



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 10:55 PM EDT

PDB ID : 6PTN
EMDB ID : EMD-20472
Title : Structure of Ctf4 trimer in complex with two CMG helicases
Authors : Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.
Deposited on : 2019-07-16
Resolution : 5.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

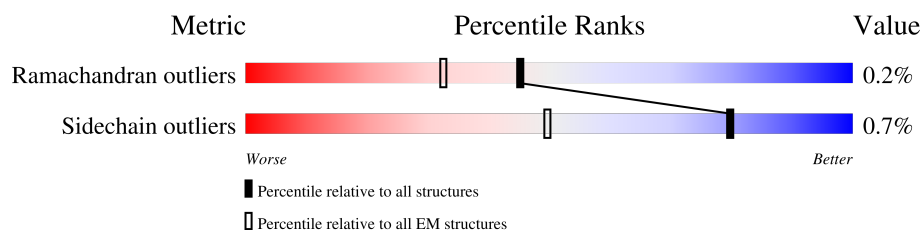
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	E	927	
1	F	927	
1	G	927	
2	A	208	
2	a	208	
3	B	213	
3	b	213	
4	C	194	
4	c	194	

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Mol	Chain	Length	Quality of chain
5	D	294	
5	d	294	
6	H	650	
6	h	650	
7	2	868	
7	i	868	
8	3	971	
8	j	971	
9	4	933	
9	k	933	
10	5	775	
10	l	775	
11	6	1017	
11	m	1017	
12	7	845	
12	n	845	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 91630 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 polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		
1	F	431	Total	C	N	O	S	1	0
			3472	2227	576	653	16		
1	G	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		
2	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		
3	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 4 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		
4	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 5 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		
5	D	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		

- Molecule 6 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		
6	H	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		
7	2	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		
8	3	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		

- Molecule 9 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		
9	4	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		

- Molecule 10 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

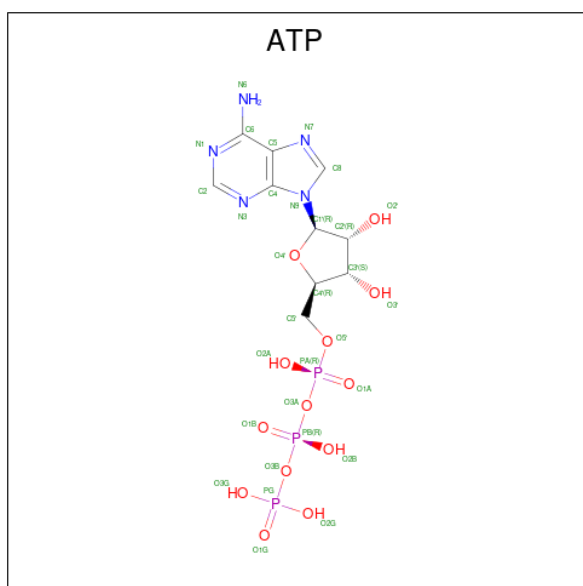
- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		
11	6	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		

- Molecule 12 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	n	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		
12	7	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



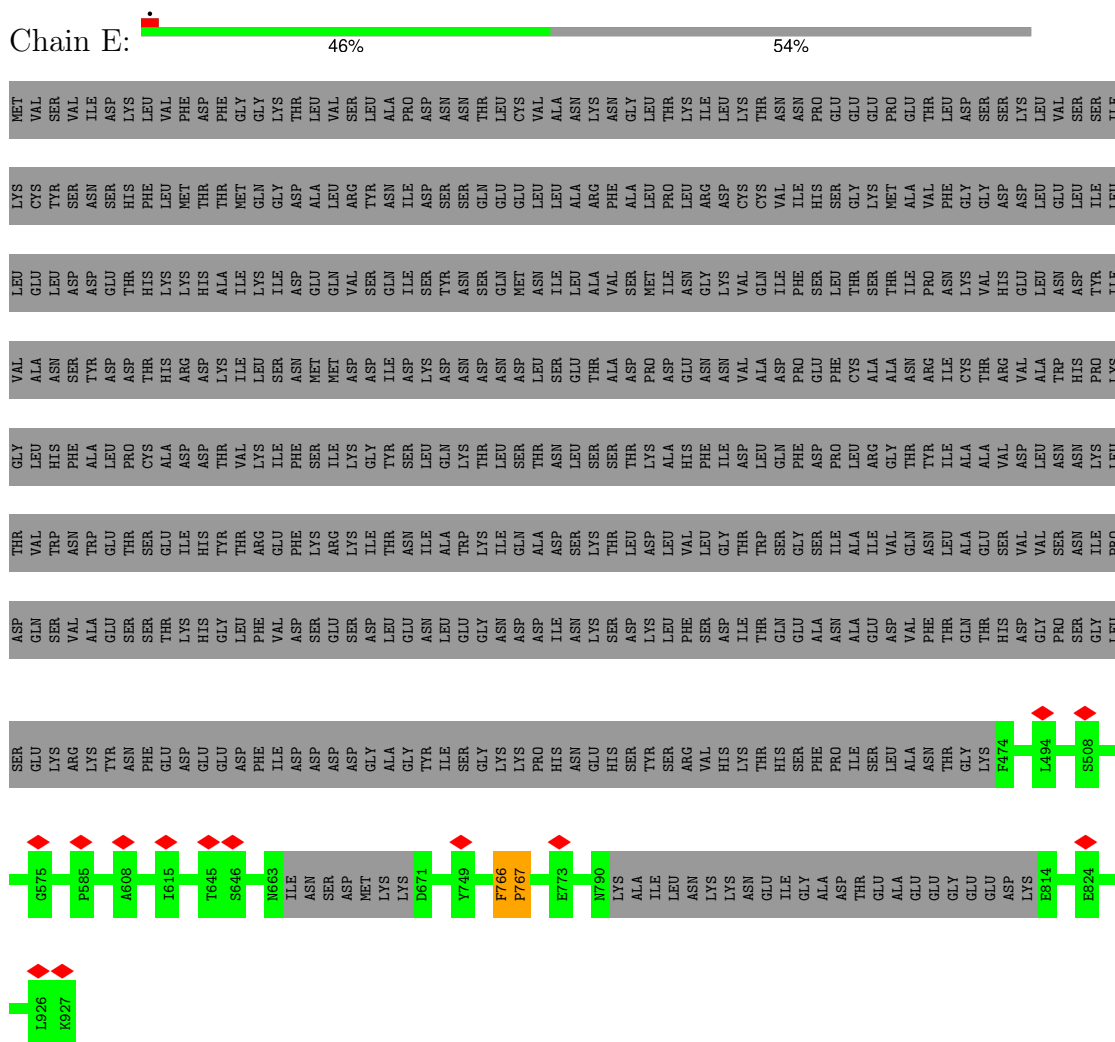
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Mol	Chain	Residues	Atoms					AltConf
13	j	1	Total 31	C 10	N 5	O 13	P 3	0
13	1	1	Total 31	C 10	N 5	O 13	P 3	0
13	2	1	Total 31	C 10	N 5	O 13	P 3	0
13	3	1	Total 31	C 10	N 5	O 13	P 3	0
13	5	1	Total 31	C 10	N 5	O 13	P 3	0

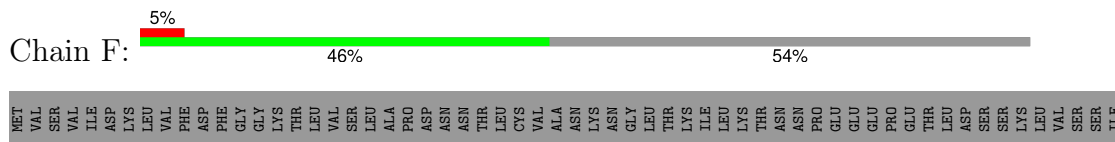
3 Residue-property plots

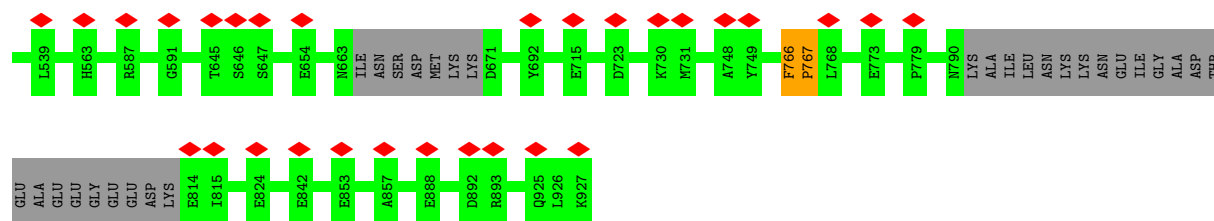
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

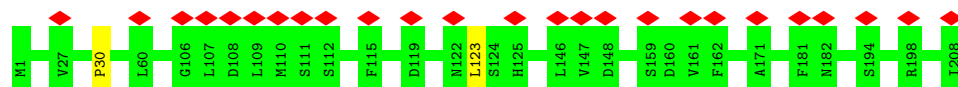


- Molecule 1: DNA polymerase alpha-binding protein

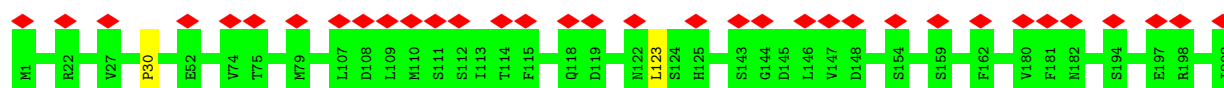




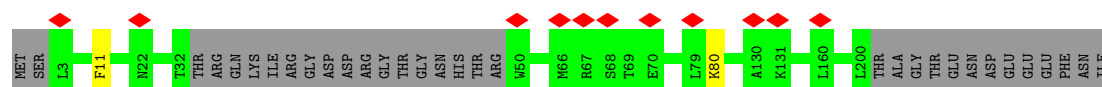
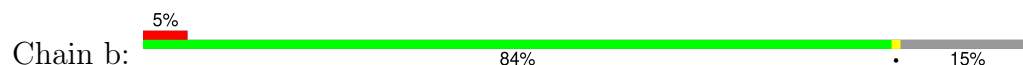
• Molecule 2: DNA replication complex GINS protein PSF1



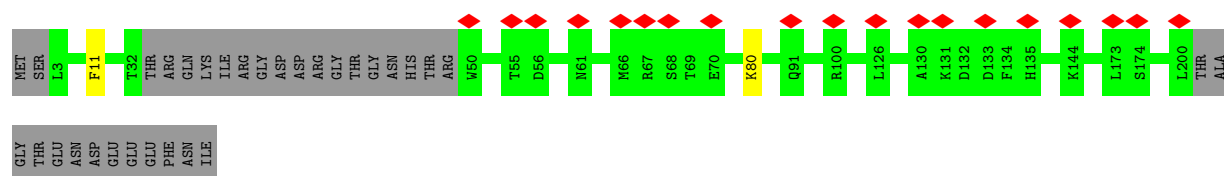
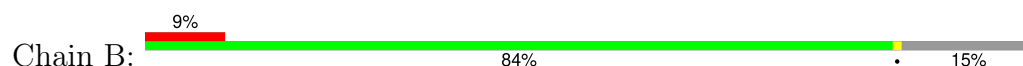
• Molecule 2: DNA replication complex GINS protein PSF1



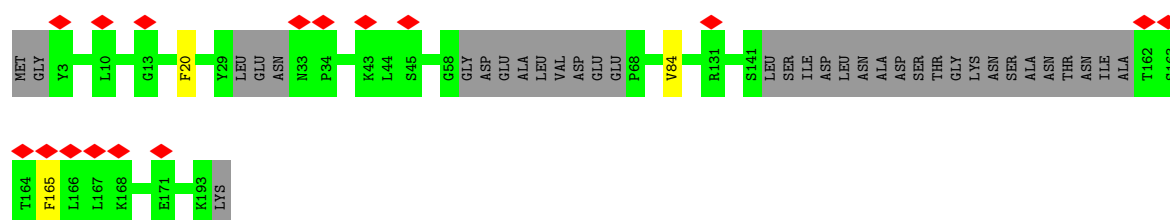
• Molecule 3: DNA replication complex GINS protein PSF2

