wwPDB EM Validation Summary Report ⓘ

Sep 25, 2023 – 10:34 am BST

PDB ID	:	8OUW
EMDB ID	:	EMD-17204
Title	:	Cryo-EM structure of CMG helicase bound to TIM-1/TIPN-1 and homodimeric DNSN-1 on fork DNA (Caenorhabditis elegans)
Authors	:	Jenkyn-Bedford, M.; Yeeles, J.T.P.; Labib, K.P.M.
Deposited on	:	2023-04-25
Resolution	:	3.75 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:

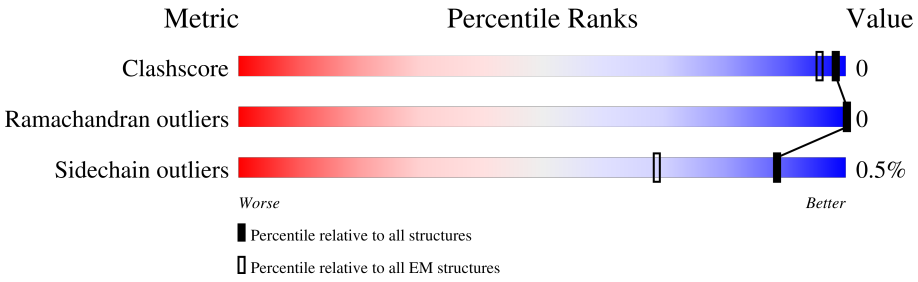
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	2	881	40% 78% · 20%
2	3	812	26% 75% · 24%
3	4	823	22% 74% · 25%
4	5	759	28% 70% · 29%
5	6	810	42% 86% · 13%
6	7	730	17% 86% · 13%
7	A	205	9% 93% · 6%
8	B	180	· 99% ·

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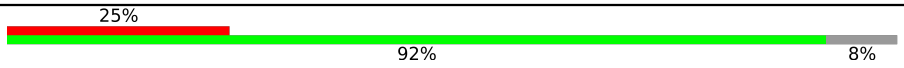
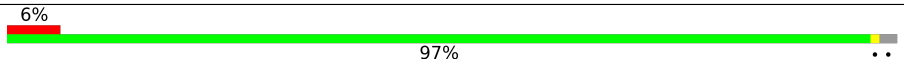
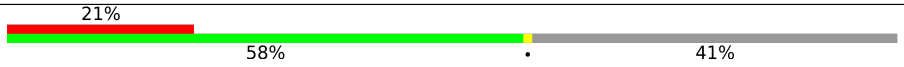
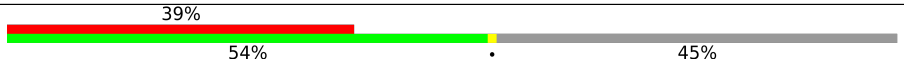
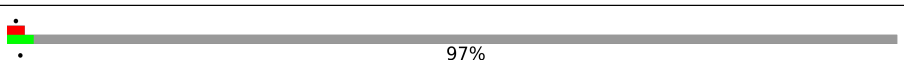
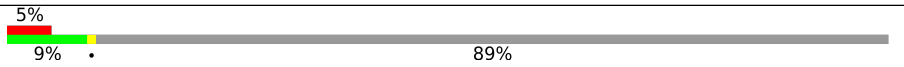
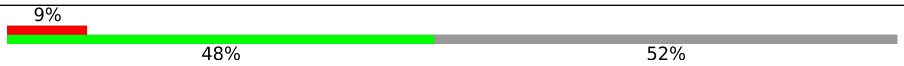
Mol	Chain	Length	Quality of chain
9	C	193	
10	D	224	
11	E	574	
12	F	594	
12	G	594	
12	H	594	
13	I	85	
13	J	85	
14	K	1353	
15	L	237	
16	M	61	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 53754 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	701	5547	3466	978	1067	36	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	619	4872	3045	871	928	28	0	0

- Molecule 3 is a protein called DNA replication licensing factor mcm-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	619	4906	3070	871	937	28	0	0

- Molecule 4 is a protein called DNA replication licensing factor mcm-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	541	4256	2708	739	786	23	0	0

- Molecule 5 is a protein called DNA replication licensing factor mcm-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	707	5595	3507	981	1072	35	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	632	4963	3103	870	952	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	193	Total	C	N	O	S	0	0
			1534	963	279	282	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q22019
A	-2	PRO	-	expression tag	UNP Q22019
A	-1	GLY	-	expression tag	UNP Q22019
A	0	SER	-	expression tag	UNP Q22019

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	180	Total	C	N	O	S	0	0
			1423	888	256	269	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	178	Total	C	N	O	S	0	0
			1404	881	237	278	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	203	Total	C	N	O	S	0	0
			1625	1017	274	320	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	563	Total	C	N	O	S	0	0
			4547	2883	782	848	34		

- Molecule 12 is a protein called Downstream Neighbor of SoN homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	348	Total	C	N	O	S	0	0
			2741	1741	462	516	22		

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Mol	Chain	Residues	Atoms	AltConf	Trace
12	G	326	Total C N O S 2564 1630 429 484 21	0	0
12	H	16	Total C N O 148 90 35 23	0	0

- Molecule 13 is a DNA chain called DNA Leading Strand Template.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	I	9	Total C N O P 180 90 18 63 9	0	0
13	J	29	Total C N O P 611 290 118 174 29	0	0

- Molecule 14 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	K	656	Total C N O S 5446 3481 952 994 19	0	0

- Molecule 15 is a protein called Protein TIPIN homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	L	82	Total C N O S 681 439 124 114 4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q9TXI0
L	-2	PRO	-	expression tag	UNP Q9TXI0
L	-1	GLY	-	expression tag	UNP Q9TXI0
L	0	SER	-	expression tag	UNP Q9TXI0

- Molecule 16 is a DNA chain called DNA Lagging Strand Template.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	M	29	Total C N O P 578 279 96 174 29	0	0

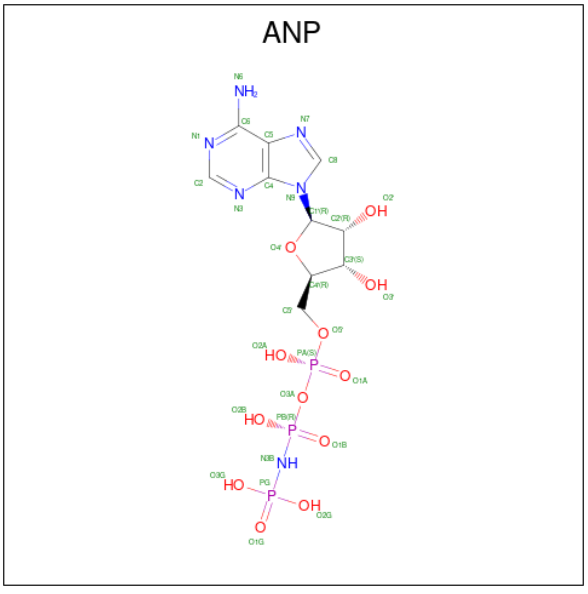
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
17	2	1	Total Zn 1 1	0
17	4	1	Total Zn 1 1	0
17	5	1	Total Zn 1 1	0
17	6	1	Total Zn 1 1	0
17	7	1	Total Zn 1 1	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
18	3	1	Total Mg 1 1	0
18	4	1	Total Mg 1 1	0
18	6	1	Total Mg 1 1	0
18	7	1	Total Mg 1 1	0

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



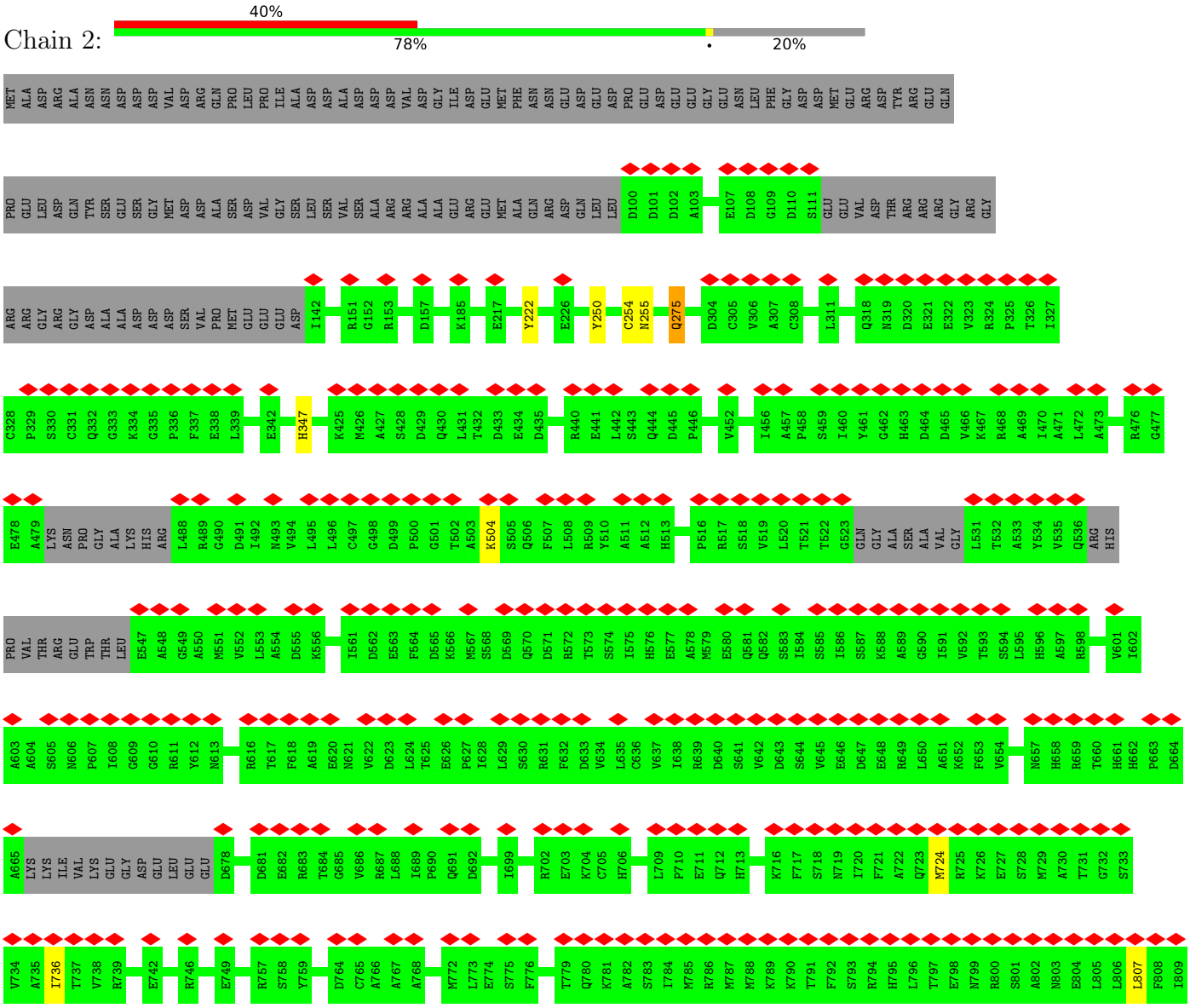
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	4	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	6	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	7	1	Total	C	N	O	P	0
			31	10	6	12	3	

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.

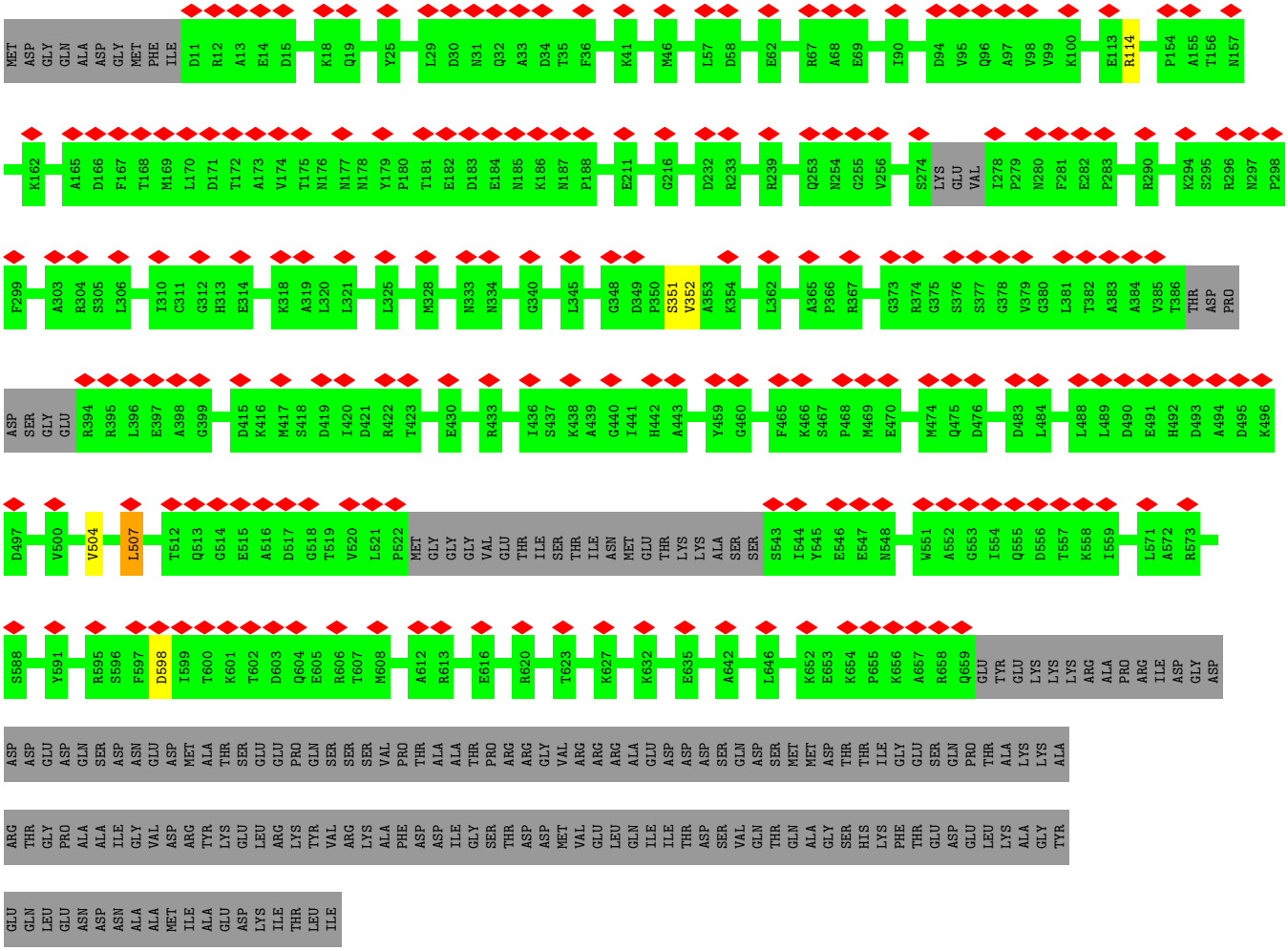
- Molecule 1: DNA replication licensing factor MCM2

