wwPDB EM Validation Summary Report (i)

Oct 5, 2026 – 02:35 PM EDT

PDB ID	:	9O34 / pdb_00009o34
EMDB ID	:	EMD-70068
Title	:	Replisome (map E)
Authors	:	Steinruecke, F.; Markert, J.; Farnung, L.
Deposited on	:	2025-04-04
Resolution	:	2.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

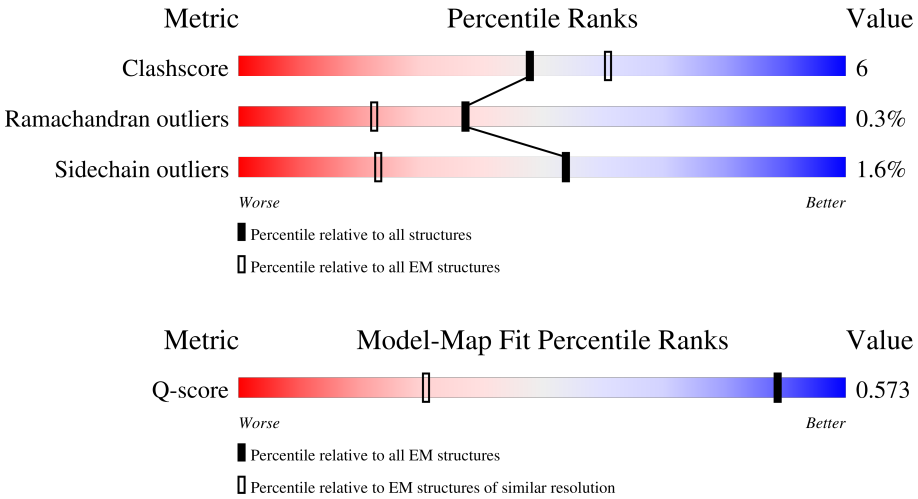
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 2.10 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.



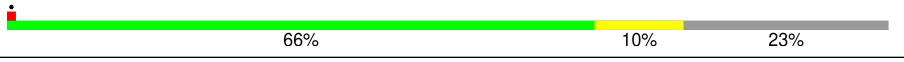
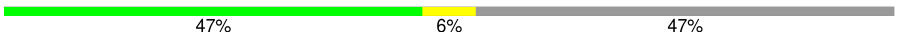
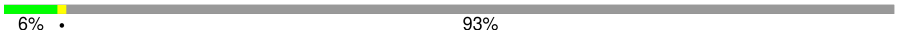
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	59% 12% • 28%
2	3	808	63% 14% • 22%
3	4	863	6% 64% 15% • 20%
4	5	734	72% 10% 18%

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	C	569	
8	D	196	
9	E	185	
10	F	216	
11	G	264	
12	H	1132	
12	I	1132	
12	J	1132	
13	K	1211	
14	L	301	
15	M	200	
16	N	182	
17	Q	1345	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 58632 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
			Total	C	N	O	S		
1	2	654	5158	3239	919	969	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	632	4962	3100	876	960	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	691	5496	3464	970	1034	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	605	4735	2968	841	891	35	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	636	5049	3170	897	956	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	617	4904	3077	873	923	31	0	0

- Molecule 7 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	534	Total	C	N	O	S	0	0
			4347	2764	745	807	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135Z	ASP	GLU	conflict	UNP O75419
C	136A	TYR	-	insertion	UNP O75419
C	136B	LYS	-	insertion	UNP O75419
C	136C	ASP	-	insertion	UNP O75419
C	136D	ASP	GLU	conflict	UNP O75419
C	136E	ASP	GLU	conflict	UNP O75419

- Molecule 8 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	196	Total	C	N	O	S	0	0
			1613	1016	290	295	12		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	176	Total	C	N	O	S	0	0
			1431	916	242	264	9		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	194	Total	C	N	O	S	0	0
			1546	979	268	293	6		

- Molecule 11 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	203	Total	C	N	O	S	0	0
			1679	1065	290	314	10		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-40	MET	-	initiating methionine	UNP Q9BRT9
G	-39	SER	-	expression tag	UNP Q9BRT9
G	-38	ALA	-	expression tag	UNP Q9BRT9
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
G	0	PRO	-	expression tag	UNP Q9BRT9

- Molecule 12 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	403	Total	C	N	O	S	0	0
			3192	2027	554	590	21		
12	I	403	Total	C	N	O	S	0	0
			3192	2027	554	590	21		
12	J	402	Total	C	N	O	S	0	0
			3183	2022	553	587	21		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	SER	-	expression tag	UNP O75717
H	-1	ASN	-	expression tag	UNP O75717
H	0	ALA	-	expression tag	UNP O75717
I	-2	SER	-	expression tag	UNP O75717
I	-1	ASN	-	expression tag	UNP O75717
I	0	ALA	-	expression tag	UNP O75717
J	-2	SER	-	expression tag	UNP O75717
J	-1	ASN	-	expression tag	UNP O75717
J	0	ALA	-	expression tag	UNP O75717

- Molecule 13 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	645	Total	C	N	O	S	0	0
			5292	3373	941	950	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	SER	-	expression tag	UNP Q9UNS1
K	-1	ASN	-	expression tag	UNP Q9UNS1
K	0	ALA	-	expression tag	UNP Q9UNS1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	87	Total	C	N	O	S	0	0
			735	471	140	121	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	34	Total	C	N	O	P	0	0
			703	340	113	216	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	23	Total	C	N	O	P	0	0
			458	221	76	138	23		

- Molecule 17 is a protein called Claspin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	98	Total	C	N	O	S	0	0
			825	524	155	144	2		

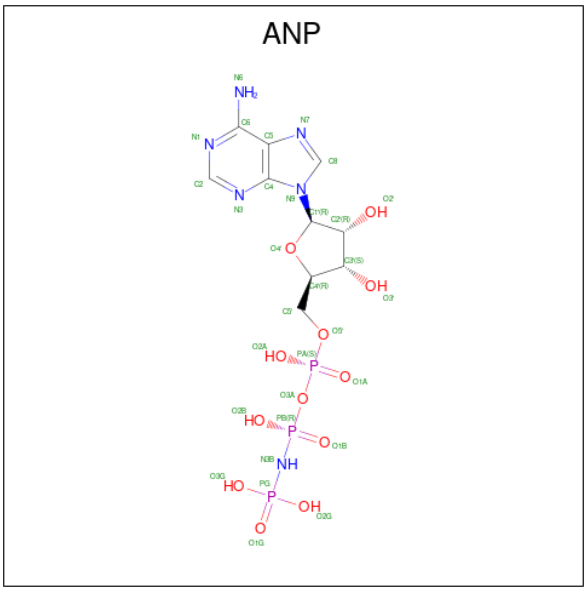
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1340	GLU	-	expression tag	UNP Q9HAW4
Q	1341	ASN	-	expression tag	UNP Q9HAW4
Q	1342	LEU	-	expression tag	UNP Q9HAW4
Q	1343	TYR	-	expression tag	UNP Q9HAW4
Q	1344	PHE	-	expression tag	UNP Q9HAW4
Q	1345	GLN	-	expression tag	UNP Q9HAW4

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	Mg	0
			1	1	
18	3	1	Total	Mg	0
			1	1	
18	5	1	Total	Mg	0
			1	1	
18	6	1	Total	Mg	0
			1	1	

- Molecule 19 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	5	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	6	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

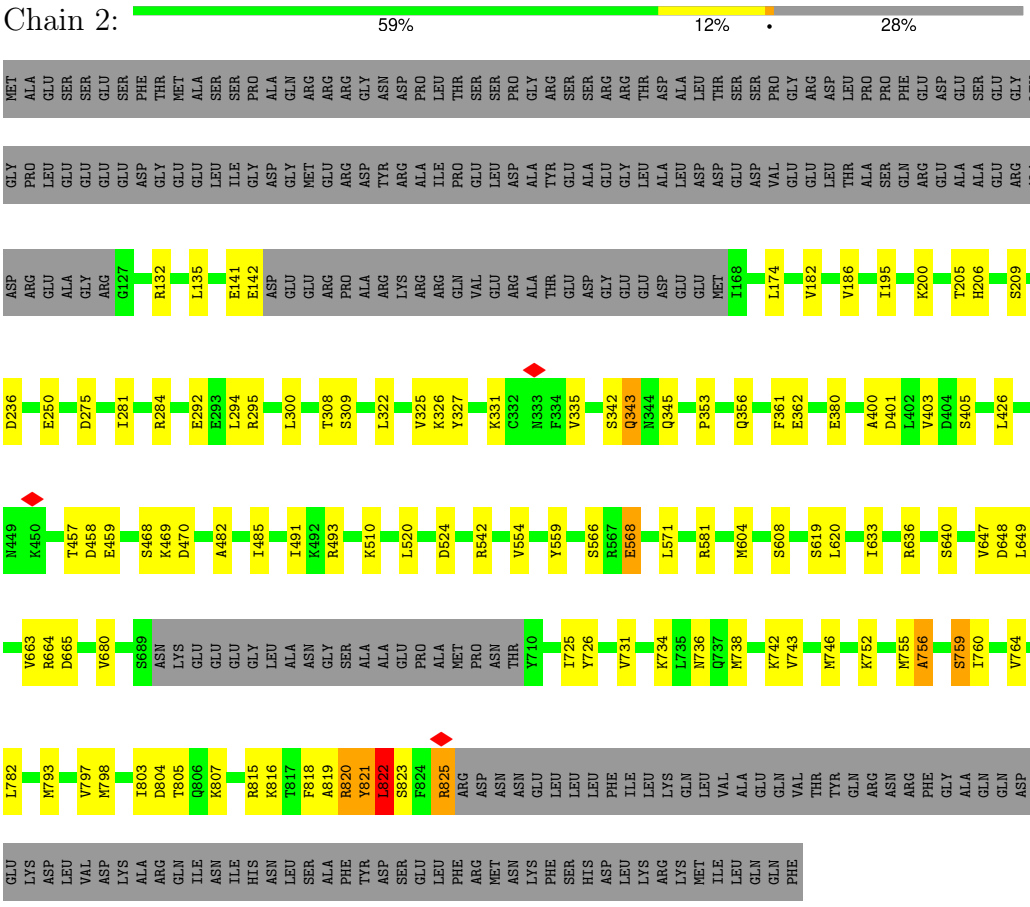
Mol	Chain	Residues	Atoms		AltConf
20	4	1	Total	Zn	0
			1	1	
20	5	1	Total	Zn	0
			1	1	
20	6	1	Total	Zn	0
			1	1	
20	7	1	Total	Zn	0
			1	1	

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.

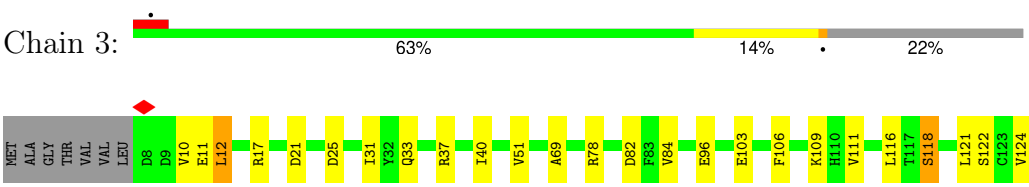
• Molecule 1: DNA replication licensing factor MCM2

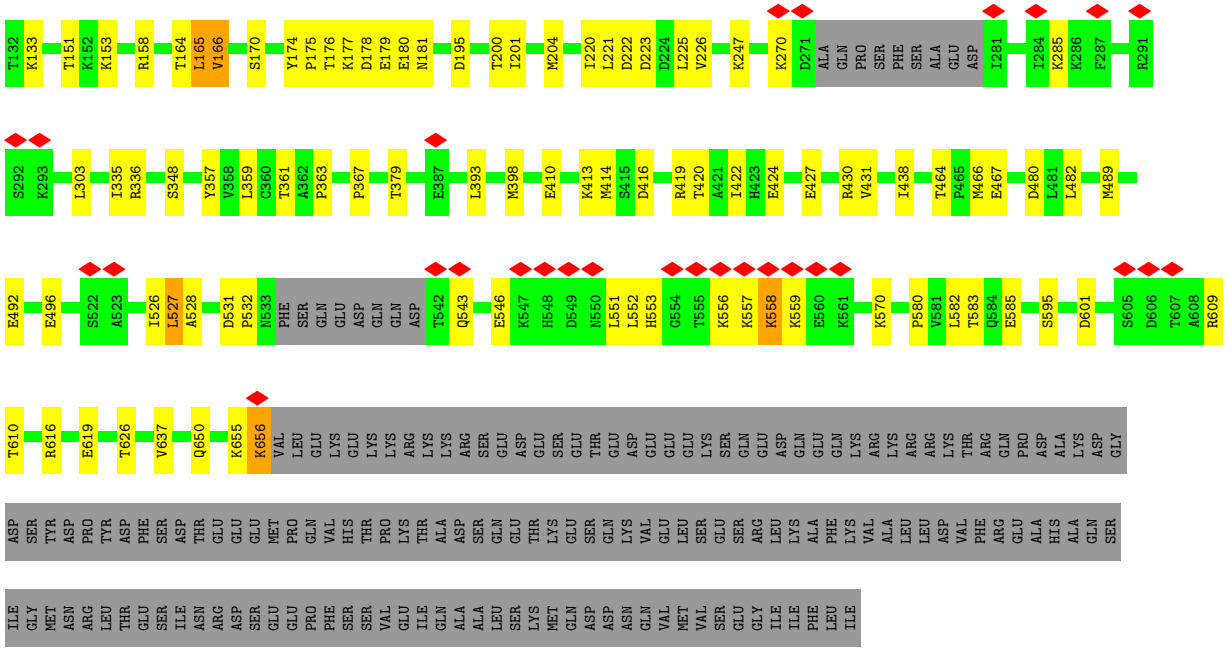
Chain 2:



• Molecule 2: DNA replication licensing factor MCM3

Chain 3:

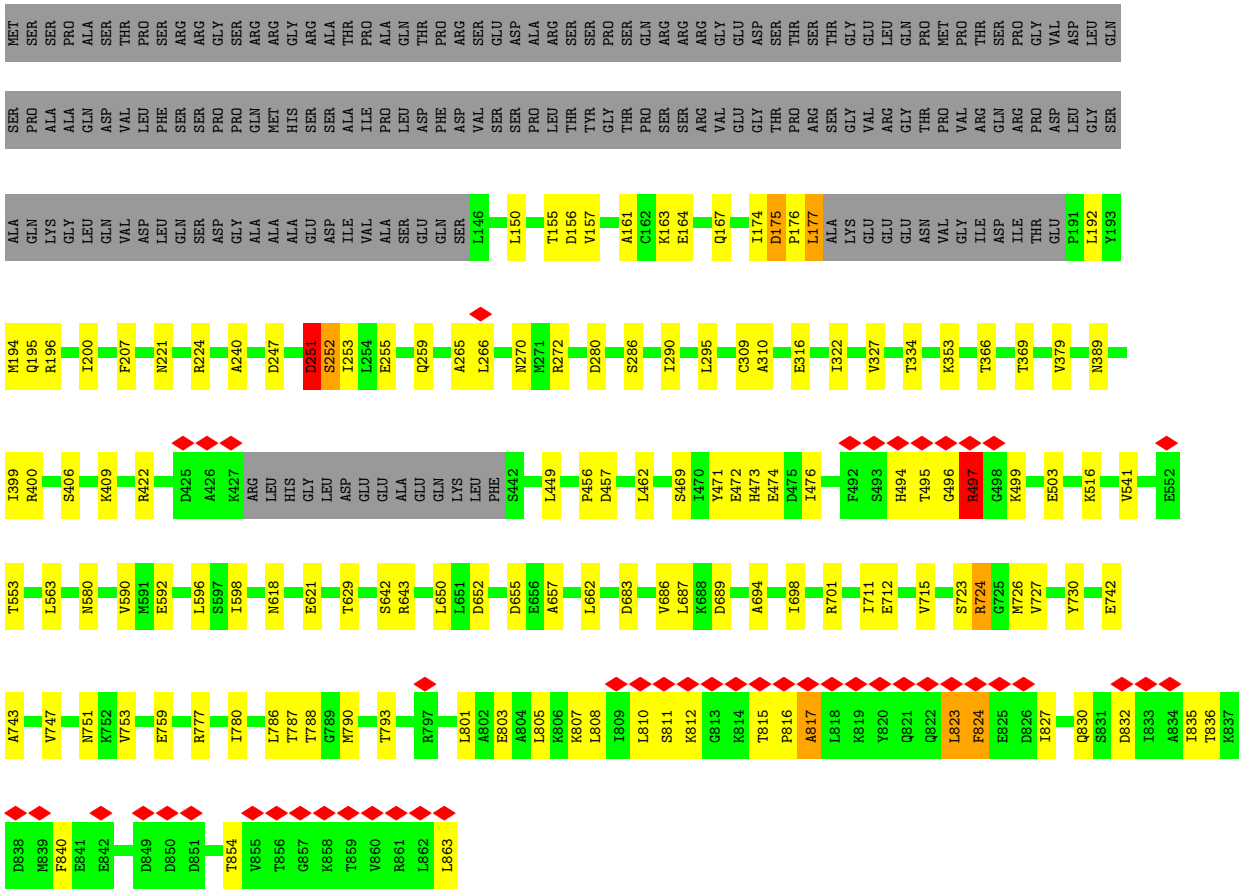




• Molecule 3: DNA replication licensing factor MCM4

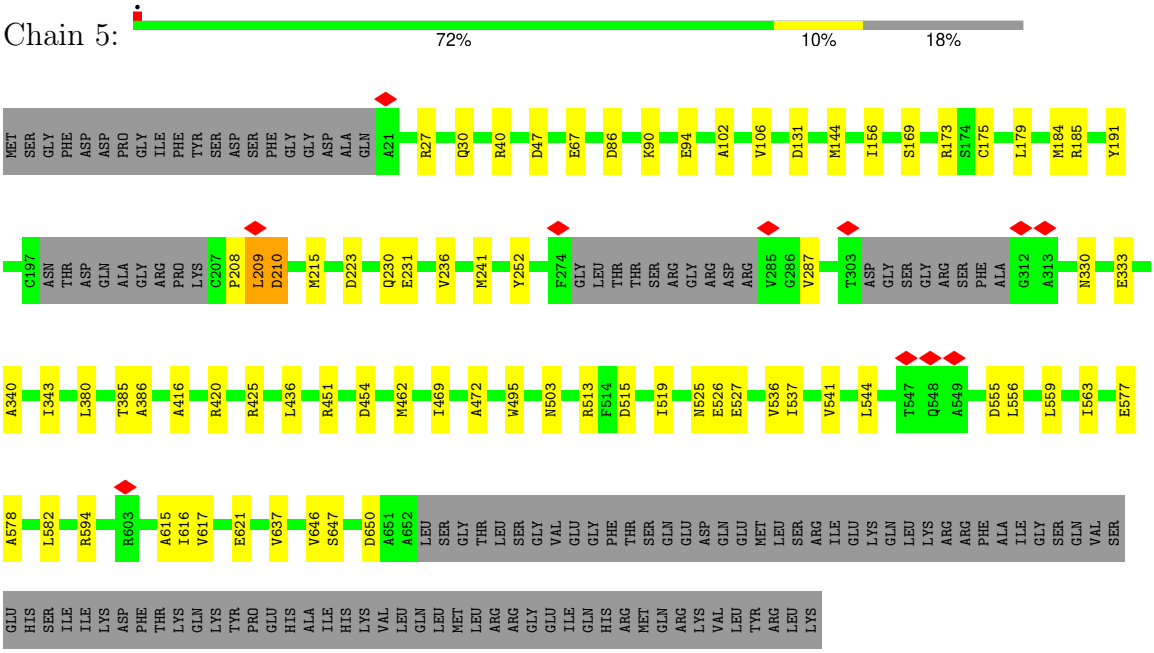
Chain 4:





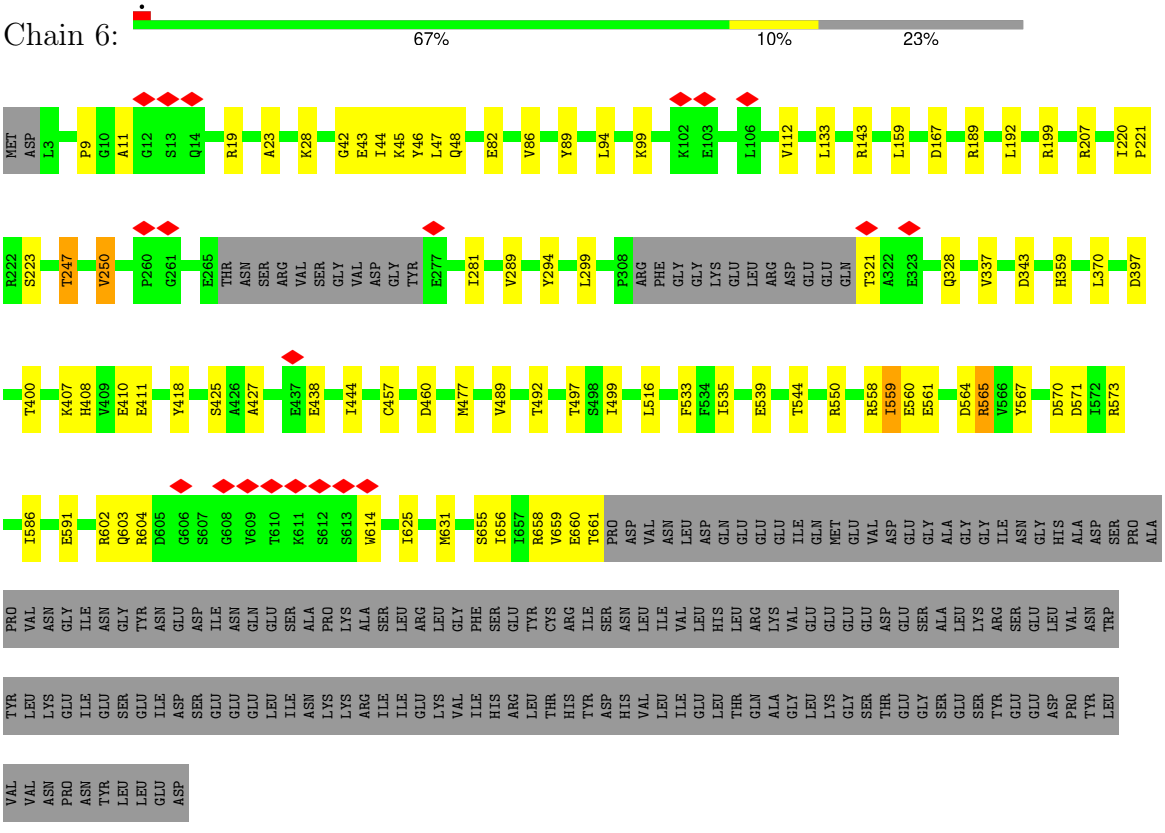
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:



• Molecule 5: DNA replication licensing factor MCM6

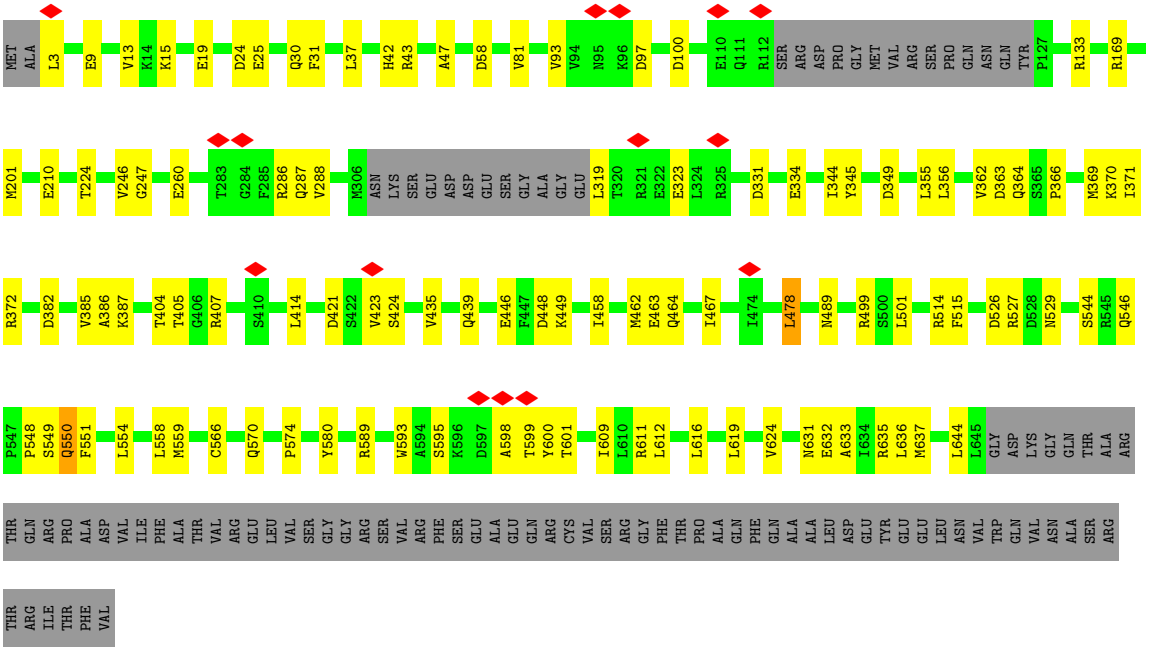
Chain 6:



• Molecule 6: DNA replication licensing factor MCM7

Chain 7:

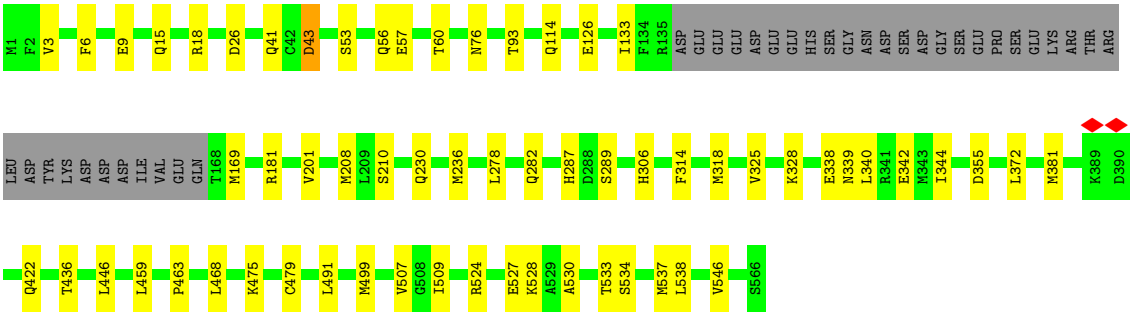




• Molecule 7: Cell division control protein 45 homolog

Chain C:

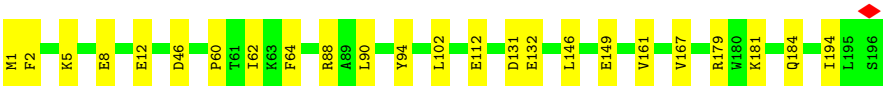




• Molecule 8: DNA replication complex GINS protein PSF1

Chain D:

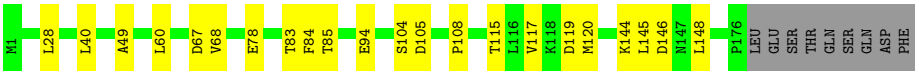




• Molecule 9: DNA replication complex GINS protein PSF2

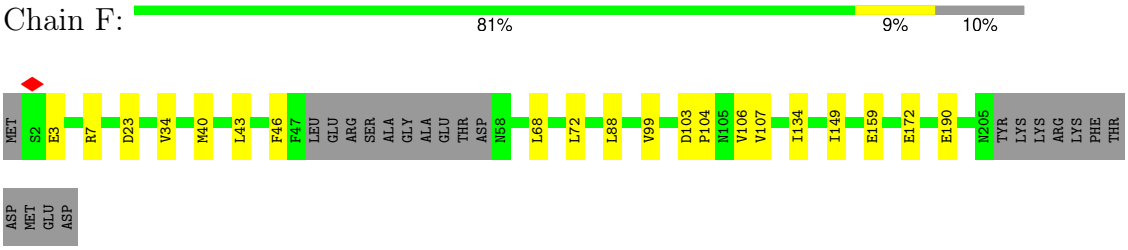
Chain E:





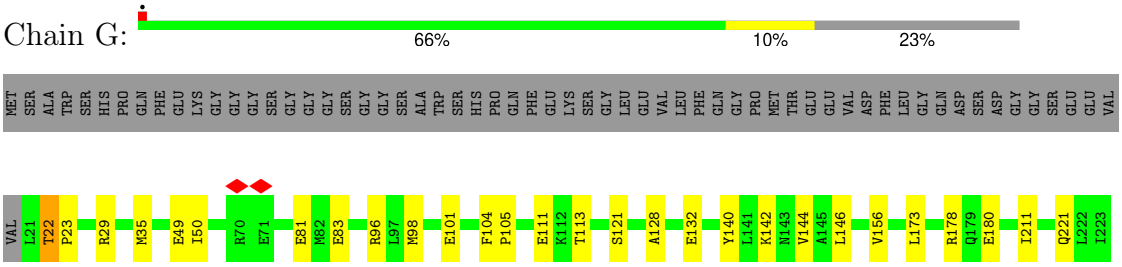
• Molecule 10: DNA replication complex GINS protein PSF3

Chain F:



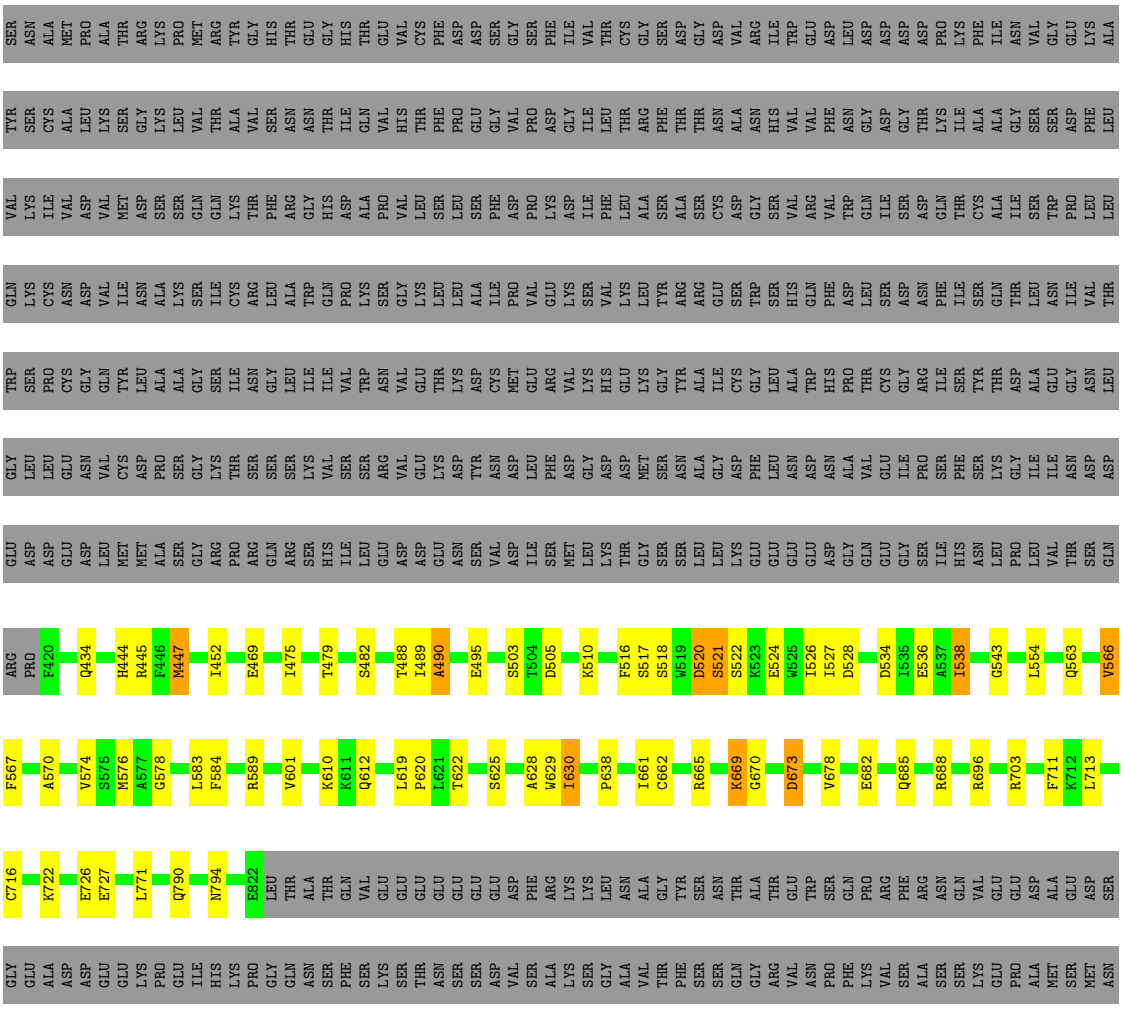
• Molecule 11: DNA replication complex GINS protein SLD5

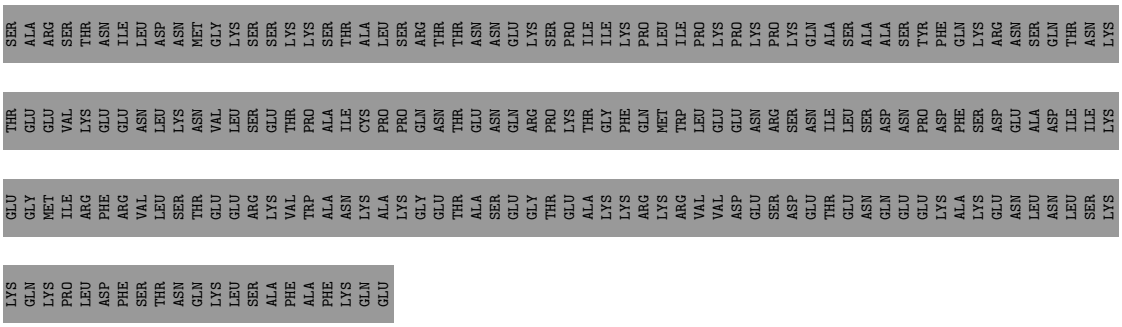
Chain G:



• Molecule 12: WD repeat and HMG-box DNA-binding protein 1

Chain H:

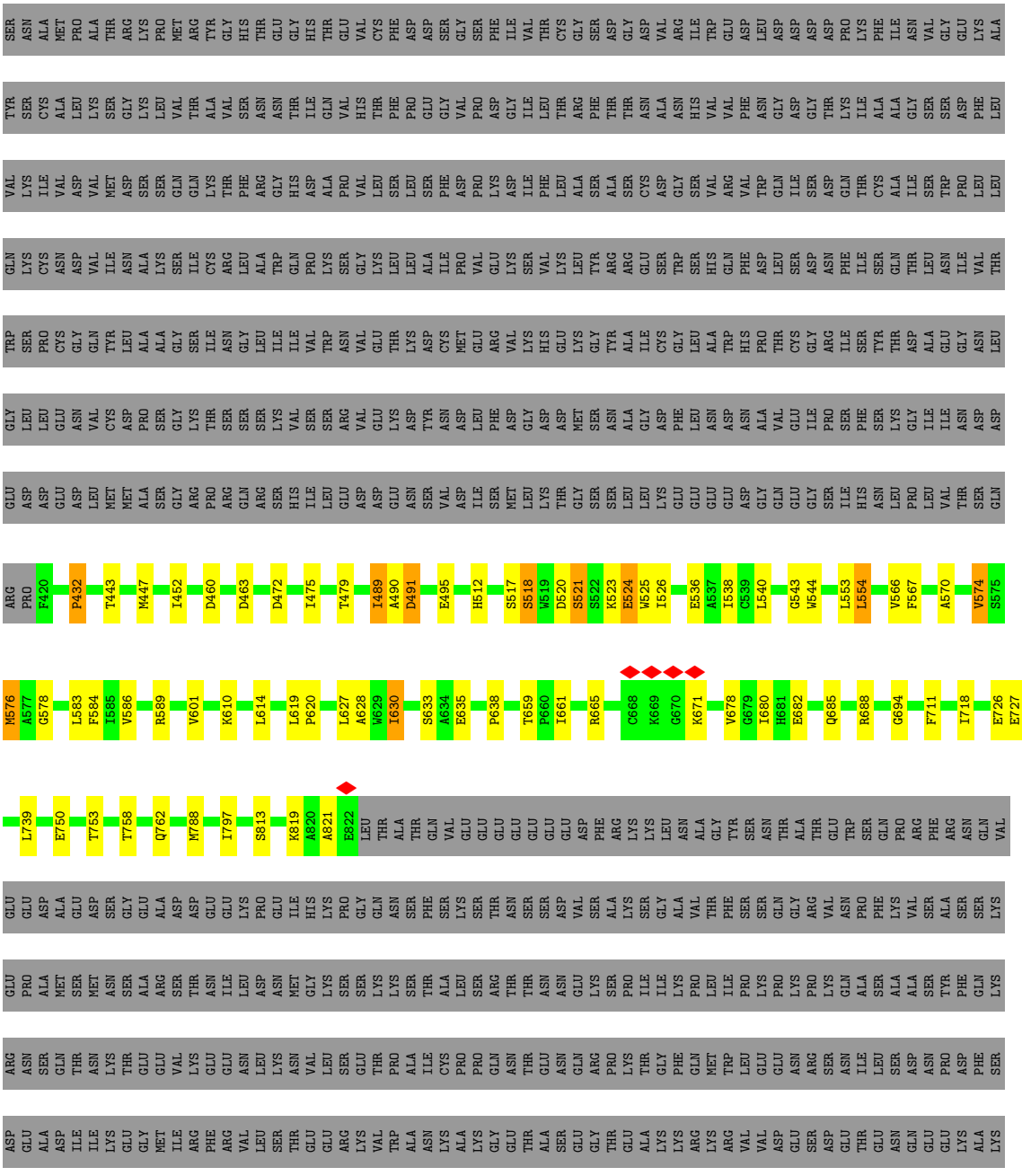




• Molecule 12: WD repeat and HMG-box DNA-binding protein 1

Chain I:

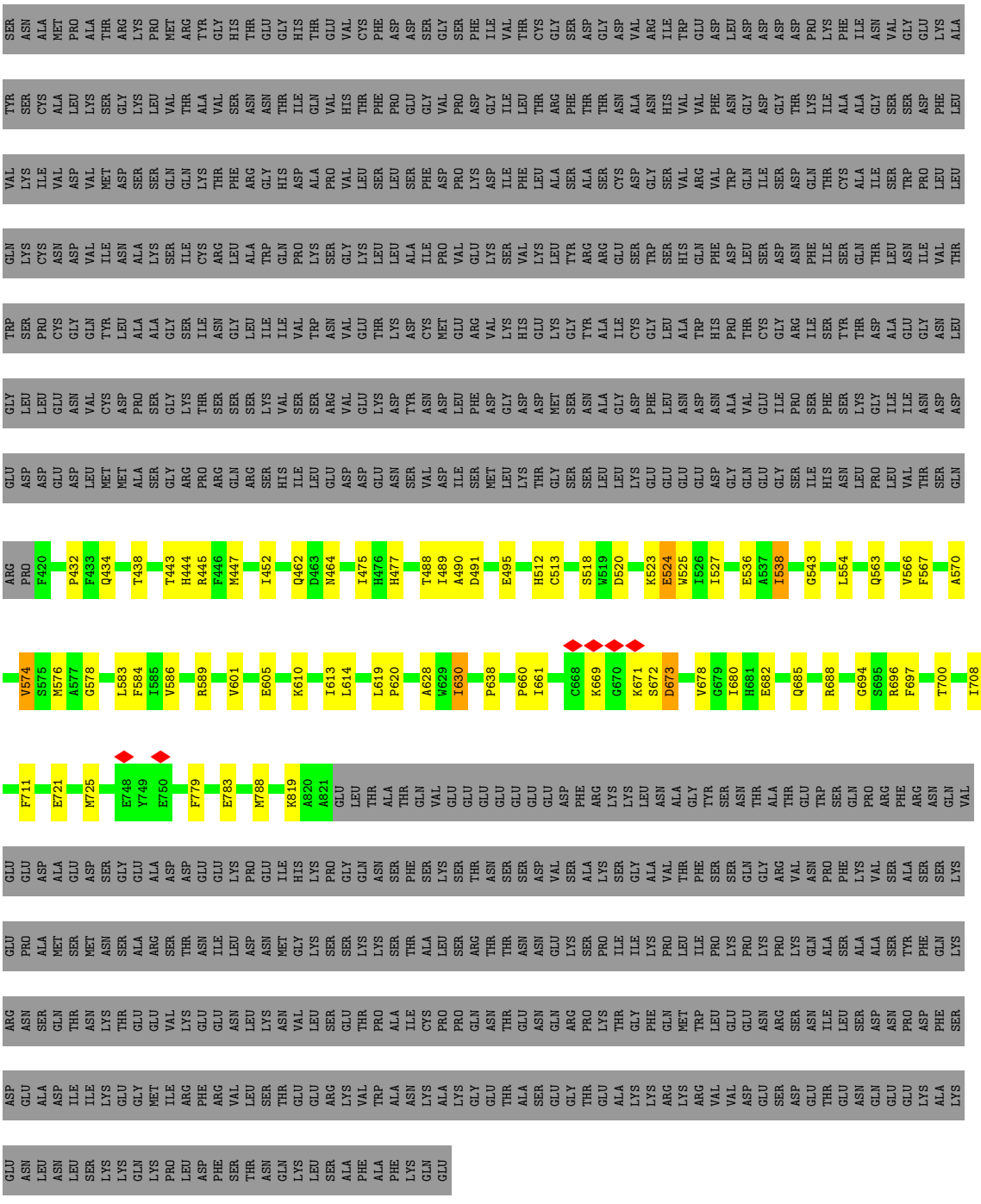




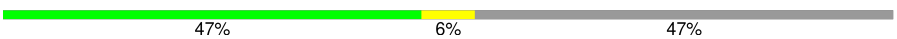


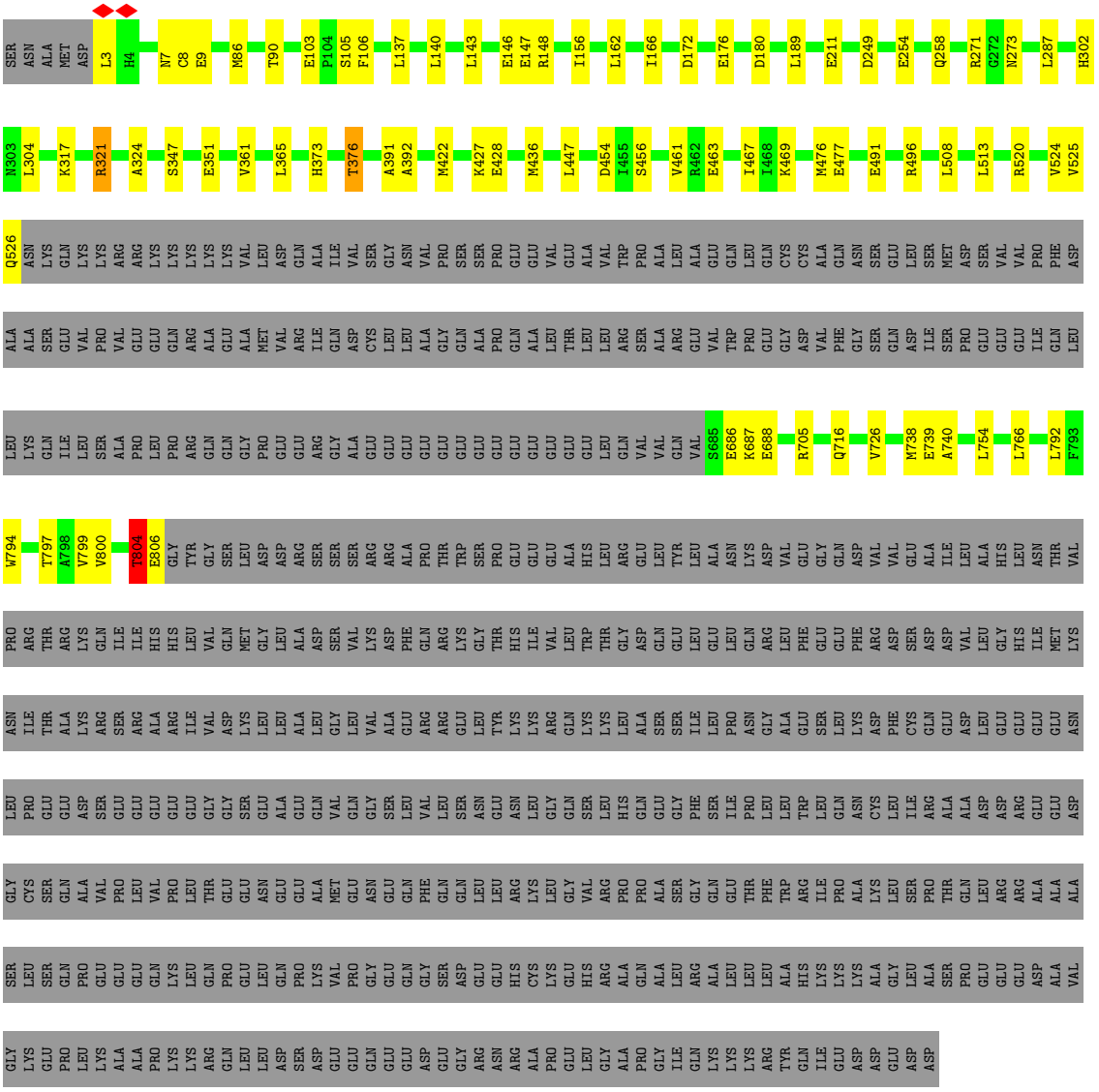
• Molecule 12: WD repeat and HMG-box DNA-binding protein 1





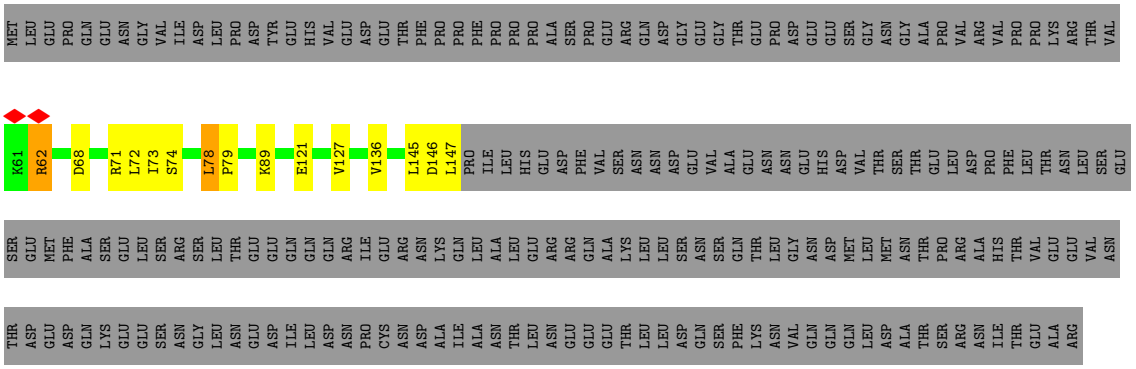
• Molecule 13: Protein timeless homolog





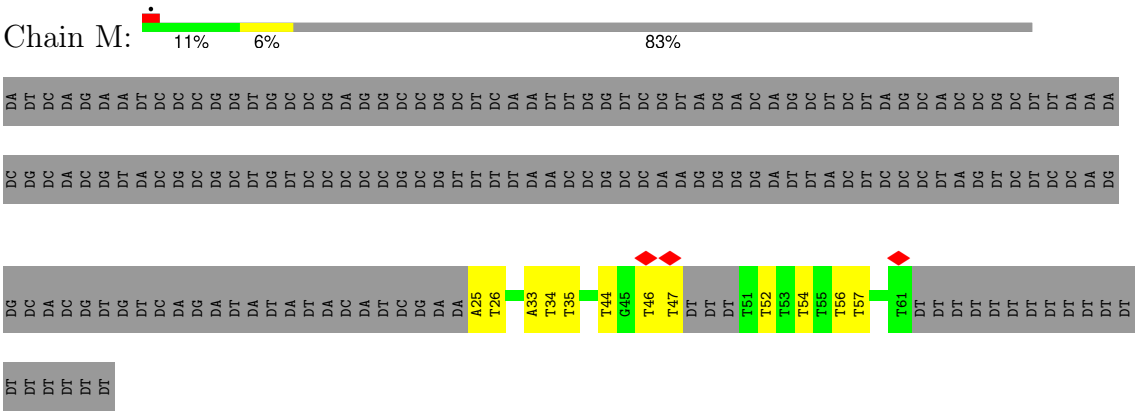
• Molecule 14: TIMELESS-interacting protein





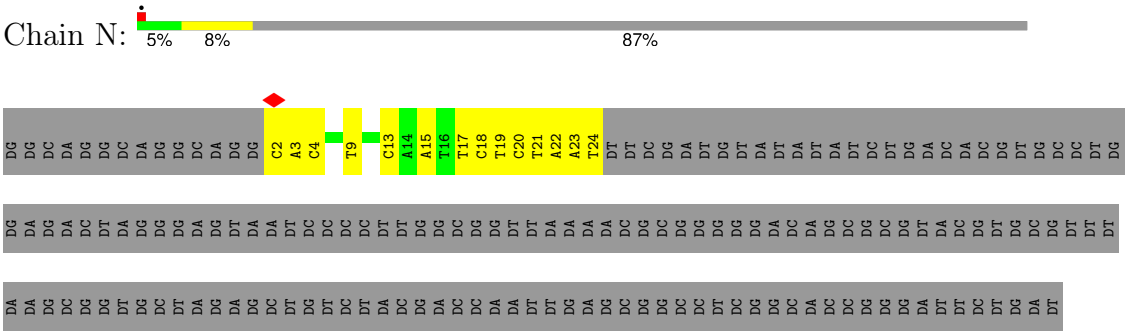
• Molecule 15: Leading Strand DNA

Chain M:



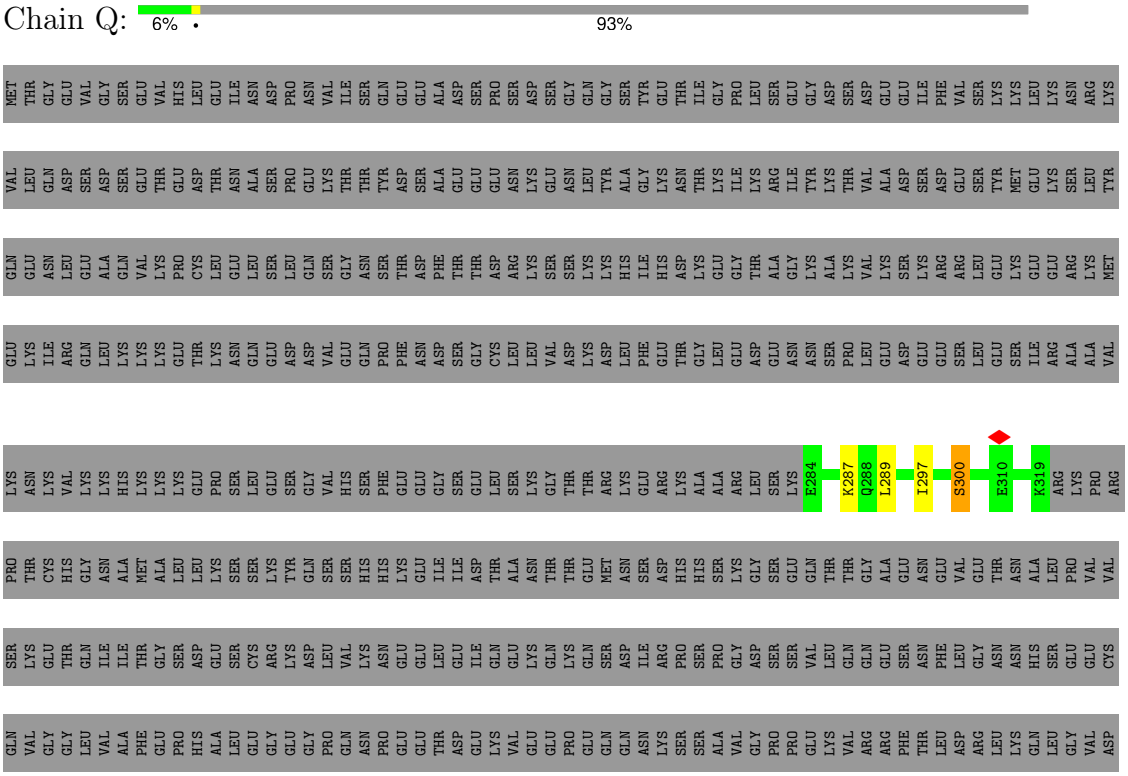
• Molecule 16: Lagging strand DNA

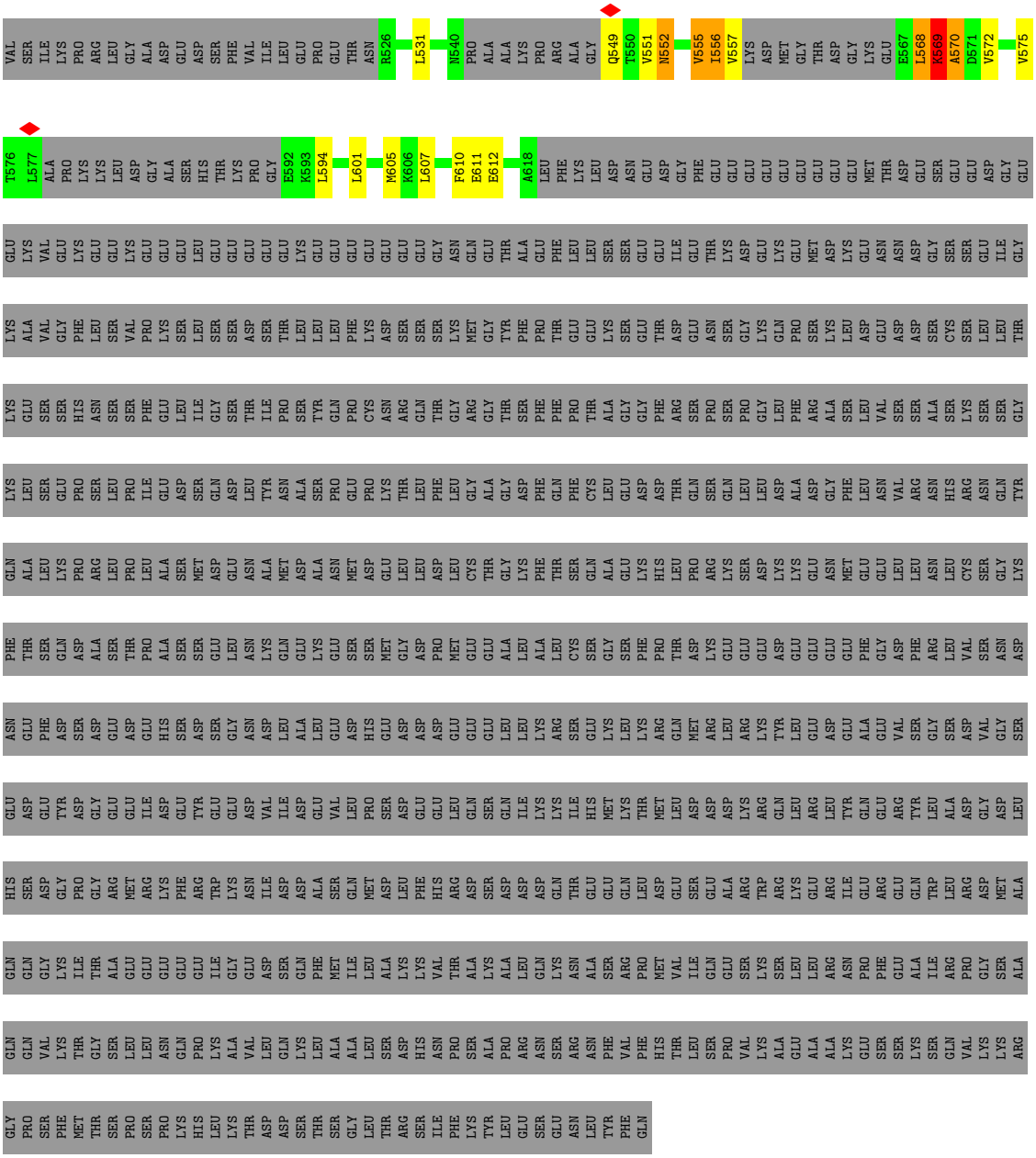
Chain N:



• Molecule 17: Claspin

Chain Q:




VAL SER ILE LYS PRO ARG LEU GLY ALA ASP GLU ASP SER PHE VAL ILE LEU GLU PRO GLU THR ASN R526 L531 N540 PRO ALA ALA LYS PRO ARG ALA GLY Q549 T550 V551 N552 V555 I556 V557 LYS ASP MET GLY THR ASP GLY LYS GLU E567 L568 K569 A570 D571 V572 V575
T576 L577 ALA PRO LYS LYS LEU ASP GLY ALA SER HIS THR LYS PRO GLY E592 K593 L594 L601 W605 K606 L607 F610 E611 E612 A618 LEU PHE LYS LEU ASP ASN GLU ASP GLY PHE GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU MET THR ASP GLU SER GLU GLU GLU ILE GLY
GLU LYS VAL GLU LYS GLU GLU LYS GLU GLU GLU LEU GLU GLU GLU GLU LYS GLU GLU GLY ASN GLN GLU THR ALA GLU PHE LEU LEU SER SER GLU GLU ILE GLU THR LYS ASP GLU LYS GLU GLU MET ASP LYS GLU ASN ASN ASP GLY SER SER GLU ILE GLY
LYS ALA VAL GLY PHE LEU SER VAL PRO LYS SER LEU SER SER ASP SER THR LEU LEU LEU PHE LYS ASP SER SER SER LYS MET GLY TYR PHE PRO THR GLU GLU LYS SER GLU THR ASP GLU ASN SER GLY LYS GLN PRO SER LYS LEU ASP GLU ASP ASP SER CYS SER LEU LEU THR
LYS GLU SER SER HIS ASN SER SER PHE GLU LEU ILE GLY SER THR ILE PRO SER TYR GLN PRO CYS ASN ARG GLN THR GLY ARG GLY THR SER PHE PHE PRO THR ALA GLY GLY PHE ARG SER PRO SER PRO GLY LEU PHE ARG ALA ALA SER LEU VAL SER SER ALA SER LYS SER SER GLY
LYS LEU SER GLU PRO SER LEU PRO ILE GLU ASP SER GLN ASP LEU TYR ASN ALA SER PRO GLU PRO LYS THR LEU PHE LEU GLY ALA ALA GLY ASP PHE GLN PHE CYS LEU GLU ASP ASP THR GLN SER GLN LEU LEU LEU ASP ALA ASP GLY PHE LEU ASN VAL ARG ASN HIS ARG ASN GLN TYR
GLN ALA LEU LYS PRO PRO ARG LEU PRO LEU ALA SER MET ASP ASP GLU ASN ALA MET ASP ALA ASN MET ASP GLU LEU LEU ASP LEU CYS THR GLY LYS PHE THR SER GLN ALA GLU LYS HIS LEU PRO ARG LYS SER ASP LYS LYS GLU ASN LEU LEU ASN HIS LEU CYS SER GLY LYS
PHE THR SER GLN ASP ALA SER THR PRO ASP SER SER GLU LEU ASN LYS GLN GLU LYS GLU SER SER MET GLY ASP PRO MET GLU GLU ALA LEU ALA LEU CYS SER GLY SER PHE PRO THR ASP LYS GLU GLU GLU ASP GLU GLU GLU GLU GLU PHE GLY ASP PHE ARG LEU VAL SER ASN ASP
ASN GLU PHE ASP SER ASP GLU ASP GLU HIS SER ASP SER GLY ASN ASP LEU ALA GLU LEU GLU ASP GLU ASP ASP GLU GLU LEU LEU LYS ARG SER GLU LYS LEU LYS ARG GLN MET ARG LEU ARG LYS TYR LEU GLU ASP GLU ALA GLU VAL SER GLY SER ASP VAL GLY SER
GLU ASP GLU TYR ASP GLY GLU GLU ILE ASP GLU TYR GLU GLU ASP VAL ILE ASP GLU VAL LEU PRO SER ASP GLU GLU LEU GLN SER GLN ILE LYS LYS ILE HIS MET LYS THR MET LEU ASP ASP ASP LYS ARG GLN LEU ARG LEU TYR GLN GLU ARG TYR LEU ALA ASP GLY ASP LEU
HIS SER ASP GLY PRO GLY ARG MET ARG LYS PHE ARG TRP LYS ASN ILE ASP ASP ALA SER GLN MET ASP LEU PHE HIS ARG ASP SER ASP ASP ASP GLN THR GLU GLU ASP GLU SER GLU ALA ARG TRP ARG LYS GLU ARG ILE GLU ARG GLU GLN ALA ILE ARG PRO GLY ASP MET ALA
GLN GLN GLY LYS ILE THR ALA GLU GLU GLU GLU GLU GLU ILE GLY GLU ASP SER GLN PHE MET ILE LEU ALA LYS LYS VAL THR ALA LYS ALA LEU ASN GLN LYS ASN ALA SER ARG PRO MET VAL ILE GLN GLU SER LYS SER LEU LEU LEU ARG ASN PRO PHE GLU ALA ILE ARG PRO GLY SER ALA
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GLY PRO SER PHE MET THR SER PRO SER ILE PHE LYS TYR LEU GLU SER GLU ASN LEU TYR PHE GLN LYS HIS LEU LYS THR ASP ASP SER THR SER GLY LEU THR ARG SER ASN PRO SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2128300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.692	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.00859	Depositor
Map size (Å)	470.0, 470.0, 470.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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, ZN, 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	0.20	0/5253	0.41	2/7095 (0.0%)
2	3	0.19	0/5037	0.45	4/6797 (0.1%)
3	4	0.20	0/5588	0.51	8/7547 (0.1%)
4	5	0.20	0/4807	0.40	0/6468
5	6	0.19	0/5131	0.36	1/6925 (0.0%)
6	7	0.18	0/4980	0.37	0/6721
7	C	0.18	0/4439	0.33	0/5992
8	D	0.19	0/1645	0.35	0/2210
9	E	0.19	0/1462	0.34	1/1981 (0.1%)
10	F	0.17	0/1580	0.30	0/2133
11	G	0.18	0/1711	0.35	0/2305
12	H	0.19	0/3269	1.28	78/4429 (1.8%)
12	I	0.19	0/3269	1.26	84/4429 (1.9%)
12	J	0.19	0/3260	1.23	78/4417 (1.8%)
13	K	0.20	0/5398	0.43	4/7273 (0.1%)
14	L	0.48	0/750	0.55	1/999 (0.1%)
15	M	0.88	0/784	1.34	0/1209
16	N	1.04	0/510	1.69	1/781 (0.1%)
17	Q	0.27	0/834	0.54	2/1112 (0.2%)
All	All	0.24	0/59707	0.67	264/80823 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
3	4	0	1
14	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	17	DT	OP1-P-O3'	-31.55	13.34	108.00
12	H	682	GLU	CA-C-N	21.93	146.39	122.26
12	H	682	GLU	C-N-CA	21.93	146.39	122.26
12	J	669	LYS	CA-C-N	21.69	140.23	121.58
12	J	669	LYS	C-N-CA	21.69	140.23	121.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	822	LEU	Peptide
3	4	251	ASP	Peptide
14	L	145	LEU	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	5158	0	5157	80	0
2	3	4962	0	4998	73	0
3	4	5496	0	5576	101	0
4	5	4735	0	4801	61	0
5	6	5049	0	5076	56	0
6	7	4904	0	4967	71	0
7	C	4347	0	4296	47	0
8	D	1613	0	1606	19	0
9	E	1431	0	1456	15	0
10	F	1546	0	1500	14	0
11	G	1679	0	1700	24	0
12	H	3192	0	3149	25	0
12	I	3192	0	3149	24	0
12	J	3183	0	3143	26	0
13	K	5292	0	5297	58	0
14	L	735	0	766	7	0
15	M	703	0	395	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	458	0	261	25	0
17	Q	825	0	858	18	0
18	2	1	0	0	0	0
18	3	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
19	2	31	0	13	0	0
19	3	31	0	13	0	0
19	5	31	0	13	0	0
19	6	31	0	13	1	0
20	4	1	0	0	0	0
20	5	1	0	0	0	0
20	6	1	0	0	0	0
20	7	1	0	0	0	0
All	All	58632	0	58203	684	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 6.

The worst 5 of 684 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)
16:N:18:DC:C6	16:N:19:DT:H72	1.79	1.16
15:M:25:DA:N6	16:N:23:DA:N6	1.96	1.13
2:3:556:LYS:O	2:3:558:LYS:NZ	1.98	0.95
17:Q:556:ILE:HG22	17:Q:568:LEU:HD22	1.47	0.93
7:C:41:GLN:NE2	8:D:149:GLU:OE1	2.06	0.89

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	648/904 (72%)	619 (96%)	26 (4%)	3 (0%)	24	22
2	3	626/808 (78%)	588 (94%)	36 (6%)	2 (0%)	36	36
3	4	685/863 (79%)	656 (96%)	26 (4%)	3 (0%)	30	28
4	5	597/734 (81%)	576 (96%)	19 (3%)	2 (0%)	36	36
5	6	630/821 (77%)	602 (96%)	27 (4%)	1 (0%)	43	44
6	7	611/719 (85%)	575 (94%)	33 (5%)	3 (0%)	24	22
7	C	530/569 (93%)	521 (98%)	9 (2%)	0	100	100
8	D	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
9	E	174/185 (94%)	173 (99%)	1 (1%)	0	100	100
10	F	190/216 (88%)	185 (97%)	5 (3%)	0	100	100
11	G	201/264 (76%)	198 (98%)	3 (2%)	0	100	100
12	H	401/1132 (35%)	393 (98%)	8 (2%)	0	100	100
12	I	401/1132 (35%)	388 (97%)	12 (3%)	1 (0%)	43	44
12	J	400/1132 (35%)	395 (99%)	5 (1%)	0	100	100
13	K	641/1211 (53%)	620 (97%)	21 (3%)	0	100	100
14	L	85/301 (28%)	79 (93%)	5 (6%)	1 (1%)	10	7
17	Q	88/1345 (6%)	85 (97%)	1 (1%)	2 (2%)	5	2
All	All	7102/12532 (57%)	6842 (96%)	242 (3%)	18 (0%)	37	36

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	756	ALA
1	2	821	TYR
3	4	497	ARG
3	4	724	ARG
4	5	209	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2	569/781 (73%)	553 (97%)	16 (3%)	38 43
2	3	546/707 (77%)	536 (98%)	10 (2%)	51 60
3	4	609/753 (81%)	592 (97%)	17 (3%)	38 43
4	5	515/625 (82%)	511 (99%)	4 (1%)	73 81
5	6	560/724 (77%)	552 (99%)	8 (1%)	59 67
6	7	535/619 (86%)	531 (99%)	4 (1%)	76 83
7	C	487/520 (94%)	482 (99%)	5 (1%)	68 76
8	D	174/174 (100%)	173 (99%)	1 (1%)	78 86
9	E	160/169 (95%)	159 (99%)	1 (1%)	78 86
10	F	167/186 (90%)	164 (98%)	3 (2%)	51 60
11	G	188/234 (80%)	187 (100%)	1 (0%)	81 88
12	H	347/989 (35%)	341 (98%)	6 (2%)	53 62
12	I	347/989 (35%)	342 (99%)	5 (1%)	59 67
12	J	346/989 (35%)	345 (100%)	1 (0%)	86 91
13	K	569/1057 (54%)	563 (99%)	6 (1%)	65 74
14	L	78/274 (28%)	73 (94%)	5 (6%)	16 14
17	Q	90/1205 (8%)	81 (90%)	9 (10%)	7 5
All	All	6287/10995 (57%)	6185 (98%)	102 (2%)	54 64

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	7	544	SER
12	H	522	SER
17	Q	556	ILE
7	C	43	ASP
9	E	104	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
6	7	30	GLN
13	K	373	HIS
7	C	283	HIS
13	K	302	HIS
13	K	507	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ANP	2	1002	18	33,33,33	1.93	13 (39%)	45,52,52	2.07	13 (28%)
19	ANP	5	801	18	33,33,33	1.85	11 (33%)	45,52,52	2.04	13 (28%)
19	ANP	3	1500	18	33,33,33	1.86	11 (33%)	45,52,52	2.07	13 (28%)
19	ANP	6	903	18	33,33,33	1.95	12 (36%)	45,52,52	2.10	13 (28%)

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
19	ANP	2	1002	18	-	3/18/38/38	0/3/3/3
19	ANP	5	801	18	-	4/18/38/38	0/3/3/3
19	ANP	3	1500	18	-	1/18/38/38	0/3/3/3
19	ANP	6	903	18	-	4/18/38/38	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1500	ANP	PB-N3B	4.62	1.75	1.63
19	6	903	ANP	PG-N3B	4.54	1.75	1.63
19	6	903	ANP	PB-N3B	4.45	1.75	1.63
19	5	801	ANP	PG-N3B	4.43	1.74	1.63
19	2	1002	ANP	PG-N3B	4.40	1.74	1.63

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	1002	ANP	C5-C4-N3	-5.94	118.54	126.72
19	5	801	ANP	C5-C4-N3	-5.71	118.86	126.72
19	3	1500	ANP	C5-C4-N3	-5.66	118.92	126.72
19	3	1500	ANP	O1G-PG-N3B	-5.53	103.63	111.77
19	2	1002	ANP	O1G-PG-N3B	-5.41	103.80	111.77

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	2	1002	ANP	PB-N3B-PG-O1G
19	2	1002	ANP	PG-N3B-PB-O1B
19	3	1500	ANP	PG-N3B-PB-O1B
19	5	801	ANP	PG-N3B-PB-O1B
19	5	801	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

