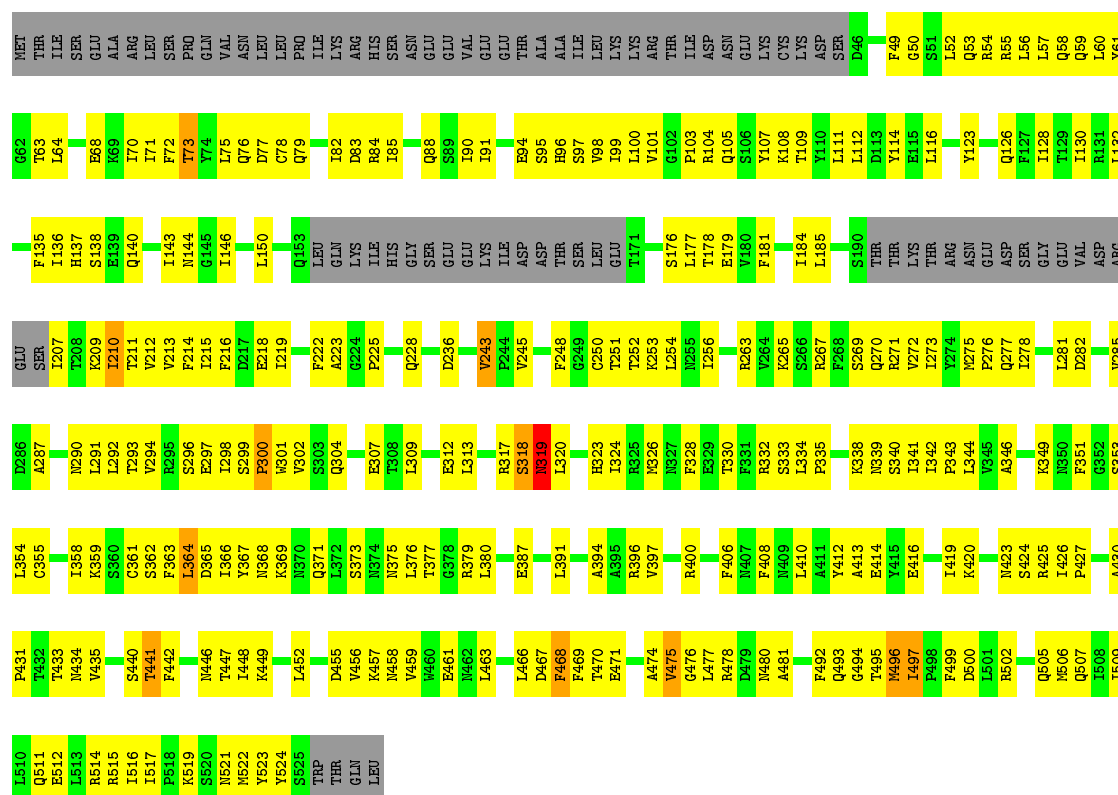
Chain C:  44% 38% 1% 17%

V933	T310	D230	Y148	H65	MET
E394	R311	E231	K149	F68	ASP
F395	R312	V232	A154	H69	LEU
R398	R313	K233	E158	V72	ASN
E399	R314	S235	H159	D73	GLN
M400	R315	L236	P160	H74	SER
A401	L316	L237	THR	I75	LVS
I402		F238	ILE	I76	MET
	K319	M239	LVS	D77	ASN
H405	M320	I240	TYR	H78	VAL
	L321	M241	GLU	I79	SER
F408	L322	T242	ASP	E80	GLU
V409	V323	M243	ILE	L83	PHE
A410	S324	L244	ASP	K84	ALA
R411	L325	S245	ASN	A85	ASP
F412	M326		ASP	B86	ALA
L413	S327	E248	GLU	I87	GLN
E414	V328		ASP	F106	ARG
E415	F329	L251	GLY	L107	SER
A416	F330	R252	ASP	L108	TYR
L417	Q331	Q253	PHE	G109	THR
		S254	THR	S110	VAL
M423	S335	T255	GLU	D111	TYR
L424	V336	L256	GLN	S112	SER
I425	F337	R257	ASN	T113	LEU
E426	L338	L258	ASP	T114	PRO
L427			V181	K115	GLN
A428	R342	K265	S182	I116	ASN
H429	V343	L266	S183	E117	ASN
M430	R344	L267	I183	L118	LVS
L431	F345	V268	D184	A119	ASN
L432	L346	S269	L185	D120	ASP
I433		S270	V188	E121	LVS
A434	D349	M271		R124	ASN
K435		K272	F191	Y125	ASP
L436	L353	G273		L128	LVS
A437	F374	T274	L199	L131	HIS
S438	V364	K275		T132	PRO
V439	V276	V277	V202	P133	PHE
L440	L367	G277	F203	K134	VAL
D441	L368	M278	M204	E135	LVS
R442	K369	Q279		S136	LEU
		L280	F205	P137	SER
C446	A372	Q281	K206	M138	LEU
	P373	Q282	D207	L141	GLY
	A374	S283	V208	R142	LVS
		F284	I211	R144	LVS
