



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:17 PM UTC

PDB ID : 8XJV / pdb_00008xjv
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:

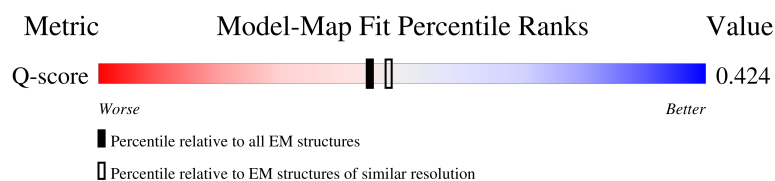
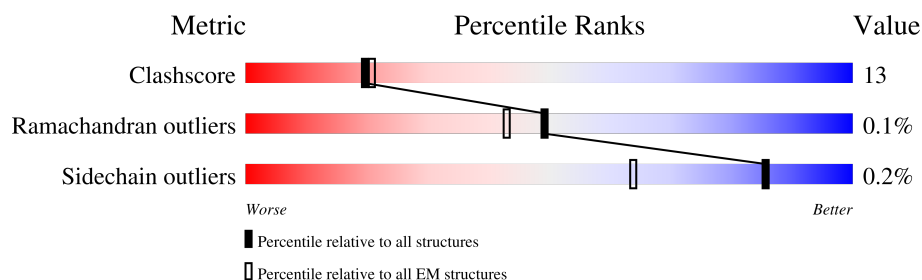
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

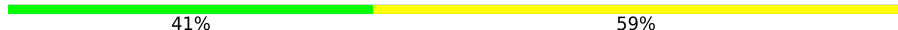
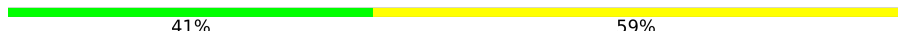
The reported resolution of this entry is 3.60 Å.

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.



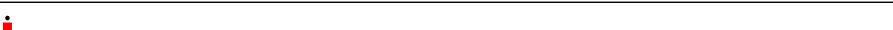
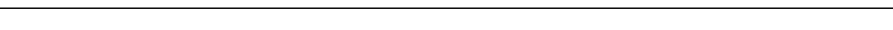
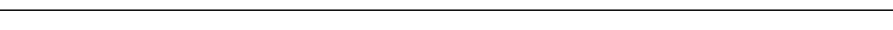
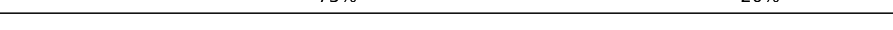
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	
2	Av	2124	
3	A	130	
3	Ae	130	

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Mol	Chain	Length	Quality of chain
3	B	130	 80% 17% .
3	C	130	 78% 20% ..
3	D	130	 88% 7% 5%
3	E	130	 82% 16% .
3	F	130	 75% 17% 8%
3	G	130	 82% 17% .
3	H	130	 78% 18% .
3	I	130	 86% 13% .
3	K	130	 78% 18% ...
3	L	130	 81% 18% .
3	aj	130	 74% 21% 5%
3	ak	130	 83% 12% 5%
3	al	130	 75% 10% 15%
3	am	130	 75% 20% ..
3	an	130	 83% 13% .
3	ao	130	 78% 18% 5%
3	ap	130	 78% 19% .
3	aq	130	 72% 18% 10%
3	ar	130	 84% 15% .
3	as	130	 77% 15% 8%
3	at	130	 78% 18% .
3	au	130	 75% 11% 15%
4	Aa	123	 66% 18% 16%
4	Ab	123	 76% 24%
4	Ac	123	 68% 13% 19%

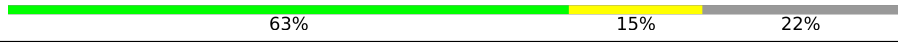
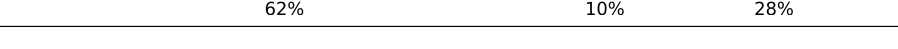
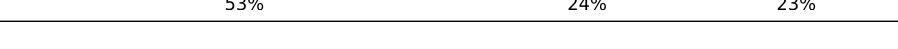
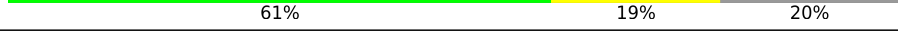
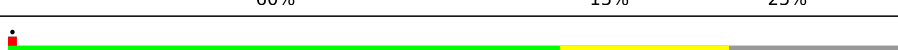
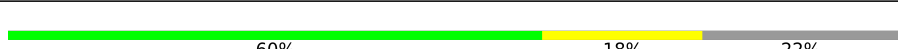
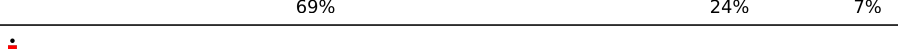
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Mol	Chain	Length	Quality of chain
4	Ad	123	
4	Af	123	
4	Ag	123	
4	At	123	
4	J	123	
4	M	123	
4	N	123	
4	O	123	
4	P	123	
4	Q	123	
4	R	123	
4	S	123	
4	T	123	
4	U	123	
4	V	123	
4	W	123	
4	av	123	
4	aw	123	
4	ax	123	
4	ay	123	
4	az	123	
5	X	136	
5	Y	136	
5	Z	136	
5	a	136	

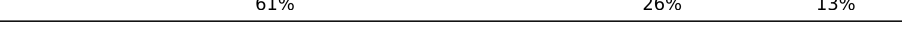
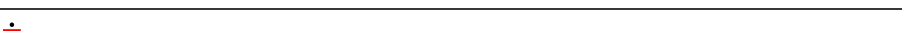
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Mol	Chain	Length	Quality of chain
5	b	136	
5	c	136	
5	d	136	
5	e	136	
5	f	136	
5	g	136	
5	h	136	
5	i	136	
5	j	136	
5	k	136	
5	l	136	
5	m	136	
5	n	136	
5	o	136	
5	p	136	
5	q	136	
5	r	136	
5	s	136	
5	t	136	
5	u	136	
6	0	103	
6	1	103	
6	2	103	
6	3	103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

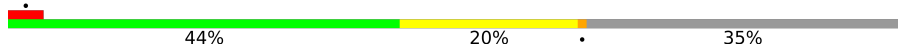
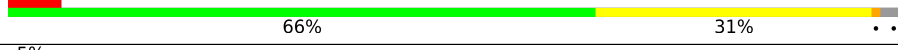
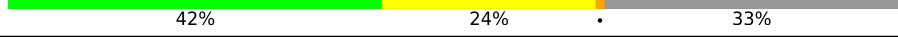
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Mol	Chain	Length	Quality of chain
6	5	103	
6	6	103	
6	7	103	
6	8	103	
6	9	103	
6	CD	103	
6	a2	103	
6	a3	103	
6	a4	103	
6	a5	103	
6	a6	103	
6	a7	103	
6	a8	103	
6	a9	103	
6	v	103	
6	w	103	
6	x	103	
6	y	103	
6	z	103	
7	Ah	196	
7	Ai	196	
7	Aj	196	
7	Ak	196	
7	Al	196	
7	Am	196	

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Mol	Chain	Length	Quality of chain
7	An	196	
7	Ao	196	
7	Ap	196	
7	Aq	196	
7	Ar	196	
7	As	196	

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

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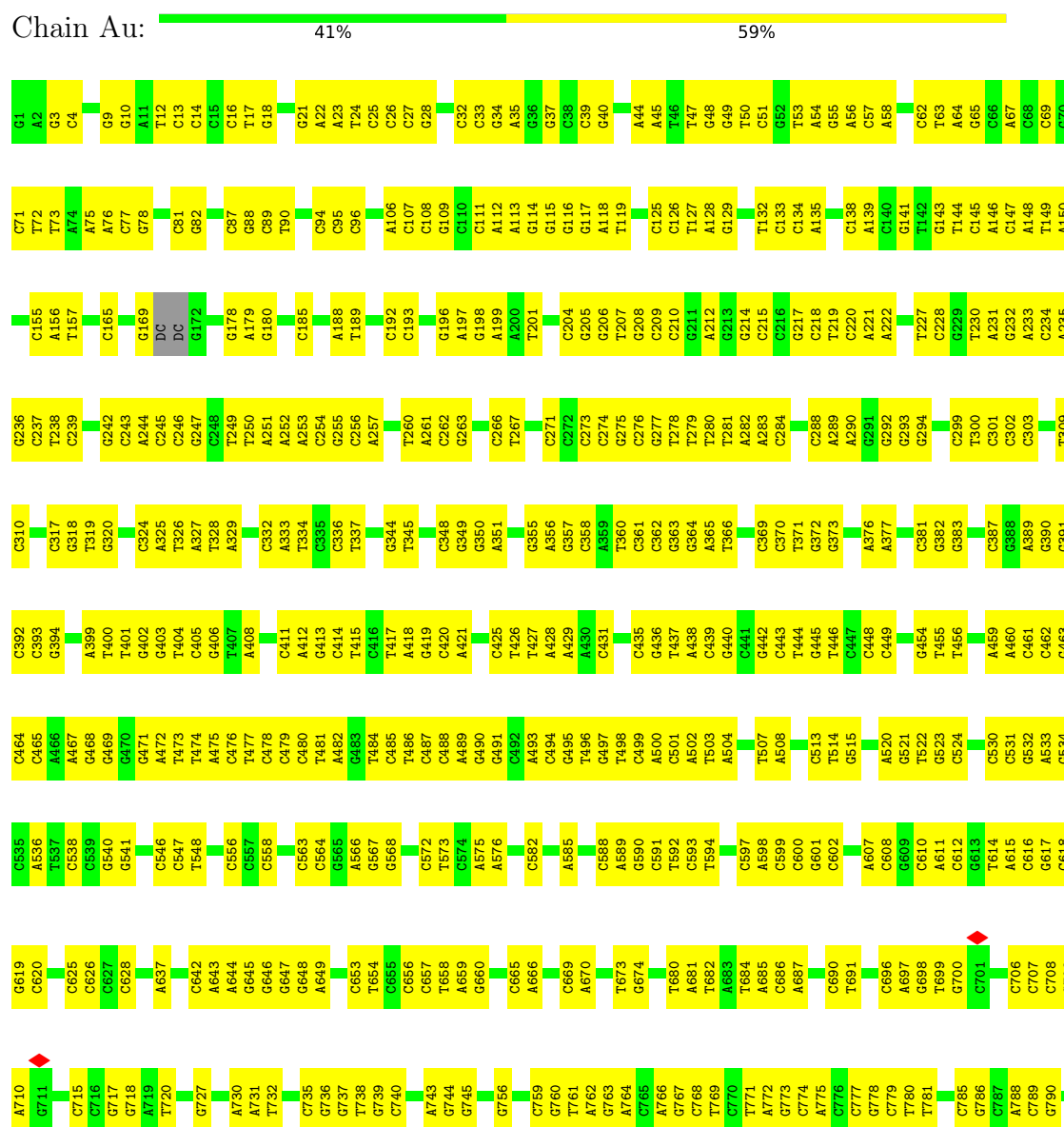
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Chain	Residue	Modelled	Actual	Comment	Reference
Aq	194	HIS	-	expression tag	UNP P02259
Aq	195	HIS	-	expression tag	UNP P02259
Ar	190	HIS	-	expression tag	UNP P02259
Ar	191	HIS	-	expression tag	UNP P02259
Ar	192	HIS	-	expression tag	UNP P02259
Ar	193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

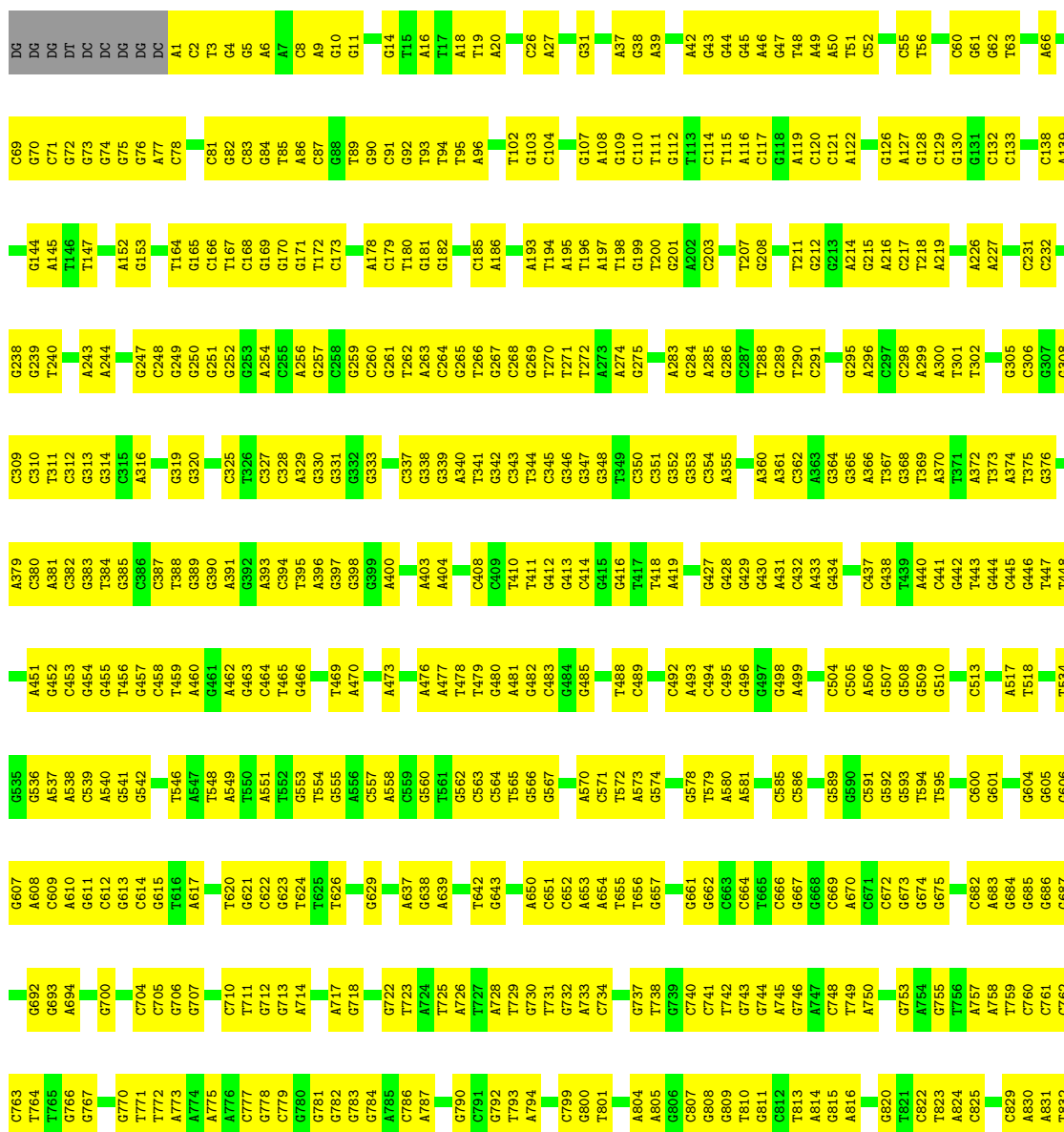
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

