



Full wwPDB EM Validation Report ⓘ

Oct 2, 2024 – 04:45 PM JST

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 Full wwPDB EM Validation 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:

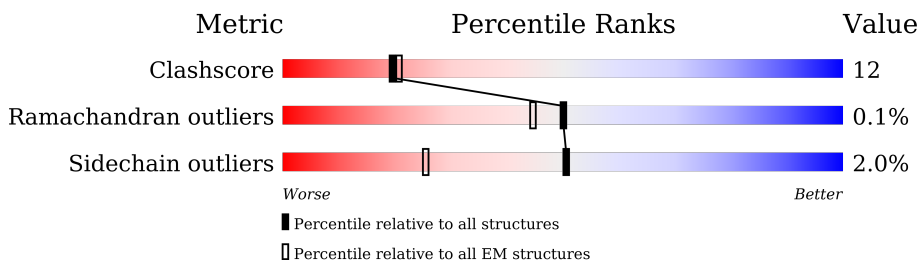
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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	
2	Av	2124	
3	A	130	
3	Ae	130	
3	B	130	
3	C	130	
3	D	130	
3	E	130	

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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	72% 11% 16%
4	M	123	85% 15%
4	N	123	66% 19% 15%
4	O	123	67% 16% 16%
4	P	123	76% 9% 15%
4	Q	123	86% 13%
4	R	123	69% 12% 19%
4	S	123	80% 20%
4	T	123	84% 16%
4	U	123	89% 10%
4	V	123	80% 20%
4	W	123	73% 26%
4	av	123	83% 16%
4	aw	123	98%
4	ax	123	98%
4	ay	123	98%
4	az	123	80% 19%
5	X	136	69% 13% 18%
5	Y	136	72% 9% 18%
5	Z	136	54% 12% 34%
5	a	136	89% 8%
5	b	136	73% 26%
5	c	136	76% 22%
5	d	136	72% 28%
5	e	136	68% 31%



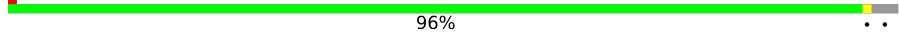

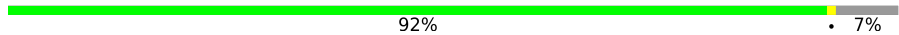

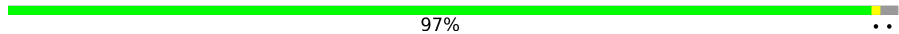
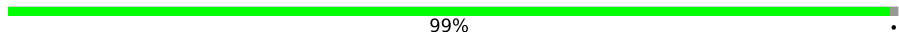


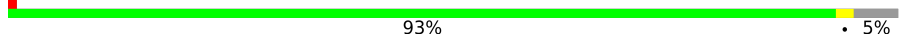
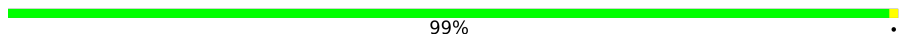
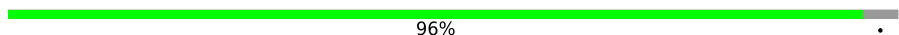
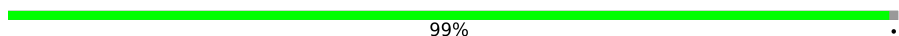










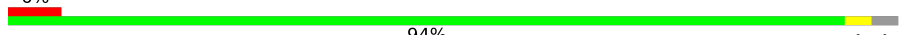
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Mol	Chain	Length	Quality of chain
5	f	136	 72% 28%
5	g	136	 74% 25%
5	h	136	 69% 29%
5	i	136	 71% 27%
5	j	136	 76% 23%
5	k	136	 72% 27%
5	l	136	 81% 16%
5	m	136	 69% 28%
5	n	136	 82% 17%
5	o	136	 79% 20%
5	p	136	 74% 25%
5	q	136	 79% 19%
5	r	136	 75% 22%
5	s	136	 70% 30%
5	t	136	 80% 19%
5	u	136	 90% 7%
6	0	103	 78% 13% 9%
6	1	103	 8% 75% 10% 16%
6	2	103	 76% 16% 8%
6	3	103	 79% 12% 10%
6	4	103	 74% 11% 16%
6	5	103	 83% 10% 8%
6	6	103	 72% 11% 17%
6	7	103	 77% 20% 3%
6	8	103	 65% 18% 17%

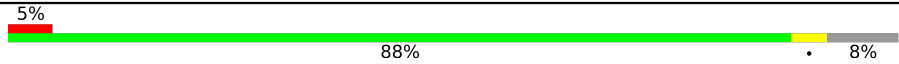

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Mol	Chain	Length	Quality of chain
6	9	103	 77% 22%
6	CD	103	 75% 17% 6%
6	a2	103	 96%
6	a3	103	 83% 16%
6	a4	103	 92% 7%
6	a5	103	 7% 88% 12%
6	a6	103	 97%
6	a7	103	 99%
6	a8	103	 7% 82% 16%
6	a9	103	 6% 85% 13%
6	v	103	 93% 5%
6	w	103	 99%
6	x	103	 96%
6	y	103	 99%
6	z	103	 81% 18%
7	Ah	196	 64% 34%
7	Ai	196	 5% 84% 13%
7	Aj	196	 49% 47%
7	Ak	196	 64% 34%
7	Al	196	 5% 52% 45%
7	Am	196	 87% 11%
7	An	196	 61% 35%
7	Ao	196	 80% 19%
7	Ap	196	 37% 63%
7	Aq	196	 6% 94%

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

2 Entry composition [i](#)

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
			Total	C	N	O	P		
1	Au	2116	43052	20433	7794	12709	2116	0	0

- Molecule 2 is a DNA chain called DNA.

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

- Molecule 3 is a protein called Histone H2A.

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

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

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

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

Continued on next page...

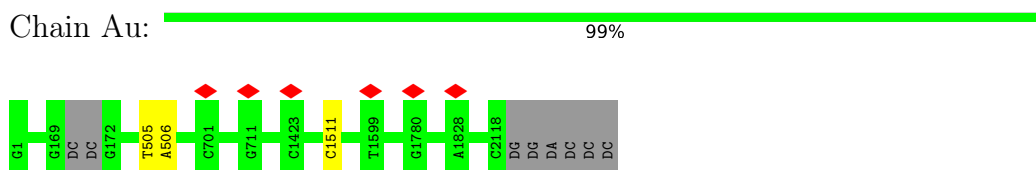
Continued from previous page...

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

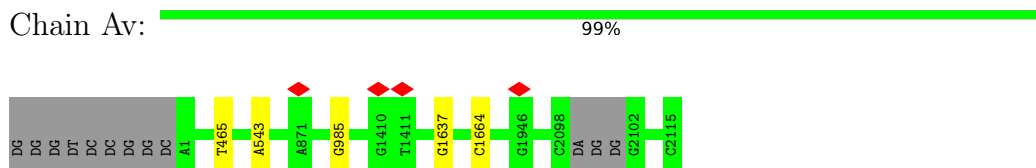
3 Residue-property plots [i](#)

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.

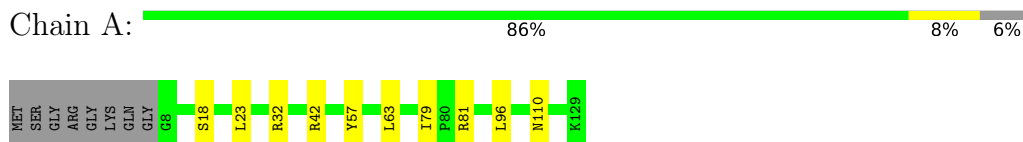
- Molecule 1: DNA



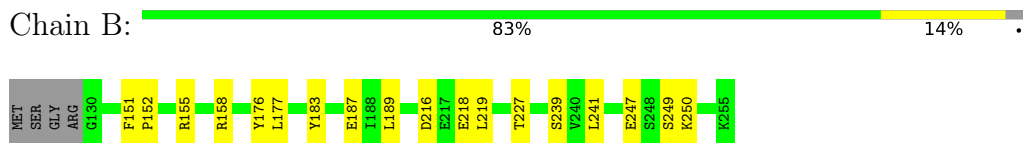
- Molecule 2: DNA



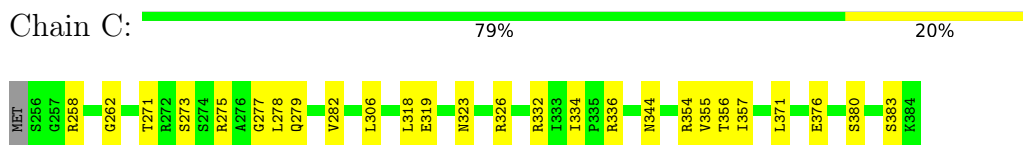
- Molecule 3: Histone H2A



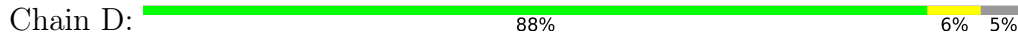
- Molecule 3: Histone H2A



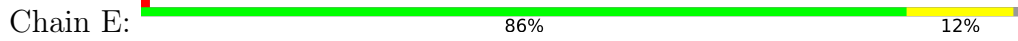
- Molecule 3: Histone H2A



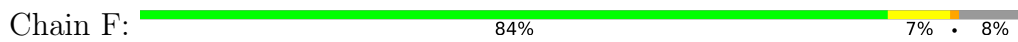
- Molecule 3: Histone H2A



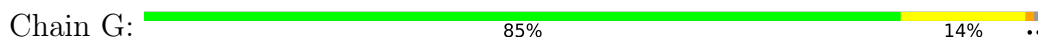
● Molecule 3: Histone H2A



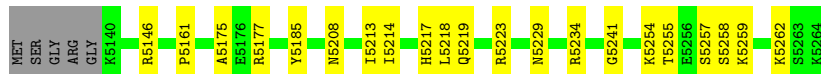
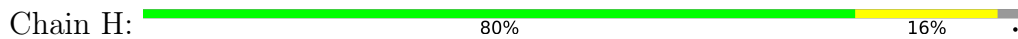
● Molecule 3: Histone H2A



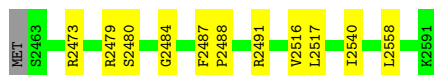
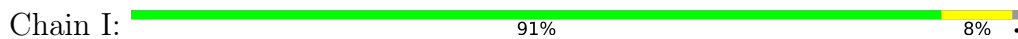
● Molecule 3: Histone H2A



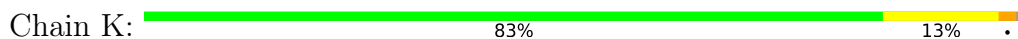
● Molecule 3: Histone H2A



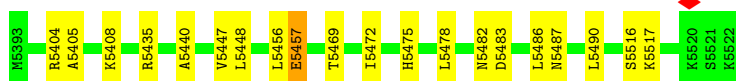
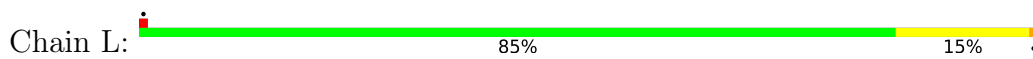
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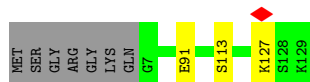
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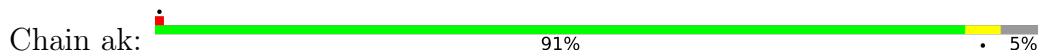
● Molecule 3: Histone H2A



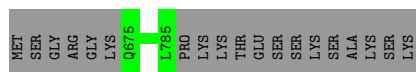
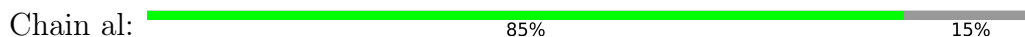
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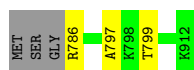
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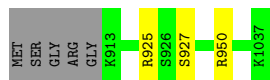
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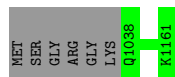
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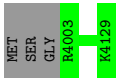
• Molecule 3: Histone H2A