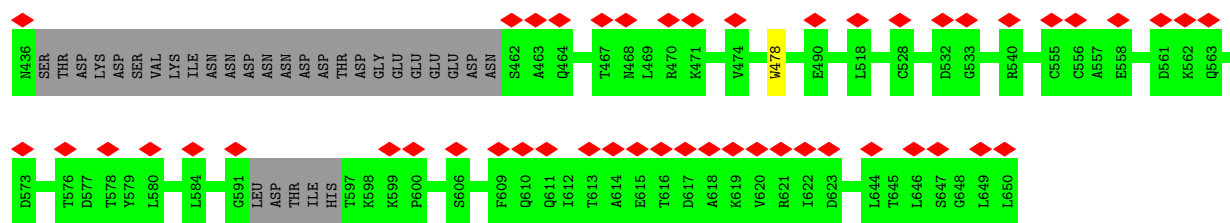


• Molecule 3: DNA replication complex GINS protein PSF2



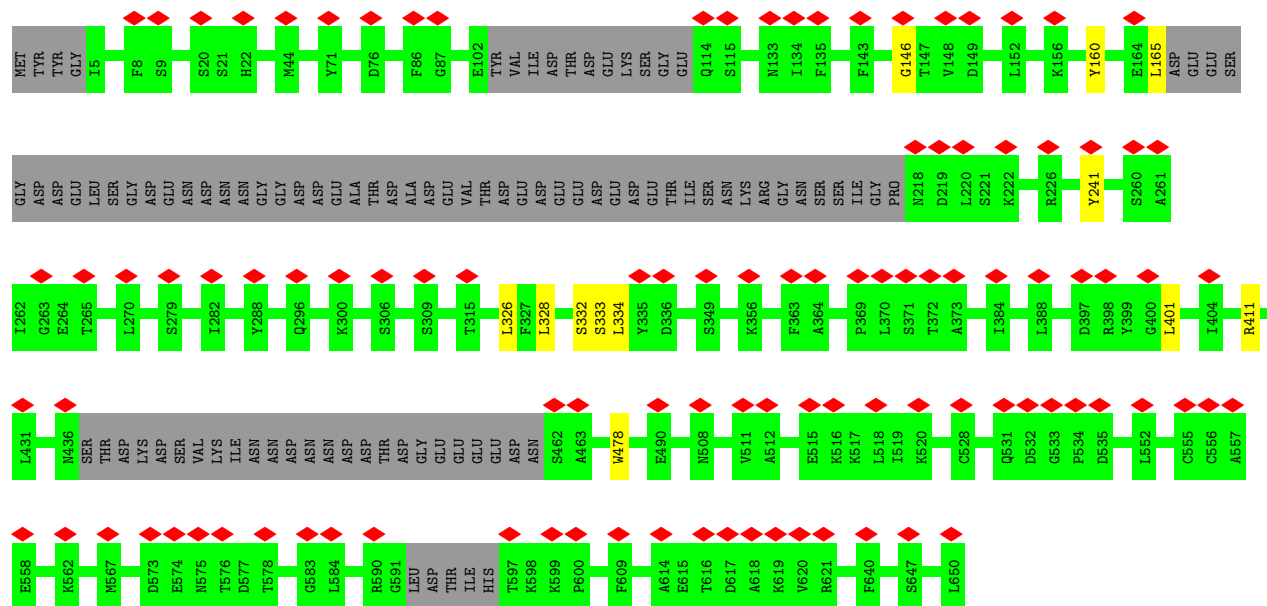
• Molecule 4: DNA replication complex GINS protein PSF3





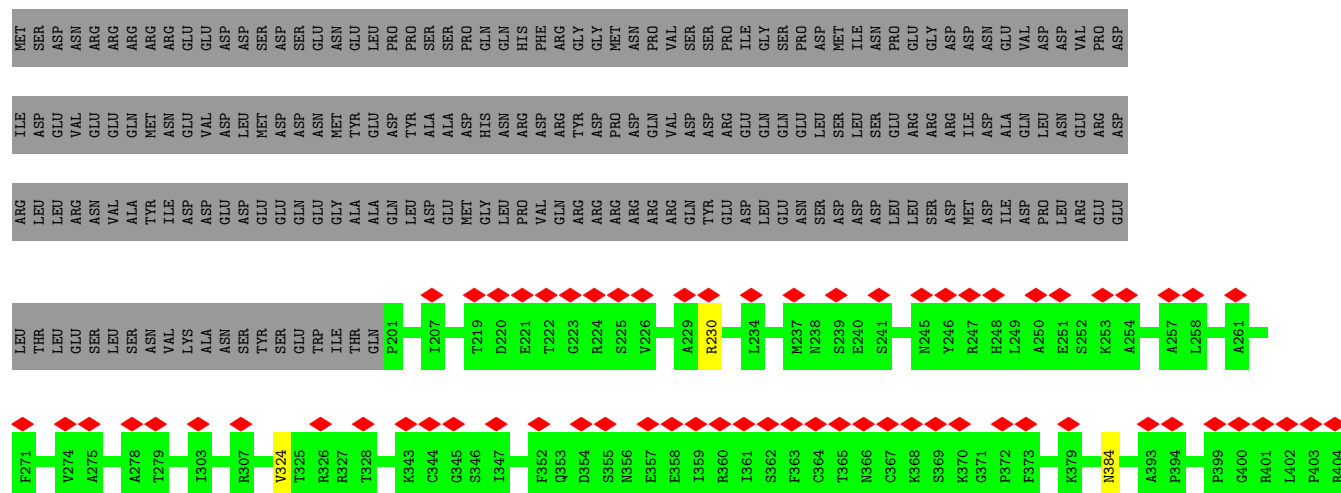
• Molecule 6: Cell division control protein 45

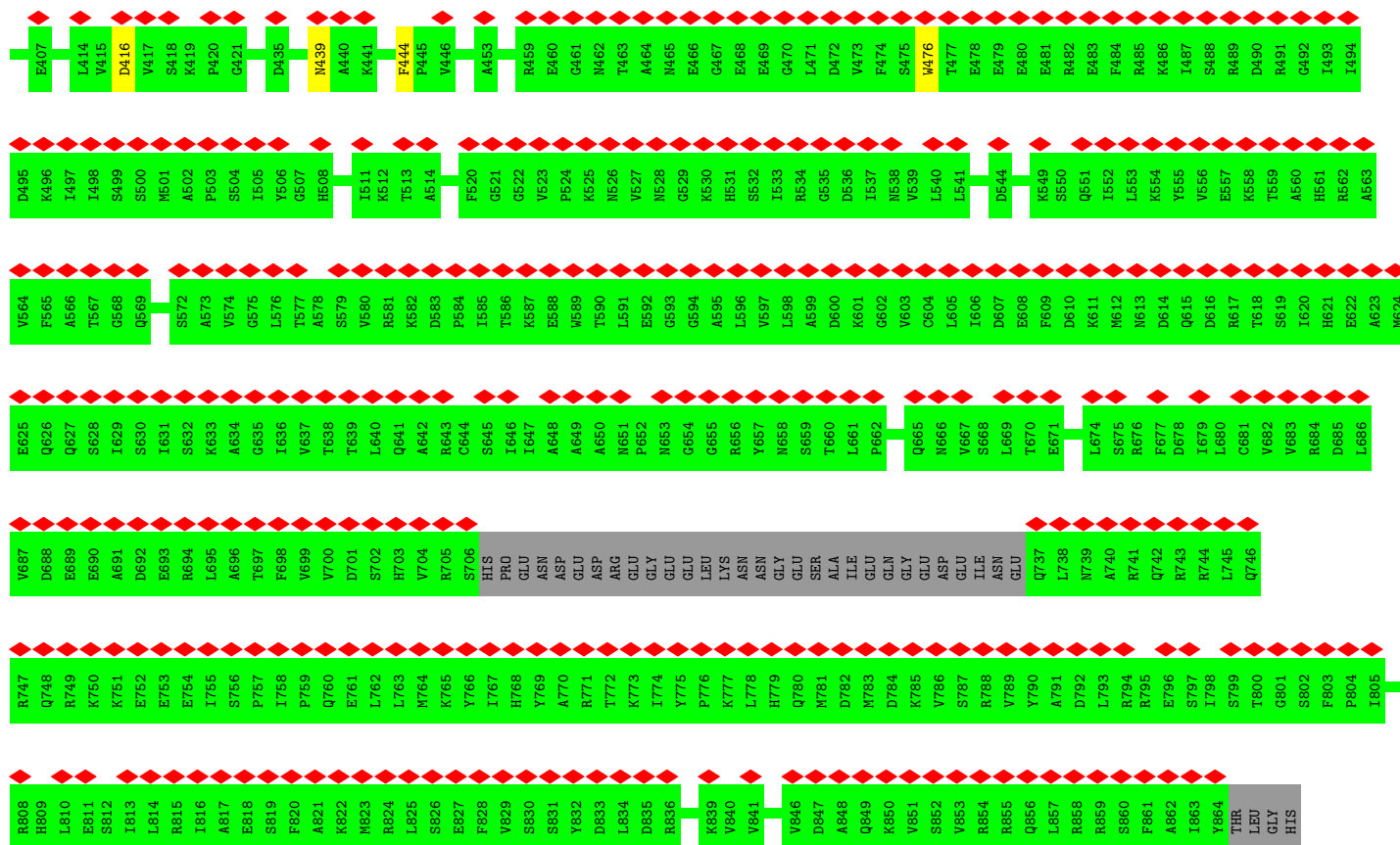
Chain H: 16% 83% 15%



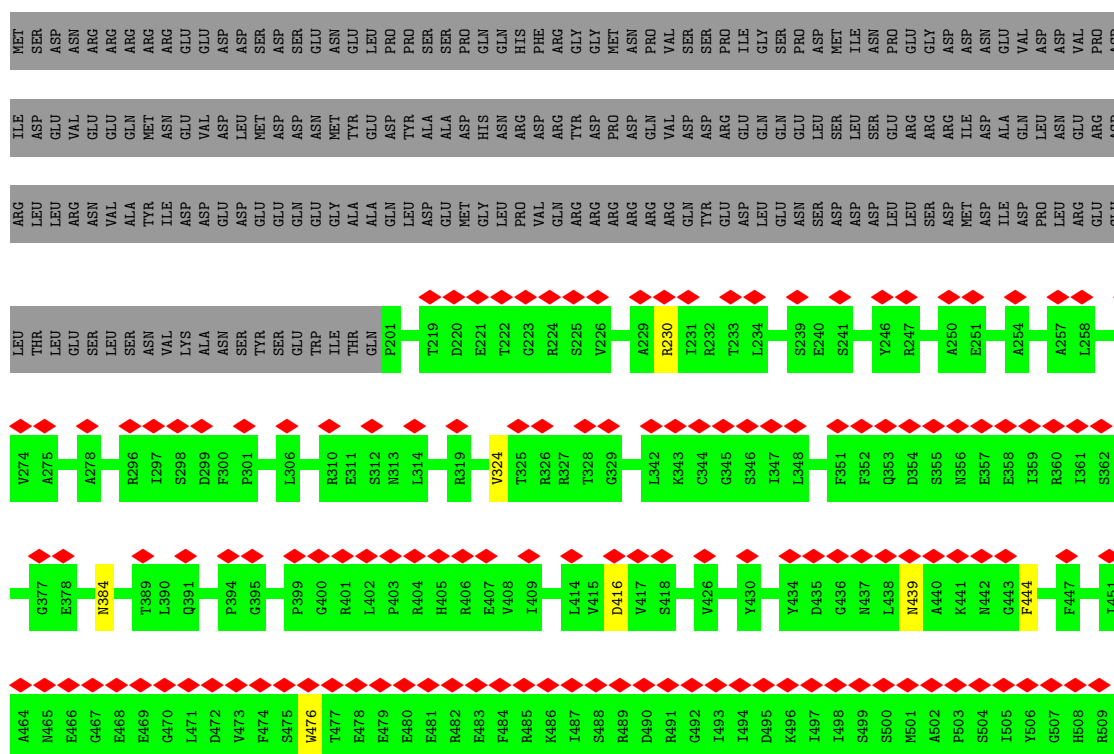
• Molecule 7: DNA replication licensing factor MCM2