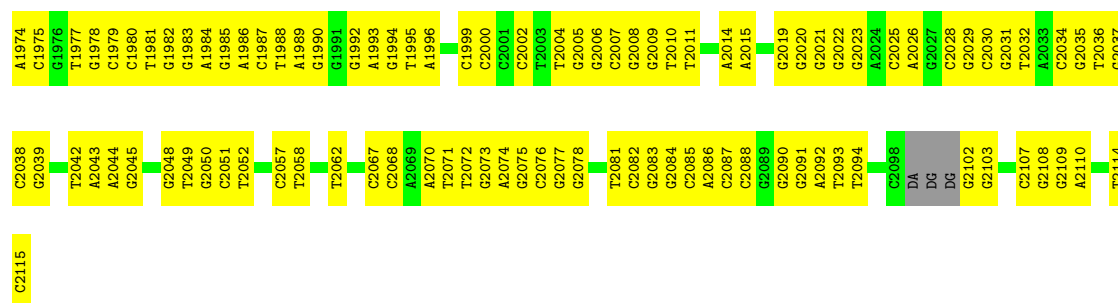


G1799	A1728	C1655	C1561	G1481	T1388	G1325	T1251	A1175	T1104	T1029	G955	T876	C793
T1800	G1729	T1656	C1562	G1481	T1389	C1326	C1252	G1176	C1105	T1030		G877	G794
G1801	G1730	A1657	C1563	C1484	T1390	C1327	C1253	G1177	A1106	A1031	T958		C802
C1802	C1731	G1658	C1564	C1485	T1391	C1328	C1254	G1178		C1032	A959	G880	
G1803	A1732	C1659	A1564	C1486	T1392	C1329	C1255	G1179	T1109	A1033	A960	G881	C805
G1804	G1733	A1660	T1565	C1486	A1393	T1329	C1255	A1180	G1110	T1034	A961	A882	C805
A1805	C1734	C1661	A1566	C1487	A1393	G1330	T1256	T1181	G1111	A1035	C962	C883	G806
G1806	T1735	C1662		T1488	C1397	T1331	G1257	T1182	C1112	T1036	G963	C884	C807
G1807	G1736	A1663	T1569	T1489	C1398	C1332	C1258	A1183	C1113	A1037	C964	C885	G808
	T1737	C1664	A1570	A1490	T1399	C1333	A1259		G1114	C1038	A965	G886	T809
C1811	C1738	T1665	A1491	A1491	G1400	C1334			T1115	A1039	C966	A887	T810
T1812	A1739	T1666	A1492	A1492	T1401	C1335	A1262	C1187		C1040	G967	G888	T811
A1815	C1740	A1667	G1583	C1493	T1402	C1336	T1263	T1189	A1118	A1041	T968	C889	T812
T1816	A1741	A1668	T1584	G1494	T1407	C1337	C1264	A1190	C1119	A1042	A890		
	T1742	A1669	C1585	C1495	G1407	C1338	C1265	G1191		T1043	C970	G891	C816
		C1670	C1586	A1496	G1408	C1339	C1266	T1192	C1122	C1043	G971		
T1820	A1745	G1671	C1587	C1497	A1413	T1341	G1267		T1123	G1046	C972	C893	C819
C1821	T1746	C1672	G1588	G1498		T1342	G1268	C1195		T1047		G894	A820
G1822	A1747	A1673	G1589		G1417		T1269	A1196	G1127	T1048	T977	G895	A821
T1823	C1748	C1674		G1502	G1417	A1345	G1270	A1197	C1128	C1049	C978	A896	G822
A1824	A1749	G1675	G1594	G1507	A1418	C1346	C1271	G1199	C1129	C1049	C978	T897	G823
G1825	T1750	T1676	A1595	T1508	G1419	C1347			A1130	G1052	C980	C898	G824
A1826		C1677	G1596	C1509	C1423	C1348	A1274		C1131	T1053	C982	C900	G825
C1827	G1754	A1678		C1510	C1424	C1349		C1202	G1132	C1056	G983	C901	A826
A1828	T1755	G1679	T1599	C1511	G1425	C1350	C1277	G1203	A1138	G1057	G985		T828
G1829	C1756	C1680	C1600	C1511	G1426	C1351	C1278	T1204	C1139	G1058			
C1830	C1757	C1681	C1601	C1512	G1427	A1352	C1280	T1206	G1140	A1059			
T1831	C1758	C1682	G1602	C1513	A1427				C1141				
C1832	A1759	T1683	G1603			G1355	T1281	A1210	C1142	G1071	T988	C912	T831
G1833	G1760	G1684	A1604	G1516	C1430	C1356	C1282	A1210	C1143	T989	T988	G912	C832
A1834	T1761	T1685	C1609	T1517	C1431	G1357	A1283	T1211	C1143	A990		G913	C833
G1835	G1762	C1686	T1610	T1518	C1432	C1358	A1284	A1212	G1072	A991		G914	C834
	C1763	C1687	G1611	C1523	T1433	T1359	T1285	T1213	A1073			C917	C835
C1841	C1764	C1688	G1612	G1524	G1434	A1360	G1287	T1215	C1148	G1001		G924	T836
T1842	G1765	C1689	G1612	G1525	C1435	C1361	G1288	A1216	C1149	G1002		G925	A836
T1843		C1690	A1613	G1525	A1436	T1362	T1289	C1217	G1150	A1003		G926	G837
A1844		G1691	G1614			C1363	C1290		C1151	T1004			
A1845	C1768	C1692	A1615	G1530	C1443	C1364	G1291	C1220	T1152	T1005		T932	G849
C1846	C1769	G1693		G1531	G1444	C1365	G1291	C1081	G1085	A1006		G933	T850
	G1771	A1698	A1628	G1532	G1445	C1366	T1292	A1082	C1087	C1007		G934	G851
C1847	A1772	A1699		G1533	G1445	A1367	A1293	T1221	G1083	C1007		G934	T852
G1848	G1773	C1700	C1631	A1534	G1450	C1368	C1294	G1223	C1156	T1008		T935	T853
A1850	C1774	C1701		T1535	A1451	G1369		C1226	C1157	C936		C936	C853
	A1775	G1702	C1634	T1536	G1452	T1369	G1298	C1227	C1158	C1010		G937	A854
C1855	T1776	C1703		A1537	G1453	C1370			C1159	C937		T938	C855
	C1777		A1637	C1538	C1454	T1371	T1302	C1227	G1160	T1012		A939	G856
G1858	C1778	A1706	A1638		G1455	C1372	G1303	G1231	C1161	A1013		G940	
C1859	G1779	G1707	T1639	C1541	C1455	C1373	G1304	C1232	C1162	C1089		A941	C863
T1860	G1780		T1640	C1542	G1456	C1374	C1305	C1233	T1163	G1090		G942	A864
G1861	A1781	T1712	G1641		C1457	G1375	A1306	G1234	T1164	A943		G944	T865
T1862	T1782	C1711	G1642	C1547	T1458	C1376		G1235	T1165	C1016		T1017	C866
C1863	C1783	T1716		T1548	G1464	C1377	G1309		C1166	C1018		C1018	T868
	C1784		T1646	C1549	G1465	C1378	C1310	G1240	T1167	G096		T946	T869
C1866				C1550	G1465	C1379	T1311	A1241	A1168	A1020		C947	G869
G1867	G1788	C1719	A1649	T1548	G1465	C1379	T1311	G1242	C1169	G1097		T948	T870
G1868				C1550	G1465	C1379	T1311	G1242	C1169	A1097		T948	T871
A1869	T1789	C1724	C1650	G1552	G1468	C1382	A1313	C1243	C1169	G1098		T948	C872
C1869	A1790	T1725	G1553	C1554	T1469	T1383	C1316	A1245	C1170	G1099		G950	C873
G1870	G1791		G1652	C1554	A1470	C1386	C1316	T1245	C1172	C1101			A874
		C1726	C1653	C1557	G1471	C1387	G1317	C1246	C1173	G1102		C953	A875
				C1557		C1388	C1319	C1247	A1174	T1027		C954	C876

- Molecule 2: DNA



G1877	A1878	T1885	A1892	A1893	A1909	C1910	C1911	G1912	G1913	G1914	A1915	T1919	C1920	C1921	A1922	G1926	A1927	T1928	C1929	G1932	C1936	T1937	C1938	G1939	G1940	G1941	G1945	G1946	A1948	C1949	T1950	G1951	G1952	A1956	G1957	G1958	A1959	T1960	G1961	A1962	A1963	A1965	T1966	G1969	T1970	G1971										
G1792	C1796	A1797	C1798	G1799	T1800	G1801	C1802	C1803	T1804	A1807	G1808	A1809	C1810	T1811	A1812	G1813	G1817	A1820	T1821	C1822	C1823	C1824	C1825	T1826	T1827	G1828	G1829	C1830	G1831	T1834	A1835	C1841	G1842	G1843	G1844	C1848	A1849	G1850	G1854	A1855	C1857	G1858	T1859	G1860	T1865	A1866	A1867	G1868								
T1717	T1718	C1722	G1723	G1724	C1725	T1726	T1727	C1728	G1729	G1730	C1731	A1732	T1739	T1742	C1743	C1744	A1745	G1746	G1747	G1748	G1749	A1750	T1751	C1752	C1753	T1757	G1758	C1759	T1760	C1761	G1762	G1763	G1764	T1765	C1766	C1767	G1768	G1769	C1770	T1773	G1774	A1779	G1780	G1781	A1782	T1783	G1784	T1785	A1786	T1787	A1788	T1791				
T1650	G1651	G1652	G1653	G1654	G1655	T1656	T1657	A1658	A1659	A1660	C1661	G1662	G1663	C1664	G1665	G1668	G1669	A1670	C1671	A1672	C1676	G1677	T1678	A1679	C1680	G1681	T1682	G1683	C1684	G1685	T1686	G1687	C1688	A1689	G1693	G1694	T1695	G1696	G1700	A1701	G1702	C1703	T1704	G1705	T1706	C1707	T1708	A1709	C1710	G1711	A1712	C1713	C1714	A1715	A1716	
G1571	G1572	A1573	T1574	G1577	G1578	A1579	T1580	G1581	C1590	G1590	G1591	G1592	C1593	T1596	G1597	G1598	A1599	T1606	G1607	C1608	T1610	A1611	T1612	A1613	C1614	G1615	T1616	C1621	G1622	T1623	G1624	C1625	C1626	T1627	G1631	A1632	C1633	T1634	A1635	G1636	G1637	G1638	A1639	G1640	T1641	A1642	T1643	T1644	C1645	C1646	C1647	T1648	T1649			
A1495	G1496	C1497	G1498	C1499	G1500	T1501	A1502	C1503	T1509	T1510	T1511	A1512	C1515	G1516	G1517	T1518	A1524	G1525	C1526	T1527	A1528	T1529	C1530	A1531	A1532	C1533	G1534	C1537	T1541	G1542	A1543	G1544	C1545	C1548	T1549	T1550	C1551	G1552	G1553	C1554	A1555	C1556	C1557	G1558	A1561	T1562	A1563	G1564	C1565	C1566	G1567	A1568	G1569	G1570		
C1416	G1420	G1421	G1422	A1423	C1424	A1425	G1426	G1427	T1433	A1434	T1435	A1436	T1437	G1438	T1439	G1440	A1441	C1444	G1445	A1453	G1454	A1455	C1456	A1457	A1458	G1459	A1460	G1461	A1462	G1463	T1464	A1465	C1470	C1471	T1472	T1473	G1474	G1475	C1476	G1477	G1478	A1481	A1484	C1485	G1488	G1489	G1490	A1493	C1494							
A1335	A1336	G1337	C1338	G1339	G1340	T1341	G1342	C1343	T1344	A1345	G1346	A1347	G1348	C1349	T1350	G1351	T1352	C1353	C1356	G1357	A1358	C1359	G1367	C1368	G1369	C1372	T1373	G1376	C1377	G1378	C1379	C1380	G1381	G1382	G1383	A1384	T1385	T1386	C1387	G1392	G1393	G1394	G1395	G1400	G1401	A1402	G1404	C1405	G1410	A1411	C1412					
G1152	C1153	T1157	A1158	G1159	G1160	C1166	T1167	G1168	A1169	G1170	G1171	T1175	C1176	A1181	G1182	C1183	A1184	T1186	G1187	G1188	A1189	G1190	C1191	G1192	G1193	C1194	G1199	C1202	C1203	G1204	G1205	C1212	C1213	G1217	T1220	C1221	C1222	G1223	T1226	T1229	C1230	G1231	C1239	T1240	C1241											
A1245	A1246	C1247	A1248	G1249	G1250	A1251	T1252	G1253	T1254	A1259	T1260	G1261	T1262	G1263	A1264	C1265	A1266	C1267	G1268	T1269	G1270	C1271	C1272	T1273	G1274	G1275	A1276	G1277	A1281	G1282	G1283	G1284	A1285	G1286	T1287	C1292	C1293	G1300	G1301	T1302	G1309	C1310	G1311	G1312	G1313	T1328	G1329	C1330	G1331	T1332	T1333	T1334				
G1086	A1087	C1088	A1089	C1090	G1091	T1092	G1093	C1094	T1095	G1096	G1097	A1098	A1099	A1100	C1101	T1102	T1103	A1104	G1105	A1111	A1112	T1113	C1114	C1115	C1116	G1117	T1118	G1121	C1122	T1125	G1126	A1127	A1128	A1129	A1130	C1131	G1132	C1133	G1134	G1135	G1136	G1137	A1138	A1139	C1140	A1141	G1142	C1143	C1144	C1145	G1146	T1147	A1148	C1149	G1150	T1151
T996	G997	T998	C999	T1000	A1004	T1009	T1010	G1013	A1014	G1015	G1016	G1100	C1020	T941	G1021	G1022	C1023	A1024	G1029	A1030	C1035	G1040	G1041	A1042	T1043	C1044	G1045	G1046	G1047	A1048	G1056	T1057	C1062	A1063	C1064	G1067	A1068	A1069	C1070	A1071	G1072	G1073	A1074	G1076	T1075	C989	T990	G914	T915	C916	C917	A991	C992	A993	G994	C995
T833	G834	A835	G836	C837	G838	G839	C840	C841	C843	C846	A847	C848	G851	G852	G853	C856	T857	G858	C859	A860	G863	G864	C867	A871	T872	G873	G877	G878	T880	C881	C882	G883	A886	G899	G907	T908	G909	A912	C913	T914	T915	C916	C917	C918	T919	G920										



• Molecule 3: Histone H2A

Chain A: 86% 8% 6%



• Molecule 3: Histone H2A

Chain B: 80% 17% .



• Molecule 3: Histone H2A

Chain C: 78% 20% ..



• Molecule 3: Histone H2A

Chain D: 88% 7% 5%



• Molecule 3: Histone H2A

Chain E: 82% 16% .



• Molecule 3: Histone H2A

Chain F: 75% 17% 8%



- Molecule 3: Histone H2A

Chain G: 82% 17% .



- Molecule 3: Histone H2A

Chain H: 78% 18% .



- Molecule 3: Histone H2A

Chain I: 86% 13% .



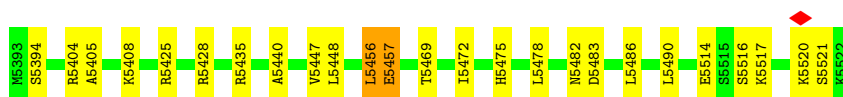
- Molecule 3: Histone H2A

Chain K: 78% 18% ...



- Molecule 3: Histone H2A

Chain L: 81% 18% .



- Molecule 3: Histone H2A

Chain aj: 74% 21% 5%



- Molecule 3: Histone H2A

Chain ak:  83% 12% 5%



- Molecule 3: Histone H2A

Chain al:  75% 10% 15%



- Molecule 3: Histone H2A

Chain am:  75% 20% 5%



- Molecule 3: Histone H2A

Chain an:  83% 13% 4%



- Molecule 3: Histone H2A

Chain ao:  78% 18% 5%



- Molecule 3: Histone H2A

Chain ap:  78% 19% 3%



- Molecule 3: Histone H2A

Chain aq:  72% 18% 10%



- Molecule 3: Histone H2A

Chain ar:  84% 15%



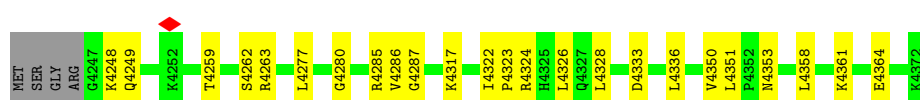
• Molecule 3: Histone H2A

Chain as:  77% 15% 8%



• Molecule 3: Histone H2A

Chain at:  78% 18%



• Molecule 3: Histone H2A

Chain au:  75% 11% 15%



• Molecule 3: Histone H2A

Chain Ae:  82% 12% 6%



• Molecule 4: Histone H2B 1.1

Chain J:  68% 15% 16%



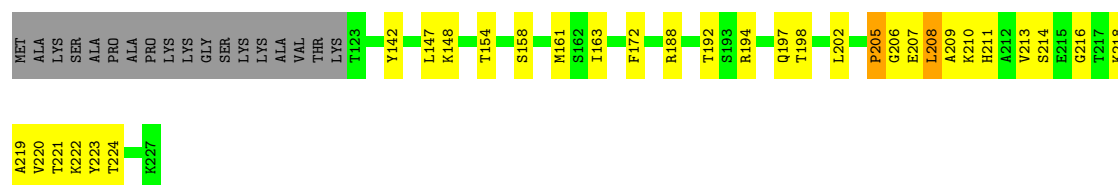
• Molecule 4: Histone H2B 1.1

Chain M:  83% 17%



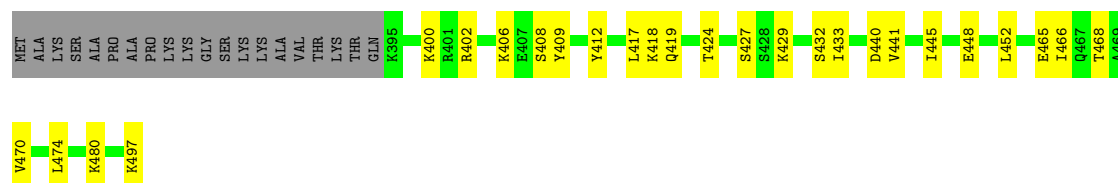
• Molecule 4: Histone H2B 1.1

Chain N:  60% 24% 15%



- Molecule 4: Histone H2B 1.1

Chain O:  63% 21% 16%



- Molecule 4: Histone H2B 1.1

Chain P:  75% 11% 15%



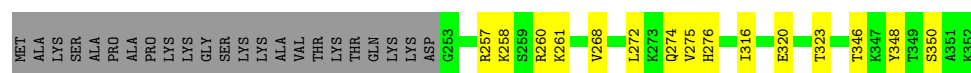
- Molecule 4: Histone H2B 1.1

Chain Q:  82% 18%



- Molecule 4: Histone H2B 1.1

Chain R:  69% 12% 19%



- Molecule 4: Histone H2B 1.1

Chain S:  79% 21%

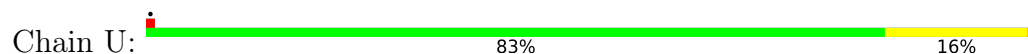


- Molecule 4: Histone H2B 1.1

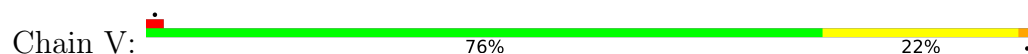
Chain T:  84% 16%



• Molecule 4: Histone H2B 1.1



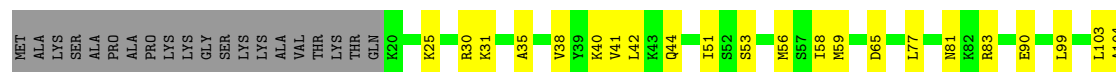
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



