



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2025 – 05:45 PM EDT

PDB ID : 6WKR
EMDB ID : EMD-21707
Title : PRC2-AEBP2-JARID2 bound to H2AK119ub1 nucleosome
Authors : Kasinath, V.; Nogales, E.; Beck, C.; Sauer, P.; Poepsel, S.; Kosmatka, J.;
Faini, M.; Toso, D.; Aebersold, R.
Deposited on : 2020-04-16
Resolution : 3.50 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

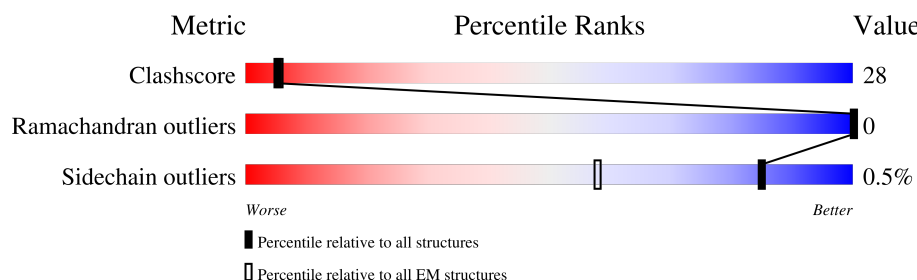
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	F	76	<div> <div>57%</div> <div>51%</div> <div>49%</div> </div>
1	T	76	<div> <div>84%</div> <div>55%</div> <div>45%</div> </div>
2	A	739	<div> <div>35%</div> <div>25%</div> <div>41%</div> </div>
3	L	441	<div> <div>41%</div> <div>41%</div> <div>18%</div> </div>
4	N	425	<div> <div>42%</div> <div>51%</div> <div>7%</div> </div>
5	C	746	<div> <div>53%</div> <div>28%</div> <div>19%</div> </div>
6	B	450	<div> <div>5%</div> <div>91%</div> </div>
6	E	450	<div> <div>6%</div> <div>7%</div> <div>92%</div> </div>

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Mol	Chain	Length	Quality of chain
7	P	295	
8	H	320	
9	I	136	
9	O	136	
10	J	103	
10	Q	103	
11	K	130	
11	R	130	
12	M	126	
12	S	126	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29296 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	76	Total	C	N	O	S	0	0
			604	379	105	118	2		
1	F	76	Total	C	N	O	S	0	0
			603	379	105	117	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	76	CYS	GLY	engineered mutation	UNP P0CG48
F	76	CYS	GLY	engineered mutation	UNP P0CG48

- Molecule 2 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	439	Total	C	N	O	S	0	0
			3340	2146	603	568	23		

- Molecule 3 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	362	Total	C	N	O	S	0	0
			2874	1822	503	528	21		

- Molecule 4 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	395	Total	C	N	O	S	0	0
			3080	1950	530	591	9		

- Molecule 5 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	606	Total	C	N	O	S	0	0
			4278	2684	779	777	38		

- Molecule 6 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	42	Total	C	N	O	S	0	0
			290	181	55	53	1		
6	E	35	Total	C	N	O		0	0
			203	125	39	39			

- Molecule 7 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	193	Total	C	N	O	S	0	0
			1346	853	260	228	5		

- Molecule 8 is a DNA chain called DNA (314-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	314	Total	C	N	O	P	0	0
			6439	3048	1191	1886	314		

- Molecule 9 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			935	586	183	163	3		
9	O	99	Total	C	N	O	S	0	0
			816	514	158	141	3		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
10	Q	87	Total	C	N	O	S	0	0
			667	419	129	118	1		

- Molecule 11 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	108	Total	C	N	O	S	0	0
			825	519	161	144	1		
11	R	108	Total	C	N	O	S	0	0
			829	522	162	144	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	99	ARG	GLY	conflict	UNP P06897
K	119	CYS	LYS	conflict	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897
R	119	CYS	LYS	conflict	UNP P06897

- Molecule 12 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	95	Total	C	N	O	S	0	0
			736	463	132	139	2		
12	S	96	Total	C	N	O	S	0	0
			741	466	133	140	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	29	THR	SER	engineered mutation	UNP P02281
S	29	THR	SER	engineered mutation	UNP P02281

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	

- Molecule 14 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total 26	C 14	N 6	O 5	S 1	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
15	P	1	Total Zn 1 1	0

THR	T358	PRO	G497	W591	LEU
F296	L359	ASN	N502	L592	GLU
A297	T362	ASN	R508	E594	GLY
Q298	GLY	ARG	Q509	T596	GLU
M299	GLU	GLN	P510	I597	SER
T300	THR	LYS	G511	T598	ALA
V301	ASN	L426	F512	F603	ALA
F302	ASP	R427	R516	V606	PRO
D303	LYS	I428	K521	N607	ASN
	SER	F429	R522	E610	GLU
R307	THR	Y430	I525	K611	GLU
L308	ALA	Q431	T526	W617	GLN
Q309	PRO	F432	L529	M618	ASN
L310	ILE		V530	L619	ASN
L311	ALA	R439	M540	H620	THR
E314	PRO	Q440	F643	V621	ALA
Y315	LEU	Q441	L544		THR
	LEU	T442	GLU		ASN
A318	THR	E443	VAL		GLY
M319	ARG	A444	GLN		LYS
Q320	ASN	R445	ARG	K650	GLU
K321	SER			L651	ALA
E322	SER			C653	LEU
GLU	GLU	C450	F543		GLU
GLU	SER		L544	F656	THR
CYS	HIS	L455	SER	M657	ASP
PRO	GLN	N456	GLU	L660	SER
ILE	GLU	C457	ASP	V661	VAL
SER	ASN	R458	GLY	S662	GLY
LYS	ASN	K459	VAL	M663	VAL
LYS	PRO	L464	GLU	H664	SER
ARG	GLY		GLN	D665	GLN
ALA	SER	K468	ARG	I674	SER
THR	VAL			D675	LYS
TRP	LYS	H471	T556	K676	LYS
GLU	PRO	S472	N562	A677	GLN
THR	THR	R473		V678	LYS
ILE	GLN	F474	Y565	T679	LEU
LEU	THR	I475	F566	K680	
ASP	ILE	F476		L681	
GLY	ALA	R477	D569		
LYS	VAL	Y477	C571		
ARG	LYS	V479	L572		
LEU	ARG	H481			
PRO	SER	P482	P576		
PRO	LEU	K483	Q577		
PHE	THR	G484	E578		
THR	GLU	A485	M579		
PHE	LEU	R486			
GLN	GLN		S583		
SER	THR	S490	E586		
Q351	ARG	T491			
G352	LYS	M492			
T354	GLU	E493			
L355	LYS	C494			
Q356	ASP	Y495			
F357	THR	D496			

• Molecule 3: Polycomb protein EED

Chain L:  41% 41% 18%

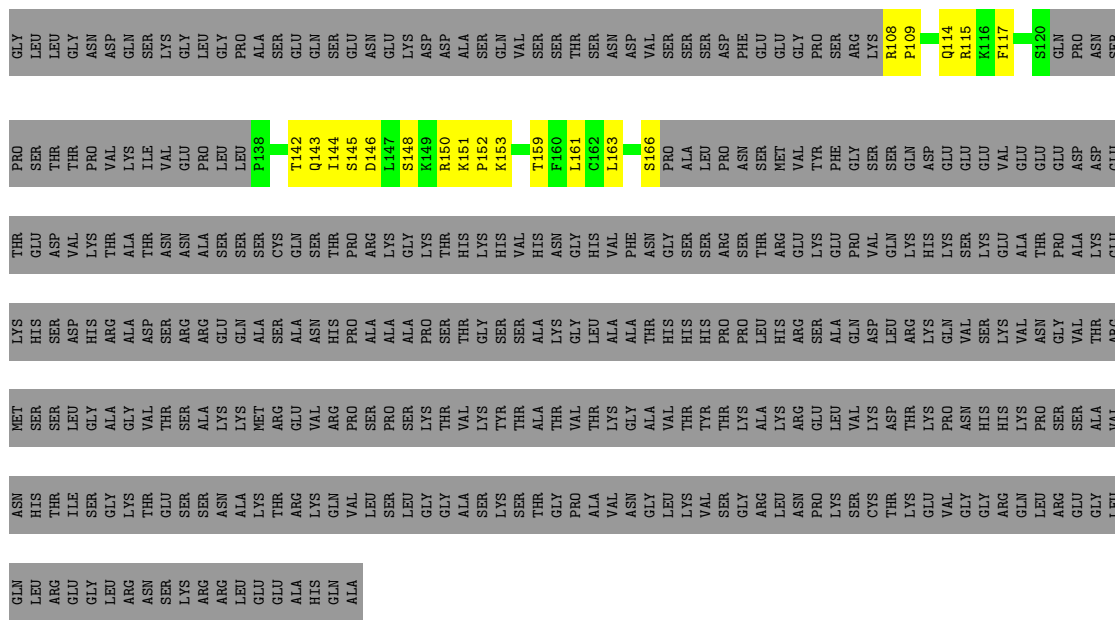
W389	D390	L391	D395	P396	A399	K400	C401	T402	T403	L404	T405	H406	K407	C408	G409	G410	T413	F418	S419	R420	D421	S422	S423	I424	L425	I426	A427	V428	D431	A432	S433	W434	W435	R436	W437	D438	R439	L440	R441																			
R313	W314	L315	D317	L318	I319	L320	S323	C324	E325	M326	A327	I328	W331	K332	P333	K334	K335	M336	E337	D338	D339	I340	S341	S342	E347	S348	R349	V350	T351	F356	D357	Y358	W359	W364	F368	S369	M370	F371	F372	W373	Q374	K375	M376	L379	G380	N381	Q382	V383	G384	K385								
T220	Q221	T222	D223	T224	L225	V226	F229	G230	G231	V232	R236	D243	Y244	D245	L246	L247	G248	E249	K250	C254	K268	R269	M270	M271	I274	K275	E276	S277	Y278	S291	Q292	H295	F296	P297	S300	T301	R302	H305	R306	N307	Y308	V309	D310	C311	V312													
L134	L135	Q136	S137	Y138	T149	C150	A151	W152	T153	Y154	S159	L162	L163	A166	T172	I175	K176	M180	Q181	L182	W183	K184	H185	Y186	V187	G188	H189	G190	N191	A192	I193	N194	E195	F198	H199	N204	L205	G117	S118	L206	L207	S208	V209	S210	K211	D212	H213	A214	L215	R216	N219							
ASN	ALA	PRO	GLY	ARG	LYS	SER	THR	TRP	GLY	LYS	LYS	LYS	LYS	ALA	ALA	CYS	LYS	Y80	S81	K83	C84	V85	N86	S87	L88	K89	E90	N93	L96	Q100	W103	H104	L111	V112	F113	A114	T115	V116	S118	N119	R120	V121	T122	L123	Y124	E125	C126	G130	R133									
MET	SER	GLU	ARG	GLY	VAL	SER	THR	THR	ALA	PRO	ALA	GLY	ALA	ALA	GLY	GLY	LYS	GLN	LYS	LEU	SER	GLY	ASP	GLU	ASN	ASN	ASN	ASP	LEU	SER	SER	GLY	ASP	GLU	ASN	ASP	ASP	ALA	ALA	VAL	SER	ILE	GLU	SER	GLY	THR	ASN	THR	GLU	ARG	PRO	ASP	THR	PRO	THR	ASN	THR	PRO