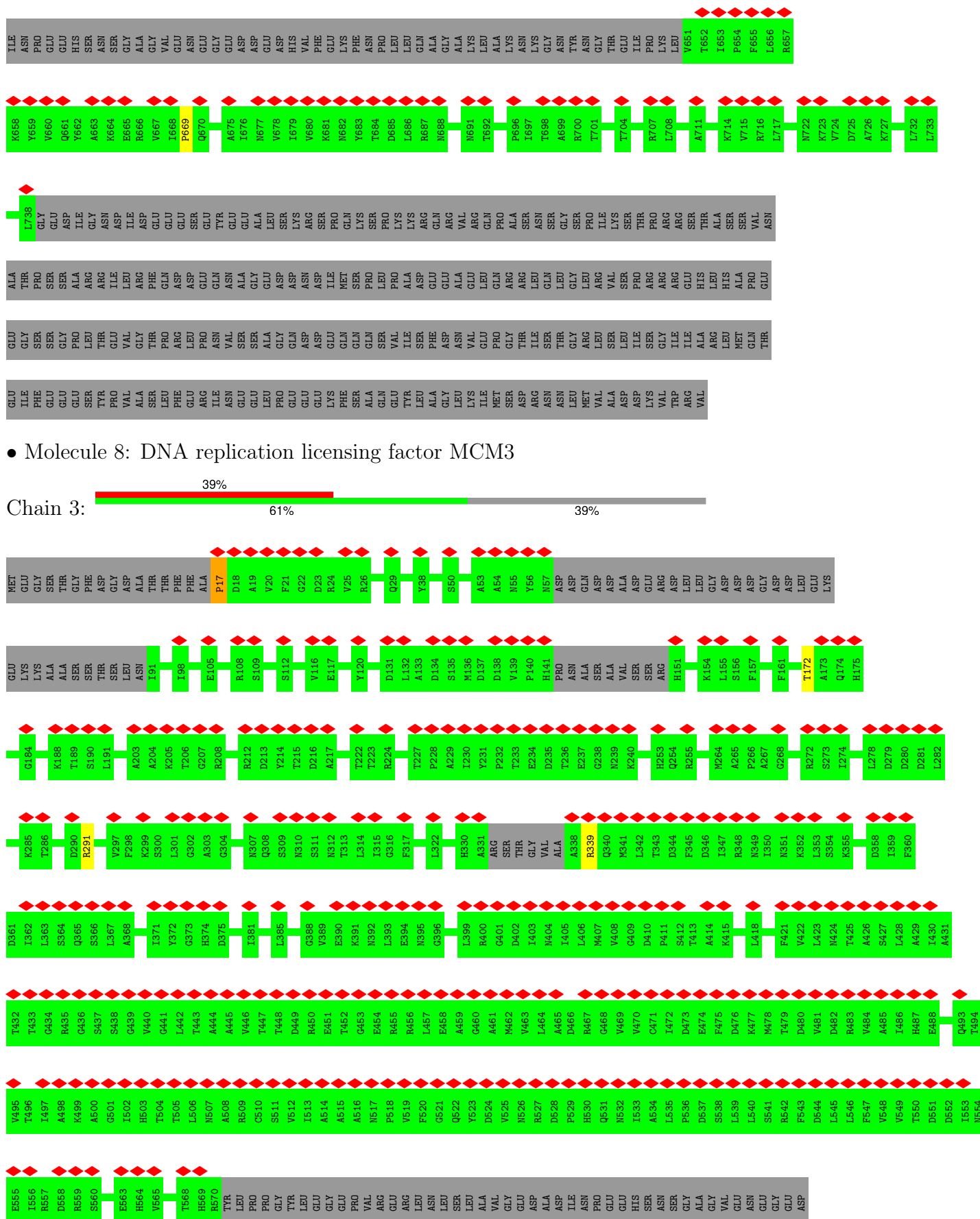
Chain i: 47% 72% 27%



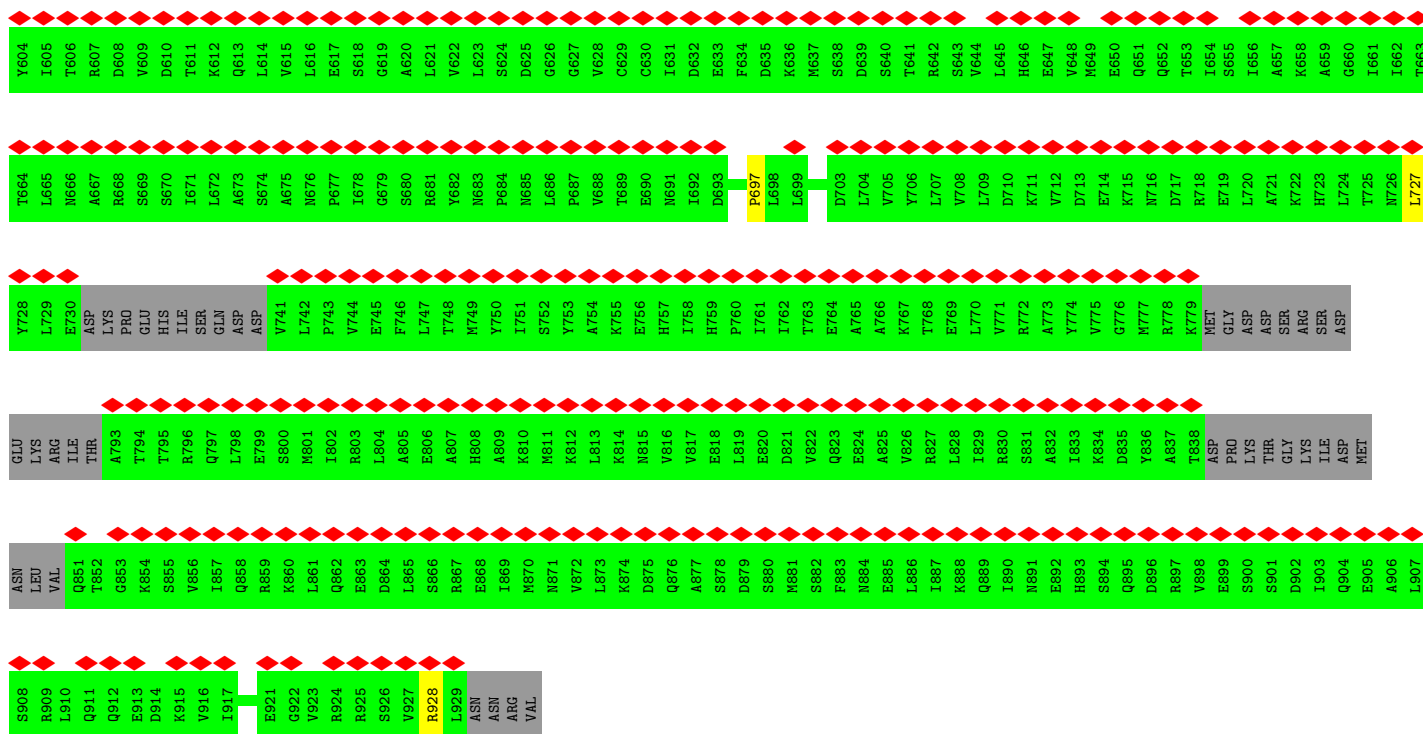


• Molecule 7: DNA replication licensing factor MCM2

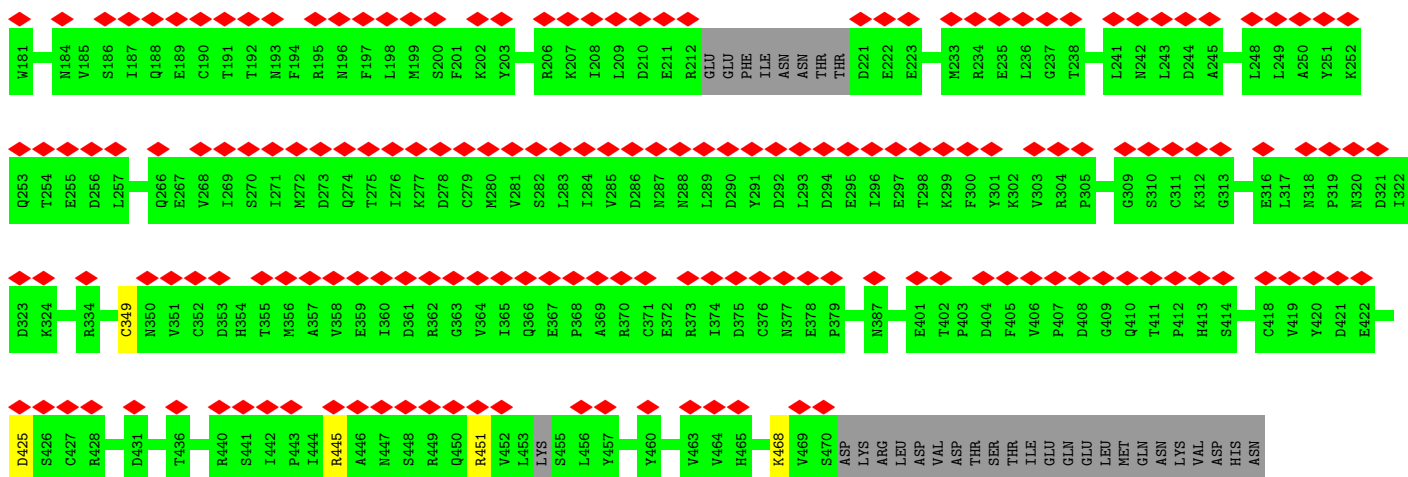
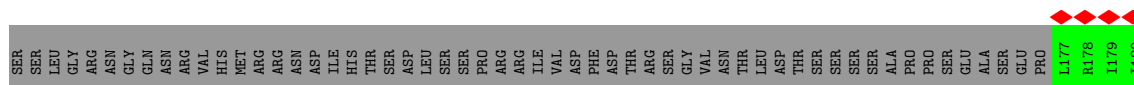
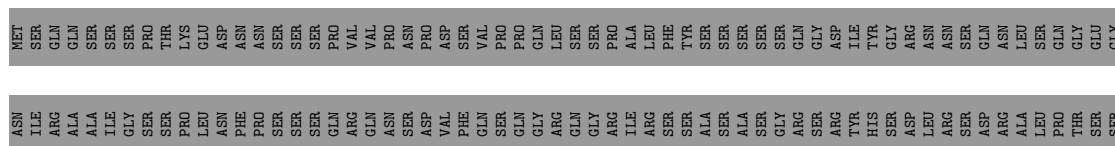
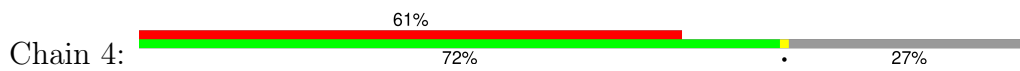


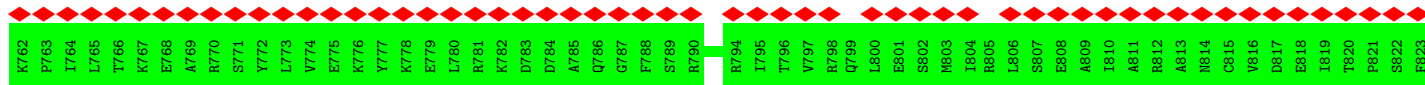


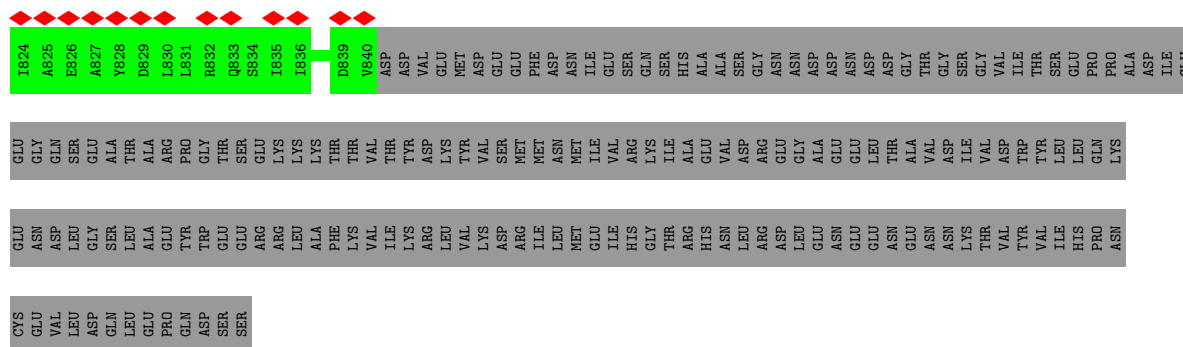




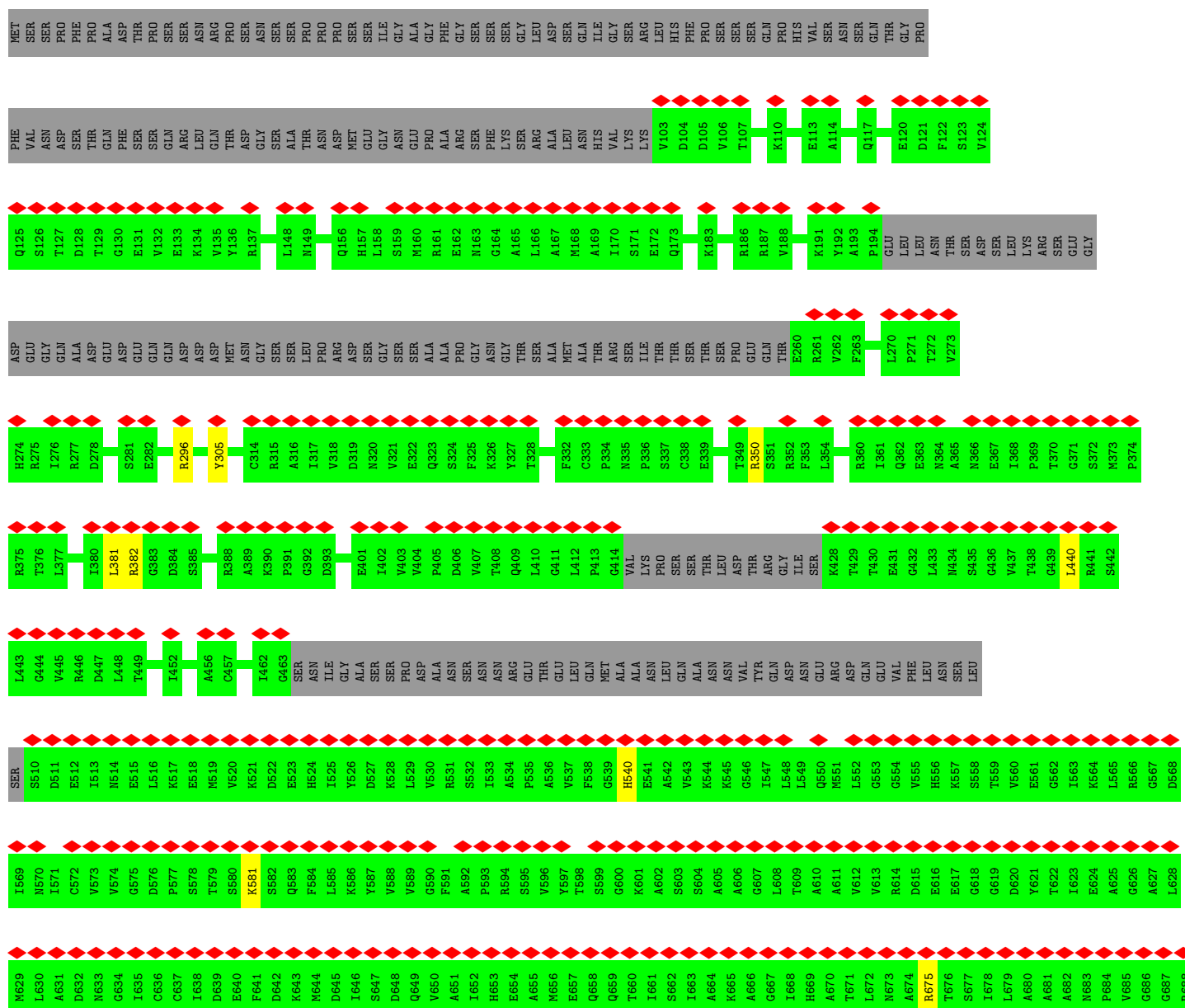
• Molecule 9: DNA replication licensing factor MCM4