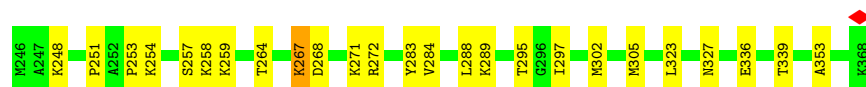
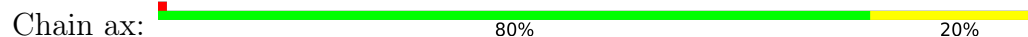
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



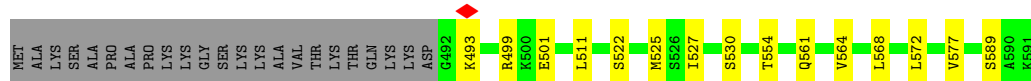
- Molecule 4: Histone H2B 1.1

Chain ay:  88% 12%



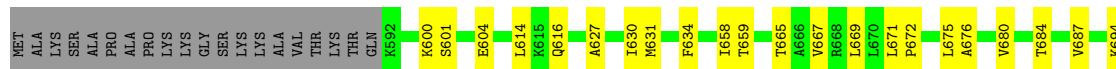
- Molecule 4: Histone H2B 1.1

Chain az:  69% 12% 19%



- Molecule 4: Histone H2B 1.1

Chain Aa:  66% 18% 16%



- Molecule 4: Histone H2B 1.1

Chain Ab:  76% 24%



- Molecule 4: Histone H2B 1.1

Chain Ac:  68% 13% 19%



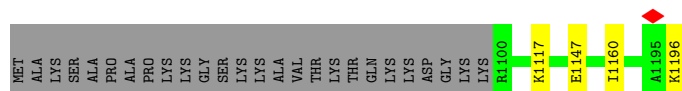
- Molecule 4: Histone H2B 1.1

Chain Ad:  68% 15% 17%



- Molecule 4: Histone H2B 1.1

Chain Af:  76% 21%



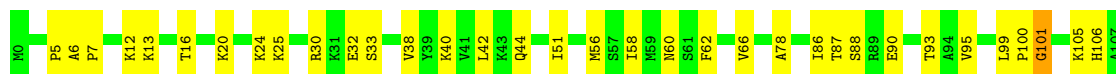
- Molecule 4: Histone H2B 1.1

Chain Ag:  76% 9% 15%



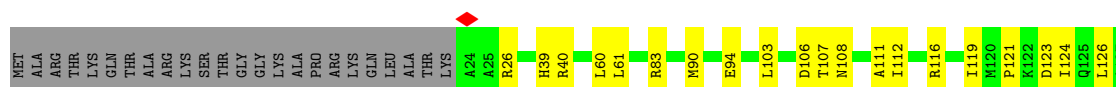
- Molecule 4: Histone H2B 1.1

Chain At:  67% 33%



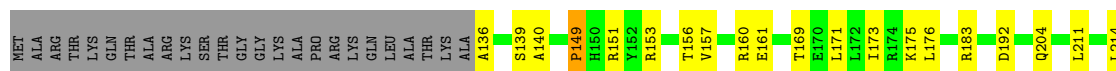
- Molecule 5: Histone H3

Chain X:  65% 17% 18%

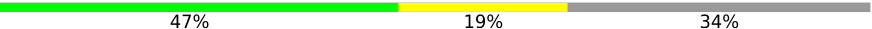


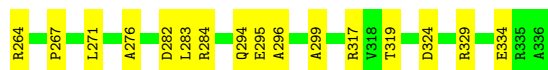
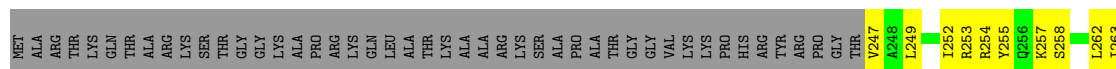
- Molecule 5: Histone H3

Chain Y:  64% 17% 18%



- Molecule 5: Histone H3

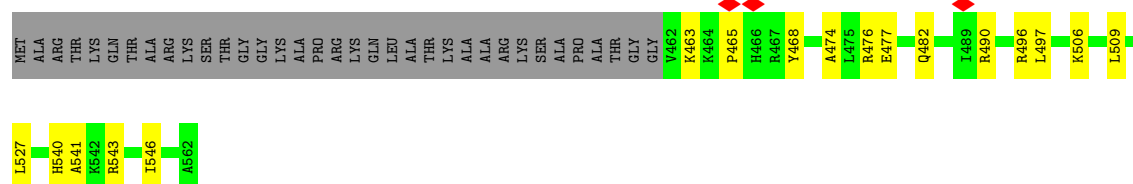
Chain Z:  47% 19% 34%



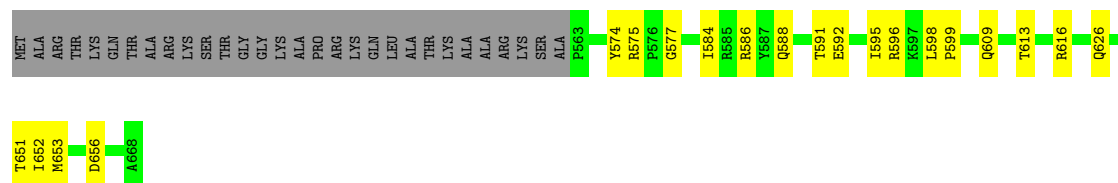
- Molecule 5: Histone H3



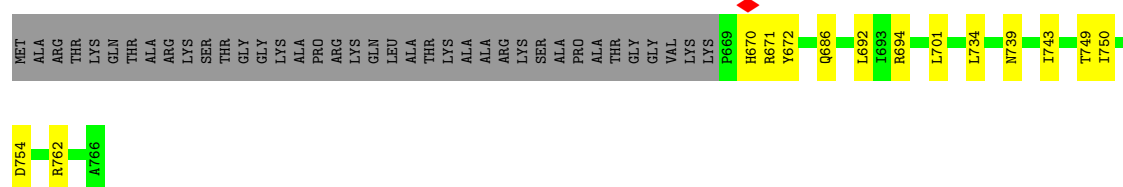
- Molecule 5: Histone H3



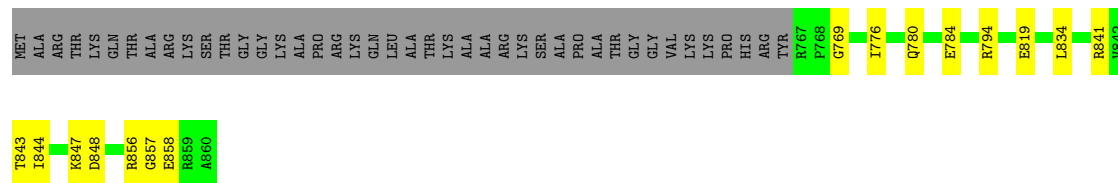
- Molecule 5: Histone H3



- Molecule 5: Histone H3

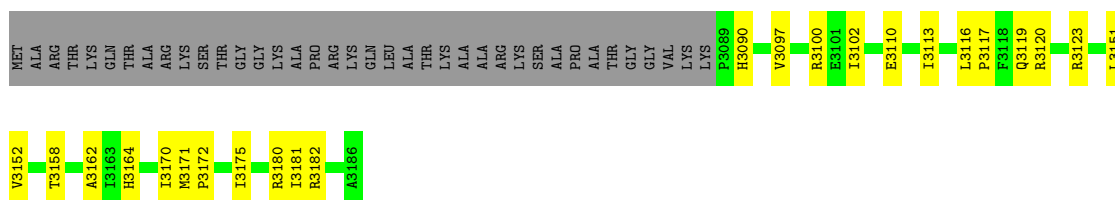


- Molecule 5: Histone H3

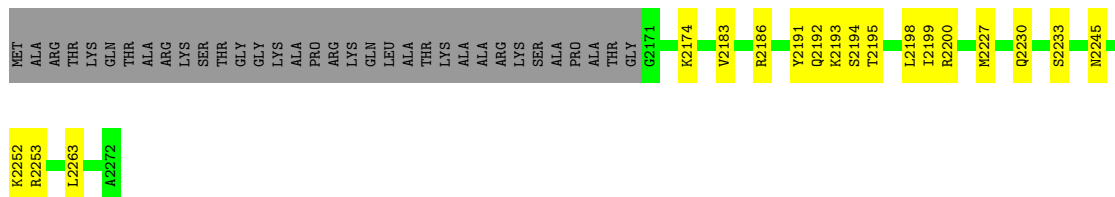


- Molecule 5: Histone H3

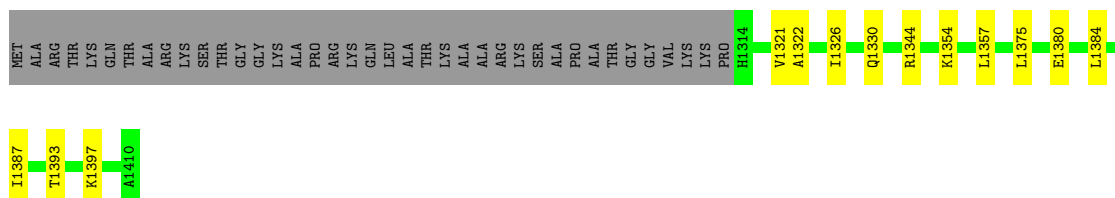




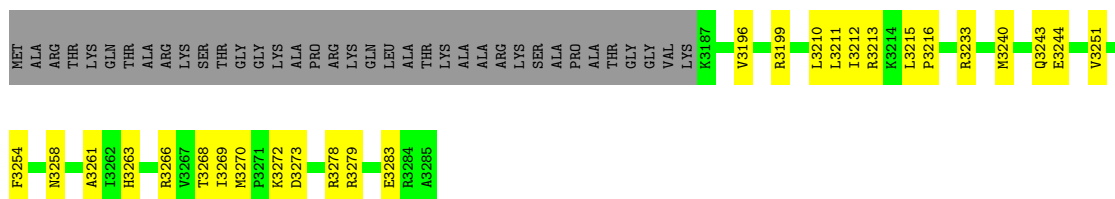
• Molecule 5: Histone H3



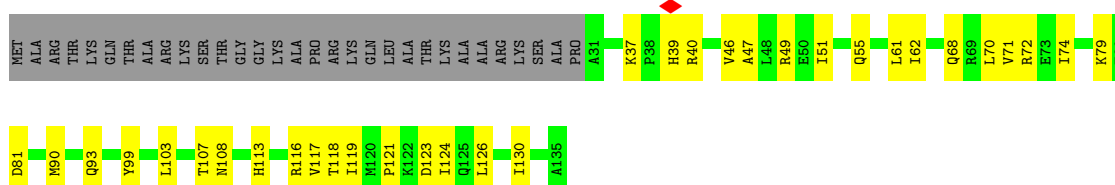
• Molecule 5: Histone H3



• Molecule 5: Histone H3

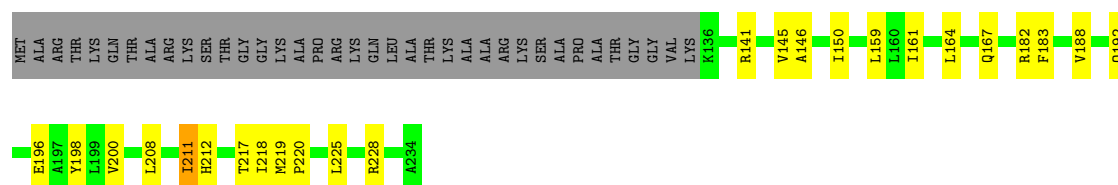


• Molecule 5: Histone H3



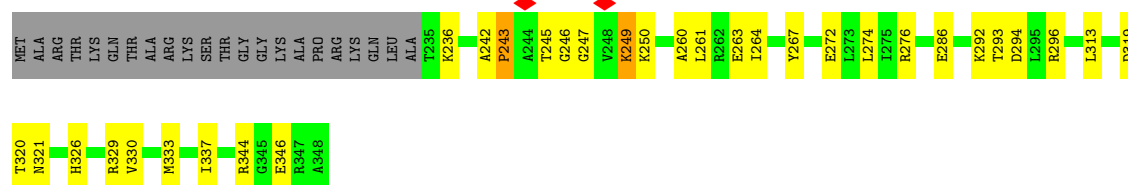
• Molecule 5: Histone H3

Chain k:  55% 17% 27%



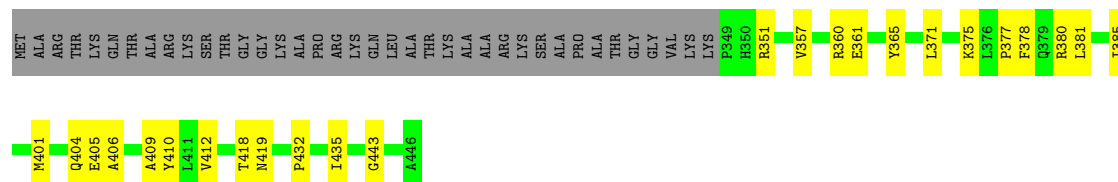
• Molecule 5: Histone H3

Chain l:  60% 22% 16%



• Molecule 5: Histone H3

Chain m:  54% 18% 28%



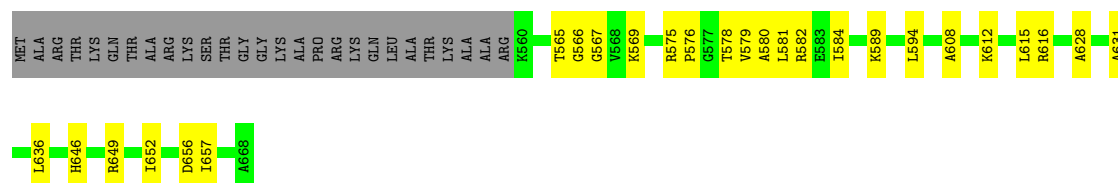
• Molecule 5: Histone H3

Chain n:  59% 24% 17%



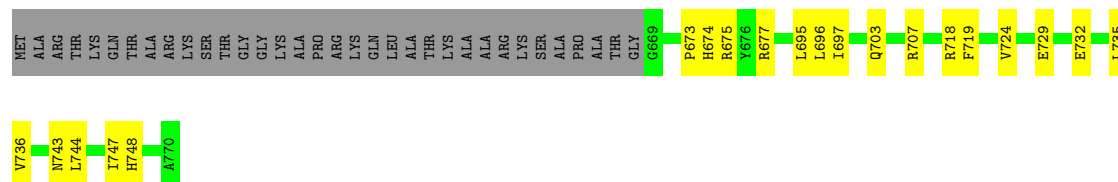
• Molecule 5: Histone H3

Chain o:  61% 19% 20%



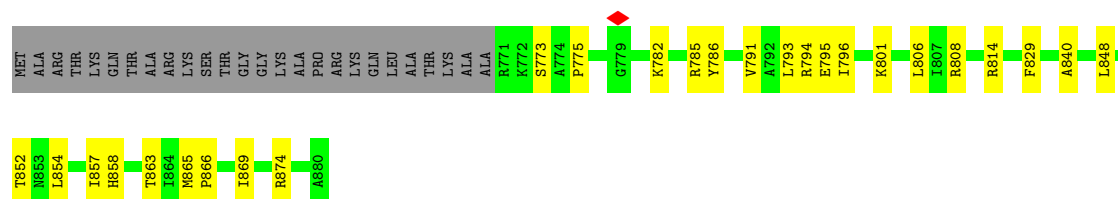
• Molecule 5: Histone H3

Chain p: 