• Molecule 4: Histone-binding protein RBBP4

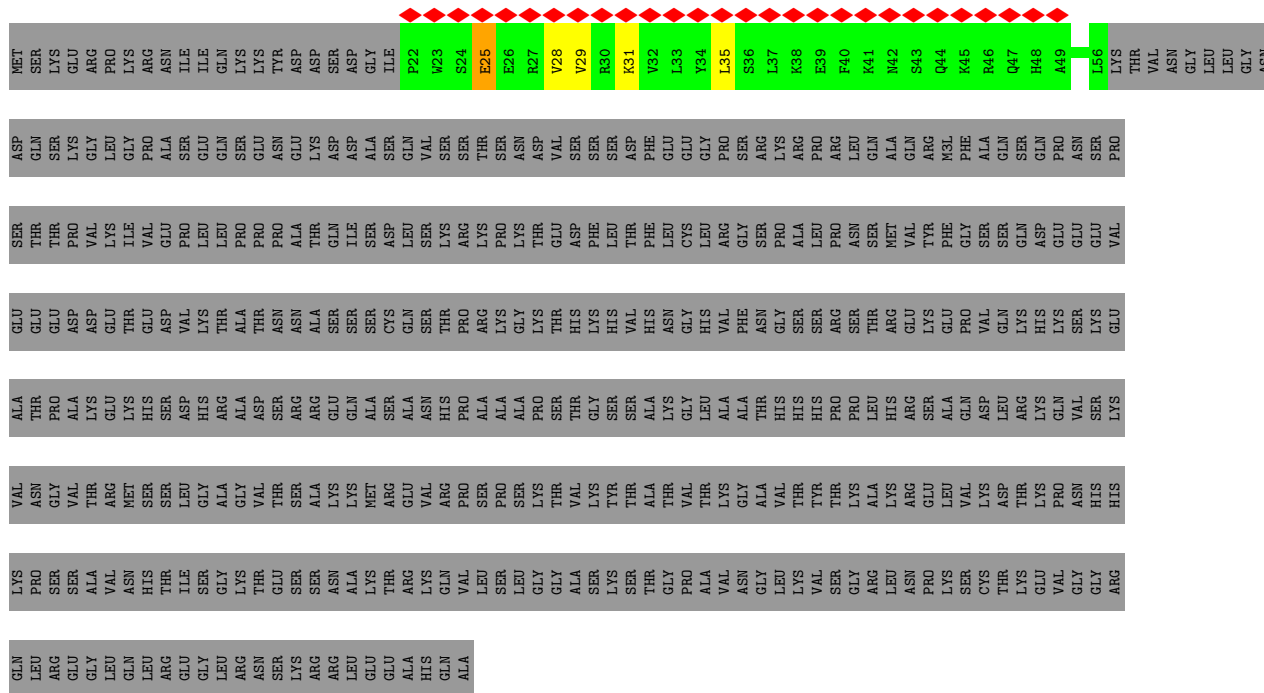
Chain N:  42% 51% 7%

MET	ALA	ASP	K4	D10	E13	E14	R15	E19	K22	K25	T28	L31	Y32	D33	L34	V35	H38	A39	L40	E41	W42	P43	S44	T46	A47	Q48	W49	L50	P51	D52	R55	P56	E57	G58	K59	F60	F61	S62	I63	H64	R65	L66	V67	L68	G69	T70	H71	T72	S73
D74	E75	Q76	N77	V80	I81	P87	N88	D89	A91	Q92	F93	ALA	SER	HIS	TYR	ASP	GLU	GLY	GLU	PHE	G106	G107	F108	E118	I119	N122	H123	E126	R129	A130	R131	Y132	M133	P134	Q135	N136	P137	C138	I139	I140	A141	T142	K143	T144	P145	D153	H154		



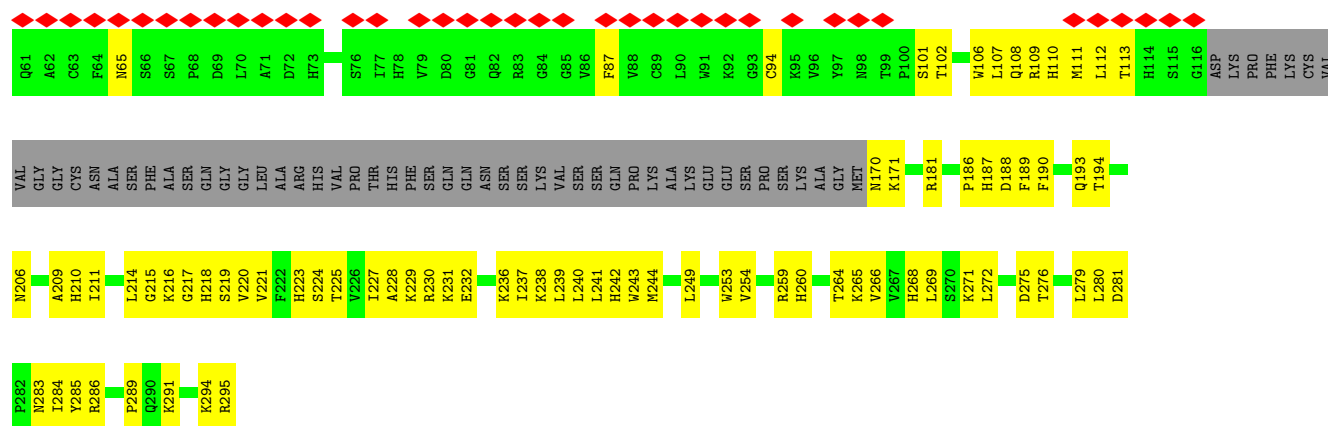


- Molecule 6: Protein Jumonji



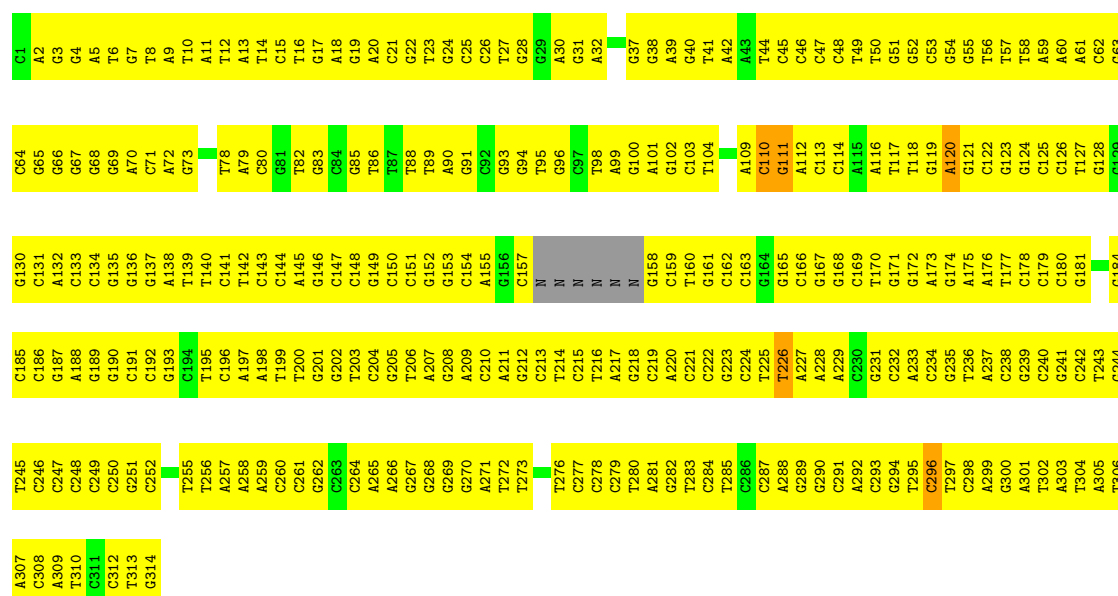
- Molecule 7: Zinc finger protein AEBP2





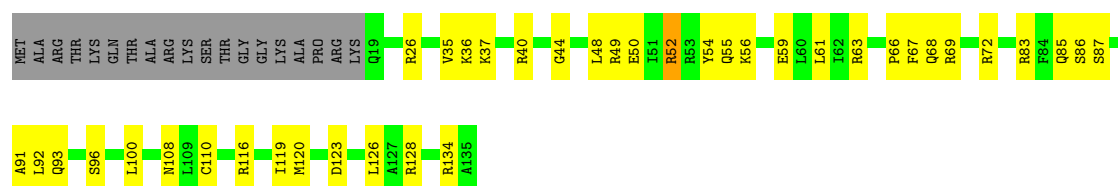
• Molecule 8: DNA (314-MER)

Chain H: 11% 86% . .



