



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:14 am GMT

PDB ID : 6HV9  
EMDB ID : EMD-0288  
Title : S. cerevisiae CMG-Pol epsilon-DNA  
Authors : Abid Ali, F.; Purkiss, A.G.; Cheung, A.; Costa, A.  
Deposited on : 2018-10-10  
Resolution : 4.98 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.2

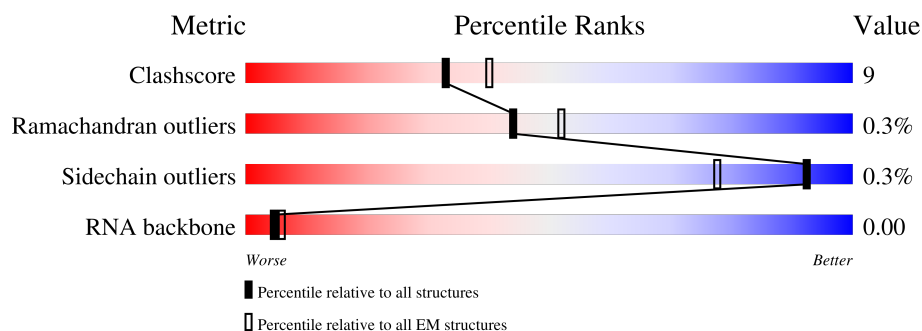
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.98 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
RNA backbone	4643	859

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  $\geq 3$ , 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	3	971	<div> <div>5%</div> <div>45%</div> <div>12%</div> <div>43%</div> </div>
2	4	933	<div> <div>16%</div> <div>51%</div> <div>12%</div> <div>37%</div> </div>
3	5	775	<div> <div>13%</div> <div>61%</div> <div>18%</div> <div>•</div> <div>19%</div> </div>
4	6	1017	<div> <div>10%</div> <div>44%</div> <div>12%</div> <div>44%</div> </div>
5	2	868	<div> <div>9%</div> <div>48%</div> <div>15%</div> <div>37%</div> </div>
6	7	845	<div> <div>25%</div> <div>58%</div> <div>15%</div> <div>27%</div> </div>
7	C	208	<div> <div>6%</div> <div>62%</div> <div>31%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
8	D	213	
9	E	194	
10	F	294	
11	G	650	
12	X	21	
13	Y	21	
14	J	7	
15	B	689	
16	A	914	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 47617 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 MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	558	Total	C	N	O	S	0	0
			4270	2689	753	818	10		

- Molecule 2 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	589	Total	C	N	O	S	0	0
			4543	2848	796	873	26		

- Molecule 3 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	628	Total	C	N	O	S	0	0
			4690	2942	820	907	21		

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	571	Total	C	N	O	S	0	0
			4307	2704	766	821	16		

- Molecule 5 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	549	Total	C	N	O	S	0	0
			4184	2639	745	785	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	616	Total	C	N	O	S	0	0
			4785	3024	820	916	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	194	Total	C	N	O	S	0	0
			1492	934	265	287	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	181	Total	C	N	O	S	0	0
			1461	935	257	265	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	159	Total	C	N	O	S	0	0
			1262	824	207	226	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	218	Total	C	N	O	S	0	0
			1743	1099	292	339	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	541	Total	C	N	O	S	0	0
			4239	2684	737	808	10		

- Molecule 12 is a RNA chain called DNA/RNA (5'-R(\*GP\*CP\*AP\*GP\*CP\*CP\*AP\*CP\*GP\*C)-D(P\*T)-R(P\*GP\*GP\*CP\*CP\*G)-D(P\*TP\*TP\*TP\*T)-R(P\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	21	Total	C	N	O	P	0	0
			425	203	76	126	20		

- Molecule 13 is a RNA chain called DNA/RNA (5'-D(P\*T)-R(P\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*CP\*G)-D(P\*T)-R(P\*GP\*GP\*C)-D(P\*T)-R(P\*GP\*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	21	Total	C	N	O	P	0	0
			433	204	84	124	21		

- Molecule 14 is a DNA chain called DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	7	Total	C	N	O	P	0	0
			140	70	14	49	7		

- Molecule 15 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	465	Total	C	N	O	S	0	0
			3661	2346	620	681	14		

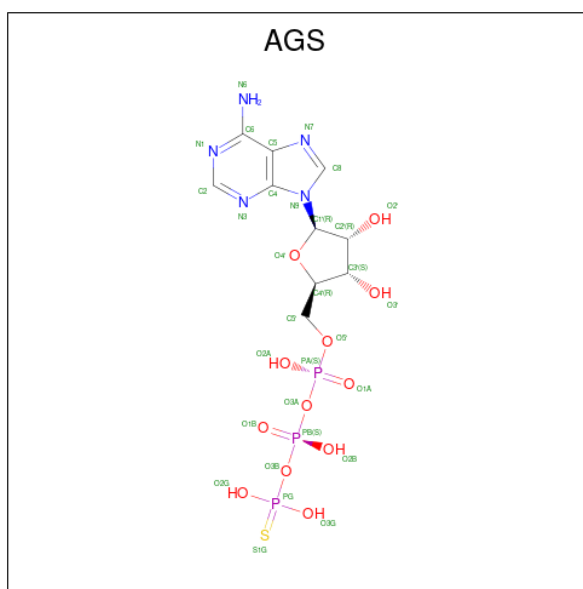
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ASN	MET	conflict	UNP P24482

- Molecule 16 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	771	Total	C	N	O	S	0	0
			5918	3797	988	1101	32		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						AltConf
17	5	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
17	5	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	





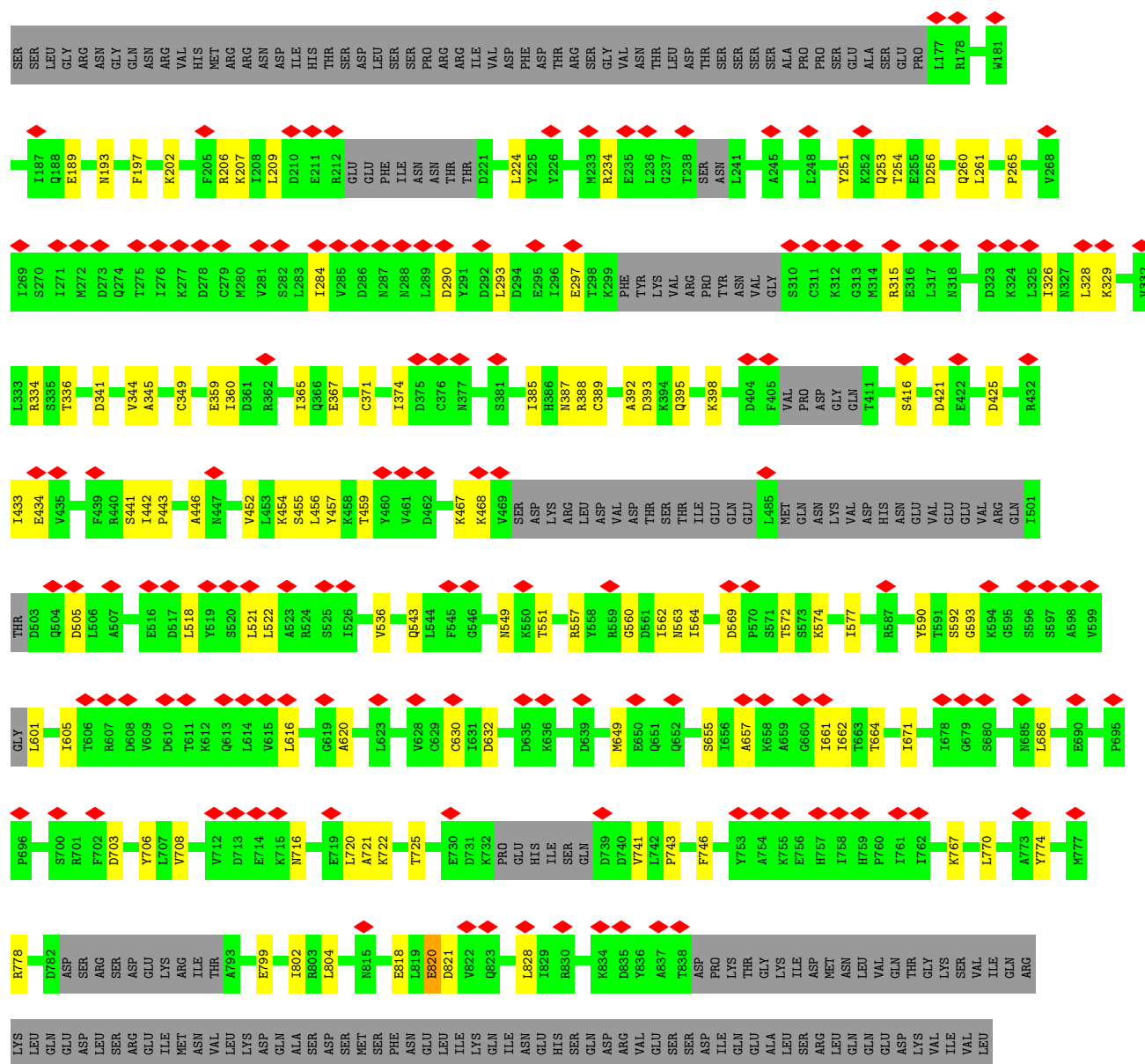
SER	GLN	VAL	GLU	TYR	LEU	ALA	PHE	ASP	ASN	VAL	GLU	PRO	LYS	THR	GLY	ASP	ASN	THR	SER	GLY	ARG	VAL	LEU	SER	LEU	ILE	ASP	ASN	GLY	VAL	TRP	ARG	ALA	ARG	LEU	GLN	MET	THR	GLU	ILE	PHE	GLU	GLU	SER	TYR	SER	PRO	VAL	ALA	SER	GLN	LEU	GLY	ASP	LEU	PHE	GLU	ARG	ILE	ASN	GLU	GLU	PRO	ASN	GLN	LEU	ALA	LEU	GLY	LYS	PHE	SER	ALA
GLN	GLU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