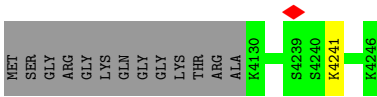
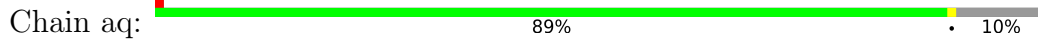
• Molecule 3: Histone H2A



• Molecule 3: Histone H2A



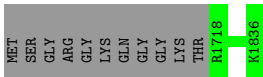
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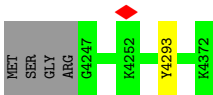
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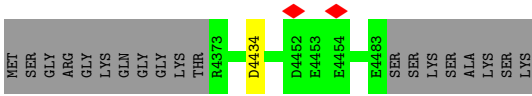
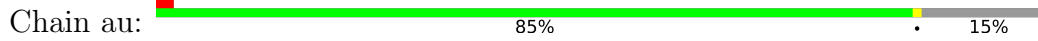
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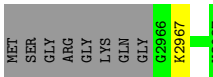
● Molecule 3: Histone H2A



● Molecule 3: Histone H2A

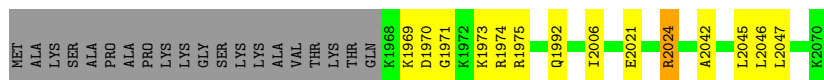


● Molecule 3: Histone H2A



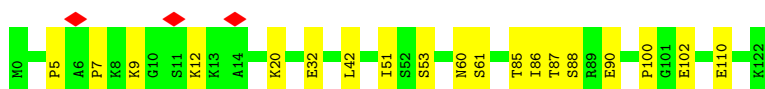
- Molecule 4: Histone H2B 1.1

Chain J:  72% 11% 16%



- Molecule 4: Histone H2B 1.1

Chain M:  85% 15%



- Molecule 4: Histone H2B 1.1

Chain N:  66% 19% 15%




- Molecule 4: Histone H2B 1.1

Chain O:  67% 16% 16%




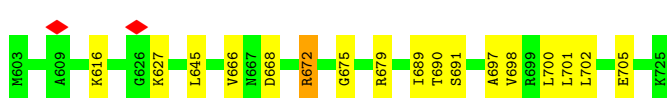
- Molecule 4: Histone H2B 1.1

Chain P:  76% 9% 15%



- Molecule 4: Histone H2B 1.1

Chain Q:  86% 13%

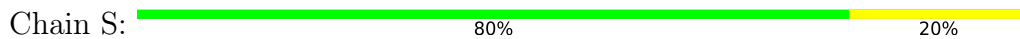


- Molecule 4: Histone H2B 1.1

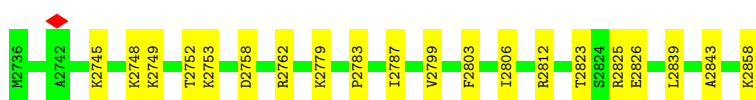
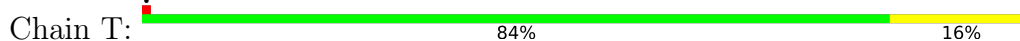
Chain R:  69% 12% 19%



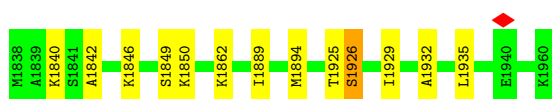
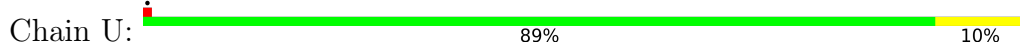
- Molecule 4: Histone H2B 1.1



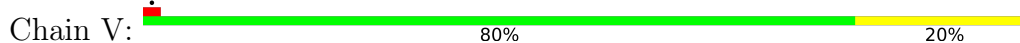
• Molecule 4: Histone H2B 1.1



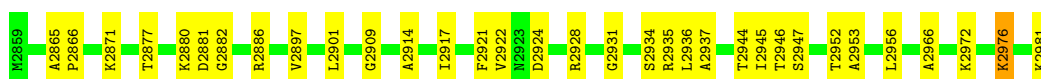
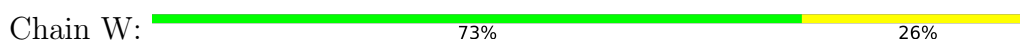
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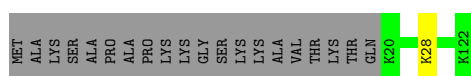
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



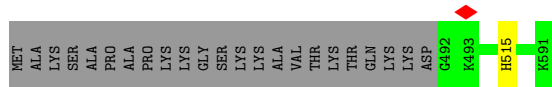
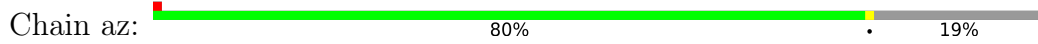
• Molecule 4: Histone H2B 1.1



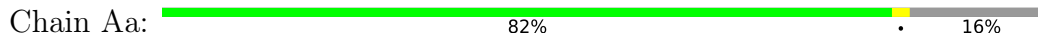
● Molecule 4: Histone H2B 1.1



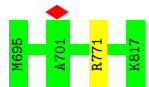
● Molecule 4: Histone H2B 1.1



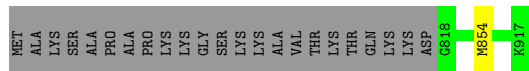
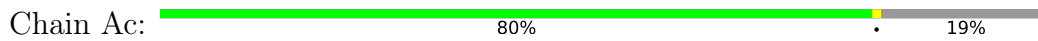
● Molecule 4: Histone H2B 1.1



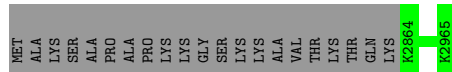
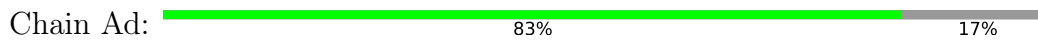
● Molecule 4: Histone H2B 1.1



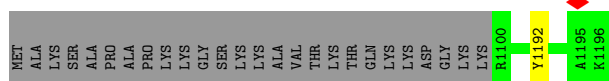
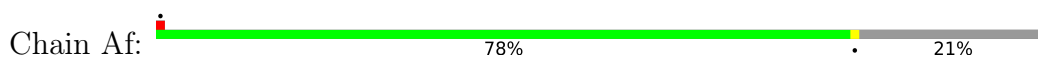
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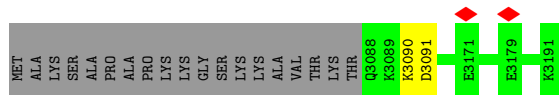
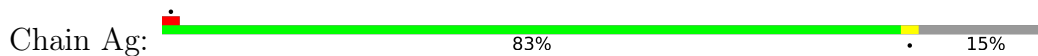
● Molecule 4: Histone H2B 1.1



● Molecule 4: Histone H2B 1.1



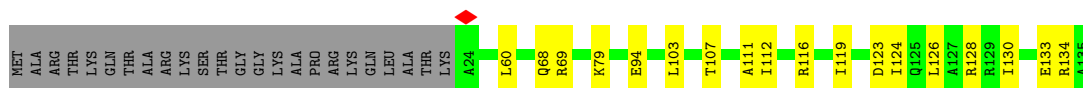
● Molecule 4: Histone H2B 1.1



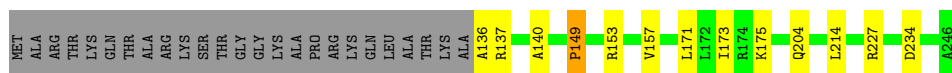
● Molecule 4: Histone H2B 1.1



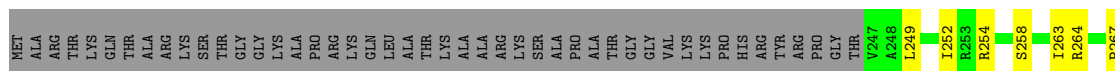
● Molecule 5: Histone H3



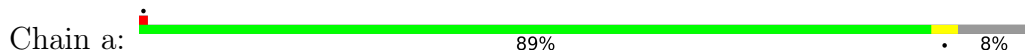
● Molecule 5: Histone H3

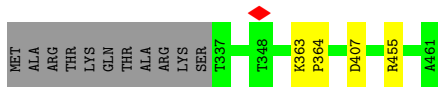


● Molecule 5: Histone H3

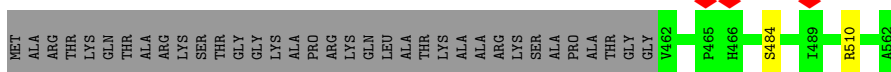


● Molecule 5: Histone H3

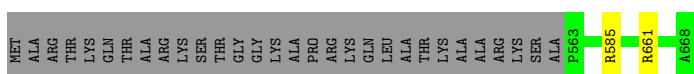




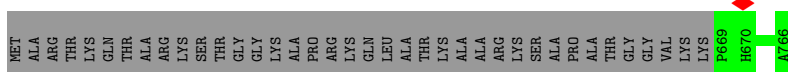
• Molecule 5: Histone H3



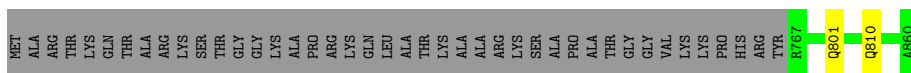
• Molecule 5: Histone H3



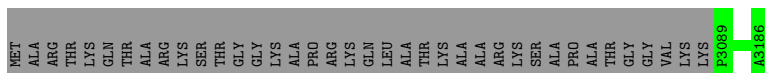
• Molecule 5: Histone H3



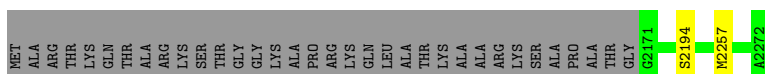
• Molecule 5: Histone H3



• Molecule 5: Histone H3

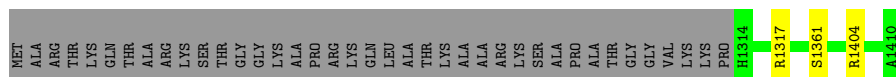


• Molecule 5: Histone H3

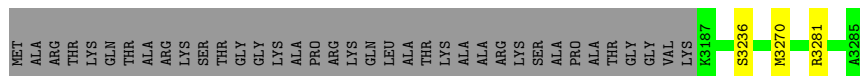


• Molecule 5: Histone H3

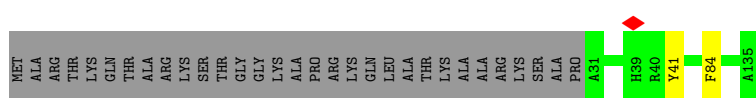




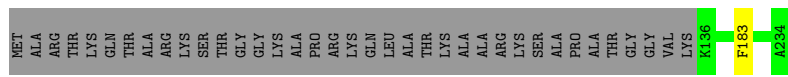
• Molecule 5: Histone H3



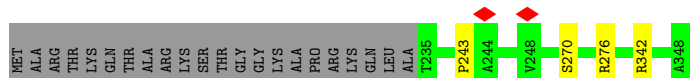
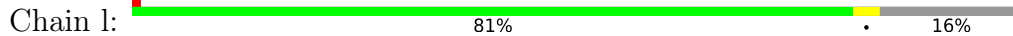
• Molecule 5: Histone H3



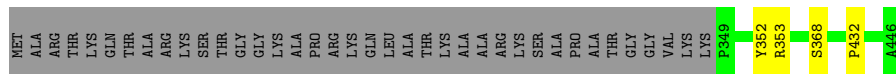
• Molecule 5: Histone H3



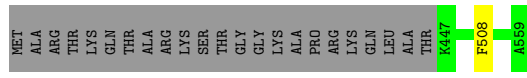
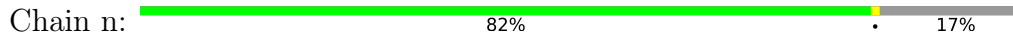
• Molecule 5: Histone H3