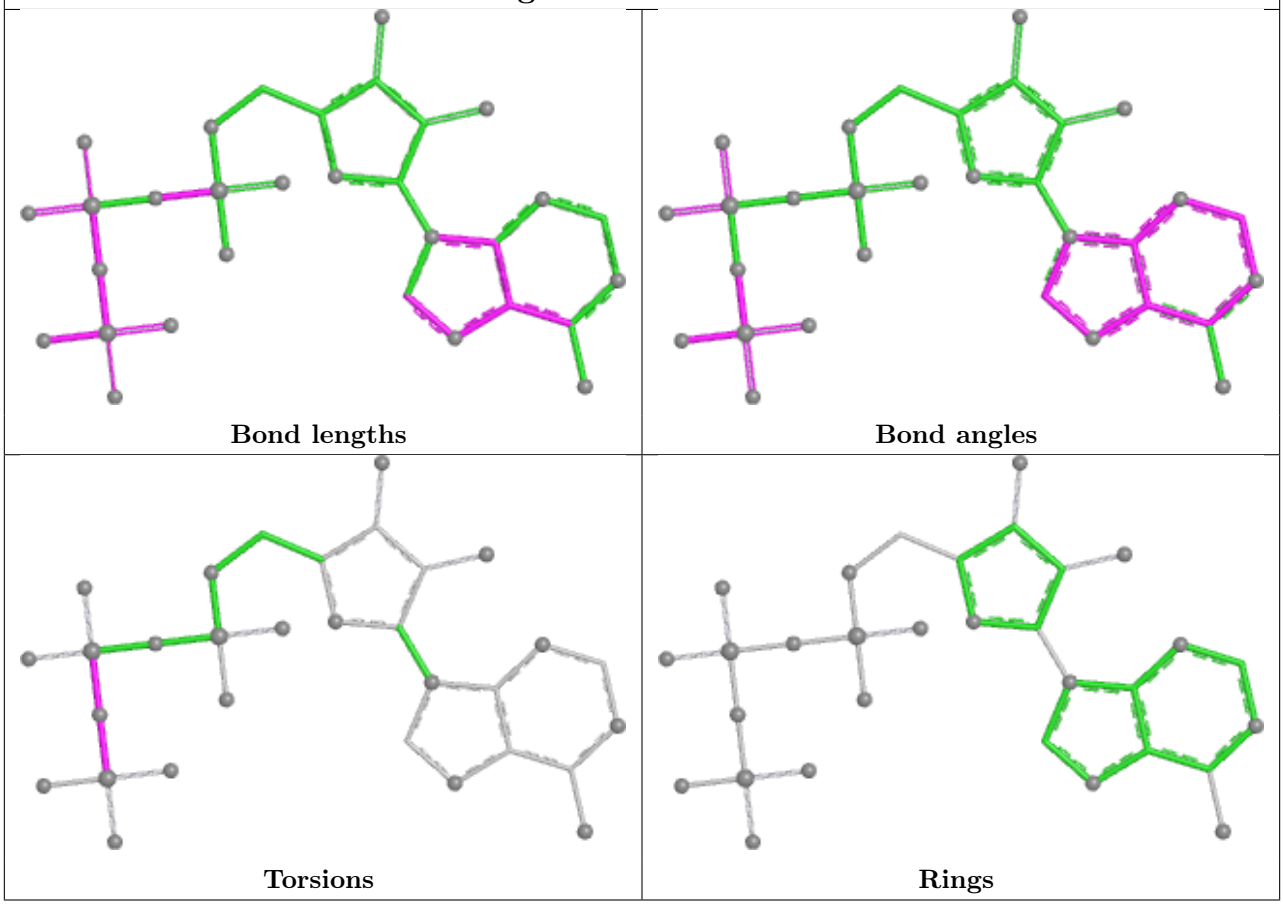
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	903	ANP	1	0

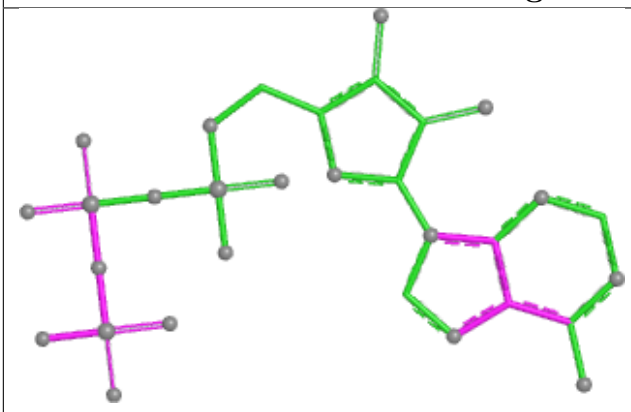
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

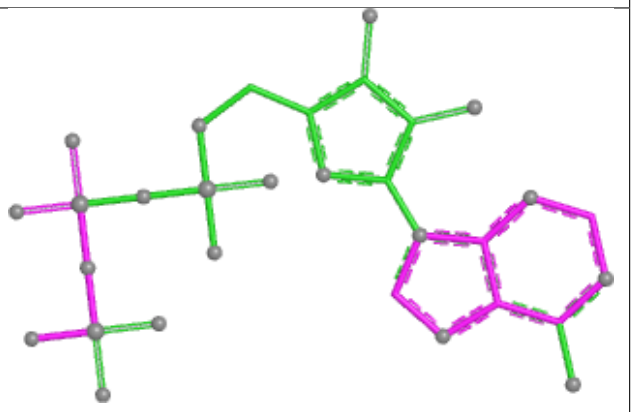
Ligand ANP 2 1002



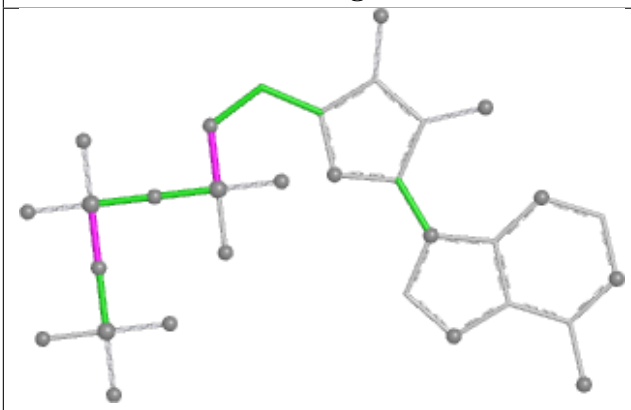
Ligand ANP 5 801



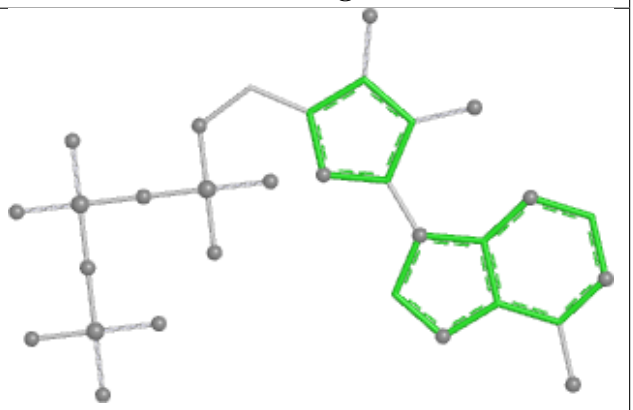
Bond lengths



Bond angles

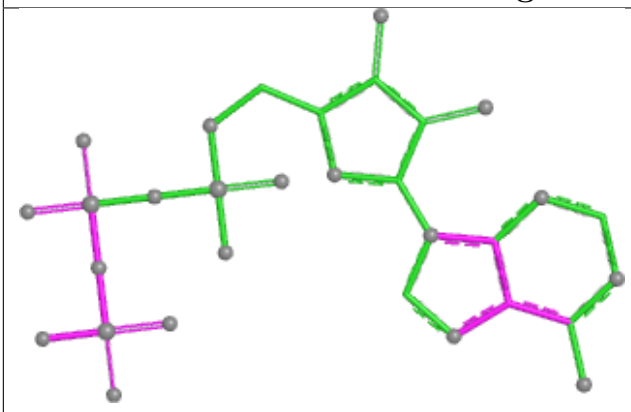


Torsions

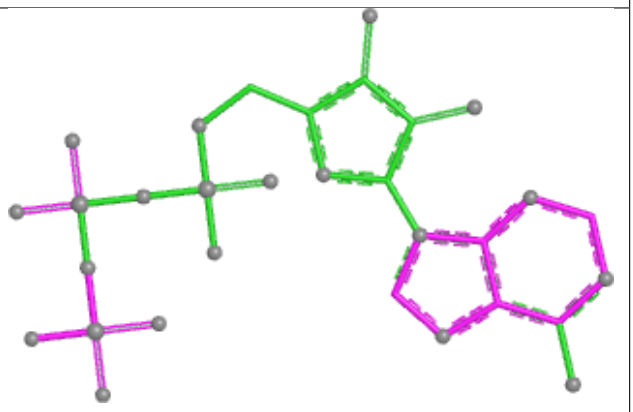


Rings

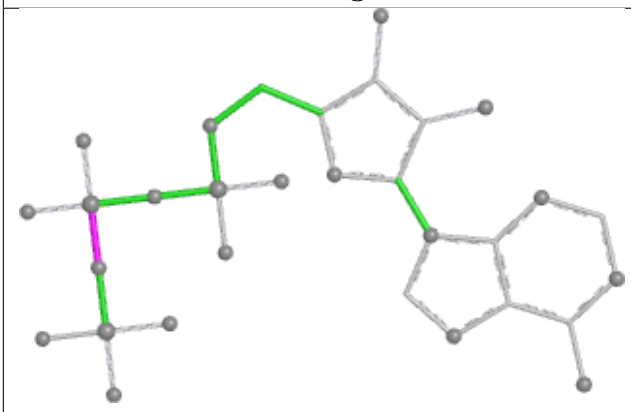
Ligand ANP 3 1500



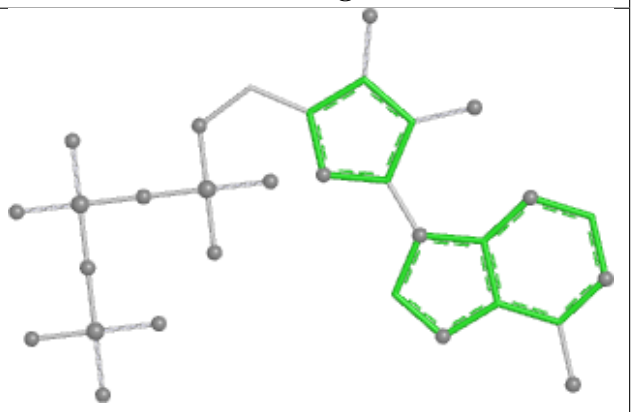
Bond lengths



Bond angles

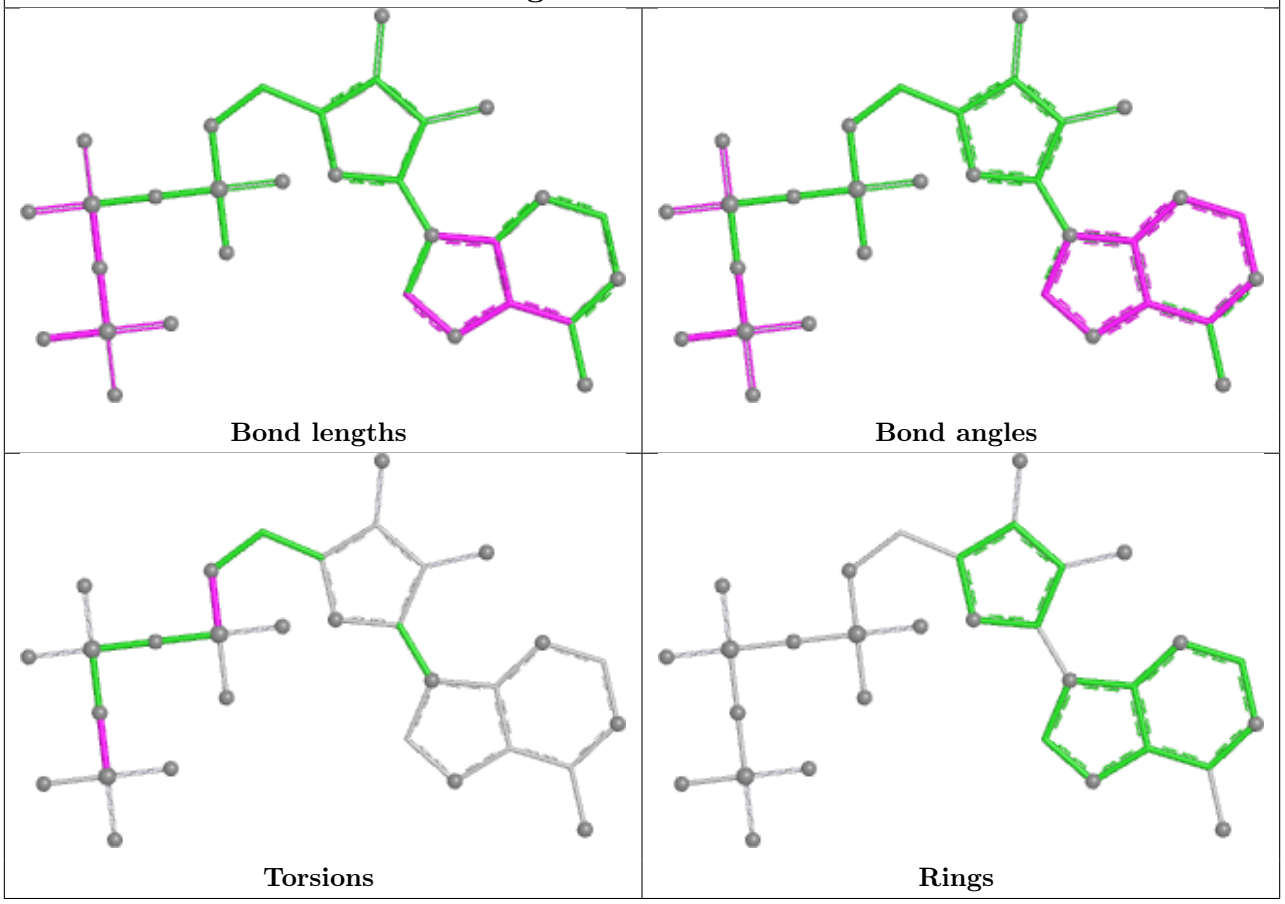


Torsions



Rings

Ligand ANP 6 903



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.