● Molecule 2: DNA replication licensing factor MCM4



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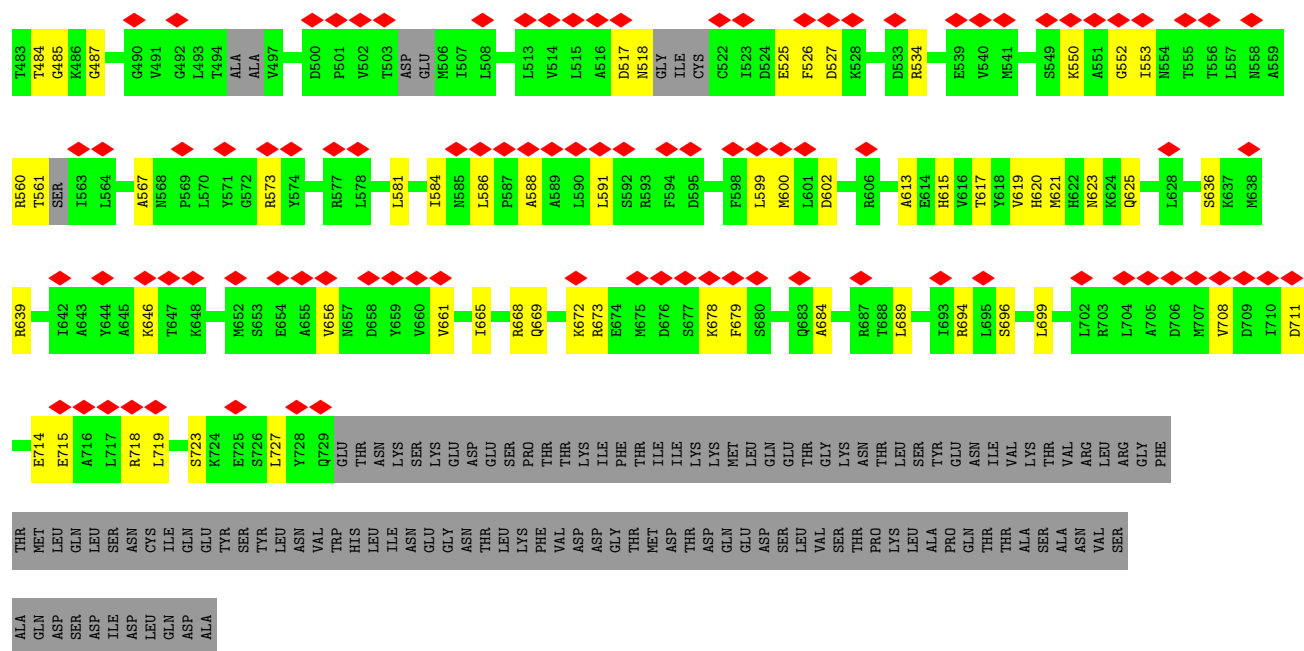
ASN	ILE	ARG	ALA	SER	ILE	GLY	SER	PRO	LYS	THR	GLY	ASP	ASN	THR	SER	GLY	ARG	VAL	LEU	SER	LEU	ILE	ASP	ASN	GLY	VAL	TRP	ARG	ALA	ARG	LEU	GLN	MET	THR	GLU	ILE	PHE	GLU	GLU	SER	TYR	SER	PRO	VAL	ALA	SER	GLN	LEU	GLY	ASP	LEU	PHE	GLU	ARG	ILE	ASN	GLU	GLU	PRO	ASN	GLN	LEU	ALA	LEU	GLY	LYS	PHE	SER	ALA
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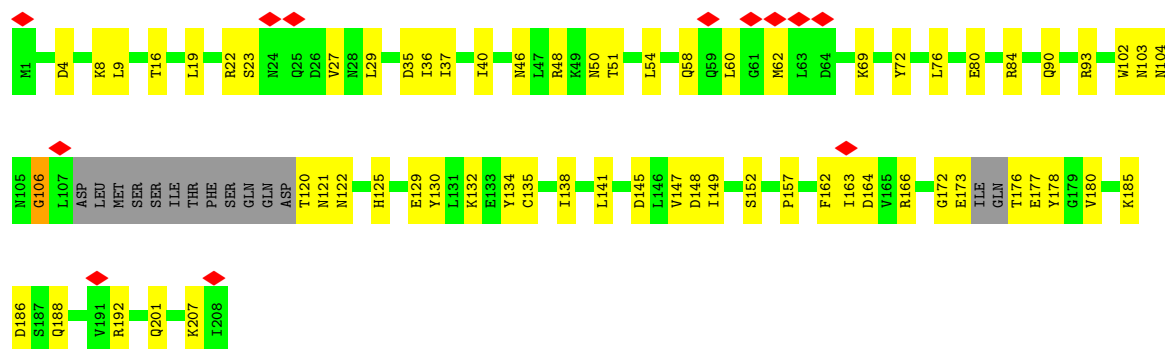




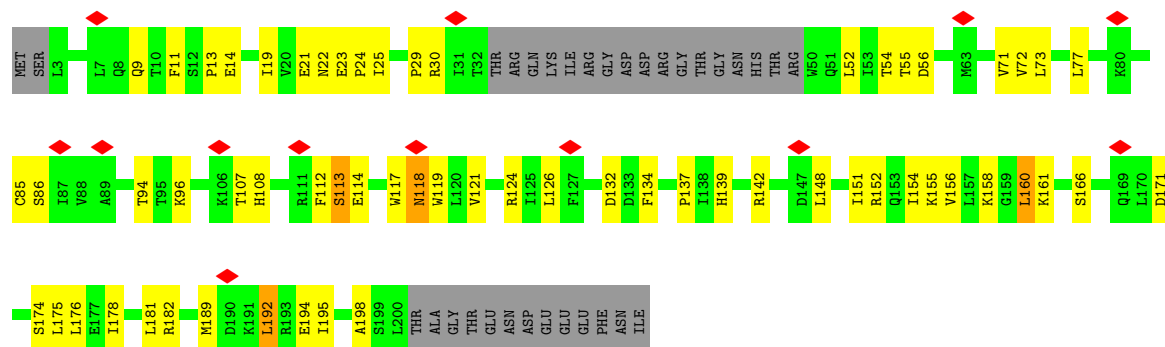




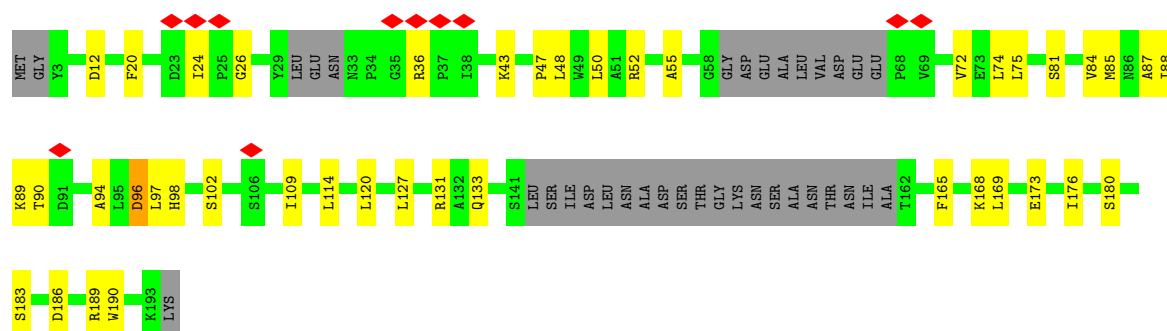
• Molecule 7: DNA replication complex GINS protein PSF1



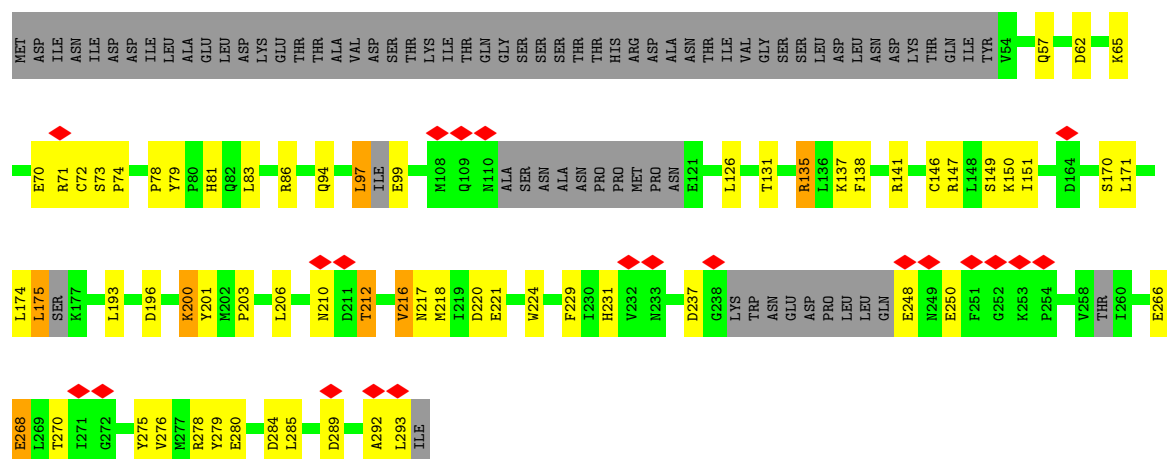
• Molecule 8: DNA replication complex GINS protein PSF2



