Full wwPDB EM Validation Report ⓘ

Jul 31, 2023 – 07:48 pm BST

PDB ID	:	8OW0
EMDB ID	:	EMD-17226
Title	:	Cryo-EM structure of CBF1-CCAN bound topologically to a centromeric 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	:	3.40 Å(reported)

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

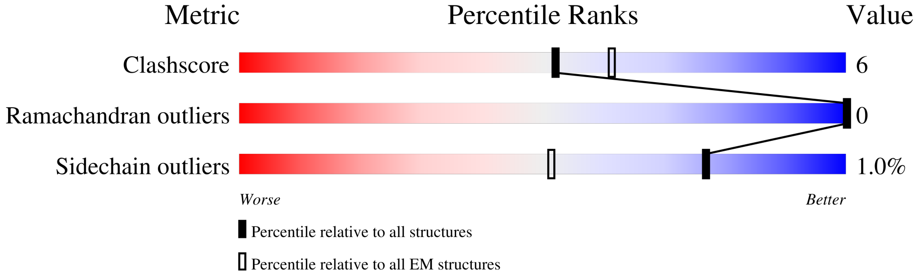
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

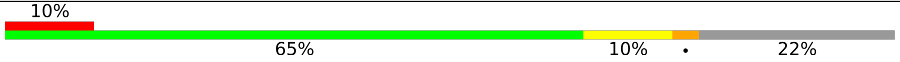
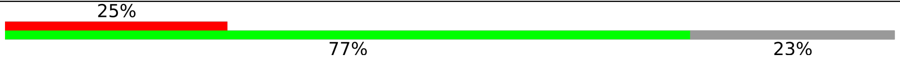
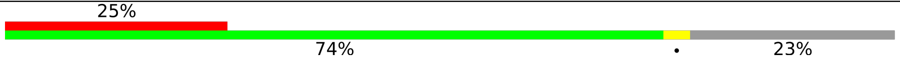
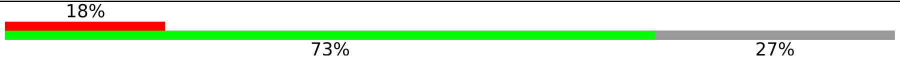
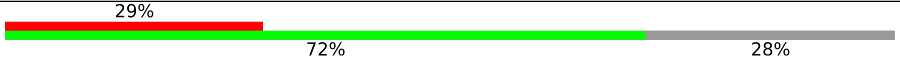
The reported resolution of this entry is 3.40 Å.

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	D	153	
2	E	153	
3	b	103	
3	f	103	
4	d	131	
4	h	131	
5	a	229	
5	e	229	

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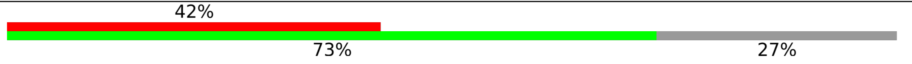
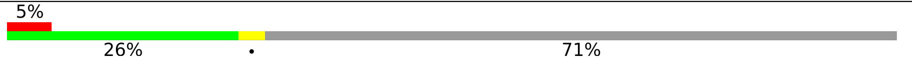
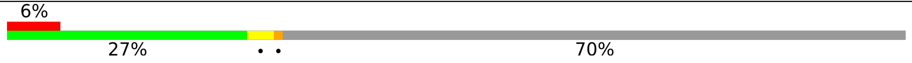
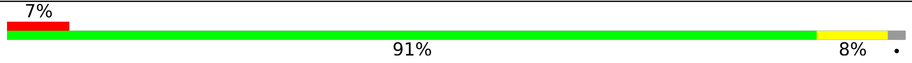
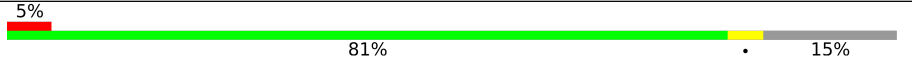
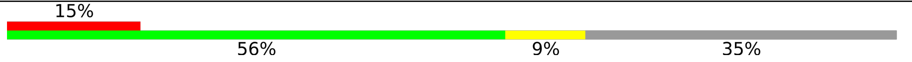
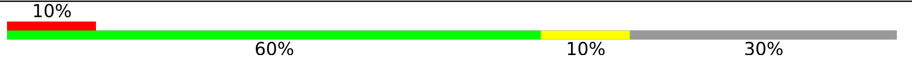
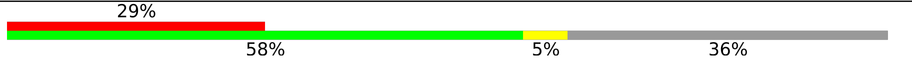
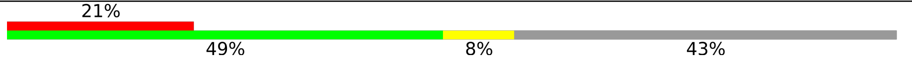
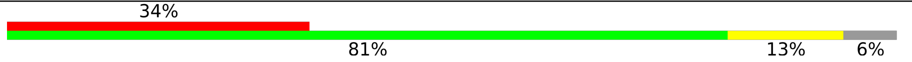
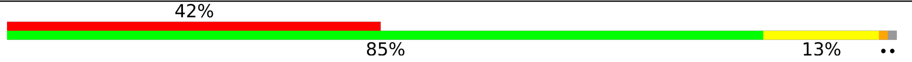
Mol	Chain	Length	Quality of chain
6	c	132	
6	g	132	
7	A	351	
7	B	351	
8	H	181	
9	I	733	
10	K	239	
11	L	245	
12	N	458	
13	O	368	
14	P	369	
15	Q	406	
16	T	361	
17	U	324	
18	W	89	
19	Y	238	
20	Z	153	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 74349 atoms, of which 36378 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 DNA chain called C0N3 DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	D	121	3839	1180	1364	446	728	121	0	0

- Molecule 2 is a DNA chain called C0N3 DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	E	120	3818	1173	1352	456	717	120	0	0

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	b	79	1283	393	658	120	112	0	0
			Total	C	H	N	O		
3	f	79	1292	395	665	120	112	0	0

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	d	95	1489	461	754	129	144	1	0	0
			Total	C	H	N	O	S		
4	h	94	1478	458	749	128	142	1	0	0

- Molecule 5 is a protein called Histone H3-like centromeric protein CSE4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	e	97	1585	498	804	139	140	4	0	0
			Total	C	H	N	O	S		
5	a	97	1585	498	804	139	140	4	0	0

- Molecule 6 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	97	Total 1530	C 467	H 785	N 146	O 132	0	0
6	c	97	Total 1518	C 464	H 776	N 146	O 132	0	0

- Molecule 7 is a protein called Centromere-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	101	Total 1668	C 507	H 846	N 152	O 161	S 2	0	0
7	B	107	Total 1773	C 542	H 897	N 161	O 171	S 2	0	0

- Molecule 8 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	171	Total 2865	C 890	H 1453	N 247	O 273	S 2	0	0

- Molecule 9 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	667	Total 10917	C 3499	H 5512	N 905	O 971	S 30	0	0

- Molecule 10 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	219	Total 3566	C 1113	H 1804	N 304	O 340	S 5	0	0

- Molecule 11 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	241	Total 3887	C 1244	H 1946	N 320	O 366	S 11	0	0

- Molecule 12 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	N	391	6373	2053	3207	537	563	13	0	0

- Molecule 13 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	O	241	3976	1277	1997	328	369	5	0	0

- Molecule 14 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	P	257	4308	1358	2192	366	378	14	0	0

- Molecule 15 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	Q	258	4347	1357	2201	375	405	9	0	0

- Molecule 16 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	T	92	1543	488	782	125	144	4	0	0

- Molecule 17 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	U	184	2965	928	1480	255	299	3	0	0

- Molecule 18 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	W	69	1111	348	560	96	105	2	0	0

- Molecule 19 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	Y	223	3308	1027	1645	281	349	6	0	0

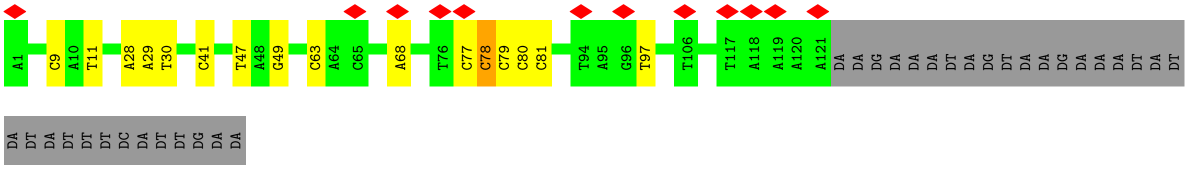
- Molecule 20 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	Z	151	2325	740	1145	204	235	1	0	0

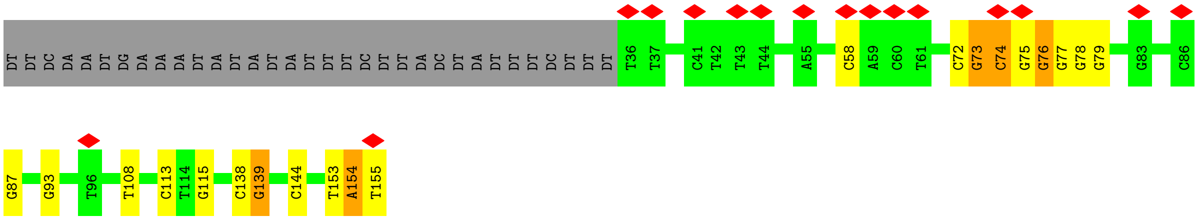
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

