wwPDB EM Validation Summary Report

Feb 19, 2024 – 12:58 PM JST

PDB ID	:	7X3T
EMDB ID	:	EMD-32992
Title	:	Cryo-EM structure of ISW1a-dinucleosome
Authors	:	Lifei, L.; Kangjing, C.; Chen, Z.
Deposited on	:	2022-03-01
Resolution	:	5.40 Å(reported)

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

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

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

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

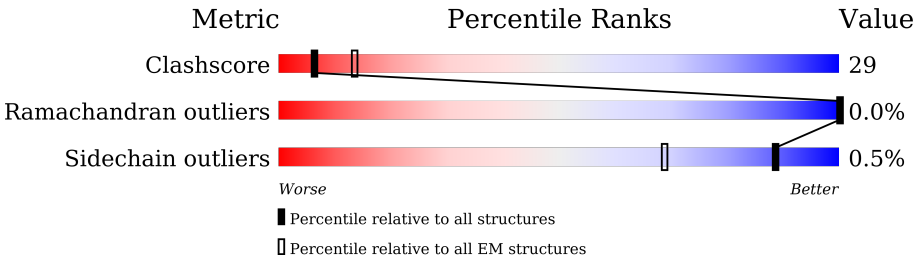
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.40 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	A	136	33% 39% 28%
1	E	136	32% 38% 30%
1	K	136	26% 46% 28%
1	O	136	35% 35% 30%
2	B	103	38% 38% 20%
2	F	103	5% 29% 54% 17%
2	L	103	23% 62% 15%
2	P	103	38% 40% 22%

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Mol	Chain	Length	Quality of chain
3	C	130	29% 53% 18%
3	G	130	38% 45% 18%
3	M	130	45% 38% 18%
3	Q	130	38% 45% 18%
4	D	126	37% 35% 26%
4	H	126	41% 32% 26%
4	N	126	29% 44% 26%
4	R	126	33% 40% 26%
5	I	354	63% 32%
6	J	354	57% 39%
7	U	624	34% 60% 5%
8	V	1062	18% 34% 41% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BEF	V	1202	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 37283 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		
1	K	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	O	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		
2	L	88	Total	C	N	O	S	0	0
			707	445	143	118	1		
2	P	80	Total	C	N	O	S	0	0
			632	398	122	111	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		
3	M	107	Total	C	N	O	0	0
			811	510	158	143		
3	Q	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
4	N	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
4	R	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 5 is a DNA chain called DNA (343-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	339	Total	C	N	O	P	0	0
			6918	3286	1256	2037	339		

- Molecule 6 is a DNA chain called DNA(343-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	339	Total	C	N	O	P	0	0
			6981	3306	1305	2031	339		

- Molecule 7 is a protein called ISWI one complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	590	Total	C	N	O	S	0	0
			4840	3114	816	895	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	126	MET	-	initiating methionine	UNP P43596

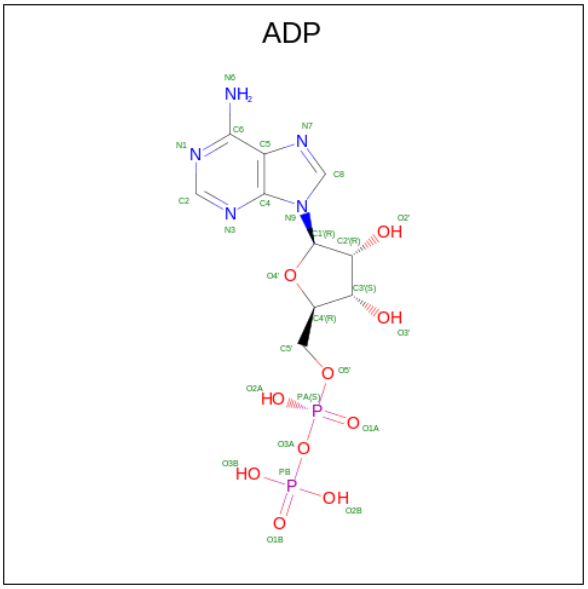
- Molecule 8 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	792	Total	C	N	O	S	0	0
			6552	4175	1132	1223	22		

There is a discrepancy between the modelled and reference sequences:

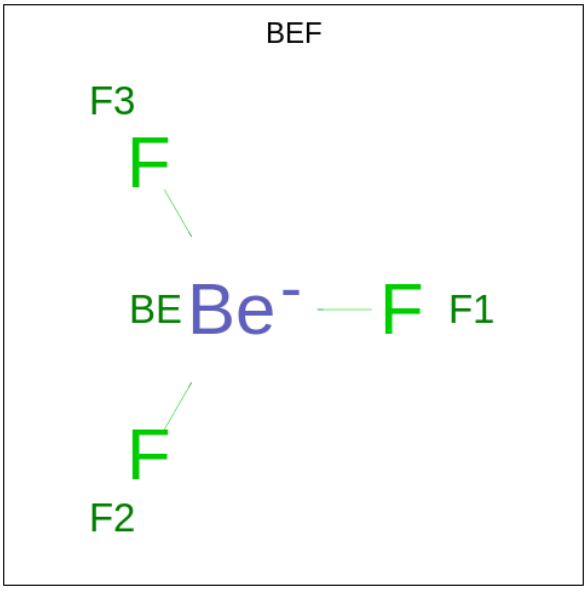
Chain	Residue	Modelled	Actual	Comment	Reference
V	68	MET	-	initiating methionine	UNP P38144

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	V	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	V	1	Total	Be	F	0
			4	1	3	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

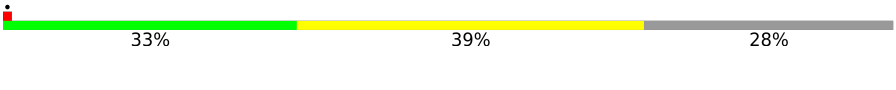
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	V	1	1	1	0

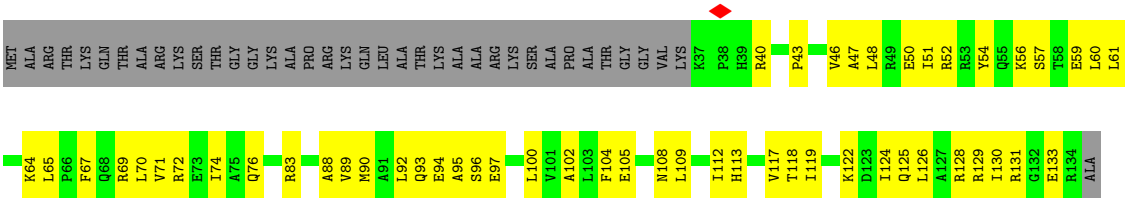
3 Residue-property plots (i)

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: Histone H3

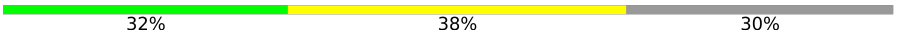
Chain A:

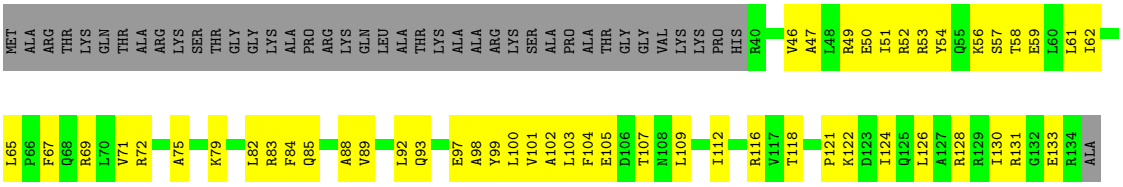




• Molecule 1: Histone H3

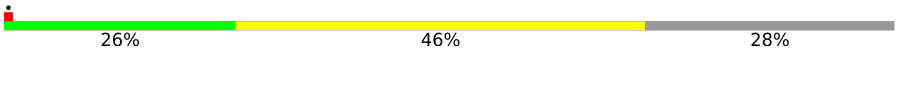
Chain E:

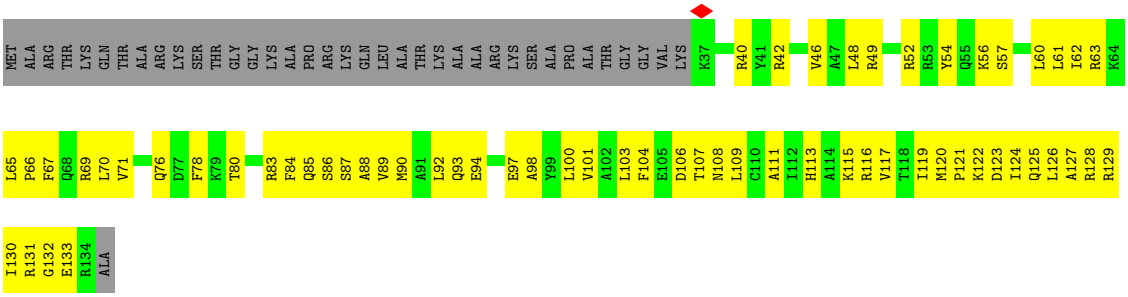




• Molecule 1: Histone H3

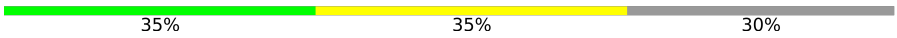
Chain K:

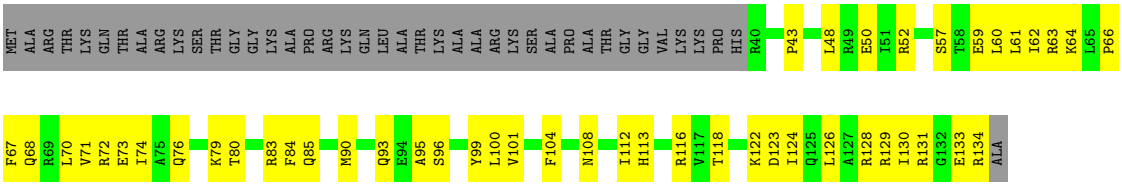




• Molecule 1: Histone H3

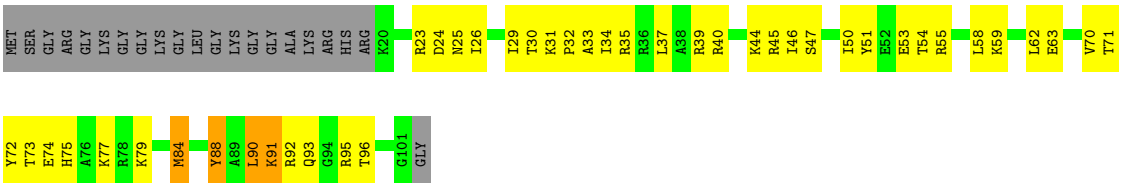
Chain O:





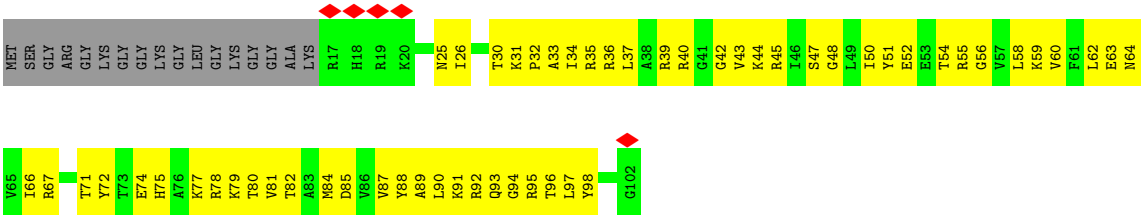
• Molecule 2: Histone H4

Chain B:



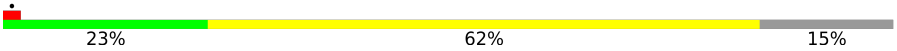
• Molecule 2: Histone H4

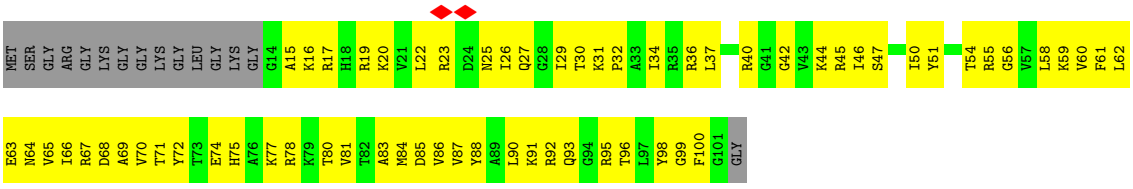
Chain F:



• Molecule 2: Histone H4

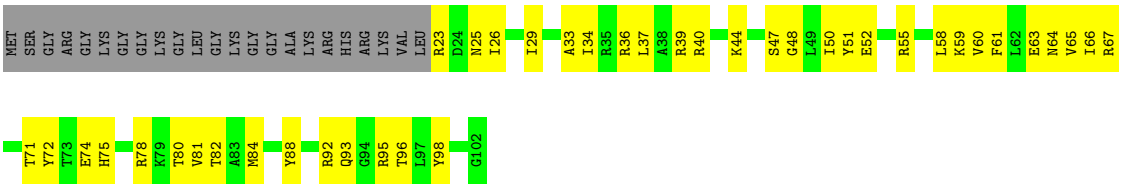
Chain L:





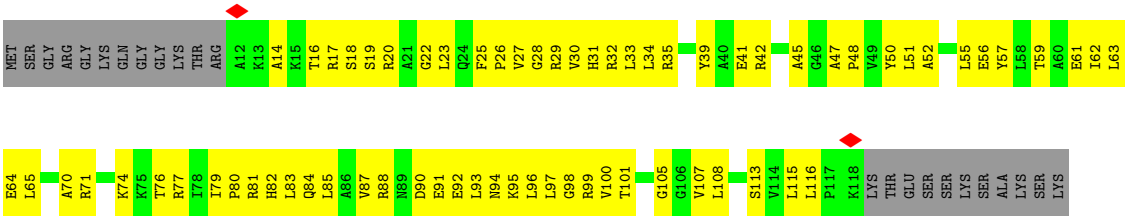
• Molecule 2: Histone H4

Chain P:



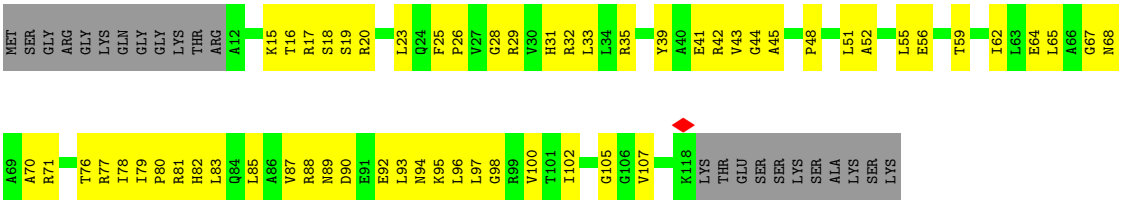
• Molecule 3: Histone H2A

Chain C:



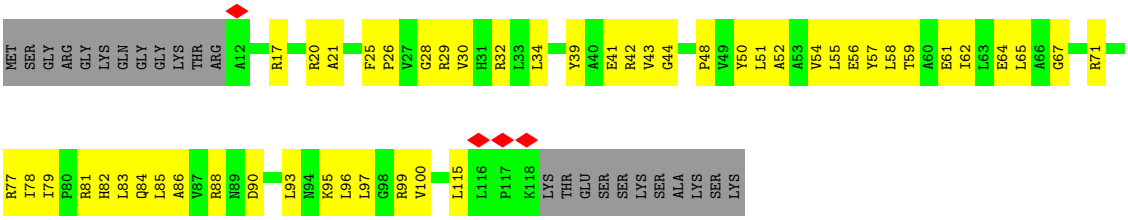
• Molecule 3: Histone H2A

Chain G:



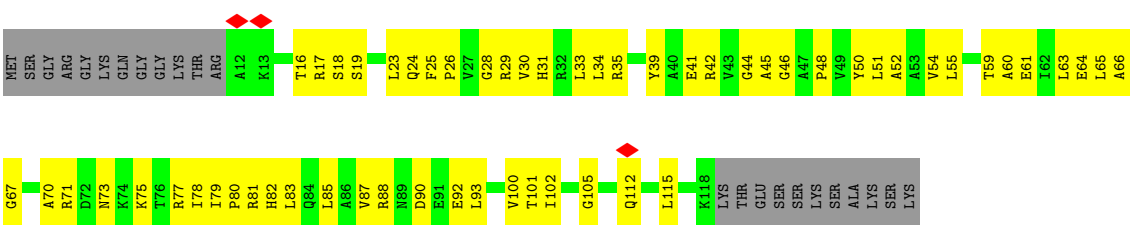
• Molecule 3: Histone H2A

Chain M:



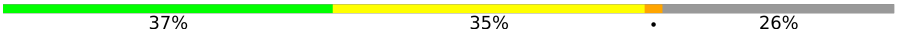
• Molecule 3: Histone H2A

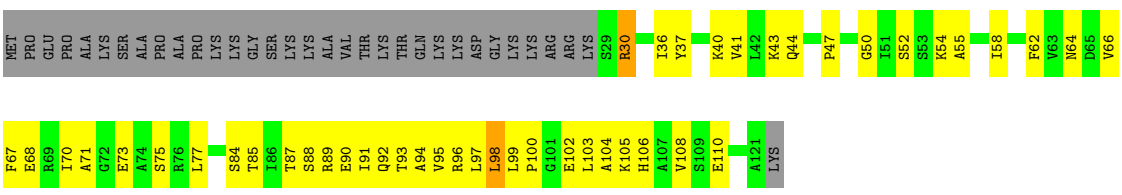
Chain Q:



• Molecule 4: Histone H2B 1.1

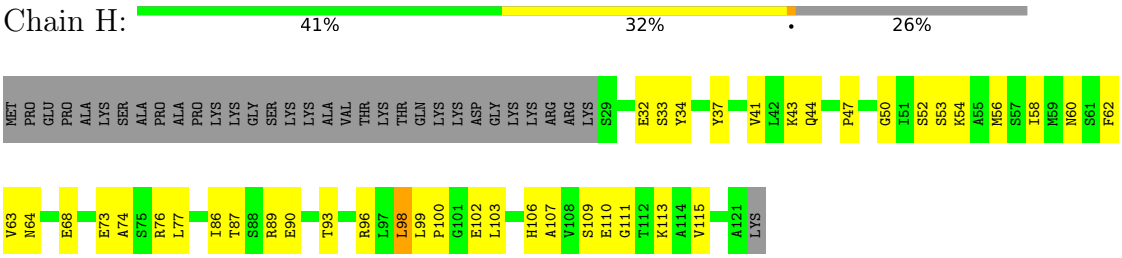
Chain D:





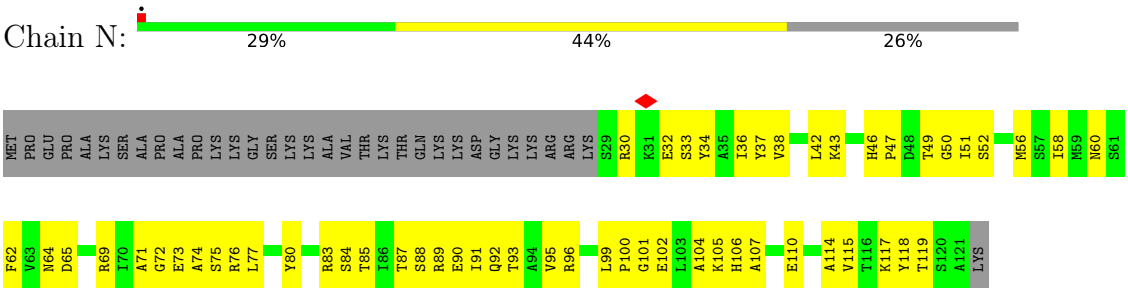
• Molecule 4: Histone H2B 1.1

Chain H:



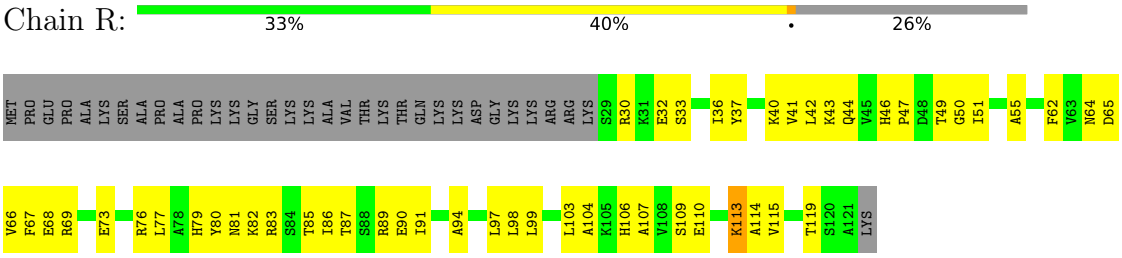
• Molecule 4: Histone H2B 1.1

Chain N:



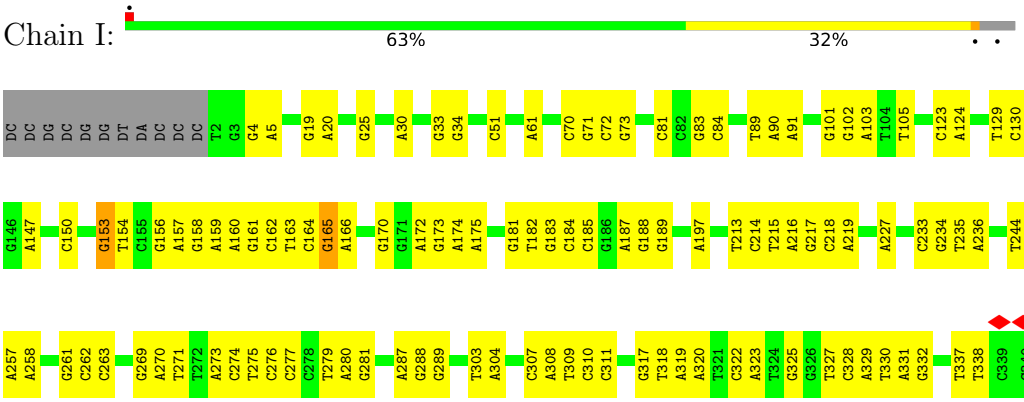
• Molecule 4: Histone H2B 1.1

Chain R:



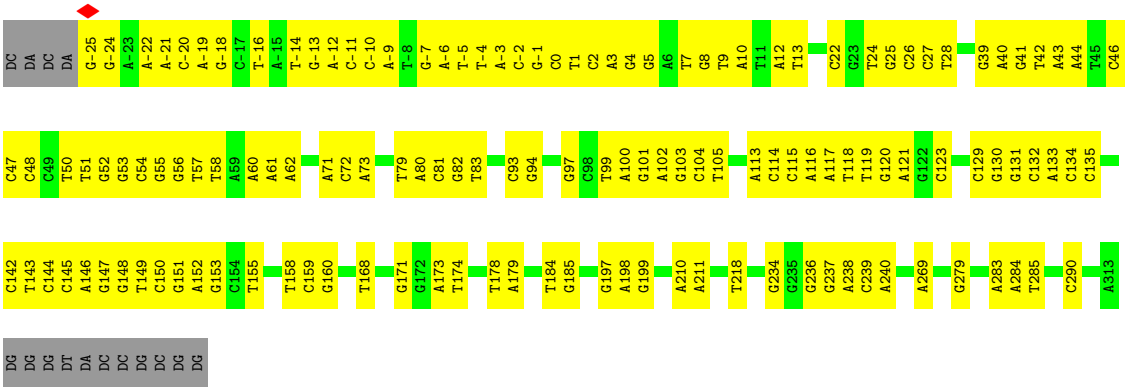
• Molecule 5: DNA (343-MER)

