



wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 06:43 PM EST

PDB ID : 8XJV
EMDB ID : EMD-38407
Title : Structural basis for the linker histone H5-nucleosome binding and chromatin compaction
Authors : Li, W.Y.; Song, F.; Zhu, P.
Deposited on : 2023-12-22
Resolution : 3.60 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.dev113
MolProbity : 4.02b-467
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) : 2.40

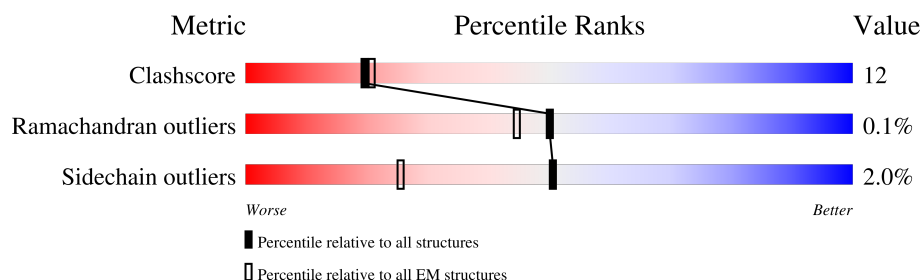
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.












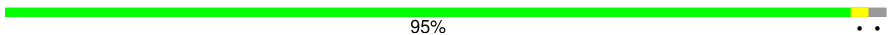
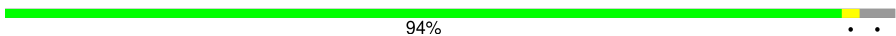
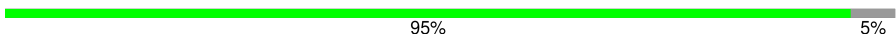
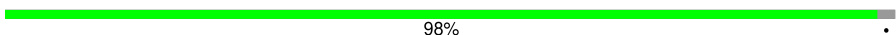



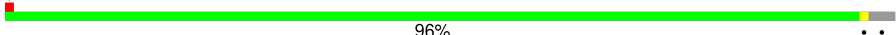


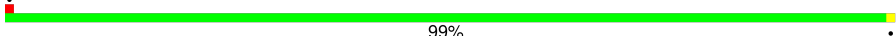




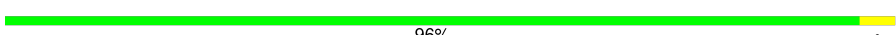
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	Au	2124	99%
2	Av	2124	99%
3	A	130	86% 8% 6%
3	Ae	130	93% 6%
3	B	130	83% 14%
3	C	130	79% 20%
3	D	130	88% 6% 5%
3	E	130	86% 12%










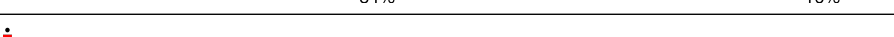
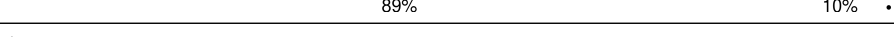




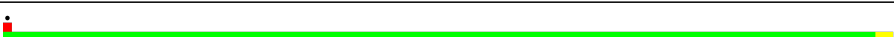
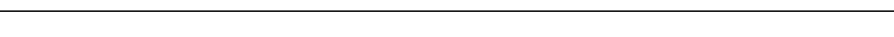
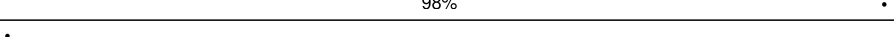
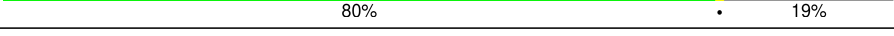






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Mol	Chain	Length	Quality of chain
3	F	130	 84%7%8%
3	G	130	 85%14%
3	H	130	 80%16%
3	I	130	 91%8%
3	K	130	 83%13%
3	L	130	 85%15%
3	aj	130	 92%5%
3	ak	130	 91%5%
3	al	130	 85%15%
3	am	130	 95%
3	an	130	 94%
3	ao	130	 95%5%
3	ap	130	 98%
3	aq	130	 89%10%
3	ar	130	 98%
3	as	130	 92%8%
3	at	130	 96%
3	au	130	 85%15%
4	Aa	123	 82%16%
4	Ab	123	 99%
4	Ac	123	 80%19%
4	Ad	123	 83%17%
4	Af	123	 78%21%
4	Ag	123	 83%15%
4	At	123	 96%














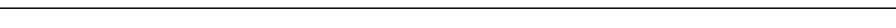











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Mol	Chain	Length	Quality of chain
4	J	123	
4	M	123	
4	N	123	
4	O	123	
4	P	123	
4	Q	123	
4	R	123	
4	S	123	
4	T	123	
4	U	123	
4	V	123	
4	W	123	
4	av	123	
4	aw	123	
4	ax	123	
4	ay	123	
4	az	123	
5	X	136	
5	Y	136	
5	Z	136	
5	a	136	
5	b	136	
5	c	136	
5	d	136	
5	e	136	



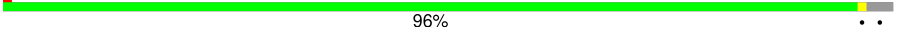



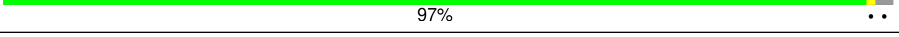
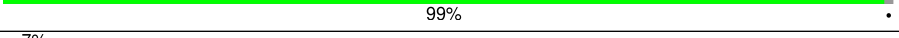
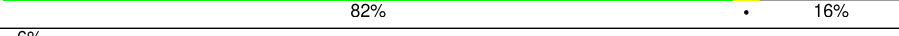

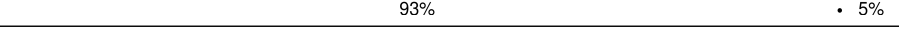
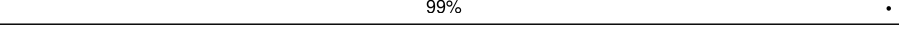
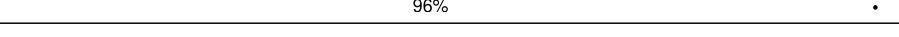
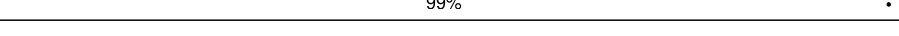


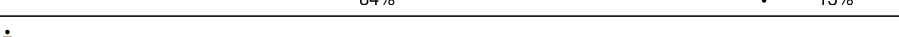
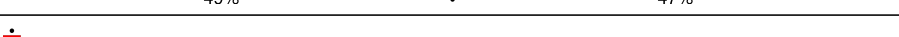
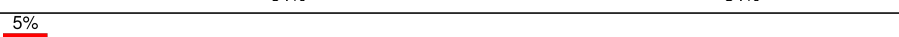






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Mol	Chain	Length	Quality of chain
5	f	136	
5	g	136	
5	h	136	
5	i	136	
5	j	136	
5	k	136	
5	l	136	
5	m	136	
5	n	136	
5	o	136	
5	p	136	
5	q	136	
5	r	136	
5	s	136	
5	t	136	
5	u	136	
6	0	103	
6	1	103	
6	2	103	
6	3	103	
6	4	103	
6	5	103	
6	6	103	
6	7	103	
6	8	103	

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Mol	Chain	Length	Quality of chain
6	9	103	
6	CD	103	
6	a2	103	
6	a3	103	
6	a4	103	
6	a5	103	
6	a6	103	
6	a7	103	
6	a8	103	
6	a9	103	
6	v	103	
6	w	103	
6	x	103	
6	y	103	
6	z	103	
7	Ah	196	
7	Ai	196	
7	Aj	196	
7	Ak	196	
7	Al	196	
7	Am	196	
7	An	196	
7	Ao	196	
7	Ap	196	
7	Aq	196	

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Mol	Chain	Length	Quality of chain
7	Ar	196	<div><div></div><div>5%</div><div>88%</div><div>8%</div></div>
7	As	196	<div><div></div><div>62%</div><div>5%</div><div>33%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 181715 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 DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Au	2116	Total	C	N	O	P	0	0
			43052	20433	7794	12709	2116		

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Av	2112	Total	C	N	O	P	0	0
			43620	20607	8241	12660	2112		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	122	Total	C	N	O		0	0
			936	585	184	167			
3	B	126	Total	C	N	O		0	0
			962	600	190	172			
3	C	129	Total	C	N	O		0	0
			983	611	196	176			
3	D	123	Total	C	N	O		0	0
			940	587	185	168			
3	E	128	Total	C	N	O		0	0
			973	605	194	174			
3	F	119	Total	C	N	O		0	0
			916	573	180	163			
3	G	129	Total	C	N	O		0	0
			983	611	196	176			
3	H	125	Total	C	N	O		0	0
			958	598	189	171			
3	I	129	Total	C	N	O		0	0
			983	611	196	176			
3	K	128	Total	C	N	O		0	0
			977	608	195	174			
3	L	130	Total	C	N	O	S	0	0
			991	616	197	177	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	aj	123	Total	C	N	O	0	0
			940	587	185	168		
3	ak	123	Total	C	N	O	0	0
			940	587	185	168		
3	al	111	Total	C	N	O	0	0
			851	533	169	149		
3	am	127	Total	C	N	O	0	0
			973	606	194	173		
3	an	125	Total	C	N	O	0	0
			958	598	189	171		
3	ao	124	Total	C	N	O	0	0
			949	592	187	170		
3	ap	127	Total	C	N	O	0	0
			973	606	194	173		
3	aq	117	Total	C	N	O	0	0
			900	564	175	161		
3	ar	129	Total	C	N	O	0	0
			983	611	196	176		
3	as	119	Total	C	N	O	0	0
			916	573	180	163		
3	at	126	Total	C	N	O	0	0
			962	600	190	172		
3	au	111	Total	C	N	O	0	0
			859	540	169	150		
3	Ae	122	Total	C	N	O	0	0
			936	585	184	167		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	103	Total	C	N	O	S	0	0
			814	510	152	150	2		
4	M	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	N	105	Total	C	N	O	S	0	0
			830	519	155	154	2		
4	O	103	Total	C	N	O	S	0	0
			814	510	152	150	2		
4	P	105	Total	C	N	O	S	0	0
			830	519	155	154	2		
4	Q	123	Total	C	N	O	S	0	0
			956	599	179	175	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	100	Total	C	N	O	S	0	0
			788	494	147	145	2		
4	S	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	T	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	U	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	V	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	W	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	av	103	Total	C	N	O	S	0	0
			814	510	152	150	2		
4	aw	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	ax	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	ay	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	az	100	Total	C	N	O	S	0	0
			788	494	147	145	2		
4	Aa	103	Total	C	N	O	S	0	0
			814	510	152	150	2		
4	Ab	123	Total	C	N	O	S	0	0
			956	599	179	175	3		
4	Ac	100	Total	C	N	O	S	0	0
			788	494	147	145	2		
4	Ad	102	Total	C	N	O	S	0	0
			805	504	150	149	2		
4	Af	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
4	Ag	104	Total	C	N	O	S	0	0
			823	515	154	152	2		
4	At	123	Total	C	N	O	S	0	0
			956	599	179	175	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1948	MET	-	initiating methionine	UNP P02281
M	0	MET	-	initiating methionine	UNP P02281
N	105	MET	-	initiating methionine	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
O	375	MET	-	initiating methionine	UNP P02281
P	480	MET	-	initiating methionine	UNP P02281
Q	603	MET	-	initiating methionine	UNP P02281
R	230	MET	-	initiating methionine	UNP P02281
S	849	MET	-	initiating methionine	UNP P02281
T	2736	MET	-	initiating methionine	UNP P02281
U	1838	MET	-	initiating methionine	UNP P02281
V	976	MET	-	initiating methionine	UNP P02281
W	2859	MET	-	initiating methionine	UNP P02281
av	0	MET	-	initiating methionine	UNP P02281
aw	123	MET	-	initiating methionine	UNP P02281
ax	246	MET	-	initiating methionine	UNP P02281
ay	369	MET	-	initiating methionine	UNP P02281
az	469	MET	-	initiating methionine	UNP P02281
Aa	572	MET	-	initiating methionine	UNP P02281
Ab	695	MET	-	initiating methionine	UNP P02281
Ac	795	MET	-	initiating methionine	UNP P02281
Ad	2843	MET	-	initiating methionine	UNP P02281
Af	1074	MET	-	initiating methionine	UNP P02281
Ag	3069	MET	-	initiating methionine	UNP P02281
At	0	MET	-	initiating methionine	UNP P02281

- Molecule 5 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	112	Total	C	N	O	S	0	0
			901	566	176	156	3		
5	Y	111	Total	C	N	O	S	0	0
			896	563	175	155	3		
5	Z	90	Total	C	N	O	S	0	0
			739	466	140	130	3		
5	a	125	Total	C	N	O	S	0	0
			995	624	196	172	3		
5	b	101	Total	C	N	O	S	0	0
			833	526	161	143	3		
5	c	106	Total	C	N	O	S	0	0
			860	542	166	149	3		
5	d	98	Total	C	N	O	S	0	0
			808	509	156	140	3		
5	e	94	Total	C	N	O	S	0	0
			768	483	147	135	3		
5	f	98	Total	C	N	O	S	0	0
			808	509	156	140	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	102	Total	C	N	O	S	0	0
			837	528	162	144	3		
5	h	97	Total	C	N	O	S	0	0
			801	504	155	139	3		
5	i	99	Total	C	N	O	S	0	0
			817	515	158	141	3		
5	j	105	Total	C	N	O	S	0	0
			853	537	165	148	3		
5	k	99	Total	C	N	O	S	0	0
			817	515	158	141	3		
5	l	114	Total	C	N	O	S	0	0
			917	576	179	159	3		
5	m	98	Total	C	N	O	S	0	0
			808	509	156	140	3		
5	n	113	Total	C	N	O	S	0	0
			910	572	178	157	3		
5	o	109	Total	C	N	O	S	0	0
			880	554	170	153	3		
5	p	102	Total	C	N	O	S	0	0
			837	528	162	144	3		
5	q	110	Total	C	N	O	S	0	0
			891	560	174	154	3		
5	r	106	Total	C	N	O	S	0	0
			860	542	166	149	3		
5	s	95	Total	C	N	O	S	0	0
			780	492	148	137	3		
5	t	110	Total	C	N	O	S	0	0
			890	560	174	153	3		
5	u	126	Total	C	N	O	S	0	0
			1001	627	197	174	3		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	v	98	Total	C	N	O	S	0	0
			767	481	156	129	1		
6	w	103	Total	C	N	O	S	0	0
			800	499	164	135	2		
6	x	99	Total	C	N	O	S	0	0
			771	483	157	130	1		
6	y	102	Total	C	N	O	S	0	0
			792	494	163	134	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	z	84	Total 673	C 424	N 133	O 115	S 1	0	0
6	0	94	Total 741	C 465	N 150	O 125	S 1	0	0
6	1	87	Total 703	C 442	N 142	O 118	S 1	0	0
6	2	95	Total 750	C 471	N 152	O 126	S 1	0	0
6	3	93	Total 736	C 463	N 149	O 123	S 1	0	0
6	4	87	Total 703	C 442	N 142	O 118	S 1	0	0
6	5	95	Total 750	C 471	N 152	O 126	S 1	0	0
6	6	85	Total 688	C 432	N 140	O 115	S 1	0	0
6	7	101	Total 786	C 491	N 162	O 132	S 1	0	0
6	8	86	Total 694	C 436	N 140	O 117	S 1	0	0
6	9	102	Total 792	C 494	N 163	O 134	S 1	0	0
6	CD	97	Total 762	C 479	N 155	O 127	S 1	0	0
6	a2	100	Total 782	C 489	N 161	O 131	S 1	0	0
6	a3	87	Total 703	C 442	N 142	O 118	S 1	0	0
6	a4	96	Total 754	C 473	N 153	O 127	S 1	0	0
6	a5	91	Total 725	C 455	N 147	O 122	S 1	0	0
6	a6	101	Total 786	C 491	N 162	O 132	S 1	0	0
6	a7	102	Total 792	C 494	N 163	O 134	S 1	0	0
6	a8	87	Total 703	C 442	N 142	O 118	S 1	0	0
6	a9	90	Total 716	C 449	N 145	O 121	S 1	0	0

