wwPDB EM Validation Summary Report

Mar 5, 2026 – 06:37 PM UTC

PDB ID	:	8B9A / pdb_00008b9a
EMDB ID	:	EMD-15309
Title	:	S. cerevisiae replisome + Ctf4, bound by pol alpha primase. Complex engaged with a fork DNA substrate containing a 60 nucleotide lagging strand.
Authors	:	Jones, M.L.; Yeeles, J.T.P.
Deposited on	:	2022-10-05
Resolution	:	3.50 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:

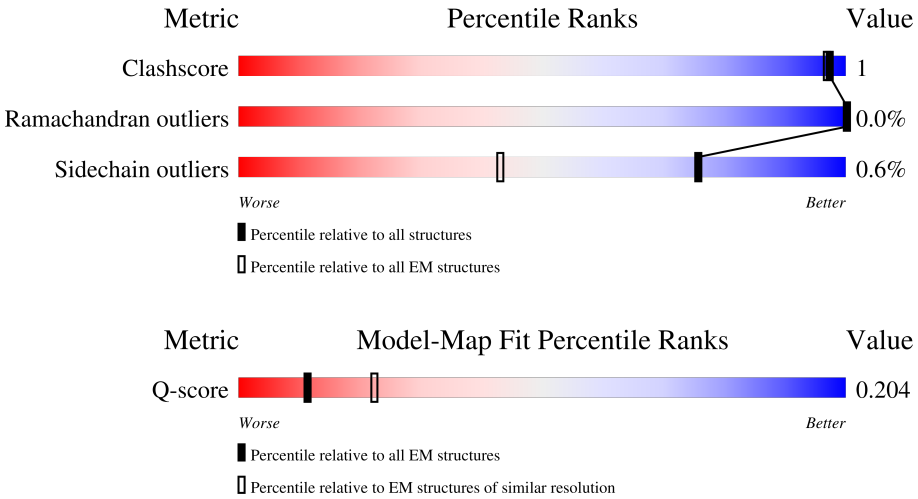
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2061 (4.14 - 5.14)

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	65% · 35%
2	3	1009	60% · 39%
3	4	933	67% 33%
4	5	775	69% 31%

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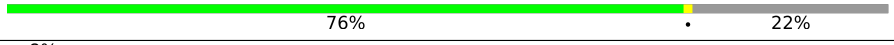
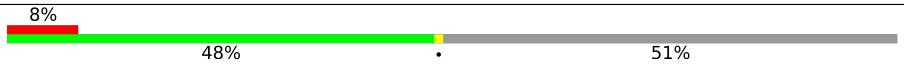
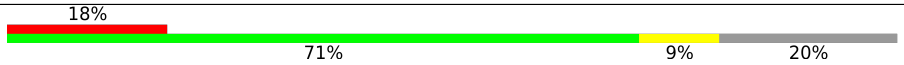
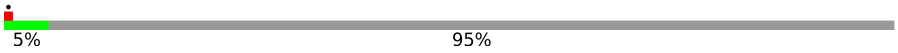
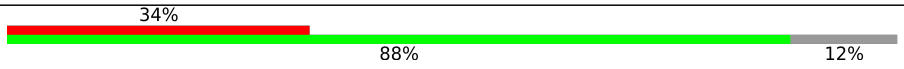
Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	528	
8	B	705	
9	C	208	
10	D	213	
11	E	217	
12	F	294	
13	G	657	
14	J	1468	
15	P	1109	
16	Q	84	
17	R	106	
18	S	444	
19	X	1238	
20	Y	319	
21	H	962	
21	K	962	
21	L	962	

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 139367 atoms, of which 69655 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	2	568	9140	2857	4606	810	853	14	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	613	9653	3023	4861	853	903	13	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-37	MET	-	initiating methionine	UNP P24279
3	-36	LYS	-	expression tag	UNP P24279
3	-35	ARG	-	expression tag	UNP P24279
3	-34	ARG	-	expression tag	UNP P24279
3	-33	TRP	-	expression tag	UNP P24279
3	-32	LYS	-	expression tag	UNP P24279
3	-31	LYS	-	expression tag	UNP P24279
3	-30	ASN	-	expression tag	UNP P24279
3	-29	PHE	-	expression tag	UNP P24279
3	-28	ILE	-	expression tag	UNP P24279
3	-27	ALA	-	expression tag	UNP P24279
3	-26	VAL	-	expression tag	UNP P24279
3	-25	SER	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	ALA	-	expression tag	UNP P24279
3	-22	ASN	-	expression tag	UNP P24279
3	-21	ARG	-	expression tag	UNP P24279
3	-20	PHE	-	expression tag	UNP P24279
3	-19	LYS	-	expression tag	UNP P24279
3	-18	LYS	-	expression tag	UNP P24279
3	-17	ILE	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-16	SER	-	expression tag	UNP P24279
3	-15	SER	-	expression tag	UNP P24279
3	-14	SER	-	expression tag	UNP P24279
3	-13	GLY	-	expression tag	UNP P24279
3	-12	ALA	-	expression tag	UNP P24279
3	-11	LEU	-	expression tag	UNP P24279
3	-10	GLU	-	expression tag	UNP P24279
3	-9	ASN	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	TYR	-	expression tag	UNP P24279
3	-6	PHE	-	expression tag	UNP P24279
3	-5	GLN	-	expression tag	UNP P24279
3	-4	GLY	-	expression tag	UNP P24279
3	-3	GLU	-	expression tag	UNP P24279
3	-2	ALA	-	expression tag	UNP P24279
3	-1	PRO	-	expression tag	UNP P24279
3	0	VAL	-	expression tag	UNP P24279

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	628	10055	3145	5065	855	961	29	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	533	8560	2670	4347	724	798	21	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	623	9908	3112	4980	860	931	25	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	656	10387	3257	5233	885	983	29	0	0

- Molecule 7 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	258	Total	C	H	N	O	S	0	0
			4382	1412	2197	363	405	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	561	Total	C	H	N	O	S	0	0
			8944	2859	4464	758	852	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	195	Total	C	H	N	O	S	0	0
			3202	1004	1603	275	311	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	188	Total	C	H	N	O	S	0	0
			3191	1010	1620	275	282	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	171	Total	C	H	N	O	S	0	0
			2775	899	1396	221	252	7		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	MET	-	initiating methionine	UNP Q12146
E	-21	GLY	-	expression tag	UNP Q12146
E	-20	SER	-	expression tag	UNP Q12146
E	-19	SER	-	expression tag	UNP Q12146
E	-18	HIS	-	expression tag	UNP Q12146
E	-17	HIS	-	expression tag	UNP Q12146
E	-16	HIS	-	expression tag	UNP Q12146
E	-15	HIS	-	expression tag	UNP Q12146
E	-14	HIS	-	expression tag	UNP Q12146
E	-13	HIS	-	expression tag	UNP Q12146
E	-12	SER	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	SER	-	expression tag	UNP Q12146
E	-10	GLY	-	expression tag	UNP Q12146
E	-9	LEU	-	expression tag	UNP Q12146
E	-8	VAL	-	expression tag	UNP Q12146
E	-7	PRO	-	expression tag	UNP Q12146
E	-6	ARG	-	expression tag	UNP Q12146
E	-5	GLY	-	expression tag	UNP Q12146
E	-4	SER	-	expression tag	UNP Q12146
E	-3	HIS	-	expression tag	UNP Q12146
E	-2	MET	-	expression tag	UNP Q12146
E	-1	ALA	-	expression tag	UNP Q12146
E	0	SER	-	expression tag	UNP Q12146

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	238	Total	C	H	N	O	S	0	0
			3928	1248	1968	321	379	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	565	Total	C	H	N	O	S	0	0
			9185	2929	4598	776	868	14		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	167G	TYR	-	linker	UNP Q08032
G	167H	LYS	-	linker	UNP Q08032
G	167I	ASP	-	linker	UNP Q08032
G	167J	ASP	-	linker	UNP Q08032
G	167K	ASP	-	linker	UNP Q08032
G	167L	GLY	-	linker	UNP Q08032
G	167M	ASP	-	linker	UNP Q08032
G	167N	TYR	-	linker	UNP Q08032
G	167O	LYS	-	linker	UNP Q08032
G	167P	ASP	-	linker	UNP Q08032
G	167Q	ASP	-	linker	UNP Q08032

- Molecule 14 is a protein called DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	J	208	Total	C	H	N	O	S	0	0
			3342	1071	1645	281	331	14		

- Molecule 15 is a protein called Mediator of replication checkpoint protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	50	Total	C	H	N	O	S	0	0
			805	258	397	68	81	1		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1097	ASP	-	expression tag	UNP P25588
P	1098	TYR	-	expression tag	UNP P25588
P	1099	LYS	-	expression tag	UNP P25588
P	1100	ASP	-	expression tag	UNP P25588
P	1101	ASP	-	expression tag	UNP P25588
P	1102	ASP	-	expression tag	UNP P25588
P	1103	GLY	-	expression tag	UNP P25588
P	1104	ASP	-	expression tag	UNP P25588
P	1105	TYR	-	expression tag	UNP P25588
P	1106	LYS	-	expression tag	UNP P25588
P	1107	ASP	-	expression tag	UNP P25588
P	1108	ASP	-	expression tag	UNP P25588
P	1109	ASP	-	expression tag	UNP P25588

- Molecule 16 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	35	Total	C	H	N	O	P	0	0
			1128	350	406	112	225	35		

- Molecule 17 is a DNA chain called Lagging strand.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	21	Total	C	H	N	O	P	0	0
			656	202	237	71	125	21		

- Molecule 18 is a protein called DNA primase small subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	391	Total	C	H	N	O	S	0	0
			6428	2055	3201	561	595	16		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-34	MET	-	initiating methionine	UNP P10363
S	-33	LYS	-	expression tag	UNP P10363
S	-32	ARG	-	expression tag	UNP P10363
S	-31	ARG	-	expression tag	UNP P10363
S	-30	TRP	-	expression tag	UNP P10363
S	-29	LYS	-	expression tag	UNP P10363
S	-28	LYS	-	expression tag	UNP P10363
S	-27	ASN	-	expression tag	UNP P10363
S	-26	PHE	-	expression tag	UNP P10363
S	-25	ILE	-	expression tag	UNP P10363
S	-24	ALA	-	expression tag	UNP P10363
S	-23	VAL	-	expression tag	UNP P10363
S	-22	SER	-	expression tag	UNP P10363
S	-21	ALA	-	expression tag	UNP P10363
S	-20	ALA	-	expression tag	UNP P10363
S	-19	ASN	-	expression tag	UNP P10363
S	-18	ARG	-	expression tag	UNP P10363
S	-17	PHE	-	expression tag	UNP P10363
S	-16	LYS	-	expression tag	UNP P10363
S	-15	LYS	-	expression tag	UNP P10363
S	-14	ILE	-	expression tag	UNP P10363
S	-13	SER	-	expression tag	UNP P10363
S	-12	SER	-	expression tag	UNP P10363
S	-11	SER	-	expression tag	UNP P10363
S	-10	GLY	-	expression tag	UNP P10363
S	-9	ALA	-	expression tag	UNP P10363
S	-8	LEU	-	expression tag	UNP P10363
S	-7	GLU	-	expression tag	UNP P10363
S	-6	ASN	-	expression tag	UNP P10363
S	-5	LEU	-	expression tag	UNP P10363
S	-4	TYR	-	expression tag	UNP P10363
S	-3	PHE	-	expression tag	UNP P10363
S	-2	GLN	-	expression tag	UNP P10363
S	-1	GLY	-	expression tag	UNP P10363
S	0	GLU	-	expression tag	UNP P10363

- Molecule 19 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	X	665	Total	C	H	N	O	S	0	0
			10978	3506	5563	911	979	19		

- Molecule 20 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Y	92	Total	C	H	N	O	S	0	0
			1575	496	806	139	131	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-1	GLY	-	expression tag	UNP Q04659
Y	0	GLU	-	expression tag	UNP Q04659

- Molecule 21 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H	437	Total	C	H	N	O	S	0	0
			6987	2255	3470	583	663	16		
21	L	437	Total	C	H	N	O	S	0	0
			6987	2255	3470	583	663	16		
21	K	437	Total	C	H	N	O	S	0	0
			6987	2255	3470	583	663	16		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-34	MET	-	initiating methionine	UNP Q01454
H	-33	LYS	-	expression tag	UNP Q01454
H	-32	ARG	-	expression tag	UNP Q01454
H	-31	ARG	-	expression tag	UNP Q01454
H	-30	TRP	-	expression tag	UNP Q01454
H	-29	LYS	-	expression tag	UNP Q01454
H	-28	LYS	-	expression tag	UNP Q01454
H	-27	ASN	-	expression tag	UNP Q01454
H	-26	PHE	-	expression tag	UNP Q01454
H	-25	ILE	-	expression tag	UNP Q01454
H	-24	ALA	-	expression tag	UNP Q01454
H	-23	VAL	-	expression tag	UNP Q01454
H	-22	SER	-	expression tag	UNP Q01454
H	-21	ALA	-	expression tag	UNP Q01454
H	-20	ALA	-	expression tag	UNP Q01454

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	ASN	-	expression tag	UNP Q01454
H	-18	ARG	-	expression tag	UNP Q01454
H	-17	PHE	-	expression tag	UNP Q01454
H	-16	LYS	-	expression tag	UNP Q01454
H	-15	LYS	-	expression tag	UNP Q01454
H	-14	ILE	-	expression tag	UNP Q01454
H	-13	SER	-	expression tag	UNP Q01454
H	-12	SER	-	expression tag	UNP Q01454
H	-11	SER	-	expression tag	UNP Q01454
H	-10	GLY	-	expression tag	UNP Q01454
H	-9	ALA	-	expression tag	UNP Q01454
H	-8	LEU	-	expression tag	UNP Q01454
H	-7	GLU	-	expression tag	UNP Q01454
H	-6	ASN	-	expression tag	UNP Q01454
H	-5	LEU	-	expression tag	UNP Q01454
H	-4	TYR	-	expression tag	UNP Q01454
H	-3	PHE	-	expression tag	UNP Q01454
H	-2	GLN	-	expression tag	UNP Q01454
H	-1	GLY	-	expression tag	UNP Q01454
H	0	GLU	-	expression tag	UNP Q01454
L	-34	MET	-	initiating methionine	UNP Q01454
L	-33	LYS	-	expression tag	UNP Q01454
L	-32	ARG	-	expression tag	UNP Q01454
L	-31	ARG	-	expression tag	UNP Q01454
L	-30	TRP	-	expression tag	UNP Q01454
L	-29	LYS	-	expression tag	UNP Q01454
L	-28	LYS	-	expression tag	UNP Q01454
L	-27	ASN	-	expression tag	UNP Q01454
L	-26	PHE	-	expression tag	UNP Q01454
L	-25	ILE	-	expression tag	UNP Q01454
L	-24	ALA	-	expression tag	UNP Q01454
L	-23	VAL	-	expression tag	UNP Q01454
L	-22	SER	-	expression tag	UNP Q01454
L	-21	ALA	-	expression tag	UNP Q01454
L	-20	ALA	-	expression tag	UNP Q01454
L	-19	ASN	-	expression tag	UNP Q01454
L	-18	ARG	-	expression tag	UNP Q01454
L	-17	PHE	-	expression tag	UNP Q01454
L	-16	LYS	-	expression tag	UNP Q01454
L	-15	LYS	-	expression tag	UNP Q01454
L	-14	ILE	-	expression tag	UNP Q01454
L	-13	SER	-	expression tag	UNP Q01454

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-12	SER	-	expression tag	UNP Q01454
L	-11	SER	-	expression tag	UNP Q01454
L	-10	GLY	-	expression tag	UNP Q01454
L	-9	ALA	-	expression tag	UNP Q01454
L	-8	LEU	-	expression tag	UNP Q01454
L	-7	GLU	-	expression tag	UNP Q01454
L	-6	ASN	-	expression tag	UNP Q01454
L	-5	LEU	-	expression tag	UNP Q01454
L	-4	TYR	-	expression tag	UNP Q01454
L	-3	PHE	-	expression tag	UNP Q01454
L	-2	GLN	-	expression tag	UNP Q01454
L	-1	GLY	-	expression tag	UNP Q01454
L	0	GLU	-	expression tag	UNP Q01454
K	-34	MET	-	initiating methionine	UNP Q01454
K	-33	LYS	-	expression tag	UNP Q01454
K	-32	ARG	-	expression tag	UNP Q01454
K	-31	ARG	-	expression tag	UNP Q01454
K	-30	TRP	-	expression tag	UNP Q01454
K	-29	LYS	-	expression tag	UNP Q01454
K	-28	LYS	-	expression tag	UNP Q01454
K	-27	ASN	-	expression tag	UNP Q01454
K	-26	PHE	-	expression tag	UNP Q01454
K	-25	ILE	-	expression tag	UNP Q01454
K	-24	ALA	-	expression tag	UNP Q01454
K	-23	VAL	-	expression tag	UNP Q01454
K	-22	SER	-	expression tag	UNP Q01454
K	-21	ALA	-	expression tag	UNP Q01454
K	-20	ALA	-	expression tag	UNP Q01454
K	-19	ASN	-	expression tag	UNP Q01454
K	-18	ARG	-	expression tag	UNP Q01454
K	-17	PHE	-	expression tag	UNP Q01454
K	-16	LYS	-	expression tag	UNP Q01454
K	-15	LYS	-	expression tag	UNP Q01454
K	-14	ILE	-	expression tag	UNP Q01454
K	-13	SER	-	expression tag	UNP Q01454
K	-12	SER	-	expression tag	UNP Q01454
K	-11	SER	-	expression tag	UNP Q01454
K	-10	GLY	-	expression tag	UNP Q01454
K	-9	ALA	-	expression tag	UNP Q01454
K	-8	LEU	-	expression tag	UNP Q01454
K	-7	GLU	-	expression tag	UNP Q01454
K	-6	ASN	-	expression tag	UNP Q01454

