wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 02:16 PM UTC

PDB ID	:	8OW1 / pdb_00008ow1
EMDB ID	:	EMD-17227
Title	:	Cryo-EM structure of the yeast Inner kinetochore bound to a CENP-A nucleosome.
Authors	:	Dendooven, T.D.; Zhang, Z.; Yang, J.; McLaughlin, S.; Schwabb, J.; Scheres, S.; Yatskevich, S.; Barford, D.
Deposited on	:	2023-04-26
Resolution	:	3.70 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

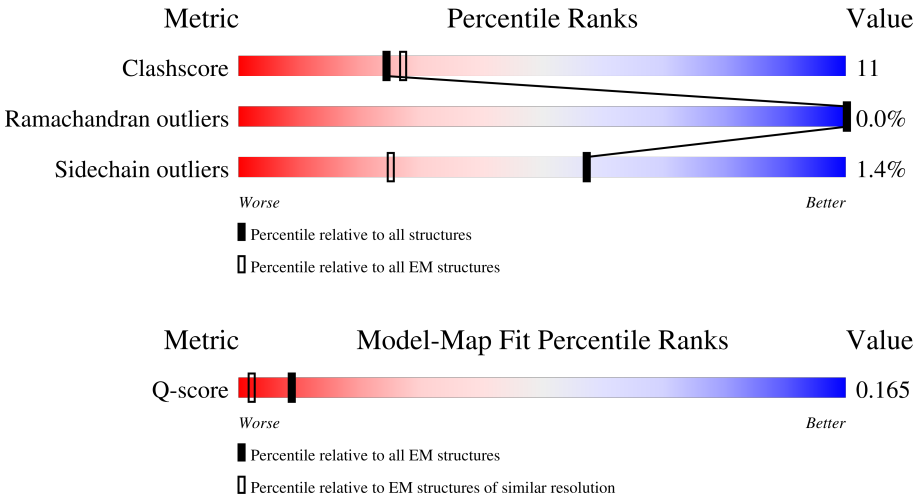
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 3.70 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	11569 (3.20 - 4.20)

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	A	351	26% 5% 69%
1	B	351	23% 10% 67%
2	I	733	61% 29% 10%
2	II	733	71% 26%

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Mol	Chain	Length	Quality of chain
3	K	239	60% 31% 8%
3	KK	239	10% 67% 28% 5%
4	H	181	48% 46% 6%
4	HH	181	66% 31%
5	L	245	66% 27%
5	LL	245	64% 29%
6	N	458	70% 15% 16%
6	NN	458	72% 12% 16%
7	CT	478	65% 17% 18%
8	CE	608	5% 73% 18% 8%
8	ce	608	72% 14% 14%
9	SK	194	64% 13% 22%
10	P	369	58% 11% 31%
10	PP	369	57% 11% 31%
11	Q	406	46% 18% 36%
11	QQ	406	43% 18% 39%
12	O	368	53% 14% 33%
12	OO	368	51% 14% 35%
13	T	361	17% 8% 75%
13	TT	361	17% 20% 5% 75%
14	U	324	41% 16% 43%
14	UU	324	40% 15% 45%
15	W	89	66% 11% 22%
15	WW	89	61% 62% 16% 22%
16	Y	238	60% 28% 5% 6%

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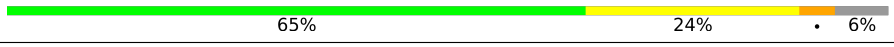
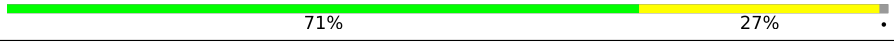
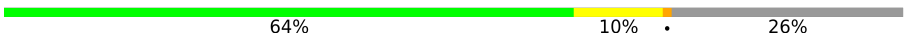
Mol	Chain	Length	Quality of chain
16	YY	238	
17	Z	153	
17	ZZ	153	
18	D	153	
19	E	153	
20	b	103	
20	f	103	
21	d	131	
21	h	131	
22	a	229	
22	e	229	
23	c	132	
23	g	132	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 78671 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 Centromere-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	110	Total	C	N	O	S	0	0
			898	554	162	179	3		
1	B	116	Total	C	N	O	S	0	0
			957	592	174	188	3		

- Molecule 2 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	659	Total	C	N	O	S	0	0
			5337	3459	890	958	30		
2	II	704	Total	C	N	O	S	0	0
			5705	3692	954	1028	31		

- Molecule 3 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	219	Total	C	N	O	S	0	0
			1762	1113	304	340	5		
3	KK	227	Total	C	N	O	S	0	0
			1805	1143	307	349	6		

- Molecule 4 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	171	Total	C	N	O	S	0	0
			1412	890	247	273	2		
4	HH	176	Total	C	N	O	S	0	0
			1449	912	252	283	2		

- Molecule 5 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LL	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		
5	L	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		

- Molecule 6 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	NN	385	Total	C	N	O	S	0	0
			3121	2021	530	557	13		
6	N	386	Total	C	N	O	S	0	0
			3129	2027	531	558	13		

- Molecule 7 is a protein called Centromere DNA-binding protein complex CBF3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CT	391	Total	C	N	O	S	0	0
			3298	2154	556	576	12		

- Molecule 8 is a protein called Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	ce	524	Total	C	N	O	S	0	0
			4352	2834	700	797	21		
8	CE	557	Total	C	N	O	S	0	0
			4608	2980	758	841	29		

- Molecule 9 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	151	Total	C	N	O	S	0	0
			1230	769	214	243	4		

- Molecule 10 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	255	Total	C	N	O	S	0	0
			2098	1348	362	374	14		
10	PP	254	Total	C	N	O	S	0	0
			2094	1346	360	374	14		

- Molecule 11 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	261	Total	C	N	O	S	0	0
			2193	1384	388	412	9		
11	QQ	247	Total	C	N	O	S	0	0
			2060	1296	364	391	9		

- Molecule 12 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	OO	240	Total	C	N	O	S	0	0
			1967	1272	323	368	4		
12	O	245	Total	C	N	O	S	0	0
			2015	1302	333	375	5		

- Molecule 13 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	92	Total	C	N	O	S	0	0
			761	488	125	144	4		
13	TT	92	Total	C	N	O	S	0	0
			761	488	125	144	4		

- Molecule 14 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	184	Total	C	N	O	S	0	0
			1485	928	255	299	3		
14	UU	179	Total	C	N	O	S	0	0
			1445	904	249	289	3		

- Molecule 15 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	69	Total	C	N	O	S	0	0
			551	348	96	105	2		
15	WW	69	Total	C	N	O	S	0	0
			550	348	96	104	2		

- Molecule 16 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	223	Total	C	N	O	S	0	0
			1663	1027	281	349	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	YY	223	Total 1663	C 1027	N 281	O 349	S 6	0	0

- Molecule 17 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	151	Total 1180	C 740	N 204	O 235	S 1	0	0
17	ZZ	151	Total 1180	C 740	N 204	O 235	S 1	0	0

- Molecule 18 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	153	Total 3139	C 1499	N 574	O 913	P 153	0	0

- Molecule 19 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	153	Total 3134	C 1499	N 559	O 923	P 153	0	0

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	79	Total 625	C 393	N 120	O 112	0	0
20	f	79	Total 627	C 395	N 120	O 112	0	0

- Molecule 21 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total 735	C 461	N 129	O 144	S 1	0	0
21	h	97	Total 745	C 467	N 129	O 148	S 1	0	0

- Molecule 22 is a protein called Histone H3-like centromeric protein CSE4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	97	Total 781	C 498	N 139	O 140	S 4	0	0
22	a	97	Total 781	C 498	N 139	O 140	S 4	0	0

- Molecule 23 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	g	98	Total 751	C 470	N 147	O 134	0	0
23	c	97	Total 742	C 464	N 146	O 132	0	0

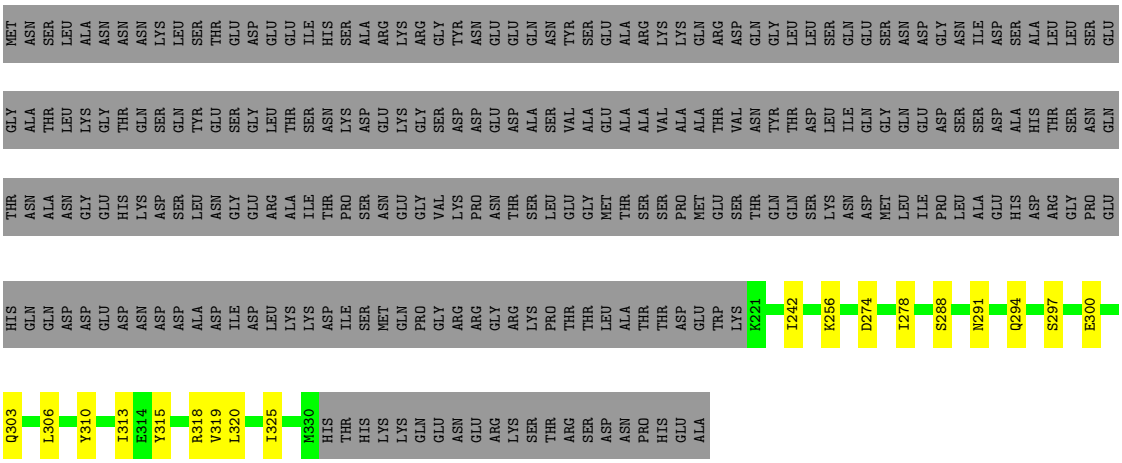
3 Residue-property plots (i)

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: Centromere-binding protein 1

Chain A:

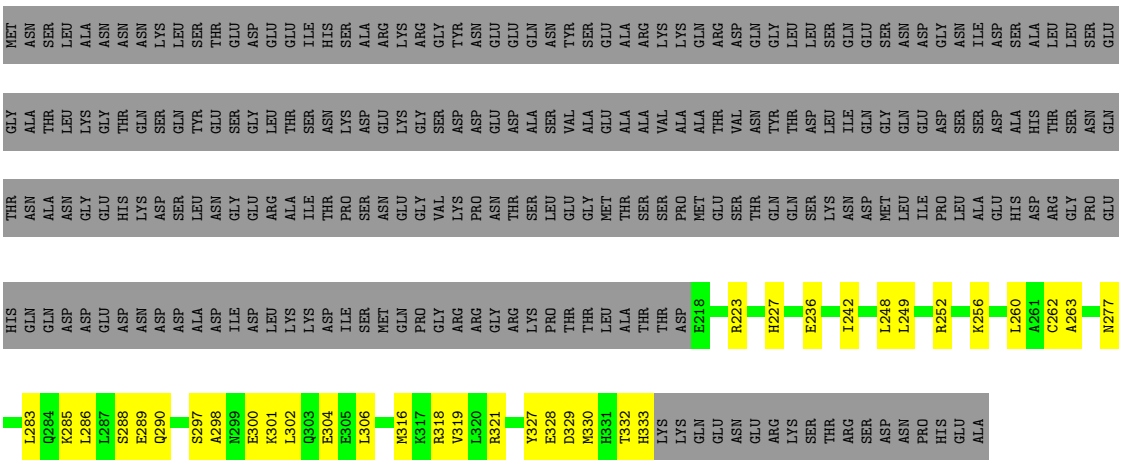




• Molecule 1: Centromere-binding protein 1

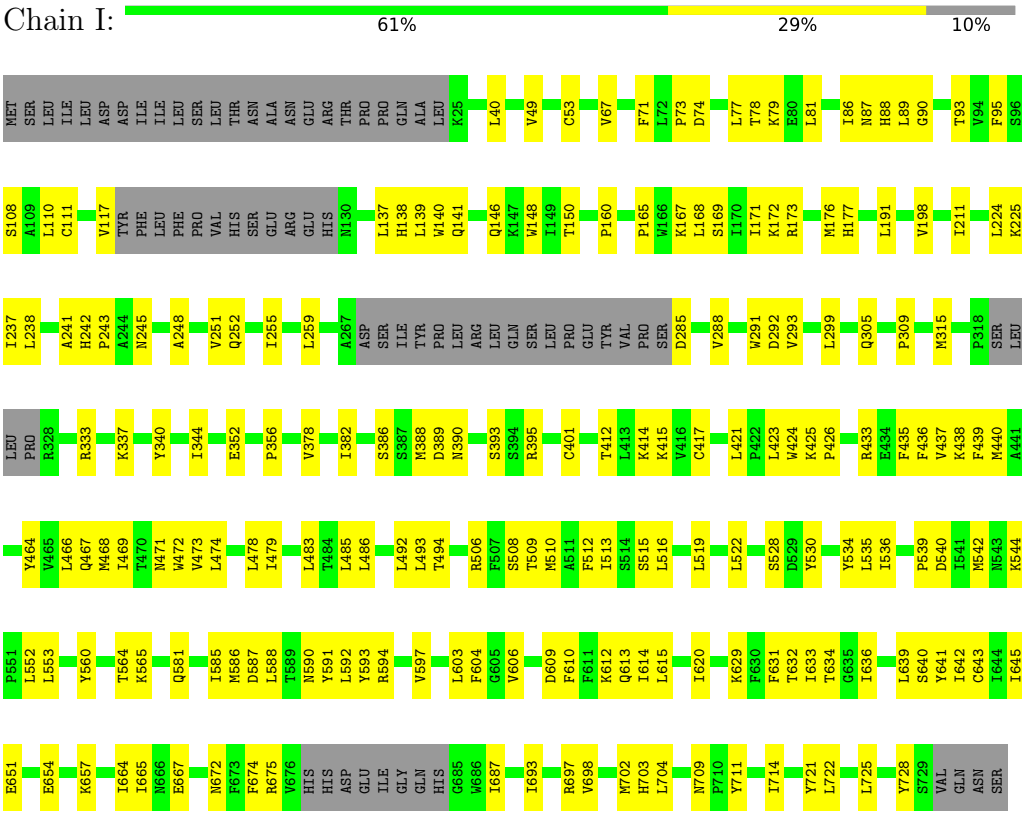
Chain B:





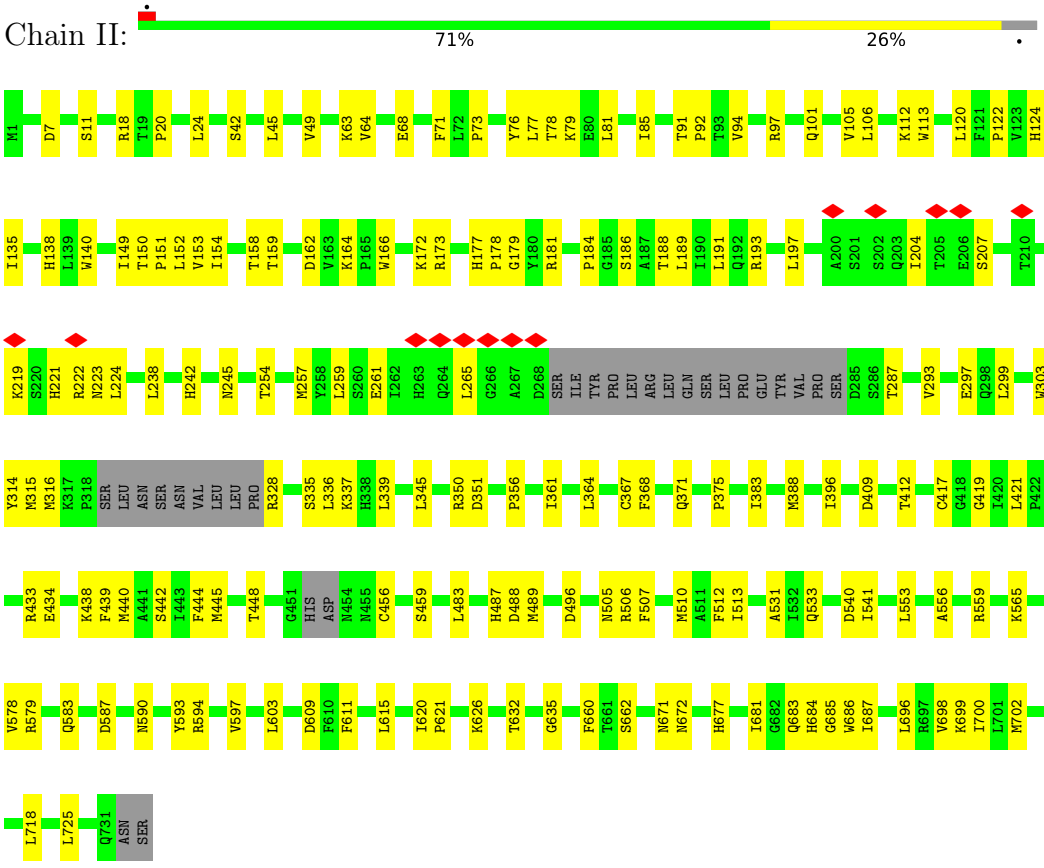
• Molecule 2: Inner kinetochore subunit CTF3

Chain I:



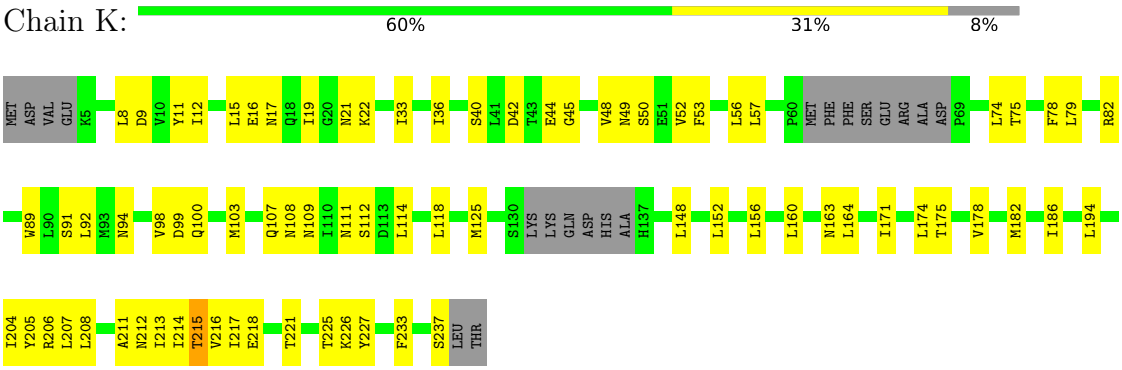
• Molecule 2: Inner kinetochore subunit CTF3

Chain II:



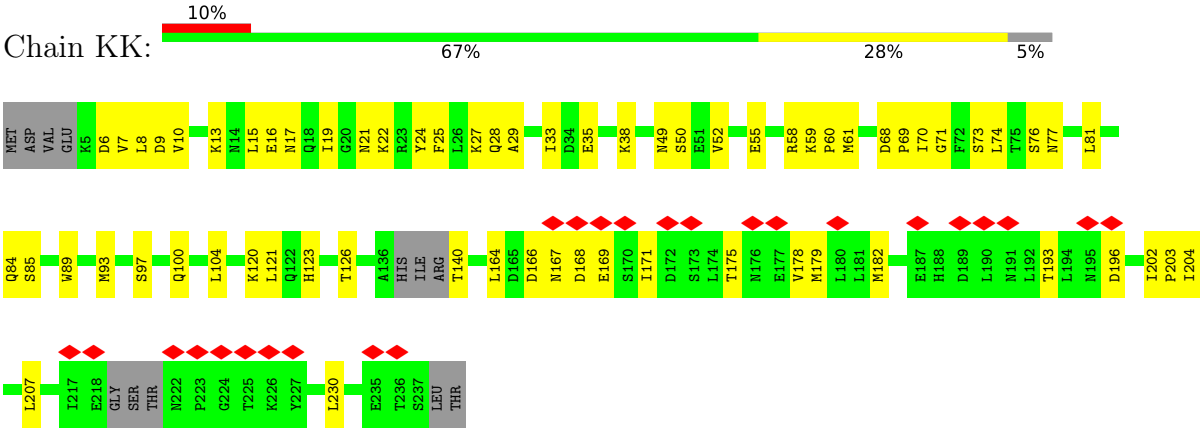
• Molecule 3: Inner kinetochore subunit MCM22

Chain K:



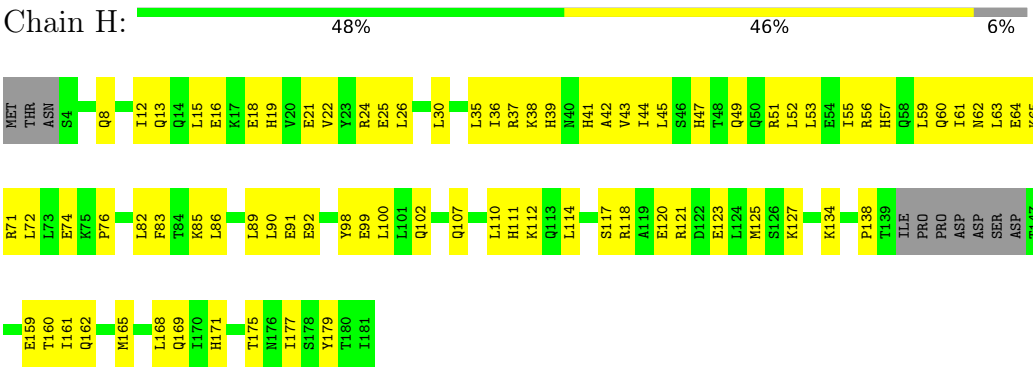
• Molecule 3: Inner kinetochore subunit MCM22

Chain KK:



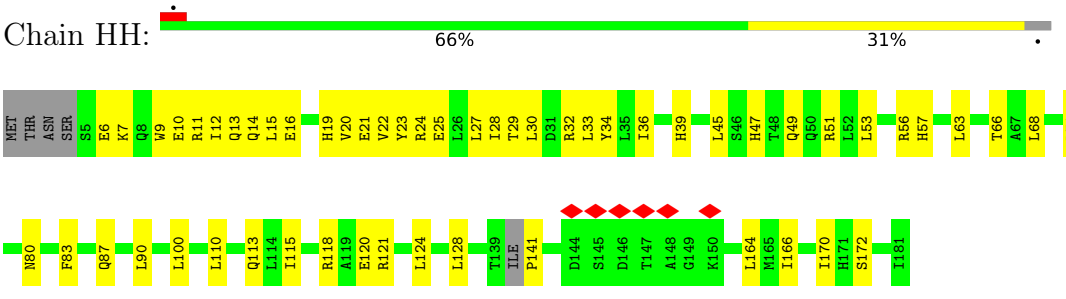
• Molecule 4: Inner kinetochore subunit MCM16

Chain H:



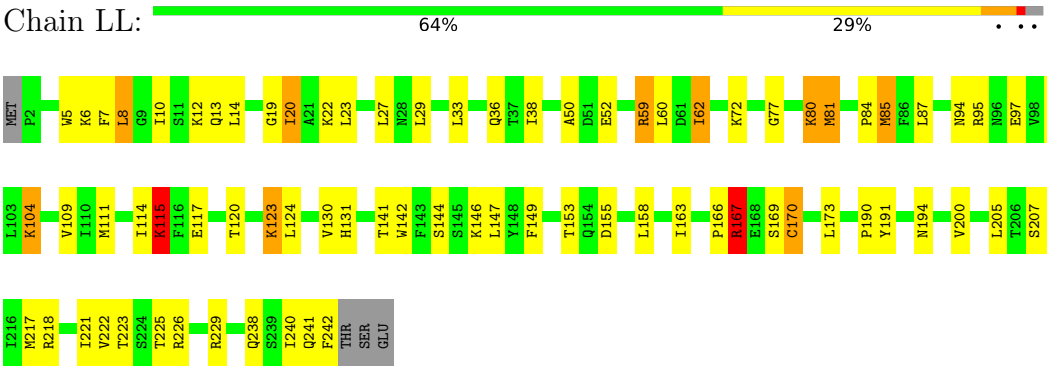
• Molecule 4: Inner kinetochore subunit MCM16

Chain HH:



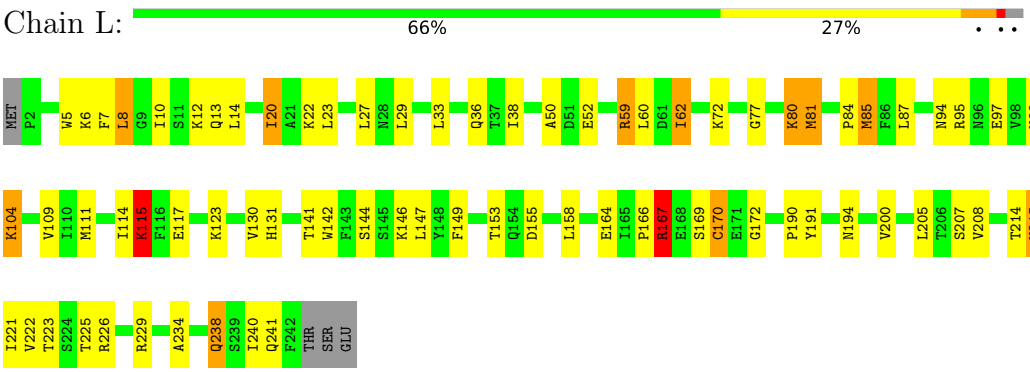
• Molecule 5: Inner kinetochore subunit IML3

Chain LL:



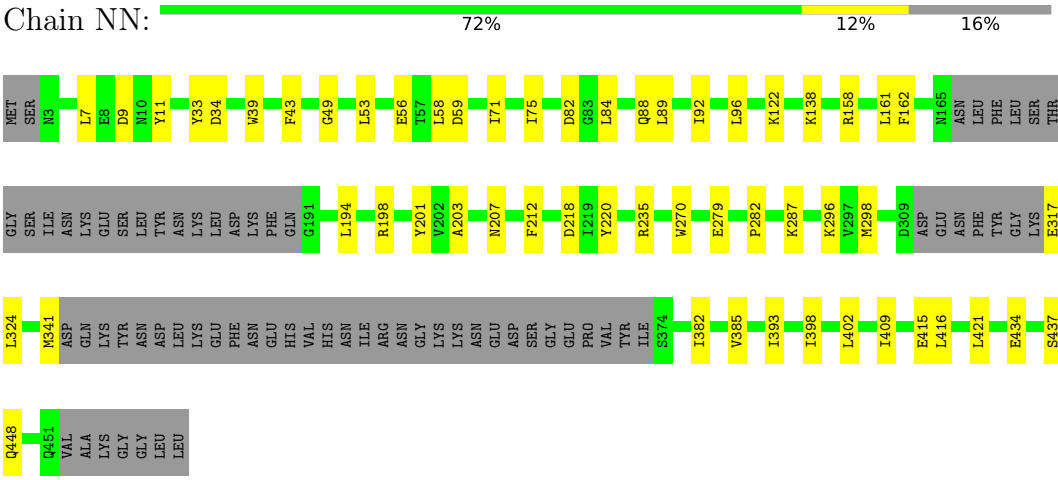
• Molecule 5: Inner kinetochore subunit IML3

Chain L:



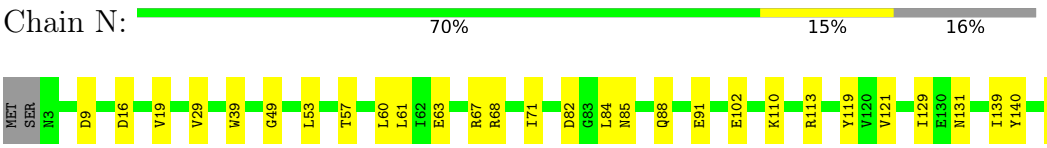
• Molecule 6: Inner kinetochore subunit CHL4

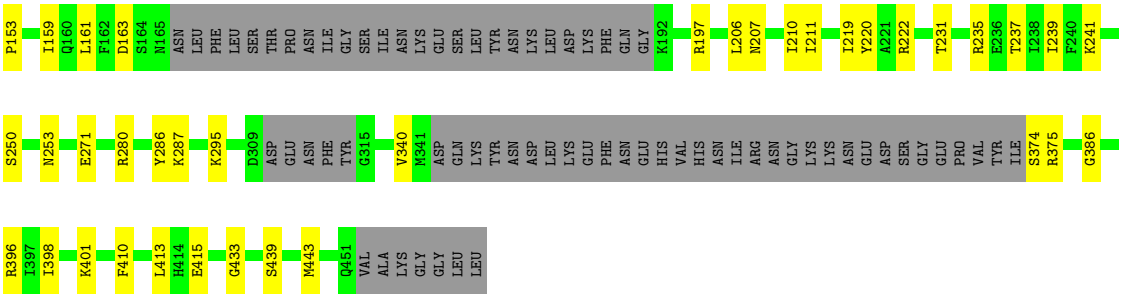
Chain NN:



• Molecule 6: Inner kinetochore subunit CHL4

Chain N:

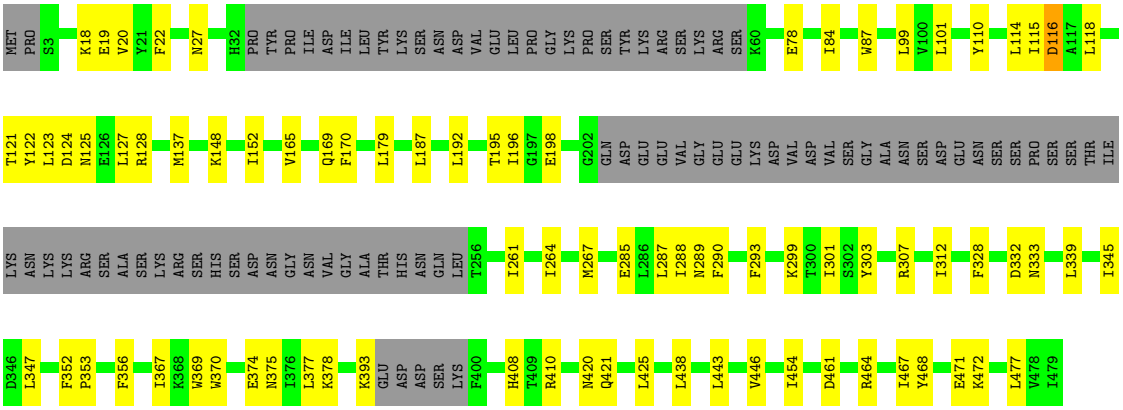




• Molecule 7: Centromere DNA-binding protein complex CBF3 subunit C

Chain CT:

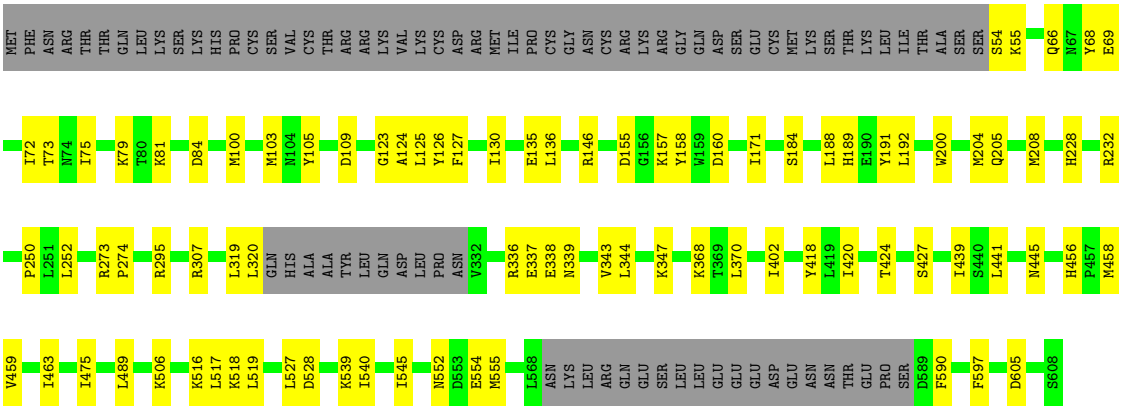




• Molecule 8: Centromere DNA-binding protein complex CBF3 subunit B

Chain ce:

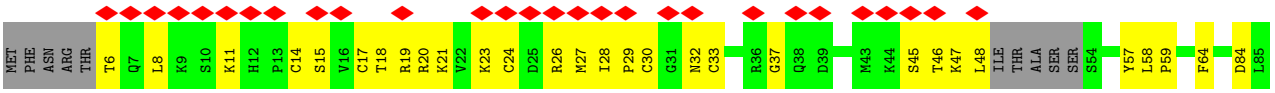


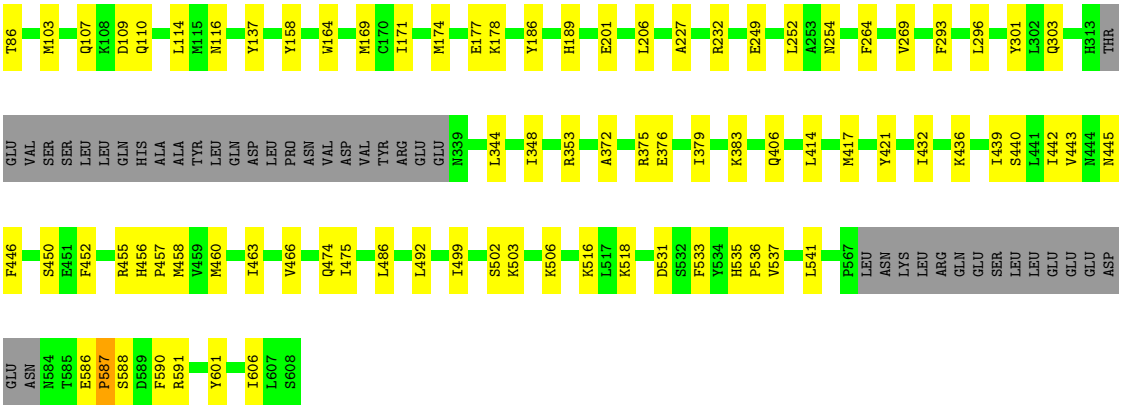


• Molecule 8: Centromere DNA-binding protein complex CBF3 subunit B

Chain CE:



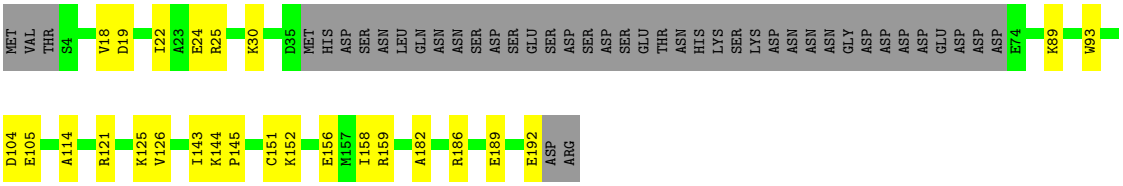




• Molecule 9: Suppressor of kinetochore protein 1

Chain SK:

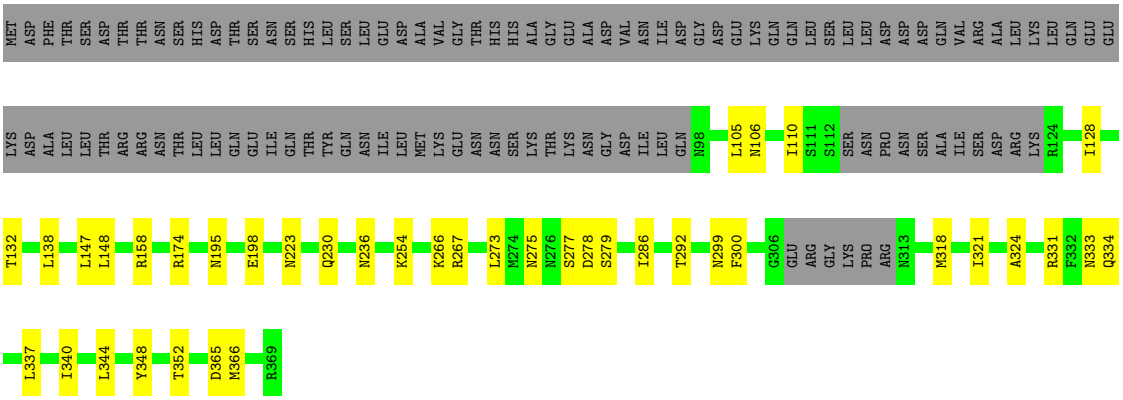




• Molecule 10: Inner kinetochore subunit CTF19

Chain P:

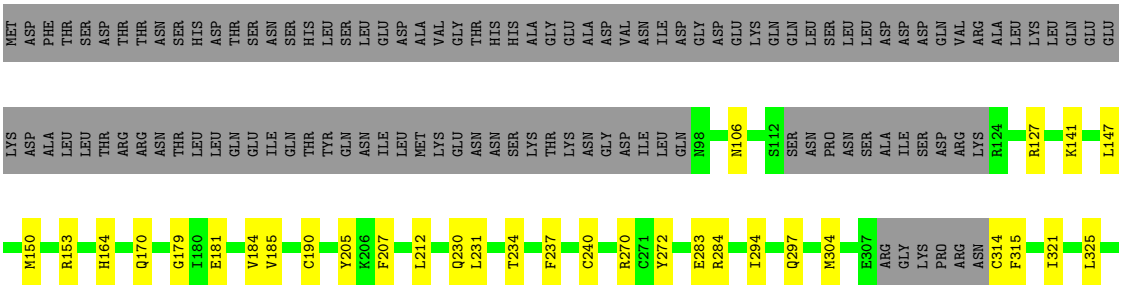


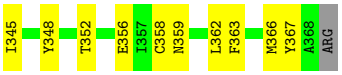


• Molecule 10: Inner kinetochore subunit CTF19

Chain PP:

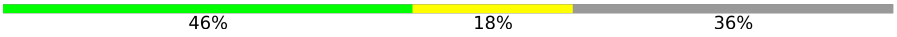


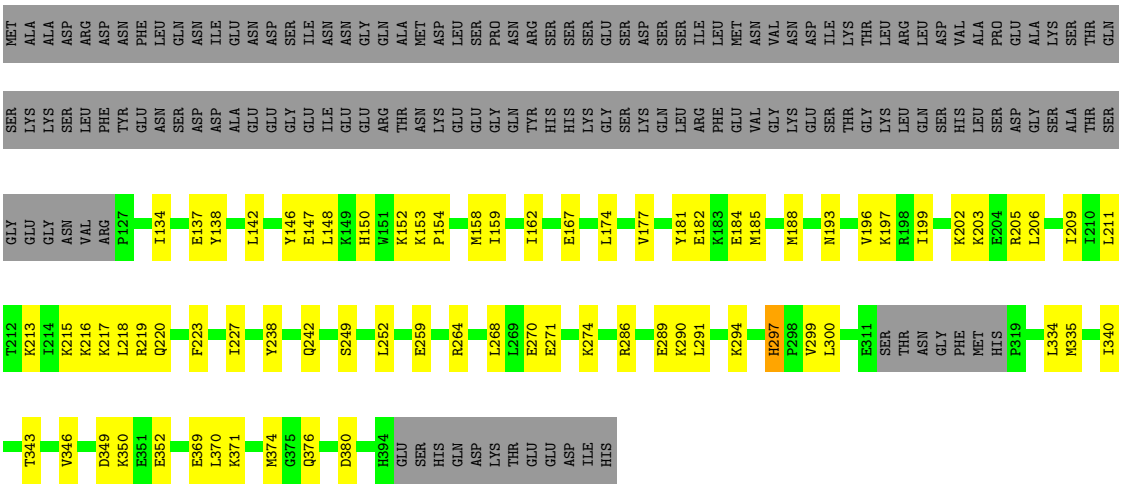




• Molecule 11: Inner kinetochore subunit OKP1

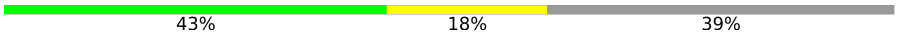
Chain Q:

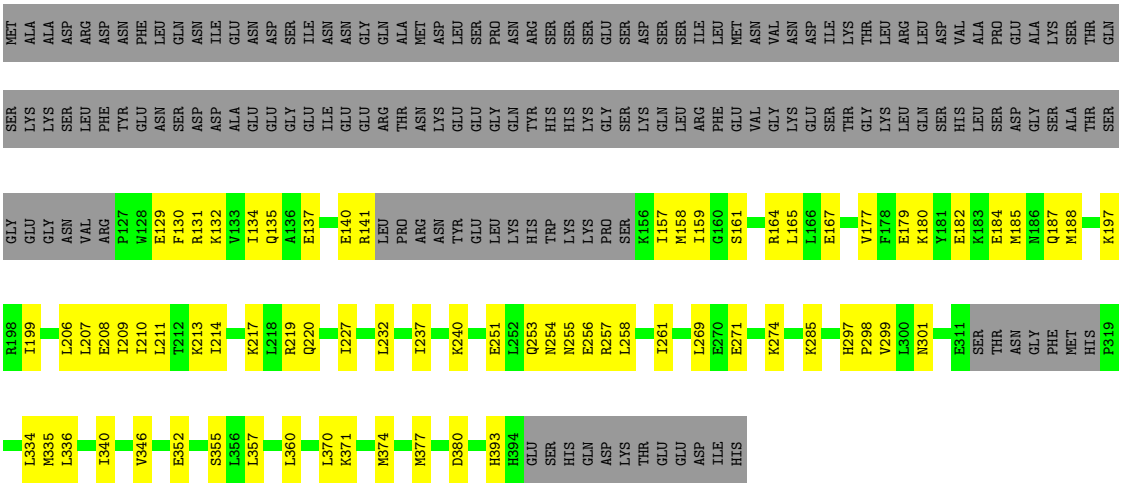




• Molecule 11: Inner kinetochore subunit OKP1

Chain QQ:

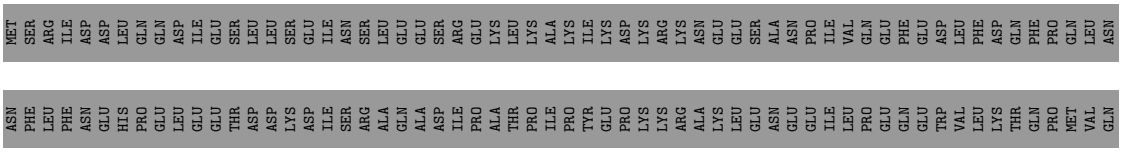


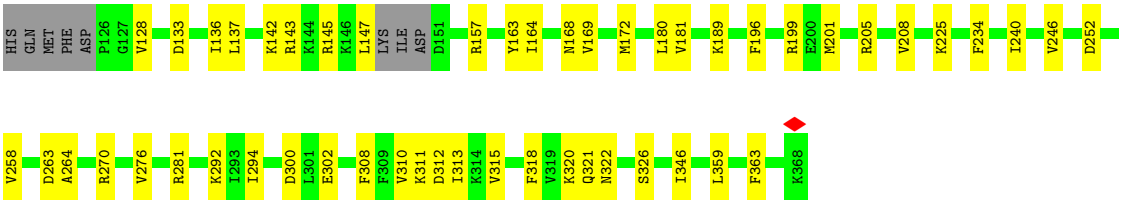


• Molecule 12: Inner kinetochore subunit MCM21

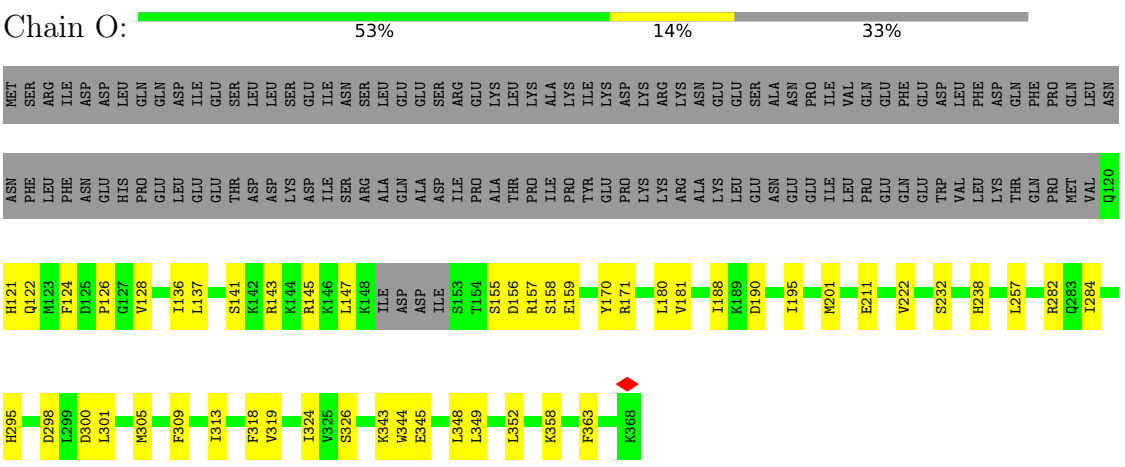
Chain OO:



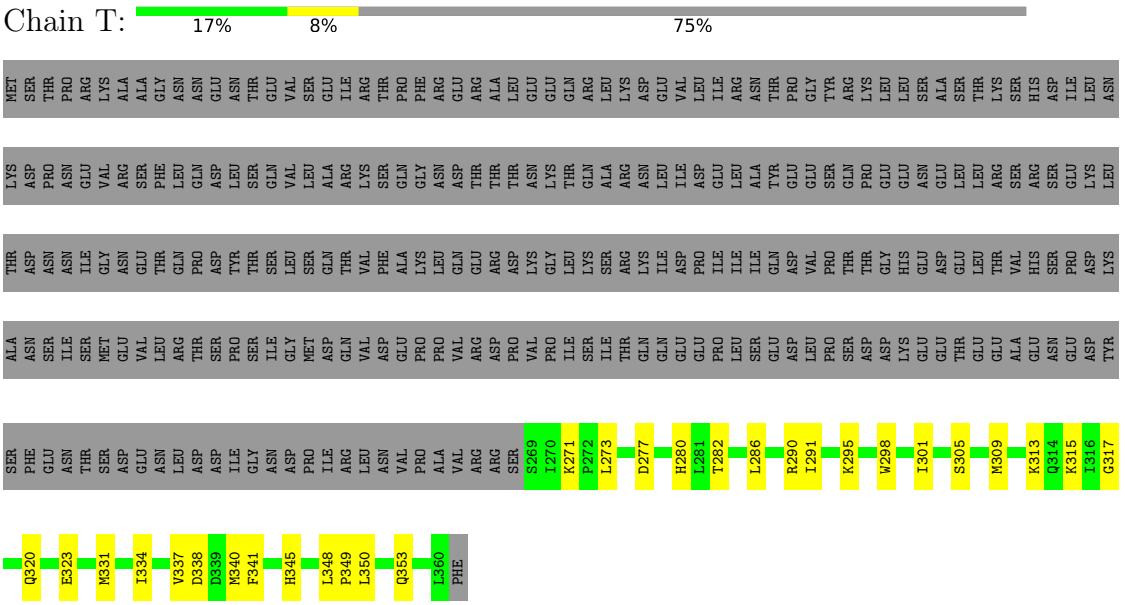




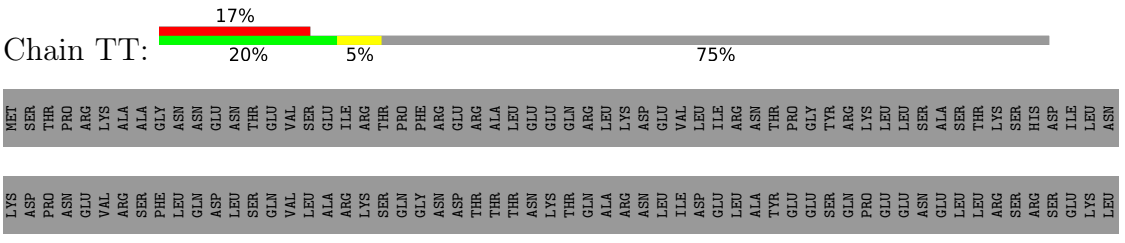
• Molecule 12: Inner kinetochore subunit MCM21

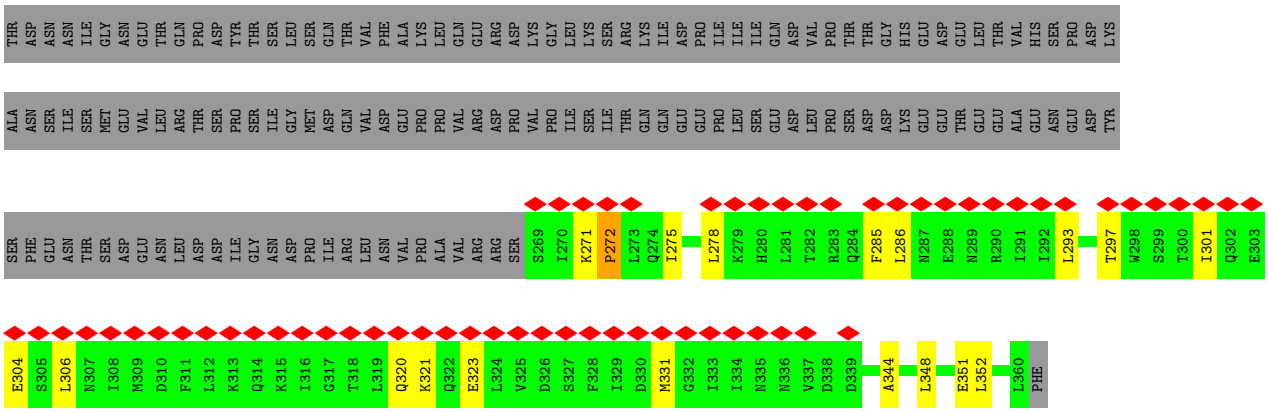


• Molecule 13: Inner kinetochore subunit CNN1



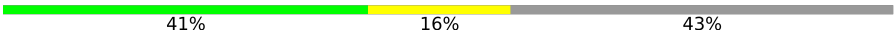
• Molecule 13: Inner kinetochore subunit CNN1

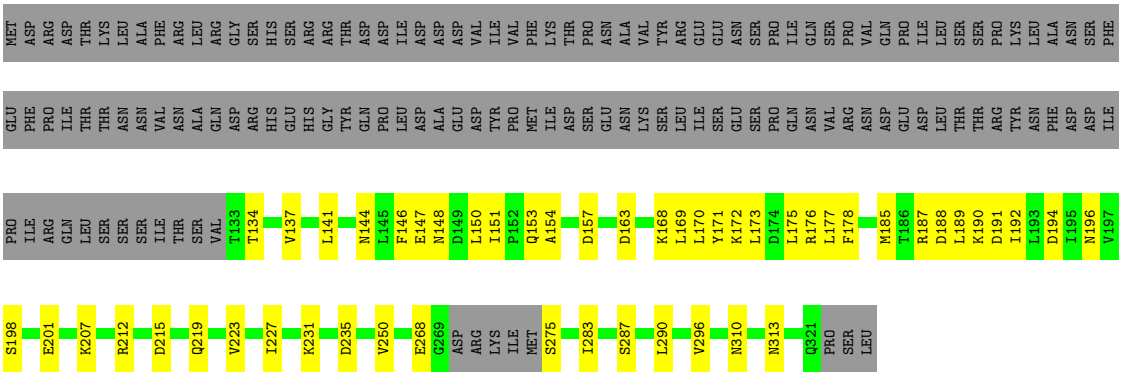




• Molecule 14: Inner kinetochore subunit AME1

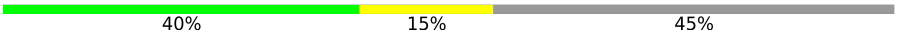
Chain U:

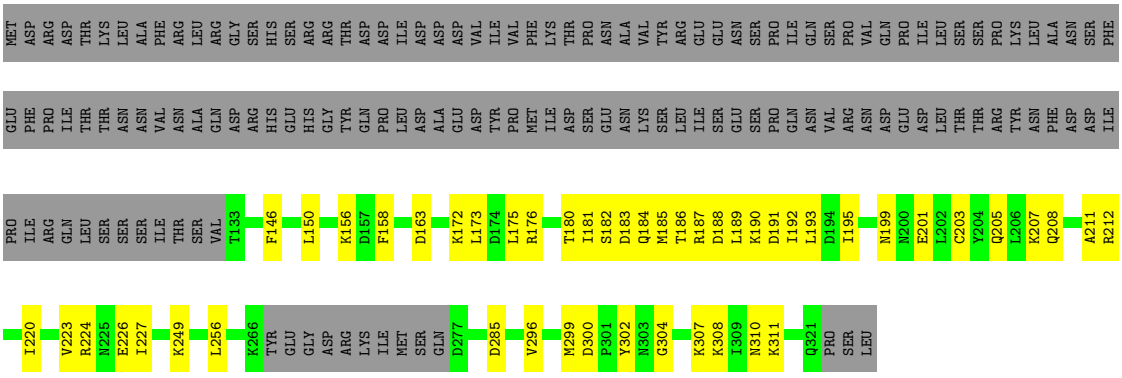




• Molecule 14: Inner kinetochore subunit AME1

Chain UU:





• Molecule 15: Inner kinetochore subunit WIP1

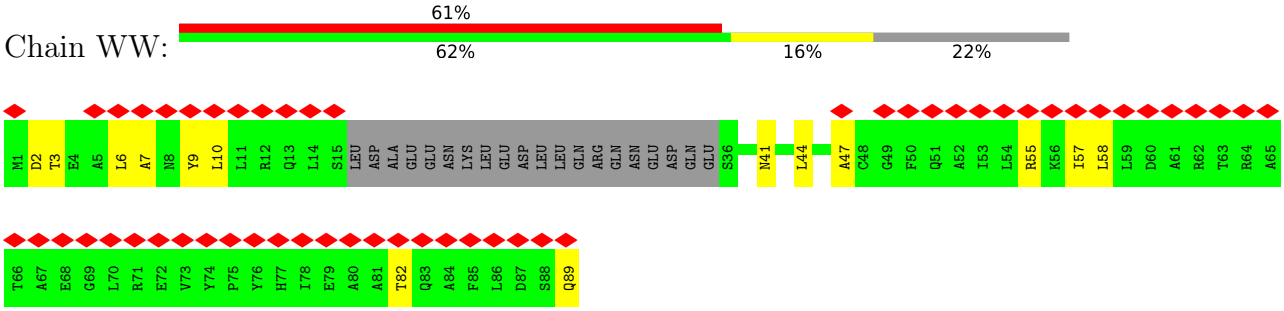
Chain W:





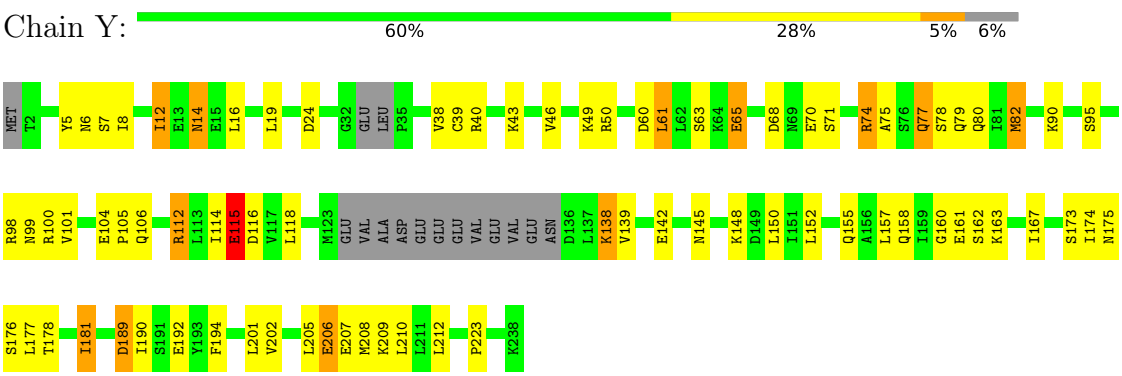
• Molecule 15: Inner kinetochore subunit WIP1

Chain WW:



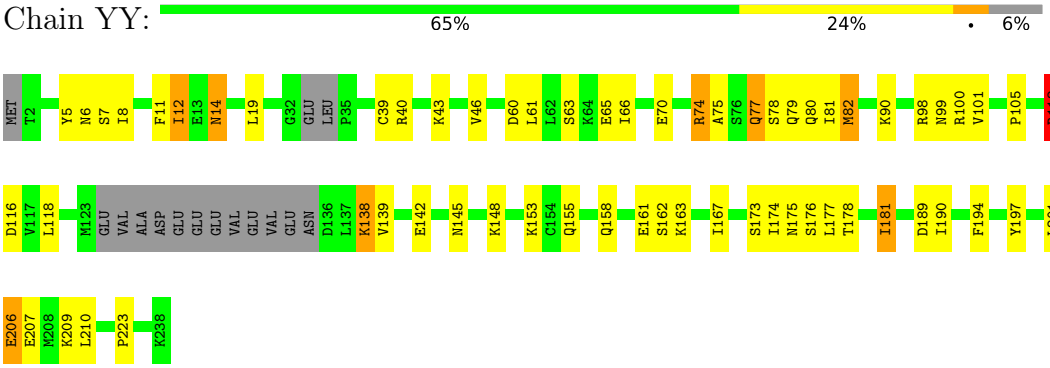
• Molecule 16: Inner kinetochore subunit NKP1

Chain Y:



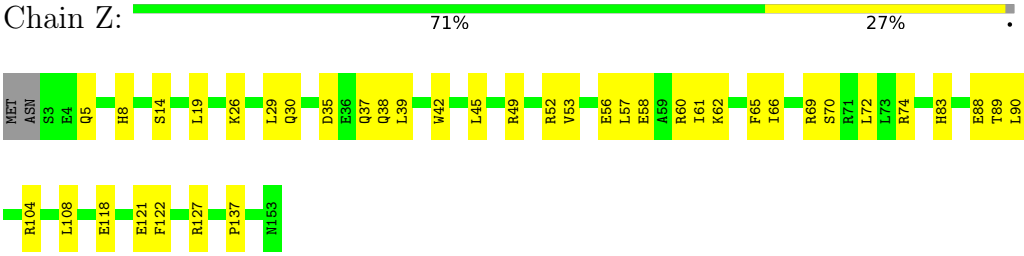
• Molecule 16: Inner kinetochore subunit NKP1

Chain YY:



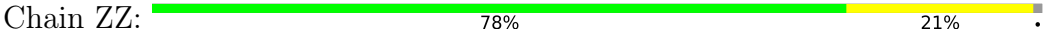
• Molecule 17: Inner kinetochore subunit NKP2

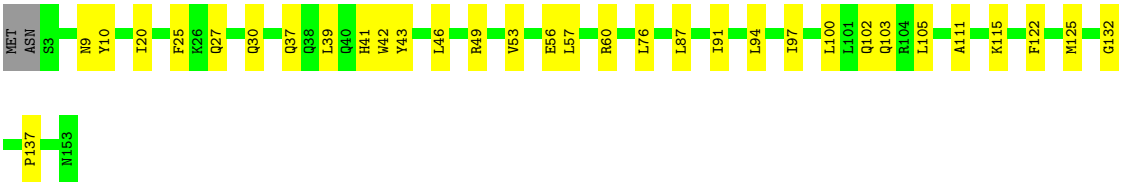
Chain Z:



• Molecule 17: Inner kinetochore subunit NKP2

Chain ZZ:

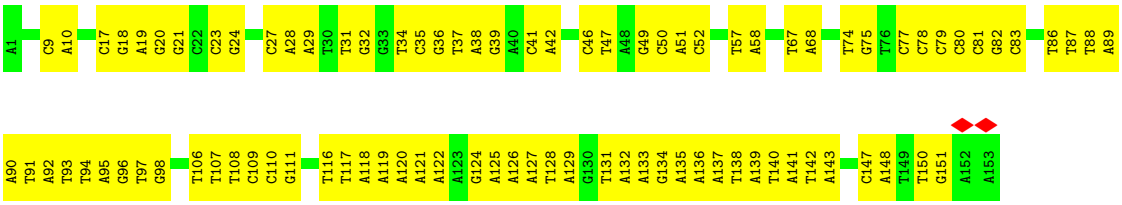




• Molecule 18: C0N3

Chain D:

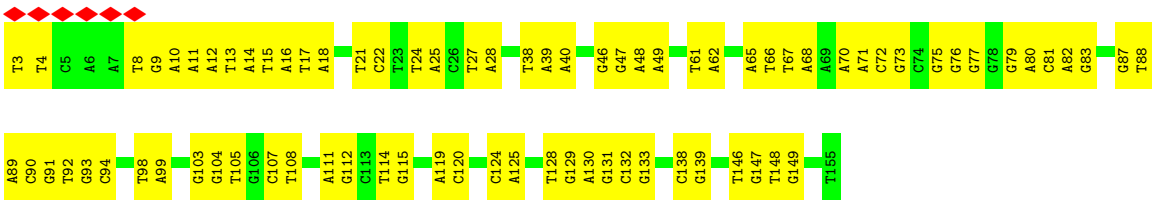




• Molecule 19: C0N3

Chain E:

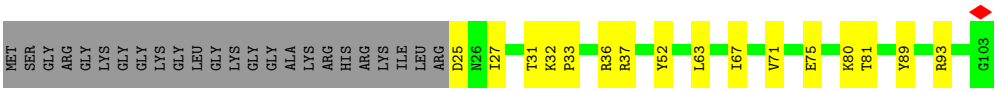




• Molecule 20: Histone H4

Chain b:

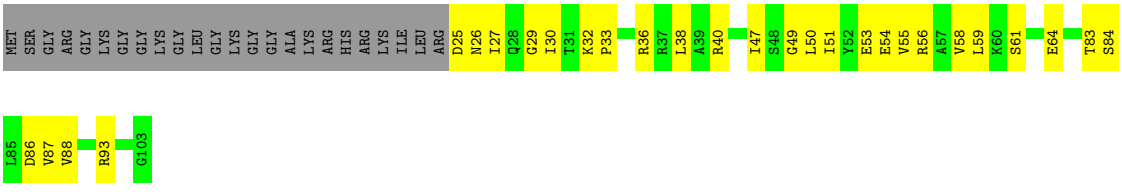




• Molecule 20: Histone H4

Chain f:

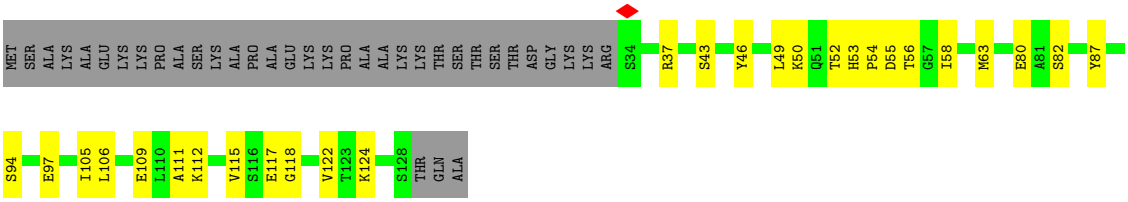




• Molecule 21: Histone H2B.1

Chain d:

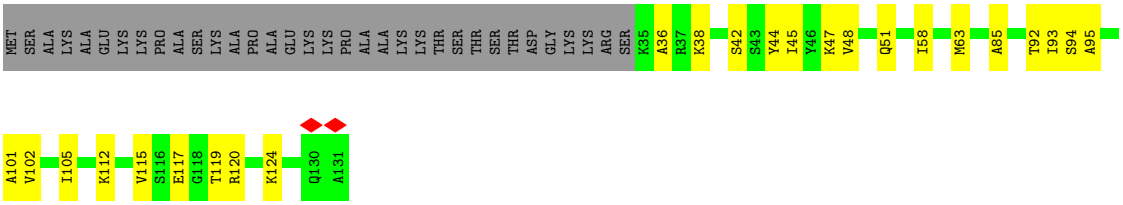




• Molecule 21: Histone H2B.1

Chain h:

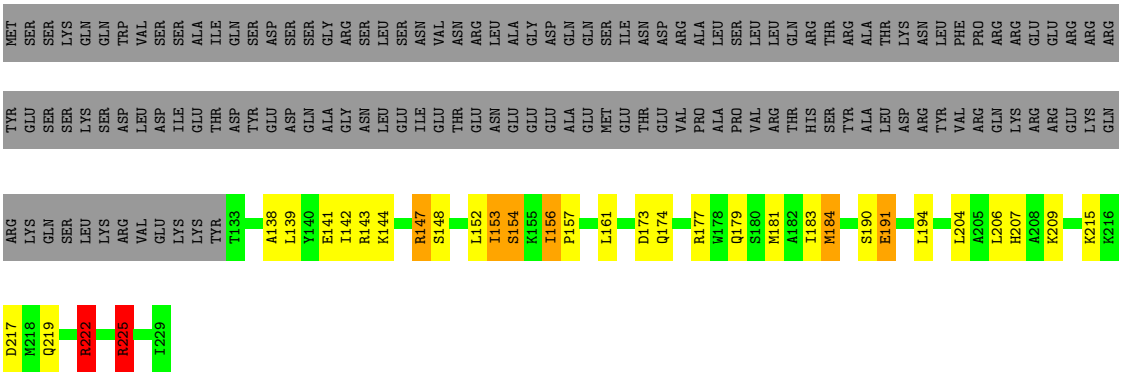




• Molecule 22: Histone H3-like centromeric protein CSE4

Chain e:

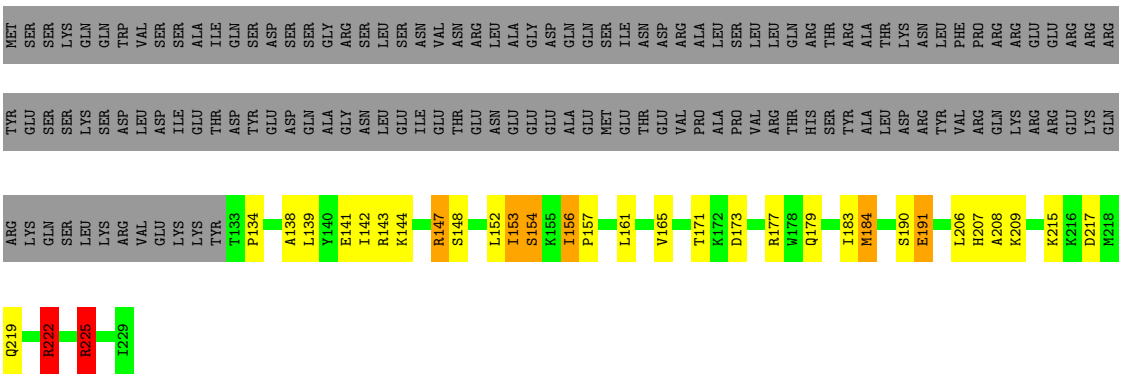




• Molecule 22: Histone H3-like centromeric protein CSE4

Chain a:





• Molecule 23: Histone H2A.1

Chain g:

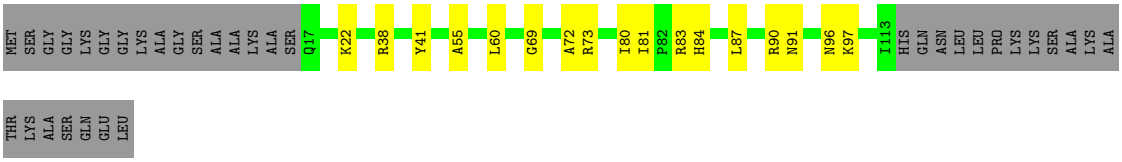




• Molecule 23: Histone H2A.1

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108672	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00271	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A	0.12	0/905	0.30	0/1210
1	B	0.15	0/968	0.36	0/1296
2	I	0.16	0/5458	0.32	0/7402
2	II	0.10	0/5837	0.28	0/7921
3	K	0.17	0/1784	0.35	0/2404
3	KK	0.14	0/1828	0.35	0/2466
4	H	0.20	0/1429	0.45	0/1923
4	HH	0.18	0/1468	0.36	0/1979
5	L	0.18	0/1981	0.51	3/2684 (0.1%)
5	LL	0.18	0/1981	0.51	3/2684 (0.1%)
6	N	0.11	0/3201	0.27	0/4322
6	NN	0.09	0/3193	0.26	0/4311
7	CT	0.10	0/3369	0.32	0/4544
8	CE	0.09	0/4716	0.27	0/6375
8	ce	0.09	0/4458	0.24	0/6038
9	SK	0.11	0/1251	0.34	0/1692
10	P	0.12	0/2131	0.28	0/2866
10	PP	0.09	0/2127	0.28	0/2860
11	Q	0.19	1/2228 (0.0%)	0.35	0/2983
11	QQ	0.13	0/2087	0.31	0/2791
12	O	0.11	0/2054	0.30	0/2761
12	OO	0.10	0/2004	0.30	0/2695
13	T	0.14	0/772	0.34	0/1040
13	TT	0.44	1/772 (0.1%)	0.67	3/1040 (0.3%)
14	U	0.16	0/1499	0.40	0/2018
14	UU	0.13	0/1458	0.36	0/1963
15	W	0.10	0/557	0.27	0/748
15	WW	0.07	0/556	0.22	0/748
16	Y	0.22	0/1672	0.65	4/2252 (0.2%)
16	YY	0.22	0/1672	0.65	4/2252 (0.2%)
17	Z	0.20	0/1195	0.49	1/1616 (0.1%)
17	ZZ	0.16	0/1195	0.36	1/1616 (0.1%)
18	D	0.18	0/3523	0.37	0/5435
19	E	0.19	0/3513	0.36	0/5420

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	b	0.17	0/632	0.38	0/845
20	f	0.15	0/634	0.39	0/848
21	d	0.14	0/745	0.37	0/1003
21	h	0.11	0/755	0.34	0/1017
22	a	0.26	0/792	0.75	7/1066 (0.7%)
22	e	0.26	0/792	0.76	7/1066 (0.7%)
23	c	0.14	0/751	0.40	0/1015
23	g	0.13	0/760	0.36	0/1027
All	All	0.15	2/80703 (0.0%)	0.37	33/110242 (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
2	I	0	4
3	K	0	1
3	KK	0	1
4	H	0	1
7	CT	0	2
11	Q	0	1
16	Y	0	1
16	YY	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	TT	272	PRO	CG-CD	-11.35	1.12	1.50
11	Q	297	HIS	C-N	5.13	1.41	1.33

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	TT	272	PRO	N-CD-CG	-14.38	81.62	103.20
13	TT	272	PRO	CA-N-CD	-9.56	98.62	112.00
16	Y	115	GLU	CA-CB-CG	9.49	133.09	114.10
16	YY	115	GLU	CA-CB-CG	9.49	133.08	114.10
13	TT	272	PRO	CA-CB-CG	-8.57	88.21	104.50

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	425	LYS	Mainchain
2	I	456	CYS	Peptide
2	I	534	TYR	Peptide
2	I	612	LYS	Peptide
3	K	215	THR	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	A	898	0	912	12	0
1	B	957	0	962	29	0
2	I	5337	0	5460	166	0
2	II	5705	0	5817	141	0
3	K	1762	0	1796	86	0
3	KK	1805	0	1809	49	0
4	H	1412	0	1451	96	0
4	HH	1449	0	1478	65	0
5	L	1941	0	1946	56	0
5	LL	1941	0	1946	58	0
6	N	3129	0	3182	50	0
6	NN	3121	0	3171	42	0
7	CT	3298	0	3368	55	0
8	CE	4608	0	4595	77	0
8	ce	4352	0	4318	54	0
9	SK	1230	0	1198	21	0
10	P	2098	0	2174	33	0
10	PP	2094	0	2172	28	0
11	Q	2193	0	2252	59	0
11	QQ	2060	0	2110	62	0
12	O	2015	0	2035	35	0
12	OO	1967	0	1993	43	0
13	T	761	0	781	27	0
13	TT	761	0	781	16	0
14	U	1485	0	1467	42	0
14	UU	1445	0	1436	42	0
15	W	551	0	559	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	WW	550	0	559	11	0
16	Y	1663	0	1588	61	0
16	YY	1663	0	1588	47	0
17	Z	1180	0	1108	38	0
17	ZZ	1180	0	1108	23	0
18	D	3139	0	1727	89	0
19	E	3134	0	1732	81	0
20	b	625	0	657	13	0
20	f	627	0	664	23	0
21	d	735	0	753	24	0
21	h	745	0	757	19	0
22	a	781	0	803	32	0
22	e	781	0	803	26	0
23	c	742	0	775	15	0
23	g	751	0	789	16	0
All	All	78671	0	76580	1648	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 11.