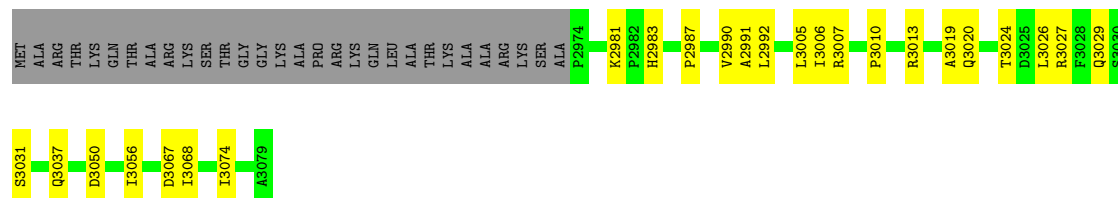
• Molecule 5: Histone H3

Chain q: 



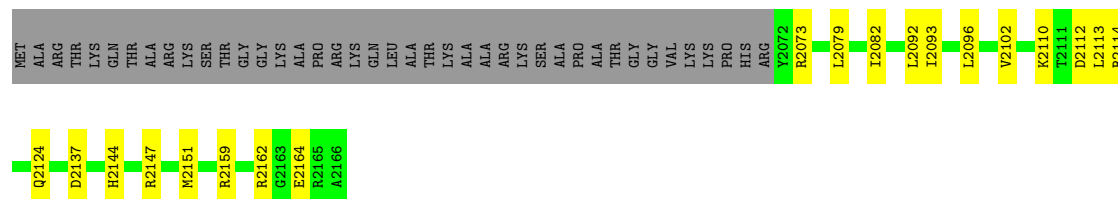
• Molecule 5: Histone H3

Chain r: 



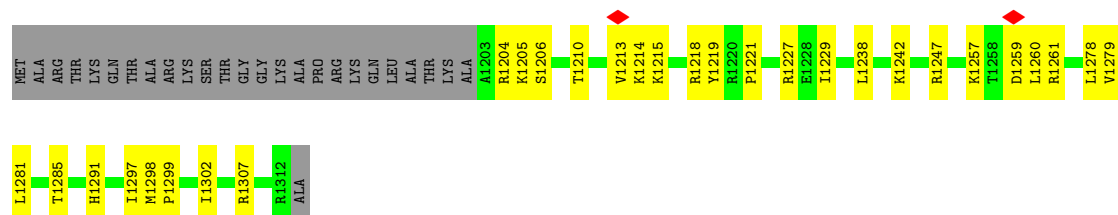
• Molecule 5: Histone H3

Chain s: 



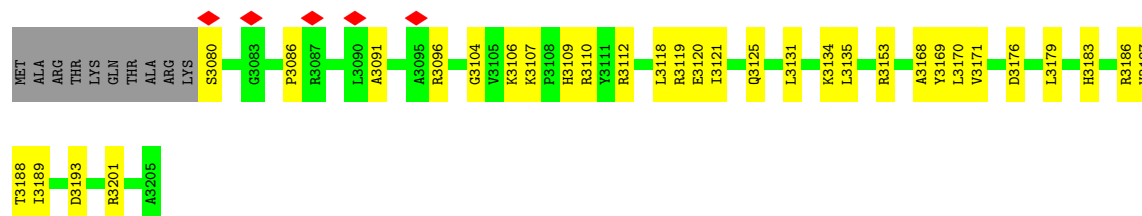
• Molecule 5: Histone H3

Chain t: 



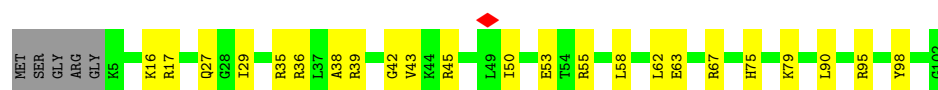
- Molecule 5: Histone H3

Chain u: 



- Molecule 6: Histone H4

Chain v: 



- Molecule 6: Histone H4

Chain w: 



- Molecule 6: Histone H4

Chain x: 



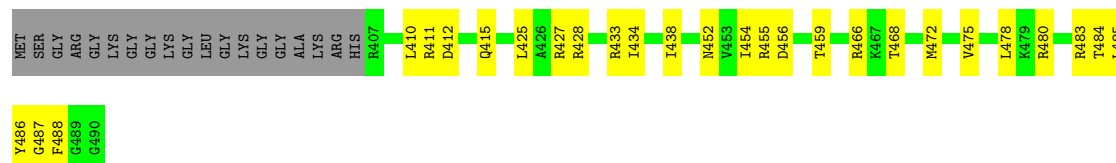
- Molecule 6: Histone H4

Chain y: 



- Molecule 6: Histone H4

Chain z: 



- Molecule 6: Histone H4

Chain 0: 



• Molecule 6: Histone H4

Chain 1: 



• Molecule 6: Histone H4

Chain 2: 



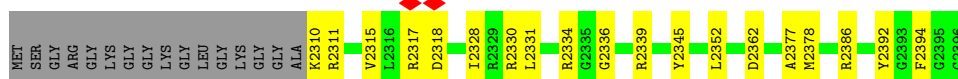
• Molecule 6: Histone H4

Chain 3: 



• Molecule 6: Histone H4

Chain 4: 



• Molecule 6: Histone H4

Chain 5: 



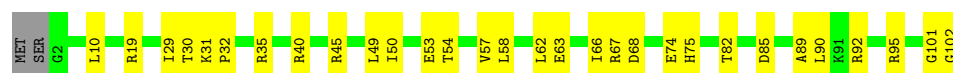
• Molecule 6: Histone H4

Chain 6: 



• Molecule 6: Histone H4

Chain 7:  69% 29% .



• Molecule 6: Histone H4

Chain 8:  61% 22% 17%



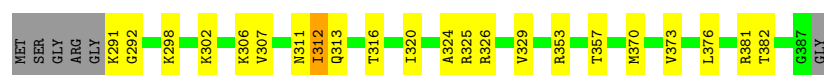
• Molecule 6: Histone H4

Chain 9:  71% 28% .



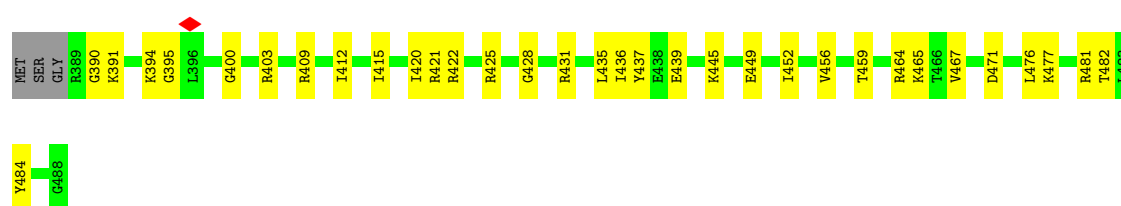
• Molecule 6: Histone H4

Chain CD:  73% 20% 6%



• Molecule 6: Histone H4

Chain a2:  65% 32% .



