



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:56 AM UTC

PDB ID : 7PMK / pdb_00007pmk
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 Full wwPDB EM Validation 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:

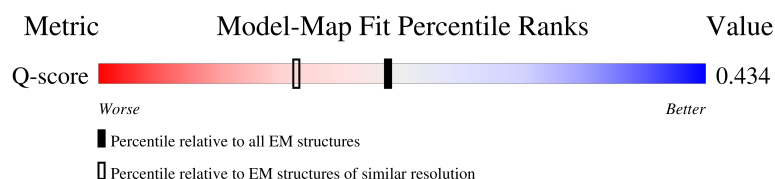
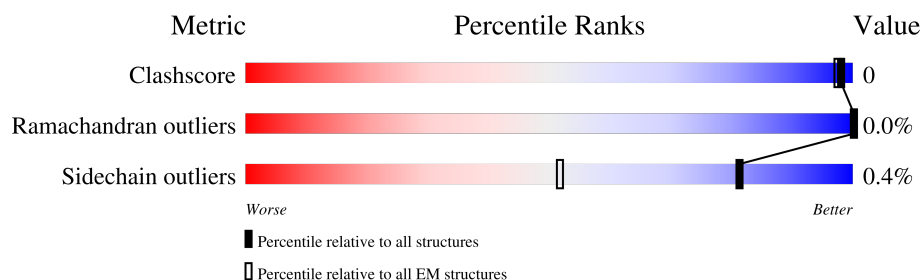
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	9% 75% 25%
2	3	1009	59% 40%
3	4	933	21% 63% 36%
4	5	775	10% 86% 13%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
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

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		

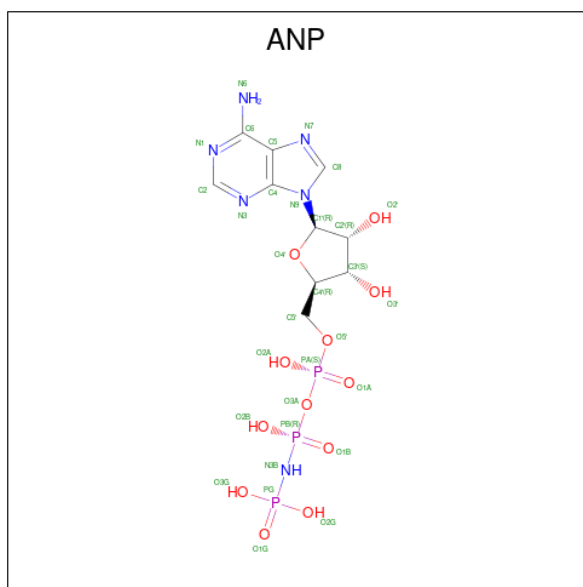
- Molecule 20 is a protein called Chromosome segregation in meiosis protein 3.

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 (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
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	

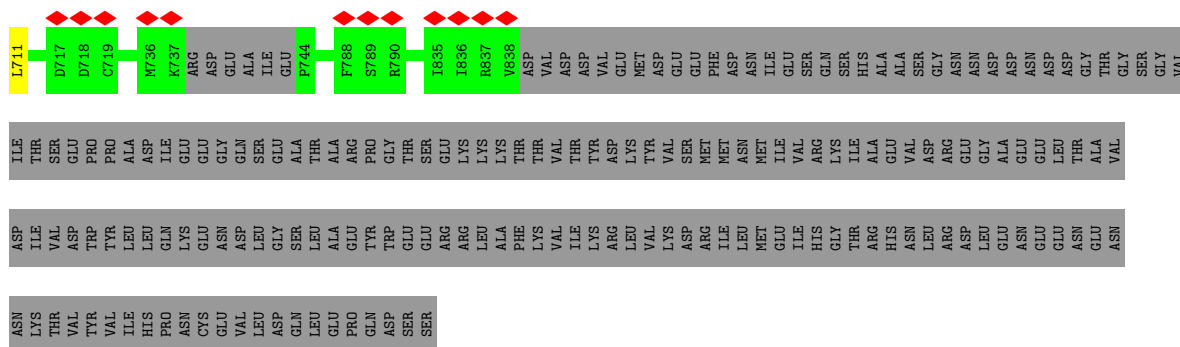
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

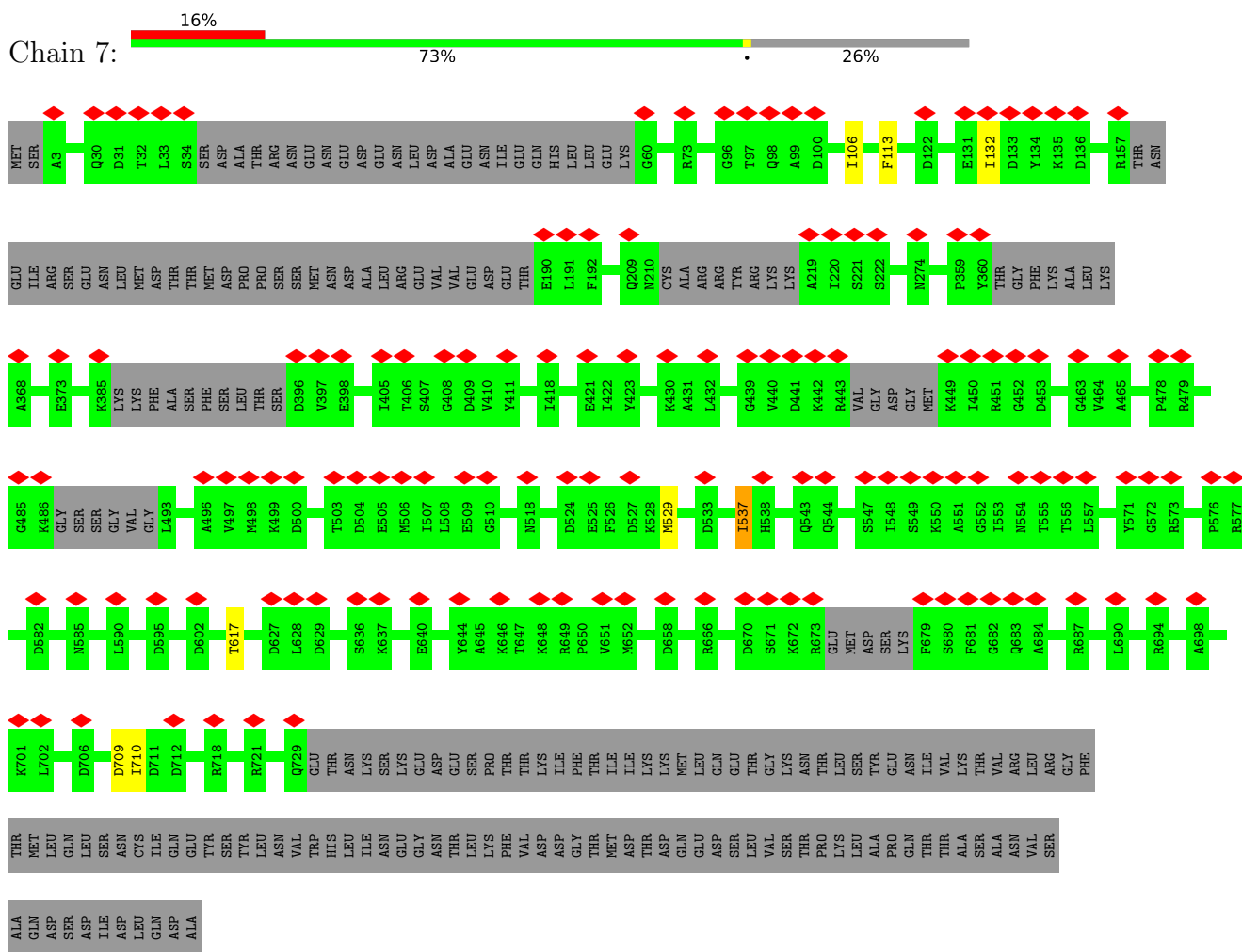
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

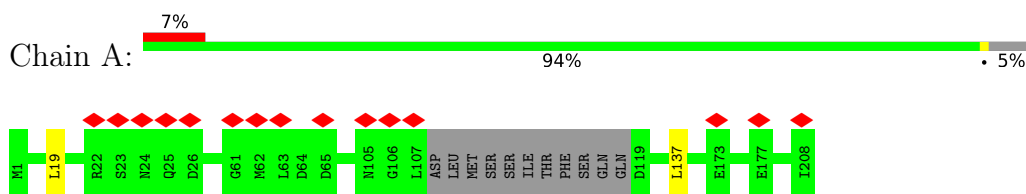




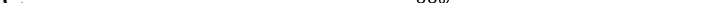
- Molecule 6: DNA replication licensing factor MCM7



- Molecule 7: DNA replication complex GINS protein PSF1



- Molecule 8: DNA replication complex GINS protein PSF2

- Chain C:  88% 12%

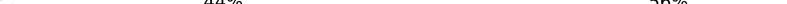
MET G2 D23 G58 ASP GLU ALA LEU VAL ASP ASP GLU P68 I144 ASP LEU ASN ALA ASP SER THR LYS ASN SER SER ALA ASN T158 K194

- Chain D:  82% 17%

- Chain E: 