- Molecule 7 is a protein called Histone H5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ah	130	Total	C	N	O	S	0	0
			992	613	206	171	2		
7	Ai	170	Total	C	N	O	S	0	0
			1298	805	274	217	2		
7	Aj	103	Total	C	N	O	S	0	0
			780	485	154	139	2		
7	Ak	129	Total	C	N	O	S	0	0
			986	610	205	169	2		
7	Al	107	Total	C	N	O	S	0	0
			808	501	161	144	2		
7	Am	175	Total	C	N	O	S	0	0
			1340	831	284	223	2		
7	An	128	Total	C	N	O	S	0	0
			975	604	201	168	2		
7	Ao	159	Total	C	N	O	S	0	0
			1215	754	255	204	2		
7	Ap	73	Total	C	N	O	S	0	0
			555	346	109	99	1		
7	Aq	190	Total	C	N	O	S	0	0
			1456	903	311	240	2		
7	Ar	180	Total	C	N	O	S	0	0
			1375	852	295	226	2		
7	As	131	Total	C	N	O	S	0	0
			999	618	207	172	2		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	541	HIS	-	expression tag	UNP P02259
Ah	542	HIS	-	expression tag	UNP P02259
Ah	543	HIS	-	expression tag	UNP P02259
Ah	544	HIS	-	expression tag	UNP P02259
Ah	545	HIS	-	expression tag	UNP P02259
Ah	546	HIS	-	expression tag	UNP P02259
Ai	190	HIS	-	expression tag	UNP P02259
Ai	191	HIS	-	expression tag	UNP P02259
Ai	192	HIS	-	expression tag	UNP P02259
Ai	193	HIS	-	expression tag	UNP P02259
Ai	194	HIS	-	expression tag	UNP P02259
Ai	195	HIS	-	expression tag	UNP P02259
Aj	323	HIS	-	expression tag	UNP P02259
Aj	324	HIS	-	expression tag	UNP P02259
Aj	325	HIS	-	expression tag	UNP P02259
Aj	326	HIS	-	expression tag	UNP P02259

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Chain	Residue	Modelled	Actual	Comment	Reference
Aj	327	HIS	-	expression tag	UNP P02259
Aj	328	HIS	-	expression tag	UNP P02259
Ak	674	HIS	-	expression tag	UNP P02259
Ak	675	HIS	-	expression tag	UNP P02259
Ak	676	HIS	-	expression tag	UNP P02259
Ak	677	HIS	-	expression tag	UNP P02259
Ak	678	HIS	-	expression tag	UNP P02259
Ak	679	HIS	-	expression tag	UNP P02259
Al	431	HIS	-	expression tag	UNP P02259
Al	432	HIS	-	expression tag	UNP P02259
Al	433	HIS	-	expression tag	UNP P02259
Al	434	HIS	-	expression tag	UNP P02259
Al	435	HIS	-	expression tag	UNP P02259
Al	436	HIS	-	expression tag	UNP P02259
Am	190	HIS	-	expression tag	UNP P02259
Am	191	HIS	-	expression tag	UNP P02259
Am	192	HIS	-	expression tag	UNP P02259
Am	193	HIS	-	expression tag	UNP P02259
Am	194	HIS	-	expression tag	UNP P02259
Am	195	HIS	-	expression tag	UNP P02259
An	190	HIS	-	expression tag	UNP P02259
An	191	HIS	-	expression tag	UNP P02259
An	192	HIS	-	expression tag	UNP P02259
An	193	HIS	-	expression tag	UNP P02259
An	194	HIS	-	expression tag	UNP P02259
An	195	HIS	-	expression tag	UNP P02259
Ao	190	HIS	-	expression tag	UNP P02259
Ao	191	HIS	-	expression tag	UNP P02259
Ao	192	HIS	-	expression tag	UNP P02259
Ao	193	HIS	-	expression tag	UNP P02259
Ao	194	HIS	-	expression tag	UNP P02259
Ao	195	HIS	-	expression tag	UNP P02259
Ap	190	HIS	-	expression tag	UNP P02259
Ap	191	HIS	-	expression tag	UNP P02259
Ap	192	HIS	-	expression tag	UNP P02259
Ap	193	HIS	-	expression tag	UNP P02259
Ap	194	HIS	-	expression tag	UNP P02259
Ap	195	HIS	-	expression tag	UNP P02259
Aq	190	HIS	-	expression tag	UNP P02259
Aq	191	HIS	-	expression tag	UNP P02259
Aq	192	HIS	-	expression tag	UNP P02259
Aq	193	HIS	-	expression tag	UNP P02259

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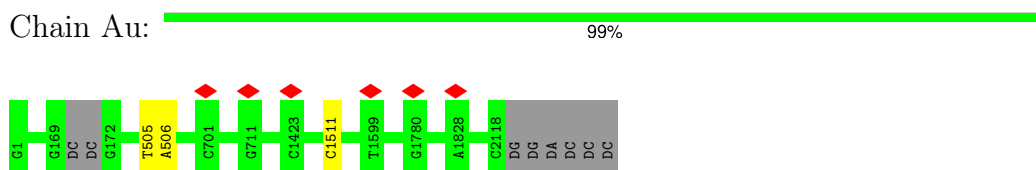
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Aq	194	HIS	-	expression tag	UNP P02259
Aq	195	HIS	-	expression tag	UNP P02259
Ar	190	HIS	-	expression tag	UNP P02259
Ar	191	HIS	-	expression tag	UNP P02259
Ar	192	HIS	-	expression tag	UNP P02259
Ar	193	HIS	-	expression tag	UNP P02259
Ar	194	HIS	-	expression tag	UNP P02259
Ar	195	HIS	-	expression tag	UNP P02259
As	190	HIS	-	expression tag	UNP P02259
As	191	HIS	-	expression tag	UNP P02259
As	192	HIS	-	expression tag	UNP P02259
As	193	HIS	-	expression tag	UNP P02259
As	194	HIS	-	expression tag	UNP P02259
As	195	HIS	-	expression tag	UNP P02259

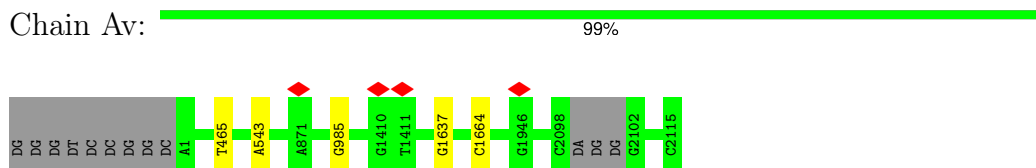
3 Residue-property plots [i](#)

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.

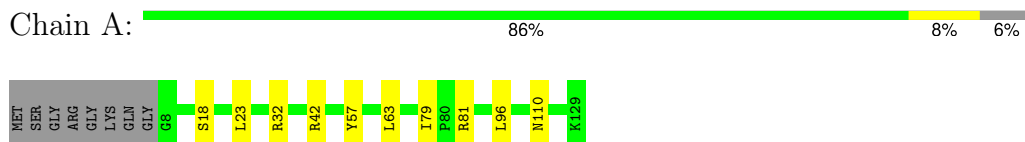
- Molecule 1: DNA



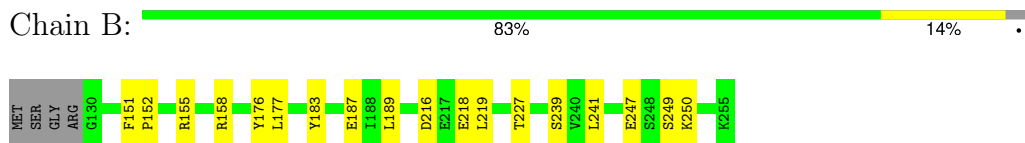
- Molecule 2: DNA



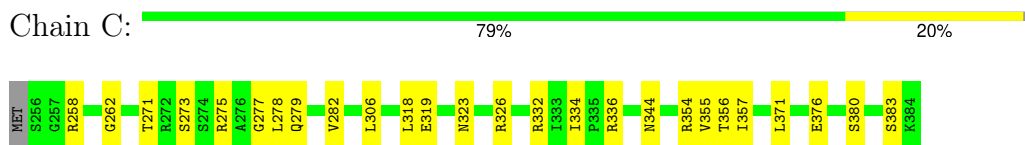
- Molecule 3: Histone H2A




- Molecule 3: Histone H2A

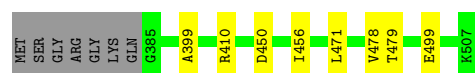


- Molecule 3: Histone H2A




- Molecule 3: Histone H2A

Chain D:  88% 6% 5%




- Molecule 3: Histone H2A

Chain E:  86% 12% •




- Molecule 3: Histone H2A

Chain F:  84% 7% • 8%




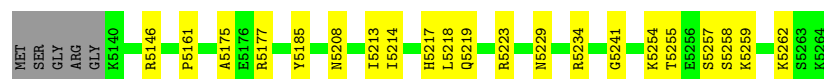
- Molecule 3: Histone H2A

Chain G:  85% 14% ••




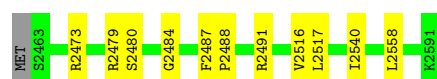
- Molecule 3: Histone H2A

Chain H:  80% 16% •




- Molecule 3: Histone H2A

Chain I:  91% 8% •




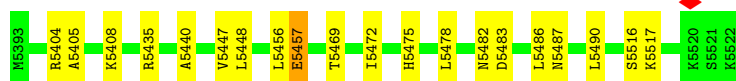
- Molecule 3: Histone H2A

Chain K:  83% 13% ••



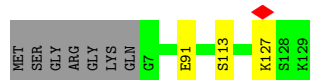
- Molecule 3: Histone H2A

Chain L:  85% 15%



- Molecule 3: Histone H2A

Chain aj:  92% 5%




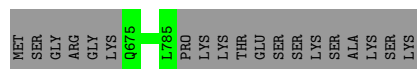
- Molecule 3: Histone H2A

Chain ak:  91% 5%



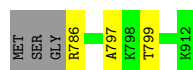
- Molecule 3: Histone H2A

Chain al:  85% 15%



- Molecule 3: Histone H2A

Chain am:  95%



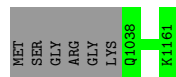
- Molecule 3: Histone H2A

Chain an:  94%



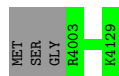
- Molecule 3: Histone H2A

Chain ao:  95% 5%




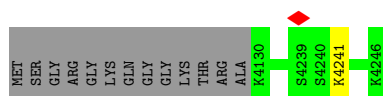
- Molecule 3: Histone H2A

Chain ap:  98% .



• Molecule 3: Histone H2A

Chain aq:  89% 10% .



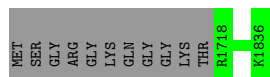
• Molecule 3: Histone H2A

Chain ar:  98% ..



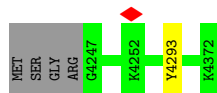
• Molecule 3: Histone H2A

Chain as:  92% 8%




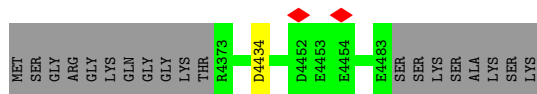
• Molecule 3: Histone H2A

Chain at:  96% ..



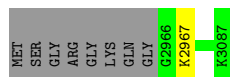
• Molecule 3: Histone H2A

Chain au:  85% 15%



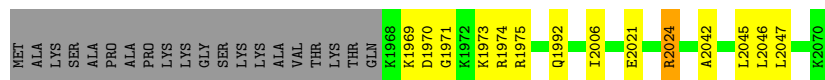
• Molecule 3: Histone H2A

Chain Ae:  93% 6%



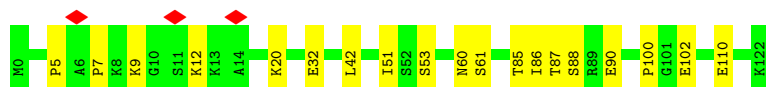
- Molecule 4: Histone H2B 1.1

Chain J: 



- Molecule 4: Histone H2B 1.1

Chain M: 



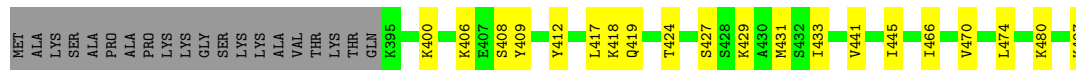
- Molecule 4: Histone H2B 1.1

Chain N: 




- Molecule 4: Histone H2B 1.1

Chain O: 




- Molecule 4: Histone H2B 1.1

Chain P: 



- Molecule 4: Histone H2B 1.1

Chain Q: 




- Molecule 4: Histone H2B 1.1

Chain R: 




- Molecule 4: Histone H2B 1.1

Chain S:  80% 20%




• Molecule 4: Histone H2B 1.1

Chain T:  84% 16%




• Molecule 4: Histone H2B 1.1

Chain U:  89% 10%



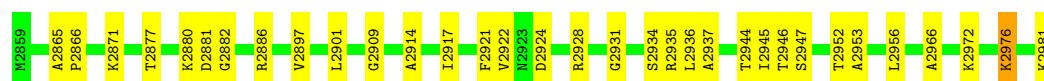
• Molecule 4: Histone H2B 1.1

Chain V:  80% 20%




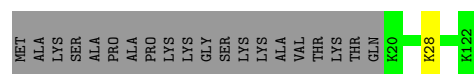
• Molecule 4: Histone H2B 1.1

Chain W:  73% 26%



• Molecule 4: Histone H2B 1.1

Chain av:  83% 16%



• Molecule 4: Histone H2B 1.1

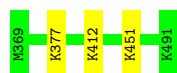
Chain aw:  98%



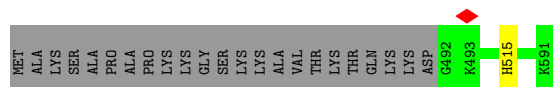
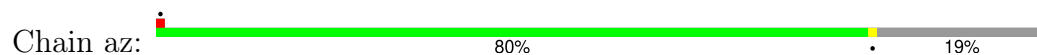
• Molecule 4: Histone H2B 1.1