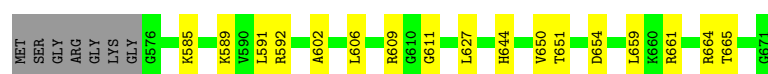
• Molecule 6: Histone H4

Chain a3:  69% 16% 16%

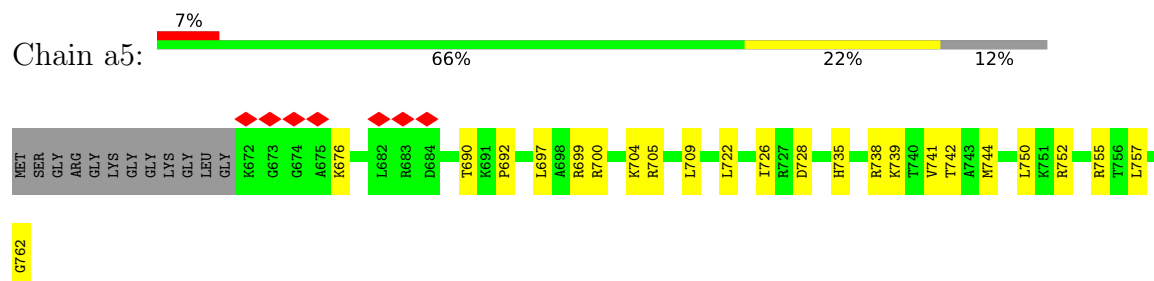


• Molecule 6: Histone H4

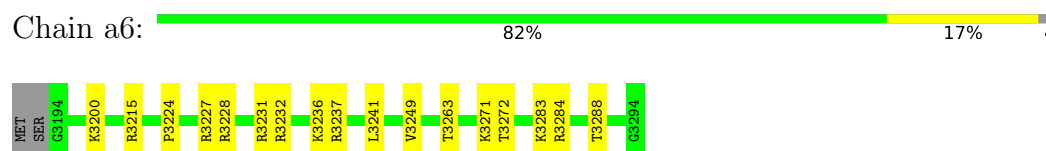
Chain a4:  77% 17% 7%



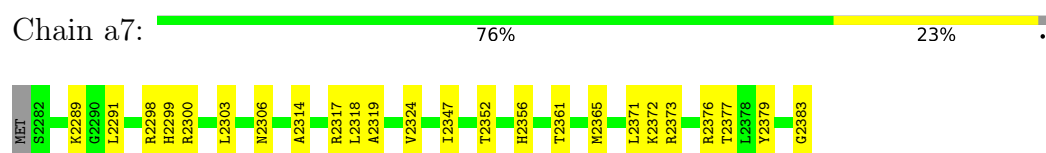
- Molecule 6: Histone H4



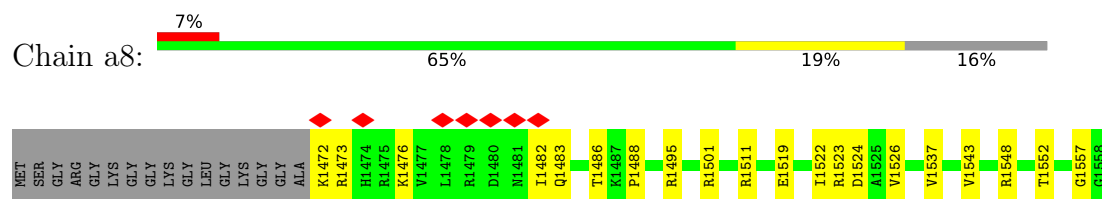
- Molecule 6: Histone H4



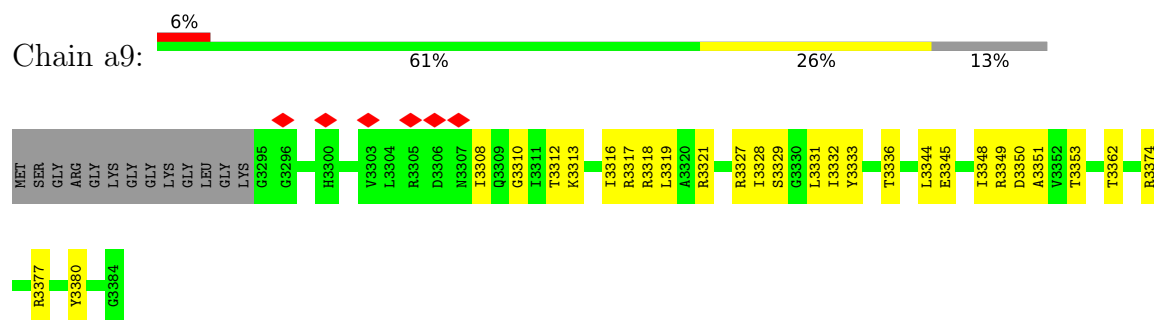
- Molecule 6: Histone H4



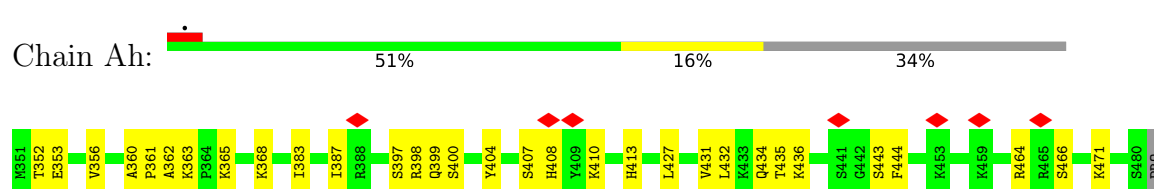
- Molecule 6: Histone H4

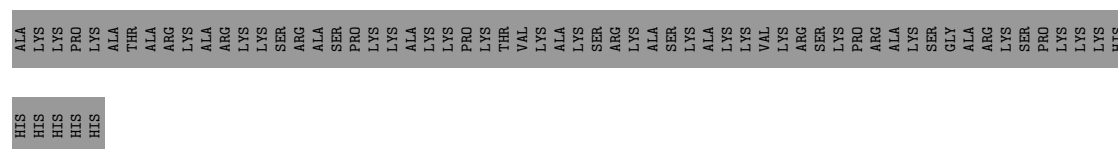


- Molecule 6: Histone H4

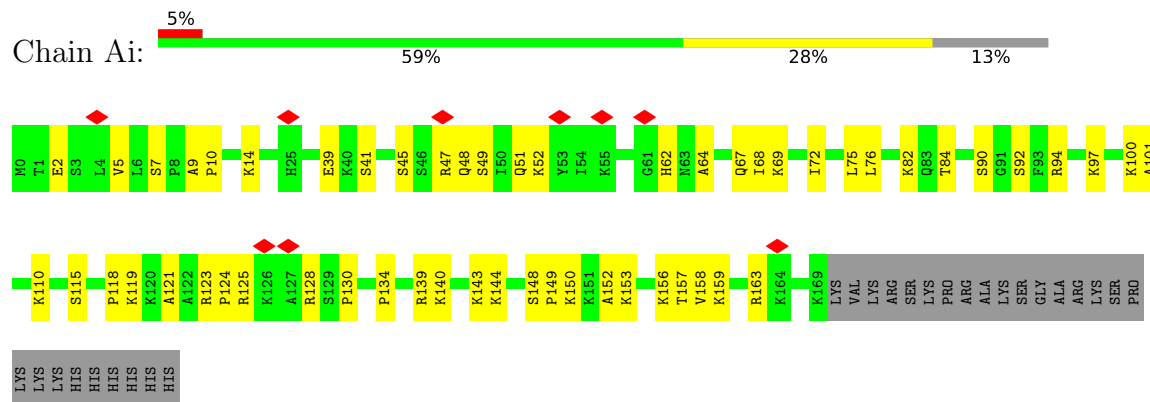


- Molecule 7: Histone H5

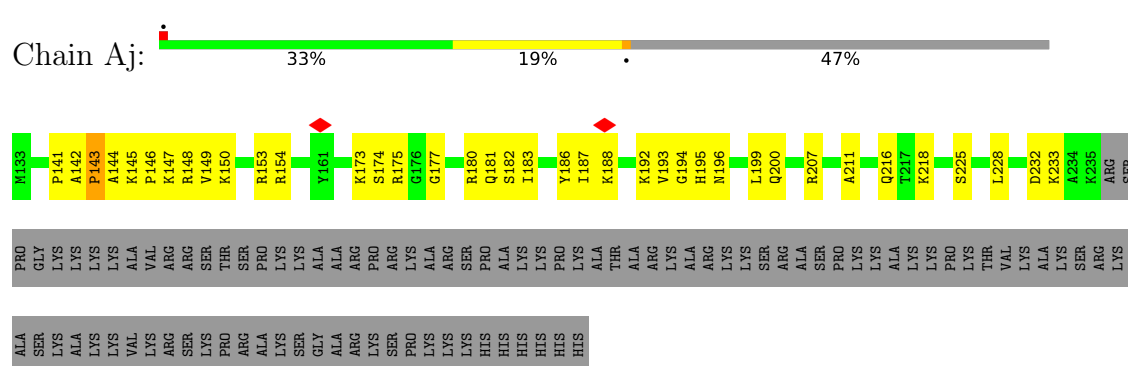




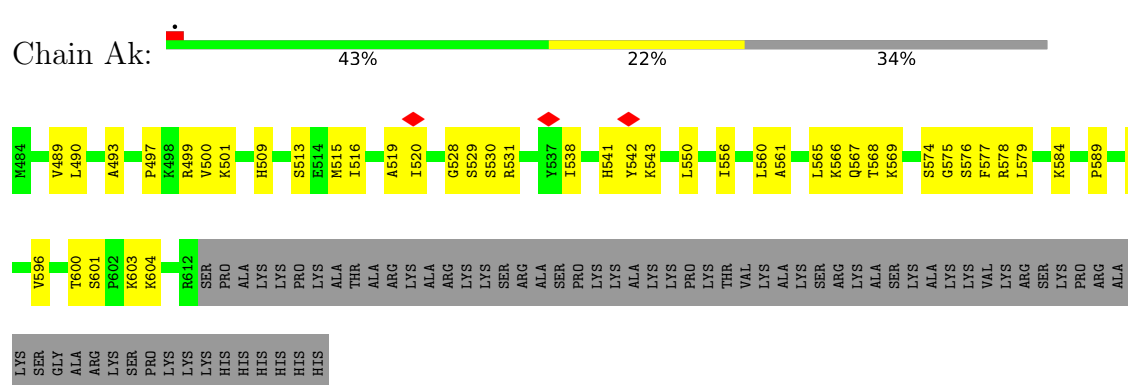
- Molecule 7: Histone H5



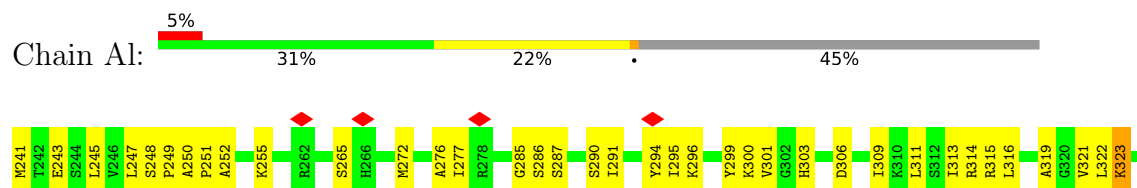
- Molecule 7: Histone H5



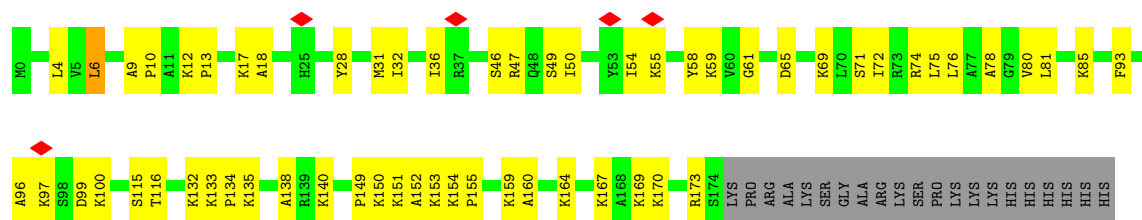
- Molecule 7: Histone H5



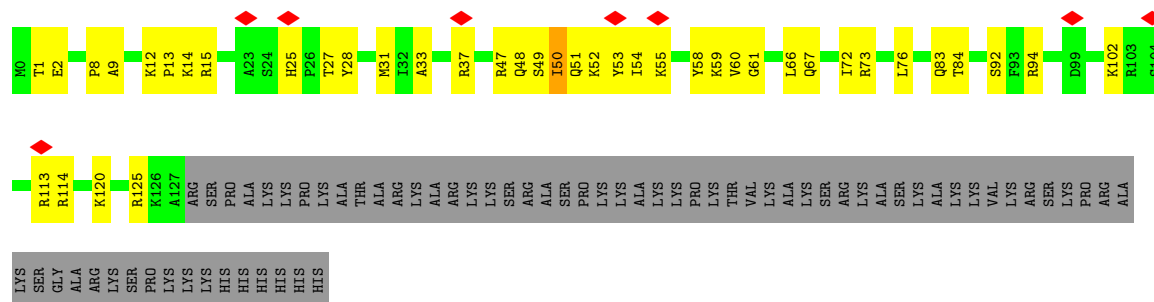
- Molecule 7: Histone H5



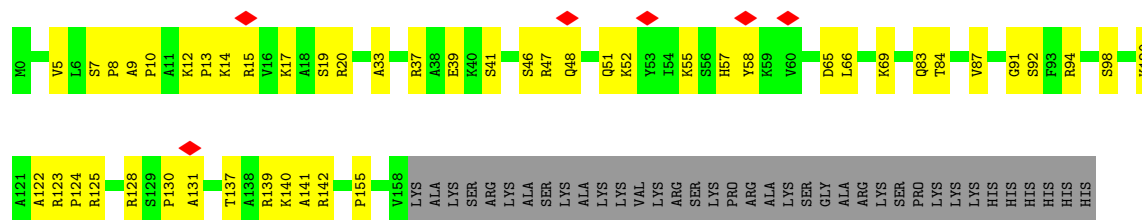
- Molecule 7: Histone H5



- Molecule 7: Histone H5

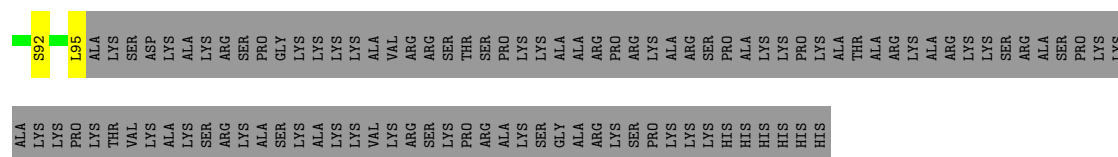


- Molecule 7: Histone H5

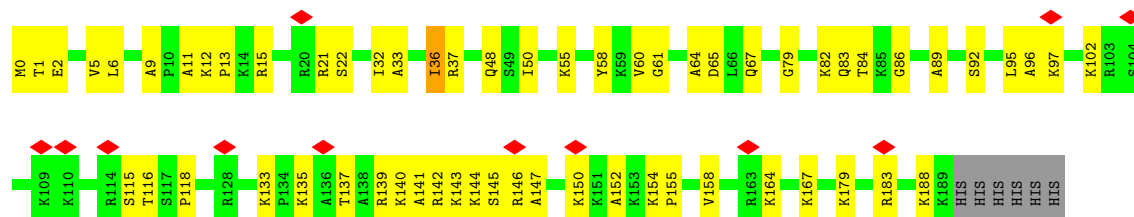


- Molecule 7: Histone H5

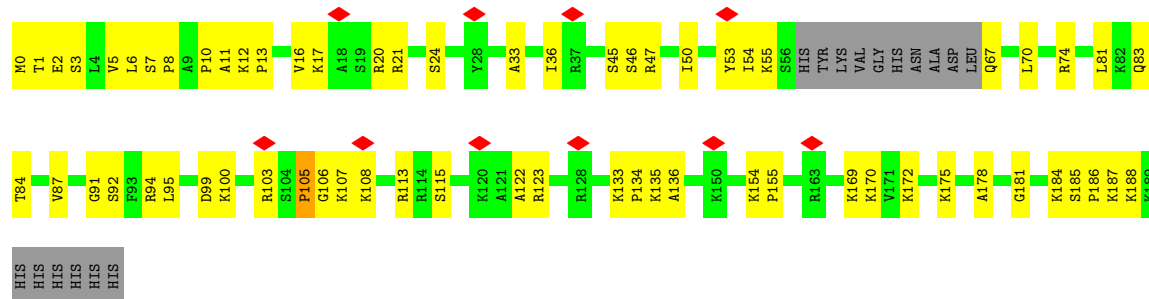




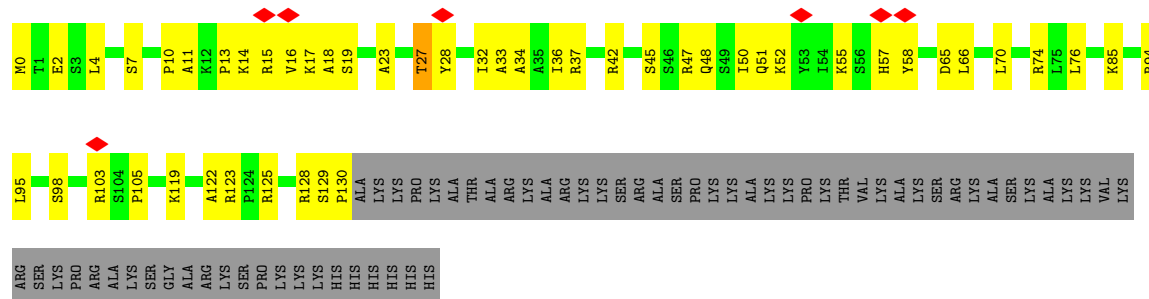
• Molecule 7: Histone H5



• Molecule 7: Histone H5



• Molecule 7: Histone H5



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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Au	0.19	0/48227	0.40	0/74345
2	Av	0.19	0/49010	0.39	0/75728
3	A	0.10	0/946	0.27	0/1269
3	Ae	0.09	0/946	0.23	0/1269
3	B	0.11	0/972	0.34	1/1302 (0.1%)
3	C	0.25	1/993 (0.1%)	0.47	3/1329 (0.2%)
3	D	0.12	0/950	0.34	0/1274
3	E	0.09	0/983	0.26	0/1318
3	F	0.08	0/926	0.28	0/1243
3	G	0.10	0/993	0.31	0/1329
3	H	0.09	0/968	0.25	0/1297
3	I	0.09	0/993	0.27	0/1329
3	K	0.69	3/987 (0.3%)	0.70	6/1321 (0.5%)
3	L	0.43	2/1001 (0.2%)	0.44	3/1339 (0.2%)
3	aj	0.30	0/950	0.46	1/1274 (0.1%)
3	ak	0.11	0/950	0.31	0/1274
3	al	0.07	0/860	0.22	0/1158
3	am	0.37	0/983	0.60	2/1316 (0.2%)
3	an	0.12	0/968	0.35	0/1297
3	ao	0.11	0/959	0.30	0/1286
3	ap	0.09	0/983	0.26	0/1316
3	aq	0.13	0/910	0.33	0/1222
3	ar	0.09	0/993	0.28	0/1329
3	as	0.09	0/926	0.26	0/1243
3	at	0.11	0/972	0.31	0/1302
3	au	0.09	0/869	0.26	0/1171
4	Aa	0.11	0/825	0.31	0/1101
4	Ab	0.10	0/969	0.30	0/1292
4	Ac	0.08	0/799	0.26	0/1068
4	Ad	0.15	0/816	0.30	0/1090
4	Af	0.07	0/777	0.22	0/1041
4	Ag	0.09	0/834	0.25	0/1113
4	At	0.46	0/969	0.59	2/1292 (0.2%)
4	J	0.08	0/825	0.26	0/1101

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	M	0.12	0/969	0.31	0/1292
4	N	0.52	0/841	0.53	1/1123 (0.1%)
4	O	0.11	0/825	0.31	0/1101
4	P	0.08	0/841	0.22	0/1123
4	Q	0.10	0/969	0.32	0/1292
4	R	0.07	0/799	0.21	0/1068
4	S	0.13	0/969	0.36	1/1292 (0.1%)
4	T	0.10	0/969	0.30	0/1292
4	U	0.11	0/969	0.33	1/1292 (0.1%)
4	V	0.20	0/969	0.38	0/1292
4	W	0.50	2/969 (0.2%)	0.35	0/1292
4	av	0.11	0/825	0.30	0/1101
4	aw	0.11	0/969	0.34	0/1292
4	ax	0.14	0/969	0.36	1/1292 (0.1%)
4	ay	0.40	2/969 (0.2%)	0.50	3/1292 (0.2%)
4	az	0.06	0/799	0.20	0/1068
5	X	0.11	0/914	0.35	0/1225
5	Y	0.13	0/909	0.38	1/1218 (0.1%)
5	Z	0.08	0/747	0.25	0/1000
5	a	0.15	0/1009	0.38	1/1351 (0.1%)
5	b	0.08	0/845	0.25	0/1132
5	c	0.08	0/873	0.23	0/1170
5	d	0.09	0/820	0.26	0/1099
5	e	0.10	0/777	0.26	0/1041
5	f	0.08	0/820	0.23	0/1099
5	g	0.08	0/849	0.25	0/1137
5	h	0.08	0/812	0.22	0/1088
5	i	0.08	0/829	0.26	0/1111
5	j	0.12	0/865	0.32	0/1159
5	k	0.08	0/829	0.27	0/1111
5	l	0.14	0/930	0.47	3/1246 (0.2%)
5	m	0.13	0/820	0.37	1/1099 (0.1%)
5	n	0.09	0/923	0.30	0/1236
5	o	0.11	0/893	0.29	0/1197
5	p	0.07	0/849	0.23	0/1137
5	q	0.13	0/904	0.24	0/1211
5	r	0.09	0/873	0.25	0/1170
5	s	0.07	0/790	0.20	0/1059
5	t	0.11	0/903	0.31	0/1211
5	u	0.12	0/1015	0.35	0/1359
6	0	0.11	0/749	0.29	0/997
6	1	0.10	0/711	0.26	0/948
6	2	0.37	1/758 (0.1%)	0.80	3/1008 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	3	0.10	0/744	0.28	0/992
6	4	0.10	0/711	0.29	0/948
6	5	0.10	0/758	0.29	0/1008
6	6	0.09	0/695	0.27	0/929
6	7	0.12	0/794	0.33	0/1053
6	8	0.11	0/702	0.35	0/937
6	9	0.11	0/800	0.35	0/1061
6	CD	0.15	0/770	0.42	0/1024
6	a2	0.12	0/790	0.27	0/1048
6	a3	0.09	0/711	0.24	0/948
6	a4	0.08	0/762	0.27	0/1013
6	a5	0.08	0/733	0.23	0/976
6	a6	0.09	0/794	0.29	0/1053
6	a7	0.09	0/800	0.29	0/1061
6	a8	0.09	0/711	0.24	0/948
6	a9	0.10	0/724	0.27	0/965
6	v	0.12	0/775	0.30	0/1029
6	w	0.08	0/808	0.22	0/1071
6	x	0.09	0/779	0.28	0/1034
6	y	0.10	0/800	0.27	0/1061
6	z	0.11	0/680	0.31	0/908
7	Ah	0.15	0/1005	0.45	0/1335
7	Ai	0.17	0/1315	0.52	0/1740
7	Aj	0.57	3/790 (0.4%)	1.10	6/1053 (0.6%)
7	Ak	0.20	0/999	0.56	1/1327 (0.1%)
7	Al	0.20	0/819	0.54	1/1092 (0.1%)
7	Am	0.19	0/1357	0.50	0/1794
7	An	0.20	0/988	0.56	1/1313 (0.1%)
7	Ao	0.17	0/1232	0.51	0/1634
7	Ap	0.20	0/562	0.47	0/749
7	Aq	0.17	0/1475	0.46	0/1947
7	Ar	0.19	0/1390	0.53	1/1830 (0.1%)
7	As	0.24	0/1013	0.65	2/1347 (0.1%)
All	All	0.19	14/193454 (0.0%)	0.39	46/278529 (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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	5284	ALA	C-N	15.64	1.55	1.33
3	K	5285	GLY	C-N	13.17	1.51	1.33
4	W	2976	LYS	C-N	13.11	1.51	1.33
7	Aj	143	PRO	CB-CG	-10.87	0.95	1.49
6	2	696	PRO	CG-CD	-9.19	1.19	1.50

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Aj	143	PRO	CA-N-CD	-17.72	87.20	112.00
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	-15.79	74.50	104.50
7	As	130	PRO	CA-N-CD	-13.25	93.45	112.00