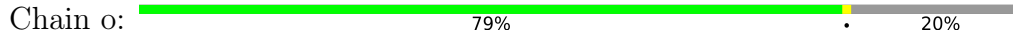
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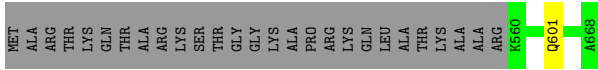


• Molecule 5: Histone H3

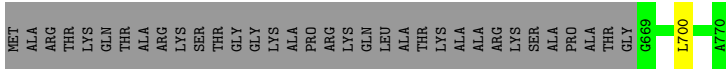


• Molecule 5: Histone H3

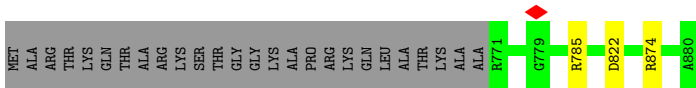
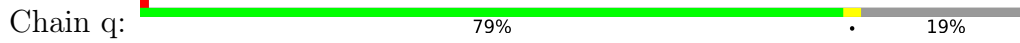




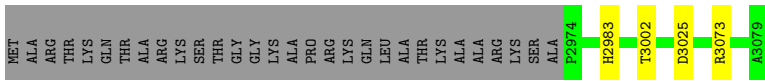
● Molecule 5: Histone H3



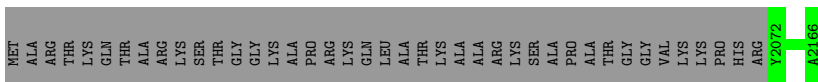
● Molecule 5: Histone H3



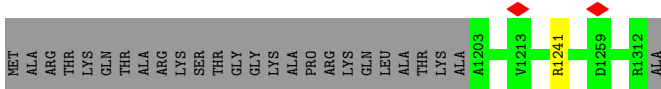
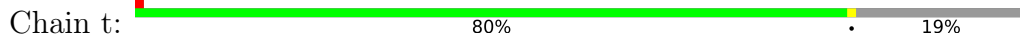
● Molecule 5: Histone H3



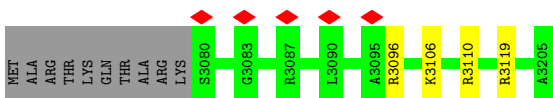
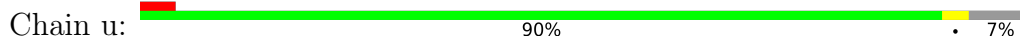
● Molecule 5: Histone H3



● Molecule 5: Histone H3

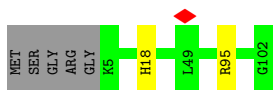


● Molecule 5: Histone H3



● Molecule 6: Histone H4





• Molecule 6: Histone H4



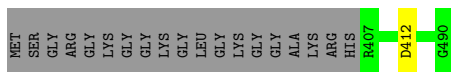
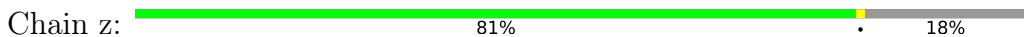
• Molecule 6: Histone H4



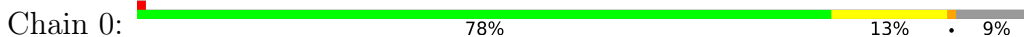
• Molecule 6: Histone H4



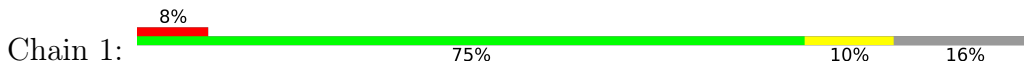
• Molecule 6: Histone H4



• Molecule 6: Histone H4

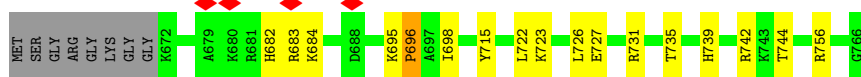


• Molecule 6: Histone H4

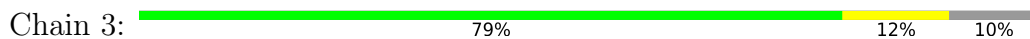


• Molecule 6: Histone H4





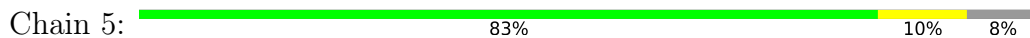
• Molecule 6: Histone H4



• Molecule 6: Histone H4



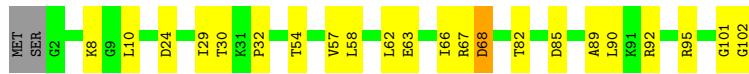
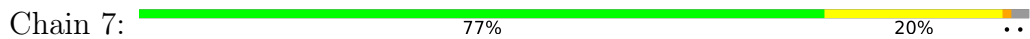
• Molecule 6: Histone H4



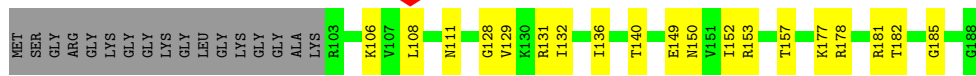
• Molecule 6: Histone H4



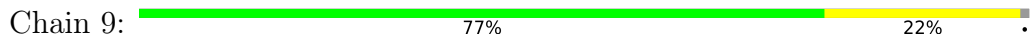
• Molecule 6: Histone H4



• Molecule 6: Histone H4

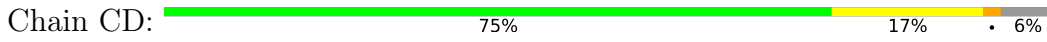


• Molecule 6: Histone H4

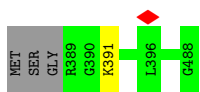




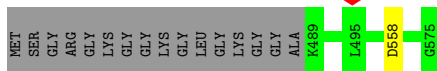
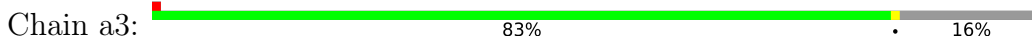
• Molecule 6: Histone H4



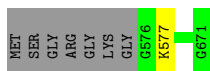
• Molecule 6: Histone H4



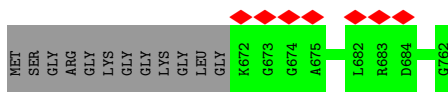
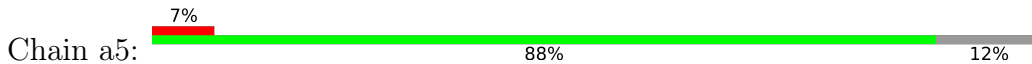
• Molecule 6: Histone H4



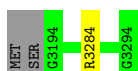
• Molecule 6: Histone H4



• Molecule 6: Histone H4



• Molecule 6: Histone H4

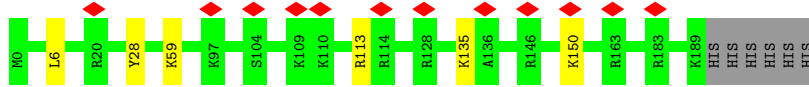


• Molecule 6: Histone H4

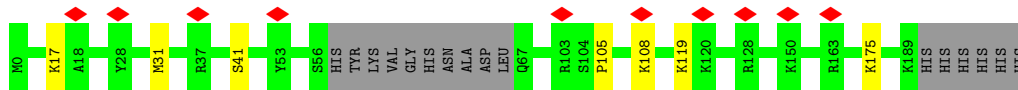
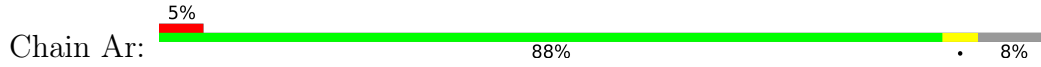


ALA
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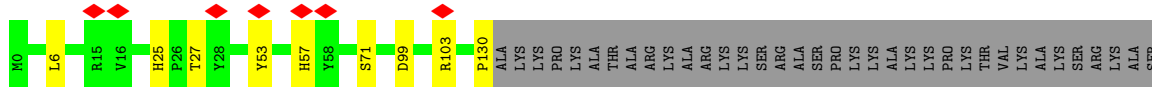
• Molecule 7: Histone H5



• Molecule 7: Histone H5



• Molecule 7: Histone H5



LYS
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PRO
ALA
LYS
SER
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HIS
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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

All (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
7	Aj	143	PRO	CA-CB	6.11	1.65	1.53
7	Aj	143	PRO	N-CD	-5.73	1.39	1.47
3	L	5457	GLU	CD-OE1	-5.52	1.19	1.25
4	ay	412	LYS	C-N	5.44	1.46	1.34
1	Au	1511	DC	C1'-N1	5.14	1.55	1.49
3	L	5457	GLU	C-N	5.05	1.45	1.34