The worst 5 of 1648 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)
18:D:82:DG:C2	19:E:75:DG:C2	2.10	1.38
18:D:82:DG:C2	19:E:75:DG:N2	1.96	1.34
18:D:82:DG:N1	19:E:75:DG:N1	1.80	1.27
18:D:80:DC:N4	19:E:76:DG:C6	2.07	1.23
18:D:82:DG:N3	19:E:75:DG:N2	1.89	1.18

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	A	108/351 (31%)	108 (100%)	0	0	100	100
1	B	114/351 (32%)	113 (99%)	1 (1%)	0	100	100
2	I	649/733 (88%)	624 (96%)	25 (4%)	0	100	100
2	II	696/733 (95%)	676 (97%)	20 (3%)	0	100	100
3	K	213/239 (89%)	207 (97%)	6 (3%)	0	100	100
3	KK	221/239 (92%)	209 (95%)	12 (5%)	0	100	100
4	H	167/181 (92%)	159 (95%)	8 (5%)	0	100	100
4	HH	172/181 (95%)	168 (98%)	4 (2%)	0	100	100
5	L	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
5	LL	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
6	N	378/458 (82%)	365 (97%)	13 (3%)	0	100	100
6	NN	377/458 (82%)	369 (98%)	8 (2%)	0	100	100
7	CT	383/478 (80%)	362 (94%)	21 (6%)	0	100	100
8	CE	549/608 (90%)	532 (97%)	16 (3%)	1 (0%)	43	72
8	ce	518/608 (85%)	506 (98%)	12 (2%)	0	100	100
9	SK	147/194 (76%)	142 (97%)	5 (3%)	0	100	100
10	P	249/369 (68%)	246 (99%)	3 (1%)	0	100	100
10	PP	248/369 (67%)	241 (97%)	7 (3%)	0	100	100
11	Q	257/406 (63%)	253 (98%)	4 (2%)	0	100	100
11	QQ	241/406 (59%)	233 (97%)	8 (3%)	0	100	100
12	O	241/368 (66%)	230 (95%)	11 (5%)	0	100	100
12	OO	236/368 (64%)	228 (97%)	8 (3%)	0	100	100
13	T	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
13	TT	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
14	U	180/324 (56%)	177 (98%)	3 (2%)	0	100	100
14	UU	175/324 (54%)	172 (98%)	3 (2%)	0	100	100
15	W	65/89 (73%)	65 (100%)	0	0	100	100
15	WW	65/89 (73%)	65 (100%)	0	0	100	100
16	Y	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
16	YY	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
17	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
17	ZZ	149/153 (97%)	148 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	b	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
20	f	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
21	d	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
21	h	95/131 (72%)	93 (98%)	2 (2%)	0	100	100
22	a	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
22	e	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
23	c	95/132 (72%)	92 (97%)	3 (3%)	0	100	100
23	g	96/132 (73%)	96 (100%)	0	0	100	100
All	All	8762/12108 (72%)	8496 (97%)	265 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	CE	587	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/305 (32%)	97 (100%)	0	100	100
1	B	103/305 (34%)	103 (100%)	0	100	100
2	I	612/683 (90%)	612 (100%)	0	100	100
2	II	654/683 (96%)	654 (100%)	0	100	100
3	K	202/223 (91%)	202 (100%)	0	100	100
3	KK	202/223 (91%)	202 (100%)	0	100	100
4	H	162/172 (94%)	162 (100%)	0	100	100
4	HH	167/172 (97%)	167 (100%)	0	100	100
5	L	217/221 (98%)	193 (89%)	24 (11%)	6	25
5	LL	217/221 (98%)	193 (89%)	24 (11%)	6	25

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	N	350/416 (84%)	350 (100%)	0	100 100
6	NN	349/416 (84%)	349 (100%)	0	100 100
7	CT	368/449 (82%)	368 (100%)	0	100 100
8	CE	521/569 (92%)	521 (100%)	0	100 100
8	ce	488/569 (86%)	488 (100%)	0	100 100
9	SK	137/179 (76%)	137 (100%)	0	100 100
10	P	240/344 (70%)	240 (100%)	0	100 100
10	PP	240/344 (70%)	239 (100%)	1 (0%)	84 81
11	Q	250/378 (66%)	250 (100%)	0	100 100
11	QQ	234/378 (62%)	234 (100%)	0	100 100
12	O	230/347 (66%)	230 (100%)	0	100 100
12	OO	225/347 (65%)	225 (100%)	0	100 100
13	T	89/339 (26%)	89 (100%)	0	100 100
13	TT	89/339 (26%)	89 (100%)	0	100 100
14	U	168/308 (54%)	168 (100%)	0	100 100
14	UU	164/308 (53%)	164 (100%)	0	100 100
15	W	57/76 (75%)	57 (100%)	0	100 100
15	WW	57/76 (75%)	57 (100%)	0	100 100
16	Y	175/219 (80%)	156 (89%)	19 (11%)	6 26
16	YY	175/219 (80%)	156 (89%)	19 (11%)	6 26
17	Z	121/143 (85%)	120 (99%)	1 (1%)	73 76
17	ZZ	121/143 (85%)	121 (100%)	0	100 100
20	b	65/81 (80%)	65 (100%)	0	100 100
20	f	66/81 (82%)	66 (100%)	0	100 100
21	d	81/109 (74%)	81 (100%)	0	100 100
21	h	81/109 (74%)	81 (100%)	0	100 100
22	a	82/207 (40%)	71 (87%)	11 (13%)	4 20
22	e	82/207 (40%)	71 (87%)	11 (13%)	4 20
23	c	75/99 (76%)	75 (100%)	0	100 100
23	g	77/99 (78%)	76 (99%)	1 (1%)	61 71
All	All	8090/11106 (73%)	7979 (99%)	111 (1%)	57 70

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Y	115	GLU
22	a	225	ARG
16	YY	19	LEU
22	a	222	ARG
23	g	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
17	Z	80	GLN
2	II	731	GLN
14	UU	148	ASN
16	YY	79	GLN
3	KK	163	ASN

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)

There are no ligands in this entry.

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.

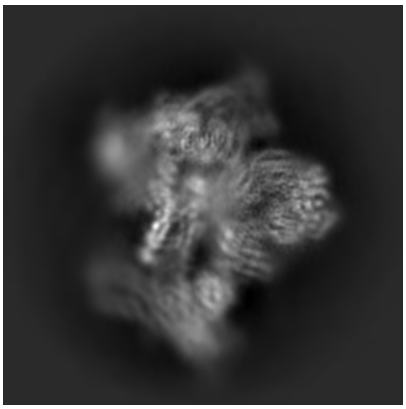
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17227. These allow visual inspection of the internal detail of the map and identification of artifacts.

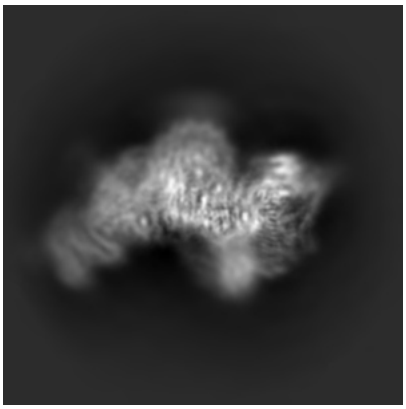
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

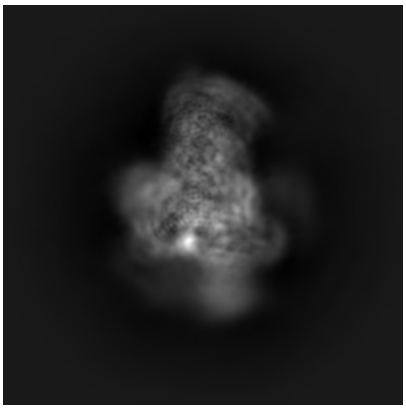
6.1.1 Primary map



X

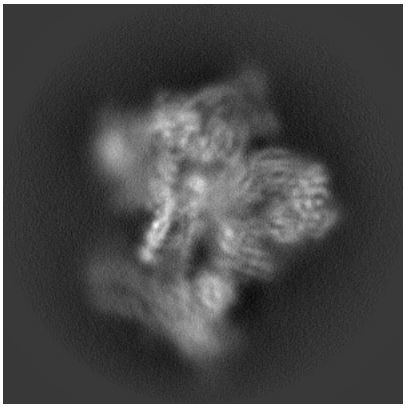


Y

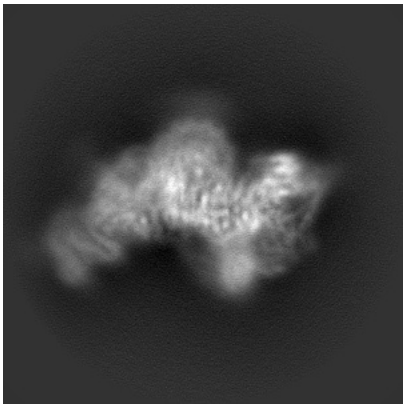


Z

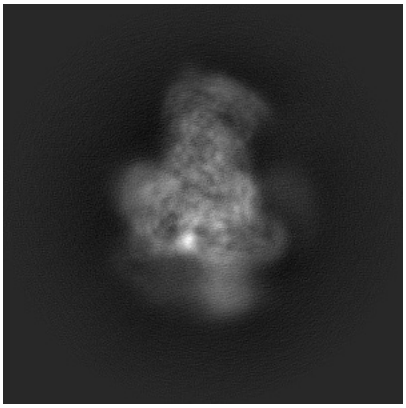
6.1.2 Raw map



X



Y

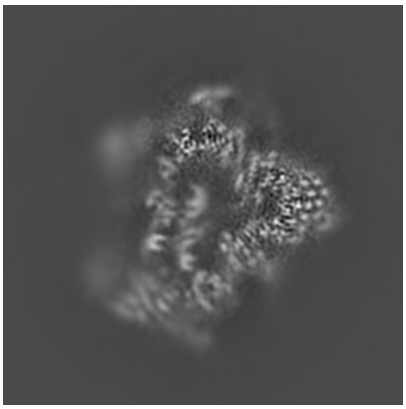


Z

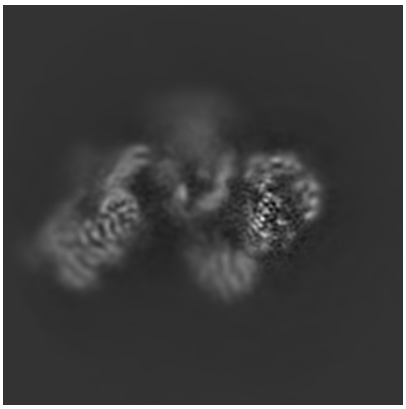
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 176

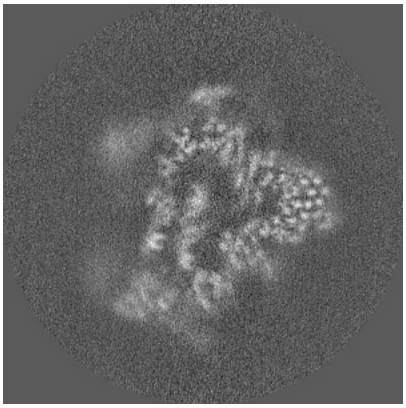


Y Index: 176

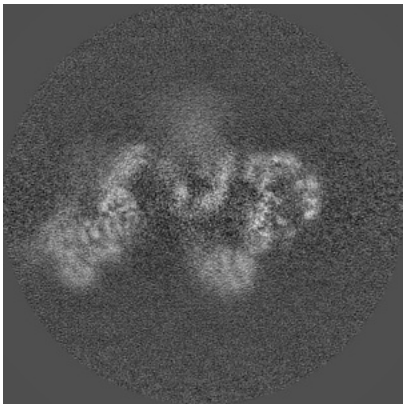


Z Index: 176

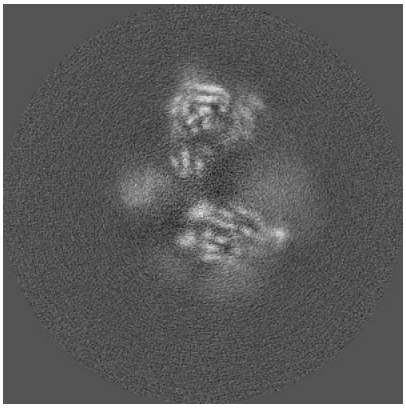
6.2.2 Raw map



X Index: 176



Y Index: 176

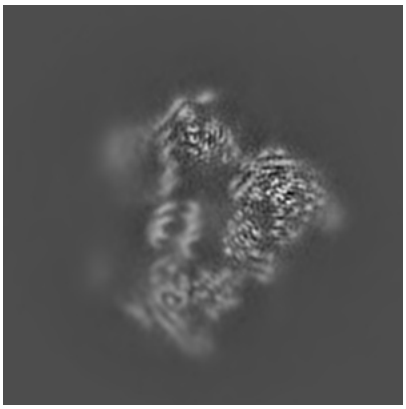


Z Index: 176

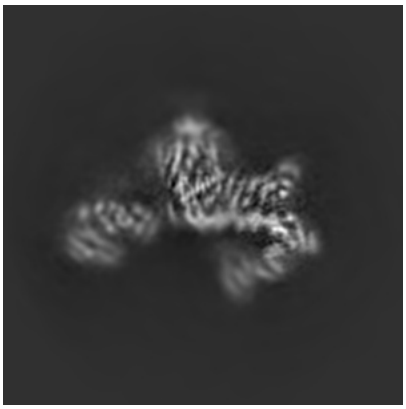
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

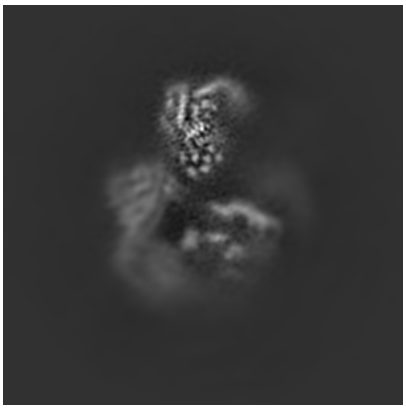
6.3.1 Primary map



X Index: 167

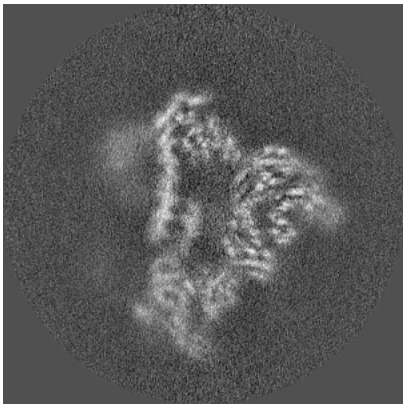


Y Index: 143

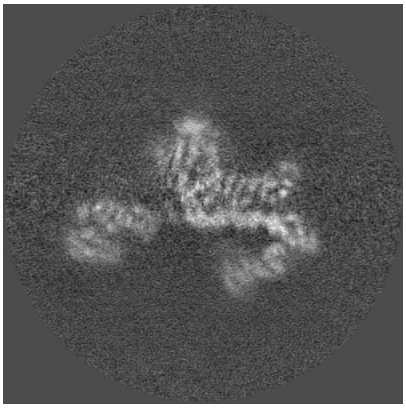


Z Index: 196

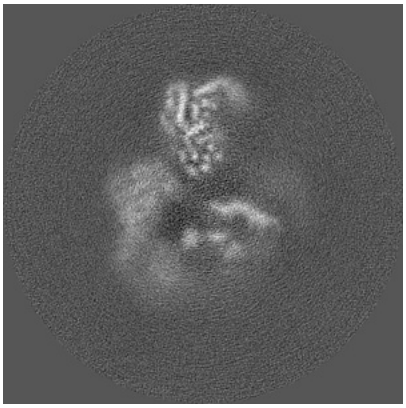
6.3.2 Raw map



X Index: 163



Y Index: 144

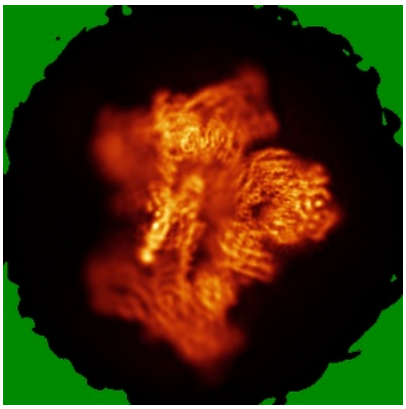


Z Index: 196

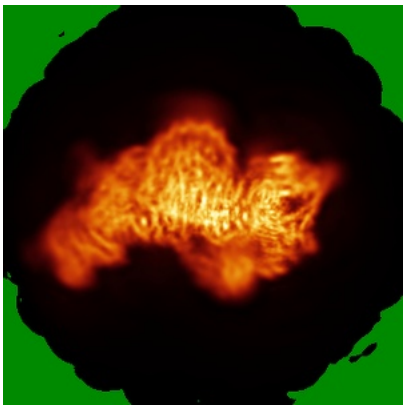
The images above show the largest variance slices of the map in three orthogonal directions.