• Molecule 9: Histone H3.2

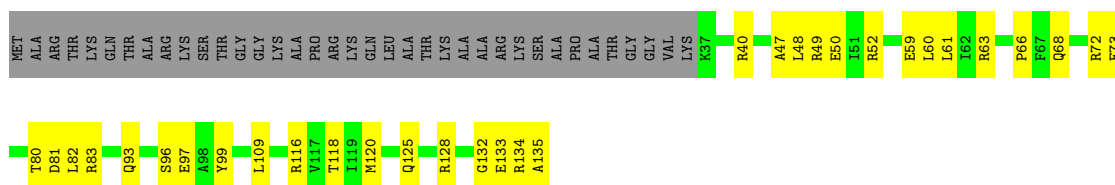
Chain I: 57% 28% 14%



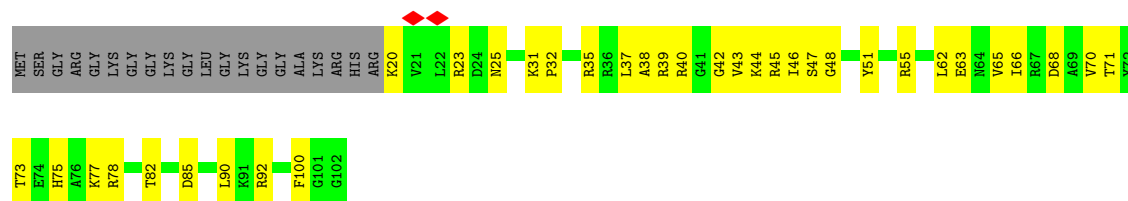
• Molecule 9: Histone H3.2

Chain O: 49% 24% 27%

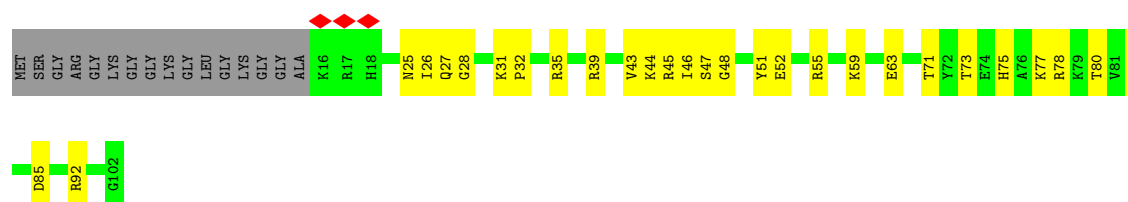




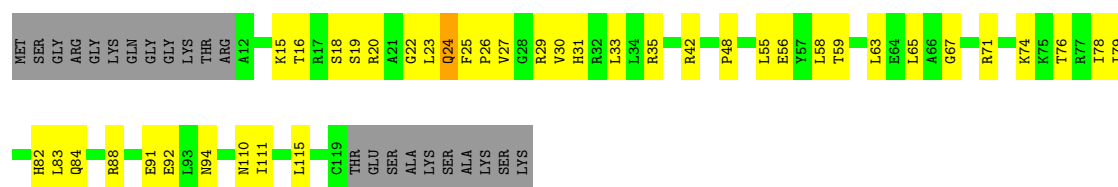
- Molecule 10: Histone H4



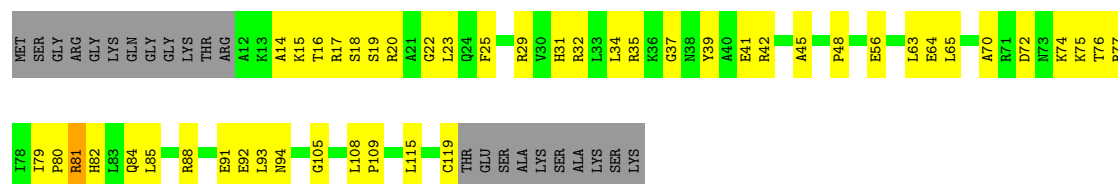
- Molecule 10: Histone H4



- Molecule 11: Histone H2A type 1

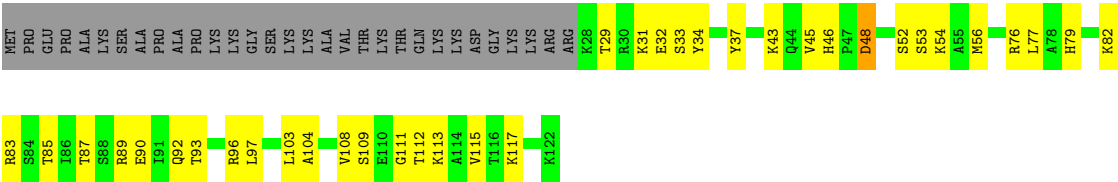


- Molecule 11: Histone H2A type 1



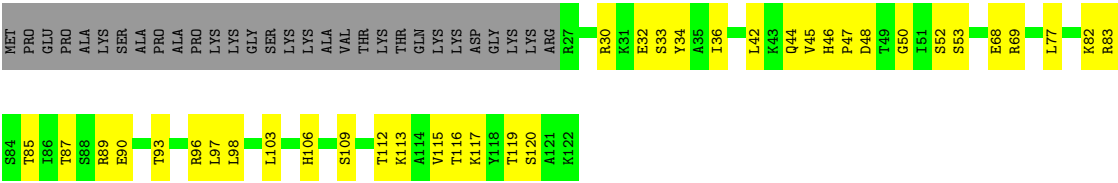
- Molecule 12: Histone H2B 1.1

Chain M: 47% 28% 25%



● Molecule 12: Histone H2B 1.1

Chain S: 47% 29% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	168601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	441.2928, 441.2928, 441.2928	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1492, 1.1492, 1.1492	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, MG, SAH, ZN

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	F	0.25	0/609	0.47	0/819
1	T	0.25	0/610	0.50	0/819
2	A	0.37	0/3419	0.47	0/4636
3	L	0.44	0/2948	0.53	0/4004
4	N	0.37	0/3165	0.50	0/4322
5	C	0.43	0/4375	0.48	0/5964
6	B	0.31	0/282	0.54	0/382
6	E	0.45	0/203	0.57	0/277
7	P	0.32	0/1376	0.49	0/1879
8	H	1.26	0/7222	1.04	6/11143 (0.1%)
9	I	0.62	0/948	0.58	0/1270
9	O	0.61	0/828	0.57	0/1109
10	J	0.75	0/669	0.61	0/894
10	Q	0.73	0/674	0.60	0/904
11	K	0.63	0/835	0.63	1/1128 (0.1%)
11	R	0.67	0/839	0.61	0/1132
12	M	0.68	0/747	0.56	0/1007
12	S	0.71	0/752	0.58	0/1014
All	All	0.74	0/30501	0.69	7/42703 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	296	DC	O4'-C4'-C3'	-7.22	101.61	104.50
8	H	110	DC	O4'-C4'-C3'	-6.96	101.72	104.50
8	H	120	DA	O4'-C4'-C3'	-5.74	102.20	104.50
11	K	24	GLN	C-N-CA	-5.37	108.28	121.70
8	H	111	DG	O4'-C4'-C3'	-5.31	102.37	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	603	0	631	29	0
1	T	604	0	631	29	0
2	A	3340	0	3106	169	0
3	L	2874	0	2735	143	0
4	N	3080	0	2895	226	0
5	C	4278	0	3675	176	0
6	B	290	0	271	19	0
6	E	203	0	154	6	0
7	P	1346	0	1188	77	0
8	H	6439	0	3521	472	0
9	I	935	0	984	43	0
9	O	816	0	856	33	0
10	J	662	0	709	38	0
10	Q	667	0	679	23	0
11	K	825	0	876	45	0
11	R	829	0	887	47	0
12	M	736	0	751	39	0
12	S	741	0	753	36	0
13	A	1	0	0	0	0
14	C	26	0	19	3	0
15	P	1	0	0	0	0
All	All	29296	0	25321	1495	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 28.

