Full wwPDB EM Validation Report ⓘ

Aug 22, 2023 – 11:14 am BST

PDB ID	:	8B9D
EMDB ID	:	EMD-15341
Title	:	Human replisome bound by Pol Alpha
Authors	:	Jones, M.L.; Yeeles, J.T.P.
Deposited on	:	2022-10-05
Resolution	:	3.40 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:

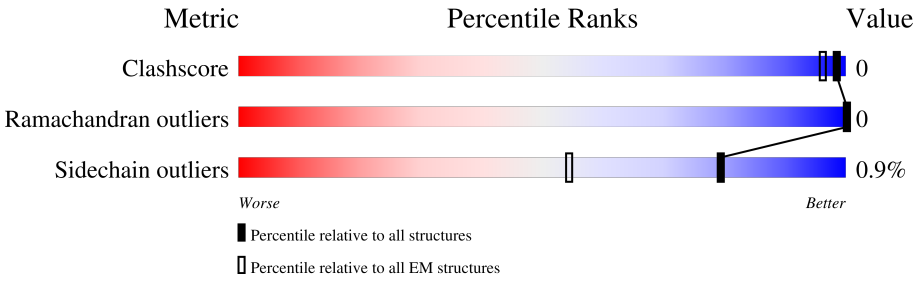
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 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	904	63% · 36%
2	3	808	70% 30%
3	4	863	78% 22%
4	5	734	81% · 19%
5	6	821	74% 26%
6	7	719	79% · 20%
7	A	598	19% 75% 25%
8	C	569	92% · 6%

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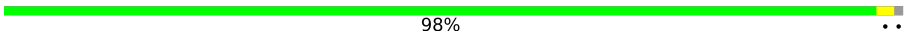
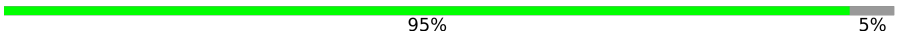
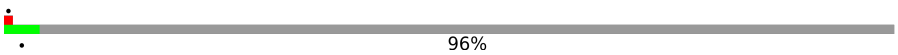
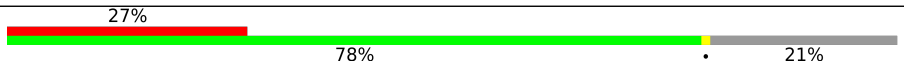
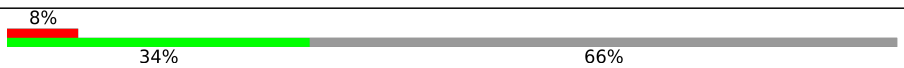
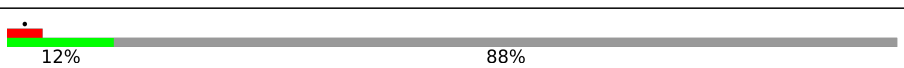
Mol	Chain	Length	Quality of chain
9	D	196	
10	E	185	
11	F	216	
12	G	261	
13	K	1209	
14	L	301	
15	M	84	
16	N	86	
17	P	509	
18	Q	1371	
19	O	462	
20	H	1160	
20	I	1160	
20	J	1160	
21	B	1504	

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 131961 atoms, of which 65802 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	2	576	9110	2856	4570	815	846	23	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	569	8989	2798	4518	794	853	26	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	677	10859	3399	5470	948	1014	28	0	0

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	597	9412	2928	4738	831	880	35	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	607	9706	3039	4870	859	912	26	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	576	9209	2874	4637	811	856	31	0	0

- Molecule 7 is a protein called DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	448	Total	C	H	N	O	S	0	0
			6958	2227	3465	572	679	15		

- Molecule 8 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	533	Total	C	H	N	O	S	0	0
			8621	2758	4285	741	806	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135A	ASP	-	linker	UNP O75419
C	135B	TYR	-	linker	UNP O75419
C	135C	LYS	-	linker	UNP O75419
C	135D	ASP	-	linker	UNP O75419
C	135E	ASP	-	linker	UNP O75419
C	135F	ASP	-	linker	UNP O75419

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	D	195	Total	C	H	N	O	S	0	0
			3207	1013	1601	289	292	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	176	Total	C	H	N	O	S	0	0
			2887	916	1456	242	264	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	187	Total	C	H	N	O	S	0	0
			2953	945	1458	261	283	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	G	203	Total	C	H	N	O	S	0	0
			3380	1065	1701	290	314	10		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-37	TRP	-	expression tag	UNP Q9BRT9
G	-36	SER	-	expression tag	UNP Q9BRT9
G	-35	HIS	-	expression tag	UNP Q9BRT9
G	-34	PRO	-	expression tag	UNP Q9BRT9
G	-33	GLN	-	expression tag	UNP Q9BRT9
G	-32	PHE	-	expression tag	UNP Q9BRT9
G	-31	GLU	-	expression tag	UNP Q9BRT9
G	-30	LYS	-	expression tag	UNP Q9BRT9
G	-29	GLY	-	expression tag	UNP Q9BRT9
G	-28	GLY	-	expression tag	UNP Q9BRT9
G	-27	GLY	-	expression tag	UNP Q9BRT9
G	-26	SER	-	expression tag	UNP Q9BRT9
G	-25	GLY	-	expression tag	UNP Q9BRT9
G	-24	GLY	-	expression tag	UNP Q9BRT9
G	-23	GLY	-	expression tag	UNP Q9BRT9
G	-22	SER	-	expression tag	UNP Q9BRT9
G	-21	GLY	-	expression tag	UNP Q9BRT9
G	-20	GLY	-	expression tag	UNP Q9BRT9
G	-19	SER	-	expression tag	UNP Q9BRT9
G	-18	ALA	-	expression tag	UNP Q9BRT9
G	-17	TRP	-	expression tag	UNP Q9BRT9
G	-16	SER	-	expression tag	UNP Q9BRT9
G	-15	HIS	-	expression tag	UNP Q9BRT9
G	-14	PRO	-	expression tag	UNP Q9BRT9
G	-13	GLN	-	expression tag	UNP Q9BRT9
G	-12	PHE	-	expression tag	UNP Q9BRT9
G	-11	GLU	-	expression tag	UNP Q9BRT9
G	-10	LYS	-	expression tag	UNP Q9BRT9
G	-9	SER	-	expression tag	UNP Q9BRT9
G	-8	GLY	-	expression tag	UNP Q9BRT9
G	-7	LEU	-	expression tag	UNP Q9BRT9
G	-6	GLU	-	expression tag	UNP Q9BRT9
G	-5	VAL	-	expression tag	UNP Q9BRT9
G	-4	LEU	-	expression tag	UNP Q9BRT9
G	-3	PHE	-	expression tag	UNP Q9BRT9
G	-2	GLN	-	expression tag	UNP Q9BRT9
G	-1	GLY	-	expression tag	UNP Q9BRT9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	PRO	-	expression tag	UNP Q9BRT9

- Molecule 13 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	638	Total	C	H	N	O	S	0	0
			10470	3332	5241	931	940	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q9UNS1

- Molecule 14 is a protein called TIMELESS-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L	87	Total	C	H	N	O	S	0	0
			1501	471	766	140	121	3		

- Molecule 15 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M	32	Total	C	H	N	O	P	0	0
			1032	320	370	106	204	32		

- Molecule 16 is a DNA chain called DNA Molecule.

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

- Molecule 17 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	241	Total	C	H	N	O	S	0	0
			4002	1279	2007	341	371	4		

- Molecule 18 is a protein called Claspin.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Q	59	Total	C	H	N	O	S	0	0
			1052	328	536	102	85	1		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1340	LEU	-	expression tag	UNP Q9HAW4
Q	1341	GLU	-	expression tag	UNP Q9HAW4
Q	1342	VAL	-	expression tag	UNP Q9HAW4
Q	1343	LEU	-	expression tag	UNP Q9HAW4
Q	1344	PHE	-	expression tag	UNP Q9HAW4
Q	1345	GLN	-	expression tag	UNP Q9HAW4
Q	1346	GLY	-	expression tag	UNP Q9HAW4
Q	1347	PRO	-	expression tag	UNP Q9HAW4
Q	1348	ASP	-	expression tag	UNP Q9HAW4
Q	1349	TYR	-	expression tag	UNP Q9HAW4
Q	1350	LYS	-	expression tag	UNP Q9HAW4
Q	1351	ASP	-	expression tag	UNP Q9HAW4
Q	1352	ASP	-	expression tag	UNP Q9HAW4
Q	1353	ASP	-	expression tag	UNP Q9HAW4
Q	1354	ASP	-	expression tag	UNP Q9HAW4
Q	1355	LYS	-	expression tag	UNP Q9HAW4
Q	1356	ASP	-	expression tag	UNP Q9HAW4
Q	1357	TYR	-	expression tag	UNP Q9HAW4
Q	1358	LYS	-	expression tag	UNP Q9HAW4
Q	1359	ASP	-	expression tag	UNP Q9HAW4
Q	1360	ASP	-	expression tag	UNP Q9HAW4
Q	1361	ASP	-	expression tag	UNP Q9HAW4
Q	1362	ASP	-	expression tag	UNP Q9HAW4
Q	1363	LYS	-	expression tag	UNP Q9HAW4
Q	1364	ASP	-	expression tag	UNP Q9HAW4
Q	1365	TYR	-	expression tag	UNP Q9HAW4
Q	1366	LYS	-	expression tag	UNP Q9HAW4
Q	1367	ASP	-	expression tag	UNP Q9HAW4
Q	1368	ASP	-	expression tag	UNP Q9HAW4
Q	1369	ASP	-	expression tag	UNP Q9HAW4
Q	1370	ASP	-	expression tag	UNP Q9HAW4
Q	1371	LYS	-	expression tag	UNP Q9HAW4

- Molecule 19 is a protein called DNA primase small subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	O	364	Total	C	H	N	O	S	0	0
			6087	1966	3035	530	543	13		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-41	MET	-	initiating methionine	UNP P49642
O	-40	ALA	-	expression tag	UNP P49642
O	-39	SER	-	expression tag	UNP P49642
O	-38	ALA	-	expression tag	UNP P49642
O	-37	TRP	-	expression tag	UNP P49642
O	-36	SER	-	expression tag	UNP P49642
O	-35	HIS	-	expression tag	UNP P49642
O	-34	PRO	-	expression tag	UNP P49642
O	-33	GLN	-	expression tag	UNP P49642
O	-32	PHE	-	expression tag	UNP P49642
O	-31	GLU	-	expression tag	UNP P49642
O	-30	LYS	-	expression tag	UNP P49642
O	-29	GLY	-	expression tag	UNP P49642
O	-28	GLY	-	expression tag	UNP P49642
O	-27	GLY	-	expression tag	UNP P49642
O	-26	SER	-	expression tag	UNP P49642
O	-25	GLY	-	expression tag	UNP P49642
O	-24	GLY	-	expression tag	UNP P49642
O	-23	GLY	-	expression tag	UNP P49642
O	-22	SER	-	expression tag	UNP P49642
O	-21	GLY	-	expression tag	UNP P49642
O	-20	GLY	-	expression tag	UNP P49642
O	-19	SER	-	expression tag	UNP P49642
O	-18	ALA	-	expression tag	UNP P49642
O	-17	TRP	-	expression tag	UNP P49642
O	-16	SER	-	expression tag	UNP P49642
O	-15	HIS	-	expression tag	UNP P49642
O	-14	PRO	-	expression tag	UNP P49642
O	-13	GLN	-	expression tag	UNP P49642
O	-12	PHE	-	expression tag	UNP P49642
O	-11	GLU	-	expression tag	UNP P49642
O	-10	LYS	-	expression tag	UNP P49642
O	-9	SER	-	expression tag	UNP P49642
O	-8	GLY	-	expression tag	UNP P49642
O	-7	LEU	-	expression tag	UNP P49642
O	-6	GLU	-	expression tag	UNP P49642
O	-5	VAL	-	expression tag	UNP P49642

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	LEU	-	expression tag	UNP P49642
O	-3	PHE	-	expression tag	UNP P49642
O	-2	GLN	-	expression tag	UNP P49642
O	-1	GLY	-	expression tag	UNP P49642
O	0	PRO	-	expression tag	UNP P49642

- Molecule 20 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	H	399	Total	C	H	N	O	S	0	0
			6286	2007	3124	550	584	21		
20	J	399	Total	C	H	N	O	S	0	0
			6286	2007	3124	550	584	21		
20	I	399	Total	C	H	N	O	S	0	0
			6286	2007	3124	550	584	21		

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-30	ASP	-	expression tag	UNP O75717
H	-29	TYR	-	expression tag	UNP O75717
H	-28	LYS	-	expression tag	UNP O75717
H	-27	ASP	-	expression tag	UNP O75717
H	-26	ASP	-	expression tag	UNP O75717
H	-25	ASP	-	expression tag	UNP O75717
H	-24	ASP	-	expression tag	UNP O75717
H	-23	LYS	-	expression tag	UNP O75717
H	-22	ASP	-	expression tag	UNP O75717
H	-21	TYR	-	expression tag	UNP O75717
H	-20	LYS	-	expression tag	UNP O75717
H	-19	ASP	-	expression tag	UNP O75717
H	-18	ASP	-	expression tag	UNP O75717
H	-17	ASP	-	expression tag	UNP O75717
H	-16	ASP	-	expression tag	UNP O75717
H	-15	LYS	-	expression tag	UNP O75717
H	-14	ASP	-	expression tag	UNP O75717
H	-13	TYR	-	expression tag	UNP O75717
H	-12	LYS	-	expression tag	UNP O75717
H	-11	ASP	-	expression tag	UNP O75717
H	-10	ASP	-	expression tag	UNP O75717
H	-9	ASP	-	expression tag	UNP O75717
H	-8	ASP	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	LYS	-	expression tag	UNP O75717
H	-6	GLU	-	expression tag	UNP O75717
H	-5	ASN	-	expression tag	UNP O75717
H	-4	LEU	-	expression tag	UNP O75717
H	-3	TYR	-	expression tag	UNP O75717
H	-2	PHE	-	expression tag	UNP O75717
H	-1	GLN	-	expression tag	UNP O75717
H	0	GLY	-	expression tag	UNP O75717
J	-30	ASP	-	expression tag	UNP O75717
J	-29	TYR	-	expression tag	UNP O75717
J	-28	LYS	-	expression tag	UNP O75717
J	-27	ASP	-	expression tag	UNP O75717
J	-26	ASP	-	expression tag	UNP O75717
J	-25	ASP	-	expression tag	UNP O75717
J	-24	ASP	-	expression tag	UNP O75717
J	-23	LYS	-	expression tag	UNP O75717
J	-22	ASP	-	expression tag	UNP O75717
J	-21	TYR	-	expression tag	UNP O75717
J	-20	LYS	-	expression tag	UNP O75717
J	-19	ASP	-	expression tag	UNP O75717
J	-18	ASP	-	expression tag	UNP O75717
J	-17	ASP	-	expression tag	UNP O75717
J	-16	ASP	-	expression tag	UNP O75717
J	-15	LYS	-	expression tag	UNP O75717
J	-14	ASP	-	expression tag	UNP O75717
J	-13	TYR	-	expression tag	UNP O75717
J	-12	LYS	-	expression tag	UNP O75717
J	-11	ASP	-	expression tag	UNP O75717
J	-10	ASP	-	expression tag	UNP O75717
J	-9	ASP	-	expression tag	UNP O75717
J	-8	ASP	-	expression tag	UNP O75717
J	-7	LYS	-	expression tag	UNP O75717
J	-6	GLU	-	expression tag	UNP O75717
J	-5	ASN	-	expression tag	UNP O75717
J	-4	LEU	-	expression tag	UNP O75717
J	-3	TYR	-	expression tag	UNP O75717
J	-2	PHE	-	expression tag	UNP O75717
J	-1	GLN	-	expression tag	UNP O75717
J	0	GLY	-	expression tag	UNP O75717
I	-30	ASP	-	expression tag	UNP O75717
I	-29	TYR	-	expression tag	UNP O75717
I	-28	LYS	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-27	ASP	-	expression tag	UNP O75717
I	-26	ASP	-	expression tag	UNP O75717
I	-25	ASP	-	expression tag	UNP O75717
I	-24	ASP	-	expression tag	UNP O75717
I	-23	LYS	-	expression tag	UNP O75717
I	-22	ASP	-	expression tag	UNP O75717
I	-21	TYR	-	expression tag	UNP O75717
I	-20	LYS	-	expression tag	UNP O75717
I	-19	ASP	-	expression tag	UNP O75717
I	-18	ASP	-	expression tag	UNP O75717
I	-17	ASP	-	expression tag	UNP O75717
I	-16	ASP	-	expression tag	UNP O75717
I	-15	LYS	-	expression tag	UNP O75717
I	-14	ASP	-	expression tag	UNP O75717
I	-13	TYR	-	expression tag	UNP O75717
I	-12	LYS	-	expression tag	UNP O75717
I	-11	ASP	-	expression tag	UNP O75717
I	-10	ASP	-	expression tag	UNP O75717
I	-9	ASP	-	expression tag	UNP O75717
I	-8	ASP	-	expression tag	UNP O75717
I	-7	LYS	-	expression tag	UNP O75717
I	-6	GLU	-	expression tag	UNP O75717
I	-5	ASN	-	expression tag	UNP O75717
I	-4	LEU	-	expression tag	UNP O75717
I	-3	TYR	-	expression tag	UNP O75717
I	-2	PHE	-	expression tag	UNP O75717
I	-1	GLN	-	expression tag	UNP O75717
I	0	GLY	-	expression tag	UNP O75717

- Molecule 21 is a protein called DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	B	178	2873	917	1430	243	268	15	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	MET	-	initiating methionine	UNP P09884
B	-40	ALA	-	expression tag	UNP P09884
B	-39	SER	-	expression tag	UNP P09884
B	-38	ALA	-	expression tag	UNP P09884