Chain I:



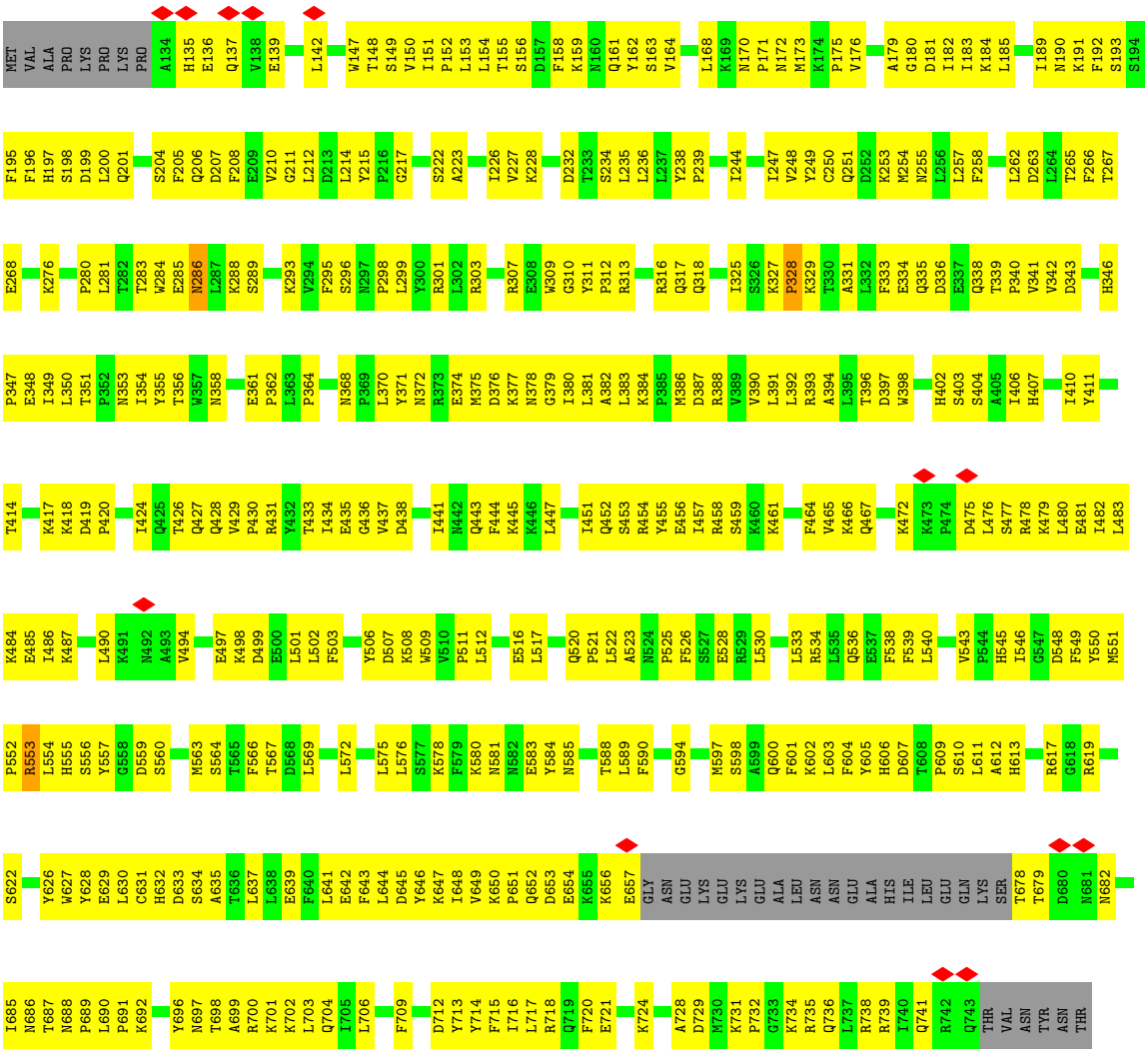
• Molecule 6: DNA(343-MER)

Chain J:



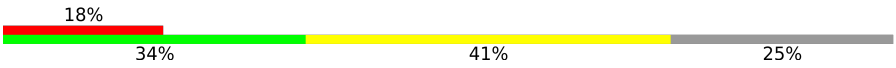
• Molecule 7: ISWI one complex protein 3

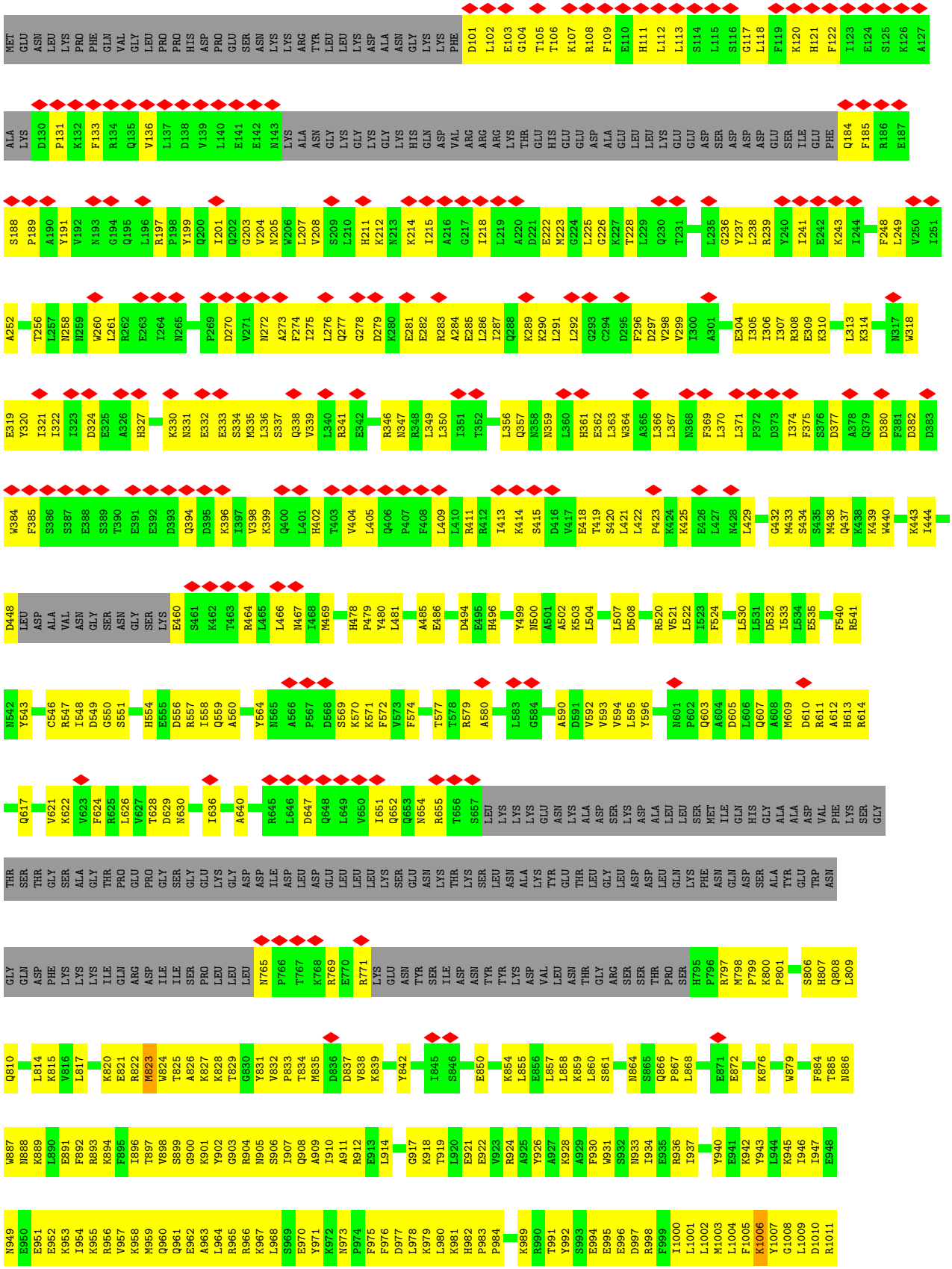
Chain U:

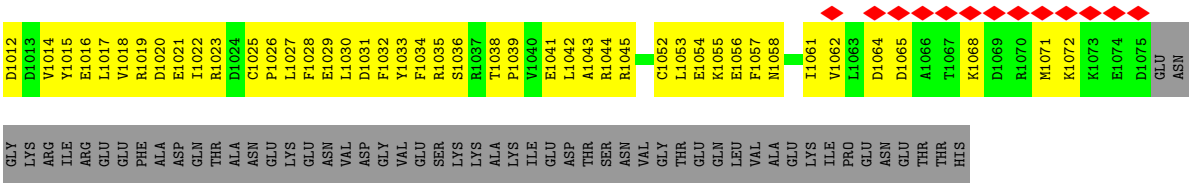


• Molecule 8: ISWI chromatin-remodeling complex ATPase ISW1

Chain V:




MET GLU ASN LEU LYS PRO PHE GLN VAL GLY LEU PRO PRO HIS ASP PRO GLU SER ASN LYS LYS ARG TYR LEU LEU LYS LYS ASP ALA ASN GLY LYS LYS PHE
D101 L102 E103 G104 T105 T106 K107 R108 F109 E110 H111 L112 L113 S114 L115 S116 G117 L118 F119 K120 H121 F122 I123 E124 S125 K126 A127
ALA LYS D130 P131 K132 F133 R134 Q135 V136 L137 D138 V139 L140 E141 E142 N143 LYS ALA ASN GLY LYS GLY LYS GLY LYS HIS GLN ASP VAL ARG ARG ARG LYS THR GLU HIS GLU GLU ASP ALA GLU LEU LEU LYS GLU GLU ASP SER ASP ASP ASP GLU SER ILE GLU PHE
Q184 F185 R186 E187
S188 P189 A190 Y191 V192 N193 G194 Q195 L196 R197 P198 Y199 Q200 I201 Q202 G203 V204 N205 W206 L207 V208 S209 L210 H211 K212 N213 K214 I215 A216 G217 I218 L219 A220 D221 E222 M223 G224 L225 G226 K227 T228 L229 Q230 T231 L235 G236 Y237 L238 R239 Y240 I241 E242 K243 I244 F248 L249 V250 I251
A252 T256 L257 N258 N259 W260 L261 R262 E263 I264 N265 P269 D270 V271 N272 A273 F274 I275 L276 Q277 G278 D279 K280 E281 E282 R283 A284 E285 L286 I287 Q288 K289 K290 L291 L292 G293 C294 D295 F296 D297 V298 V299 I300 A301 E304 I305 I306 I307 R308 E309 K310 L313 K314 N317 W318
E319 Y320 I321 I322 I323 D324 E325 A326 H327 K330 N331 E332 E333 S334 M335 L336 S337 Q338 V339 L340 R341 E342 R346 N347 R348 L349 L350 I351 T352 L356 Q357 N358 N359 L360 H361 E362 L363 W364 A365 L366 L367 N368 F369 L370 L371 P372 D373 I374 F375 S376 D377 A378 Q379 D380 F381 D382 D383
W384 F385 S386 S387 E388 S389 T390 E391 E392 D393 Q394 D395 K396 I397 V398 K399 Q400 L401 H402 T403 V404 L405 Q406 P407 F408 L409 L410 R411 R412 I413 K414 S415 D416 V417 E418 T419 S420 L421 L422 P423 K424 K425 E426 L427 N428 L429 G432 M433 S434 S435 M436 Q437 K438 K439 W440 K443 I444
D448 LEU ASP ALA VAL ASN GLY SER ASN GLY SER LYS E460 S461 K462 T463 R464 L465 L466 N467 I468 M469 H478 P479 Y480 L481 A485 E486 D494 E495 H496 Y499 N500 A501 A502 K503 L504 L507 D508 R520 V521 L522 I523 F524 L530 L531 D532 I533 L534 E535 F540 R541
N542 Y543 C546 R547 I548 D549 G550 S551 H554 E555 D556 R557 I558 Q559 A560 Y564 N565 A566 P567 D568 S569 K570 K571 F572 V573 F574 T577 T578 R579 A580 L583 G584 A590 D591 V592 V593 V594 L595 Y596 N601 P602 Q603 A604 D605 L606 Q607 A608 M609 D610 R611 A612 H613 R614
Q617 V621 K622 V623 F624 R625 L626 V627 T628 D629 N630 I636 A640 R645 L646 D647 Q648 L649 V650 I651 Q652 Q653 N654 R655 T656 S657 LEU LYS LYS LYS GLU ASN LYS ALA ASP SER LYS ASP ALA LEU LEU SER MET ILE GLN HIS GLY ALA ALA ASP VAL PHE LYS SER GLY
THR SER THR GLY SER ALA GLY THR PRO GLU PRO GLY SER GLY GLU LYS GLY ASP ASP ILE ASP LEU ASP GLU LEU LEU LEU LYS SER GLU ASN LYS THR LYS SER LEU ASN ALA LYS TYR GLU THR LEU GLY LEU ASP ASP LEU GLN LYS PHE ASN GLN ASP SER ALA TYR GLU TRP ASN
GLY GLN ASP PHE LYS LYS LYS ILE GLN ARG ASP ILE ILE SER PRO LEU LEU LEU N765 P766 T767 K768 R769 E770 R771 LYS GLU ASN TYR SER ILE ASP ASN TYR TYR LYS ASP VAL LEU ASN THR GLY ARG SER SER THR PRO SER H795 P796 R797 M798 P799 K800 P801 S806 H807 Q808 L809
Q810 L814 K815 V816 L817 K820 E821 R822 M823 W824 T825 A826 K827 K828 T829 G830 Y831 V832 P833 T834 M835 D836 D837 V838 K839 Y842 I845 S846 E850 K854 L855 E856 L857 L858 K859 L860 S861 N864 S865 Q866 P867 L868 E871 E872 K876 W879 F884 T885 N886
W887 N888 K889 L890 E891 F892 R893 K894 F895 I896 T897 V898 S899 Q900 K901 Y902 Q903 R904 N905 S906 I907 Q908 A909 I910 A911 R912 E913 L914 G917 K918 T919 L920 E921 E922 V923 R924 A925 Y926 A927 K928 A929 F930 W931 S932 N933 I934 E935 R936 I937 Y940 E941 K942 Y943 L944 K945 I946 F947 E948
N949 E950 E951 E952 K953 I954 K955 R956 V957 K958 M959 Q960 Q961 E962 A963 L964 R965 R966 K967 L968 S969 E970 Y971 K972 N973 P974 F975 F976 D977 L978 K979 L980 K981 H982 P983 P984 K989 R990 T991 Y992 S993 E994 E995 E996 D997 R998 F999 I1000 L1001 L1002 M1003 L1004 F1005 K1006 Y1007 G1008 L1009 D1010 R1011


D1012 D1013 V1014 Y1015 E1016 L1017 V1018 R1019 D1020 E1021 I1022 R1023 D1024 C1025 P1026 L1027 F1028 E1029 L1030 D1031 F1032 Y1033 F1034 R1035 S1036 R1037 T1038 P1039 V1040 E1041 L1042 A1043 R1044 R1045 C1052 L1053 E1054 K1055 E1056 F1057 N1058 I1061 V1062 L1063 D1064 D1065 A1066 T1067 K1068 D1069 R1070 M1071 K1072 K1073 E1074 D1075 GLU ASN
GLY LYS ARG ILE ARG GLU GLU PHE ALA ASP GLN THR ALA ASN GLU LYS GLU ASN VAL ASP GLY VAL GLU SER LYS LYS ALA LYS ILE GLU ASP THR SER ASN VAL GLY THR GLU GLN LEU VAL ALA GLU LYS ILE PRO GLU ASN GLU THR THR HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0048	Depositor
Map size (Å)	389.69998, 389.69998, 389.69998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.48	0/813	0.68	0/1093
1	E	0.47	0/789	0.59	0/1059
1	K	0.40	0/813	0.57	0/1093
1	O	0.39	0/789	0.53	0/1059
2	B	0.51	0/660	0.64	0/885
2	F	0.54	0/680	0.70	0/912
2	L	0.45	0/715	0.65	0/955
2	P	0.35	0/639	0.56	0/855
3	C	0.48	0/821	0.64	0/1112
3	G	0.44	0/825	0.64	0/1116
3	M	0.37	0/821	0.58	0/1112
3	Q	0.34	0/825	0.56	0/1116
4	D	0.55	0/728	0.73	2/983 (0.2%)
4	H	0.48	0/736	0.67	1/991 (0.1%)
4	N	0.39	0/728	0.57	0/983
4	R	0.38	0/736	0.56	0/991
5	I	0.64	1/7753 (0.0%)	0.87	2/11956 (0.0%)
6	J	0.59	2/7839 (0.0%)	0.85	0/12105
7	U	0.39	0/4962	0.57	0/6709
8	V	0.31	0/6680	0.53	1/8996 (0.0%)
All	All	0.49	3/39352 (0.0%)	0.72	6/56081 (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
8	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	22	DC	O3'-P	5.85	1.68	1.61
5	I	213	DT	O3'-P	5.41	1.67	1.61
6	J	211	DA	O3'-P	5.04	1.67	1.61

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	98	LEU	C-N-CA	-8.35	100.83	121.70
4	D	98	LEU	C-N-CA	-7.14	103.86	121.70
5	I	165	DG	O4'-C4'-C3'	-6.13	102.05	104.50
5	I	153	DG	O4'-C1'-N9	5.54	111.87	108.00
4	D	30	ARG	NE-CZ-NH2	-5.47	117.56	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	V	1006	LYS	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	801	0	831	60	0
1	E	779	0	815	59	0
1	K	801	0	831	80	0
1	O	779	0	815	65	0
2	B	653	0	695	41	0
2	F	672	0	698	70	0
2	L	707	0	760	88	0
2	P	632	0	665	49	0
3	C	811	0	849	74	0
3	G	815	0	860	66	0
3	M	811	0	849	65	0
3	Q	815	0	860	57	0
4	D	717	0	723	57	0
4	H	725	0	745	44	0
4	N	717	0	723	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	725	0	745	55	0
5	I	6918	0	3807	147	0
6	J	6981	0	3802	182	0
7	U	4840	0	4833	402	0
8	V	6552	0	6584	469	0
9	V	27	0	12	6	0
10	V	4	0	0	3	0
11	V	1	0	0	0	0
All	All	37283	0	31502	1885	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 29.

The worst 5 of 1885 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:284:DA:H2"	6:J:285:DT:C5'	1.72	1.19
6:J:284:DA:H2"	6:J:285:DT:H5'	1.17	1.14
6:J:283:DA:H2"	6:J:284:DA:OP2	1.40	1.11
8:V:364:TRP:HA	8:V:367:LEU:HB3	1.46	0.97
2:L:29:ILE:HD11	2:L:55:ARG:HG2	1.47	0.94

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	96/136 (71%)	91 (95%)	5 (5%)	0	100	100
1	E	93/136 (68%)	89 (96%)	4 (4%)	0	100	100
1	K	96/136 (71%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
2	B	80/103 (78%)	76 (95%)	4 (5%)	0	100	100
2	F	84/103 (82%)	83 (99%)	1 (1%)	0	100	100
2	L	86/103 (84%)	82 (95%)	4 (5%)	0	100	100
2	P	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
3	C	105/130 (81%)	104 (99%)	1 (1%)	0	100	100
3	G	105/130 (81%)	105 (100%)	0	0	100	100
3	M	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
3	Q	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
4	D	91/126 (72%)	87 (96%)	4 (4%)	0	100	100
4	H	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
4	N	91/126 (72%)	85 (93%)	6 (7%)	0	100	100
4	R	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
7	U	586/624 (94%)	523 (89%)	62 (11%)	1 (0%)	47	81
8	V	780/1062 (73%)	713 (91%)	67 (9%)	0	100	100
All	All	2856/3666 (78%)	2677 (94%)	178 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	U	328	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	84/111 (76%)	84 (100%)	0	100	100
1	E	82/111 (74%)	82 (100%)	0	100	100
1	K	84/111 (76%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	82/111 (74%)	82 (100%)	0	100 100
2	B	67/79 (85%)	58 (87%)	9 (13%)	4 18
2	F	67/79 (85%)	67 (100%)	0	100 100
2	L	72/79 (91%)	72 (100%)	0	100 100
2	P	64/79 (81%)	64 (100%)	0	100 100
3	C	81/102 (79%)	81 (100%)	0	100 100
3	G	82/102 (80%)	82 (100%)	0	100 100
3	M	81/102 (79%)	81 (100%)	0	100 100
3	Q	82/102 (80%)	82 (100%)	0	100 100
4	D	77/106 (73%)	77 (100%)	0	100 100
4	H	79/106 (74%)	79 (100%)	0	100 100
4	N	77/106 (73%)	77 (100%)	0	100 100
4	R	79/106 (74%)	78 (99%)	1 (1%)	69 82
7	U	541/571 (95%)	539 (100%)	2 (0%)	91 94
8	V	724/959 (76%)	724 (100%)	0	100 100
All	All	2505/3122 (80%)	2493 (100%)	12 (0%)	89 93

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	95	ARG
2	B	96	THR
4	R	113	LYS
7	U	286	ASN
2	B	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	46	HIS
8	V	402	HIS
8	V	258	ASN
8	V	496	HIS
3	G	31	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	BEF	V	1202	-	0,3,3	-	-	-		
9	ADP	V	1201	11	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	V	1201	11	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1201	ADP	C5-C4	2.42	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1201	ADP	PA-O3A-PB	-3.90	119.45	132.83
9	V	1201	ADP	N3-C2-N1	-3.25	123.60	128.68
9	V	1201	ADP	C3'-C2'-C1'	2.81	105.21	100.98
9	V	1201	ADP	C4-C5-N7	-2.58	106.70	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1201	ADP	O4'-C4'-C5'-O5'
9	V	1201	ADP	C3'-C4'-C5'-O5'
9	V	1201	ADP	PB-O3A-PA-O1A
9	V	1201	ADP	PB-O3A-PA-O2A

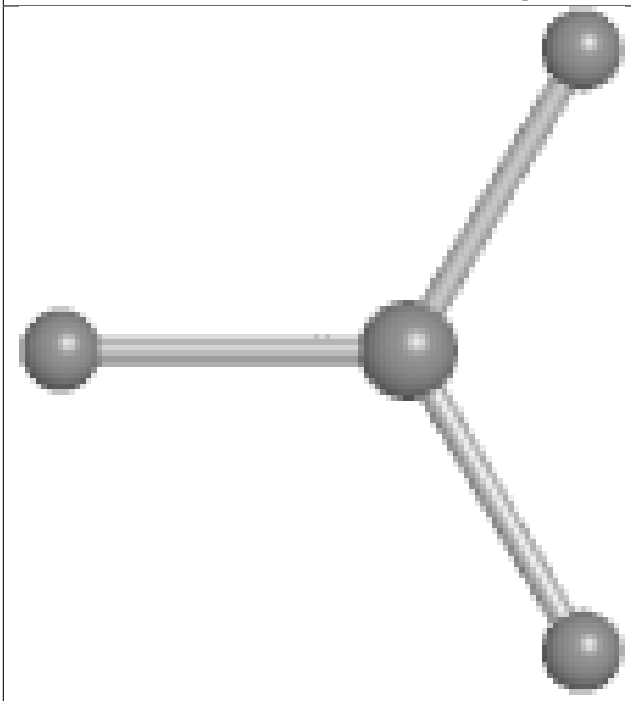
There are no ring outliers.