D451	L377	L285		S146	GLU
A452	L380	D286	L216	V139	SER
K453		T287	D217	R140	GLU
F454	R383	L292	M218	M141	V52
A455		M293	L222	M142	N53
	G387	F298		L143	V54
H459	L388		A226	R144	E55
T460	E399		F227	R145	K56
I461	E390	I302	K228	V147	R57
F462	F391	V205	E259		L60
GLN					



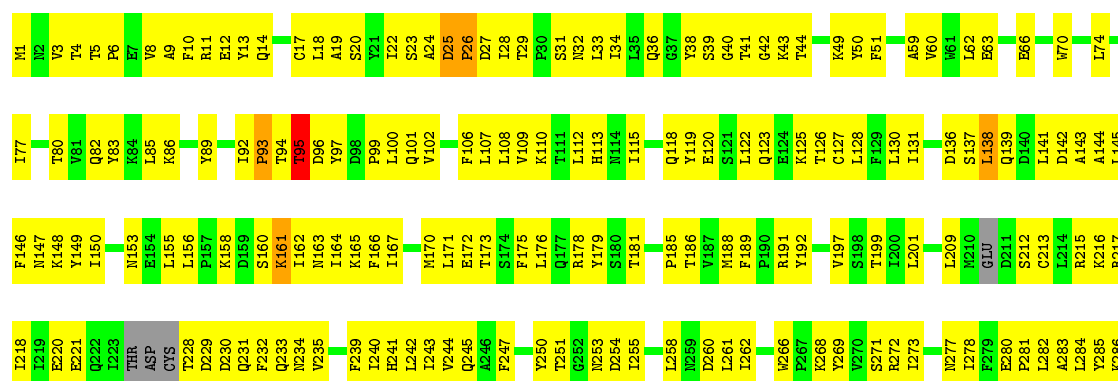
• Molecule 12: Origin recognition complex subunit 4

Chain D: 37% 45% 16%



• Molecule 13: Origin recognition complex subunit 5

Chain E: 35% 49% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	304288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	2	0.33	0/4830	0.57	0/6520
10	B	0.29	0/2693	0.55	2/3635 (0.1%)
11	C	0.30	0/4324	0.54	1/5835 (0.0%)
12	D	0.47	0/3678	0.75	4/4976 (0.1%)
13	E	0.49	0/3498	0.75	3/4752 (0.1%)
14	F	0.23	0/137	0.45	0/183
15	M	0.52	0/886	0.98	0/1366
16	N	0.55	0/906	0.81	0/1395
2	3	0.26	0/5261	0.52	2/7124 (0.0%)
3	4	0.41	0/6049	0.73	6/8168 (0.1%)
4	5	0.24	0/4587	0.50	0/6193
5	6	0.50	0/5474	0.76	5/7389 (0.1%)
6	7	0.29	0/5825	0.57	1/7864 (0.0%)
7	8	0.34	0/4240	0.63	0/5743
8	9	0.27	0/3048	0.51	0/4100
9	A	0.35	0/3004	0.63	0/4046
All	All	0.37	0/58440	0.64	24/79289 (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	2	0	2
13	E	0	3
2	3	0	1
3	4	0	2
4	5	0	1
5	6	0	5
6	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	8	0	3
8	9	0	3
All	All	0	21