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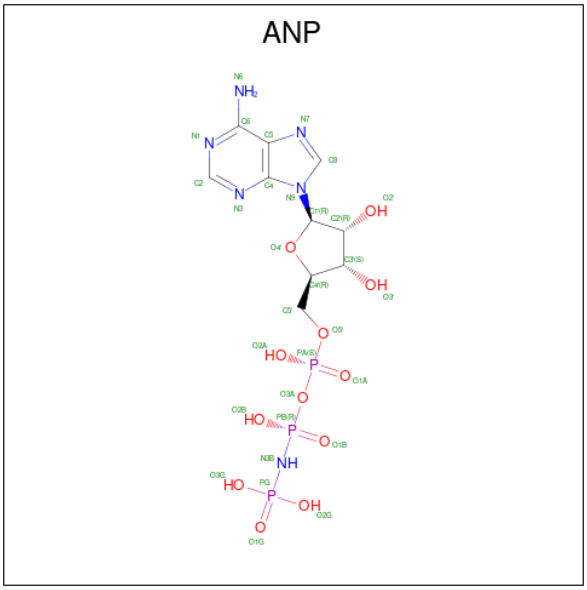
Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	LEU	-	expression tag	UNP Q01454
K	-4	TYR	-	expression tag	UNP Q01454
K	-3	PHE	-	expression tag	UNP Q01454
K	-2	GLN	-	expression tag	UNP Q01454
K	-1	GLY	-	expression tag	UNP Q01454
K	0	GLU	-	expression tag	UNP Q01454

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
22	2	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
22	3	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
22	4	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
22	7	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	2	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
23	4	1	Total Mg 1 1	0
23	5	1	Total Mg 1 1	0
23	7	1	Total Mg 1 1	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
24	4	1	Total Zn 1 1	0
24	5	1	Total Zn 1 1	0
24	6	1	Total Zn 1 1	0
24	7	1	Total Zn 1 1	0

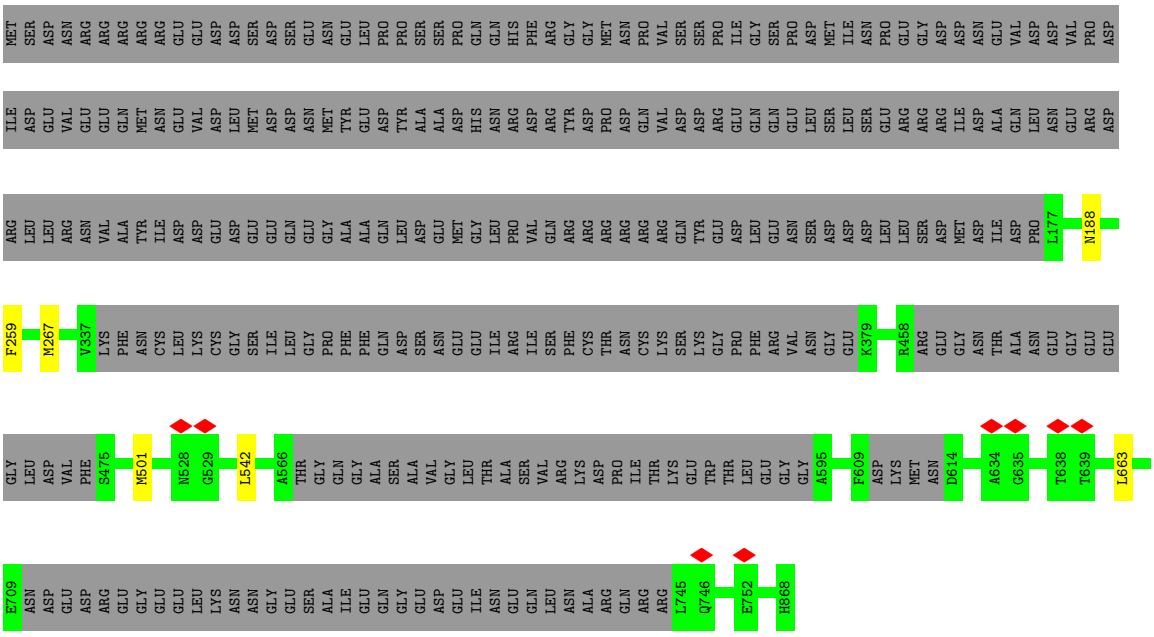
3 Residue-property plots (i)

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

• Molecule 1: DNA replication licensing factor MCM2

Chain 2:

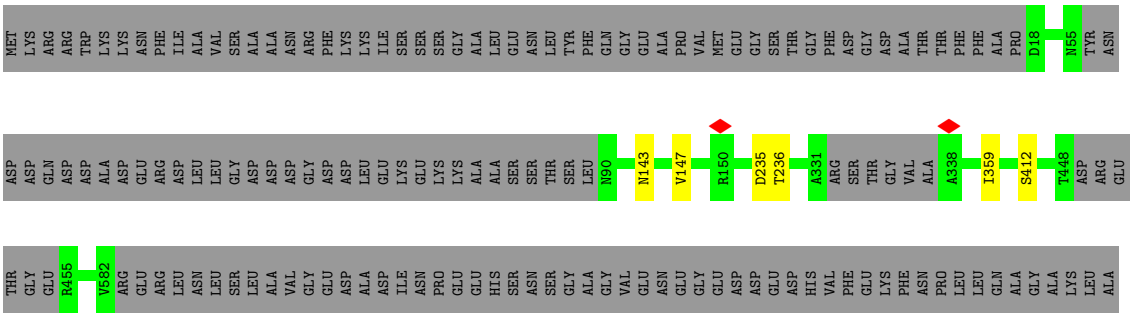


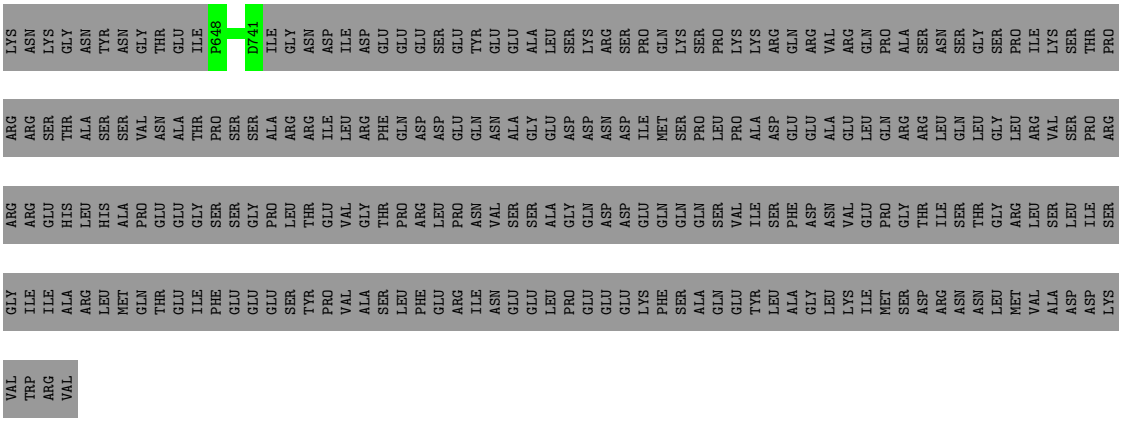


• Molecule 2: DNA replication licensing factor MCM3

Chain 3:







• Molecule 3: DNA replication licensing factor MCM4

Chain 4:

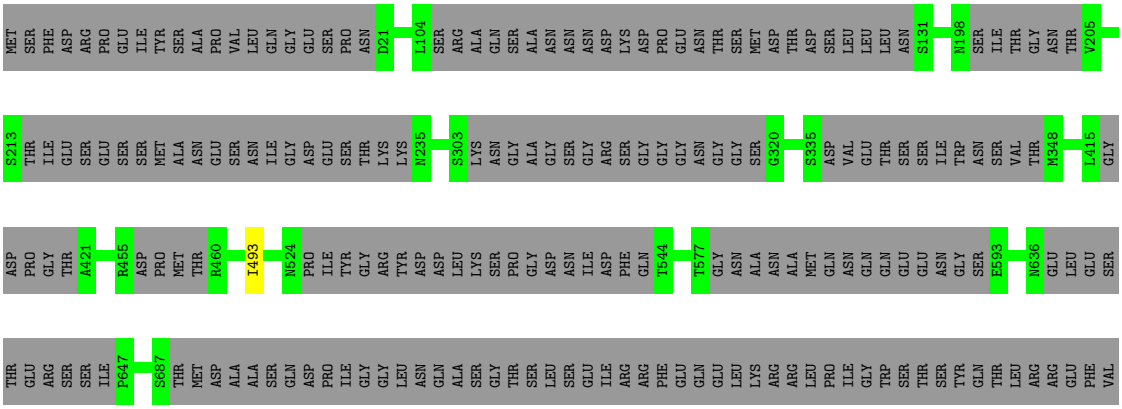




• Molecule 4: Minichromosome maintenance protein 5

Chain 5:



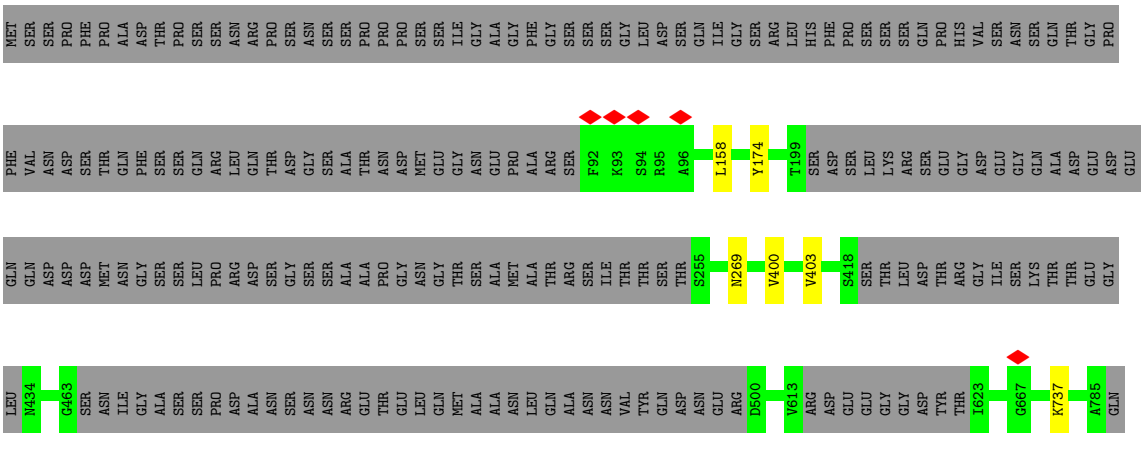




• Molecule 5: DNA replication licensing factor MCM6

Chain 6:

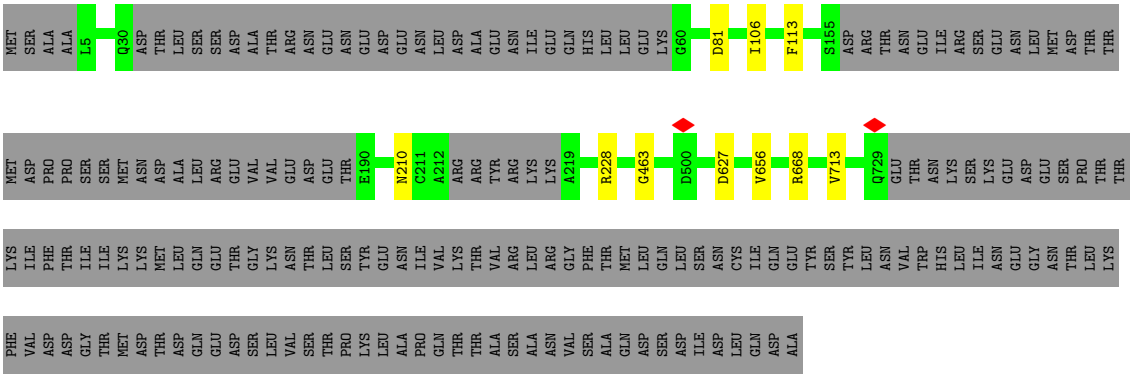




• Molecule 6: DNA replication licensing factor MCM7

Chain 7:

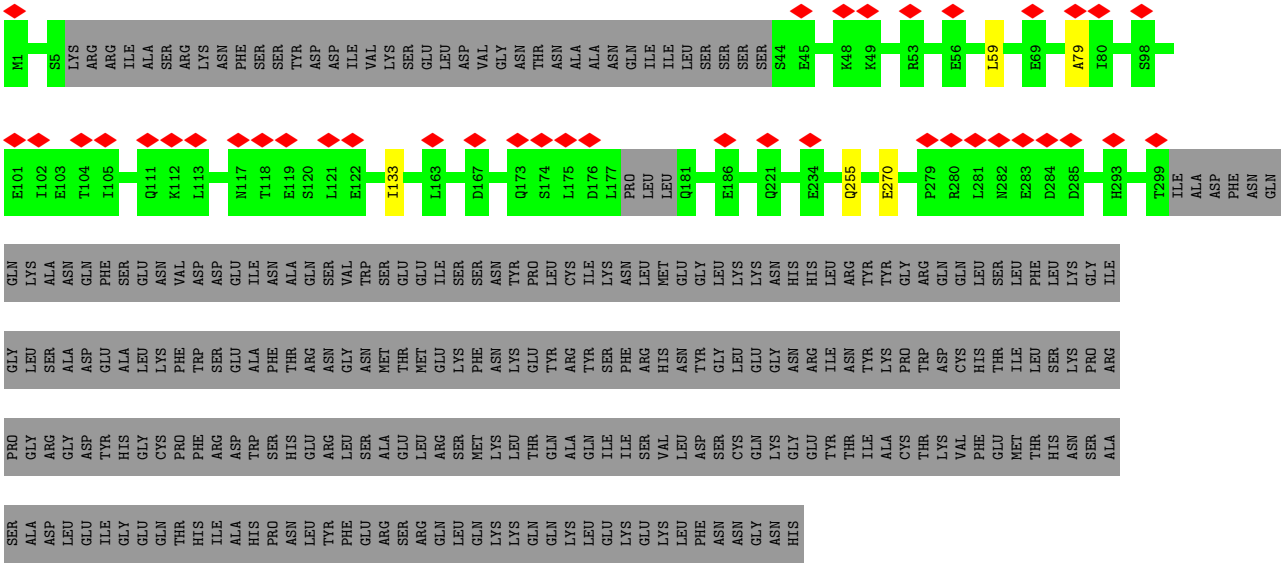




• Molecule 7: DNA primase large subunit

Chain A:

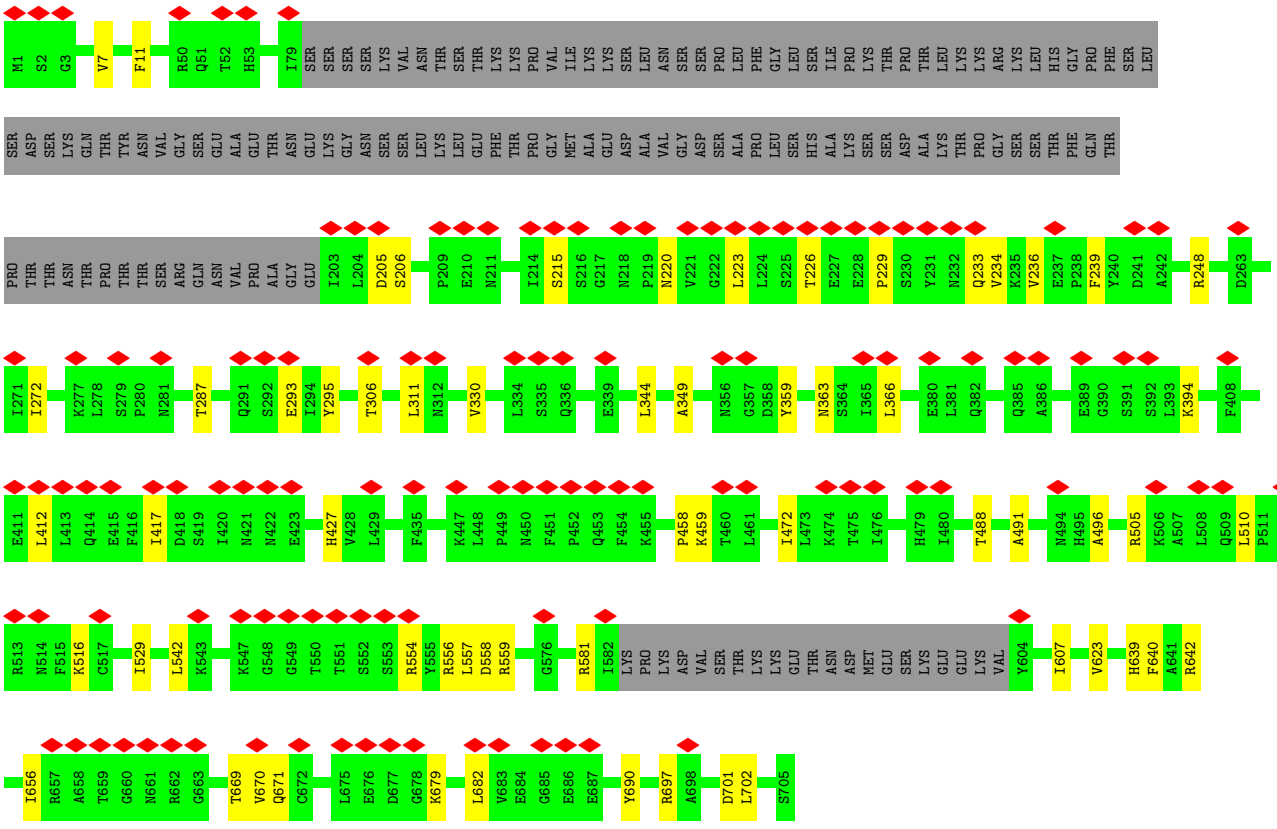




• Molecule 8: DNA polymerase alpha subunit B

Chain B:





• Molecule 9: DNA replication complex GINS protein PSF1

Chain C:

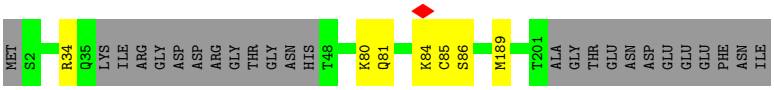




• Molecule 10: DNA replication complex GINS protein PSF2

Chain D:

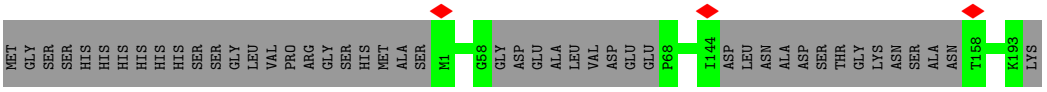




• Molecule 11: DNA replication complex GINS protein PSF3

Chain E:

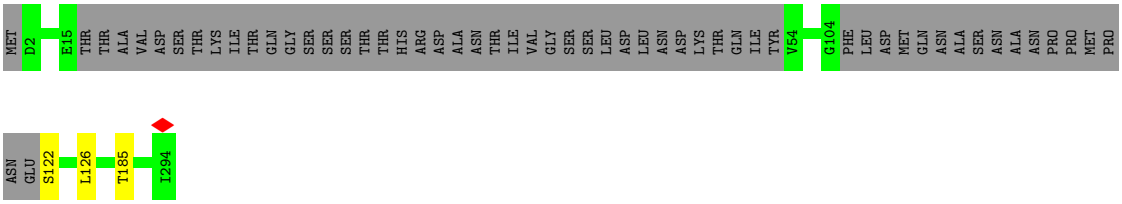




• Molecule 12: DNA replication complex GINS protein SLD5

Chain F:

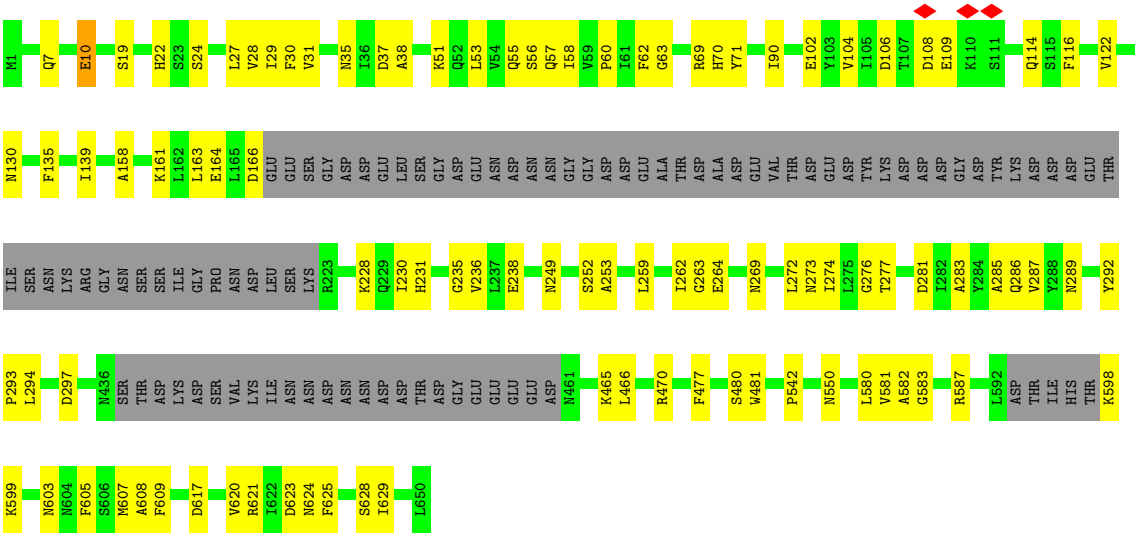




• Molecule 13: Cell division control protein 45

Chain G:

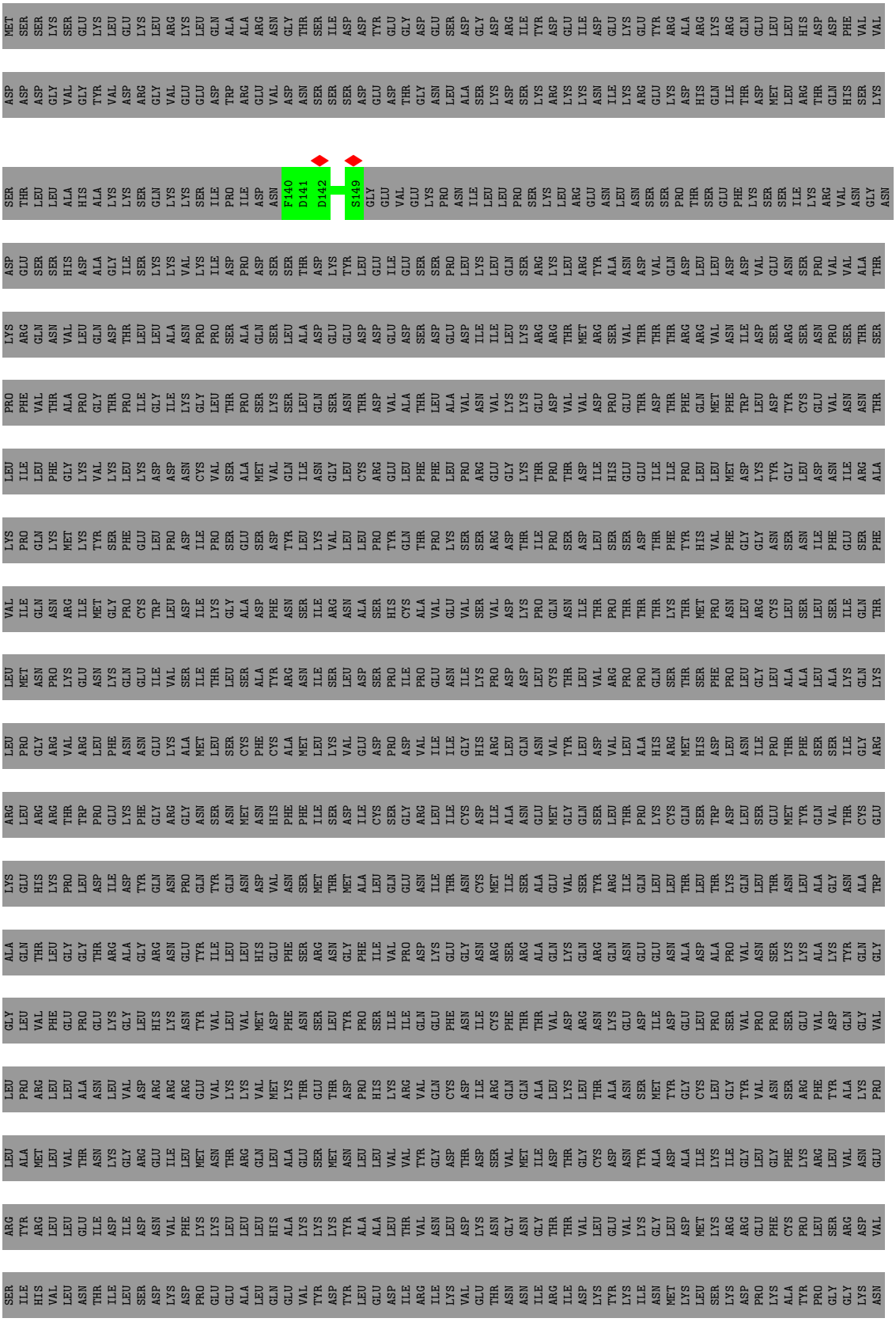


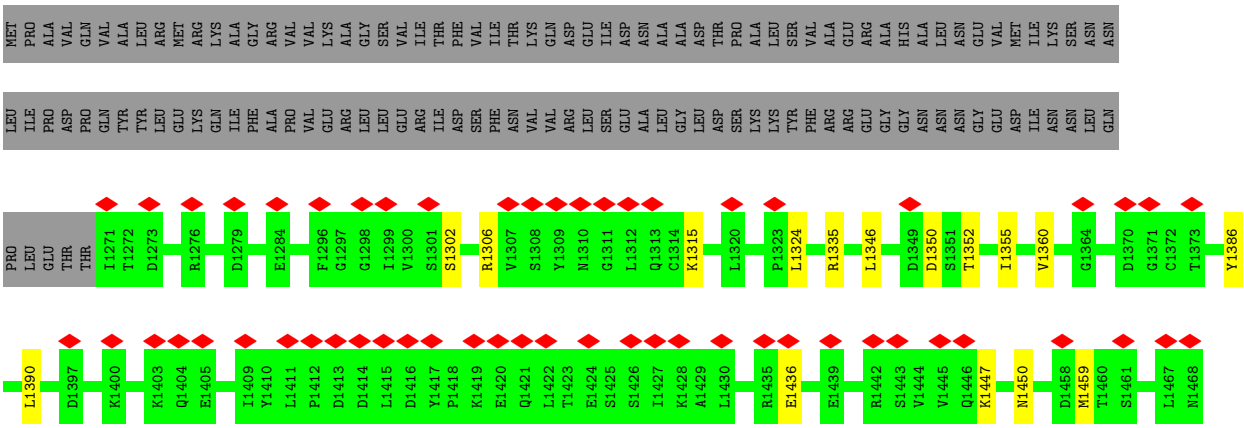


• Molecule 14: DNA polymerase alpha catalytic subunit A

Chain J:

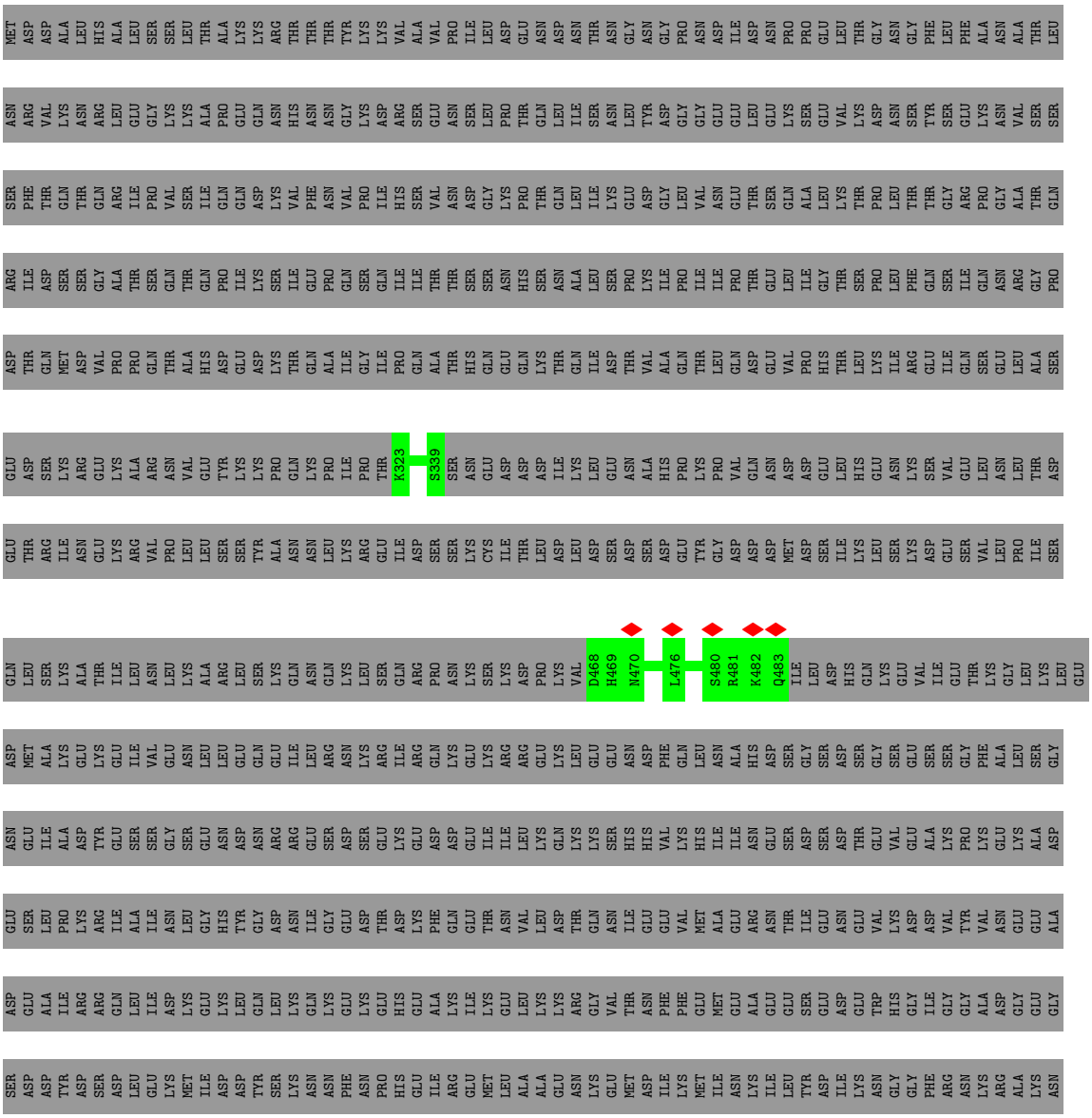

13%
86%

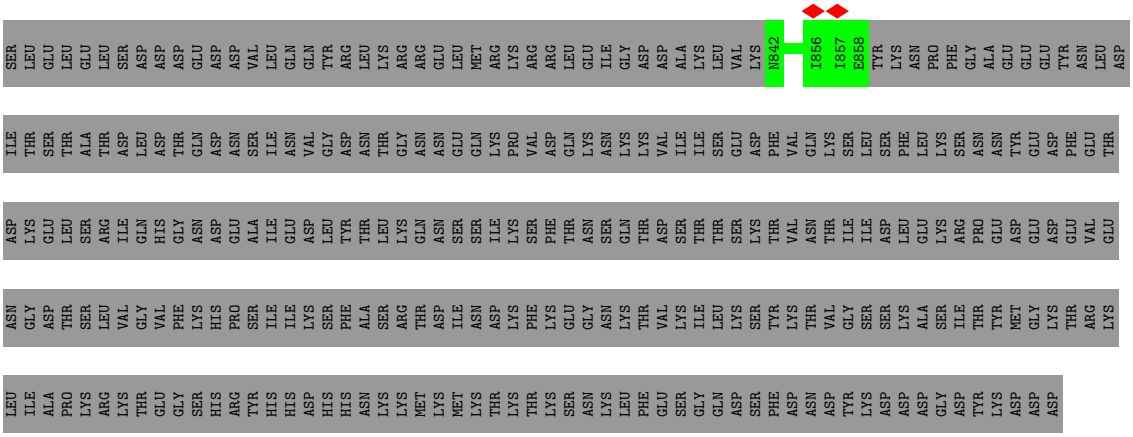

MET SER SER LYS SER GLU LYS LEU LYS LEU GLU LEU ARG LYS LEU GLN ALA ALA ARG ASN GLY THR SER ILE ASP ASP TYR GLU GLY ASP GLU SER ASP GLY ASP ARG ILE TYR ASP GLU ILE ASP GLU LYS GLU TYR ARG ALA ARG LYS GLN GLU LEU LEU HIS ASP ASP PHE VAL VAL
ASP ASP GLY VAL GLY TYR VAL ASP ARG GLY VAL GLU GLU ASP TRP ARG GLU VAL ASP ASN SER SER SER ASP GLU ASP THR GLY ASN LEU ALA SER LYS ASP SER LYS ARG LYS LYS ASN ILE LYS ARG GLU LYS ASP HIS GLN ILE THR ASP MET LEU ARG THR GLN HIS SER LYS
SER THR LEU LEU ALA HIS ALA LYS LYS SER GLN LYS LYS SER ILE PRO ILE ASP ASN F140 D141 D142 S149 GLY GLU VAL GLU LYS PRO ASN ILE LEU LEU LEU PRO SER LYS LEU ARG GLU ASN LEU ASN SER SER PRO THR SER GLU PHE LYS SER SER ILE LYS ARG VAL ASN GLY ASN
ASP GLU SER SER HIS ASP ALA GLY ILE SER LYS LYS VAL LYS ILE ASP PRO ASP SER SER THR ASP LYS TYR LEU GLU ILE GLU SER SER PRO LEU GLU SER ARG TYR ALA ASN ASP VAL GLN ASP LEU LEU ASP ASP VAL GLU ASN SER PRO VAL VAL ALA THR
LYS ARG GLN ASN VAL LEU GLN ASP THR LEU LEU ALA ASN PRO PRO SER ALA GLN SER LEU ALA ASP GLU GLU ASP ASP GLU ASP GLU ASP SER ASP GLU ASP ILE ILE LEU LYS ARG ARG THR MET ARG SER VAL THR THR THR ARG ARG VAL ASN ILE ASP SER ARG SER ASN PRO SER THR SER
PRO PHE VAL THR ALA PRO GLY THR PRO ILE GLY ILE LYS GLY LEU THR PRO SER LYS SER LEU GLN SER ASN THR ASP VAL ALA THR LEU ALA VAL ASN VAL LYS LYS GLU ASP VAL VAL ASP PRO GLU THR ASP THR PHE GLN MET PHE TRP LEU ASP TYR CYS GLU VAL ASN ASN THR
LEU ILE LEU PHE GLY LYS VAL LYS LEU LYS ASP ASP ASN CYS VAL SER ALA MET VAL GLN ILE ASN GLY GLY LEU CYS ARG GLU LEU PHE PHE LEU PRO ARG GLU GLY LYS THR PRO THR ASP ILE HIS GLU GLU ILE ILE PRO LEU LEU MET ASP LYS TYR GLY LEU ASP ASN ILE ARG ALA
LYS PRO GLN LYS MET LYS TYR SER PHE GLU LEU PRO ASP ILE PRO SER GLU GLU SER ASP TYR LEU LYS VAL LEU LEU PRO TYR GLN THR PRO LYS SER SER ARG ASP THR ILE PRO SER ASP LEU SER SER ASP THR PHE TYR HIS VAL PHE GLY GLY ASN SER ASN ILE PHE GLU SER PHE
VAL ILE GLN ASN ARG ILE MET GLY PRO CYS TRP LEU ASP ILE LYS GLY ALA ASP PHE ASN SER ILE ARG ASN ALA SER HIS CYS ALA VAL GLU VAL SER VAL ASP LYS PRO GLN ASN ILE THR PRO THR THR THR LYS THR MET PRO ASN LEU ARG CYS LEU SER LEU SER ILE GLN THR
LEU MET ASN PRO LYS GLU ASN LYS GLN GLU ILE VAL SER ILE THR LEU SER SER ALA TYR ARG ASN ILE SER LEU ASP SER PRO ILE PRO PRO GLU ASN ILE LYS PRO ASP ASP LEU CYS THR LEU VAL VAL ARG PRO PRO GLN SER THR SER PHE PRO LEU GLY LEU ALA ALA LEU SER ILE LYS GLN LYS
LEU PRO GLY ARG VAL ARG LEU PHE ASN ASN GLU LYS ALA MET LEU SER CYS PHE CYS ALA MET LEU LYS VAL GLU ASP PRO ASP VAL ILE ILE GLY HIS ARG LEU GLN ASN VAL TYR LEU ASP VAL LEU ALA HIS ARG MET HIS ASP LEU ASN LEU ARG ILE LEU SER GLY GLY ARG
ARG LEU ARG ARG THR TRP PRO GLU LYS PHE GLY ARG GLY ASN SER ASN MET ASN HIS PHE PHE ILE SER ASP ILE CYS SER GLY ARG LEU ILE CYS ASP ILE ALA ASN GLU MET GLY GLN SER LEU THR PRO LYS CYS GLN SER TRP ASP LEU SER GLU MET TYR GLN VAL THR CYS GLU
LYS GLU HIS LYS PRO LEU ASP ILE ASP TYR GLN GLN ASN PRO GLN TYR GLN ASN ASP VAL ASN SER MET THR MET ALA LEU GLN LEU GLU ASN ILE THR ASN CYS MET ILE SER ALA GLU VAL SER TYR ARG ILE GLN LEU LEU THR LEU THR LYS GLN LEU THR ASN LEU ALA GLY ASN ALA TRP
ALA GLN THR LEU GLY GLY THR ARG ARG GLY ASN GLU TYR ILE LEU LEU HIS GLU PHE SER ARG ASN GLY PHE ILE VAL PRO ASP LYS GLU GLY ASN ARG SER ARG ALA GLN LYS GLN ARG ASN GLU GLU GLU ASN ALA ASP ALA PRO VAL ASN SER LYS LYS ARG GLN GLY
GLY LEU VAL PHE GLU PRO GLU LYS GLY LEU HIS LYS ASN TYR VAL LEU VAL MET ASP PHE ASN SER LEU TYR PRO SER ILE ILE GLN GLU PHE ASN ILE CYS PHE THR THR VAL ASP ARG ASN LYS GLU ASP ILE ASP GLU LEU PRO SER VAL PRO PRO SER GLU VAL ASP GLN GLY VAL
LEU PRO ARG LEU LEU ALA ASN LEU VAL ASP ARG ARG GLU VAL LYS LYS VAL MET LYS THR GLU THR ASP PRO HIS LYS ARG VAL GLN CYS ASP ILE ARG GLN GLN ALA LEU LYS LEU THR ALA ASN SER MET TYR GLY CYS LEU GLY TYR VAL ASN SER ARG PHE TYR ALA LYS PRO
LEU ALA MET LEU VAL THR ASN LYS GLY ARG GLU ILE LEU MET ASN THR ARG GLN LEU ALA GLU SER MET ASN LEU LEU VAL VAL TYR GLY ASP THR ASP TYR ASN SER ASP ALA ILE LYS ILE LEU GLY ARG LEU VAL ASN GLU
ARG TYR ARG LEU LEU GLU ILE ASP ILE ASP ASN VAL PHE LYS LYS LEU LEU LEU HIS ALA LYS LYS LYS TYR ALA ALA LEU THR VAL ASN LEU ASP LYS ASN GLY ASN GLY THR THR VAL LEU GLU VAL LYS GLY LEU ASP MET LYS ARG ARG GLU PHE CYS PRO LEU SER ARG ASP VAL
SER ILE HIS VAL LEU ASN THR ILE LEU GLU ALA LEU GLU ASP PRO GLU ILE ARG ILE LYS VAL GLU THR ASN ASN ILE ARG ILE ASP LYS TYR LYS ILE ASN MET LYS LEU SER LYS ASP PRO LYS ALA TYR PRO GLY GLY LYS ASN



• Molecule 15: Mediator of replication checkpoint protein 1

Chain P: 5% 95%

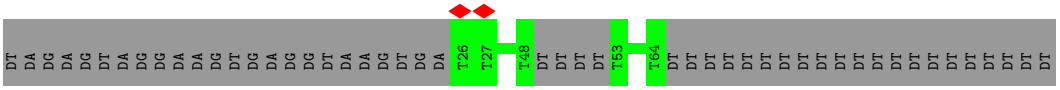




• Molecule 16: Leading strand DNA

Chain Q:

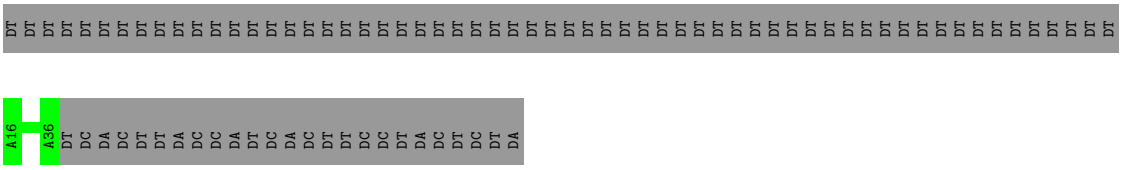




• Molecule 17: Lagging strand

Chain R:

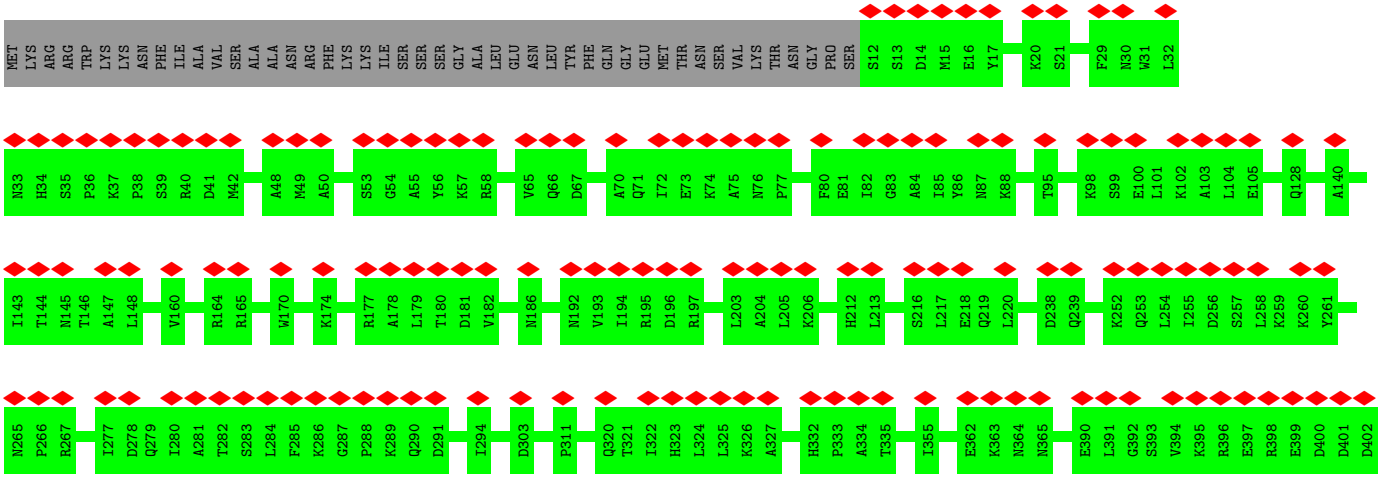


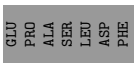


• Molecule 18: DNA primase small subunit

Chain S:



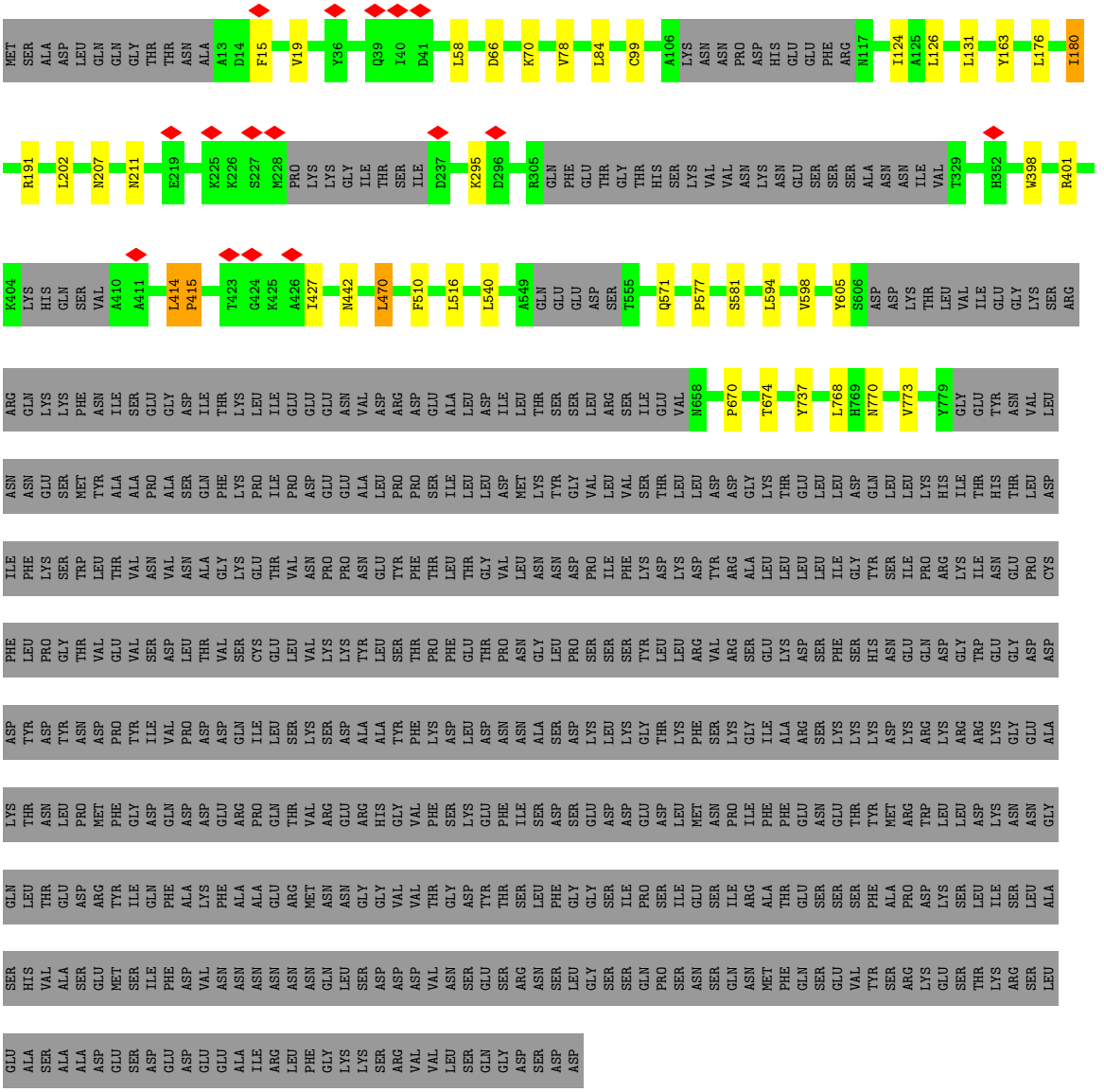




• Molecule 19: Topoisomerase 1-associated factor 1

Chain X:

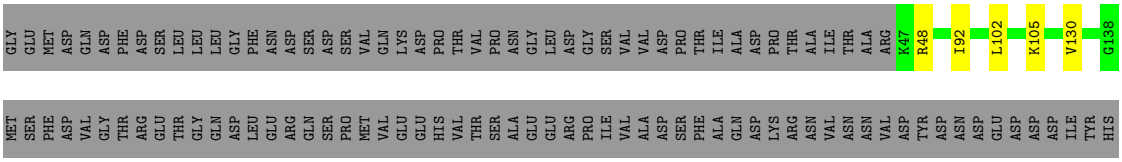


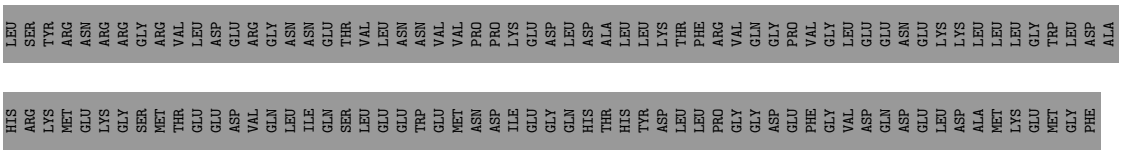


• Molecule 20: Chromosome segregation in meiosis protein 3

Chain Y:



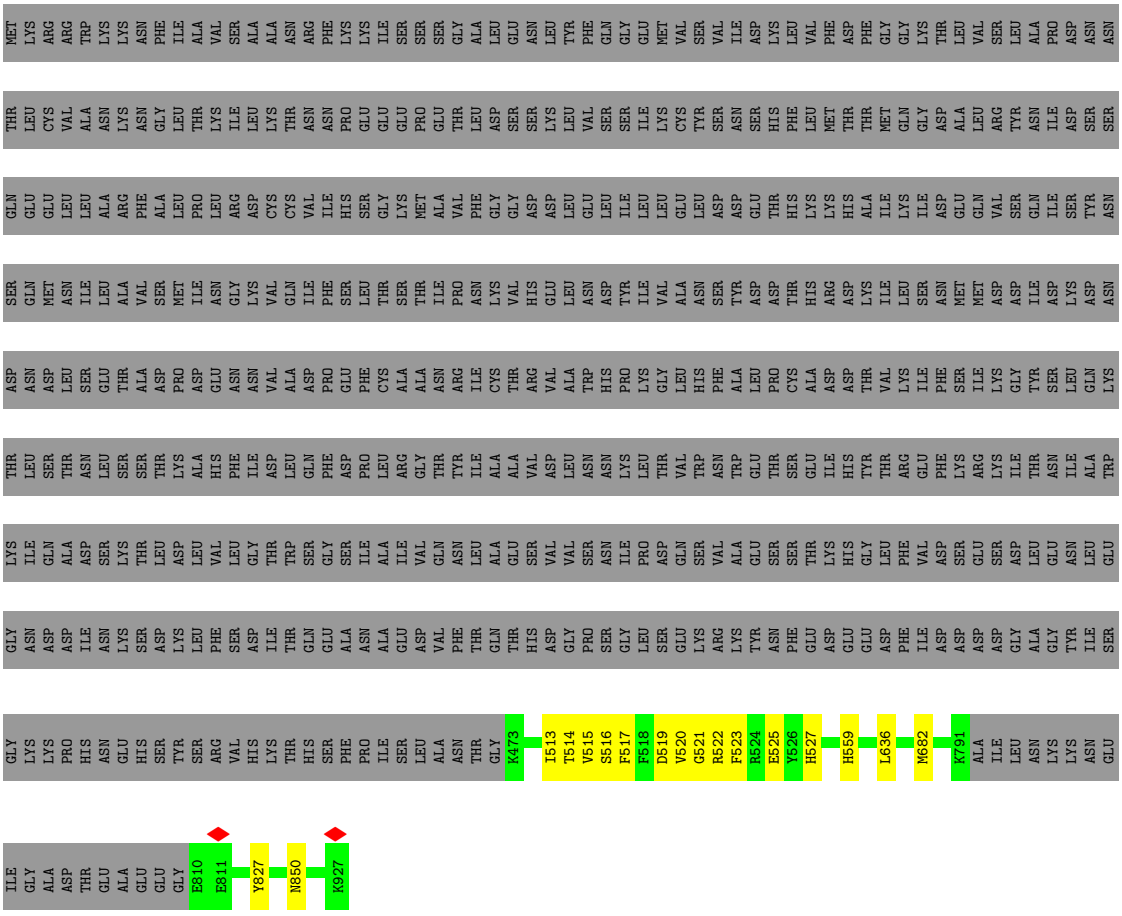




• Molecule 21: DNA polymerase alpha-binding protein

Chain H:

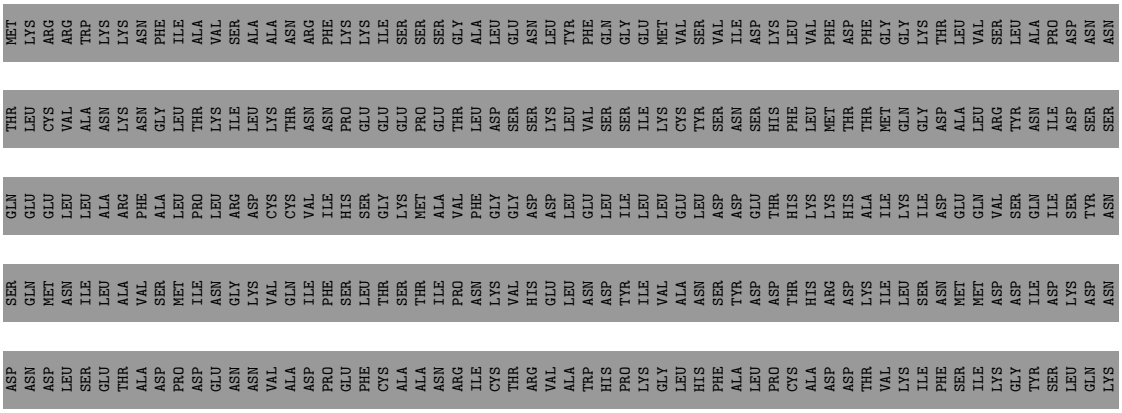


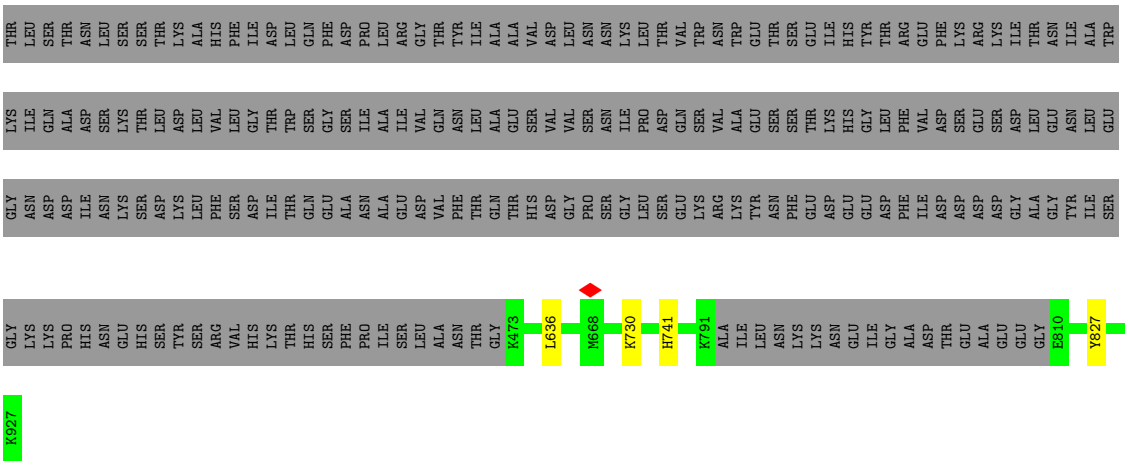


• Molecule 21: DNA polymerase alpha-binding protein

Chain L:



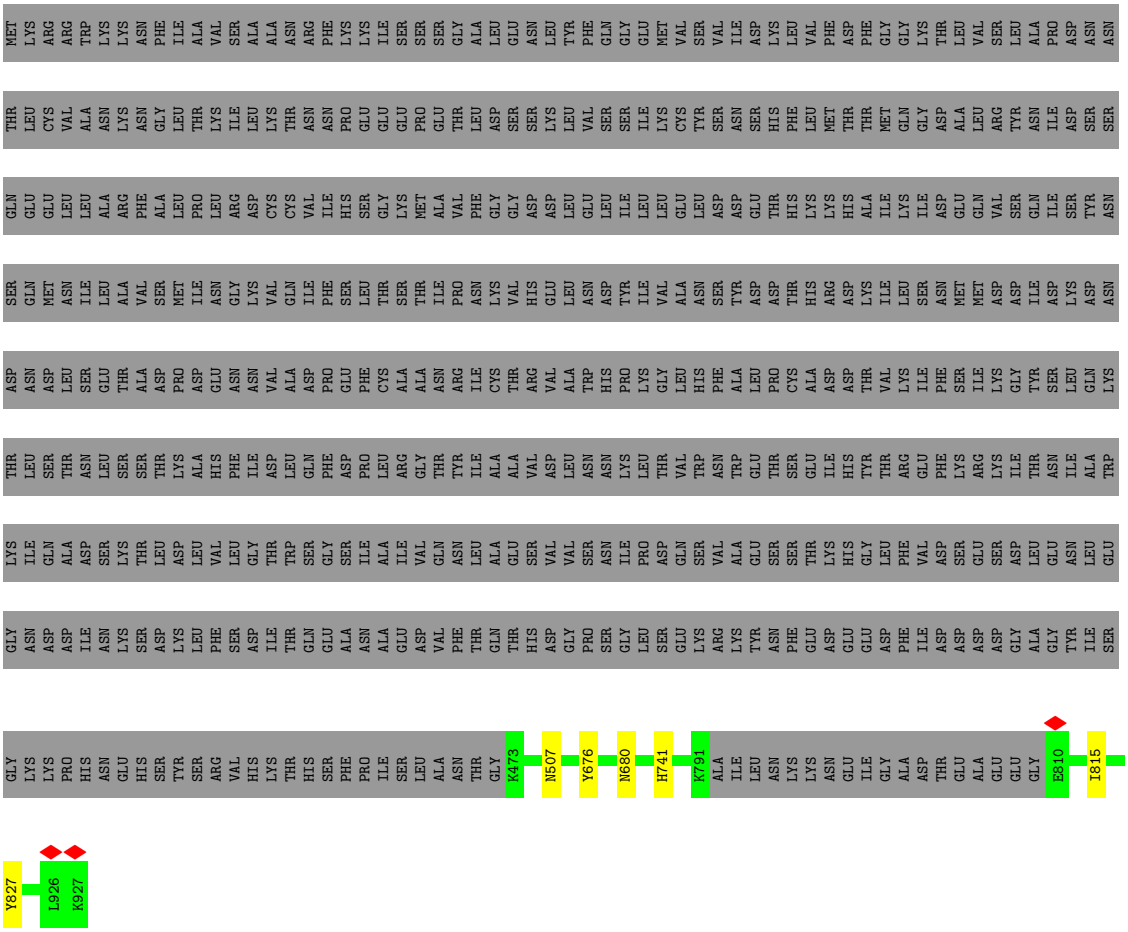




• Molecule 21: DNA polymerase alpha-binding protein

Chain K:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54970	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 ($e^-/Å^2$)	39.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.684	Depositor
Minimum map value	-3.501	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.360	Depositor
Recommended contour level	1.43	Depositor
Map size (Å)	498.8, 498.8, 498.8	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2672727, 2.2672727, 2.2672727	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.41	0/4608	0.66	0/6221
2	3	0.42	0/4877	0.67	0/6616
3	4	0.44	0/5066	0.66	0/6850
4	5	0.45	0/4265	0.66	0/5750
5	6	0.43	0/5008	0.66	0/6755
6	7	0.45	0/5235	0.67	0/7077
7	A	0.27	0/2228	0.54	0/2993
8	B	0.27	0/4579	0.48	0/6211
9	C	0.64	0/1619	0.97	21/2178 (1.0%)
10	D	0.50	0/1603	0.73	6/2170 (0.3%)
11	E	0.39	0/1412	0.57	0/1910
12	F	0.46	0/1995	0.66	4/2694 (0.1%)
13	G	1.36	26/4672 (0.6%)	1.66	157/6320 (2.5%)
14	J	0.28	0/1730	0.51	0/2330
15	P	0.29	0/413	0.59	0/547
16	Q	0.37	0/804	0.71	0/1240
17	R	0.38	0/467	0.64	0/715
18	S	0.24	0/3304	0.52	0/4462
19	X	0.44	1/5519 (0.0%)	0.82	5/7441 (0.1%)
20	Y	0.36	0/785	0.74	0/1050
21	H	0.64	8/3603 (0.2%)	0.82	23/4874 (0.5%)
21	K	0.31	0/3603	0.57	0/4874
21	L	0.30	0/3603	0.58	0/4874
All	All	0.53	35/70998 (0.0%)	0.77	216/96152 (0.2%)

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
5	6	0	1
6	7	0	5
13	G	0	1
19	X	0	2
20	Y	0	1
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	470	LEU	CG-CD1	-9.30	1.21	1.52
21	H	559	HIS	CE1-NE2	-8.83	1.23	1.32
21	H	527	HIS	CE1-NE2	-8.74	1.23	1.32
13	G	70	HIS	CE1-NE2	-8.59	1.24	1.32
13	G	22	HIS	ND1-CE1	-8.23	1.24	1.32

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	30	PHE	CA-CB-CG	8.96	122.75	113.80
9	C	189	PHE	CA-CB-CG	7.89	121.69	113.80
19	X	295	LYS	CA-C-N	7.81	133.84	122.36
19	X	295	LYS	C-N-CA	7.81	133.84	122.36
13	G	609	PHE	CA-CB-CG	7.81	121.61	113.80

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	6	737	LYS	Mainchain
6	7	210	ASN	Mainchain
6	7	228	ARG	Sidechain
6	7	627	ASP	Mainchain
6	7	81	ASP	Mainchain

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	4534	4606	4599	3	0
2	3	4792	4861	4857	4	0
3	4	4990	5065	5057	2	0
4	5	4213	4347	4335	0	0
5	6	4928	4980	4970	1	0
6	7	5154	5233	5224	3	0
7	A	2185	2197	2194	1	0
8	B	4480	4464	4461	37	0
9	C	1599	1603	1601	1	0
10	D	1571	1620	1618	2	0
11	E	1379	1396	1397	0	0
12	F	1960	1968	1965	1	0
13	G	4587	4598	4594	4	0
14	J	1697	1645	1643	12	0
15	P	408	397	394	0	0
16	Q	722	406	408	0	0
17	R	419	237	238	0	0
18	S	3227	3201	3199	0	0
19	X	5415	5563	5556	17	0
20	Y	769	806	805	2	0
21	H	3517	3470	3468	2	0
21	K	3517	3470	3468	1	0
21	L	3517	3470	3468	0	0
22	2	31	13	13	0	0
22	3	31	13	13	2	0
22	4	31	13	13	2	0
22	7	31	13	13	1	0
23	2	1	0	0	0	0
23	4	1	0	0	0	0
23	5	1	0	0	0	0
23	7	1	0	0	0	0
24	4	1	0	0	0	0
24	5	1	0	0	0	0
24	6	1	0	0	0	0
24	7	1	0	0	0	0
All	All	69712	69655	69571	82	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 1.

The worst 5 of 82 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)
19:X:414:LEU:HD11	19:X:470:LEU:CD1	2.05	0.86
8:B:488:THR:O	14:J:1335:ARG:NH1	2.13	0.80
8:B:417:ILE:HD12	8:B:472:ILE:HG22	1.69	0.74
8:B:459:LYS:NZ	14:J:1436:GLU:OE2	2.22	0.72
8:B:236:VAL:O	8:B:516:LYS:NZ	2.23	0.71

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	556/868 (64%)	547 (98%)	9 (2%)	0	100	100
2	3	603/1009 (60%)	588 (98%)	15 (2%)	0	100	100
3	4	620/933 (66%)	603 (97%)	17 (3%)	0	100	100
4	5	511/775 (66%)	497 (97%)	14 (3%)	0	100	100
5	6	611/1017 (60%)	602 (98%)	9 (2%)	0	100	100
6	7	648/845 (77%)	633 (98%)	15 (2%)	0	100	100
7	A	252/528 (48%)	248 (98%)	3 (1%)	1 (0%)	30	62
8	B	555/705 (79%)	541 (98%)	14 (2%)	0	100	100
9	C	191/208 (92%)	190 (100%)	1 (0%)	0	100	100
10	D	184/213 (86%)	183 (100%)	1 (0%)	0	100	100
11	E	165/217 (76%)	162 (98%)	3 (2%)	0	100	100
12	F	232/294 (79%)	228 (98%)	4 (2%)	0	100	100
13	G	557/657 (85%)	541 (97%)	16 (3%)	0	100	100
14	J	204/1468 (14%)	201 (98%)	3 (2%)	0	100	100
15	P	44/1109 (4%)	42 (96%)	2 (4%)	0	100	100
18	S	389/444 (88%)	382 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	X	651/1238 (53%)	635 (98%)	16 (2%)	0	100	100
20	Y	90/319 (28%)	88 (98%)	2 (2%)	0	100	100
21	H	433/962 (45%)	418 (96%)	15 (4%)	0	100	100
21	K	433/962 (45%)	420 (97%)	13 (3%)	0	100	100
21	L	433/962 (45%)	426 (98%)	7 (2%)	0	100	100
All	All	8362/15733 (53%)	8175 (98%)	186 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	255	GLN

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	503/770 (65%)	501 (100%)	2 (0%)	84	81
2	3	530/866 (61%)	529 (100%)	1 (0%)	87	85
3	4	568/848 (67%)	568 (100%)	0	100	100
4	5	482/688 (70%)	481 (100%)	1 (0%)	87	85
5	6	545/886 (62%)	542 (99%)	3 (1%)	78	79
6	7	578/753 (77%)	578 (100%)	0	100	100
7	A	246/488 (50%)	244 (99%)	2 (1%)	73	77
8	B	508/637 (80%)	506 (100%)	2 (0%)	84	81
9	C	181/193 (94%)	181 (100%)	0	100	100
10	D	178/198 (90%)	177 (99%)	1 (1%)	78	79
11	E	155/192 (81%)	155 (100%)	0	100	100
12	F	229/279 (82%)	229 (100%)	0	100	100
13	G	510/592 (86%)	508 (100%)	2 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	J	194/1334 (14%)	193 (100%)	1 (0%)	81 80
15	P	47/1015 (5%)	47 (100%)	0	100 100
18	S	357/402 (89%)	357 (100%)	0	100 100
19	X	607/1125 (54%)	592 (98%)	15 (2%)	42 63
20	Y	85/286 (30%)	82 (96%)	3 (4%)	32 57
21	H	389/854 (46%)	387 (100%)	2 (0%)	81 80
21	K	389/854 (46%)	385 (99%)	4 (1%)	68 75
21	L	389/854 (46%)	385 (99%)	4 (1%)	68 75
All	All	7670/14114 (54%)	7627 (99%)	43 (1%)	76 79

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	X	605	TYR
21	L	636	LEU
19	X	737	TYR
20	Y	102	LEU
21	L	741	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
13	G	18	ASN
14	J	1316	HIS
13	G	52	GLN
13	G	141	GLN
18	S	219	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, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	ANP	3	1500	23	33,33,33	1.13	4 (12%)	45,52,52	0.86	1 (2%)
22	ANP	7	901	23	33,33,33	1.02	4 (12%)	45,52,52	0.66	1 (2%)
22	ANP	2	1500	23	33,33,33	0.96	4 (12%)	45,52,52	0.69	1 (2%)
22	ANP	4	1001	23	33,33,33	0.95	3 (9%)	45,52,52	0.56	0

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
22	ANP	3	1500	23	-	5/18/38/38	0/3/3/3
22	ANP	7	901	23	-	3/18/38/38	0/3/3/3
22	ANP	2	1500	23	-	7/18/38/38	0/3/3/3
22	ANP	4	1001	23	-	3/18/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	1500	ANP	PB-O3A	-3.96	1.54	1.59
22	3	1500	ANP	PA-O3A	-3.57	1.55	1.59
22	7	901	ANP	PB-O3A	-3.56	1.54	1.59
22	4	1001	ANP	PB-O3A	-3.49	1.54	1.59
22	7	901	ANP	PA-O3A	-2.84	1.56	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	1500	ANP	O3A-PB-N3B	-3.25	97.57	106.59
22	2	1500	ANP	O1G-PG-N3B	-2.23	108.49	111.77
22	7	901	ANP	O3A-PB-N3B	-2.19	100.51	106.59

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2	1500	ANP	PB-N3B-PG-O1G
22	2	1500	ANP	PG-N3B-PB-O1B
22	2	1500	ANP	O4'-C1'-N9-C8
22	2	1500	ANP	O4'-C1'-N9-C4
22	3	1500	ANP	PB-N3B-PG-O1G

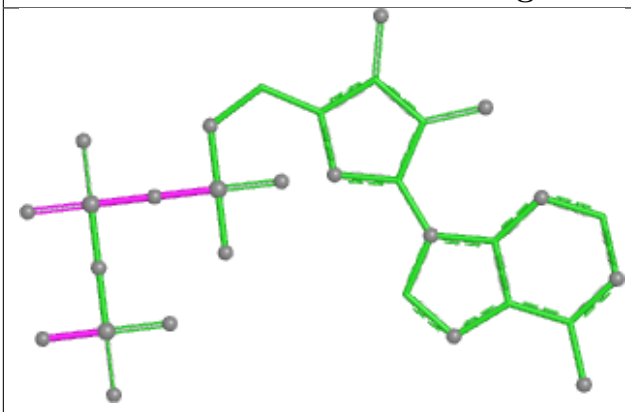
There are no ring outliers.