All (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
7	Aj	142	ALA	C-N-CD	10.06	149.53	128.40
6	2	696	PRO	CA-CB-CG	-9.08	86.75	104.00
6	2	696	PRO	CA-N-CD	-8.43	99.70	111.50
3	K	5284	ALA	O-C-N	7.83	136.51	123.20
5	m	432	PRO	CA-N-CD	-7.11	101.55	111.50
7	Aj	141	PRO	CA-N-CD	-6.76	102.04	111.50
7	As	130	PRO	N-CD-CG	-6.55	93.37	103.20
7	An	8	PRO	CA-N-CD	-6.52	102.37	111.50
3	K	5285	GLY	O-C-N	-6.47	112.34	122.70
4	S	854	PRO	CA-N-CD	-6.21	102.80	111.50
3	K	5284	ALA	CA-C-N	-6.13	103.94	116.20
2	Av	1637	DG	O4'-C4'-C3'	-5.92	102.13	104.50
7	Ar	105	PRO	CA-N-CD	-5.91	103.23	111.50
3	C	278	LEU	O-C-N	5.84	132.05	122.70
3	K	5360	LEU	CA-CB-CG	5.80	128.64	115.30
3	K	5284	ALA	C-N-CA	-5.76	110.20	122.30
2	Av	465	DT	O4'-C4'-C3'	-5.75	102.20	104.50
7	An	66	LEU	CA-CB-CG	5.64	128.28	115.30
7	Aj	141	PRO	N-CD-CG	-5.61	94.78	103.20
2	Av	543	DA	O4'-C4'-C3'	-5.48	102.31	104.50
1	Au	506	DA	O4'-C1'-N9	5.39	111.78	108.00
7	Ak	589	PRO	CA-N-CD	-5.34	104.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	364	PRO	CA-N-CD	-5.30	104.09	111.50
5	l	243	PRO	CA-N-CD	-5.23	104.18	111.50
2	Av	985	DG	O4'-C1'-N9	5.09	111.56	108.00
5	Y	149	PRO	CA-N-CD	-5.09	104.38	111.50
2	Av	1664	DC	O4'-C1'-N1	5.06	111.54	108.00
7	As	6	LEU	CA-CB-CG	5.05	126.93	115.30
1	Au	505	DT	O4'-C1'-N1	5.05	111.54	108.00
4	ax	253	PRO	CA-N-CD	-5.04	104.45	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
3:C:279:GLN:NE2	4:O:419:GLN:HE22	1.50	0.94
3:B:218:GLU:HB3	4:N:208:LEU:HD11	1.50	0.92
3:C:279:GLN:HE21	4:O:419:GLN:HE22	1.18	0.91
6:7:30:THR:HG22	6:7:32:PRO:HD2	1.53	0.89
3:C:279:GLN:CD	4:O:419:GLN:OE1	2.13	0.86
4:M:9:LYS:HA	4:M:12:LYS:HE2	1.65	0.78
6:3:3174:LYS:HZ3	6:3:3179:ASN:HA	1.49	0.78
3:B:227:THR:HG21	6:8:181:ARG:HH21	1.51	0.75
5:Z:276:ALA:HB1	5:Z:283:LEU:HD13	1.68	0.74
3:C:279:GLN:OE1	4:O:419:GLN:OE1	2.05	0.73
5:X:60:LEU:HD21	5:X:94:GLU:HG2	1.74	0.70
4:U:1849:SER:OG	4:U:1850:LYS:N	2.25	0.69
3:A:63:LEU:HD13	4:M:42:LEU:HB2	1.75	0.68
3:L:5456:LEU:HD22	4:W:2901:LEU:HD12	1.74	0.68
3:C:334:ILE:HG22	3:C:336:ARG:H	1.58	0.68
5:Y:149:PRO:O	5:Y:153:ARG:NH2	2.23	0.68
4:O:445:ILE:HD11	4:O:466:ILE:HG23	1.76	0.66
3:A:42:ARG:HB2	4:M:85:THR:HG22	1.76	0.66
6:2:682:HIS:O	6:2:682:HIS:HD2	1.77	0.66
4:N:205:PRO:HD2	4:N:208:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:2745:LYS:O	4:T:2748:LYS:NZ	2.27	0.66
3:H:5213:ILE:HB	4:S:900:ILE:HG13	1.77	0.65
6:8:106:LYS:HA	6:8:106:LYS:HE3	1.79	0.65
5:Z:317:ARG:NH2	5:Z:324:ASP:OD2	2.29	0.65
6:2:682:HIS:CD2	6:2:683:ARG:HG2	2.31	0.65
4:Q:697:ALA:HA	4:Q:700:LEU:HD12	1.78	0.65
4:N:211:HIS:O	4:N:214:SER:HB2	1.97	0.64
4:S:849:MET:N	4:S:849:MET:SD	2.71	0.64
4:M:5:PRO:HB2	4:M:7:PRO:HD2	1.79	0.64
6:CD:291:LYS:O	6:CD:298:LYS:NZ	2.30	0.64
5:X:107:THR:HG22	5:X:119:ILE:HB	1.80	0.64
5:Z:249:LEU:HA	5:Z:252:ILE:HG12	1.80	0.64
5:Y:227:ARG:NH2	5:Y:234:ASP:OD2	2.32	0.63
5:X:103:LEU:HD21	5:X:124:ILE:HG23	1.81	0.63
3:K:5342:ILE:HG22	3:K:5344:ARG:H	1.64	0.62
6:6:3261:ARG:HB3	6:6:3265:ARG:HD2	1.81	0.62
6:4:2362:ASP:OD2	6:4:2386:ARG:NH1	2.32	0.62
4:Q:616:LYS:HD2	4:Q:627:LYS:HB3	1.80	0.61
4:W:2871:LYS:HE3	4:W:2886:ARG:HD3	1.80	0.61
4:P:531:ILE:HD13	4:P:536:MET:HG3	1.80	0.61
5:X:126:LEU:O	5:X:130:ILE:HG12	2.00	0.61
5:Y:173:ILE:O	5:Y:204:GLN:NE2	2.34	0.61
4:N:206:GLY:O	4:N:208:LEU:HD12	2.01	0.61
3:D:456:ILE:HB	4:P:531:ILE:HG13	1.83	0.60
4:N:206:GLY:C	4:N:208:LEU:H	2.05	0.60
3:H:5254:LYS:HG2	3:H:5255:THR:HG22	1.83	0.60
6:5:1483:ARG:NH2	6:5:1490:ASP:OD2	2.35	0.60
3:C:319:GLU:O	3:C:323:ASN:ND2	2.34	0.60
4:W:2914:ALA:HA	4:W:2917:ILE:HD12	1.84	0.60
6:9:285:LEU:HG	6:9:287:GLY:H	1.67	0.60
6:3:3181:GLN:OE1	6:3:3209:ARG:NH1	2.35	0.59
3:F:748:SER:OG	3:F:749:LYS:N	2.31	0.59
3:L:5404:ARG:NH1	4:W:2981:LYS:O	2.35	0.59
6:1:642:THR:HG21	6:1:650:VAL:HG22	1.85	0.59
4:V:1067:ILE:O	4:V:1071:VAL:HG23	2.03	0.58
3:C:279:GLN:HE21	4:O:419:GLN:NE2	1.78	0.58
4:T:2779:LYS:HA	4:T:2783:PRO:HA	1.85	0.58
4:S:935:ILE:HG23	4:S:939:GLU:HB2	1.83	0.58
4:S:944:VAL:HG13	4:S:948:LEU:HD13	1.85	0.58
6:8:150:ASN:OD1	6:8:153:ARG:NH2	2.36	0.58
3:A:63:LEU:HB3	4:M:42:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:682:HIS:O	6:2:682:HIS:CD2	2.56	0.58
6:2:731:ARG:O	6:2:735:THR:OG1	2.17	0.58
6:CD:306:LYS:HA	6:CD:306:LYS:HE3	1.85	0.58
3:B:189:LEU:HD22	4:N:147:LEU:HD13	1.86	0.58
6:CD:298:LYS:HD2	6:CD:298:LYS:O	2.04	0.58
3:C:356:THR:OG1	6:9:283:ARG:NH1	2.37	0.58
4:J:2042:ALA:HA	4:J:2045:LEU:HD12	1.86	0.58
6:7:62:LEU:O	6:7:66:ILE:HG23	2.04	0.57
4:V:1075:LEU:HB2	4:V:1080:ALA:HB2	1.86	0.57
3:H:5223:ARG:NH1	3:H:5229:ASN:OD1	2.38	0.57
3:G:755:SER:O	3:G:757:ARG:NH2	2.39	0.56
3:G:763:LYS:HG3	3:G:764:THR:H	1.70	0.56
3:G:867:SER:HB2	3:G:876:SER:HB3	1.87	0.56
4:O:418:LYS:NZ	4:O:424:THR:O	2.36	0.56
4:R:316:ILE:HG23	4:R:320:GLU:HB2	1.87	0.56
6:2:698:ILE:HD12	6:2:715:TYR:HD1	1.70	0.56
3:G:778:GLN:NE2	4:R:274:GLN:OE1	2.38	0.56
3:G:865:ILE:HD12	3:G:870:LEU:HD11	1.87	0.56
6:CD:353:ARG:O	6:CD:357:THR:OG1	2.19	0.55
3:D:399:ALA:HB2	4:P:598:TYR:HB2	1.88	0.55
3:E:599:GLU:OE2	4:Q:705:GLU:N	2.39	0.55
3:I:2540:ILE:HB	4:T:2787:ILE:HD12	1.87	0.55
3:K:5332:ALA:O	3:K:5336:ASN:ND2	2.39	0.55
4:S:968:THR:HG22	4:S:969:SER:H	1.72	0.55
5:Y:136:ALA:HA	5:Y:140:ALA:HB3	1.87	0.55
3:G:834:PRO:HA	3:G:837:LEU:HD12	1.89	0.55
3:F:652:VAL:HG13	3:F:673:PRO:HB2	1.89	0.55
4:W:2953:ALA:HA	4:W:2956:LEU:HD12	1.87	0.55
5:Z:263:ILE:HD11	5:Z:294:GLN:HG3	1.88	0.54
3:C:323:ASN:OD1	3:C:326:ARG:NH1	2.41	0.54
3:E:562:LEU:HD22	4:Q:666:VAL:HG13	1.88	0.54
4:S:914:ASP:OD2	4:S:918:ARG:NH2	2.41	0.54
5:X:116:ARG:NH2	5:X:123:ASP:OD1	2.28	0.54
3:F:736:ILE:HD11	3:F:741:LEU:HD13	1.90	0.54
3:D:479:THR:HG21	6:CD:381:ARG:HH21	1.73	0.54
4:J:1992:GLN:HB3	4:S:962:LYS:HG2	1.90	0.54
4:Q:698:VAL:HG13	4:Q:702:LEU:HD12	1.89	0.54
3:E:570:LEU:HD22	4:Q:645:LEU:HD13	1.90	0.53
4:Q:690:THR:OG1	4:Q:691:SER:N	2.40	0.53
3:C:277:GLY:O	4:W:2976:LYS:NZ	2.33	0.53
3:G:876:SER:O	3:G:883:LYS:NZ	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5457:GLU:OE2	4:O:480:LYS:HD2	2.07	0.53
4:W:2937:ALA:HB2	4:W:2945:ILE:HD11	1.90	0.53
3:B:176:TYR:OH	4:N:213:VAL:HA	2.08	0.53
6:6:3300:LEU:O	6:6:3304:LEU:HG	2.09	0.53
6:7:68:ASP:HB3	6:7:89:ALA:HB1	1.91	0.53
6:8:132:ILE:HG21	6:8:136:ILE:HG21	1.90	0.53
3:K:5295:ARG:NH2	4:V:1008:GLU:OE2	2.42	0.53
4:O:470:VAL:HG13	4:O:474:LEU:HD12	1.92	0.52
6:2:723:LYS:NZ	6:2:727:GLU:OE2	2.42	0.52
3:G:818:GLU:OE1	4:R:276:HIS:NE2	2.43	0.52
3:L:5405:ALA:HB1	3:L:5408:LYS:HB2	1.92	0.52
3:I:2558:LEU:HD22	4:T:2839:LEU:HD21	1.91	0.52
4:O:441:VAL:O	4:O:445:ILE:HG22	2.10	0.52
4:N:197:GLN:NE2	4:N:213:VAL:HG13	2.24	0.52
4:J:2006:ILE:HG23	6:4:2392:TYR:HB3	1.92	0.52
4:Q:697:ALA:O	4:Q:701:LEU:HD12	2.10	0.52
4:T:2823:THR:HG23	4:T:2825:ARG:H	1.75	0.52
3:B:218:GLU:CB	4:N:208:LEU:HD11	2.34	0.51
3:B:239:SER:O	3:B:241:LEU:N	2.41	0.51
6:9:217:ILE:O	6:9:243:ARG:NH2	2.40	0.51
3:K:5297:LEU:HA	3:K:5302:TYR:HD2	1.76	0.51
6:0:560:ARG:NH2	6:0:567:ASP:OD2	2.44	0.51
3:C:319:GLU:OE2	3:C:323:ASN:ND2	2.38	0.51
3:K:5326:LEU:HD22	4:V:1018:LEU:HD13	1.93	0.51
4:Q:675:GLY:O	4:Q:679:ARG:NH1	2.43	0.51
4:W:2936:LEU:HD21	6:6:3314:TYR:HE1	1.75	0.51
6:4:2317:ARG:HG3	6:4:2318:ASP:H	1.76	0.51
3:C:258:ARG:HH11	3:C:262:GLY:HA3	1.75	0.51
4:S:942:THR:HG21	6:2:739:HIS:HB2	1.93	0.51
3:H:5214:ILE:HG12	3:H:5217:HIS:CE1	2.46	0.50
3:A:32:ARG:NH2	4:M:32:GLU:OE1	2.33	0.50
4:J:2021:GLU:OE2	4:J:2024:ARG:NH2	2.44	0.50
6:CD:376:LEU:HB3	6:CD:381:ARG:O	2.12	0.50
3:E:531:GLN:N	3:E:563:GLU:OE2	2.44	0.50
3:H:5258:SER:OG	3:H:5259:LYS:N	2.44	0.50
6:CD:311:ASN:O	6:CD:312:ILE:HG22	2.10	0.50
4:R:260:ARG:NH1	4:R:261:LYS:O	2.45	0.50
6:9:247:LYS:NZ	6:9:251:GLU:OE2	2.43	0.50
6:6:3332:LEU:HB3	6:6:3337:ARG:O	2.12	0.50
3:L:5448:LEU:HD22	4:W:2922:VAL:HG13	1.93	0.49
6:9:226:ALA:HB1	6:9:231:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:218:LYS:O	4:N:222:LYS:HG2	2.12	0.49
4:S:908:MET:O	4:S:912:VAL:HG23	2.12	0.49
6:2:722:LEU:O	6:2:726:LEU:HG	2.12	0.49
3:E:570:LEU:HD13	4:Q:645:LEU:HB2	1.93	0.49
3:L:5516:SER:OG	3:L:5517:LYS:N	2.45	0.49
3:C:380:SER:O	3:C:383:SER:OG	2.29	0.49
3:G:809:LEU:O	3:G:813:THR:HG23	2.12	0.49
3:G:817:LEU:HD11	4:R:268:VAL:HG13	1.93	0.49
4:J:1970:ASP:OD1	4:J:1971:GLY:N	2.45	0.49
4:N:163:ILE:HG13	6:8:185:GLY:HA2	1.94	0.49
4:U:1932:ALA:HA	4:U:1935:LEU:HD12	1.94	0.49
3:E:516:LYS:HB3	3:E:519:ALA:HB3	1.94	0.49
4:J:1974:ARG:O	4:J:1975:ARG:NH1	2.46	0.49
6:3:3219:VAL:HG22	6:3:3247:GLN:HE22	1.77	0.49
6:7:63:GLU:OE1	6:7:67:ARG:NH2	2.45	0.48
6:8:108:LEU:HD13	6:8:111:ASN:HD22	1.78	0.48
3:A:79:ILE:HD11	3:A:81:ARG:HB3	1.95	0.48
3:E:518:ARG:HB3	3:E:527:ARG:HH21	1.76	0.48
4:O:419:GLN:HB3	4:W:2972:LYS:HG2	1.93	0.48
6:8:136:ILE:HG12	6:8:140:THR:HG23	1.94	0.48
3:L:5456:LEU:HD13	4:W:2901:LEU:HB2	1.95	0.48
4:R:323:THR:HG23	6:1:640:THR:HG22	1.96	0.48
6:5:1424:ARG:NH1	6:5:1429:ASP:OD2	2.45	0.48
3:I:2516:VAL:HG22	4:T:2843:ALA:HB1	1.94	0.48
6:3:3200:ILE:HB	6:3:3204:ILE:HG21	1.95	0.48
3:I:2488:PRO:HB2	3:I:2491:ARG:HG3	1.95	0.48
4:O:406:LYS:HZ3	4:O:408:SER:HG	1.59	0.48
5:Z:254:ARG:O	5:Z:258:SER:OG	2.30	0.48