M1	Y2	E10	L45	L82	D106	T107	D108	GLU	LYS	S111	G112	S137	D166	GLU	GLU	GLU	SER	SER	GLY	ASP	ASP	GLU	GLU	LEU	SER	SER	GLY	ASP	GLU	ASN	ASN	ASN	GLY	GLY	ASP	ASP	GLU	GLU	THR	ASP	ALA	ASP	ASP	GLU	VAL	ALA	LYS	ASP	ASP	ASP	GLY	ASP	TYR	TYR
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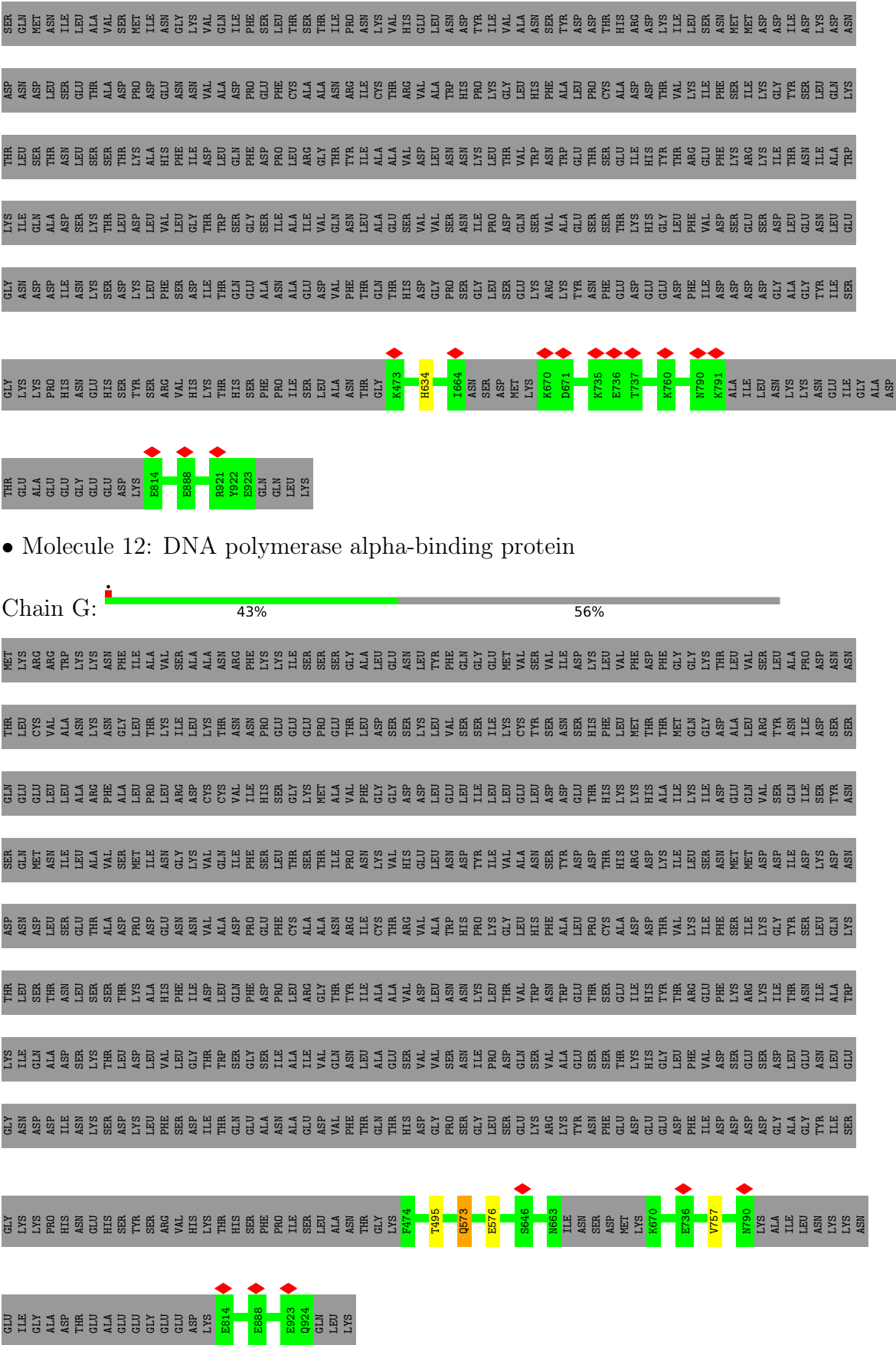
Lys	Asp	Asp	Asp	Glu	Thr	Ile	Ser	Ser	Asn	Arg	Gly	Asn	Ser	Ser	Gly	Pro	Asn	Asp	Leu	Ser	Lys	R223	R224	Q225	R307	N308	S309	M436	Ser	Thr	Asp	Lys	Asp	Val	Lys	Ile	Asn	Asn	Asp	Asn	Asp	Thr	Asp	Gly	Glu	Glu	Glu	Asp	N461	S462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930
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- Chain F: 

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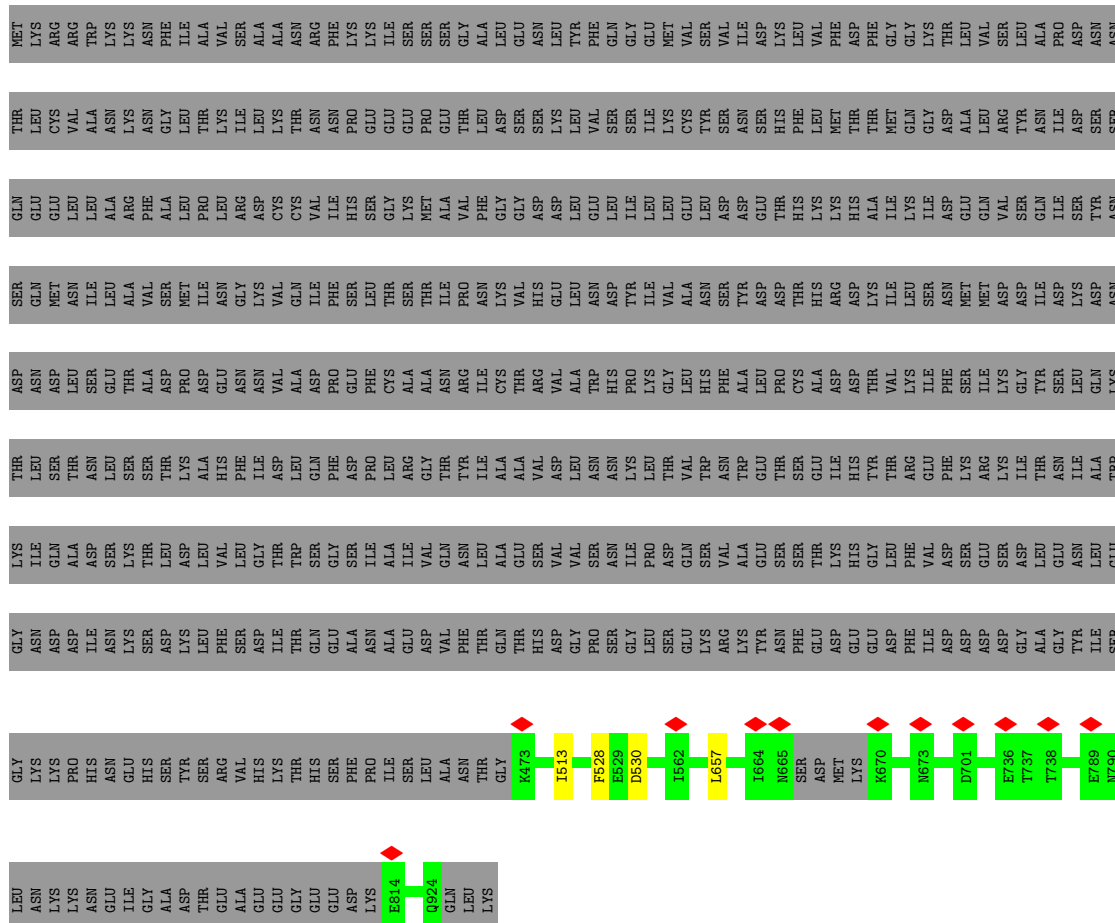
THR	LEU	CYS	VAL	ALA	ASN	LYS	GLY	LEU	THR	LYS	ILE	LEU	LEU	THR	ASN	PRO	GLU	GLU	GLY	GLU	PRO	GLU	THR	LEU	SER	SER	LYS	SER	VAL	SER	SER	SER	ILE	CYS	LYS	THR	THR	THR	MET	LEU	PHE	HIS	SER	ASP	ASP	GLN	GLY	ASP	ALA	LEU	ARG	TYR	ASN	ASP	ASP	SER
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GLN	GLU	GLU	LEU	LEU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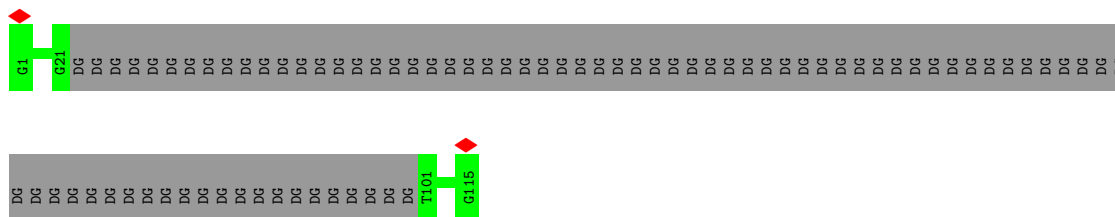