The worst 5 of 1495 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:103:DC:O2	8:H:212:DG:N2	1.92	1.02
8:H:110:DC:O2	8:H:205:DG:N2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:DC:O2	8:H:161:DG:N2	1.96	0.98
8:H:53:DC:O2	8:H:262:DG:N2	1.98	0.97
8:H:110:DC:N3	8:H:205:DG:N1	2.13	0.96

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	F	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
1	T	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	A	423/739 (57%)	378 (89%)	45 (11%)	0	100	100
3	L	360/441 (82%)	317 (88%)	43 (12%)	0	100	100
4	N	391/425 (92%)	348 (89%)	43 (11%)	0	100	100
5	C	600/746 (80%)	515 (86%)	85 (14%)	0	100	100
6	B	37/450 (8%)	27 (73%)	10 (27%)	0	100	100
6	E	33/450 (7%)	30 (91%)	3 (9%)	0	100	100
7	P	189/295 (64%)	163 (86%)	26 (14%)	0	100	100
9	I	115/136 (85%)	107 (93%)	8 (7%)	0	100	100
9	O	97/136 (71%)	85 (88%)	12 (12%)	0	100	100
10	J	81/103 (79%)	66 (82%)	15 (18%)	0	100	100
10	Q	85/103 (82%)	74 (87%)	11 (13%)	0	100	100
11	K	106/130 (82%)	99 (93%)	7 (7%)	0	100	100
11	R	106/130 (82%)	98 (92%)	8 (8%)	0	100	100
12	M	93/126 (74%)	81 (87%)	12 (13%)	0	100	100
12	S	94/126 (75%)	81 (86%)	13 (14%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2958/4688 (63%)	2612 (88%)	346 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	69/69 (100%)	69 (100%)	0	100	100
1	T	69/69 (100%)	69 (100%)	0	100	100
2	A	326/646 (50%)	326 (100%)	0	100	100
3	L	309/392 (79%)	309 (100%)	0	100	100
4	N	332/375 (88%)	332 (100%)	0	100	100
5	C	373/667 (56%)	369 (99%)	4 (1%)	70	83
6	B	25/387 (6%)	25 (100%)	0	100	100
6	E	11/387 (3%)	9 (82%)	2 (18%)	1	7
7	P	111/263 (42%)	111 (100%)	0	100	100
9	I	96/111 (86%)	95 (99%)	1 (1%)	73	84
9	O	86/111 (78%)	86 (100%)	0	100	100
10	J	68/79 (86%)	67 (98%)	1 (2%)	60	77
10	Q	64/79 (81%)	63 (98%)	1 (2%)	58	76
11	K	84/101 (83%)	84 (100%)	0	100	100
11	R	85/101 (84%)	84 (99%)	1 (1%)	67	82
12	M	79/106 (74%)	78 (99%)	1 (1%)	65	81
12	S	79/106 (74%)	79 (100%)	0	100	100
All	All	2266/4049 (56%)	2255 (100%)	11 (0%)	85	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	Q	78	ARG
11	R	81	ARG
6	E	29	VAL
6	E	25	GLU
9	I	52	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	273	GLN
9	I	68	GLN
1	F	25	ASN
5	C	507	GLN
7	P	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
6	M3L	B	116	6	10,11,12	0.53	0	9,14,16	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	M3L	B	116	6	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
14	SAH	C	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.89	3 (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
14	SAH	C	801	-	-	8/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	801	SAH	C2-N3	3.77	1.37	1.32
14	C	801	SAH	OXT-C	-2.40	1.23	1.30
14	C	801	SAH	C2-N1	2.17	1.37	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	801	SAH	N3-C2-N1	-5.83	120.76	128.67
14	C	801	SAH	C5'-SD-CG	-4.13	89.99	102.26
14	C	801	SAH	OXT-C-O	-2.66	118.05	124.08

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

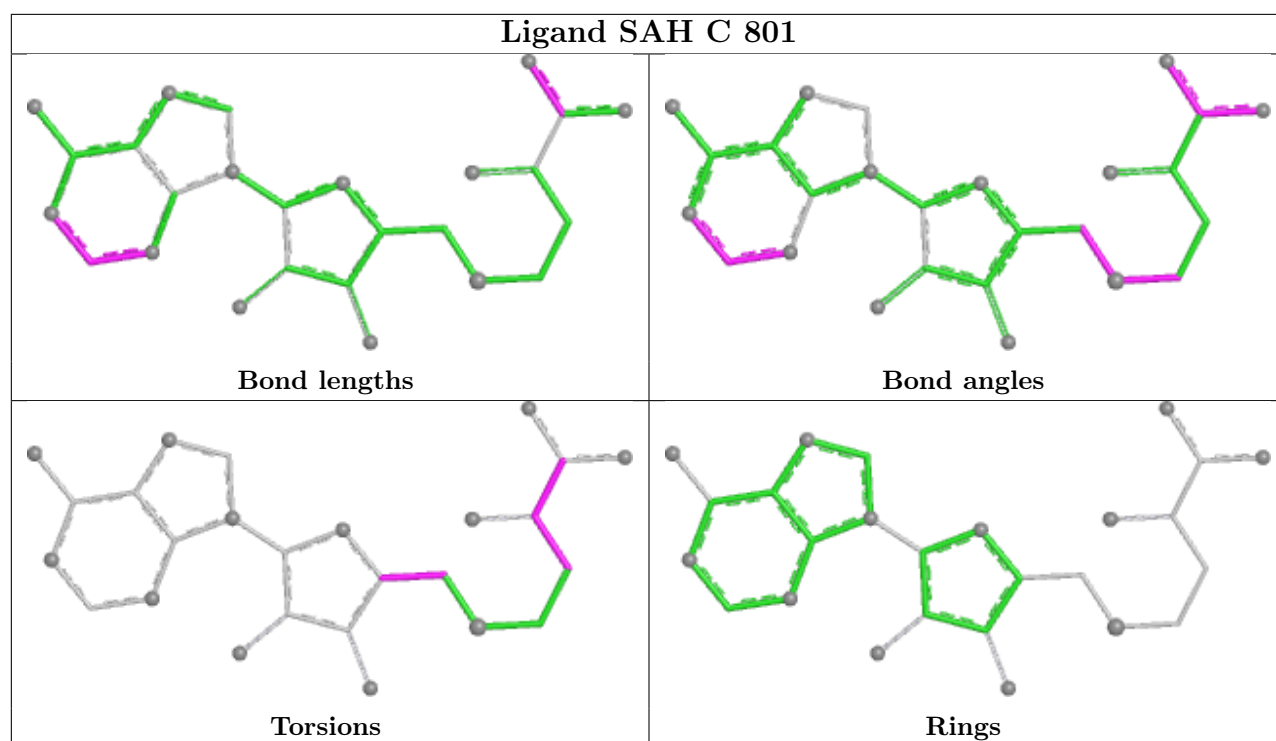
Mol	Chain	Res	Type	Atoms
14	C	801	SAH	N-CA-CB-CG
14	C	801	SAH	O-C-CA-N
14	C	801	SAH	OXT-C-CA-N
14	C	801	SAH	C-CA-CB-CG
14	C	801	SAH	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	801	SAH	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

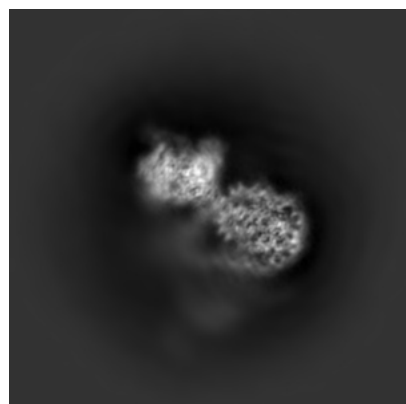
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21707. These allow visual inspection of the internal detail of the map and identification of artifacts.

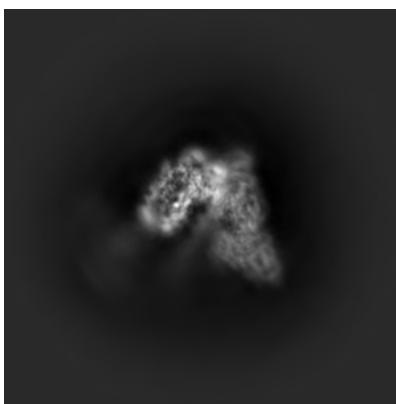
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

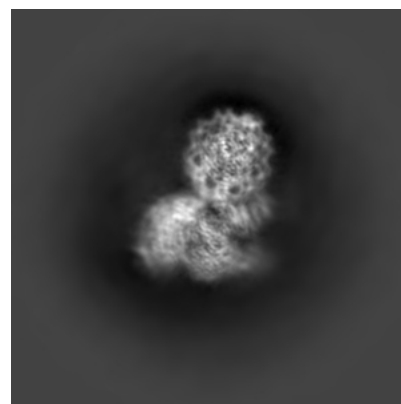
6.1.1 Primary map



X

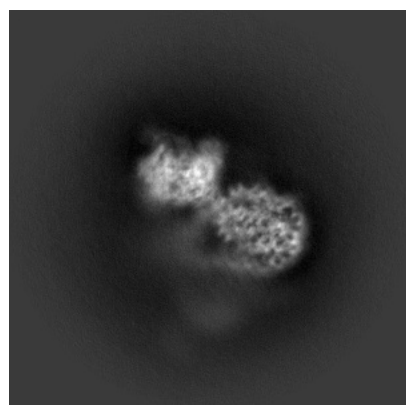


Y

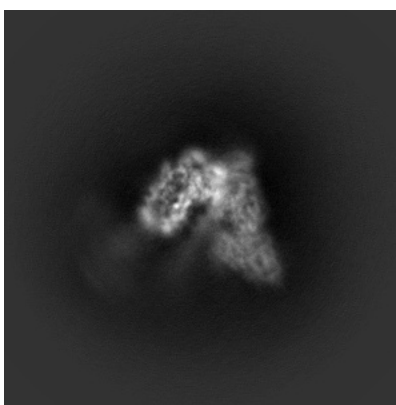


Z

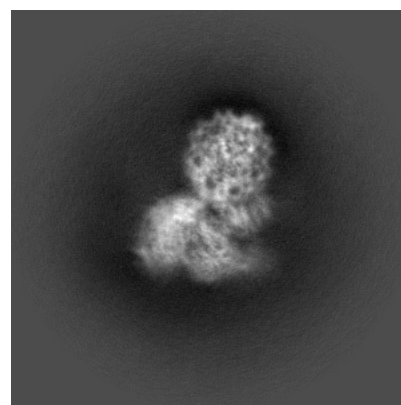
6.1.2 Raw map



X



Y

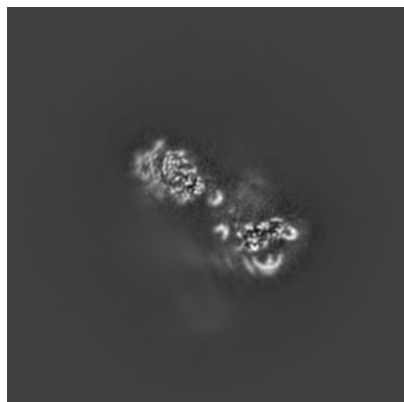


Z

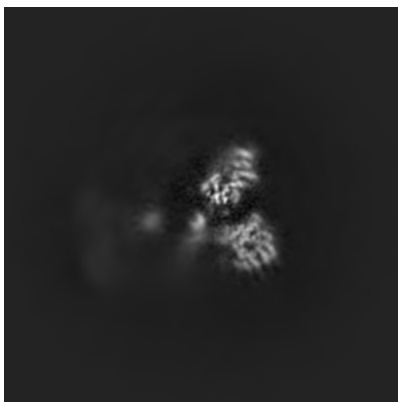
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