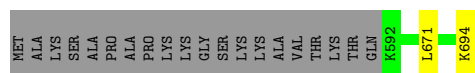
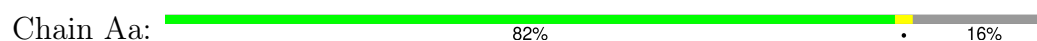
- Molecule 4: Histone H2B 1.1



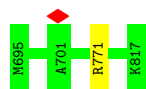
- Molecule 4: Histone H2B 1.1



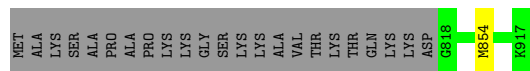
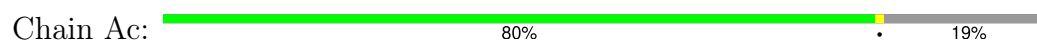
- Molecule 4: Histone H2B 1.1



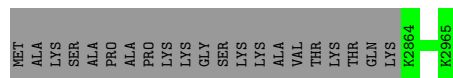
- Molecule 4: Histone H2B 1.1



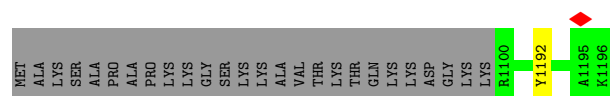
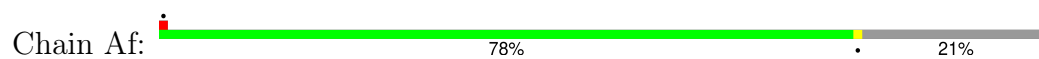
- Molecule 4: Histone H2B 1.1



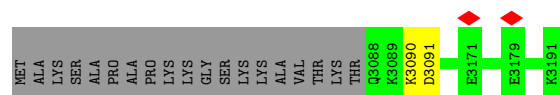
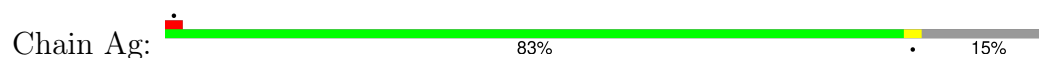
- Molecule 4: Histone H2B 1.1



- Molecule 4: Histone H2B 1.1



- Molecule 4: Histone H2B 1.1



- Molecule 4: Histone H2B 1.1



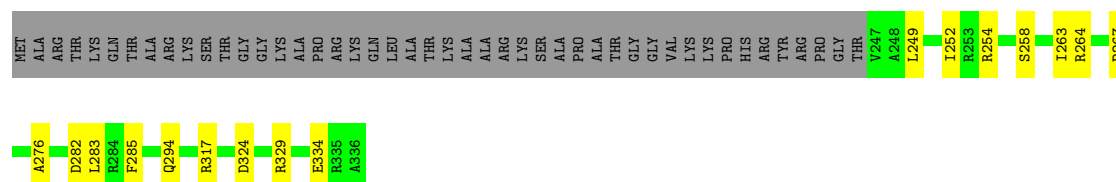
- Molecule 5: Histone H3



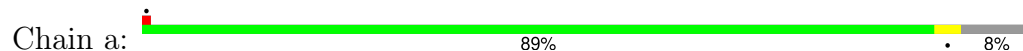
- Molecule 5: Histone H3

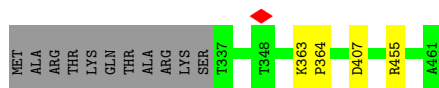


- Molecule 5: Histone H3

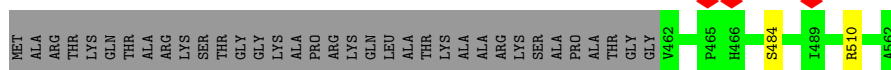


- Molecule 5: Histone H3

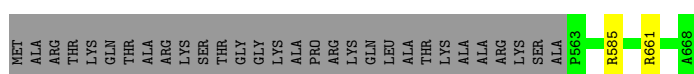
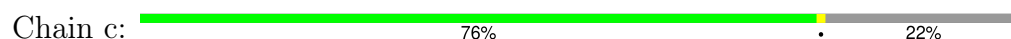




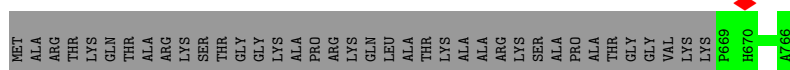
- Molecule 5: Histone H3



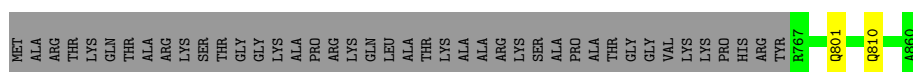
- Molecule 5: Histone H3



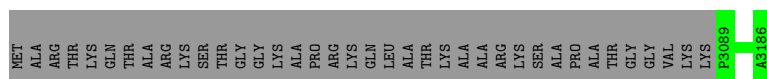
- Molecule 5: Histone H3



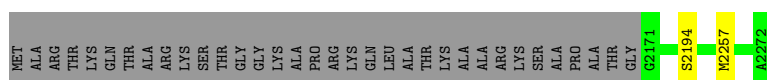
- Molecule 5: Histone H3



- Molecule 5: Histone H3

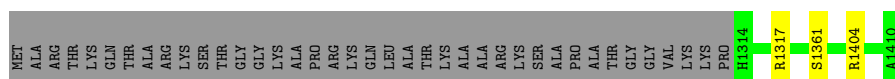


- Molecule 5: Histone H3

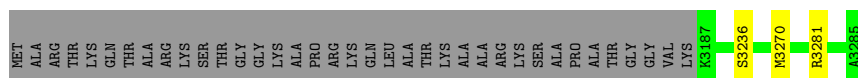


- Molecule 5: Histone H3

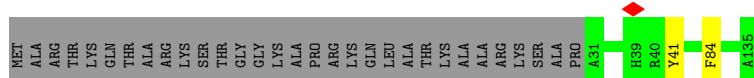
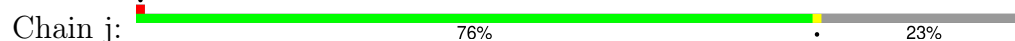




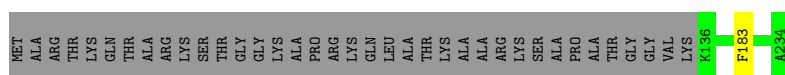
• Molecule 5: Histone H3



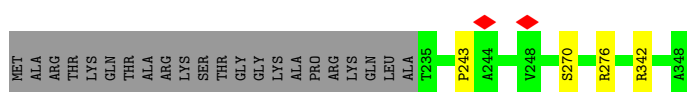
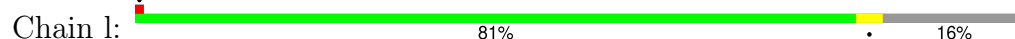
• Molecule 5: Histone H3



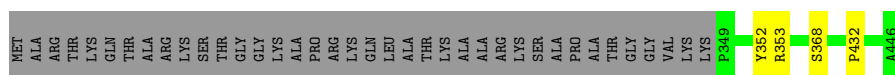
• Molecule 5: Histone H3



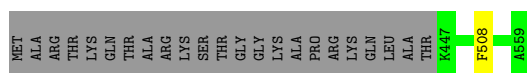
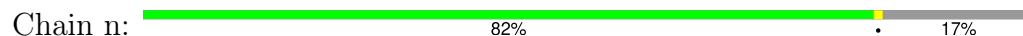
• Molecule 5: Histone H3



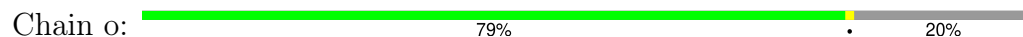
• Molecule 5: Histone H3

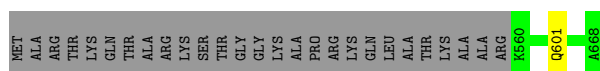


• Molecule 5: Histone H3

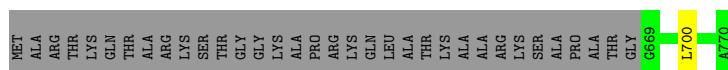


• Molecule 5: Histone H3

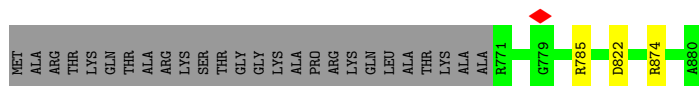
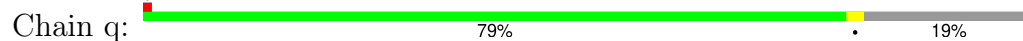




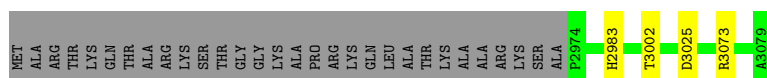
● Molecule 5: Histone H3



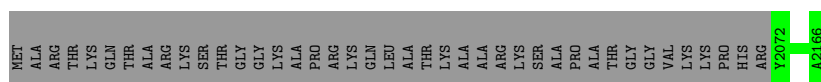
● Molecule 5: Histone H3



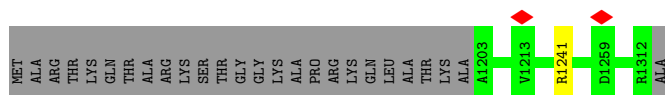
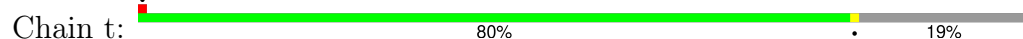
● Molecule 5: Histone H3



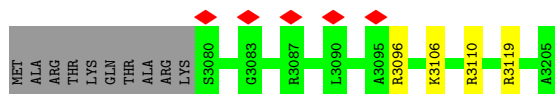
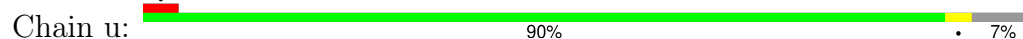
● Molecule 5: Histone H3