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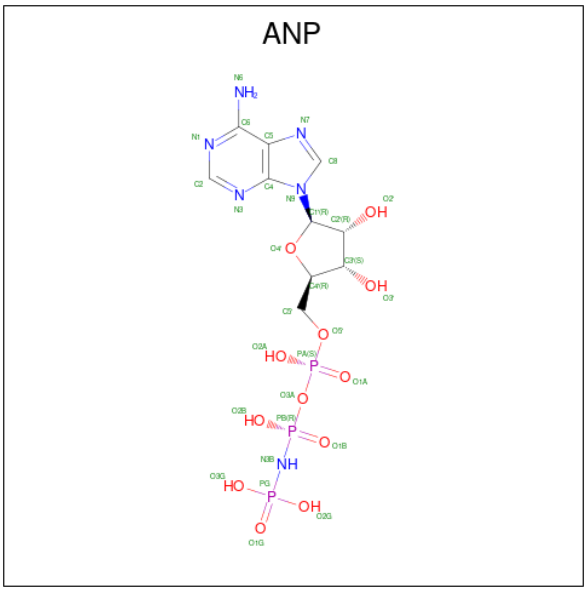
Chain	Residue	Modelled	Actual	Comment	Reference
B	-37	TRP	-	expression tag	UNP P09884
B	-36	SER	-	expression tag	UNP P09884
B	-35	HIS	-	expression tag	UNP P09884
B	-34	PRO	-	expression tag	UNP P09884
B	-33	GLN	-	expression tag	UNP P09884
B	-32	PHE	-	expression tag	UNP P09884
B	-31	GLU	-	expression tag	UNP P09884
B	-30	LYS	-	expression tag	UNP P09884
B	-29	GLY	-	expression tag	UNP P09884
B	-28	GLY	-	expression tag	UNP P09884
B	-27	GLY	-	expression tag	UNP P09884
B	-26	SER	-	expression tag	UNP P09884
B	-25	GLY	-	expression tag	UNP P09884
B	-24	GLY	-	expression tag	UNP P09884
B	-23	GLY	-	expression tag	UNP P09884
B	-22	SER	-	expression tag	UNP P09884
B	-21	GLY	-	expression tag	UNP P09884
B	-20	GLY	-	expression tag	UNP P09884
B	-19	SER	-	expression tag	UNP P09884
B	-18	ALA	-	expression tag	UNP P09884
B	-17	TRP	-	expression tag	UNP P09884
B	-16	SER	-	expression tag	UNP P09884
B	-15	HIS	-	expression tag	UNP P09884
B	-14	PRO	-	expression tag	UNP P09884
B	-13	GLN	-	expression tag	UNP P09884
B	-12	PHE	-	expression tag	UNP P09884
B	-11	GLU	-	expression tag	UNP P09884
B	-10	LYS	-	expression tag	UNP P09884
B	-9	SER	-	expression tag	UNP P09884
B	-8	GLY	-	expression tag	UNP P09884
B	-7	LEU	-	expression tag	UNP P09884
B	-6	GLU	-	expression tag	UNP P09884
B	-5	VAL	-	expression tag	UNP P09884
B	-4	LEU	-	expression tag	UNP P09884
B	-3	PHE	-	expression tag	UNP P09884
B	-2	GLN	-	expression tag	UNP P09884
B	-1	GLY	-	expression tag	UNP P09884
B	0	PRO	-	expression tag	UNP P09884

- Molecule 22 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
22	2	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
22	3	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
22	5	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

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

Mol	Chain	Residues	Atoms		AltConf
23	2	1	Total	Mg	0
			1	1	
23	3	1	Total	Mg	0
			1	1	
23	5	1	Total	Mg	0
			1	1	

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

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

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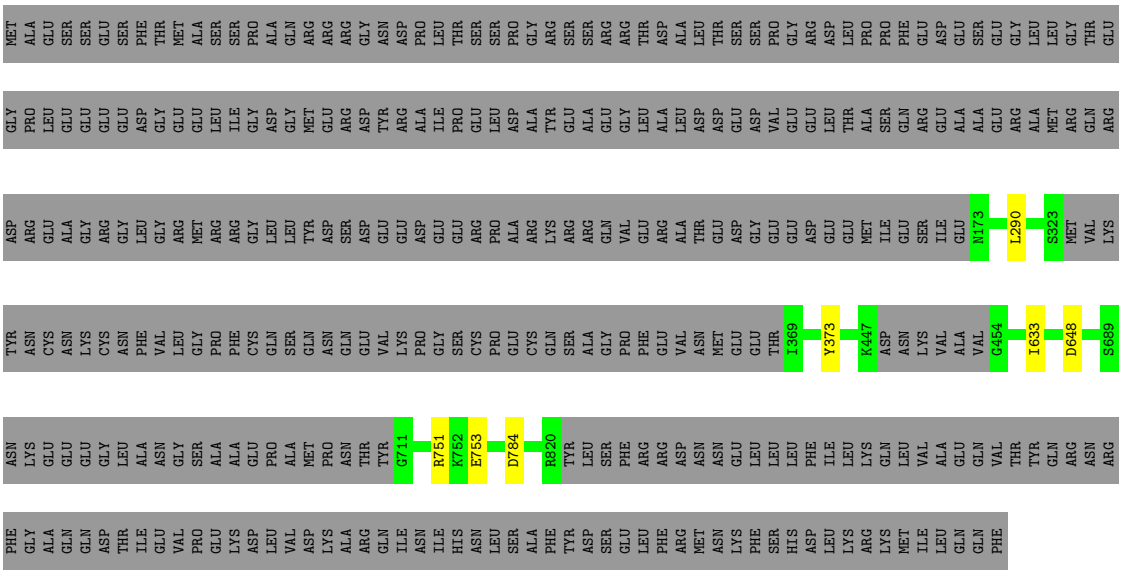
Mol	Chain	Residues	Atoms	AltConf
24	6	1	Total Zn 1 1	0
24	7	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

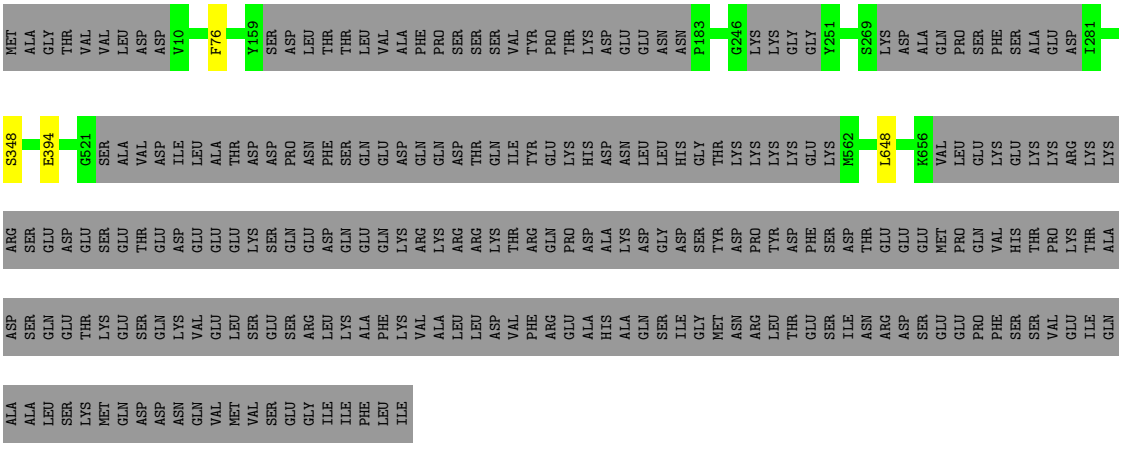
• Molecule 1: DNA replication licensing factor MCM2

Chain 2:



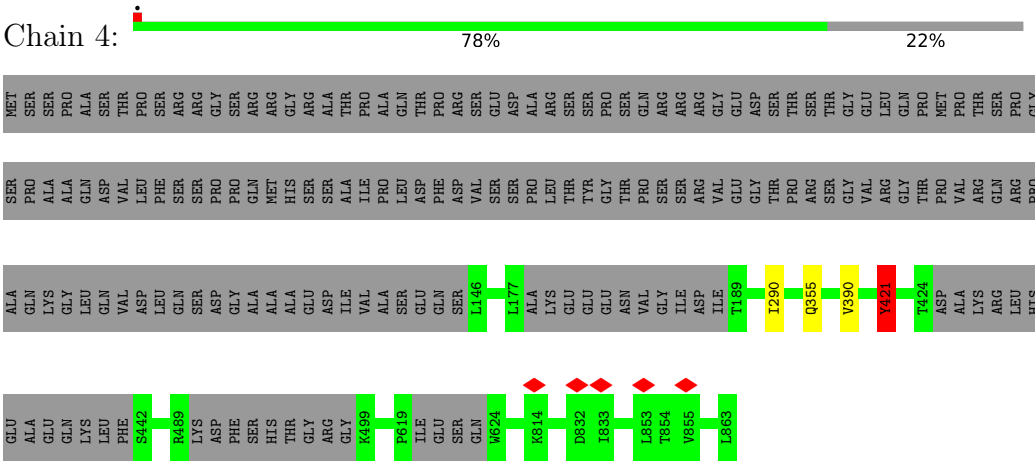
• Molecule 2: DNA replication licensing factor MCM3

Chain 3:



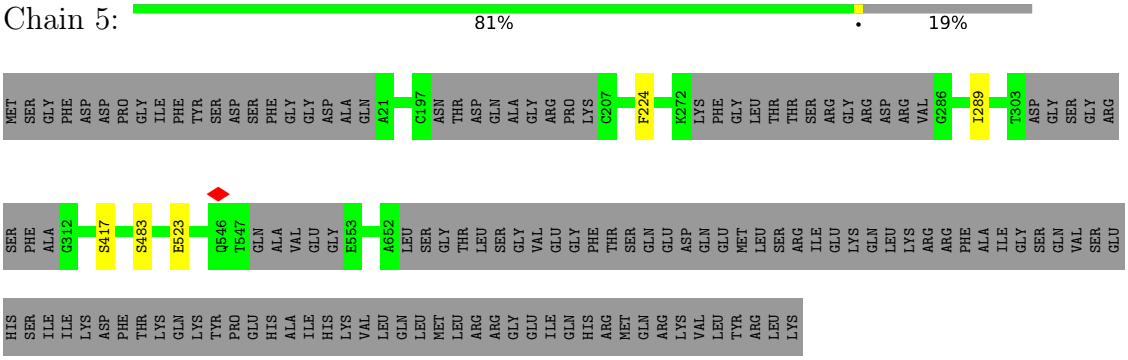
• Molecule 3: DNA replication licensing factor MCM4

Chain 4:



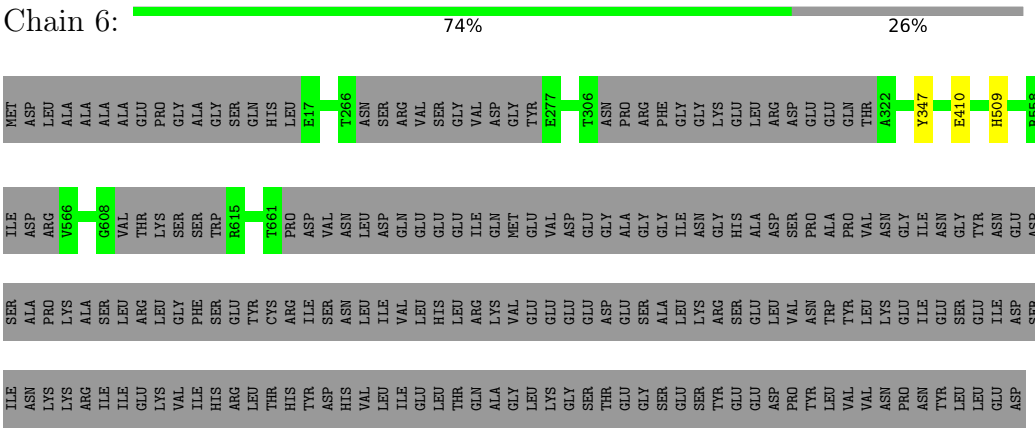
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:



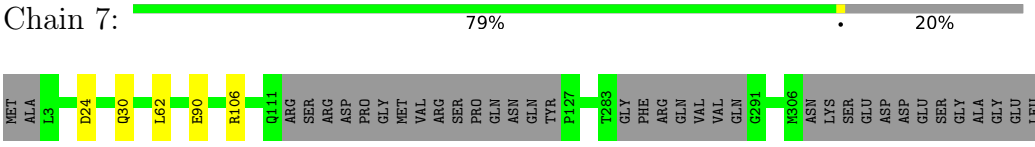
• Molecule 5: DNA replication licensing factor MCM6

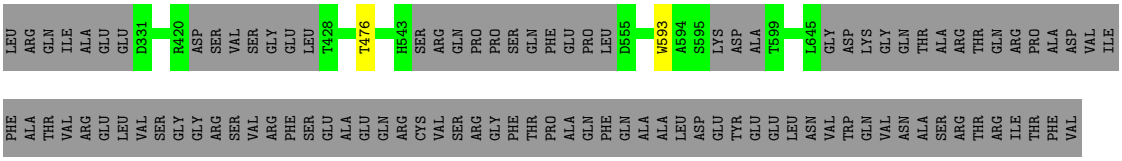
Chain 6:



• Molecule 6: DNA replication licensing factor MCM7

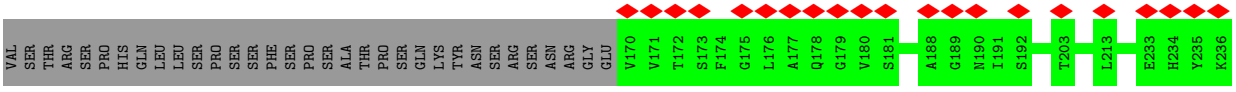
Chain 7:

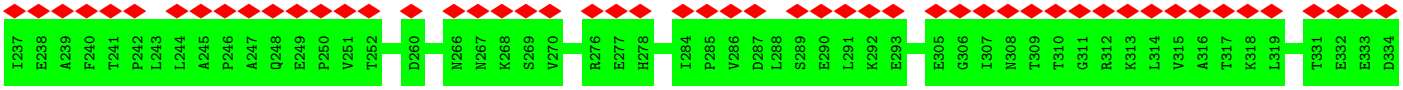


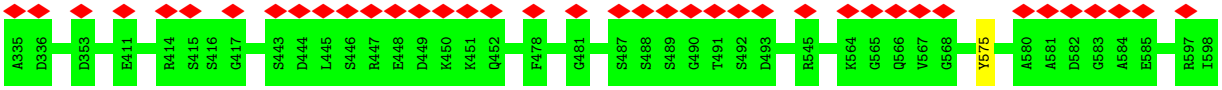


• Molecule 7: DNA polymerase alpha subunit B

Chain A:

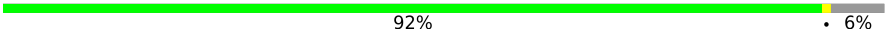






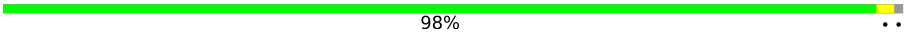
• Molecule 8: Cell division control protein 45 homolog

Chain C:



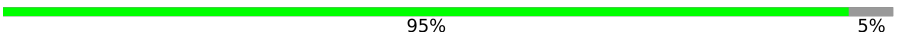
• Molecule 9: DNA replication complex GINS protein PSF1

Chain D:



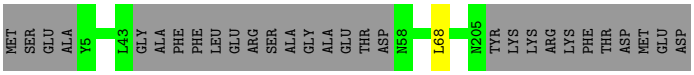
• Molecule 10: DNA replication complex GINS protein PSF2

Chain E:



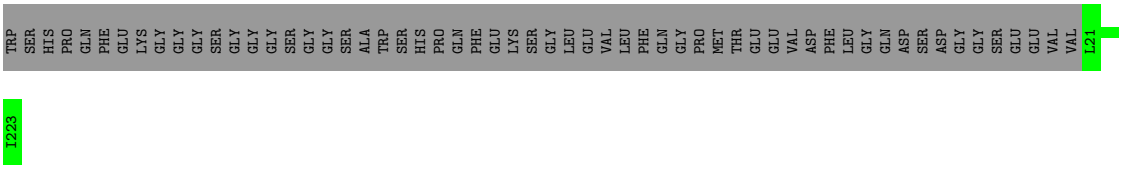
• Molecule 11: DNA replication complex GINS protein PSF3

Chain F:



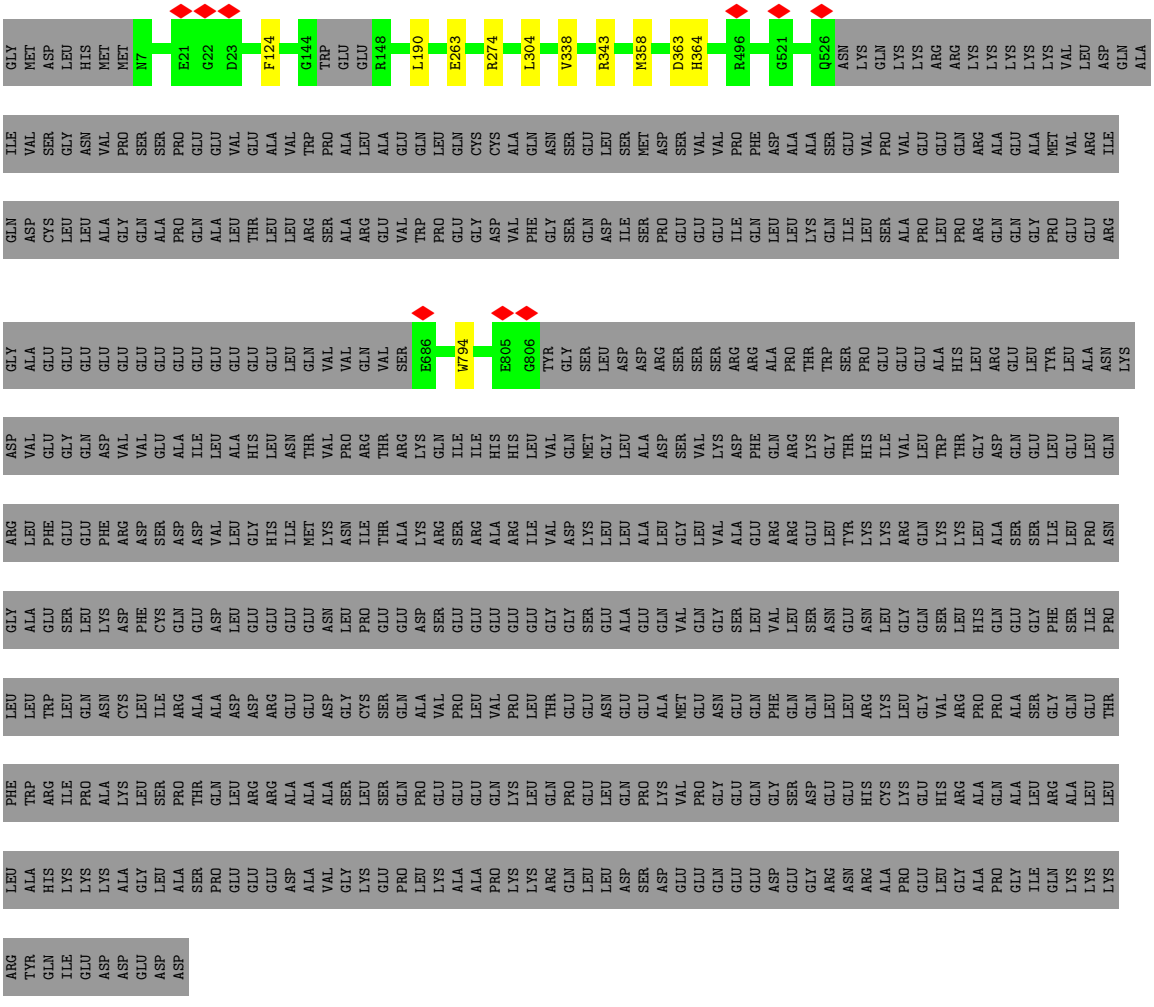
• Molecule 12: DNA replication complex GINS protein SLD5