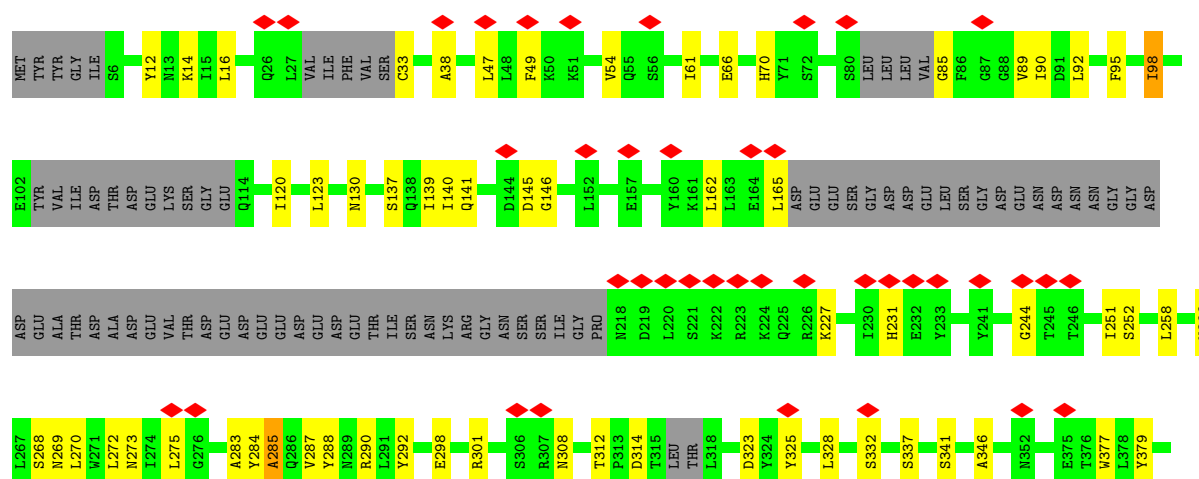
• Molecule 9: DNA replication complex GINS protein PSF3

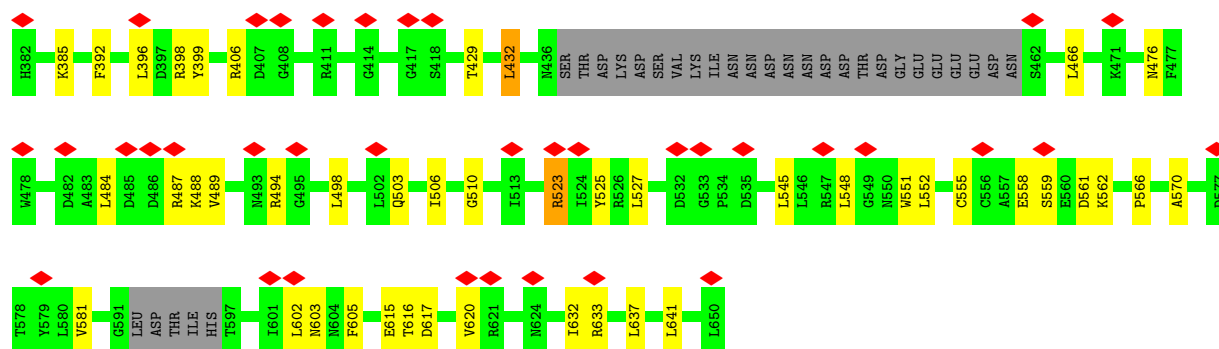


- Molecule 10: DNA replication complex GINS protein SLD5

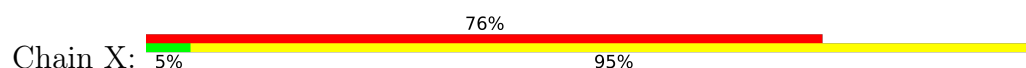


- Molecule 11: Cell division control protein 45

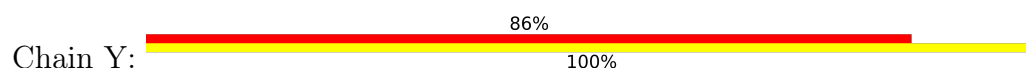




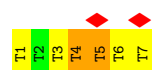
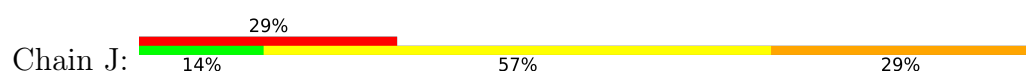
- Molecule 12: DNA/RNA (5'-R(\*GP\*CP\*AP\*GP\*CP\*CP\*AP\*CP\*GP\*C)-D(P\*T)-R(P\*GP\*GP\*CP\*CP\*G)-D(P\*TP\*TP\*TP\*T)-R(P\*A)-3')



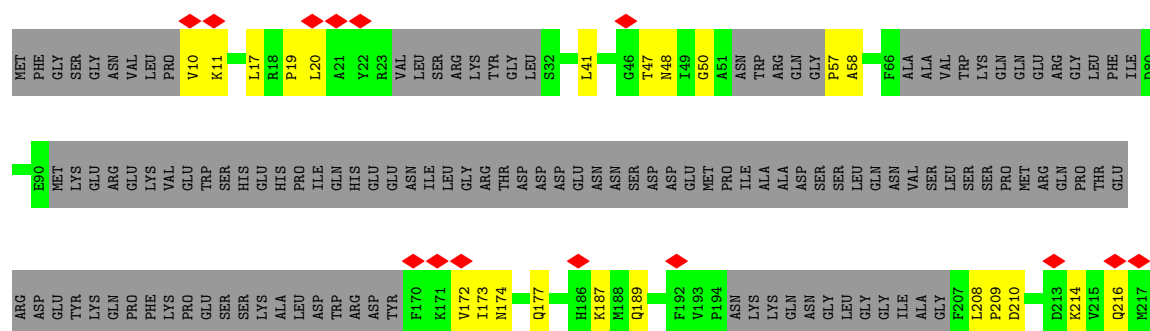
- Molecule 13: DNA/RNA (5'-D(P\*T)-R(P\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*CP\*G)-D(P\*T)-R(P\*GP\*GP\*C)-D(P\*T)-R(P\*GP\*C)-3')

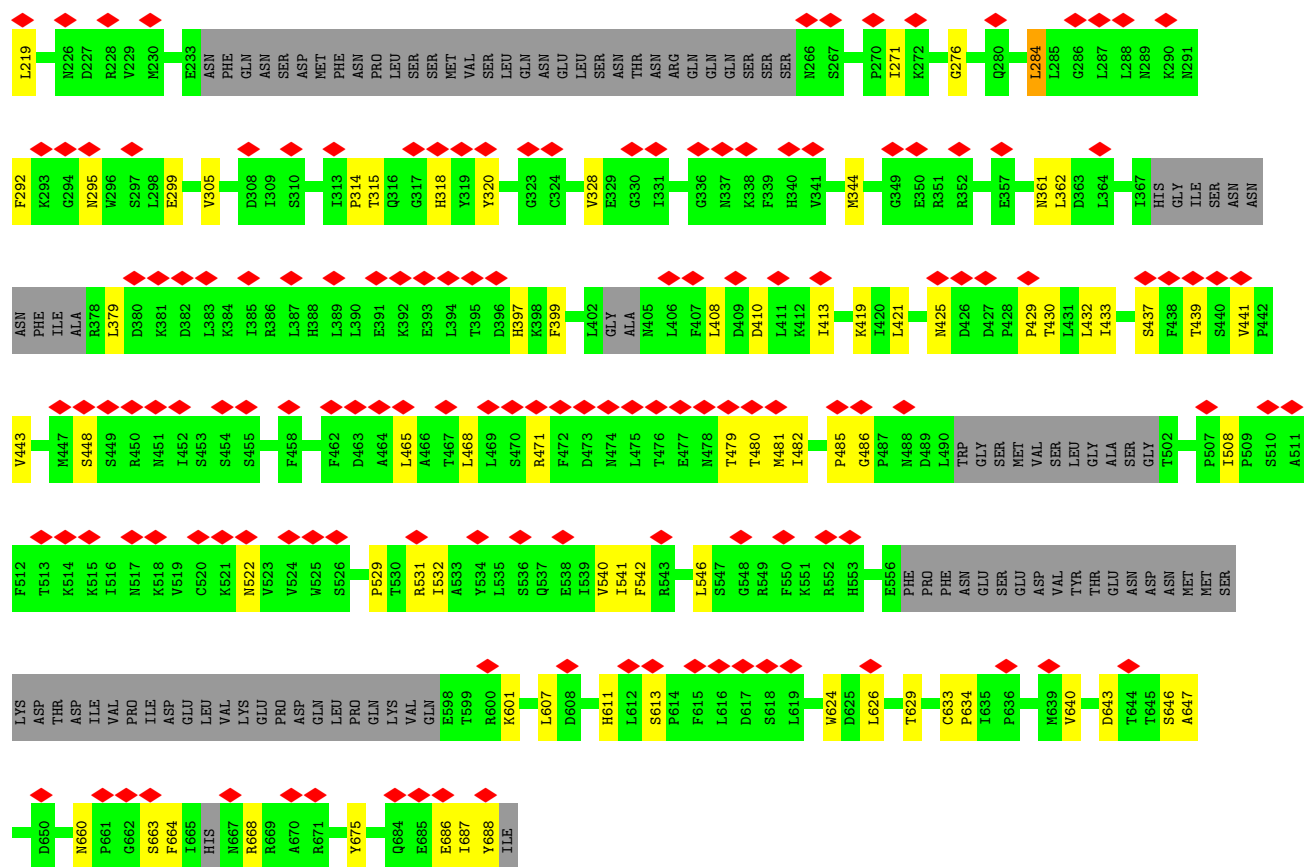


- Molecule 14: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3')

