



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:27 AM UTC

PDB ID : 8OUW / pdb_00008ouw
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

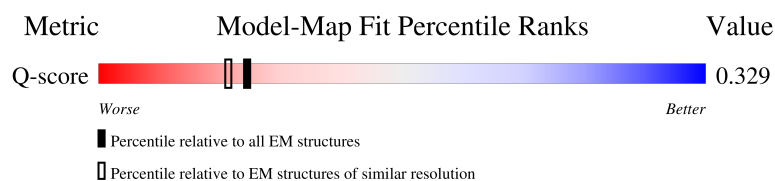
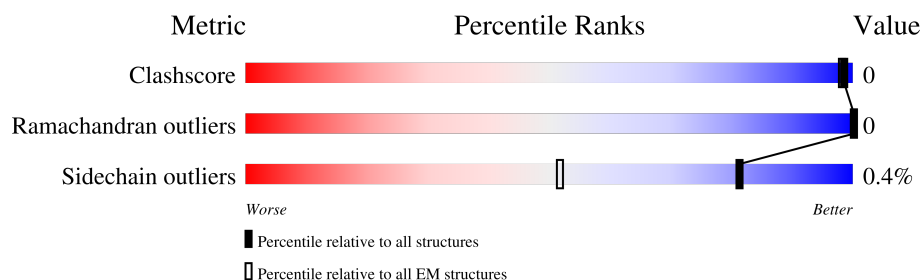
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10301 (3.25 - 4.25)

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	2	881	40% 79% 20%
2	3	812	26% 75% 24%
3	4	823	22% 74% 25%
4	5	759	28% 70% 29%

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Mol	Chain	Length	Quality of chain
5	6	810	
6	7	730	
7	A	205	
8	B	180	
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

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
1	2	701	Total	C	N	O	S	0	0
			5547	3466	978	1067	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	619	Total	C	N	O	S	0	0
			4872	3045	871	928	28		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	707	Total	C	N	O	S	0	0
			5595	3507	981	1072	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	632	Total	C	N	O	S	0	0
			4963	3103	870	952	38		

- 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	0	0
			2564	1630	429	484	21		
12	H	16	Total	C	N	O		0	0
			148	90	35	23			

- 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	0	0
			180	90	18	63	9		
13	J	29	Total	C	N	O	P	0	0
			611	290	118	174	29		

- Molecule 14 is a protein called Protein timeless homolog.

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

- Molecule 15 is a protein called Protein TIPIN homolog.

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

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	0	0
			578	279	96	174	29		

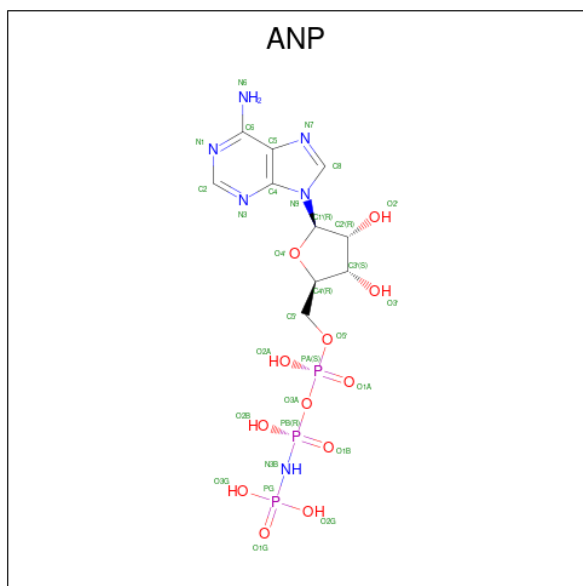
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

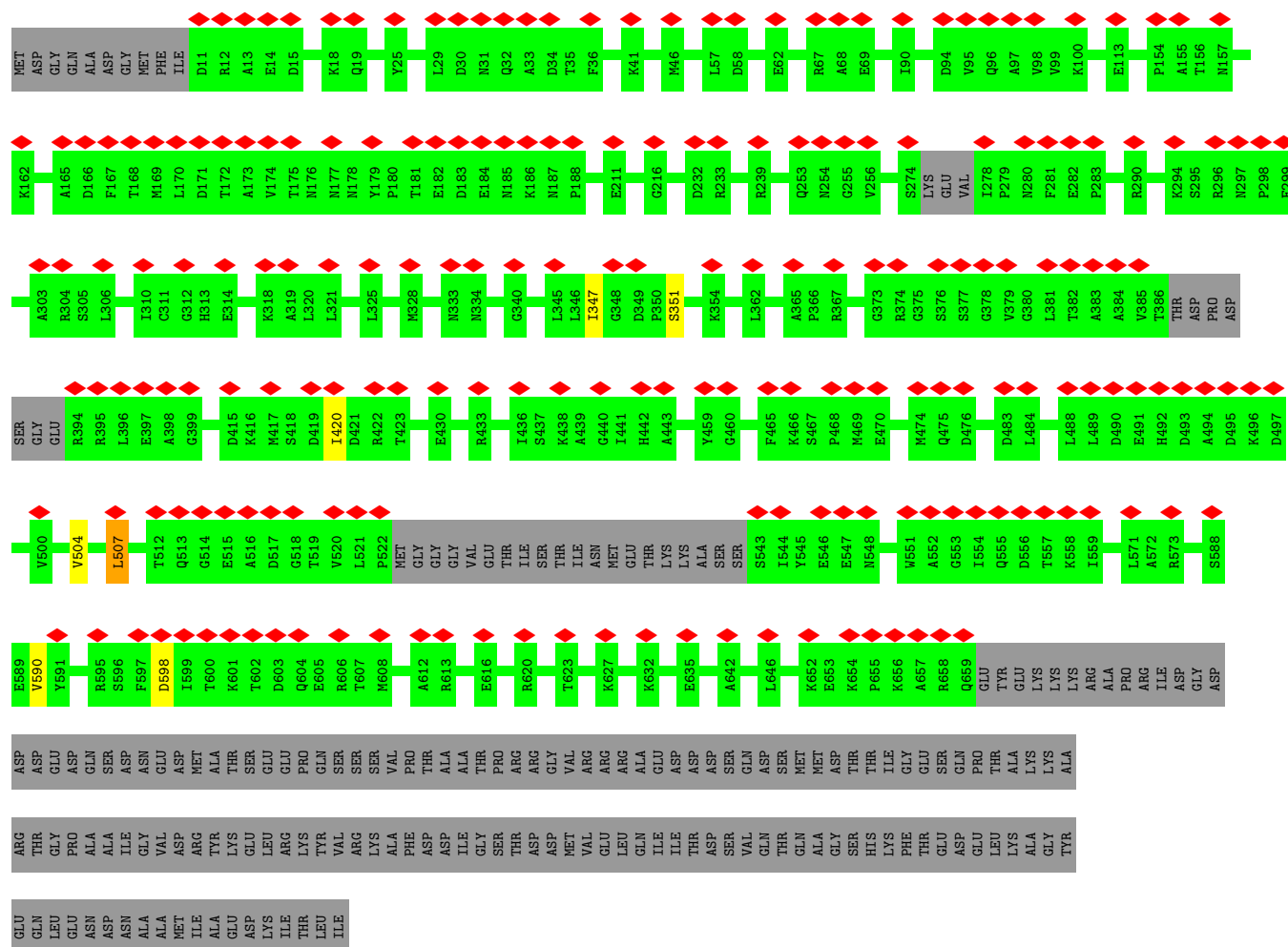
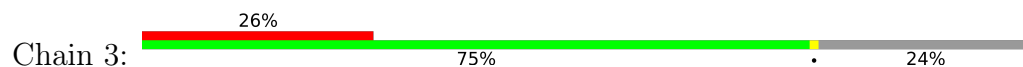
Mol	Chain	Residues	Atoms		AltConf
18	3	1	Total	Mg	0
			1	1	
18	4	1	Total	Mg	0
			1	1	
18	6	1	Total	Mg	0
			1	1	
18	7	1	Total	Mg	0
			1	1	

- Molecule 19 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

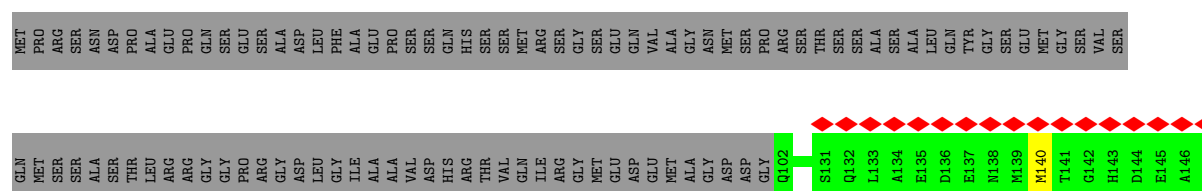
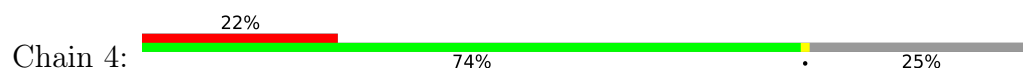


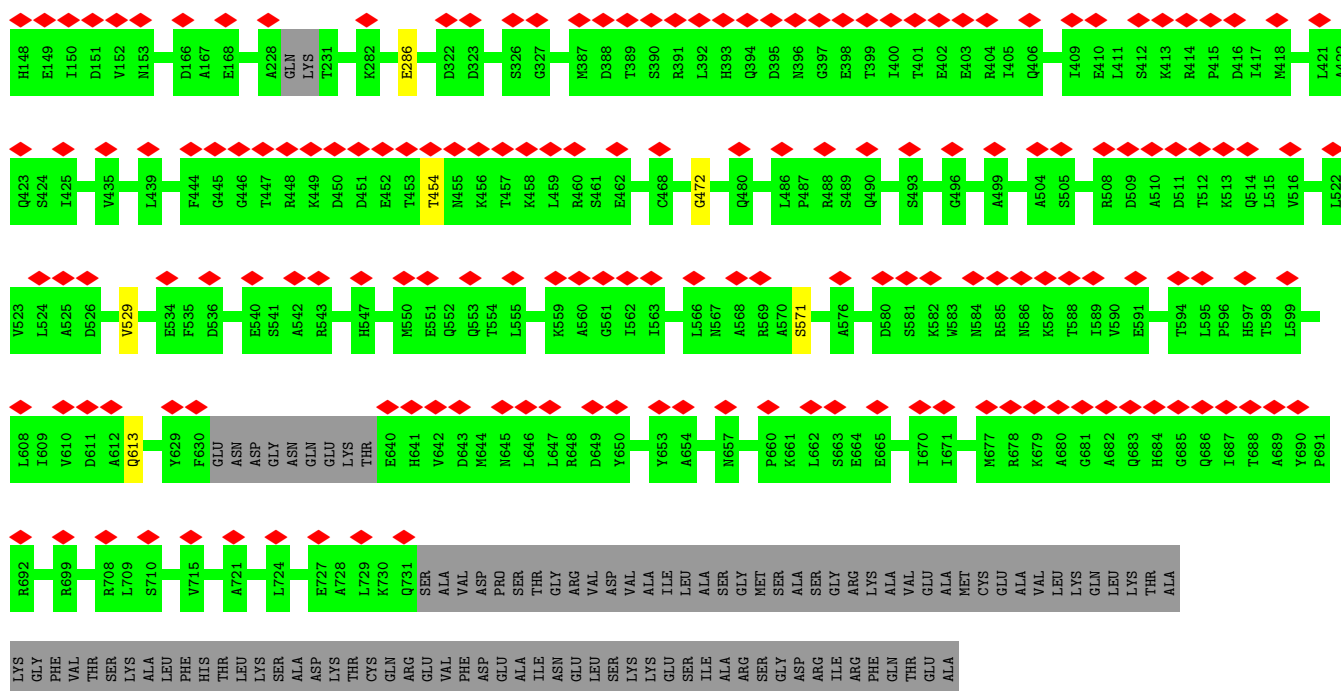
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	4	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	6	1	Total	C	N	O	P	0
			31	10	6	12	3	
19	7	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 2: DNA replication licensing factor MCM3

