wwPDB EM Validation Summary Report

Jan 27, 2022 – 03:43 pm GMT

PDB ID	:	7PMK
EMDB ID	:	EMD-13537
Title	:	S. cerevisiae replisome-SCF(Dia2) complex bound to double-stranded DNA (conformation I)
Authors	:	Jenkyn-Bedford, M.; Yeeles, J.T.P.; Deegan, T.D.
Deposited on	:	2021-09-02
Resolution	:	3.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

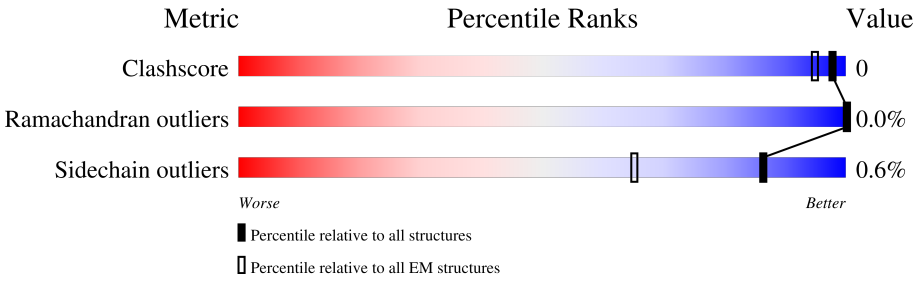
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	9% 74% · 25%
2	3	1009	· 59% · 40%
3	4	933	21% 63% · 36%
4	5	775	10% 86% · 13%
5	6	1017	7% 61% · 37%
6	7	845	16% 73% · 26%
7	A	208	7% 94% · 5%
8	B	213	88% · 10%

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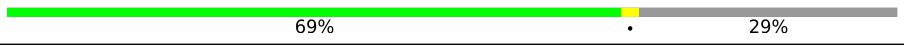
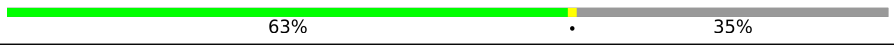
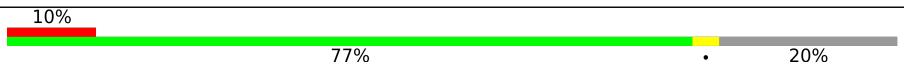
Mol	Chain	Length	Quality of chain
9	C	194	
10	D	294	
11	E	657	
12	F	962	
12	G	962	
12	H	962	
13	I	115	
14	J	122	
15	K	194	
16	L	735	
17	Q	2222	
18	R	689	
19	X	1238	
20	Y	319	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 74697 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	655	Total	C	N	O	S	0	0
			5175	3257	929	970	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	607	Total	C	N	O	S	0	0
			4759	3007	847	892	13		

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
3	4	597	Total	C	N	O	S	0	0
			4749	2996	818	907	28		

- Molecule 4 is a protein called DNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	673	Total	C	N	O	S	0	0
			5332	3351	927	1030	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	637	Total	C	N	O	S	0	0
			5013	3162	881	945	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	629	Total	C	N	O	S	0	0
			4914	3109	853	926	26		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	171	Total	C	N	O	S	0	0
			1381	900	223	252	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	564	Total	C	N	O	S	0	0
			4569	2916	772	867	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167F	ASP	-	expression tag	UNP Q08032
E	167G	TYR	-	expression tag	UNP Q08032
E	167H	LYS	-	expression tag	UNP Q08032
E	167I	ASP	-	expression tag	UNP Q08032
E	167J	ASP	-	expression tag	UNP Q08032
E	167K	ASP	-	expression tag	UNP Q08032
E	167L	GLY	-	expression tag	UNP Q08032
E	167M	ASP	-	expression tag	UNP Q08032
E	167N	TYR	-	expression tag	UNP Q08032
E	167O	LYS	-	expression tag	UNP Q08032

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Chain	Residue	Modelled	Actual	Comment	Reference
E	167P	ASP	-	expression tag	UNP Q08032
E	167Q	ASP	-	expression tag	UNP Q08032

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

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

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	MET	-	initiating methionine	UNP A0A6A5Q5Y5
F	-33	LYS	-	expression tag	UNP A0A6A5Q5Y5
F	-32	ARG	-	expression tag	UNP A0A6A5Q5Y5
F	-31	ARG	-	expression tag	UNP A0A6A5Q5Y5
F	-30	TRP	-	expression tag	UNP A0A6A5Q5Y5
F	-29	LYS	-	expression tag	UNP A0A6A5Q5Y5
F	-28	LYS	-	expression tag	UNP A0A6A5Q5Y5
F	-27	ASN	-	expression tag	UNP A0A6A5Q5Y5
F	-26	PHE	-	expression tag	UNP A0A6A5Q5Y5
F	-25	ILE	-	expression tag	UNP A0A6A5Q5Y5
F	-24	ALA	-	expression tag	UNP A0A6A5Q5Y5
F	-23	VAL	-	expression tag	UNP A0A6A5Q5Y5
F	-22	SER	-	expression tag	UNP A0A6A5Q5Y5
F	-21	ALA	-	expression tag	UNP A0A6A5Q5Y5
F	-20	ALA	-	expression tag	UNP A0A6A5Q5Y5
F	-19	ASN	-	expression tag	UNP A0A6A5Q5Y5
F	-18	ARG	-	expression tag	UNP A0A6A5Q5Y5
F	-17	PHE	-	expression tag	UNP A0A6A5Q5Y5
F	-16	LYS	-	expression tag	UNP A0A6A5Q5Y5
F	-15	LYS	-	expression tag	UNP A0A6A5Q5Y5
F	-14	ILE	-	expression tag	UNP A0A6A5Q5Y5
F	-13	SER	-	expression tag	UNP A0A6A5Q5Y5
F	-12	SER	-	expression tag	UNP A0A6A5Q5Y5
F	-11	SER	-	expression tag	UNP A0A6A5Q5Y5
F	-10	GLY	-	expression tag	UNP A0A6A5Q5Y5
F	-9	ALA	-	expression tag	UNP A0A6A5Q5Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	LEU	-	expression tag	UNP A0A6A5Q5Y5
F	-7	GLU	-	expression tag	UNP A0A6A5Q5Y5
F	-6	ASN	-	expression tag	UNP A0A6A5Q5Y5
F	-5	LEU	-	expression tag	UNP A0A6A5Q5Y5
F	-4	TYR	-	expression tag	UNP A0A6A5Q5Y5
F	-3	PHE	-	expression tag	UNP A0A6A5Q5Y5
F	-2	GLN	-	expression tag	UNP A0A6A5Q5Y5
F	-1	GLY	-	expression tag	UNP A0A6A5Q5Y5
F	0	GLU	-	expression tag	UNP A0A6A5Q5Y5
G	-34	MET	-	initiating methionine	UNP A0A6A5Q5Y5
G	-33	LYS	-	expression tag	UNP A0A6A5Q5Y5
G	-32	ARG	-	expression tag	UNP A0A6A5Q5Y5
G	-31	ARG	-	expression tag	UNP A0A6A5Q5Y5
G	-30	TRP	-	expression tag	UNP A0A6A5Q5Y5
G	-29	LYS	-	expression tag	UNP A0A6A5Q5Y5
G	-28	LYS	-	expression tag	UNP A0A6A5Q5Y5
G	-27	ASN	-	expression tag	UNP A0A6A5Q5Y5
G	-26	PHE	-	expression tag	UNP A0A6A5Q5Y5
G	-25	ILE	-	expression tag	UNP A0A6A5Q5Y5
G	-24	ALA	-	expression tag	UNP A0A6A5Q5Y5
G	-23	VAL	-	expression tag	UNP A0A6A5Q5Y5
G	-22	SER	-	expression tag	UNP A0A6A5Q5Y5
G	-21	ALA	-	expression tag	UNP A0A6A5Q5Y5
G	-20	ALA	-	expression tag	UNP A0A6A5Q5Y5
G	-19	ASN	-	expression tag	UNP A0A6A5Q5Y5
G	-18	ARG	-	expression tag	UNP A0A6A5Q5Y5
G	-17	PHE	-	expression tag	UNP A0A6A5Q5Y5
G	-16	LYS	-	expression tag	UNP A0A6A5Q5Y5
G	-15	LYS	-	expression tag	UNP A0A6A5Q5Y5
G	-14	ILE	-	expression tag	UNP A0A6A5Q5Y5
G	-13	SER	-	expression tag	UNP A0A6A5Q5Y5
G	-12	SER	-	expression tag	UNP A0A6A5Q5Y5
G	-11	SER	-	expression tag	UNP A0A6A5Q5Y5
G	-10	GLY	-	expression tag	UNP A0A6A5Q5Y5
G	-9	ALA	-	expression tag	UNP A0A6A5Q5Y5
G	-8	LEU	-	expression tag	UNP A0A6A5Q5Y5
G	-7	GLU	-	expression tag	UNP A0A6A5Q5Y5
G	-6	ASN	-	expression tag	UNP A0A6A5Q5Y5
G	-5	LEU	-	expression tag	UNP A0A6A5Q5Y5
G	-4	TYR	-	expression tag	UNP A0A6A5Q5Y5
G	-3	PHE	-	expression tag	UNP A0A6A5Q5Y5
G	-2	GLN	-	expression tag	UNP A0A6A5Q5Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP A0A6A5Q5Y5
G	0	GLU	-	expression tag	UNP A0A6A5Q5Y5
H	-34	MET	-	initiating methionine	UNP A0A6A5Q5Y5
H	-33	LYS	-	expression tag	UNP A0A6A5Q5Y5
H	-32	ARG	-	expression tag	UNP A0A6A5Q5Y5
H	-31	ARG	-	expression tag	UNP A0A6A5Q5Y5
H	-30	TRP	-	expression tag	UNP A0A6A5Q5Y5
H	-29	LYS	-	expression tag	UNP A0A6A5Q5Y5
H	-28	LYS	-	expression tag	UNP A0A6A5Q5Y5
H	-27	ASN	-	expression tag	UNP A0A6A5Q5Y5
H	-26	PHE	-	expression tag	UNP A0A6A5Q5Y5
H	-25	ILE	-	expression tag	UNP A0A6A5Q5Y5
H	-24	ALA	-	expression tag	UNP A0A6A5Q5Y5
H	-23	VAL	-	expression tag	UNP A0A6A5Q5Y5
H	-22	SER	-	expression tag	UNP A0A6A5Q5Y5
H	-21	ALA	-	expression tag	UNP A0A6A5Q5Y5
H	-20	ALA	-	expression tag	UNP A0A6A5Q5Y5
H	-19	ASN	-	expression tag	UNP A0A6A5Q5Y5
H	-18	ARG	-	expression tag	UNP A0A6A5Q5Y5
H	-17	PHE	-	expression tag	UNP A0A6A5Q5Y5
H	-16	LYS	-	expression tag	UNP A0A6A5Q5Y5
H	-15	LYS	-	expression tag	UNP A0A6A5Q5Y5
H	-14	ILE	-	expression tag	UNP A0A6A5Q5Y5
H	-13	SER	-	expression tag	UNP A0A6A5Q5Y5
H	-12	SER	-	expression tag	UNP A0A6A5Q5Y5
H	-11	SER	-	expression tag	UNP A0A6A5Q5Y5
H	-10	GLY	-	expression tag	UNP A0A6A5Q5Y5
H	-9	ALA	-	expression tag	UNP A0A6A5Q5Y5
H	-8	LEU	-	expression tag	UNP A0A6A5Q5Y5
H	-7	GLU	-	expression tag	UNP A0A6A5Q5Y5
H	-6	ASN	-	expression tag	UNP A0A6A5Q5Y5
H	-5	LEU	-	expression tag	UNP A0A6A5Q5Y5
H	-4	TYR	-	expression tag	UNP A0A6A5Q5Y5
H	-3	PHE	-	expression tag	UNP A0A6A5Q5Y5
H	-2	GLN	-	expression tag	UNP A0A6A5Q5Y5
H	-1	GLY	-	expression tag	UNP A0A6A5Q5Y5
H	0	GLU	-	expression tag	UNP A0A6A5Q5Y5

- Molecule 13 is a DNA chain called Leading strand template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	36	Total	C	N	O	P	0	0
			782	360	165	221	36		

- Molecule 14 is a DNA chain called Lagging strand template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	33	Total	C	N	O	P	0	0
			629	298	101	197	33		

- Molecule 15 is a protein called E3 ubiquitin ligase complex SCF subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1120	709	195	212	4		

- Molecule 16 is a protein called Protein DIA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	475	Total	C	N	O	S	0	0
			3921	2533	654	710	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	GLY	-	expression tag	UNP Q08496
L	-1	ALA	-	expression tag	UNP Q08496
L	0	GLY	-	expression tag	UNP Q08496

- Molecule 17 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	766	Total	C	N	O	S	0	0
			6203	4028	1015	1124	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	290	ALA	ASP	variant	UNP P21951
Q	292	ALA	GLU	variant	UNP P21951

- Molecule 18 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	552	Total	C	N	O	S	0	0
			4427	2843	759	807	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	665	Total	C	N	O	S	0	0
			5410	3505	912	974	19		

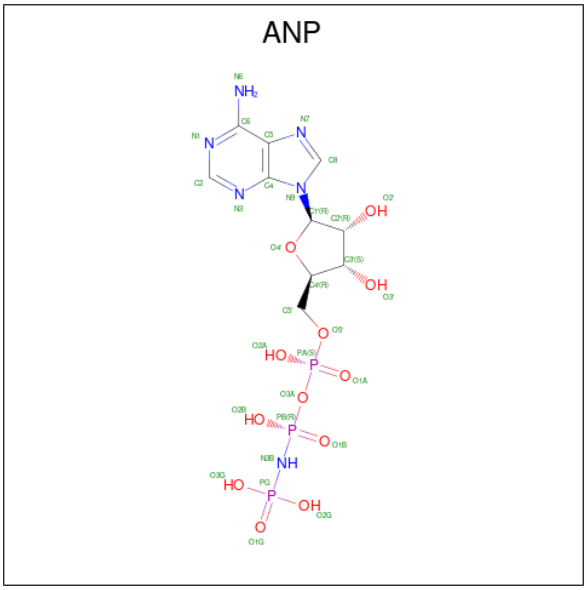
- Molecule 20 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	98	Total	C	N	O	S	0	0
			791	511	138	138	4		