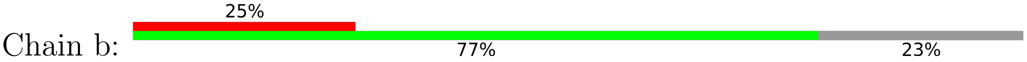
- Molecule 1: C0N3 DNA

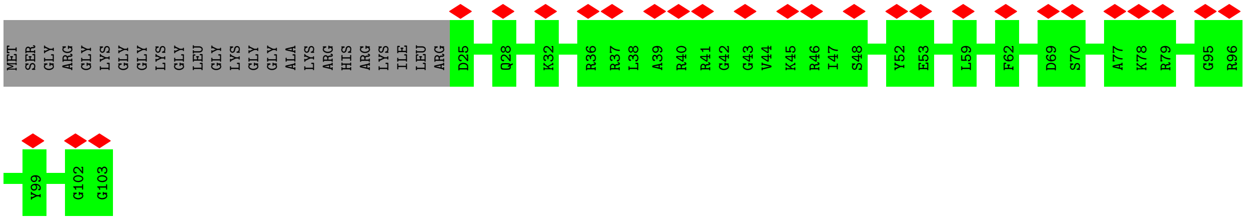


- Molecule 2: C0N3 DNA

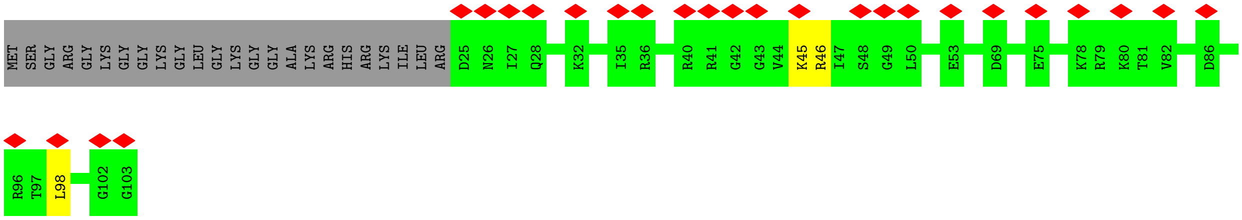


- Molecule 3: Histone H4

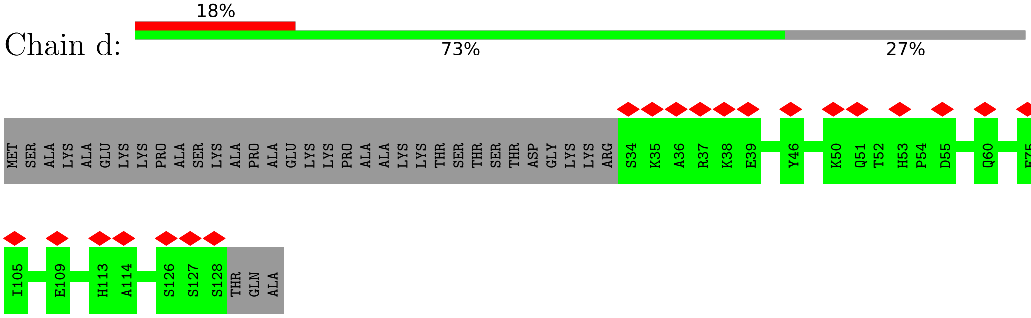




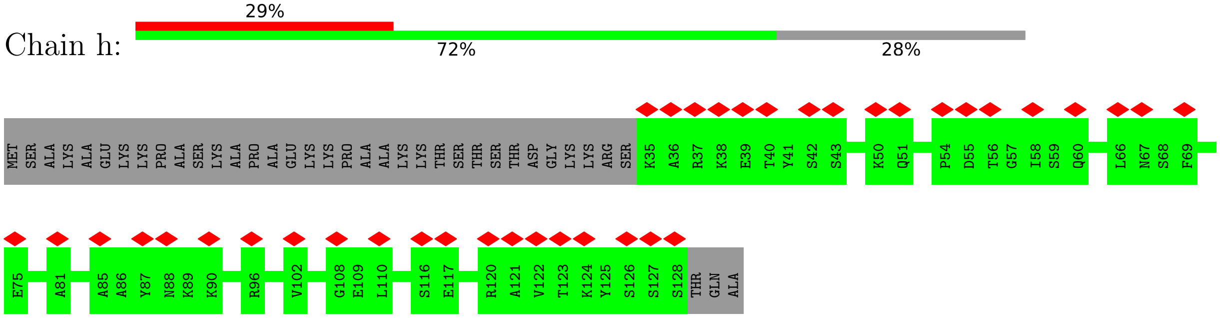
- Molecule 3: Histone H4



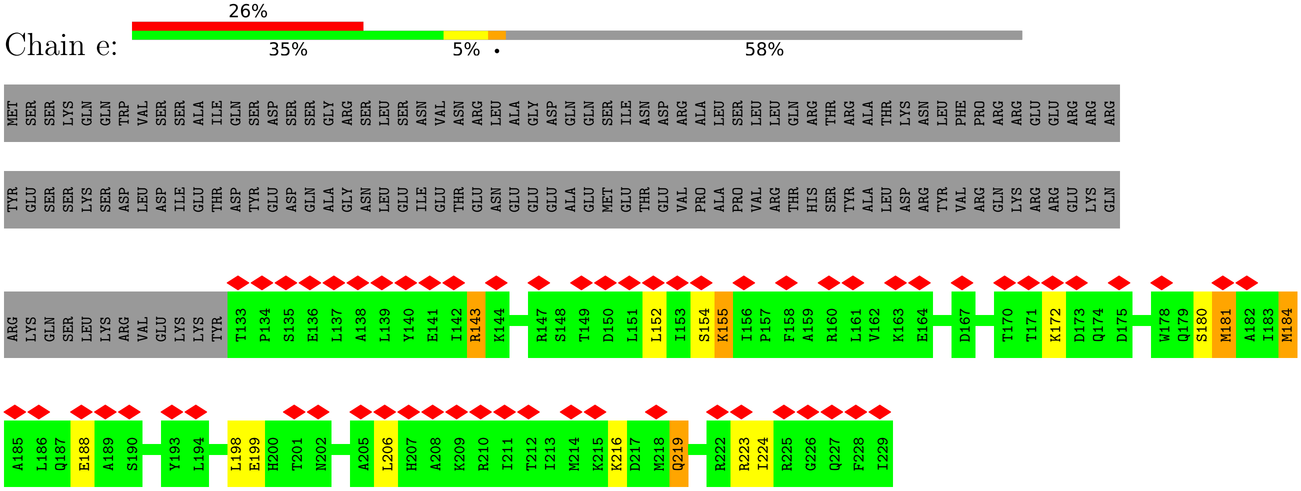
- Molecule 4: Histone H2B.1



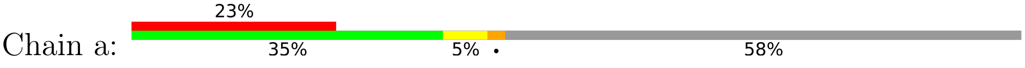
- Molecule 4: Histone H2B.1

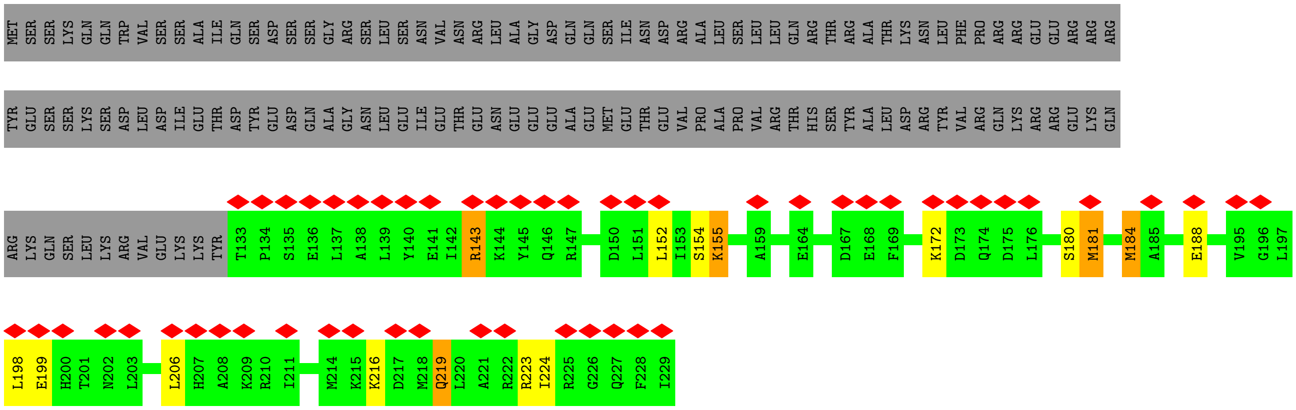


- Molecule 5: Histone H3-like centromeric protein CSE4

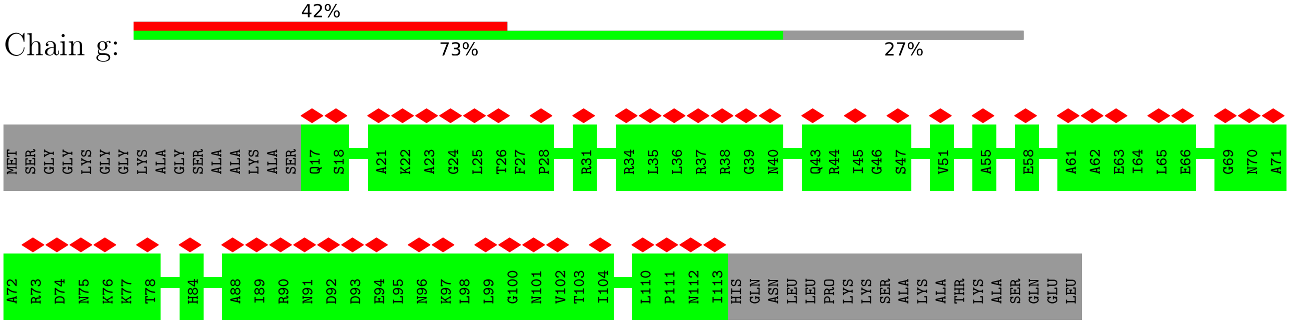


- Molecule 5: Histone H3-like centromeric protein CSE4

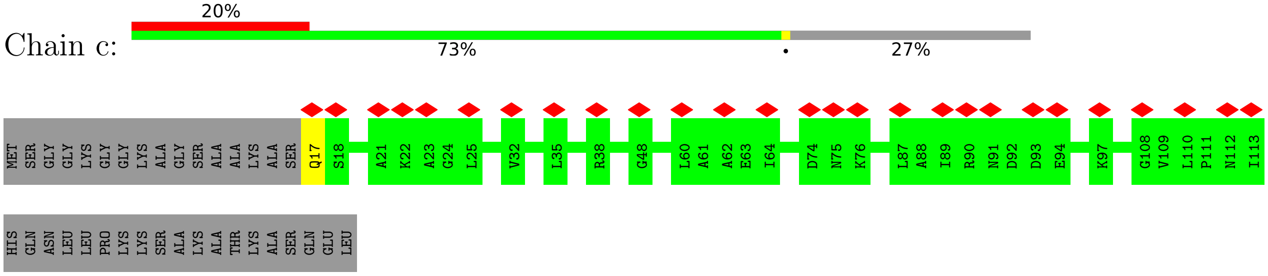




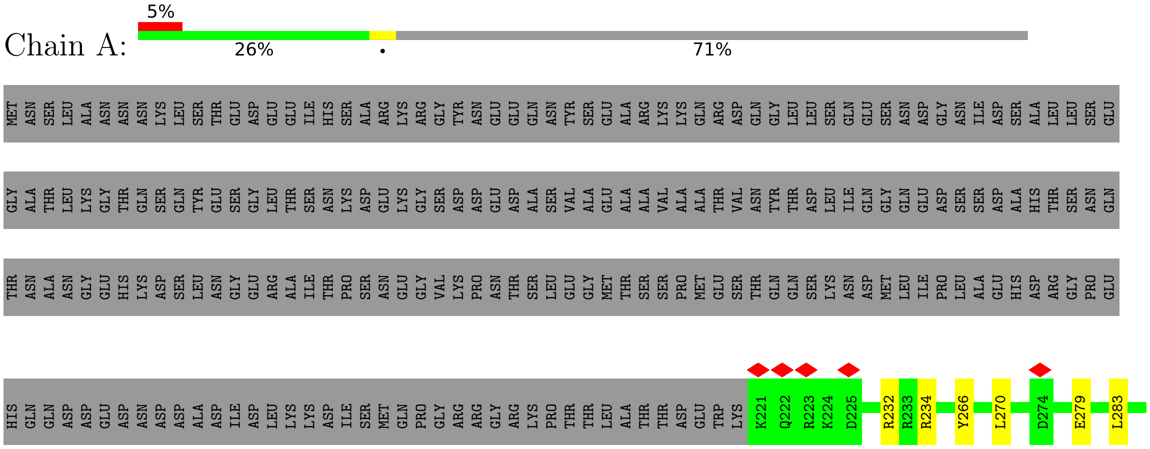
- Molecule 6: Histone H2A.1

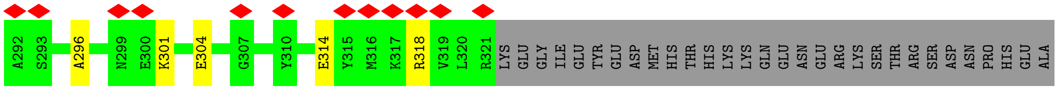


- Molecule 6: Histone H2A.1



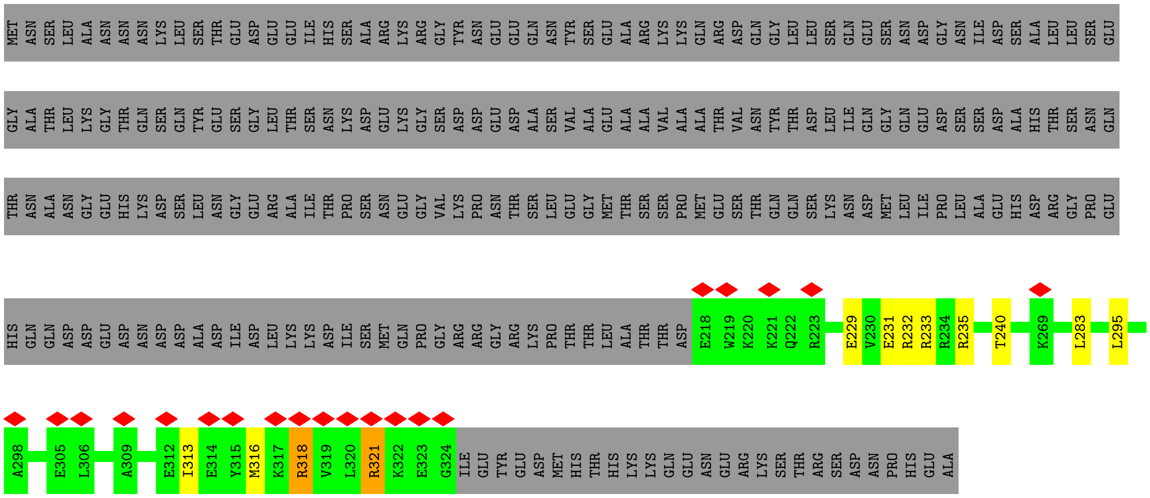
- Molecule 7: Centromere-binding protein 1





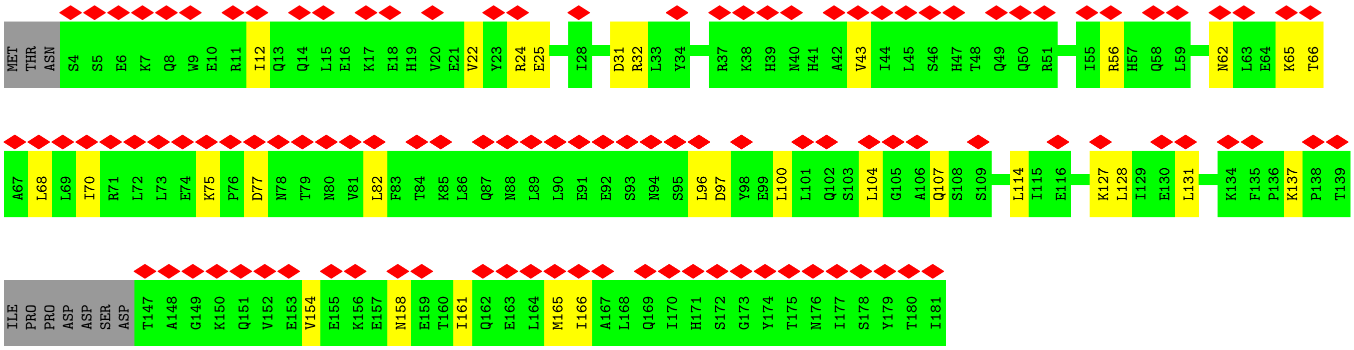
- Molecule 7: Centromere-binding protein 1

Chain B:



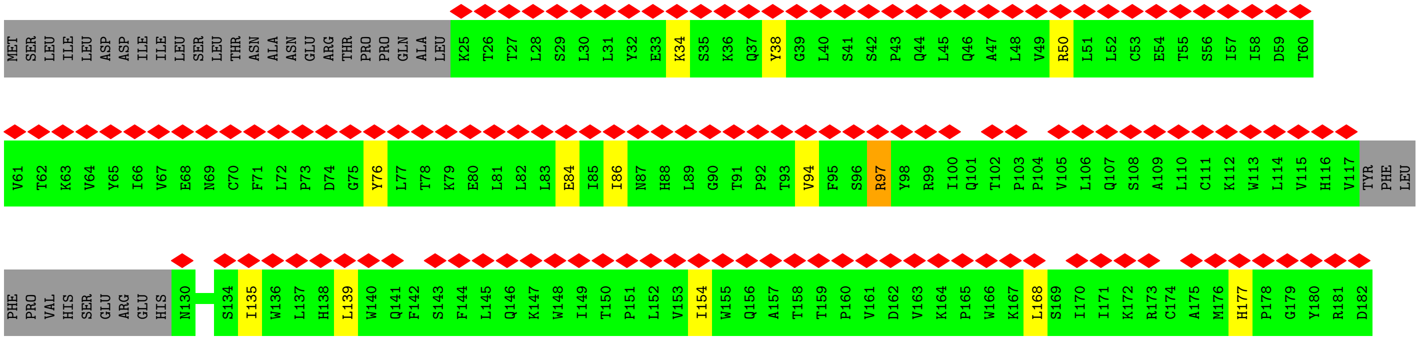
- Molecule 8: Inner kinetochore subunit MCM16

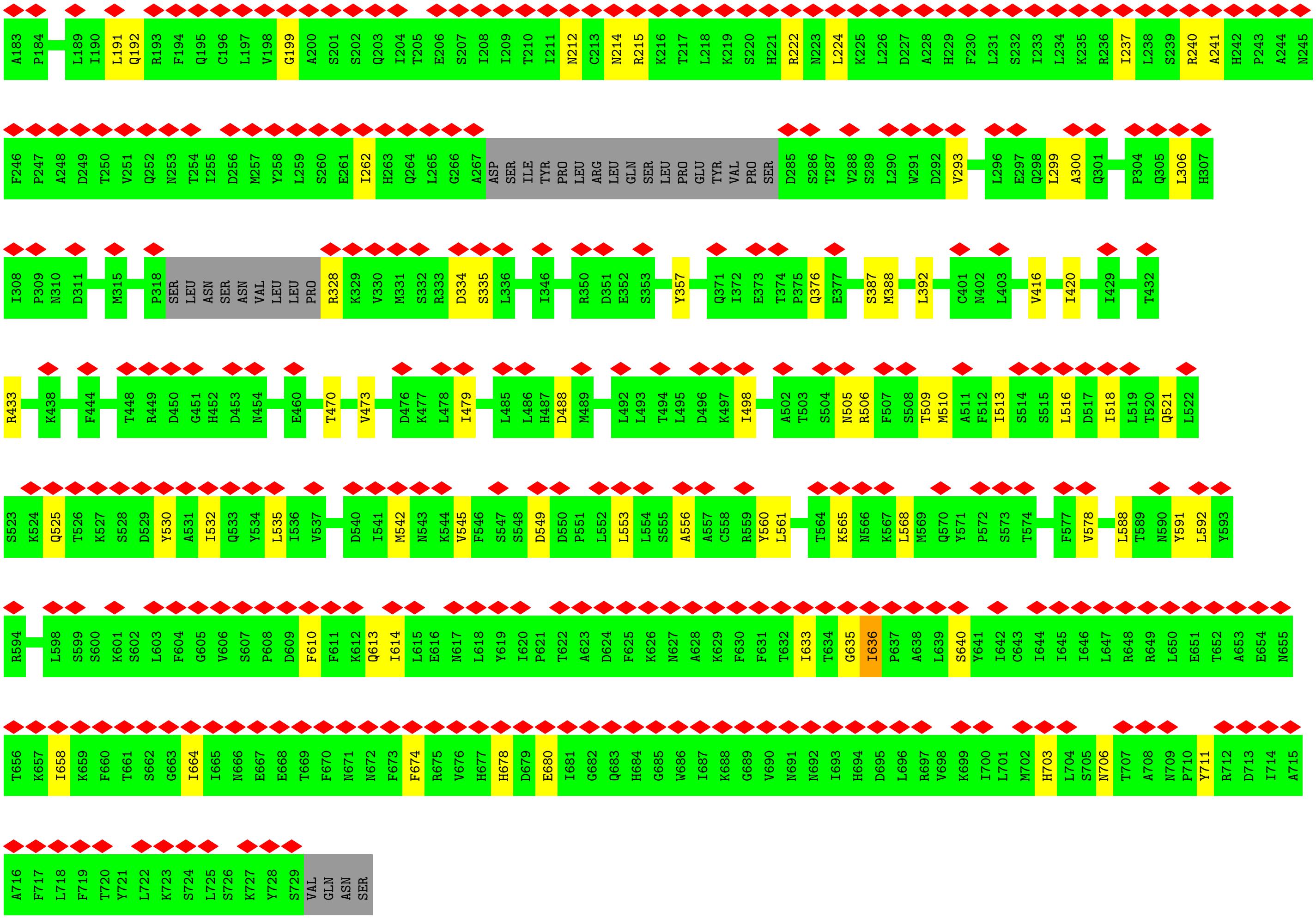
Chain H:



- Molecule 9: Inner kinetochore subunit CTF3

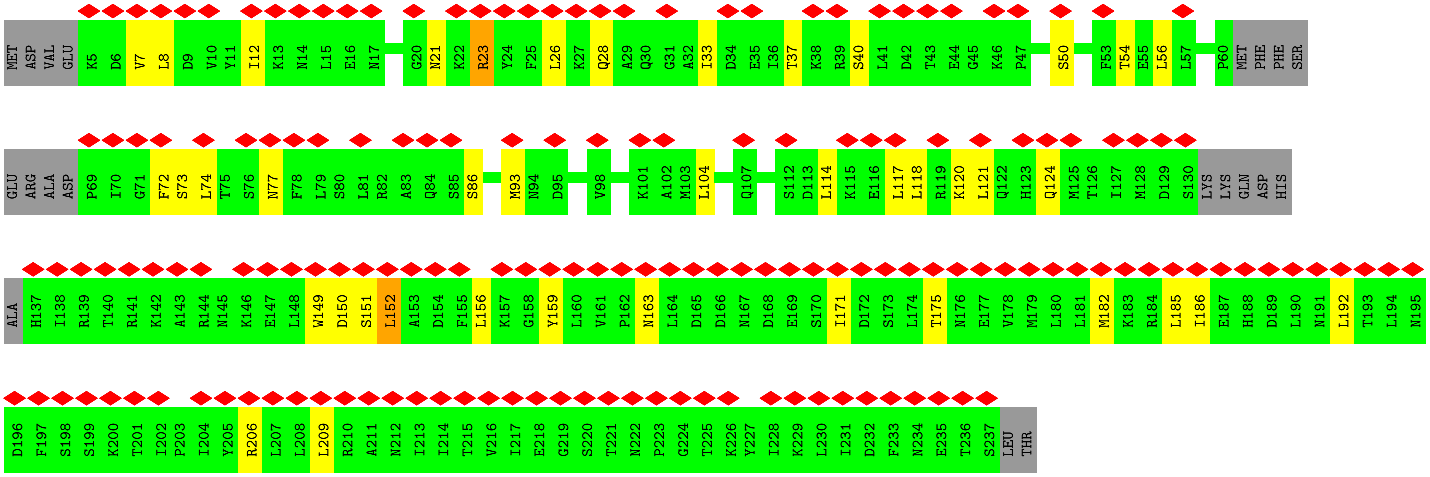
Chain I:





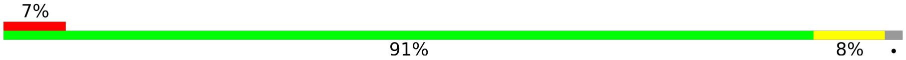
- Molecule 10: Inner kinetochore subunit MCM22

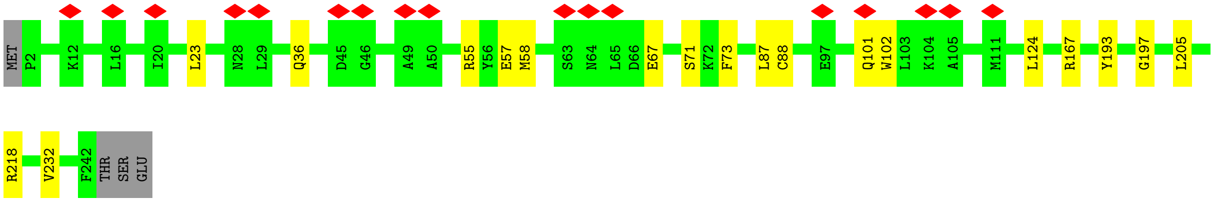
Chain K:



- Molecule 11: Inner kinetochore subunit IML3

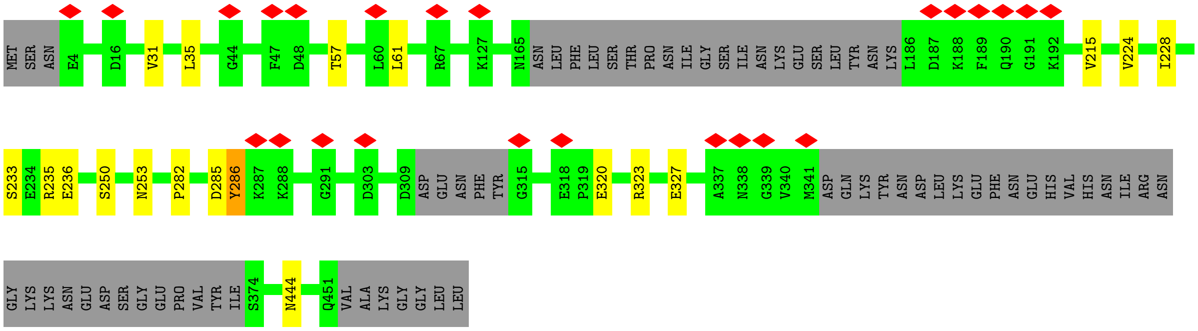
Chain L:





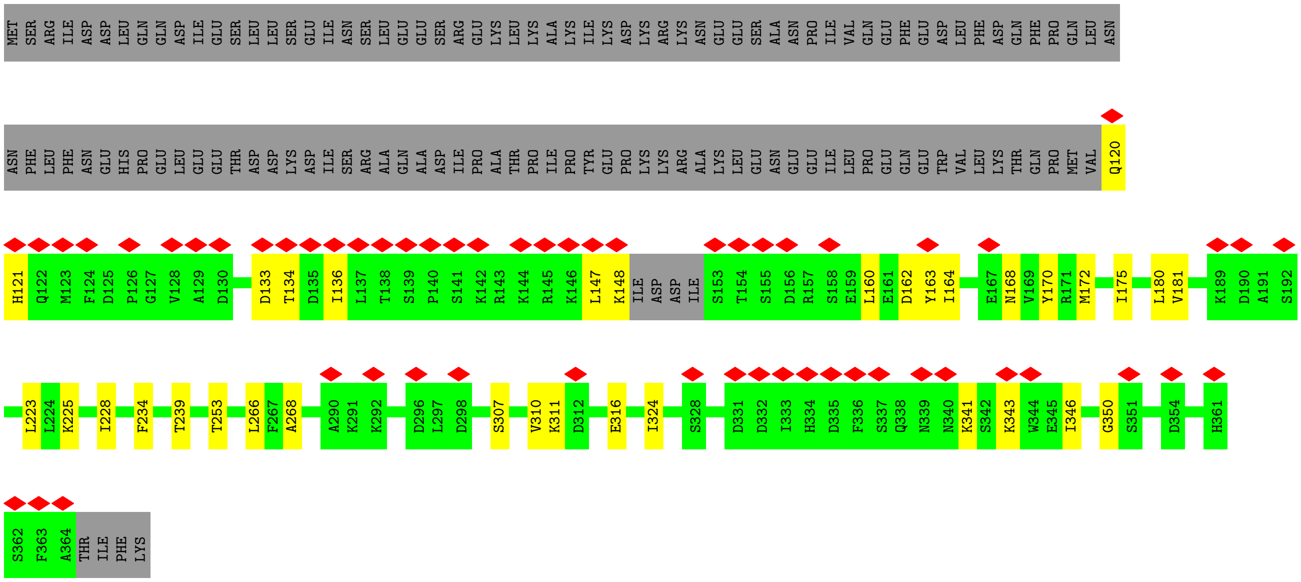
- Molecule 12: Inner kinetochore subunit CHL4

Chain N:



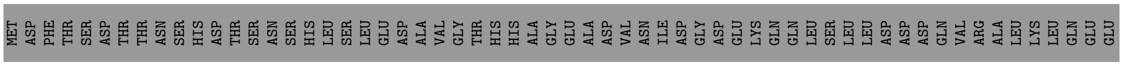
- Molecule 13: Inner kinetochore subunit MCM21

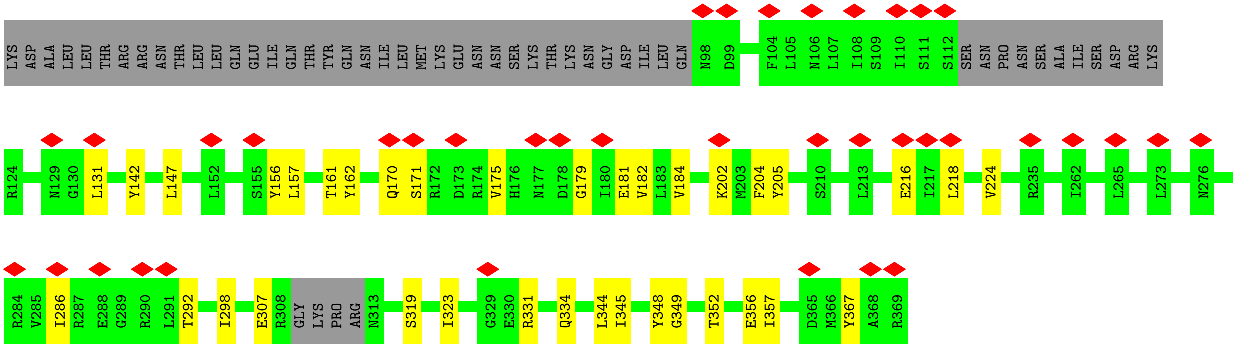
Chain O:



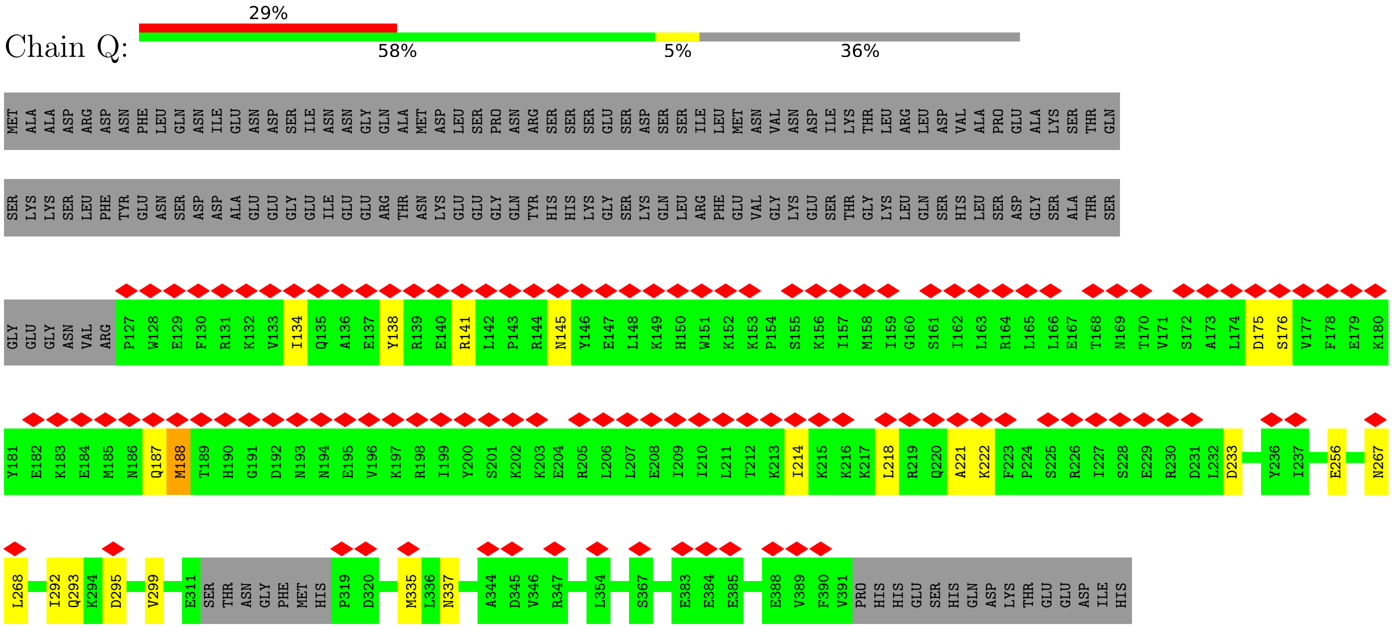
- Molecule 14: Inner kinetochore subunit CTF19

Chain P:

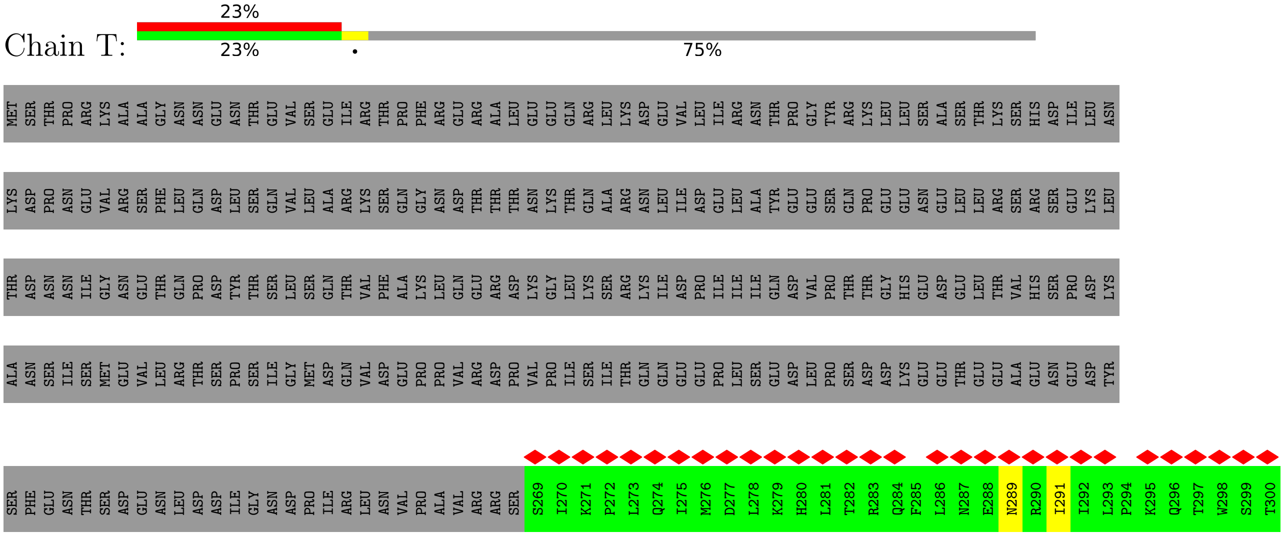


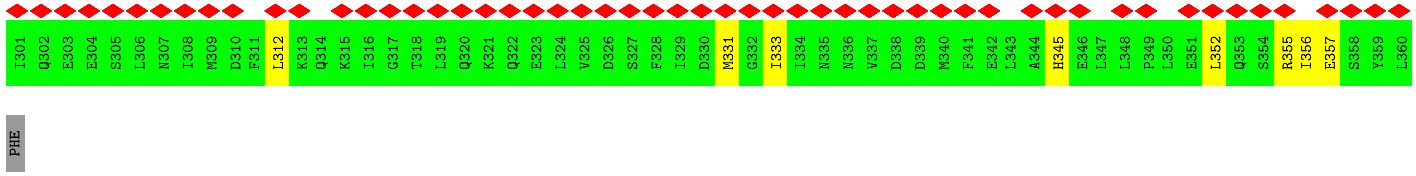


- Molecule 15: Inner kinetochore subunit OKP1



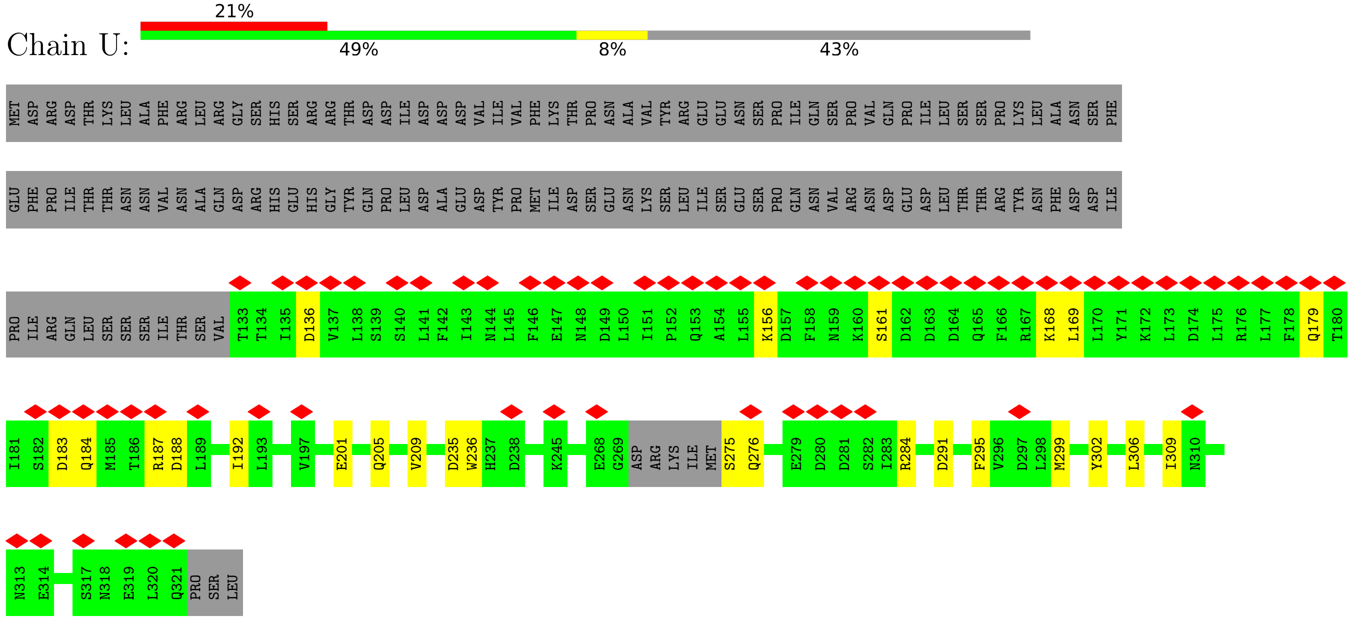
- Molecule 16: Inner kinetochore subunit CNN1





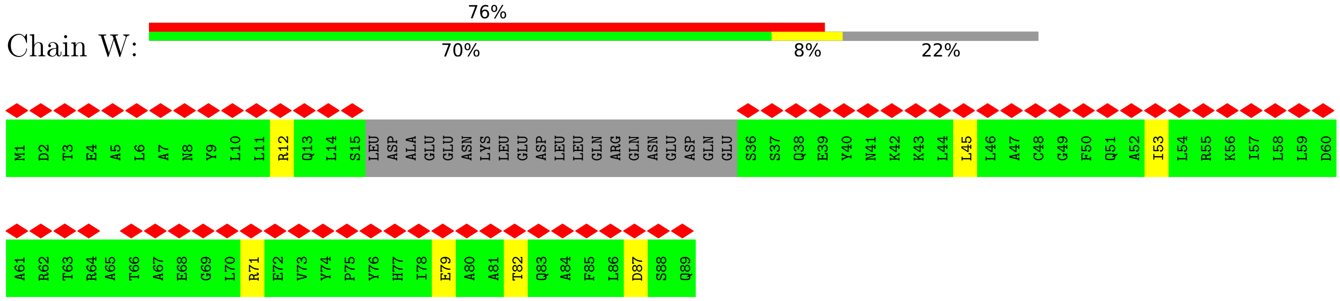
- Molecule 17: Inner kinetochore subunit AME1

Chain U:



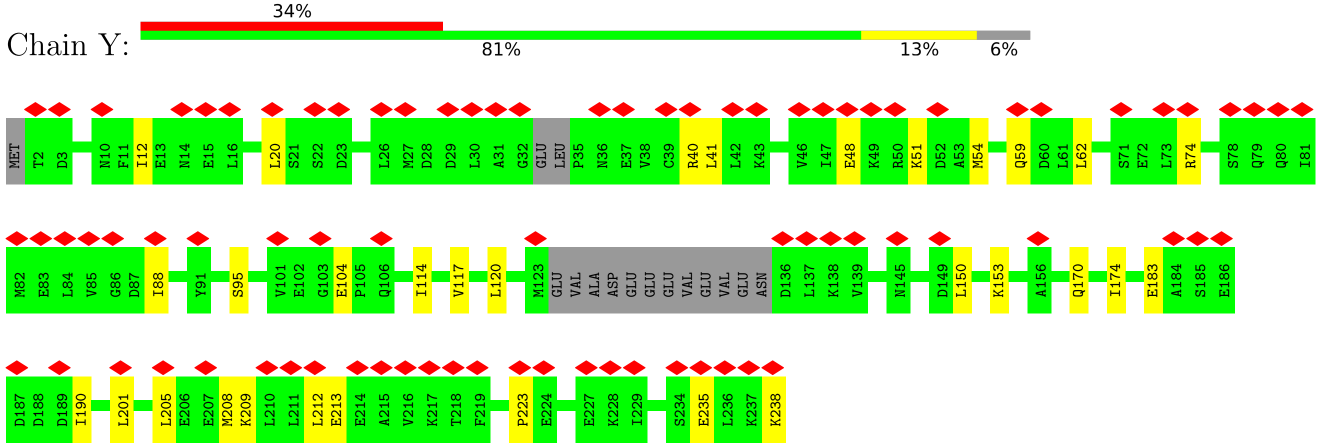
- Molecule 18: Inner kinetochore subunit WIP1

Chain W:



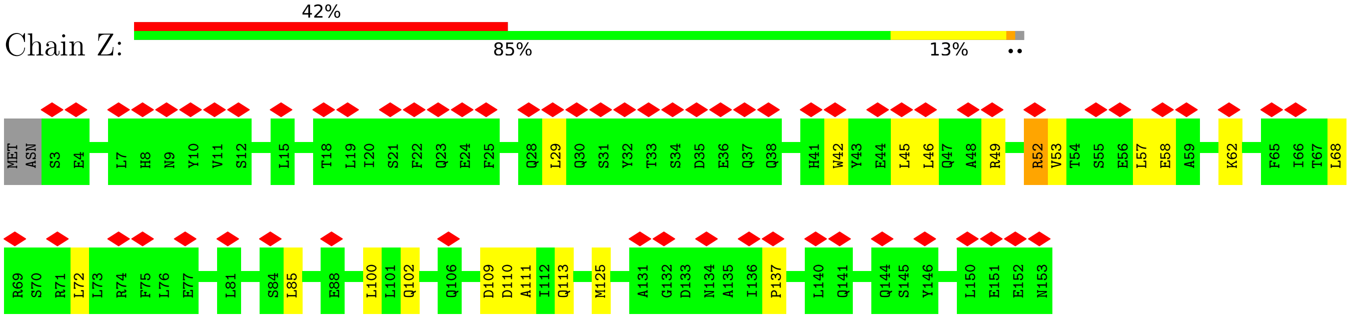
- Molecule 19: Inner kinetochore subunit NKP1

Chain Y:



- Molecule 20: Inner kinetochore subunit NKP2

Chain Z:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100311	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 ($e^-/\text{Å}^2$)	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	0.975	Depositor
Minimum map value	-0.638	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	307.08, 307.08, 307.08	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.853, 0.853, 0.853	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	D	0.68	1/2774 (0.0%)	1.07	1/4278 (0.0%)
2	E	0.65	0/2768	1.08	7/4271 (0.2%)
3	b	0.34	0/632	0.66	0/845
3	f	0.48	0/634	0.67	0/848
4	d	0.31	0/745	0.50	0/1003
4	h	0.28	0/739	0.54	0/995
5	a	0.51	0/792	1.23	12/1066 (1.1%)
5	e	0.52	0/792	1.23	12/1066 (1.1%)
6	c	0.30	0/751	0.54	0/1015
6	g	0.28	0/754	0.57	0/1019
7	A	0.29	0/828	0.55	0/1108
7	B	0.32	0/884	0.65	2/1182 (0.2%)
8	H	0.28	0/1429	0.53	0/1923
9	I	0.26	0/5530	0.47	0/7501
10	K	0.26	0/1784	0.54	2/2404 (0.1%)
11	L	0.27	0/1981	0.53	0/2684
12	N	0.31	1/3239 (0.0%)	0.52	1/4372 (0.0%)
13	O	0.29	0/2017	0.51	0/2713
14	P	0.32	0/2149	0.57	0/2888
15	Q	0.28	0/2178	0.55	2/2917 (0.1%)
16	T	0.28	0/772	0.50	0/1040
17	U	0.28	0/1499	0.53	1/2018 (0.0%)
18	W	0.28	0/557	0.50	0/748
19	Y	0.28	0/1672	0.54	1/2252 (0.0%)
20	Z	0.28	0/1195	0.52	1/1616 (0.1%)
All	All	0.38	2/39095 (0.0%)	0.69	42/53772 (0.1%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	f	0	1
5	a	0	1
5	e	0	1
9	I	0	2
14	P	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	286	TYR	CD1-CE1	-7.54	1.28	1.39
1	D	47	DT	C1'-N1	5.12	1.55	1.49

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	143	ARG	CG-CD-NE	13.29	139.71	111.80
5	e	143	ARG	CG-CD-NE	13.29	139.70	111.80
5	a	181	MET	CB-CG-SD	11.22	146.07	112.40
5	e	181	MET	CB-CG-SD	11.22	146.05	112.40
2	E	154	DA	P-O3'-C3'	-10.29	107.36	119.70
2	E	76	DG	P-O3'-C3'	-9.35	108.49	119.70
5	e	206	LEU	CB-CG-CD1	8.55	125.54	111.00
5	a	206	LEU	CB-CG-CD1	8.53	125.49	111.00
5	e	143	ARG	CB-CG-CD	8.27	133.10	111.60
5	a	143	ARG	CB-CG-CD	8.26	133.09	111.60
2	E	154	DA	OP1-P-O3'	8.00	122.81	105.20
5	a	152	LEU	CA-CB-CG	7.71	133.03	115.30
5	e	152	LEU	CA-CB-CG	7.69	132.98	115.30
15	Q	188	MET	CG-SD-CE	-7.41	88.35	100.20
1	D	78	DC	P-O3'-C3'	-6.89	111.43	119.70
15	Q	188	MET	CB-CG-SD	6.46	131.78	112.40
5	a	219	GLN	C-N-CA	6.41	137.72	121.70
5	e	219	GLN	C-N-CA	6.39	137.67	121.70
5	e	219	GLN	CB-CA-C	-6.24	97.92	110.40
5	a	219	GLN	CB-CA-C	-6.21	97.97	110.40
2	E	74	DC	P-O3'-C3'	-6.03	112.47	119.70
2	E	73	DG	P-O3'-C3'	-5.86	112.67	119.70
19	Y	223	PRO	N-CA-CB	5.62	110.04	103.30
20	Z	137	PRO	N-CA-CB	5.56	109.98	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	181	MET	CA-CB-CG	5.54	122.71	113.30
5	e	181	MET	CA-CB-CG	5.53	122.70	113.30
5	a	219	GLN	N-CA-C	-5.48	96.21	111.00
5	e	219	GLN	N-CA-C	-5.46	96.27	111.00
7	B	318	ARG	NE-CZ-NH2	-5.39	117.61	120.30
5	e	184	MET	CB-CG-SD	-5.38	96.26	112.40
5	a	184	MET	CB-CG-SD	-5.38	96.26	112.40
5	e	155	LYS	CA-CB-CG	5.38	125.22	113.40
5	a	155	LYS	CA-CB-CG	5.37	125.22	113.40
5	a	184	MET	CA-CB-CG	5.29	122.29	113.30
2	E	139	DG	O4'-C1'-N9	5.25	111.68	108.00
5	e	184	MET	CA-CB-CG	5.25	122.23	113.30
10	K	23	ARG	NE-CZ-NH2	-5.24	117.68	120.30
10	K	152	LEU	CA-CB-CG	5.20	127.26	115.30
17	U	291	ASP	CB-CG-OD2	5.20	122.98	118.30
7	B	321	ARG	CG-CD-NE	5.18	122.69	111.80
12	N	285	ASP	CB-CG-OD1	5.02	122.82	118.30
2	E	113	DC	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	241	ALA	Mainchain
9	I	636	ILE	Peptide
14	P	307	GLU	Mainchain
5	a	154	SER	Peptide
5	e	154	SER	Peptide
3	f	98	LEU	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	D	2475	1364	1365	22	0
2	E	2466	1352	1351	29	0
3	b	625	658	657	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	627	665	664	0	0
4	d	735	754	753	0	0
4	h	729	749	748	0	0
5	a	781	804	803	0	0
5	e	781	804	803	0	0
6	c	742	776	775	0	0
6	g	745	785	784	0	0
7	A	822	846	845	7	0
7	B	876	897	896	7	0
8	H	1412	1453	1451	44	0
9	I	5405	5512	5514	61	0
10	K	1762	1804	1796	46	0
11	L	1941	1946	1946	12	0
12	N	3166	3207	3220	14	0
13	O	1979	1997	1995	28	0
14	P	2116	2192	2189	28	0
15	Q	2146	2201	2201	16	0
16	T	761	782	781	11	0
17	U	1485	1480	1467	15	0
18	W	551	560	559	8	0
19	Y	1663	1645	1588	25	0
20	Z	1180	1145	1108	19	0
All	All	37971	36378	36259	296	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 6.