● Molecule 12: DNA polymerase alpha-binding protein

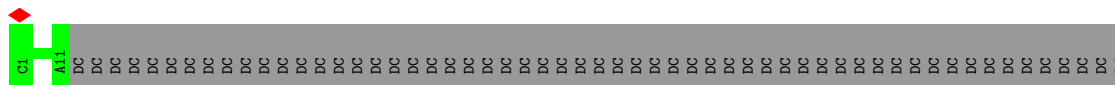
- Molecule 12: DNA polymerase alpha-binding protein



- Molecule 13: Leading strand template DNA

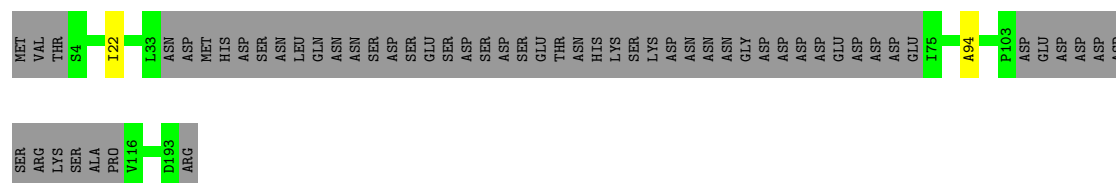


- Molecule 14: Lagging strand template DNA



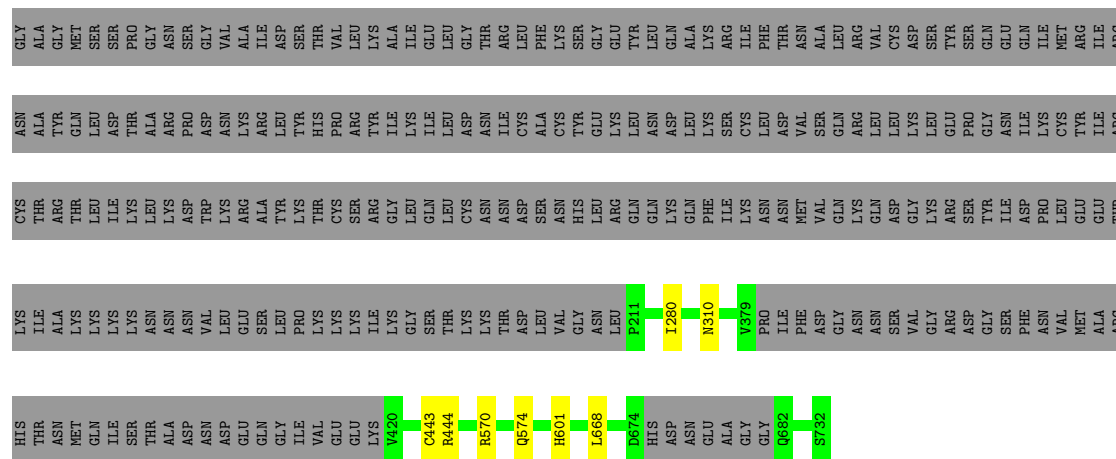
- Molecule 15: E3 ubiquitin ligase complex SCF subunit

Chain K:  70% : 29%



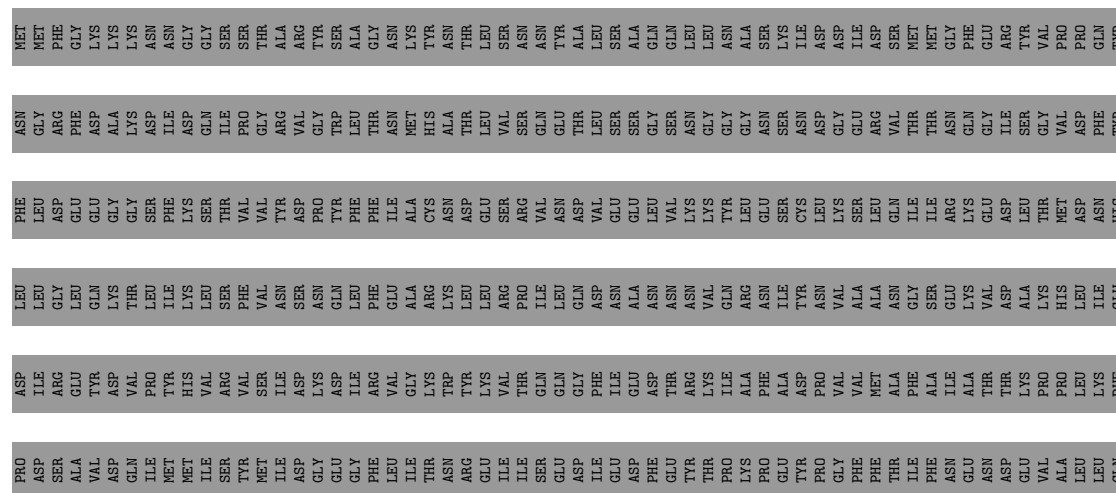
- Molecule 16: Protein DIA2

Chain L: 64% 35%



- Molecule 17: DNA polymerase epsilon catalytic subunit A

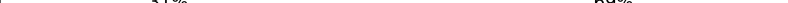
Chain Q: 34% 66%





LYS	ARG	SER	LEU	GLU	ALA	SER	ALA	ALA	ASP	GLU	SER	ASP	GLU	ASP	GLU	GLU	ALA	ILE	ARG	LEU	PHE	GLY	LYS	LYS	SER	ARG	VAL	VAL	LEU	SER	GLN	GLY	ASP	SER	ASP	ASP
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- Molecule 20: Chromosome segregation in meiosis protein 3

Chain Y:  31% 69%

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

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 ($e^-/\text{\AA}^2$)	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: MG, ANP, ZN

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	0.30	0/5264	0.53	0/7111
2	3	0.28	0/4843	0.50	0/6565
3	4	0.27	0/4819	0.54	0/6512
4	5	0.31	0/5407	0.55	1/7300 (0.0%)
5	6	0.28	0/5095	0.52	0/6875
6	7	0.27	0/4987	0.51	0/6747
7	A	0.27	0/1631	0.54	0/2194
8	B	0.26	0/1642	0.48	0/2221
9	C	0.27	0/1414	0.48	0/1911
10	D	0.25	0/2040	0.47	0/2755
11	E	0.25	0/4653	0.49	0/6297
12	F	0.25	0/3489	0.49	0/4724
12	G	0.25	0/3465	0.51	0/4696
12	H	0.26	0/3496	0.50	0/4735
13	I	0.36	0/883	0.78	0/1371
14	J	0.54	0/694	0.92	0/1053
15	K	0.31	0/1139	0.59	0/1539
16	L	0.31	0/3996	0.60	0/5395
17	Q	0.28	0/6332	0.54	0/8548
18	R	0.31	0/4526	0.59	0/6125
19	X	0.28	0/5512	0.52	0/7426
20	Y	0.31	0/807	0.54	0/1084
All	All	0.28	0/76134	0.54	1/103184 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	343	TRP	CA-CB-CG	5.09	123.28	113.60

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

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	8	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	5	0
7	A	1611	0	1615	2	0
8	B	1609	0	1662	2	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	1120	0	1111	1	0
16	L	3921	0	4025	3	0
17	Q	6203	0	6270	4	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	59	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.