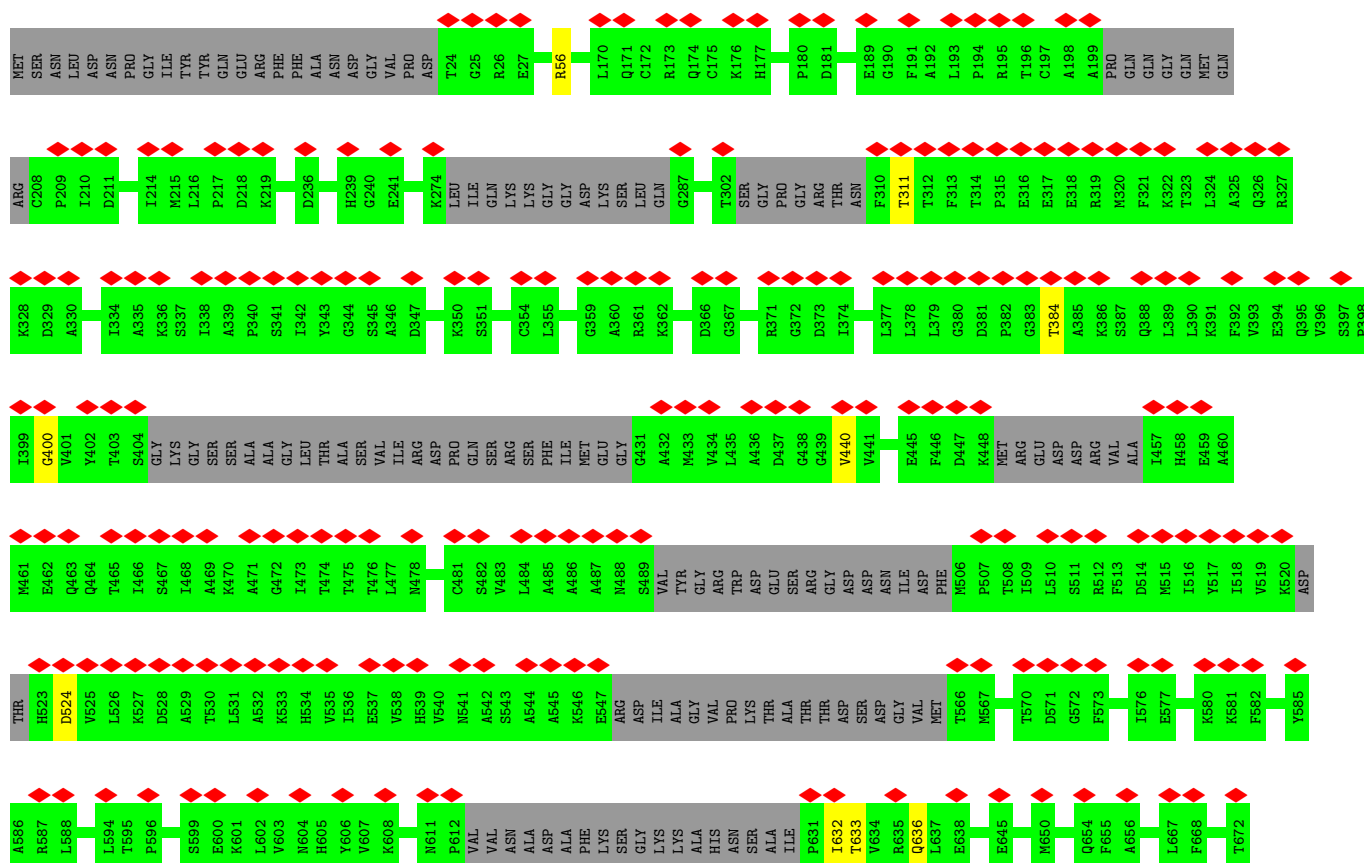


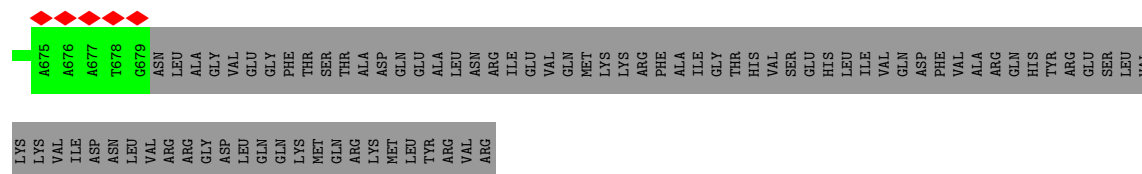
- Molecule 3: DNA replication licensing factor mcm-4





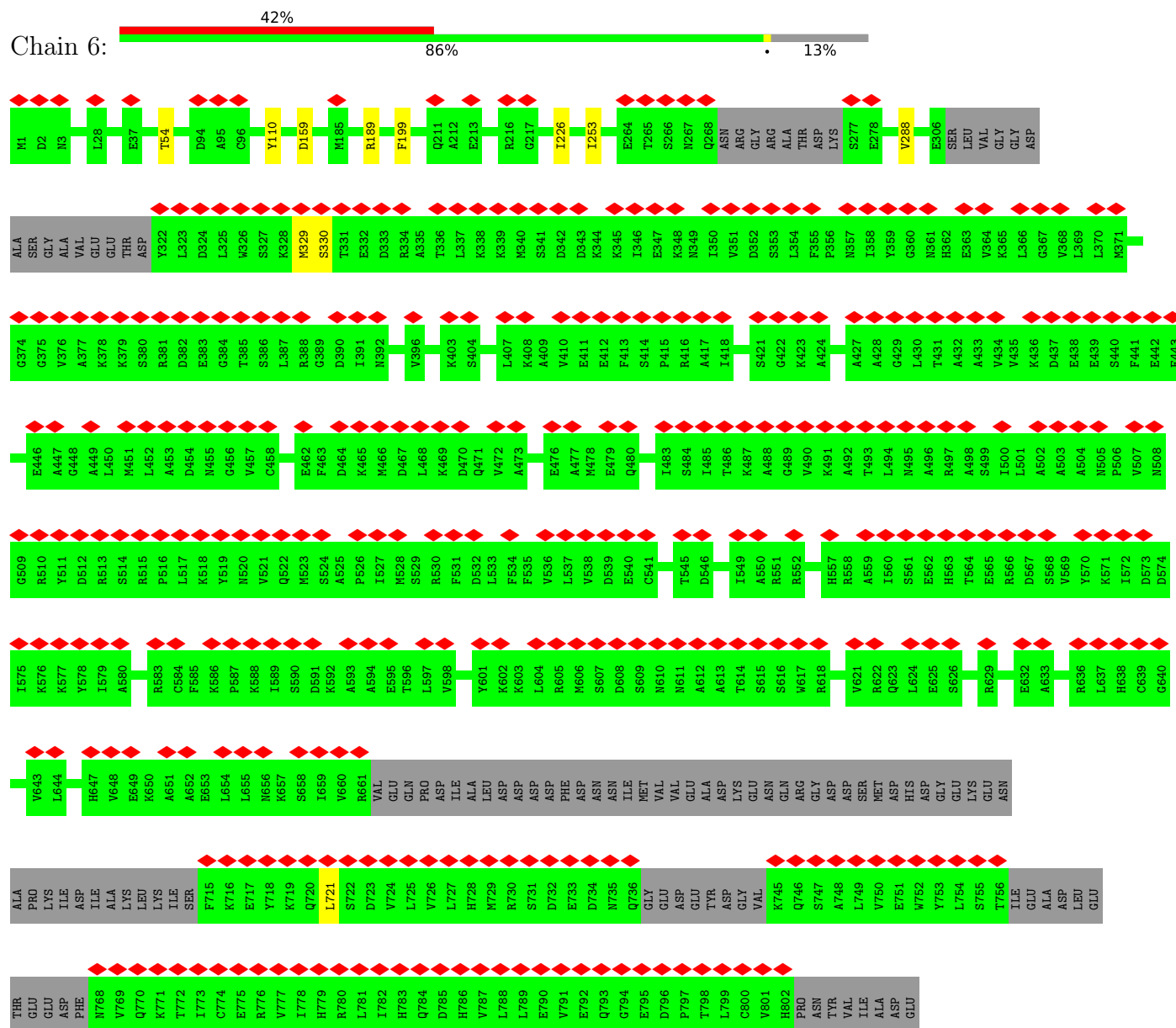
• Molecule 4: DNA replication licensing factor mcm-5



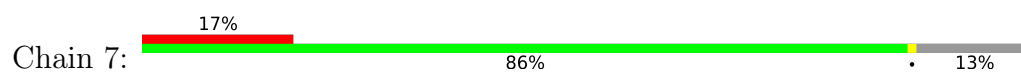


• Molecule 5: DNA replication licensing factor mcm-6

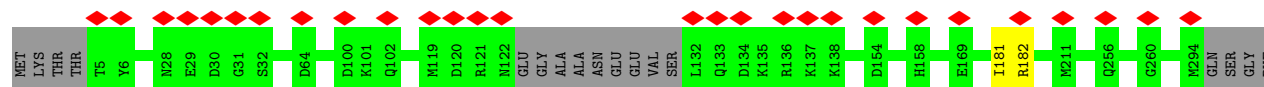
Chain 6:

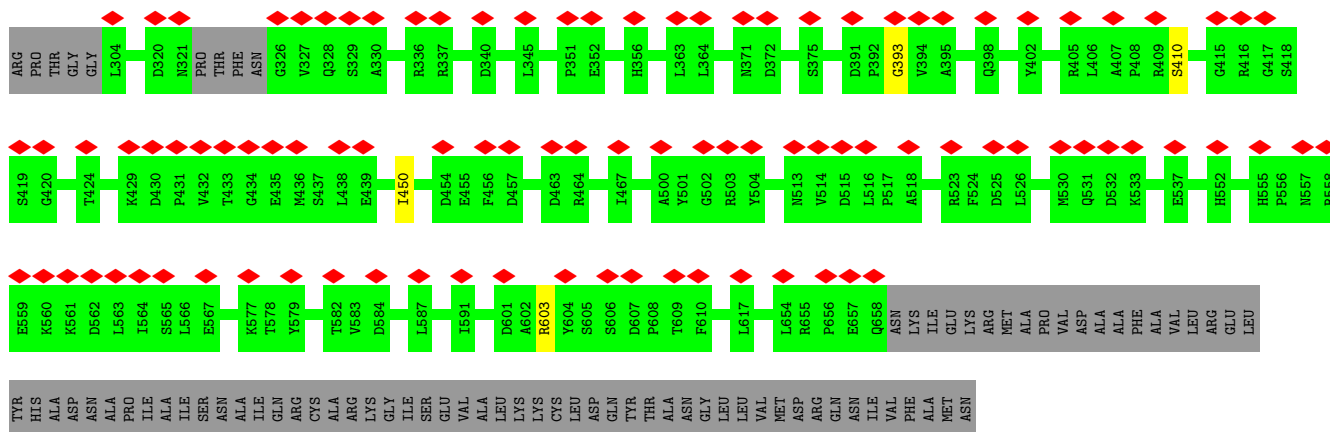


• Molecule 6: DNA replication licensing factor MCM7

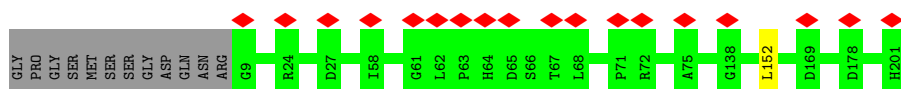


Chain 7:

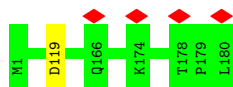




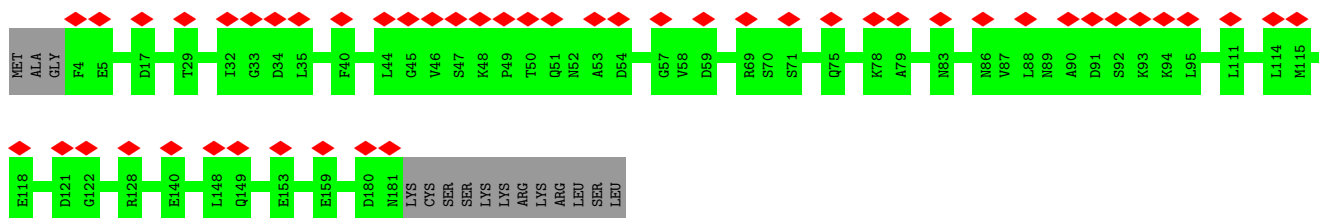
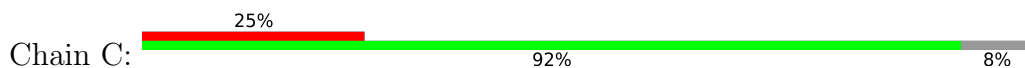
• Molecule 7: Probable DNA replication complex GINS protein PSF1



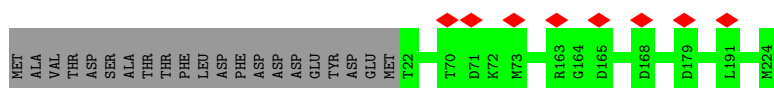
• Molecule 8: Probable DNA replication complex GINS protein PSF2