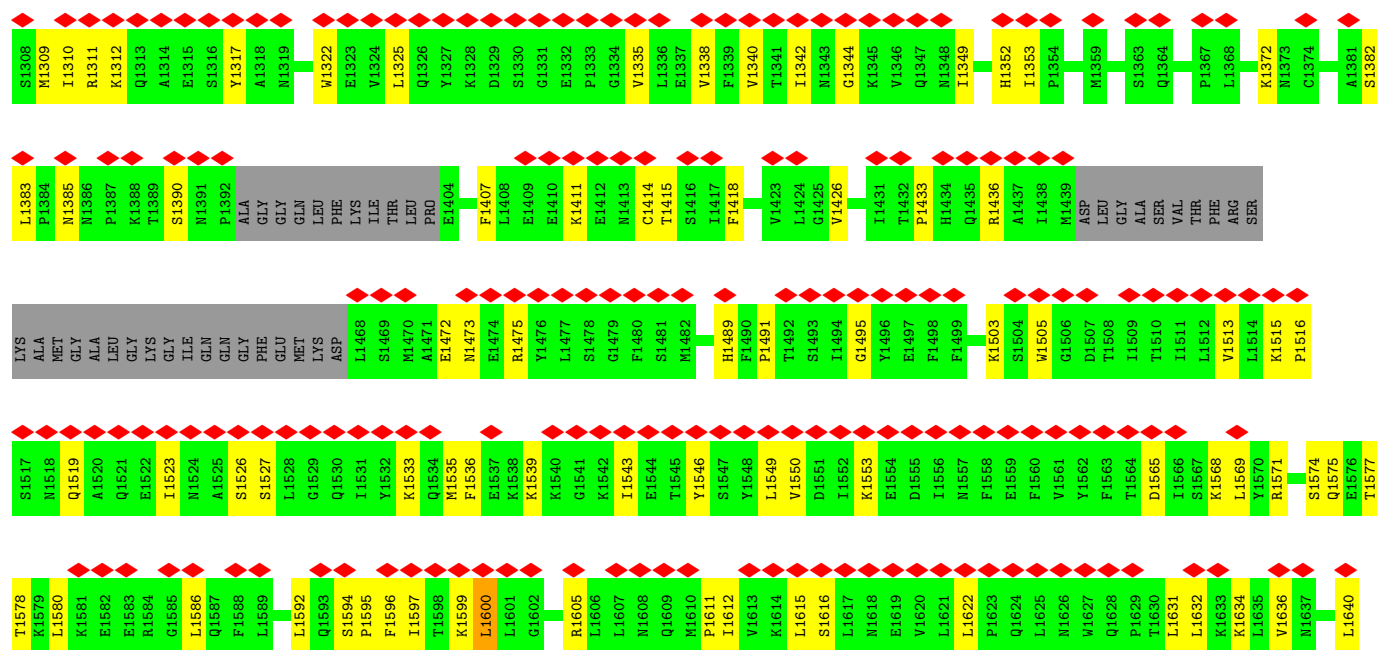
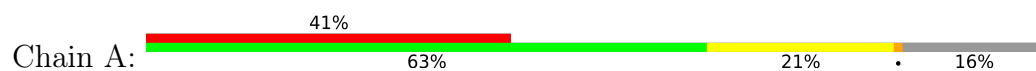


- Molecule 15: DNA polymerase epsilon subunit B

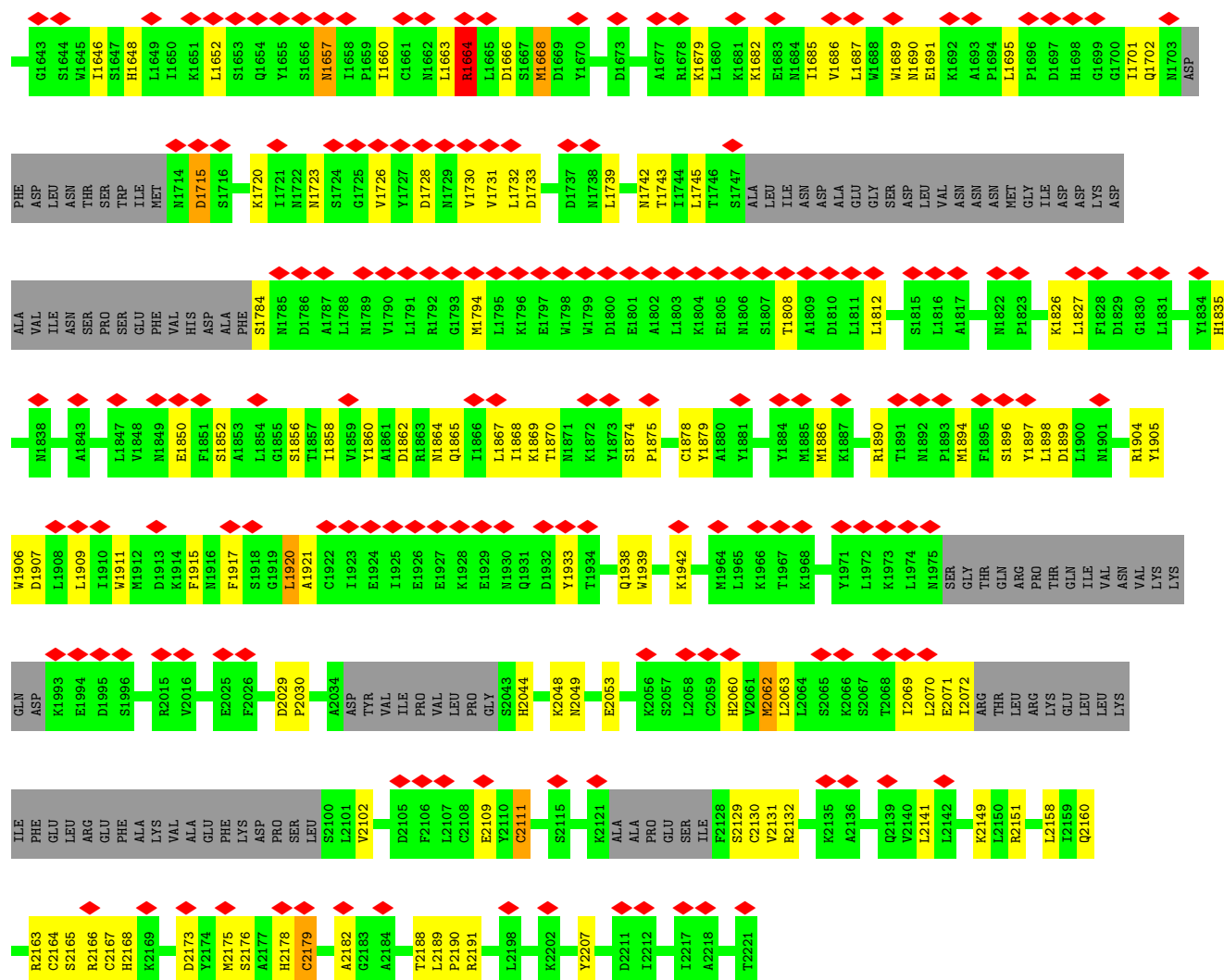




• Molecule 16: DNA polymerase epsilon catalytic subunit A







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78556	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 ( $e^-/\text{\AA}^2$ )	4.2	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	5.270	Depositor
Minimum map value	-2.822	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.184	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	3	0.59	1/4330 (0.0%)	0.95	9/5872 (0.2%)
2	4	0.42	0/4594	0.79	5/6203 (0.1%)
3	5	0.75	3/4741 (0.1%)	1.13	24/6405 (0.4%)
4	6	0.50	0/4359	0.83	3/5882 (0.1%)
5	2	0.65	2/4241 (0.0%)	0.99	10/5720 (0.2%)
6	7	0.44	0/4853	0.76	2/6553 (0.0%)
7	C	0.57	0/1511	1.07	9/2039 (0.4%)
8	D	0.64	0/1489	1.10	5/2016 (0.2%)
9	E	0.64	0/1294	1.00	4/1750 (0.2%)
10	F	0.54	0/1771	1.01	8/2386 (0.3%)
11	G	0.52	0/4311	0.98	17/5832 (0.3%)
12	X	0.85	0/475	1.00	0/731
13	Y	0.83	0/486	0.93	0/748
14	J	1.53	3/153 (2.0%)	1.78	3/234 (1.3%)
15	B	0.47	0/3727	0.84	3/5041 (0.1%)
16	A	0.47	1/6029 (0.0%)	0.92	16/8179 (0.2%)
All	All	0.56	10/48364 (0.0%)	0.94	118/65591 (0.2%)

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
10	F	0	4
11	G	0	3
All	All	0	7

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	269	GLU	C-N	-10.85	1.09	1.34
3	5	606	CYS	CB-SG	-7.06	1.70	1.82
5	2	622	GLU	CB-CG	-6.66	1.39	1.52
5	2	397	VAL	CB-CG2	-6.61	1.39	1.52
14	J	3	DT	P-O5'	6.34	1.66	1.59

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	98	ILE	C-N-CA	10.63	148.27	121.70
14	J	3	DT	O4'-C1'-N1	-9.61	101.27	108.00
14	J	5	DT	O4'-C1'-N1	9.34	114.54	108.00
3	5	137	LEU	CA-CB-CG	9.03	136.07	115.30
2	4	821	ASP	CB-CG-OD1	8.88	126.30	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	F	212	THR	Peptide,Mainchain
10	F	216	VAL	Peptide,Mainchain
11	G	523	ARG	Sidechain
11	G	98	ILE	Peptide,Mainchain

## 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	3	4270	0	4258	82	0
2	4	4543	0	4517	75	0
3	5	4690	0	4526	101	0
4	6	4307	0	4166	86	0
5	2	4184	0	4126	82	0
6	7	4785	0	4761	80	0
7	C	1492	0	1394	37	0
8	D	1461	0	1445	45	0
9	E	1262	0	1240	31	0
10	F	1743	0	1671	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	4239	0	4082	51	0
12	X	425	0	238	18	0
13	Y	433	0	235	19	0
14	J	140	0	85	7	0
15	B	3661	0	3656	56	0
16	A	5918	0	5682	121	0
17	5	62	0	24	8	0
18	A	2	0	0	0	0
All	All	47617	0	46106	856	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 9.