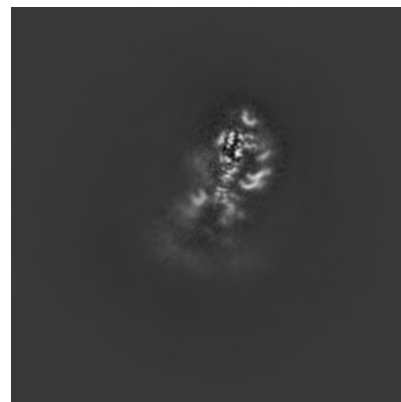
6.2.1 Primary map



X Index: 192

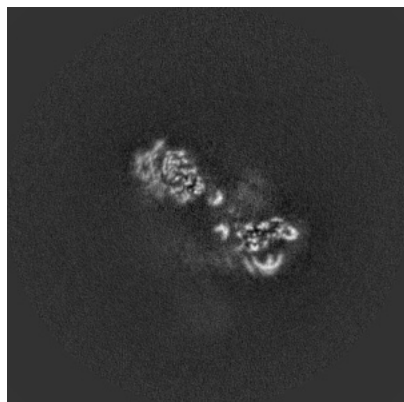


Y Index: 192

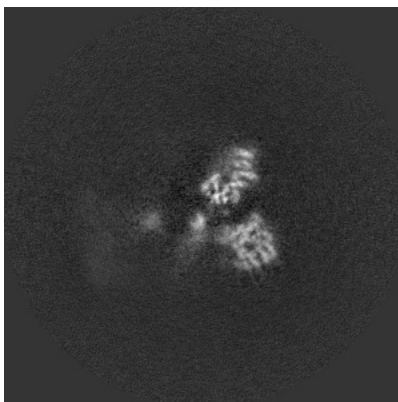


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

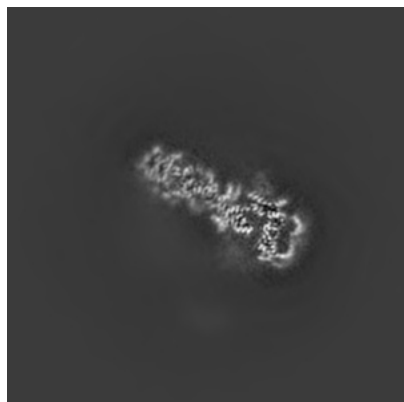


Z Index: 192

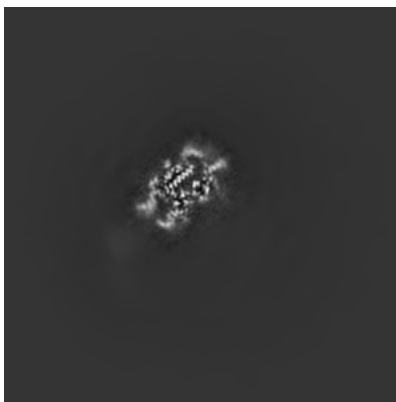
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

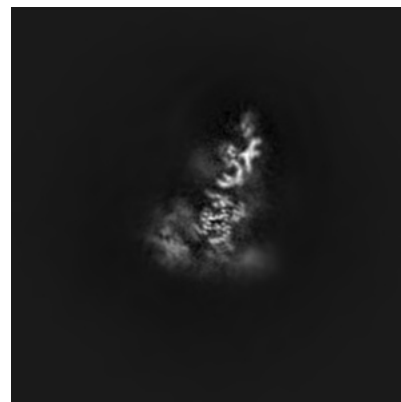
6.3.1 Primary map



X Index: 205

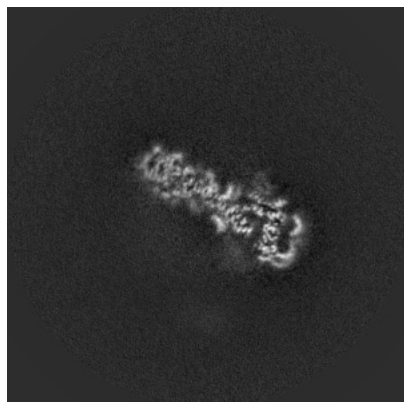


Y Index: 252

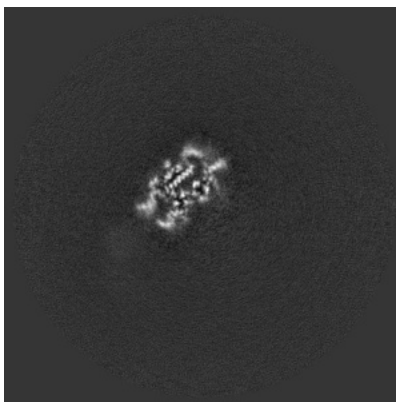


Z Index: 206

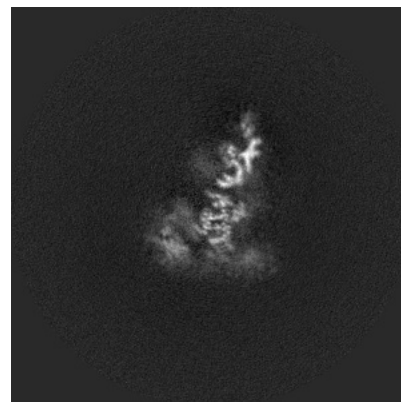
6.3.2 Raw map



X Index: 204



Y Index: 252

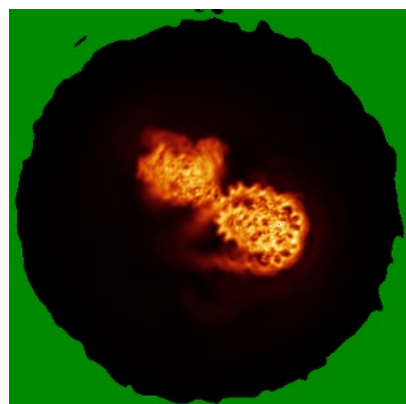


Z Index: 206

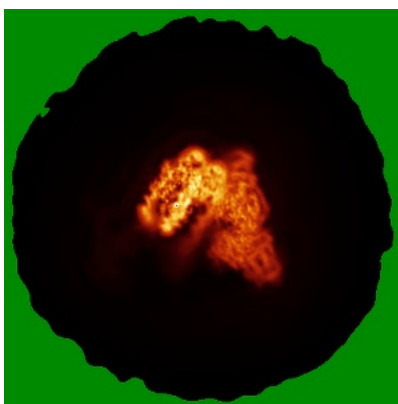
The images above show the largest variance slices of the map in three orthogonal directions.

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

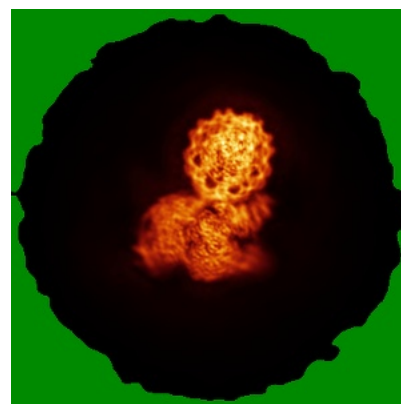
6.4.1 Primary map



X

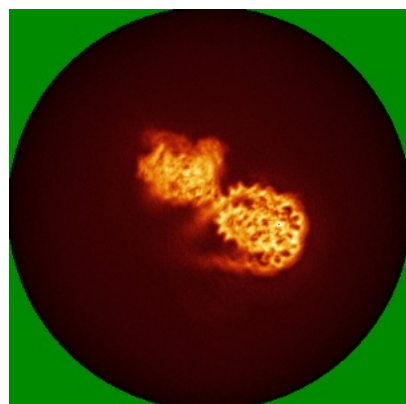


Y



Z

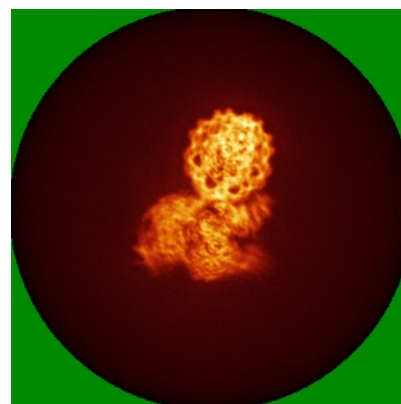
6.4.2 Raw map



X



Y



Z

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

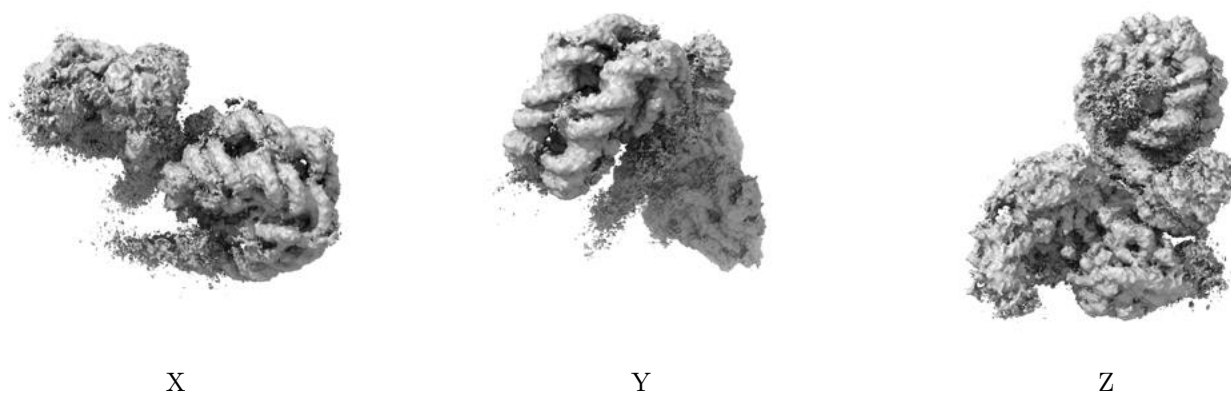
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