3 monomers are involved in 5 short contacts:

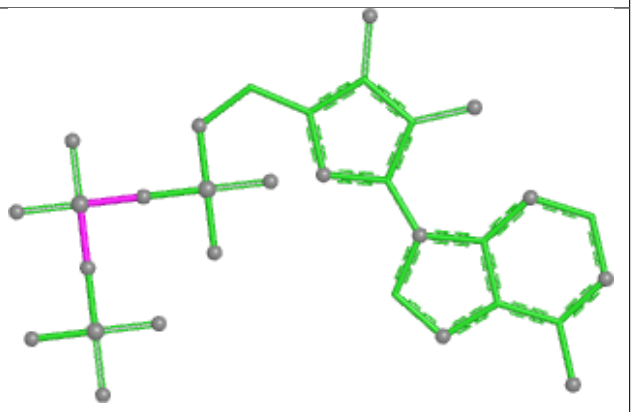
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	1500	ANP	2	0
22	7	901	ANP	1	0
22	4	1001	ANP	2	0

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

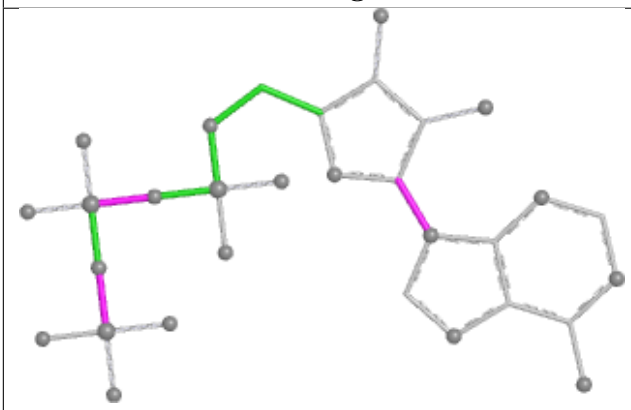
Ligand ANP 3 1500



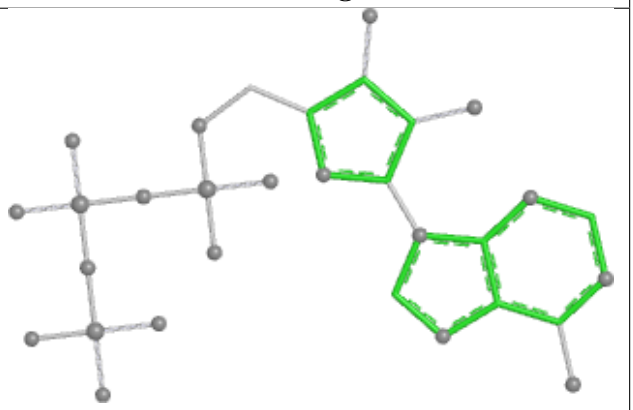
Bond lengths



Bond angles

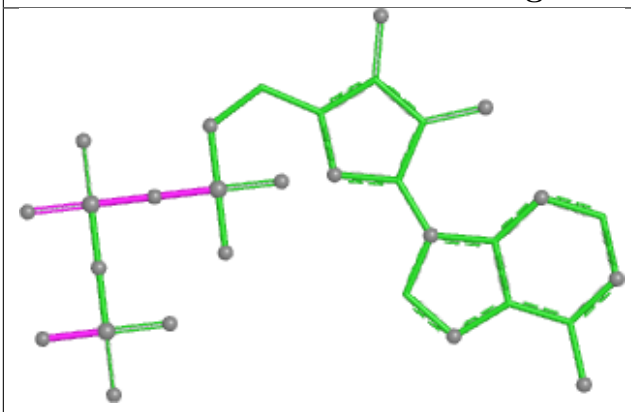


Torsions

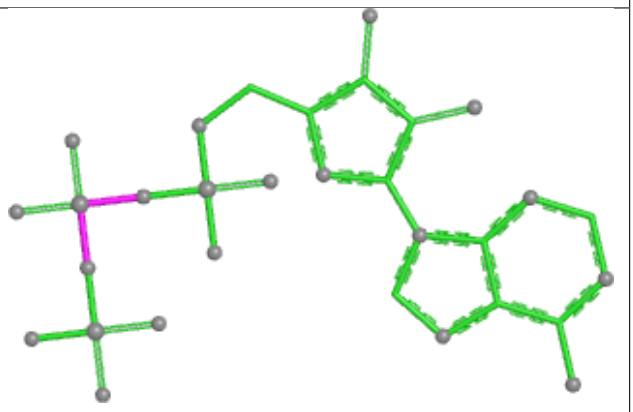


Rings

Ligand ANP 7 901



Bond lengths



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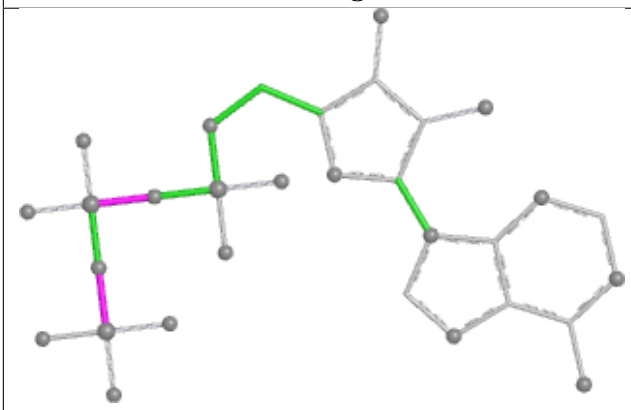
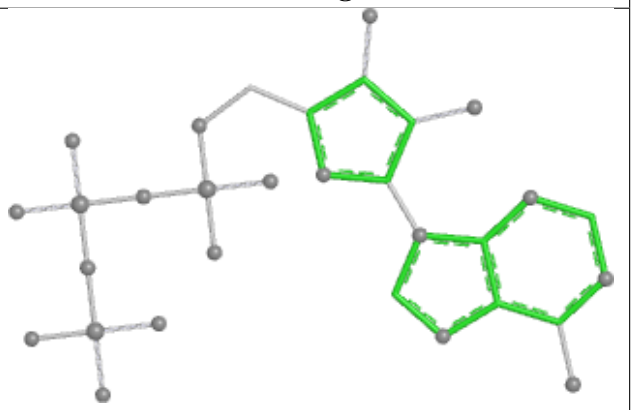
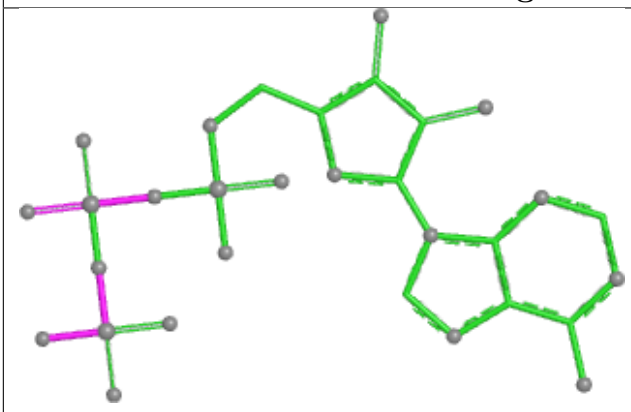


Torsions

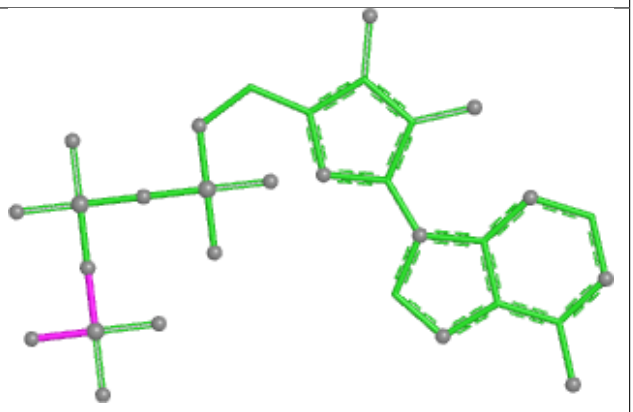


Rings

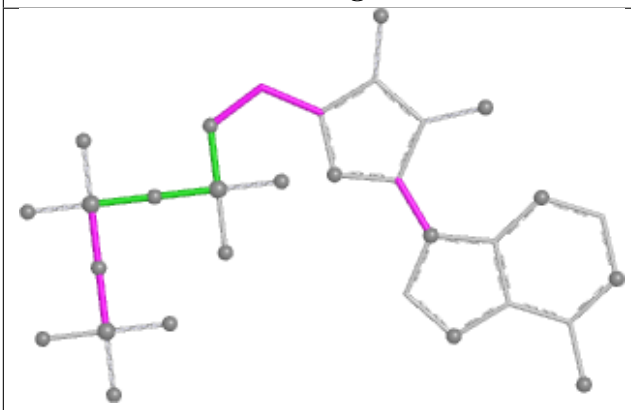
Ligand ANP 2 1500



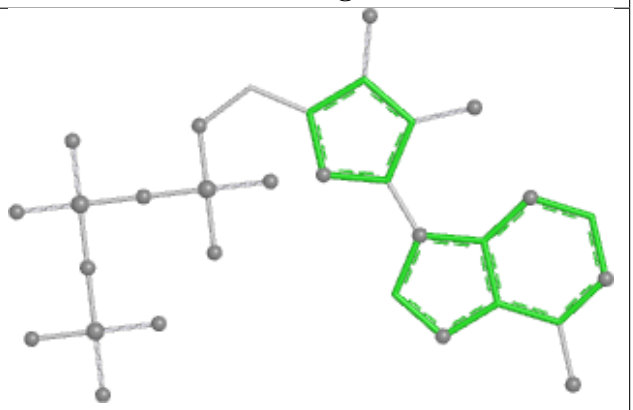
Bond lengths



Bond angles

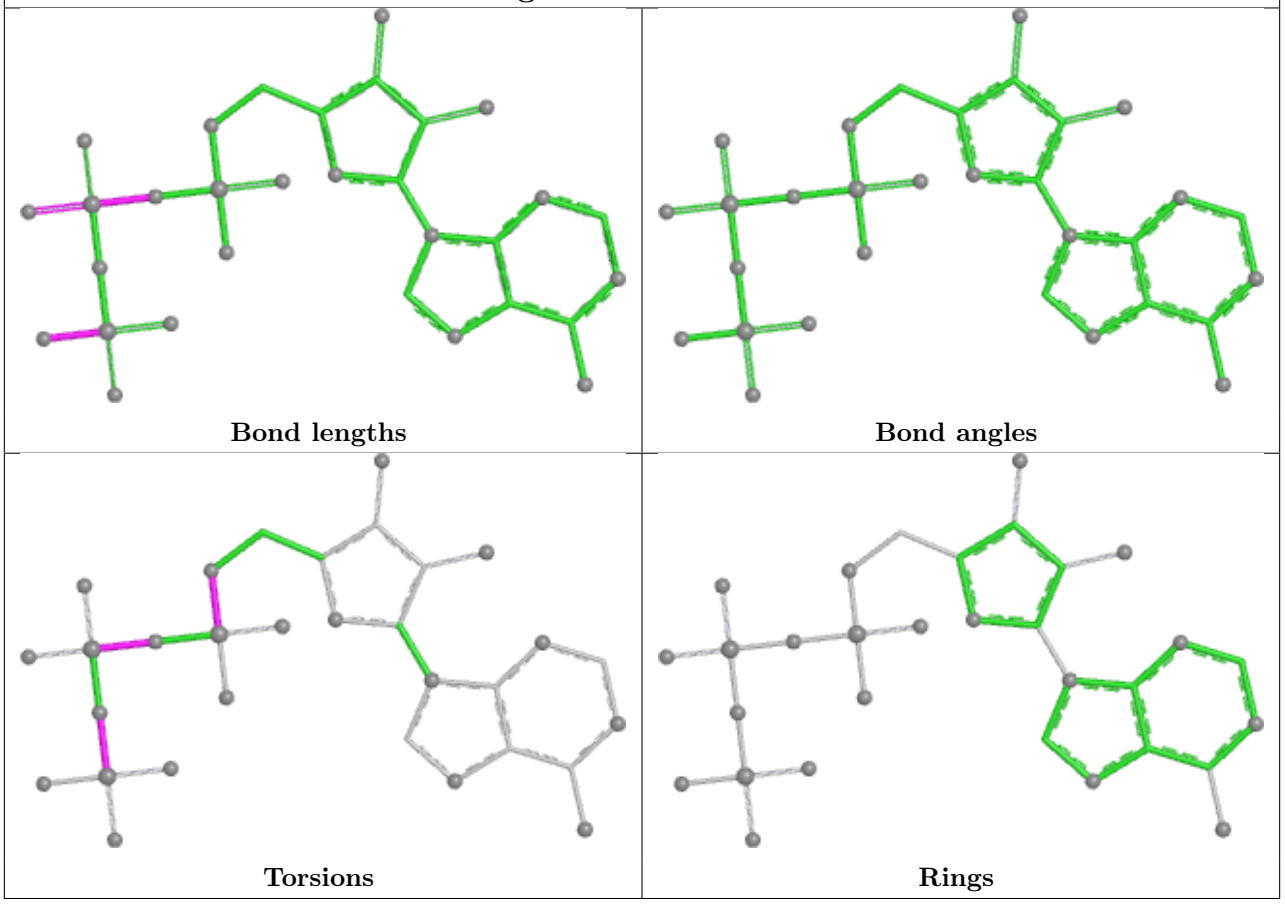


Torsions



Rings

Ligand ANP 4 1001



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.

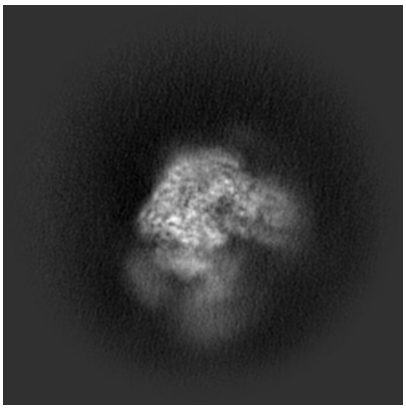
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15309. These allow visual inspection of the internal detail of the map and identification of artifacts.

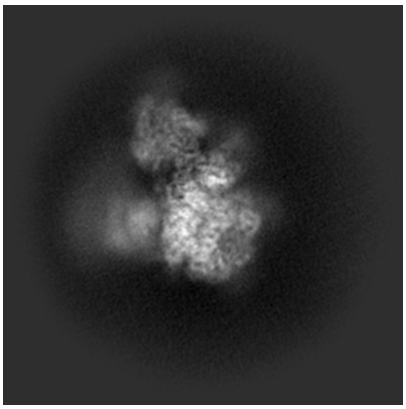
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

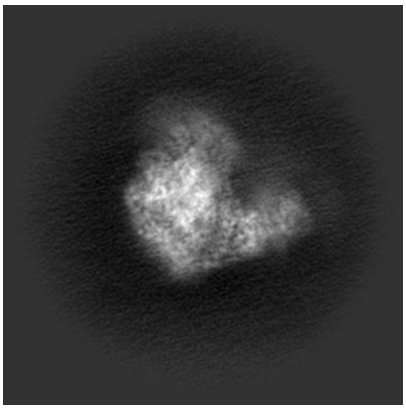
6.1.1 Primary map



X

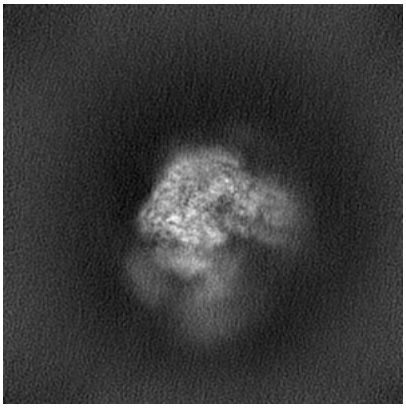


Y

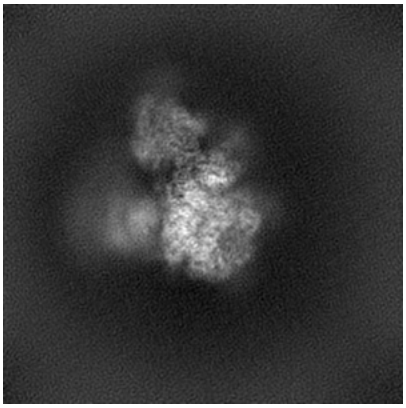


Z

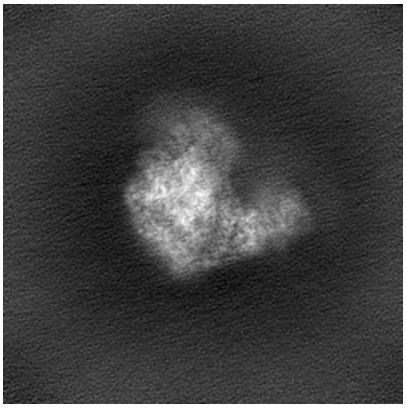
6.1.2 Raw map



X



Y

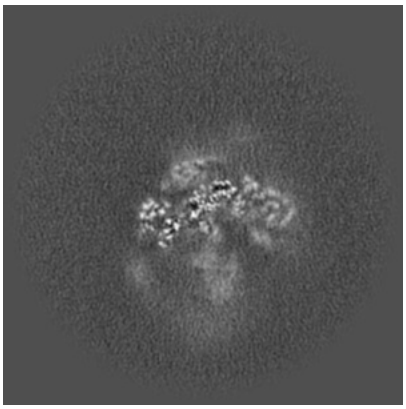


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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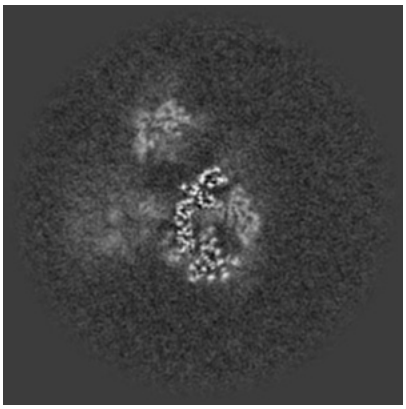