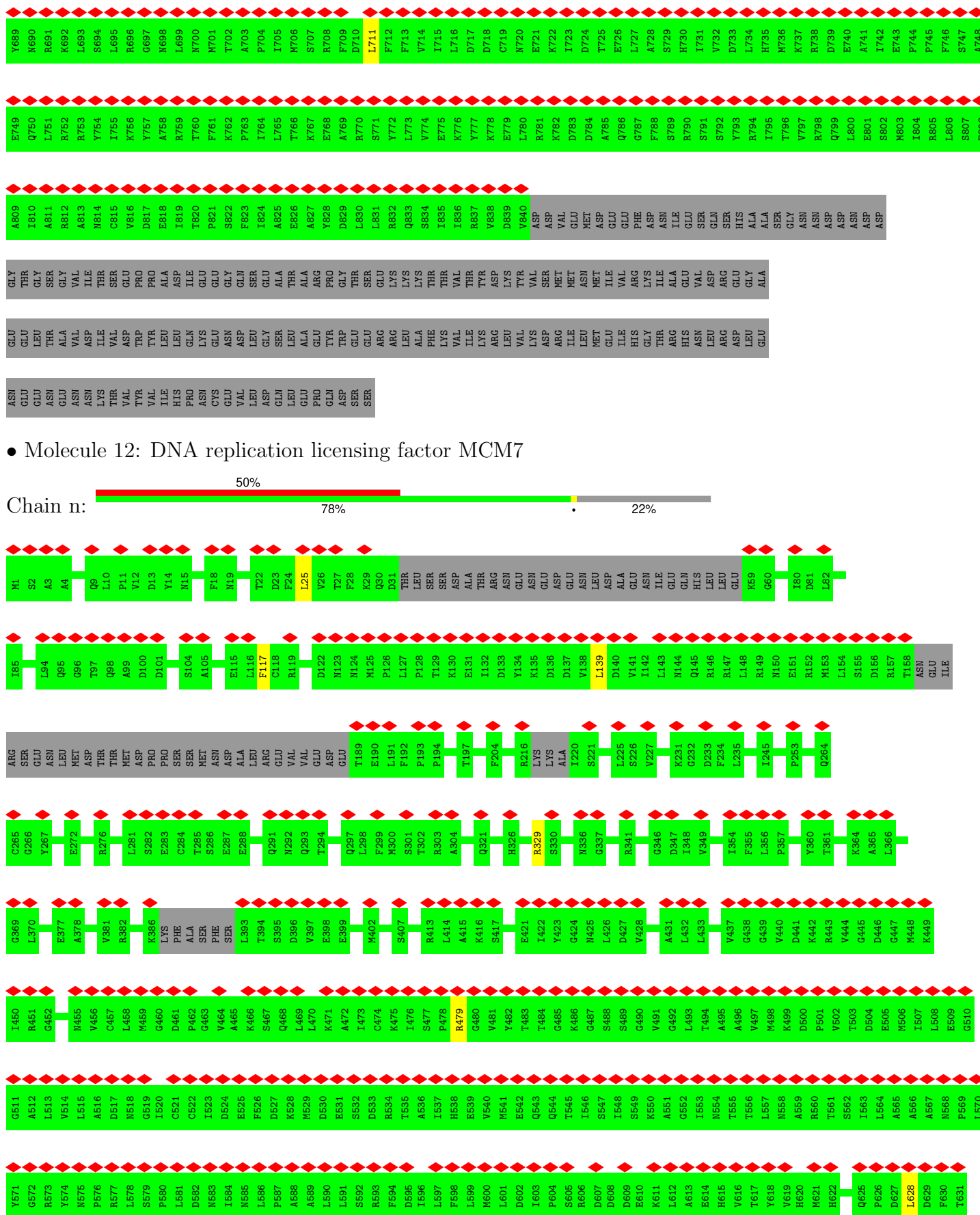


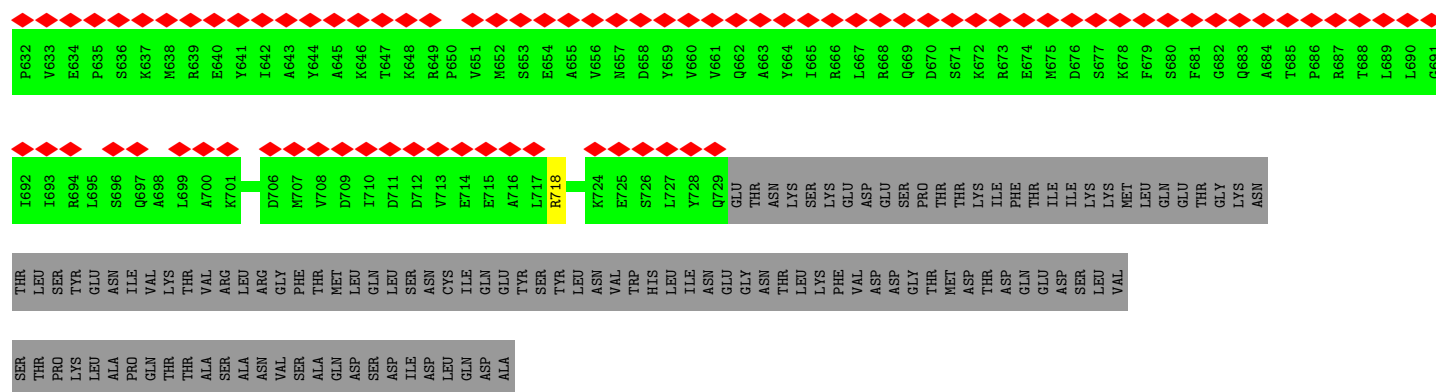




• Molecule 11: DNA replication licensing factor MCM6

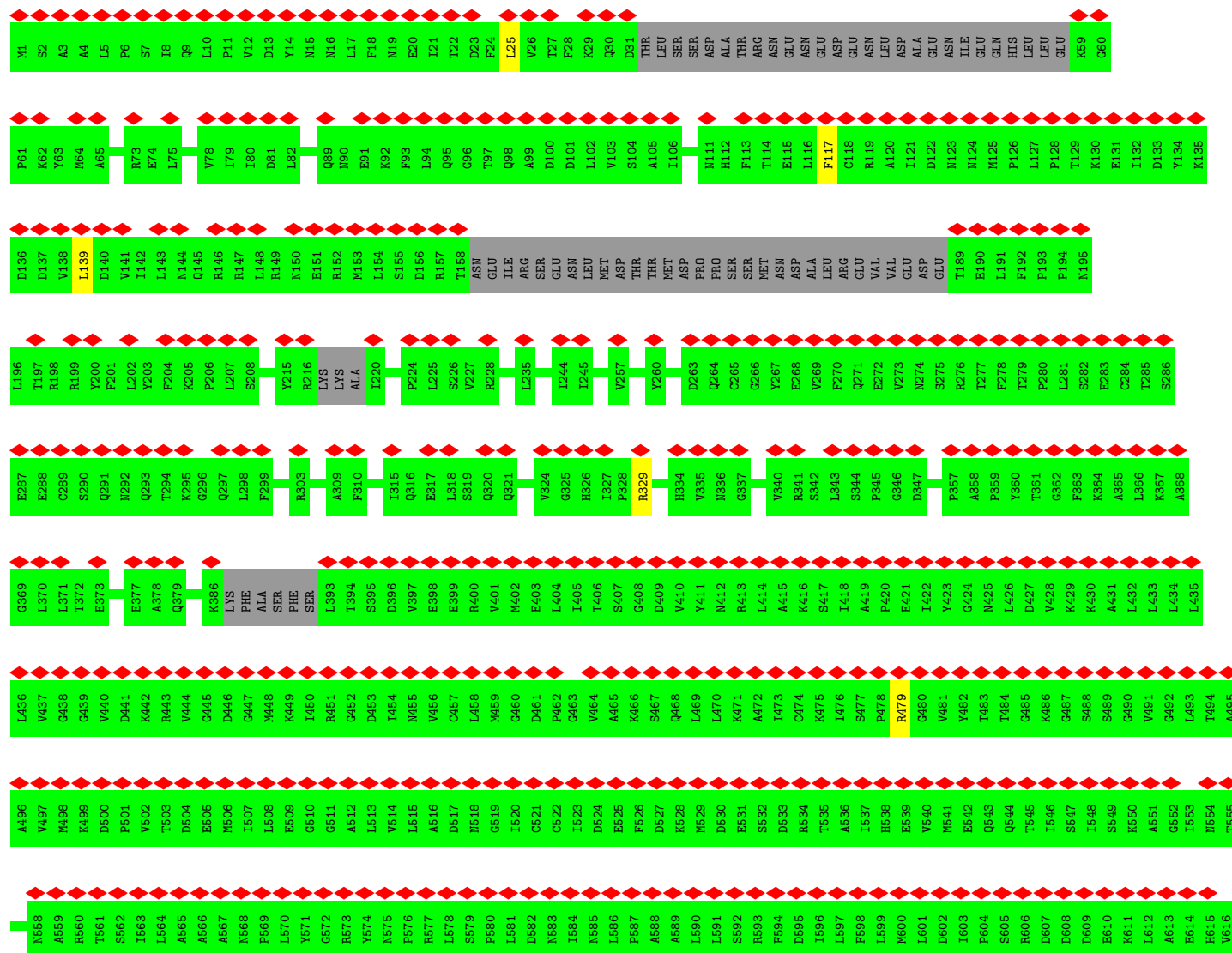






Molecule 12: DNA replication licensing factor MCM7

Chain 7:



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0246	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	E	0.41	0/3501	0.60	3/4741 (0.1%)
1	F	0.40	0/3558	0.61	3/4817 (0.1%)
1	G	0.40	0/3500	0.62	3/4738 (0.1%)
2	A	0.42	0/1718	0.66	2/2314 (0.1%)
2	a	0.43	0/1718	0.66	2/2314 (0.1%)
3	B	0.46	1/1545 (0.1%)	0.65	0/2092
3	b	0.46	1/1545 (0.1%)	0.65	0/2092
4	C	0.47	0/1320	0.63	1/1784 (0.1%)
4	c	0.47	0/1320	0.63	1/1784 (0.1%)
5	D	0.43	0/1956	0.58	0/2638
5	d	0.43	0/1956	0.58	0/2638
6	H	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	h	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
7	2	0.45	0/5051	0.64	1/6821 (0.0%)
7	i	0.45	0/5051	0.64	1/6821 (0.0%)
8	3	0.44	0/4739	0.78	3/6425 (0.0%)
8	j	0.44	0/4739	0.78	3/6425 (0.0%)
9	4	0.37	0/5479	0.62	2/7392 (0.0%)
9	k	0.37	0/5479	0.61	2/7392 (0.0%)
10	5	0.47	0/4750	0.69	4/6412 (0.1%)
10	l	0.47	0/4750	0.69	4/6412 (0.1%)
11	6	0.43	0/4789	0.65	3/6466 (0.0%)
11	m	0.43	0/4789	0.65	3/6466 (0.0%)
12	7	0.37	0/5299	0.61	3/7160 (0.0%)
12	n	0.37	0/5299	0.61	3/7160 (0.0%)
All	All	0.43	4/92977 (0.0%)	0.65	57/125650 (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
1	E	0	1
1	F	0	1
1	G	0	1
8	3	0	1
8	j	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	478	TRP	CB-CG	-6.12	1.39	1.50
6	H	478	TRP	CB-CG	-6.07	1.39	1.50
3	B	11	PHE	C-N	-5.28	1.22	1.34
3	b	11	PHE	C-N	-5.25	1.22	1.34

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	17	PRO	CA-C-O	-29.18	50.16	120.20
8	3	17	PRO	CA-C-O	-29.18	50.17	120.20
8	3	17	PRO	CA-C-N	15.27	150.80	117.20
8	j	17	PRO	CA-C-N	15.23	150.72	117.20
1	G	766	PHE	C-N-CD	-13.93	89.95	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	3	17	PRO	Mainchain
1	E	766	PHE	Peptide
1	F	766	PHE	Peptide
1	G	766	PHE	Peptide
8	j	17	PRO	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	E	419/927 (45%)	407 (97%)	11 (3%)	1 (0%)	44	78
1	F	428/927 (46%)	415 (97%)	12 (3%)	1 (0%)	44	78
1	G	417/927 (45%)	407 (98%)	9 (2%)	1 (0%)	44	78
2	A	206/208 (99%)	179 (87%)	26 (13%)	1 (0%)	25	65
2	a	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	25	65
3	B	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	b	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
4	C	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
4	c	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
5	D	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	d	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
6	H	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	22	61
6	h	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	22	61
7	2	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
7	i	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
8	3	584/971 (60%)	506 (87%)	77 (13%)	1 (0%)	44	78
8	j	584/971 (60%)	506 (87%)	76 (13%)	2 (0%)	37	73
9	4	668/933 (72%)	579 (87%)	89 (13%)	0	100	100
9	k	668/933 (72%)	578 (86%)	90 (14%)	0	100	100
10	5	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	44	78
10	l	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	44	78
11	6	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	44	78
11	m	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	44	78
12	7	653/845 (77%)	556 (85%)	97 (15%)	0	100	100
12	n	653/845 (77%)	554 (85%)	99 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11318/16717 (68%)	9873 (87%)	1427 (13%)	18 (0%)	45 78