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



Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	5	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
22	2	1	Total Mg 1 1	0
22	3	1	Total Mg 1 1	0
22	5	1	Total Mg 1 1	0

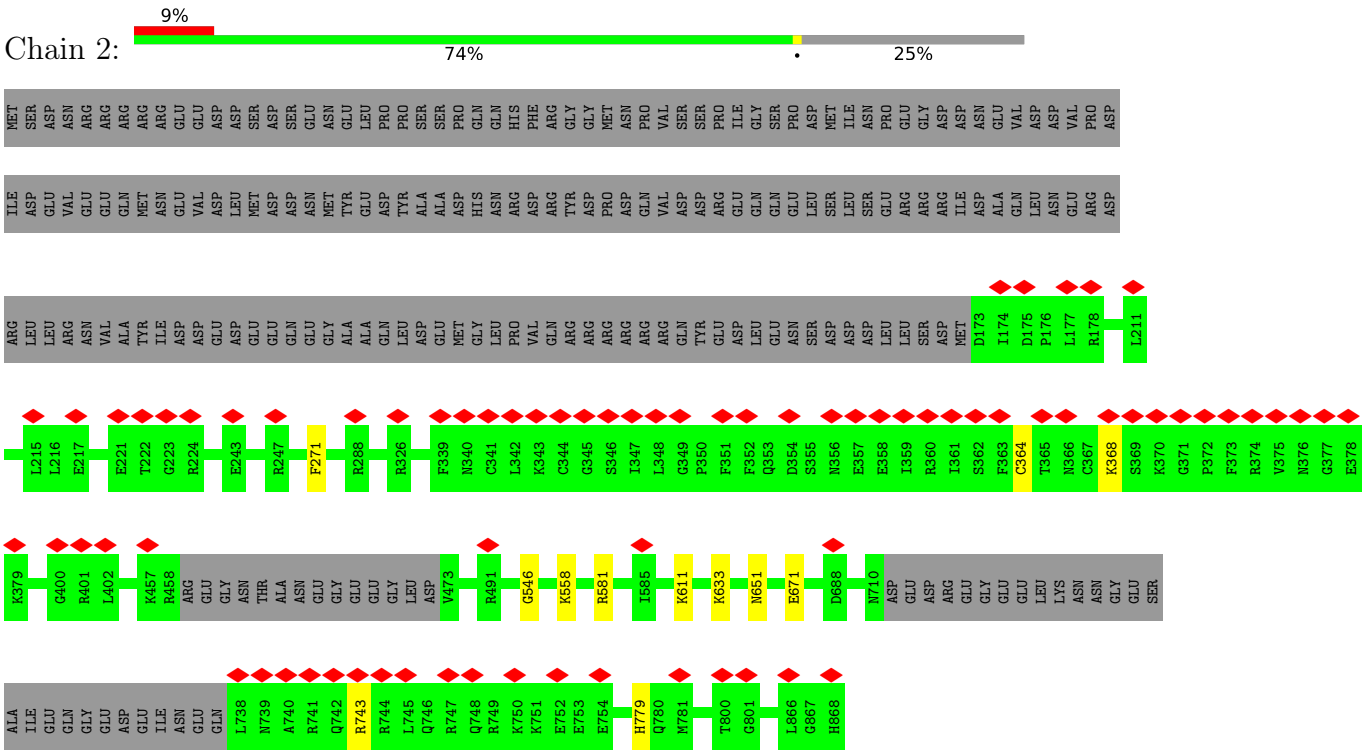
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
23	2	1	Total Zn 1 1	0
23	4	1	Total Zn 1 1	0
23	5	1	Total Zn 1 1	0
23	6	1	Total Zn 1 1	0
23	7	1	Total Zn 1 1	0
23	Q	2	Total Zn 2 2	0

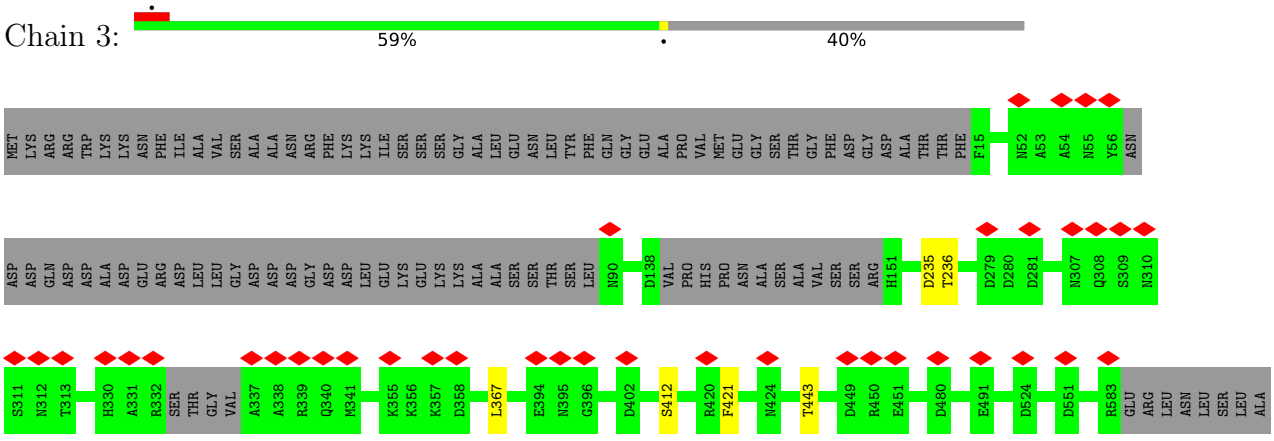
3 Residue-property plots (i)

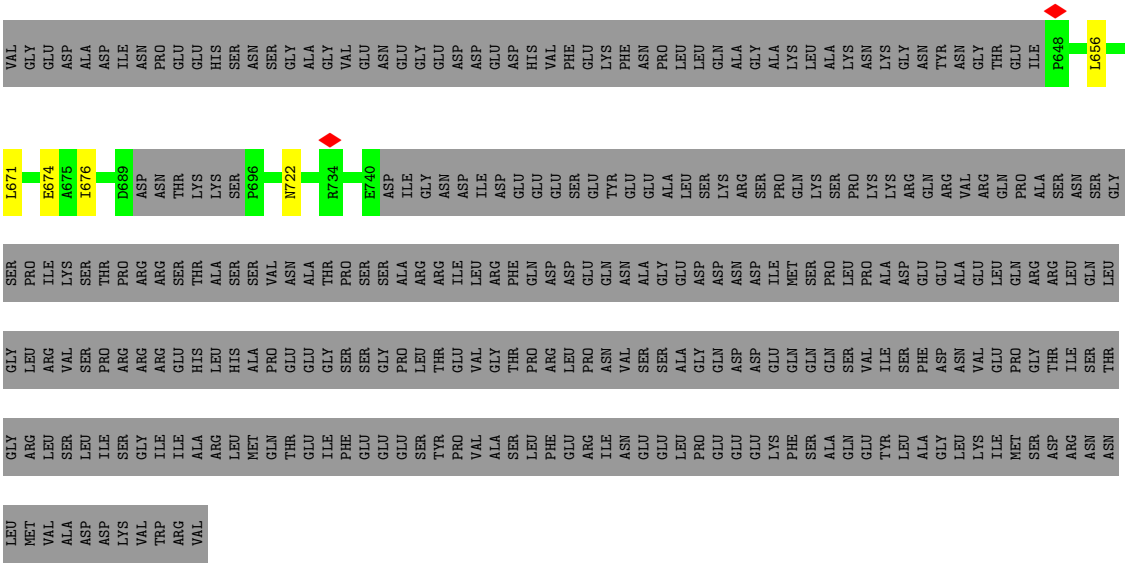
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



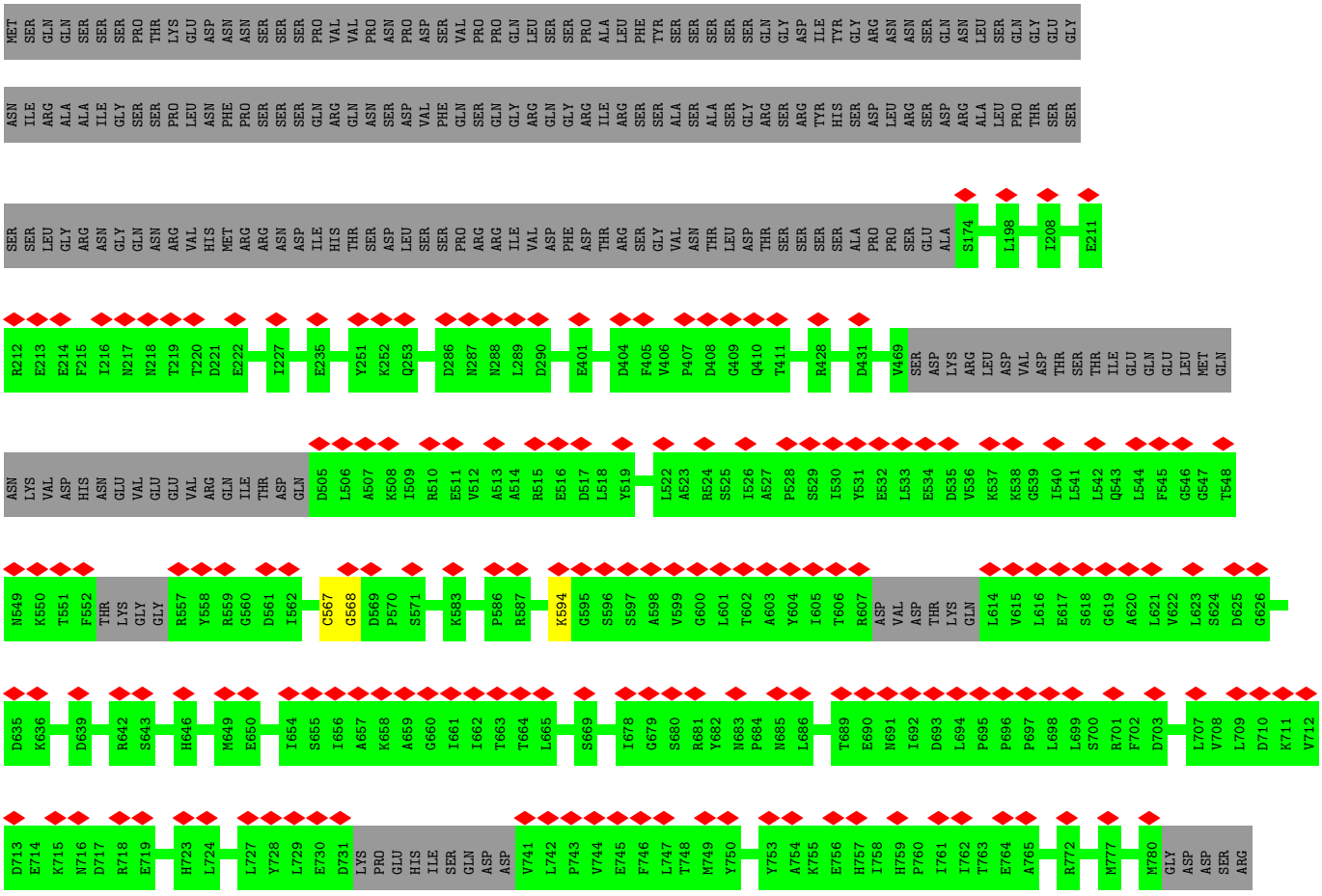
• Molecule 2: DNA replication licensing factor MCM3

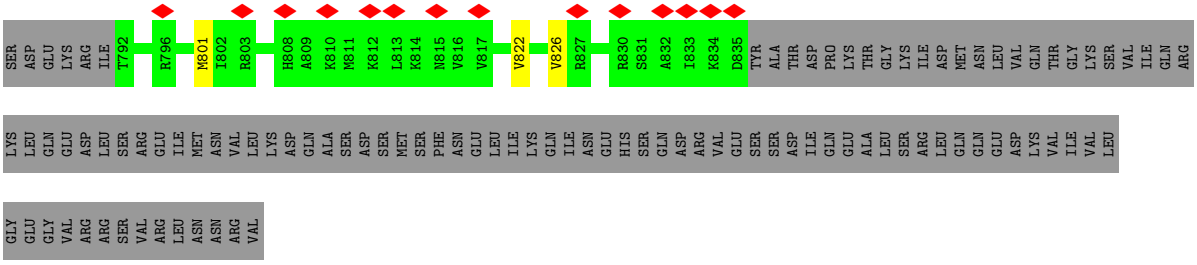




• Molecule 3: DNA replication licensing factor MCM4

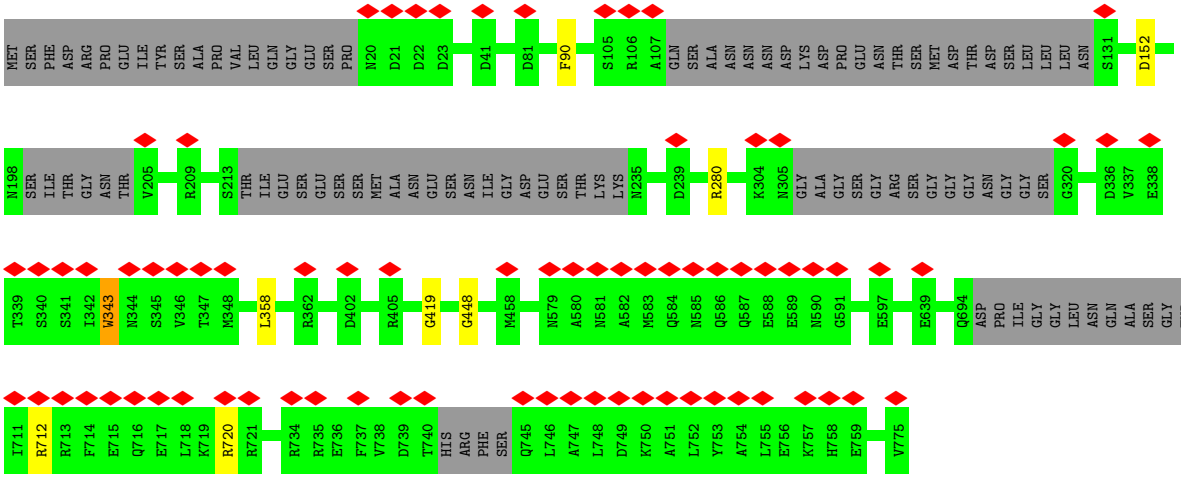
Chain 4:





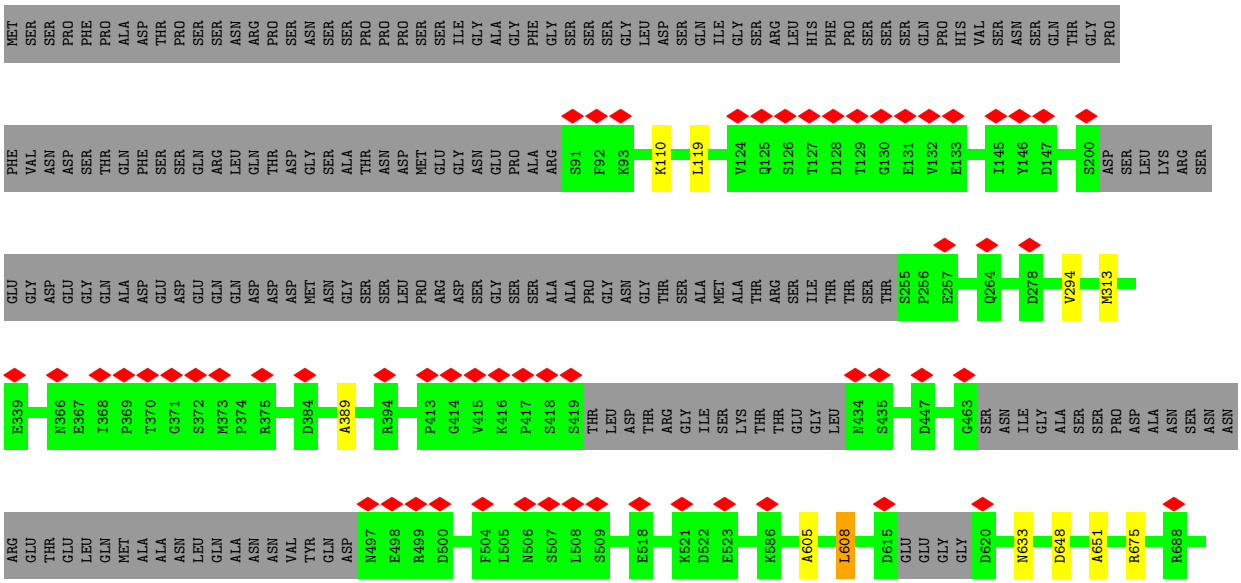
• Molecule 4: DNA helicase

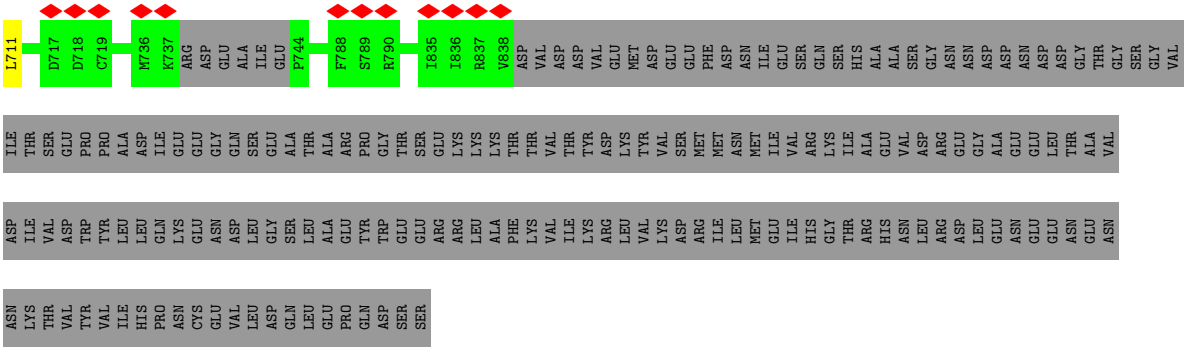
Chain 5:



• Molecule 5: DNA replication licensing factor MCM6

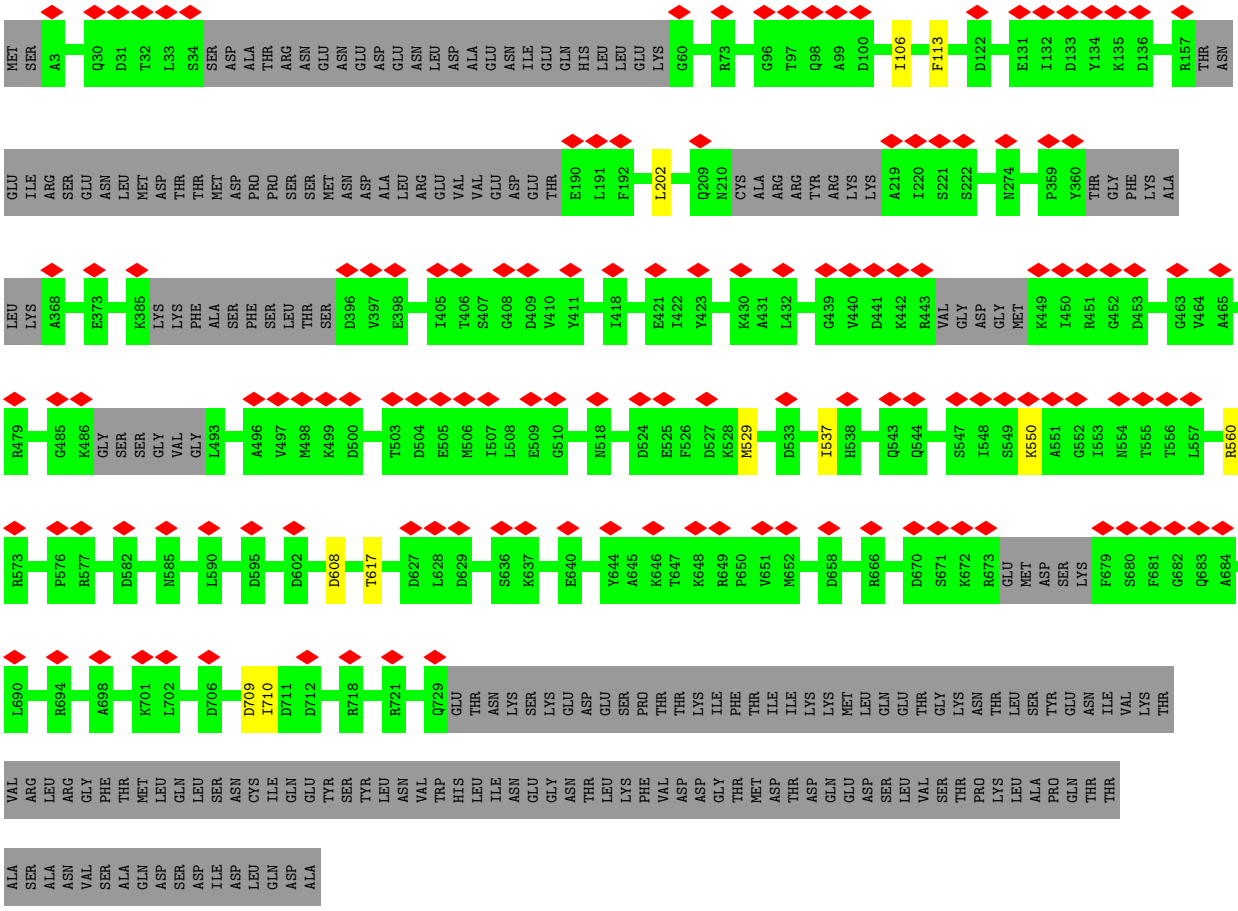
Chain 6:





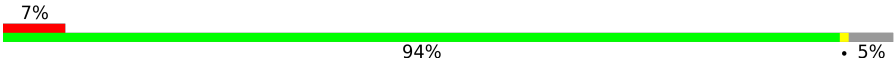
• Molecule 6: DNA replication licensing factor MCM7

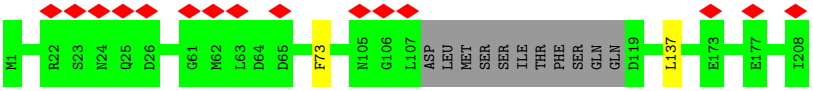
Chain 7:



• Molecule 7: DNA replication complex GINS protein PSF1

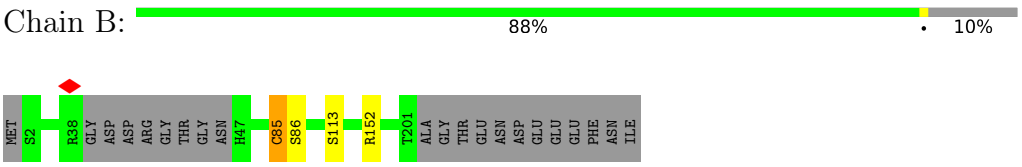
Chain A:





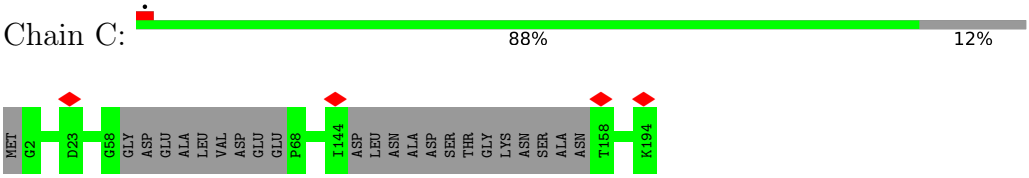
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B:



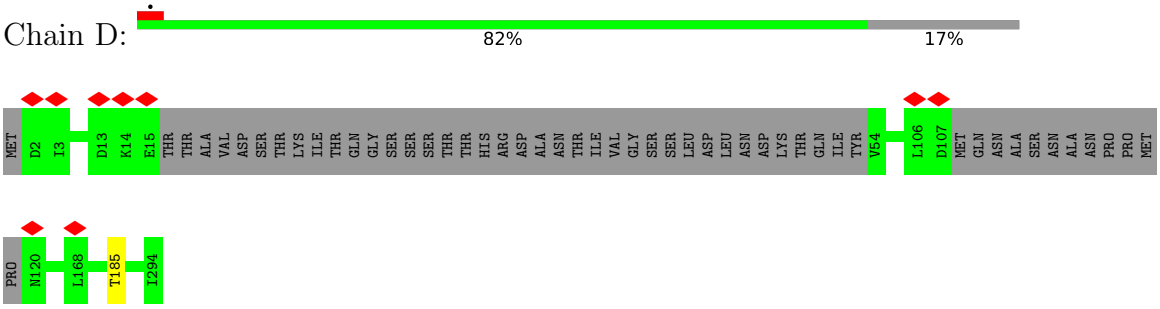
• Molecule 9: DNA replication complex GINS protein PSF3

Chain C:



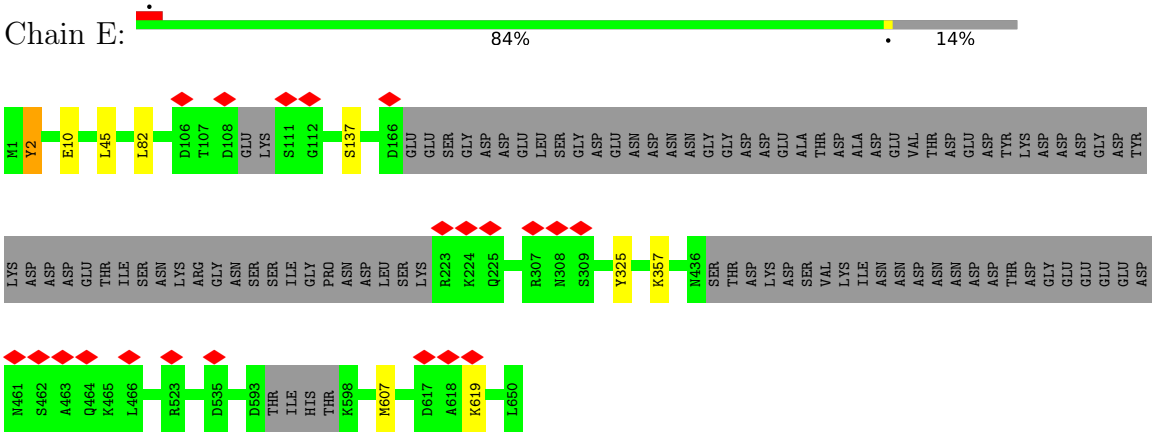
• Molecule 10: DNA replication complex GINS protein SLD5

Chain D:



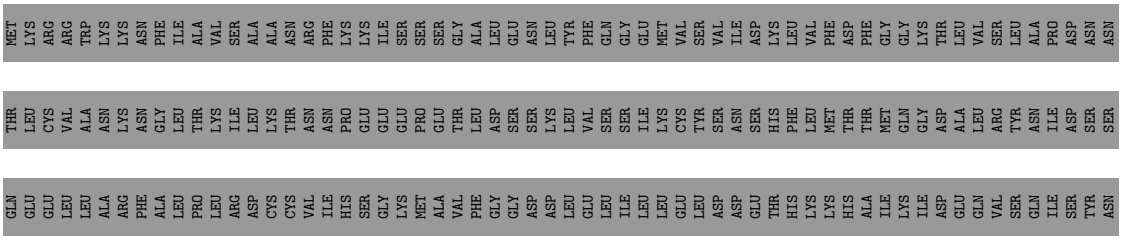
• Molecule 11: Cell division control protein 45,Cell division control protein 45