• Molecule 9: DNA replication complex GINS protein PSF3

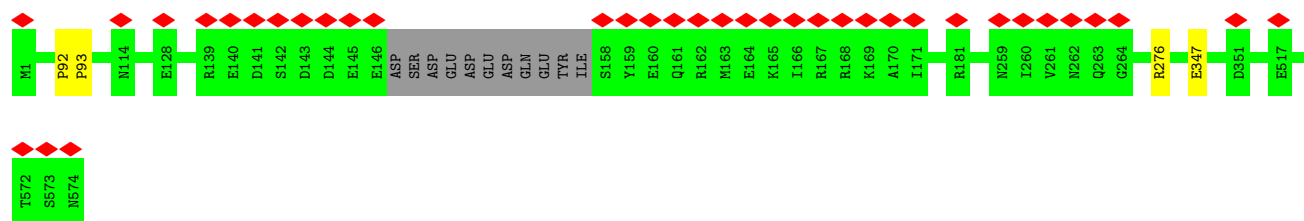


• Molecule 10: DNA replication complex GINS protein SLD5

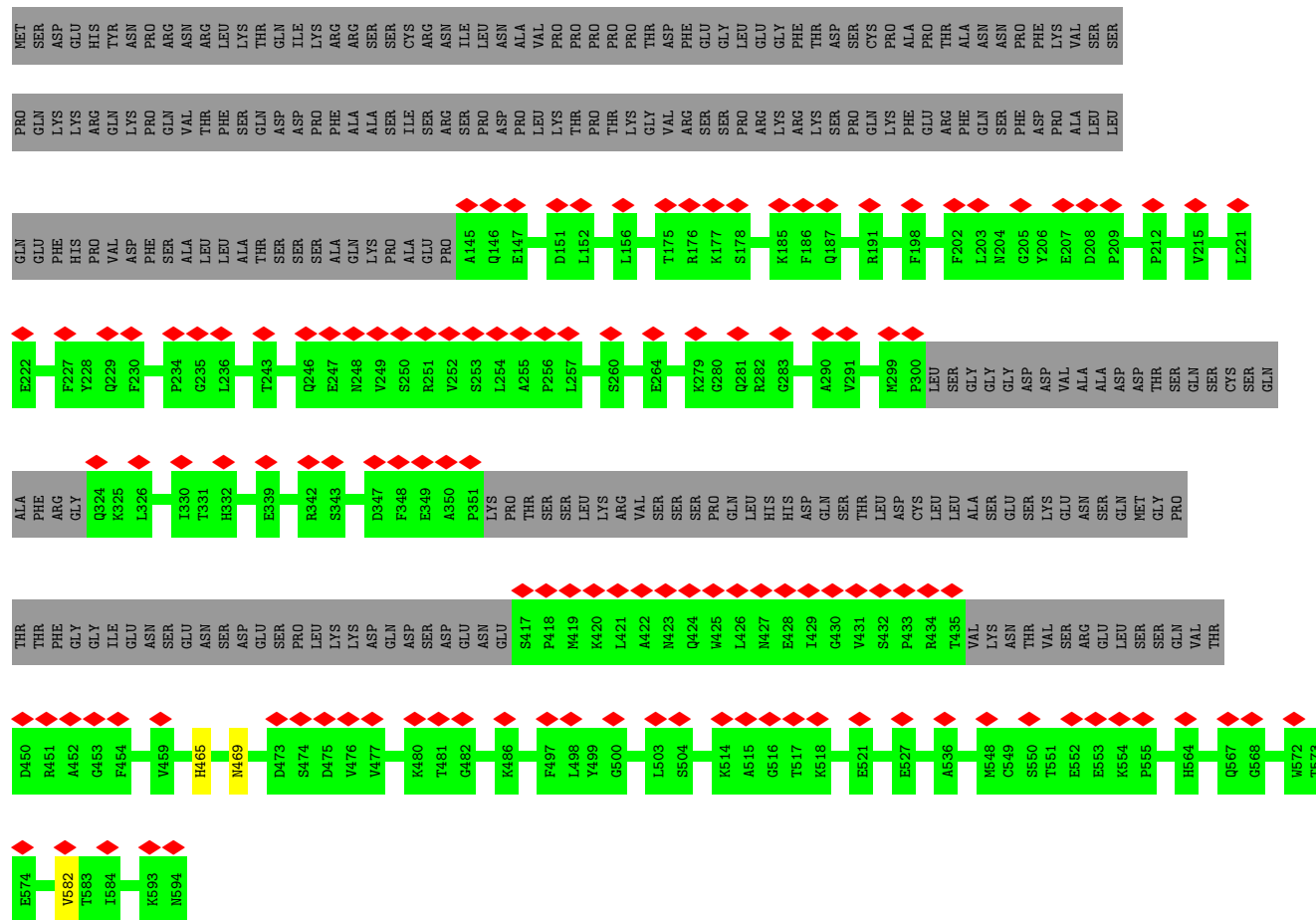


• Molecule 11: Cell division control protein 45 homolog

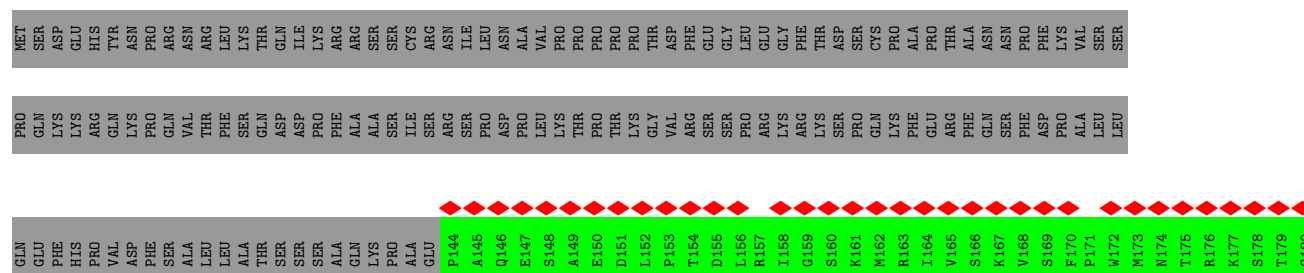
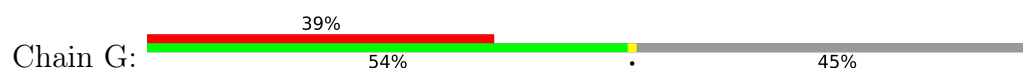


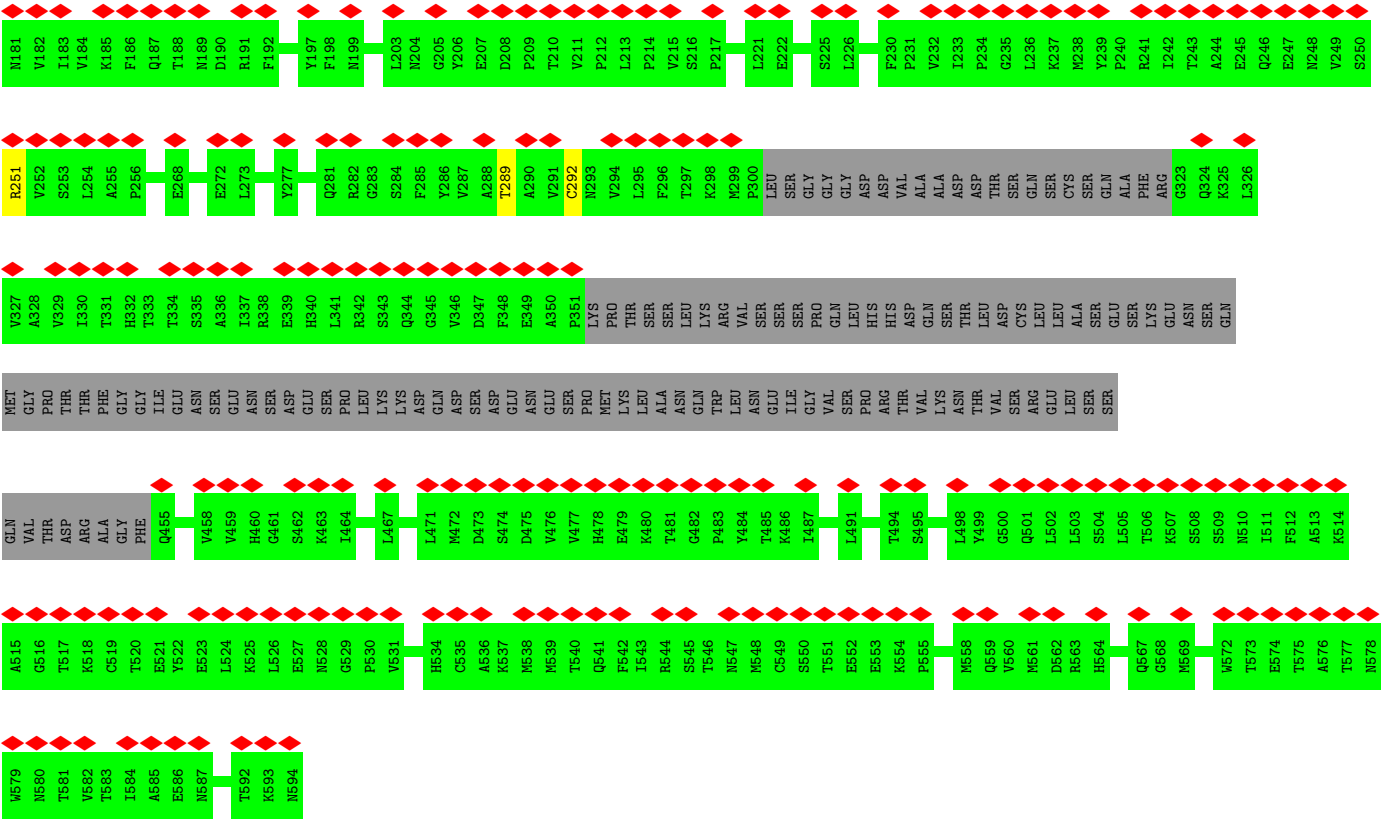


• Molecule 12: Downstream Neighbor of SoN homolog

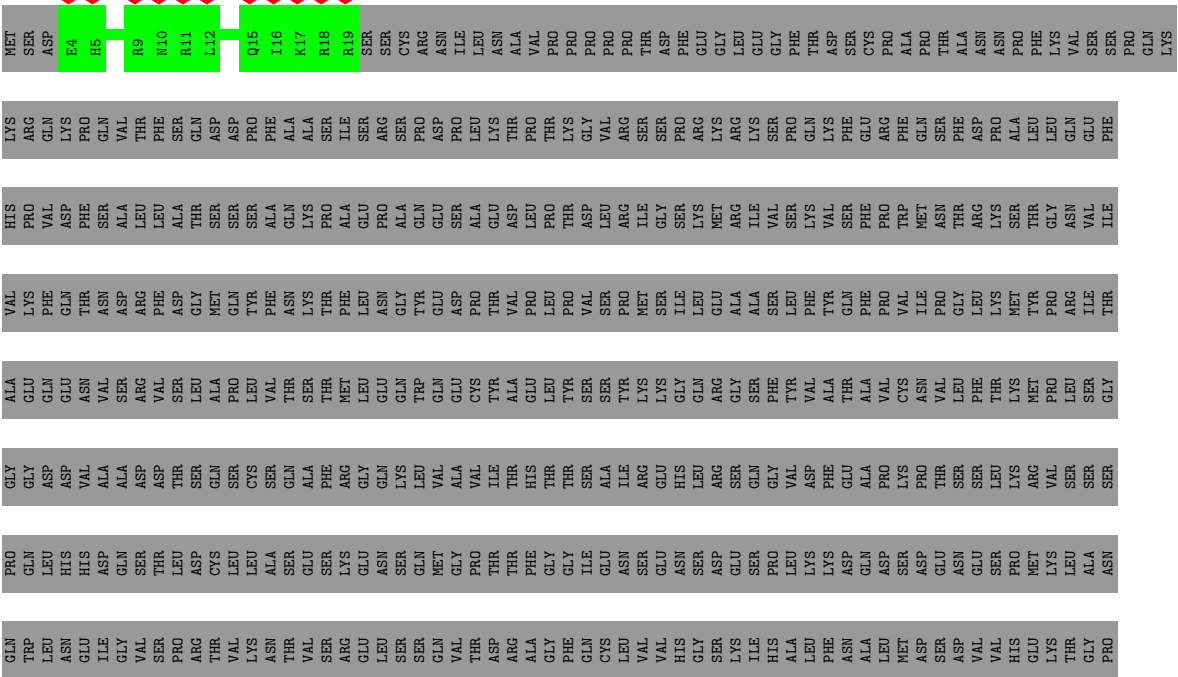


• Molecule 12: Downstream Neighbor of SoN homolog





● Molecule 12: Downstream Neighbor of SoN homolog



[illegible]

- Molecule 13: DNA Leading Strand Template

[illegible]

- Molecule 13: DNA Leading Strand Template

[illegible]

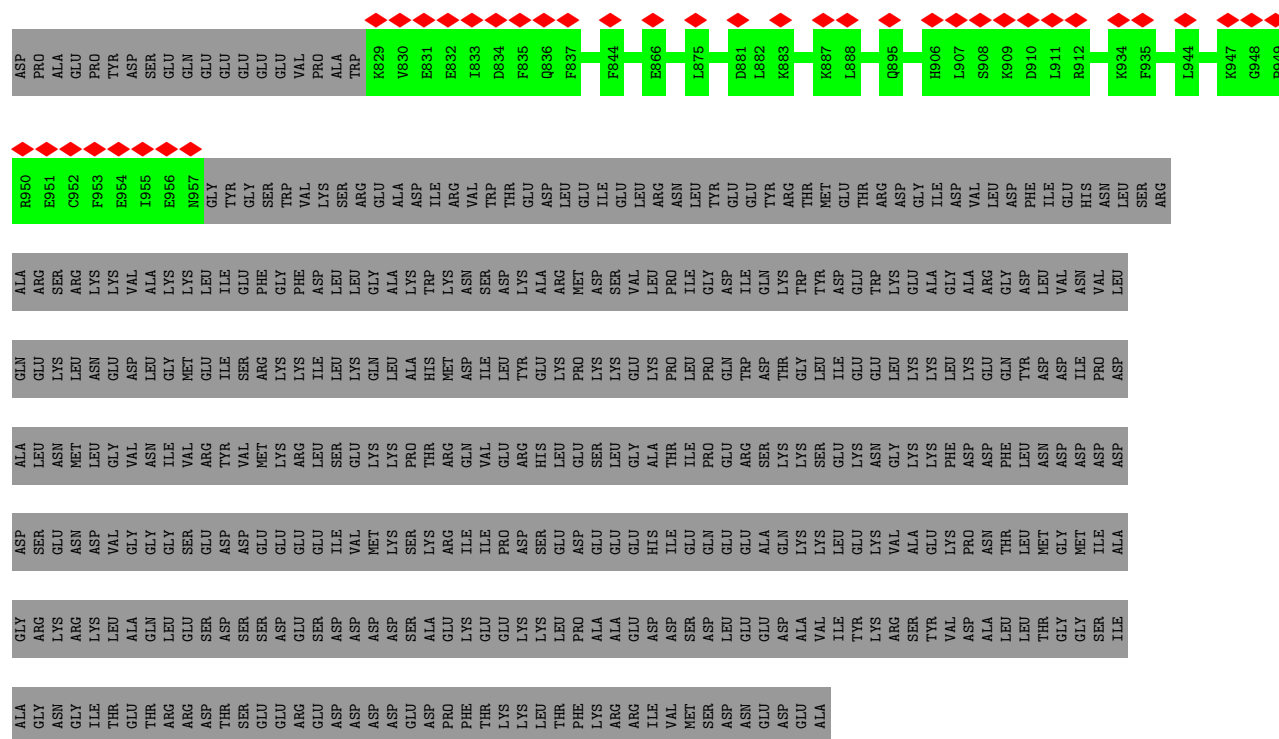
- Molecule 14: Protein timeless homolog

[illegible]