6:1:596:GLN:HG3	6:1:624:ARG:HB3	1.94	0.48
3:B:247:GLU:HG3	3:B:249:SER:H	1.77	0.48
3:C:318:LEU:HD13	4:O:417:LEU:HB2	1.96	0.48
3:K:5281:SER:OG	3:K:5286:LEU:O	2.32	0.48
3:K:5284:ALA:HB2	4:V:1094:TYR:HB2	1.96	0.48
3:F:744:LYS:NZ	3:F:747:SER:O	2.47	0.48
3:G:817:LEU:HD13	4:R:272:LEU:HB2	1.97	0.47
6:7:82:THR:OG1	6:7:85:ASP:OD1	2.32	0.47
4:V:1080:ALA:O	4:V:1084:VAL:HG23	2.14	0.47
6:3:3175:VAL:HG13	6:3:3177:ARG:HE	1.79	0.47
3:H:5208:ASN:HD22	3:H:5217:HIS:CD2	2.32	0.47
3:I:2480:SER:O	3:I:2484:GLY:N	2.47	0.47
4:W:2931:GLY:O	4:W:2935:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:227:THR:HG21	6:8:181:ARG:NH2	2.26	0.47
4:N:206:GLY:C	4:N:208:LEU:N	2.68	0.47
4:V:1035:MET:O	4:V:1039:VAL:HG23	2.15	0.47
4:V:1069:THR:HG23	6:5:1476:THR:HG22	1.96	0.47
6:0:512:THR:OG1	6:0:513:LYS:N	2.48	0.47
3:K:5366:ALA:HB3	4:V:1034:ILE:HD11	1.96	0.47
6:0:532:ILE:O	6:0:536:THR:OG1	2.24	0.47
5:Y:153:ARG:O	5:Y:157:VAL:HG23	2.15	0.46
6:0:534:GLU:OE2	6:0:537:ARG:NH2	2.44	0.46
4:T:2758:ASP:N	4:T:2758:ASP:OD1	2.48	0.46
3:B:218:GLU:HB3	4:N:208:LEU:CD1	2.34	0.46
6:5:1435:THR:HG22	6:5:1436:LYS:H	1.81	0.46
3:E:550:VAL:HA	4:Q:689:ILE:HG22	1.98	0.46
4:J:1973:LYS:HD2	4:J:1973:LYS:HA	1.80	0.46
6:7:68:ASP:OD2	6:7:92:ARG:NE	2.48	0.46
6:CD:370:MET:O	6:CD:373:VAL:HG12	2.14	0.46
4:O:433:ILE:HG13	6:9:287:GLY:HA2	1.97	0.46
6:1:589:LYS:HG3	6:1:591:LEU:H	1.81	0.46
6:CD:302:LYS:HE2	6:CD:302:LYS:HA	1.98	0.46
3:B:216:ASP:HB3	3:B:219:LEU:HD12	1.96	0.46
3:G:818:GLU:OE2	3:G:822:ASN:ND2	2.49	0.46
3:L:5435:ARG:HB2	4:W:2944:THR:HG22	1.96	0.46
3:L:5472:ILE:HG12	3:L:5475:HIS:CE1	2.51	0.46
6:0:513:LYS:HG3	6:0:533:TYR:CZ	2.51	0.46
3:G:775:ALA:HB2	4:R:348:TYR:HB2	1.96	0.46
4:S:900:ILE:HD13	4:S:905:MET:SD	2.55	0.46
5:Z:264:ARG:HB3	5:Z:267:PRO:HD2	1.98	0.46
3:L:5469:THR:O	4:W:2909:GLY:N	2.41	0.46
5:X:107:THR:HG23	5:X:123:ASP:HB2	1.98	0.46
3:B:177:LEU:HD21	4:N:172:PHE:HD1	1.81	0.45
3:I:2473:ARG:HD2	4:T:2858:LYS:HZ3	1.81	0.45
4:P:574:ALA:HA	4:P:577:LEU:HD12	1.98	0.45
4:U:1925:THR:OG1	4:U:1926:SER:N	2.49	0.45
6:2:695:LYS:HG3	6:2:715:TYR:CE1	2.51	0.45
4:W:2924:ASP:OD2	4:W:2928:ARG:NH2	2.50	0.45
3:L:5478:LEU:O	3:L:5482:ASN:ND2	2.49	0.45
4:S:946:LEU:O	6:2:756:ARG:NH2	2.49	0.45
3:B:250:LYS:HD3	3:B:250:LYS:HA	1.86	0.44
4:J:2046:LEU:HG	4:J:2047:LEU:HD23	1.99	0.44
6:4:2315:VAL:O	6:4:2315:VAL:HG13	2.17	0.44
3:C:275:ARG:NH1	4:O:497:LYS:OXT	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:171:LEU:HB2	5:Y:175:LYS:NZ	2.33	0.44
6:8:149:GLU:HA	6:8:152:ILE:HG22	2.00	0.44
4:T:2752:THR:O	4:T:2753:LYS:HG2	2.17	0.44
3:C:273:SER:HB2	3:C:282:VAL:HG22	2.00	0.44
3:H:5257:SER:HB2	3:H:5262:LYS:C	2.38	0.44
3:L:5440:ALA:HB2	4:W:2946:THR:HA	1.99	0.44
6:6:3277:ARG:O	6:6:3281:ARG:HG2	2.17	0.44
6:7:90:LEU:HB3	6:7:95:ARG:O	2.18	0.44
4:S:921:GLY:O	4:S:925:ARG:HG2	2.18	0.44
4:T:2749:LYS:HB3	4:T:2762:ARG:HA	1.99	0.44
5:X:111:ALA:HB2	5:X:119:ILE:HA	2.00	0.44
5:X:128:ARG:CZ	5:X:133:GLU:HB3	2.48	0.44
6:4:2317:ARG:HD3	6:4:2317:ARG:HA	1.81	0.44
3:I:2517:LEU:HD22	4:T:2799:VAL:HG13	1.99	0.43
4:V:1077:GLY:C	4:V:1079:LEU:H	2.21	0.43
3:B:241:LEU:HD13	6:8:128:GLY:O	2.18	0.43
4:W:2952:THR:HG21	6:6:3317:HIS:HB2	2.01	0.43
6:5:1415:LEU:HD12	6:5:1415:LEU:HA	1.85	0.43
6:8:177:LYS:HB2	6:8:182:THR:HG23	2.00	0.43
3:H:5213:ILE:H	4:S:900:ILE:HA	1.84	0.43
3:K:5340:ARG:HD3	4:V:1028:SER:HB3	1.99	0.43
4:M:20:LYS:HD2	4:M:20:LYS:HA	1.76	0.43
4:N:209:ALA:O	4:N:210:LYS:C	2.56	0.43
4:N:216:GLY:O	4:N:220:VAL:HG23	2.19	0.43
4:V:988:LYS:HD3	4:V:1000:LYS:NZ	2.32	0.43
4:J:1969:LYS:HA	4:J:1969:LYS:HD2	1.73	0.43
3:K:5365:ILE:HD13	3:K:5365:ILE:HA	1.90	0.43
4:M:42:LEU:HD13	4:M:51:ILE:HD11	2.00	0.43
4:M:61:SER:OG	6:7:101:GLY:O	2.25	0.43
4:N:219:ALA:O	4:N:223:TYR:HB2	2.19	0.43
4:R:346:THR:O	4:R:350:SER:OG	2.28	0.43
4:V:1098:LYS:HE2	4:V:1098:LYS:O	2.18	0.43
3:B:183:TYR:O	3:B:187:GLU:HG2	2.19	0.43
3:C:306:LEU:HD13	4:O:445:ILE:HD13	2.01	0.43
4:J:1973:LYS:HG3	4:J:1974:ARG:H	1.82	0.43
6:9:271:ALA:O	6:9:275:VAL:HG23	2.18	0.43
3:L:5490:LEU:HD21	4:W:2921:PHE:HE1	1.84	0.43
4:U:1846:LYS:HE3	4:U:1849:SER:HB2	2.01	0.43
4:V:1075:LEU:HD12	4:V:1080:ALA:HA	2.01	0.43
3:L:5456:LEU:HD11	4:W:2897:VAL:HG13	2.00	0.43
4:U:1889:ILE:HG12	4:U:1894:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:1070:ALA:HA	4:V:1073:LEU:HD12	2.00	0.43
6:1:659:LEU:HB3	6:1:664:ARG:O	2.19	0.43
6:7:29:ILE:HG13	6:7:58:LEU:HD23	2.01	0.43
4:N:221:THR:O	4:N:224:THR:OG1	2.36	0.43
3:H:5185:TYR:CE1	4:S:960:GLY:HA3	2.54	0.43
3:H:5219:GLN:OE1	3:H:5241:GLY:N	2.50	0.43
6:9:270:THR:OG1	6:9:271:ALA:N	2.52	0.43
3:A:57:TYR:CD1	4:M:110:GLU:HG3	2.54	0.42
3:L:5447:VAL:HG22	4:W:2966:ALA:HB1	2.01	0.42
6:2:682:HIS:CD2	6:2:682:HIS:C	2.92	0.42
6:3:3164:LEU:H	6:3:3164:LEU:HD12	1.84	0.42
3:H:5161:PRO:HG3	4:S:886:TYR:CZ	2.54	0.42
6:0:548:ILE:O	6:0:552:VAL:HG12	2.19	0.42
6:5:1484:LYS:HB3	6:5:1484:LYS:HE2	1.81	0.42
3:A:96:LEU:HD13	4:M:100:PRO:HD3	2.01	0.42
6:4:2377:ALA:HB1	6:4:2394:PHE:HB3	2.02	0.42
4:T:2826:GLU:HA	6:3:3229:HIS:HE1	1.85	0.42
3:C:271:THR:HG22	3:C:273:SER:H	1.85	0.42
6:8:129:VAL:HG11	6:8:132:ILE:HD11	2.01	0.42
6:9:191:ARG:HB2	6:9:200:LYS:HE2	2.01	0.42
6:CD:291:LYS:HD3	6:CD:292:GLY:N	2.35	0.42
4:N:206:GLY:O	4:N:207:GLU:HB3	2.19	0.42
4:U:1929:ILE:HA	4:U:1932:ALA:HB3	2.01	0.42
4:W:2946:THR:OG1	4:W:2947:SER:N	2.52	0.42
3:K:5326:LEU:HD13	4:V:1018:LEU:HB2	2.02	0.42
4:P:575:VAL:HG13	4:P:579:LEU:HD12	2.01	0.42
6:0:546:ASN:HB3	6:0:575:GLN:HE22	1.85	0.42
4:O:433:ILE:HA	6:9:286:TYR:O	2.20	0.42
4:U:1840:LYS:HG2	4:U:1842:ALA:H	1.84	0.42
4:W:2877:THR:OG1	4:W:2880:LYS:O	2.33	0.42
6:9:266:ARG:O	6:9:267:LYS:HG2	2.20	0.42
3:K:5359:LEU:HD23	3:K:5360:LEU:N	2.35	0.41
4:M:86:ILE:HD13	4:M:90:GLU:HG2	2.02	0.41
4:T:2749:LYS:HA	4:T:2749:LYS:HD3	1.88	0.41
6:9:197:GLY:HA3	6:9:200:LYS:HE3	2.02	0.41
3:A:18:SER:O	3:A:23:LEU:N	2.42	0.41
3:C:271:THR:O	3:C:275:ARG:HB2	2.20	0.41
3:L:5517:LYS:HB2	3:L:5517:LYS:HE3	1.90	0.41
4:M:60:ASN:ND2	6:7:102:GLY:OXT	2.54	0.41
3:C:332:ARG:HD3	4:O:427:SER:HB3	2.01	0.41
3:H:5175:ALA:HB2	4:S:935:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:5328:LEU:HB3	3:K:5349:ALA:HB1	2.02	0.41
4:N:192:THR:HG23	4:N:194:ARG:H	1.85	0.41
6:7:54:THR:HA	6:7:57:VAL:HG12	2.03	0.41
6:8:153:ARG:O	6:8:157:THR:OG1	2.32	0.41
6:CD:324:ALA:HB1	6:CD:329:VAL:HG11	2.03	0.41
3:C:357:ILE:HG23	4:O:433:ILE:HG21	2.03	0.41
4:W:2934:SER:HB3	4:W:2935:ARG:NH1	2.36	0.41
6:9:246:LEU:O	6:9:250:LEU:HG	2.20	0.41
3:G:759:LYS:HA	3:G:759:LYS:HD2	1.83	0.41
3:D:478:VAL:HG13	6:CD:382:THR:HG23	2.02	0.41
3:L:5483:ASP:HB3	3:L:5486:LEU:HB2	2.03	0.41
6:7:10:LEU:HD23	6:7:10:LEU:H	1.84	0.41
3:B:152:PRO:HD3	4:N:142:TYR:CG	2.55	0.41
3:B:155:ARG:HG2	3:B:158:ARG:NH2	2.36	0.41
3:C:355:VAL:HG22	6:9:284:THR:HB	2.01	0.41
3:D:410:ARG:NH2	4:P:512:GLU:OE2	2.54	0.41
4:M:42:LEU:HD22	4:M:51:ILE:HD11	2.03	0.41
4:O:433:ILE:H	4:O:433:ILE:HD12	1.85	0.41
4:Q:668:ASP:OD1	4:Q:672:ARG:NH1	2.54	0.41
4:S:926:LEU:HD12	6:2:739:HIS:CG	2.56	0.41
4:W:2865:ALA:HB3	4:W:2866:PRO:HD3	2.02	0.41
5:Z:329:ARG:HH21	5:Z:334:GLU:HB3	1.86	0.41
6:2:695:LYS:HB3	6:2:696:PRO:HD2	2.01	0.41
6:4:2328:ILE:HD13	6:4:2345:TYR:HA	2.02	0.41
6:CD:320:ILE:H	6:CD:320:ILE:HD12	1.86	0.41
3:C:371:LEU:HD11	3:C:376:GLU:O	2.21	0.41
3:E:541:LEU:HD13	3:E:550:VAL:HG11	2.03	0.41
5:Y:214:LEU:HD23	5:Y:214:LEU:HA	1.81	0.41
6:CD:316:THR:O	6:CD:320:ILE:HD12	2.21	0.41
4:U:1862:LYS:HD3	4:U:1862:LYS:HA	1.97	0.40
4:V:1063:THR:OG1	4:V:1066:GLU:OE1	2.23	0.40
4:W:2881:ASP:OD1	4:W:2882:GLY:N	2.53	0.40
5:Z:249:LEU:HA	5:Z:252:ILE:CG1	2.49	0.40
3:F:750:SER:OG	3:F:751:ALA:N	2.54	0.40
3:G:818:GLU:HB2	4:R:275:VAL:HG11	2.03	0.40
4:M:87:THR:OG1	4:M:88:SER:N	2.55	0.40
4:V:991:VAL:HG23	4:V:993:LYS:HE2	2.03	0.40
6:2:742:ARG:NH1	6:2:744:THR:O	2.44	0.40
6:5:1471:ILE:HD12	6:5:1471:ILE:HA	1.97	0.40
6:CD:311:ASN:C	6:CD:313:GLN:H	2.22	0.40
3:E:586:ILE:HG12	3:E:589:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:604:LEU:HB3	3:E:607:VAL:HG21	2.03	0.40
4:O:409:TYR:HA	4:O:412:TYR:HD2	1.86	0.40
4:T:2803:PHE:HA	4:T:2806:ILE:HG22	2.04	0.40
5:X:112:ILE:HD13	5:X:112:ILE:HA	1.87	0.40
5:Z:329:ARG:NE	5:Z:334:GLU:OE1	2.54	0.40
3:B:176:TYR:CZ	4:N:197:GLN:HG2	2.56	0.40
3:D:471:LEU:HD23	4:P:583:LEU:HD11	2.03	0.40
3:K:5320:TYR:HE2	4:V:1079:LEU:HD12	1.87	0.40
6:1:596:GLN:HB2	6:1:624:ARG:HD3	2.02	0.40
4:O:400:LYS:HG2	4:O:400:LYS:O	2.21	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	205	PRO
6	0	499	ARG
3	am	797	ALA
4	At	20	LYS
6	CD	312	ILE
7	Ao	57	HIS
4	At	101	GLY
4	ax	267	LYS
7	As	27	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	97/102 (95%)	96 (99%)	1 (1%)	73	85
3	Ae	97/102 (95%)	96 (99%)	1 (1%)	73	85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	110	ASN
3	B	151	PHE
3	C	344	ASN
3	C	354	ARG
3	D	450	ASP
3	D	499	GLU
3	E	606	ARG
3	F	748	SER
3	G	759	LYS
3	H	5146	ARG
3	H	5177	ARG
3	H	5218	LEU
3	H	5234	ARG
3	I	2479	ARG
3	I	2487	PHE
4	J	2024	ARG
3	L	5487	ASN
4	M	53	SER
4	M	102	GLU
4	O	429	LYS
4	O	431	MET
4	P	506	ARG
4	P	532	SER
4	Q	672	ARG
4	R	283	SER
4	R	287	SER
4	S	897	ASP
4	S	932	ARG
4	T	2812	ARG