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	h	334	LEU
6	H	334	LEU
1	G	767	PRO
6	h	332	SER
10	l	147	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	377/825 (46%)	377 (100%)	0	100	100
1	F	384/825 (46%)	384 (100%)	0	100	100
1	G	377/825 (46%)	377 (100%)	0	100	100
2	A	193/193 (100%)	193 (100%)	0	100	100
2	a	193/193 (100%)	193 (100%)	0	100	100
3	B	171/198 (86%)	170 (99%)	1 (1%)	84	88
3	b	171/198 (86%)	170 (99%)	1 (1%)	84	88
4	C	144/173 (83%)	142 (99%)	2 (1%)	62	75
4	c	144/173 (83%)	142 (99%)	2 (1%)	62	75
5	D	225/279 (81%)	225 (100%)	0	100	100
5	d	225/279 (81%)	225 (100%)	0	100	100
6	H	499/586 (85%)	496 (99%)	3 (1%)	84	88
6	h	499/586 (85%)	496 (99%)	3 (1%)	84	88
7	2	535/770 (70%)	529 (99%)	6 (1%)	70	80
7	i	535/770 (70%)	529 (99%)	6 (1%)	70	80
8	3	515/835 (62%)	512 (99%)	3 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	j	515/835 (62%)	512 (99%)	3 (1%)	84	88
9	4	610/848 (72%)	604 (99%)	6 (1%)	73	82
9	k	610/848 (72%)	605 (99%)	5 (1%)	79	85
10	5	534/688 (78%)	527 (99%)	7 (1%)	65	77
10	l	534/688 (78%)	527 (99%)	7 (1%)	65	77
11	6	493/886 (56%)	487 (99%)	6 (1%)	67	78
11	m	493/886 (56%)	487 (99%)	6 (1%)	67	78
12	7	585/753 (78%)	581 (99%)	4 (1%)	81	87
12	n	585/753 (78%)	581 (99%)	4 (1%)	81	87
All	All	10146/14893 (68%)	10071 (99%)	75 (1%)	80	87

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	4	928	ARG
12	7	117	PHE
10	5	275	THR
11	6	296	ARG
10	l	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
7	2	333	GLN
10	5	561	ASN
7	2	551	GLN
8	3	554	ASN
11	6	750	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
13	ATP	i	901	-	28,33,33	0.81	0	34,52,52	1.20	3 (8%)
13	ATP	3	1001	-	28,33,33	0.89	0	34,52,52	1.27	3 (8%)
13	ATP	1	801	-	28,33,33	0.73	0	34,52,52	1.68	5 (14%)
13	ATP	5	801	-	28,33,33	0.74	0	34,52,52	1.68	5 (14%)
13	ATP	j	1001	-	28,33,33	0.89	0	34,52,52	1.26	3 (8%)
13	ATP	2	901	-	28,33,33	0.82	0	34,52,52	1.21	3 (8%)

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
13	ATP	i	901	-	-	6/18/38/38	0/3/3/3
13	ATP	3	1001	-	-	4/18/38/38	0/3/3/3
13	ATP	1	801	-	-	4/18/38/38	0/3/3/3
13	ATP	5	801	-	-	4/18/38/38	0/3/3/3
13	ATP	j	1001	-	-	5/18/38/38	0/3/3/3
13	ATP	2	901	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	801	ATP	C4'-O4'-C1'	-4.97	105.37	109.92
13	l	801	ATP	C4'-O4'-C1'	-4.92	105.42	109.92
13	5	801	ATP	N3-C2-N1	-4.26	122.89	128.67
13	l	801	ATP	N3-C2-N1	-4.24	122.92	128.67
13	l	801	ATP	O4'-C1'-N9	3.91	113.93	108.75

There are no chirality outliers.

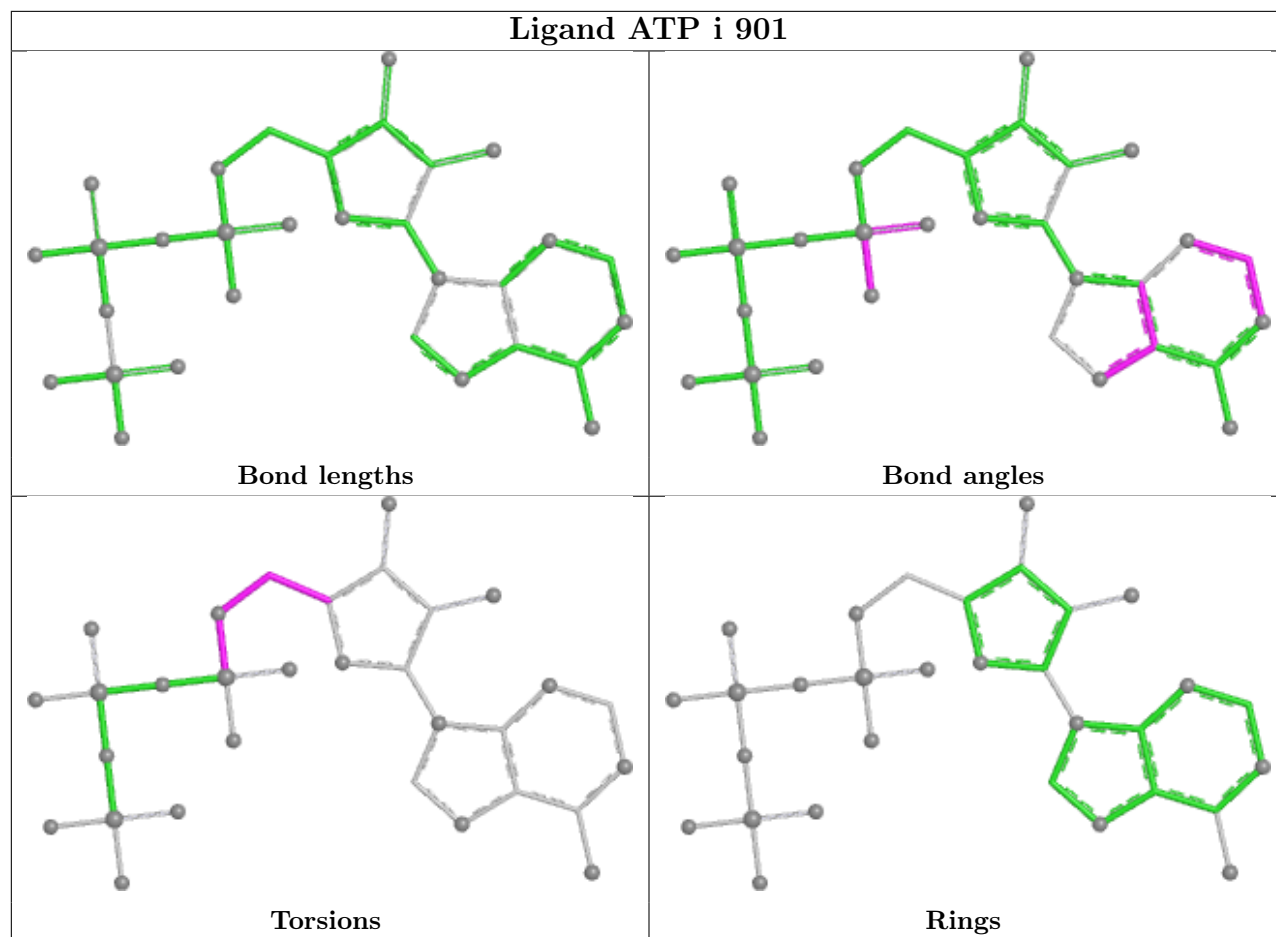
5 of 29 torsion outliers are listed below:

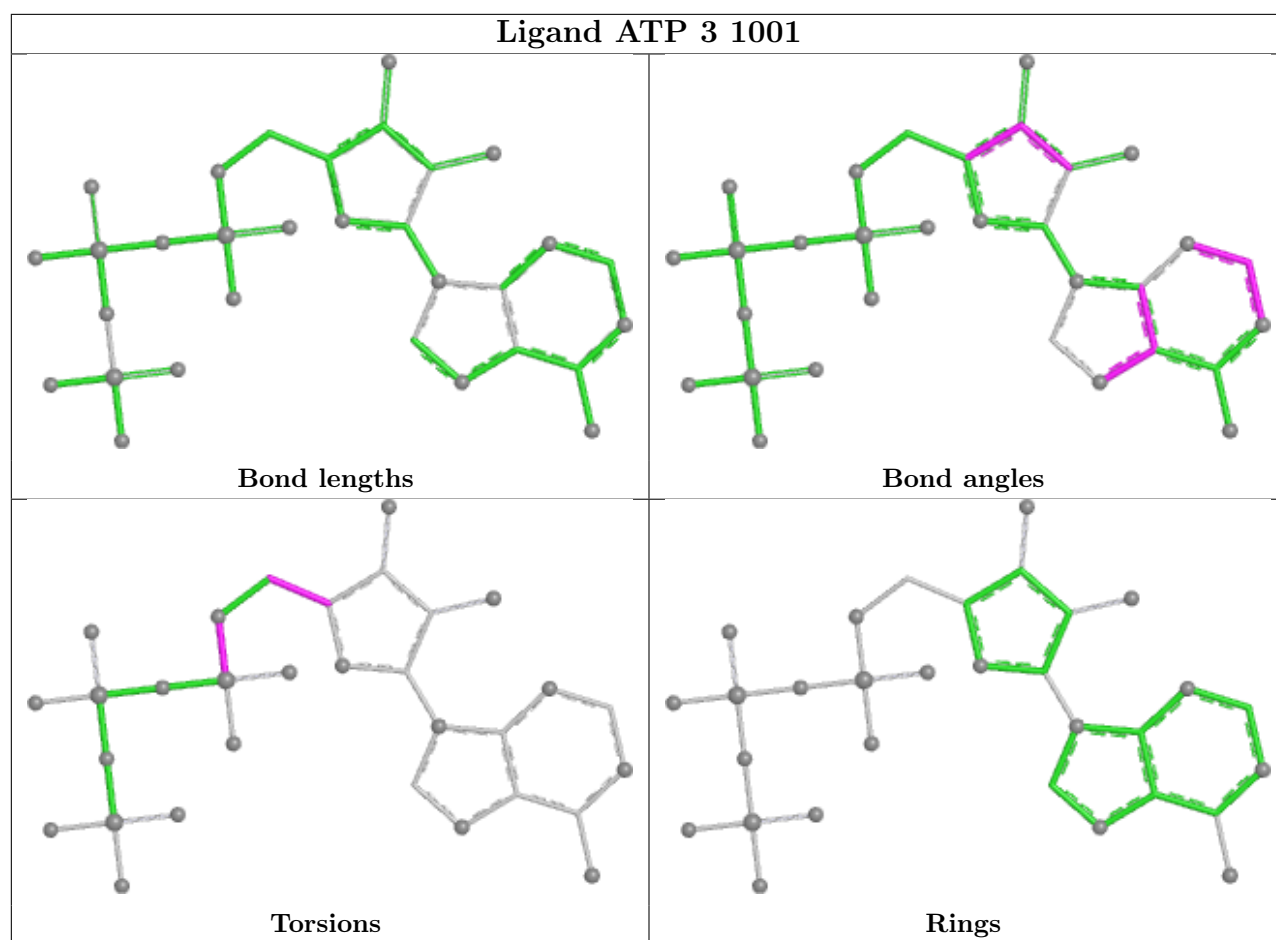
Mol	Chain	Res	Type	Atoms
13	i	901	ATP	C5'-O5'-PA-O1A
13	i	901	ATP	C5'-O5'-PA-O2A
13	i	901	ATP	C5'-O5'-PA-O3A
13	j	1001	ATP	C5'-O5'-PA-O2A
13	j	1001	ATP	C5'-O5'-PA-O3A

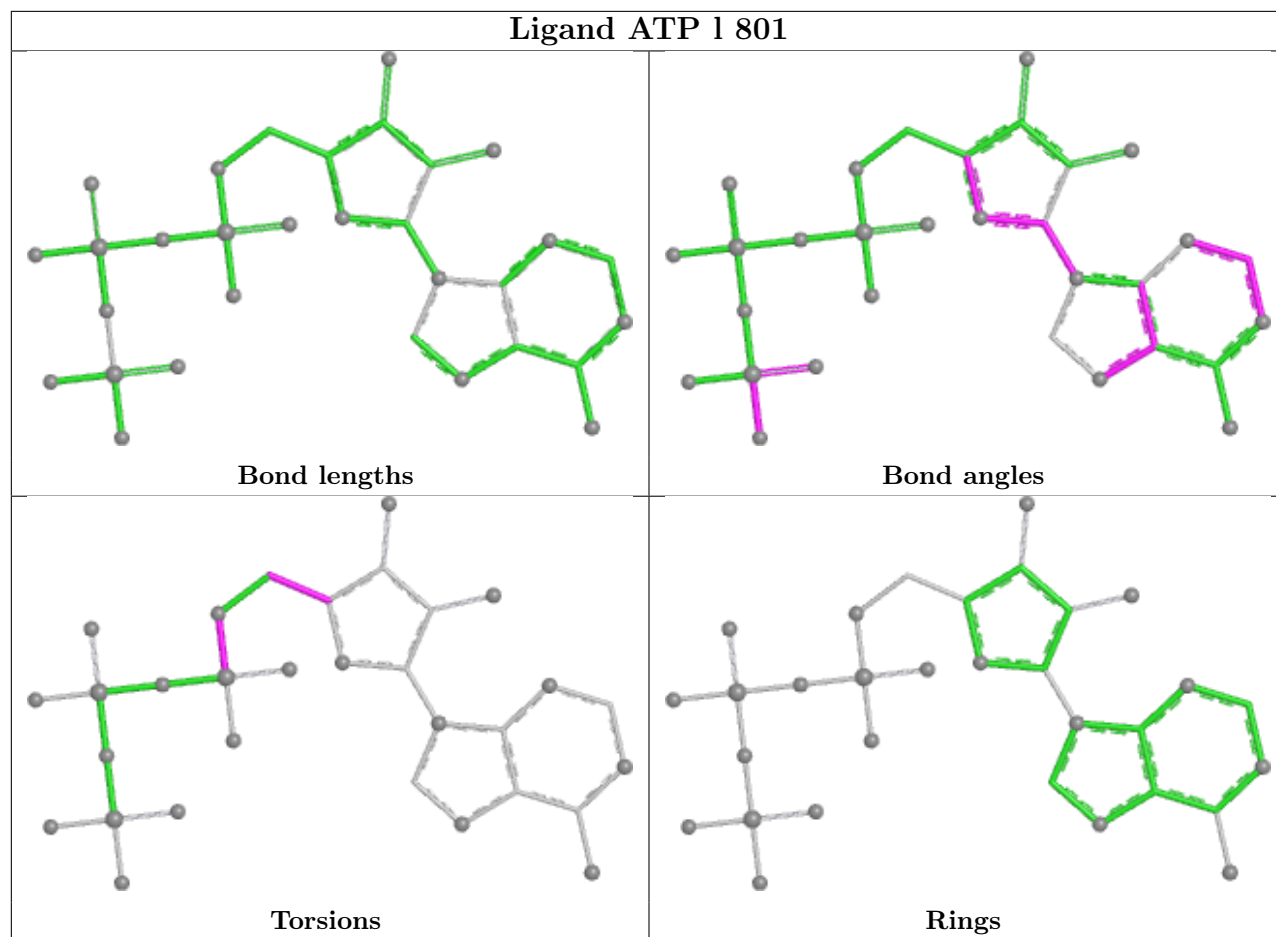
There are no ring outliers.