The worst 5 of 856 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:460:GLY:HA3	6:7:600:MET:HB2	1.62	0.81
5:2:617:ARG:O	5:2:621:HIS:HB2	1.84	0.77
7:C:102:TRP:HE1	7:C:134:TYR:HH	1.33	0.76
9:E:48:LEU:O	9:E:52:ARG:HB2	1.85	0.76
11:G:244:GLY:HA3	11:G:603:ASN:HB2	1.67	0.76

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	3	542/971 (56%)	500 (92%)	40 (7%)	2 (0%)	34	72
2	4	569/933 (61%)	508 (89%)	60 (10%)	1 (0%)	47	81
3	5	598/775 (77%)	547 (92%)	51 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	6	551/1017 (54%)	496 (90%)	55 (10%)	0	100	100
5	2	527/868 (61%)	483 (92%)	44 (8%)	0	100	100
6	7	588/845 (70%)	539 (92%)	48 (8%)	1 (0%)	47	81
7	C	188/208 (90%)	177 (94%)	10 (5%)	1 (0%)	29	68
8	D	177/213 (83%)	164 (93%)	10 (6%)	3 (2%)	9	43
9	E	151/194 (78%)	143 (95%)	8 (5%)	0	100	100
10	F	206/294 (70%)	184 (89%)	21 (10%)	1 (0%)	29	68
11	G	525/650 (81%)	478 (91%)	44 (8%)	3 (1%)	25	65
15	B	441/689 (64%)	390 (88%)	50 (11%)	1 (0%)	47	81
16	A	751/914 (82%)	553 (74%)	193 (26%)	5 (1%)	22	62
All	All	5814/8571 (68%)	5162 (89%)	634 (11%)	18 (0%)	44	76

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	374	ILE
8	D	54	THR
8	D	113	SER
8	D	171	ASP
11	G	284	TYR

### 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	3	458/835 (55%)	457 (100%)	1 (0%)	93	96
2	4	493/848 (58%)	492 (100%)	1 (0%)	93	96
3	5	488/688 (71%)	488 (100%)	0	100	100
4	6	435/886 (49%)	434 (100%)	1 (0%)	93	96
5	2	435/770 (56%)	435 (100%)	0	100	100
6	7	524/753 (70%)	524 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	C	149/193 (77%)	148 (99%)	1 (1%)	84	90
8	D	156/198 (79%)	155 (99%)	1 (1%)	86	92
9	E	135/173 (78%)	135 (100%)	0	100	100
10	F	194/279 (70%)	194 (100%)	0	100	100
11	G	443/586 (76%)	442 (100%)	1 (0%)	93	96
15	B	409/629 (65%)	407 (100%)	2 (0%)	88	93
16	A	624/837 (75%)	615 (99%)	9 (1%)	67	81
All	All	4943/7675 (64%)	4926 (100%)	17 (0%)	92	95

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	A	1668	MET
16	A	2062	MET
15	B	48	ASN
16	A	1309	MET
16	A	1312	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
7	C	202	GLN
11	G	273	ASN
8	D	22	ASN
9	E	133	GLN
15	B	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	X	0/21	-	-
13	Y	0/21	-	-
All	All	0/42	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
17	AGS	5	801	3	26,33,33	0.75	1 (3%)	26,52,52	1.19	3 (11%)
17	AGS	5	802	3	26,33,33	0.91	0	26,52,52	1.92	5 (19%)

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
17	AGS	5	801	3	-	8/17/38/38	0/3/3/3
17	AGS	5	802	3	-	3/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	801	AGS	PG-S1G	2.24	1.95	1.90

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



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	802	AGS	O4'-C1'-C2'	-5.71	98.58	106.93
17	5	802	AGS	PA-O3A-PB	-4.91	115.99	132.83
17	5	802	AGS	C1'-N9-C4	3.47	132.73	126.64
17	5	801	AGS	PA-O3A-PB	-2.96	122.67	132.83
17	5	802	AGS	C3'-C2'-C1'	-2.39	97.38	100.98

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

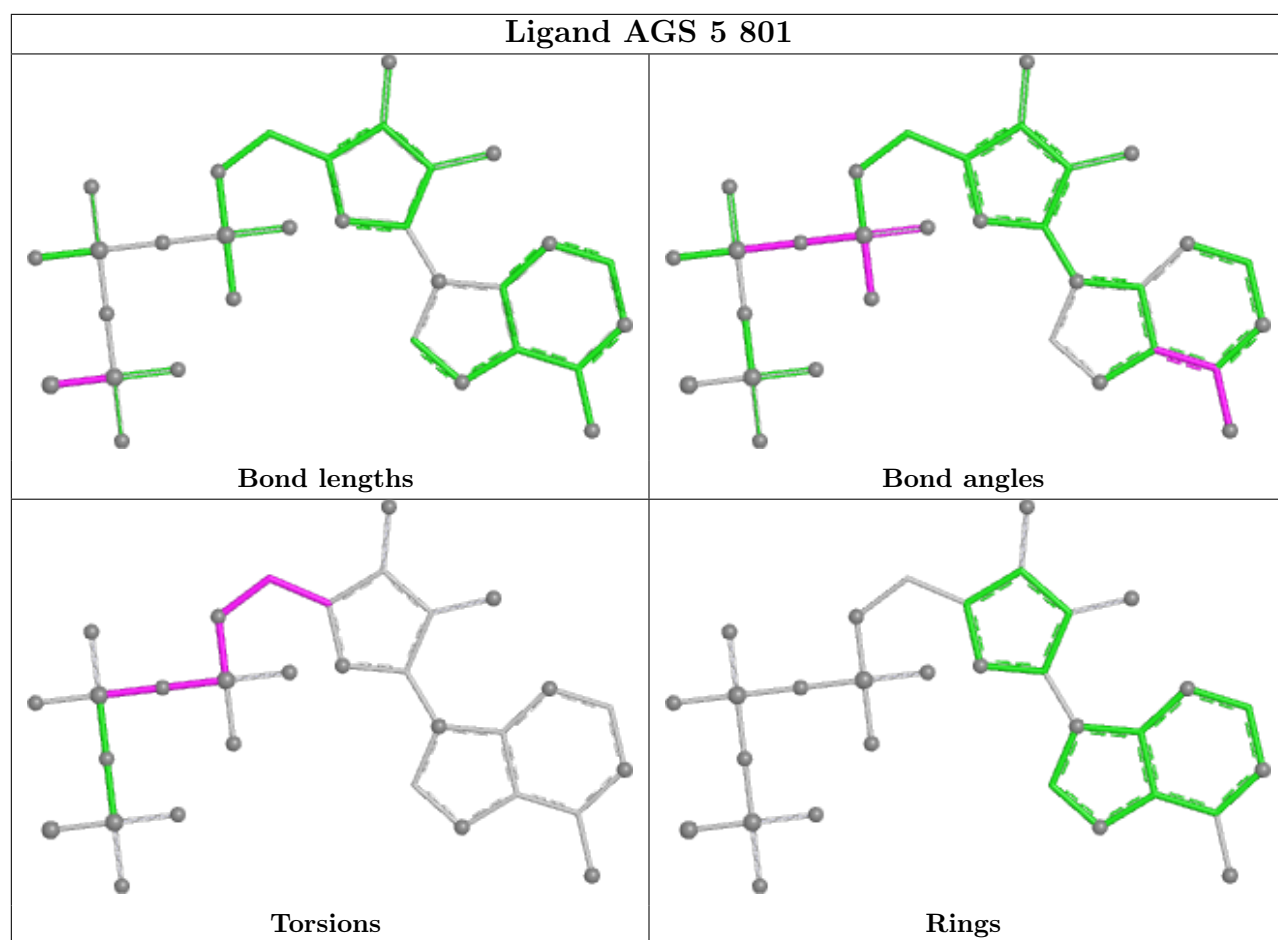
Mol	Chain	Res	Type	Atoms
17	5	801	AGS	C5'-O5'-PA-O1A
17	5	801	AGS	C5'-O5'-PA-O2A
17	5	802	AGS	C5'-O5'-PA-O1A
17	5	802	AGS	C5'-O5'-PA-O2A
17	5	801	AGS	C4'-C5'-O5'-PA