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Mol	Chain	Res	Type
4	U	1926	SER
4	V	976	MET
4	V	1098	LYS
5	X	68	GLN
5	X	69	ARG
5	X	79	LYS
5	X	134	ARG
5	Y	137	ARG
5	Z	282	ASP
5	Z	285	PHE
5	a	363	LYS
5	a	407	ASP
5	a	455	ARG
5	b	484	SER
5	b	510	ARG
5	c	585	ARG
5	c	661	ARG
5	e	801	GLN
5	e	810	GLN
5	g	2194	SER
5	g	2257	MET
5	h	1317	ARG
5	h	1361	SER
5	h	1404	ARG
5	i	3236	SER
5	i	3270	MET
5	i	3281	ARG
5	j	41	TYR
5	j	84	PHE
5	k	183	PHE
5	l	270	SER
5	l	276	ARG
5	l	342	ARG
5	m	352	TYR
5	m	353	ARG
5	m	368	SER
5	n	508	PHE
5	o	601	GLN
5	p	700	LEU
5	q	785	ARG
5	q	822	ASP
5	q	874	ARG

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Mol	Chain	Res	Type
5	r	2983	HIS
5	r	3002	THR
5	r	3025	ASP
5	r	3073	ARG
5	t	1241	ARG
5	u	3096	ARG
5	u	3106	LYS
5	u	3110	ARG
5	u	3119	ARG
6	v	18	HIS
6	v	95	ARG
6	w	113	LEU
6	z	412	ASP
6	0	499	ARG
6	1	637	ASP
6	2	684	LYS
6	4	2372	ARG
6	6	3262	LYS
6	7	8	LYS
6	7	24	ASP
6	7	68	ASP
6	8	131	ARG
6	8	178	ARG
6	9	193	LYS
6	9	262	GLU
6	CD	294	LYS
6	CD	298	LYS
6	a2	391	LYS
6	a3	558	ASP
6	a4	577	LYS
6	a6	3284	ARG
6	a8	1472	LYS
6	a8	1476	LYS
6	a8	1524	ASP
6	a9	3305	ARG
6	a9	3318	ARG
3	aj	91	GLU
3	aj	113	SER
3	aj	127	LYS
3	ak	155	ARG
3	ak	214	GLU
3	ak	236	SER

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Mol	Chain	Res	Type
3	ak	238	LEU
3	ak	239	LEU
3	am	786	ARG
3	am	799	THR
3	an	925	ARG
3	an	927	SER
3	an	950	ARG
3	aq	4241	LYS
3	ar	2606	LYS
3	ar	2607	THR
3	at	4293	TYR
3	au	4434	ASP
4	av	28	LYS
4	aw	131	LYS
4	aw	179	MET
4	ax	268	ASP
4	ay	377	LYS
4	ay	451	LYS
4	az	515	HIS
4	Aa	671	LEU
4	Aa	694	LYS
4	Ab	771	ARG
4	Ac	854	MET
3	Ae	2967	LYS
4	Af	1192	TYR
4	Ag	3090	LYS
4	Ag	3091	ASP
7	Ah	351	MET
7	Ah	379	TYR
7	Ah	404	TYR
7	Ah	417	LEU
7	Ah	461	LYS
7	Ai	4	LEU
7	Ai	14	LYS
7	Ai	56	SER
7	Ai	125	ARG
7	Ai	139	ARG
7	Ai	157	THR
7	Aj	147	LYS
7	Aj	190	HIS
7	Aj	199	LEU
7	Ak	549	ASP

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Mol	Chain	Res	Type
7	Ak	550	LEU
7	Al	288	ARG
7	Al	289	GLN
7	Al	294	TYR
7	Al	299	TYR
7	Al	323	LYS
7	Am	28	TYR
7	Am	57	HIS
7	Am	62	HIS
7	Am	154	LYS
7	An	53	TYR
7	An	58	TYR
7	An	59	LYS
7	An	90	SER
7	An	98	SER
7	An	115	SER
7	Ao	71	SER
7	Ap	48	GLN
7	Aq	6	LEU
7	Aq	28	TYR
7	Aq	59	LYS
7	Aq	113	ARG
7	Aq	135	LYS
7	Aq	150	LYS
7	Ar	17	LYS
7	Ar	31	MET
7	Ar	41	SER
7	Ar	108	LYS
7	Ar	119	LYS
7	Ar	175	LYS
7	As	25	HIS
7	As	53	TYR
7	As	57	HIS
7	As	71	SER
7	As	99	ASP
7	As	103	ARG
4	At	2	LYS
4	At	31	LYS
4	At	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	157	HIS
3	C	279	GLN
3	C	339	GLN
3	C	344	ASN
3	E	545	ASN
3	E	611	GLN
3	F	729	GLN
3	G	778	GLN
3	G	792	ASN
3	H	5208	ASN
3	I	2574	GLN
3	L	5487	ASN
4	N	165	ASN
4	N	184	HIS
4	N	197	GLN
4	P	499	GLN
4	P	524	GLN
4	R	274	GLN
4	T	2828	GLN
4	V	1055	HIS
4	V	1057	ASN
4	W	2940	ASN
5	Y	219	ASN
5	Y	224	HIS
5	Y	236	GLN
5	Z	314	HIS
5	c	572	HIS
5	c	609	GLN
5	d	670	HIS
5	e	850	GLN
5	f	3119	GLN
5	g	2245	ASN
5	i	3258	ASN
5	j	113	HIS
5	l	281	GLN
5	l	306	GLN
5	l	321	ASN
5	m	404	GLN
5	m	419	ASN
5	n	509	GLN
5	n	517	GLN
5	n	532	ASN
5	o	658	GLN

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Mol	Chain	Res	Type
5	p	711	GLN
5	p	728	GLN
5	q	853	ASN
5	q	870	GLN
5	r	3020	GLN
5	r	3029	GLN
5	r	3052	ASN
5	s	2139	ASN
5	t	1217	HIS
5	t	1291	HIS
5	u	3089	GLN
5	u	3138	GLN
6	x	266	ASN
6	y	329	ASN
6	0	575	GLN
6	2	689	ASN
6	2	739	HIS
6	3	3247	GLN
6	6	3317	HIS
6	9	263	HIS
6	a4	633	ASN
6	a7	2356	HIS
6	a8	1481	ASN
6	a9	3357	HIS
3	aj	73	ASN
3	am	821	ASN
3	am	893	ASN
3	an	932	GLN
3	an	981	ASN
3	an	990	HIS
3	ao	1114	HIS
3	ap	4082	HIS
3	aq	4141	GLN
3	aq	4190	ASN
3	as	1789	HIS
3	at	4249	GLN
3	au	4430	ASN
3	au	4435	ASN
4	aw	169	HIS
4	ay	429	ASN
4	ay	448	HIS
4	az	513	GLN

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Mol	Chain	Res	Type
4	az	561	GLN
3	Ae	3070	GLN
4	Af	1153	HIS
4	Ag	3161	GLN
7	Al	303	HIS
7	Ap	67	GLN
4	At	64	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

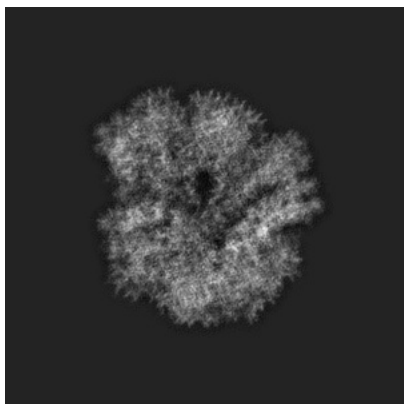
6 Map visualisation [i](#)

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.