2 monomers are involved in 8 short contacts:

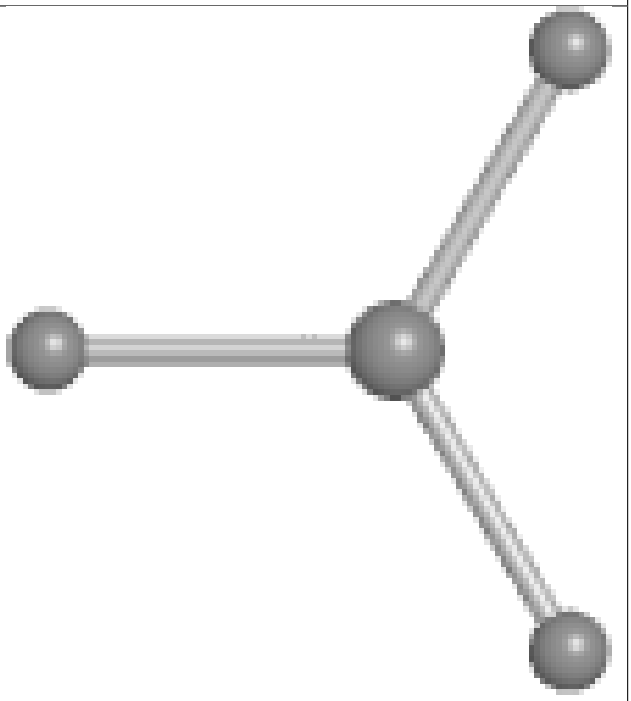
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	V	1202	BEF	3	0
9	V	1201	ADP	6	0

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

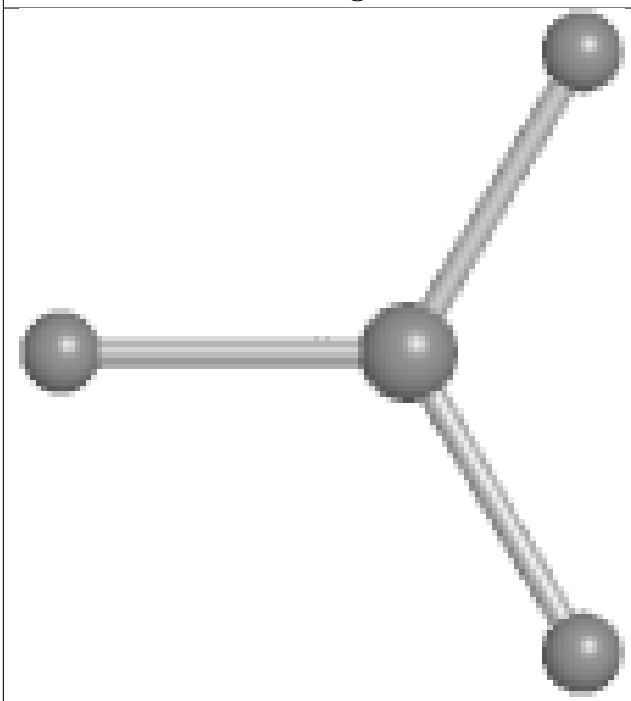
Ligand BEF V 1202



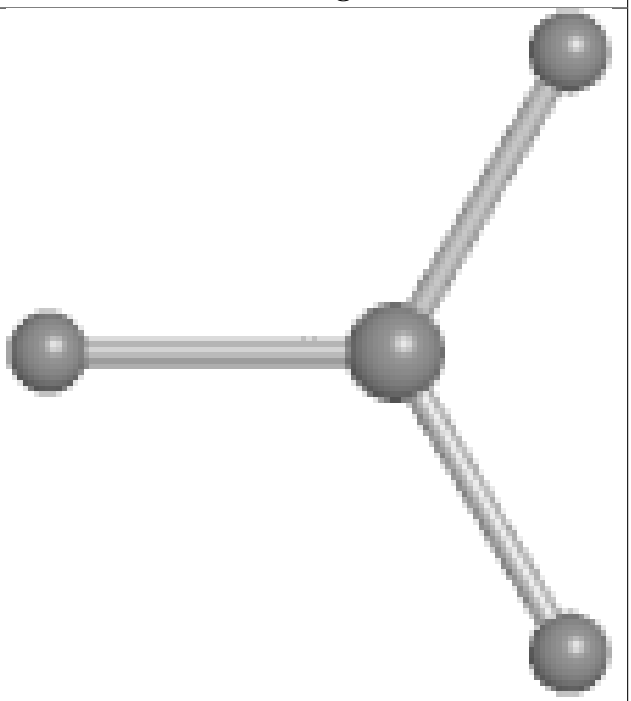
Bond lengths



Bond angles

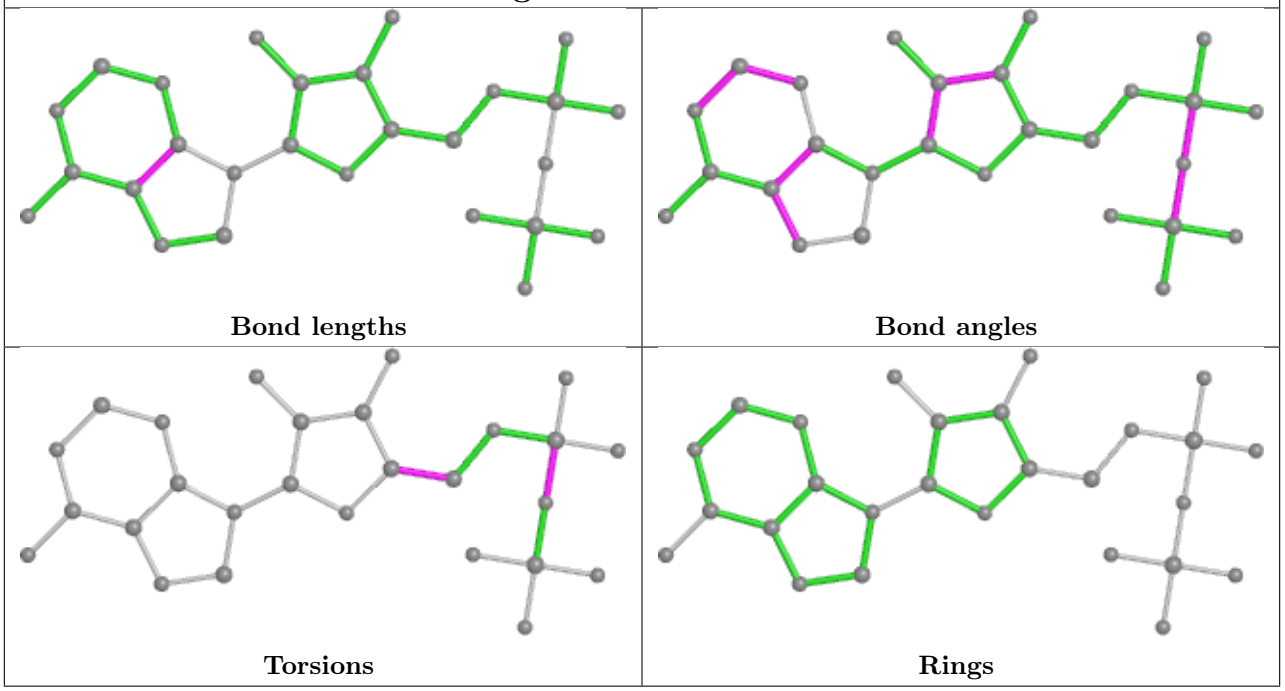


Torsions



Rings

Ligand ADP V 1201



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.

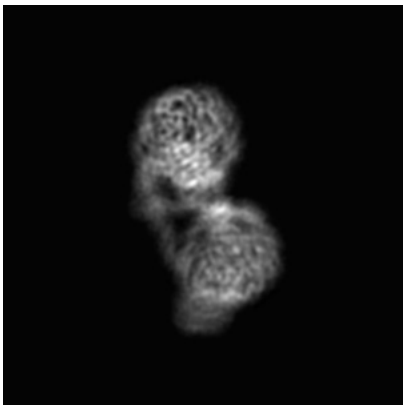
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32992. These allow visual inspection of the internal detail of the map and identification of artifacts.

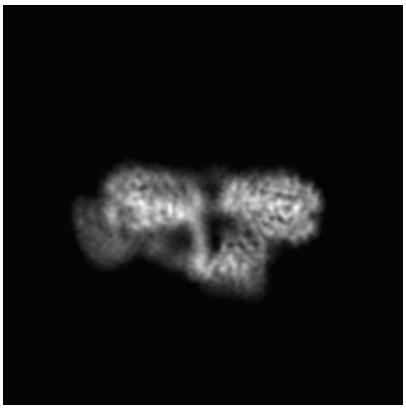
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

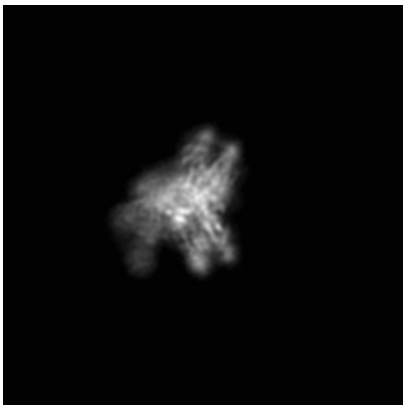
6.1.1 Primary map



X

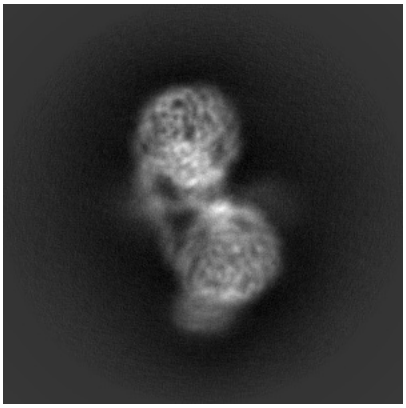


Y



Z

6.1.2 Raw map



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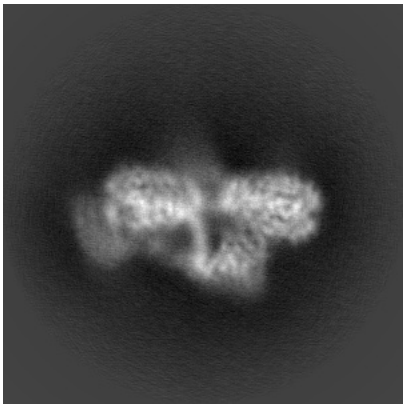
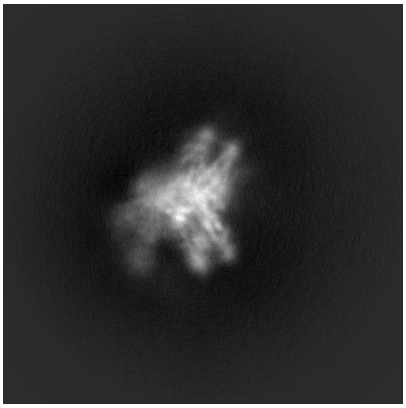