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	1365	0
2	Av	43620	0	23665	1432	0
3	A	936	0	1008	10	0
3	Ae	936	0	1008	15	0
3	B	962	0	1035	22	0
3	C	983	0	1056	33	0
3	D	940	0	1011	11	0
3	E	973	0	1043	17	0
3	F	916	0	985	23	0
3	G	983	0	1056	19	0
3	H	958	0	1032	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	983	0	1056	15	0
3	K	977	0	1051	20	0
3	L	991	0	1065	27	0
3	aj	940	0	1011	20	0
3	ak	940	0	1011	14	0
3	al	851	0	909	10	0
3	am	973	0	1048	24	0
3	an	958	0	1032	16	0
3	ao	949	0	1019	21	0
3	ap	973	0	1048	23	0
3	aq	900	0	967	21	0
3	ar	983	0	1056	12	0
3	as	916	0	985	15	0
3	at	962	0	1035	18	0
3	au	859	0	921	12	0
4	Aa	814	0	856	24	0
4	Ab	956	0	1021	27	0
4	Ac	788	0	826	18	0
4	Ad	805	0	843	15	0
4	Af	766	0	797	5	0
4	Ag	823	0	864	9	0
4	At	956	0	1024	33	0
4	J	814	0	856	18	0
4	M	956	0	1024	20	0
4	N	830	0	871	29	0
4	O	814	0	856	33	0
4	P	830	0	871	13	0
4	Q	956	0	1021	16	0
4	R	788	0	826	13	0
4	S	956	0	1021	20	0
4	T	956	0	1021	15	0
4	U	956	0	1021	19	0
4	V	956	0	1021	24	0
4	W	956	0	1021	29	0
4	av	814	0	856	20	0
4	aw	956	0	1021	16	0
4	ax	956	0	1021	21	0
4	ay	956	0	1021	8	0
4	az	788	0	826	13	0
5	X	901	0	951	21	0
5	Y	896	0	946	24	0
5	Z	739	0	779	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	a	995	0	1059	21	0
5	b	833	0	880	15	0
5	c	860	0	906	21	0
5	d	808	0	846	11	0
5	e	768	0	809	14	0
5	f	808	0	846	17	0
5	g	837	0	883	16	0
5	h	801	0	838	13	0
5	i	817	0	858	24	0
5	j	853	0	898	31	0
5	k	817	0	858	24	0
5	l	917	0	971	28	0
5	m	808	0	846	16	0
5	n	910	0	964	30	0
5	o	880	0	928	22	0
5	p	837	0	883	19	0
5	q	891	0	941	23	0
5	r	860	0	906	23	0
5	s	780	0	818	16	0
5	t	890	0	941	31	0
5	u	1001	0	1064	37	0
6	0	741	0	796	19	0
6	1	703	0	755	13	0
6	2	750	0	809	28	0
6	3	736	0	793	17	0
6	4	703	0	755	17	0
6	5	750	0	809	14	0
6	6	688	0	745	15	0
6	7	786	0	847	26	0
6	8	694	0	742	24	0
6	9	792	0	852	27	0
6	CD	762	0	825	24	0
6	a2	782	0	844	28	0
6	a3	703	0	755	15	0
6	a4	754	0	812	14	0
6	a5	725	0	779	21	0
6	a6	786	0	847	16	0
6	a7	792	0	852	19	0
6	a8	703	0	755	18	0
6	a9	716	0	766	25	0
6	v	767	0	828	19	0
6	w	800	0	861	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	x	771	0	831	26	0
6	y	792	0	852	13	0
6	z	673	0	722	23	0
7	Ah	992	0	1087	23	0
7	Ai	1298	0	1466	47	0
7	Aj	780	0	838	30	0
7	Ak	986	0	1082	36	0
7	Al	808	0	866	39	0
7	Am	1340	0	1519	52	0
7	An	975	0	1072	36	0
7	Ao	1215	0	1363	48	0
7	Ap	555	0	584	19	0
7	Aq	1456	0	1660	62	0
7	Ar	1375	0	1585	57	0
7	As	999	0	1097	50	0
All	All	181715	0	149311	3933	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 13.

The worst 5 of 3933 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	1.56
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	1.27
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	49
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	35
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%)	12	45
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	49
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%)	11	43
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%)	11	43
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%)	21	54
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	49
All	All	11912/14160 (84%)	11227 (94%)	676 (6%)	9 (0%)	49	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%)	97 (100%)	0	100	100
3	Ae	97/102 (95%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	99/102 (97%)	99 (100%)	0	100	100
3	C	101/102 (99%)	100 (99%)	1 (1%)	68	75
3	D	97/102 (95%)	97 (100%)	0	100	100
3	E	100/102 (98%)	100 (100%)	0	100	100
3	F	95/102 (93%)	95 (100%)	0	100	100
3	G	101/102 (99%)	101 (100%)	0	100	100
3	H	99/102 (97%)	99 (100%)	0	100	100
3	I	101/102 (99%)	101 (100%)	0	100	100
3	K	100/102 (98%)	100 (100%)	0	100	100
3	L	102/102 (100%)	102 (100%)	0	100	100
3	aj	97/102 (95%)	97 (100%)	0	100	100
3	ak	97/102 (95%)	96 (99%)	1 (1%)	68	75
3	al	86/102 (84%)	86 (100%)	0	100	100
3	am	100/102 (98%)	98 (98%)	2 (2%)	48	66
3	an	99/102 (97%)	99 (100%)	0	100	100
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%)	94 (100%)	0	100	100
3	ar	101/102 (99%)	100 (99%)	1 (1%)	68	75
3	as	95/102 (93%)	95 (100%)	0	100	100
3	at	99/102 (97%)	99 (100%)	0	100	100
3	au	88/102 (86%)	88 (100%)	0	100	100
4	Aa	88/103 (85%)	88 (100%)	0	100	100
4	Ab	103/103 (100%)	103 (100%)	0	100	100
4	Ac	85/103 (82%)	85 (100%)	0	100	100
4	Ad	87/103 (84%)	87 (100%)	0	100	100
4	Af	83/103 (81%)	83 (100%)	0	100	100
4	Ag	89/103 (86%)	88 (99%)	1 (1%)	65	74
4	At	103/103 (100%)	102 (99%)	1 (1%)	68	75
4	J	88/103 (85%)	88 (100%)	0	100	100
4	M	103/103 (100%)	103 (100%)	0	100	100

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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%)	87 (99%)	1 (1%)	65	74
4	P	90/103 (87%)	90 (100%)	0	100	100
4	Q	103/103 (100%)	102 (99%)	1 (1%)	68	75
4	R	85/103 (82%)	85 (100%)	0	100	100
4	S	103/103 (100%)	102 (99%)	1 (1%)	68	75
4	T	103/103 (100%)	103 (100%)	0	100	100
4	U	103/103 (100%)	103 (100%)	0	100	100
4	V	103/103 (100%)	101 (98%)	2 (2%)	50	67
4	W	103/103 (100%)	103 (100%)	0	100	100
4	av	88/103 (85%)	88 (100%)	0	100	100
4	aw	103/103 (100%)	103 (100%)	0	100	100
4	ax	103/103 (100%)	103 (100%)	0	100	100
4	ay	103/103 (100%)	103 (100%)	0	100	100
4	az	85/103 (82%)	85 (100%)	0	100	100
5	X	93/111 (84%)	93 (100%)	0	100	100
5	Y	93/111 (84%)	93 (100%)	0	100	100
5	Z	78/111 (70%)	78 (100%)	0	100	100
5	a	102/111 (92%)	102 (100%)	0	100	100
5	b	88/111 (79%)	88 (100%)	0	100	100
5	c	90/111 (81%)	90 (100%)	0	100	100
5	d	85/111 (77%)	84 (99%)	1 (1%)	63	73
5	e	81/111 (73%)	81 (100%)	0	100	100
5	f	85/111 (77%)	85 (100%)	0	100	100
5	g	88/111 (79%)	88 (100%)	0	100	100
5	h	84/111 (76%)	84 (100%)	0	100	100
5	i	86/111 (78%)	86 (100%)	0	100	100
5	j	89/111 (80%)	89 (100%)	0	100	100
5	k	86/111 (78%)	85 (99%)	1 (1%)	63	73
5	l	95/111 (86%)	95 (100%)	0	100	100
5	m	85/111 (77%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	n	94/111 (85%)	94 (100%)	0	100	100
5	o	92/111 (83%)	92 (100%)	0	100	100
5	p	88/111 (79%)	88 (100%)	0	100	100
5	q	93/111 (84%)	93 (100%)	0	100	100
5	r	90/111 (81%)	90 (100%)	0	100	100
5	s	82/111 (74%)	82 (100%)	0	100	100
5	t	93/111 (84%)	93 (100%)	0	100	100
5	u	103/111 (93%)	103 (100%)	0	100	100
6	0	74/79 (94%)	74 (100%)	0	100	100
6	1	72/79 (91%)	72 (100%)	0	100	100
6	2	75/79 (95%)	75 (100%)	0	100	100
6	3	74/79 (94%)	73 (99%)	1 (1%)	59	71
6	4	72/79 (91%)	72 (100%)	0	100	100
6	5	75/79 (95%)	75 (100%)	0	100	100
6	6	71/79 (90%)	70 (99%)	1 (1%)	59	71
6	7	77/79 (98%)	76 (99%)	1 (1%)	61	72
6	8	71/79 (90%)	71 (100%)	0	100	100
6	9	78/79 (99%)	78 (100%)	0	100	100
6	CD	76/79 (96%)	76 (100%)	0	100	100
6	a2	77/79 (98%)	77 (100%)	0	100	100
6	a3	72/79 (91%)	72 (100%)	0	100	100
6	a4	75/79 (95%)	75 (100%)	0	100	100
6	a5	73/79 (92%)	73 (100%)	0	100	100
6	a6	77/79 (98%)	77 (100%)	0	100	100
6	a7	78/79 (99%)	78 (100%)	0	100	100
6	a8	72/79 (91%)	72 (100%)	0	100	100
6	a9	72/79 (91%)	72 (100%)	0	100	100
6	v	76/79 (96%)	76 (100%)	0	100	100
6	w	79/79 (100%)	79 (100%)	0	100	100
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%)	69 (100%)	0	100	100
7	Ah	104/158 (66%)	103 (99%)	1 (1%)	68	75
7	Ai	135/158 (85%)	134 (99%)	1 (1%)	76	78
7	Aj	82/158 (52%)	82 (100%)	0	100	100
7	Ak	103/158 (65%)	103 (100%)	0	100	100
7	Al	85/158 (54%)	84 (99%)	1 (1%)	63	73
7	Am	140/158 (89%)	139 (99%)	1 (1%)	76	78
7	An	102/158 (65%)	101 (99%)	1 (1%)	68	75
7	Ao	127/158 (80%)	127 (100%)	0	100	100
7	Ap	57/158 (36%)	56 (98%)	1 (2%)	51	68
7	Aq	152/158 (96%)	151 (99%)	1 (1%)	76	78
7	Ar	144/158 (91%)	144 (100%)	0	100	100
7	As	105/158 (66%)	105 (100%)	0	100	100
All	All	9893/11376 (87%)	9869 (100%)	24 (0%)	85	85

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	ar	2607	THR
7	Ai	157	THR
7	Ah	413	HIS
7	Al	323	LYS
5	d	750	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
4	az	513	GLN
4	Ab	787	GLN
5	l	321	ASN
5	l	306	GLN
4	Ag	3133	ASN

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.

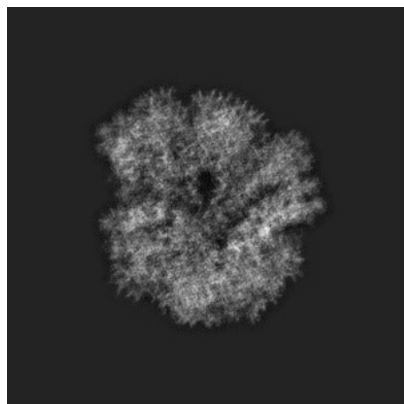
6 Map visualisation [i](#)

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.

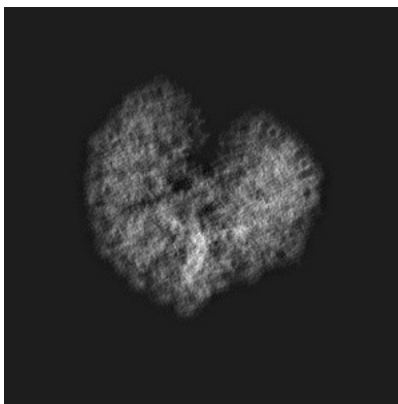
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

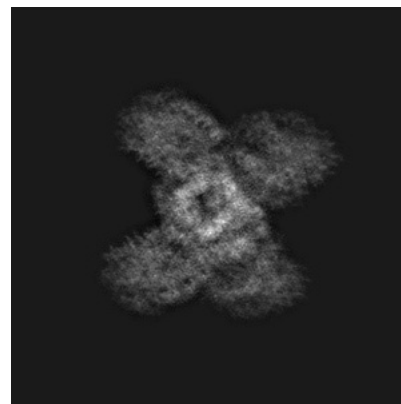
6.1.1 Primary map



X

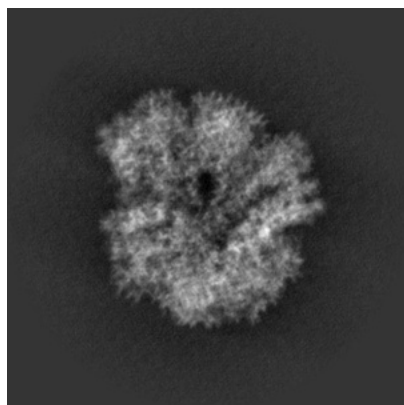


Y

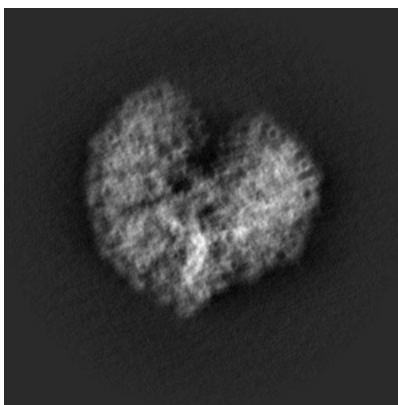


Z

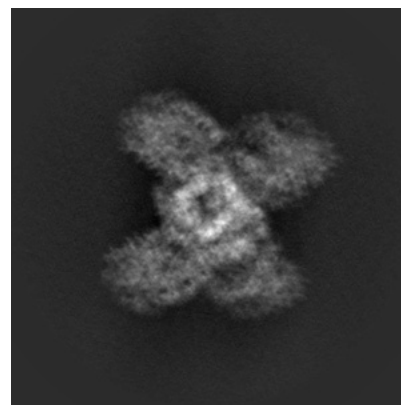
6.1.2 Raw map



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

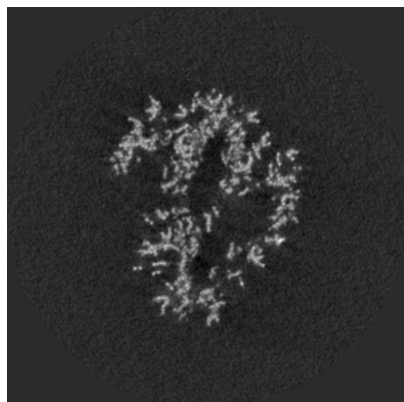


Y Index: 144

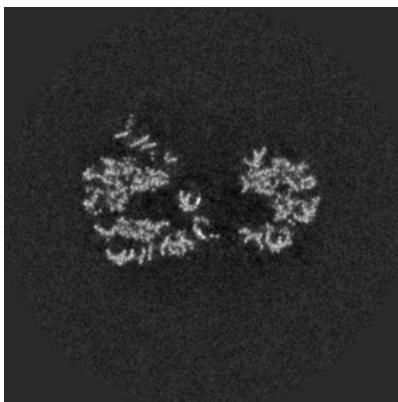


Z Index: 144

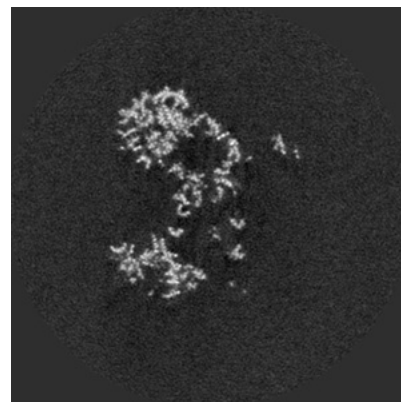
6.2.2 Raw map



X Index: 144



Y Index: 144

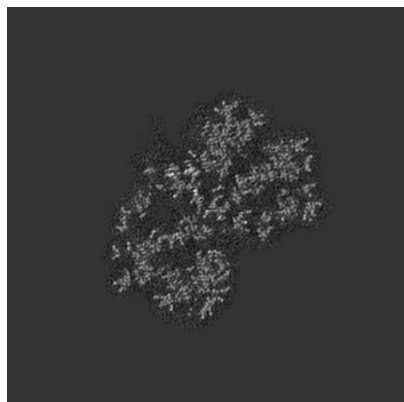


Z Index: 144

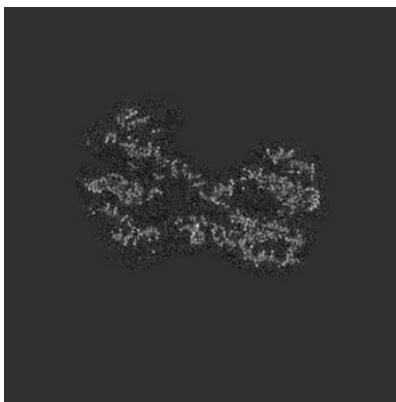
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 125