Chain G:



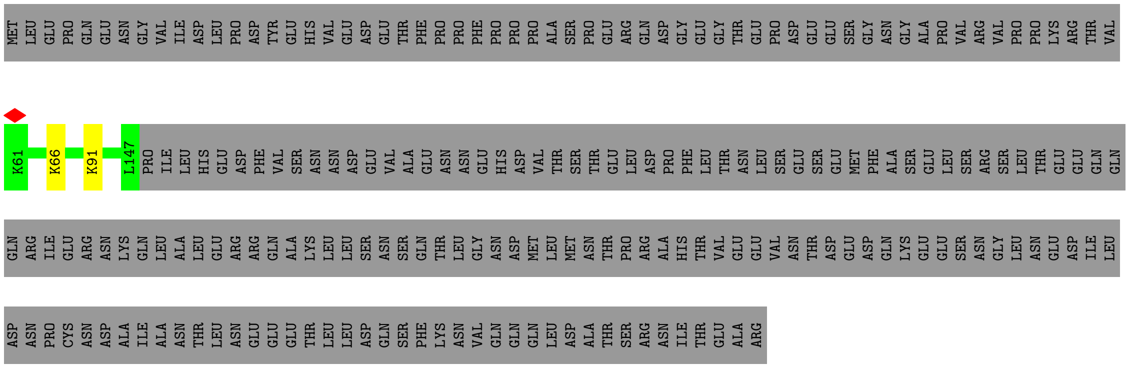
• Molecule 13: Protein timeless homolog

Chain K:



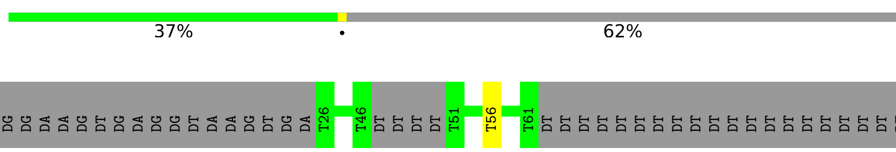
• Molecule 14: TIMELESS-interacting protein

Chain L:



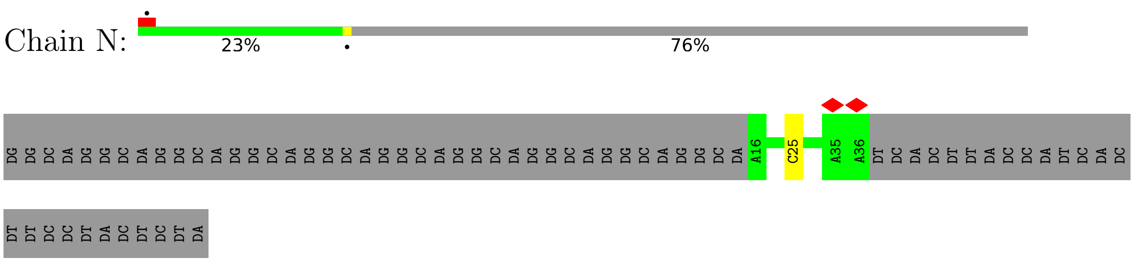
• Molecule 15: Leading strand DNA

Chain M:



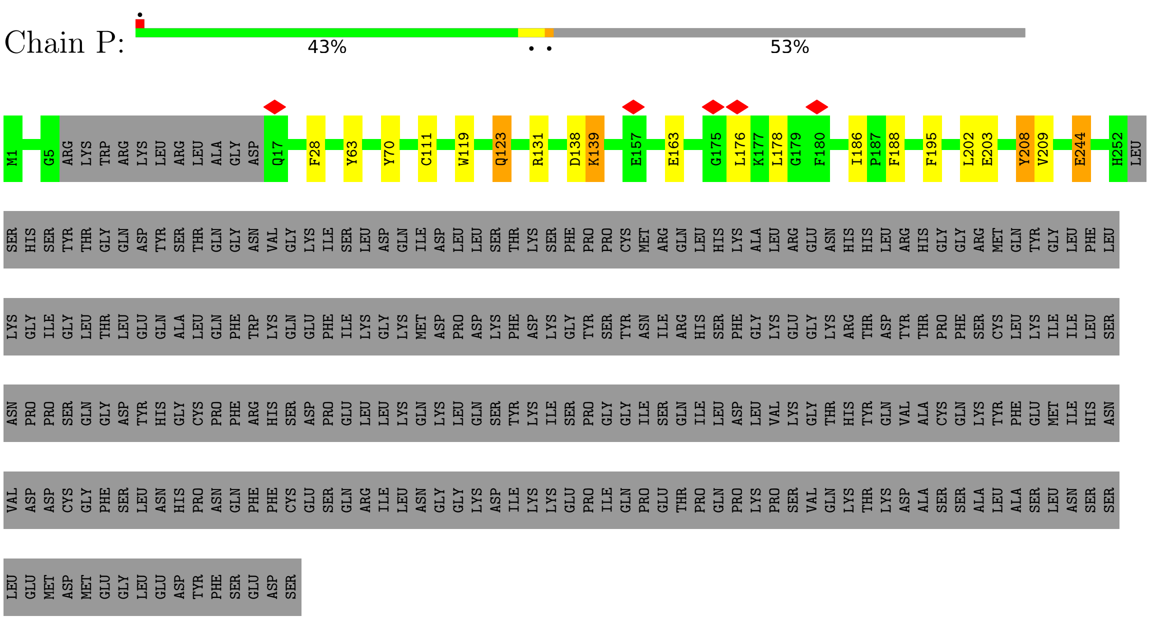
• Molecule 16: DNA Molecule

Chain N:



• Molecule 17: DNA primase large subunit

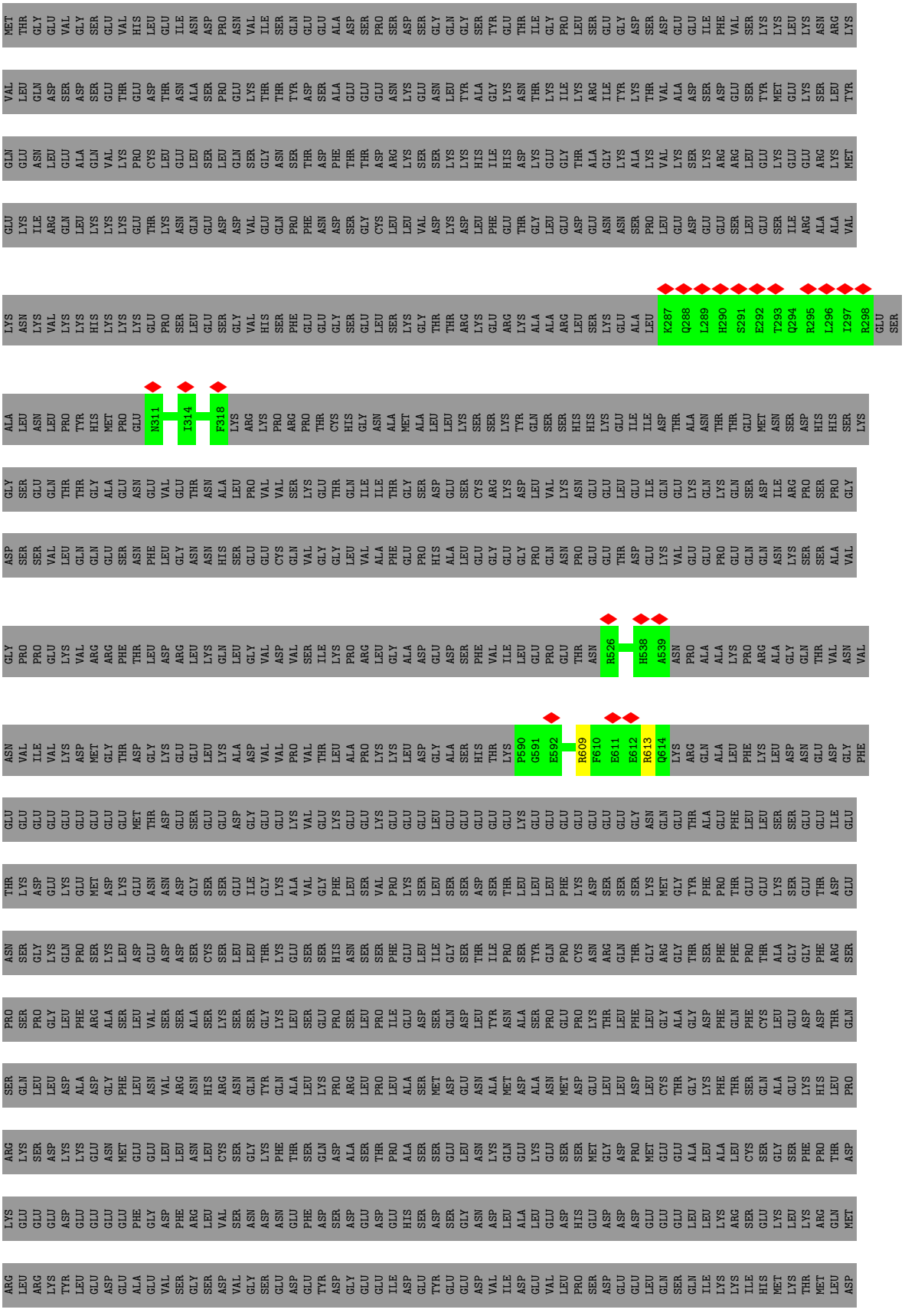
Chain P:

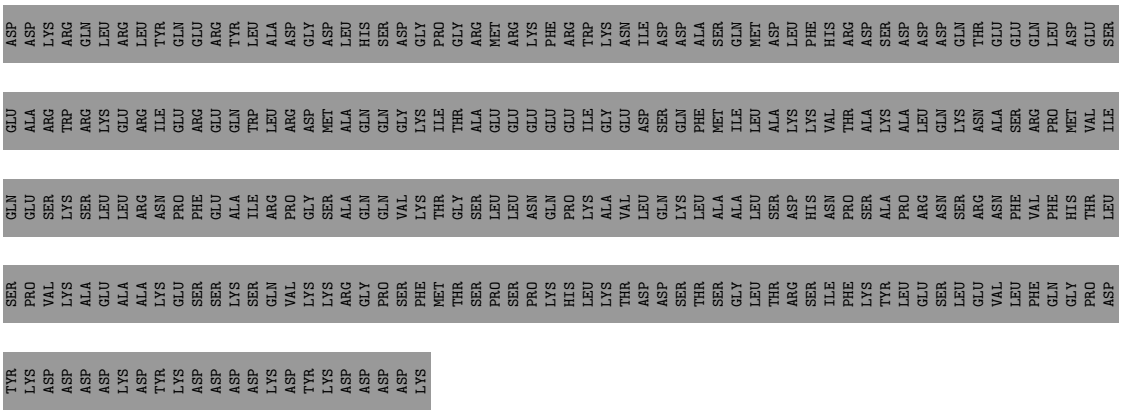


• Molecule 18: Claspin

Chain Q:

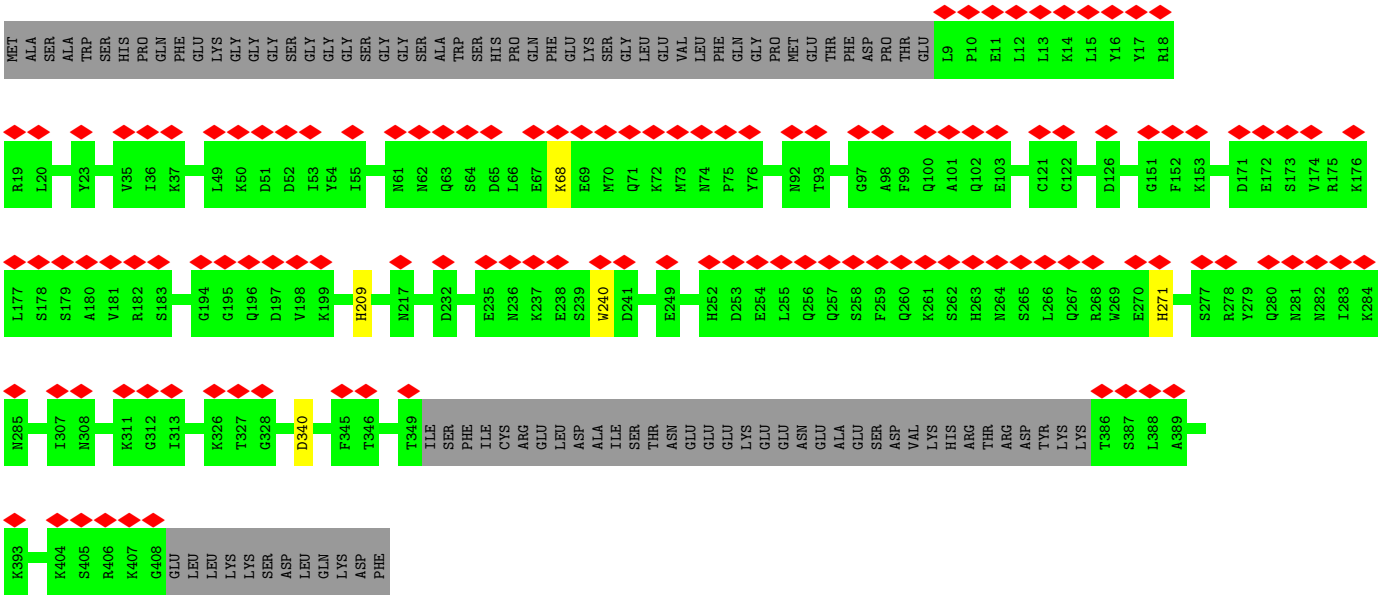

96%


K287
Q288
L289
H290
S291
E292
T293
Q294
R295
L296
I297
R298
N311
I314
F318
R526
H538
A539
P590
G591
E592
R609
F610
E611
E612
R613
Q614



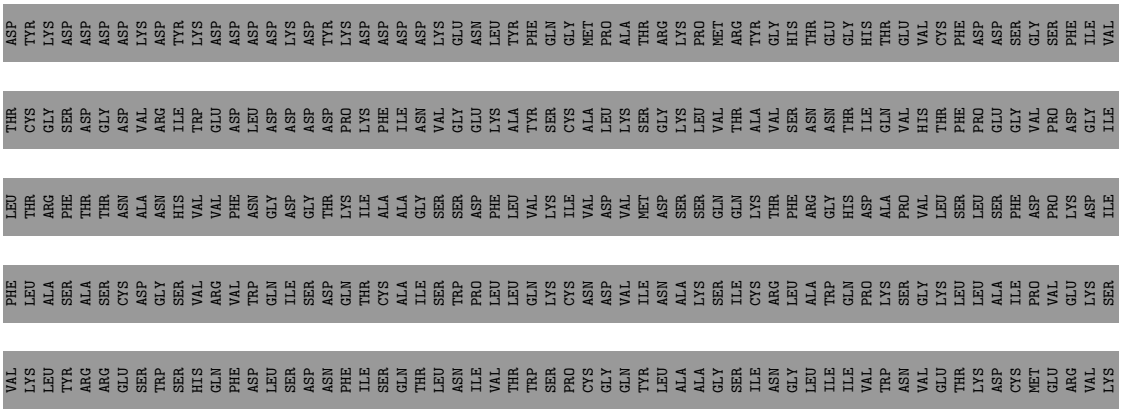
• Molecule 19: DNA primase small subunit