All (296) 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)
8:H:104:LEU:HD12	9:I:510:MET:HE3	1.46	0.97
8:H:128:LEU:HD11	10:K:114:LEU:HD21	1.47	0.94
15:Q:256:GLU:OE1	19:Y:74:ARG:NH2	2.11	0.83
8:H:166:ILE:HG23	9:I:135:ILE:HD13	1.62	0.81
14:P:344:LEU:HD12	14:P:357:ILE:HD13	1.64	0.79
15:Q:145:ASN:ND2	18:W:87:ASP:O	2.16	0.78
9:I:50:ARG:NH2	9:I:84:GLU:OE1	2.18	0.76
8:H:165:MET:HE3	10:K:152:LEU:HD12	1.67	0.76
13:O:160:LEU:HD22	14:P:131:LEU:HD23	1.67	0.76
1:D:68:DA:N6	2:E:87:DG:O6	2.18	0.75
16:T:312:LEU:HD21	18:W:53:ILE:HD13	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:73:SER:O	10:K:77:ASN:ND2	2.20	0.74
12:N:235:ARG:NH2	19:Y:95:SER:OG	2.19	0.74
15:Q:138:TYR:OH	15:Q:222:LYS:O	2.05	0.73
14:P:286:ILE:N	14:P:292:THR:O	2.22	0.72
1:D:97:DT:O4	2:E:58:DC:N4	2.23	0.72
13:O:307:SER:OG	13:O:316:GLU:OE1	2.06	0.72
14:P:344:LEU:HD13	14:P:356:GLU:OE1	1.91	0.71
12:N:327:GLU:OE2	14:P:142:TYR:OH	2.10	0.70
17:U:179:GLN:OE1	19:Y:40:ARG:NE	2.26	0.69
17:U:201:GLU:O	17:U:205:GLN:NE2	2.24	0.69
17:U:302:TYR:OH	19:Y:183:GLU:OE2	2.09	0.69
2:E:153:DT:C2	2:E:154:DA:C2	2.81	0.68
9:I:237:ILE:O	9:I:240:ARG:NH1	2.27	0.68
20:Z:58:GLU:OE1	20:Z:62:LYS:NZ	2.27	0.67
19:Y:209:LYS:NZ	19:Y:213:GLU:OE1	2.26	0.67
8:H:104:LEU:HD12	9:I:510:MET:CE	2.25	0.66
12:N:233:SER:OG	12:N:236:GLU:O	2.08	0.66
14:P:348:TYR:O	14:P:352:THR:OG1	2.12	0.66
9:I:521:GLN:O	9:I:525:GLN:NE2	2.28	0.66
14:P:171:SER:OG	14:P:184:VAL:HG12	1.96	0.66
8:H:114:LEU:HD12	10:K:104:LEU:HD22	1.79	0.65
19:Y:190:ILE:HG23	20:Z:125:MET:CE	2.27	0.65
9:I:498:ILE:O	9:I:505:ASN:ND2	2.30	0.64
1:D:11:DT:OP2	18:W:71:ARG:NH1	2.29	0.64
8:H:104:LEU:CD1	9:I:510:MET:HE3	2.24	0.64
19:Y:153:LYS:NZ	20:Z:102:GLN:OE1	2.31	0.63
8:H:161:ILE:HG23	10:K:152:LEU:HD13	1.80	0.63
12:N:286:TYR:HE1	13:O:164:ILE:HG21	1.62	0.63
9:I:636:ILE:O	9:I:640:SER:N	2.31	0.63
19:Y:190:ILE:HG23	20:Z:125:MET:HE1	1.80	0.62
12:N:320:GLU:OE2	12:N:323:ARG:NH2	2.31	0.62
7:A:314:GLU:OE2	7:A:318:ARG:NH1	2.32	0.62
9:I:674:PHE:O	9:I:678:HIS:N	2.32	0.62
10:K:171:ILE:O	10:K:175:THR:OG1	2.11	0.62
14:P:181:GLU:OE1	14:P:205:TYR:OH	2.11	0.61
14:P:344:LEU:HD12	14:P:357:ILE:CD1	2.30	0.61
15:Q:337:ASN:OD1	17:U:284:ARG:NH2	2.33	0.61
9:I:510:MET:SD	9:I:513:ILE:HD11	2.41	0.61
12:N:286:TYR:CE1	13:O:164:ILE:HG21	2.35	0.61
9:I:199:GLY:O	11:L:101:GLN:NE2	2.32	0.61
10:K:37:THR:O	10:K:40:SER:OG	2.19	0.60

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
11:L:87:LEU:HD23	11:L:88:CYS:N	2.17	0.60
12:N:224:VAL:O	12:N:228:ILE:HD12	2.01	0.60
13:O:180:LEU:HD13	13:O:223:LEU:HD22	1.83	0.60
12:N:57:THR:O	12:N:61:LEU:HG	2.02	0.60
11:L:55:ARG:NE	11:L:57:GLU:OE2	2.34	0.60
19:Y:12:ILE:HG12	19:Y:62:LEU:HD11	1.83	0.59
2:E:154:DA:C5	2:E:155:DT:C4	2.91	0.59
20:Z:110:ASP:OD1	20:Z:111:ALA:N	2.35	0.59
14:P:156:TYR:O	14:P:161:THR:HG22	2.03	0.59
8:H:161:ILE:HG13	10:K:186:ILE:HD11	1.85	0.59
11:L:124:LEU:HD11	11:L:232:VAL:HG13	1.85	0.59
8:H:25:GLU:OE2	10:K:26:LEU:HD22	2.03	0.58
9:I:545:VAL:HB	9:I:553:LEU:HD21	1.85	0.58
8:H:68:LEU:HD22	10:K:72:PHE:H	1.69	0.58
13:O:310:VAL:HG23	13:O:311:LYS:H	1.69	0.58
9:I:376:GLN:OE1	9:I:376:GLN:N	2.36	0.58
1:D:77:DC:C4	1:D:78:DC:C4	2.92	0.58
16:T:289:ASN:O	16:T:291:ILE:HD12	2.03	0.58
9:I:94:VAL:HG11	16:T:357:GLU:HG3	1.86	0.57
9:I:610:PHE:O	9:I:613:GLN:N	2.38	0.56
8:H:25:GLU:OE1	10:K:26:LEU:HD13	2.05	0.56
2:E:138:DC:N4	2:E:139:DG:O6	2.38	0.56
8:H:104:LEU:CD1	9:I:510:MET:CE	2.83	0.56
10:K:50:SER:O	10:K:54:THR:N	2.36	0.56
11:L:205:LEU:O	11:L:218:ARG:NH2	2.38	0.56
13:O:160:LEU:O	13:O:164:ILE:HG22	2.05	0.56
16:T:331:MET:HG3	18:W:53:ILE:HD11	1.87	0.56
16:T:352:LEU:O	16:T:356:ILE:HD12	2.06	0.55
2:E:77:DG:C5	2:E:78:DG:C6	2.94	0.55
7:B:318:ARG:HG3	7:B:321:ARG:HH21	1.72	0.55
8:H:70:ILE:HD13	9:I:664:ILE:HD13	1.89	0.55
8:H:128:LEU:CD1	10:K:114:LEU:HD21	2.31	0.55
10:K:8:LEU:O	10:K:12:ILE:HG23	2.07	0.54
14:P:202:LYS:HE3	14:P:218:LEU:HD11	1.90	0.54
15:Q:267:ASN:OD1	15:Q:268:LEU:N	2.40	0.54
13:O:346:ILE:HD11	20:Z:100:LEU:HD22	1.88	0.54
1:D:79:DC:C2	2:E:78:DG:N2	2.76	0.54
8:H:96:LEU:HD13	10:K:86:SER:CB	2.38	0.54
12:N:250:SER:OG	12:N:253:ASN:OD1	2.24	0.54
8:H:56:ARG:NH1	10:K:56:LEU:O	2.41	0.54
19:Y:117:VAL:HA	19:Y:120:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:201:LEU:O	19:Y:205:LEU:HD23	2.07	0.53
9:I:561:LEU:O	9:I:565:LYS:N	2.41	0.53
8:H:97:ASP:OD2	9:I:711:TYR:OH	2.25	0.53
2:E:78:DG:C5	2:E:79:DG:C6	2.96	0.53
20:Z:68:LEU:O	20:Z:72:LEU:HD23	2.08	0.53
8:H:32:ARG:HH12	10:K:33:ILE:HG23	1.72	0.53
19:Y:170:GLN:O	19:Y:174:ILE:HD12	2.09	0.53
14:P:367:TYR:OH	15:Q:299:VAL:N	2.41	0.52
16:T:312:LEU:CD2	18:W:53:ILE:HD13	2.37	0.52
1:D:81:DC:C2	2:E:76:DG:N2	2.78	0.52
9:I:76:TYR:HH	9:I:328:ARG:N	2.07	0.52
7:A:279:GLU:O	7:A:283:LEU:HD23	2.09	0.52
8:H:82:LEU:HD21	10:K:8:LEU:HD11	1.91	0.52
19:Y:41:LEU:HD23	20:Z:29:LEU:CD2	2.40	0.52
20:Z:85:LEU:H	20:Z:85:LEU:HD23	1.75	0.52
9:I:300:ALA:HB1	10:K:124:GLN:OE1	2.10	0.52
9:I:387:SER:OG	9:I:388:MET:SD	2.66	0.52
13:O:225:LYS:O	13:O:234:PHE:N	2.38	0.52
13:O:341:LYS:NZ	19:Y:104:GLU:OE2	2.43	0.51
1:D:28:DA:C5	1:D:29:DA:C6	2.99	0.51
10:K:117:LEU:O	10:K:121:LEU:N	2.39	0.51
17:U:161:SER:OG	17:U:168:LYS:N	2.43	0.51
8:H:22:VAL:HB	10:K:23:ARG:HH22	1.74	0.51
19:Y:117:VAL:HG21	19:Y:150:LEU:HD21	1.91	0.51
9:I:470:THR:HG22	9:I:518:ILE:HD12	1.91	0.51
13:O:170:TYR:HB3	14:P:157:LEU:HD13	1.92	0.51
13:O:181:VAL:HG12	14:P:147:LEU:HD21	1.92	0.51
20:Z:53:VAL:O	20:Z:57:LEU:N	2.39	0.51
8:H:100:LEU:HB3	9:I:510:MET:HE2	1.92	0.51
9:I:506:ARG:O	9:I:509:THR:N	2.43	0.51
8:H:96:LEU:HD11	9:I:506:ARG:NH1	2.26	0.51
8:H:65:LYS:NZ	9:I:549:ASP:OD1	2.43	0.50
17:U:183:ASP:OD1	17:U:184:GLN:N	2.44	0.50
19:Y:117:VAL:HG21	19:Y:150:LEU:CD2	2.41	0.50
15:Q:134:ILE:HD12	15:Q:221:ALA:HB1	1.91	0.50
12:N:282:PRO:O	13:O:168:ASN:ND2	2.45	0.50
9:I:38:TYR:O	9:I:240:ARG:NH2	2.44	0.50
20:Z:42:TRP:O	20:Z:46:LEU:N	2.45	0.49
2:E:74:DC:C2	2:E:75:DG:C5	3.00	0.49
2:E:144:DC:OP2	7:A:234:ARG:NH1	2.46	0.49
7:B:229:GLU:OE1	7:B:232:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:212:ASN:ND2	9:I:214:ASN:OD1	2.45	0.49
1:D:79:DC:H1'	1:D:80:DC:C5	2.48	0.49
8:H:31:ASP:OD1	8:H:32:ARG:N	2.44	0.49
19:Y:88:ILE:HB	20:Z:85:LEU:HD21	1.93	0.49
1:D:79:DC:C2	1:D:80:DC:C4	3.00	0.49
8:H:128:LEU:HD11	10:K:114:LEU:CD2	2.31	0.49
12:N:444:ASN:O	13:O:228:ILE:HD12	2.12	0.49
9:I:94:VAL:O	9:I:97:ARG:NH1	2.45	0.49
18:W:79:GLU:O	18:W:82:THR:OG1	2.22	0.49
10:K:21:ASN:HD22	13:O:136:ILE:HD12	1.77	0.48
15:Q:141:ARG:NH2	17:U:136:ASP:OD1	2.44	0.48
7:A:301:LYS:O	7:A:304:GLU:N	2.46	0.48
16:T:356:ILE:HG21	18:W:45:LEU:HD21	1.94	0.48
20:Z:109:ASP:O	20:Z:113:GLN:NE2	2.46	0.48
1:D:78:DC:C2	1:D:79:DC:C4	3.01	0.48
9:I:610:PHE:O	9:I:614:ILE:N	2.38	0.48
14:P:323:ILE:O	14:P:334:GLN:NE2	2.44	0.48
2:E:72:DC:N4	2:E:73:DG:O6	2.46	0.48
13:O:162:ASP:OD1	13:O:163:TYR:N	2.46	0.48
13:O:160:LEU:HD22	14:P:131:LEU:CD2	2.41	0.47
2:E:78:DG:H1'	2:E:79:DG:C8	2.49	0.47
14:P:175:VAL:O	14:P:179:GLY:N	2.44	0.47
20:Z:45:LEU:O	20:Z:49:ARG:N	2.39	0.47
8:H:166:ILE:CG2	9:I:135:ILE:HD13	2.39	0.47
10:K:149:TRP:CH2	10:K:186:ILE:HD13	2.50	0.47
20:Z:45:LEU:HD23	20:Z:49:ARG:HD2	1.94	0.47
14:P:170:GLN:HB2	14:P:184:VAL:HG13	1.95	0.47
7:A:296:ALA:HB2	7:B:295:LEU:HD21	1.97	0.47
8:H:75:LYS:O	8:H:77:ASP:N	2.47	0.47
13:O:134:THR:O	13:O:134:THR:HG22	2.15	0.47
8:H:96:LEU:HD13	10:K:86:SER:HB2	1.95	0.47
19:Y:54:MET:O	19:Y:59:GLN:NE2	2.47	0.47
19:Y:208:MET:SD	19:Y:212:LEU:HD22	2.55	0.47
10:K:23:ARG:NE	10:K:23:ARG:HA	2.29	0.47
19:Y:41:LEU:HD23	20:Z:29:LEU:HD23	1.95	0.47
15:Q:175:ASP:OD1	15:Q:176:SER:N	2.48	0.46
13:O:120:GLN:OE1	13:O:121:HIS:N	2.49	0.46
9:I:592:LEU:HD22	9:I:633:ILE:HG22	1.97	0.46
1:D:80:DC:N3	2:E:77:DG:N2	2.63	0.46
7:B:240:THR:OG1	11:L:167:ARG:NH2	2.49	0.46
12:N:250:SER:O	12:N:253:ASN:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:DC:OP1	7:A:232:ARG:NH1	2.46	0.46
1:D:30:DT:H5'	1:D:30:DT:C6	2.50	0.46
1:D:77:DC:C4	1:D:78:DC:N4	2.84	0.46
13:O:175:ILE:O	14:P:162:TYR:OH	2.28	0.46
1:D:63:DC:O2	2:E:93:DG:N2	2.22	0.46
9:I:224:LEU:HD22	9:I:262:ILE:HG21	1.97	0.46
19:Y:114:ILE:HA	19:Y:117:VAL:HG22	1.98	0.46
8:H:131:LEU:HB2	10:K:121:LEU:HD23	1.98	0.46
10:K:156:LEU:HD11	10:K:182:MET:HG2	1.97	0.46
14:P:345:ILE:O	14:P:349:GLY:N	2.49	0.46
16:T:333:ILE:HD11	18:W:53:ILE:HG13	1.98	0.46
11:L:193:TYR:O	11:L:197:GLY:N	2.43	0.45
2:E:74:DC:H2"	2:E:75:DG:C8	2.52	0.45
8:H:107:GLN:HB2	10:K:93:MET:HE2	1.97	0.45
8:H:62:ASN:ND2	9:I:591:TYR:OH	2.48	0.45
19:Y:235:GLU:O	19:Y:238:LYS:N	2.47	0.45
8:H:165:MET:CE	10:K:152:LEU:HD12	2.42	0.45
9:I:357:TYR:CD1	9:I:392:LEU:HD12	2.52	0.45
12:N:215:VAL:O	12:N:215:VAL:HG13	2.16	0.45
1:D:41:DC:O2	2:E:115:DG:N1	2.49	0.45
10:K:159:TYR:O	10:K:163:ASN:ND2	2.49	0.45
12:N:31:VAL:O	12:N:35:LEU:HD13	2.16	0.45
9:I:212:ASN:O	9:I:215:ARG:NE	2.46	0.45
9:I:293:VAL:HG11	9:I:299:LEU:HD23	1.99	0.45
13:O:147:LEU:HD23	13:O:148:LYS:HG3	1.97	0.45
1:D:29:DA:H1'	1:D:30:DT:C5	2.52	0.45
9:I:532:ILE:HA	9:I:535:LEU:HD12	1.99	0.45
2:E:73:DG:C5	2:E:74:DC:N4	2.84	0.44
2:E:153:DT:H2"	2:E:154:DA:C5	2.51	0.44
8:H:128:LEU:HD23	10:K:121:LEU:HD22	1.98	0.44
9:I:416:VAL:O	9:I:420:ILE:HD12	2.17	0.44
2:E:75:DG:H2"	2:E:76:DG:C8	2.52	0.44
9:I:703:HIS:O	9:I:706:ASN:ND2	2.50	0.44
11:L:58:MET:O	11:L:73:PHE:N	2.45	0.44
13:O:346:ILE:HD11	20:Z:100:LEU:CD2	2.47	0.44
13:O:175:ILE:HD11	13:O:268:ALA:HB1	1.98	0.44
17:U:205:GLN:O	17:U:209:VAL:HG23	2.17	0.44
8:H:127:LYS:HB2	10:K:118:LEU:HD11	1.98	0.44
14:P:331:ARG:NH2	14:P:334:GLN:OE1	2.50	0.44
2:E:153:DT:H2"	2:E:154:DA:N7	2.32	0.44
2:E:154:DA:C8	2:E:155:DT:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:67:GLU:O	11:L:71:SER:N	2.50	0.44
9:I:516:LEU:HD22	9:I:556:ALA:HB1	2.00	0.44
14:P:182:VAL:HG22	14:P:204:PHE:CD1	2.53	0.44
14:P:319:SER:O	15:Q:335:MET:N	2.41	0.44
8:H:43:VAL:HG22	8:H:43:VAL:O	2.18	0.44
19:Y:20:LEU:HD11	19:Y:54:MET:CE	2.47	0.44
1:D:28:DA:C5	1:D:29:DA:N6	2.87	0.43
9:I:293:VAL:HG21	9:I:306:LEU:HD12	1.99	0.43
9:I:433:ARG:NH2	9:I:488:ASP:OD2	2.51	0.43
10:K:185:LEU:HA	10:K:192:LEU:HD11	1.99	0.43
1:D:80:DC:N3	2:E:76:DG:C2	2.86	0.43
10:K:120:LYS:O	10:K:124:GLN:NE2	2.51	0.43
10:K:28:GLN:OE1	13:O:133:ASP:N	2.46	0.43
11:L:23:LEU:HD13	11:L:102:TRP:CE3	2.53	0.43
17:U:161:SER:HB3	17:U:168:LYS:HA	2.01	0.43
2:E:153:DT:H1'	2:E:154:DA:C4	2.54	0.43
9:I:34:LYS:O	9:I:38:TYR:N	2.50	0.43
9:I:658:ILE:HD11	9:I:680:GLU:OE2	2.19	0.43
11:L:73:PHE:CD2	11:L:87:LEU:HD21	2.53	0.43
9:I:542:MET:HA	9:I:545:VAL:HG22	2.00	0.43
7:A:266:TYR:CE2	7:A:270:LEU:HD11	2.54	0.42
14:P:202:LYS:N	14:P:216:GLU:O	2.45	0.42
20:Z:49:ARG:HB2	20:Z:52:ARG:NH2	2.34	0.42
8:H:82:LEU:HD21	10:K:8:LEU:CD1	2.48	0.42
9:I:192:GLN:OE1	9:I:222:ARG:NH2	2.53	0.42
13:O:168:ASN:O	13:O:172:MET:HG2	2.19	0.42
14:P:298:ILE:HG23	14:P:323:ILE:HG22	2.01	0.42
9:I:588:LEU:HD11	9:I:592:LEU:HD11	2.01	0.42
15:Q:188:MET:SD	17:U:169:LEU:HD22	2.59	0.42
8:H:12:ILE:HG13	10:K:12:ILE:HG22	2.01	0.42
15:Q:293:GLN:NE2	15:Q:295:ASP:OD2	2.48	0.42
9:I:154:ILE:HG21	9:I:262:ILE:HD13	2.02	0.42
13:O:324:ILE:HD12	13:O:350:GLY:O	2.19	0.42
16:T:352:LEU:O	16:T:355:ARG:N	2.53	0.42
17:U:188:ASP:O	17:U:192:ILE:HG23	2.20	0.42
1:D:80:DC:N3	2:E:76:DG:N2	2.67	0.42
2:E:76:DG:H2"	2:E:77:DG:C5	2.54	0.42
8:H:128:LEU:CD2	10:K:121:LEU:HD22	2.50	0.42
1:D:79:DC:H1'	1:D:80:DC:C6	2.55	0.42
7:B:283:LEU:HD11	15:Q:292:ILE:HD11	2.01	0.42
13:O:239:THR:O	13:O:239:THR:HG22	2.20	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
9:I:214:ASN:OD1	9:I:215:ARG:N	2.52	0.41
15:Q:233:ASP:N	15:Q:233:ASP:OD1	2.52	0.41
9:I:168:LEU:HD22	9:I:191:LEU:HD13	2.01	0.41
9:I:334:ASP:OD1	9:I:335:SER:N	2.53	0.41
14:P:224:VAL:HG22	14:P:224:VAL:O	2.19	0.41
2:E:76:DG:H1’	2:E:77:DG:C4	2.56	0.41
8:H:68:LEU:HD22	10:K:72:PHE:N	2.33	0.41
10:K:171:ILE:O	10:K:175:THR:CB	2.69	0.41
8:H:22:VAL:HA	8:H:25:GLU:HG3	2.02	0.41
10:K:114:LEU:O	10:K:114:LEU:HD23	2.20	0.41
10:K:150:ASP:OD1	10:K:151:SER:N	2.53	0.41
19:Y:48:GLU:O	19:Y:51:LYS:NZ	2.31	0.41
7:B:231:GLU:OE1	7:B:235:ARG:NH1	2.54	0.41
9:I:473:VAL:O	9:I:479:ILE:HD12	2.20	0.41
9:I:530:TYR:HB2	9:I:535:LEU:HD11	2.03	0.41
9:I:568:LEU:HD11	9:I:578:VAL:HG13	2.03	0.41
13:O:253:THR:HG22	13:O:266:LEU:HD22	2.02	0.41
1:D:49:DG:N2	2:E:108:DT:O2	2.54	0.41
2:E:78:DG:C4’	2:E:79:DG:H5’	2.50	0.41
8:H:24:ARG:HH12	10:K:74:LEU:HD21	1.86	0.41
8:H:66:THR:HG23	9:I:635:GLY:O	2.21	0.41
11:L:36:GLN:NE2	11:L:57:GLU:OE1	2.54	0.41
14:P:182:VAL:HG13	14:P:204:PHE:CE1	2.56	0.41
14:P:184:VAL:HG21	14:P:218:LEU:HD12	2.02	0.41
15:Q:187:GLN:OE1	15:Q:187:GLN:N	2.46	0.41
17:U:275:SER:OG	17:U:276:GLN:N	2.53	0.41
20:Z:49:ARG:O	20:Z:52:ARG:HD3	2.21	0.41
15:Q:214:ILE:O	15:Q:218:LEU:N	2.51	0.41
17:U:235:ASP:OD1	17:U:236:TRP:N	2.54	0.41
9:I:86:ILE:HG23	9:I:139:LEU:HD21	2.03	0.40
9:I:177:HIS:NE2	16:T:345:HIS:O	2.53	0.40
17:U:295:PHE:CE2	17:U:299:MET:HG3	2.56	0.40
17:U:306:LEU:HA	17:U:309:ILE:HG22	2.03	0.40
8:H:154:VAL:O	8:H:158:ASN:ND2	2.55	0.40
7:B:313:ILE:O	7:B:316:MET:HB3	2.22	0.40
10:K:209:LEU:O	16:T:345:HIS:NE2	2.54	0.40
9:I:516:LEU:HD21	9:I:560:TYR:HB2	2.02	0.40
10:K:7:VAL:HG13	10:K:8:LEU:HD22	2.02	0.40
19:Y:20:LEU:HD11	19:Y:54:MET:HE2	2.03	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	
3	b	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
3	f	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
4	d	93/131 (71%)	92 (99%)	1 (1%)	0	100	100
4	h	92/131 (70%)	91 (99%)	1 (1%)	0	100	100
5	a	95/229 (42%)	84 (88%)	11 (12%)	0	100	100
5	e	95/229 (42%)	84 (88%)	11 (12%)	0	100	100
6	c	95/132 (72%)	93 (98%)	2 (2%)	0	100	100
6	g	95/132 (72%)	93 (98%)	2 (2%)	0	100	100
7	A	99/351 (28%)	92 (93%)	7 (7%)	0	100	100
7	B	105/351 (30%)	105 (100%)	0	0	100	100
8	H	167/181 (92%)	165 (99%)	2 (1%)	0	100	100
9	I	659/733 (90%)	640 (97%)	19 (3%)	0	100	100
10	K	213/239 (89%)	202 (95%)	11 (5%)	0	100	100
11	L	239/245 (98%)	235 (98%)	4 (2%)	0	100	100
12	N	383/458 (84%)	361 (94%)	22 (6%)	0	100	100
13	O	237/368 (64%)	225 (95%)	12 (5%)	0	100	100
14	P	251/369 (68%)	237 (94%)	14 (6%)	0	100	100
15	Q	254/406 (63%)	248 (98%)	6 (2%)	0	100	100
16	T	90/361 (25%)	88 (98%)	2 (2%)	0	100	100
17	U	180/324 (56%)	177 (98%)	3 (2%)	0	100	100
18	W	65/89 (73%)	64 (98%)	1 (2%)	0	100	100
19	Y	217/238 (91%)	206 (95%)	11 (5%)	0	100	100
20	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
All	All	4027/6056 (66%)	3872 (96%)	155 (4%)	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	
3	b	65/81 (80%)	65 (100%)	0	100	100
3	f	66/81 (82%)	64 (97%)	2 (3%)	41	68
4	d	81/109 (74%)	81 (100%)	0	100	100
4	h	80/109 (73%)	80 (100%)	0	100	100
5	a	82/207 (40%)	69 (84%)	13 (16%)	2	10
5	e	82/207 (40%)	69 (84%)	13 (16%)	2	10
6	c	75/99 (76%)	74 (99%)	1 (1%)	69	84
6	g	76/99 (77%)	76 (100%)	0	100	100
7	A	89/305 (29%)	89 (100%)	0	100	100
7	B	94/305 (31%)	93 (99%)	1 (1%)	73	86
8	H	162/172 (94%)	161 (99%)	1 (1%)	86	94
9	I	619/683 (91%)	618 (100%)	1 (0%)	93	98
10	K	202/223 (91%)	201 (100%)	1 (0%)	88	94
11	L	217/221 (98%)	217 (100%)	0	100	100
12	N	353/416 (85%)	353 (100%)	0	100	100
13	O	226/347 (65%)	225 (100%)	1 (0%)	91	95
14	P	241/344 (70%)	241 (100%)	0	100	100
15	Q	243/378 (64%)	243 (100%)	0	100	100
16	T	89/339 (26%)	89 (100%)	0	100	100
17	U	168/308 (54%)	166 (99%)	2 (1%)	71	85
18	W	57/76 (75%)	56 (98%)	1 (2%)	59	79
19	Y	175/219 (80%)	175 (100%)	0	100	100
20	Z	121/143 (85%)	120 (99%)	1 (1%)	81	91
All	All	3663/5471 (67%)	3625 (99%)	38 (1%)	77	88