● Molecule 5: Histone H3

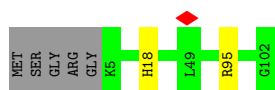


● Molecule 5: Histone H3



● Molecule 6: Histone H4





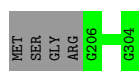
• Molecule 6: Histone H4

Chain w: 99%



• Molecule 6: Histone H4

Chain x: 96%



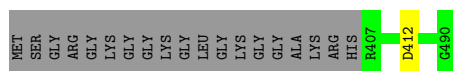
• Molecule 6: Histone H4

Chain y: 99%



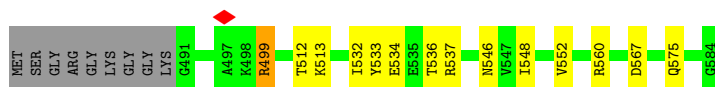
• Molecule 6: Histone H4

Chain z: 81% 18%



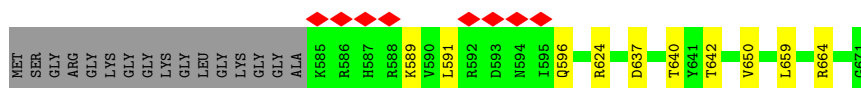
• Molecule 6: Histone H4

Chain 0: 78% 13% 9%



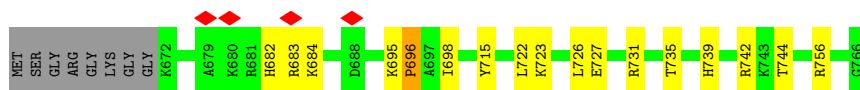
• Molecule 6: Histone H4

Chain 1: 8% 75% 10% 16%

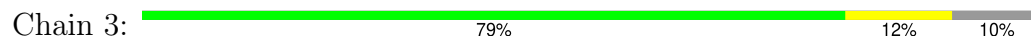


• Molecule 6: Histone H4

Chain 2: 76% 16% 8%



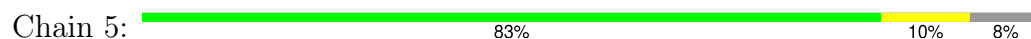
- Molecule 6: Histone H4



- Molecule 6: Histone H4



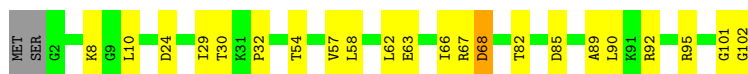
- Molecule 6: Histone H4



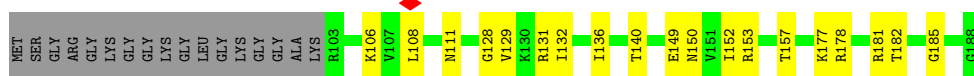
- Molecule 6: Histone H4



- Molecule 6: Histone H4

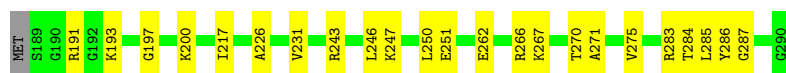


- Molecule 6: Histone H4



- Molecule 6: Histone H4





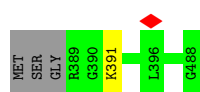
- Molecule 6: Histone H4

Chain CD: 75% 17% 6%



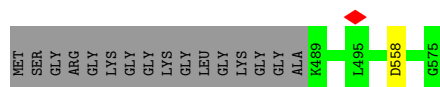
- Molecule 6: Histone H4

Chain a2: 96%



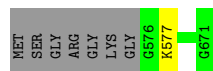
- Molecule 6: Histone H4

Chain a3: 83% 16%



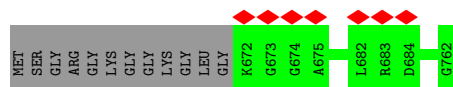
- Molecule 6: Histone H4

Chain a4: 92% 7%



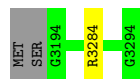
- Molecule 6: Histone H4

Chain a5: 7% 88% 12%



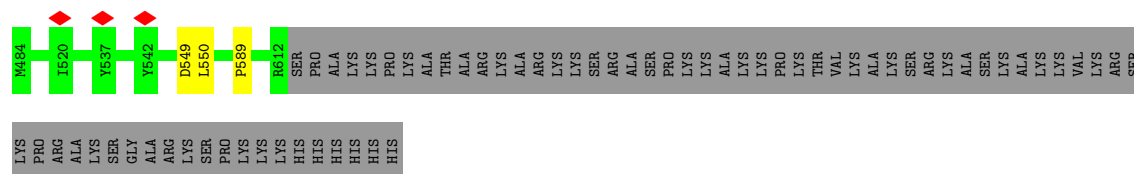
- Molecule 6: Histone H4

Chain a6: 97%

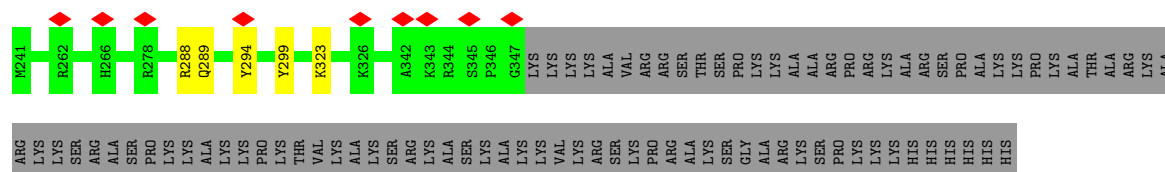


- Molecule 6: Histone H4

Chain a7: 99%



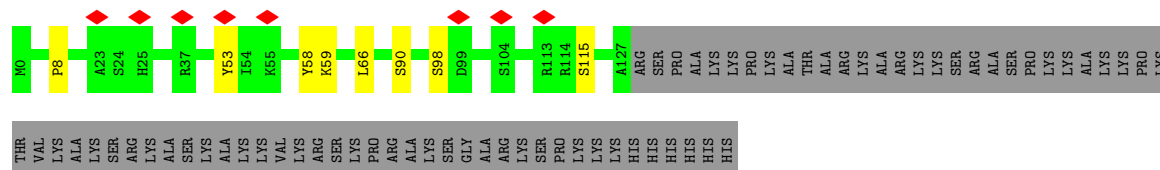
• Molecule 7: Histone H5



• Molecule 7: Histone H5

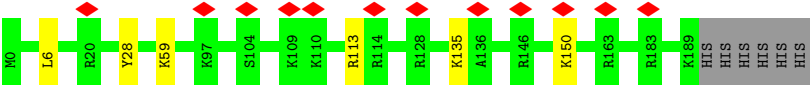


• Molecule 7: Histone H5

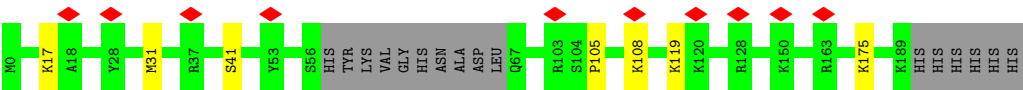
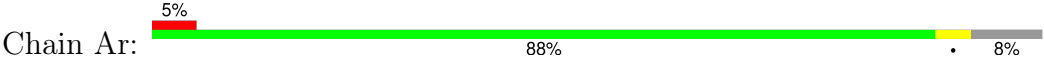


ALA
ARG
LYS
SER
PRO
LYS
LYS
HIS
HIS
HIS
HIS
HIS
HIS

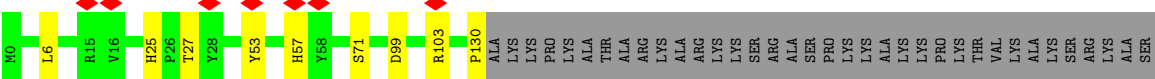
• Molecule 7: Histone H5



• Molecule 7: Histone H5



• Molecule 7: Histone H5



LYS
ALA
LYS
LYS
VAL
LYS
ARG
SER
LYS
PRO
ARG
ALA
LYS
SER
GLY
ALA
ARG
LYS
SER
PRO
LYS
LYS
LYS
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13670	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0293	Depositor
Map size (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.76, 1.76, 1.76	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	Au	0.54	1/48227 (0.0%)	0.92	2/74345 (0.0%)
2	Av	0.52	0/49010	0.90	5/75728 (0.0%)
3	A	0.24	0/946	0.53	0/1269
3	Ae	0.23	0/946	0.48	0/1269
3	B	0.23	0/972	0.50	0/1302
3	C	0.28	0/993	0.58	1/1329 (0.1%)
3	D	0.25	0/950	0.53	0/1274
3	E	0.24	0/983	0.52	0/1318
3	F	0.23	0/926	0.50	0/1243
3	G	0.23	0/993	0.52	0/1329
3	H	0.24	0/968	0.50	0/1297
3	I	0.24	0/993	0.50	0/1329
3	K	0.54	2/987 (0.2%)	0.70	5/1321 (0.4%)
3	L	0.42	2/1001 (0.2%)	0.55	0/1339
3	aj	0.28	0/950	0.53	0/1274
3	ak	0.23	0/950	0.54	0/1274
3	al	0.23	0/860	0.49	0/1158
3	am	0.32	0/983	0.54	0/1316
3	an	0.24	0/968	0.52	0/1297
3	ao	0.23	0/959	0.51	0/1286
3	ap	0.23	0/983	0.51	0/1316
3	aq	0.25	0/910	0.52	0/1222
3	ar	0.23	0/993	0.53	0/1329
3	as	0.24	0/926	0.51	0/1243
3	at	0.24	0/972	0.53	0/1302
3	au	0.23	0/869	0.51	0/1171
4	Aa	0.24	0/825	0.49	0/1101
4	Ab	0.23	0/969	0.46	0/1292
4	Ac	0.23	0/799	0.47	0/1068
4	Ad	0.24	0/816	0.47	0/1090
4	Af	0.23	0/777	0.46	0/1041
4	Ag	0.23	0/834	0.46	0/1113
4	At	0.35	0/969	0.55	0/1292
4	J	0.23	0/825	0.49	0/1101

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	M	0.25	0/969	0.47	0/1292
4	N	0.37	0/841	0.53	0/1123
4	O	0.23	0/825	0.50	0/1101
4	P	0.23	0/841	0.45	0/1123
4	Q	0.24	0/969	0.47	0/1292
4	R	0.23	0/799	0.45	0/1068
4	S	0.25	0/969	0.52	1/1292 (0.1%)
4	T	0.23	0/969	0.48	0/1292
4	U	0.24	0/969	0.50	0/1292
4	V	0.26	0/969	0.48	0/1292
4	W	0.37	1/969 (0.1%)	0.47	0/1292
4	av	0.24	0/825	0.50	0/1101
4	aw	0.24	0/969	0.48	0/1292
4	ax	0.25	0/969	0.50	1/1292 (0.1%)
4	ay	0.34	1/969 (0.1%)	0.54	0/1292
4	az	0.23	0/799	0.45	0/1068
5	X	0.24	0/914	0.53	0/1225
5	Y	0.25	0/909	0.57	1/1218 (0.1%)
5	Z	0.23	0/747	0.50	0/1000
5	a	0.26	0/1009	0.58	1/1351 (0.1%)
5	b	0.23	0/845	0.53	0/1132
5	c	0.23	0/873	0.51	0/1170
5	d	0.23	0/820	0.51	0/1099
5	e	0.24	0/777	0.52	0/1041
5	f	0.23	0/820	0.50	0/1099
5	g	0.23	0/849	0.51	0/1137
5	h	0.24	0/812	0.52	0/1088
5	i	0.23	0/829	0.52	0/1111
5	j	0.24	0/865	0.54	0/1159
5	k	0.23	0/829	0.52	0/1111
5	l	0.25	0/930	0.58	1/1246 (0.1%)
5	m	0.25	0/820	0.58	1/1099 (0.1%)
5	n	0.23	0/923	0.52	0/1236
5	o	0.24	0/893	0.52	0/1197
5	p	0.23	0/849	0.53	0/1137
5	q	0.27	0/904	0.52	0/1211
5	r	0.23	0/873	0.50	0/1170
5	s	0.23	0/790	0.50	0/1059
5	t	0.23	0/903	0.52	0/1211
5	u	0.24	0/1015	0.55	0/1359
6	0	0.23	0/749	0.56	0/997
6	1	0.23	0/711	0.56	0/948
6	2	0.43	1/758 (0.1%)	0.88	3/1008 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	3	0.24	0/744	0.56	0/992
6	4	0.23	0/711	0.55	0/948
6	5	0.23	0/758	0.56	0/1008
6	6	0.23	0/695	0.57	0/929
6	7	0.25	0/794	0.58	0/1053
6	8	0.24	0/702	0.58	0/937
6	9	0.23	0/800	0.56	0/1061
6	CD	0.25	0/770	0.59	0/1024
6	a2	0.24	0/790	0.57	0/1048
6	a3	0.23	0/711	0.54	0/948
6	a4	0.23	0/762	0.54	0/1013
6	a5	0.24	0/733	0.56	0/976
6	a6	0.24	0/794	0.58	0/1053
6	a7	0.23	0/800	0.55	0/1061
6	a8	0.24	0/711	0.54	0/948
6	a9	0.24	0/724	0.57	0/965
6	v	0.24	0/775	0.59	0/1029
6	w	0.24	0/808	0.55	0/1071
6	x	0.23	0/779	0.55	0/1034
6	y	0.24	0/800	0.55	0/1061
6	z	0.24	0/680	0.58	0/908
7	Ah	0.26	0/1005	0.63	0/1335
7	Ai	0.25	0/1315	0.65	0/1740
7	Aj	0.58	3/790 (0.4%)	1.17	6/1053 (0.6%)
7	Ak	0.27	0/999	0.67	1/1327 (0.1%)
7	Al	0.27	0/819	0.63	0/1092
7	Am	0.26	0/1357	0.64	0/1794
7	An	0.27	0/988	0.67	2/1313 (0.2%)
7	Ao	0.25	0/1232	0.63	0/1634
7	Ap	0.26	0/562	0.61	0/749
7	Aq	0.26	0/1475	0.62	0/1947
7	Ar	0.26	0/1390	0.65	1/1830 (0.1%)
7	As	0.30	0/1013	0.75	3/1347 (0.2%)
All	All	0.42	11/193454 (0.0%)	0.77	35/278529 (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
3	K	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	5284	ALA	C-N	12.67	1.55	1.33
7	Aj	143	PRO	CB-CG	-10.93	0.95	1.50
6	2	696	PRO	CG-CD	-9.43	1.19	1.50
4	W	2976	LYS	C-N	7.70	1.51	1.34
3	K	5285	GLY	C-N	7.39	1.51	1.34

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Aj	143	PRO	CA-N-CD	-17.36	87.20	111.50
7	Aj	143	PRO	N-CD-CG	-15.91	79.33	103.20
6	2	696	PRO	N-CD-CG	-15.83	79.45	103.20
7	Aj	143	PRO	CA-CB-CG	-15.53	74.50	104.00
7	As	130	PRO	CA-N-CD	-12.89	93.45	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	5285	GLY	Mainchain

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	Au	43052	0	23722	0	0
2	Av	43620	0	23665	0	0
3	A	936	0	1008	8	0
3	Ae	936	0	1008	0	0
3	B	962	0	1035	17	0
3	C	983	0	1056	28	0
3	D	940	0	1011	6	0
3	E	973	0	1043	11	0
3	F	916	0	985	5	0
3	G	983	0	1056	15	0
3	H	958	0	1032	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	983	0	1056	7	0
3	K	977	0	1051	14	0
3	L	991	0	1065	17	0
3	aj	940	0	1011	0	0
3	ak	940	0	1011	0	0
3	al	851	0	909	0	0
3	am	973	0	1048	0	0
3	an	958	0	1032	0	0
3	ao	949	0	1019	0	0
3	ap	973	0	1048	0	0
3	aq	900	0	967	0	0
3	ar	983	0	1056	0	0
3	as	916	0	985	0	0
3	at	962	0	1035	0	0
3	au	859	0	921	0	0
4	Aa	814	0	856	0	0
4	Ab	956	0	1021	0	0
4	Ac	788	0	826	0	0
4	Ad	805	0	843	0	0
4	Af	766	0	797	0	0
4	Ag	823	0	864	0	0
4	At	956	0	1024	0	0
4	J	814	0	856	10	0
4	M	956	0	1024	15	0
4	N	830	0	871	22	0
4	O	814	0	856	27	0
4	P	830	0	871	7	0
4	Q	956	0	1021	12	0
4	R	788	0	826	10	0
4	S	956	0	1021	17	0
4	T	956	0	1021	14	0
4	U	956	0	1021	8	0
4	V	956	0	1021	19	0
4	W	956	0	1021	25	0
4	av	814	0	856	0	0
4	aw	956	0	1021	0	0
4	ax	956	0	1021	0	0
4	ay	956	0	1021	0	0
4	az	788	0	826	0	0
5	X	901	0	951	9	0
5	Y	896	0	946	7	0
5	Z	739	0	779	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	a	995	0	1059	0	0
5	b	833	0	880	0	0
5	c	860	0	906	0	0
5	d	808	0	846	0	0
5	e	768	0	809	0	0
5	f	808	0	846	0	0
5	g	837	0	883	0	0
5	h	801	0	838	0	0
5	i	817	0	858	0	0
5	j	853	0	898	0	0
5	k	817	0	858	0	0
5	l	917	0	971	0	0
5	m	808	0	846	0	0
5	n	910	0	964	0	0
5	o	880	0	928	0	0
5	p	837	0	883	0	0
5	q	891	0	941	0	0
5	r	860	0	906	0	0
5	s	780	0	818	0	0
5	t	890	0	941	0	0
5	u	1001	0	1064	0	0
6	0	741	0	796	7	0
6	1	703	0	755	6	0
6	2	750	0	809	14	0
6	3	736	0	793	7	0
6	4	703	0	755	7	0
6	5	750	0	809	7	0
6	6	688	0	745	6	0
6	7	786	0	847	12	0
6	8	694	0	742	13	0
6	9	792	0	852	14	0
6	CD	762	0	825	15	0
6	a2	782	0	844	0	0
6	a3	703	0	755	0	0
6	a4	754	0	812	0	0
6	a5	725	0	779	0	0
6	a6	786	0	847	0	0
6	a7	792	0	852	0	0
6	a8	703	0	755	0	0
6	a9	716	0	766	0	0
6	v	767	0	828	0	0
6	w	800	0	861	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	x	771	0	831	0	0
6	y	792	0	852	0	0
6	z	673	0	722	0	0
7	Ah	992	0	1087	0	0
7	Ai	1298	0	1466	0	0
7	Aj	780	0	838	0	0
7	Ak	986	0	1082	0	0
7	Al	808	0	866	0	0
7	Am	1340	0	1519	0	0
7	An	975	0	1072	0	0
7	Ao	1215	0	1363	0	0
7	Ap	555	0	584	0	0
7	Aq	1456	0	1660	0	0
7	Ar	1375	0	1585	0	0
7	As	999	0	1097	0	0
All	All	181715	0	149311	363	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 12.