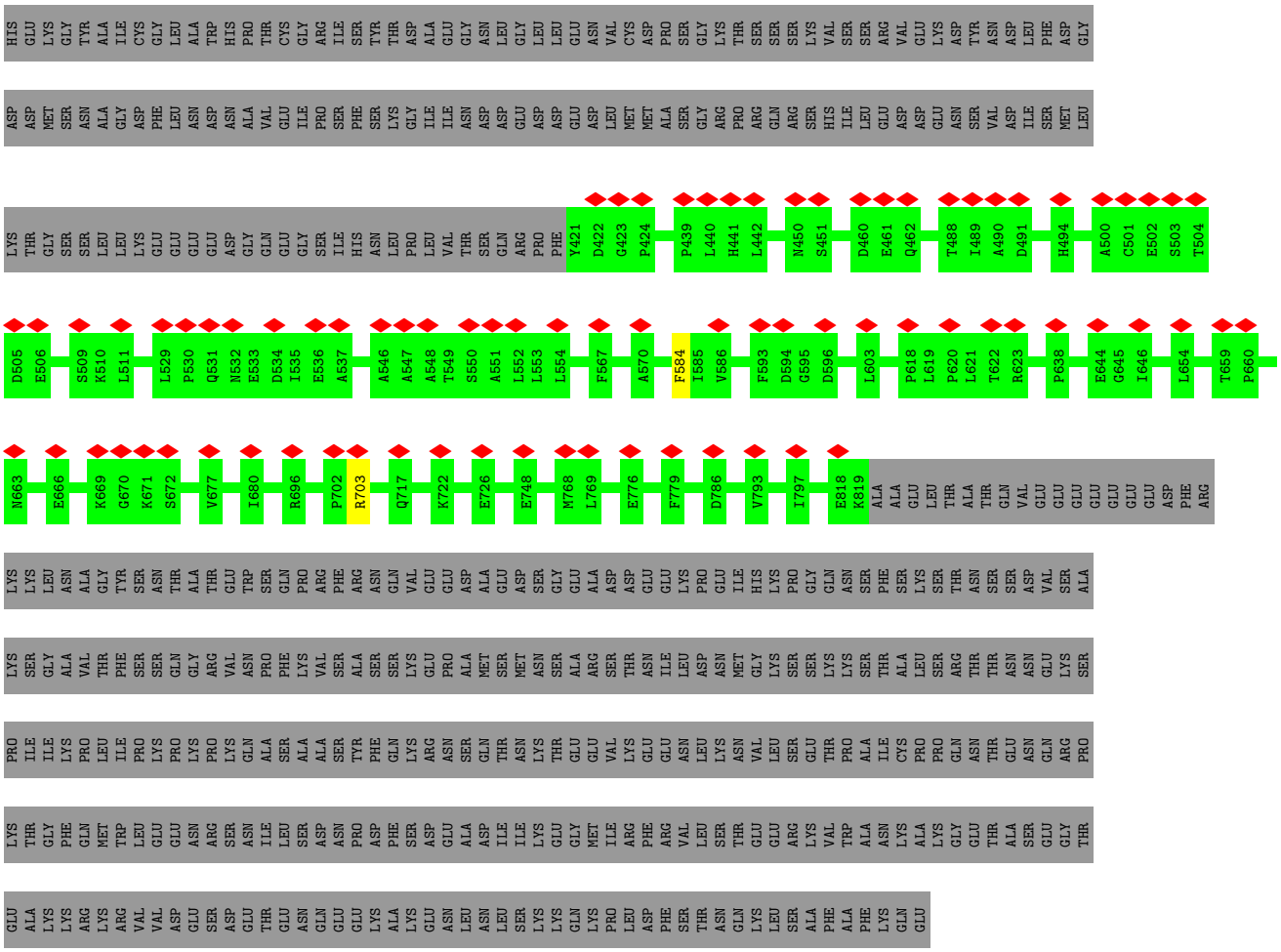
Chain O:



• Molecule 20: WD repeat and HMG-box DNA-binding protein 1

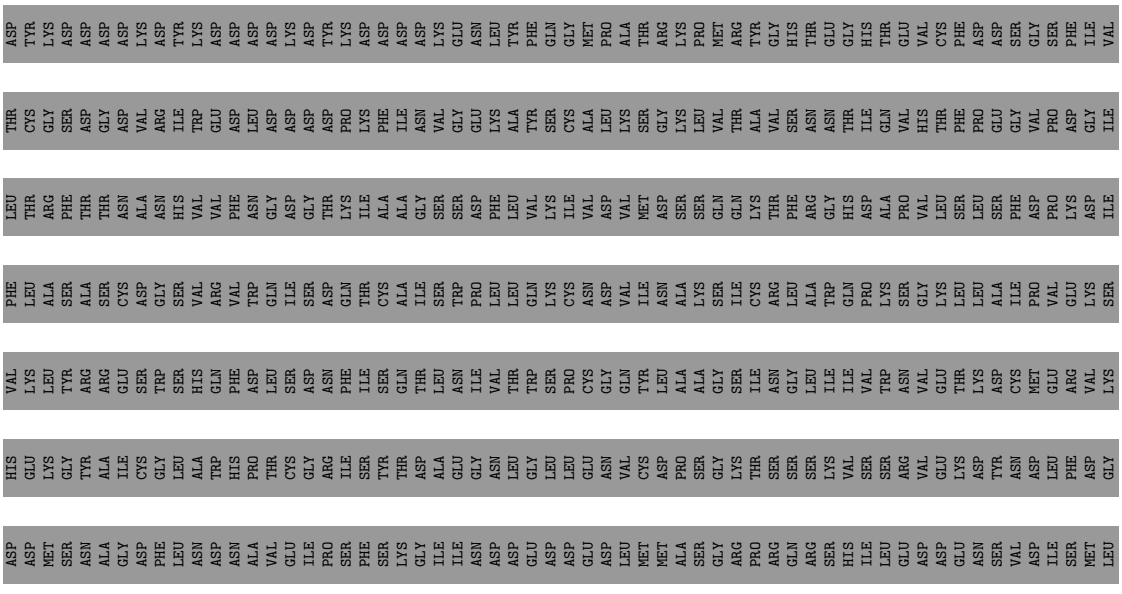
Chain H:

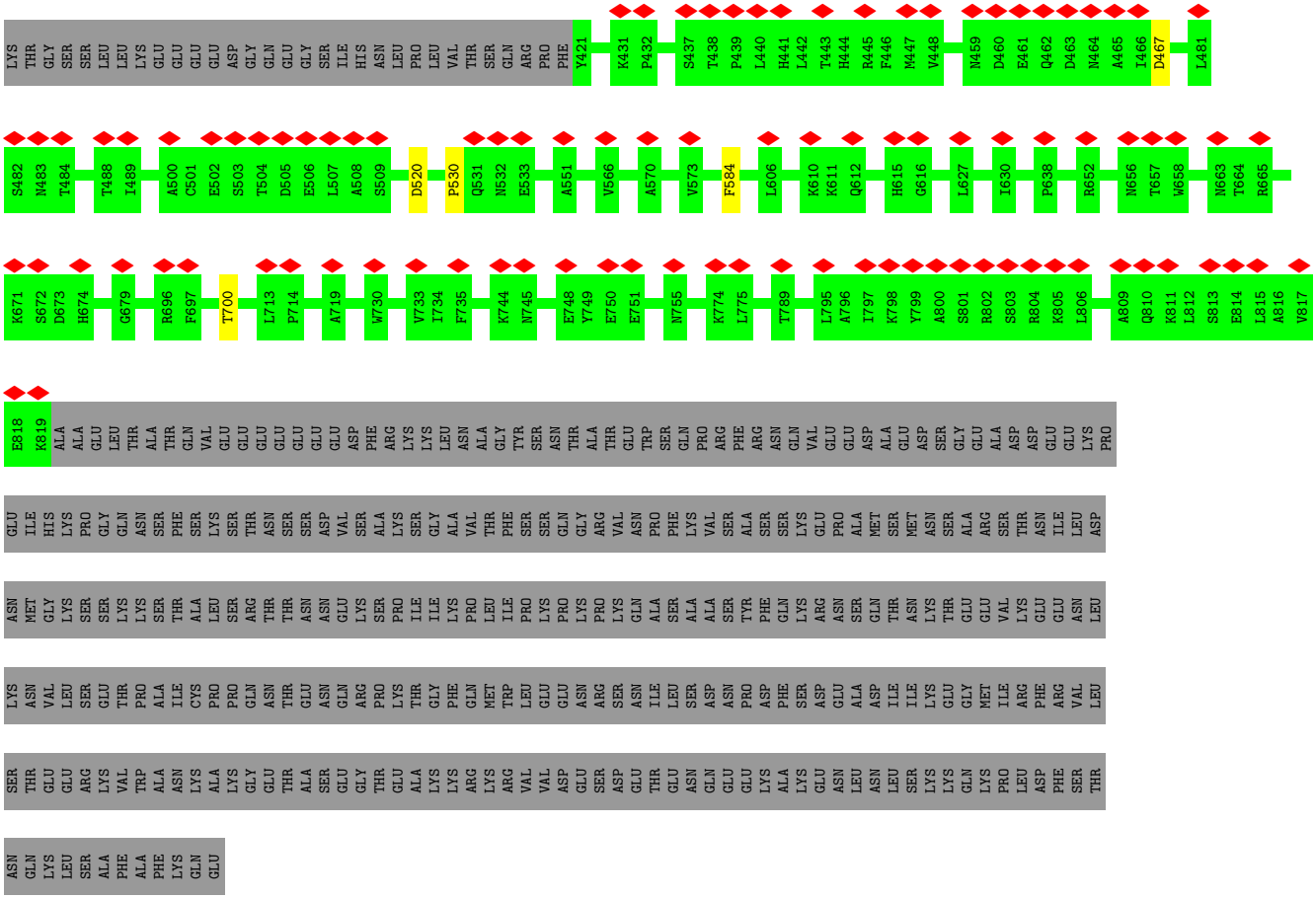




• Molecule 20: WD repeat and HMG-box DNA-binding protein 1

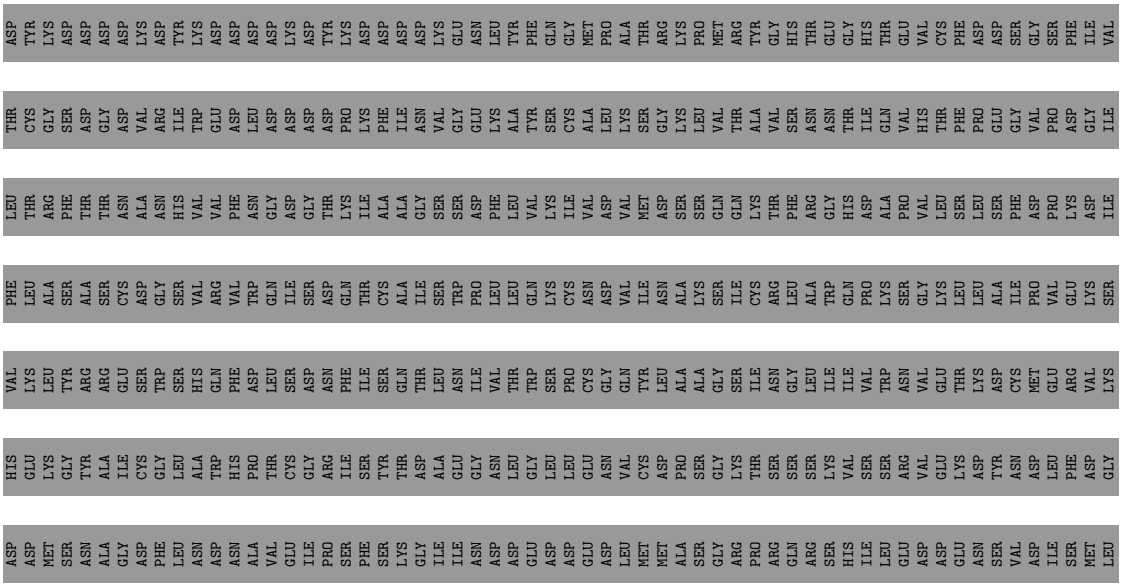
Chain J:

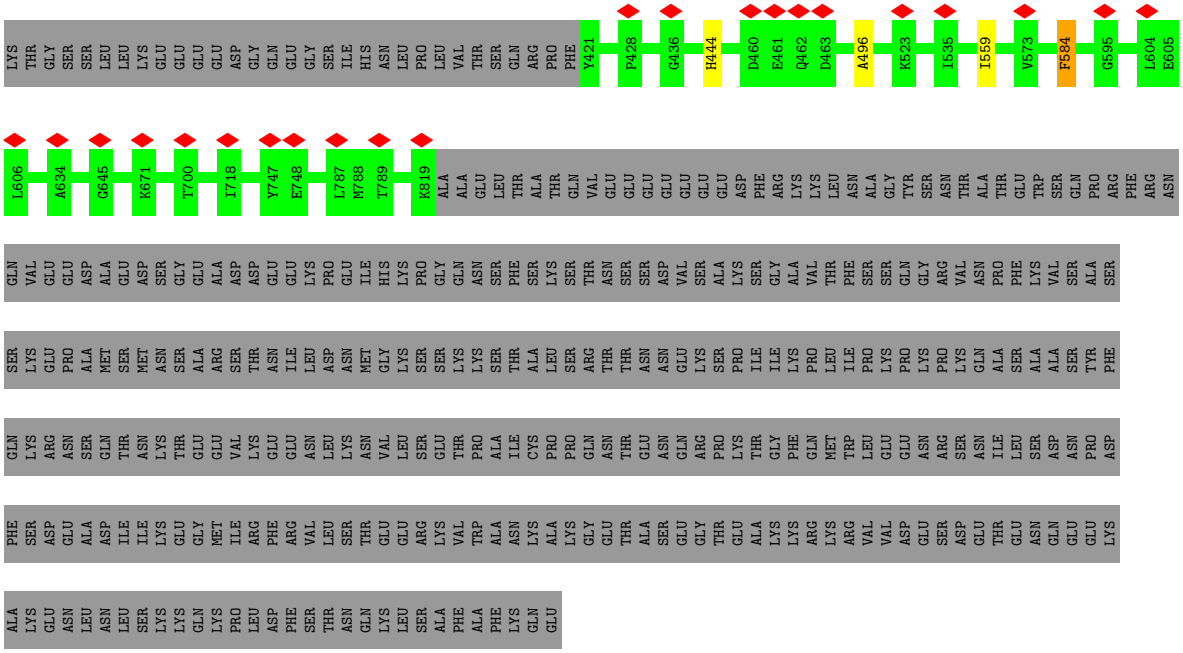




• Molecule 20: WD repeat and HMG-box DNA-binding protein 1

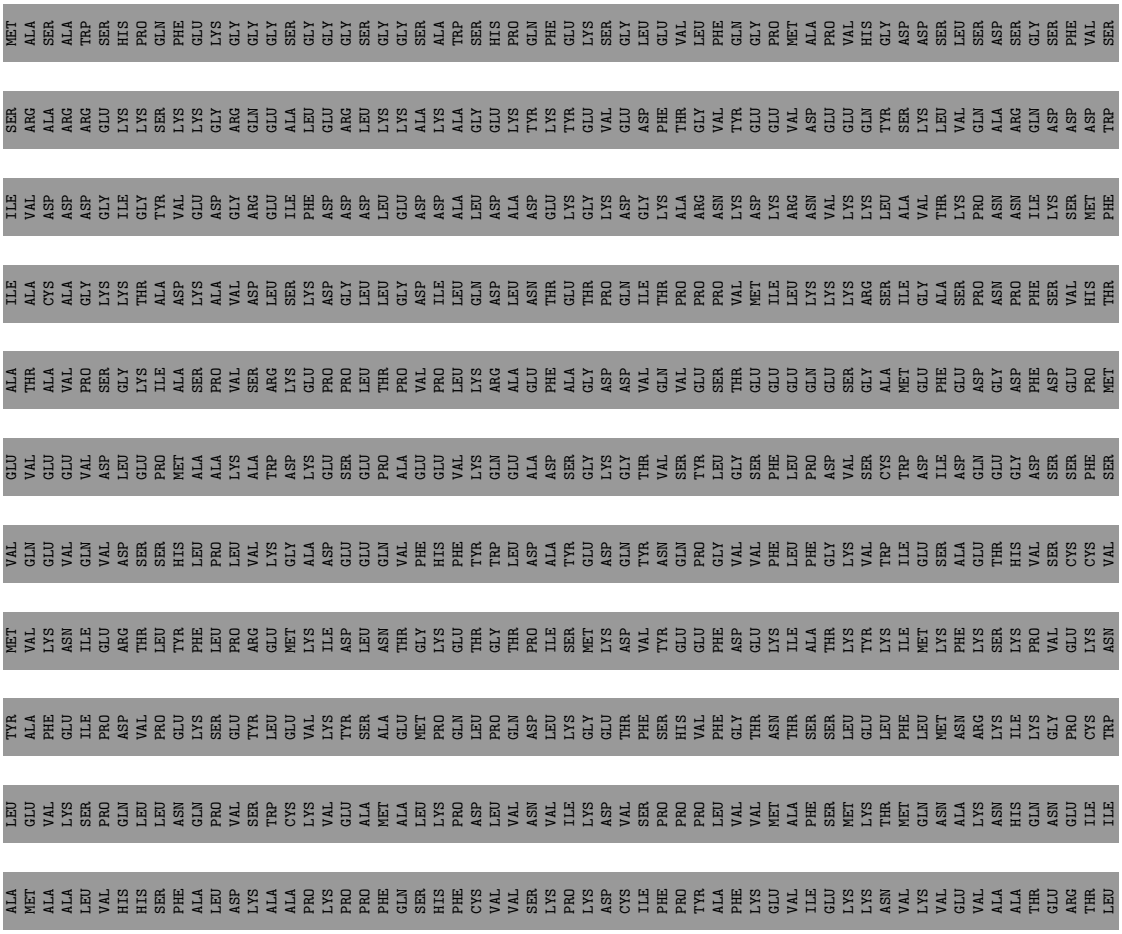
Chain I:

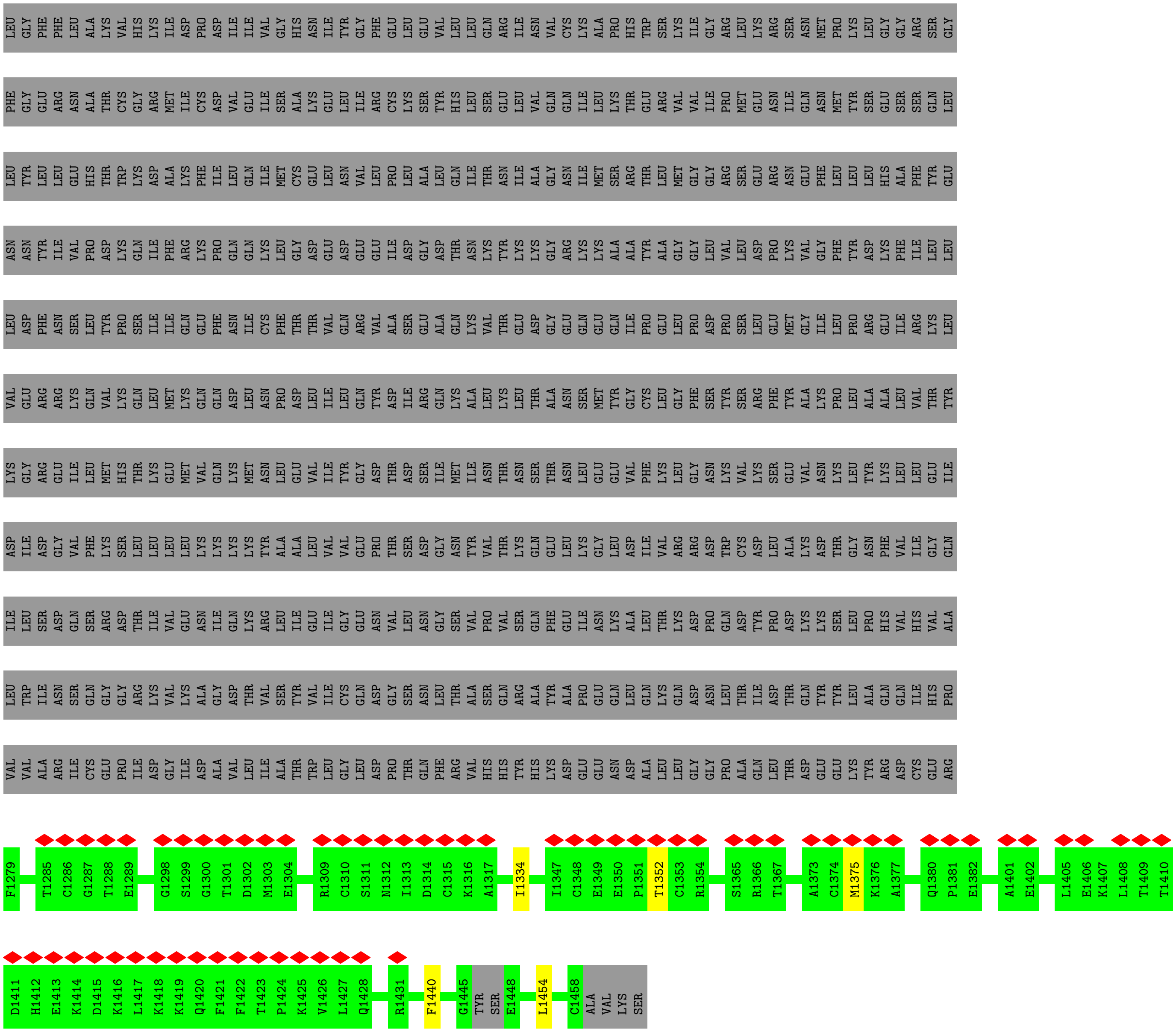




• Molecule 21: DNA polymerase alpha catalytic subunit

Chain B:




LEU GLY PHE PHE LEU ALA LYS VAL HIS LYS ILE ASP PRO ASP ILE ILE VAL GLY HIS ASN ILE TYR GLY PHE GLU LEU GLU VAL LEU LEU GLN ARG ILE ASN VAL CYS LYS ALA PRO HIS TRP SER LYS ILE GLY ARG LEU LYS ARG SER ASN MET PRO LYS LEU GLY GLY ARG SER GLY
PHE GLY GLU ARG ASN ALA THR CYS GLY ARG MET ILE CYS ASP VAL GLU ILE SER ALA LYS GLU LEU ILE ARG CYS LYS SER TYR HIS LEU SER GLU LEU VAL GLN GLN ILE LEU LYS THR GLU ARG VAL VAL ILE PRO MET GLU ASN ILE GLN ASN MET TYR SER GLU SER SER GLN LEU
LEU TYR LEU LEU GLU HIS THR TRP LYS ASP ALA LYS PHE ILE LEU GLN ILE MET CYS GLU LEU ASN VAL LEU PRO LEU ALA LEU GLN ILE THR ASN ILE ALA GLY ASN ILE MET SER ARG THR LEU MET GLY GLY ARG SER GLU ARG ASN GLU PHE LEU LEU LEU HIS ALA PHE TYR GLU
ASN ASN TYR ILE VAL PRO ASP LYS GLN ILE PHE ARG LYS PRO GLN GLN LYS LEU GLY ASP GLU ASP GLU GLU ILE ASP GLY ASP THR ASN LYS TYR LYS LYS GLY ARG LYS LYS ALA ALA TYR ALA GLY GLY LEU VAL LEU ASP PRO LYS VAL GLY PHE TYR ASP LYS PHE ILE LEU LEU
LEU ASP PHE ASN SER LEU TYR PRO SER ILE ILE GLN GLU PHE ASN ILE CYS PHE THR THR VAL GLN ARG VAL ALA SER GLU ALA GLN LYS VAL THR GLU ASP GLY GLU GLN GLU GLN ILE PRO GLU LEU PRO ASP PRO SER LEU GLU MET GLY ILE LEU PRO ARG GLU ILE ARG LYS LEU
VAL GLU ARG ARG LYS GLN VAL LYS GLN LEU MET LYS GLN GLN ASP LEU ASN PRO ASP LEU ILE LEU GLN TYR ASP ILE ARG GLN LYS ALA LEU LYS LEU THR ALA ASN SER MET TYR GLY CYS LEU GLY PHE SER TYR SER ARG PHE TYR ALA LYS PRO LEU ALA ALA LEU VAL THR TYR
LYS GLY ARG GLU ILE LEU MET HIS THR LYS GLU MET VAL GLN LYS MET ASN LEU GLU VAL ILE TYR GLY ASP THR ASP SER ILE MET ILE ASN THR ASN SER THR ASN LEU GLU GLU VAL PHE LYS LEU GLY ASN LYS VAL LYS SER GLU VAL ASN LYS LEU TYR TYR LYS LEU LEU GLU ILE
ASP ILE ASP GLY VAL PHE LYS SER LEU LEU LEU LEU LYS LYS LYS TYR ALA ALA LEU VAL VAL GLU PRO THR SER ASP GLY ASN TYR VAL THR LYS GLN GLU LEU LYS GLY LEU ASP ILE VAL ARG ARG ASP TRP CYS ASP LEU ALA LYS ASP THR GLY ASN PHE VAL ILE GLY GLN
ILE LEU SER ASP GLN SER ARG ASP THR ILE VAL GLU ASN ILE GLN LYS ARG LEU ILE GLU ILE GLY GLU ASN VAL LEU ASN GLY SER VAL PRO VAL SER GLN PHE GLU ILE ASN LYS ALA LEU THR LYS ASP PRO GLN ASP TYR PRO ASP LYS LYS SER LEU PRO HIS VAL HIS VAL ALA
LEU TRP ILE ASN SER GLN GLY GLY ARG LYS VAL LYS ALA GLY ASP THR VAL SER TYR VAL ILE CYS GLN ASP GLY SER ASN LEU THR ALA SER GLN ARG ALA TYR ALA PRO GLU GLN LEU GLN LYS GLN ASP ASN LEU THR ILE ASP THR GLN TYR TYR LEU ALA GLN GLN ILE HIS PRO
VAL VAL ALA ARG ILE CYS GLU PRO ILE ASP GLY ILE ASP ALA ALA VAL LEU ILE ALA THR TRP LEU GLY LEU ASP PRO THR GLN PHE ARG VAL HIS HIS TYR HIS LYS ASP GLU GLU ASN ASP ALA LEU LEU GLY GLY PRO ALA GLN LEU THR ASP GLU GLU LYS TYR ARG ASP CYS GLU ARG
F1279 T1285 C1286 G1287 T1288 E1289 G1298 S1299 G1300 T1301 D1302 M1303 E1304 R1309 C1310 S1311 N1312 I1313 D1314 C1315 K1316 A1317 I1334 I1347 C1348 E1349 E1350 P1351 T1352 C1353 R1354 S1365 R1366 T1367 A1373 C1374 M1375 K1376 A1377 Q1380 P1381 E1382 A1401 E1402 L1405 E1406 K1407 L1408 T1409 T1410
D1411 H1412 E1413 K1414 D1415 K1416 L1417 K1418 K1419 Q1420 F1421 F1422 T1423 P1424 K1425 V1426 L1427 Q1428 R1431 F1440 G1445 TYR SER E1448 L1454 C1458 ALA VAL LYS SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174696	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 ($e^-/Å^2$)	37.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.092	Depositor
Minimum map value	-2.479	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.137	Depositor
Map size (Å)	395.616, 395.616, 395.616	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2363, 1.2363, 1.2363	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, MG, ANP

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	0.42	0/4622	0.70	0/6244
2	3	0.42	0/4536	0.70	0/6116
3	4	0.43	0/5477	0.68	1/7397 (0.0%)
4	5	0.43	0/4744	0.71	0/6382
5	6	0.42	0/4911	0.70	0/6621
6	7	0.39	0/4639	0.70	0/6255
7	A	0.35	0/3569	0.61	0/4850
8	C	0.42	0/4428	0.67	1/5978 (0.0%)
9	D	0.42	0/1638	0.73	0/2202
10	E	0.43	0/1462	0.66	0/1981
11	F	0.38	0/1527	0.68	0/2062
12	G	0.41	0/1711	0.70	0/2305
13	K	0.46	0/5331	0.68	0/7181
14	L	0.45	0/750	0.73	0/999
15	M	0.87	1/738 (0.1%)	1.18	1/1138 (0.1%)
16	N	0.93	1/467 (0.2%)	1.07	0/715
17	P	0.42	0/2034	0.75	1/2736 (0.0%)
18	Q	0.41	0/522	0.67	0/686
19	O	0.36	0/3132	0.66	0/4226
20	H	0.40	0/3238	0.65	2/4387 (0.0%)
20	I	0.39	0/3238	0.66	2/4387 (0.0%)
20	J	0.40	0/3238	0.65	3/4387 (0.1%)
21	B	0.34	0/1475	0.62	0/1987
All	All	0.43	2/67427 (0.0%)	0.69	11/91222 (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
6	7	0	1
17	P	0	1
20	J	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	56	DT	C3'-O3'	5.30	1.50	1.44
16	N	25	DC	C1'-N1	5.20	1.56	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	584	PHE	CB-CG-CD2	-5.87	116.69	120.80
8	C	279	VAL	C-N-CA	5.83	136.28	121.70
20	I	584	PHE	CB-CG-CD2	-5.78	116.75	120.80
20	H	584	PHE	CB-CG-CD1	5.66	124.76	120.80
20	I	584	PHE	CB-CG-CD1	5.62	124.73	120.80
3	4	421	TYR	CA-CB-CG	5.56	123.96	113.40
17	P	208	TYR	CA-CB-CG	-5.42	103.10	113.40
20	J	584	PHE	CB-CG-CD2	-5.30	117.09	120.80
20	J	584	PHE	CB-CG-CD1	5.19	124.43	120.80
20	J	520	ASP	CB-CG-OD1	5.13	122.92	118.30
15	M	56	DT	P-O3'-C3'	5.04	125.75	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	7	90	GLU	Mainchain
20	J	530	PRO	Peptide
17	P	208	TYR	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	4540	4570	4570	4	0
2	3	4471	4518	4518	2	0
3	4	5389	5470	5470	2	0
4	5	4674	4738	4738	2	0
5	6	4836	4870	4870	0	0
6	7	4572	4637	4637	1	0
7	A	3493	3465	3465	0	0
8	C	4336	4285	4283	2	0
9	D	1606	1601	1601	0	0
10	E	1431	1456	1456	0	0
11	F	1495	1458	1458	0	0
12	G	1679	1701	1700	0	0
13	K	5229	5241	5241	1	0
14	L	735	766	766	0	0
15	M	662	370	372	0	0
16	N	419	237	238	0	0
17	P	1995	2007	2007	5	0
18	Q	516	536	536	0	0
19	O	3052	3035	3035	0	0
20	H	3162	3124	3124	0	0
20	I	3162	3124	3124	1	0
20	J	3162	3124	3124	0	0
21	B	1443	1430	1430	1	0
22	2	31	13	13	0	0
22	3	31	13	13	2	0
22	5	31	13	13	0	0
23	2	1	0	0	0	0
23	3	1	0	0	0	0
23	5	1	0	0	0	0
24	4	1	0	0	0	0
24	5	1	0	0	0	0
24	6	1	0	0	0	0
24	7	1	0	0	0	0
All	All	66159	65802	65802	19	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 (19) 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)
2:3:348:SER:H	22:3:1000:ANP:HNB1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:24:ASP:OD1	6:7:30:GLN:N	2.38	0.55
17:P:119:TRP:O	17:P:123:GLN:NE2	2.47	0.47
17:P:244:GLU:OE1	17:P:244:GLU:N	2.47	0.47
1:2:290:LEU:O	1:2:290:LEU:HD12	2.16	0.45
1:2:633:ILE:HD11	1:2:648:ASP:HB2	1.99	0.45
8:C:514:ASP:OD1	8:C:515:SER:N	2.50	0.45
1:2:373:TYR:CE2	4:5:289:ILE:HD11	2.53	0.43
13:K:190:LEU:HD12	13:K:338:VAL:HG13	2.00	0.43
17:P:138:ASP:OD1	17:P:139:LYS:N	2.52	0.43
21:B:1334:ILE:HG21	21:B:1440:PHE:CD2	2.54	0.42
3:4:390:VAL:HG22	3:4:421:TYR:HB3	2.01	0.42
2:3:348:SER:N	22:3:1000:ANP:HNB1	2.16	0.41
1:2:751:ARG:NH2	4:5:523:GLU:O	2.53	0.41
3:4:290:ILE:CD1	3:4:355:GLN:HB2	2.50	0.41
20:I:496:ALA:HB3	20:I:559:ILE:HD11	2.03	0.41
17:P:163:GLU:HB2	17:P:178:LEU:HD22	2.03	0.41
8:C:470:SER:OG	8:C:509:ILE:HD11	2.21	0.40
17:P:186:ILE:HD11	17:P:209:VAL:HG11	2.02	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	568/904 (63%)	553 (97%)	15 (3%)	0	100	100
2	3	559/808 (69%)	541 (97%)	18 (3%)	0	100	100
3	4	667/863 (77%)	652 (98%)	15 (2%)	0	100	100
4	5	587/734 (80%)	571 (97%)	16 (3%)	0	100	100
5	6	597/821 (73%)	581 (97%)	16 (3%)	0	100	100
6	7	562/719 (78%)	549 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	444/598 (74%)	436 (98%)	8 (2%)	0	100	100
8	C	529/569 (93%)	516 (98%)	13 (2%)	0	100	100
9	D	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
10	E	174/185 (94%)	171 (98%)	3 (2%)	0	100	100
11	F	183/216 (85%)	179 (98%)	4 (2%)	0	100	100
12	G	201/261 (77%)	198 (98%)	3 (2%)	0	100	100
13	K	632/1209 (52%)	625 (99%)	7 (1%)	0	100	100
14	L	85/301 (28%)	82 (96%)	3 (4%)	0	100	100
17	P	237/509 (47%)	226 (95%)	11 (5%)	0	100	100
18	Q	51/1371 (4%)	51 (100%)	0	0	100	100
19	O	360/462 (78%)	350 (97%)	10 (3%)	0	100	100
20	H	397/1160 (34%)	390 (98%)	7 (2%)	0	100	100
20	I	397/1160 (34%)	388 (98%)	9 (2%)	0	100	100
20	J	397/1160 (34%)	393 (99%)	4 (1%)	0	100	100
21	B	174/1504 (12%)	170 (98%)	4 (2%)	0	100	100
All	All	7994/15710 (51%)	7813 (98%)	181 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	499/781 (64%)	497 (100%)	2 (0%)	91	95
2	3	489/707 (69%)	486 (99%)	3 (1%)	86	94
3	4	598/753 (79%)	597 (100%)	1 (0%)	93	98
4	5	509/625 (81%)	506 (99%)	3 (1%)	86	94
5	6	538/724 (74%)	535 (99%)	3 (1%)	86	94
6	7	498/619 (80%)	494 (99%)	4 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	A	396/527 (75%)	395 (100%)	1 (0%)	92 97
8	C	486/520 (94%)	483 (99%)	3 (1%)	86 94
9	D	173/174 (99%)	170 (98%)	3 (2%)	60 80
10	E	160/169 (95%)	160 (100%)	0	100 100
11	F	163/186 (88%)	162 (99%)	1 (1%)	86 94
12	G	188/232 (81%)	188 (100%)	0	100 100
13	K	562/1055 (53%)	553 (98%)	9 (2%)	62 81
14	L	78/274 (28%)	76 (97%)	2 (3%)	46 72
17	P	220/459 (48%)	207 (94%)	13 (6%)	19 49
18	Q	54/1230 (4%)	52 (96%)	2 (4%)	34 62
19	O	339/422 (80%)	334 (98%)	5 (2%)	65 82
20	H	345/1017 (34%)	344 (100%)	1 (0%)	92 97
20	I	345/1017 (34%)	343 (99%)	2 (1%)	86 94
20	J	345/1017 (34%)	343 (99%)	2 (1%)	86 94
21	B	164/1328 (12%)	161 (98%)	3 (2%)	59 79
All	All	7149/13836 (52%)	7086 (99%)	63 (1%)	79 90

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	753	GLU
1	2	784	ASP
2	3	76	PHE
2	3	394	GLU
2	3	648	LEU
3	4	421	TYR
4	5	224	PHE
4	5	417	SER
4	5	483	SER
5	6	347	TYR
5	6	410	GLU
5	6	509	HIS
6	7	62	LEU
6	7	106	ARG
6	7	476	THR
6	7	593	TRP
7	A	575	TYR

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Mol	Chain	Res	Type
8	C	247	ARG
8	C	280	LEU
8	C	284	TRP
9	D	88	ARG
9	D	94	TYR
9	D	193	HIS
11	F	68	LEU
13	K	124	PHE
13	K	263	GLU
13	K	274	ARG
13	K	304	LEU
13	K	343	ARG
13	K	358	MET
13	K	363	ASP
13	K	364	HIS
13	K	794	TRP
14	L	66	LYS
14	L	91	LYS
17	P	28	PHE
17	P	63	TYR
17	P	70	TYR
17	P	111	CYS
17	P	123	GLN
17	P	131	ARG
17	P	139	LYS
17	P	176	LEU
17	P	188	PHE
17	P	195	PHE
17	P	202	LEU
17	P	203	GLU
17	P	244	GLU
18	Q	609	ARG
18	Q	613	ARG
19	O	68	LYS
19	O	209	HIS
19	O	240	TRP
19	O	271	HIS
19	O	340	ASP
20	H	703	ARG
21	B	1352	THR
21	B	1375	MET
21	B	1454	LEU