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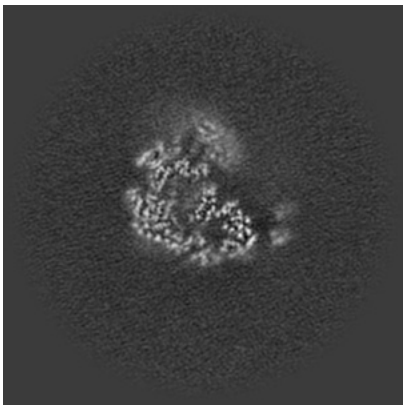

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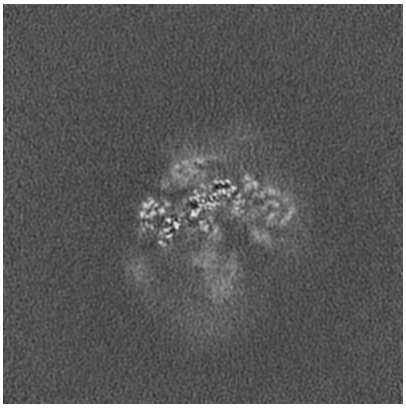
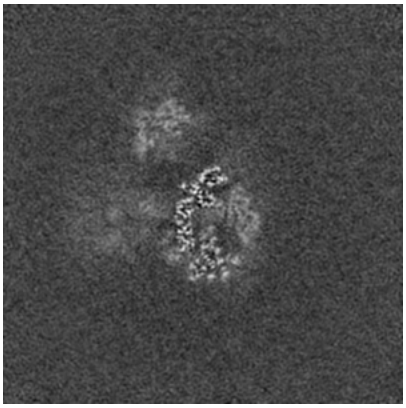
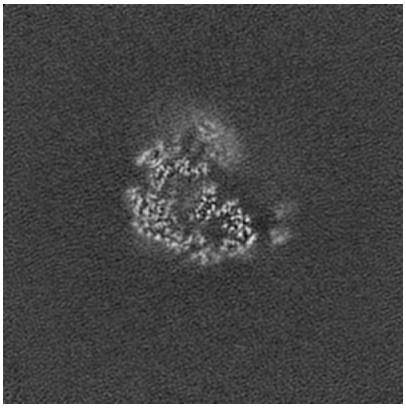
6.2.2 Raw map



X Index: 110



Y Index: 110

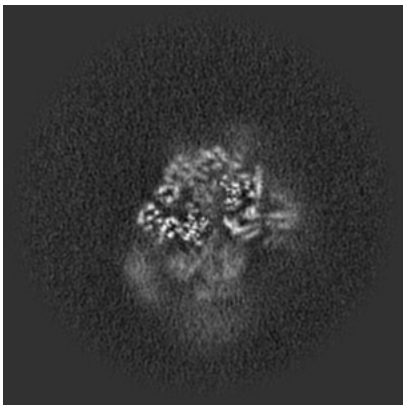


Z Index: 110

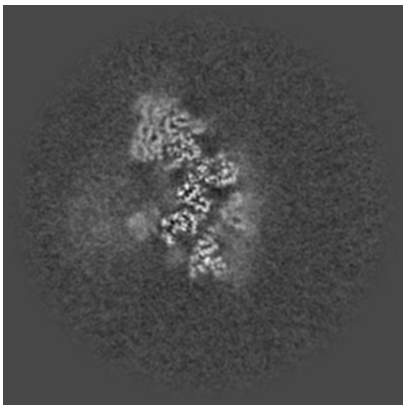
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

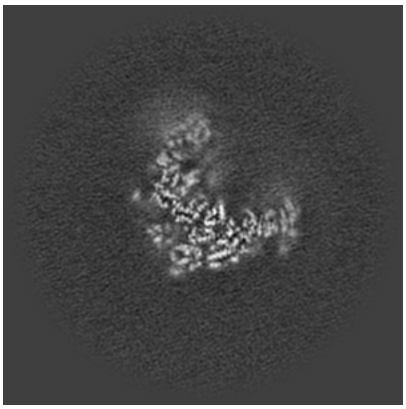
6.3.1 Primary map



X Index: 104

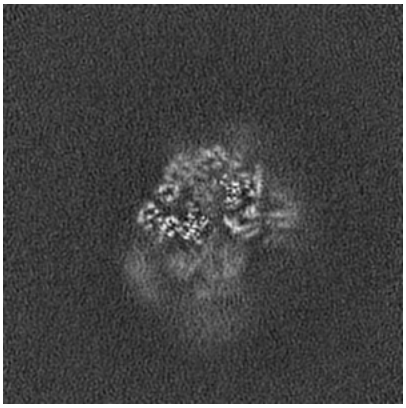


Y Index: 103

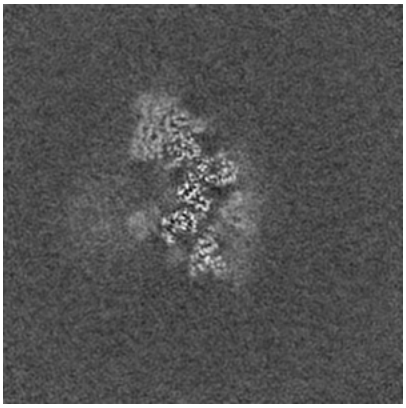


Z Index: 100

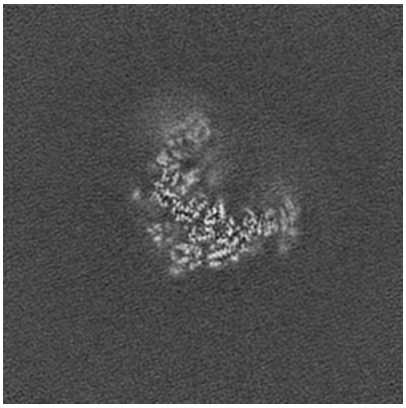
6.3.2 Raw map



X Index: 104



Y Index: 103

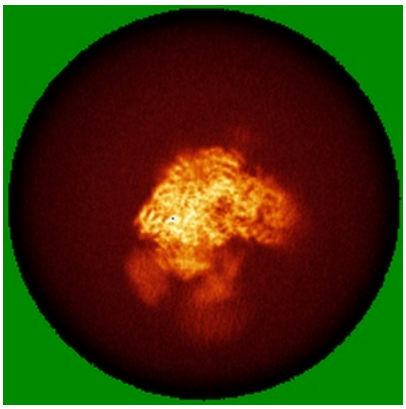


Z Index: 100

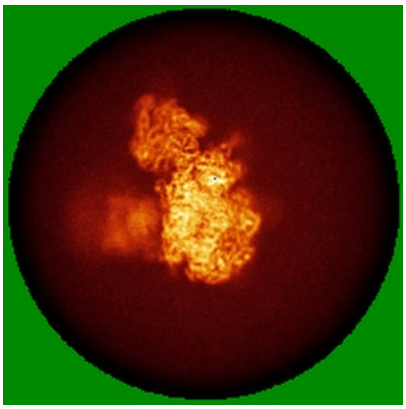
The images above show the largest variance slices of the map in three orthogonal directions.

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

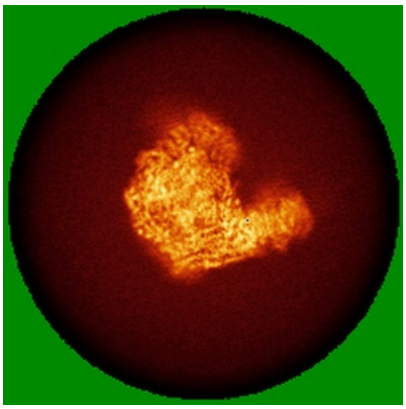
6.4.1 Primary map



X

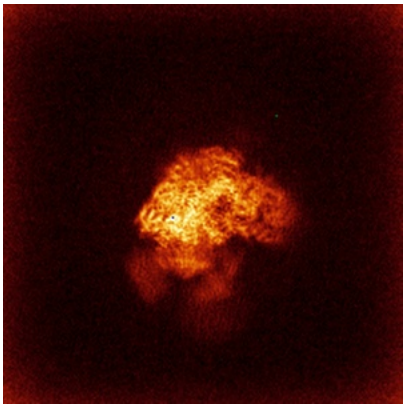


Y

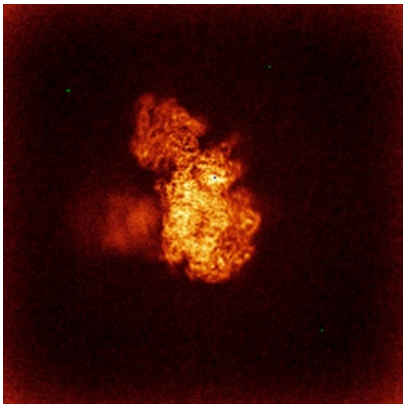


Z

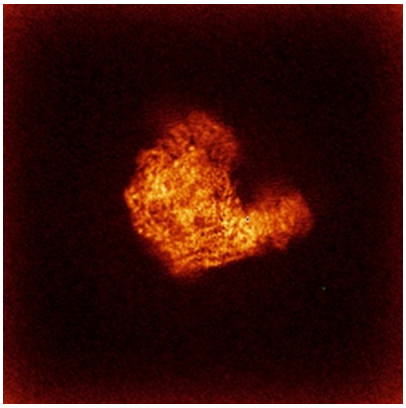
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

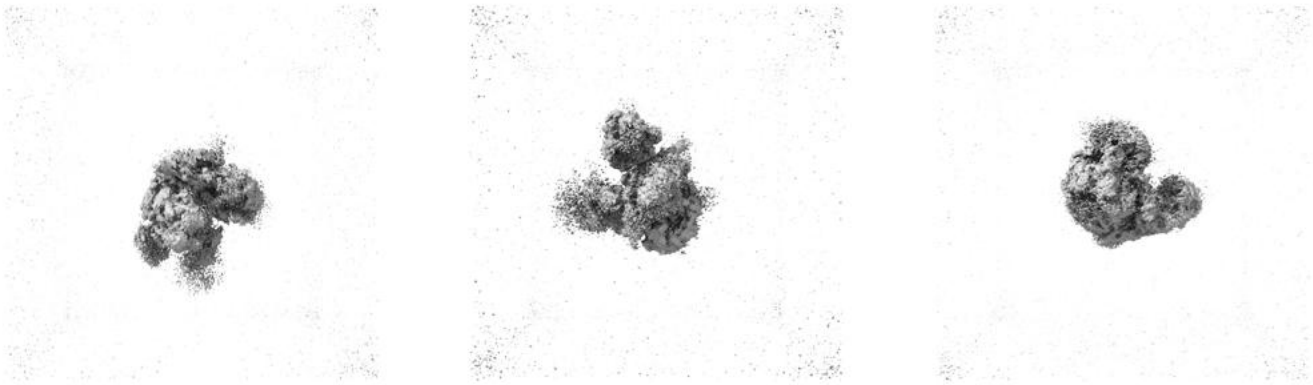
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

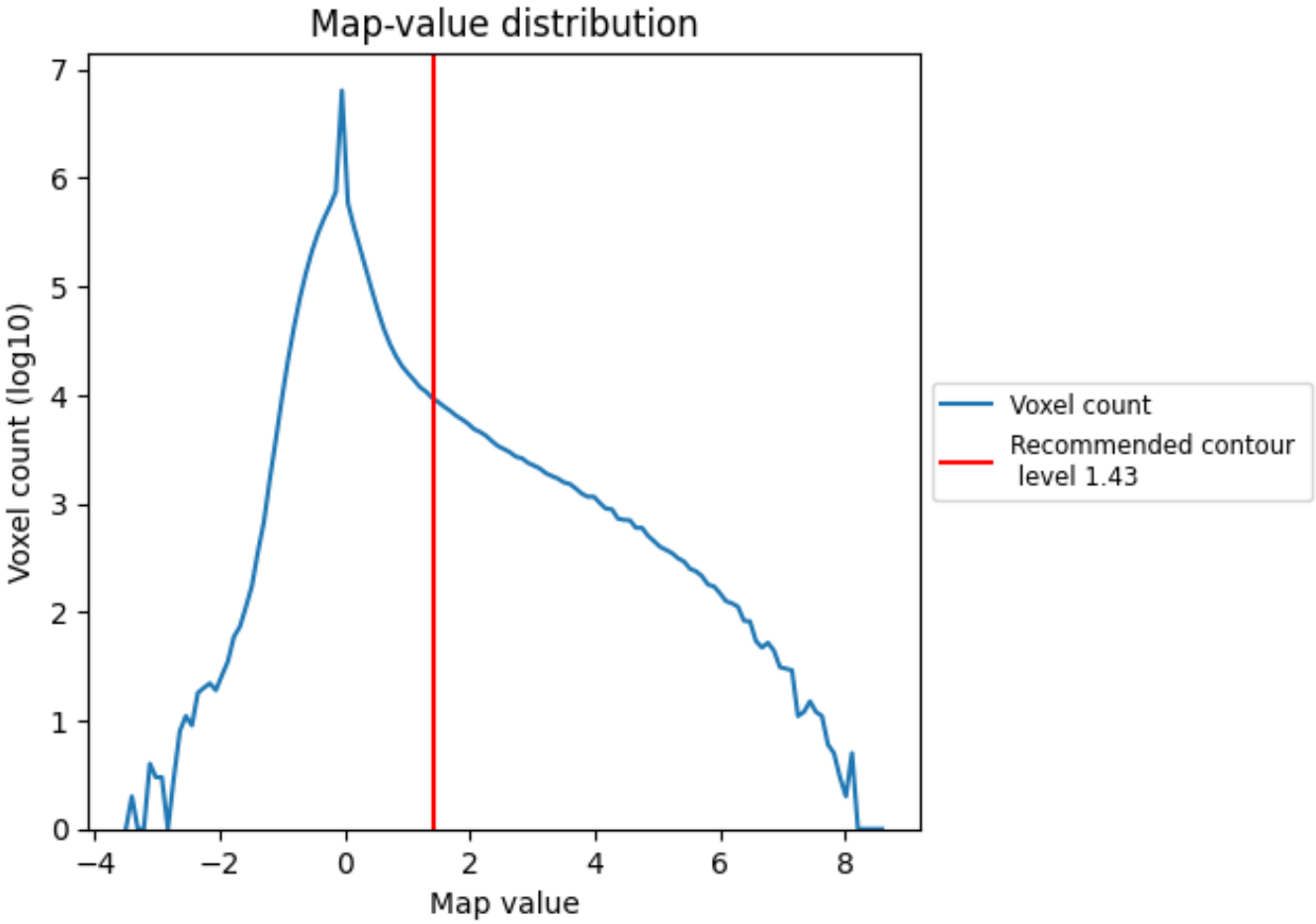
6.6 Mask visualisation (i)

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

7 Map analysis

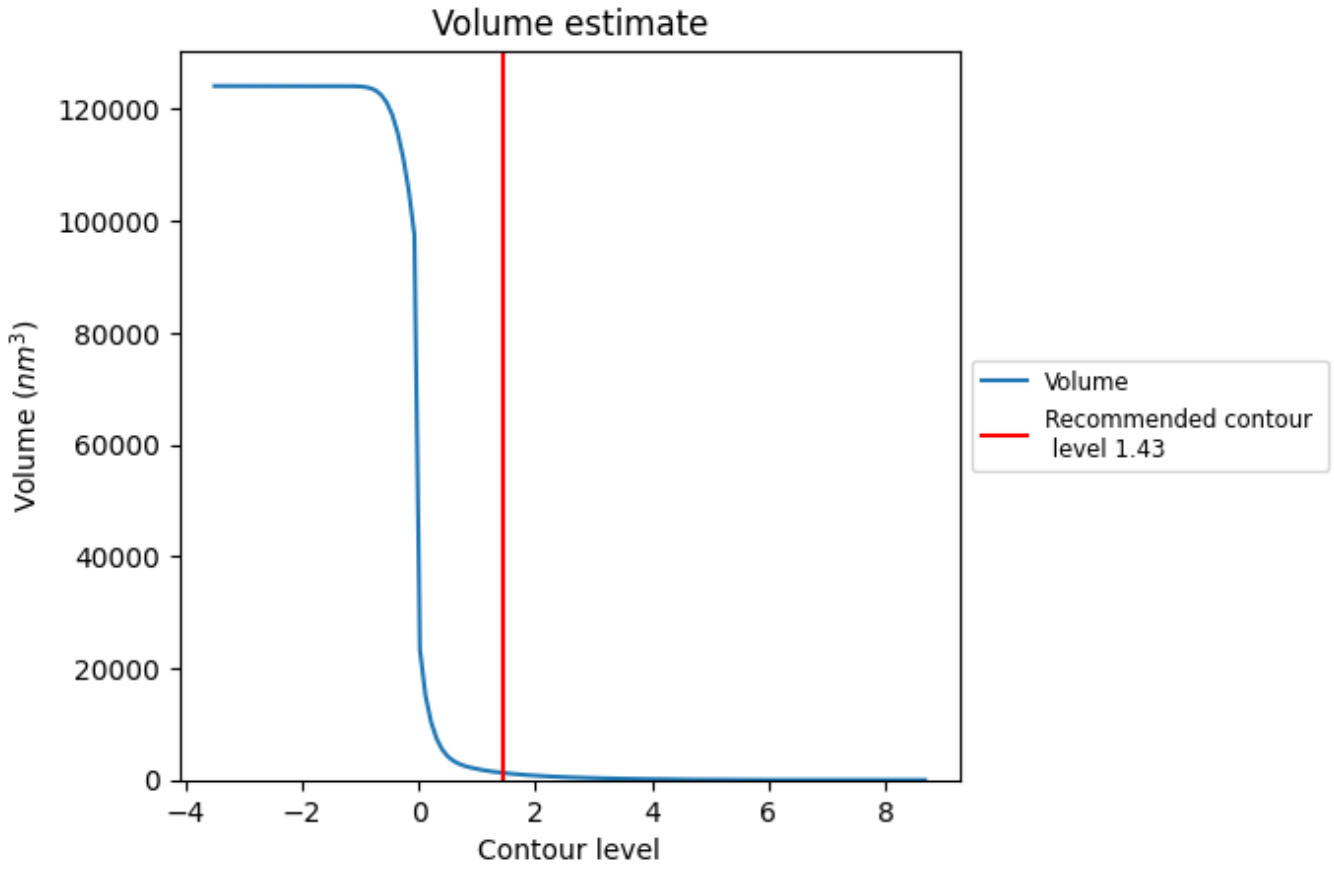
This section contains the results of statistical analysis of the map.