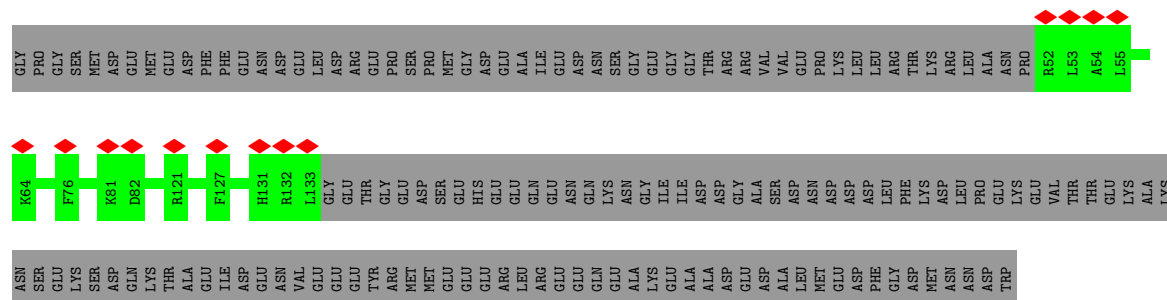
LEU LYS LYS GLU VAL PRO PRO GLU MET MET ARG GLY MET MET ASN PRO PRO ILE ASP SER GLN LEU ASP VAL VAL VAL ASP ASP ALA ALA GLN GLN LYS PHE PHE LYS LEU SER SER ILE TLE ARG ARG LEU ARG ARG GLY GLY PHE PRO ALA ALA VAL VAL LEU TYR HIS HIS SER SER ARG ARG ALA LEU LEU TRP TRP PRO PRO GLU GLU SER SER PHE

lys	arg	gly	leu	thr	asp	asn	gln	asp	ser	pro	gly	glu	glu	asp	gln	leu	leu	glu	leu	glu	asp	met	lys	lys	val	ala	ala	lys	asp	leu	lys	lys	cys	lys	thr	cys	glu	glu	asp	asp	pro	ala	ala	tyr	lys	lys	thr	lys	thr	asp	lys	met	asp	ala	ala	thr	ala	lys
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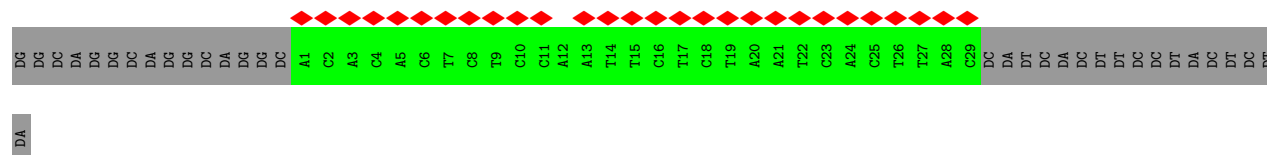
[illegible][illegible]



- Molecule 15: Protein TIPIN homolog



- Molecule 16: DNA Lagging Strand Template



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.29	0/5637	0.61	0/7608
2	3	0.30	0/4945	0.62	0/6672
3	4	0.29	0/4988	0.63	0/6748
4	5	0.31	0/4323	0.64	0/5828
5	6	0.30	0/5675	0.61	2/7648 (0.0%)
6	7	0.29	0/5043	0.61	0/6814
7	A	0.32	0/1562	0.61	0/2107
8	B	0.31	0/1447	0.64	0/1954
9	C	0.31	0/1428	0.56	0/1924
10	D	0.33	0/1652	0.57	0/2230
11	E	0.29	0/4637	0.61	0/6262
12	F	0.33	0/2803	0.65	0/3801
12	G	0.34	0/2623	0.63	0/3558
12	H	0.28	0/150	0.65	0/198
13	I	0.27	0/197	0.66	0/302
13	J	0.29	0/688	0.59	0/1064
14	K	0.35	0/5554	0.63	0/7467
15	L	0.30	0/695	0.64	0/931
16	M	0.29	0/644	0.61	0/987
All	All	0.31	0/54691	0.62	2/74103 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	288	VAL	N-CA-C	-6.71	107.34	113.71
5	6	330	SER	N-CA-C	5.70	117.36	111.03

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 ⓘ

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
17	2	1	0	0	0	0
17	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
6:7:181:ILE:HG22	6:7:182:ARG:HG3	1.90	0.54
5:6:159:ASP:OD2	5:6:189:ARG:NH2	2.42	0.53
4:5:56:ARG:NH1	8:B:119:ASP:OD1	2.40	0.49
2:3:598:ASP:OD1	2:3:598:ASP:N	2.50	0.44
4:5:400:GLY:HA2	4:5:440:VAL:O	2.17	0.44
2:3:504:VAL:HA	2:3:507:LEU:HD23	2.00	0.43
1:2:254:CYS:SG	1:2:255:ASN:N	2.91	0.43
3:4:529:VAL:HG22	3:4:571:SER:HB2	2.01	0.42
4:5:633:THR:OG1	4:5:636:GLN:OE1	2.37	0.42
1:2:275:GLN:NE2	5:6:199:PHE:O	2.51	0.42
11:E:92:PRO:HA	11:E:93:PRO:HD3	1.90	0.42
12:F:465:HIS:O	12:F:469:ASN:ND2	2.51	0.42
1:2:724:MET:HB3	1:2:736:ILE:HD12	2.01	0.42
3:4:613:GLN:HB3	6:7:603:ARG:HE	1.86	0.40
6:7:410:SER:HA	6:7:450:ILE:O	2.22	0.40

There are no symmetry-related clashes.

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	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%)	613 (99%)	4 (1%)	78	79
2	3	538/700 (77%)	534 (99%)	4 (1%)	76	77
3	4	546/710 (77%)	543 (100%)	3 (0%)	81	81
4	5	468/650 (72%)	465 (99%)	3 (1%)	78	79
5	6	623/709 (88%)	620 (100%)	3 (0%)	81	81
6	7	545/623 (88%)	545 (100%)	0	100	100
7	A	167/176 (95%)	166 (99%)	1 (1%)	78	79
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%)	509 (100%)	0	100	100
12	F	310/532 (58%)	309 (100%)	1 (0%)	86	84
12	G	291/532 (55%)	288 (99%)	3 (1%)	68	73
12	H	16/532 (3%)	16 (100%)	0	100	100
14	K	601/1213 (50%)	601 (100%)	0	100	100
15	L	74/209 (35%)	74 (100%)	0	100	100
All	All	5806/8405 (69%)	5784 (100%)	22 (0%)	81	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	275	GLN
1	2	347	HIS
1	2	807	LEU
1	2	876	ILE
2	3	347	ILE
2	3	420	ILE
2	3	507	LEU
2	3	590	VAL
3	4	140	MET
3	4	286	GLU
3	4	454	THR
4	5	311	THR
4	5	384	THR
4	5	632	ILE
5	6	226	ILE
5	6	253	ILE

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Mol	Chain	Res	Type
5	6	721	LEU
7	A	152	LEU
12	F	582	VAL
12	G	251	ARG
12	G	289	THR
12	G	292	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	200	ASN
1	2	275	GLN
1	2	355	GLN
1	2	406	GLN
1	2	444	GLN
1	2	447	ASN
2	3	104	HIS
2	3	128	ASN
2	3	195	HIS
2	3	207	GLN
2	3	426	HIS
2	3	431	GLN
2	3	442	HIS
2	3	456	ASN
2	3	513	GLN
2	3	548	ASN
3	4	180	ASN
3	4	304	HIS
3	4	394	GLN
4	5	488	ASN
5	6	89	HIS
5	6	175	GLN
5	6	211	GLN
5	6	255	GLN
5	6	610	ASN
6	7	221	ASN
6	7	531	GLN
7	A	145	HIS
7	A	186	GLN
8	B	139	ASN
8	B	143	HIS
8	B	166	GLN

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Mol	Chain	Res	Type
10	D	189	GLN
10	D	222	GLN
11	E	122	ASN
11	E	414	ASN
11	E	547	ASN
12	F	293	ASN
12	F	332	HIS
12	F	427	ASN
12	F	578	ASN
12	G	564	HIS
14	K	388	GLN
14	K	922	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 oligosaccharides 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	6	903	18	33,33,33	0.96	4 (12%)	45,52,52	0.60	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	ANP	4	1502	18	33,33,33	0.94	4 (12%)	45,52,52	0.57	0
19	ANP	7	1500	18	33,33,33	0.94	4 (12%)	45,52,52	0.52	0
19	ANP	3	1502	18	33,33,33	0.91	3 (9%)	45,52,52	0.80	0

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	6	903	18	-	2/18/38/38	0/3/3/3
19	ANP	4	1502	18	-	2/18/38/38	0/3/3/3
19	ANP	7	1500	18	-	3/18/38/38	0/3/3/3
19	ANP	3	1502	18	-	8/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	903	ANP	PB-O3A	-2.94	1.55	1.59
19	4	1502	ANP	PB-O3A	-2.54	1.55	1.59
19	7	1500	ANP	PG-O1G	2.53	1.50	1.46
19	3	1502	ANP	PG-O1G	2.51	1.50	1.46
19	7	1500	ANP	PB-O3A	-2.51	1.56	1.59
19	4	1502	ANP	PG-O1G	2.46	1.49	1.46
19	3	1502	ANP	PG-N3B	2.45	1.69	1.63
19	7	1500	ANP	PG-N3B	2.43	1.69	1.63
19	6	903	ANP	PG-O1G	2.43	1.49	1.46
19	4	1502	ANP	PG-N3B	2.41	1.69	1.63
19	6	903	ANP	PB-O1B	2.36	1.49	1.46
19	7	1500	ANP	PB-O1B	2.34	1.49	1.46
19	3	1502	ANP	PB-O1B	2.34	1.49	1.46
19	6	903	ANP	PG-N3B	2.26	1.69	1.63
19	4	1502	ANP	PB-O1B	2.24	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	903	ANP	O1G-PG-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (15) 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	O4'-C1'-N9-C8
19	3	1502	ANP	O4'-C1'-N9-C4
19	4	1502	ANP	PB-N3B-PG-O1G
19	4	1502	ANP	C5'-O5'-PA-O1A
19	6	903	ANP	PG-N3B-PB-O1B
19	6	903	ANP	PG-N3B-PB-O3A
19	7	1500	ANP	PB-N3B-PG-O1G
19	7	1500	ANP	PA-O3A-PB-O2B
19	3	1502	ANP	O4'-C4'-C5'-O5'
19	3	1502	ANP	C3'-C4'-C5'-O5'
19	3	1502	ANP	C4'-C5'-O5'-PA
19	3	1502	ANP	PA-O3A-PB-O1B
19	7	1500	ANP	PA-O3A-PB-O1B

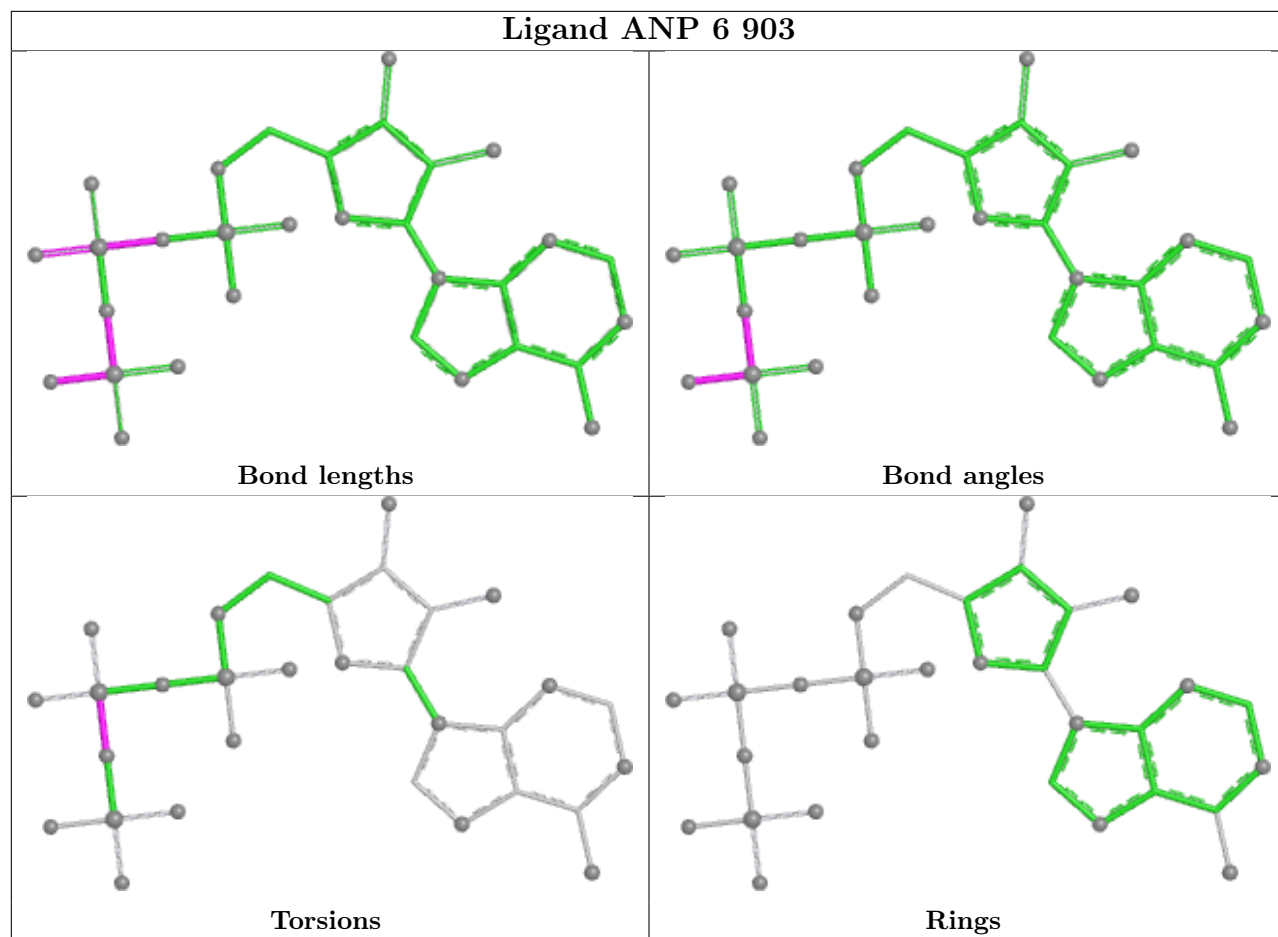
There are no ring outliers.