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Mol	Chain	Res	Type
20	J	467	ASP
20	J	700	THR
20	I	444	HIS
20	I	584	PHE

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

Mol	Chain	Res	Type
10	E	37	ASN

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 10 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
22	ANP	5	1001	23	29,33,33	1.09	3 (10%)	31,52,52	1.20	2 (6%)
22	ANP	3	1000	23	29,33,33	1.04	3 (10%)	31,52,52	1.20	3 (9%)
22	ANP	2	1000	23	29,33,33	1.11	3 (10%)	31,52,52	1.12	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
22	ANP	5	1001	23	-	2/14/38/38	0/3/3/3
22	ANP	3	1000	23	-	3/14/38/38	0/3/3/3
22	ANP	2	1000	23	-	2/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	1001	ANP	PB-O3A	-3.50	1.54	1.59
22	2	1000	ANP	PB-O3A	-3.45	1.54	1.59
22	3	1000	ANP	PB-O3A	-3.18	1.55	1.59
22	5	1001	ANP	PG-O1G	2.37	1.49	1.46
22	2	1000	ANP	PB-O1B	2.28	1.49	1.46
22	2	1000	ANP	PG-O1G	2.28	1.49	1.46
22	3	1000	ANP	PB-O1B	2.19	1.49	1.46
22	3	1000	ANP	PG-O1G	2.16	1.49	1.46
22	5	1001	ANP	PB-O1B	2.10	1.49	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	1001	ANP	PB-O3A-PA	-4.33	117.38	132.62
22	2	1000	ANP	PB-O3A-PA	-3.94	118.73	132.62
22	3	1000	ANP	PB-O3A-PA	-3.65	119.78	132.62
22	3	1000	ANP	O1G-PG-N3B	-3.03	107.31	111.77
22	2	1000	ANP	C5-C6-N6	2.14	123.61	120.35
22	5	1001	ANP	O3A-PB-N3B	-2.04	100.94	106.59
22	3	1000	ANP	C5-C6-N6	2.03	123.43	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2	1000	ANP	PB-N3B-PG-O1G
22	2	1000	ANP	PG-N3B-PB-O1B
22	3	1000	ANP	PB-N3B-PG-O1G
22	3	1000	ANP	PA-O3A-PB-O1B
22	3	1000	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
22	5	1001	ANP	PB-N3B-PG-O1G
22	5	1001	ANP	PG-N3B-PB-O1B

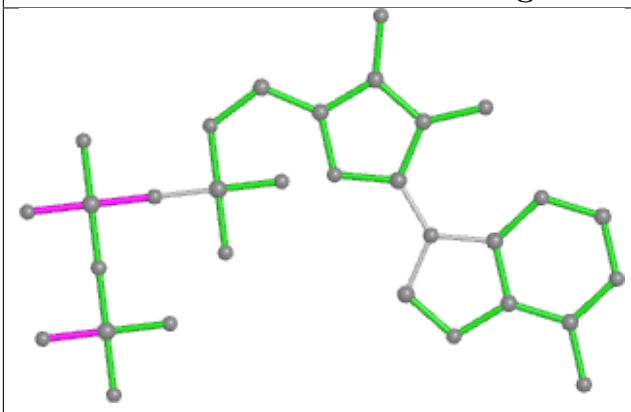
There are no ring outliers.

1 monomer is involved in 2 short contacts:

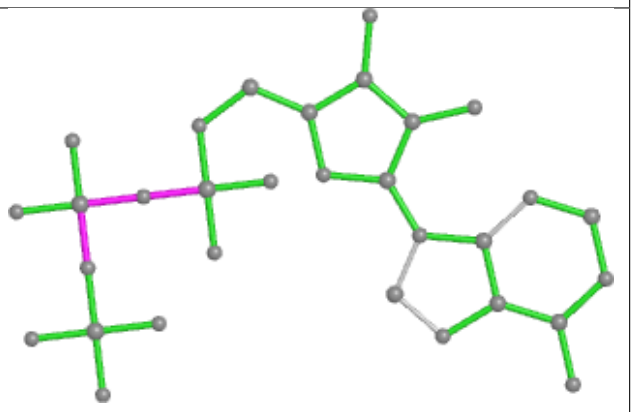
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	1000	ANP	2	0

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.

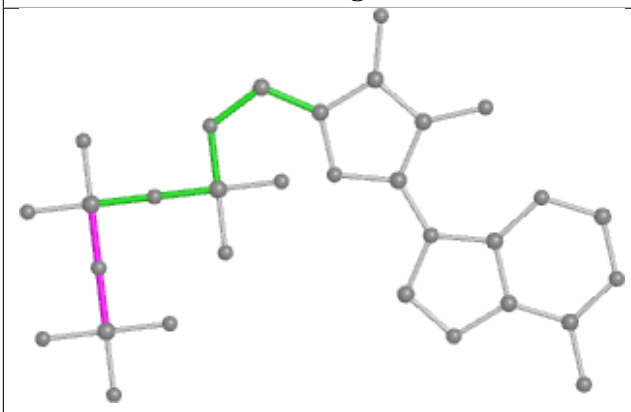
Ligand ANP 5 1001



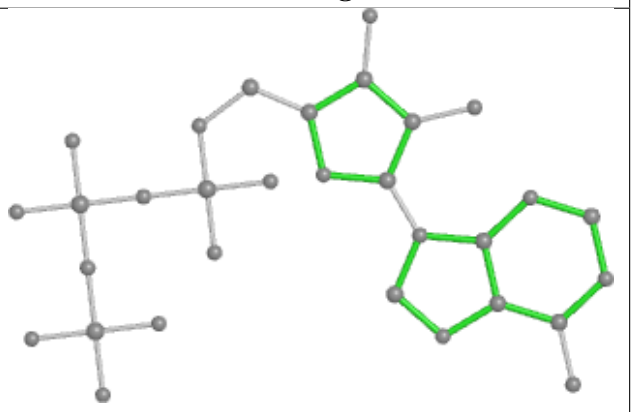
Bond lengths



Bond angles

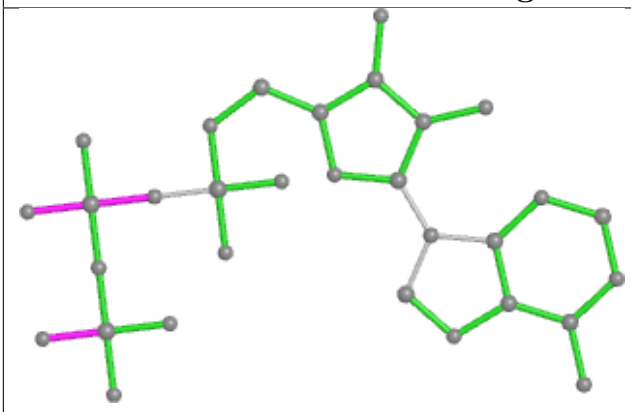


Torsions

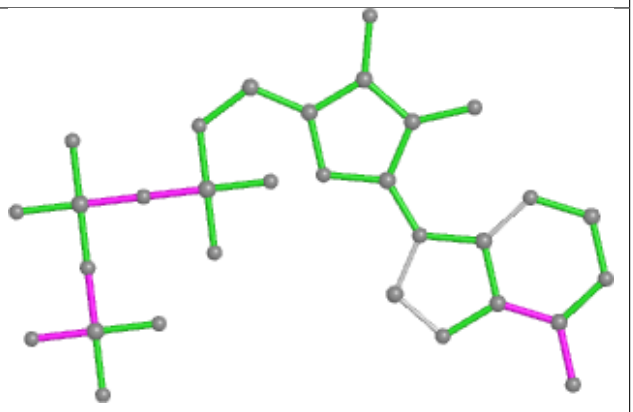


Rings

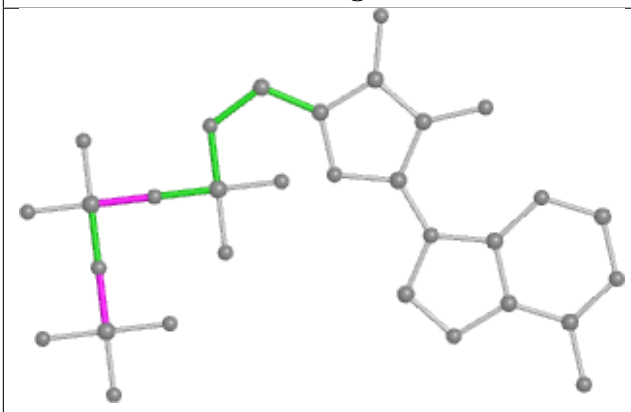
Ligand ANP 3 1000



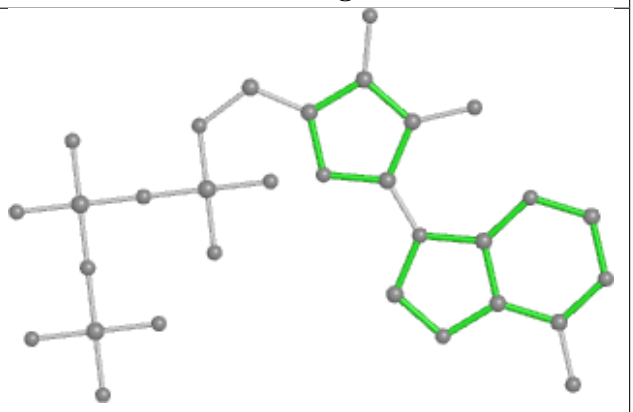
Bond lengths



Bond angles

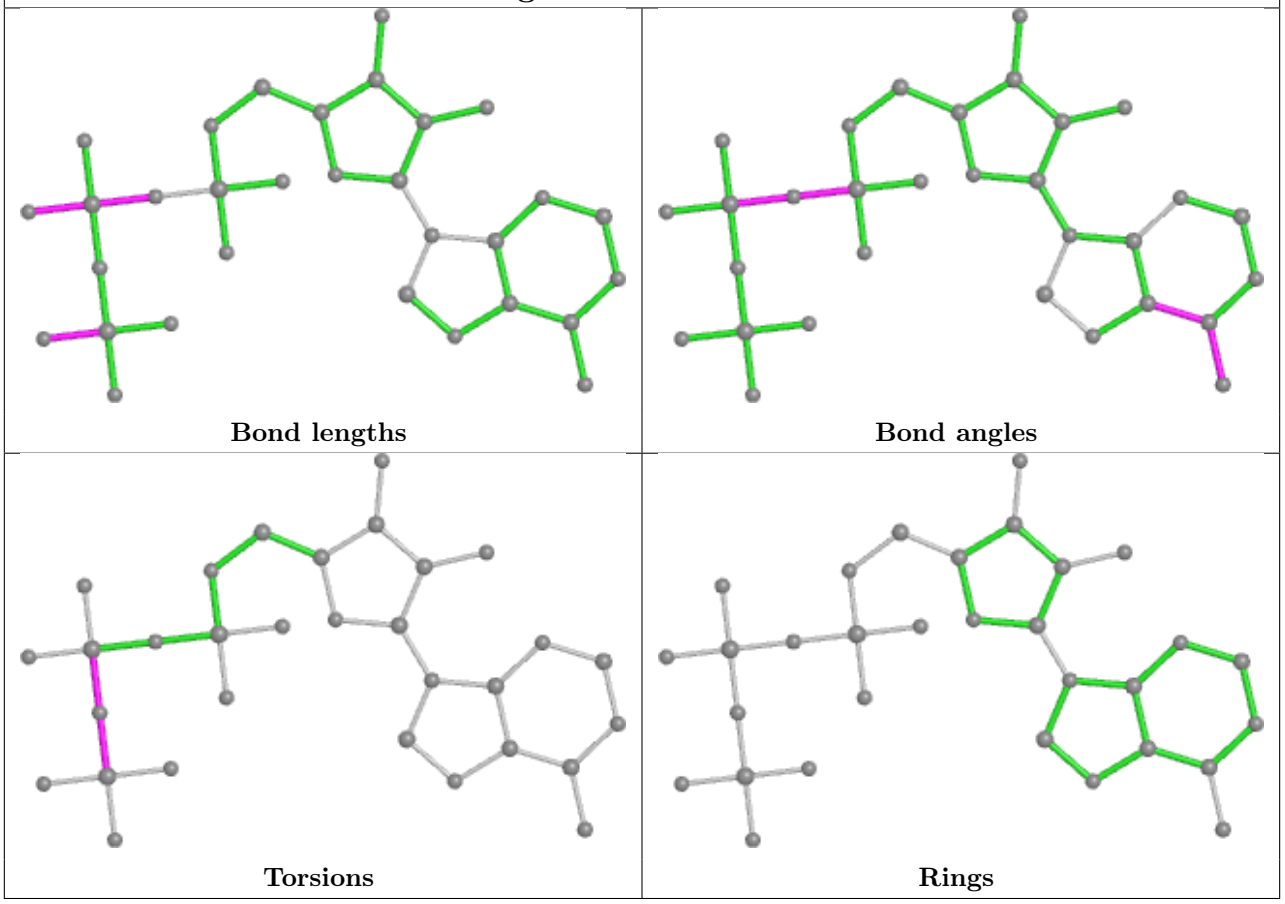


Torsions



Rings

Ligand ANP 2 1000



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.

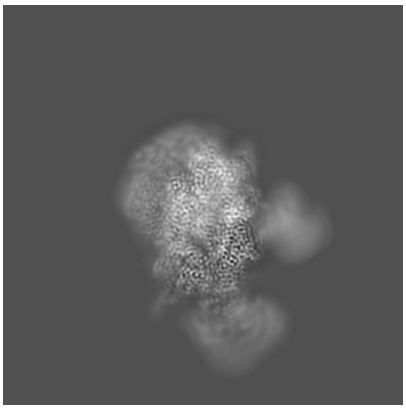
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15341. These allow visual inspection of the internal detail of the map and identification of artifacts.

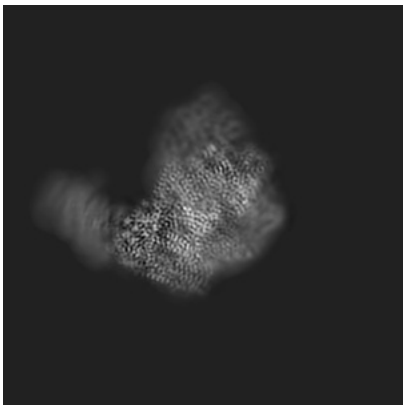
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

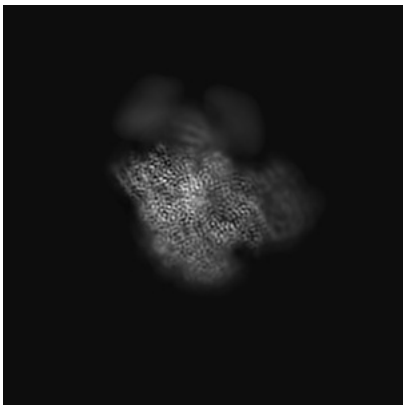
6.1.1 Primary map



X

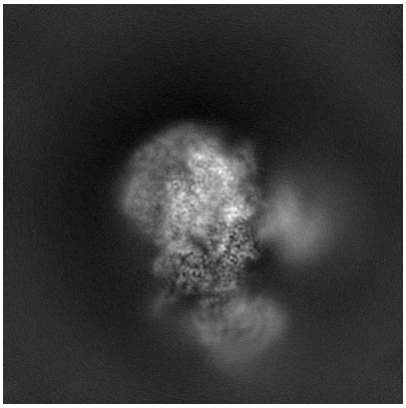


Y

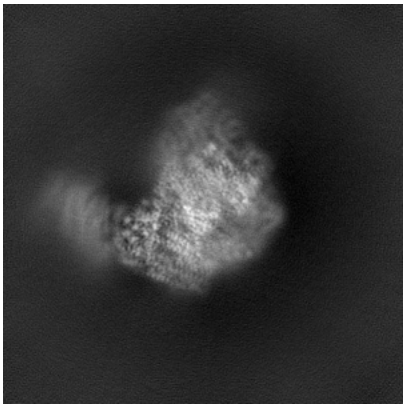


Z

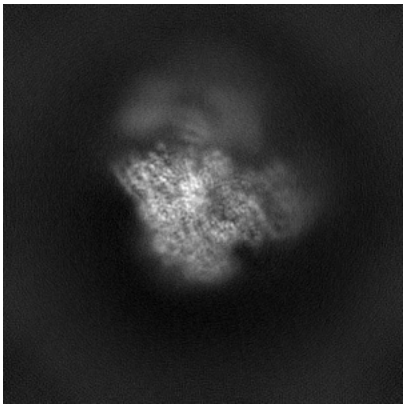
6.1.2 Raw map



X



Y

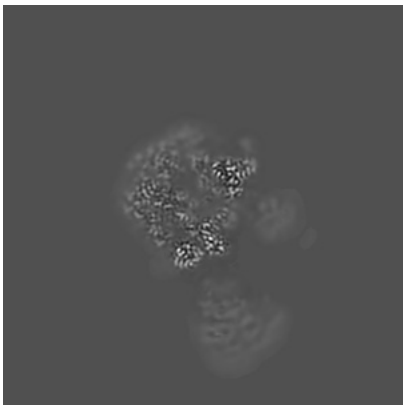


Z

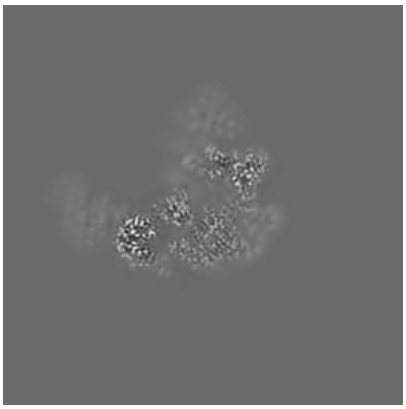
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