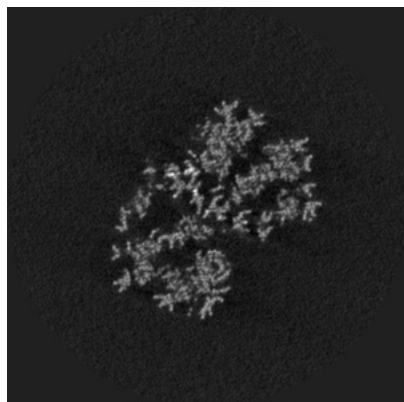


Y Index: 153

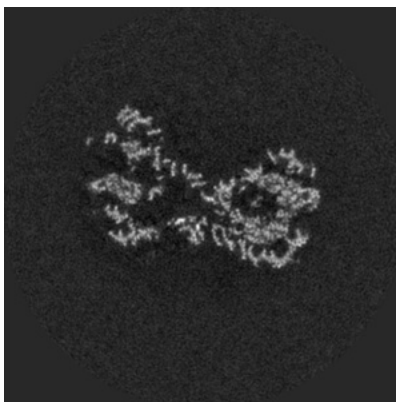


Z Index: 139

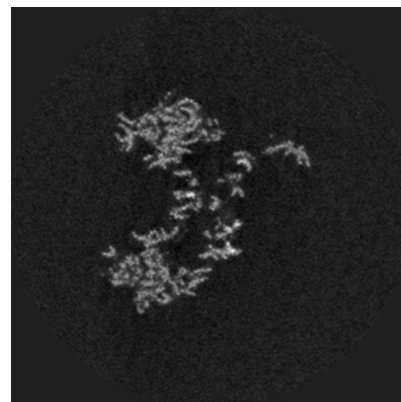
6.3.2 Raw map



X Index: 125



Y Index: 154

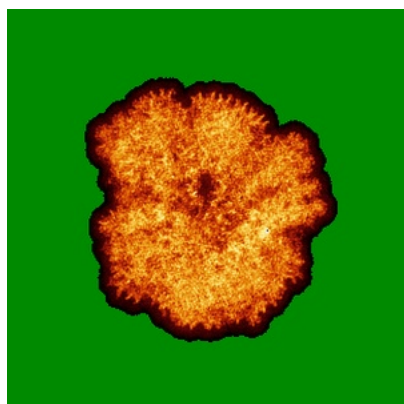


Z Index: 138

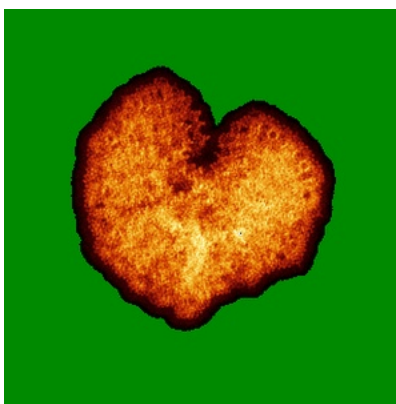
The images above show the largest variance slices of the map in three orthogonal directions.

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

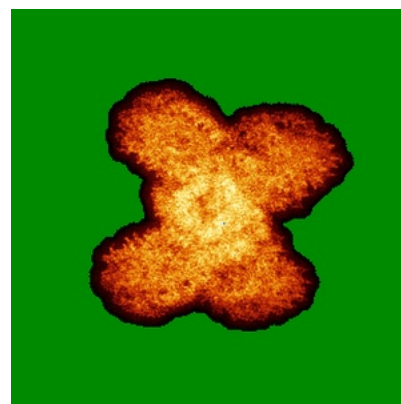
6.4.1 Primary map



X

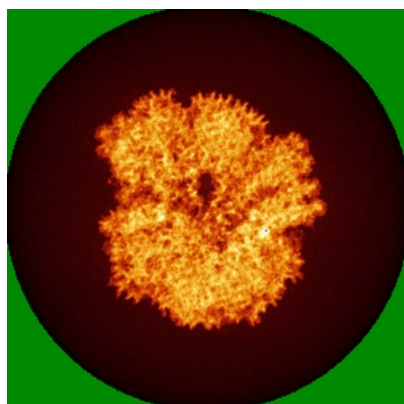


Y

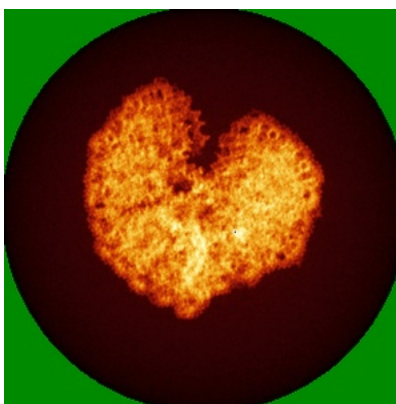


Z

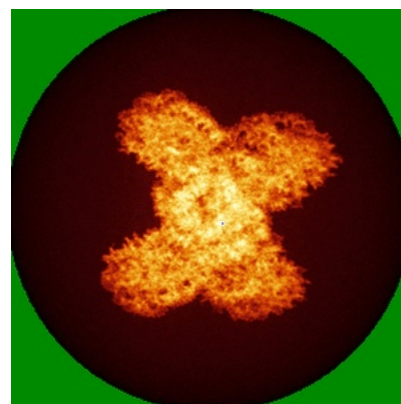
6.4.2 Raw map



X



Y

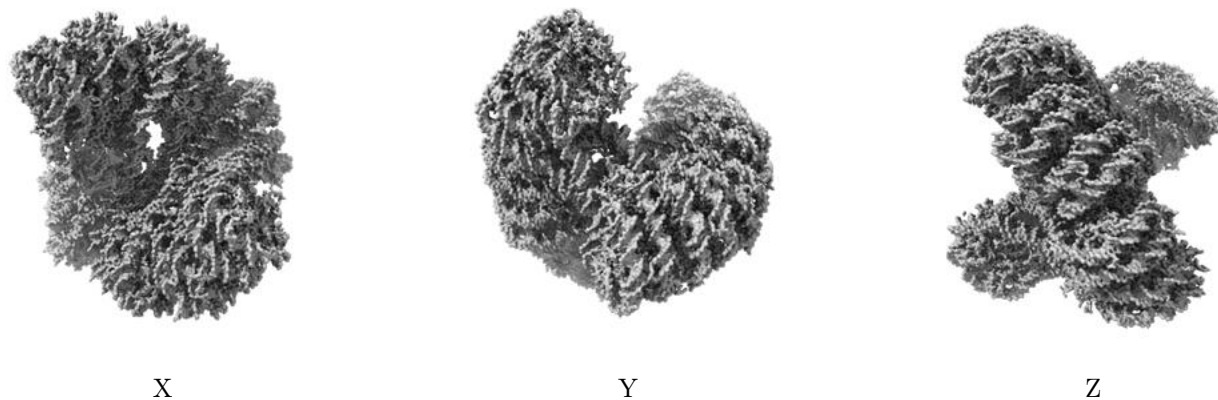


Z

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.

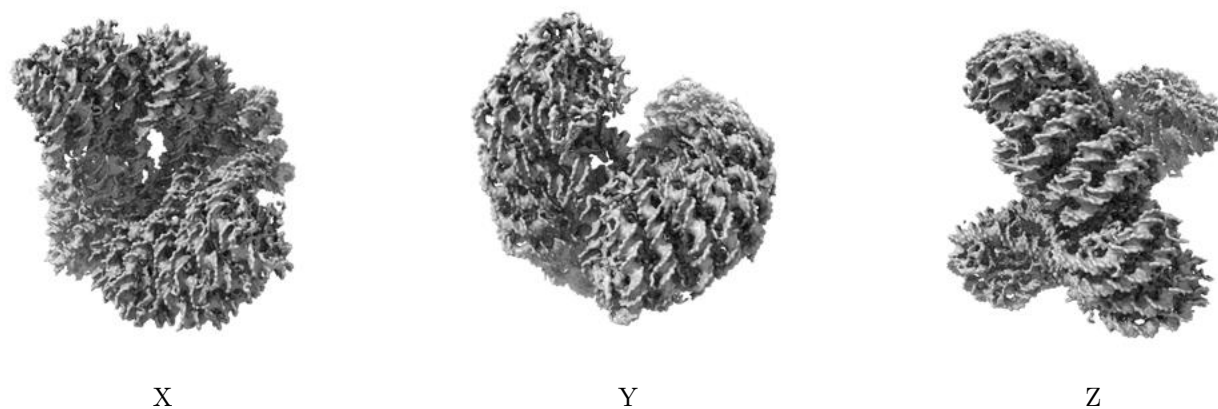
6.5 Orthogonal surface views [i](#)

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.

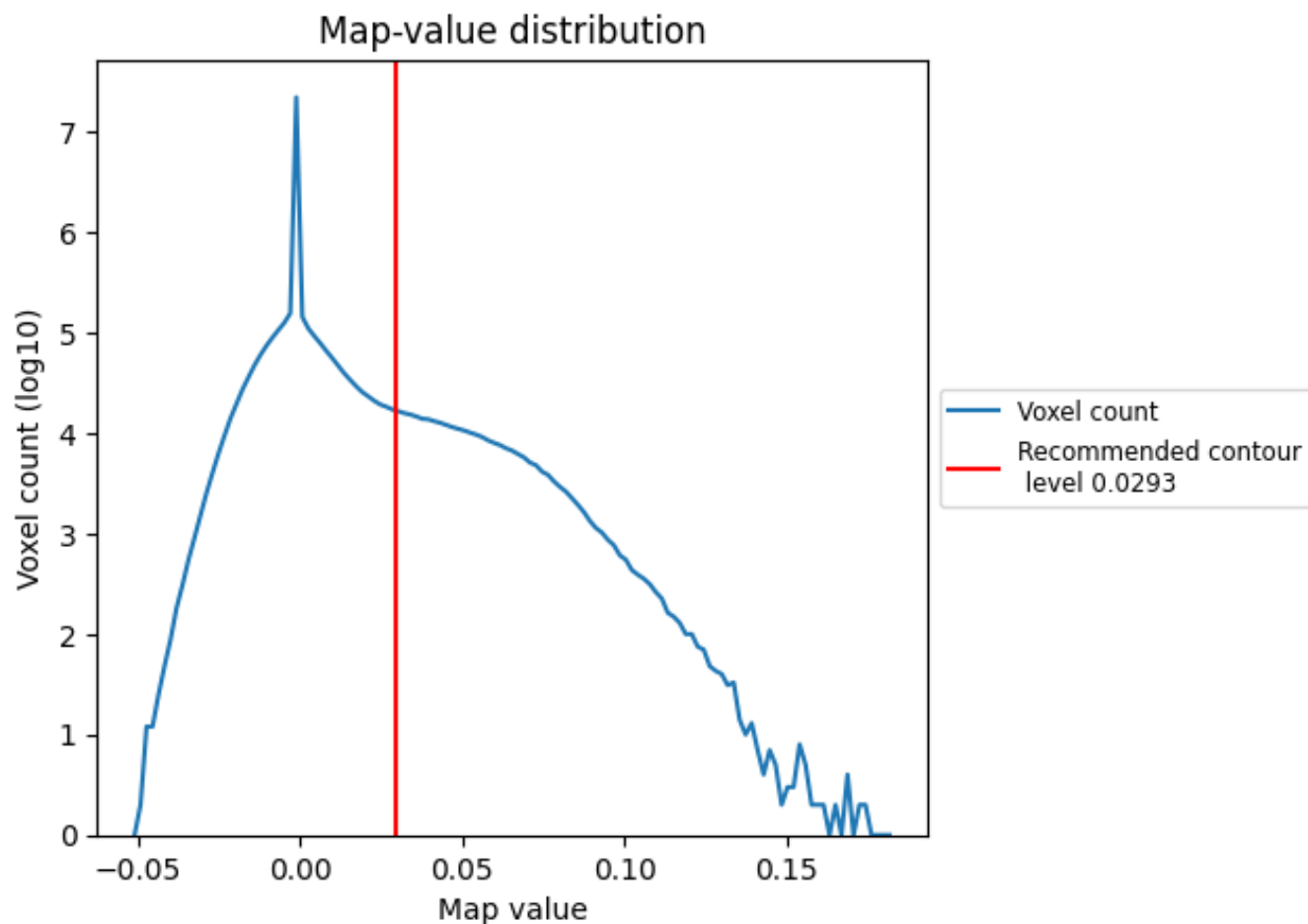
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

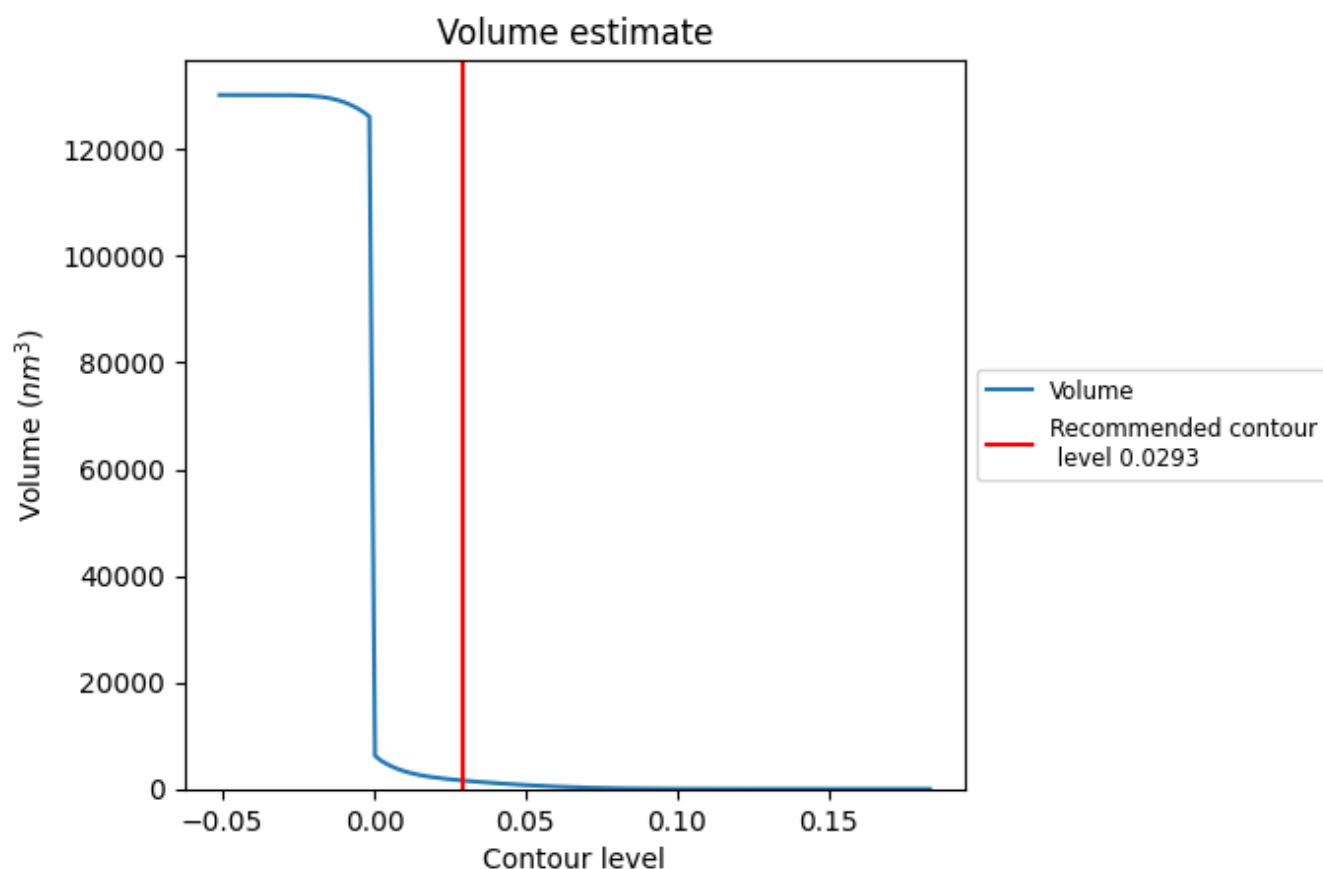
This section contains the results of statistical analysis of the map.

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.