The worst 5 of 363 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)
3:C:279:GLN:HE22	4:O:419:GLN:CD	1.10	1.51
3:C:279:GLN:NE2	4:O:419:GLN:NE2	1.80	1.28
3:C:279:GLN:NE2	4:O:419:GLN:CD	1.92	1.22
3:C:279:GLN:HE22	4:O:419:GLN:NE2	1.38	1.18
3:C:279:GLN:NE2	4:O:419:GLN:OE1	1.80	1.11

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	
3	A	120/130 (92%)	110 (92%)	10 (8%)	0	100	100
3	Ae	120/130 (92%)	113 (94%)	7 (6%)	0	100	100
3	B	124/130 (95%)	115 (93%)	9 (7%)	0	100	100
3	C	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
3	D	121/130 (93%)	115 (95%)	6 (5%)	0	100	100
3	E	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
3	F	117/130 (90%)	110 (94%)	7 (6%)	0	100	100
3	G	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
3	H	123/130 (95%)	119 (97%)	4 (3%)	0	100	100
3	I	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
3	K	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
3	L	128/130 (98%)	124 (97%)	4 (3%)	0	100	100
3	aj	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
3	ak	121/130 (93%)	114 (94%)	7 (6%)	0	100	100
3	al	109/130 (84%)	106 (97%)	3 (3%)	0	100	100
3	am	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	51
3	an	123/130 (95%)	112 (91%)	11 (9%)	0	100	100
3	ao	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
3	ap	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
3	aq	115/130 (88%)	111 (96%)	4 (4%)	0	100	100
3	ar	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
3	as	117/130 (90%)	113 (97%)	4 (3%)	0	100	100
3	at	124/130 (95%)	114 (92%)	10 (8%)	0	100	100
3	au	109/130 (84%)	104 (95%)	5 (5%)	0	100	100
4	Aa	101/123 (82%)	97 (96%)	4 (4%)	0	100	100
4	Ab	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
4	Ac	98/123 (80%)	98 (100%)	0	0	100	100
4	Ad	100/123 (81%)	97 (97%)	3 (3%)	0	100	100
4	Af	95/123 (77%)	92 (97%)	3 (3%)	0	100	100
4	Ag	102/123 (83%)	99 (97%)	3 (3%)	0	100	100
4	At	121/123 (98%)	112 (93%)	7 (6%)	2 (2%)	7	37
4	J	101/123 (82%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
4	N	103/123 (84%)	97 (94%)	5 (5%)	1 (1%)	13	46
4	O	101/123 (82%)	94 (93%)	7 (7%)	0	100	100
4	P	103/123 (84%)	101 (98%)	2 (2%)	0	100	100
4	Q	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
4	R	98/123 (80%)	94 (96%)	4 (4%)	0	100	100
4	S	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
4	T	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
4	U	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
4	V	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
4	W	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
4	av	101/123 (82%)	96 (95%)	5 (5%)	0	100	100
4	aw	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
4	ax	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	16	51
4	ay	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
4	az	98/123 (80%)	96 (98%)	2 (2%)	0	100	100
5	X	110/136 (81%)	105 (96%)	5 (4%)	0	100	100
5	Y	109/136 (80%)	105 (96%)	4 (4%)	0	100	100
5	Z	88/136 (65%)	87 (99%)	1 (1%)	0	100	100
5	a	123/136 (90%)	116 (94%)	7 (6%)	0	100	100
5	b	99/136 (73%)	97 (98%)	2 (2%)	0	100	100
5	c	104/136 (76%)	101 (97%)	3 (3%)	0	100	100
5	d	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
5	e	92/136 (68%)	89 (97%)	3 (3%)	0	100	100
5	f	96/136 (71%)	96 (100%)	0	0	100	100
5	g	100/136 (74%)	98 (98%)	2 (2%)	0	100	100
5	h	95/136 (70%)	95 (100%)	0	0	100	100
5	i	97/136 (71%)	95 (98%)	2 (2%)	0	100	100
5	j	103/136 (76%)	100 (97%)	3 (3%)	0	100	100
5	k	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
5	l	112/136 (82%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	m	96/136 (71%)	90 (94%)	6 (6%)	0	100	100
5	n	111/136 (82%)	104 (94%)	7 (6%)	0	100	100
5	o	107/136 (79%)	100 (94%)	7 (6%)	0	100	100
5	p	100/136 (74%)	98 (98%)	2 (2%)	0	100	100
5	q	108/136 (79%)	101 (94%)	7 (6%)	0	100	100
5	r	104/136 (76%)	100 (96%)	4 (4%)	0	100	100
5	s	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
5	t	108/136 (79%)	101 (94%)	7 (6%)	0	100	100
5	u	124/136 (91%)	120 (97%)	4 (3%)	0	100	100
6	0	92/103 (89%)	90 (98%)	1 (1%)	1 (1%)	12	45
6	1	85/103 (82%)	84 (99%)	1 (1%)	0	100	100
6	2	93/103 (90%)	85 (91%)	8 (9%)	0	100	100
6	3	91/103 (88%)	88 (97%)	3 (3%)	0	100	100
6	4	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
6	5	93/103 (90%)	89 (96%)	4 (4%)	0	100	100
6	6	83/103 (81%)	81 (98%)	2 (2%)	0	100	100
6	7	99/103 (96%)	95 (96%)	4 (4%)	0	100	100
6	8	84/103 (82%)	82 (98%)	2 (2%)	0	100	100
6	9	100/103 (97%)	95 (95%)	5 (5%)	0	100	100
6	CD	95/103 (92%)	85 (90%)	9 (10%)	1 (1%)	12	45
6	a2	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
6	a3	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
6	a4	94/103 (91%)	90 (96%)	4 (4%)	0	100	100
6	a5	89/103 (86%)	88 (99%)	1 (1%)	0	100	100
6	a6	99/103 (96%)	96 (97%)	3 (3%)	0	100	100
6	a7	100/103 (97%)	91 (91%)	9 (9%)	0	100	100
6	a8	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
6	a9	88/103 (85%)	86 (98%)	2 (2%)	0	100	100
6	v	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
6	w	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
6	x	97/103 (94%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	y	100/103 (97%)	95 (95%)	5 (5%)	0	100	100
6	z	82/103 (80%)	79 (96%)	3 (4%)	0	100	100
7	Ah	128/196 (65%)	119 (93%)	9 (7%)	0	100	100
7	Ai	168/196 (86%)	147 (88%)	21 (12%)	0	100	100
7	Aj	101/196 (52%)	92 (91%)	9 (9%)	0	100	100
7	Ak	127/196 (65%)	114 (90%)	13 (10%)	0	100	100
7	Al	105/196 (54%)	94 (90%)	11 (10%)	0	100	100
7	Am	173/196 (88%)	150 (87%)	23 (13%)	0	100	100
7	An	126/196 (64%)	110 (87%)	16 (13%)	0	100	100
7	Ao	157/196 (80%)	138 (88%)	18 (12%)	1 (1%)	22	55
7	Ap	71/196 (36%)	67 (94%)	4 (6%)	0	100	100
7	Aq	188/196 (96%)	172 (92%)	16 (8%)	0	100	100
7	Ar	176/196 (90%)	144 (82%)	32 (18%)	0	100	100
7	As	129/196 (66%)	111 (86%)	17 (13%)	1 (1%)	16	51
All	All	11912/14160 (84%)	11227 (94%)	676 (6%)	9 (0%)	50	79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	205	PRO
6	O	499	ARG
3	am	797	ALA
4	At	20	LYS
6	CD	312	ILE

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	A	97/102 (95%)	96 (99%)	1 (1%)	73	85
3	Ae	97/102 (95%)	96 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	99/102 (97%)	98 (99%)	1 (1%)	73	85
3	C	101/102 (99%)	99 (98%)	2 (2%)	50	72
3	D	97/102 (95%)	95 (98%)	2 (2%)	48	71
3	E	100/102 (98%)	99 (99%)	1 (1%)	73	85
3	F	95/102 (93%)	94 (99%)	1 (1%)	70	83
3	G	101/102 (99%)	100 (99%)	1 (1%)	73	85
3	H	99/102 (97%)	95 (96%)	4 (4%)	27	56
3	I	101/102 (99%)	99 (98%)	2 (2%)	50	72
3	K	100/102 (98%)	100 (100%)	0	100	100
3	L	102/102 (100%)	101 (99%)	1 (1%)	73	85
3	aj	97/102 (95%)	94 (97%)	3 (3%)	35	62
3	ak	97/102 (95%)	92 (95%)	5 (5%)	19	49
3	al	86/102 (84%)	86 (100%)	0	100	100
3	am	100/102 (98%)	98 (98%)	2 (2%)	50	72
3	an	99/102 (97%)	96 (97%)	3 (3%)	36	63
3	ao	98/102 (96%)	98 (100%)	0	100	100
3	ap	100/102 (98%)	100 (100%)	0	100	100
3	aq	94/102 (92%)	93 (99%)	1 (1%)	70	83
3	ar	101/102 (99%)	99 (98%)	2 (2%)	50	72
3	as	95/102 (93%)	95 (100%)	0	100	100
3	at	99/102 (97%)	98 (99%)	1 (1%)	73	85
3	au	88/102 (86%)	87 (99%)	1 (1%)	70	83
4	Aa	88/103 (85%)	86 (98%)	2 (2%)	45	68
4	Ab	103/103 (100%)	102 (99%)	1 (1%)	73	85
4	Ac	85/103 (82%)	84 (99%)	1 (1%)	67	82
4	Ad	87/103 (84%)	87 (100%)	0	100	100
4	Af	83/103 (81%)	82 (99%)	1 (1%)	67	82
4	Ag	89/103 (86%)	87 (98%)	2 (2%)	47	69
4	At	103/103 (100%)	100 (97%)	3 (3%)	37	63
4	J	88/103 (85%)	87 (99%)	1 (1%)	70	83
4	M	103/103 (100%)	101 (98%)	2 (2%)	52	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	90/103 (87%)	90 (100%)	0	100	100
4	O	88/103 (85%)	86 (98%)	2 (2%)	45	68
4	P	90/103 (87%)	88 (98%)	2 (2%)	47	69
4	Q	103/103 (100%)	102 (99%)	1 (1%)	73	85
4	R	85/103 (82%)	83 (98%)	2 (2%)	44	67
4	S	103/103 (100%)	101 (98%)	2 (2%)	52	73
4	T	103/103 (100%)	102 (99%)	1 (1%)	73	85
4	U	103/103 (100%)	102 (99%)	1 (1%)	73	85
4	V	103/103 (100%)	101 (98%)	2 (2%)	52	73
4	W	103/103 (100%)	103 (100%)	0	100	100
4	av	88/103 (85%)	87 (99%)	1 (1%)	70	83
4	aw	103/103 (100%)	101 (98%)	2 (2%)	52	73
4	ax	103/103 (100%)	102 (99%)	1 (1%)	73	85
4	ay	103/103 (100%)	101 (98%)	2 (2%)	52	73
4	az	85/103 (82%)	84 (99%)	1 (1%)	67	82
5	X	93/111 (84%)	89 (96%)	4 (4%)	25	54
5	Y	93/111 (84%)	92 (99%)	1 (1%)	70	83
5	Z	78/111 (70%)	76 (97%)	2 (3%)	41	65
5	a	102/111 (92%)	99 (97%)	3 (3%)	37	63
5	b	88/111 (79%)	86 (98%)	2 (2%)	45	68
5	c	90/111 (81%)	88 (98%)	2 (2%)	47	69
5	d	85/111 (77%)	85 (100%)	0	100	100
5	e	81/111 (73%)	79 (98%)	2 (2%)	42	66
5	f	85/111 (77%)	85 (100%)	0	100	100
5	g	88/111 (79%)	86 (98%)	2 (2%)	45	68
5	h	84/111 (76%)	81 (96%)	3 (4%)	30	59
5	i	86/111 (78%)	83 (96%)	3 (4%)	31	60
5	j	89/111 (80%)	87 (98%)	2 (2%)	47	69
5	k	86/111 (78%)	85 (99%)	1 (1%)	67	82
5	l	95/111 (86%)	92 (97%)	3 (3%)	34	61
5	m	85/111 (77%)	82 (96%)	3 (4%)	31	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	n	94/111 (85%)	93 (99%)	1 (1%)	70	83
5	o	92/111 (83%)	91 (99%)	1 (1%)	70	83
5	p	88/111 (79%)	87 (99%)	1 (1%)	70	83
5	q	93/111 (84%)	90 (97%)	3 (3%)	34	61
5	r	90/111 (81%)	86 (96%)	4 (4%)	24	53
5	s	82/111 (74%)	82 (100%)	0	100	100
5	t	93/111 (84%)	92 (99%)	1 (1%)	70	83
5	u	103/111 (93%)	99 (96%)	4 (4%)	27	57
6	0	74/79 (94%)	73 (99%)	1 (1%)	62	79
6	1	72/79 (91%)	71 (99%)	1 (1%)	62	79
6	2	75/79 (95%)	74 (99%)	1 (1%)	65	81
6	3	74/79 (94%)	74 (100%)	0	100	100
6	4	72/79 (91%)	71 (99%)	1 (1%)	62	79
6	5	75/79 (95%)	75 (100%)	0	100	100
6	6	71/79 (90%)	70 (99%)	1 (1%)	62	79
6	7	77/79 (98%)	74 (96%)	3 (4%)	27	57
6	8	71/79 (90%)	69 (97%)	2 (3%)	38	64
6	9	78/79 (99%)	76 (97%)	2 (3%)	41	65
6	CD	76/79 (96%)	74 (97%)	2 (3%)	41	65
6	a2	77/79 (98%)	76 (99%)	1 (1%)	65	81
6	a3	72/79 (91%)	71 (99%)	1 (1%)	62	79
6	a4	75/79 (95%)	74 (99%)	1 (1%)	65	81
6	a5	73/79 (92%)	73 (100%)	0	100	100
6	a6	77/79 (98%)	76 (99%)	1 (1%)	65	81
6	a7	78/79 (99%)	78 (100%)	0	100	100
6	a8	72/79 (91%)	69 (96%)	3 (4%)	25	54
6	a9	72/79 (91%)	70 (97%)	2 (3%)	38	64
6	v	76/79 (96%)	74 (97%)	2 (3%)	41	65
6	w	79/79 (100%)	78 (99%)	1 (1%)	65	81
6	x	76/79 (96%)	76 (100%)	0	100	100
6	y	78/79 (99%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	z	69/79 (87%)	68 (99%)	1 (1%)	62	79
7	Ah	104/158 (66%)	99 (95%)	5 (5%)	21	51
7	Ai	135/158 (85%)	129 (96%)	6 (4%)	24	53
7	Aj	82/158 (52%)	79 (96%)	3 (4%)	29	58
7	Ak	103/158 (65%)	101 (98%)	2 (2%)	52	73
7	Al	85/158 (54%)	80 (94%)	5 (6%)	16	45
7	Am	140/158 (89%)	136 (97%)	4 (3%)	37	63
7	An	102/158 (65%)	96 (94%)	6 (6%)	16	45
7	Ao	127/158 (80%)	126 (99%)	1 (1%)	79	88
7	Ap	57/158 (36%)	56 (98%)	1 (2%)	54	74
7	Aq	152/158 (96%)	146 (96%)	6 (4%)	27	57
7	Ar	144/158 (91%)	138 (96%)	6 (4%)	25	54
7	As	105/158 (66%)	99 (94%)	6 (6%)	17	46
All	All	9893/11376 (87%)	9699 (98%)	194 (2%)	50	72

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	am	786	ARG
7	Ah	417	LEU
3	an	950	ARG
4	ay	451	LYS
7	Ai	157	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
6	0	575	GLN
3	an	981	ASN
6	2	739	HIS
6	a8	1481	ASN
3	aq	4141	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

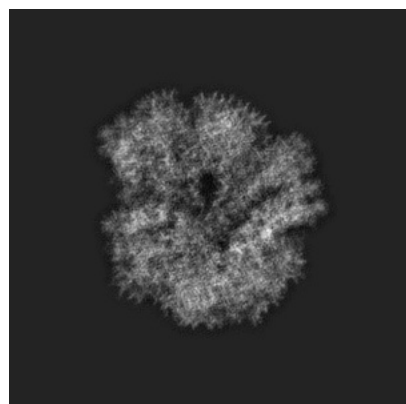
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38407. These allow visual inspection of the internal detail of the map and identification of artifacts.