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	143	ARG
5	e	155	LYS
5	e	172	LYS
5	e	180	SER
5	e	181	MET
5	e	184	MET
5	e	188	GLU
5	e	198	LEU
5	e	199	GLU
5	e	216	LYS
5	e	219	GLN
5	e	223	ARG
5	e	224	ILE
3	f	45	LYS
3	f	46	ARG
6	c	17	GLN
5	a	143	ARG
5	a	155	LYS
5	a	172	LYS
5	a	180	SER
5	a	181	MET
5	a	184	MET
5	a	188	GLU
5	a	198	LEU
5	a	199	GLU
5	a	216	LYS
5	a	219	GLN
5	a	223	ARG
5	a	224	ILE
7	B	233	ARG
8	H	137	LYS
9	I	97	ARG
10	K	206	ARG
13	O	343	LYS
17	U	156	LYS
17	U	187	ARG
18	W	12	ARG
20	Z	52	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	525	GLN
10	K	77	ASN
17	U	205	GLN
20	Z	113	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)

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.

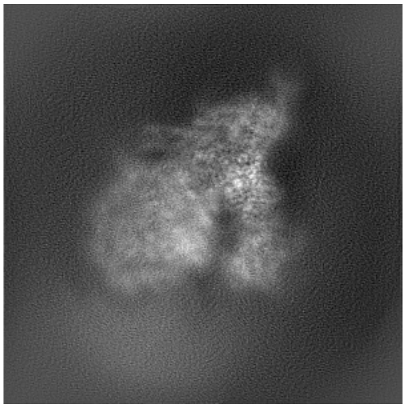
6 Map visualisation ⓘ

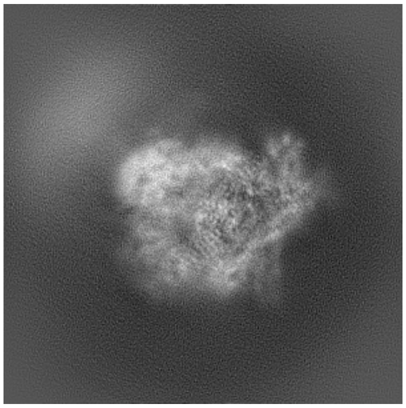
This section contains visualisations of the EMDB entry EMD-17226. These allow visual inspection of the internal detail of the map and identification of artifacts.

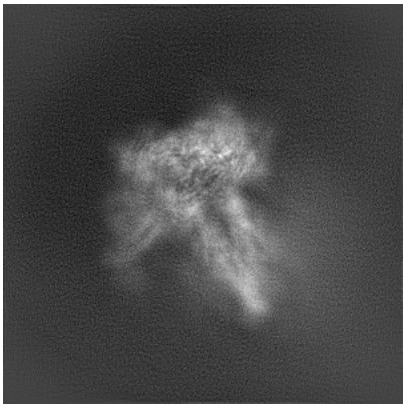
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

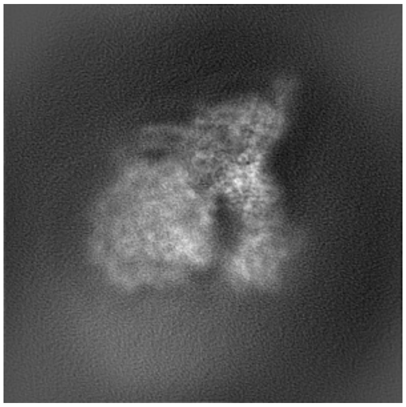
6.1.1 Primary map

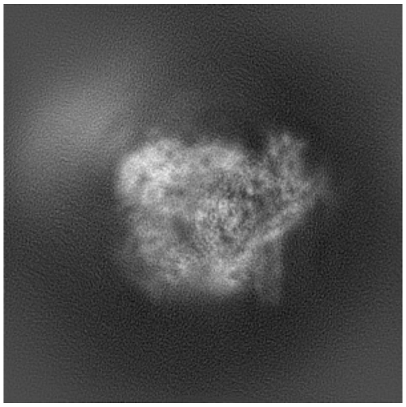

X

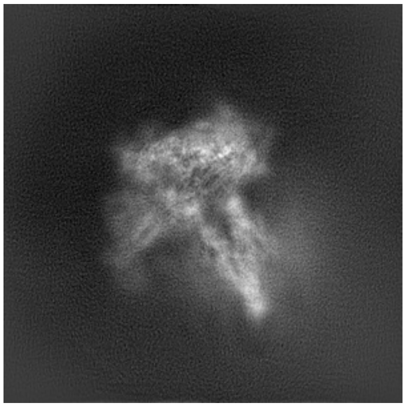

Y


Z

6.1.2 Raw map


X

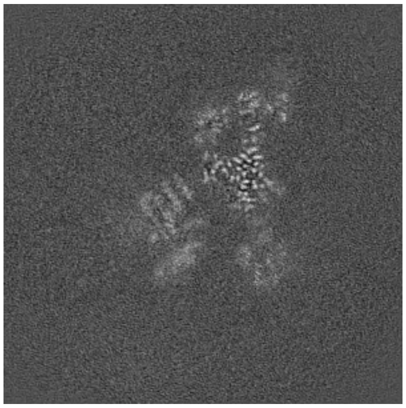

Y

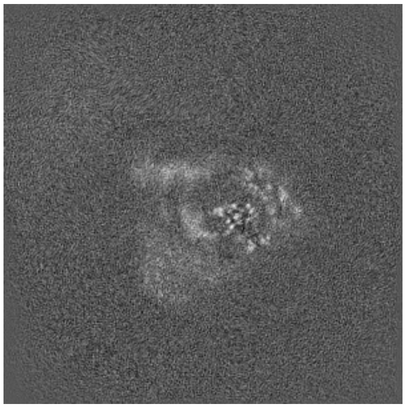

Z

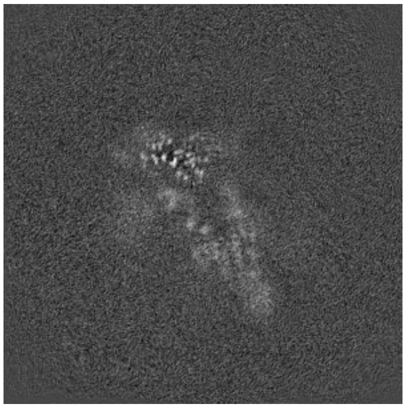
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