Chain 2:



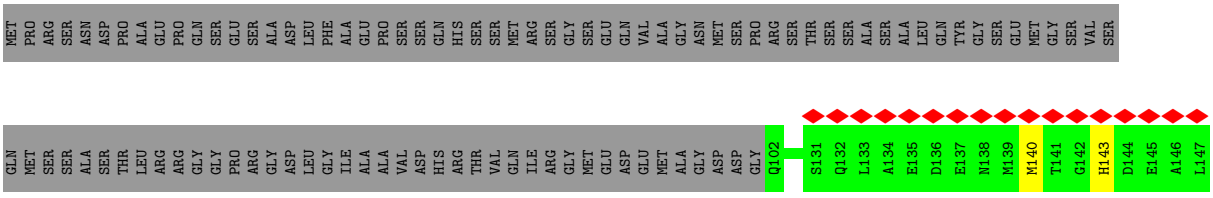
• Molecule 2: DNA replication licensing factor MCM3

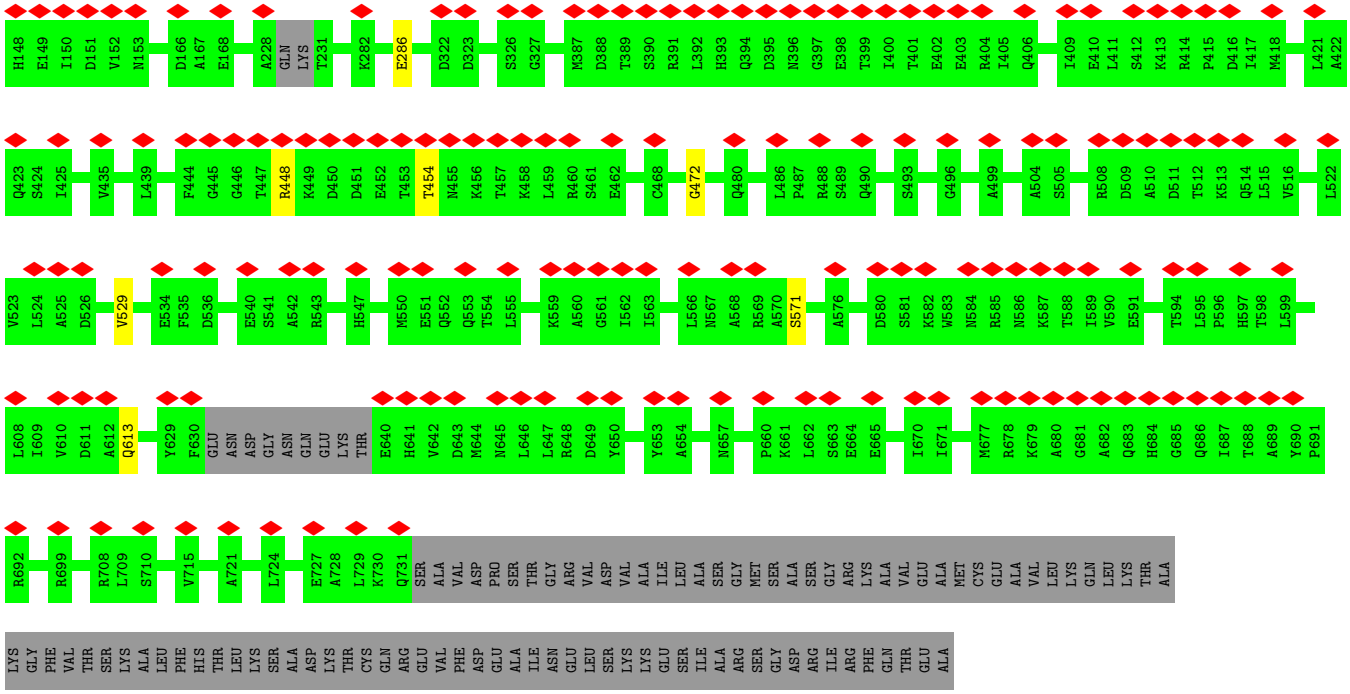
Chain 3:



• Molecule 3: DNA replication licensing factor mcm-4

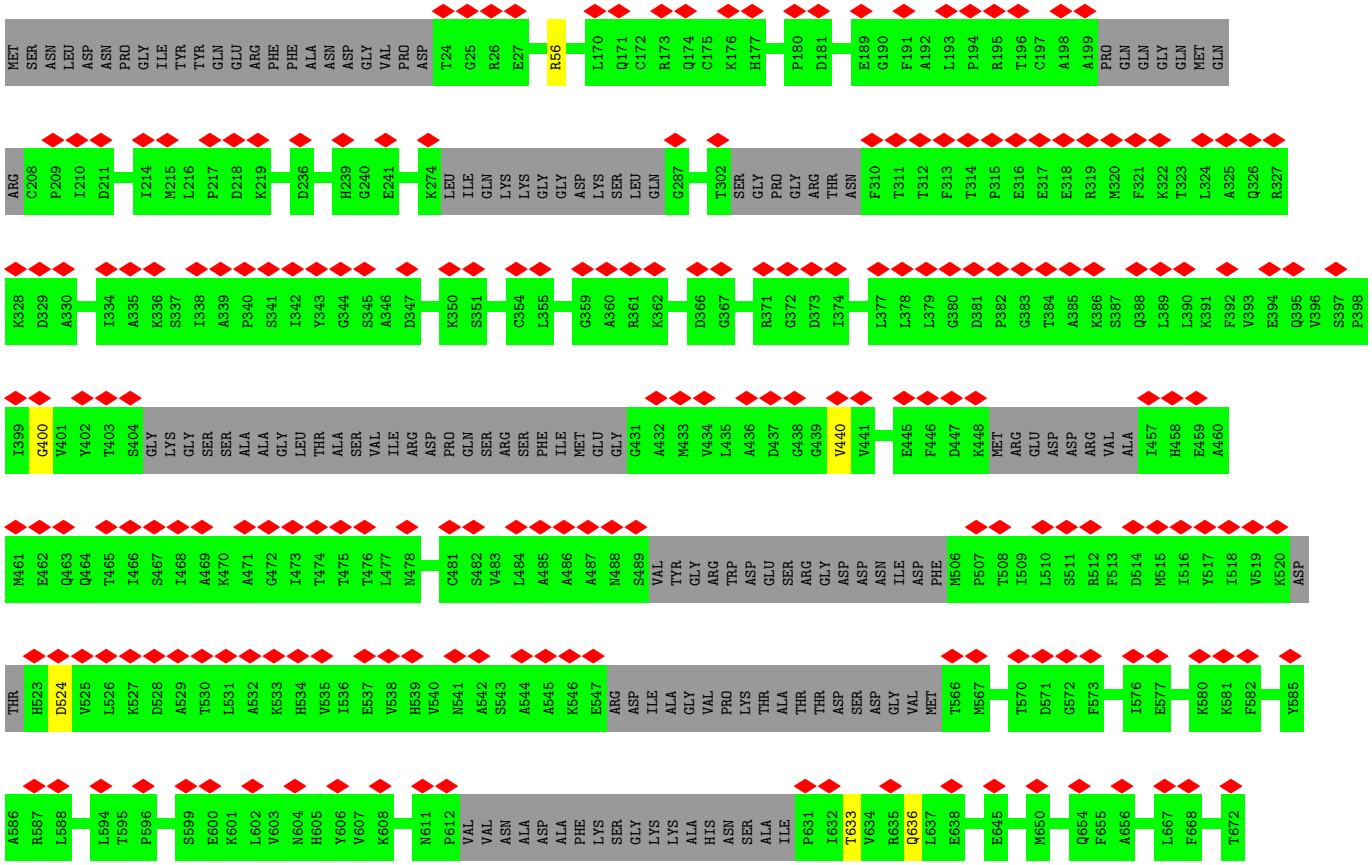
Chain 4:

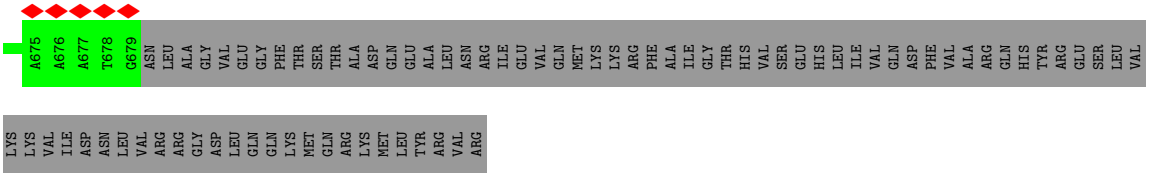




• Molecule 4: DNA replication licensing factor mcm-5

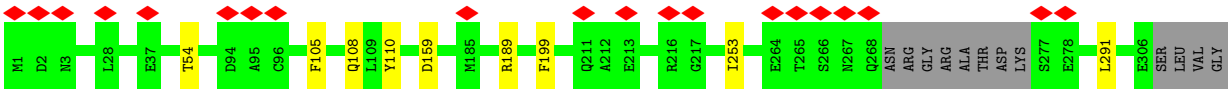
Chain 5:

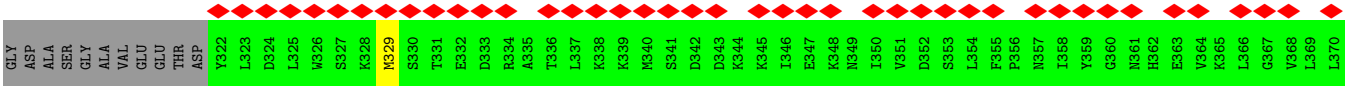


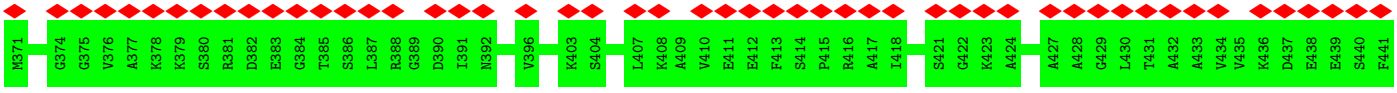


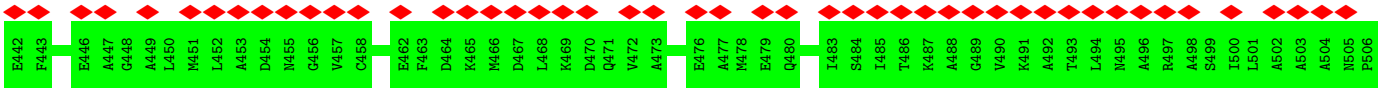
• Molecule 5: DNA replication licensing factor mcm-6

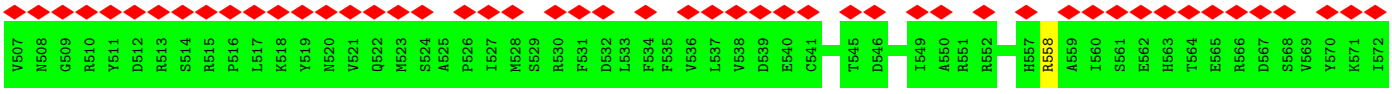
Chain 6:

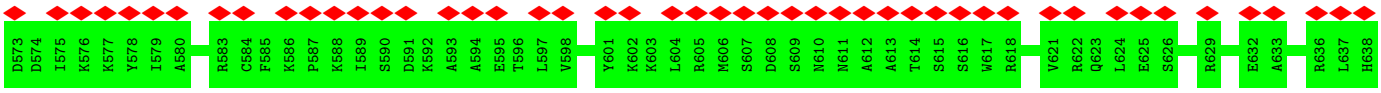


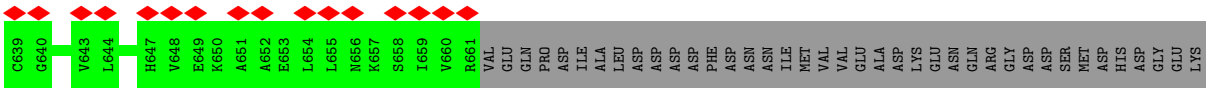


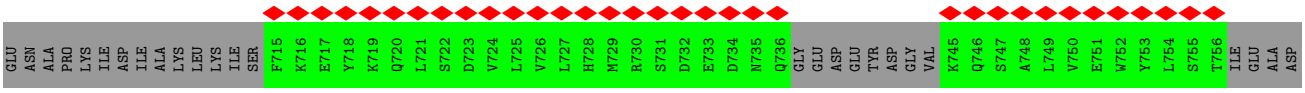


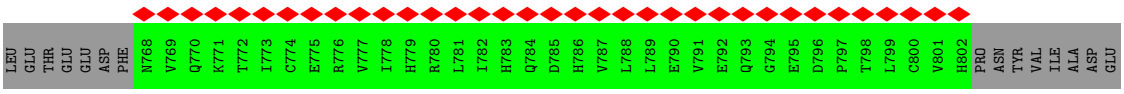






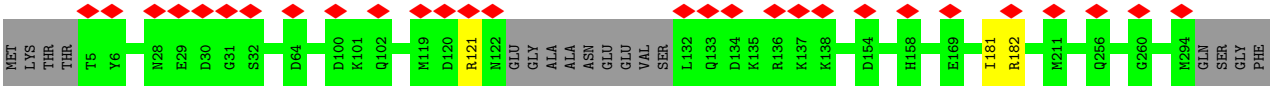


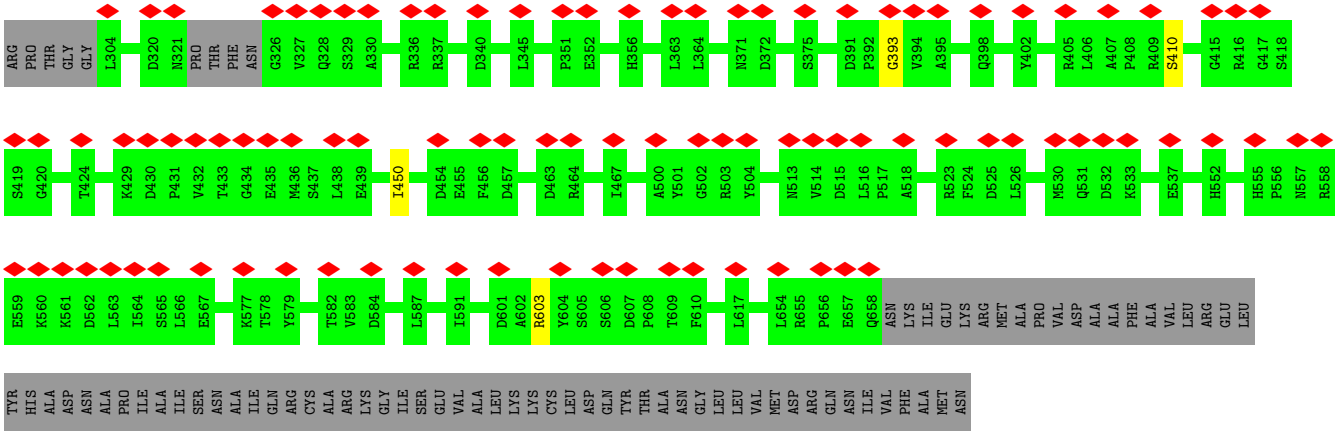




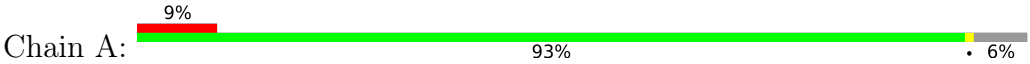
• Molecule 6: DNA replication licensing factor MCM7