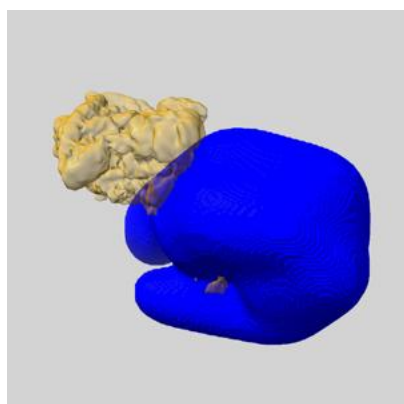
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

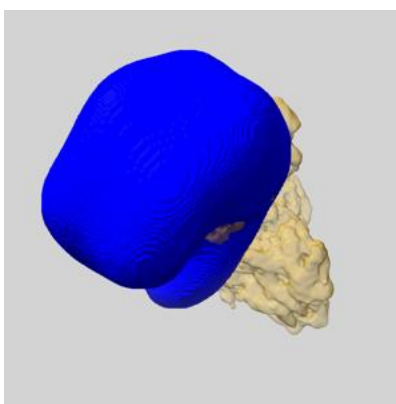
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

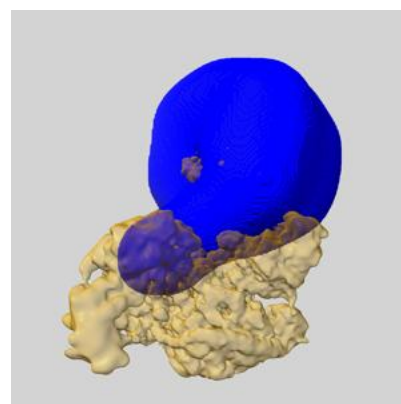
6.6.1 emd_21707_msk_2.map [i](#)



X

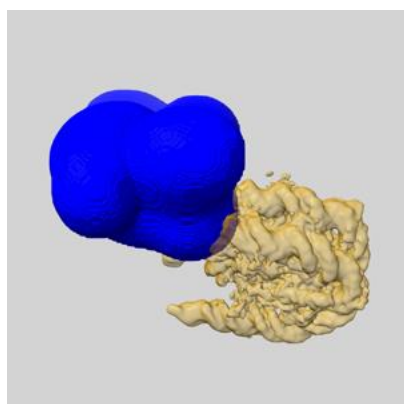


Y

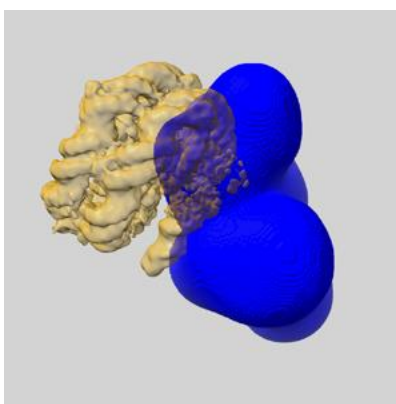


Z

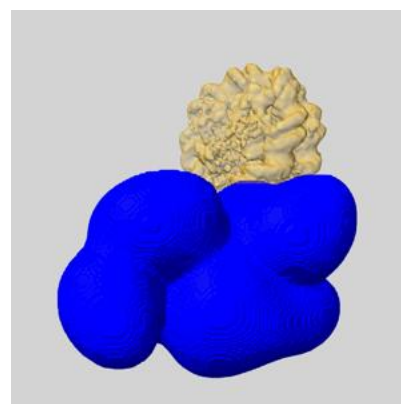
6.6.2 emd_21707_msk_1.map [i](#)