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

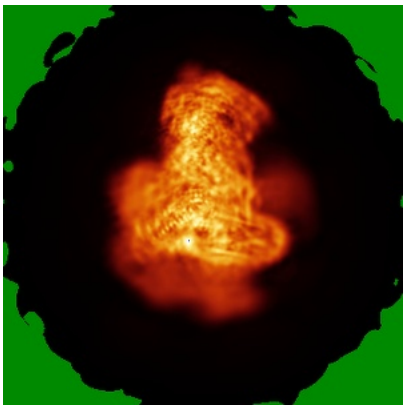
6.4.1 Primary map



X

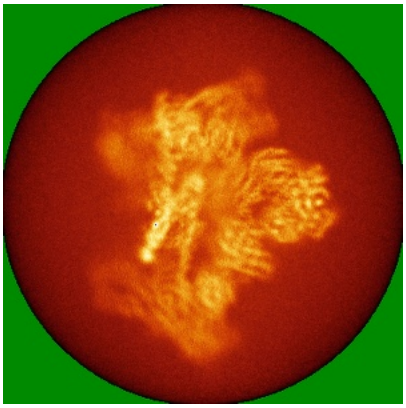


Y

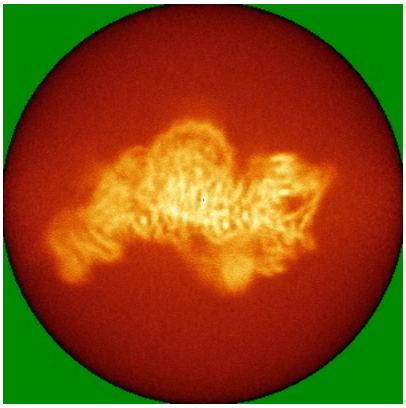


Z

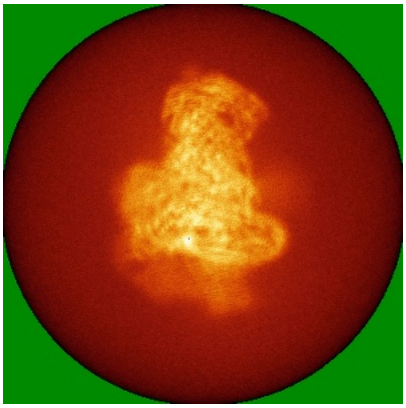
6.4.2 Raw map



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)

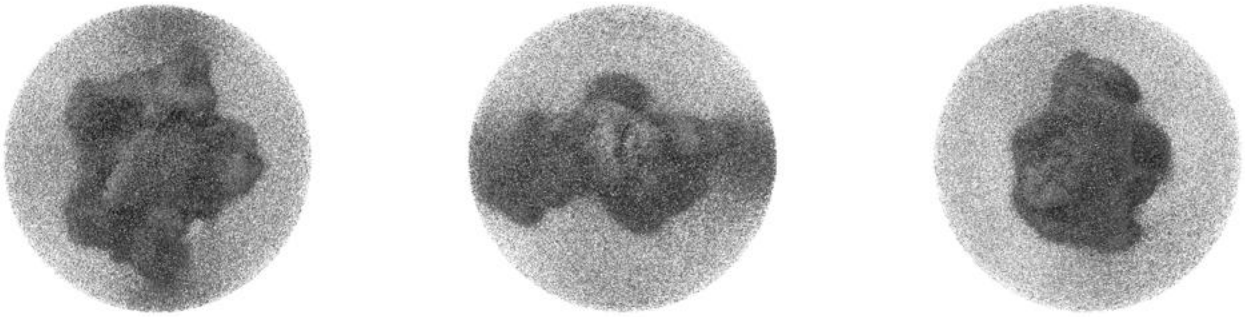
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00271. 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.

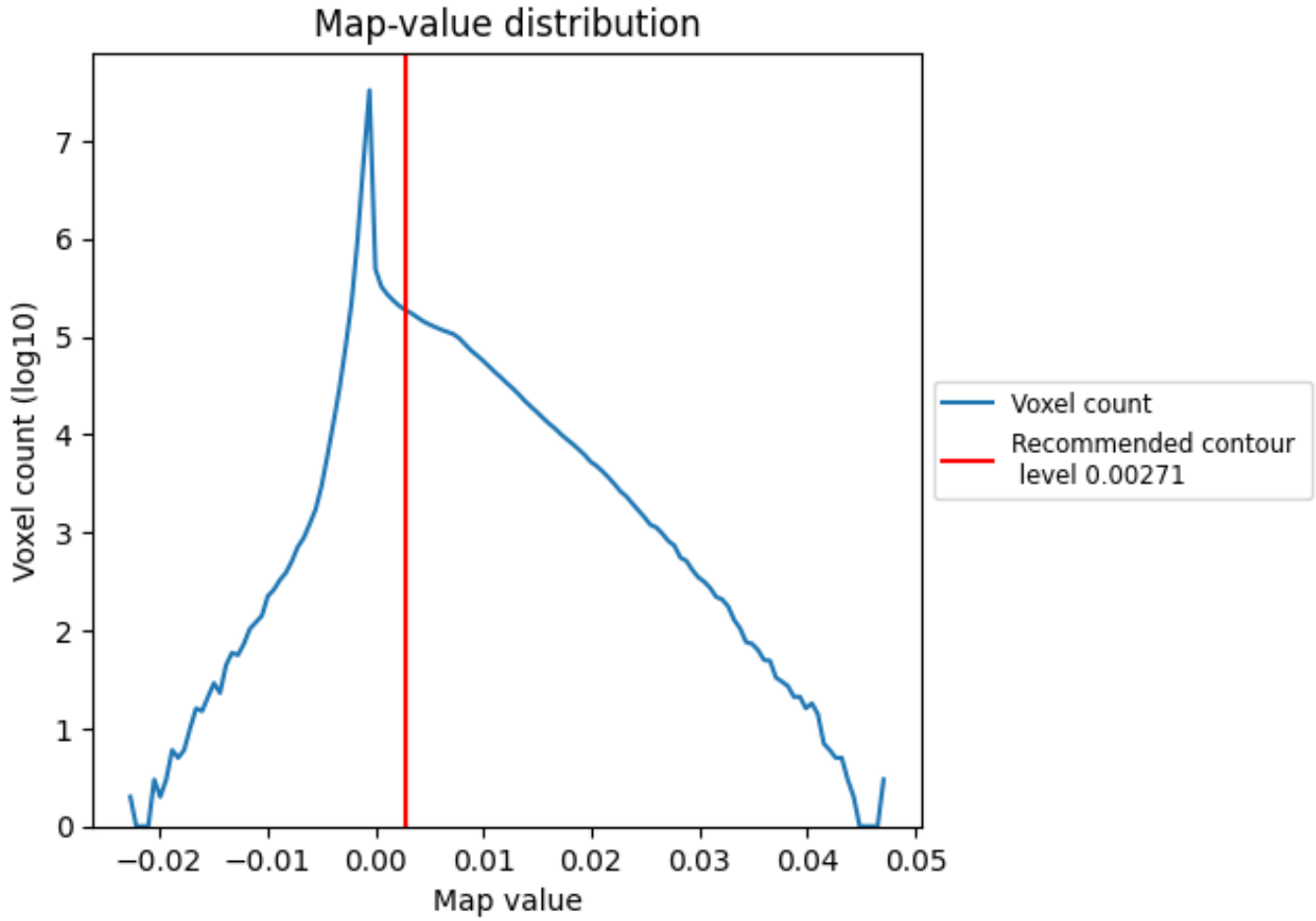
6.6 Mask visualisation (i)

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

7 Map analysis

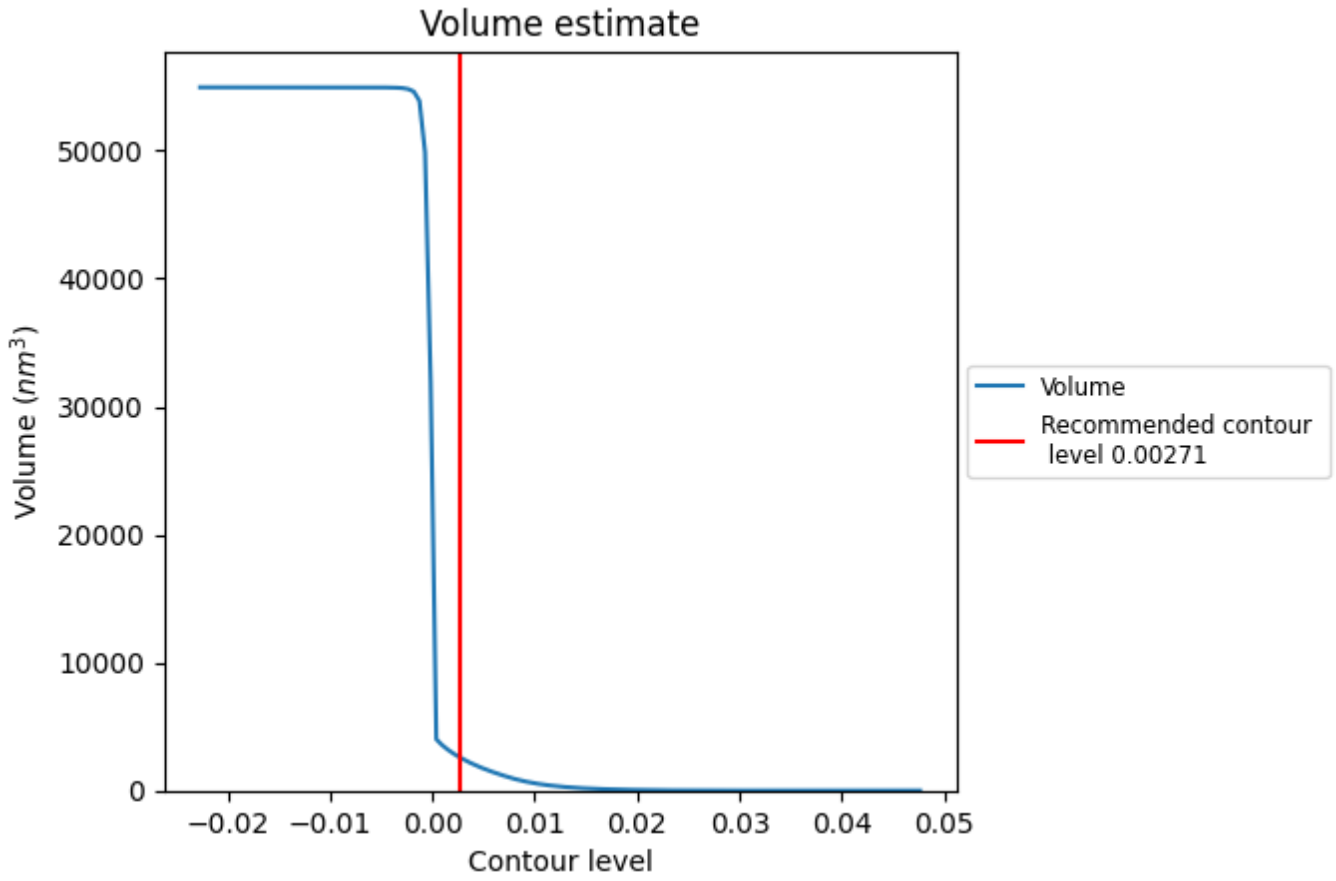
This section contains the results of statistical analysis of the map.

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.

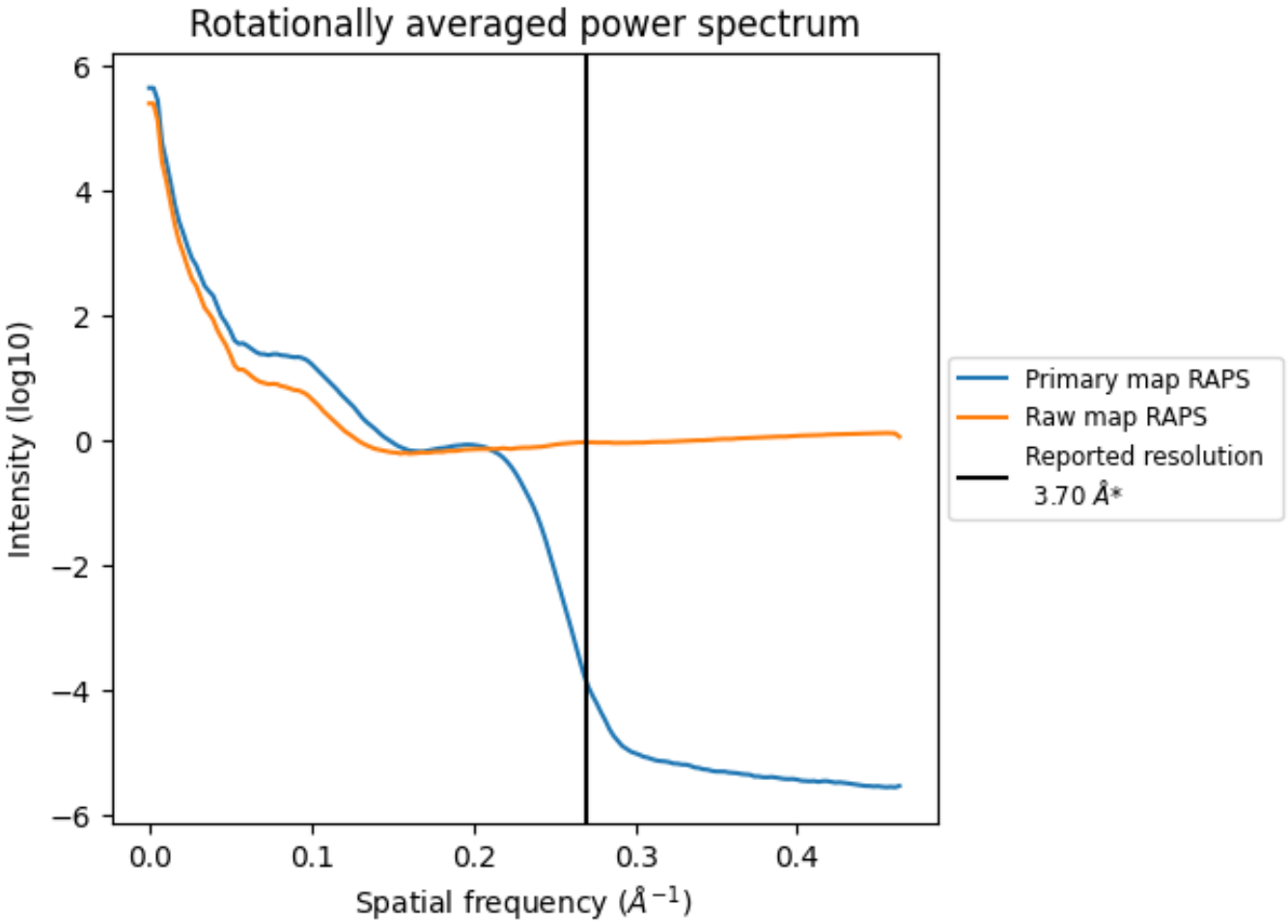
7.2 Volume estimate (i)