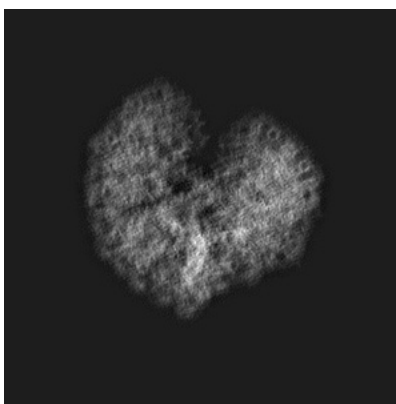
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

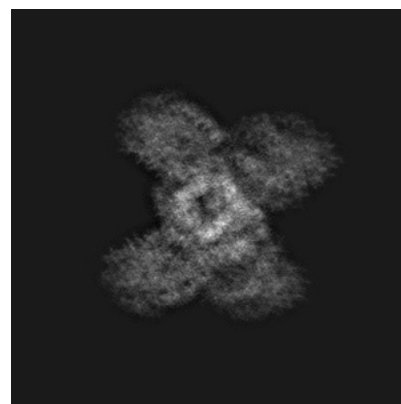
6.1.1 Primary map



X

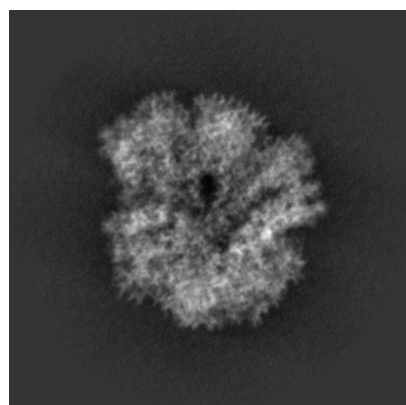


Y

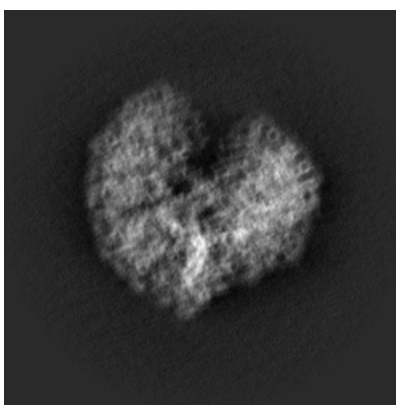


Z

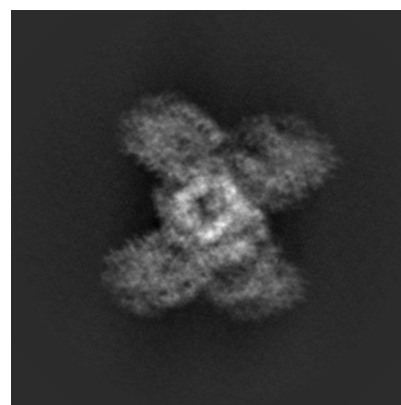
6.1.2 Raw map



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: 144

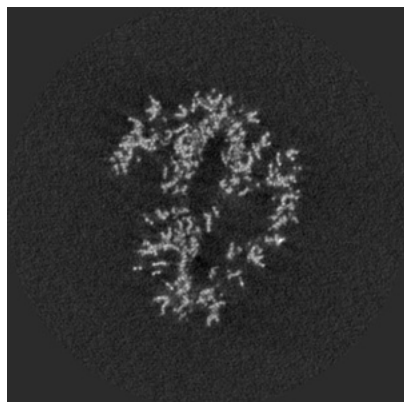


Y Index: 144

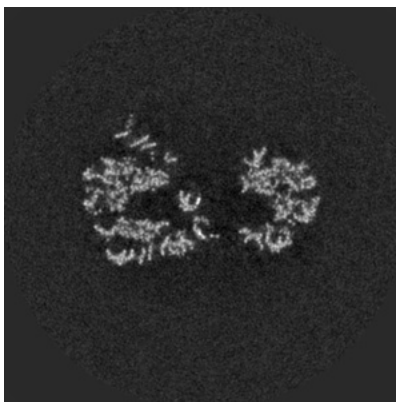


Z Index: 144

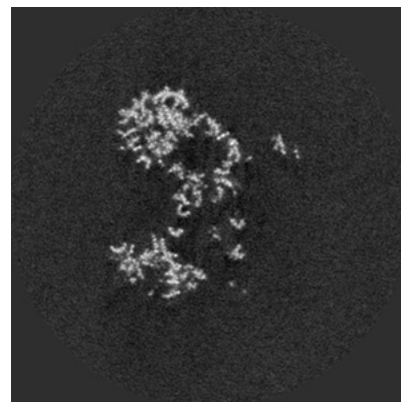
6.2.2 Raw map



X Index: 144



Y Index: 144

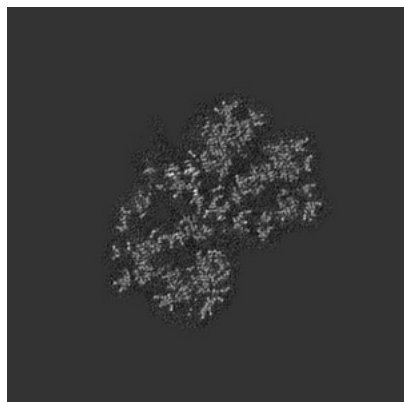


Z Index: 144

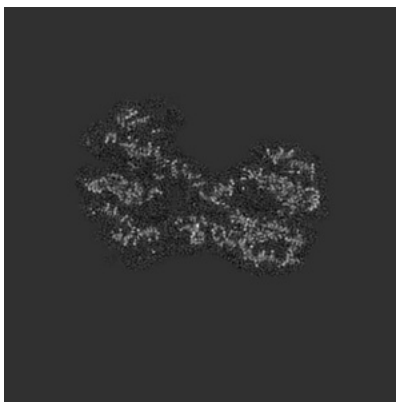
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

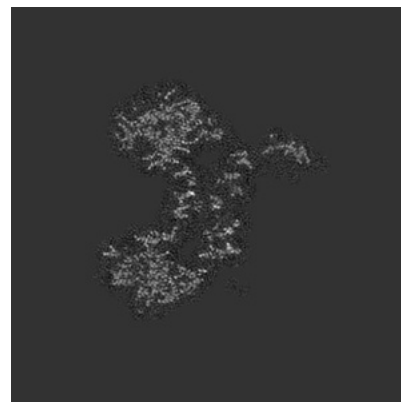
6.3.1 Primary map



X Index: 125

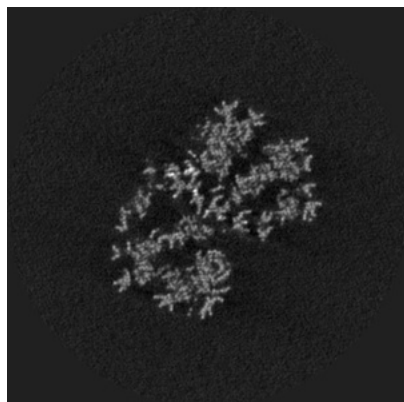


Y Index: 153

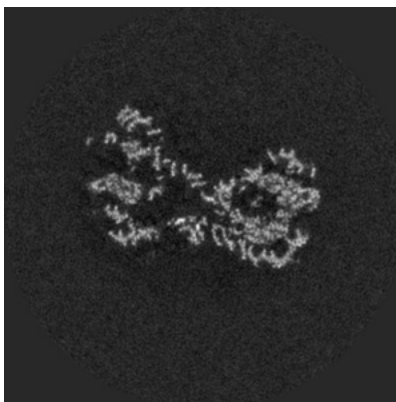


Z Index: 139

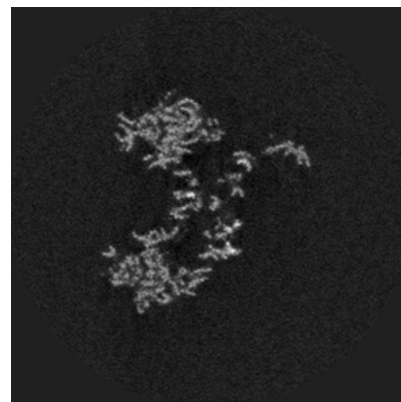
6.3.2 Raw map



X Index: 125



Y Index: 154

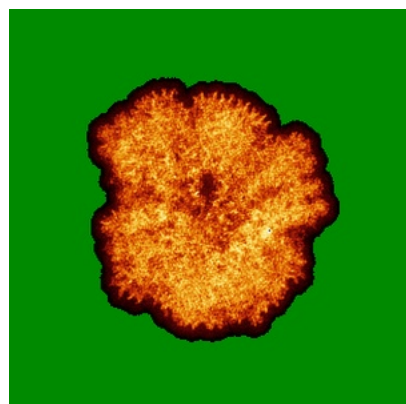


Z Index: 138

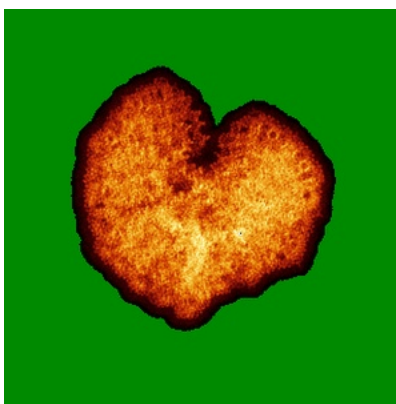
The images above show the largest variance slices of the map in three orthogonal directions.

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

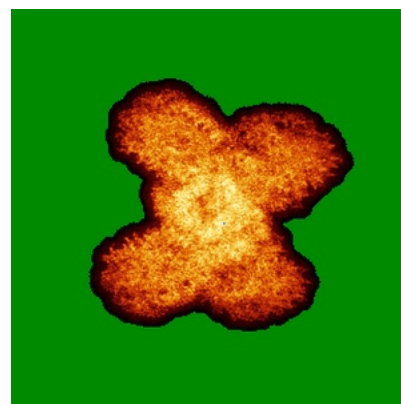
6.4.1 Primary map



X

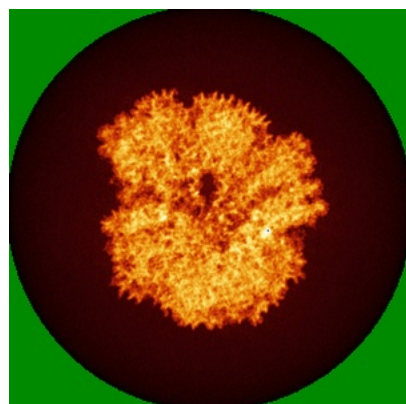


Y

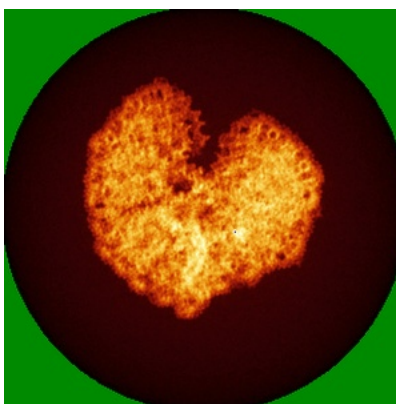


Z

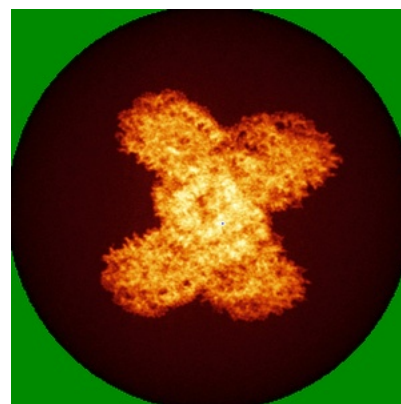
6.4.2 Raw map



X



Y

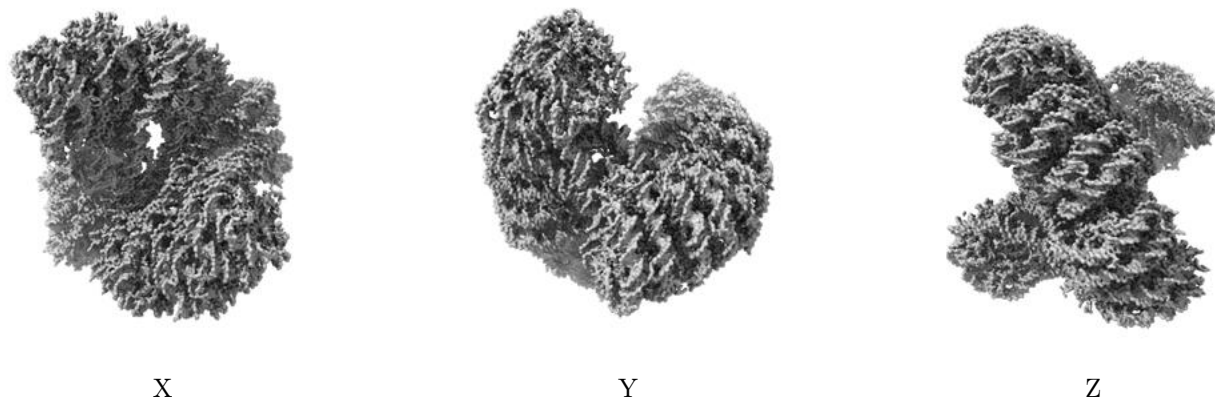


Z

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.