X



Y

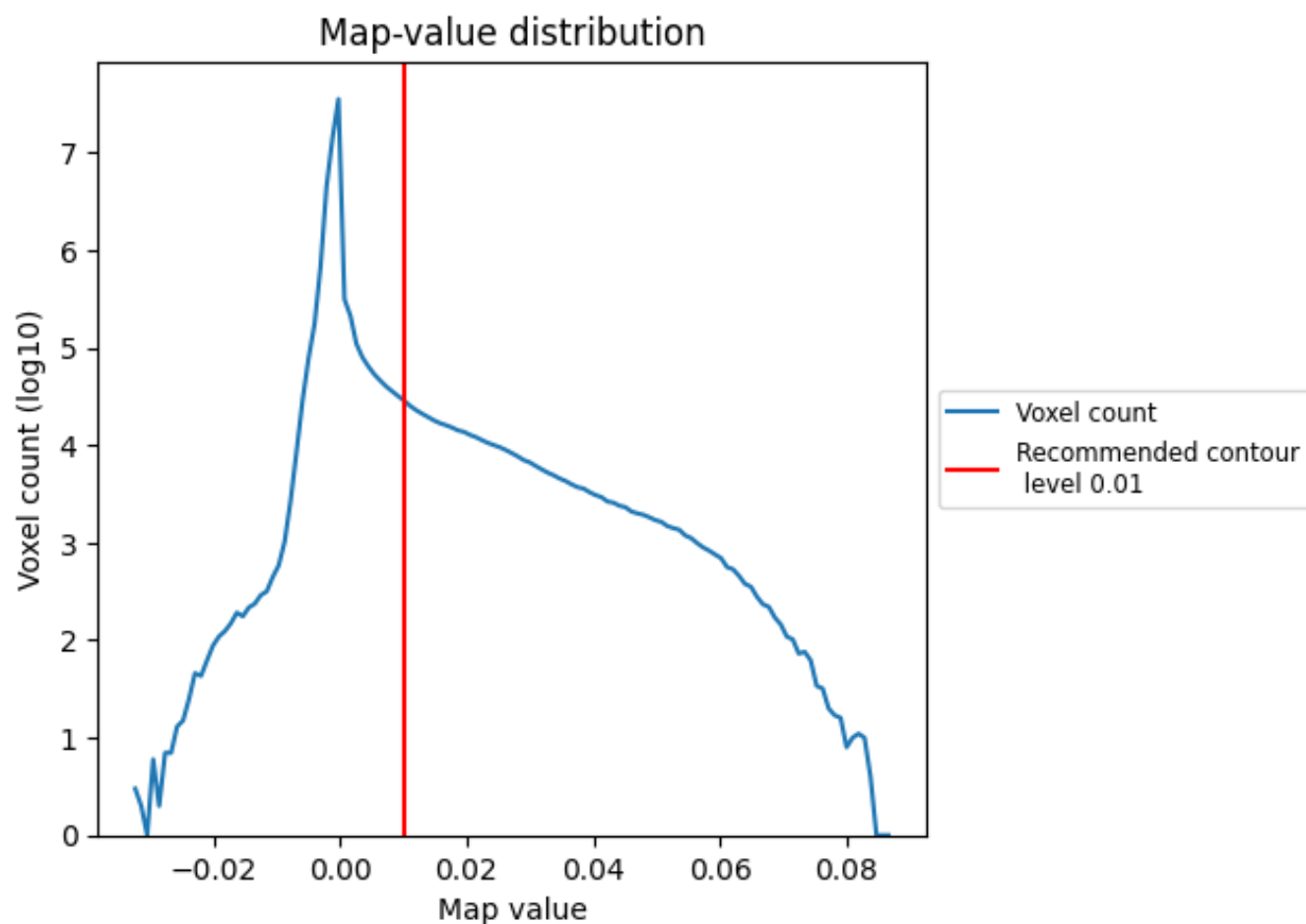


Z

7 Map analysis [i](#)

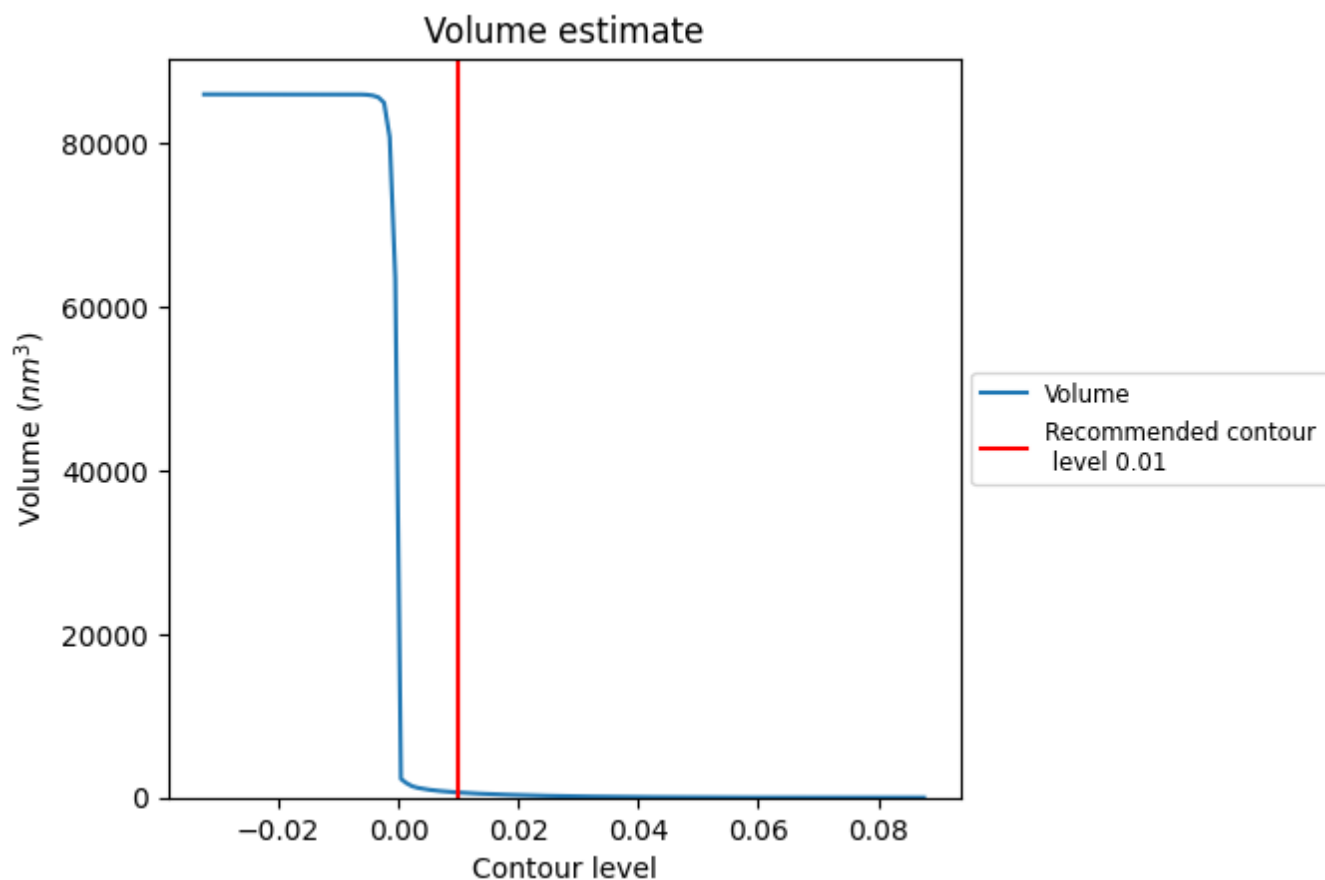
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

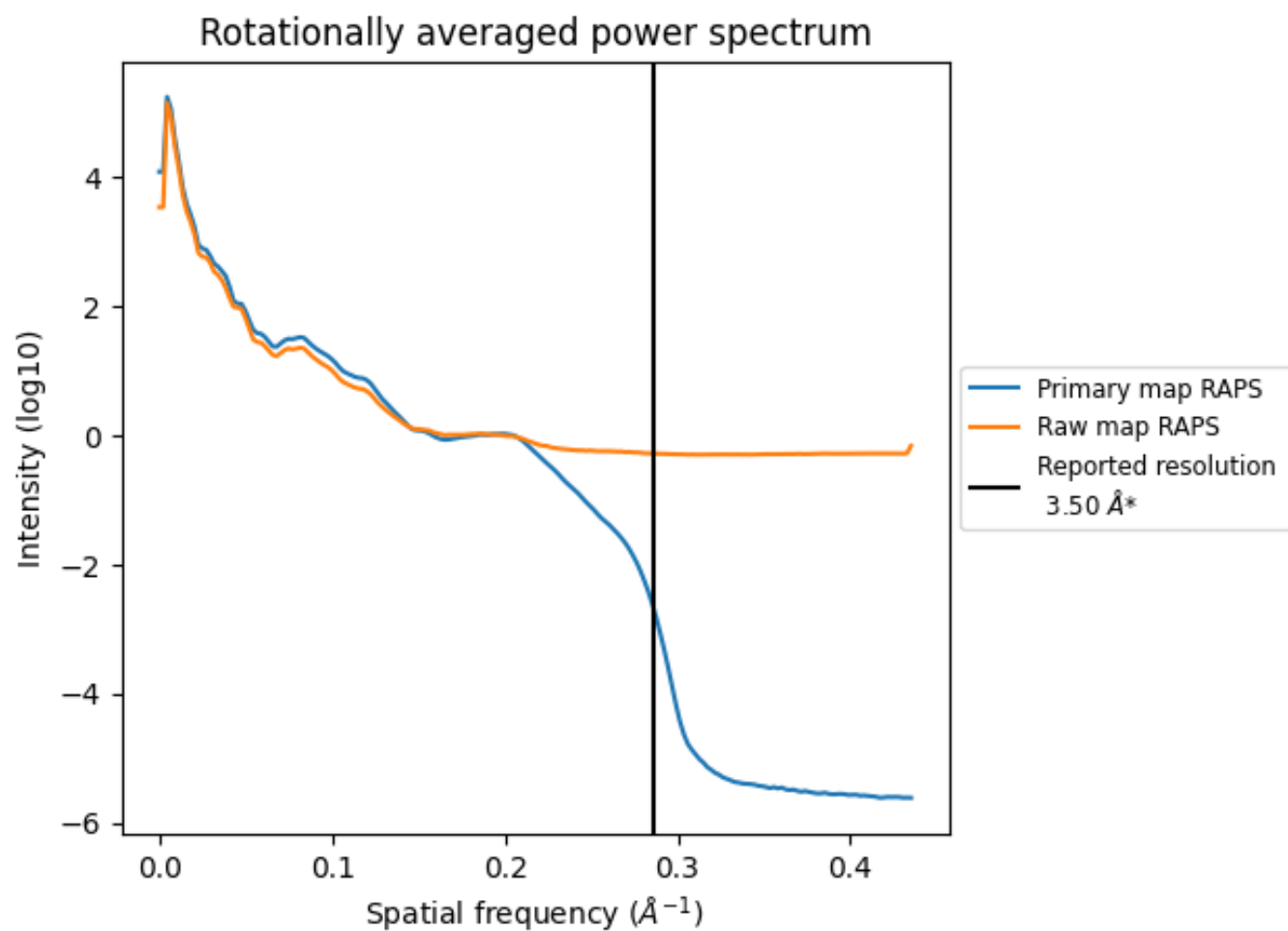
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619 nm³; this corresponds to an approximate mass of 559 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 ⓘ