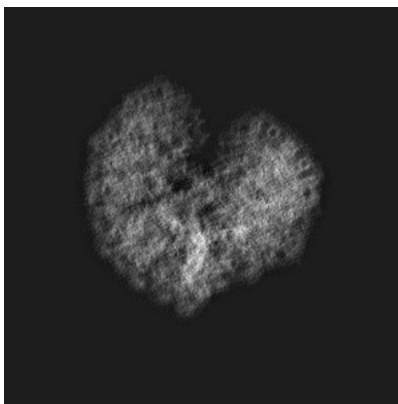
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

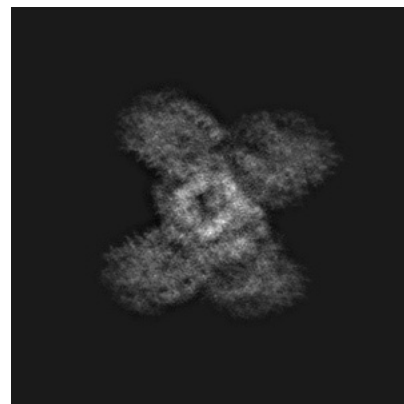
6.1.1 Primary map



X

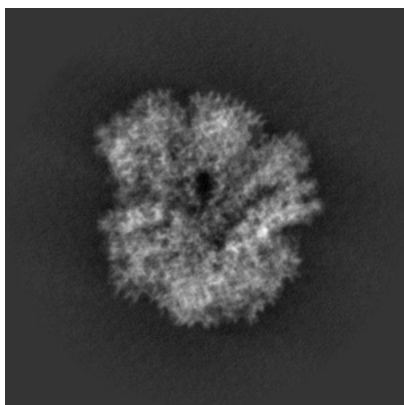


Y

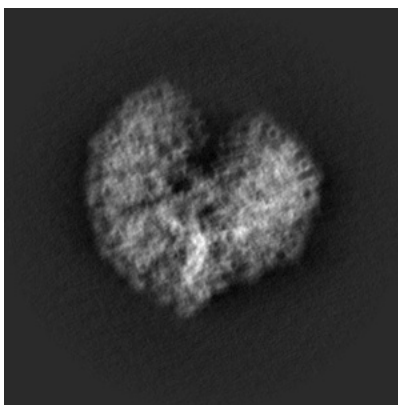


Z

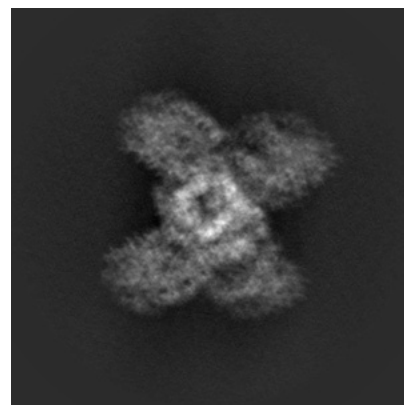
6.1.2 Raw map



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

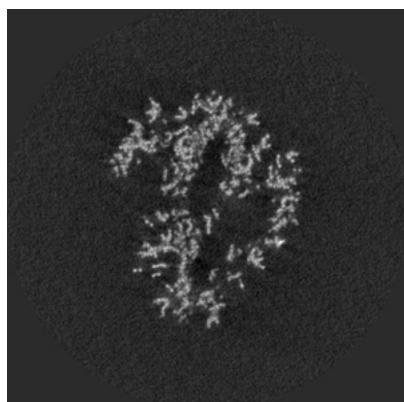


Y Index: 144

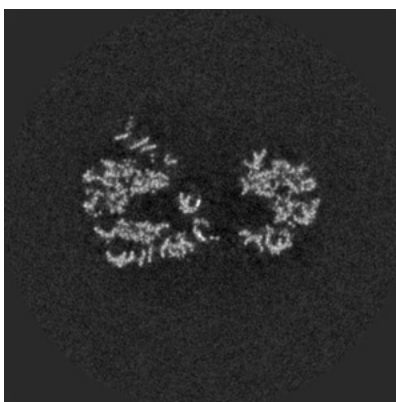


Z Index: 144

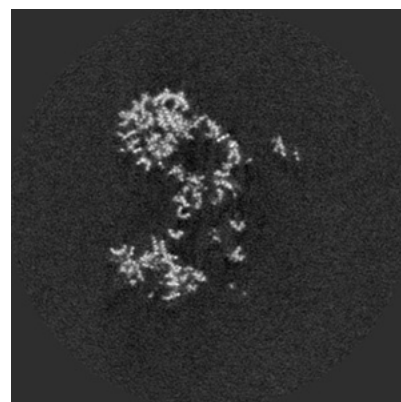
6.2.2 Raw map



X Index: 144



Y Index: 144

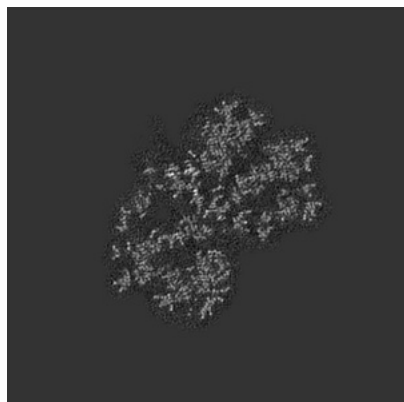


Z Index: 144

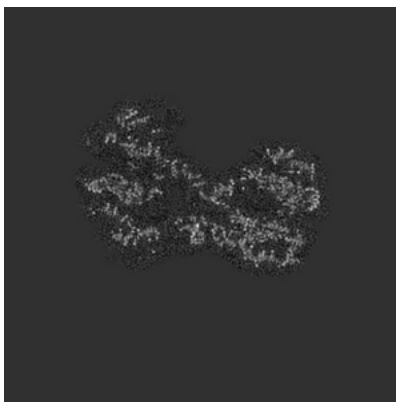
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

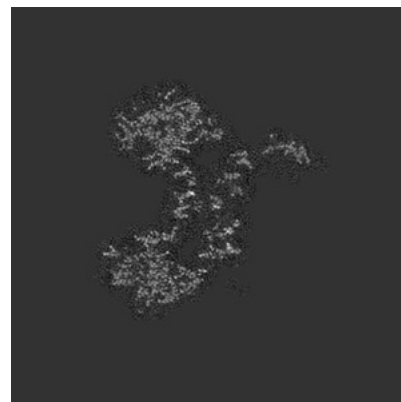
6.3.1 Primary map



X Index: 125

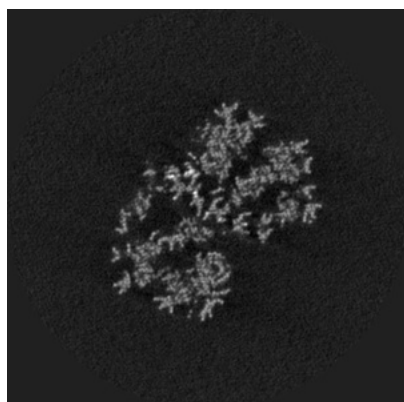


Y Index: 153

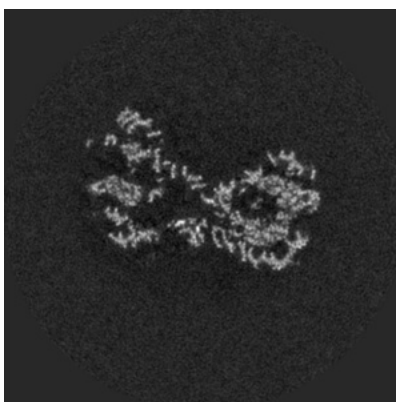


Z Index: 139

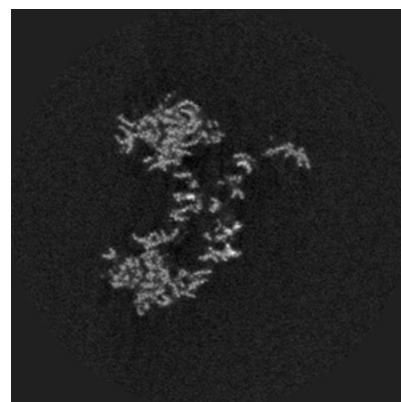
6.3.2 Raw map



X Index: 125



Y Index: 154

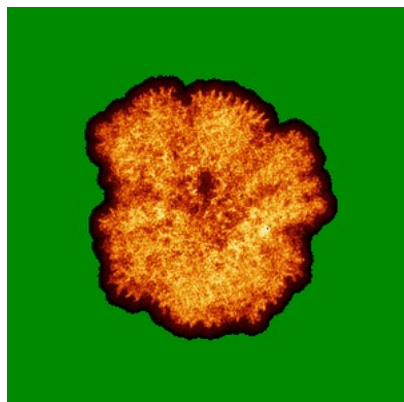


Z Index: 138

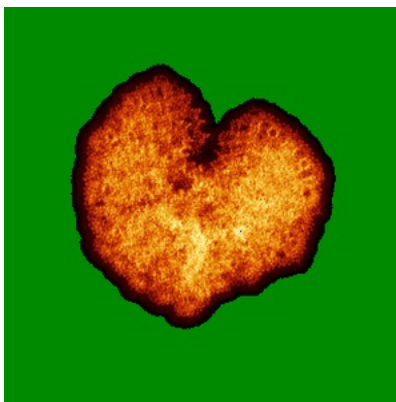
The images above show the largest variance slices of the map in three orthogonal directions.