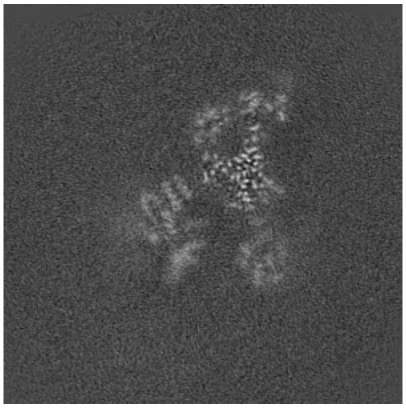
6.2.1 Primary map

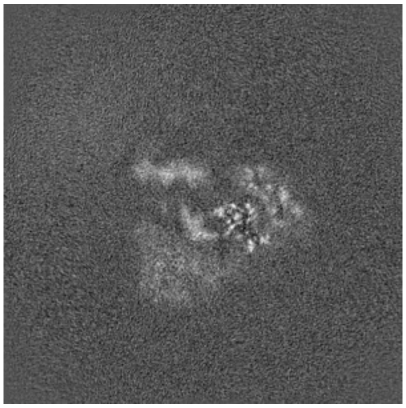

X Index: 180

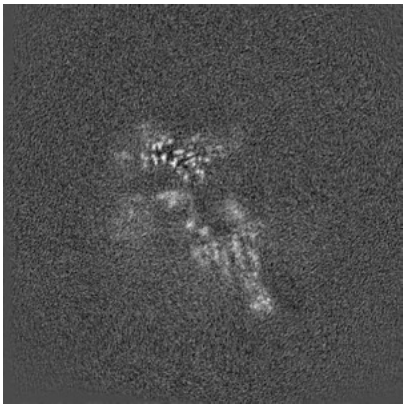

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

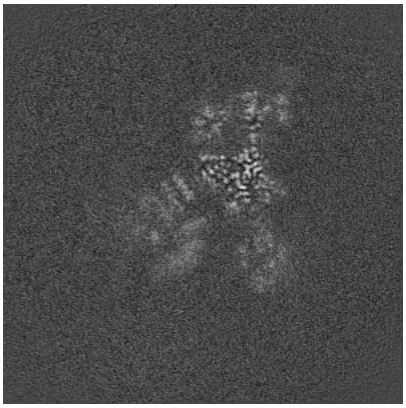

Y Index: 180


Z Index: 180

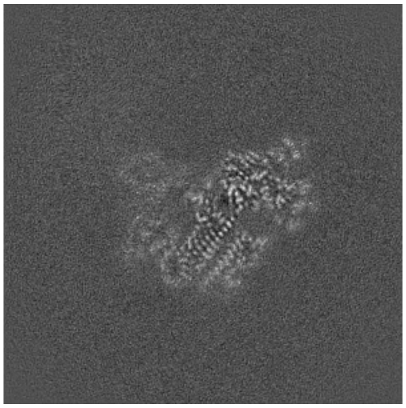
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

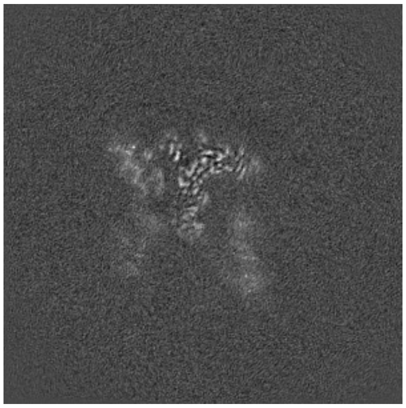
6.3.1 Primary map



X Index: 178

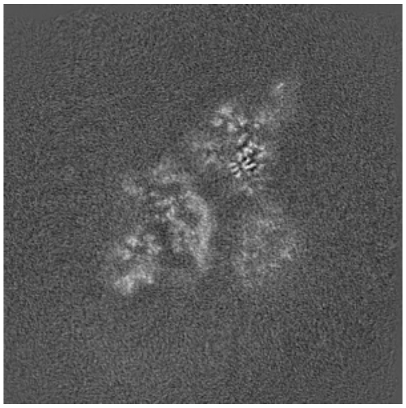


Y Index: 223

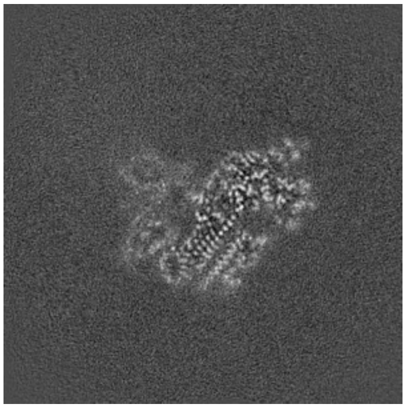


Z Index: 200

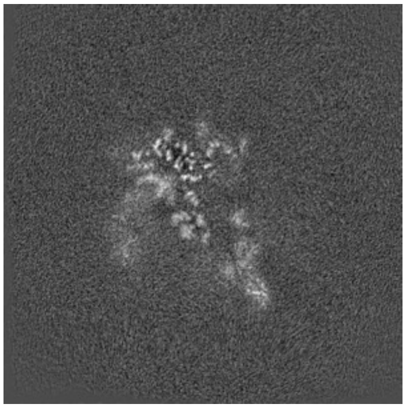
6.3.2 Raw map



X Index: 207



Y Index: 223

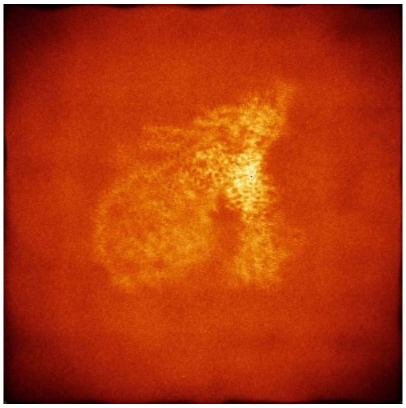


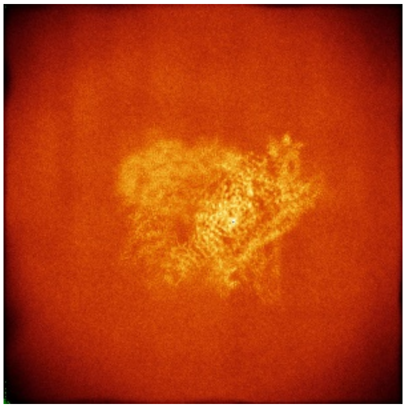
Z Index: 191

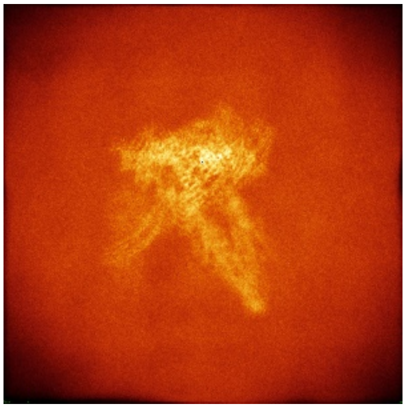
The images above show the largest variance slices of the map in three orthogonal directions.

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

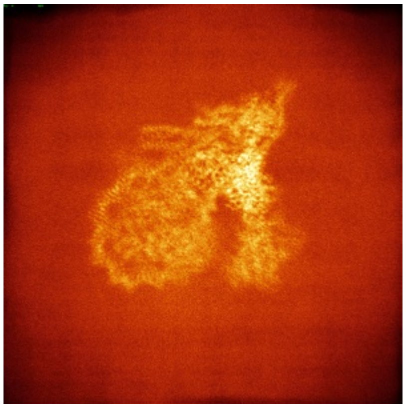
6.4.1 Primary map

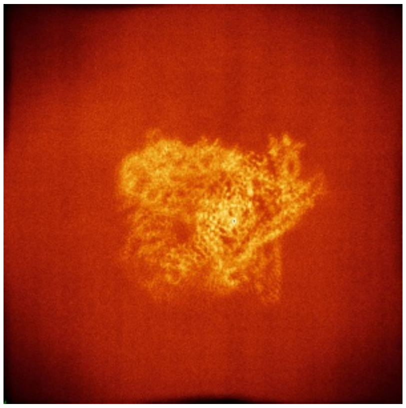

X

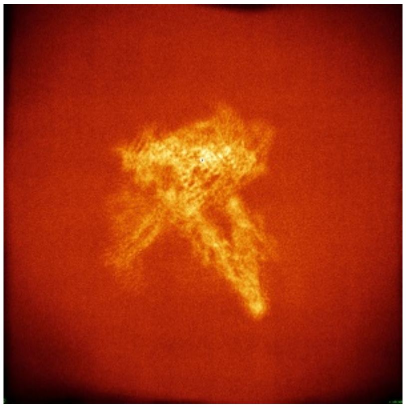

Y


Z

6.4.2 Raw map


X


Y

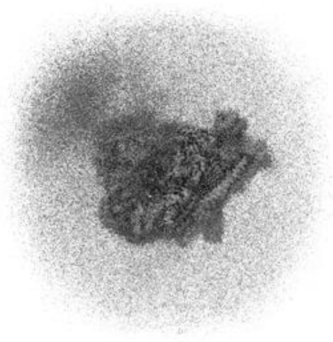

Z

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

6.5.1 Primary map


X


Y

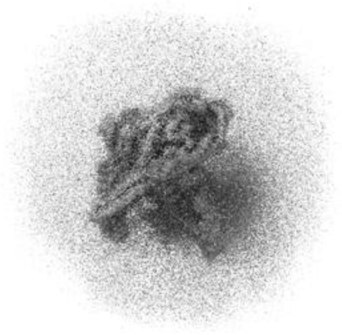

Z

The images above show the 3D surface view of the map at the recommended contour level 0.149. 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.

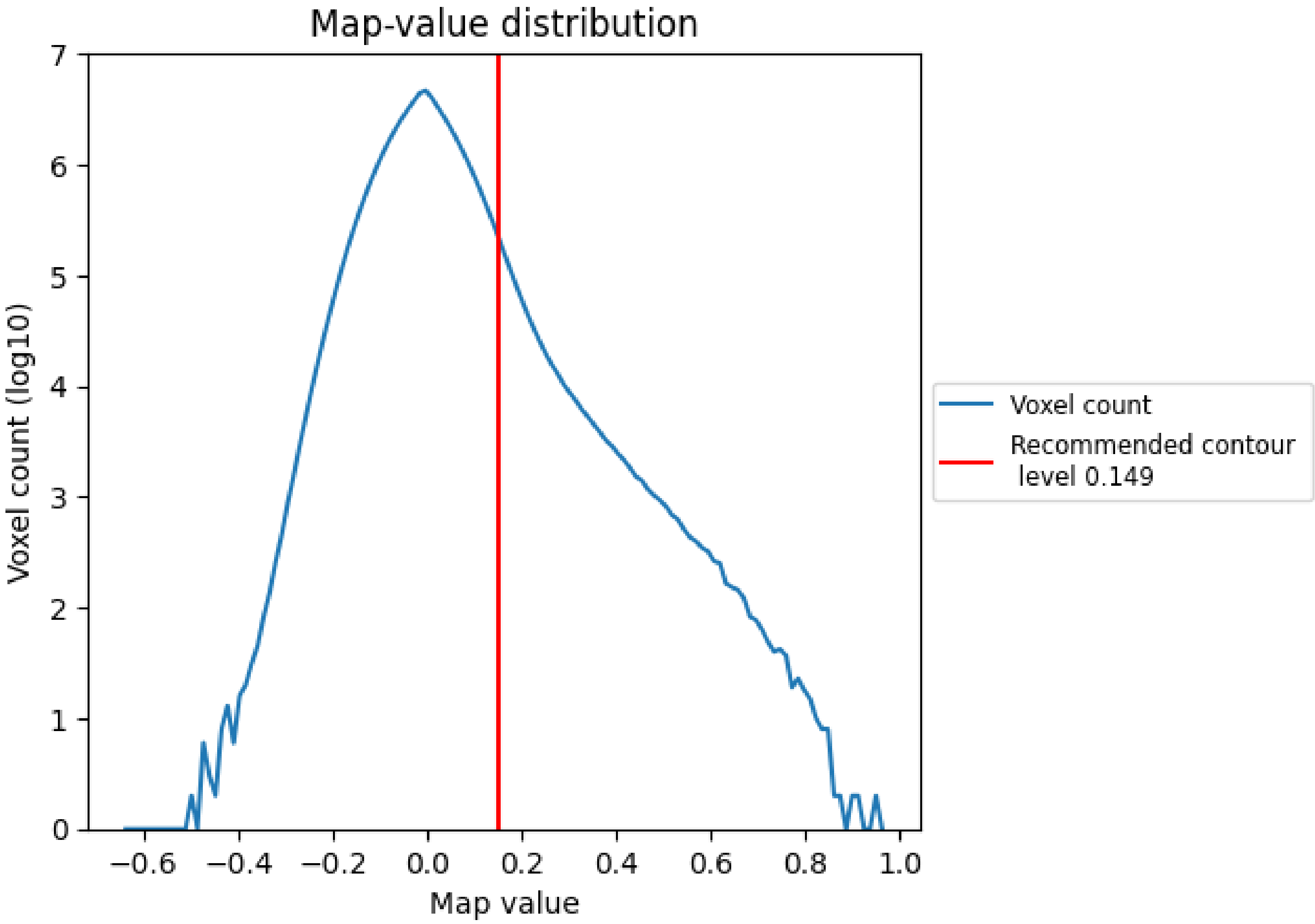
6.6 Mask visualisation

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

7 Map analysis ⓘ

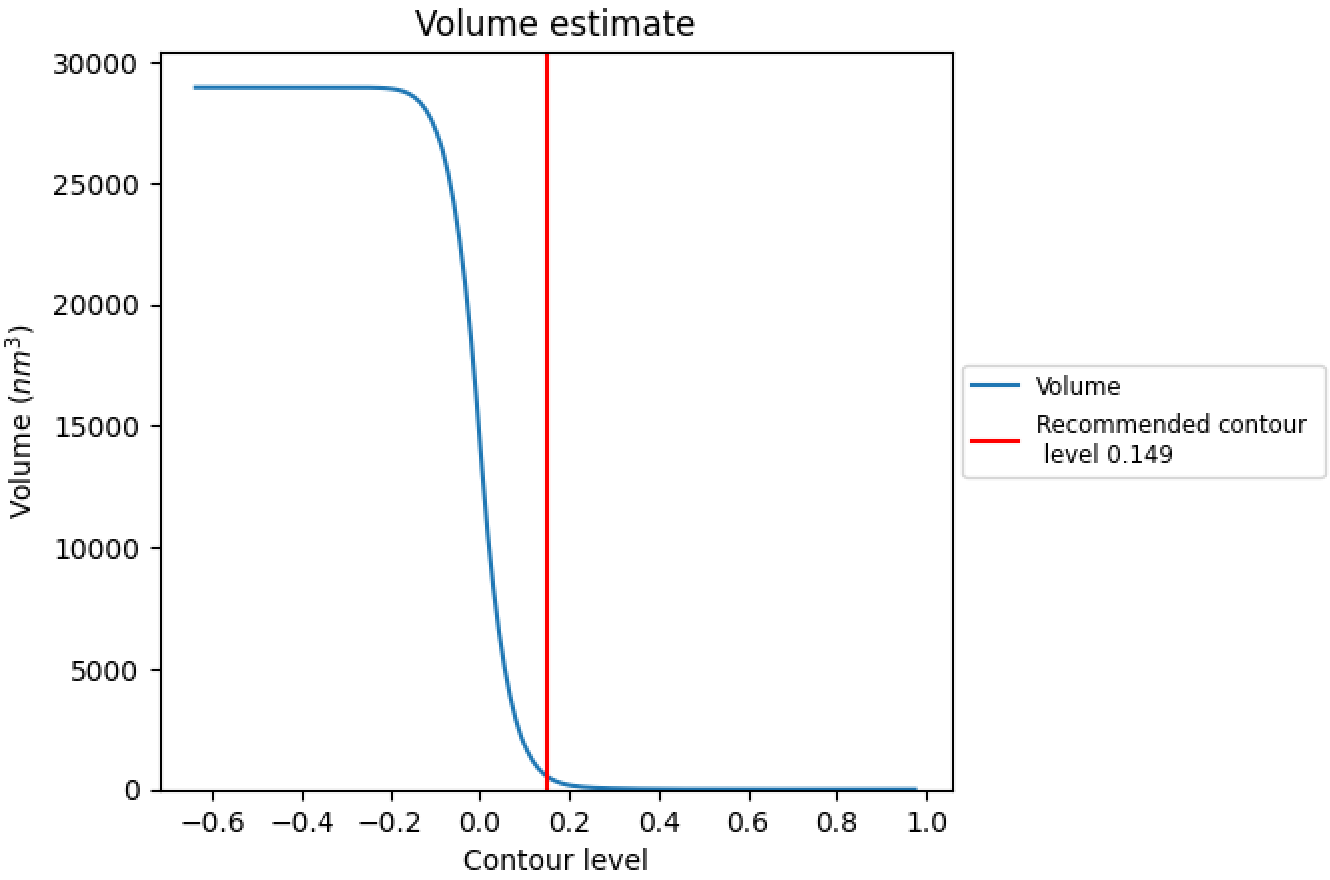
This section contains the results of statistical analysis of the map.