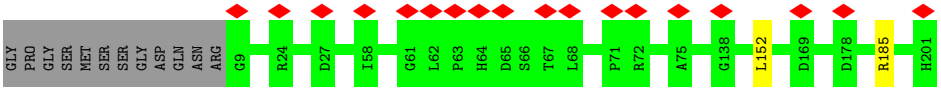
Chain 7:



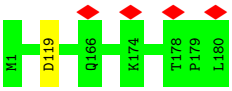


• Molecule 7: Probable DNA replication complex GINS protein PSF1

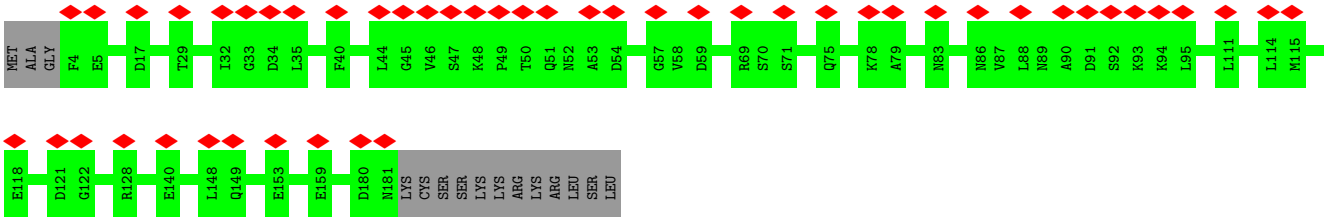




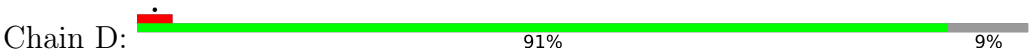
• Molecule 8: Probable DNA replication complex GINS protein PSF2

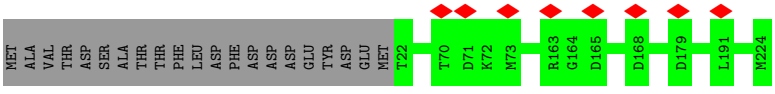


• Molecule 9: DNA replication complex GINS protein PSF3

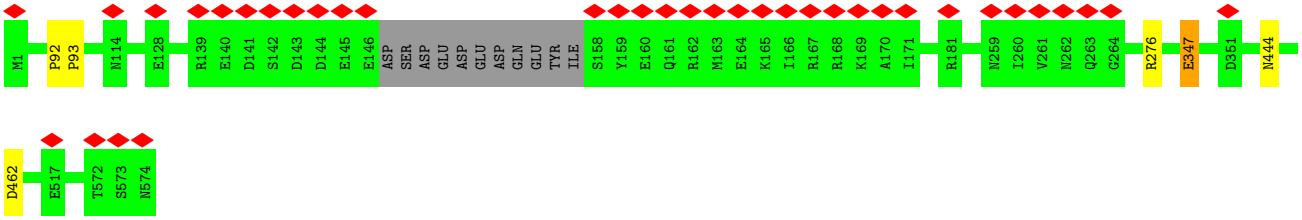


• Molecule 10: DNA replication complex GINS protein SLD5

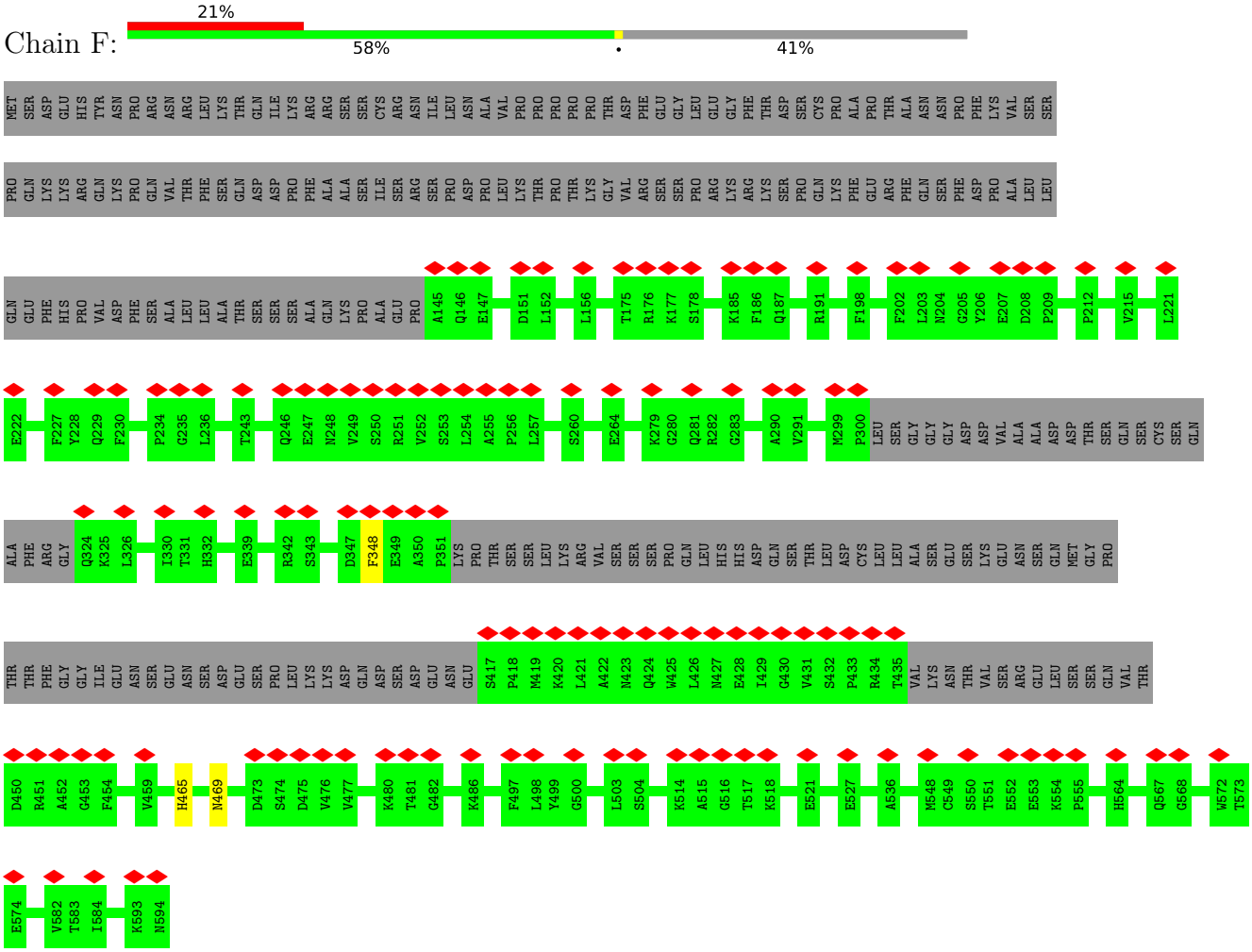




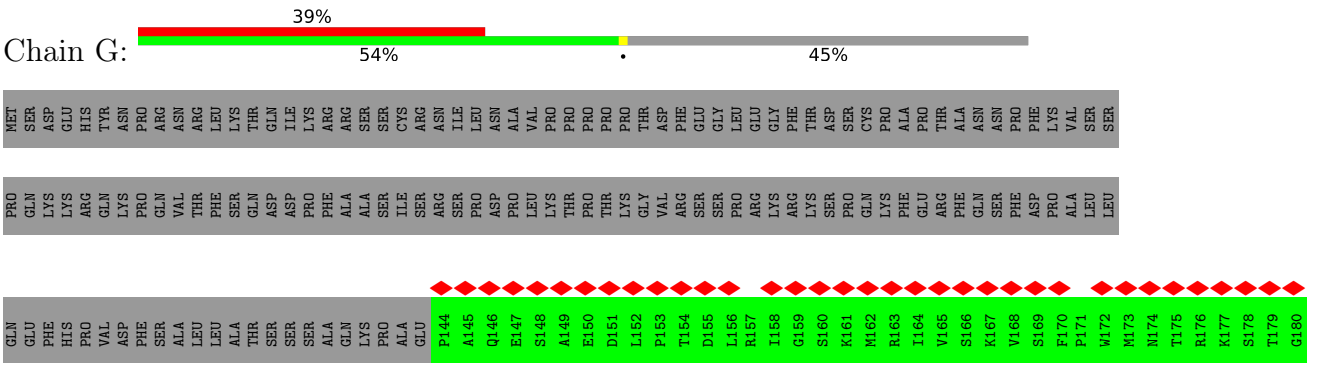
• Molecule 11: Cell division control protein 45 homolog

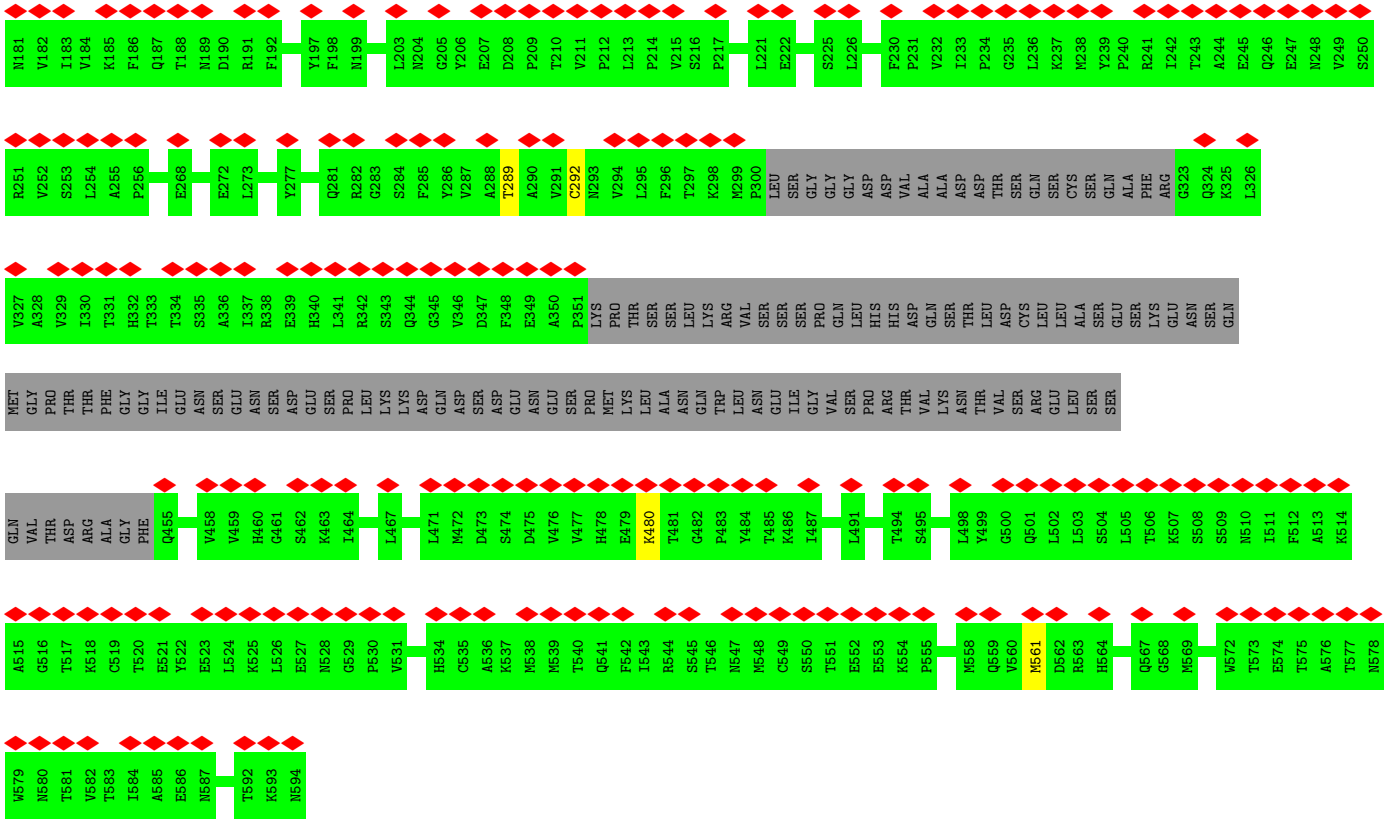


• Molecule 12: Downstream Neighbor of SoN homolog



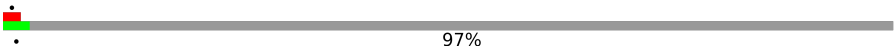
• Molecule 12: Downstream Neighbor of SoN homolog

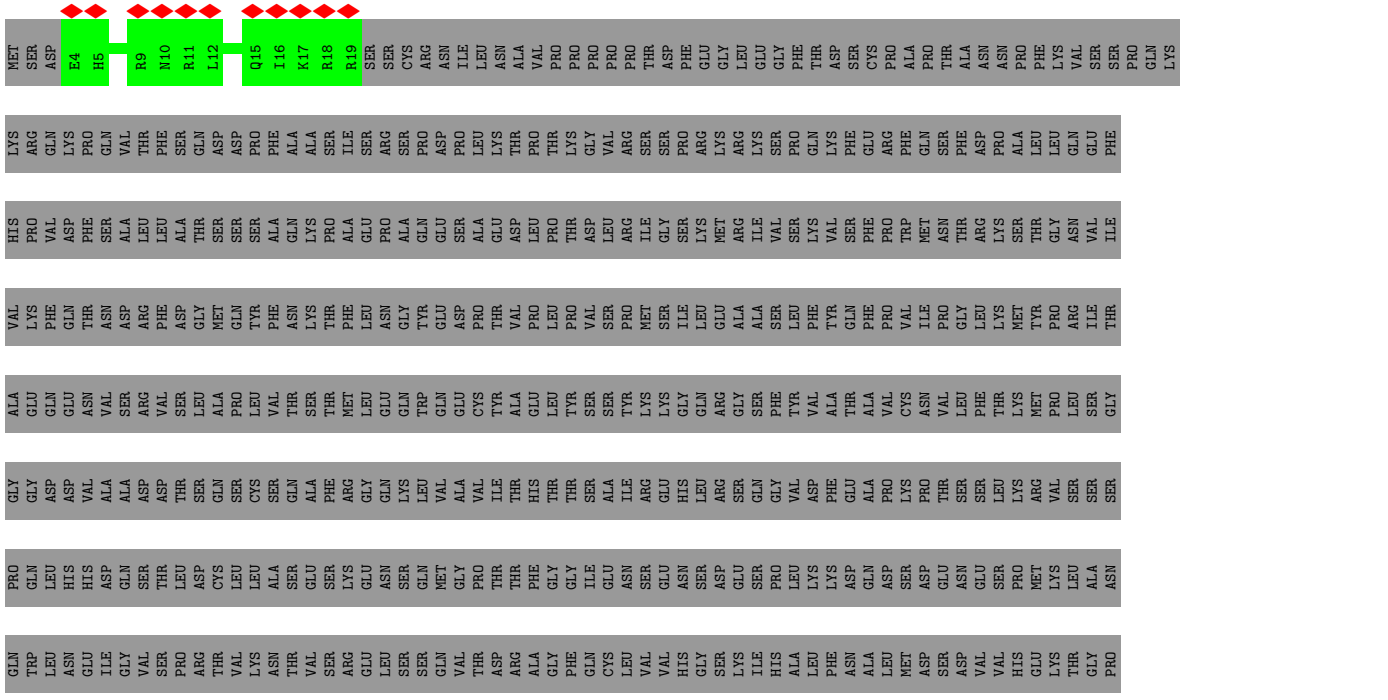


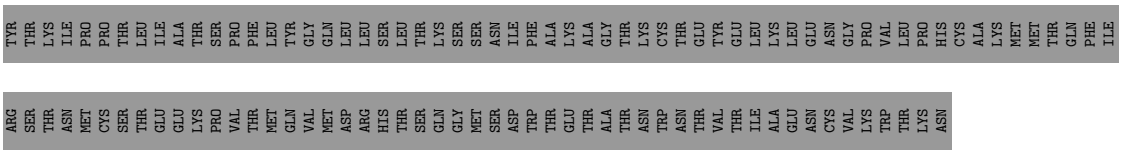


• Molecule 12: Downstream Neighbor of SoN homolog

Chain H:

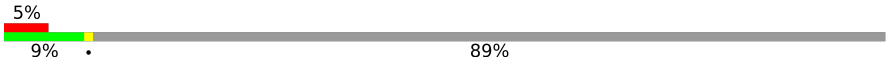


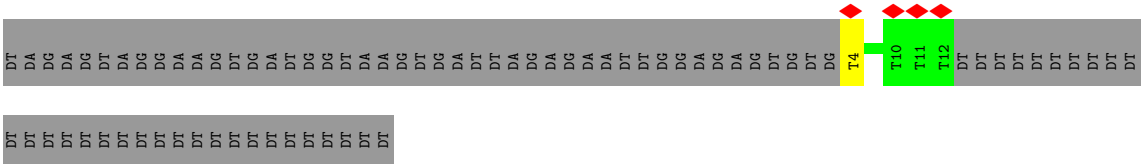




• Molecule 13: DNA Leading Strand Template

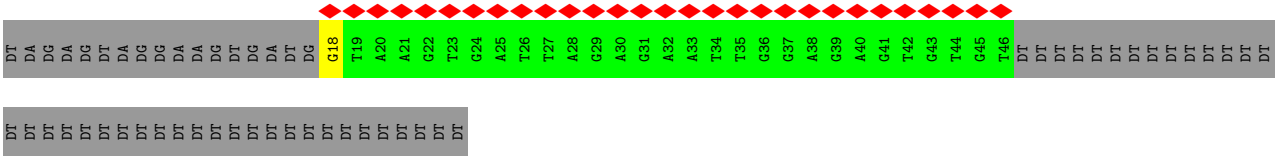
Chain I:





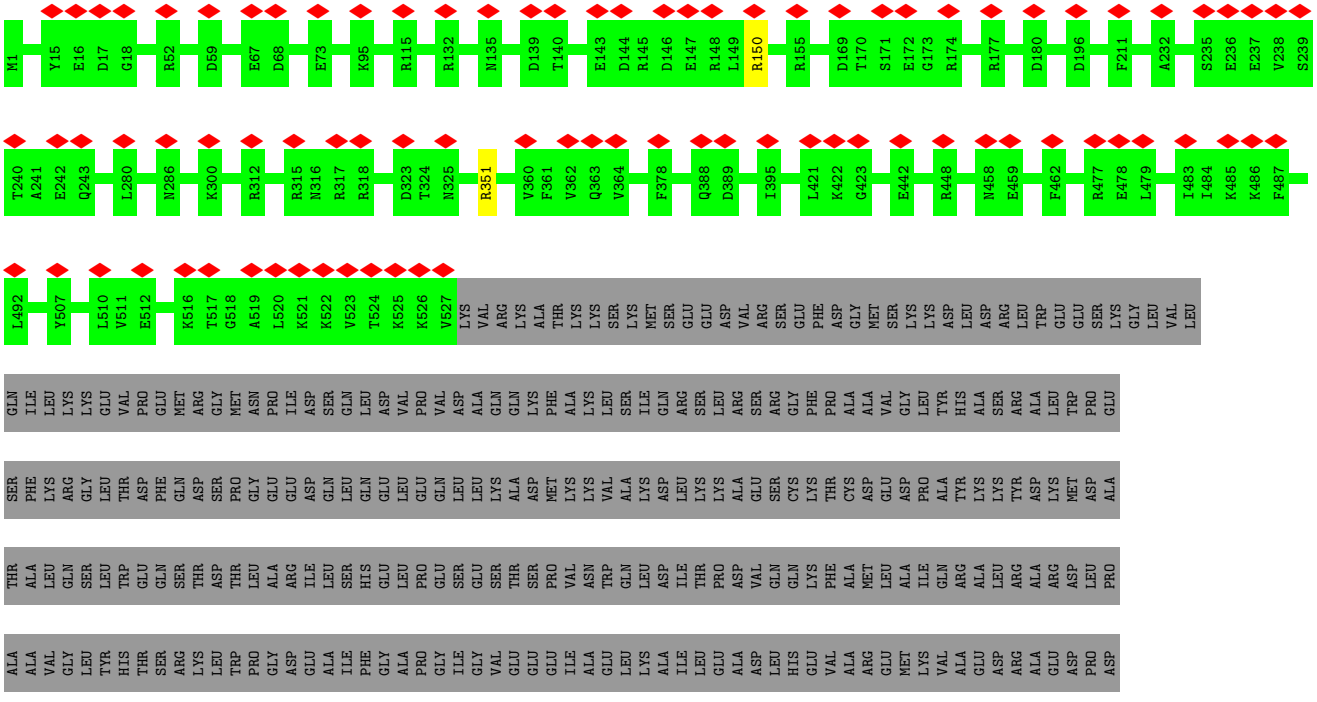
• Molecule 13: DNA Leading Strand Template

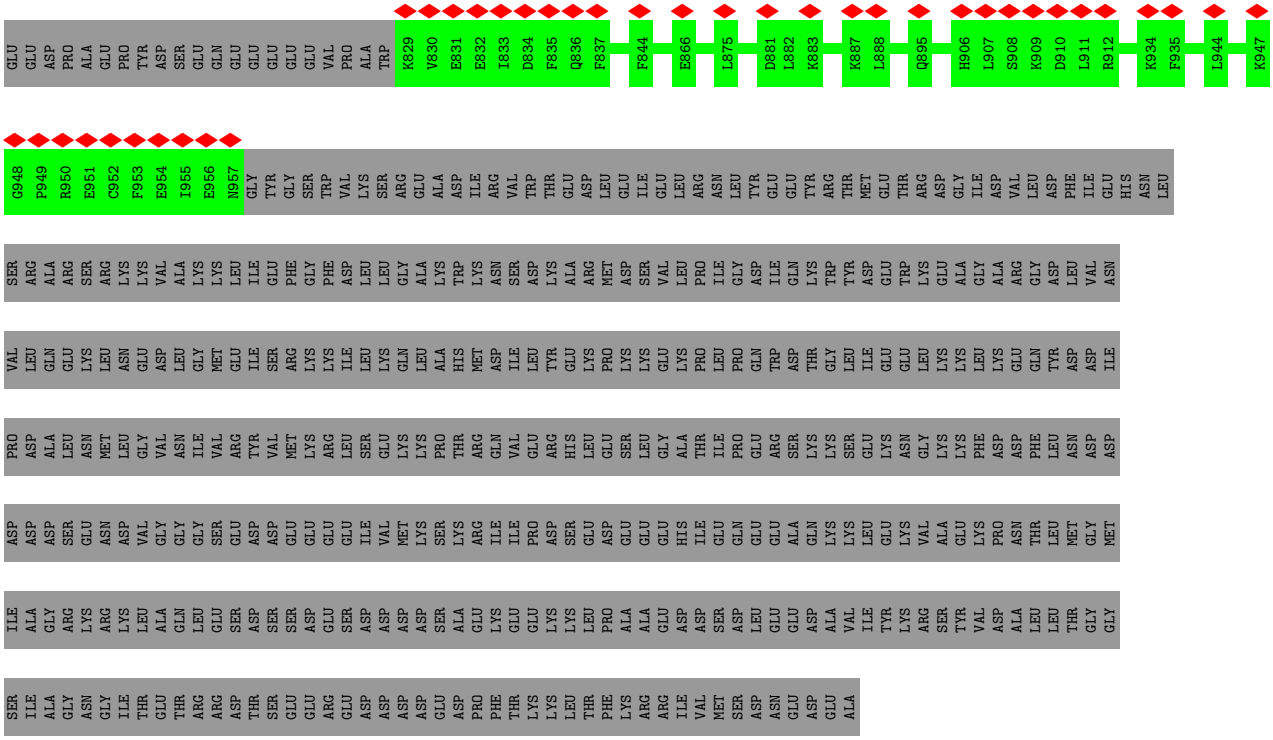
Chain J:



• Molecule 14: Protein timeless homolog

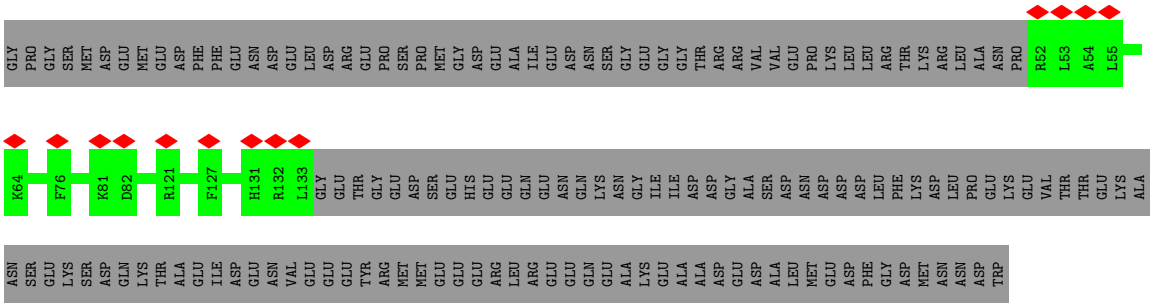
Chain K:





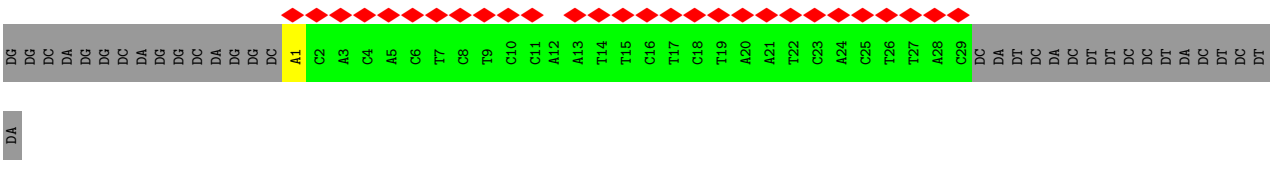
• Molecule 15: Protein TIPIN homolog

Chain L:



• Molecule 16: DNA Lagging Strand Template

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0128	Depositor
Map size (Å)	409.22, 409.22, 409.22	wwPDB
Map dimensions	316, 316, 316	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.295, 1.295, 1.295	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/5637	0.59	0/7608
2	3	0.31	0/4945	0.61	1/6672 (0.0%)
3	4	0.32	0/4988	0.62	0/6748
4	5	0.32	0/4323	0.60	0/5828
5	6	0.32	0/5675	0.59	0/7648
6	7	0.31	0/5043	0.59	0/6814
7	A	0.33	0/1562	0.60	0/2107
8	B	0.31	0/1447	0.58	0/1954
9	C	0.33	0/1428	0.52	0/1924
10	D	0.32	0/1652	0.53	0/2230
11	E	0.31	0/4637	0.59	0/6262
12	F	0.33	0/2803	0.61	0/3801
12	G	0.35	0/2623	0.60	0/3558
12	H	0.28	0/150	0.62	0/198
13	I	0.68	0/197	1.37	1/302 (0.3%)
13	J	0.73	0/688	1.11	1/1064 (0.1%)
14	K	0.36	0/5554	0.57	0/7467
15	L	0.32	0/695	0.60	0/931
16	M	0.72	0/644	1.19	1/987 (0.1%)
All	All	0.34	0/54691	0.62	4/74103 (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
4	5	0	1
5	6	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	18	DG	OP1-P-OP2	-6.71	109.54	119.60
13	I	4	DT	OP1-P-OP2	-6.69	109.57	119.60
16	M	1	DA	OP1-P-OP2	-6.36	110.06	119.60
2	3	352	VAL	CG1-CB-CG2	-6.22	100.95	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	5	524	ASP	Peptide
5	6	329	MET	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	5547	0	5494	3	0
2	3	4872	0	4915	3	0
3	4	4906	0	4888	3	0
4	5	4256	0	4370	3	0
5	6	5595	0	5632	3	0
6	7	4963	0	4951	4	0
7	A	1534	0	1540	0	0
8	B	1423	0	1429	1	0
9	C	1404	0	1374	0	0
10	D	1625	0	1611	0	0
11	E	4547	0	4549	2	0
12	F	2741	0	2730	1	0
12	G	2564	0	2556	0	0
12	H	148	0	155	0	0
13	I	180	0	109	0	0
13	J	611	0	329	0	0
14	K	5446	0	5480	0	0
15	L	681	0	722	0	0
16	M	578	0	329	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	3	1	0	0	0	0
18	4	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
19	3	31	0	13	1	0
19	4	31	0	13	1	0
19	6	31	0	13	0	0
19	7	31	0	13	1	0
All	All	53754	0	53215	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:351:SER:H	19:3:1502:ANP:HNB1	1.43	0.66
6:7:393:GLY:H	19:7:1500:ANP:HNB1	1.46	0.62
3:4:472:GLY:H	19:4:1502:ANP:HNB1	1.49	0.58
11:E:276:ARG:NH2	11:E:347:GLU:OE2	2.39	0.55
5:6:54:THR:HG22	5:6:110:TYR:HB2	1.87	0.55