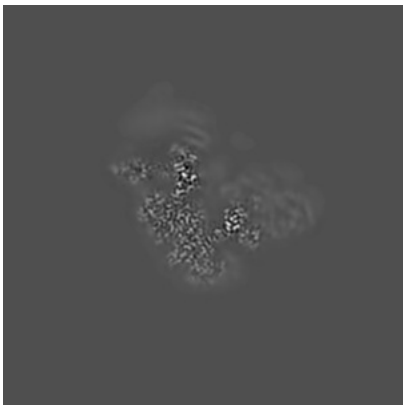
6.2.1 Primary map



X Index: 160

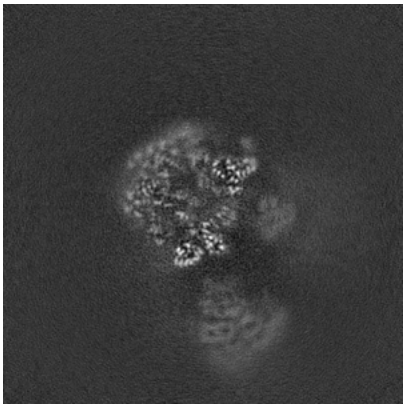


Y Index: 160

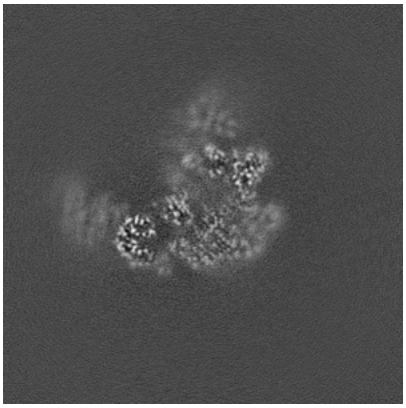


Z Index: 160

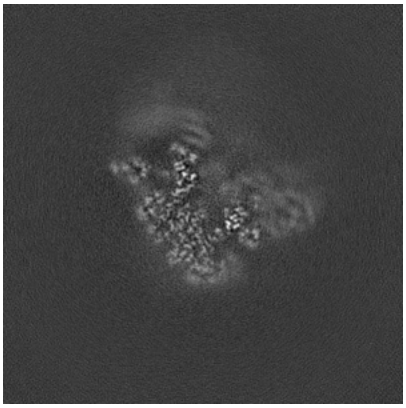
6.2.2 Raw map



X Index: 160



Y Index: 160

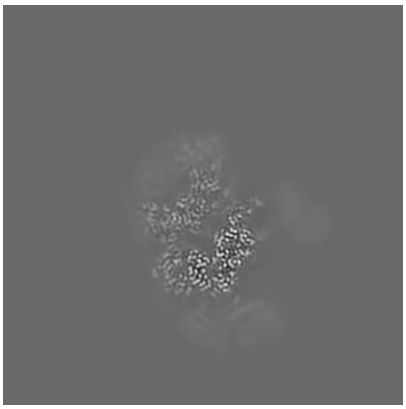


Z Index: 160

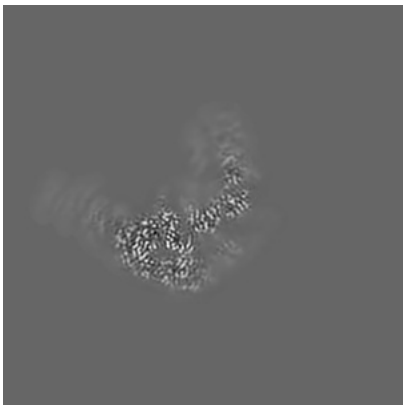
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

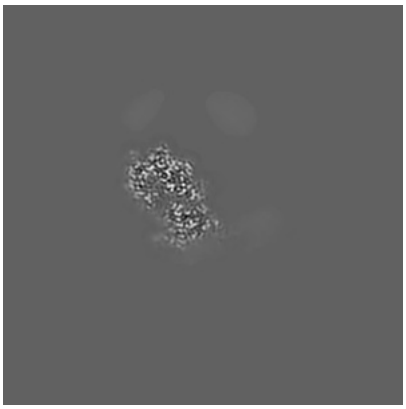
6.3.1 Primary map



X Index: 135

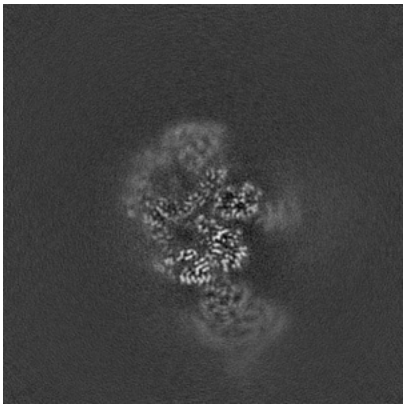


Y Index: 180

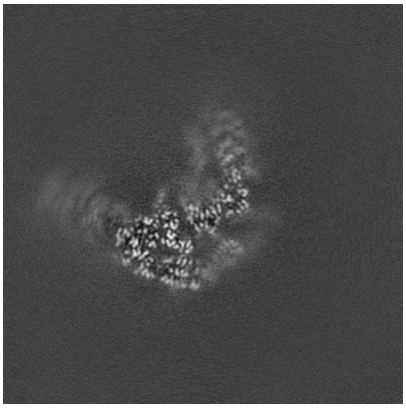


Z Index: 120

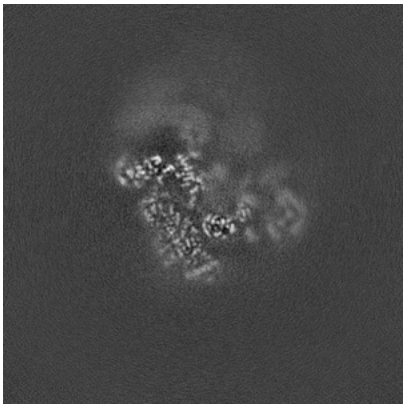
6.3.2 Raw map



X Index: 147



Y Index: 179

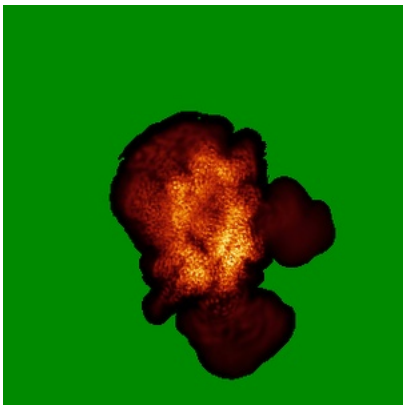


Z Index: 151

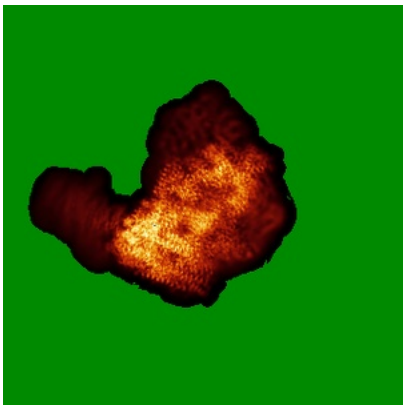
The images above show the largest variance slices of the map in three orthogonal directions.

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

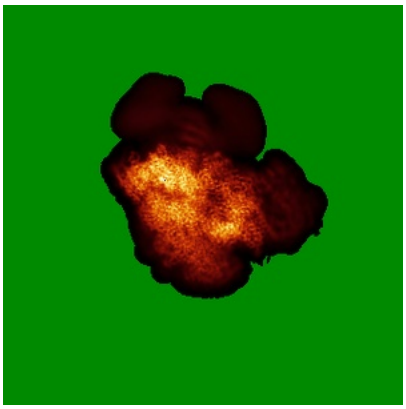
6.4.1 Primary map



X

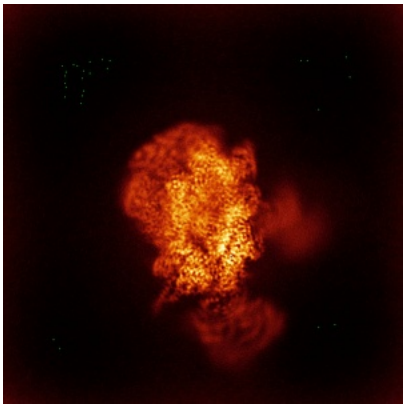


Y

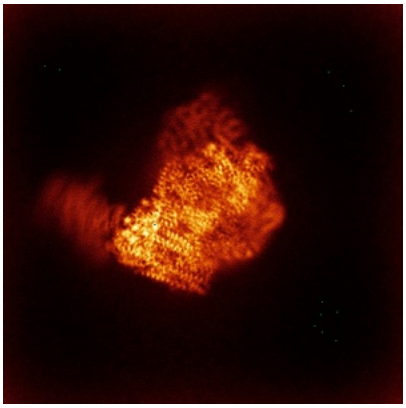


Z

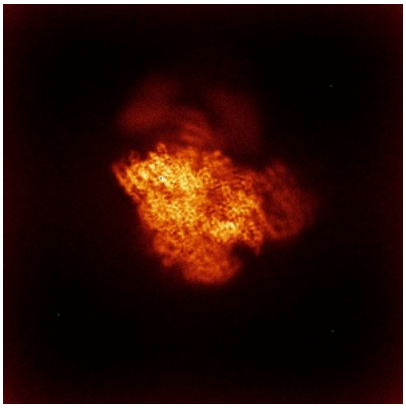
6.4.2 Raw map



X



Y

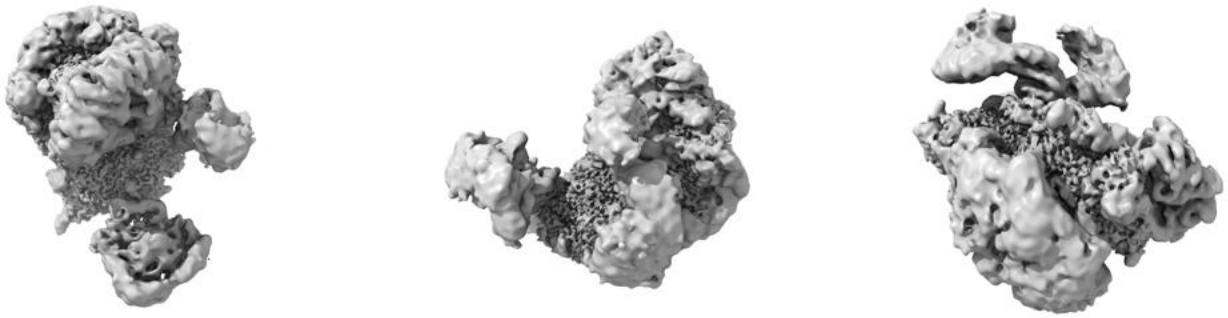


Z

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

6.5 Orthogonal surface views (i)

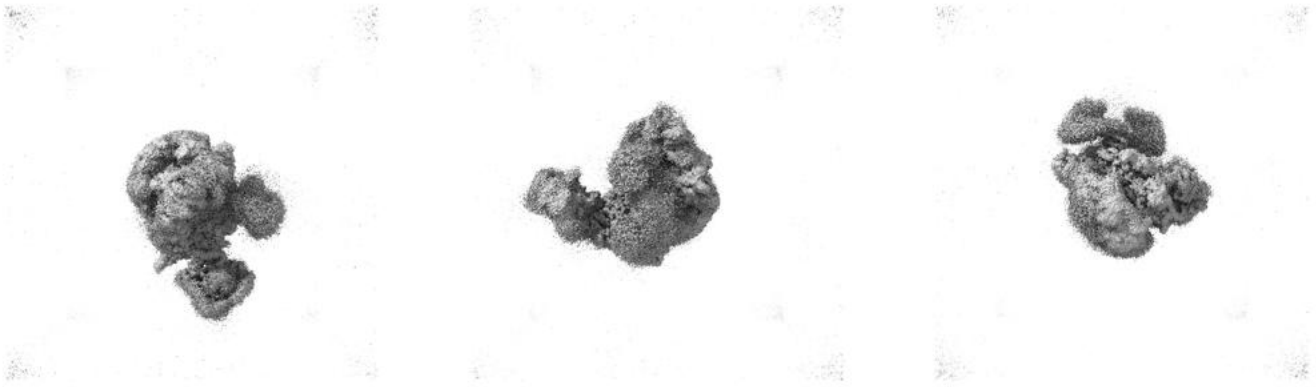
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.137. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

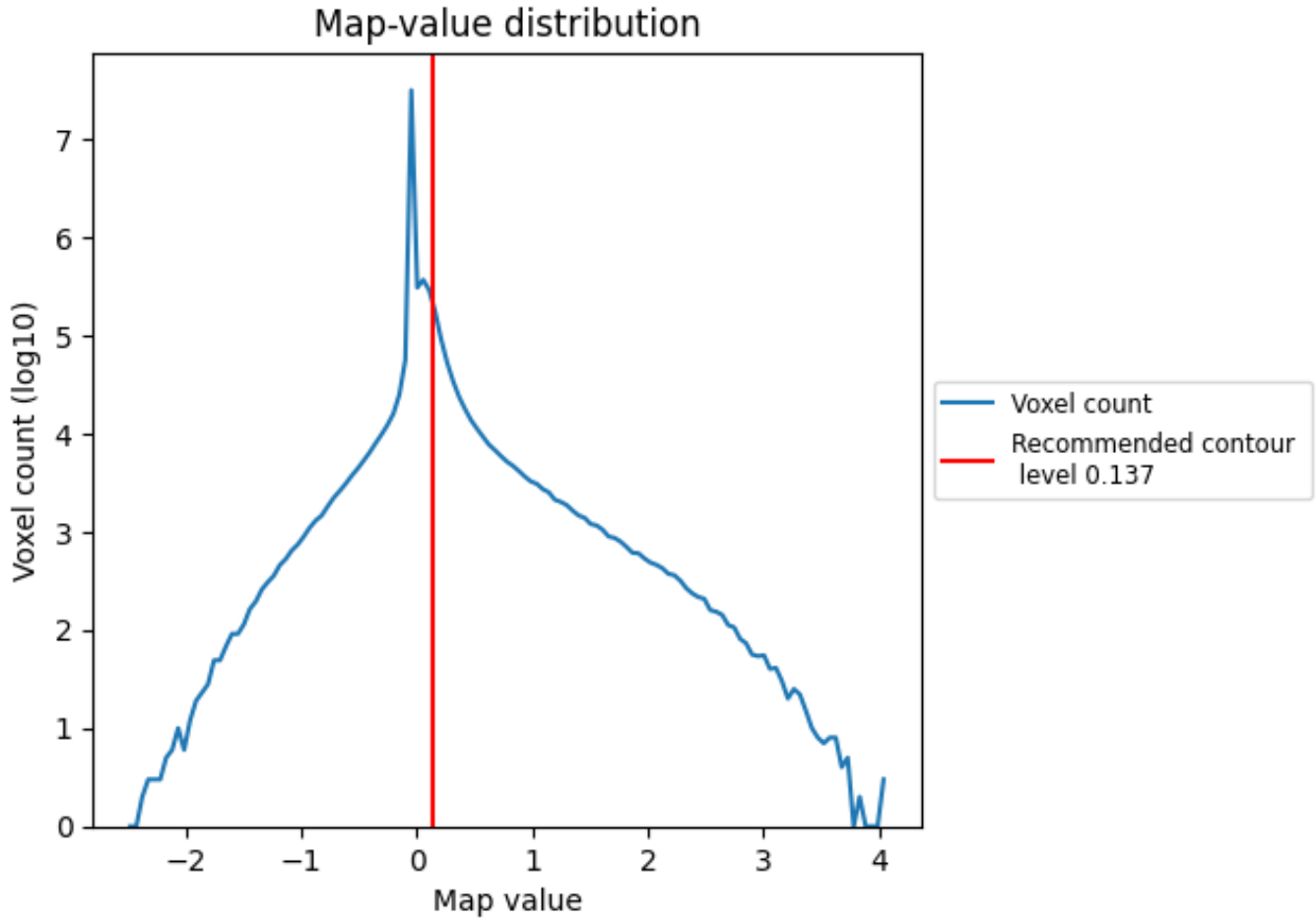
6.6 Mask visualisation (i)

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

7 Map analysis

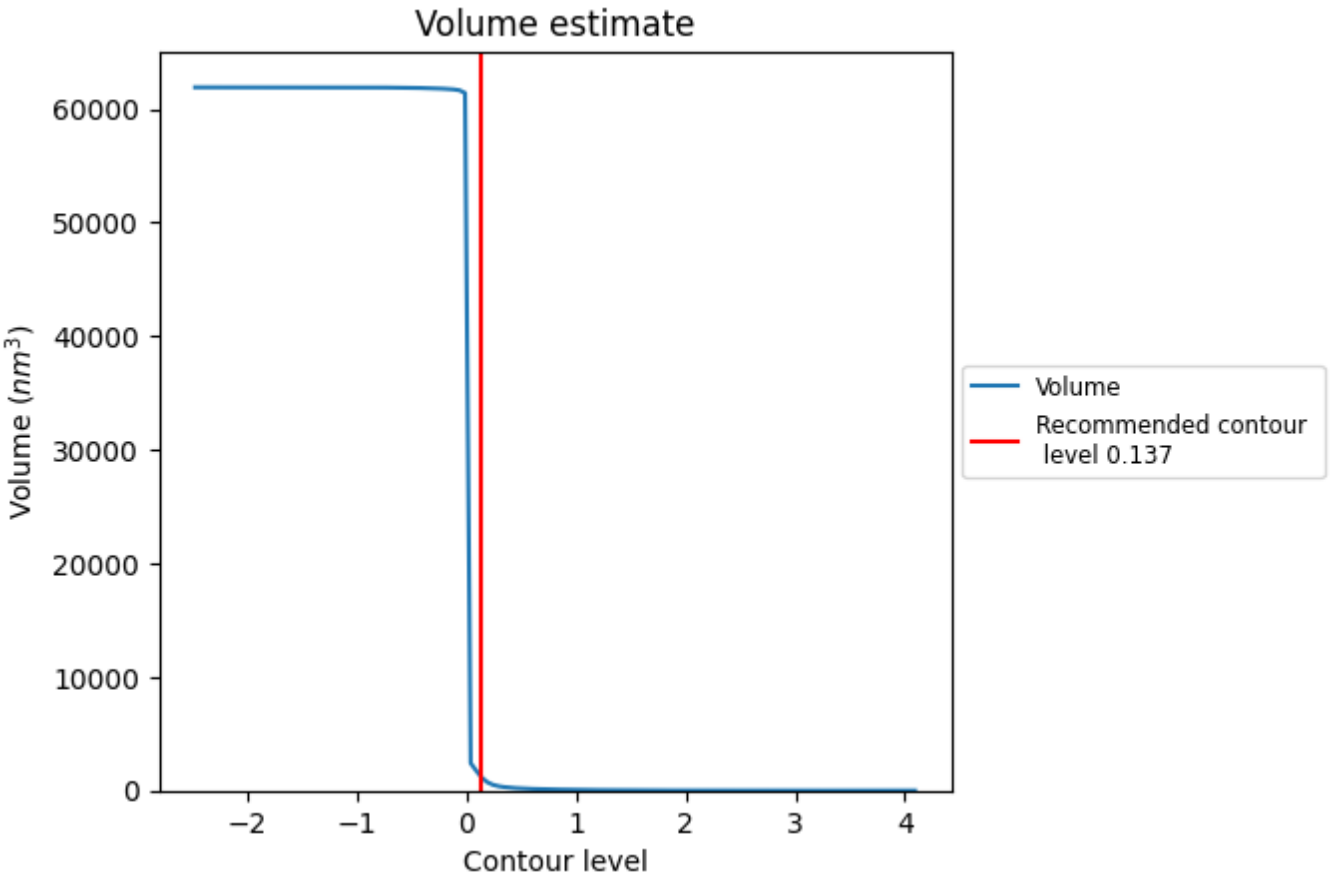
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