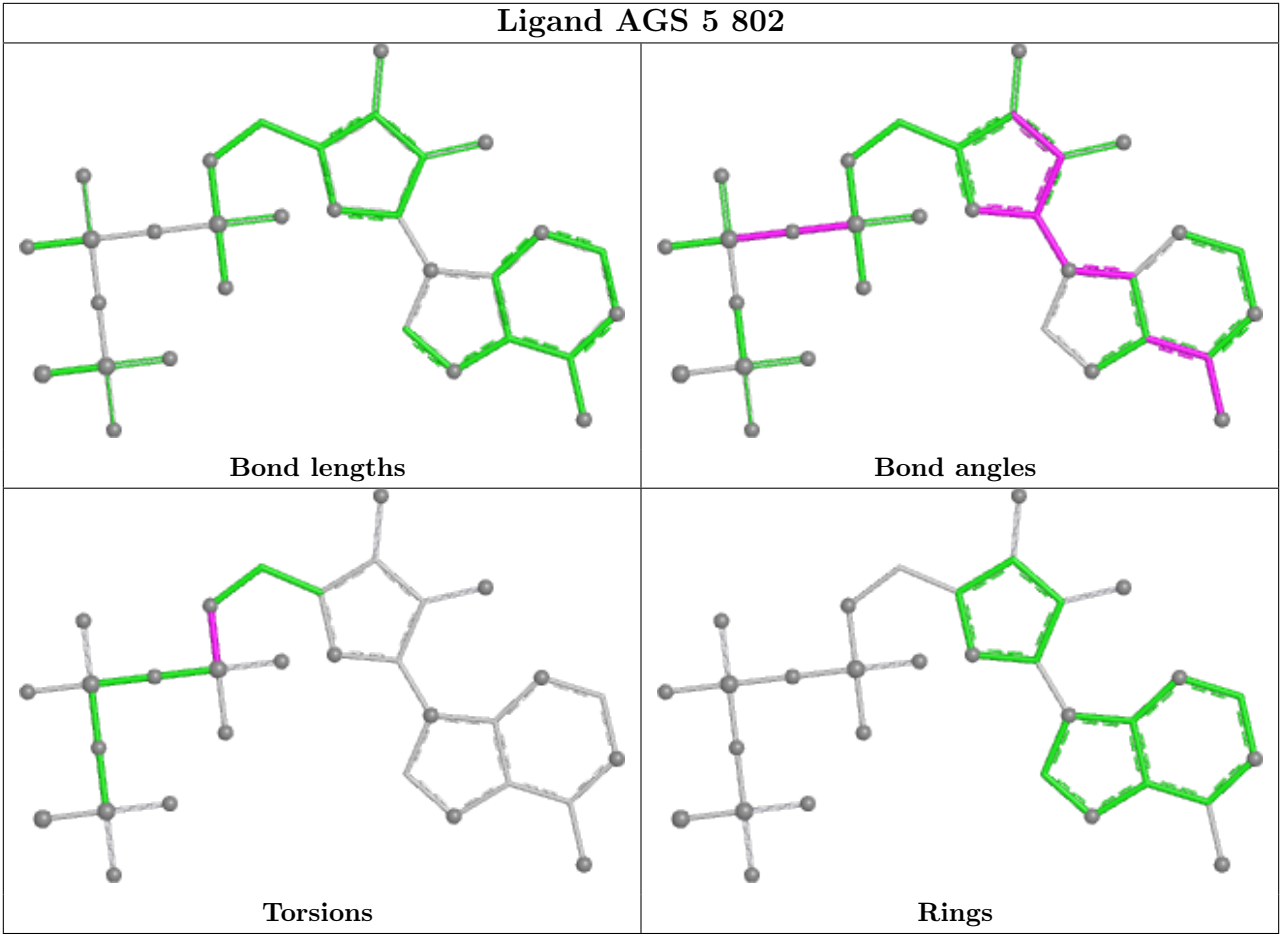
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	5	801	AGS	5	0
17	5	802	AGS	3	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	A	1
15	B	1
3	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2060:HIS	C	2061:VAL	N	14.58
1	B	280:GLN	C	281:ASN	N	5.05
1	5	269:GLU	C	270:MET	N	1.09

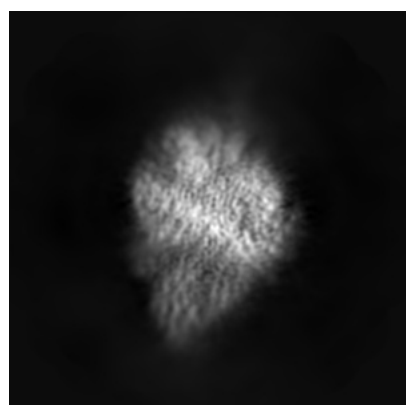
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0288. These allow visual inspection of the internal detail of the map and identification of artifacts.

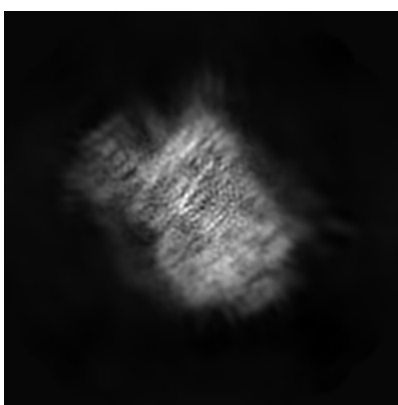
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

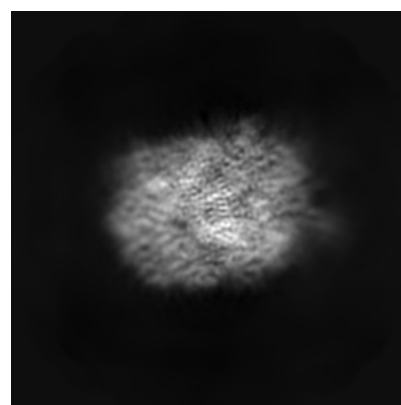
#### 6.1.1 Primary map



X



Y

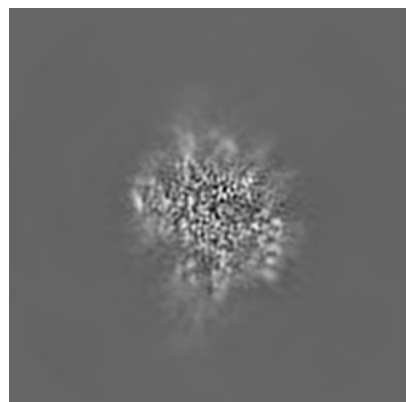


Z

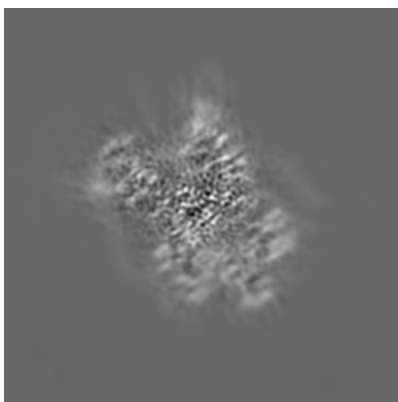
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

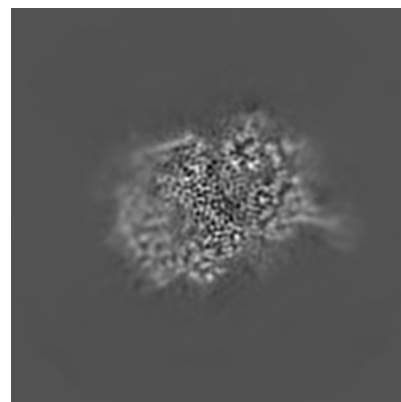
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

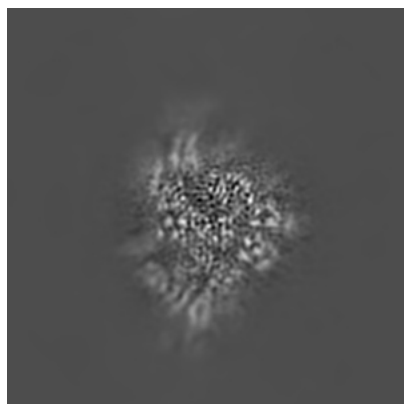


Z Index: 128

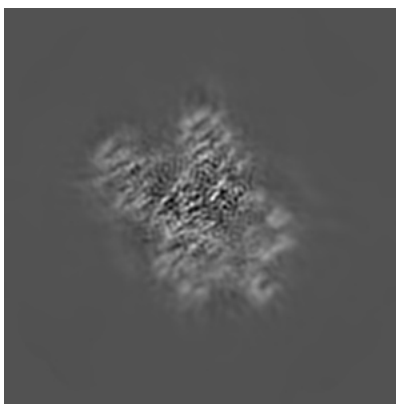
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

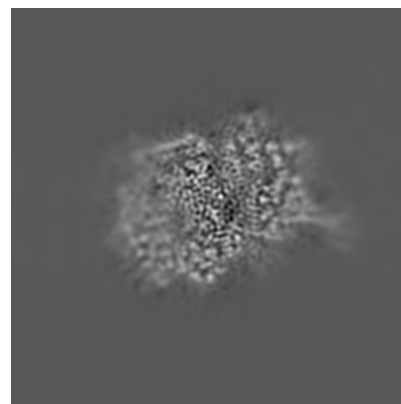
### 6.3.1 Primary map



X Index: 139



Y Index: 132

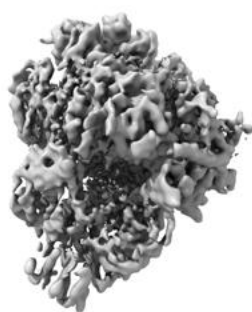


Z Index: 129

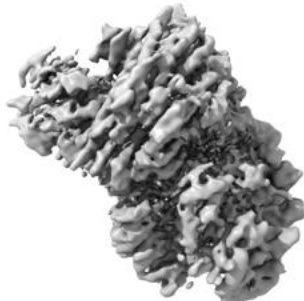
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

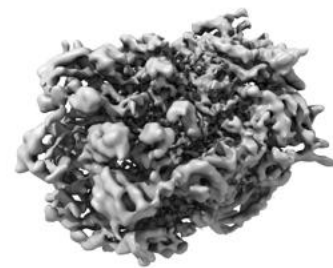
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