All (59) 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)
6:7:529:MET:HE1	6:7:537:ILE:HD12	1.48	0.95
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
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
7:A:137:LEU:HD13	10:D:185:THR:HG21	1.91	0.52
18:R:503:LEU:HD11	18:R:542:PHE:CE1	2.45	0.51
11:E:45:LEU:HD21	11:E:82:LEU:HD22	1.93	0.51
3:4:801:MET:SD	3:4:826:VAL:HG22	2.51	0.51
8:B:85:CYS:SG	8:B:86:SER:N	2.84	0.51
16:L:443:CYS:SG	16:L:444:ARG:N	2.84	0.51
4:5:419:GLY:H	21:5:1500:ANP:HNB1	1.58	0.50
19:X:694:PHE:CZ	19:X:738:VAL:HG22	2.47	0.50
2:3:676:ILE:HD12	6:7:617:THR:HB	1.93	0.50
18:R:503:LEU:O	18:R:505:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:605:ALA:HB2	5:6:648:ASP:HA	1.93	0.49
4:5:419:GLY:N	21:5:1500:ANP:HNB1	2.10	0.49
2:3:674:GLU:OE2	2:3:722:ASN:ND2	2.44	0.49
11:E:2:TYR:OH	11:E:137:SER:O	2.22	0.48
17:Q:1676:TYR:CD1	17:Q:1794:MET:HE1	2.48	0.48
1:2:546:GLY:N	21:2:1500:ANP:HNB1	2.12	0.48
19:X:734:SER:O	19:X:738:VAL:HG23	2.15	0.47
5:6:605:ALA:HB1	5:6:651:ALA:HB2	1.97	0.46
8:B:113:SER:O	8:B:152:ARG:NH2	2.48	0.46
18:R:523:VAL:HG11	18:R:525:TRP:CZ2	2.51	0.46
6:7:106:ILE:HG22	6:7:113:PHE:CD1	2.51	0.46
2:3:671:LEU:HG	2:3:676:ILE:HD11	1.98	0.45
7:A:137:LEU:HD13	10:D:185:THR:CG2	2.47	0.44
1:2:671:GLU:OE1	1:2:671:GLU:N	2.50	0.44
15:K:22:ILE:HG23	15:K:94:ALA:HB1	2.00	0.44
17:Q:1794:MET:HE3	17:Q:1798:TRP:CH2	2.52	0.44
2:3:367:LEU:HD22	2:3:421:PHE:HE2	1.82	0.44
2:3:367:LEU:HD23	2:3:656:LEU:HD21	1.99	0.44
3:4:822:VAL:O	3:4:826:VAL:HG23	2.18	0.43
18:R:361:ASN:ND2	18:R:379:LEU:O	2.52	0.43
12:F:634:HIS:NE2	12:H:657:LEU:O	2.51	0.43
12:H:513:ILE:N	12:H:528:PHE:O	2.50	0.43
18:R:324:CYS:SG	18:R:609:GLN:NE2	2.92	0.43
2:3:386:MET:HE3	2:3:663:ALA:CB	2.49	0.43
18:R:528:ASN:HB3	18:R:529:PRO:HD3	2.01	0.43
17:Q:1574:SER:O	17:Q:1578:THR:HG23	2.18	0.42
18:R:503:LEU:HD13	18:R:620:ARG:NH2	2.34	0.42
1:2:364:CYS:O	1:2:368:LYS:N	2.51	0.42
18:R:503:LEU:O	18:R:503:LEU:HD12	2.19	0.42
6:7:709:ASP:OD1	6:7:710:ILE:N	2.52	0.42
1:2:611:LYS:NZ	1:2:651:ASN:OD1	2.52	0.41
5:6:294:VAL:HG21	5:6:389:ALA:HB1	2.02	0.41
5:6:608:LEU:HD23	5:6:608:LEU:HA	1.82	0.41
16:L:570:ARG:NH2	16:L:574:GLN:OE1	2.52	0.41
17:Q:1743:THR:HG21	17:Q:1840:THR:HA	2.02	0.41
18:R:404:ALA:HB2	18:R:642:CYS:SG	2.61	0.41
19:X:421:SER:O	19:X:586:GLN:NE2	2.51	0.41
2:3:235:ASP:OD1	2:3:236:THR:N	2.52	0.41
12:G:573:GLN:NE2	12:G:576:GLU:OE1	2.54	0.41
3:4:567:CYS:SG	3:4:568:GLY:N	2.92	0.41
11:E:10:GLU:OE1	11:E:10:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:280:ILE:HG22	16:L:310:ASN:HB2	2.02	0.40
5:6:633:ASN:N	5:6:675:ARG:O	2.54	0.40
1:2:633:LYS:HA	4:5:448:GLY:HA3	2.03	0.40

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%)	43	73
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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	
3	4	379/848 (45%)	378 (100%)	1 (0%)	86	88
4	5	415/688 (60%)	415 (100%)	0	100	100
5	6	550/886 (62%)	545 (99%)	5 (1%)	70	81
6	7	542/753 (72%)	540 (100%)	2 (0%)	84	86
7	A	182/193 (94%)	181 (100%)	1 (0%)	81	85
8	B	182/198 (92%)	181 (100%)	1 (0%)	81	85
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%)	505 (100%)	2 (0%)	84	86
12	F	375/854 (44%)	375 (100%)	0	100	100
12	G	372/854 (44%)	369 (99%)	3 (1%)	73	82
12	H	375/854 (44%)	374 (100%)	1 (0%)	86	88
15	K	124/179 (69%)	124 (100%)	0	100	100
16	L	456/686 (66%)	455 (100%)	1 (0%)	87	89
17	Q	701/2012 (35%)	699 (100%)	2 (0%)	86	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	498/629 (79%)	497 (100%)	1 (0%)	87	89
19	X	607/1125 (54%)	603 (99%)	4 (1%)	76	83
20	Y	85/286 (30%)	85 (100%)	0	100	100
All	All	6738/12089 (56%)	6714 (100%)	24 (0%)	81	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	594	LYS
5	6	119	LEU
5	6	313	MET
5	6	400	VAL
5	6	608	LEU
5	6	711	LEU
6	7	132	ILE
6	7	537	ILE
7	A	19	LEU
8	B	85	CYS
11	E	2	TYR
11	E	619	LYS
12	G	495	THR
12	G	573	GLN
12	G	757	VAL
12	H	530	ASP
16	L	668	LEU
17	Q	1353	ILE
17	Q	1484	ILE
18	R	545	ASP
19	X	219	GLU
19	X	383	VAL
19	X	414	LEU
19	X	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	543	GLN
3	4	651	GLN
3	4	759	HIS
4	5	155	HIS

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Mol	Chain	Res	Type
4	5	195	ASN
4	5	196	ASN
4	5	590	ASN
5	6	364	ASN
5	6	524	HIS
5	6	659	GLN
5	6	673	ASN
5	6	730	HIS
6	7	145	GLN
6	7	297	GLN
7	A	104	ASN
8	B	51	GLN
9	C	103	HIS
9	C	133	GLN
9	C	136	ASN
10	D	249	ASN
11	E	52	GLN
11	E	500	GLN
12	F	565	ASN
12	F	680	ASN
12	G	555	GLN
12	G	887	HIS
12	H	761	HIS
15	K	81	ASN
15	K	101	ASN
15	K	188	ASN
16	L	597	ASN
16	L	610	ASN
17	Q	1343	ASN
17	Q	1413	ASN
17	Q	2134	HIS
18	R	186	HIS
18	R	199	ASN
18	R	340	HIS
18	R	368	HIS
18	R	648	GLN
19	X	258	HIS
19	X	298	ASN
20	Y	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	5	1500	-	33,33,33	0.96	4 (12%)	45,52,52	0.50	0
21	ANP	2	1500	-	33,33,33	1.05	5 (15%)	45,52,52	0.51	0
21	ANP	3	1500	-	33,33,33	1.09	5 (15%)	45,52,52	0.57	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
21	ANP	5	1500	-	-	5/18/38/38	0/3/3/3
21	ANP	2	1500	-	-	3/18/38/38	0/3/3/3
21	ANP	3	1500	-	-	3/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	1500	ANP	PB-O3A	-3.43	1.54	1.59
21	2	1500	ANP	PB-O3A	-3.24	1.55	1.59
21	5	1500	ANP	PB-O3A	-2.86	1.55	1.59
21	3	1500	ANP	PA-O3A	-2.75	1.56	1.59
21	2	1500	ANP	PG-O1G	2.49	1.50	1.46
21	3	1500	ANP	PG-O1G	2.48	1.49	1.46
21	5	1500	ANP	PG-O1G	2.40	1.49	1.46
21	2	1500	ANP	PB-O1B	2.39	1.49	1.46
21	5	1500	ANP	PB-O1B	2.28	1.49	1.46
21	3	1500	ANP	PB-O1B	2.27	1.49	1.46
21	2	1500	ANP	PA-O3A	-2.25	1.57	1.59
21	5	1500	ANP	PG-N3B	2.24	1.69	1.63
21	2	1500	ANP	PG-N3B	2.22	1.69	1.63
21	3	1500	ANP	PG-N3B	2.08	1.68	1.63

There are no bond angle outliers.

There are no chirality outliers.

All (11) 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-O2B
21	3	1500	ANP	PB-N3B-PG-O1G
21	3	1500	ANP	PA-O3A-PB-O2B
21	5	1500	ANP	PB-N3B-PG-O1G
21	5	1500	ANP	O4'-C4'-C5'-O5'
21	5	1500	ANP	C3'-C4'-C5'-O5'
21	5	1500	ANP	PA-O3A-PB-O2B
21	2	1500	ANP	PA-O3A-PB-O1B
21	3	1500	ANP	PA-O3A-PB-O1B
21	5	1500	ANP	PA-O3A-PB-O1B