Y

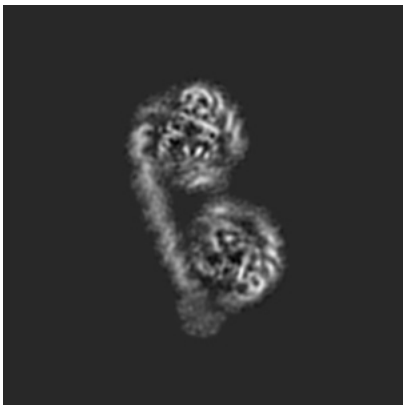


Z

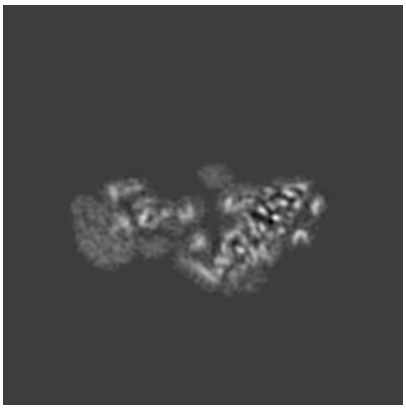
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

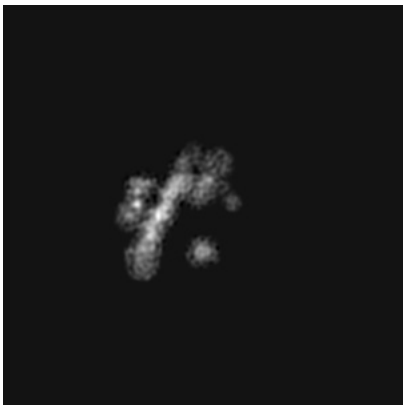
6.2.1 Primary map



X Index: 180

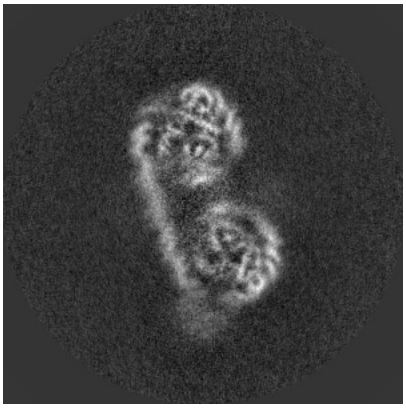


Y Index: 180

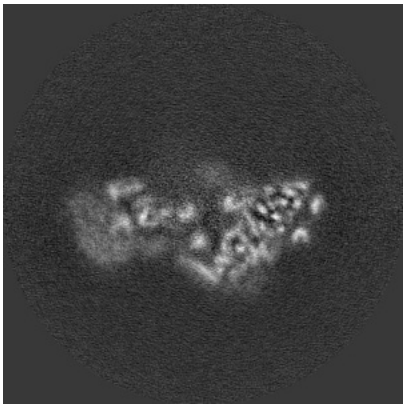


Z Index: 180

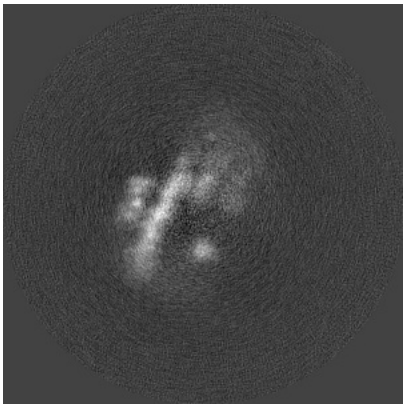
6.2.2 Raw map



X Index: 180



Y Index: 180

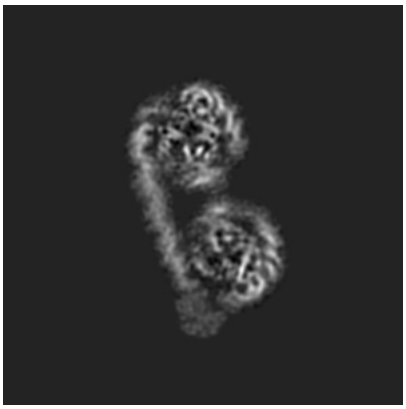


Z Index: 180

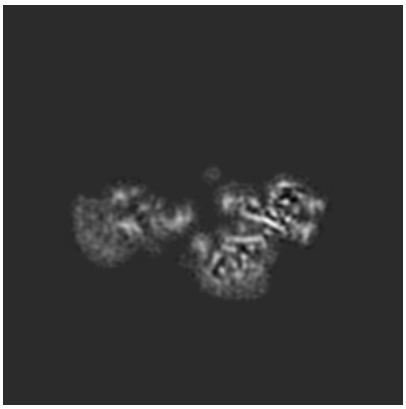
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

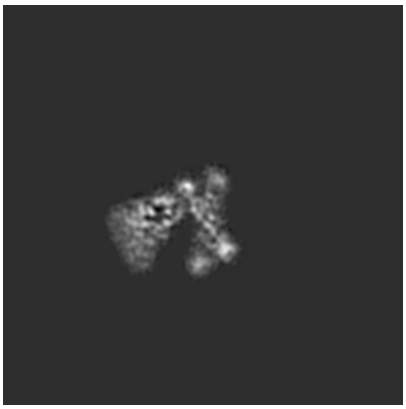
6.3.1 Primary map



X Index: 179

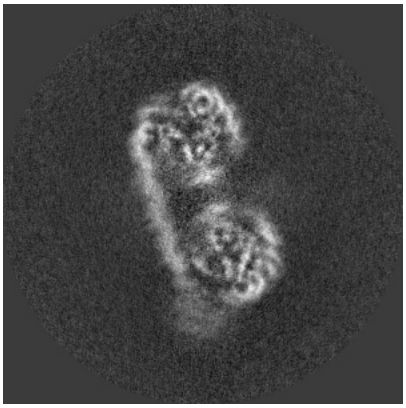


Y Index: 174

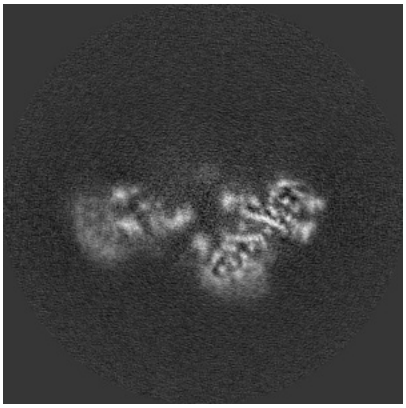


Z Index: 217

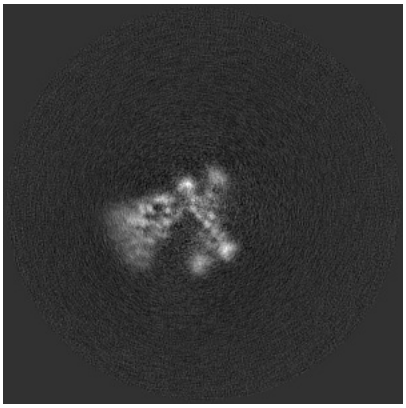
6.3.2 Raw map



X Index: 178



Y Index: 174

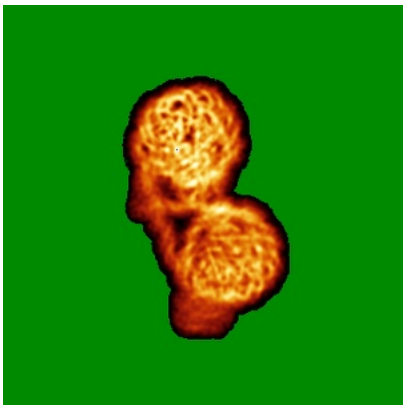


Z Index: 218

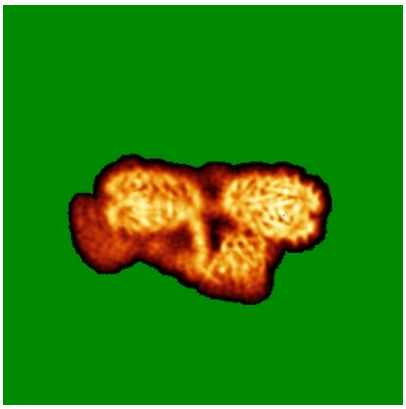
The images above show the largest variance slices of the map in three orthogonal directions.

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

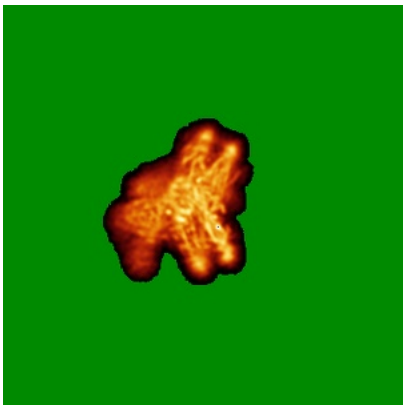
6.4.1 Primary map



X

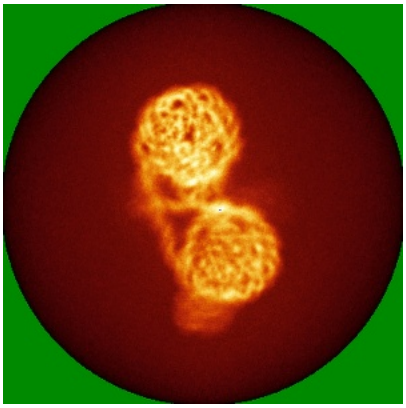


Y

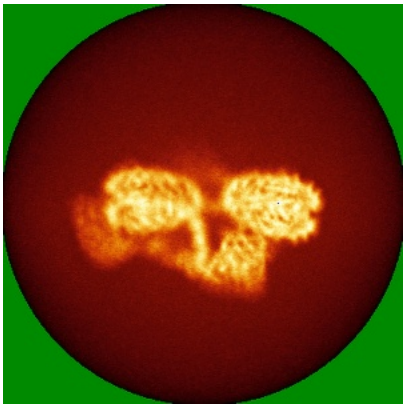


Z

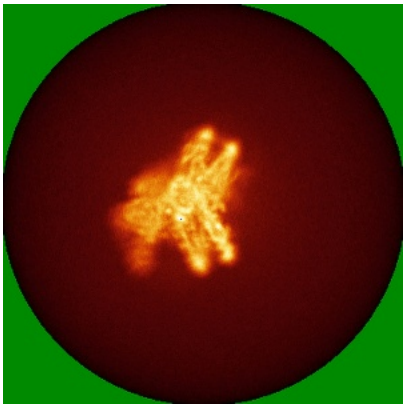
6.4.2 Raw map



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.

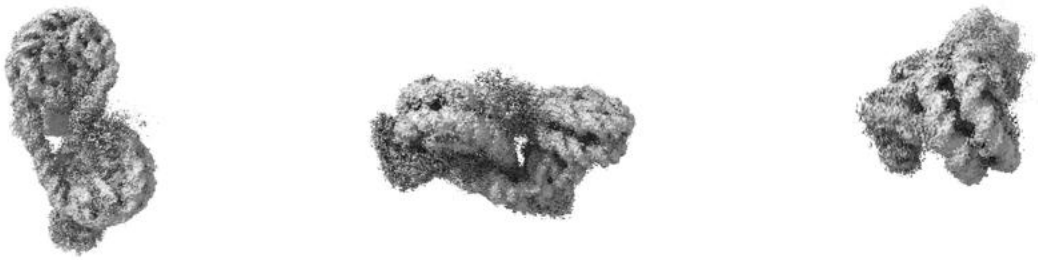
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0048. 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.