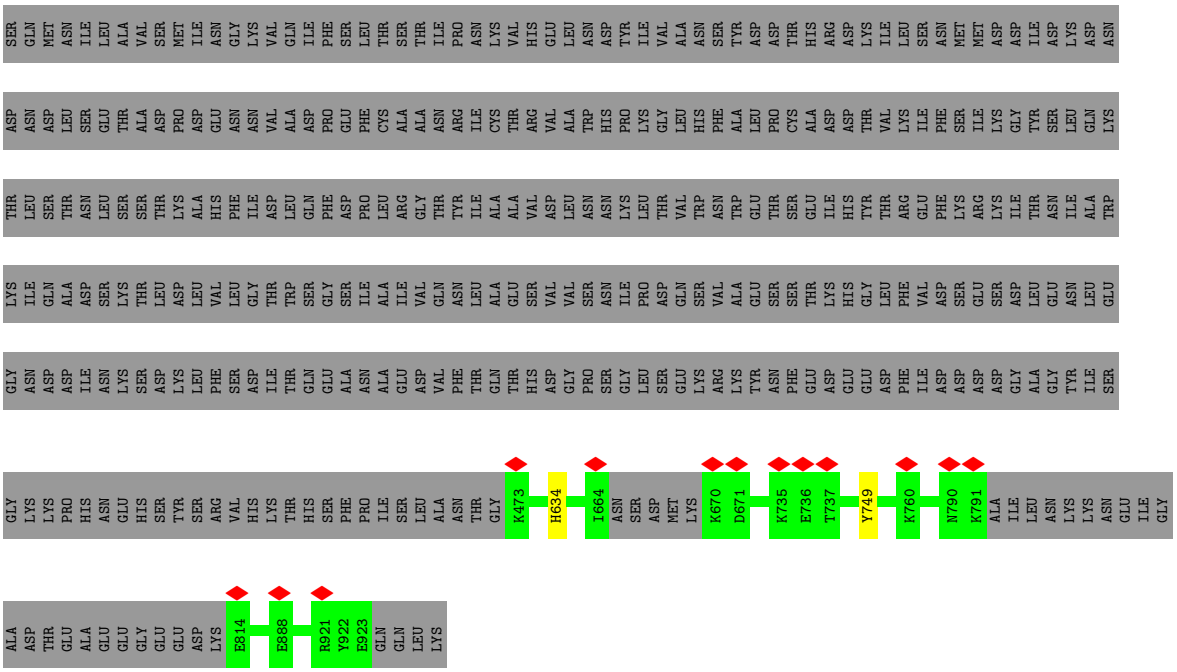
Chain E:



• Molecule 12: DNA polymerase alpha-binding protein

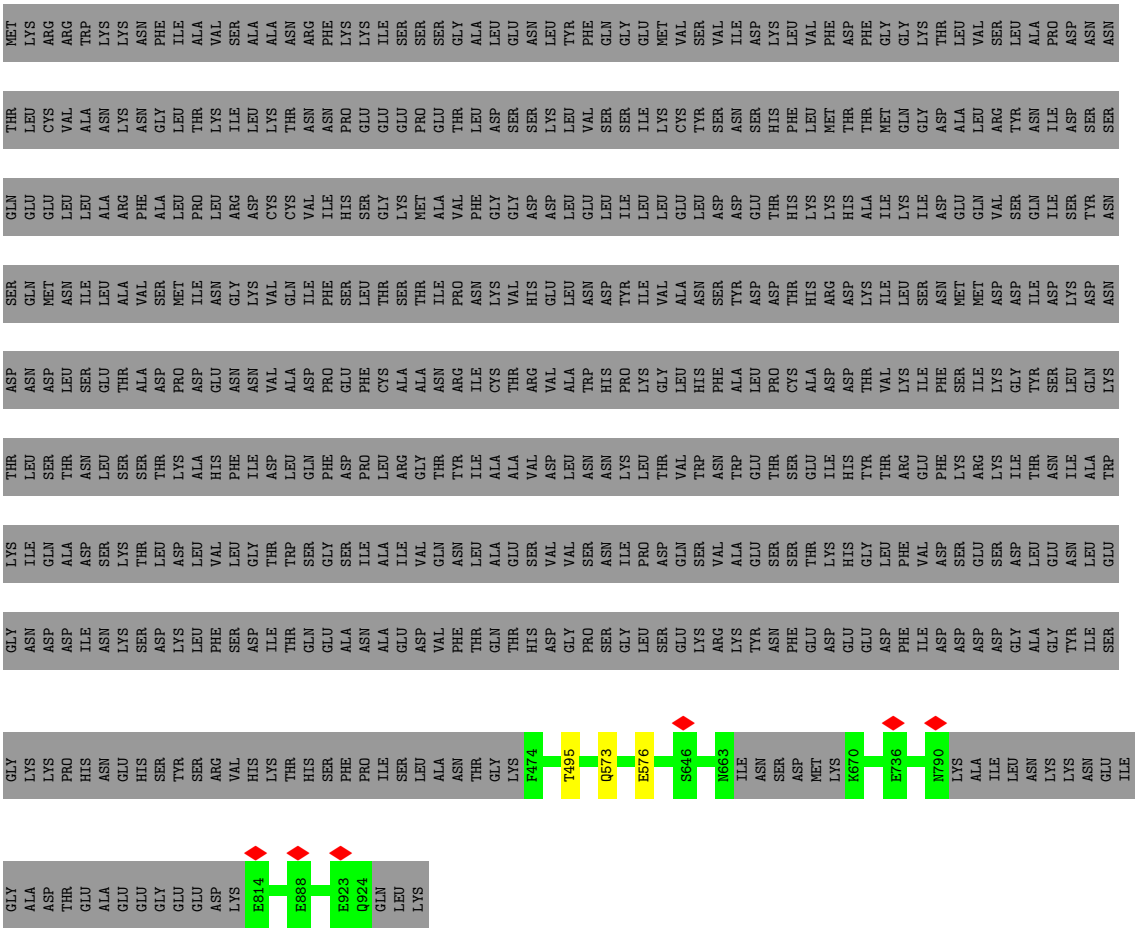
Chain F:





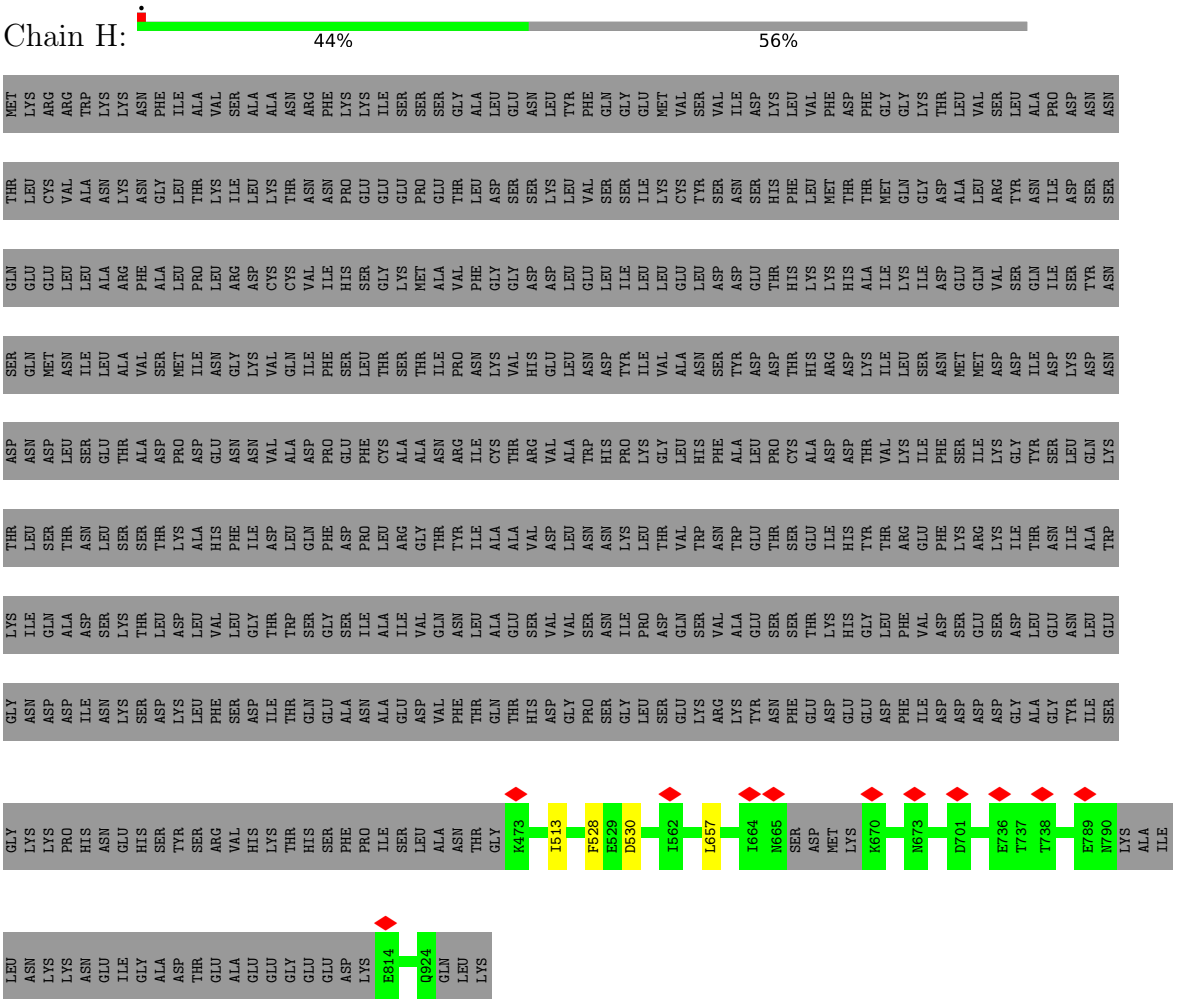
• Molecule 12: DNA polymerase alpha-binding protein

Chain G:



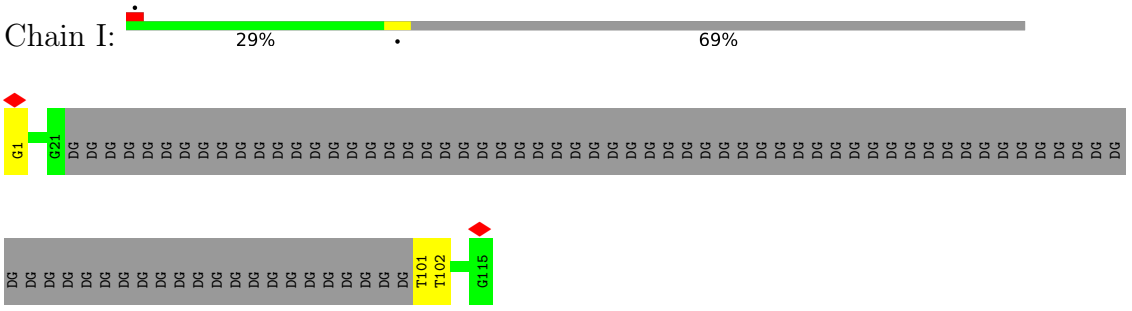
• Molecule 12: DNA polymerase alpha-binding protein

Chain H:



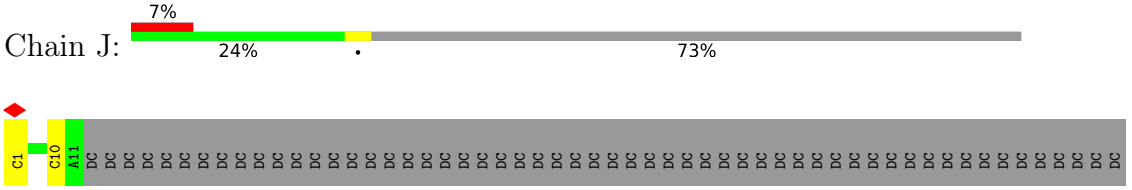
• Molecule 13: Leading strand template DNA

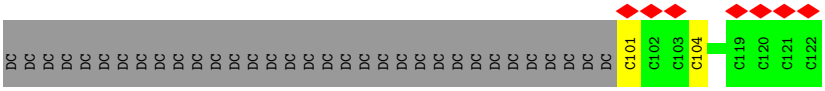
Chain I:



• Molecule 14: Lagging strand template DNA

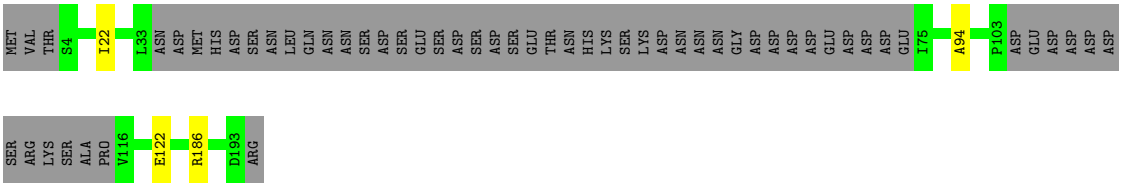
Chain J:





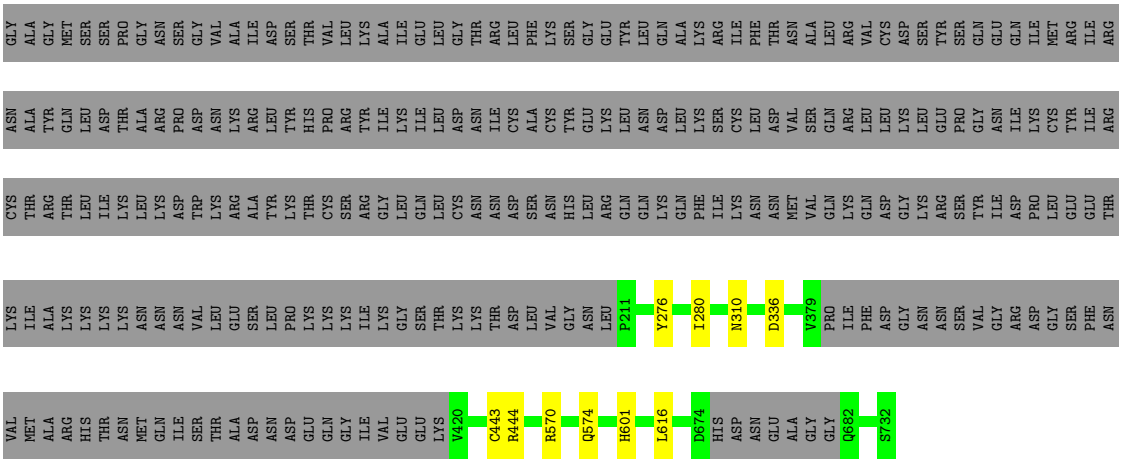
• Molecule 15: E3 ubiquitin ligase complex SCF subunit