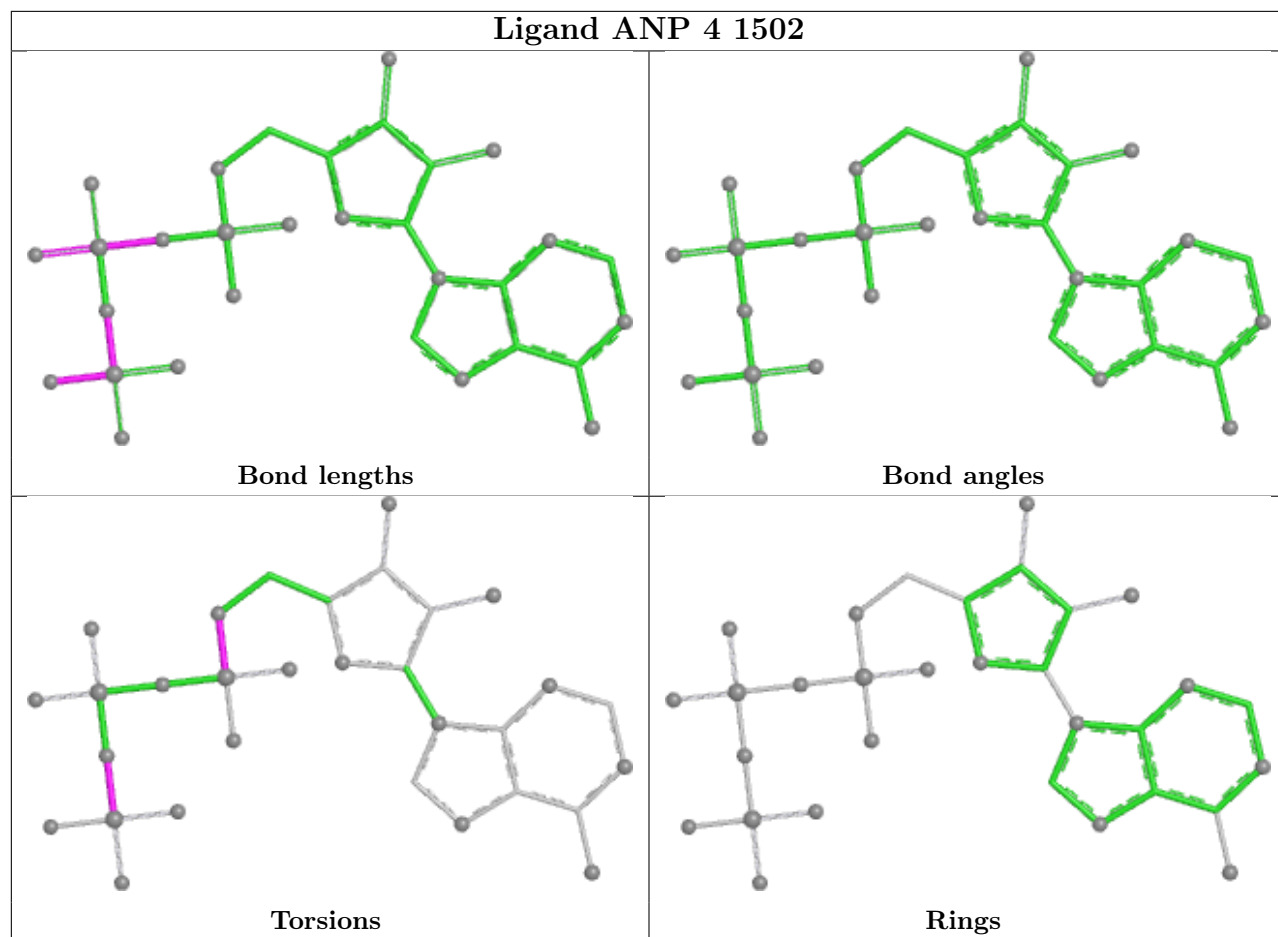
3 monomers are involved in 3 short contacts:

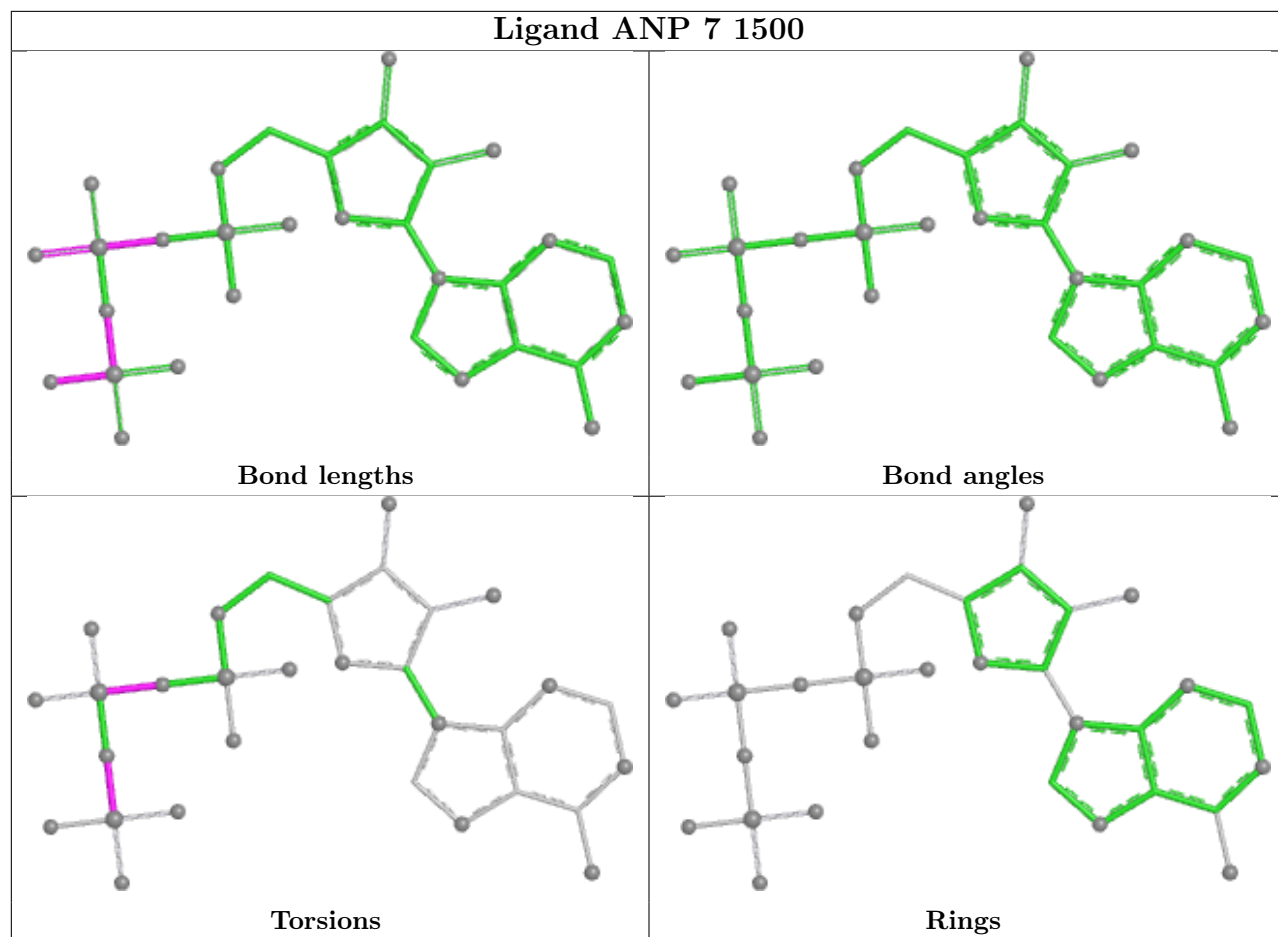
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	1502	ANP	1	0
19	7	1500	ANP	1	0
19	3	1502	ANP	1	0

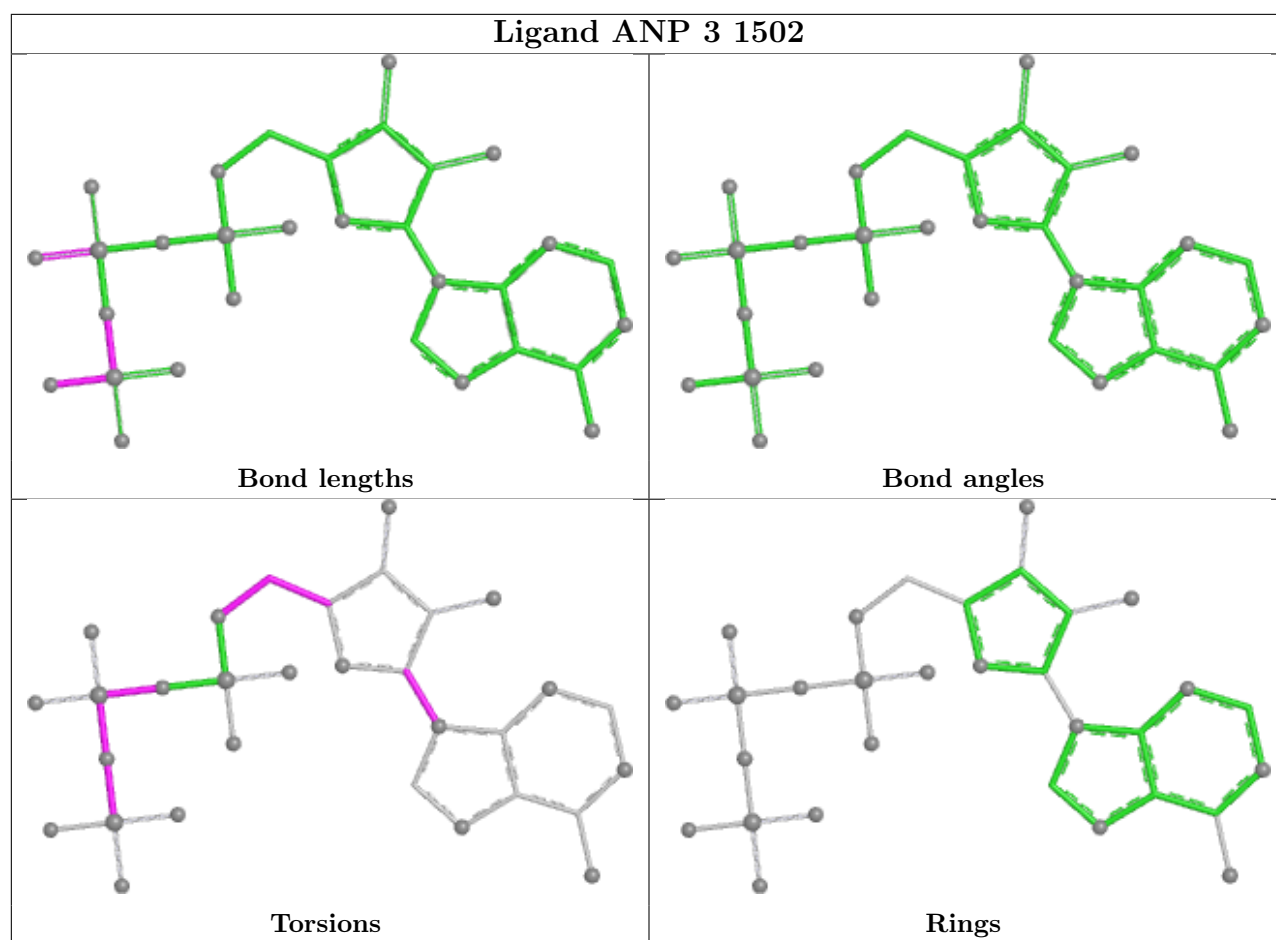
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ANP 6 903









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

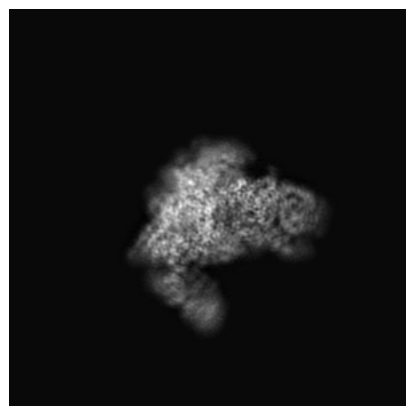
6 Map visualisation [i](#)

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.