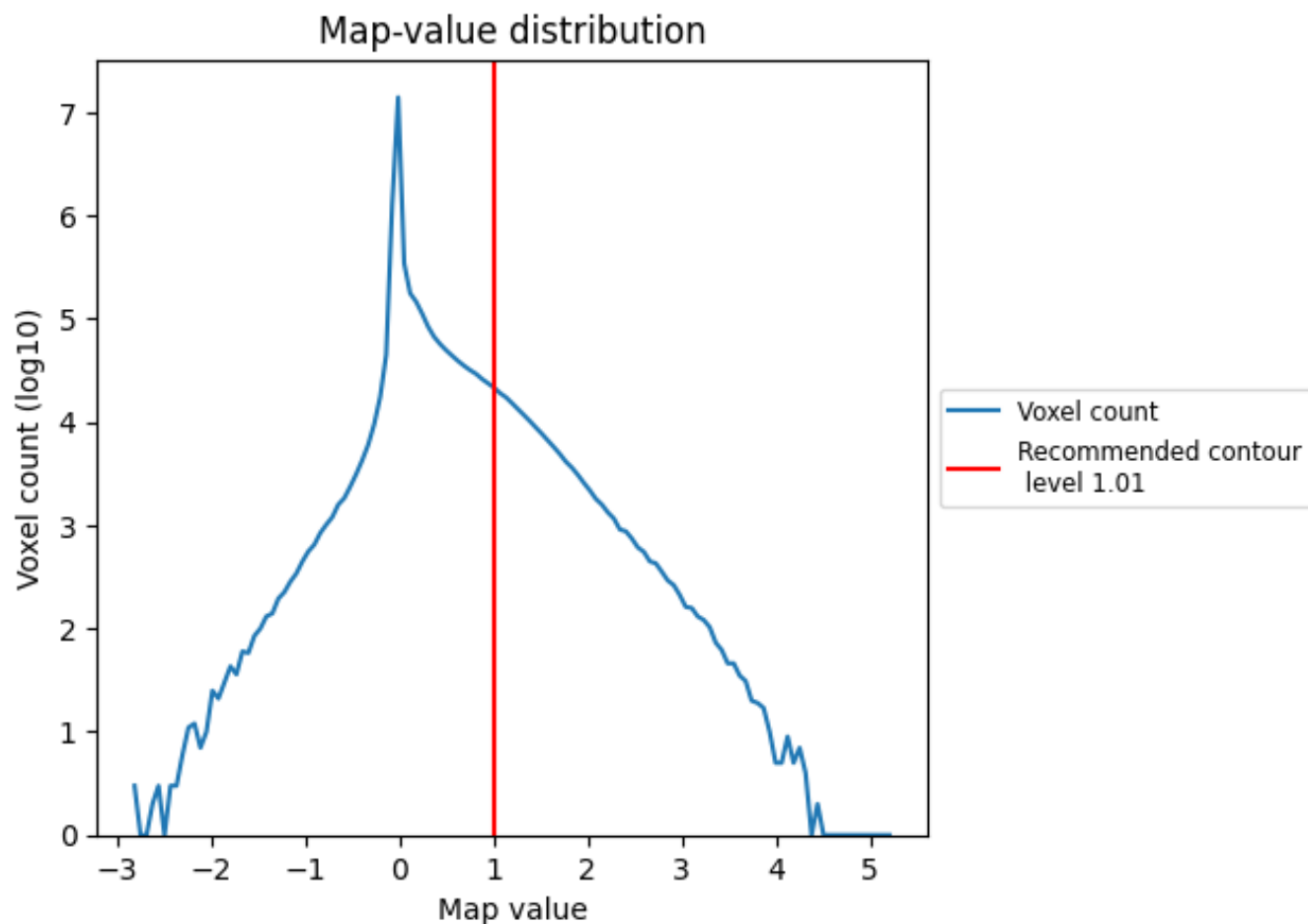
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

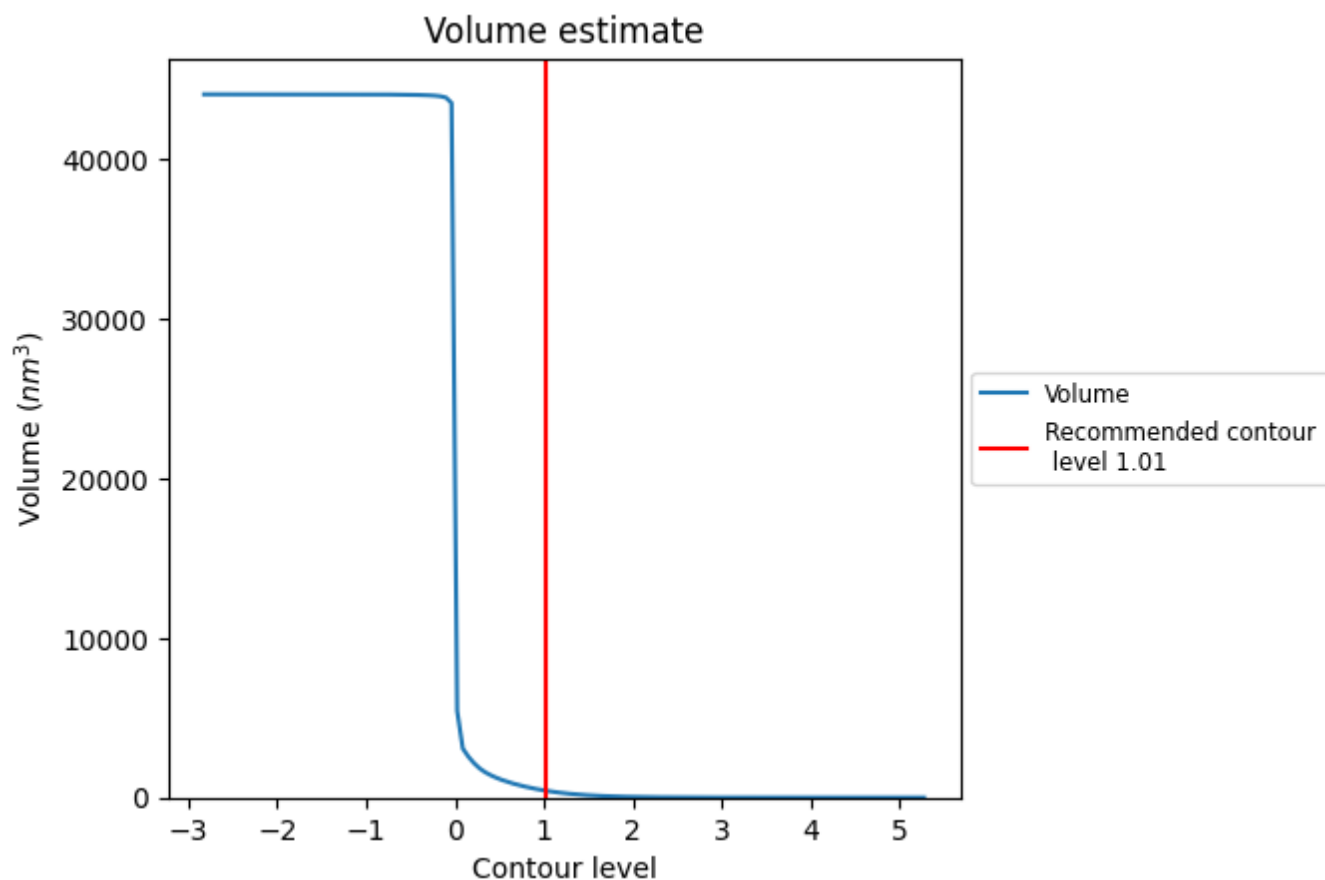
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

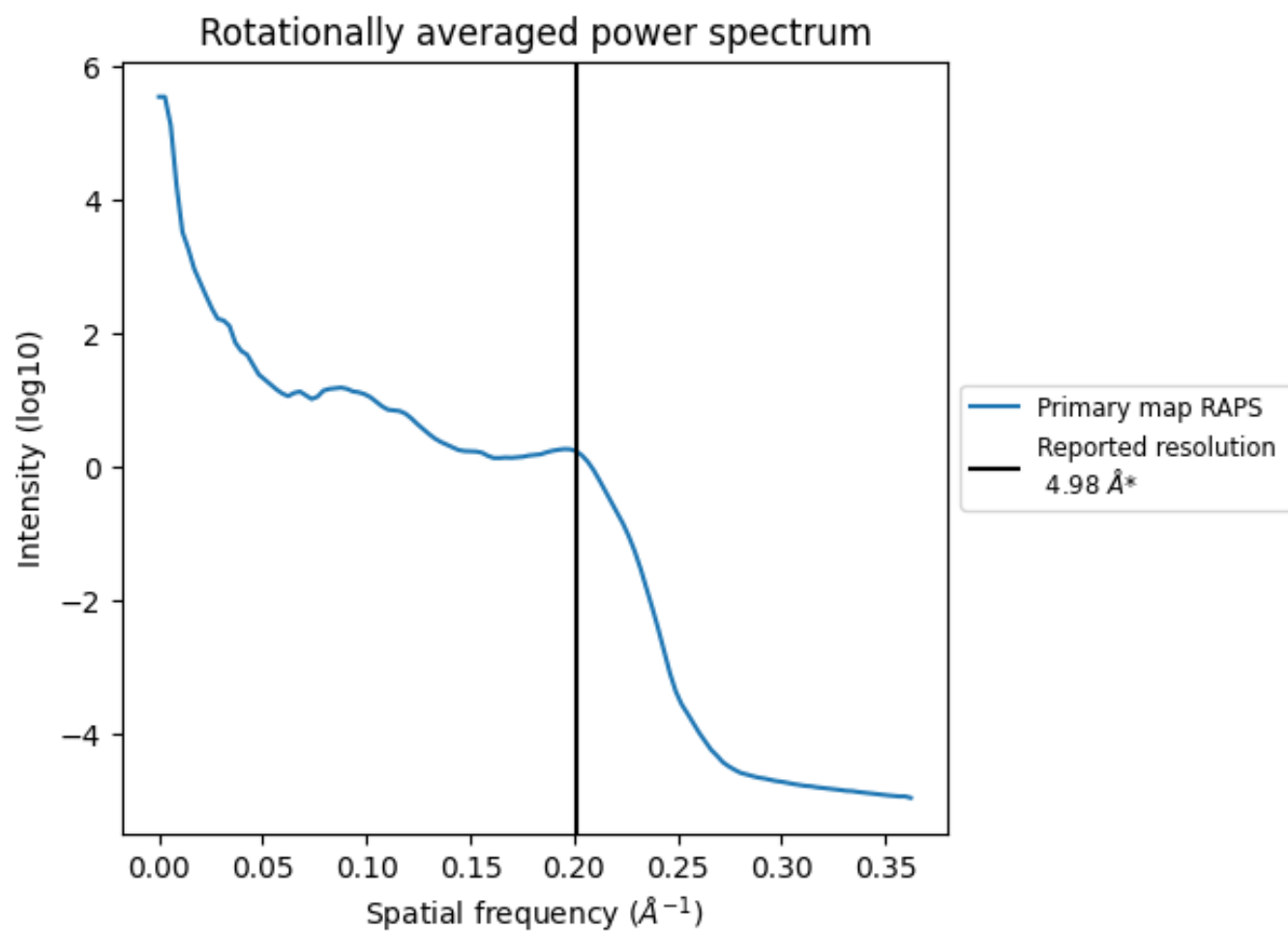


The volume at the recommended contour level is 440 nm<sup>3</sup>; this corresponds to an approximate mass of 397 kDa.