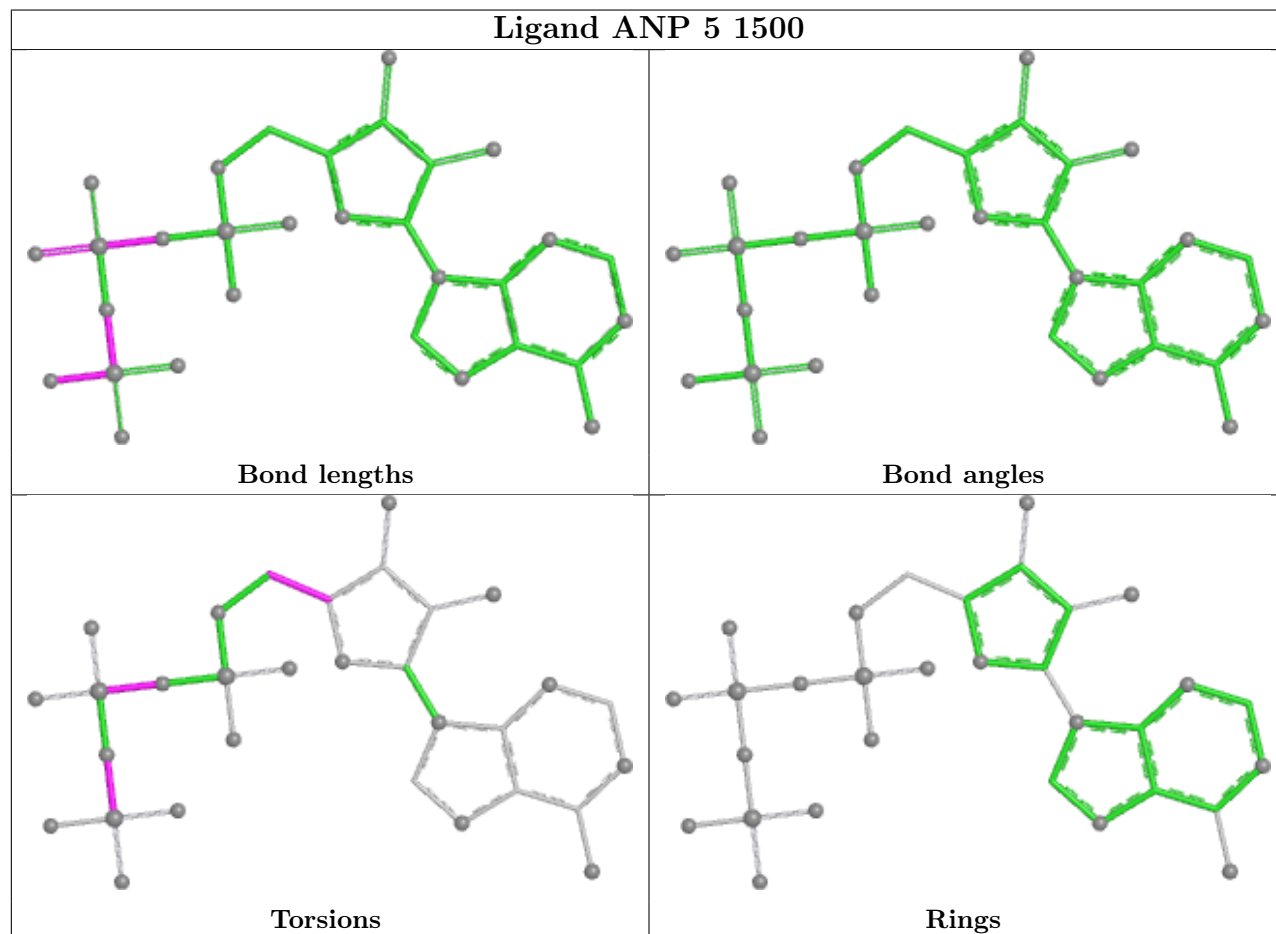
There are no ring outliers.

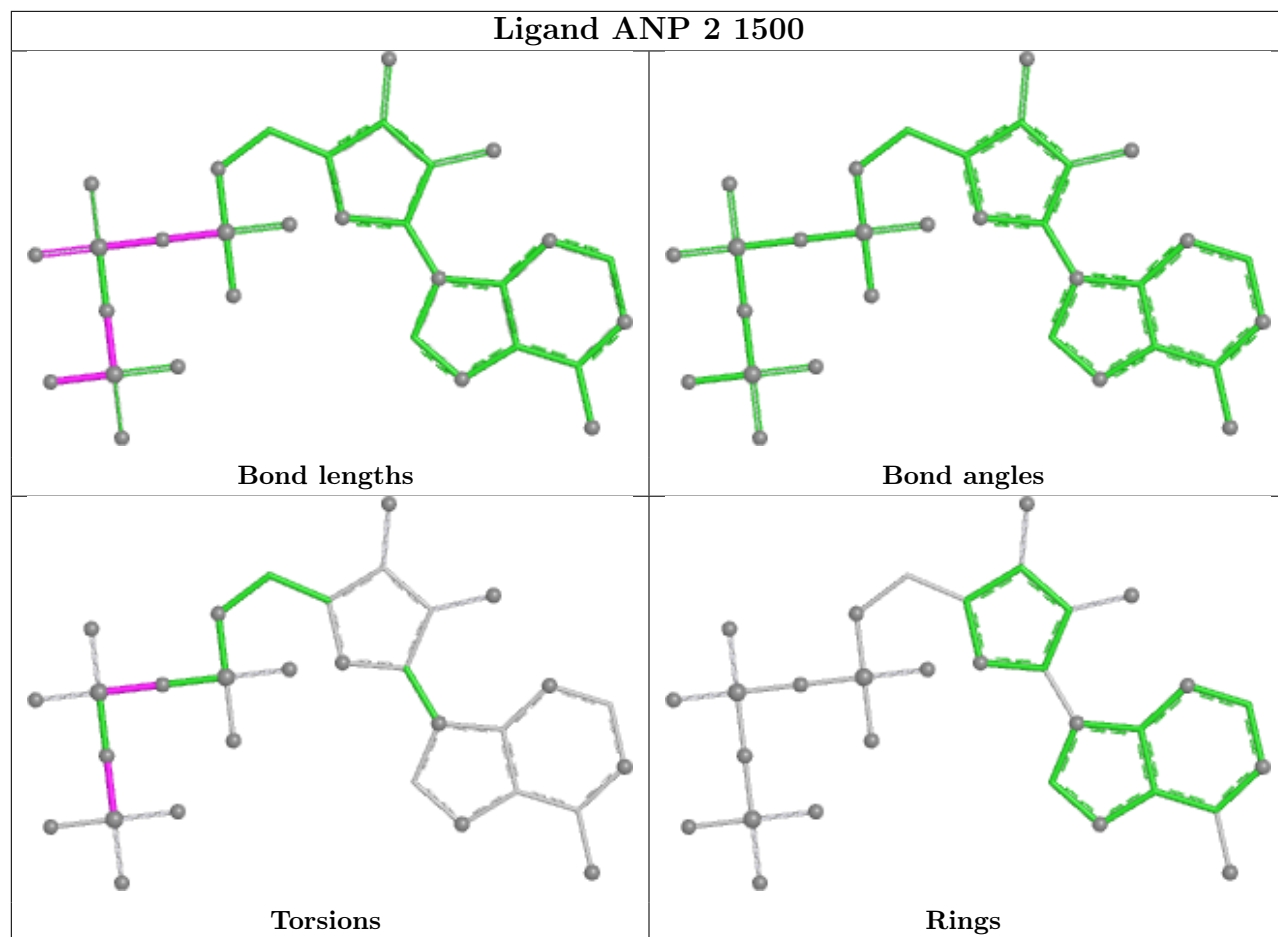
3 monomers are involved in 5 short contacts:

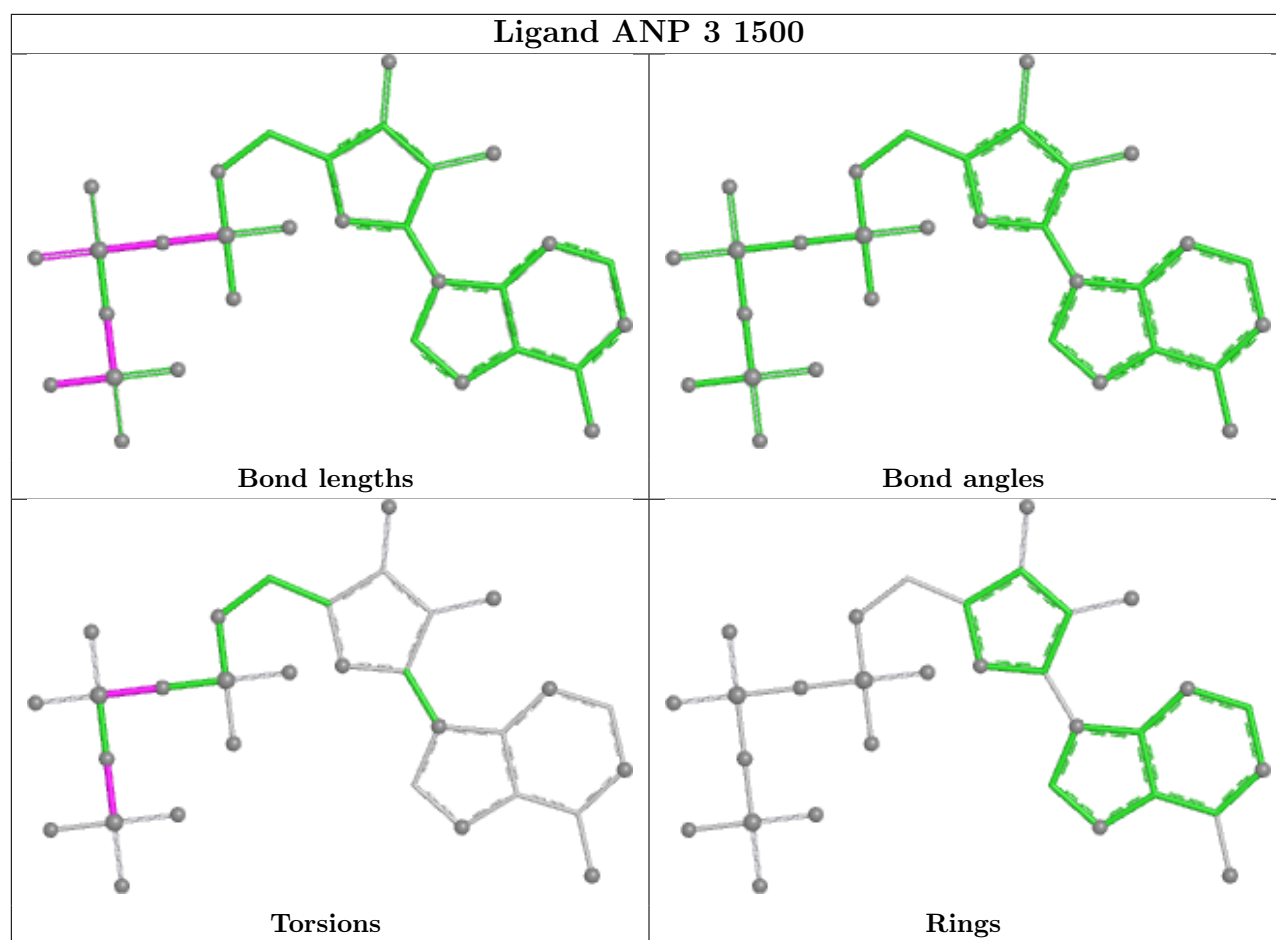
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	5	1500	ANP	2	0
21	2	1500	ANP	2	0
21	3	1500	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