Chain K:



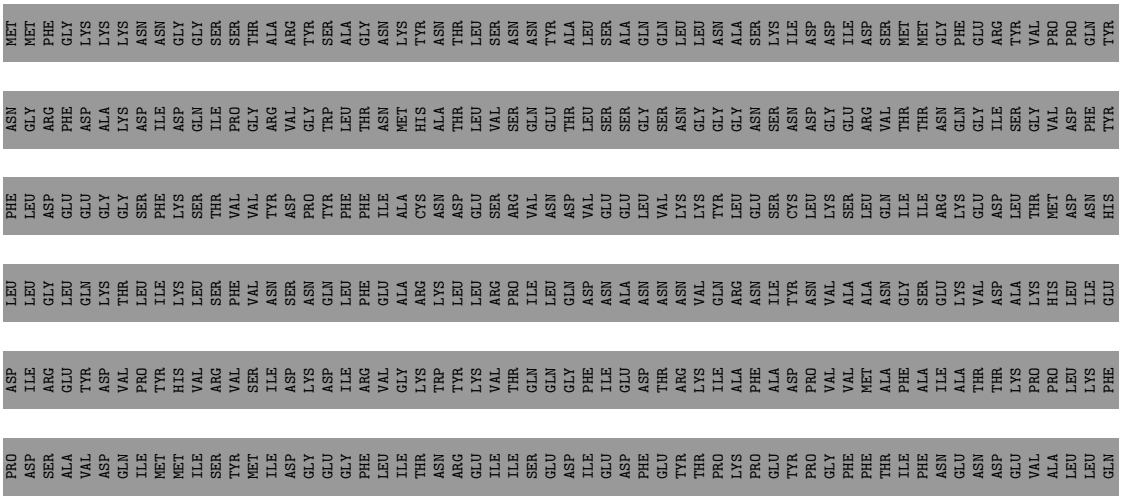
• Molecule 16: Protein DIA2

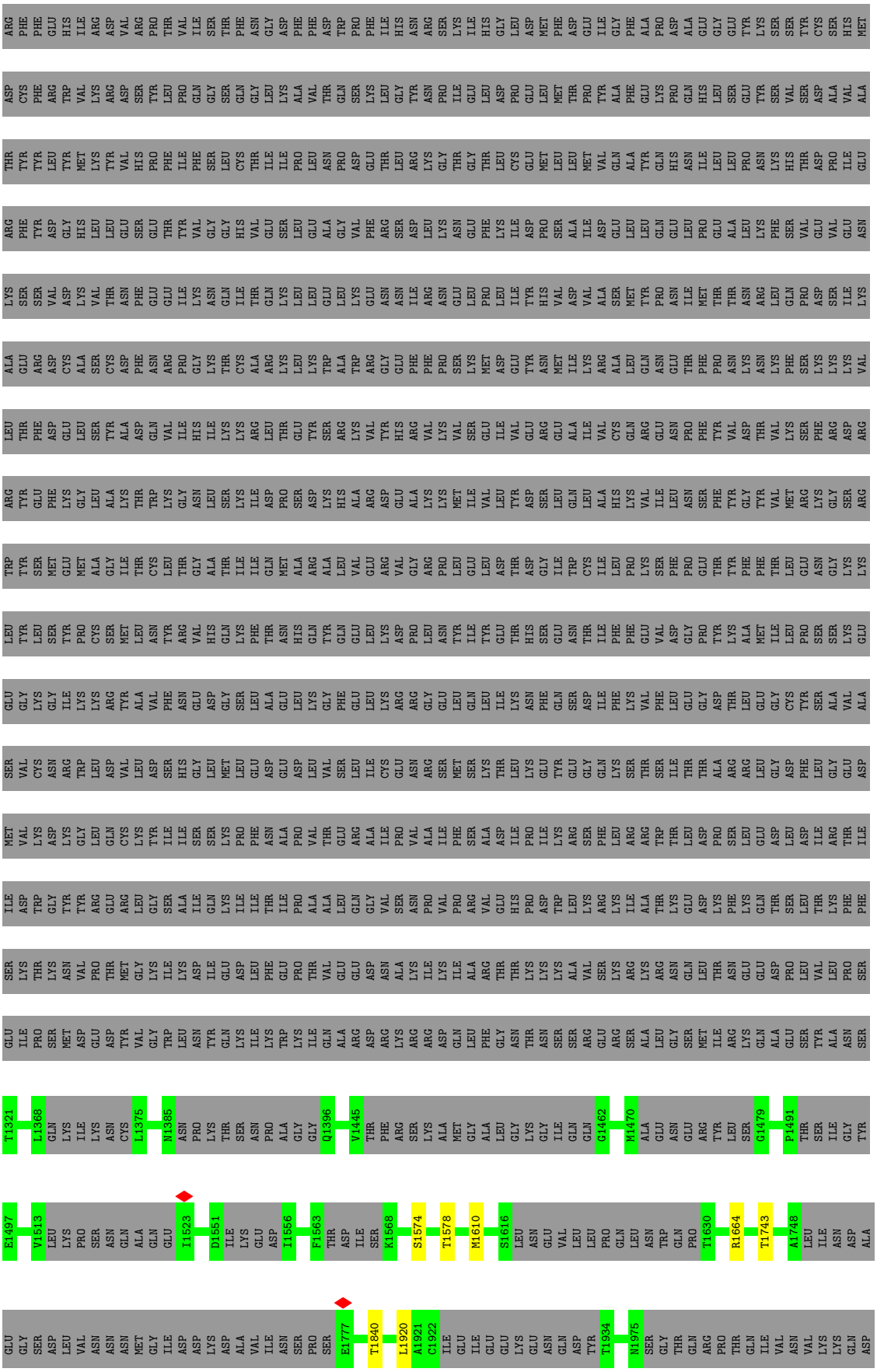
Chain L:

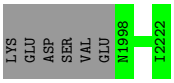


• Molecule 17: DNA polymerase epsilon catalytic subunit A

Chain Q:

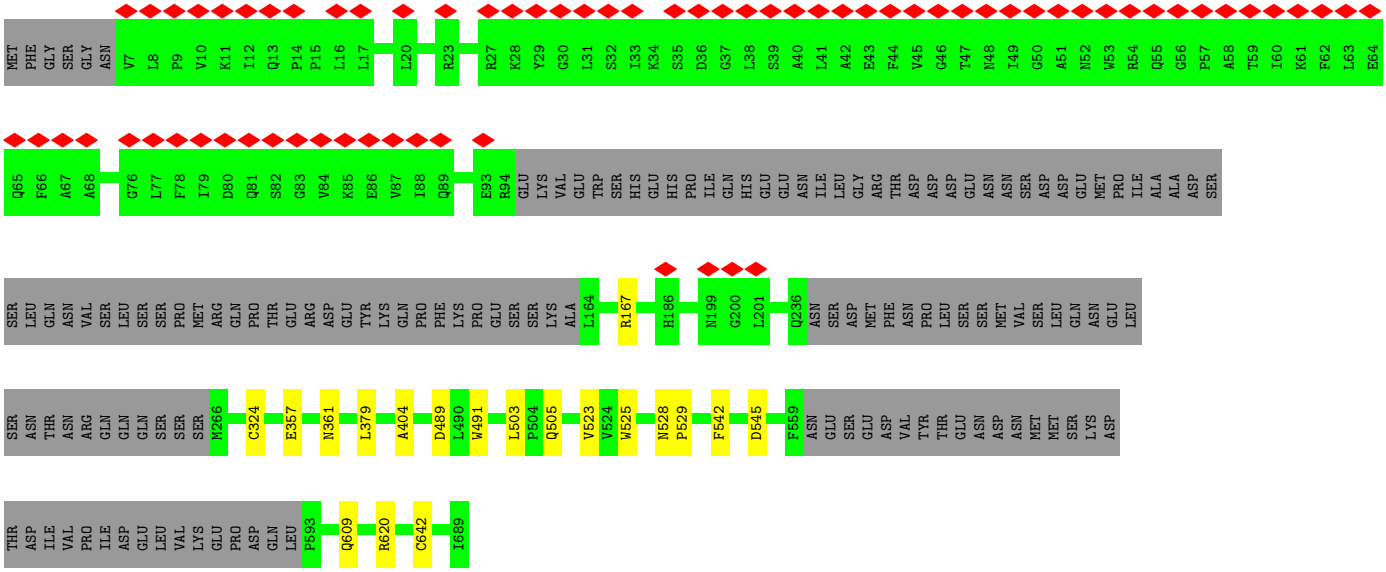



T1321
L1368
L1375
N1385
Q1396
V1445
G1462
M1470
G1479
P1491
E1497
Y1513
I1523
D1551
T1556
F1563
K1568
S1574
T1578
M1610
S1616
T1630
R1664
T1743
A1748
E1777
T1840
L1920
A1921
C1922
T1934
M1975



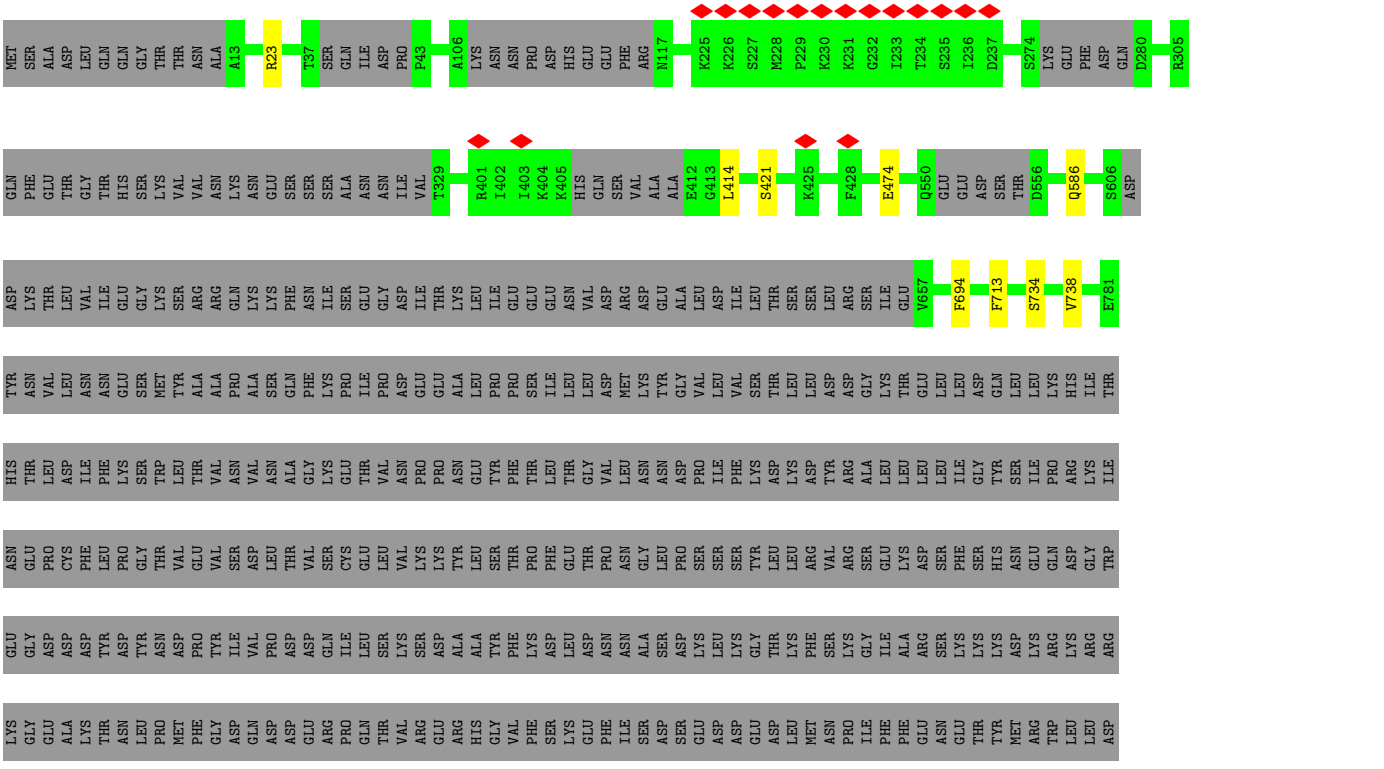
• Molecule 18: DNA polymerase epsilon subunit B

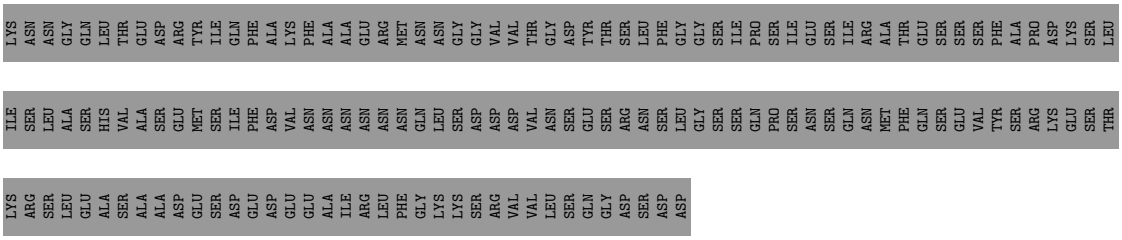
Chain R:



• Molecule 19: Topoisomerase 1-associated factor 1

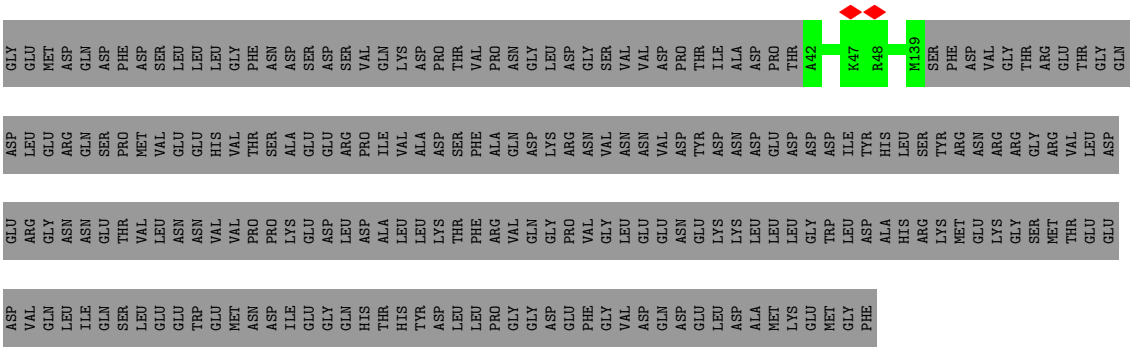
Chain X:





• Molecule 20: Chromosome segregation in meiosis protein 3

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	369254	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 ($e^-/Å^2$)	38.8	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	72.258	Depositor
Minimum map value	-40.891	Depositor
Average map value	0.048	Depositor
Map value standard deviation	1.677	Depositor
Recommended contour level	7.09	Depositor
Map size (Å)	398.55997, 398.55997, 398.55997	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.34	0/5264	0.68	0/7111
2	3	0.31	0/4843	0.65	0/6565
3	4	0.32	0/4819	0.67	0/6512
4	5	0.34	0/5407	0.67	2/7300 (0.0%)
5	6	0.32	0/5095	0.67	0/6875
6	7	0.31	0/4987	0.64	0/6747
7	A	0.32	0/1631	0.65	0/2194
8	B	0.30	0/1642	0.63	0/2221
9	C	0.32	0/1414	0.56	0/1911
10	D	0.32	0/2040	0.60	0/2755
11	E	0.31	0/4653	0.64	0/6297
12	F	0.31	0/3489	0.63	0/4724
12	G	0.31	0/3465	0.63	0/4696
12	H	0.32	0/3496	0.62	0/4735
13	I	0.79	0/883	1.18	3/1371 (0.2%)
14	J	1.22	1/694 (0.1%)	1.39	3/1053 (0.3%)
15	K	0.34	0/1139	0.68	0/1539
16	L	0.36	0/3996	0.66	0/5395
17	Q	0.33	0/6332	0.61	0/8548
18	R	0.34	0/4526	0.65	0/6125
19	X	0.33	0/5512	0.61	0/7426
20	Y	0.33	0/807	0.61	0/1084
All	All	0.35	1/76134 (0.0%)	0.67	8/103184 (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
16	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	104	DC	C1'-N1	7.01	1.58	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	101	DT	OP1-P-OP2	-7.19	108.81	119.60
13	I	1	DG	OP1-P-OP2	-6.54	109.80	119.60
14	J	1	DC	OP1-P-OP2	-6.38	110.04	119.60
14	J	101	DC	OP1-P-OP2	-6.17	110.35	119.60
13	I	102	DT	P-O3'-C3'	5.67	126.50	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	L	601	HIS	Peptide
18	R	489	ASP	Peptide

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	5175	0	5219	6	0
2	3	4759	0	4819	7	0
3	4	4749	0	4816	3	0
4	5	5332	0	5397	3	0
5	6	5013	0	5022	5	0
6	7	4914	0	4949	6	0
7	A	1611	0	1615	2	0
8	B	1609	0	1662	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1381	0	1394	0	0
10	D	2004	0	2001	2	0
11	E	4569	0	4556	3	0
12	F	3404	0	3352	1	0
12	G	3380	0	3310	1	0
12	H	3411	0	3355	2	0
13	I	782	0	403	0	0
14	J	629	0	365	0	0
15	K	1120	0	1111	1	0
16	L	3921	0	4025	3	0
17	Q	6203	0	6270	2	0
18	R	4427	0	4480	10	0
19	X	5410	0	5573	3	0
20	Y	791	0	811	0	0
21	2	31	0	13	2	0
21	3	31	0	13	1	0
21	5	31	0	13	2	0
22	2	1	0	0	0	0
22	3	1	0	0	0	0
22	5	1	0	0	0	0
23	2	1	0	0	0	0
23	4	1	0	0	0	0
23	5	1	0	0	0	0
23	6	1	0	0	0	0
23	7	1	0	0	0	0
23	Q	2	0	0	0	0
All	All	74697	0	74544	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:412:SER:H	21:3:1500:ANP:HNB1	1.44	0.66
6:7:106:ILE:HG22	6:7:113:PHE:CG	2.41	0.55
6:7:529:MET:HE1	6:7:537:ILE:HD12	1.88	0.55
1:2:546:GLY:H	21:2:1500:ANP:HNB1	1.55	0.53
18:R:503:LEU:HD11	18:R:542:PHE:HE1	1.73	0.53

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	649/868 (75%)	636 (98%)	13 (2%)	0	100	100
2	3	595/1009 (59%)	584 (98%)	10 (2%)	1 (0%)	47	79
3	4	585/933 (63%)	573 (98%)	12 (2%)	0	100	100
4	5	659/775 (85%)	641 (97%)	18 (3%)	0	100	100
5	6	625/1017 (62%)	602 (96%)	23 (4%)	0	100	100
6	7	611/845 (72%)	597 (98%)	14 (2%)	0	100	100
7	A	193/208 (93%)	187 (97%)	6 (3%)	0	100	100
8	B	188/213 (88%)	182 (97%)	6 (3%)	0	100	100
9	C	165/194 (85%)	163 (99%)	2 (1%)	0	100	100
10	D	237/294 (81%)	232 (98%)	5 (2%)	0	100	100
11	E	554/657 (84%)	547 (99%)	7 (1%)	0	100	100
12	F	418/962 (44%)	407 (97%)	11 (3%)	0	100	100
12	G	416/962 (43%)	404 (97%)	12 (3%)	0	100	100
12	H	419/962 (44%)	410 (98%)	9 (2%)	0	100	100
15	K	131/194 (68%)	123 (94%)	8 (6%)	0	100	100
16	L	469/735 (64%)	445 (95%)	24 (5%)	0	100	100
17	Q	740/2222 (33%)	720 (97%)	20 (3%)	0	100	100
18	R	544/689 (79%)	530 (97%)	14 (3%)	0	100	100
19	X	649/1238 (52%)	636 (98%)	13 (2%)	0	100	100
20	Y	96/319 (30%)	95 (99%)	1 (1%)	0	100	100
All	All	8943/15296 (58%)	8714 (97%)	228 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	443	THR

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	569/770 (74%)	564 (99%)	5 (1%)	78 91
2	3	522/866 (60%)	522 (100%)	0	100 100
3	4	539/848 (64%)	538 (100%)	1 (0%)	93 98
4	5	604/688 (88%)	598 (99%)	6 (1%)	76 90
5	6	550/886 (62%)	545 (99%)	5 (1%)	78 91
6	7	542/753 (72%)	538 (99%)	4 (1%)	84 94
7	A	182/193 (94%)	181 (100%)	1 (0%)	88 95
8	B	182/198 (92%)	181 (100%)	1 (0%)	88 95
9	C	154/173 (89%)	154 (100%)	0	100 100
10	D	234/279 (84%)	234 (100%)	0	100 100
11	E	507/592 (86%)	502 (99%)	5 (1%)	76 90
12	F	375/854 (44%)	374 (100%)	1 (0%)	92 96
12	G	372/854 (44%)	371 (100%)	1 (0%)	92 96
12	H	375/854 (44%)	374 (100%)	1 (0%)	92 96
15	K	124/179 (69%)	122 (98%)	2 (2%)	62 84
16	L	456/686 (66%)	453 (99%)	3 (1%)	84 94
17	Q	701/2012 (35%)	698 (100%)	3 (0%)	91 95
18	R	498/629 (79%)	494 (99%)	4 (1%)	81 93
19	X	607/1125 (54%)	603 (99%)	4 (1%)	84 94
20	Y	85/286 (30%)	85 (100%)	0	100 100
All	All	8178/13725 (60%)	8131 (99%)	47 (1%)	86 94

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	F	749	TYR
16	L	616	LEU
12	G	495	THR

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Mol	Chain	Res	Type
15	K	186	ARG
17	Q	1664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
18	R	609	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	ANP	2	1500	-	29,33,33	1.12	4 (13%)	31,52,52	0.98	2 (6%)
21	ANP	3	1500	-	29,33,33	1.13	4 (13%)	31,52,52	1.00	2 (6%)
21	ANP	5	1500	-	29,33,33	1.09	4 (13%)	31,52,52	1.04	2 (6%)

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
21	ANP	2	1500	-	-	3/14/38/38	0/3/3/3
21	ANP	3	1500	-	-	3/14/38/38	0/3/3/3
21	ANP	5	1500	-	-	4/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	1500	ANP	PB-O3A	-3.38	1.54	1.59
21	2	1500	ANP	PB-O3A	-3.19	1.55	1.59
21	5	1500	ANP	PB-O3A	-2.81	1.55	1.59
21	2	1500	ANP	PG-O1G	2.40	1.50	1.46
21	3	1500	ANP	PG-O1G	2.39	1.49	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	1500	ANP	PB-O3A-PA	-3.60	119.93	132.62
21	2	1500	ANP	PB-O3A-PA	-3.09	121.72	132.62
21	3	1500	ANP	PB-O3A-PA	-2.89	122.44	132.62
21	5	1500	ANP	C5-C6-N6	2.35	123.93	120.35
21	3	1500	ANP	C5-C6-N6	2.30	123.84	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	2	1500	ANP	PB-N3B-PG-O1G
21	2	1500	ANP	PA-O3A-PB-O1B
21	2	1500	ANP	PA-O3A-PB-O2B
21	3	1500	ANP	PB-N3B-PG-O1G
21	3	1500	ANP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	1500	ANP	2	0
21	3	1500	ANP	1	0

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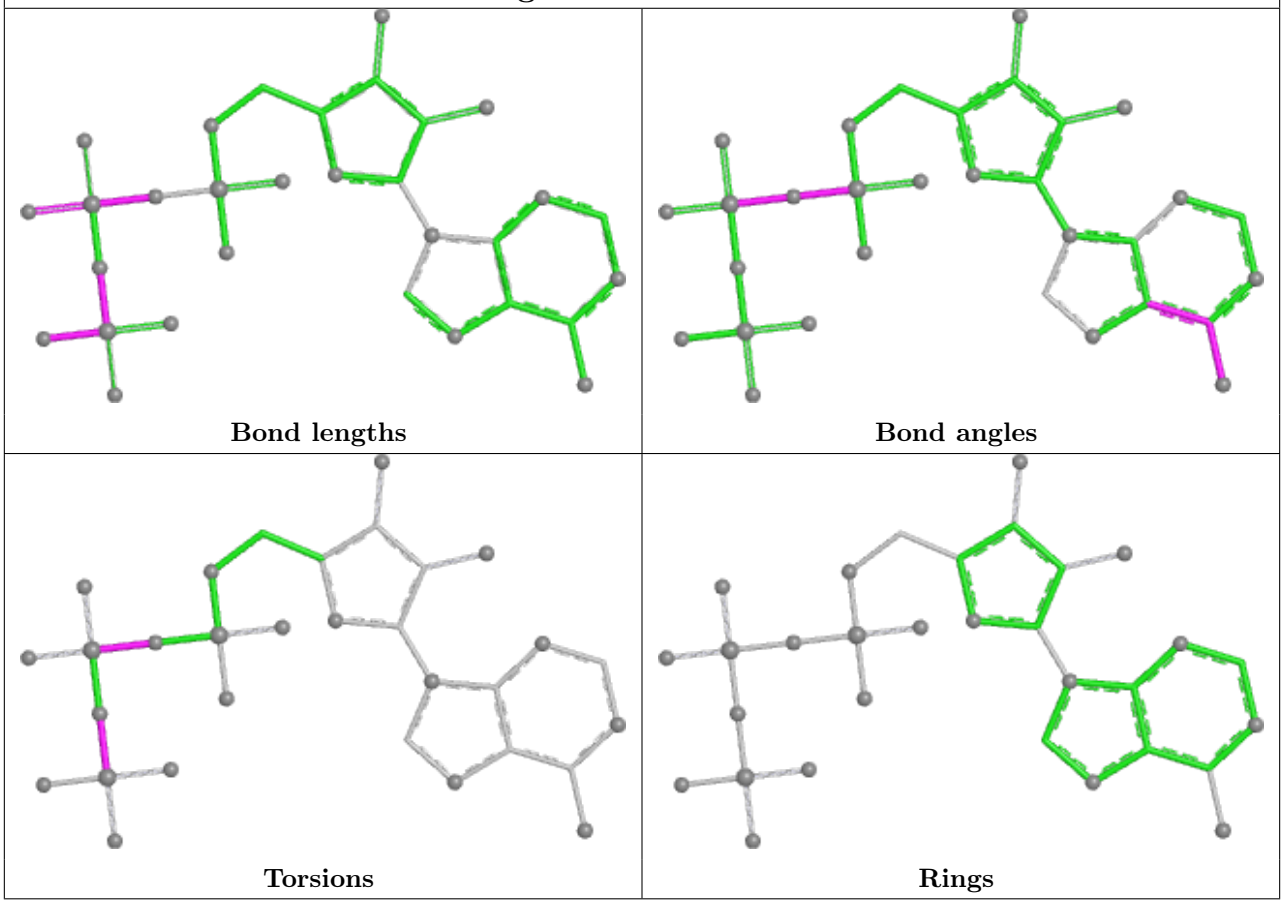
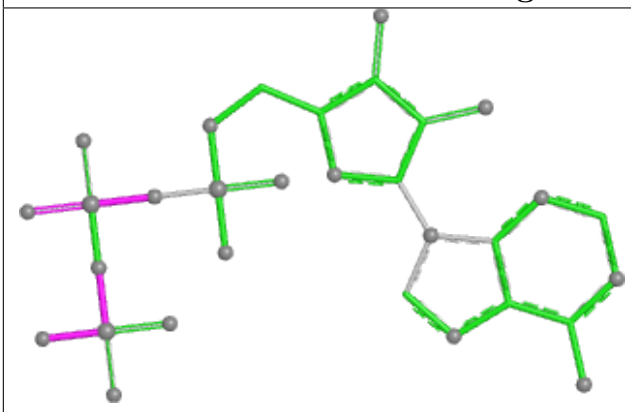
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	5	1500	ANP	2	0

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.