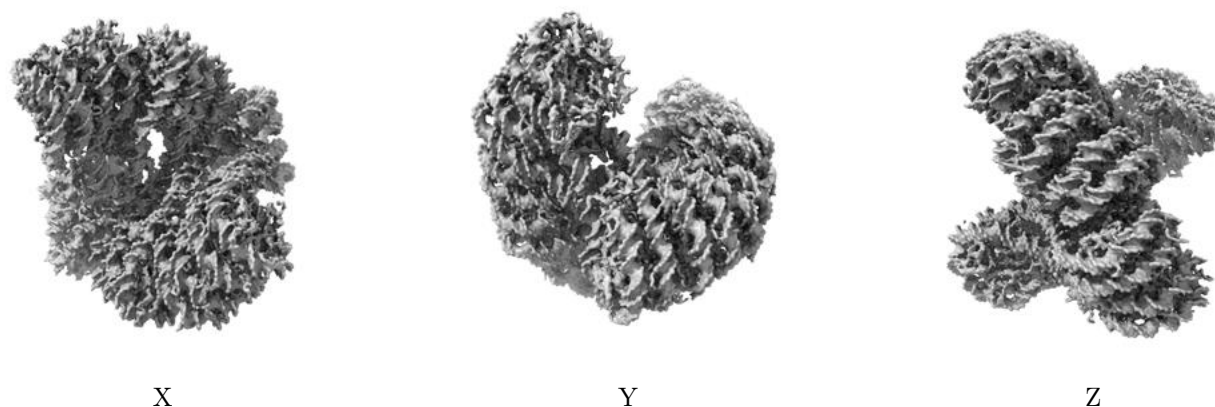
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0293. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

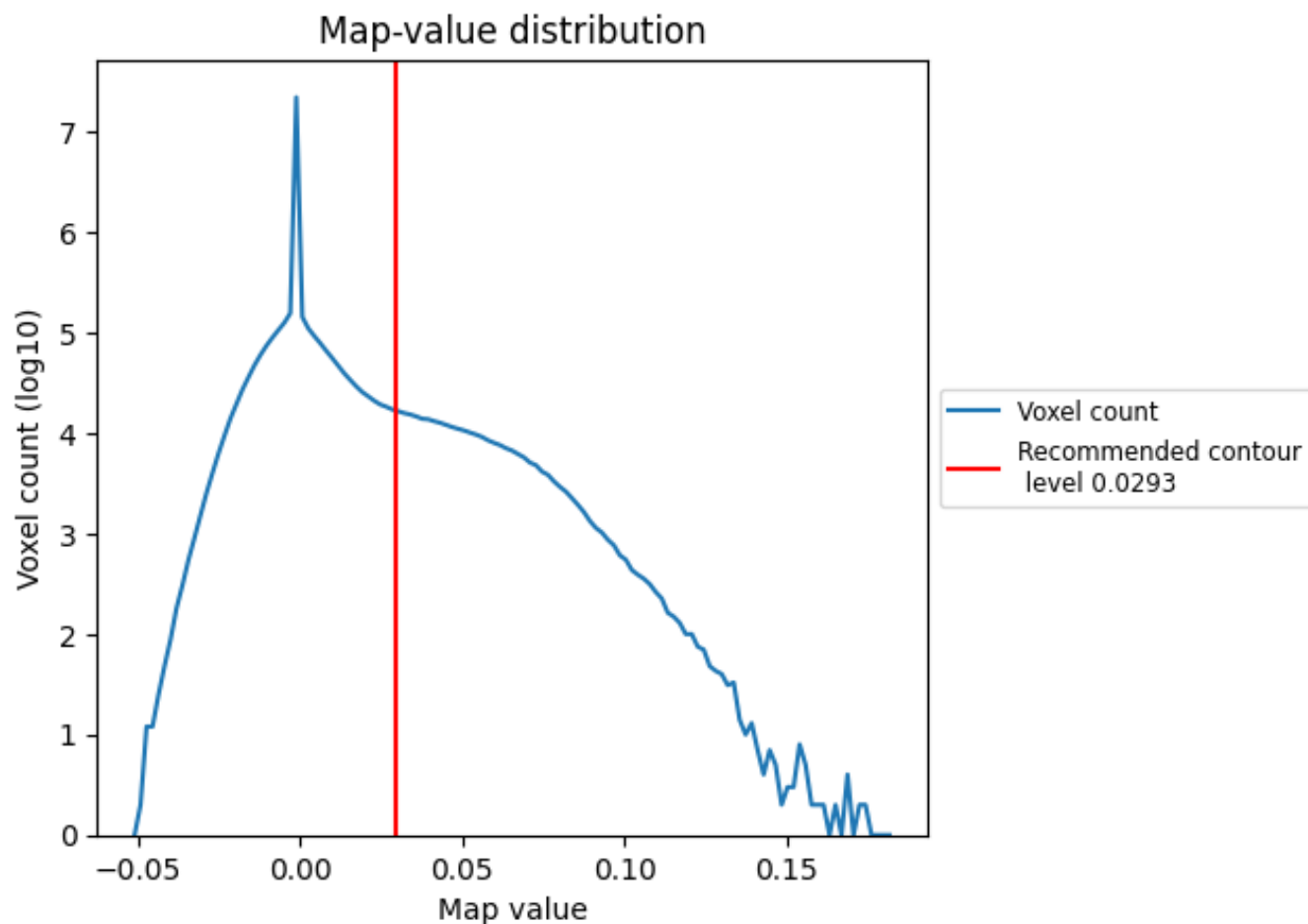
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

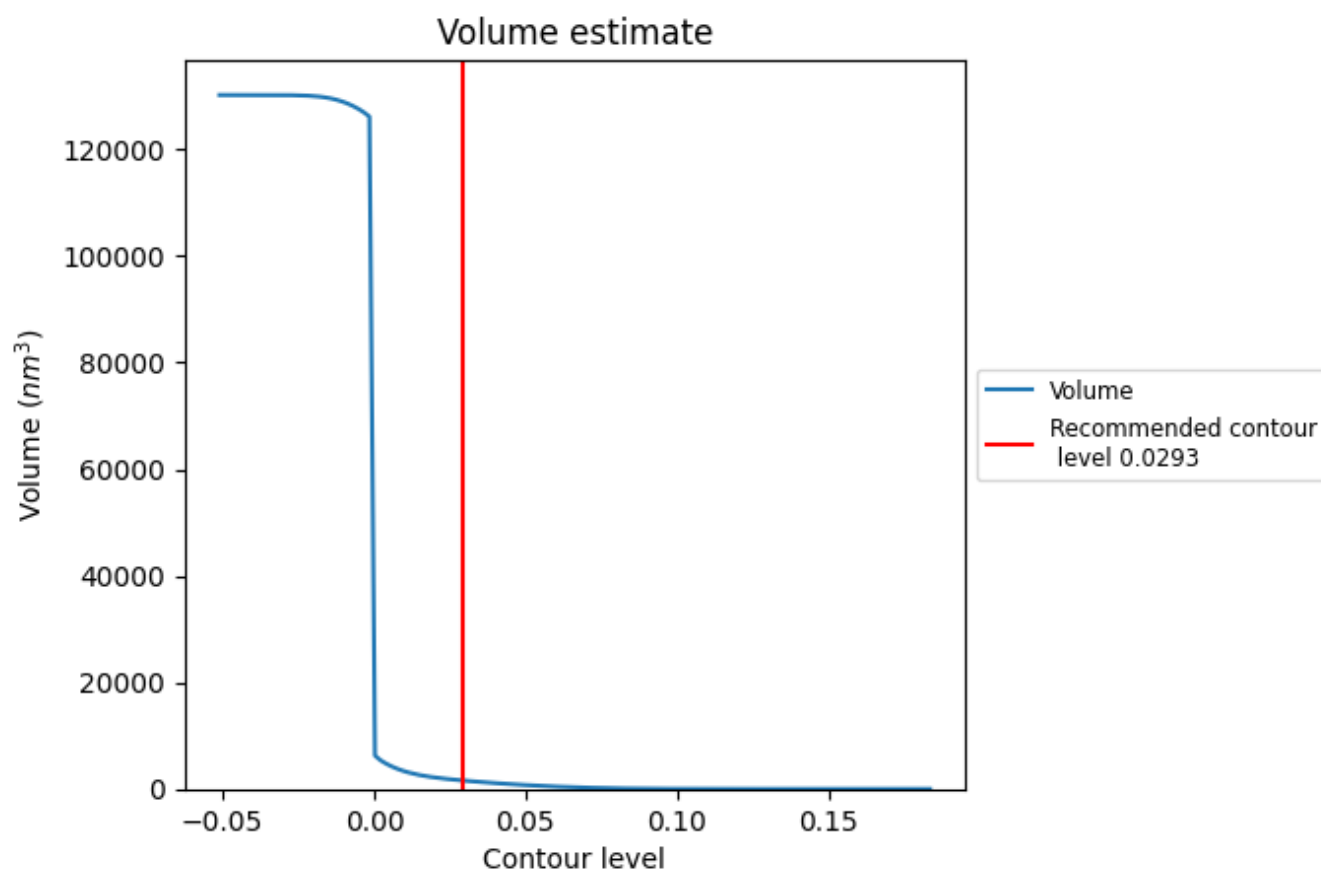
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

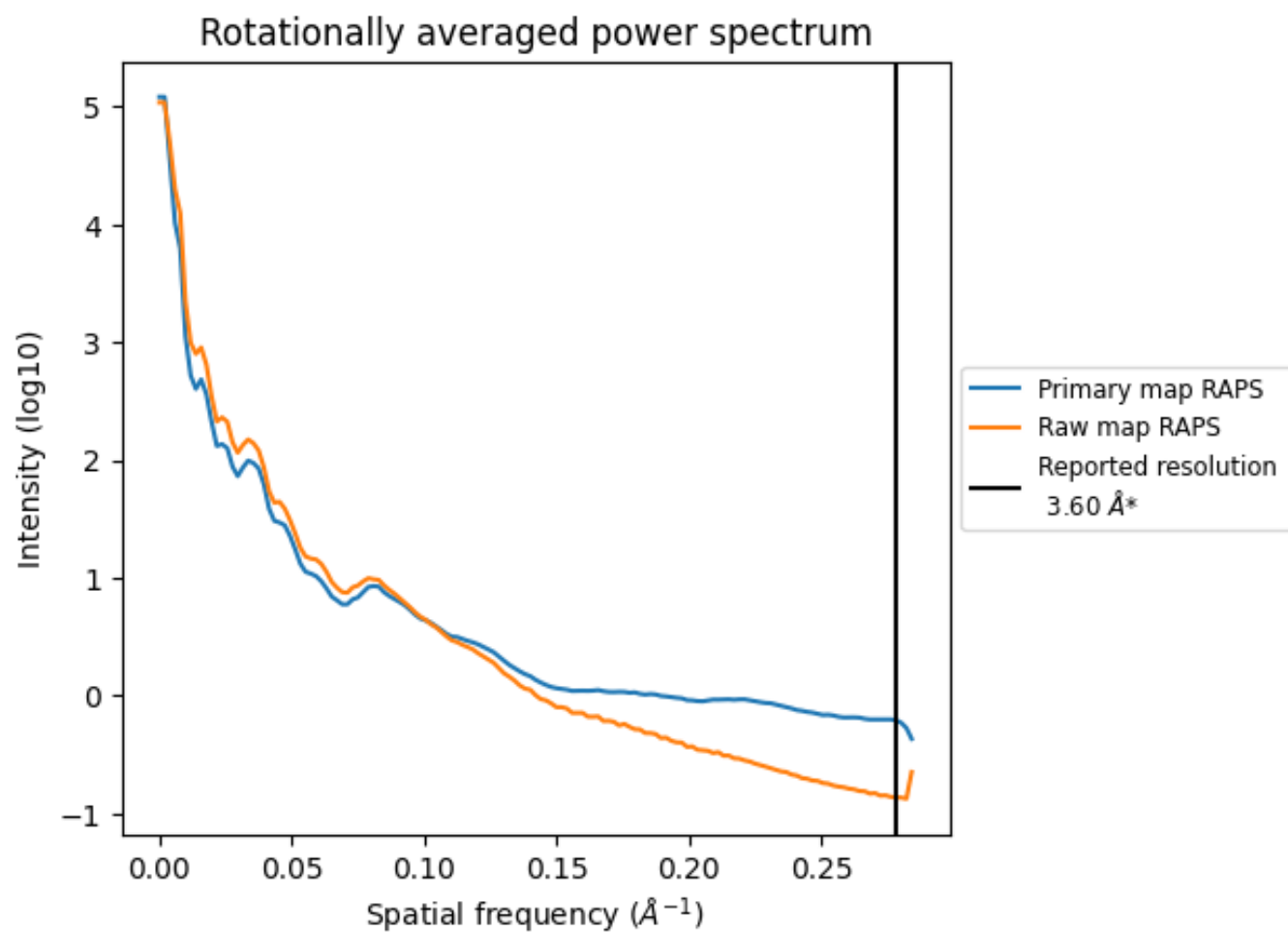
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1585 nm^3 ; this corresponds to an approximate mass of 1431 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](#)