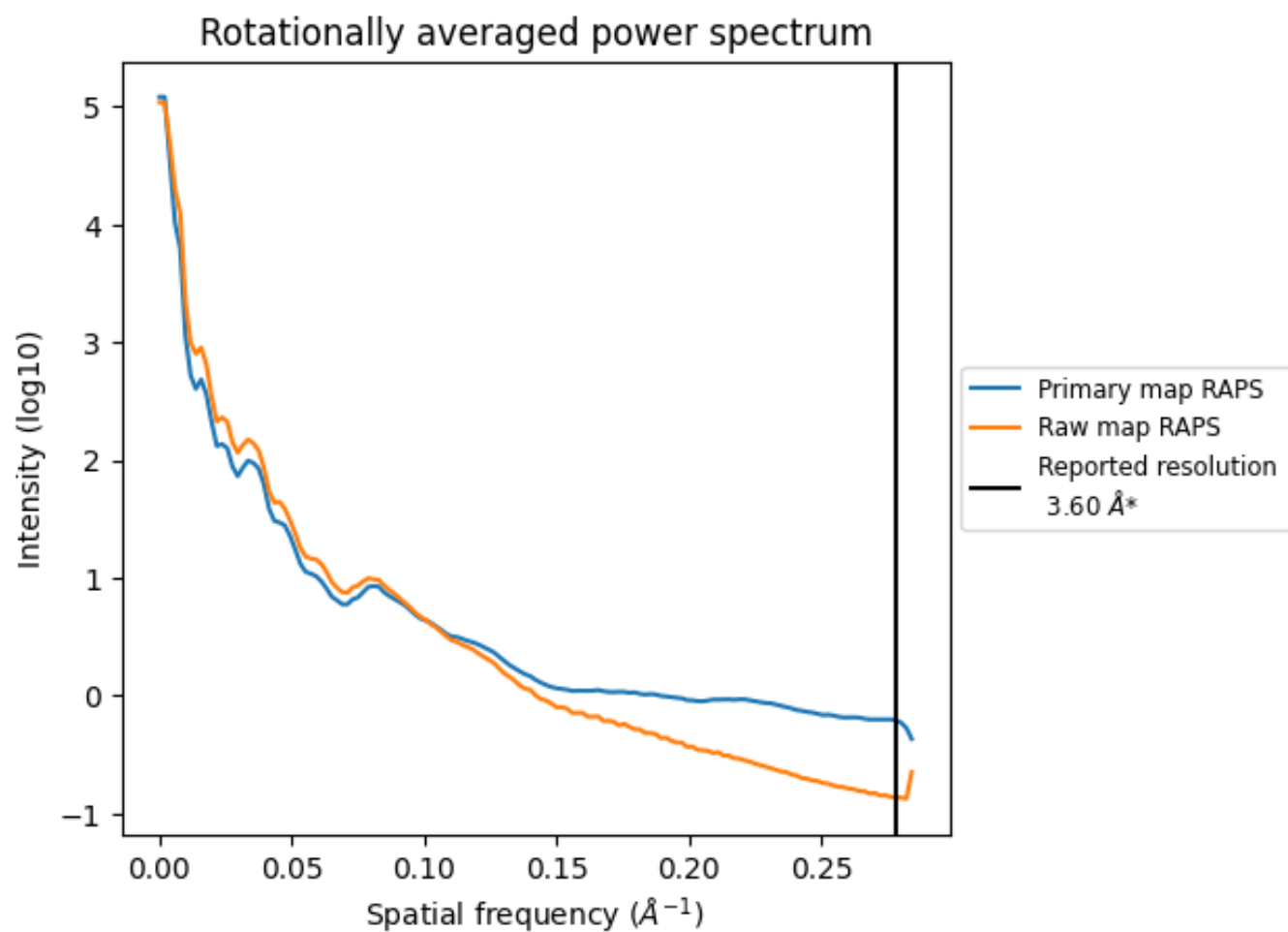
7.2 Volume estimate [i](#)



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](#)

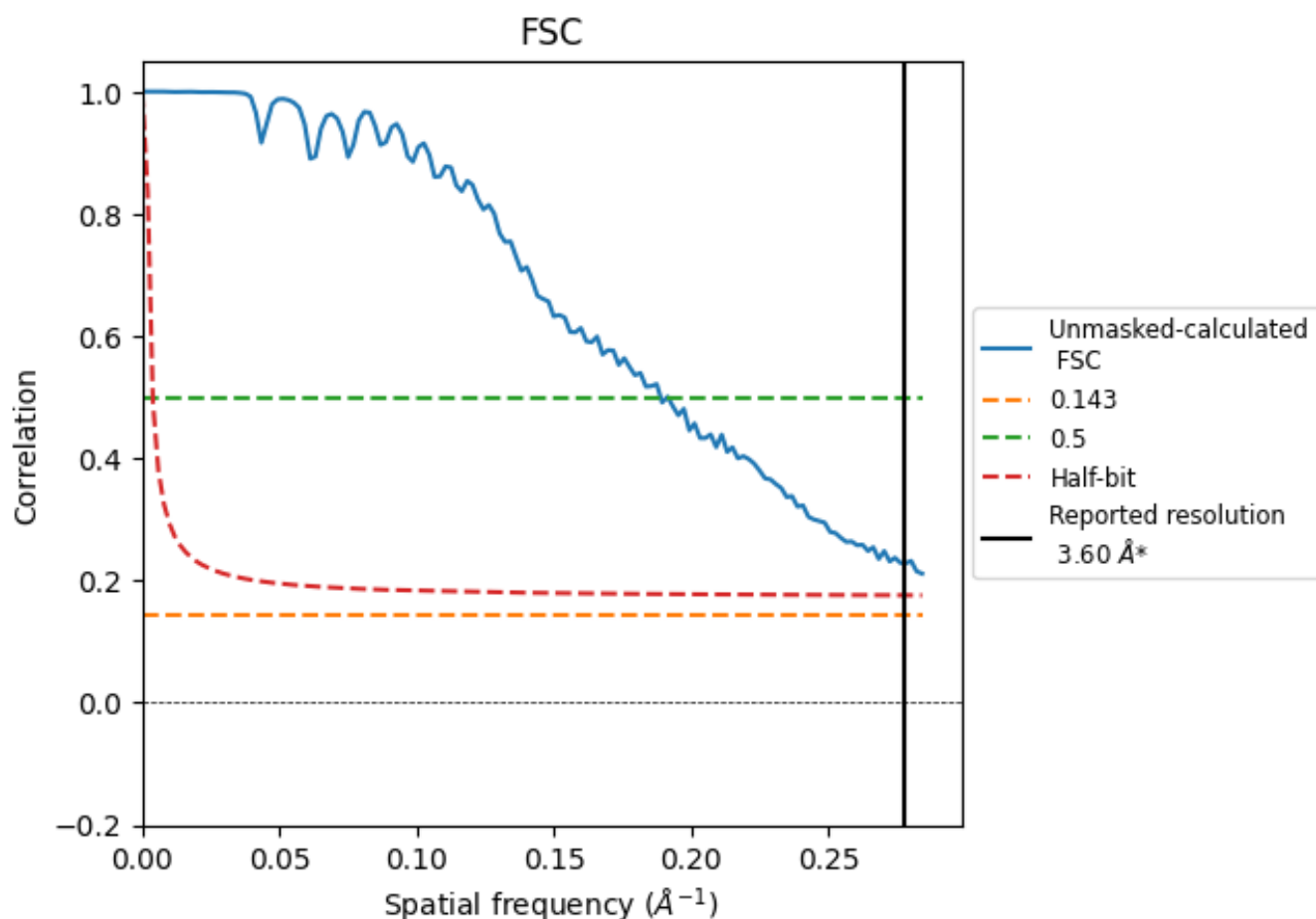


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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](#)

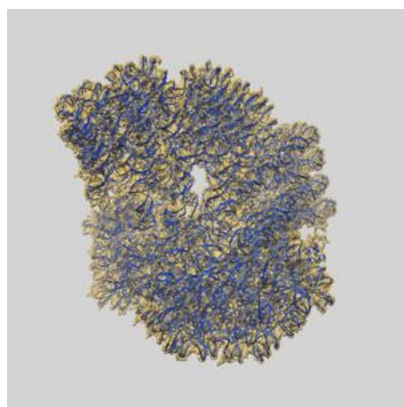
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	5.30	-

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

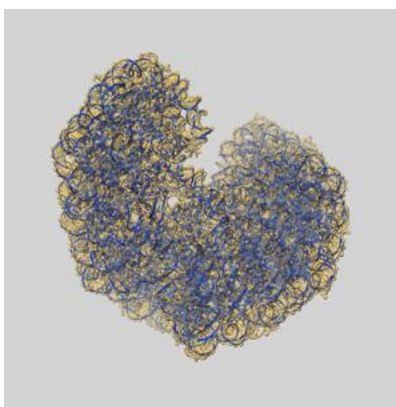
9 Map-model fit [i](#)

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](#).

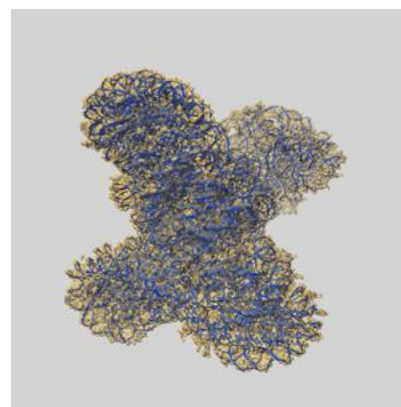
9.1 Map-model overlay [i](#)



X



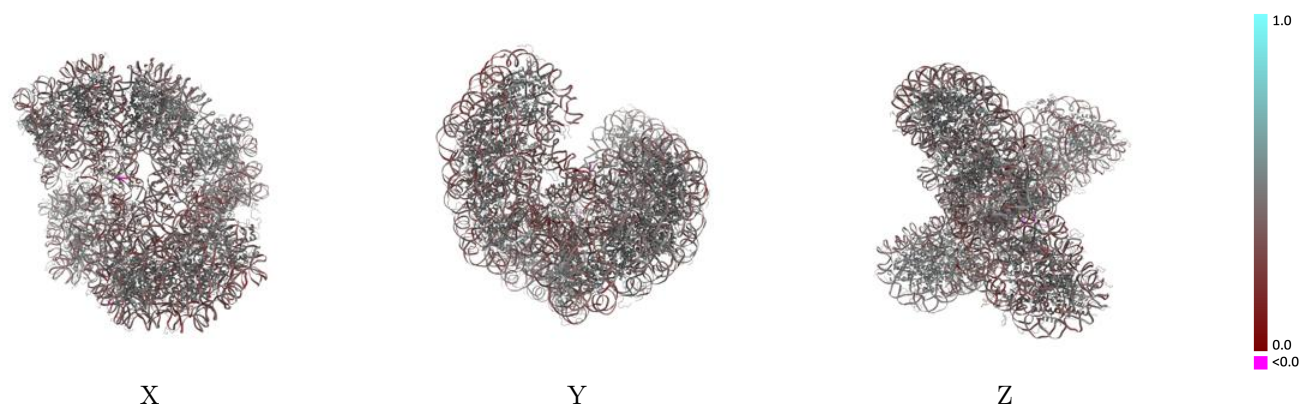
Y



Z

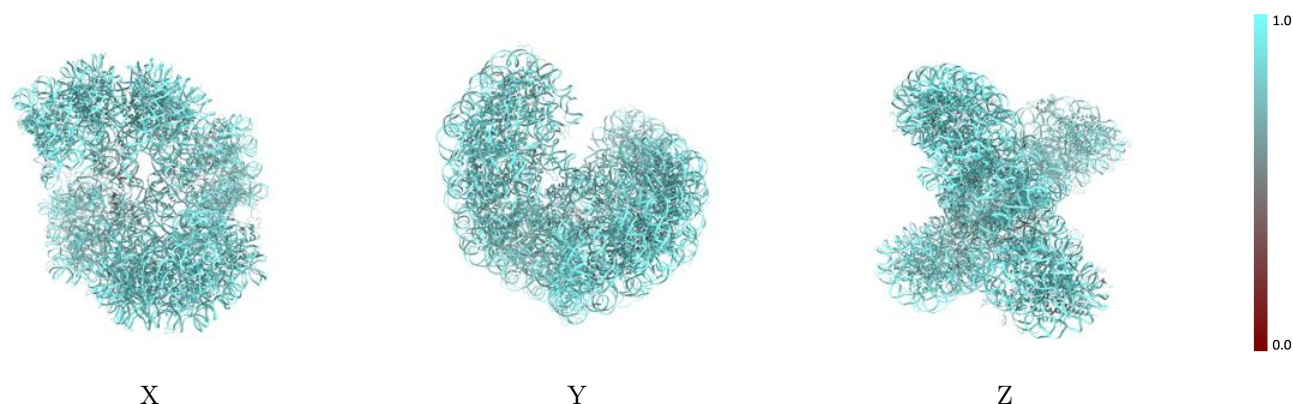
The images above show the 3D surface view of the map at the recommended contour level 0.0293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



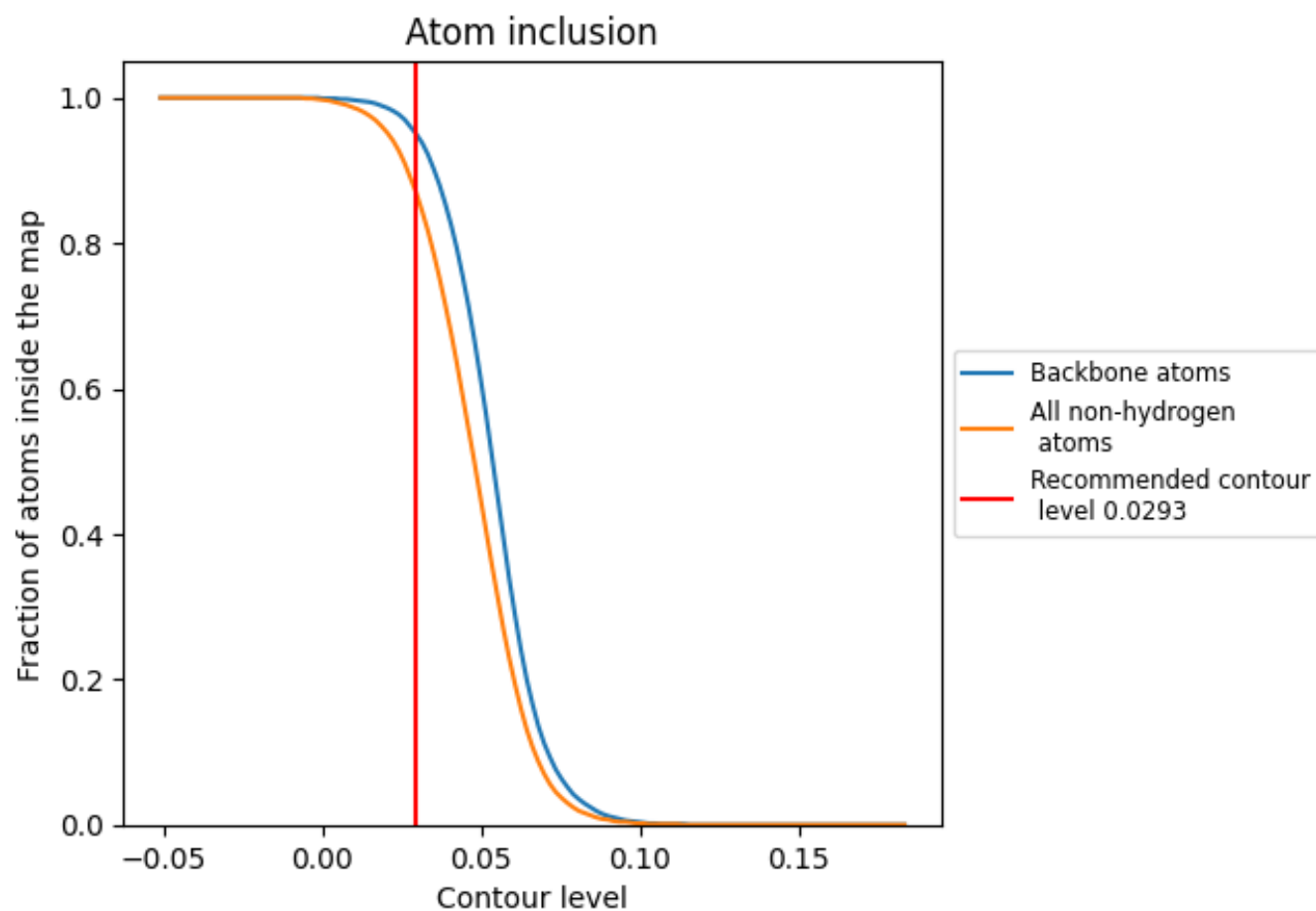
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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