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	685/881 (78%)	679 (99%)	6 (1%)	0	100	100
2	3	611/812 (75%)	597 (98%)	14 (2%)	0	100	100
3	4	613/823 (74%)	597 (97%)	16 (3%)	0	100	100
4	5	521/759 (69%)	509 (98%)	12 (2%)	0	100	100
5	6	695/810 (86%)	679 (98%)	16 (2%)	0	100	100
6	7	624/730 (86%)	615 (99%)	9 (1%)	0	100	100
7	A	191/205 (93%)	186 (97%)	5 (3%)	0	100	100
8	B	178/180 (99%)	173 (97%)	5 (3%)	0	100	100
9	C	176/193 (91%)	172 (98%)	4 (2%)	0	100	100
10	D	201/224 (90%)	197 (98%)	4 (2%)	0	100	100
11	E	559/574 (97%)	547 (98%)	12 (2%)	0	100	100
12	F	340/594 (57%)	334 (98%)	6 (2%)	0	100	100
12	G	320/594 (54%)	315 (98%)	5 (2%)	0	100	100
12	H	14/594 (2%)	14 (100%)	0	0	100	100
14	K	652/1353 (48%)	640 (98%)	12 (2%)	0	100	100
15	L	80/237 (34%)	80 (100%)	0	0	100	100
All	All	6460/9563 (68%)	6334 (98%)	126 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2	617/766 (80%)	611 (99%)	6 (1%)	76	86
2	3	538/700 (77%)	536 (100%)	2 (0%)	91	95
3	4	546/710 (77%)	541 (99%)	5 (1%)	78	88
4	5	468/650 (72%)	468 (100%)	0	100	100
5	6	623/709 (88%)	618 (99%)	5 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	7	545/623 (88%)	544 (100%)	1 (0%)	93 97
7	A	167/176 (95%)	165 (99%)	2 (1%)	71 84
8	B	158/158 (100%)	158 (100%)	0	100 100
9	C	158/171 (92%)	158 (100%)	0	100 100
10	D	185/204 (91%)	185 (100%)	0	100 100
11	E	509/520 (98%)	506 (99%)	3 (1%)	86 93
12	F	310/532 (58%)	309 (100%)	1 (0%)	92 96
12	G	291/532 (55%)	287 (99%)	4 (1%)	67 82
12	H	16/532 (3%)	16 (100%)	0	100 100
14	K	601/1213 (50%)	599 (100%)	2 (0%)	92 96
15	L	74/209 (35%)	74 (100%)	0	100 100
All	All	5806/8405 (69%)	5775 (100%)	31 (0%)	89 94

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	108	GLN
12	G	480	LYS
5	6	558	ARG
14	K	150	ARG
12	F	348	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	145	HIS
7	A	186	GLN
12	F	578	ASN
8	B	139	ASN
3	4	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 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	3	1502	18	29,33,33	1.05	3 (10%)	31,52,52	1.18	3 (9%)
19	ANP	7	1500	18	29,33,33	1.09	4 (13%)	31,52,52	1.02	2 (6%)
19	ANP	6	903	18	29,33,33	1.09	4 (13%)	31,52,52	1.12	3 (9%)
19	ANP	4	1502	18	29,33,33	1.08	4 (13%)	31,52,52	1.08	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ANP	3	1502	18	-	5/14/38/38	0/3/3/3
19	ANP	7	1500	18	-	3/14/38/38	0/3/3/3
19	ANP	6	903	18	-	2/14/38/38	0/3/3/3
19	ANP	4	1502	18	-	4/14/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	903	ANP	PB-O3A	-2.89	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1502	ANP	PB-O3A	-2.49	1.55	1.59
19	7	1500	ANP	PB-O3A	-2.47	1.56	1.59
19	3	1502	ANP	PG-N3B	2.45	1.69	1.63
19	7	1500	ANP	PG-O1G	2.44	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	1502	ANP	PB-O3A-PA	-3.74	119.43	132.62
19	6	903	ANP	PB-O3A-PA	-3.73	119.48	132.62
19	7	1500	ANP	PB-O3A-PA	-3.41	120.59	132.62
19	3	1502	ANP	PB-O3A-PA	-3.20	121.35	132.62
19	3	1502	ANP	C1'-N9-C4	2.59	131.19	126.64

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	3	1502	ANP	PB-N3B-PG-O1G
19	3	1502	ANP	PG-N3B-PB-O3A
19	3	1502	ANP	C3'-C4'-C5'-O5'
19	4	1502	ANP	PB-N3B-PG-O1G
19	4	1502	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

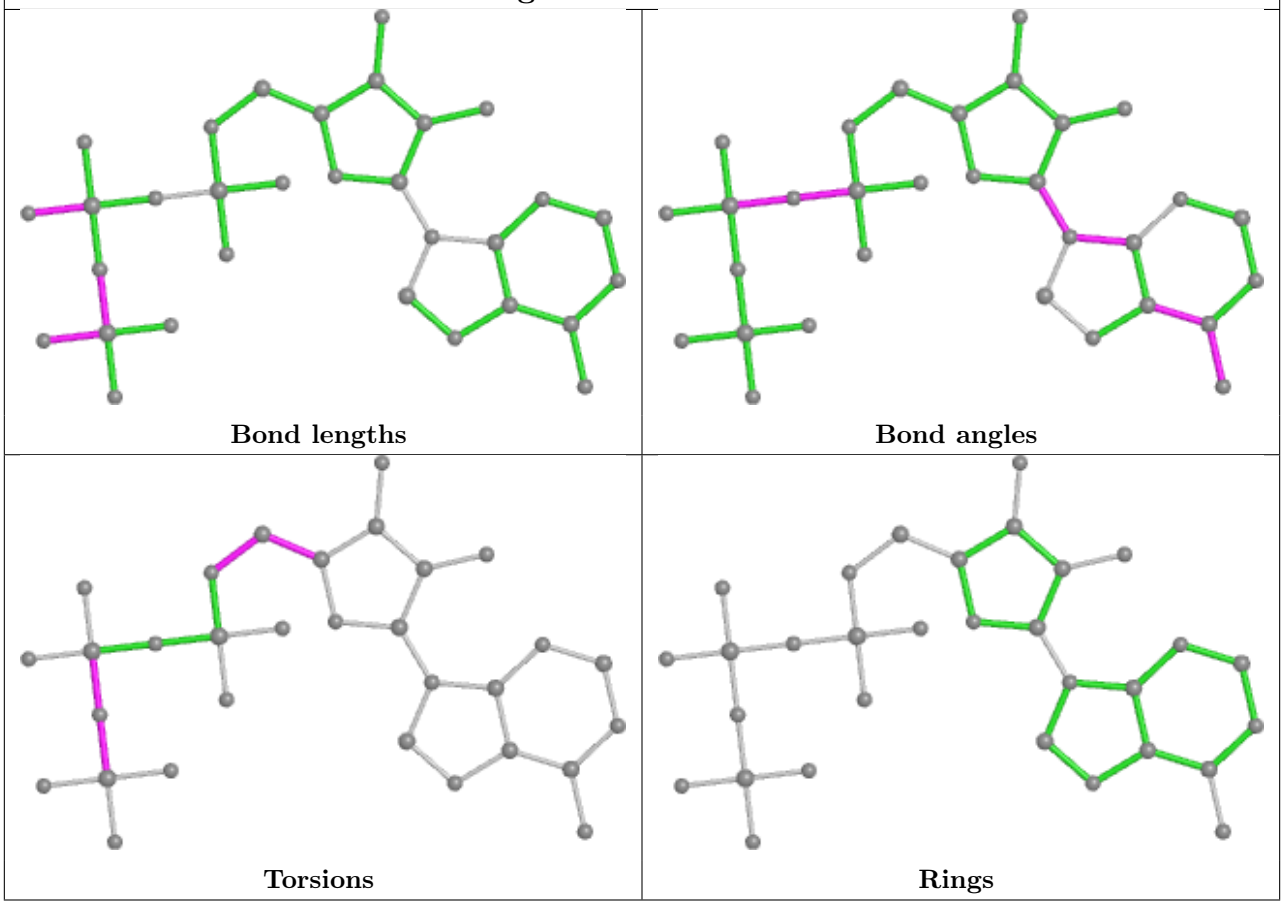
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	1502	ANP	1	0
19	7	1500	ANP	1	0
19	4	1502	ANP	1	0

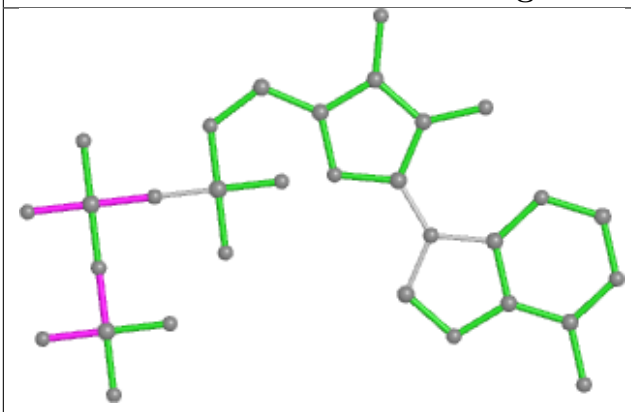
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