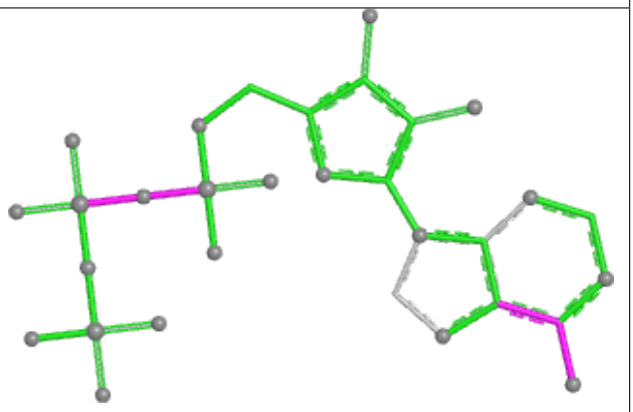
Ligand ANP 2 1500



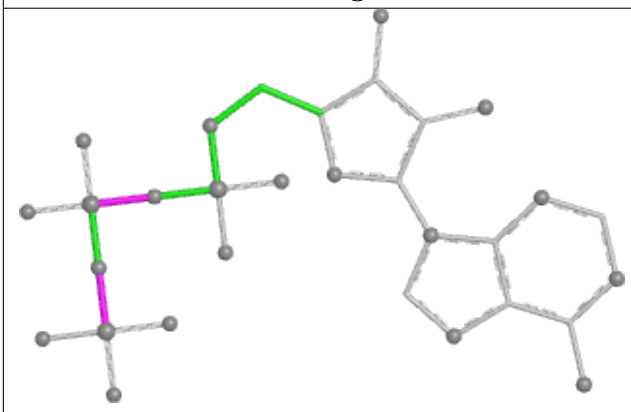
Ligand ANP 3 1500



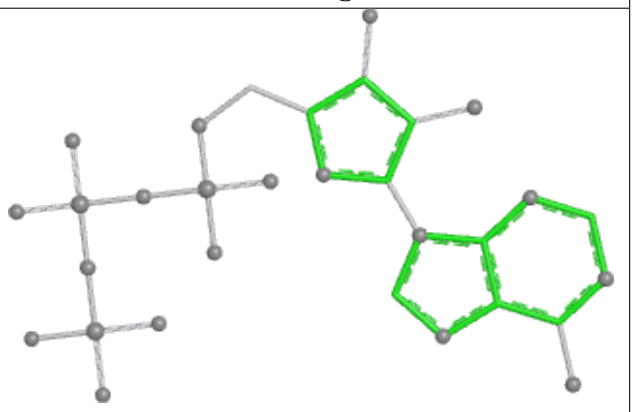
Bond lengths



Bond angles

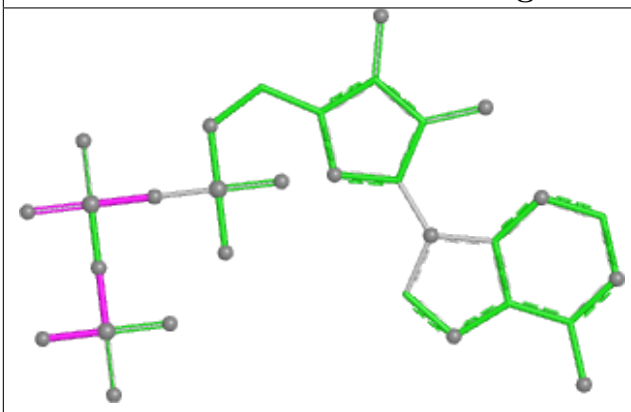


Torsions

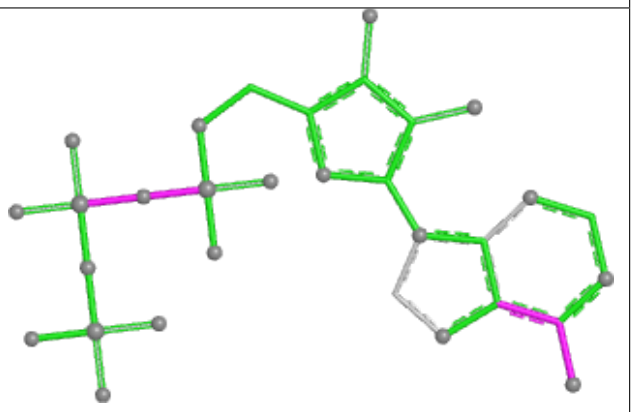


Rings

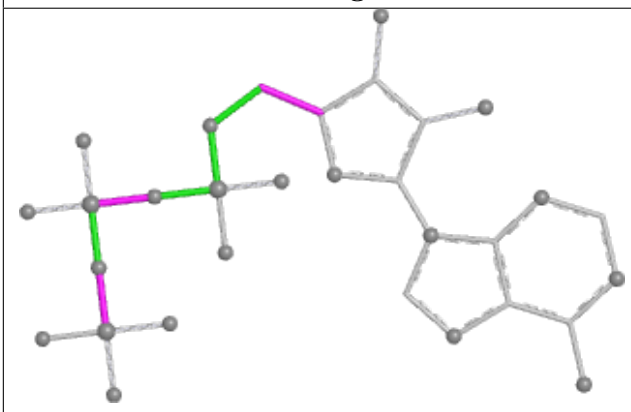
Ligand ANP 5 1500



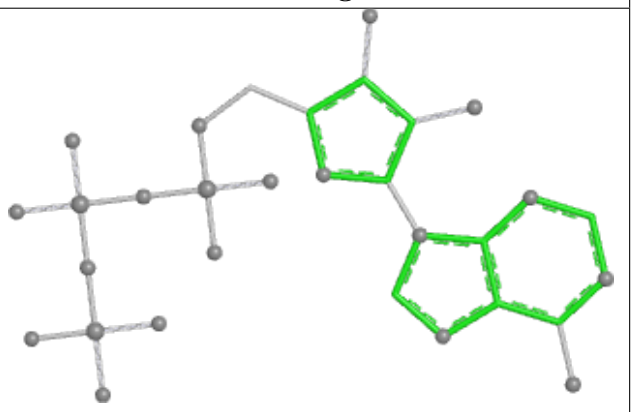
Bond lengths



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.

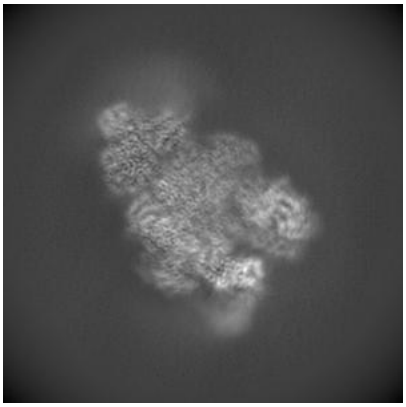
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13537. These allow visual inspection of the internal detail of the map and identification of artifacts.

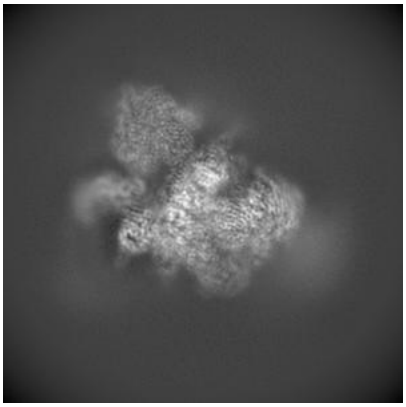
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

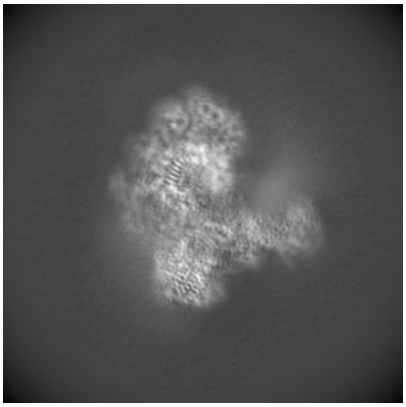
6.1.1 Primary map



X



Y

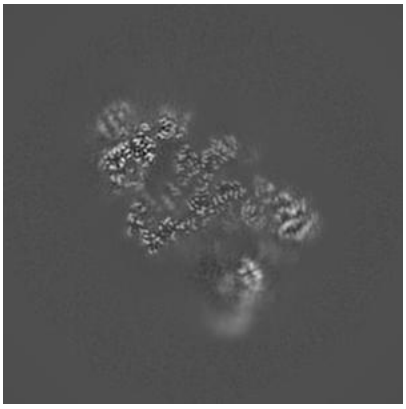


Z

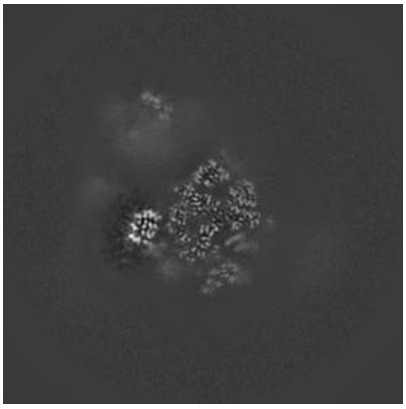
The images above show the map projected in three orthogonal directions.

6.2 Central slices

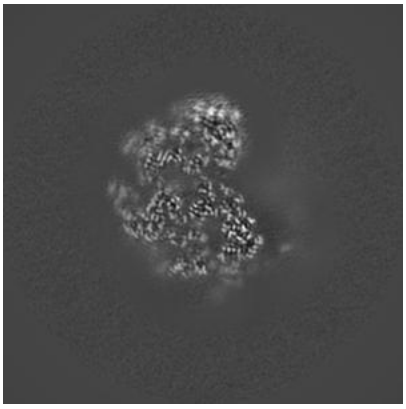
6.2.1 Primary map



X Index: 188



Y Index: 188

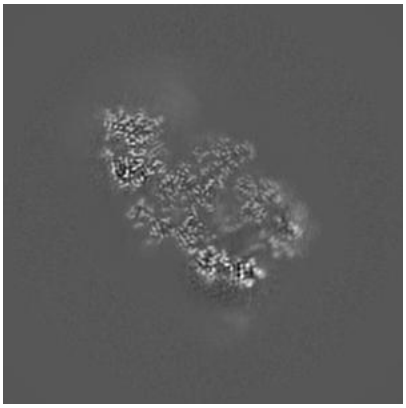


Z Index: 188

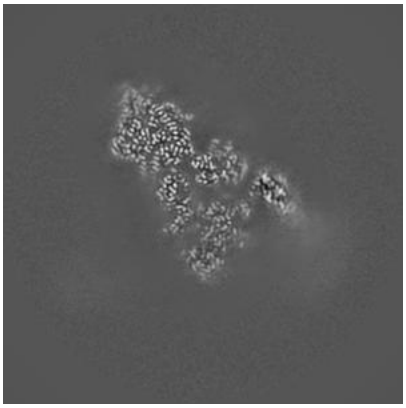
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

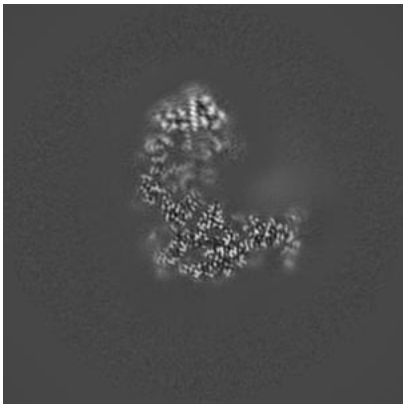
6.3.1 Primary map



X Index: 166



Y Index: 161



Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 7.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

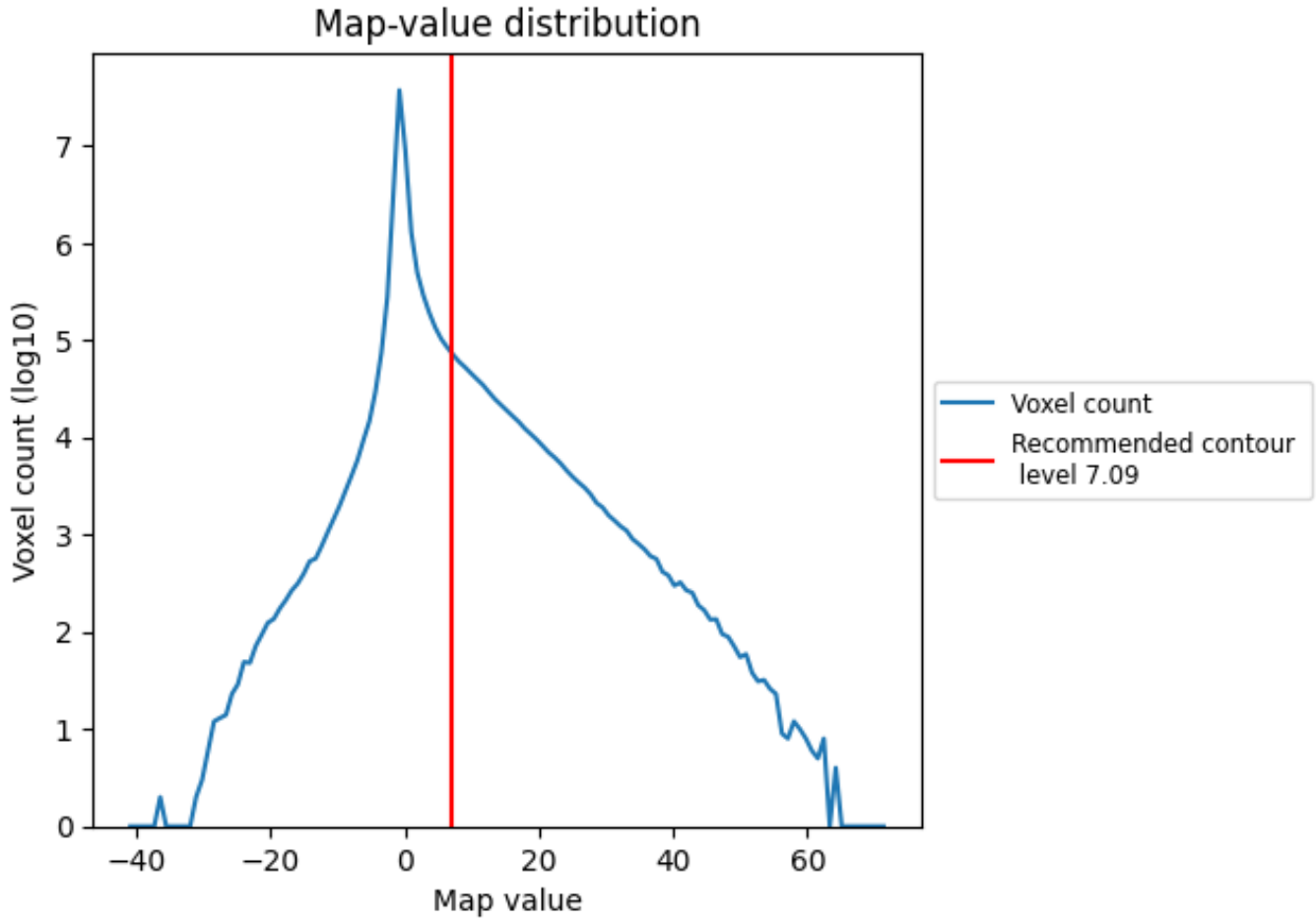
6.5 Mask visualisation (i)