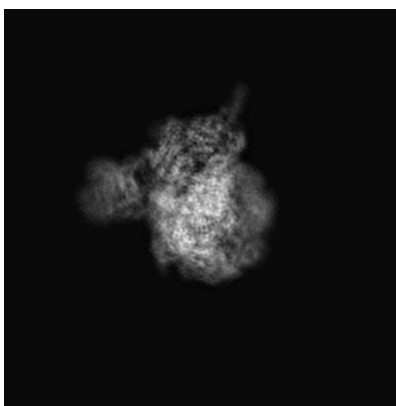
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

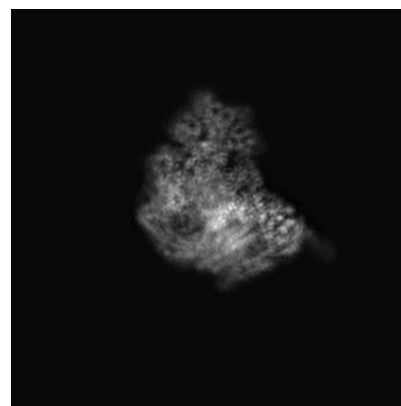
6.1.1 Primary map



X

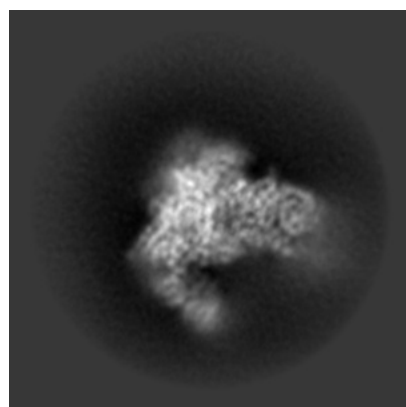


Y

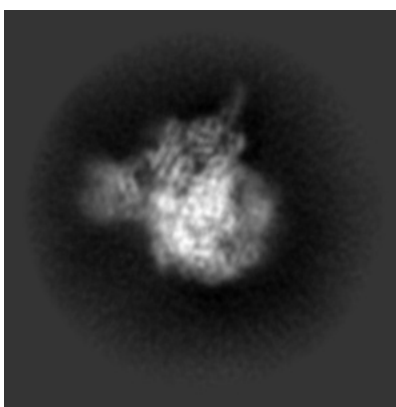


Z

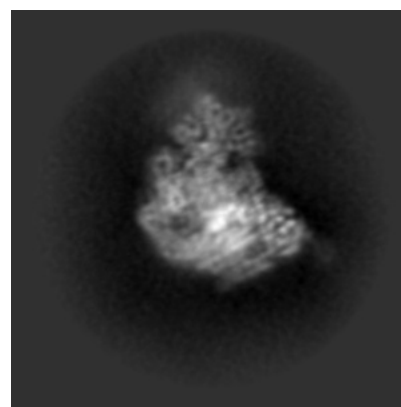
6.1.2 Raw map



X



Y

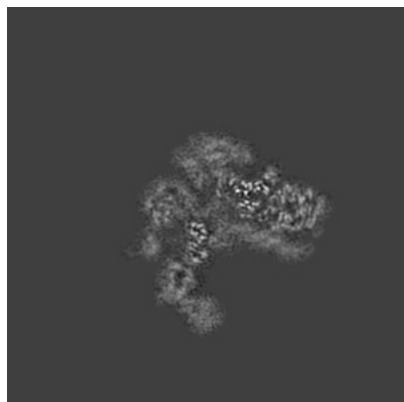


Z

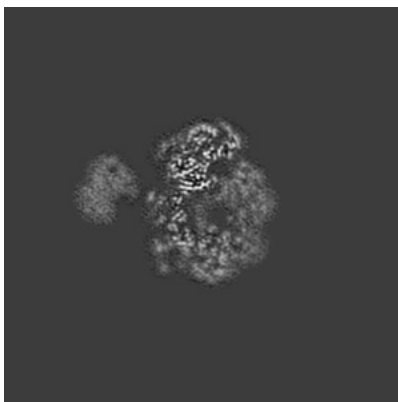
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

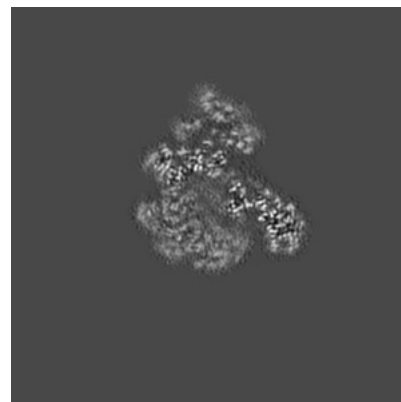
6.2.1 Primary map



X Index: 158

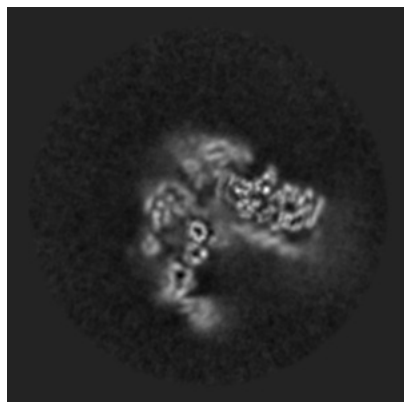


Y Index: 158

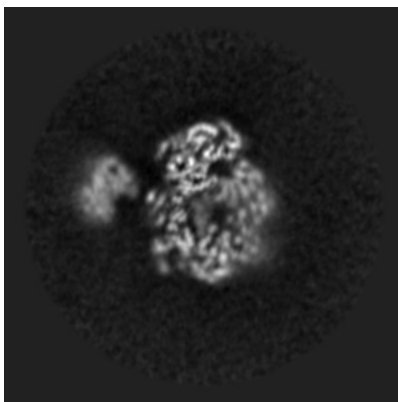


Z Index: 158

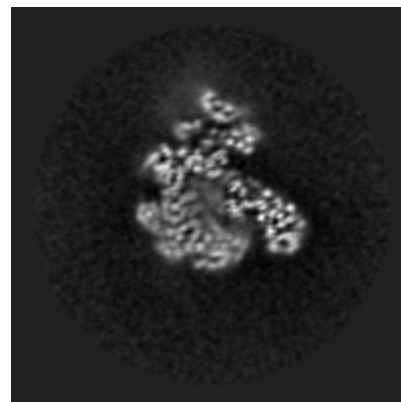
6.2.2 Raw map



X Index: 158



Y Index: 158

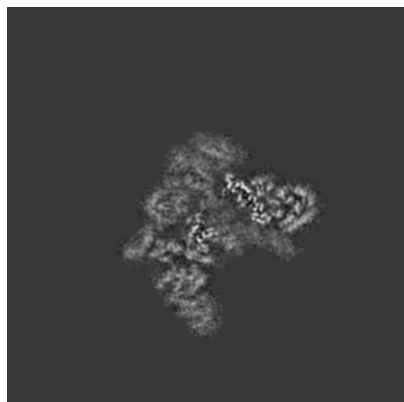


Z Index: 158

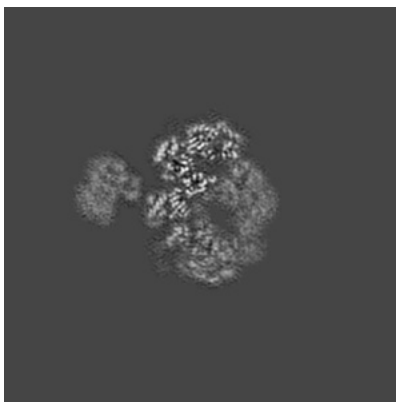
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

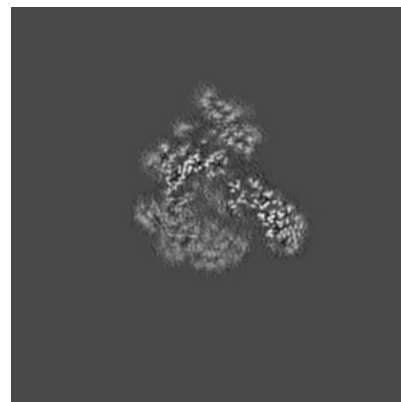
6.3.1 Primary map



X Index: 165

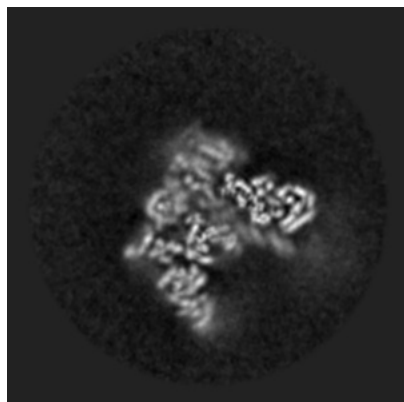


Y Index: 155

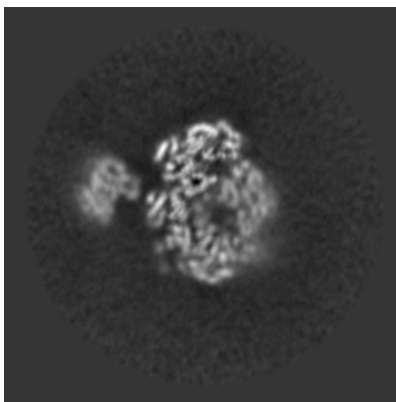


Z Index: 160

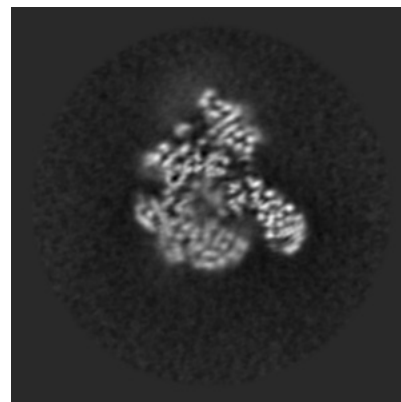
6.3.2 Raw map



X Index: 165



Y Index: 156

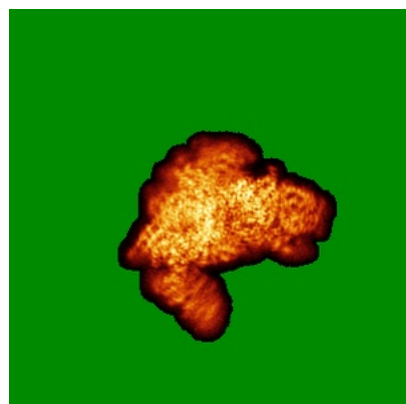


Z Index: 161

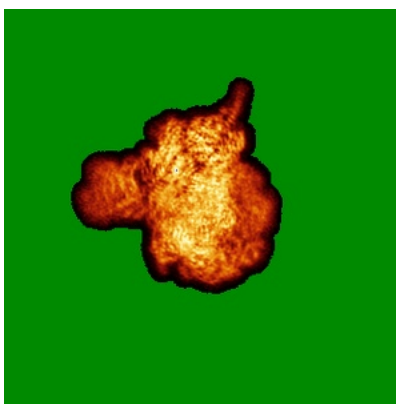
The images above show the largest variance slices of the map in three orthogonal directions.

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

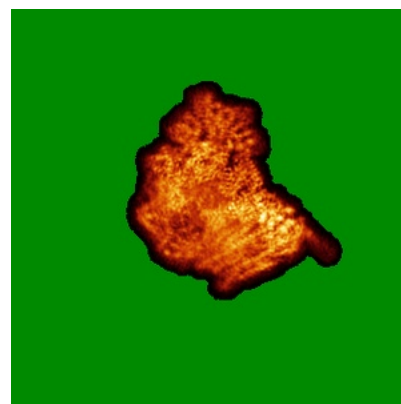
6.4.1 Primary map



X

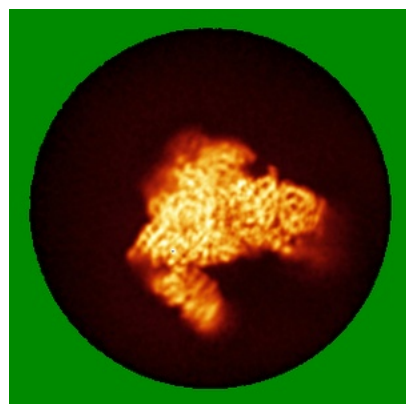


Y

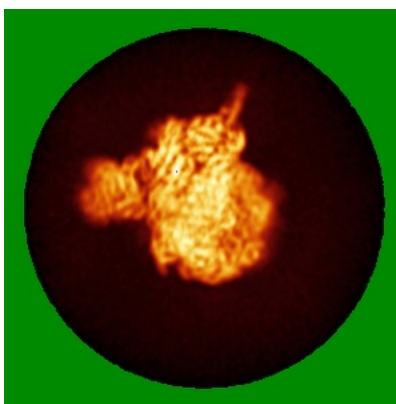


Z

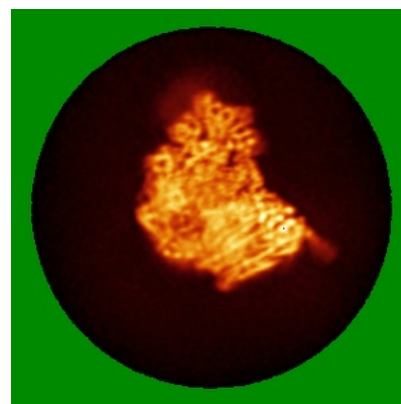
6.4.2 Raw map



X



Y

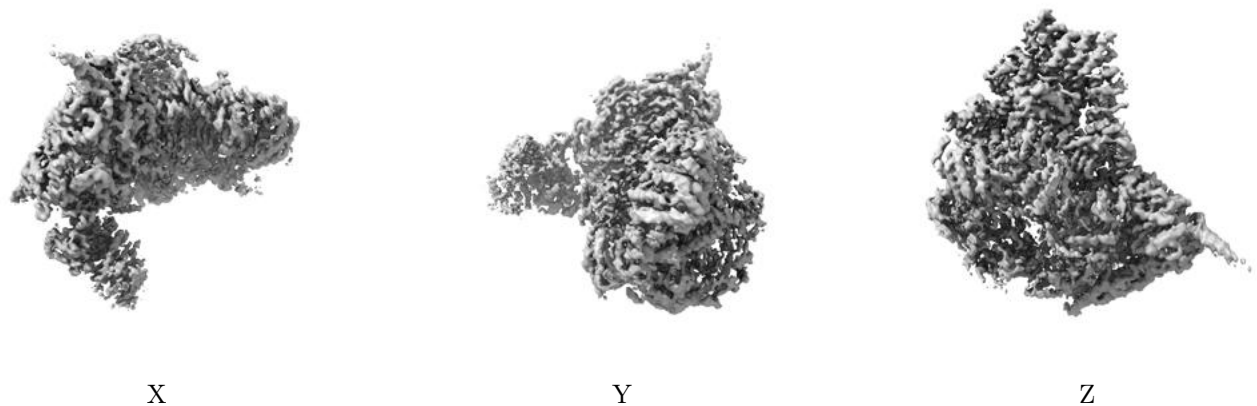


Z

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.