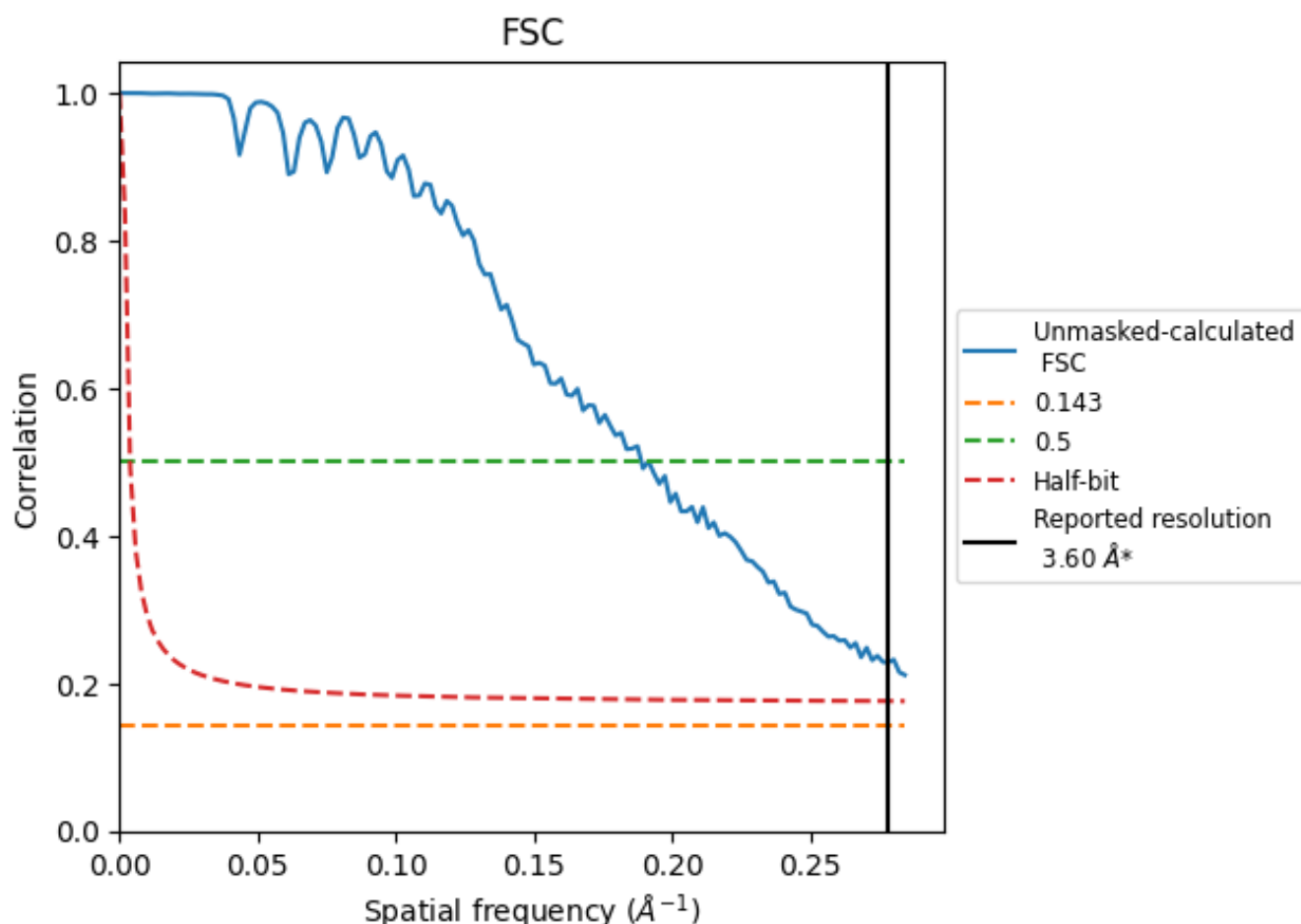


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

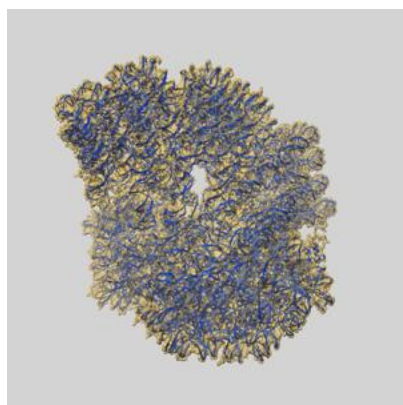
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	5.30	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

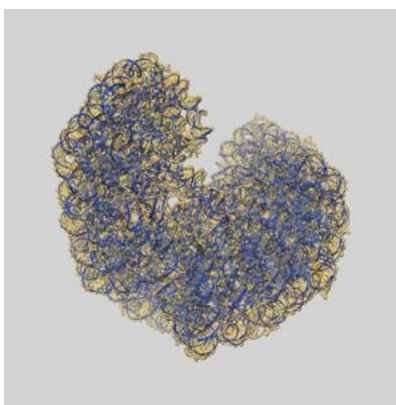
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38407 and PDB model 8XJV. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

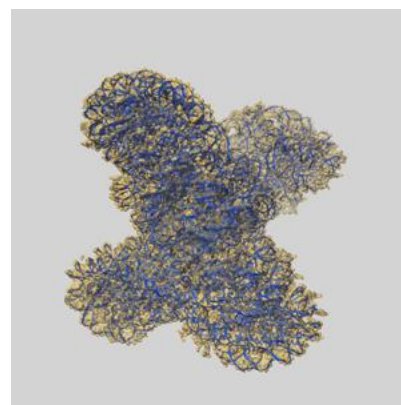
9.1 Map-model overlay [i](#)



X



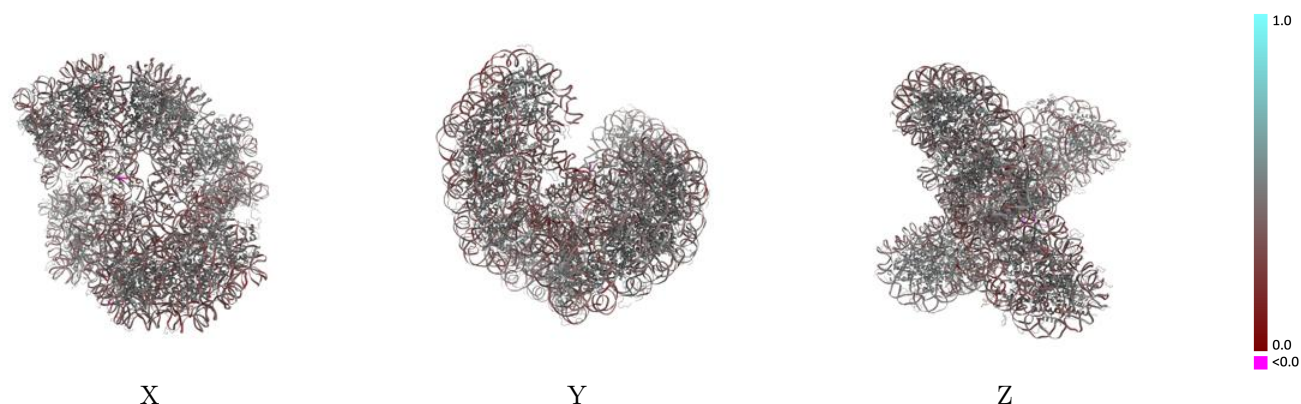
Y



Z

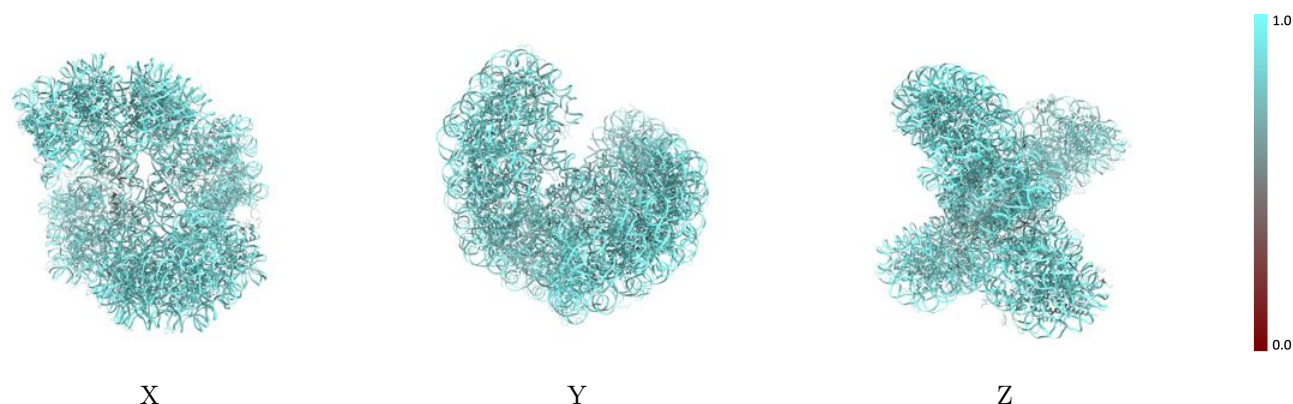
The images above show the 3D surface view of the map at the recommended contour level 0.0293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



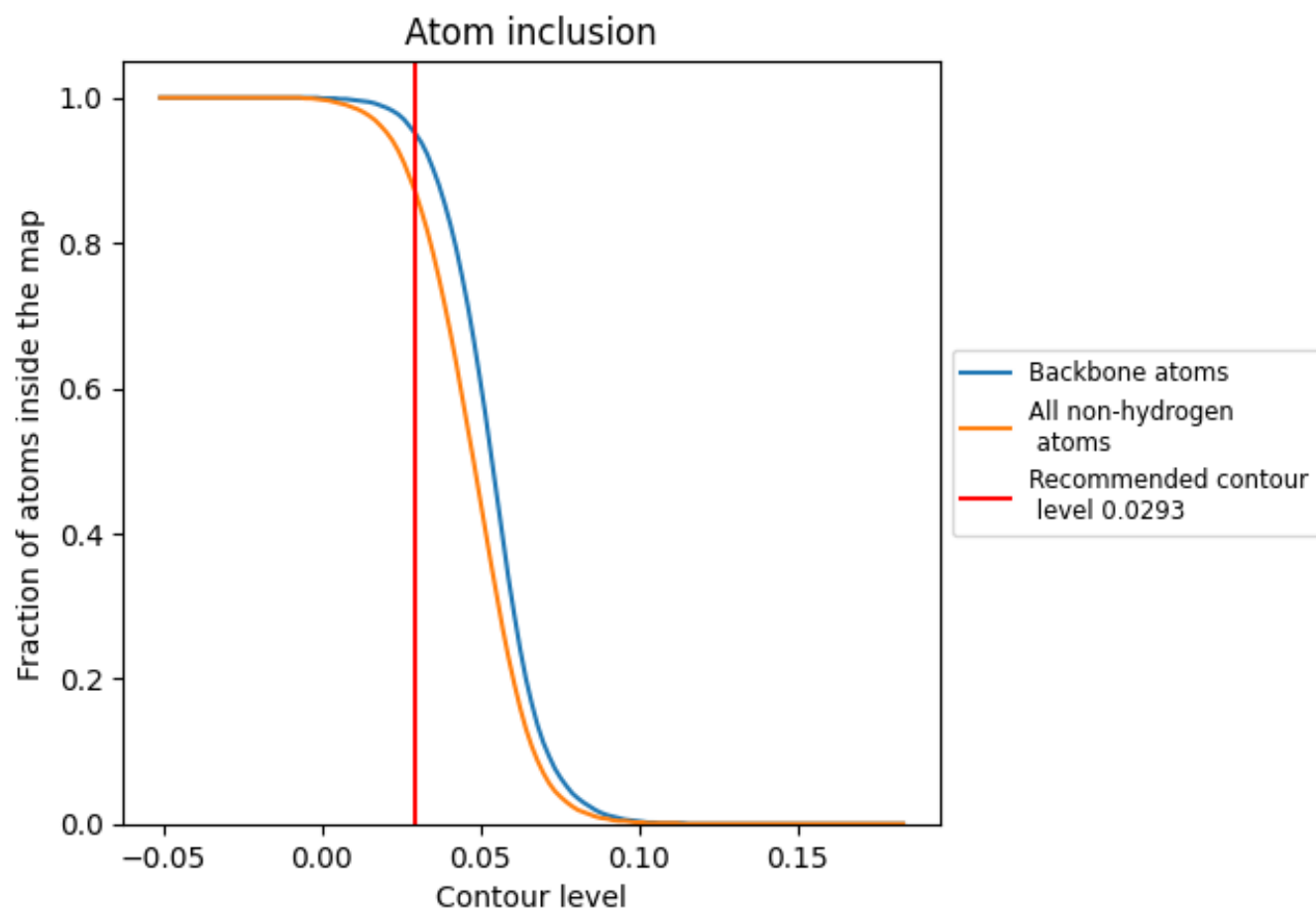
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0293).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.0293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.4240
0	 0.9070	 0.4750
1	 0.8100	 0.4720
2	 0.8650	 0.4430
3	 0.8950	 0.4770
4	 0.9020	 0.4890
5	 0.8970	 0.4900
6	 0.9040	 0.4700
7	 0.8970	 0.4640
8	 0.8890	 0.4680
9	 0.8960	 0.4720
A	 0.8140	 0.4670
Aa	 0.8920	 0.4720
Ab	 0.8650	 0.4650
Ac	 0.8970	 0.4690
Ad	 0.9080	 0.4860
Ae	 0.8740	 0.4860
Af	 0.9020	 0.4770
Ag	 0.8810	 0.4810
Ah	 0.7590	 0.4280
Ai	 0.7400	 0.4050
Aj	 0.8010	 0.4340
Ak	 0.7830	 0.4280
Al	 0.7160	 0.4070
Am	 0.7550	 0.4180
An	 0.7800	 0.4260
Ao	 0.7500	 0.4200
Ap	 0.7740	 0.4140
Aq	 0.7420	 0.4000
Ar	 0.7520	 0.4060
As	 0.7480	 0.3970
At	 0.8820	 0.4810
Au	 0.8820	 0.3730
Av	 0.8800	 0.3760
B	 0.8900	 0.5000







































































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Chain	Atom inclusion	Q-score
C	 0.9000	 0.5050
CD	 0.8740	 0.4630
D	 0.8850	 0.4740
E	 0.8020	 0.4670
F	 0.8990	 0.4880
G	 0.8870	 0.4880
H	 0.8840	 0.4740
I	 0.8830	 0.4770
J	 0.9290	 0.4860
K	 0.8780	 0.4930
L	 0.8440	 0.4840
M	 0.7980	 0.4500
N	 0.9120	 0.5040
O	 0.8850	 0.4940
P	 0.9160	 0.4930
Q	 0.8040	 0.4750
R	 0.9020	 0.4670
S	 0.8780	 0.4620
T	 0.8770	 0.4580
U	 0.8710	 0.4660
V	 0.8770	 0.4790
W	 0.8770	 0.4810
X	 0.8570	 0.4680
Y	 0.9040	 0.4800
Z	 0.9370	 0.4810
a	 0.8900	 0.4630
a2	 0.8690	 0.4540
a3	 0.8830	 0.4850
a4	 0.9160	 0.4870
a5	 0.8650	 0.4720
a6	 0.9070	 0.4910
a7	 0.8820	 0.4840
a8	 0.8380	 0.4770
a9	 0.8460	 0.4730
aj	 0.8780	 0.4850
ak	 0.8660	 0.4950
al	 0.8980	 0.5070
am	 0.8860	 0.5050
an	 0.8570	 0.4590
ao	 0.8730	 0.4820
ap	 0.8900	 0.4800
aq	 0.8590	 0.4680

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Chain	Atom inclusion	Q-score
ar	 0.8970	 0.4910
as	 0.8770	 0.4920
at	 0.8620	 0.4880
au	 0.8650	 0.4760
av	 0.9150	 0.4830
aw	 0.8880	 0.4820
ax	 0.8950	 0.4850
ay	 0.8730	 0.4890
az	 0.9200	 0.4860
b	 0.8070	 0.4510
c	 0.9090	 0.4850
d	 0.9020	 0.4740
e	 0.9110	 0.4890
f	 0.9200	 0.4770
g	 0.9120	 0.4910
h	 0.9260	 0.4800
i	 0.9330	 0.4960
j	 0.9050	 0.4690
k	 0.9060	 0.4890
l	 0.8790	 0.4600
m	 0.9320	 0.4970
n	 0.8690	 0.4740
o	 0.9080	 0.4860
p	 0.9190	 0.4920
q	 0.8860	 0.4760
r	 0.8900	 0.4740
s	 0.9110	 0.4810
t	 0.9090	 0.4670
u	 0.8680	 0.4580
v	 0.8140	 0.4370
w	 0.8920	 0.4860
x	 0.9100	 0.4910
y	 0.9130	 0.4900
z	 0.8190	 0.4590