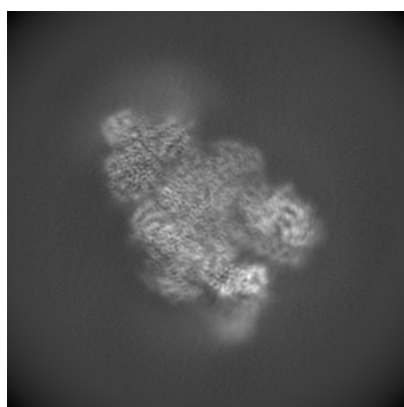
6 Map visualisation [i](#)

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.

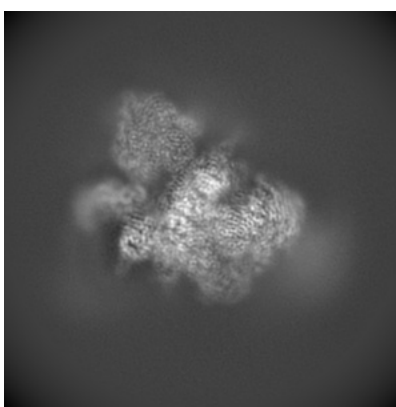
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

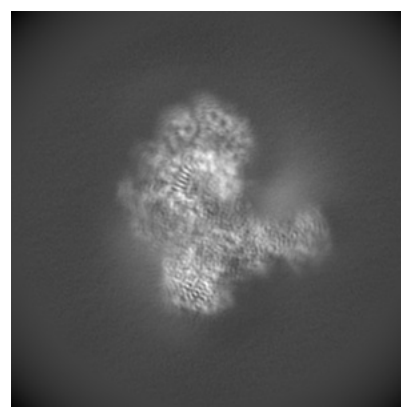
6.1.1 Primary map



X



Y

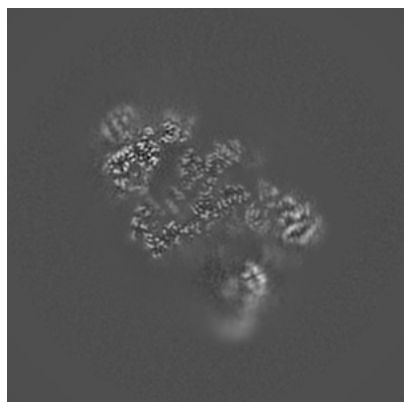


Z

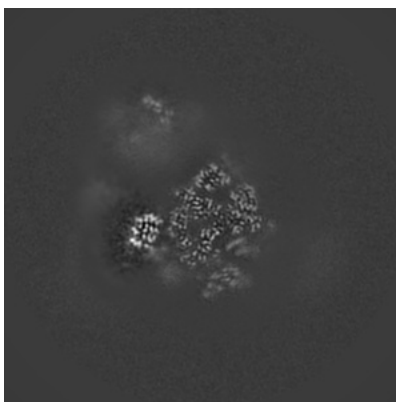
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

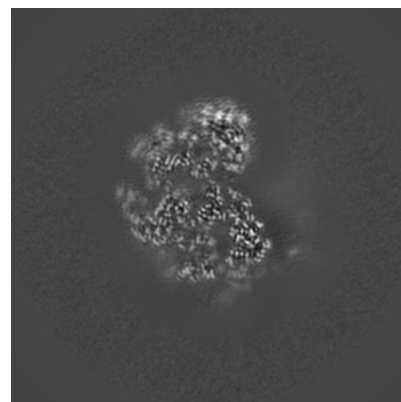
6.2.1 Primary map



X Index: 188



Y Index: 188

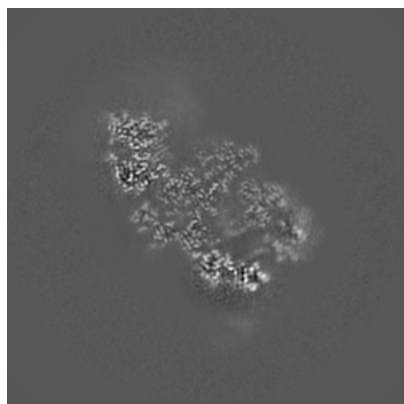


Z Index: 188

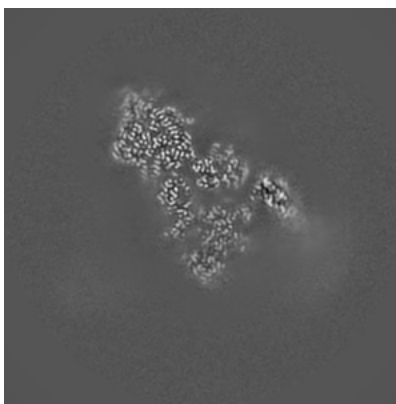
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

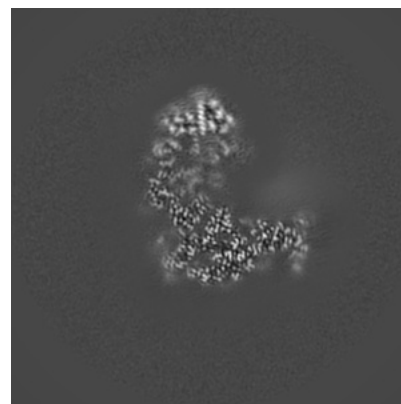
6.3.1 Primary map



X Index: 166



Y Index: 161

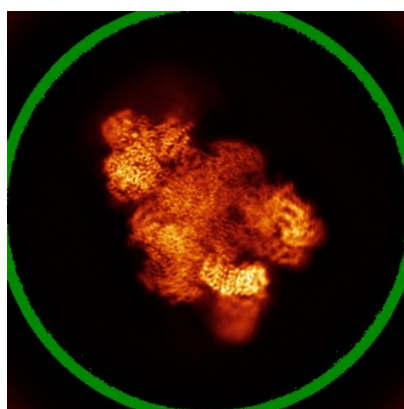


Z Index: 167

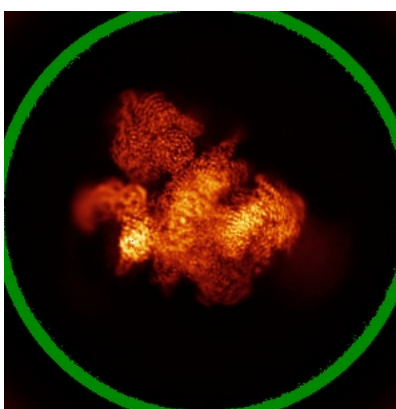
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

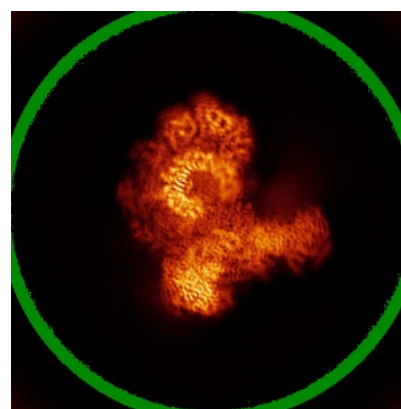
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