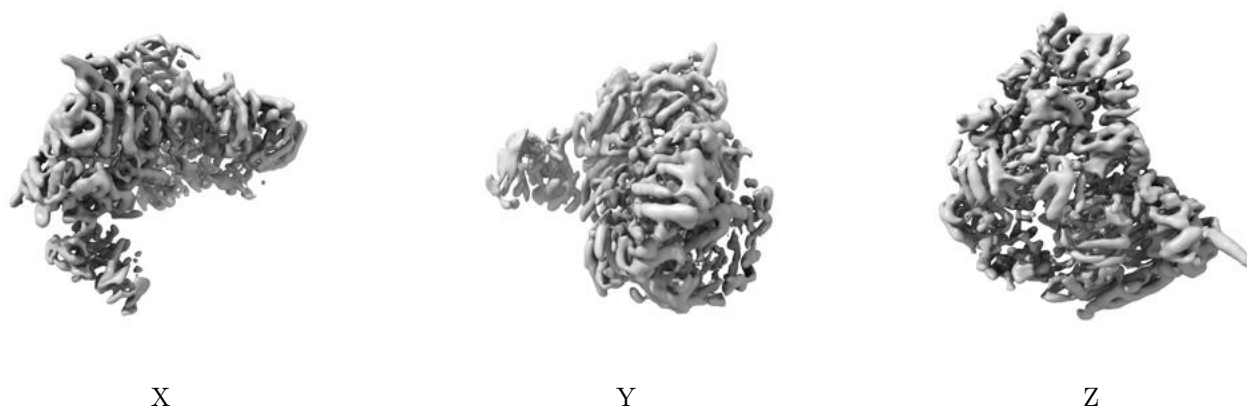
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

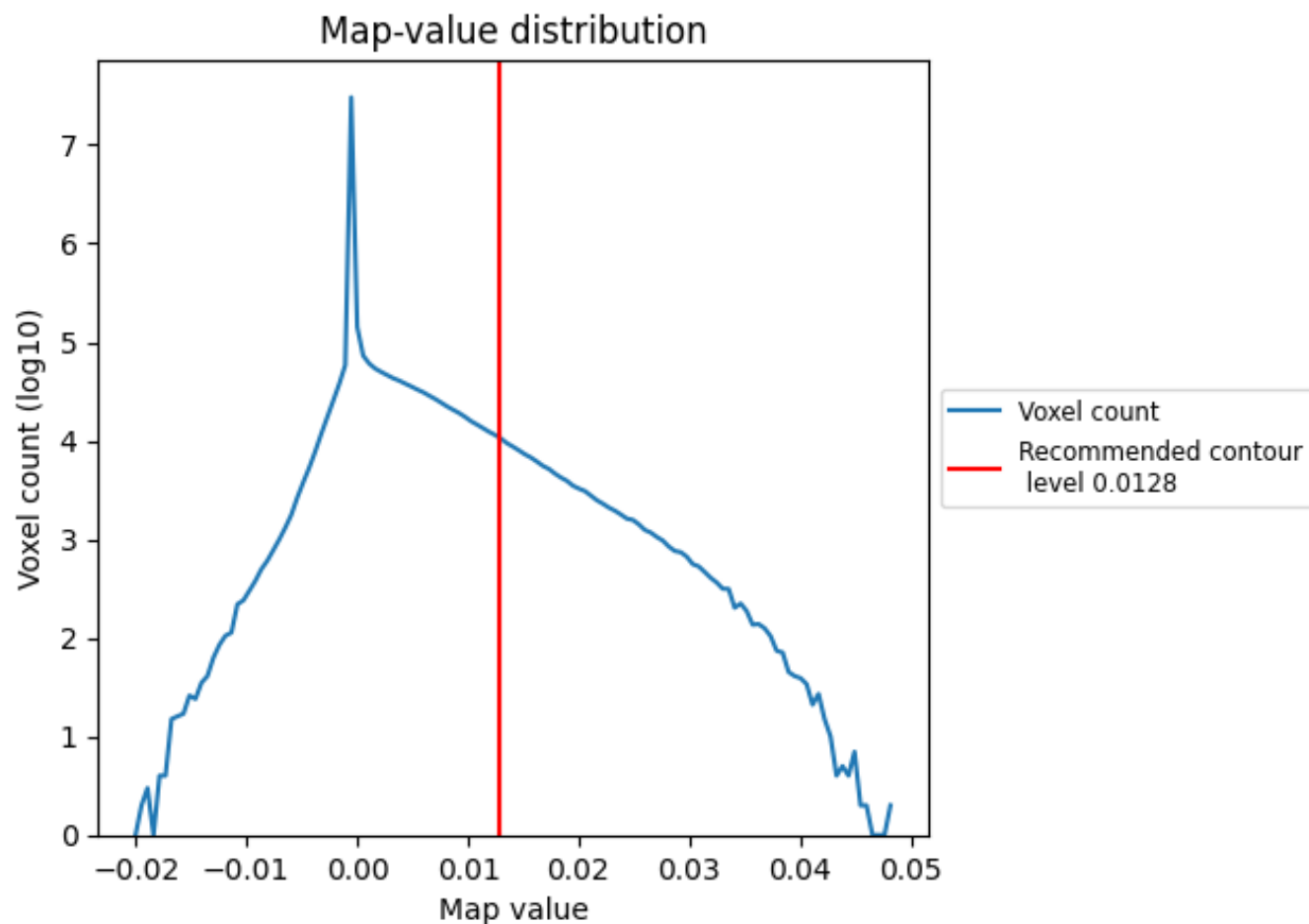
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

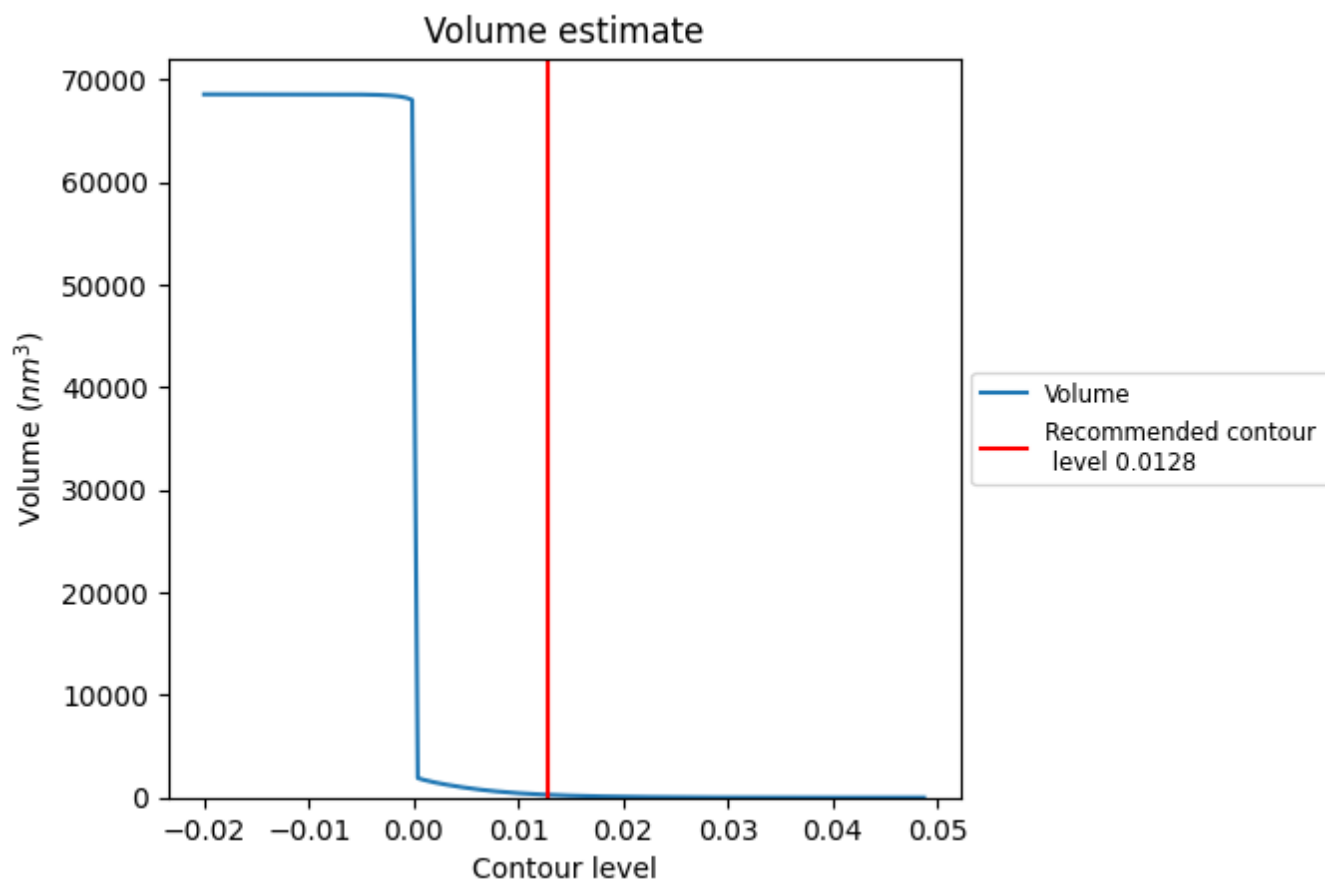
This section contains the results of statistical analysis of the map.

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.

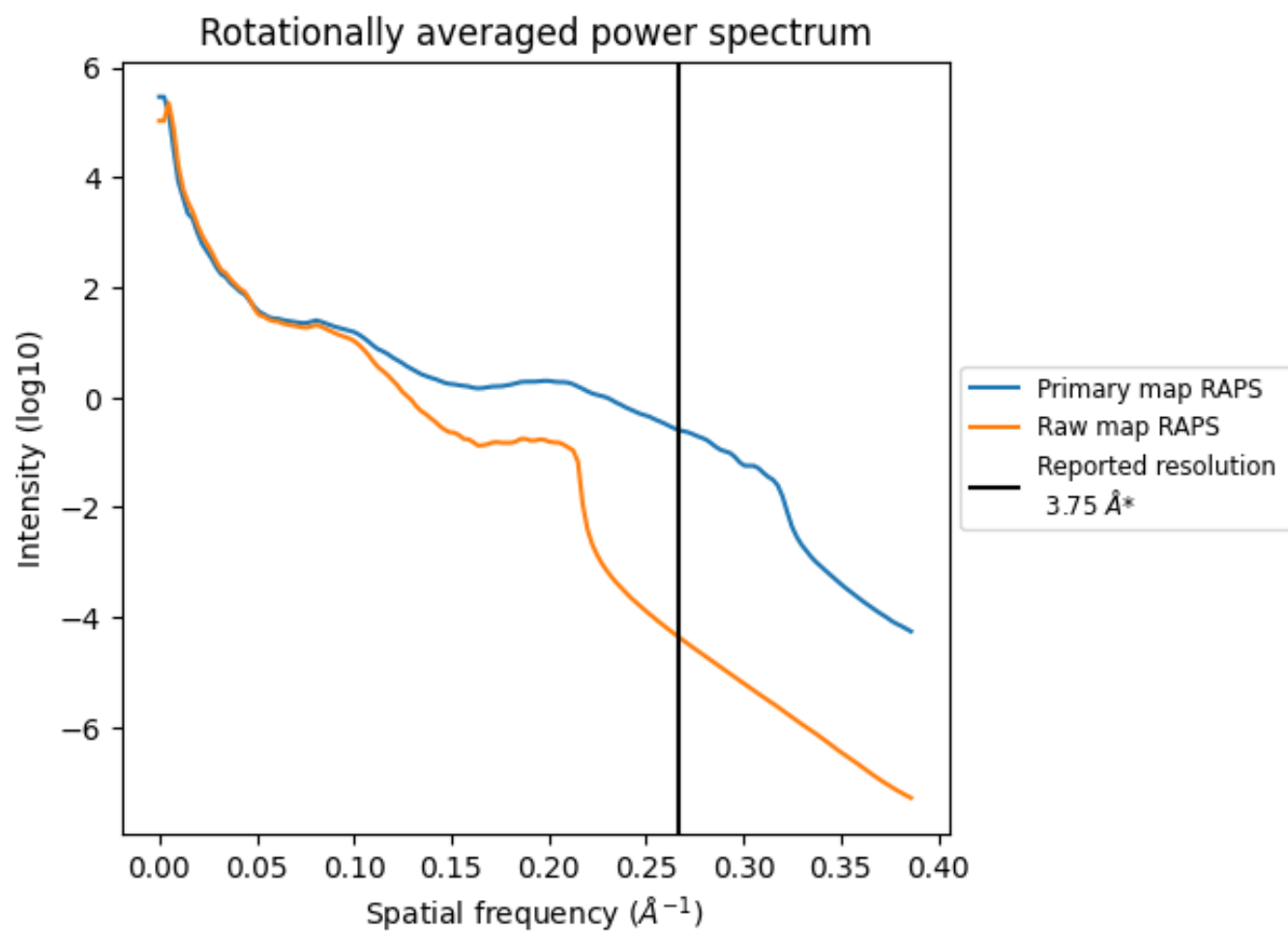
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; 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 ⓘ