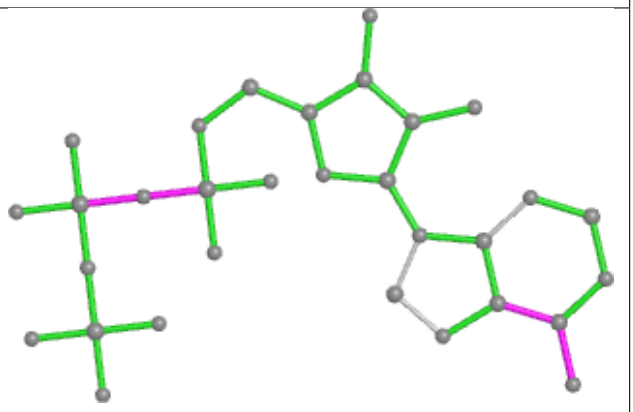
Ligand ANP 3 1502



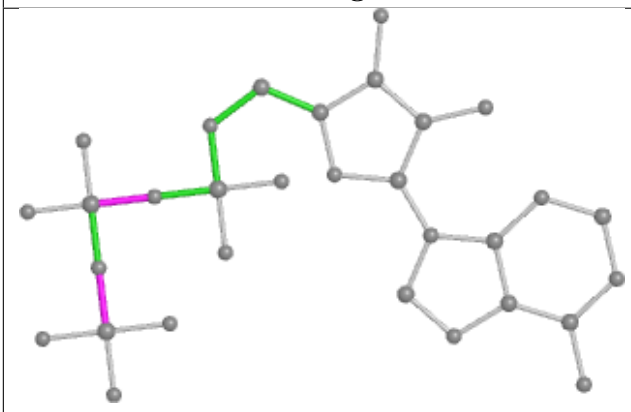
Ligand ANP 7 1500



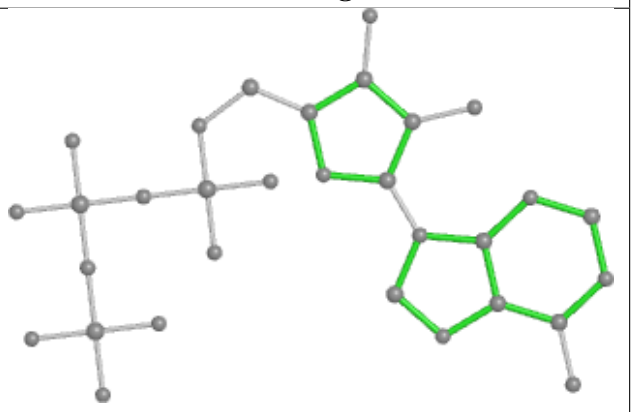
Bond lengths



Bond angles

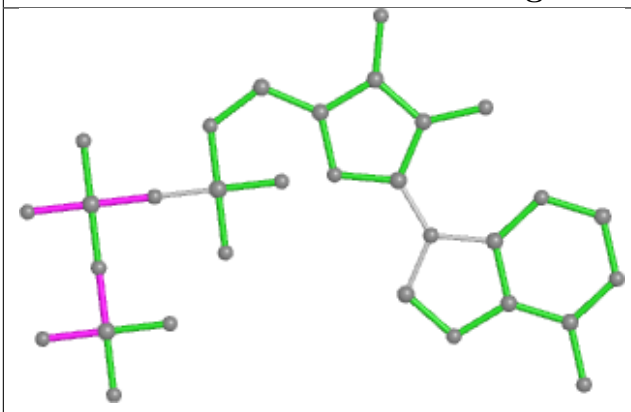


Torsions

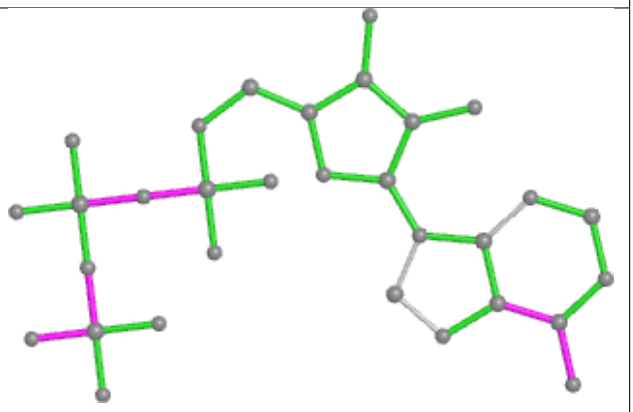


Rings

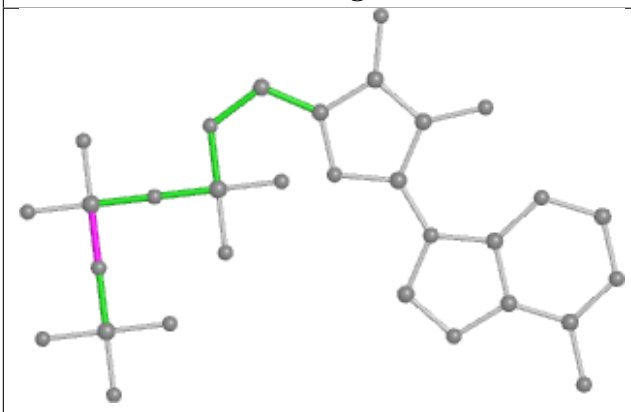
Ligand ANP 6 903



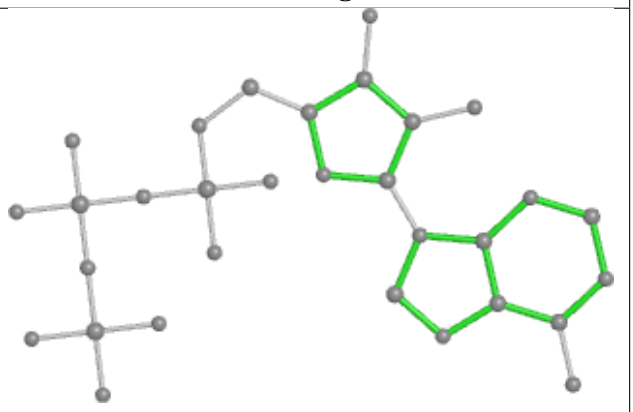
Bond lengths



Bond angles

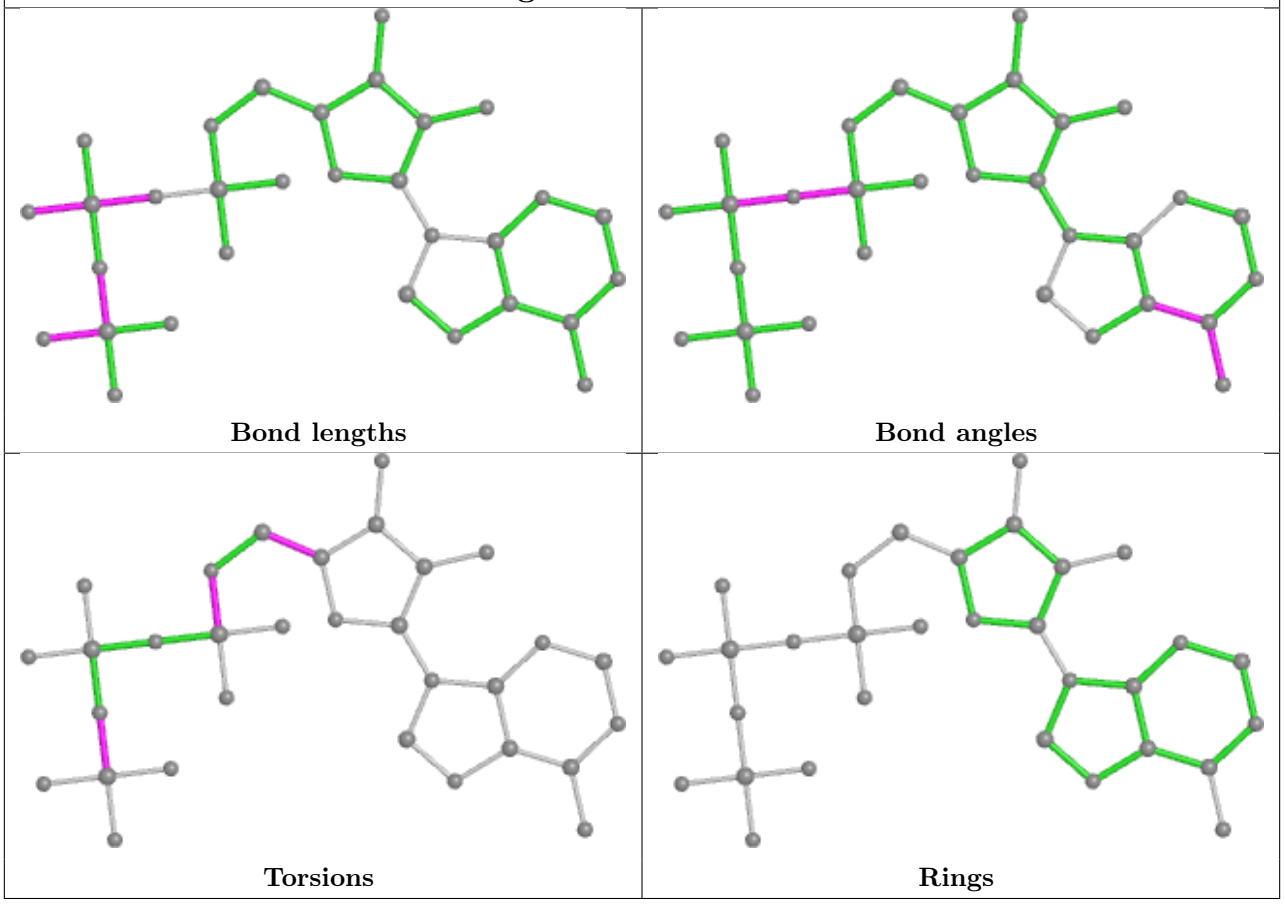


Torsions



Rings

Ligand ANP 4 1502



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.

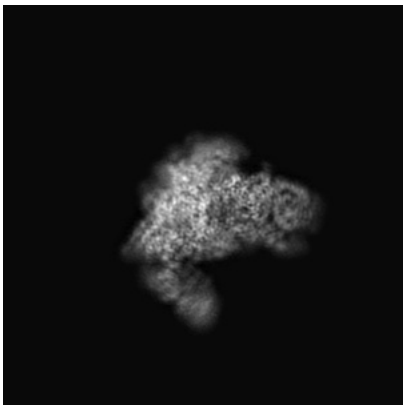
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17204. These allow visual inspection of the internal detail of the map and identification of artifacts.

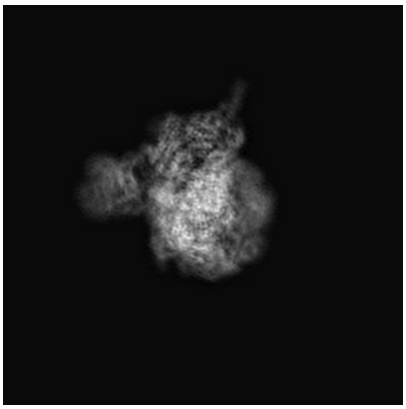
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

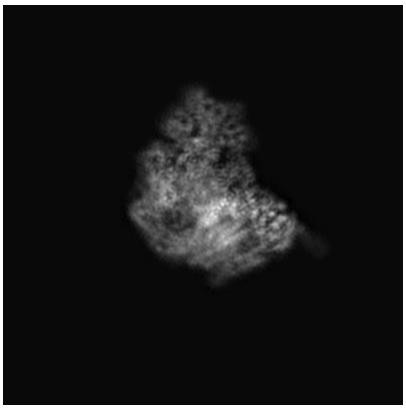
6.1.1 Primary map



X

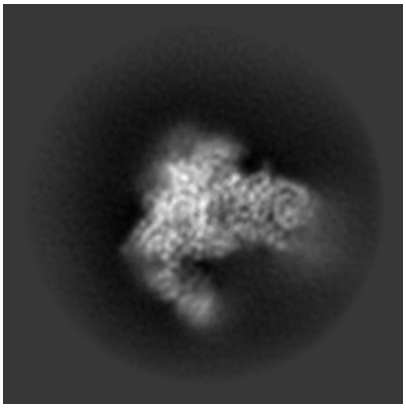


Y

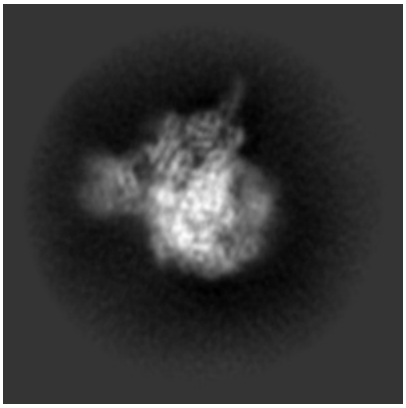


Z

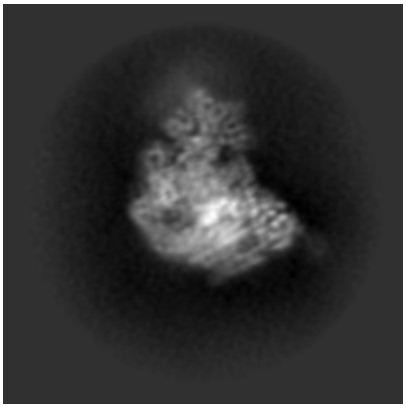
6.1.2 Raw map



X



Y

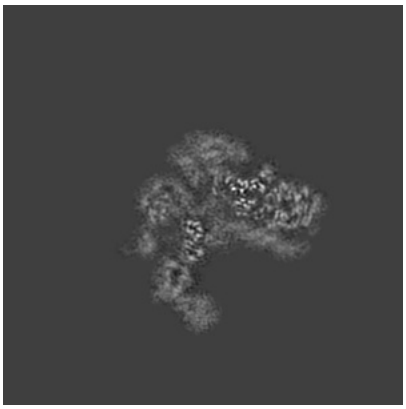


Z

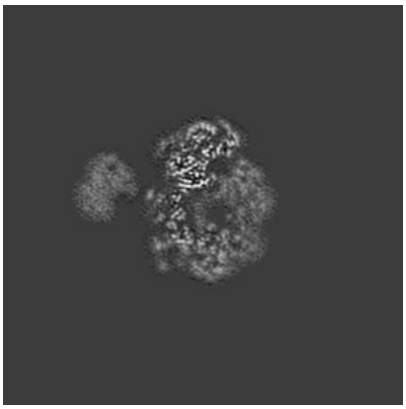
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

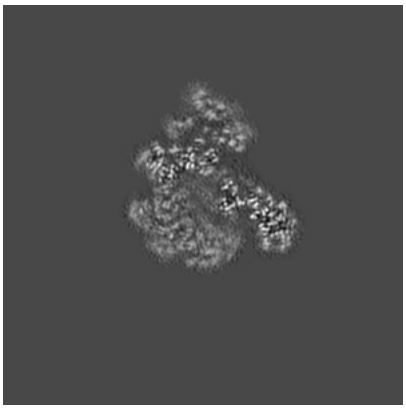
6.2.1 Primary map



X Index: 158

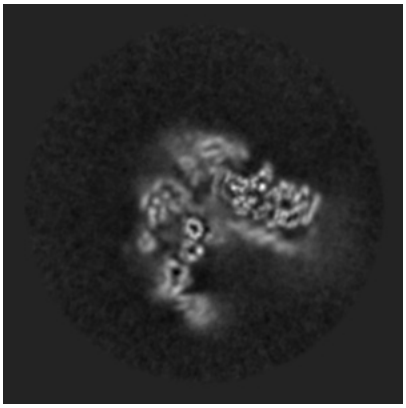


Y Index: 158

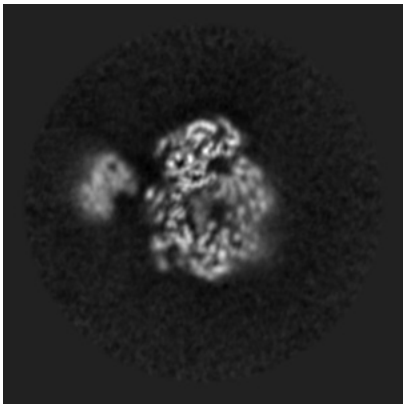


Z Index: 158

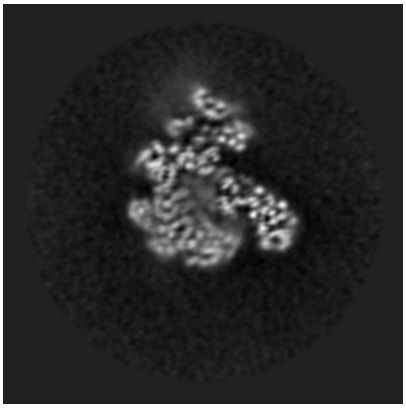
6.2.2 Raw map



X Index: 158



Y Index: 158

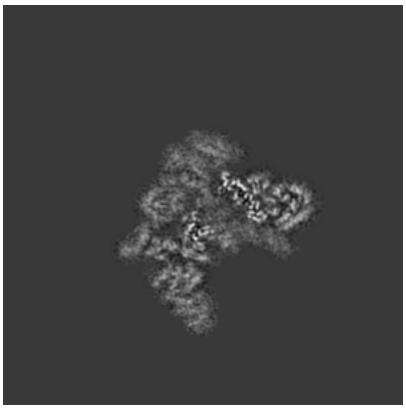


Z Index: 158

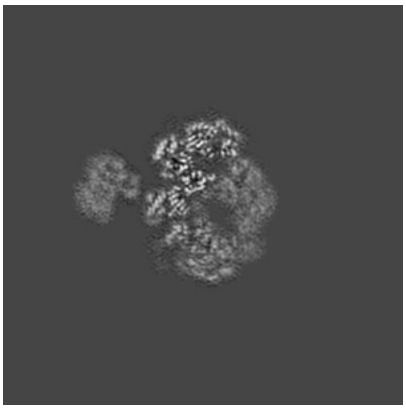
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

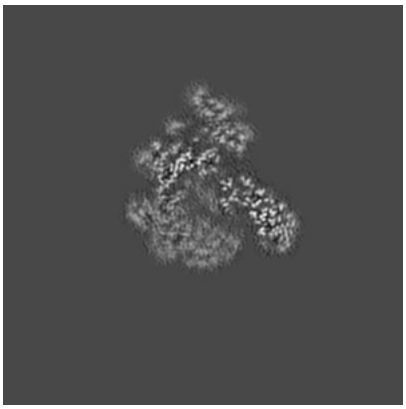
6.3.1 Primary map



X Index: 165

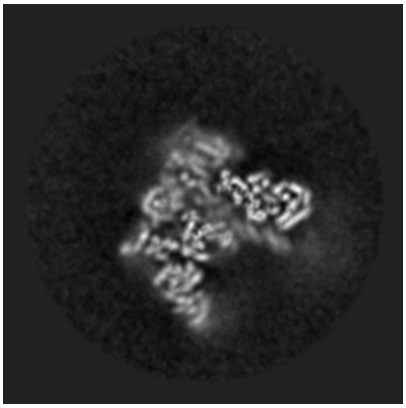


Y Index: 155

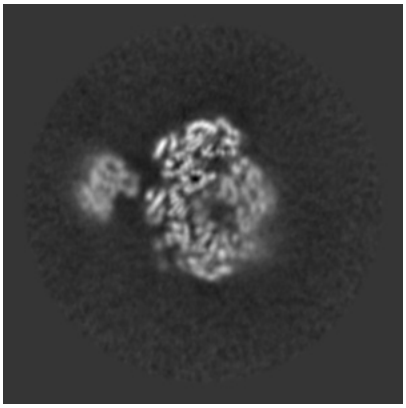


Z Index: 160

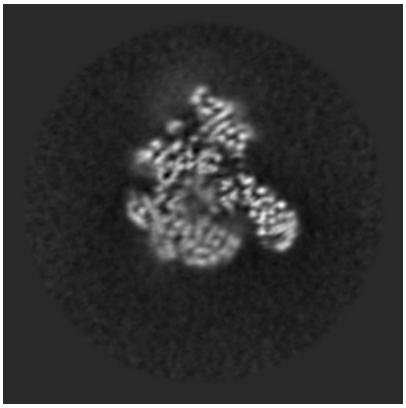
6.3.2 Raw map



X Index: 165



Y Index: 156

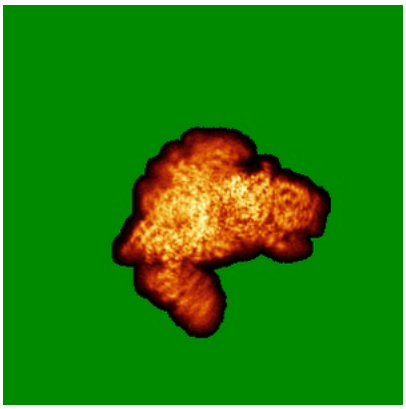


Z Index: 161

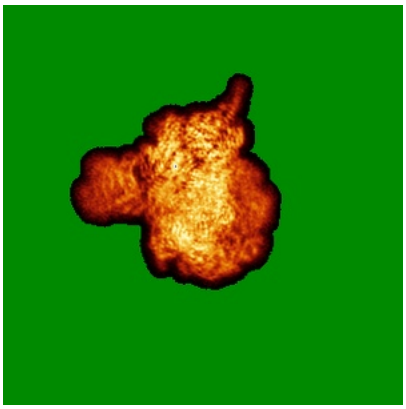
The images above show the largest variance slices of the map in three orthogonal directions.