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.

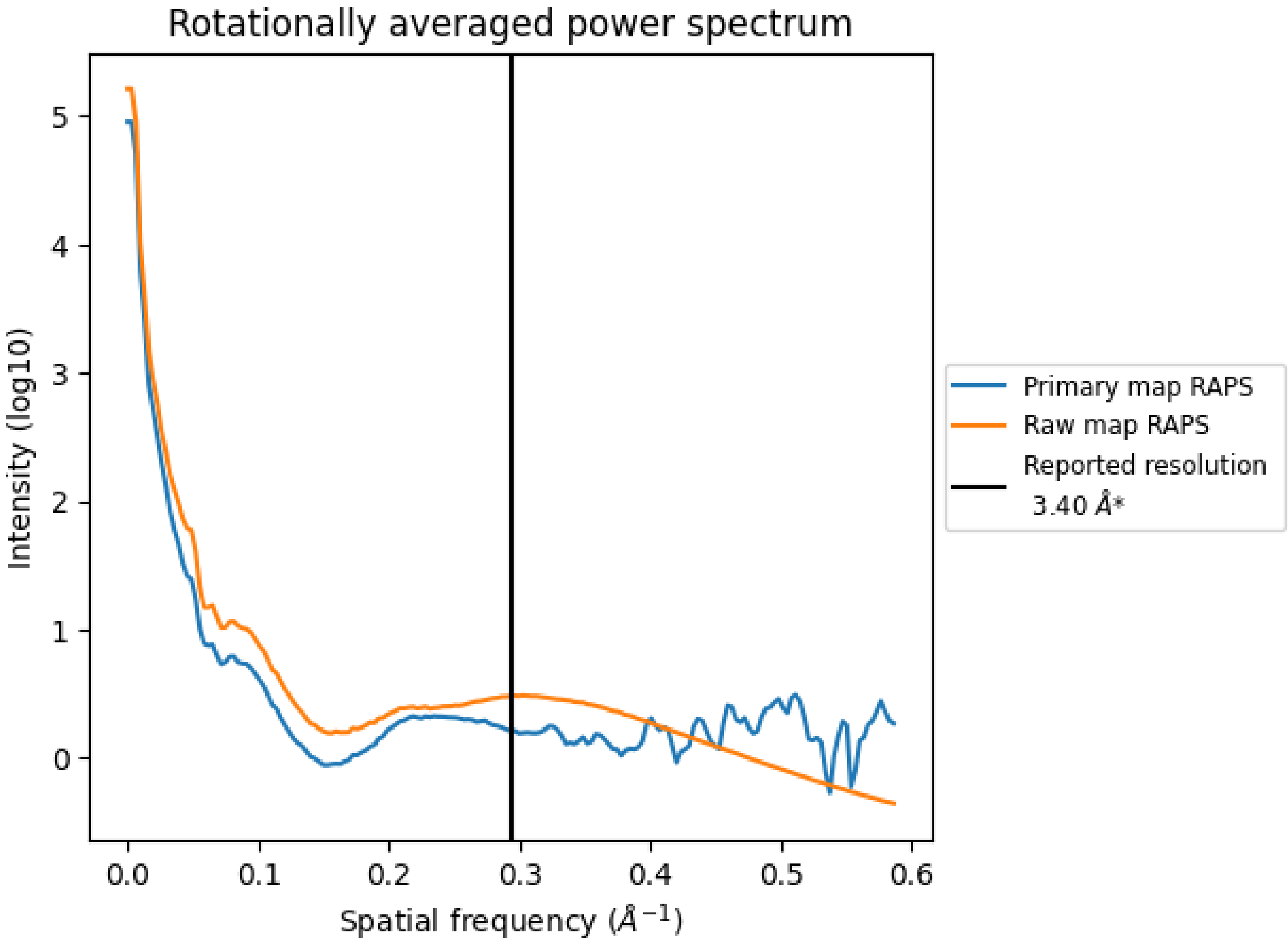
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 558 nm^3; this corresponds to an approximate mass of 504 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 0.294 $Å^{-1}$

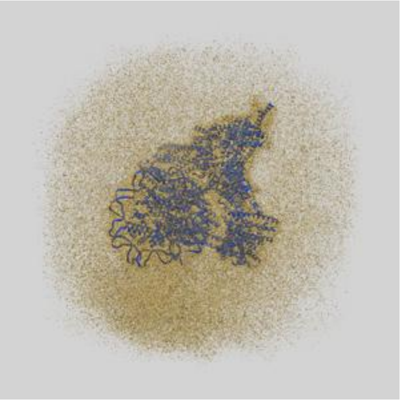
8 Fourier-Shell correlation ⓘ

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

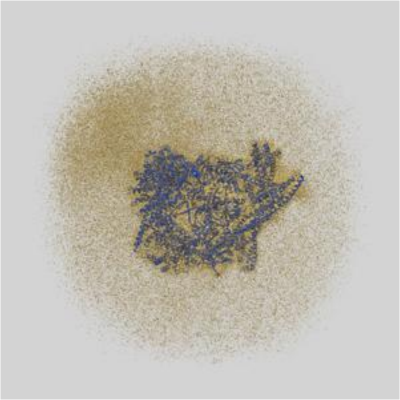
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17226 and PDB model 8OW0. Per-residue inclusion information can be found in section 3 on page 8.

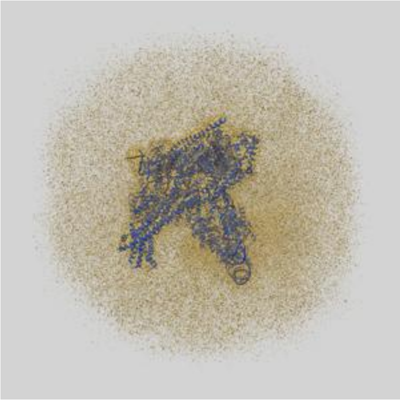
9.1 Map-model overlay (i)



X



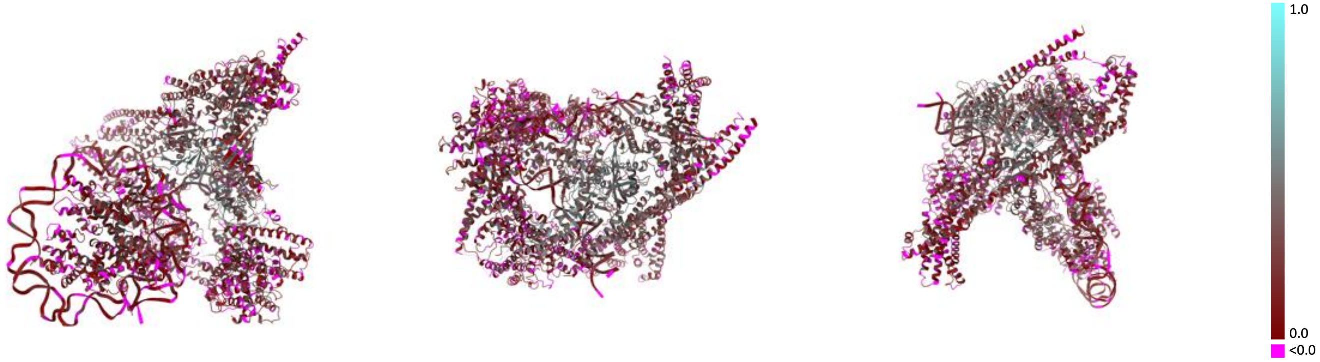
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.149 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.

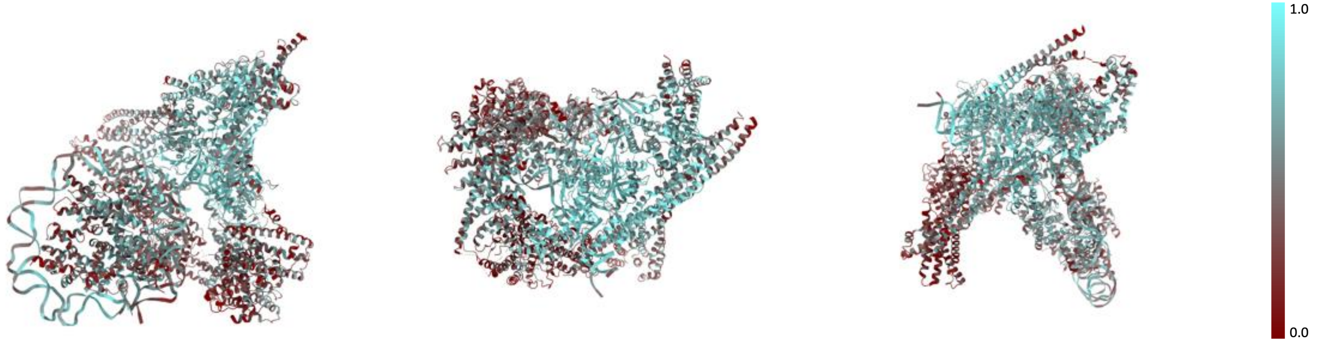
9.2 Q-score mapped to coordinate model ⓘ



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.

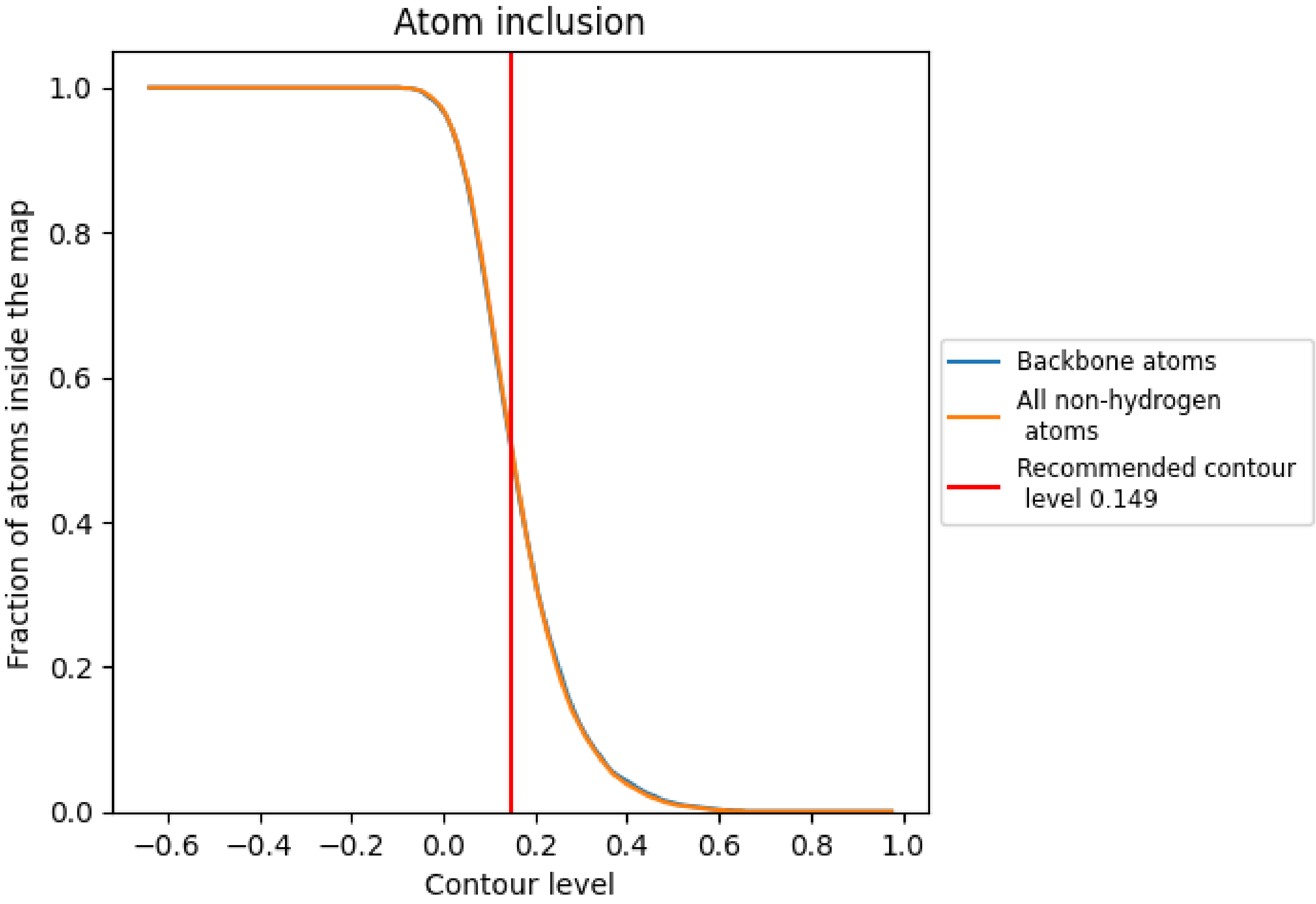
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.149).

9.4 Atom inclusion ⓘ



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.2000
A	0.6230	0.2460
B	0.6160	0.2560
D	0.6500	0.1180
E	0.6310	0.1180
H	0.3430	0.1690
I	0.3090	0.1390
K	0.2700	0.1110
L	0.7110	0.3680
N	0.7610	0.3930
O	0.5950	0.2980
P	0.6370	0.2680
Q	0.4470	0.1870
T	0.1620	0.0820
U	0.4960	0.2180
W	0.1680	0.0750
Y	0.5140	0.2100
Z	0.4550	0.1870
a	0.3850	0.0900
b	0.5060	0.1370
c	0.5620	0.2270
d	0.5720	0.2160
e	0.3810	0.1090
f	0.5220	0.1800
g	0.3920	0.1290
h	0.4620	0.1600