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	319	ASN	N-CA-C	-8.77	87.33	111.00
12	D	319	ASN	N-CA-CB	8.07	125.12	110.60
10	B	429	GLY	C-N-CD	-7.91	103.20	120.60
5	6	585	LEU	CA-CB-CG	-7.19	98.76	115.30
3	4	298	THR	N-CA-C	6.82	129.40	111.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	355	SER	Peptide
1	2	524	PRO	Peptide
2	3	163	ALA	Peptide
3	4	408	ASP	Peptide
3	4	628	VAL	Peptide

5.2 Too-close contacts

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	4755	0	4774	375	0
2	3	5177	0	5231	354	0
3	4	5969	0	6014	618	0
4	5	4527	0	4641	166	0
5	6	5394	0	5338	494	0
6	7	5740	0	5839	322	0
7	8	4163	0	4232	247	0
8	9	3005	0	3134	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2963	0	3019	244	0
10	B	2636	0	2633	204	0
11	C	4234	0	4200	284	0
12	D	3615	0	3664	414	0
13	E	3417	0	3422	443	0
14	F	135	0	132	5	0
15	M	795	0	448	24	0
16	N	804	0	436	37	0
17	2	31	0	11	10	0
17	3	31	0	9	2	0
17	6	31	0	12	10	0
17	7	31	0	12	9	0
17	9	31	0	12	8	0
17	A	31	0	12	6	0
17	D	31	0	11	6	0
17	E	31	0	12	2	0
All	All	57577	0	57248	3976	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 35.

The worst 5 of 3976 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)
12:D:300:PRO:HD2	12:D:301:TRP:CE3	1.29	1.60
2:3:31:PHE:CE1	2:3:35:PHE:CE2	1.80	1.60
10:B:321:SER:HB2	10:B:486:SER:CB	1.12	1.59
1:2:246:TYR:CZ	1:2:300:PHE:HE1	1.22	1.56
10:B:321:SER:CB	10:B:486:SER:HB2	1.31	1.55

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	597/868 (69%)	545 (91%)	51 (8%)	1 (0%)	52	86
2	3	645/971 (66%)	599 (93%)	43 (7%)	3 (0%)	34	76
3	4	749/933 (80%)	633 (84%)	100 (13%)	16 (2%)	9	51
4	5	568/775 (73%)	538 (95%)	29 (5%)	1 (0%)	52	86
5	6	683/1017 (67%)	609 (89%)	63 (9%)	11 (2%)	12	56
6	7	716/845 (85%)	643 (90%)	58 (8%)	15 (2%)	9	51
7	8	509/604 (84%)	445 (87%)	56 (11%)	8 (2%)	12	56
8	9	368/513 (72%)	333 (90%)	30 (8%)	5 (1%)	14	58
9	A	362/914 (40%)	311 (86%)	47 (13%)	4 (1%)	17	63
10	B	309/620 (50%)	288 (93%)	17 (6%)	4 (1%)	15	59
11	C	502/616 (82%)	452 (90%)	41 (8%)	9 (2%)	11	54
12	D	441/529 (83%)	382 (87%)	45 (10%)	14 (3%)	5	43
13	E	407/479 (85%)	356 (88%)	44 (11%)	7 (2%)	11	55
14	F	13/435 (3%)	13 (100%)	0	0	100	100
All	All	6869/10119 (68%)	6147 (90%)	624 (9%)	98 (1%)	19	58

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	189	GLU
3	4	491	ASP
3	4	779	LYS
3	4	896	ASP
5	6	317	ILE