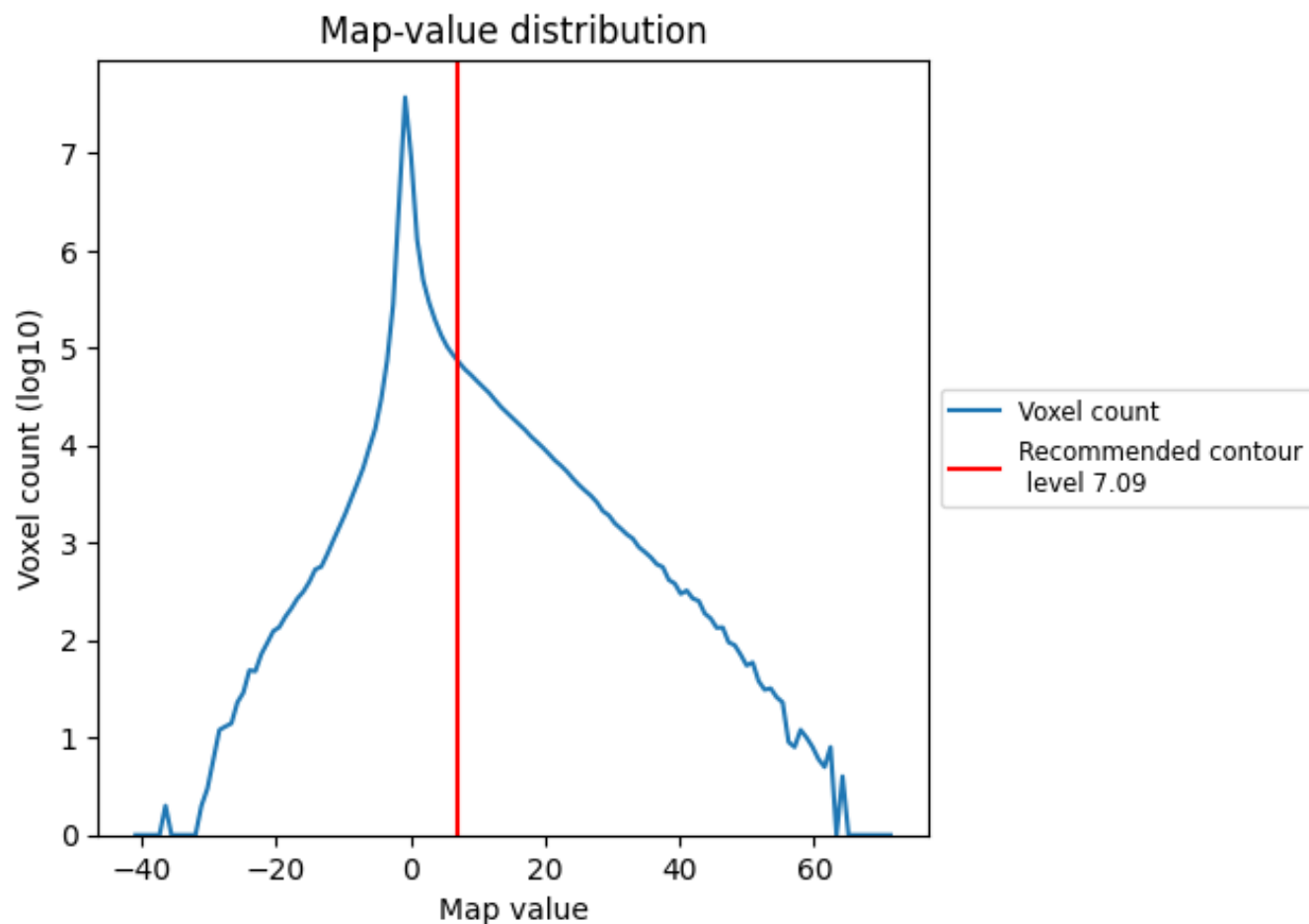
6.6 Mask visualisation

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

7 Map analysis [i](#)

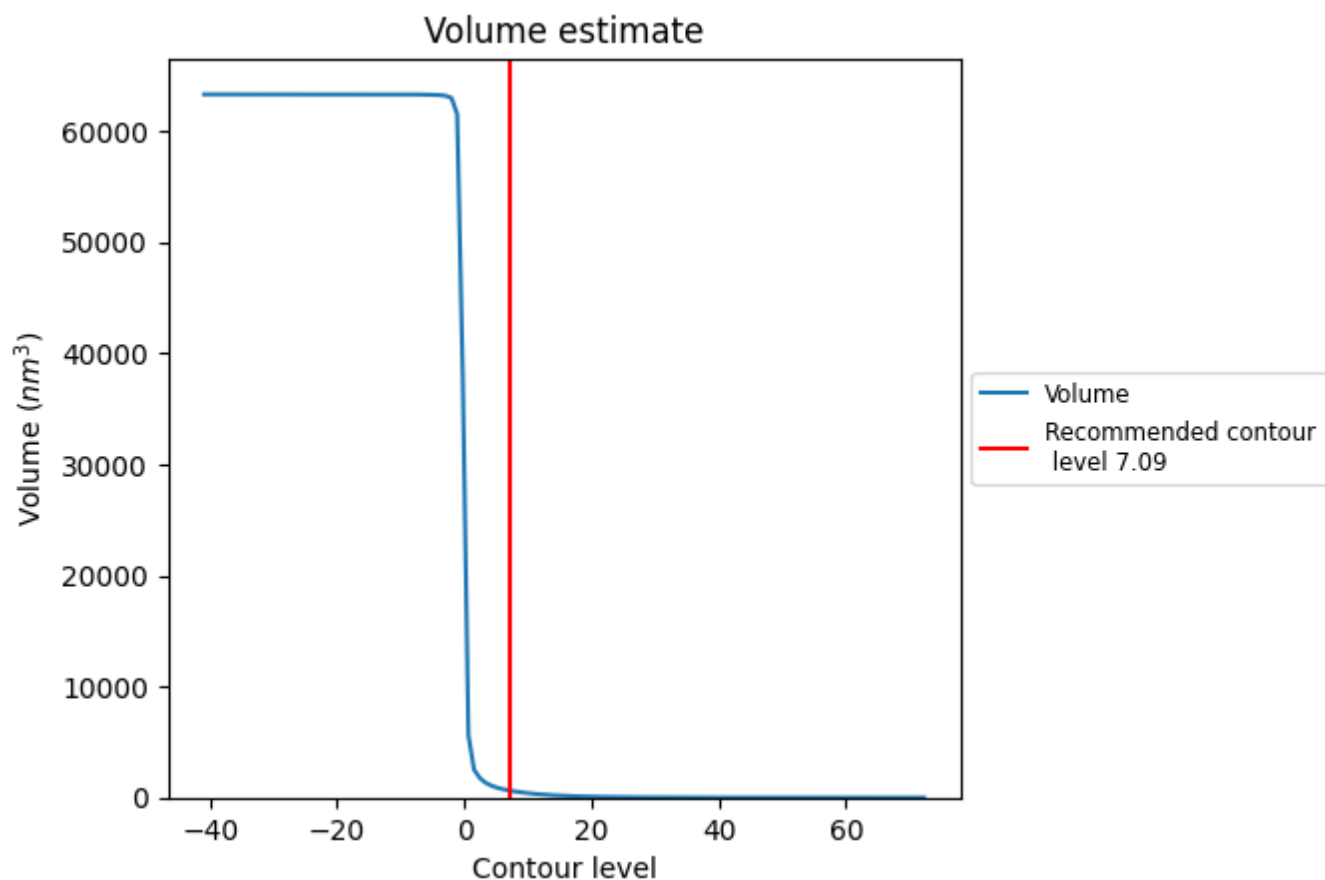
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

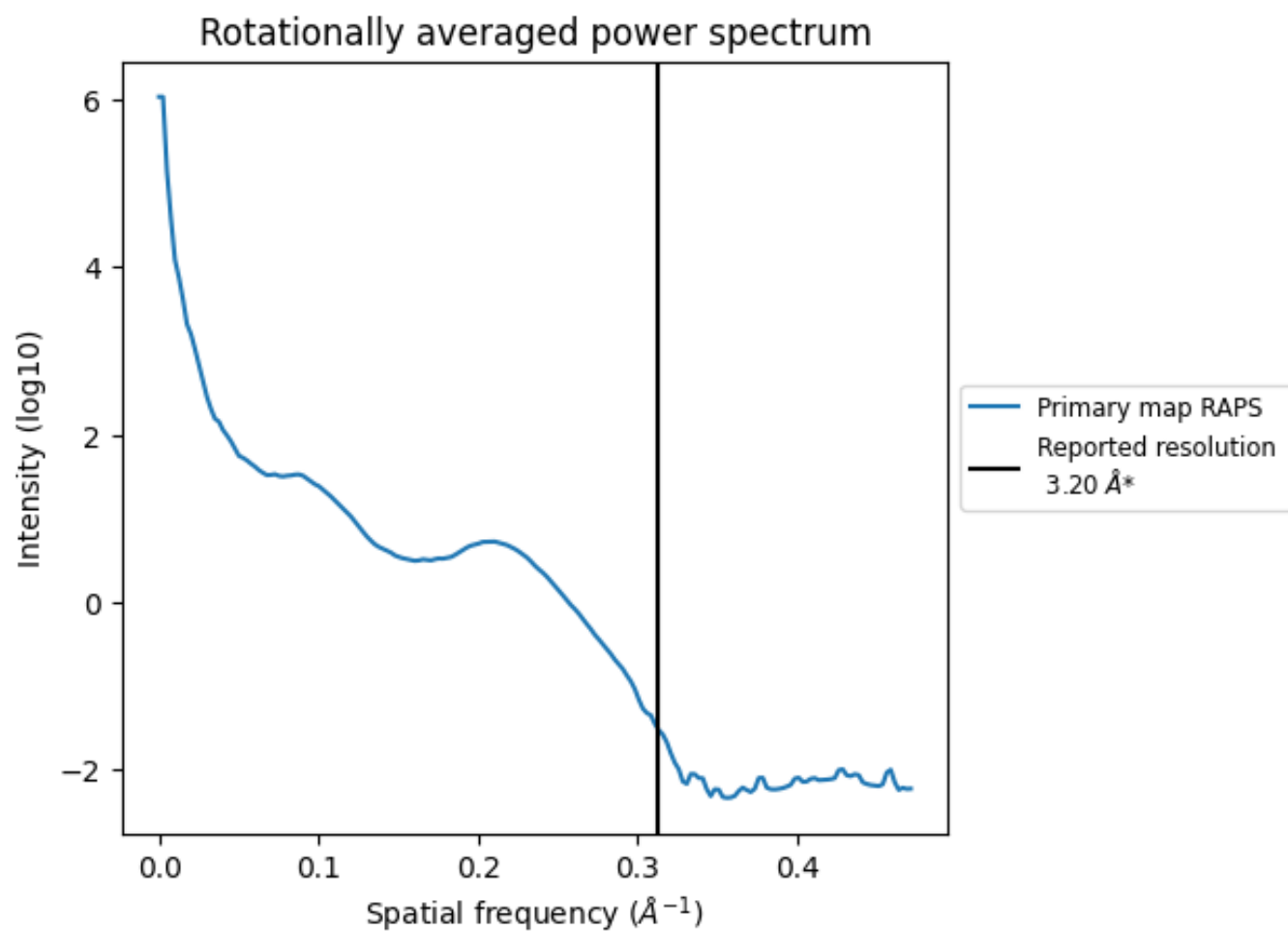
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 636 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