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 0.201 Å<sup>-1</sup>

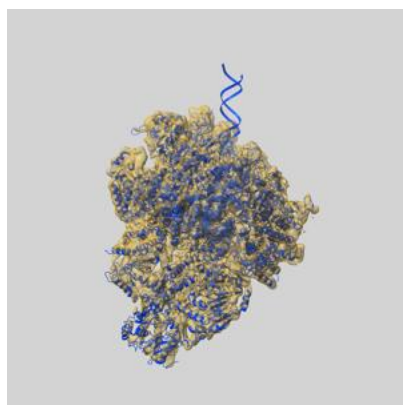
## 8 Fourier-Shell correlation ⓘ

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

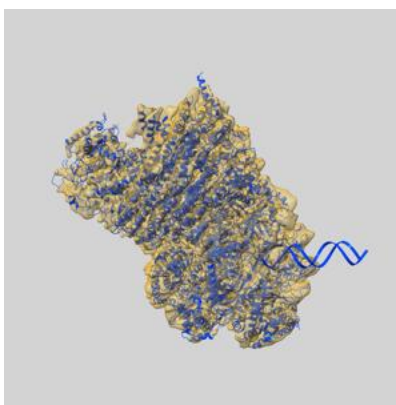
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0288 and PDB model 6HV9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

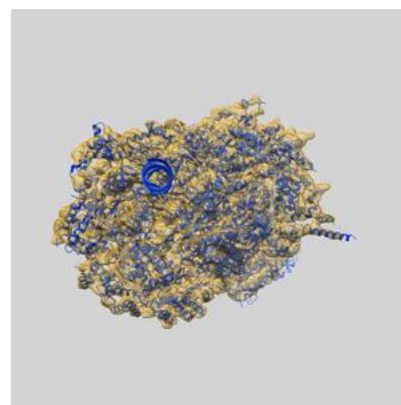
### 9.1 Map-model overlay [i](#)



X



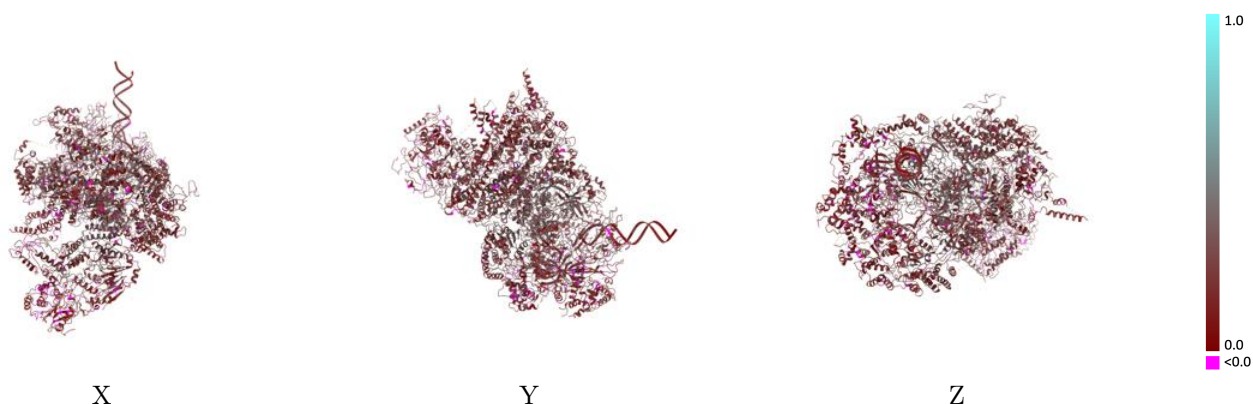
Y



Z

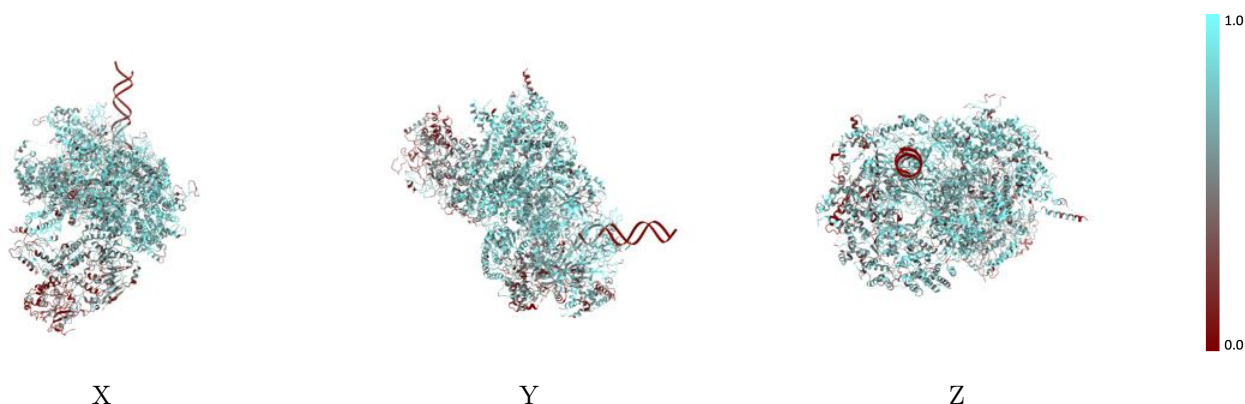
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



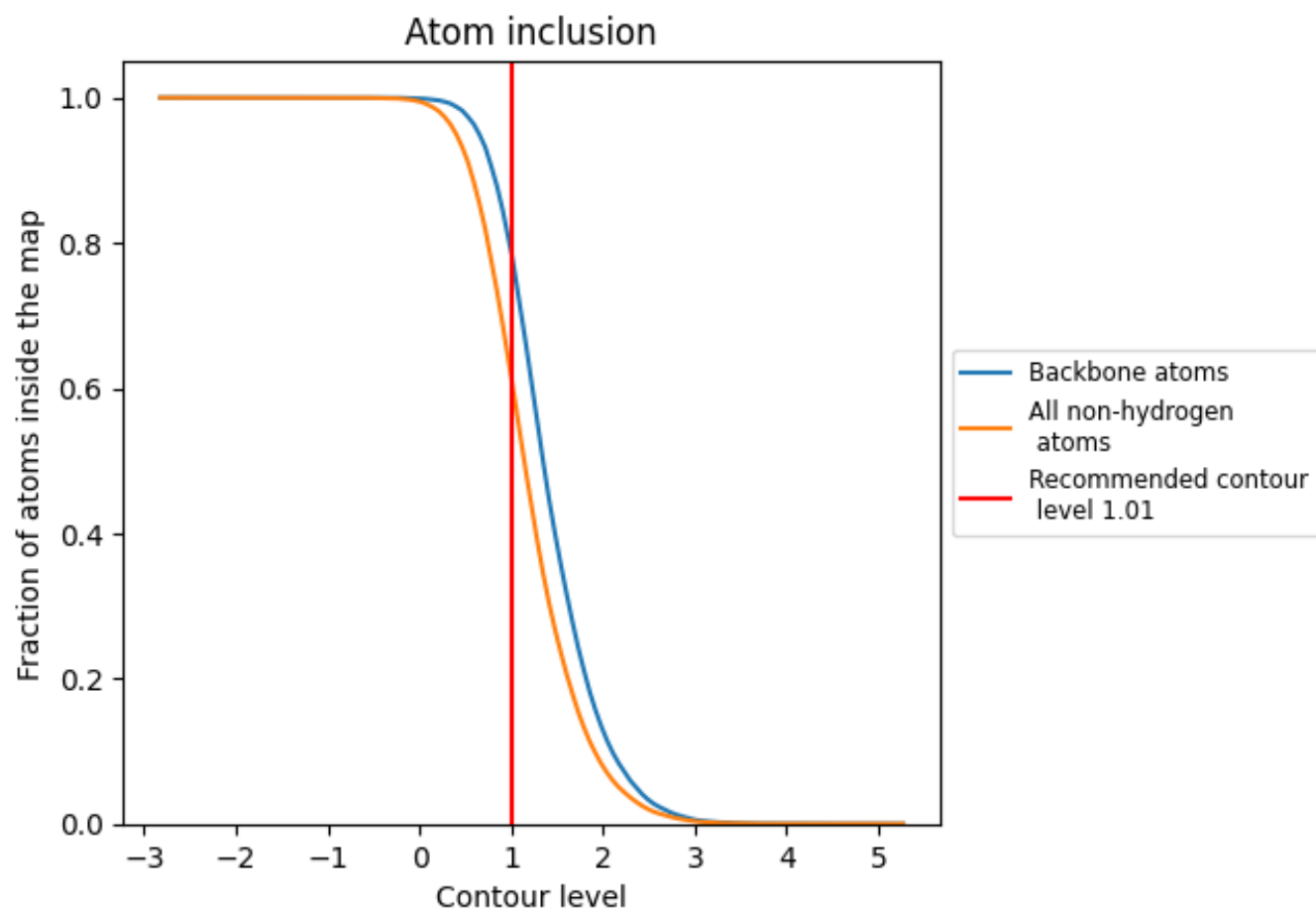
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6086	 0.2310
2	 0.6910	 0.2780
3	 0.7391	 0.2870
4	 0.5713	 0.1860
5	 0.6921	 0.3050
6	 0.6496	 0.2140
7	 0.5230	 0.1890
A	 0.4213	 0.1710
B	 0.5137	 0.2290
C	 0.7016	 0.2280
D	 0.7350	 0.2480
E	 0.7438	 0.2690
F	 0.6929	 0.2300
G	 0.6864	 0.2410
J	 0.5714	 0.2480
X	 0.1647	 0.1690
Y	 0.1524	 0.1610