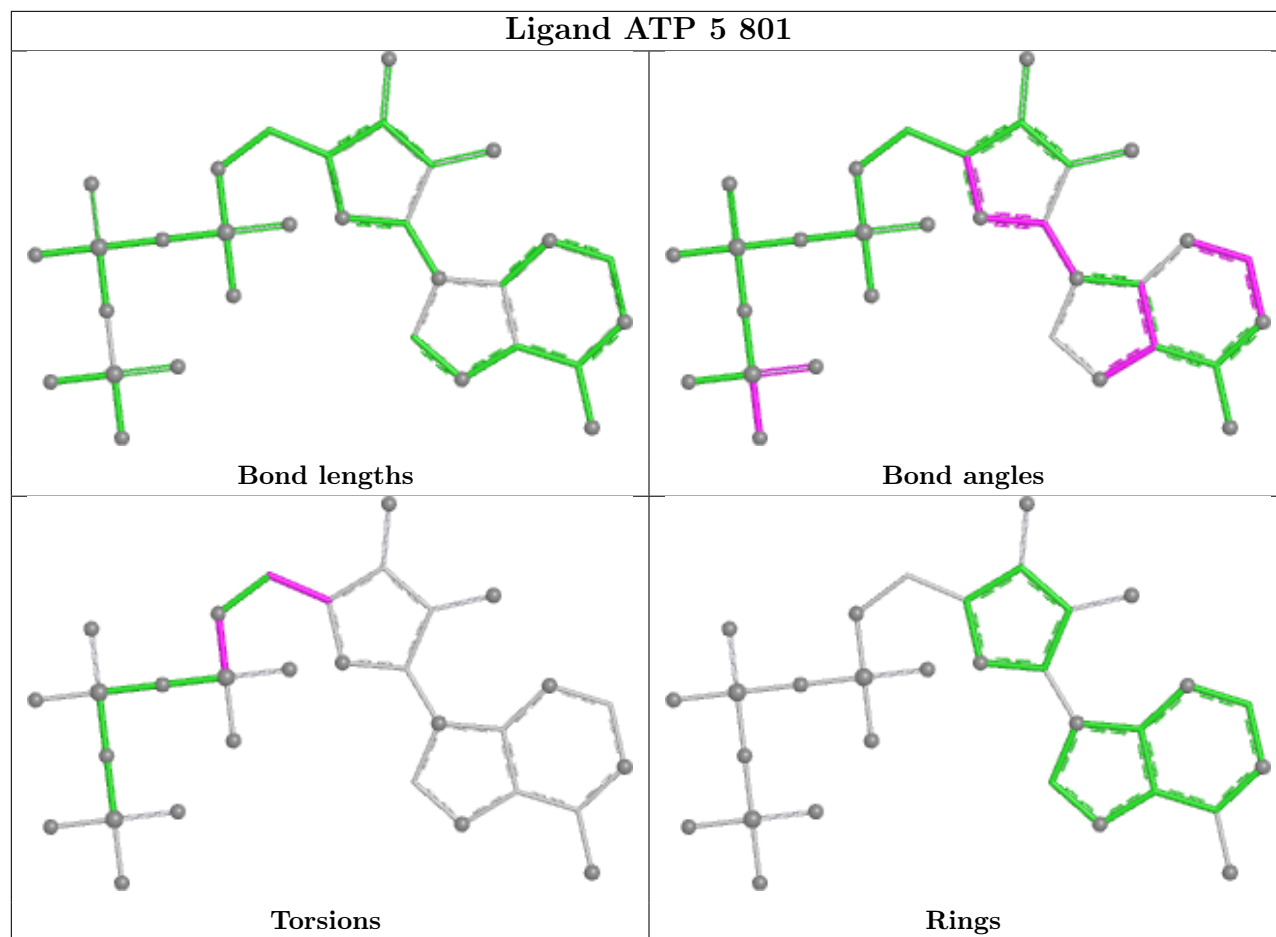
No monomer is involved in short contacts.

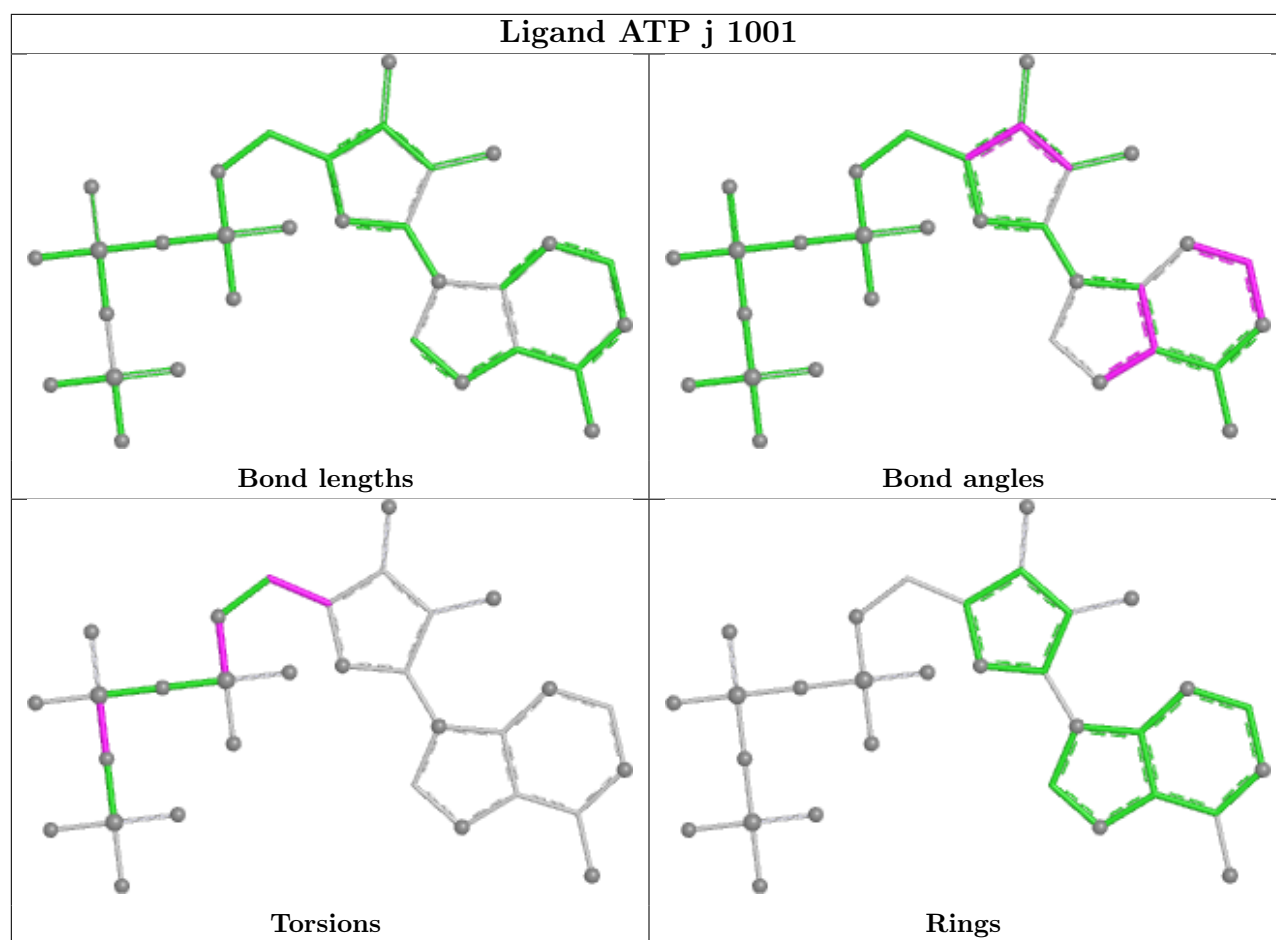
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

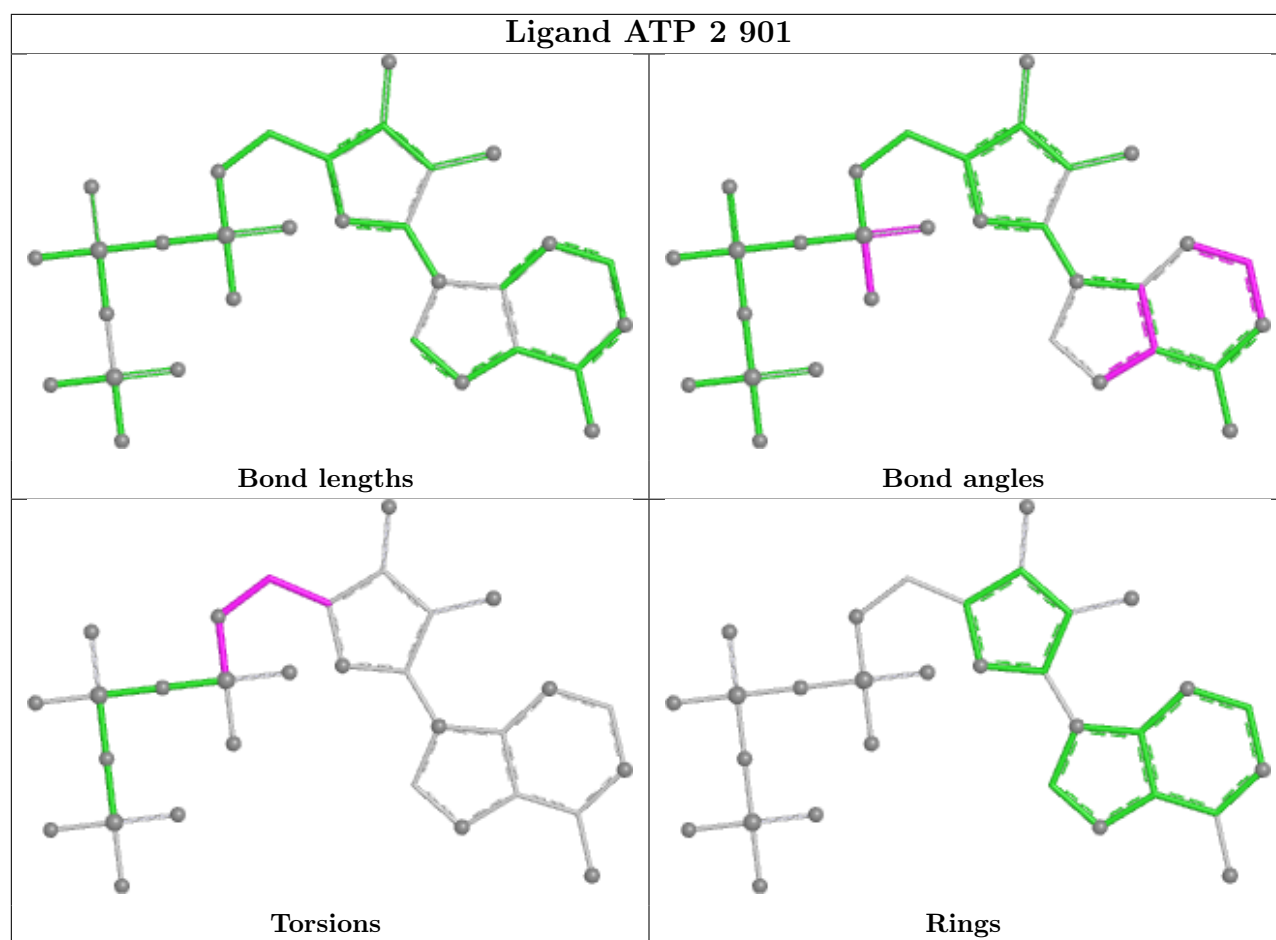












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	776:ILE	C	777:ARG	N	2.04

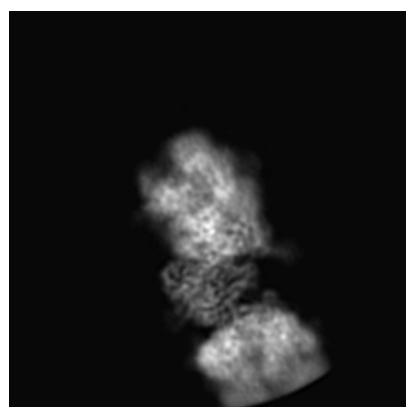
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20472. These allow visual inspection of the internal detail of the map and identification of artifacts.