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

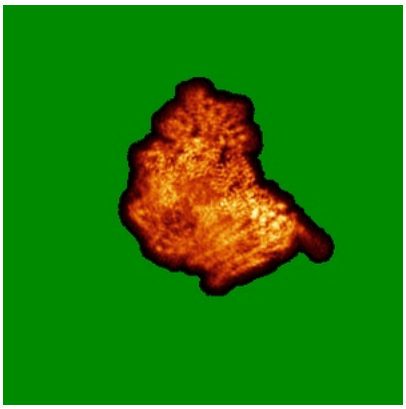
6.4.1 Primary map



X

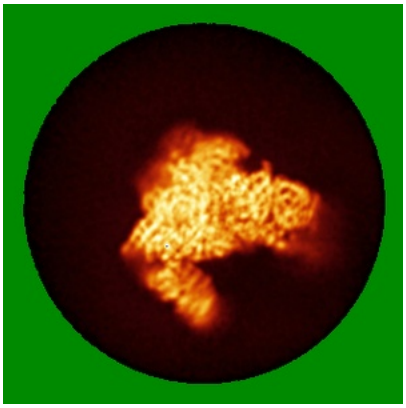


Y

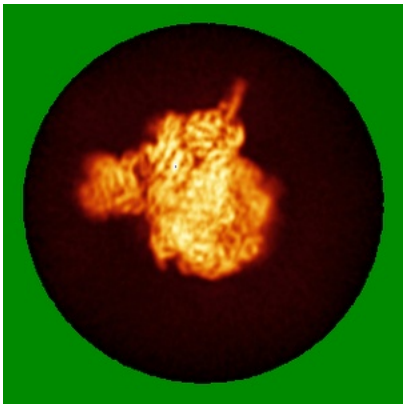


Z

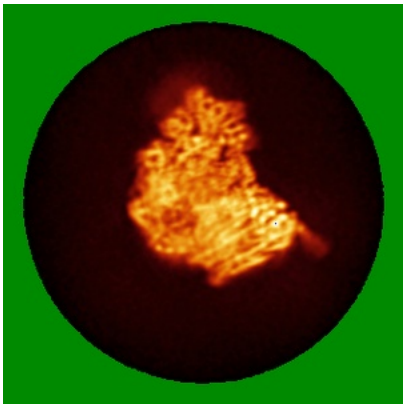
6.4.2 Raw map



X



Y

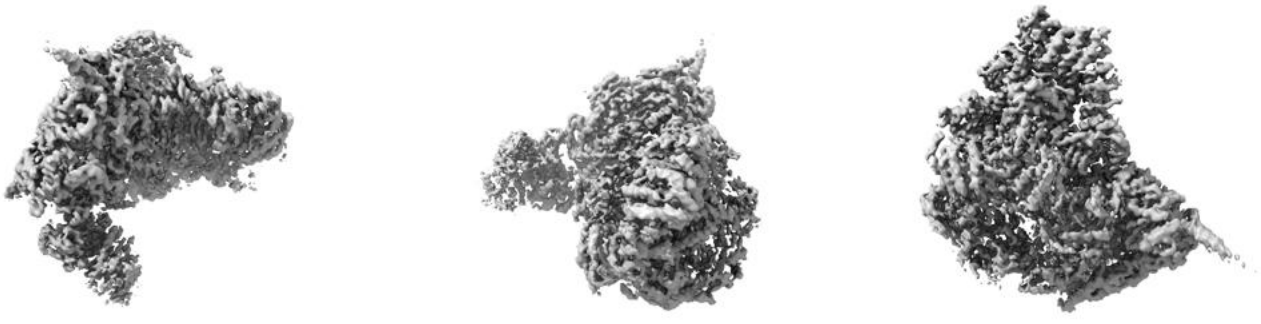


Z

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

6.5 Orthogonal surface views (i)

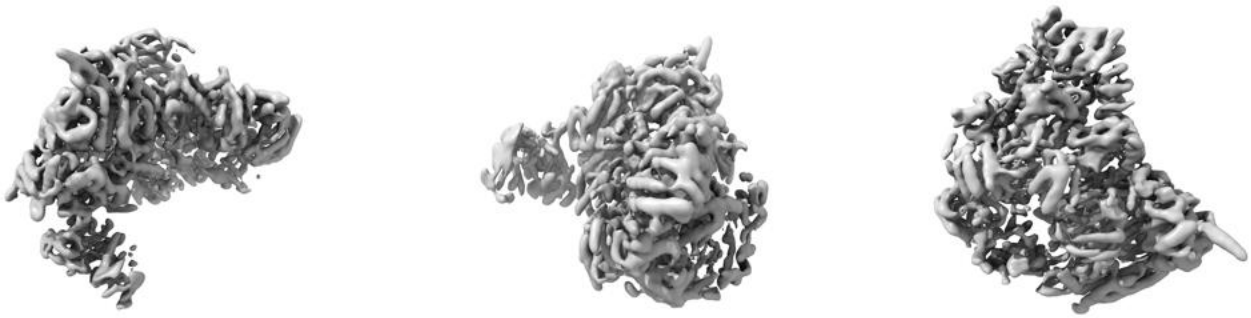
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

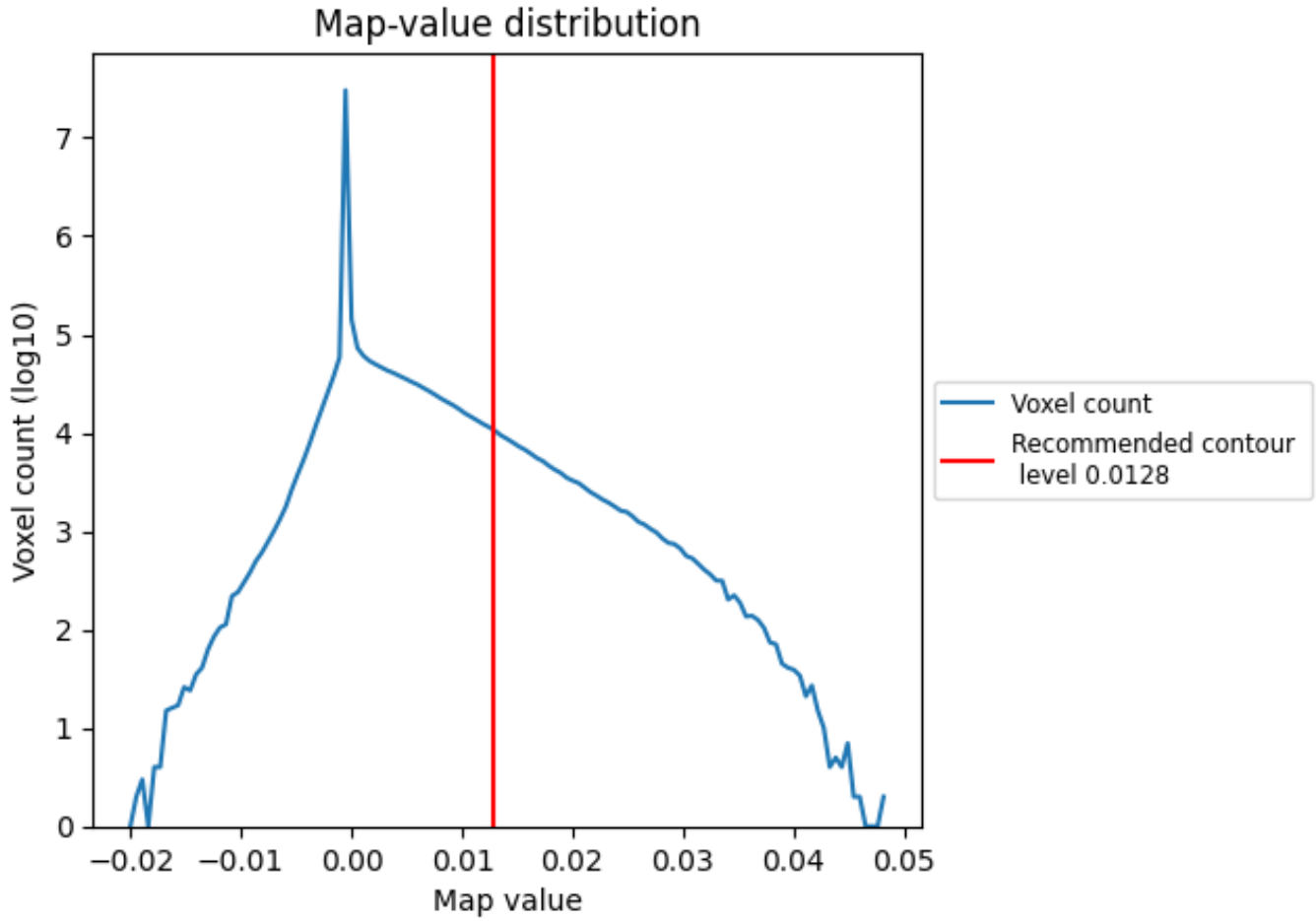
6.6 Mask visualisation (i)

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

7 Map analysis

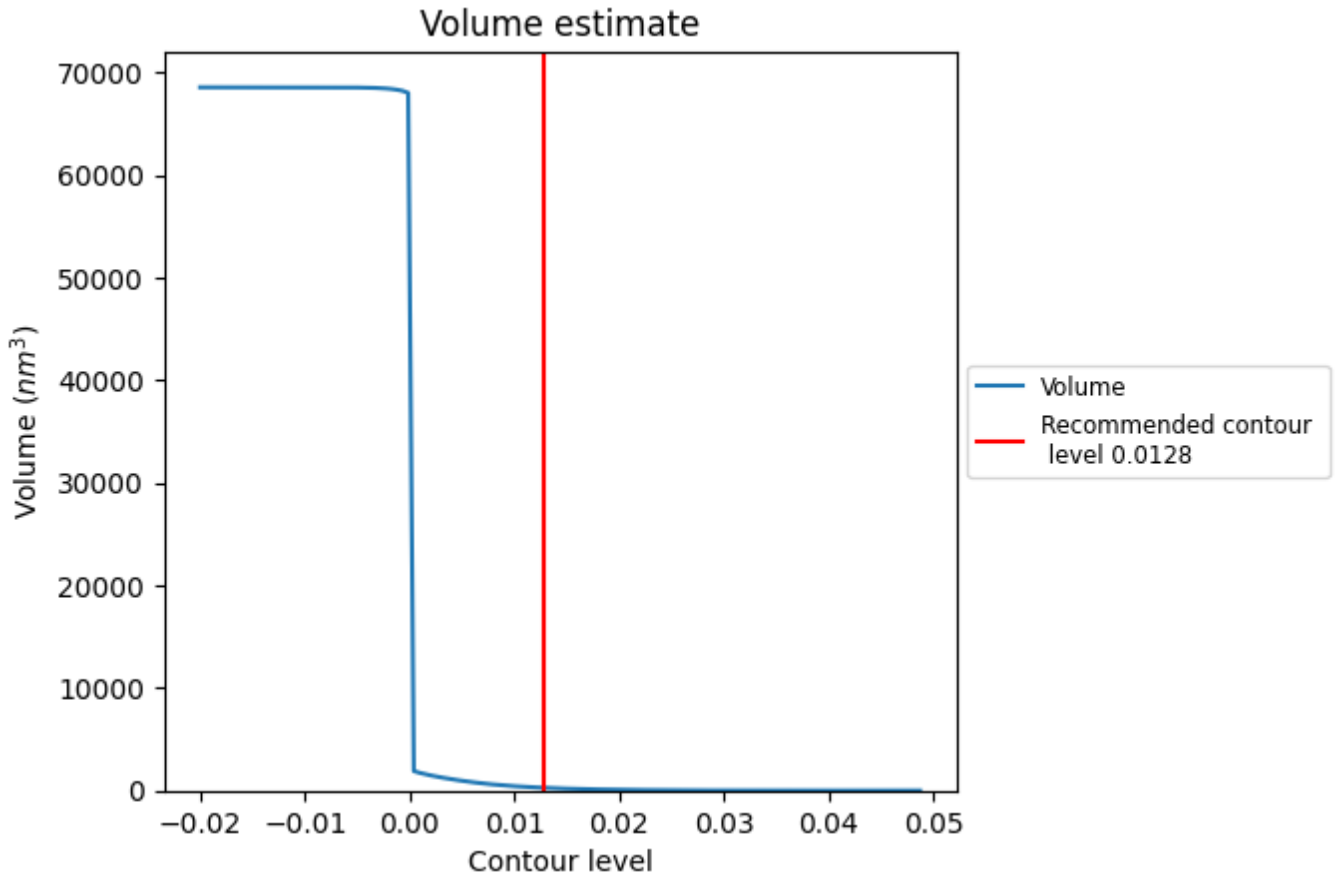
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

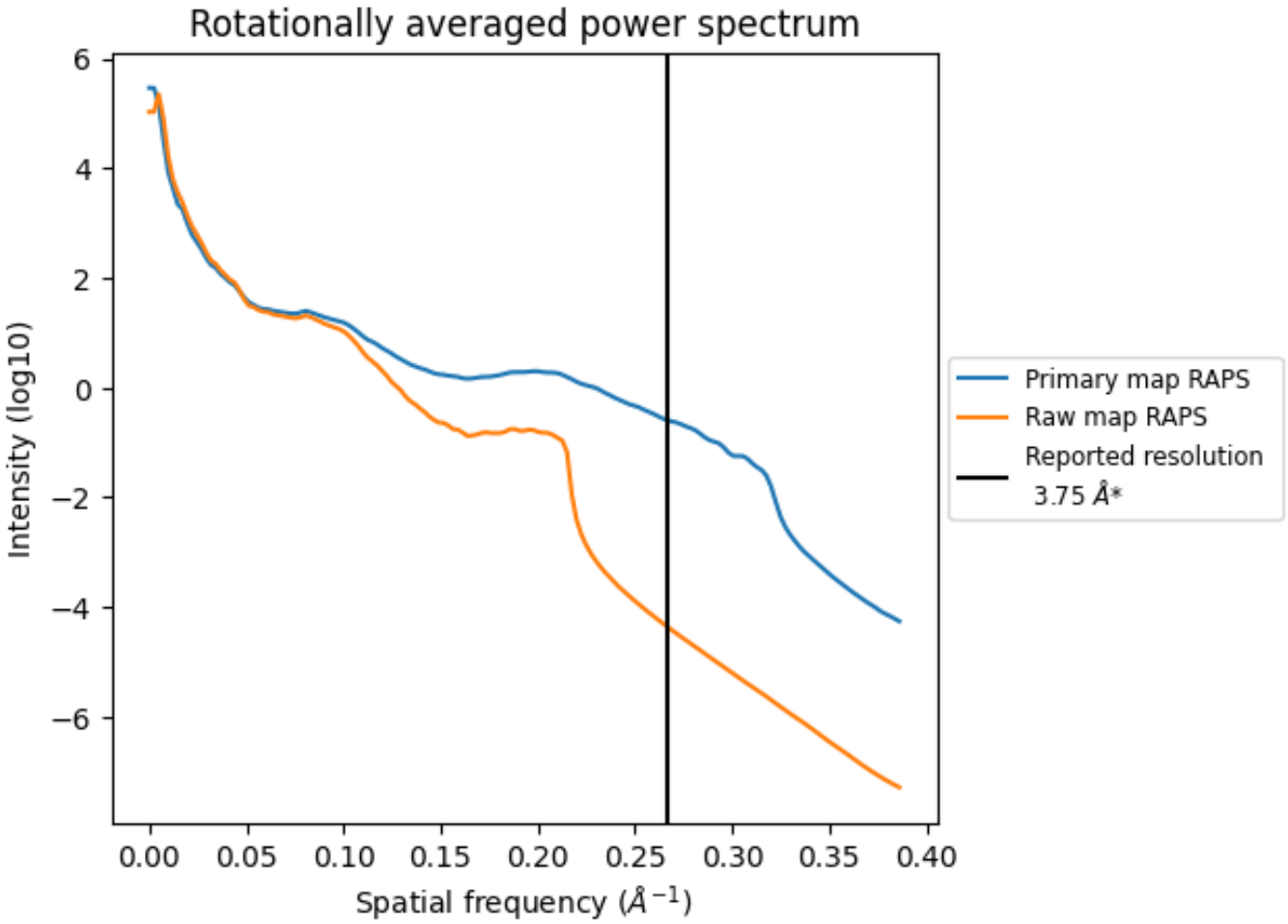
7.2 Volume estimate (i)