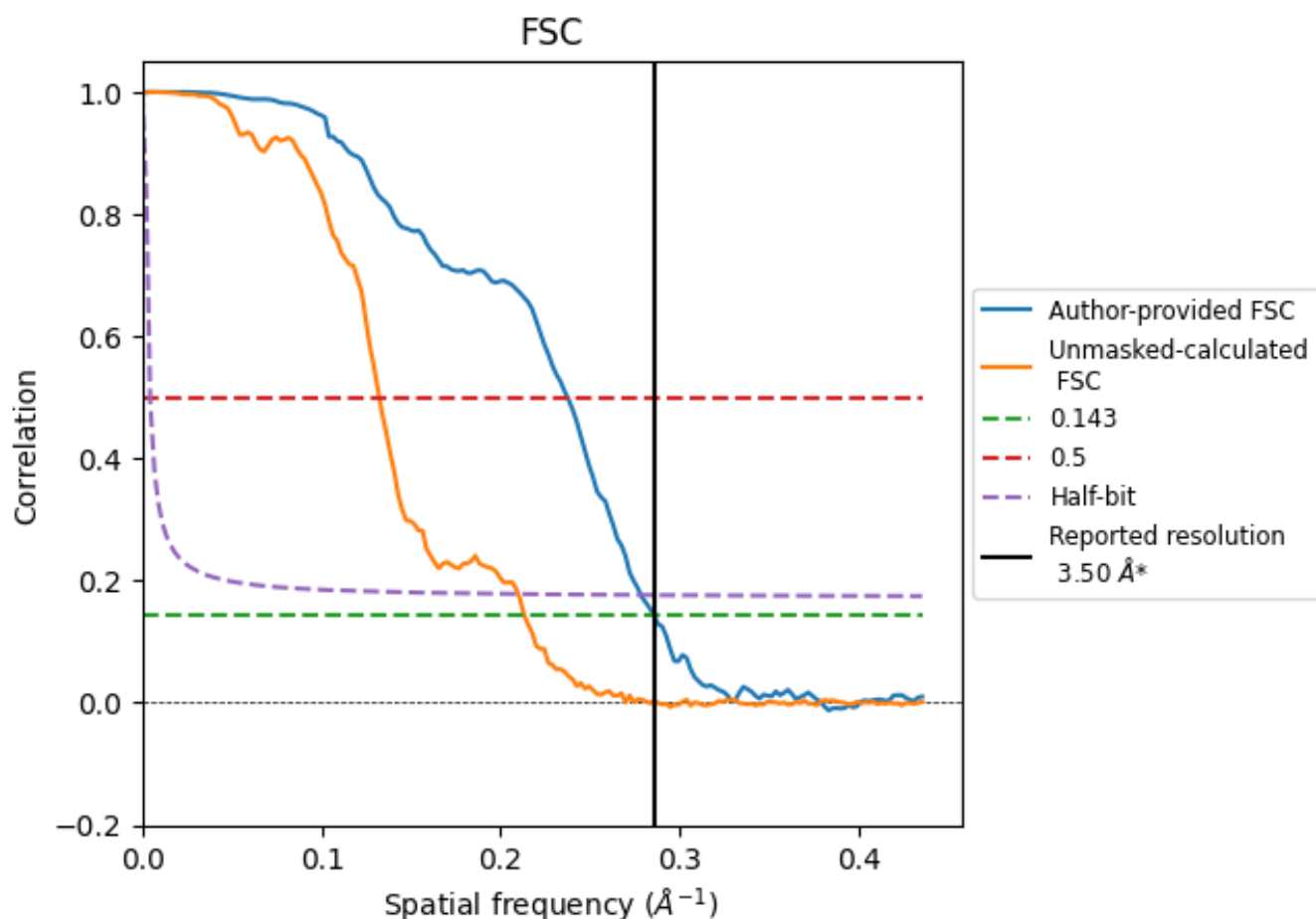


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

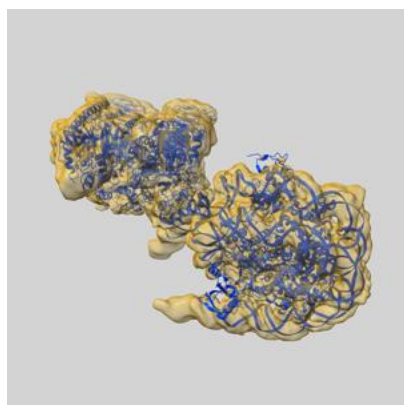
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.21	3.59
Unmasked-calculated*	4.69	7.56	4.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.69 differs from the reported value 3.5 by more than 10 %

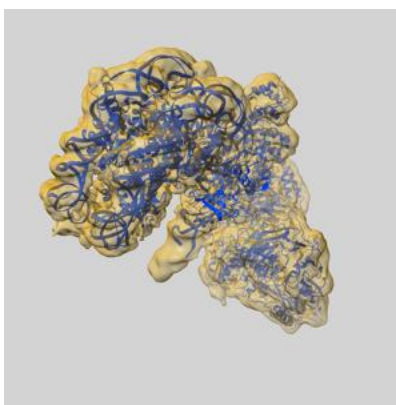
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21707 and PDB model 6WKR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

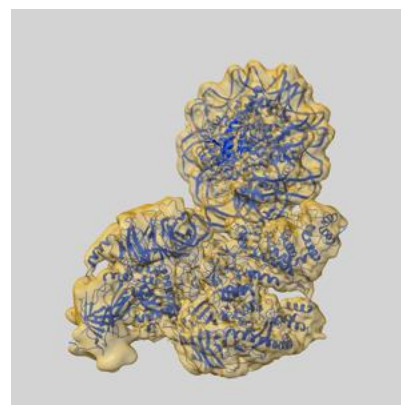
9.1 Map-model overlay [i](#)



X



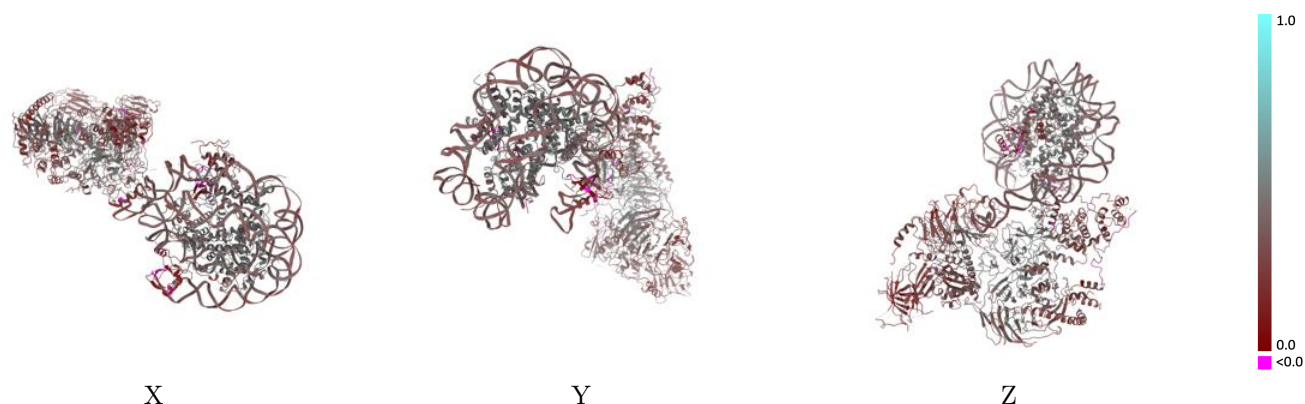
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



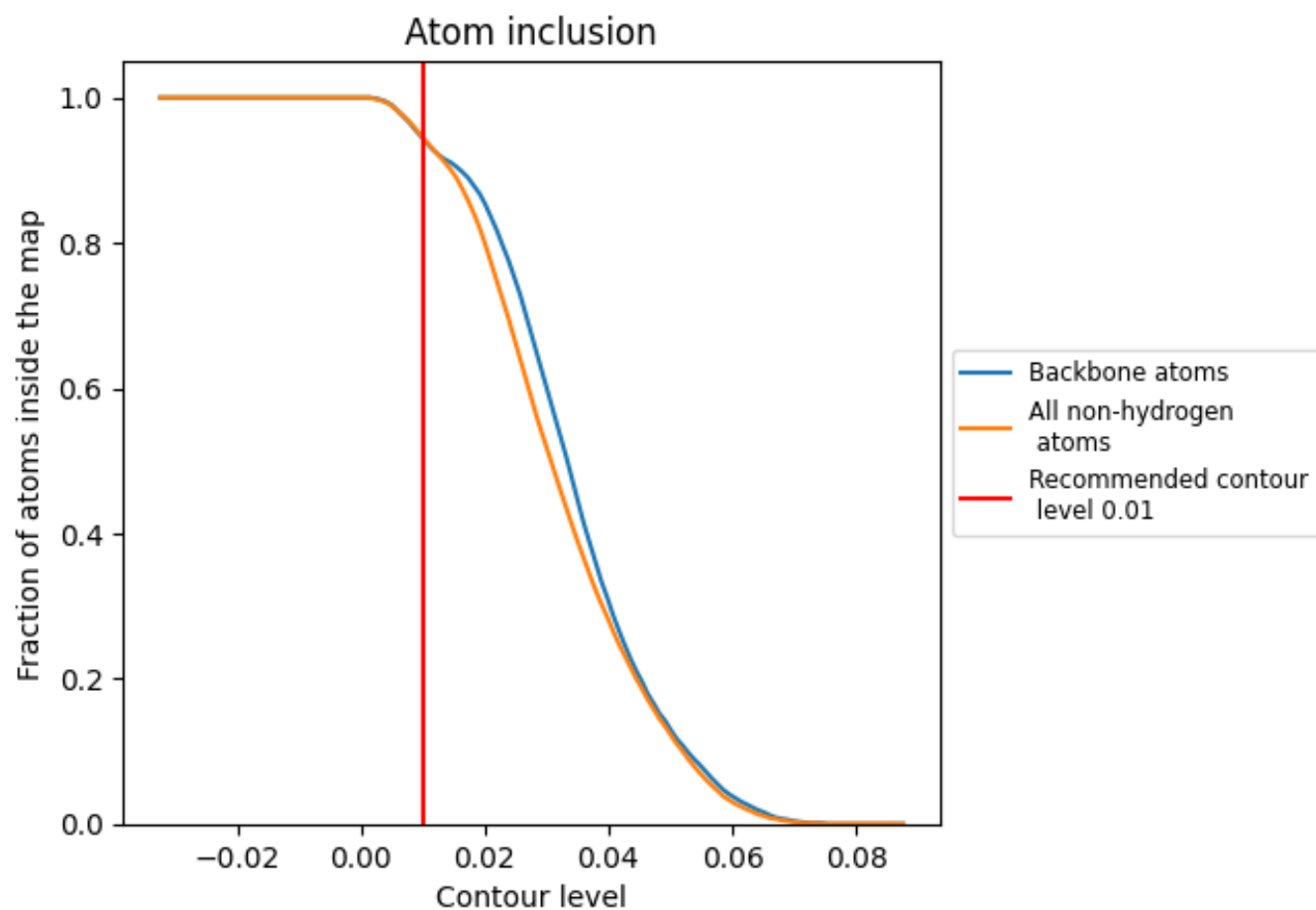
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9450	<div></div> 0.3620
A	<div></div> 0.9870	<div></div> 0.3290
B	<div></div> 1.0000	<div></div> 0.3330
C	<div></div> 0.9800	<div></div> 0.3560
E	<div></div> 0.1640	<div></div> 0.2400
F	<div></div> 0.4090	<div></div> 0.1670
H	<div></div> 1.0000	<div></div> 0.3480
I	<div></div> 0.9850	<div></div> 0.4510
J	<div></div> 0.9610	<div></div> 0.4460
K	<div></div> 0.9890	<div></div> 0.4610
L	<div></div> 0.9950	<div></div> 0.4020
M	<div></div> 0.9930	<div></div> 0.4610
N	<div></div> 0.9960	<div></div> 0.3340
O	<div></div> 0.9860	<div></div> 0.4450
P	<div></div> 0.7700	<div></div> 0.2980
Q	<div></div> 0.9720	<div></div> 0.4610
R	<div></div> 0.9910	<div></div> 0.4640
S	<div></div> 0.9860	<div></div> 0.4560
T	<div></div> 0.1430	<div></div> 0.1450