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

7 Map analysis

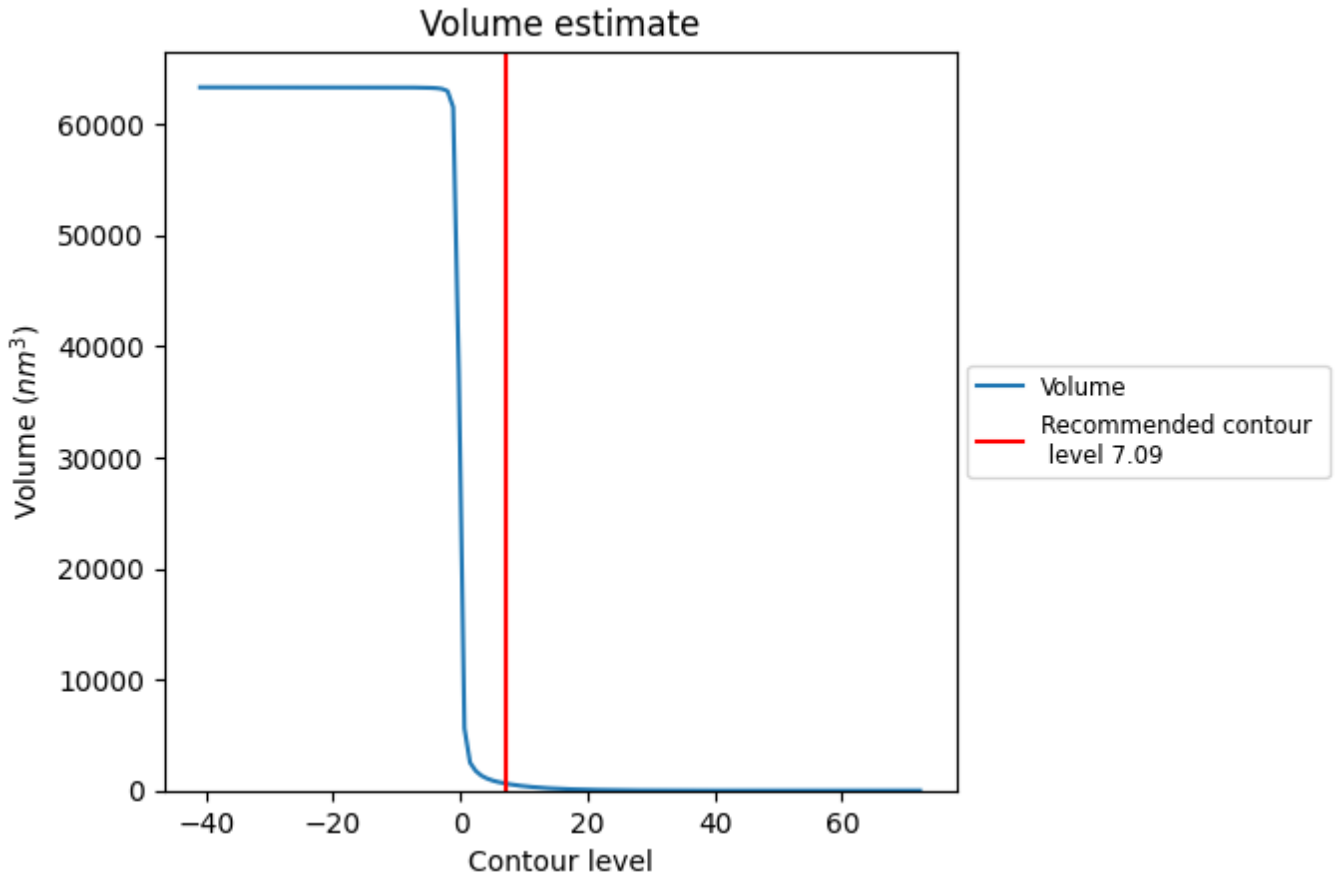
This section contains the results of statistical analysis of the map.

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.

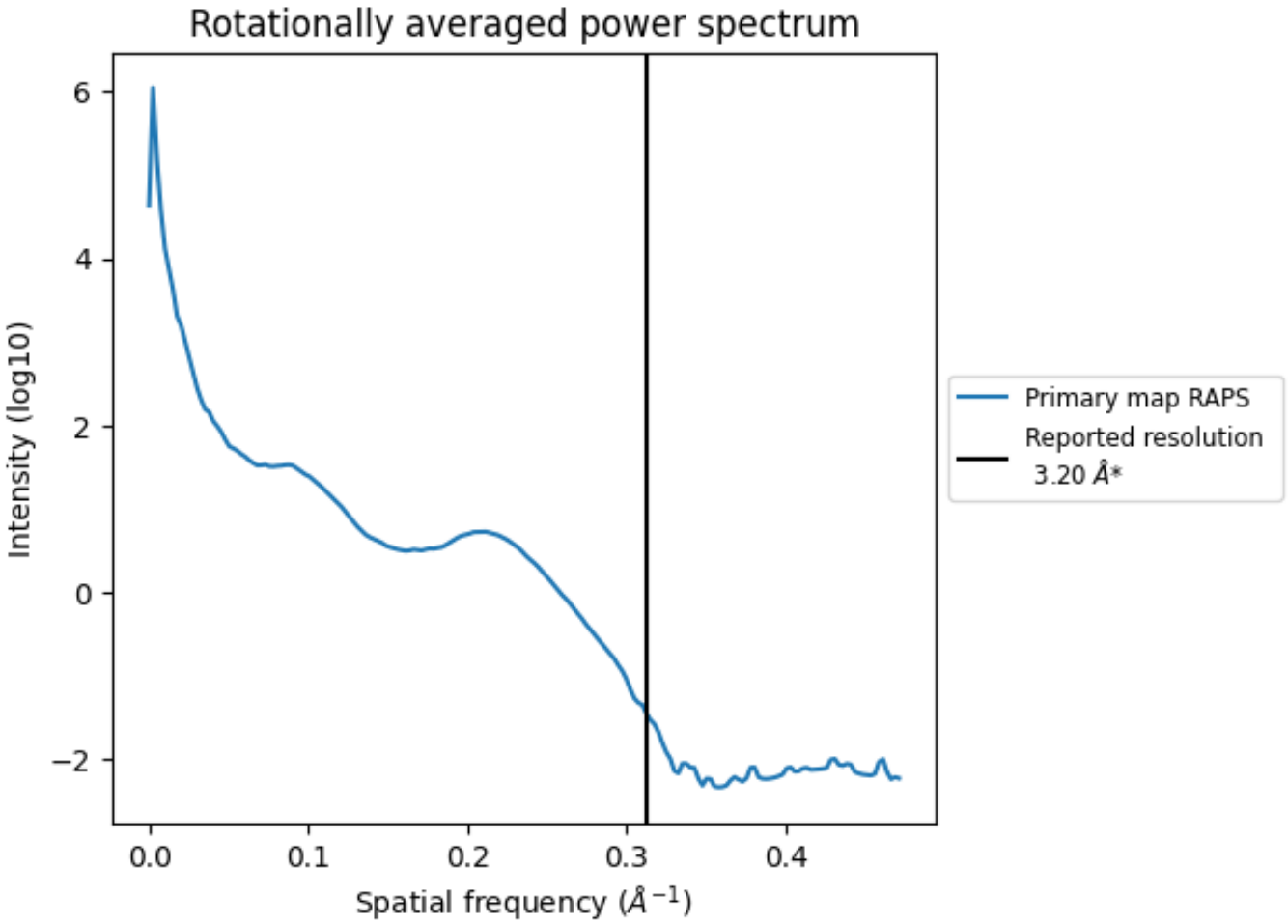
7.2 Volume estimate (i)



The volume at the recommended contour level is 636 nm^3; this corresponds to an approximate mass of 575 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 0.312 $Å^{-1}$

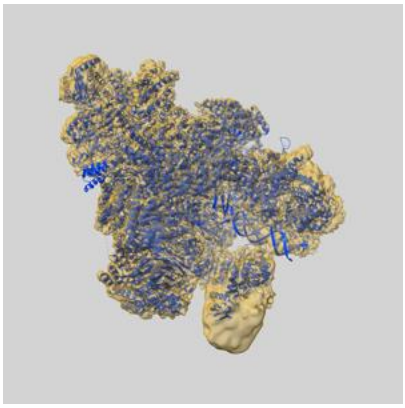
8 Fourier-Shell correlation (i)

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

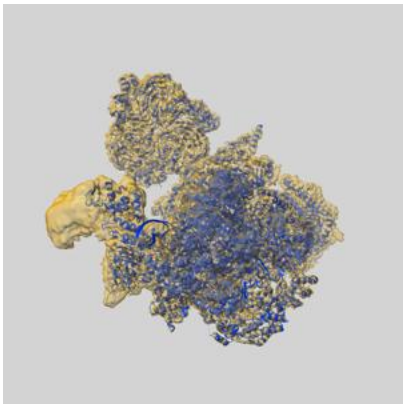
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13537 and PDB model 7PMK. Per-residue inclusion information can be found in section 3 on page 13.

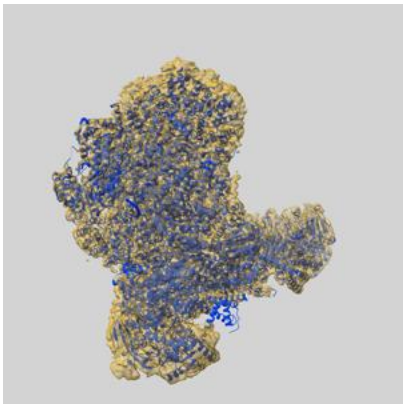
9.1 Map-model overlay



X



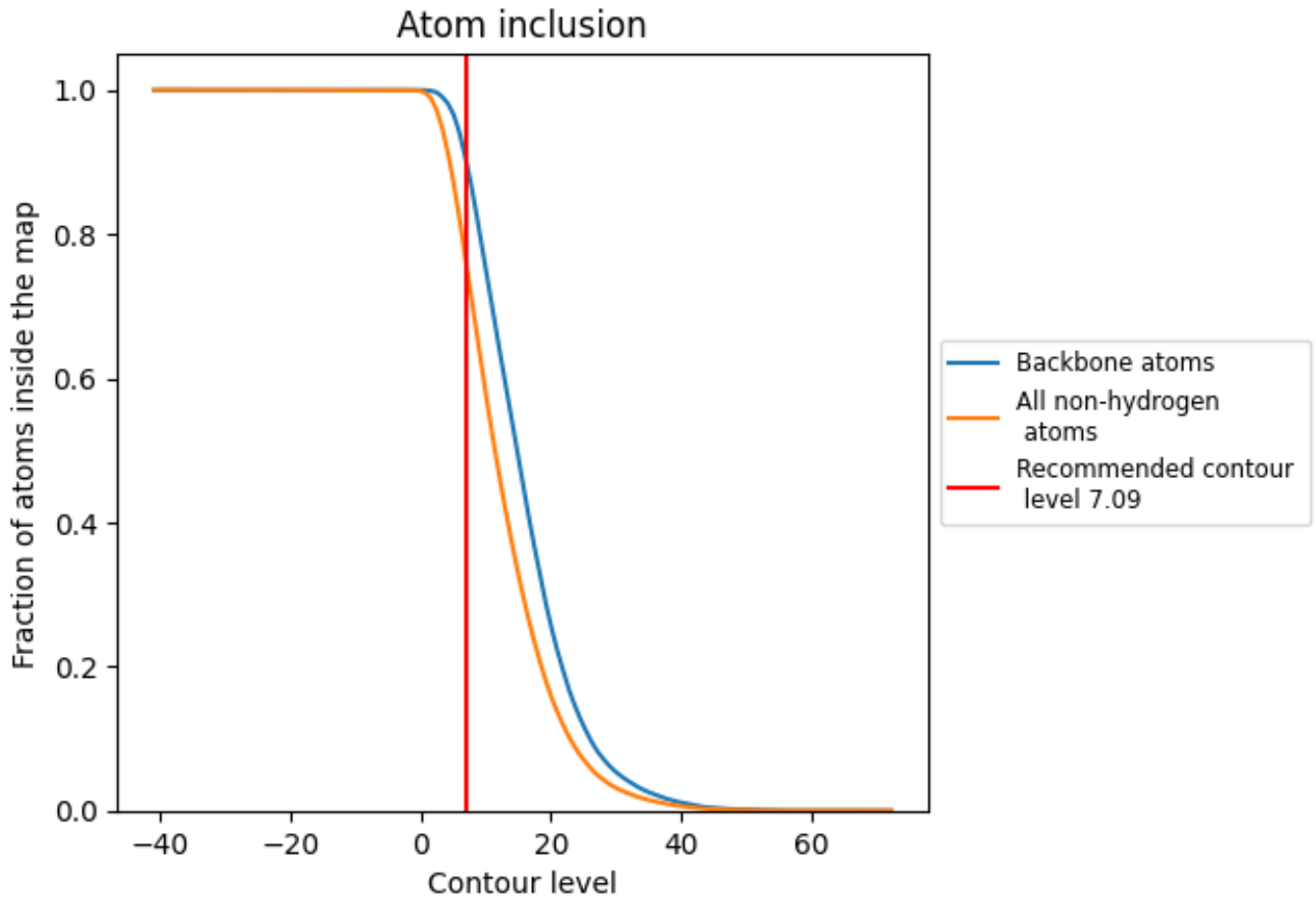
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.09 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 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.