5.3.2 Protein sidechains ⓘ

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	512/770 (66%)	510 (100%)	2 (0%)	93	97
2	3	573/835 (69%)	572 (100%)	1 (0%)	95	97
3	4	677/848 (80%)	676 (100%)	1 (0%)	95	97
4	5	516/688 (75%)	516 (100%)	0	100	100
5	6	569/886 (64%)	566 (100%)	3 (0%)	92	96
6	7	647/753 (86%)	647 (100%)	0	100	100
7	8	474/545 (87%)	473 (100%)	1 (0%)	95	97
8	9	343/470 (73%)	342 (100%)	1 (0%)	94	97
9	A	328/813 (40%)	327 (100%)	1 (0%)	94	97
10	B	296/573 (52%)	295 (100%)	1 (0%)	94	97
11	C	476/576 (83%)	476 (100%)	0	100	100
12	D	411/488 (84%)	410 (100%)	1 (0%)	95	97
13	E	388/440 (88%)	386 (100%)	2 (0%)	92	96
14	F	15/406 (4%)	15 (100%)	0	100	100
All	All	6225/9091 (68%)	6211 (100%)	14 (0%)	95	97

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

Mol	Chain	Res	Type
5	6	788	PHE
7	8	520	LEU
12	D	468	PHE
5	6	712	PHE
10	B	475	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
7	8	244	HIS
9	A	851	GLN
12	D	407	ASN
7	8	396	ASN
7	8	543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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$
17	AGS	2	2001	1,5	26,33,33	1.03	1 (3%)	24,52,52	1.77	4 (16%)
17	AGS	3	2001	2,6	26,33,33	0.84	2 (7%)	24,52,52	1.33	1 (4%)
17	AGS	6	1101	5	26,33,33	1.23	2 (7%)	24,52,52	1.03	2 (8%)
17	AGS	7	2001	6	26,33,33	0.87	1 (3%)	24,52,52	1.31	1 (4%)
17	AGS	9	2001	-	26,33,33	1.11	1 (3%)	24,52,52	0.67	1 (4%)
17	AGS	A	2001	9	26,33,33	0.80	1 (3%)	24,52,52	0.94	1 (4%)
17	AGS	D	2001	12	26,33,33	0.98	2 (7%)	24,52,52	0.90	1 (4%)
17	AGS	E	2001	-	26,33,33	0.80	1 (3%)	24,52,52	1.34	1 (4%)

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
17	AGS	2	2001	1,5	-	0/17/38/38	0/3/3/3
17	AGS	3	2001	2,6	-	0/17/38/38	0/3/3/3
17	AGS	6	1101	5	-	0/17/38/38	0/3/3/3
17	AGS	7	2001	6	-	0/17/38/38	0/3/3/3
17	AGS	9	2001	-	-	0/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	AGS	A	2001	9	-	0/17/38/38	0/3/3/3
17	AGS	D	2001	12	-	0/17/38/38	0/3/3/3
17	AGS	E	2001	-	-	0/17/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	2001	AGS	C8-N7	-2.08	1.30	1.34
17	D	2001	AGS	C8-N7	-2.01	1.30	1.34
17	3	2001	AGS	PG-S1G	2.07	1.94	1.90
17	A	2001	AGS	PG-S1G	2.31	1.94	1.90
17	E	2001	AGS	PG-S1G	2.47	1.95	1.90

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	2001	AGS	PB-O3B-PG	-7.04	107.19	132.71
17	E	2001	AGS	PB-O3B-PG	-5.70	112.04	132.71
17	3	2001	AGS	PB-O3B-PG	-5.50	112.75	132.71
17	7	2001	AGS	PB-O3B-PG	-5.06	114.37	132.71
17	A	2001	AGS	PB-O3B-PG	-4.22	117.39	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	2001	AGS	10	0
17	3	2001	AGS	2	0
17	6	1101	AGS	10	0
17	7	2001	AGS	9	0
17	9	2001	AGS	8	0
17	A	2001	AGS	6	0
17	D	2001	AGS	6	0
17	E	2001	AGS	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.