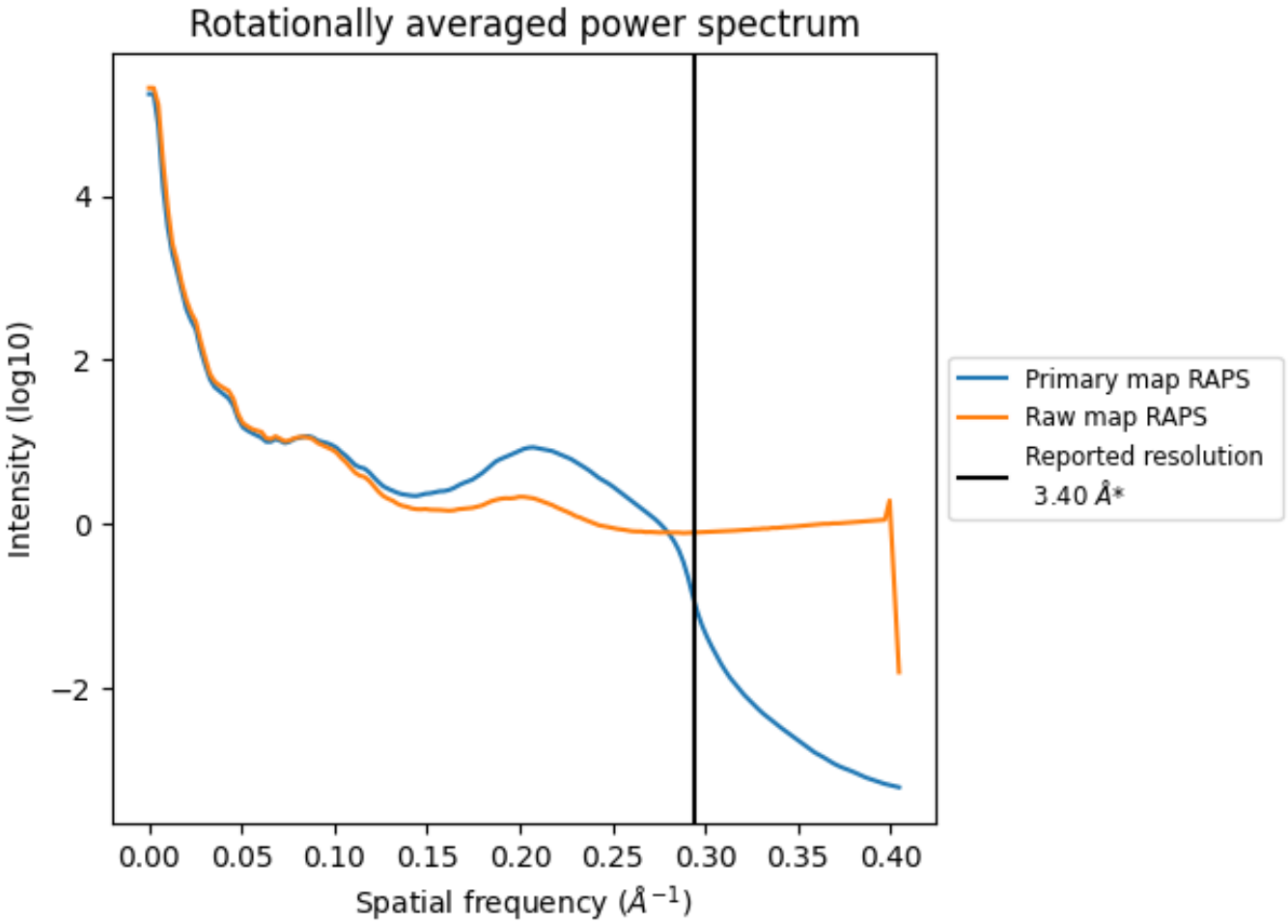
7.2 Volume estimate



The volume at the recommended contour level is 1147 nm^3; this corresponds to an approximate mass of 1036 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)

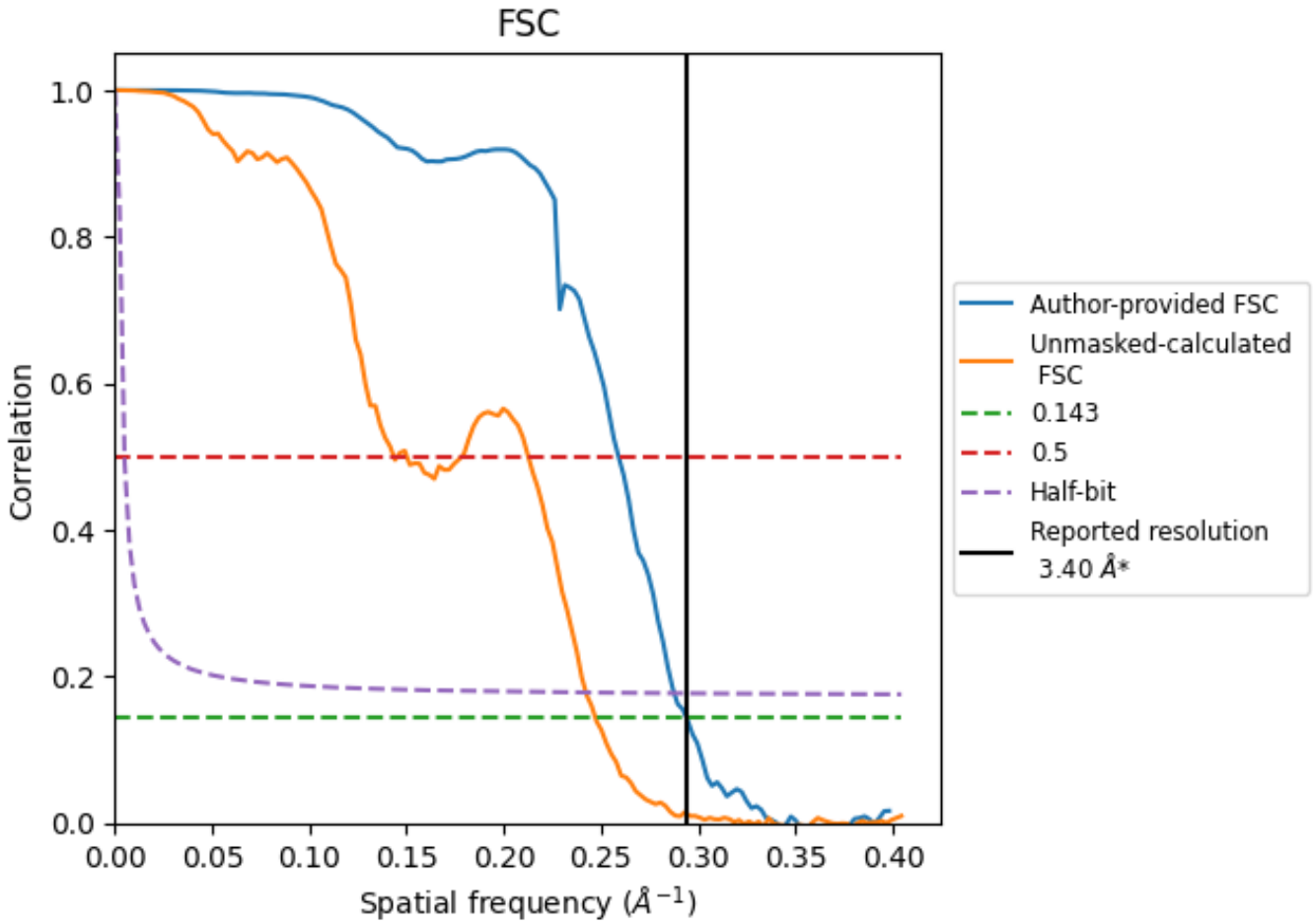


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

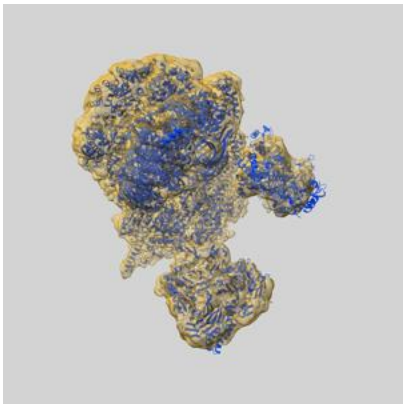
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.86	3.48
Unmasked-calculated*	4.05	6.97	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

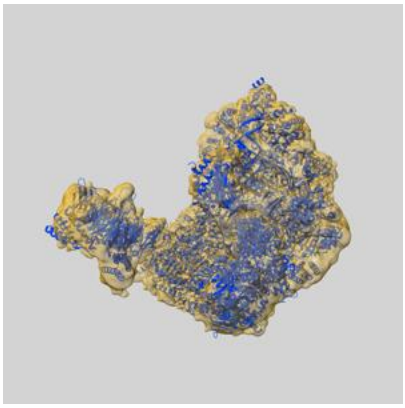
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15341 and PDB model 8B9D. Per-residue inclusion information can be found in section 3 on page 16.

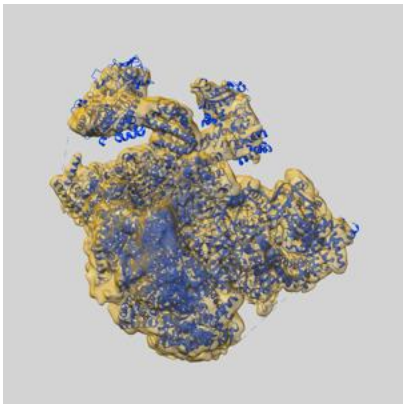
9.1 Map-model overlay



X



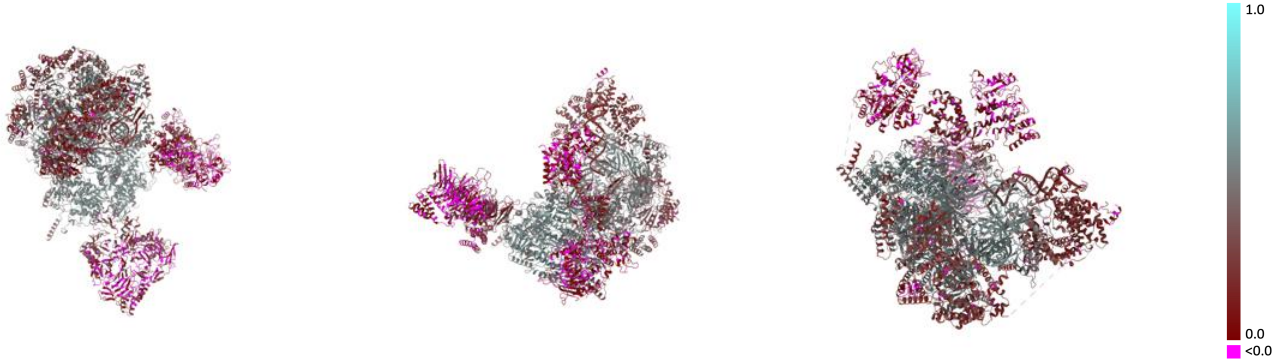
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.137 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

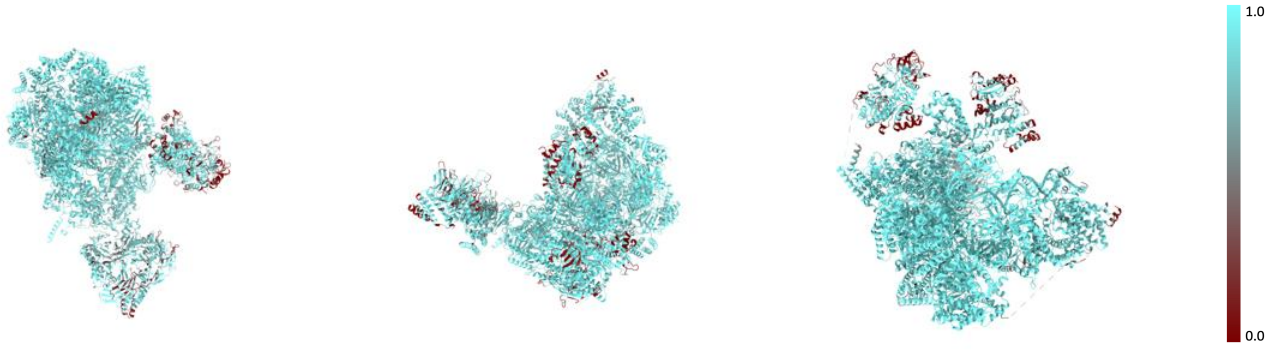
9.2 Q-score mapped to coordinate model



X Y Z

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

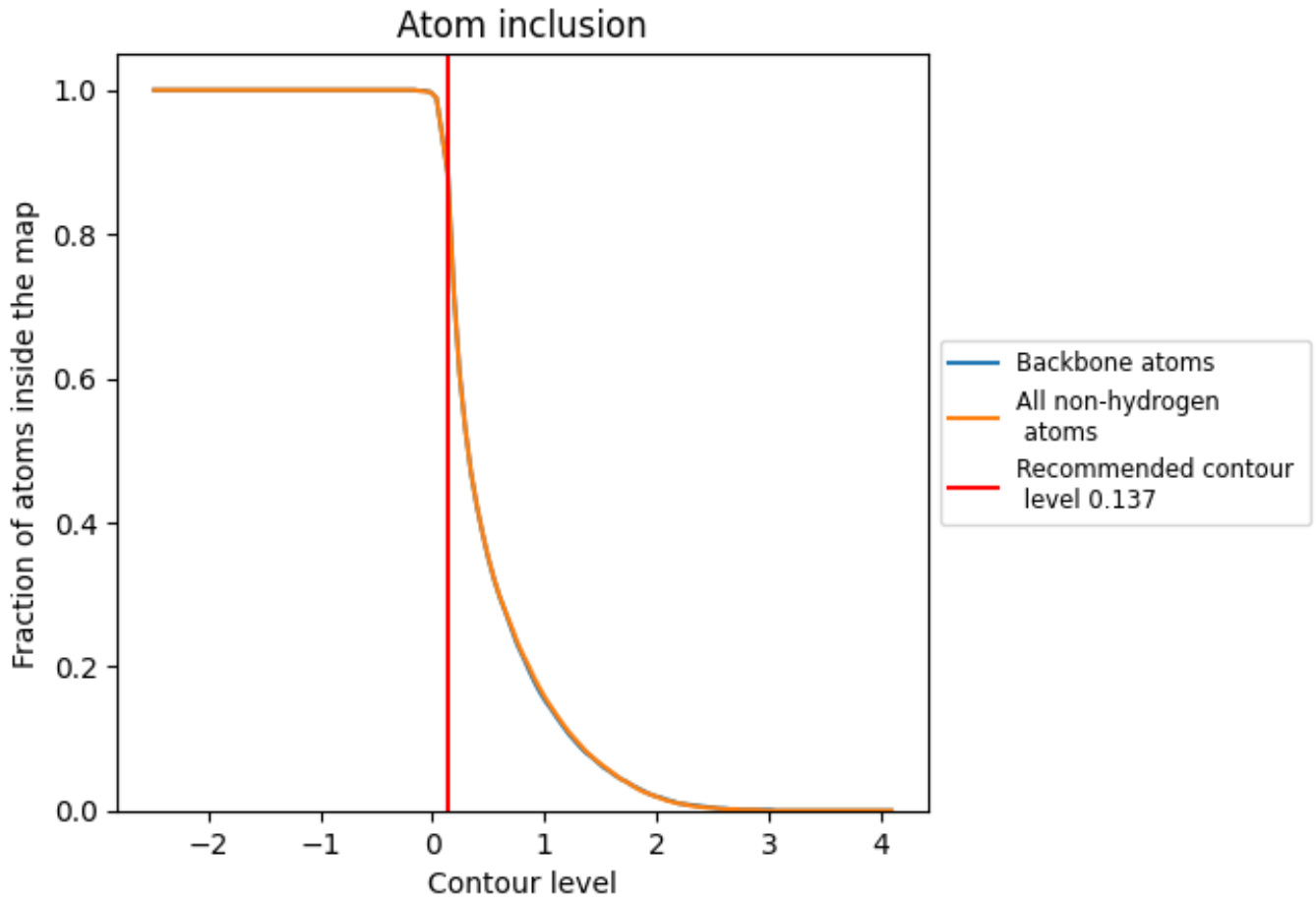
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.137).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.3100
2	0.9650	0.4870
3	0.9760	0.4410
4	0.9650	0.3500
5	0.9620	0.4750
6	0.9710	0.4110
7	0.9770	0.3510
A	0.7150	0.0570
B	0.6210	0.0700
C	0.9740	0.4900
D	0.9760	0.4960
E	0.9790	0.5540
F	0.9800	0.5320
G	0.9650	0.5230
H	0.7340	0.0550
I	0.8150	0.1640
J	0.6930	0.0500
K	0.8830	0.2060
L	0.8870	0.2180
M	0.9030	0.3040
N	0.8880	0.2380
O	0.6130	0.0530
P	0.9140	0.1520
Q	0.5410	0.1250