The volume at the recommended contour level is 269 nm^3; this corresponds to an approximate mass of 243 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)

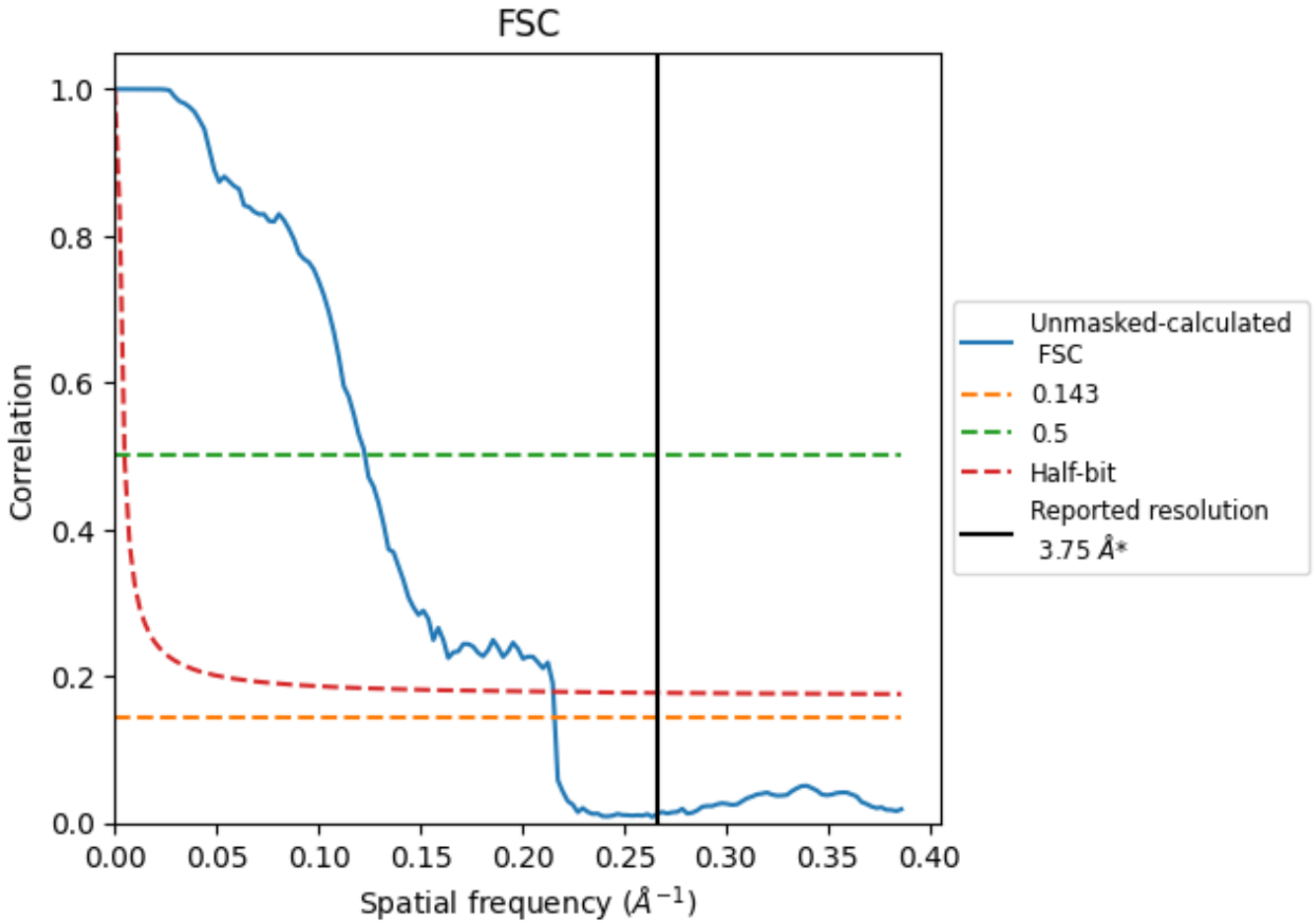


*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

8.2 Resolution estimates (i)

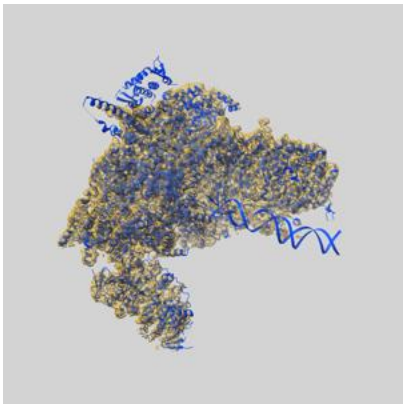
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.63	8.14	4.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.63 differs from the reported value 3.75 by more than 10 %

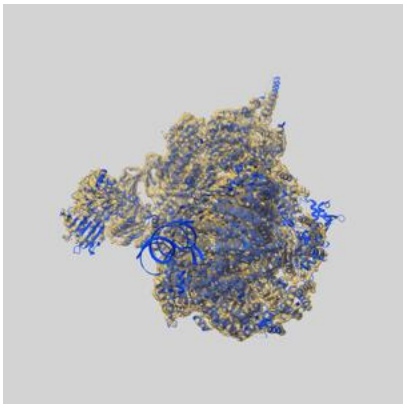
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17204 and PDB model 8OUW. Per-residue inclusion information can be found in section 3 on page 9.

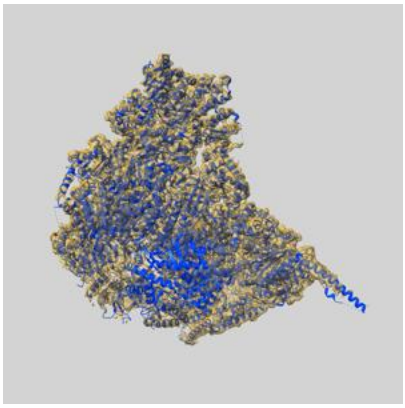
9.1 Map-model overlay



X



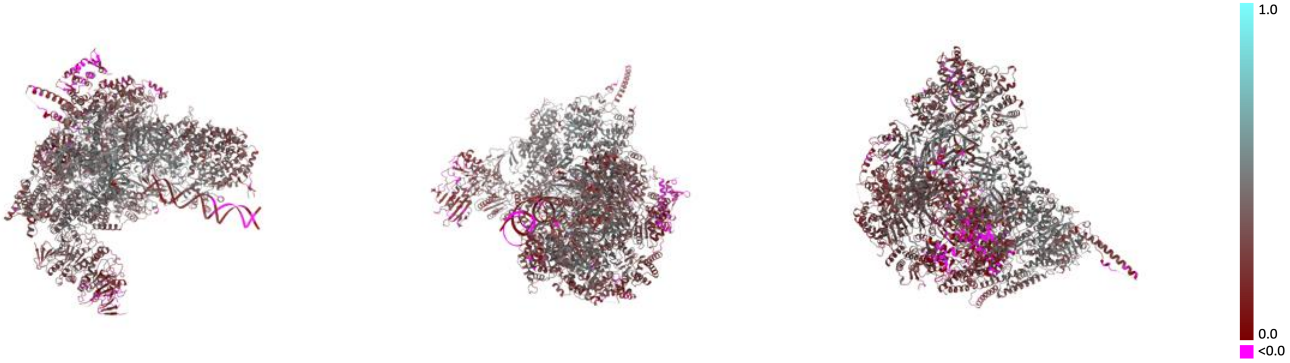
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0128 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.

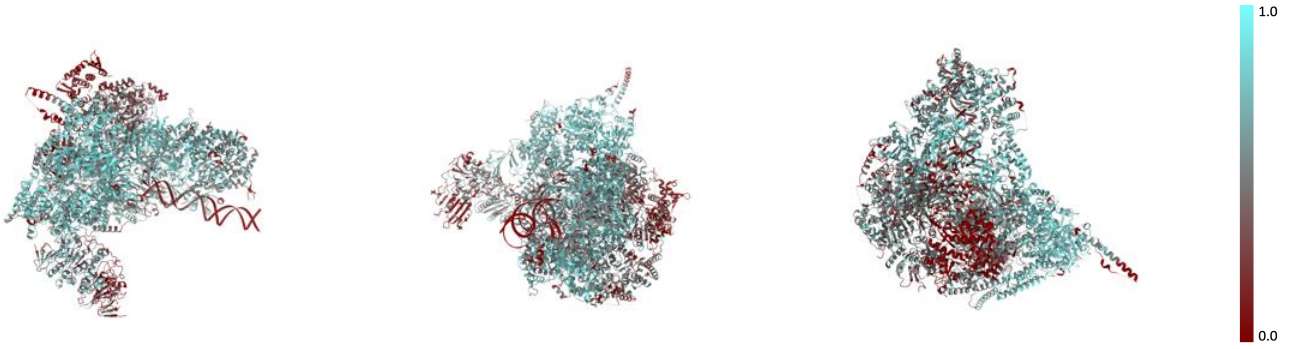
9.2 Q-score mapped to coordinate model (i)



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.

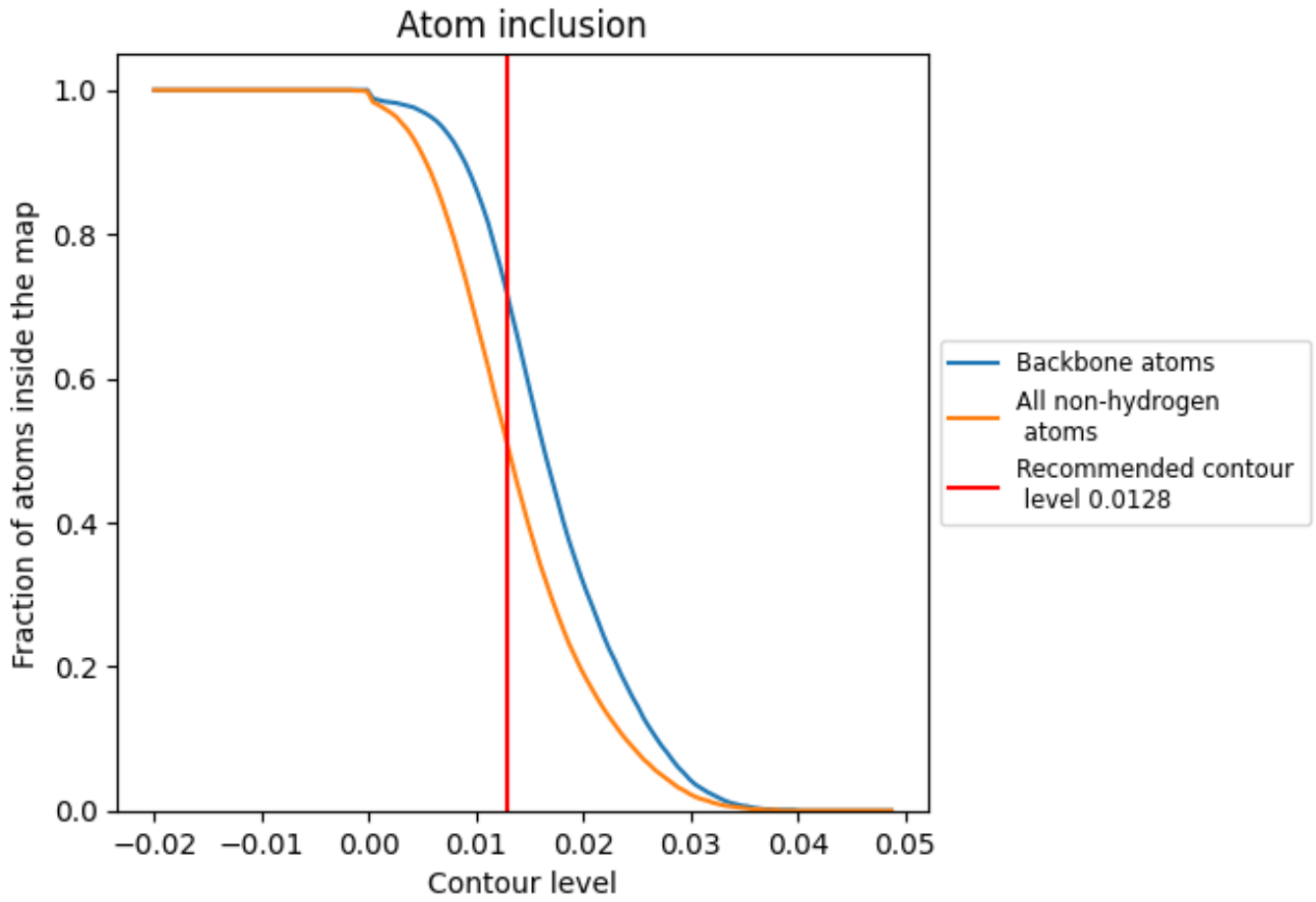
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0128).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 51% 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 (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5140	0.3290
2	0.4090	0.2920
3	0.4840	0.3240
4	0.5330	0.3480
5	0.4940	0.3410
6	0.4210	0.2940
7	0.5740	0.3520
A	0.6940	0.3740
B	0.7390	0.4400
C	0.5580	0.3420
D	0.7020	0.3990
E	0.7300	0.4220
F	0.4740	0.2990
G	0.2510	0.1890
H	0.2660	0.2330
I	0.3940	0.4000
J	0.0970	0.0640
K	0.5760	0.3530
L	0.5840	0.3260
M	0.0780	0.0890