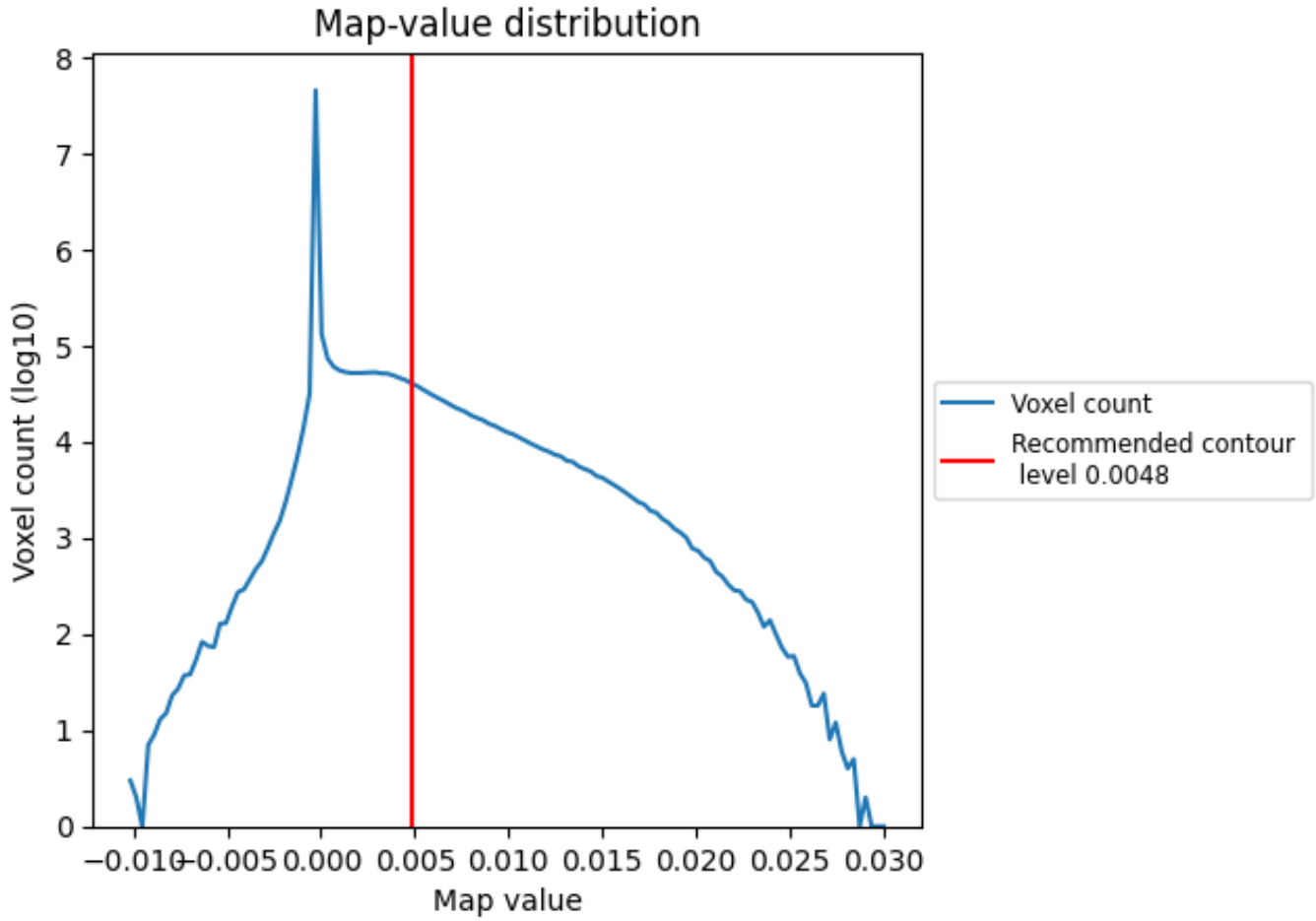
6.6 Mask visualisation (i)

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

7 Map analysis

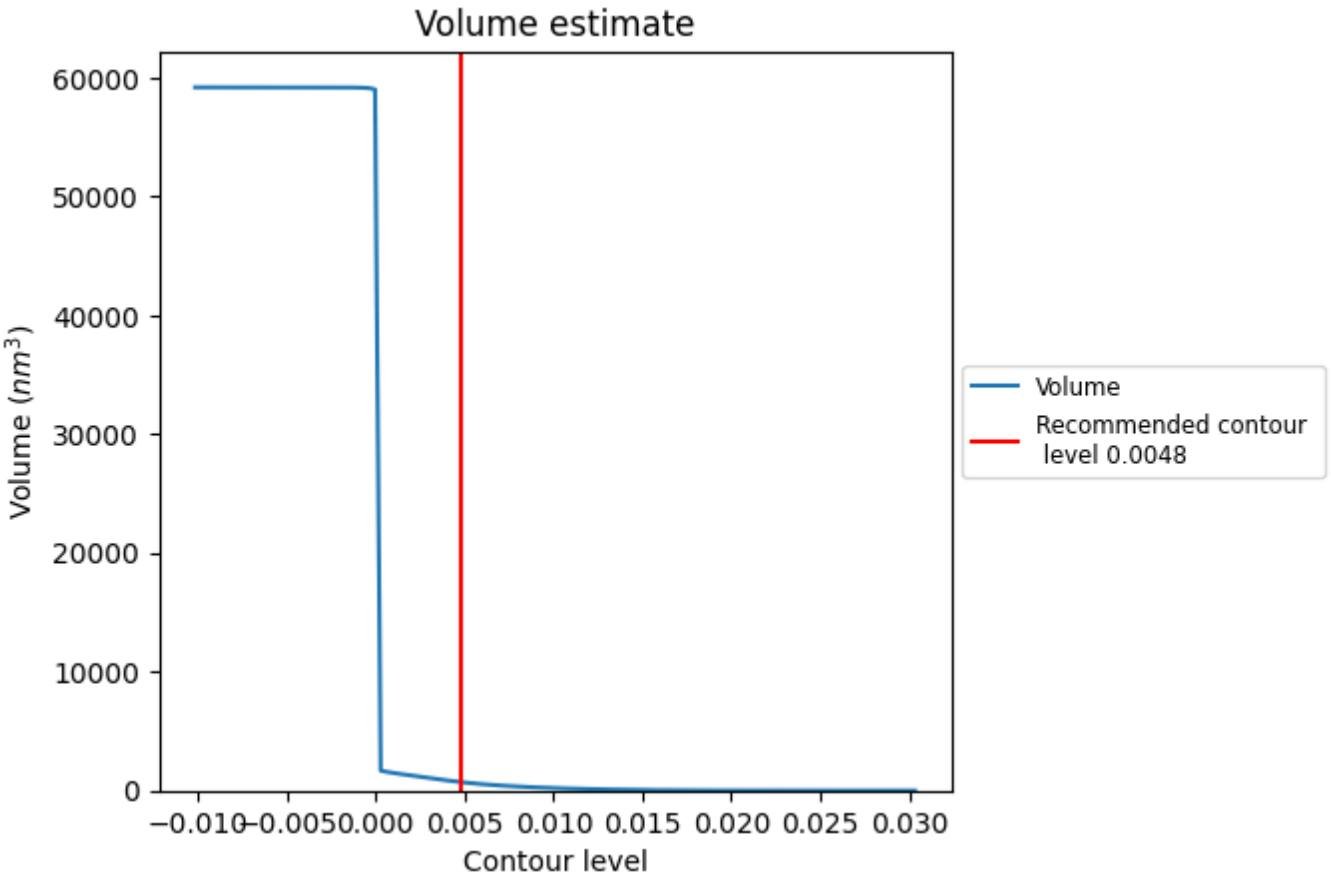
This section contains the results of statistical analysis of the map.

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.

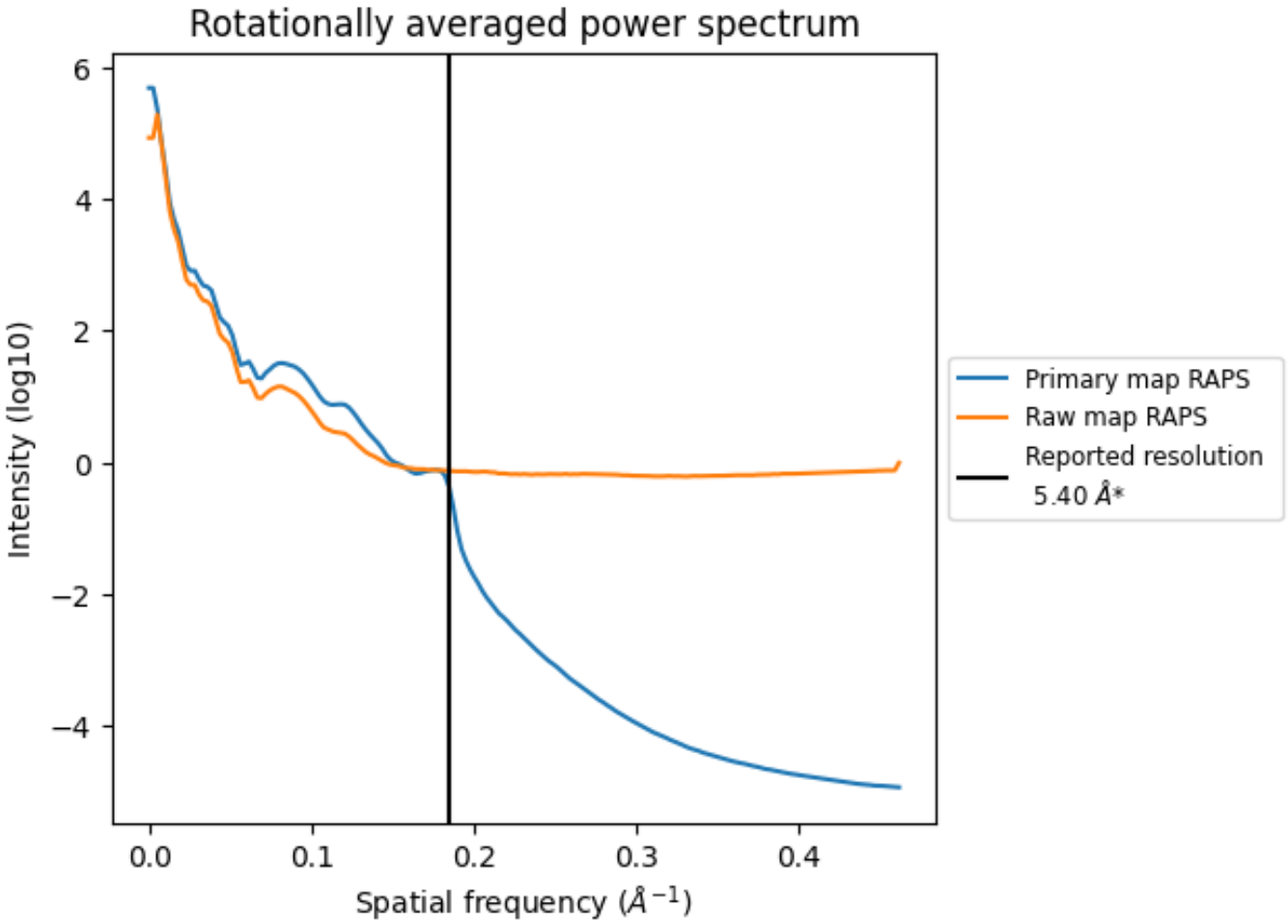
7.2 Volume estimate (i)



The volume at the recommended contour level is 711 nm^3; this corresponds to an approximate mass of 643 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)