The volume at the recommended contour level is 2581 nm^3; this corresponds to an approximate mass of 2331 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)

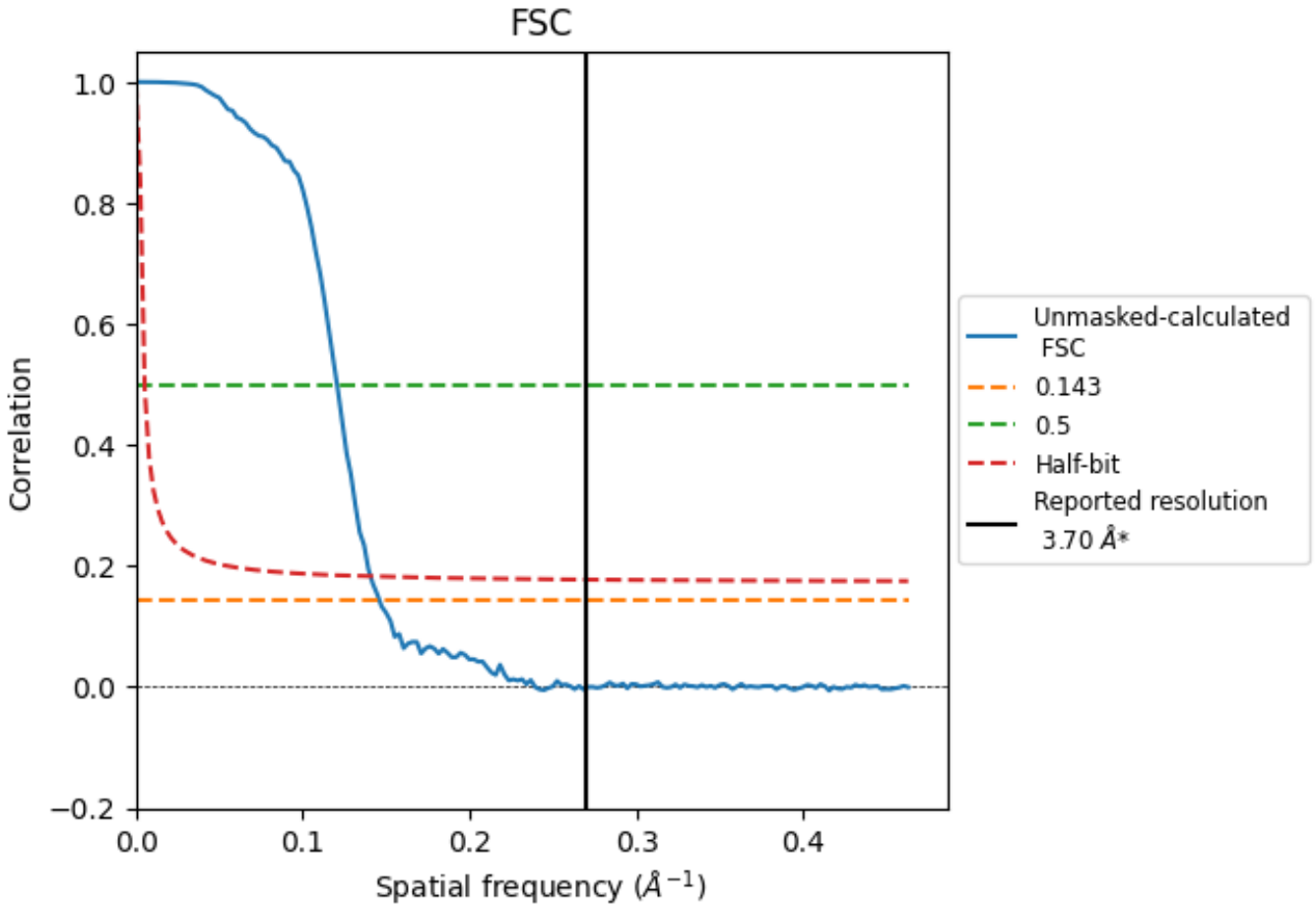


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

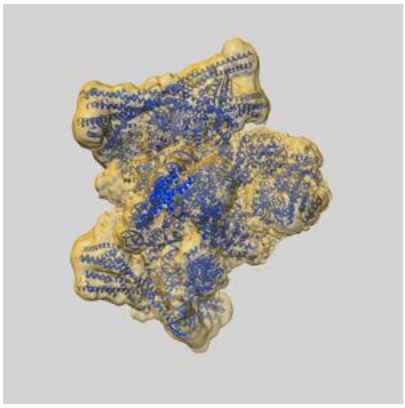
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.85	8.29	7.11

*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 6.85 differs from the reported value 3.7 by more than 10 %

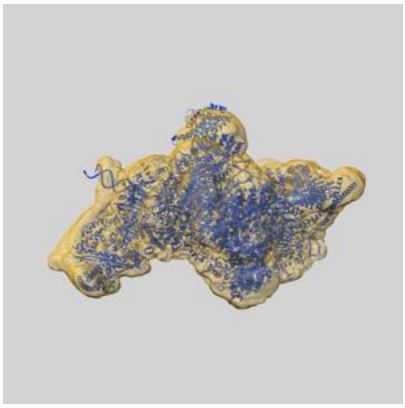
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17227 and PDB model 8OW1. Per-residue inclusion information can be found in section 3 on page 10.

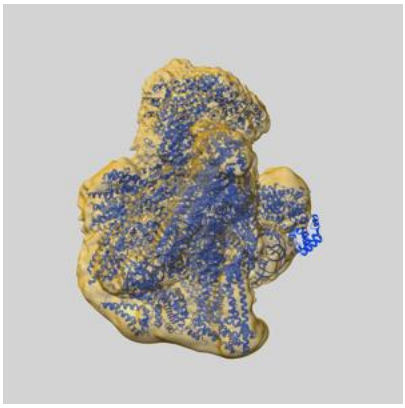
9.1 Map-model overlay



X



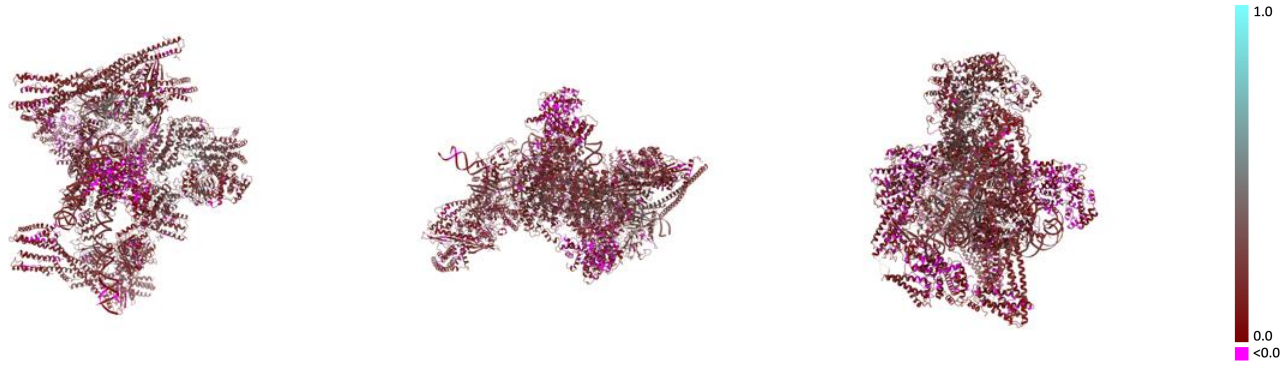
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00271 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.

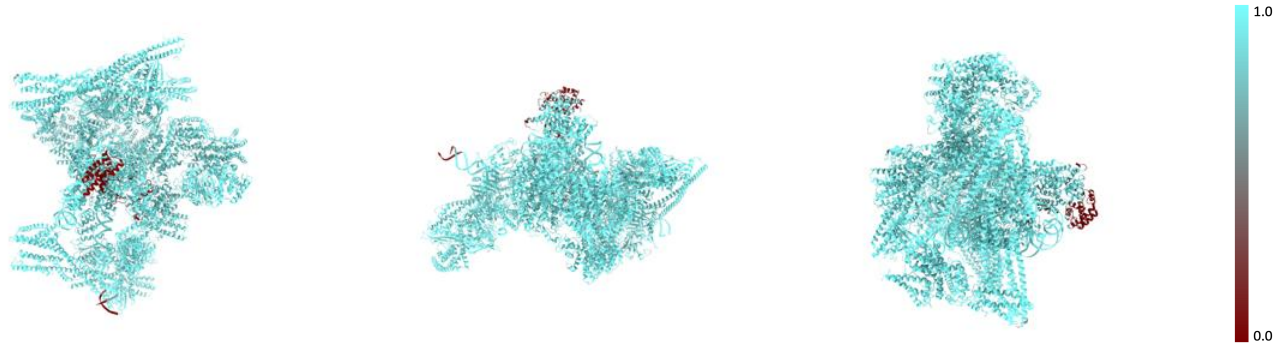
9.2 Q-score mapped to coordinate model (i)



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.

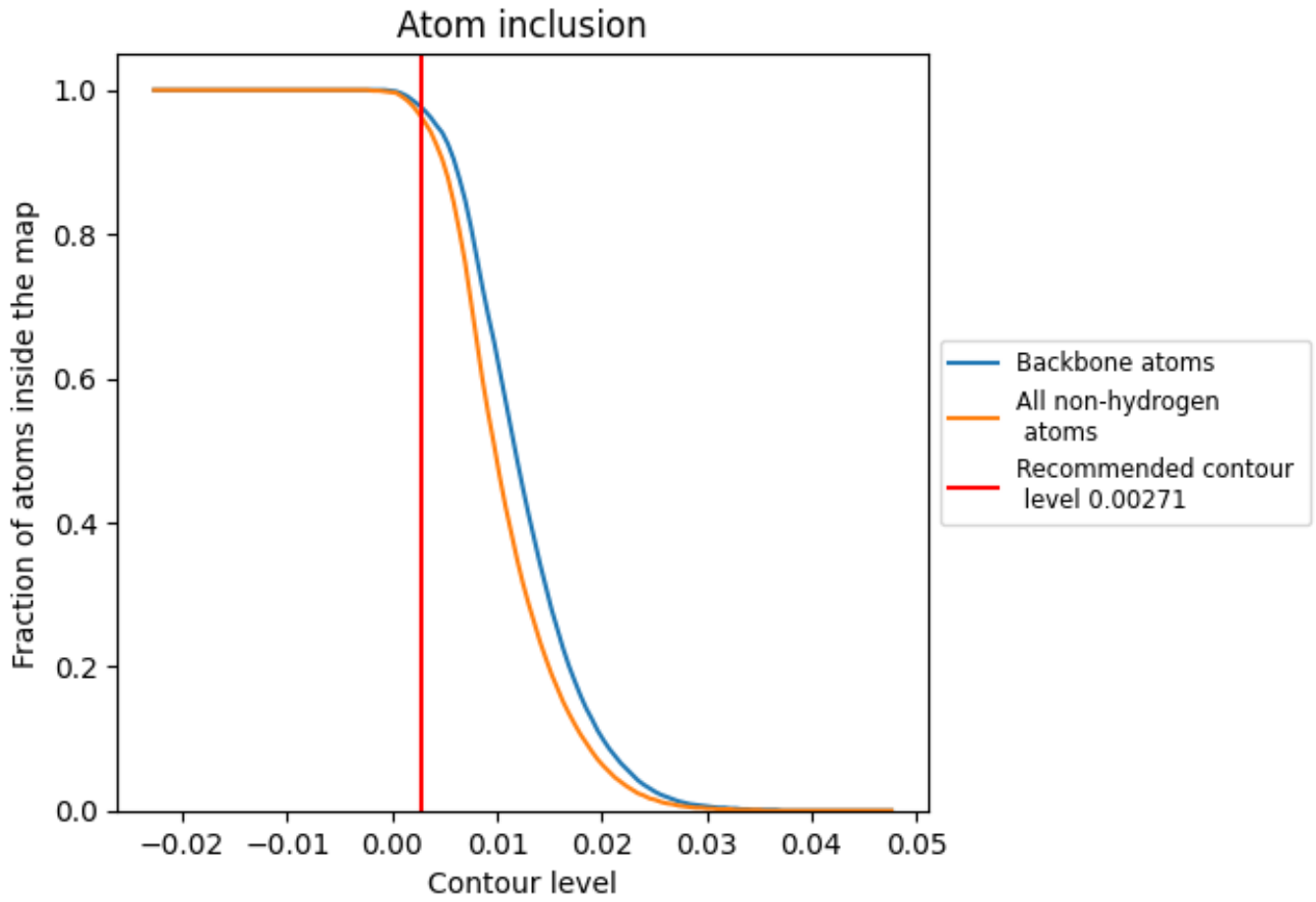
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00271).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.00271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9640	0.1650
A	0.9900	0.1660
B	0.9880	0.2000
CE	0.9230	0.2300
CT	0.9840	0.2070
D	0.9780	0.1910
E	0.9630	0.1940
H	0.9990	0.0860
HH	0.9440	0.1480
I	0.9990	0.0650
II	0.9650	0.1480
K	0.9970	0.0900
KK	0.8670	0.1080
L	0.9850	0.1950
LL	0.9900	0.1570
N	0.9600	0.2510
NN	0.9910	0.1860
O	0.9690	0.2320
OO	0.9840	0.1560
P	0.9880	0.1810
PP	0.9960	0.1480
Q	0.9960	0.1390
QQ	1.0000	0.1290
SK	0.9930	0.1920
T	0.9970	0.0560
TT	0.3070	-0.0000
U	0.9970	0.1460
UU	0.9980	0.1240
W	1.0000	0.0940
WW	0.2070	0.0250
Y	0.9950	0.1540
YY	0.9950	0.1510
Z	0.9830	0.1560
ZZ	0.9970	0.1470
a	0.9750	0.1650



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.9670	0.2090
c	0.9610	0.2250
ce	0.9750	0.2360
d	0.9570	0.2170
e	0.9650	0.1700
f	0.9670	0.1920
g	0.9780	0.1810
h	0.9600	0.1950