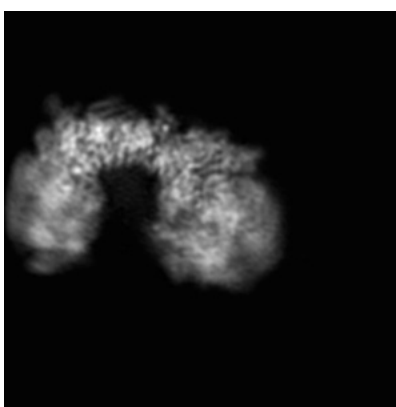
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

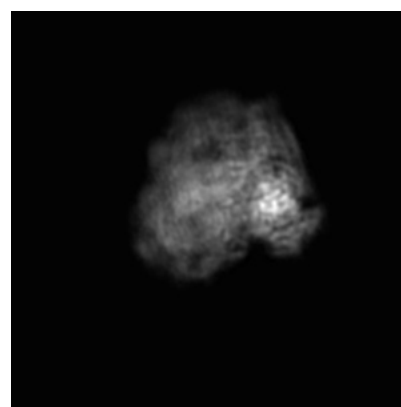
6.1.1 Primary map



X



Y

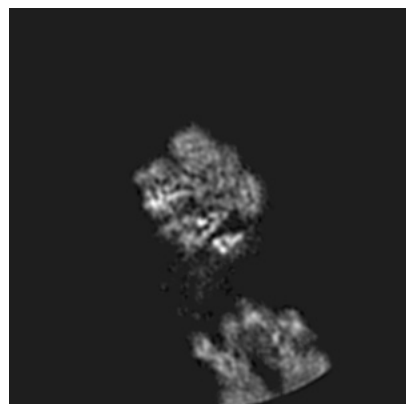


Z

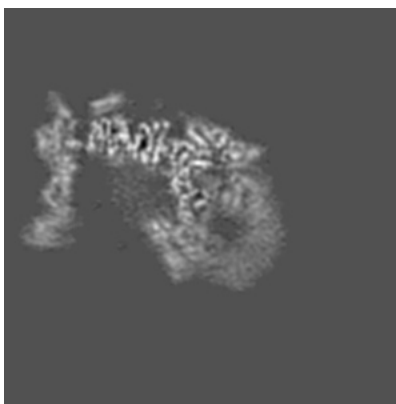
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

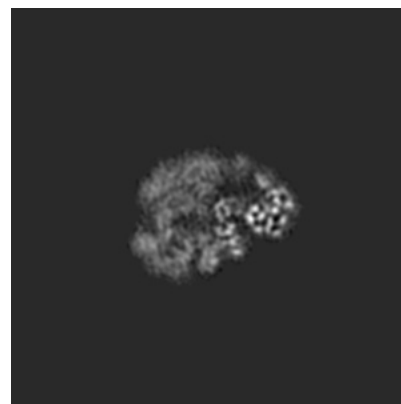
6.2.1 Primary map



X Index: 200



Y Index: 200

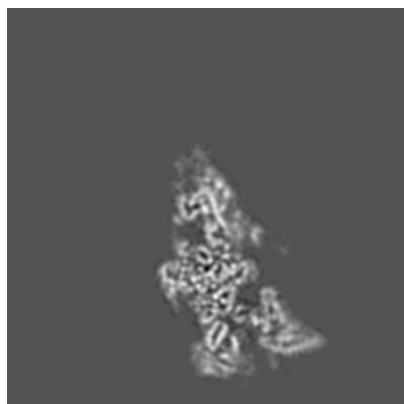


Z Index: 200

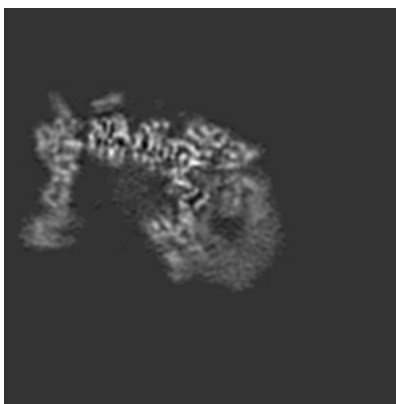
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

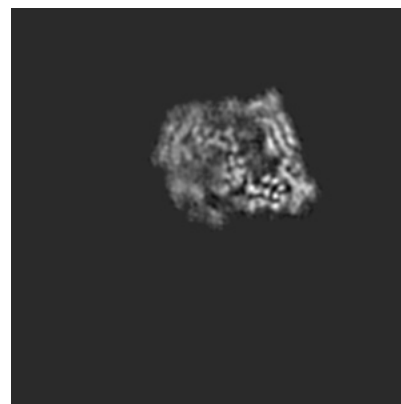
6.3.1 Primary map



X Index: 264



Y Index: 202

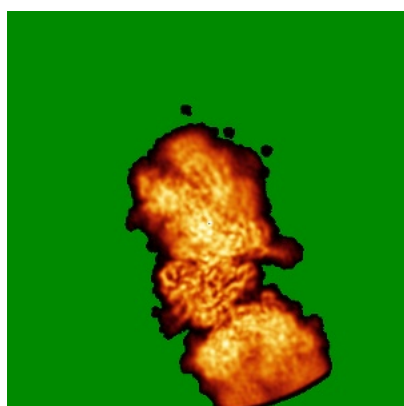


Z Index: 68

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

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

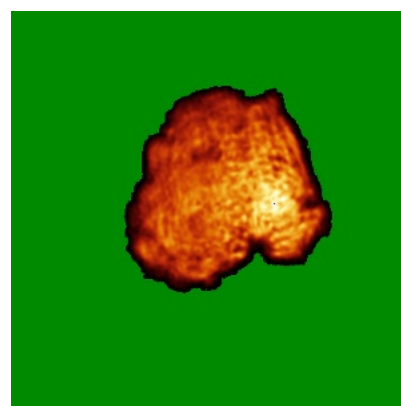
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0246. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

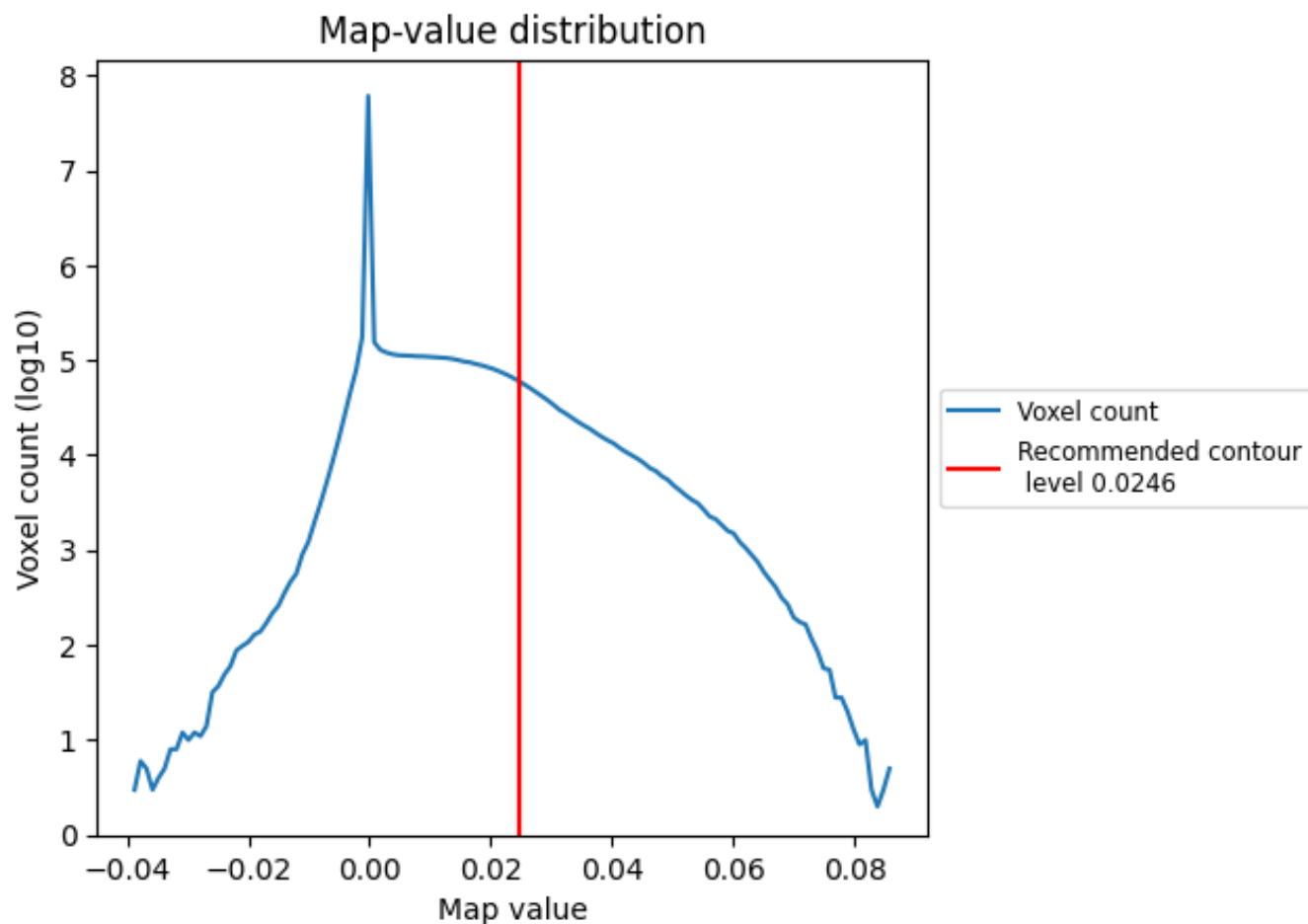
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

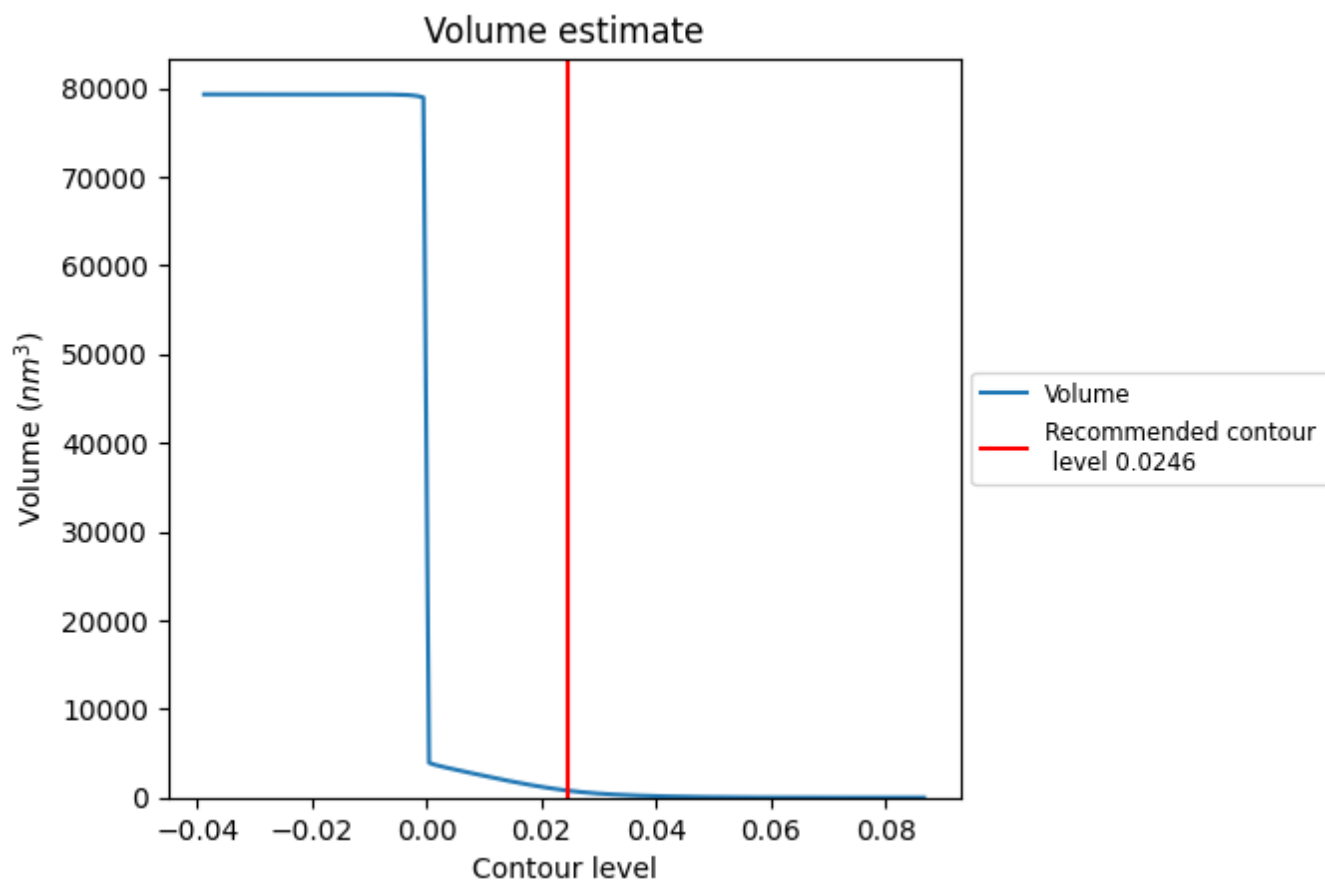
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