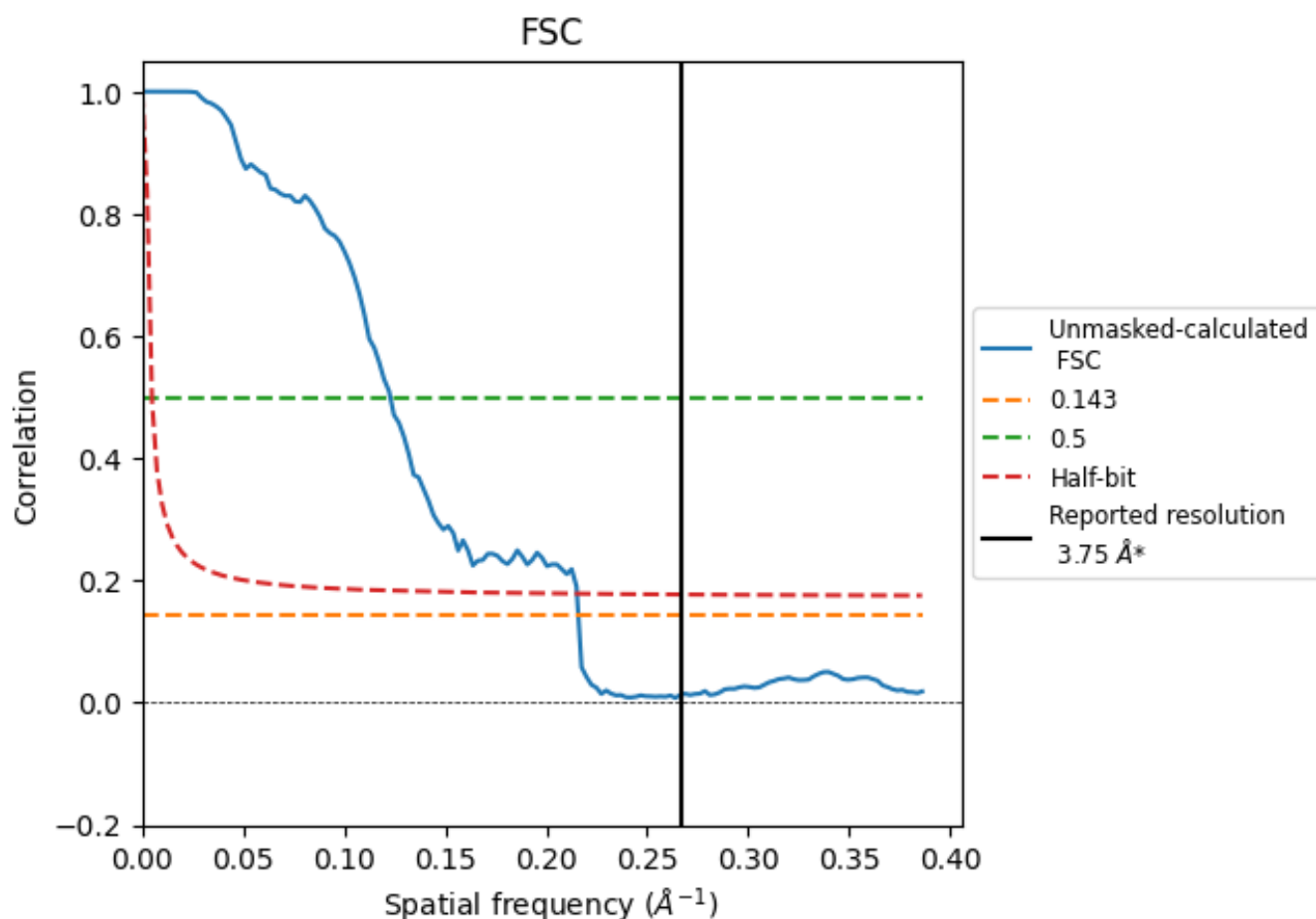


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.267 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

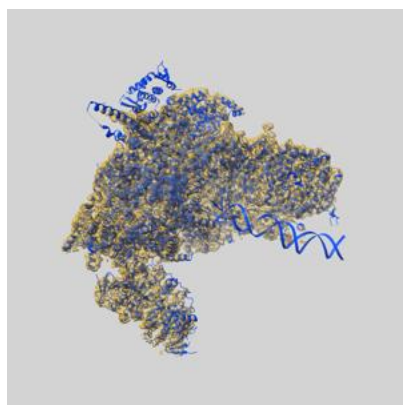
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.63	8.14	4.64

*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 %

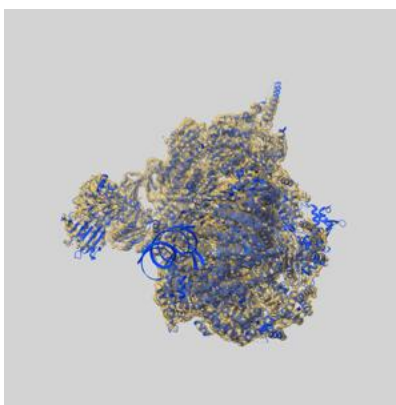
9 Map-model fit [i](#)

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](#).

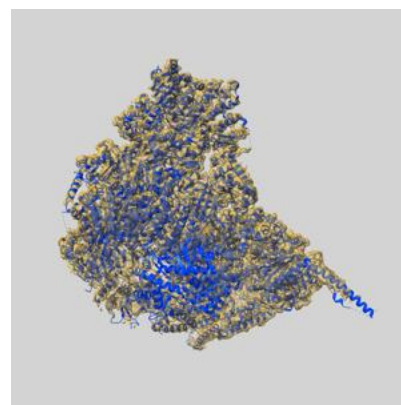
9.1 Map-model overlay [i](#)



X



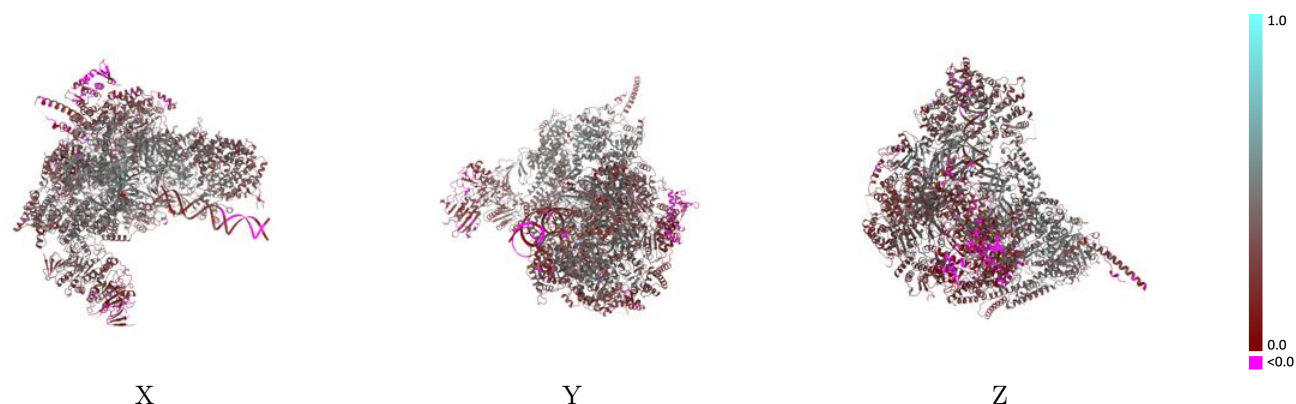
Y



Z

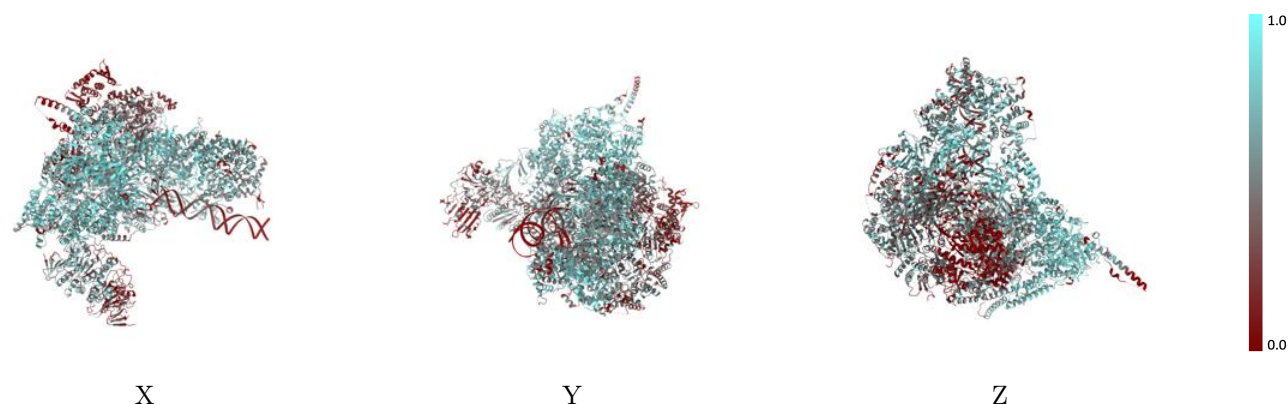
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



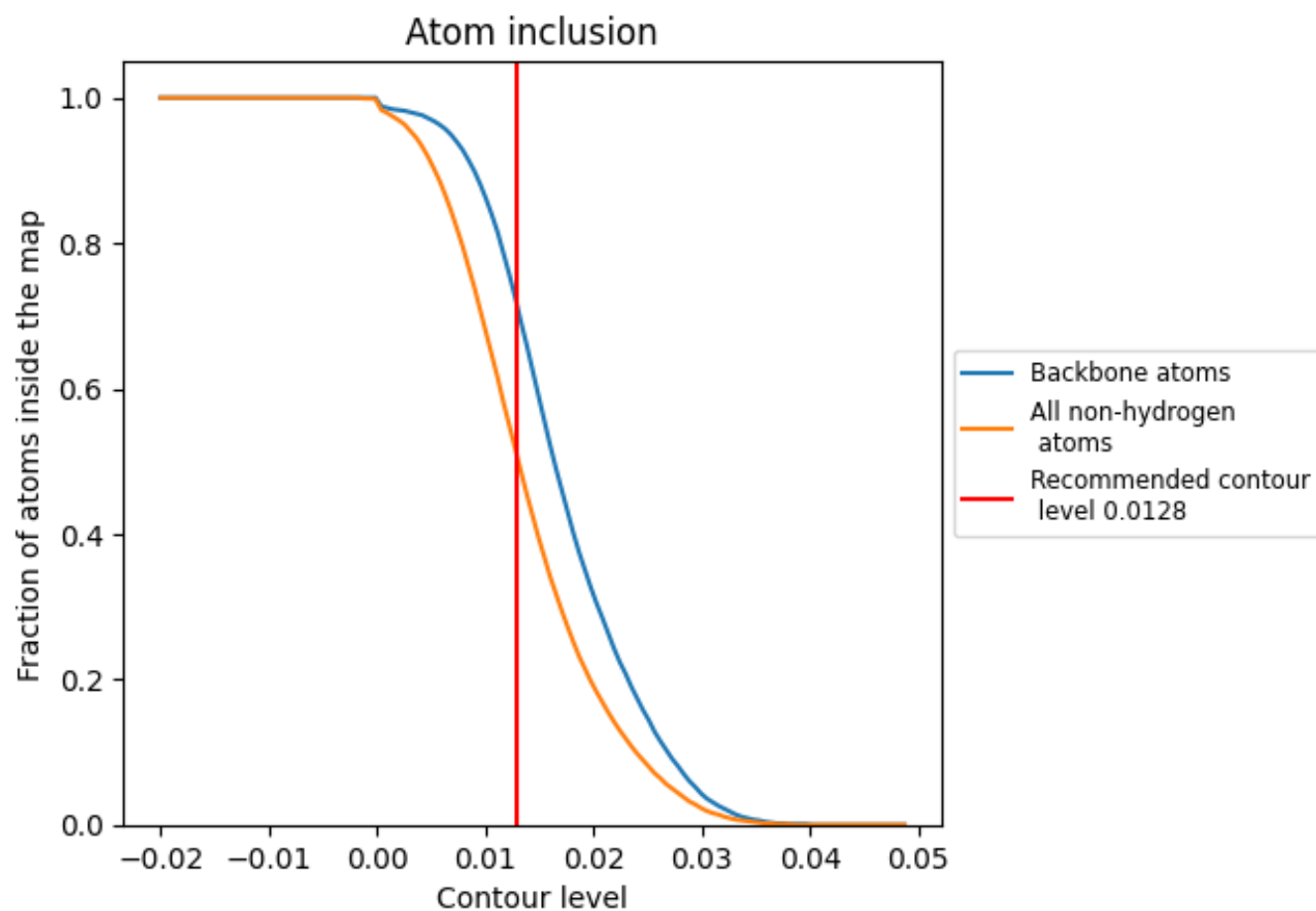
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0128).

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