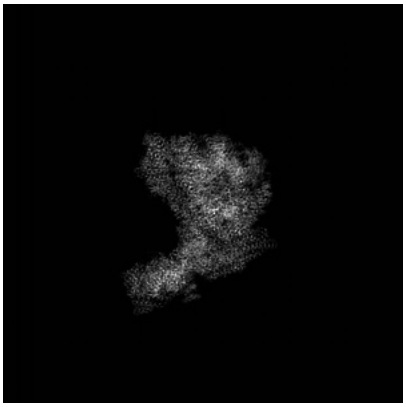
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70068. These allow visual inspection of the internal detail of the map and identification of artifacts.

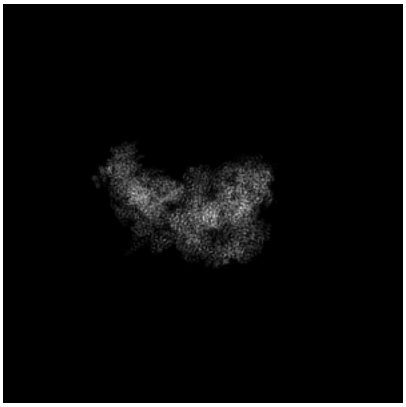
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

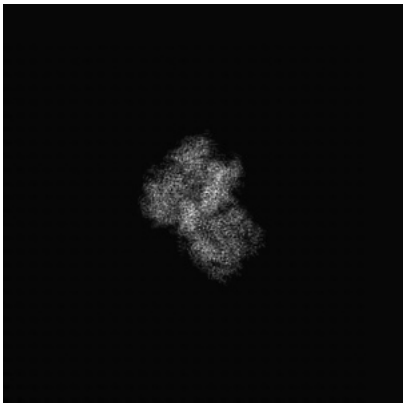
6.1.1 Primary map



X



Y

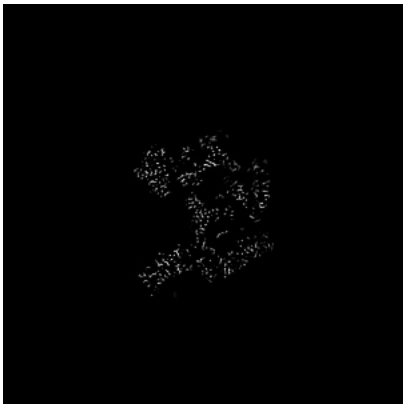


Z

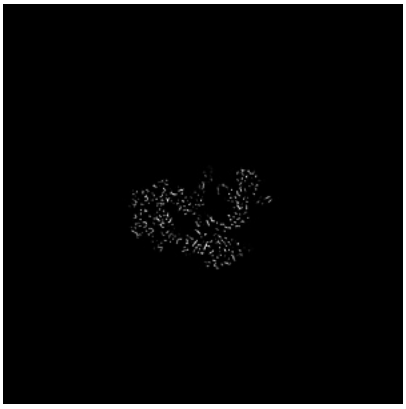
The images above show the map projected in three orthogonal directions.

6.2 Central slices

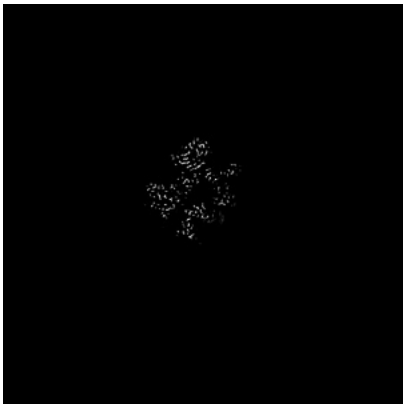
6.2.1 Primary map



X Index: 250



Y Index: 250



Z Index: 250

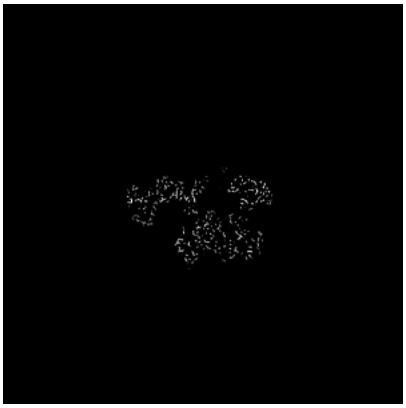
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

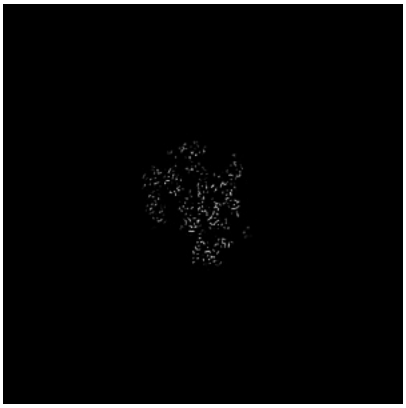
6.3.1 Primary map



X Index: 263



Y Index: 264

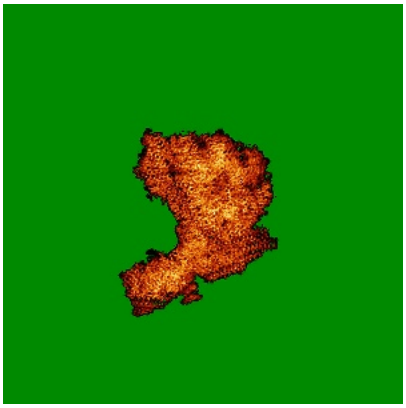


Z Index: 297

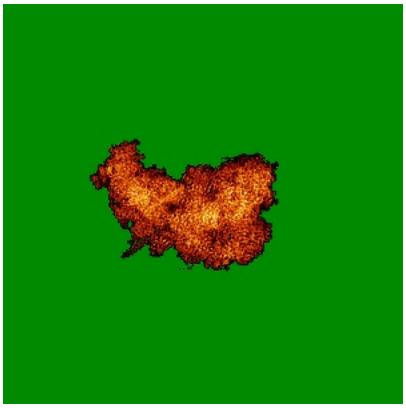
The images above show the largest variance slices of the map in three orthogonal directions.

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

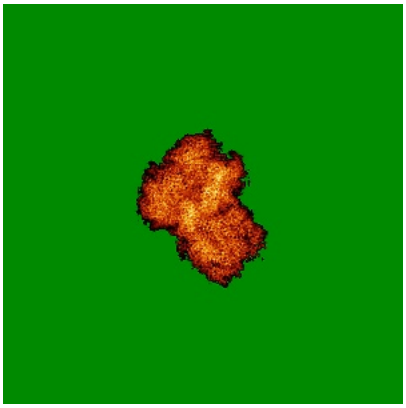
6.4.1 Primary map



X



Y

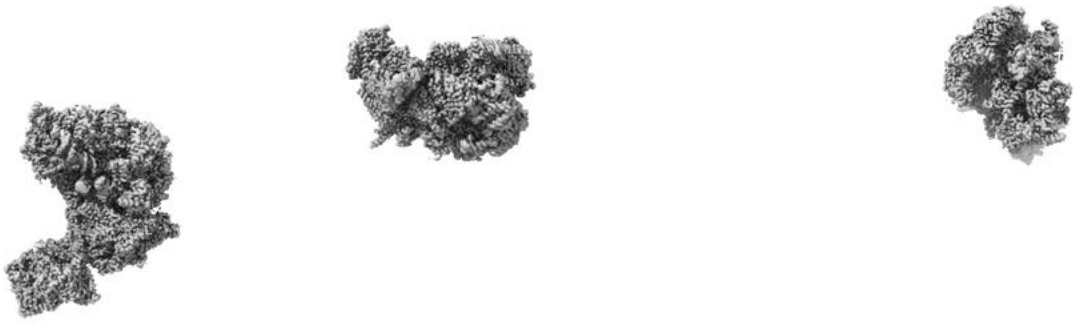


Z

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 (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 0.00859. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

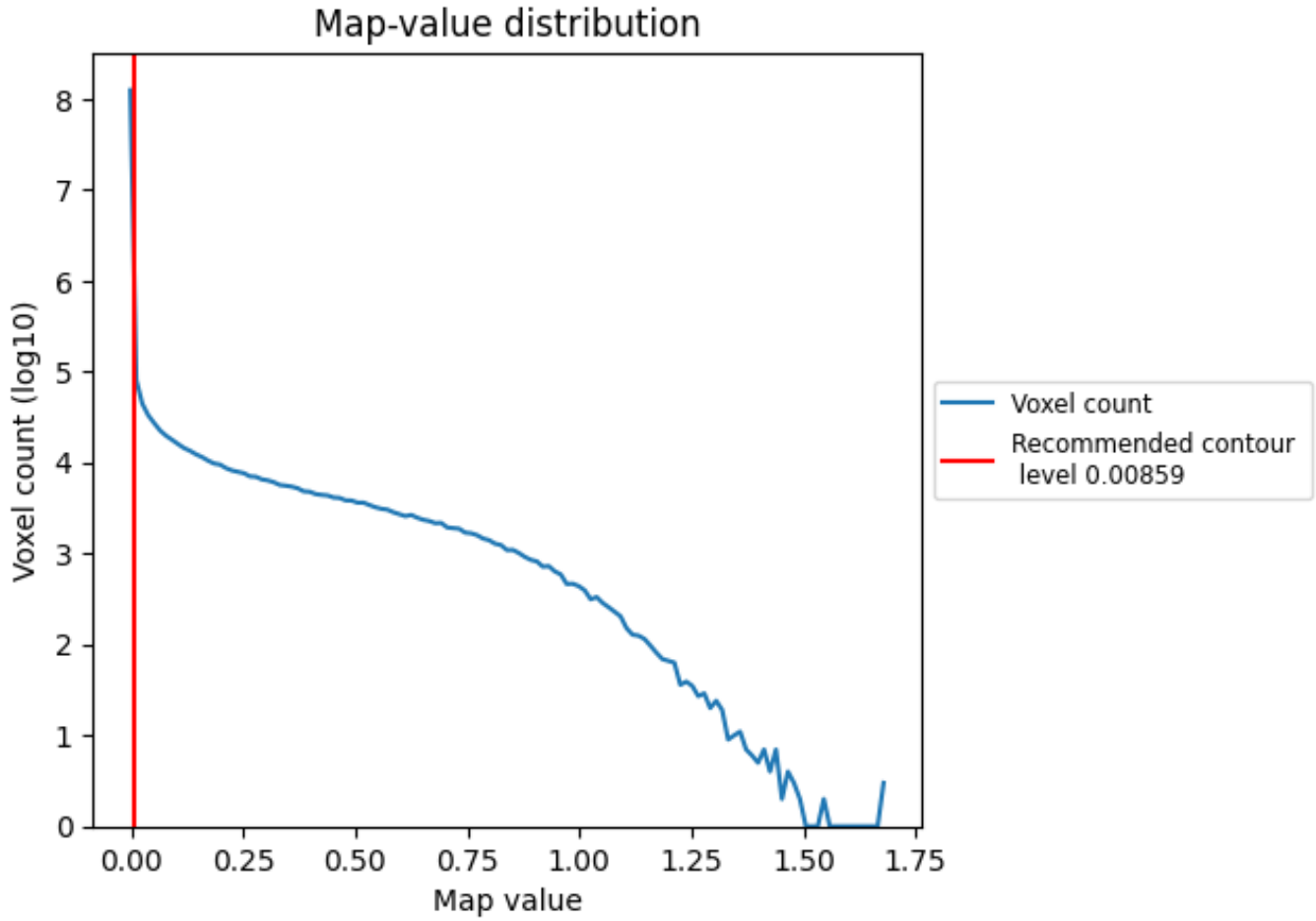
6.6 Mask visualisation (i)

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

7 Map analysis

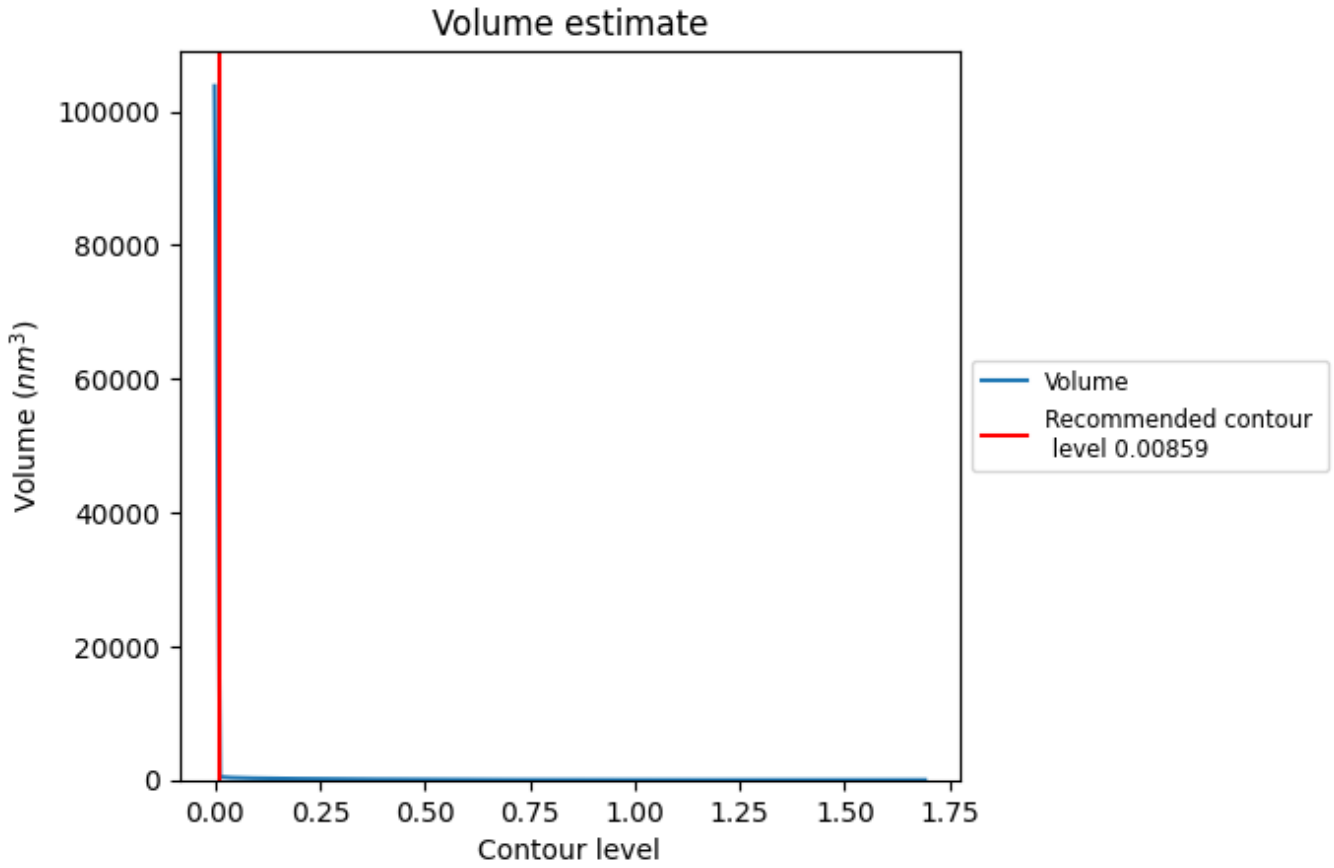
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