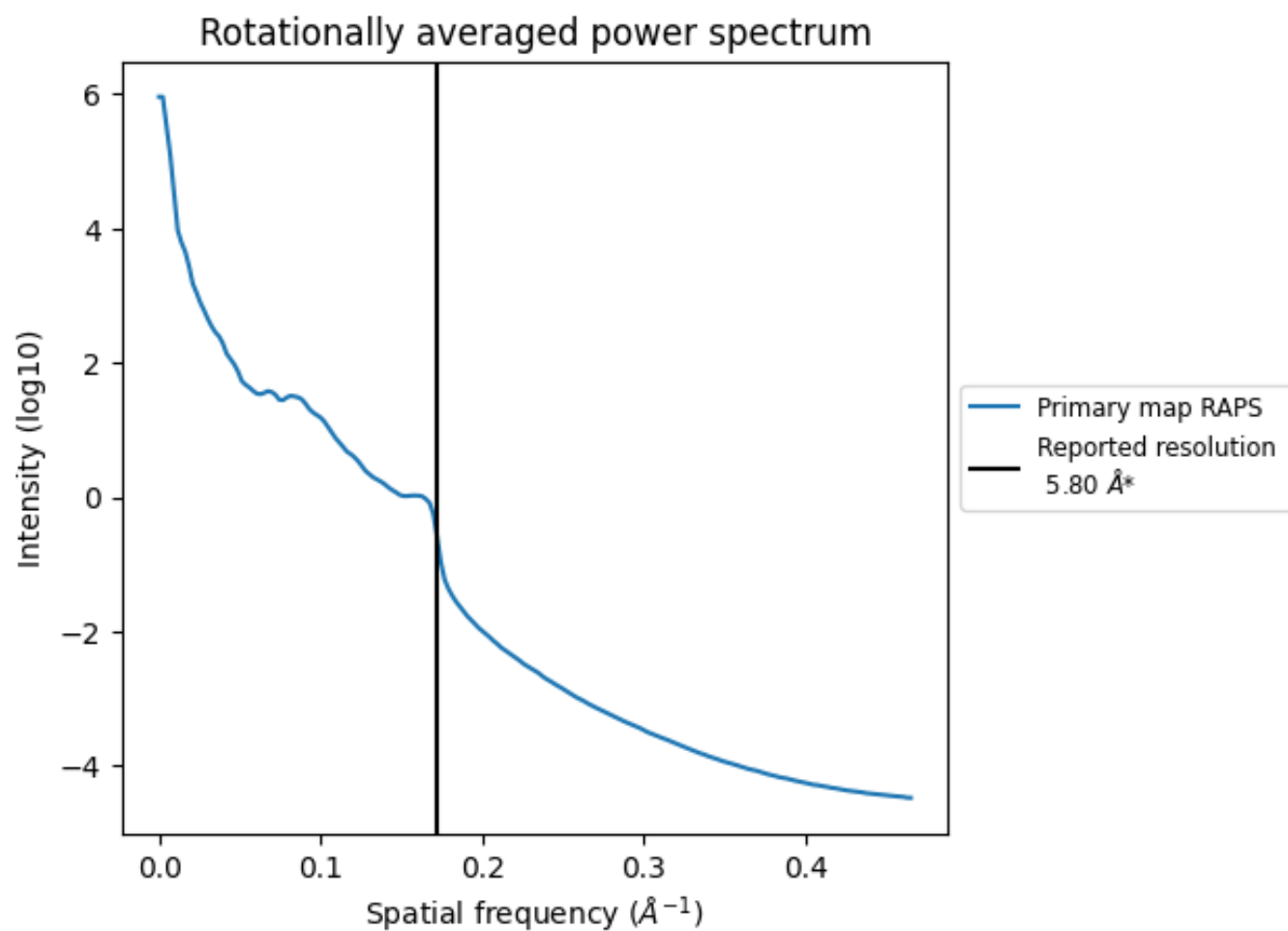
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790 nm³; this corresponds to an approximate mass of 713 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

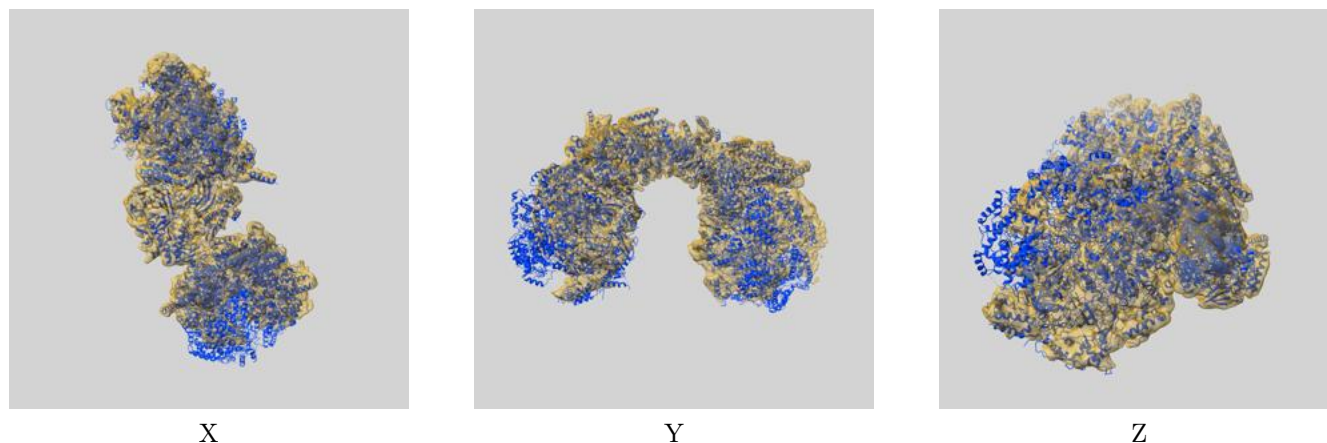
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

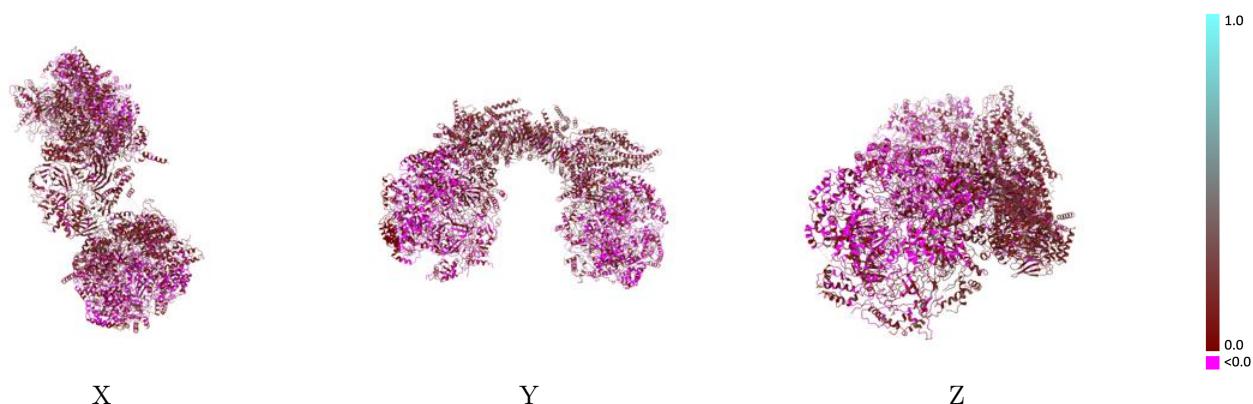
This section contains information regarding the fit between EMDB map EMD-20472 and PDB model 6PTN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



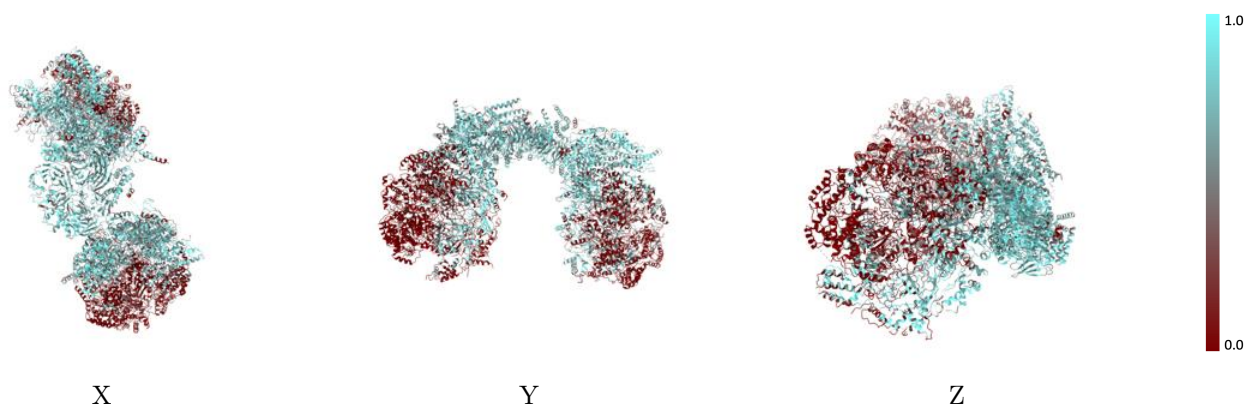
The images above show the 3D surface view of the map at the recommended contour level 0.0246 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



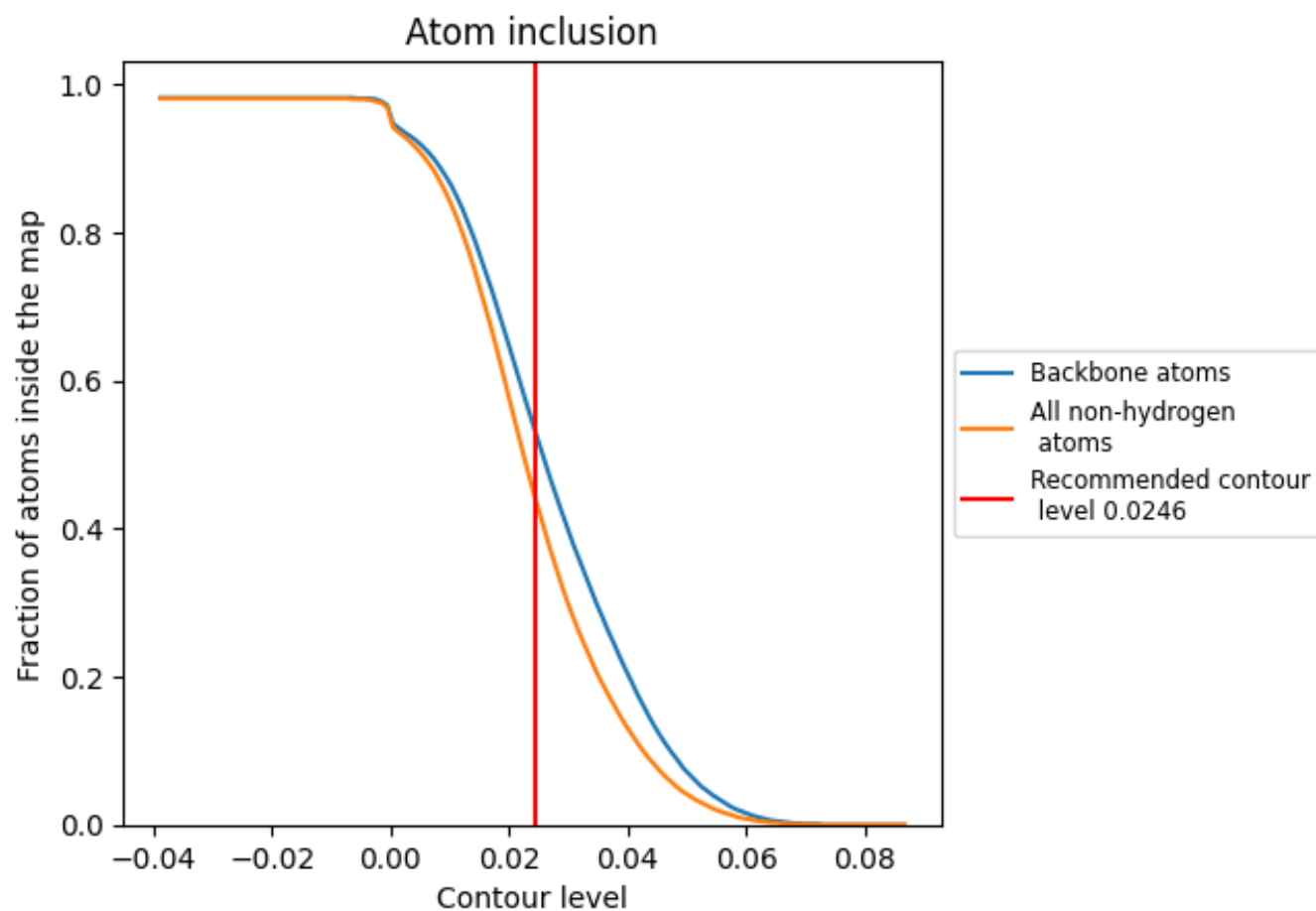
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.0246).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 44% 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 (0.0246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4360	 0.0870
2	 0.2410	 0.0390
3	 0.3320	 0.0510
4	 0.1460	 0.0300
5	 0.3520	 0.0660
6	 0.1940	 0.0320
7	 0.1580	 0.0300
A	 0.6820	 0.1640
B	 0.6730	 0.1620
C	 0.6840	 0.1410
D	 0.7090	 0.1630
E	 0.7120	 0.1720
F	 0.7070	 0.1510
G	 0.7170	 0.1680
H	 0.6800	 0.1390
a	 0.7450	 0.1660
b	 0.7480	 0.1750
c	 0.7360	 0.1620
d	 0.7480	 0.1740
h	 0.6770	 0.1390
i	 0.3080	 0.0380
j	 0.4640	 0.0880
k	 0.2590	 0.0460
l	 0.4060	 0.0750
m	 0.3480	 0.0570
n	 0.3290	 0.0540