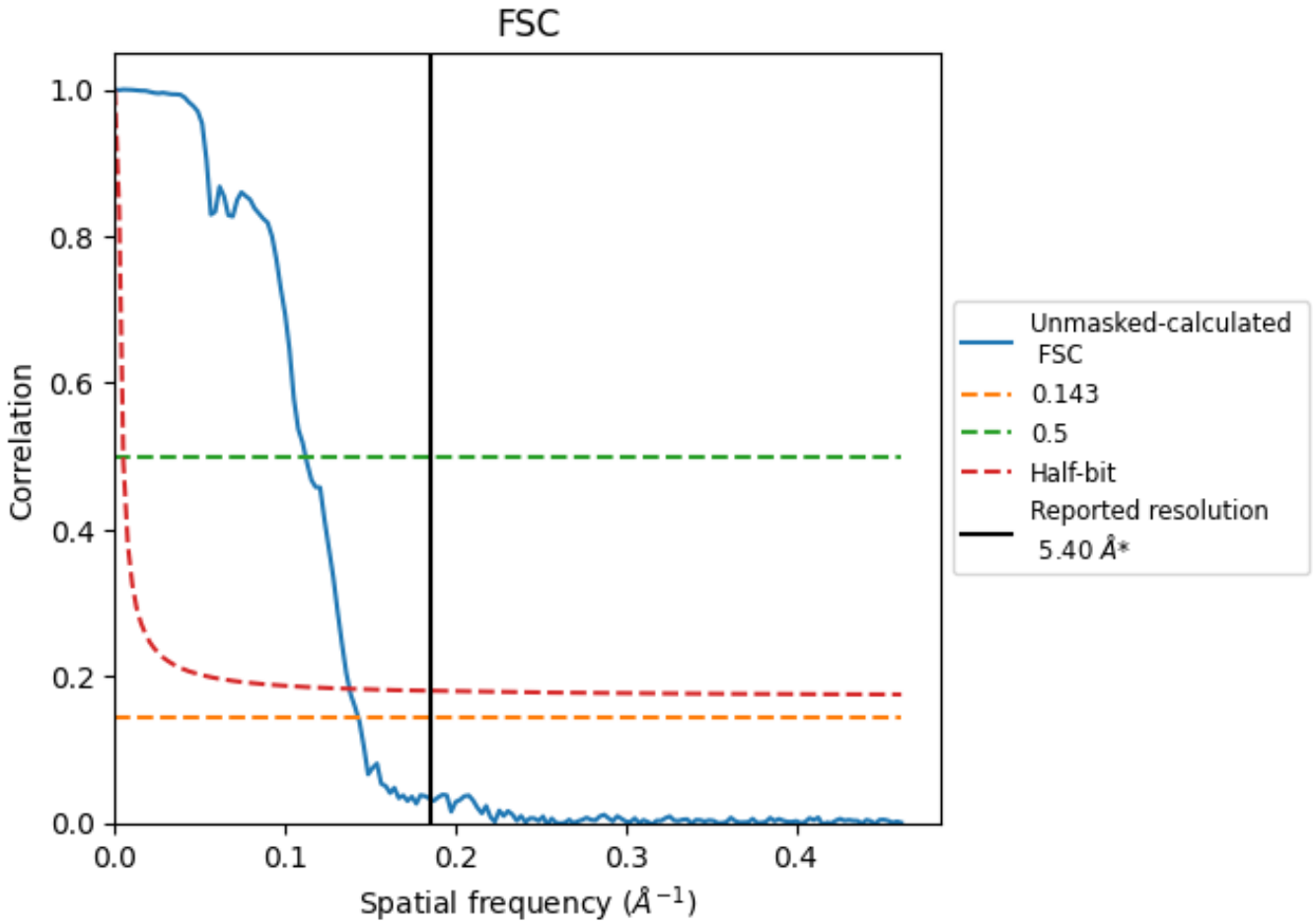


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

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 0.185 Å^{-1}

8.2 Resolution estimates (i)

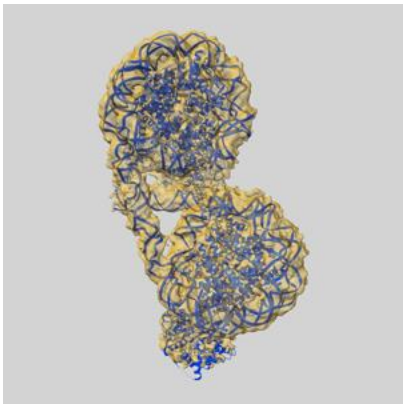
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.99	8.92	7.25

*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 6.99 differs from the reported value 5.4 by more than 10 %

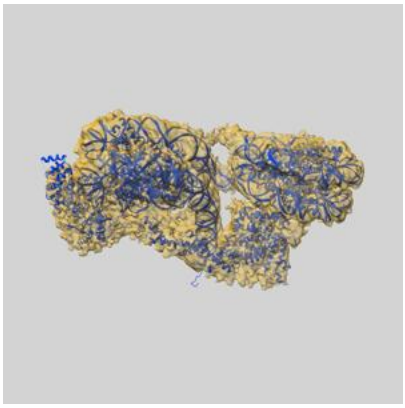
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32992 and PDB model 7X3T. Per-residue inclusion information can be found in section 3 on page 8.

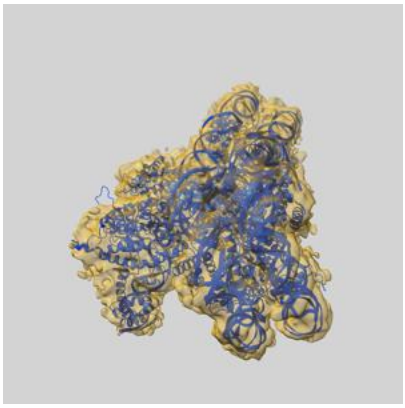
9.1 Map-model overlay



X



Y



Z

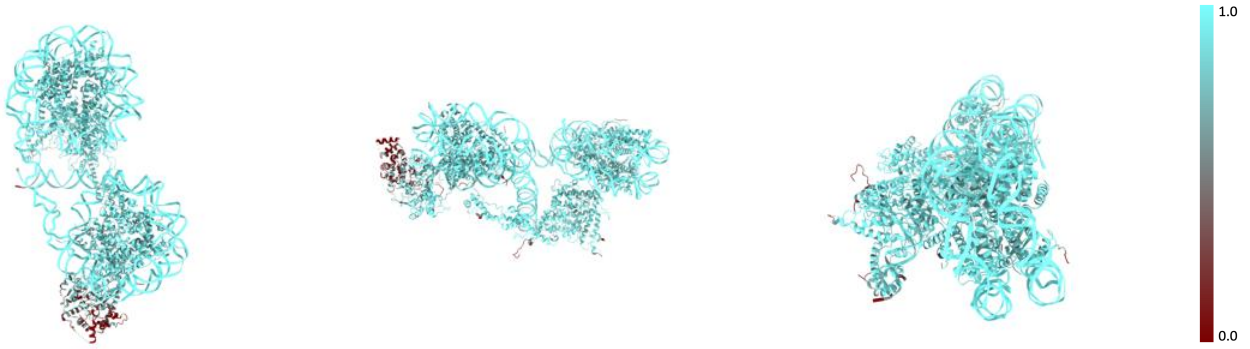
The images above show the 3D surface view of the map at the recommended contour level 0.0048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

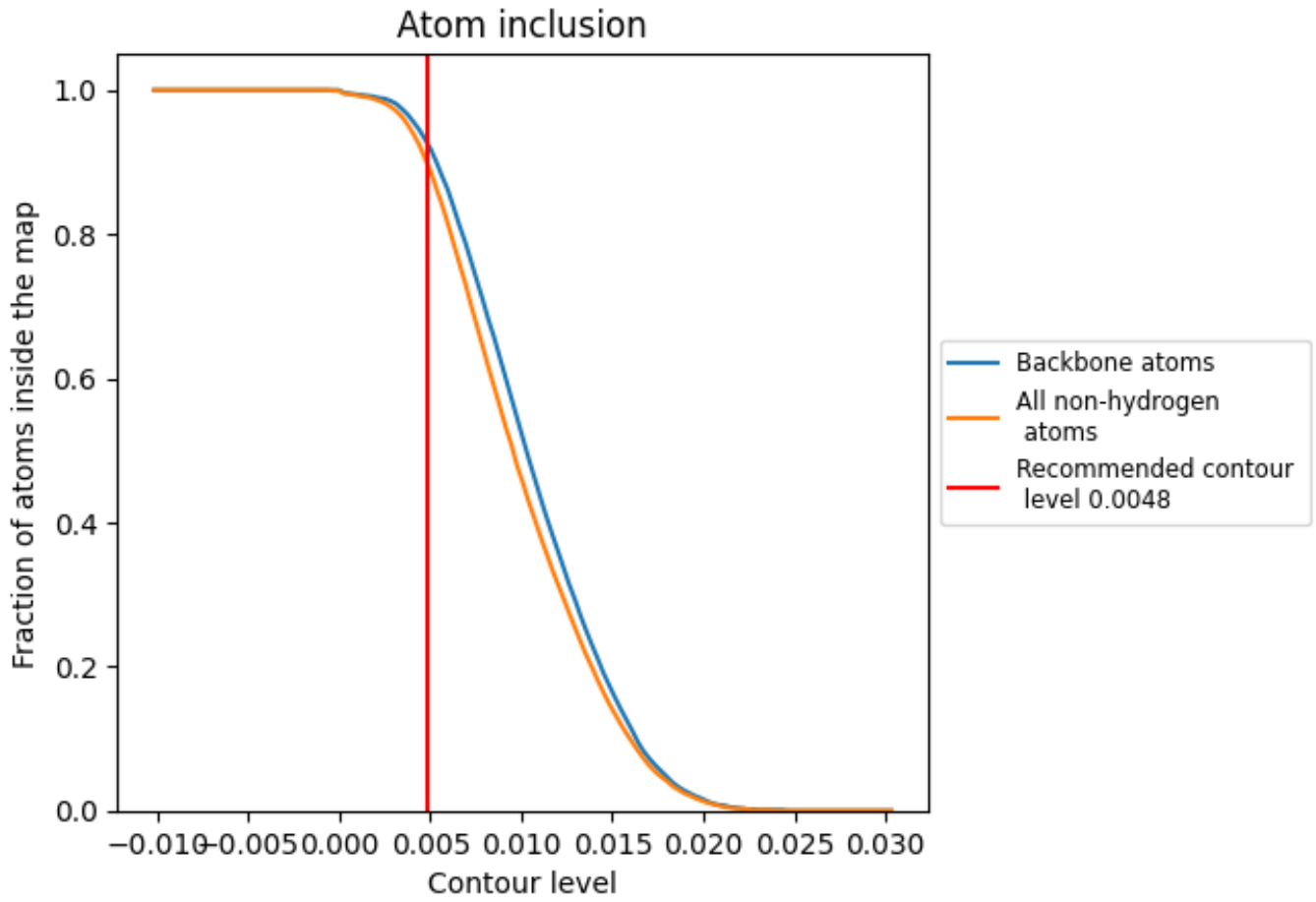
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0048).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.0048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.1920
A	0.9470	0.2150
B	0.9170	0.2360
C	0.9130	0.2480
D	0.9290	0.2540
E	0.9150	0.2110
F	0.8830	0.2310
G	0.9320	0.2430
H	0.9150	0.2410
I	0.9720	0.2000
J	0.9720	0.2020
K	0.8910	0.2100
L	0.8980	0.2230
M	0.8920	0.2070
N	0.9030	0.2150
O	0.9320	0.1900
P	0.9290	0.1870
Q	0.8920	0.2050
R	0.9360	0.2220
U	0.9200	0.1950
V	0.7080	0.1190