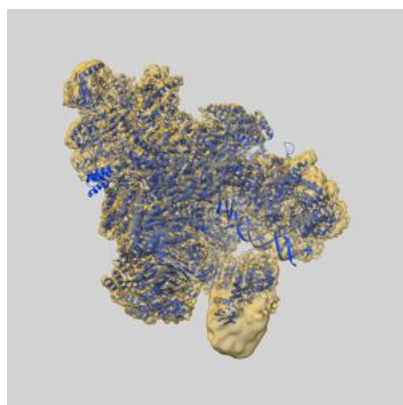
8 Fourier-Shell correlation ⓘ

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

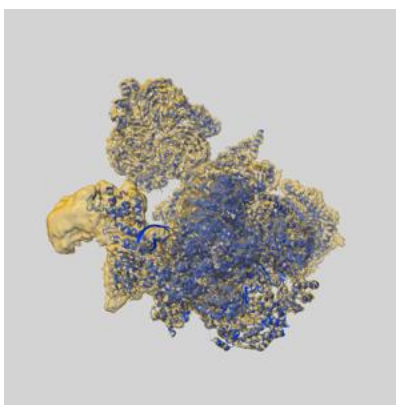
9 Map-model fit [i](#)

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

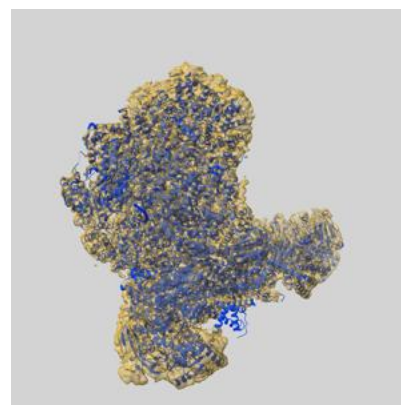
9.1 Map-model overlay [i](#)



X



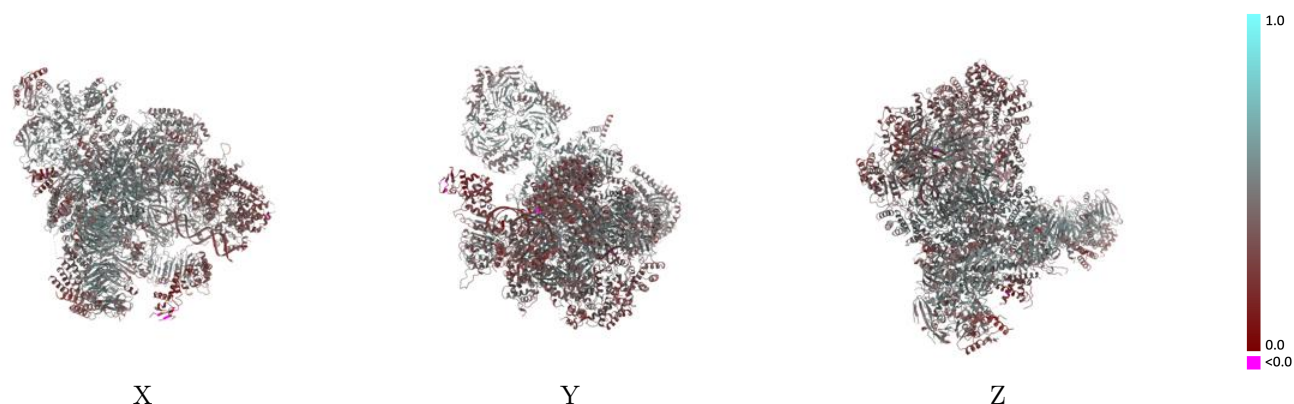
Y



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

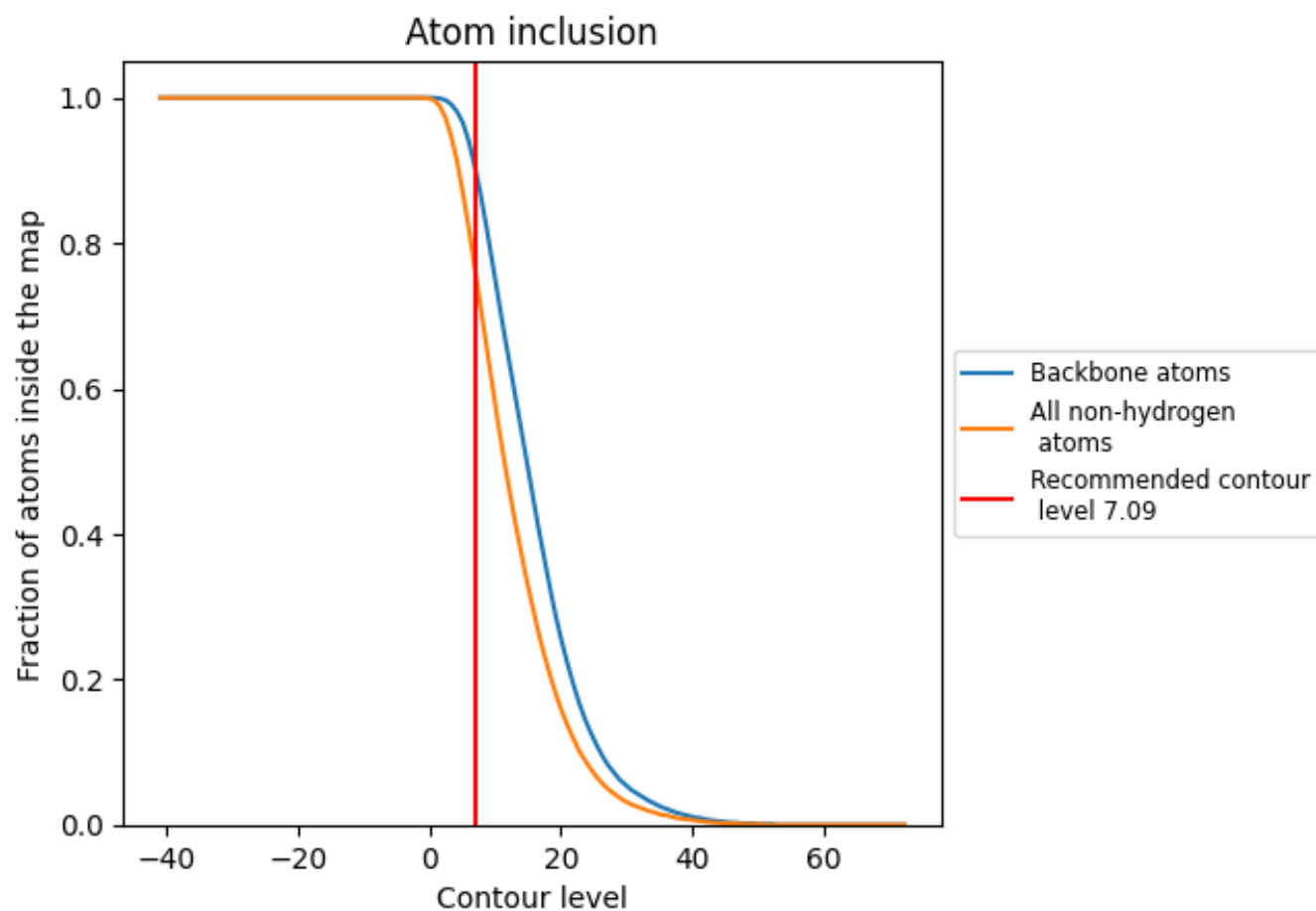


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (7.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.4340
2	 0.6790	 0.4580
3	 0.7160	 0.4780
4	 0.5180	 0.3820
5	 0.6960	 0.4780
6	 0.6550	 0.4360
7	 0.5750	 0.4100
A	 0.7000	 0.4420
B	 0.8300	 0.5280
C	 0.7920	 0.4840
D	 0.7810	 0.4800
E	 0.7940	 0.4810
F	 0.7990	 0.4850
G	 0.8080	 0.4410
H	 0.8080	 0.4460
I	 0.7650	 0.3230
J	 0.6300	 0.3140
K	 0.9570	 0.2080
L	 0.9270	 0.4080
Q	 0.8970	 0.4360
R	 0.7990	 0.4550
X	 0.8470	 0.3470
Y	 0.8350	 0.3350