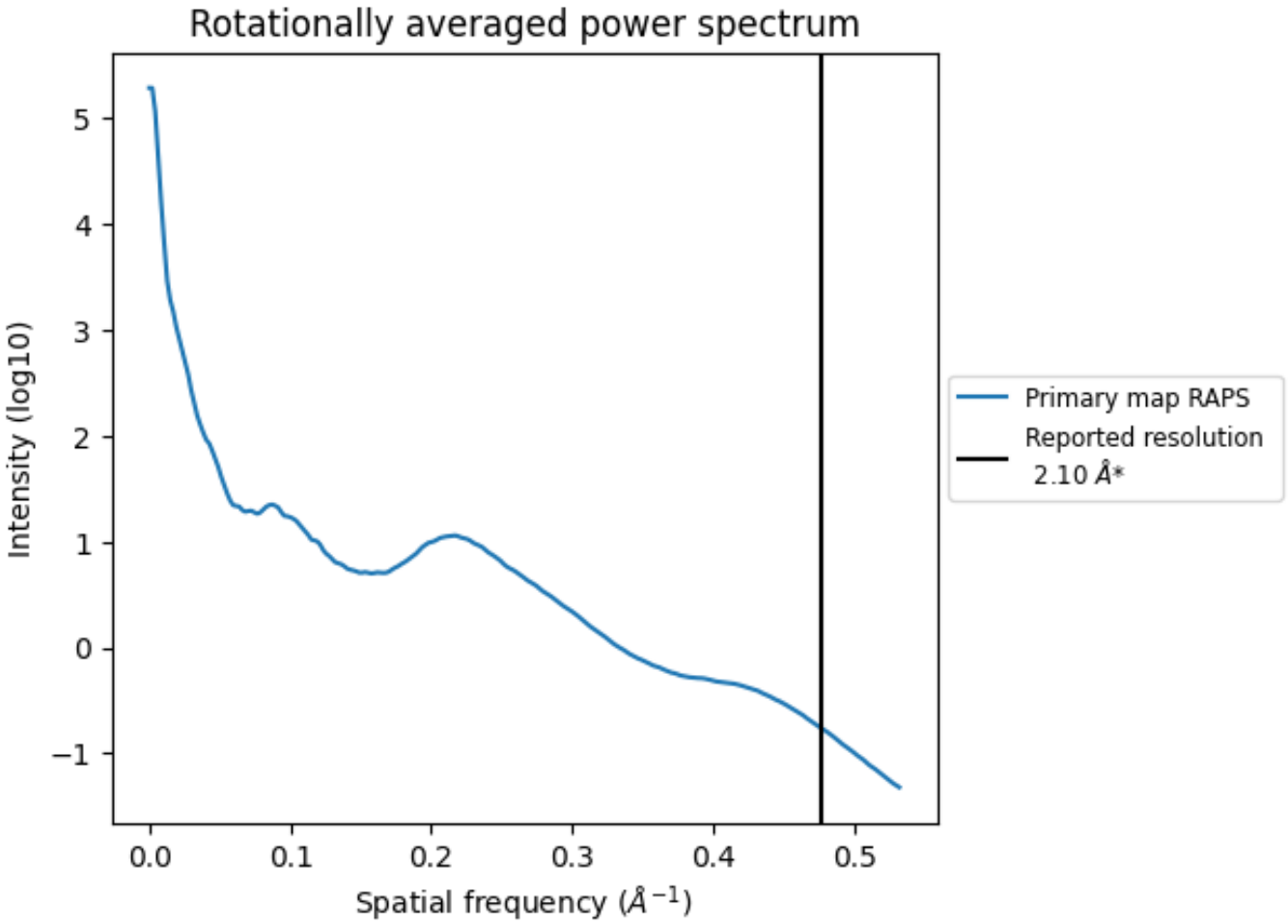
7.2 Volume estimate (i)



The volume at the recommended contour level is 22140 nm^3; this corresponds to an approximate mass of 20000 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 0.476 Å^{-1}

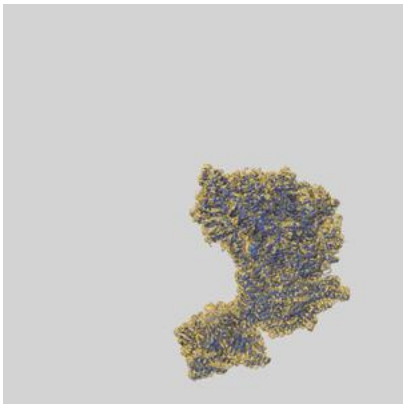
8 Fourier-Shell correlation

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

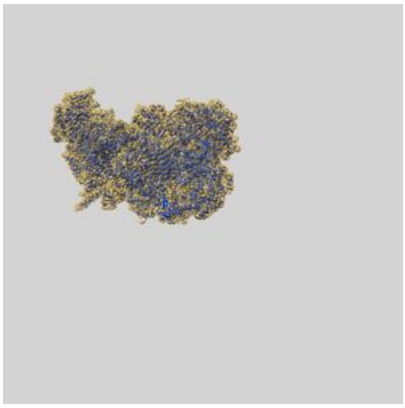
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70068 and PDB model 9O34. Per-residue inclusion information can be found in section 3 on page 10.

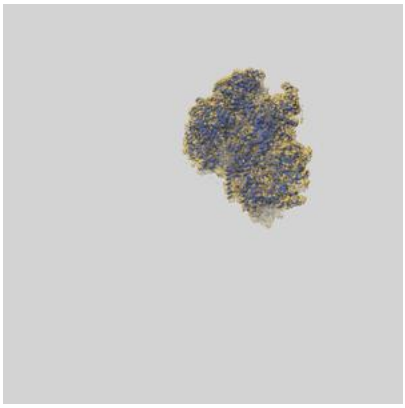
9.1 Map-model overlay



X



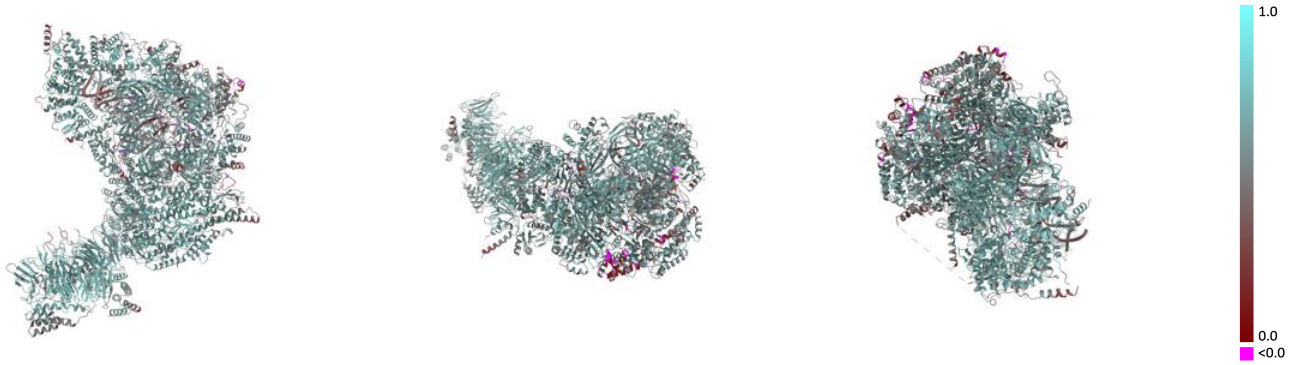
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00859 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.

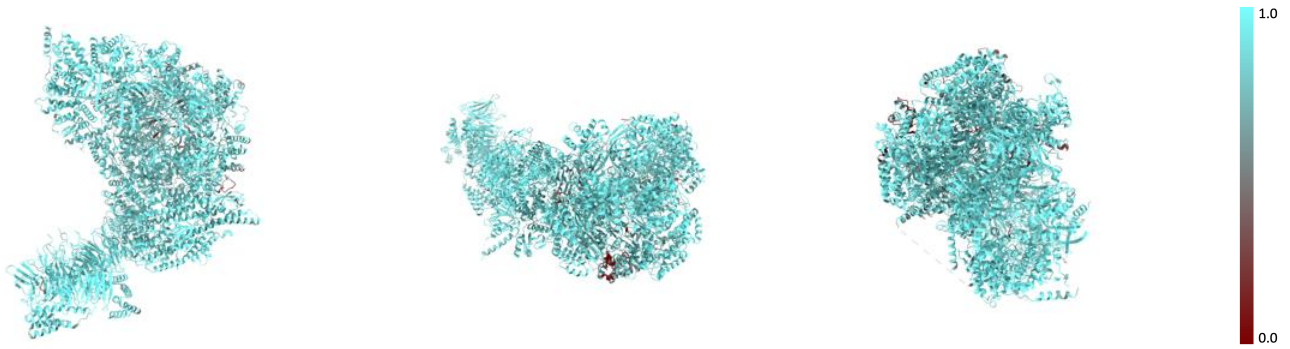
9.2 Q-score mapped to coordinate model



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.

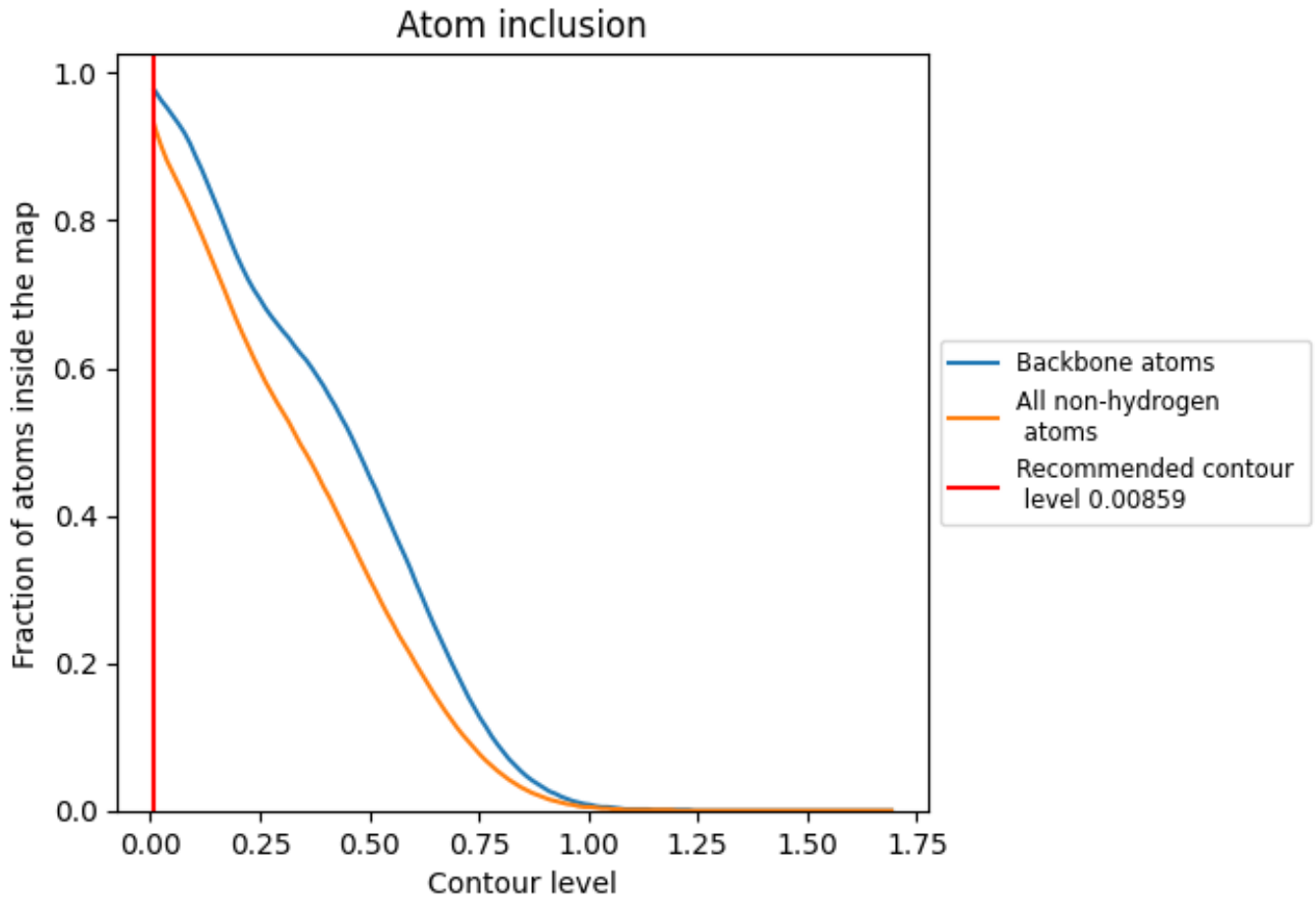
9.3 Atom inclusion mapped to coordinate model



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 (0.00859).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.00859) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.5730
2	0.9520	0.5960
3	0.9100	0.5590
4	0.8740	0.5070
5	0.9450	0.5980
6	0.9250	0.5670
7	0.9110	0.5120
C	0.9530	0.5920
D	0.9430	0.5710
E	0.9670	0.6490
F	0.9400	0.6010
G	0.9530	0.6100
H	0.9530	0.6110
I	0.9380	0.5910
J	0.9390	0.6100
K	0.9590	0.6100
L	0.9130	0.5580
M	0.8690	0.4550
N	0.8840	0.4110
Q	0.8300	0.4430