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.

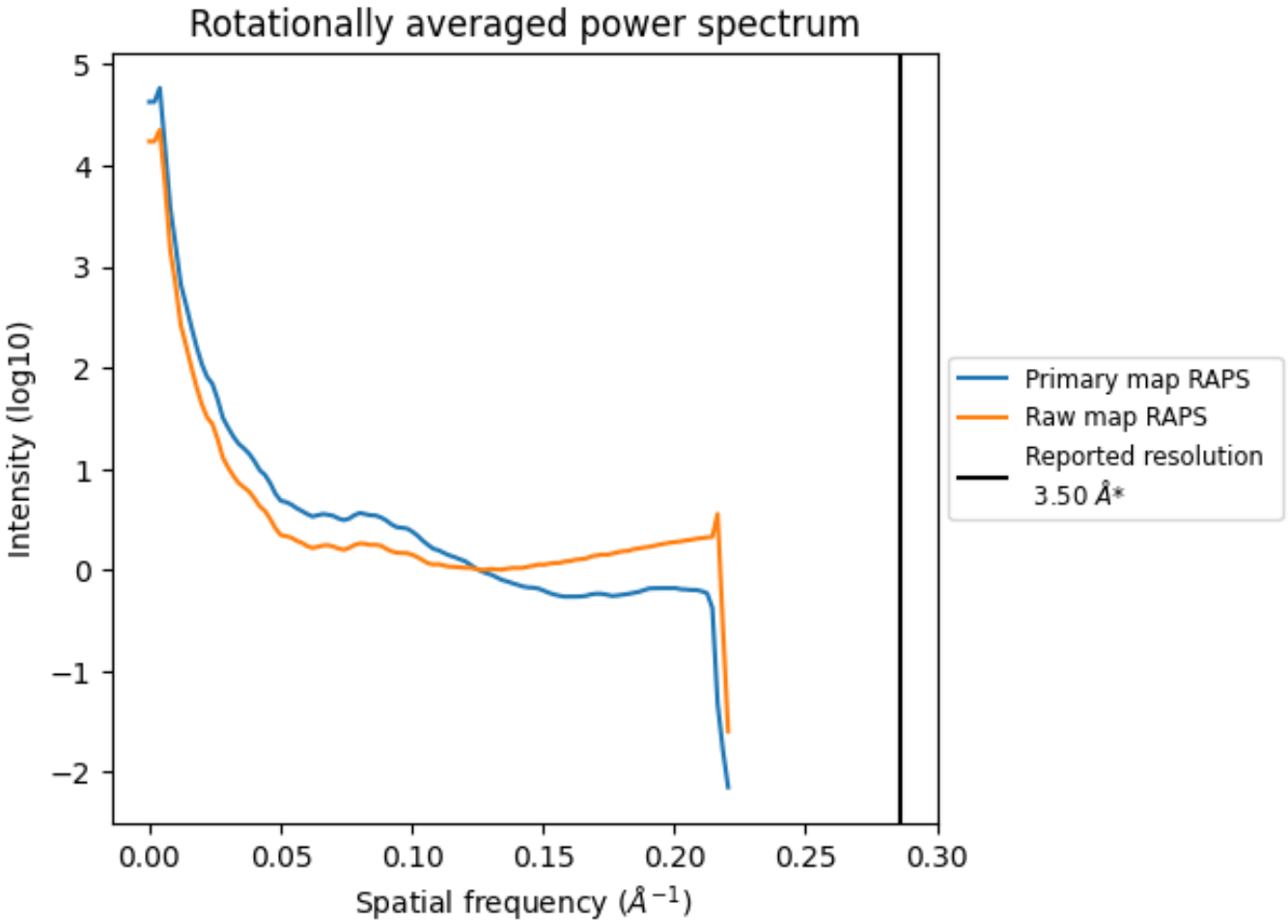
7.2 Volume estimate (i)



The volume at the recommended contour level is 1285 nm^3; this corresponds to an approximate mass of 1161 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)

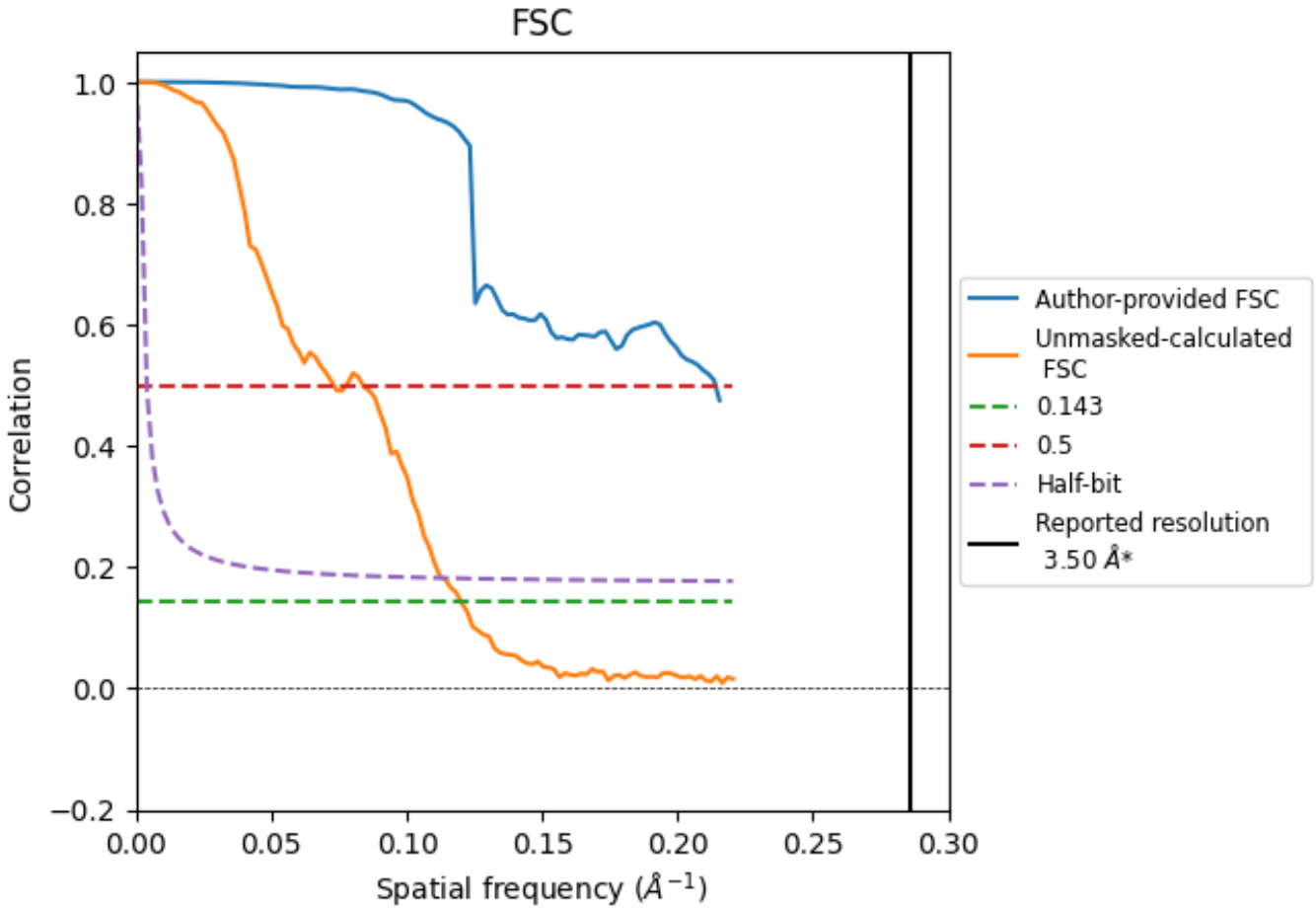


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

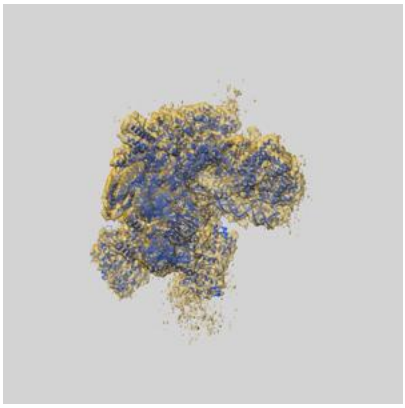
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	4.67	-
Unmasked-calculated*	8.33	13.70	8.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.33 differs from the reported value 3.5 by more than 10 %

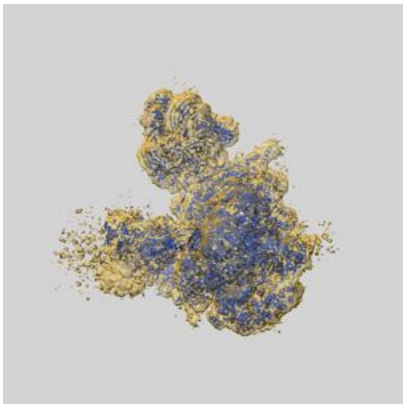
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15309 and PDB model 8B9A. Per-residue inclusion information can be found in section 3 on page 15.

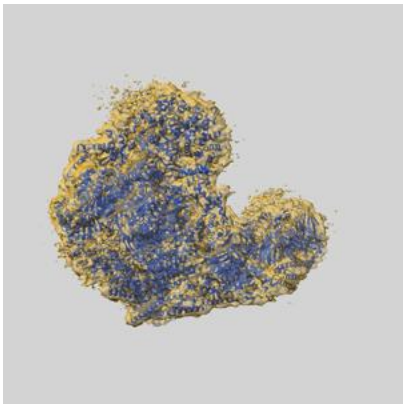
9.1 Map-model overlay



X



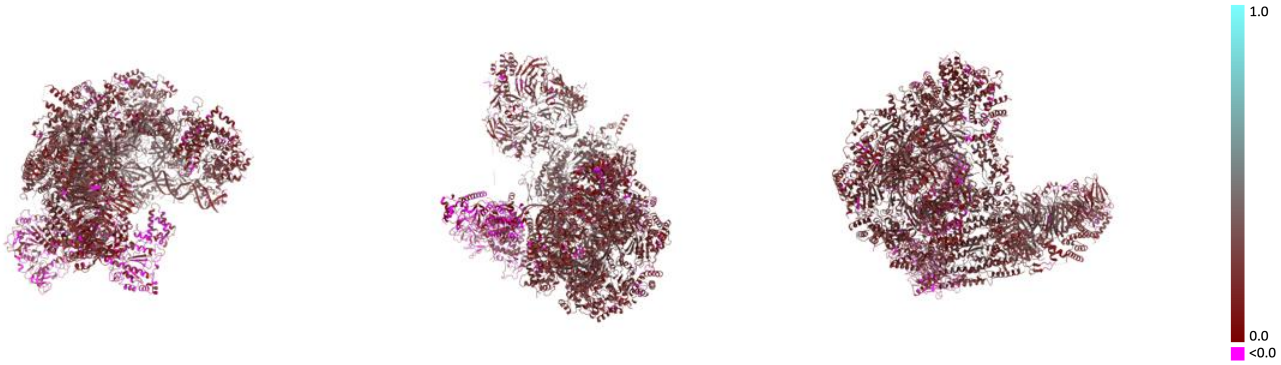
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.43 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.

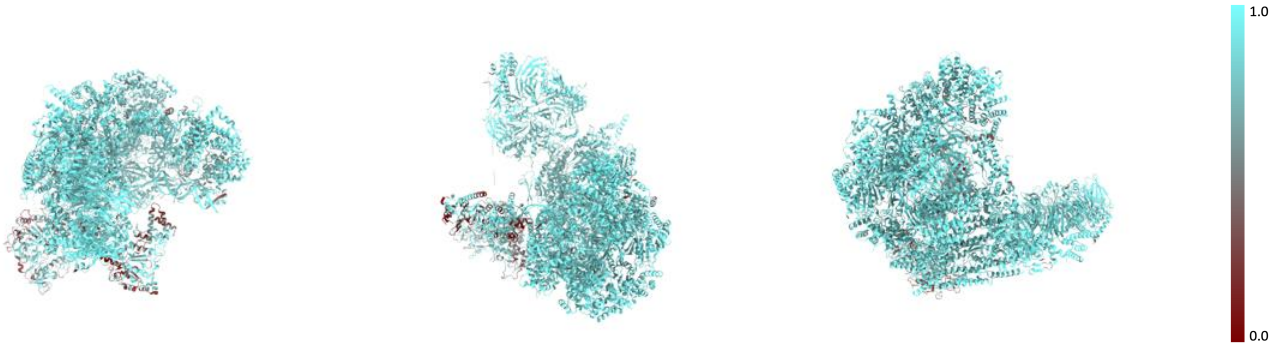
9.2 Q-score mapped to coordinate model



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.

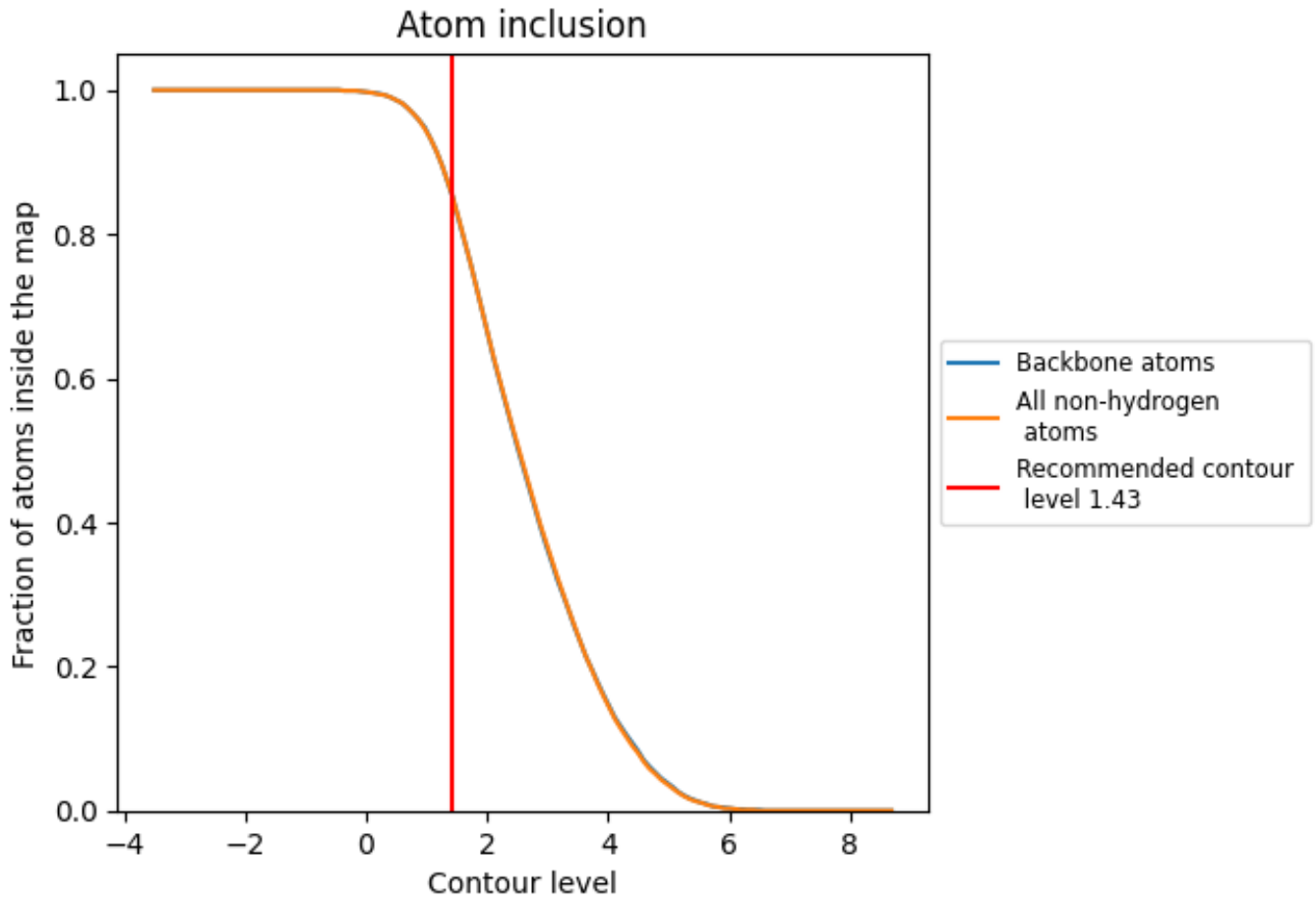
9.3 Atom inclusion mapped to coordinate model



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 (1.43).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (1.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.2040
2	0.9010	0.2170
3	0.8970	0.2560
4	0.9050	0.2310
5	0.9040	0.2650
6	0.8980	0.2270
7	0.8920	0.2340
A	0.7480	0.1050
B	0.6640	0.0700
C	0.8830	0.2350
D	0.8550	0.2700
E	0.8640	0.2630
F	0.8900	0.2660
G	0.9080	0.2640
H	0.9080	0.2720
J	0.6200	0.0660
K	0.9310	0.1880
L	0.9320	0.1980
P	0.7750	0.1310
Q	0.9220	0.2320
R	0.9500	0.2260
S	0.5760	0.0300
X	0.8660	0.1800
Y	0.8590	0.1980