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

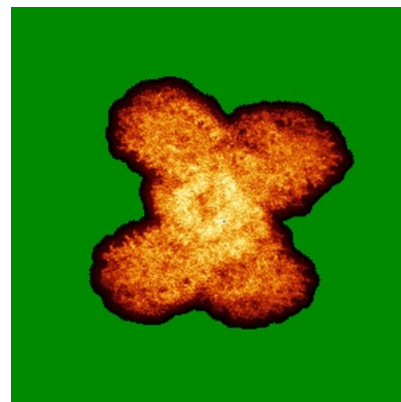
6.4.1 Primary map



X

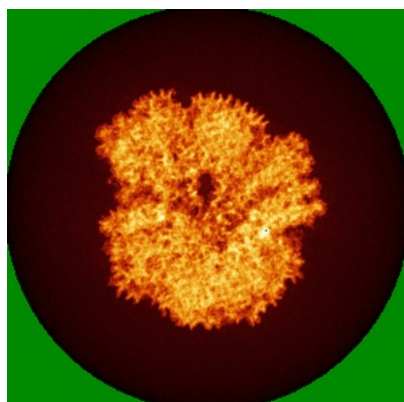


Y

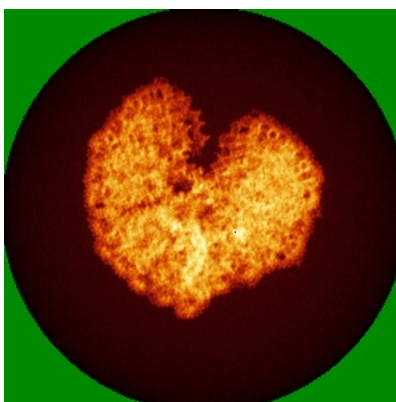


Z

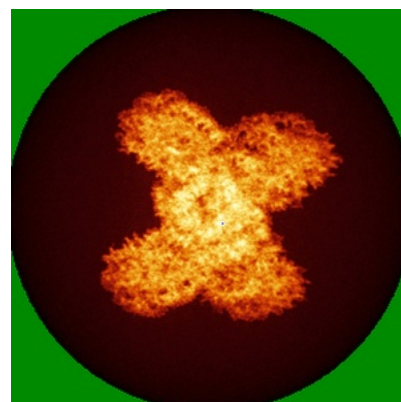
6.4.2 Raw map



X



Y

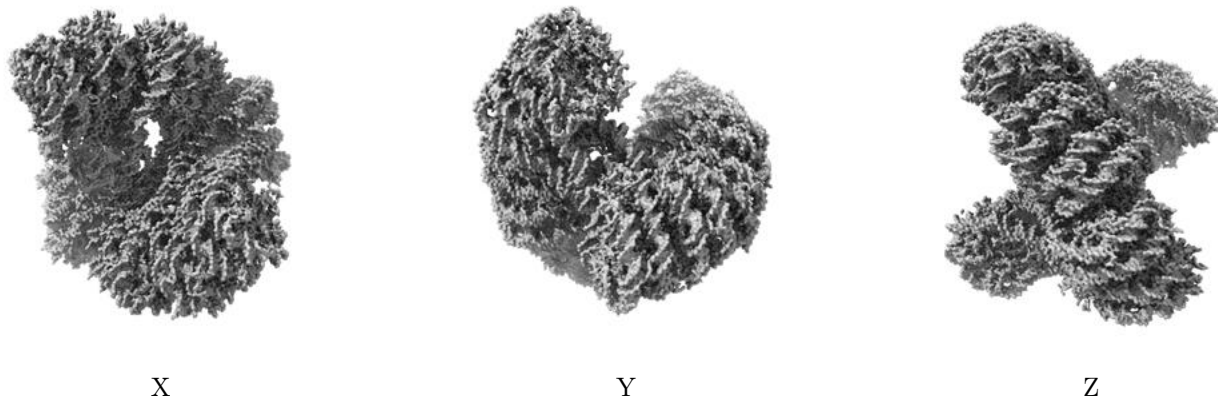


Z

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.

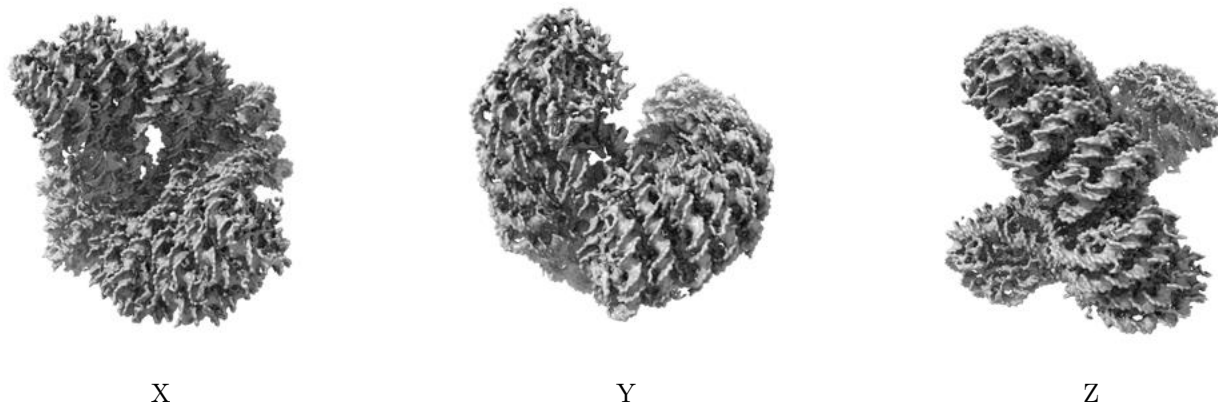
6.5 Orthogonal surface views [i](#)

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.

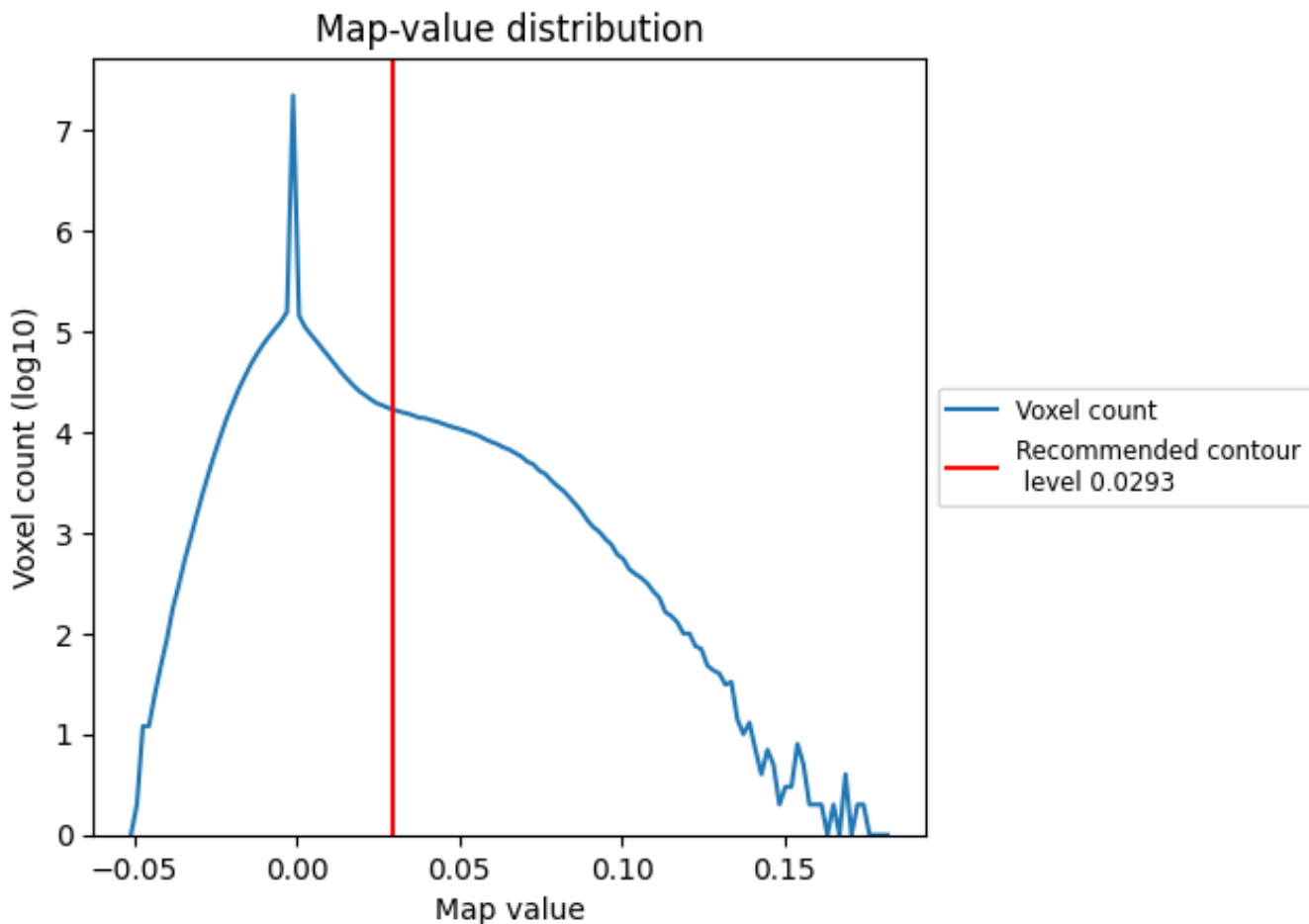
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

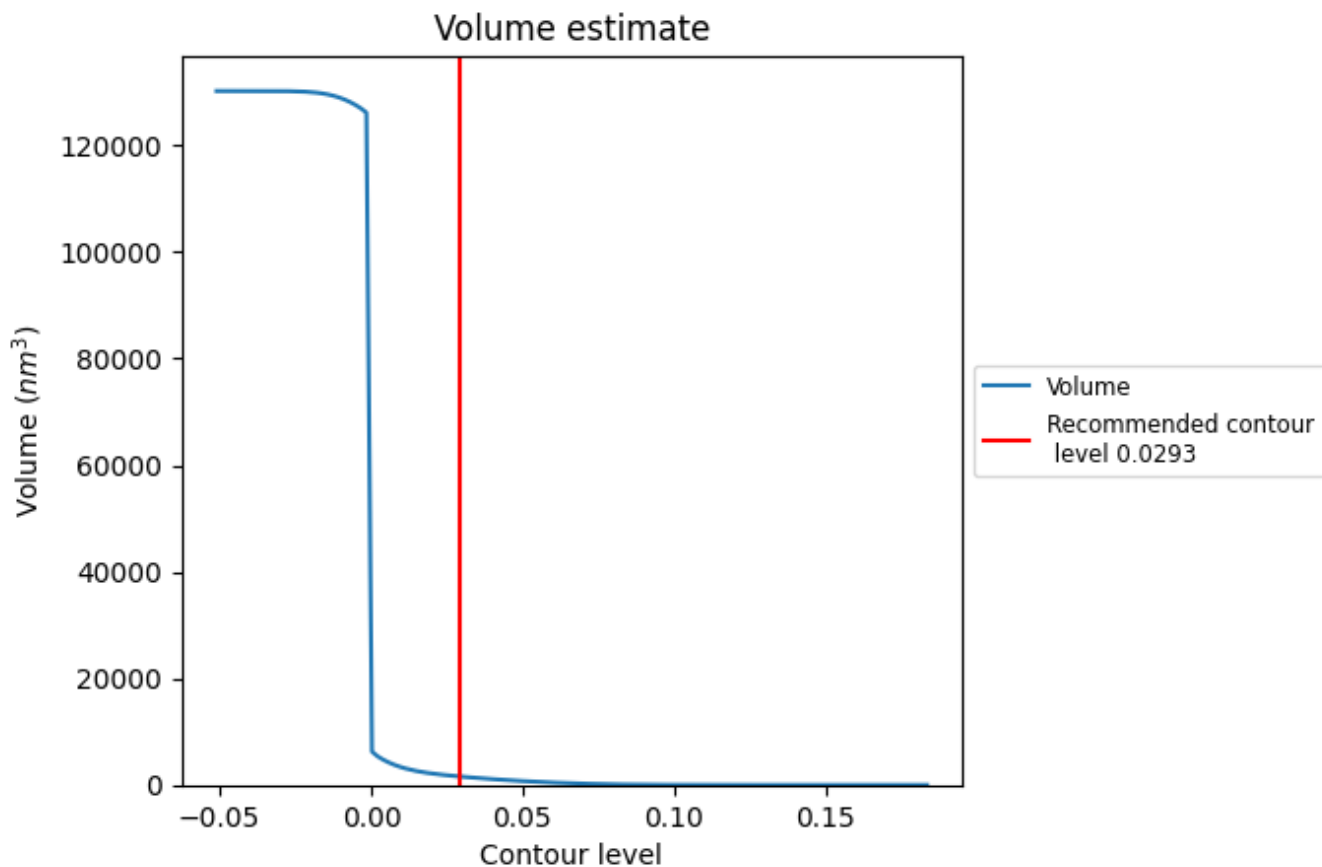
This section contains the results of statistical analysis of the map.

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.

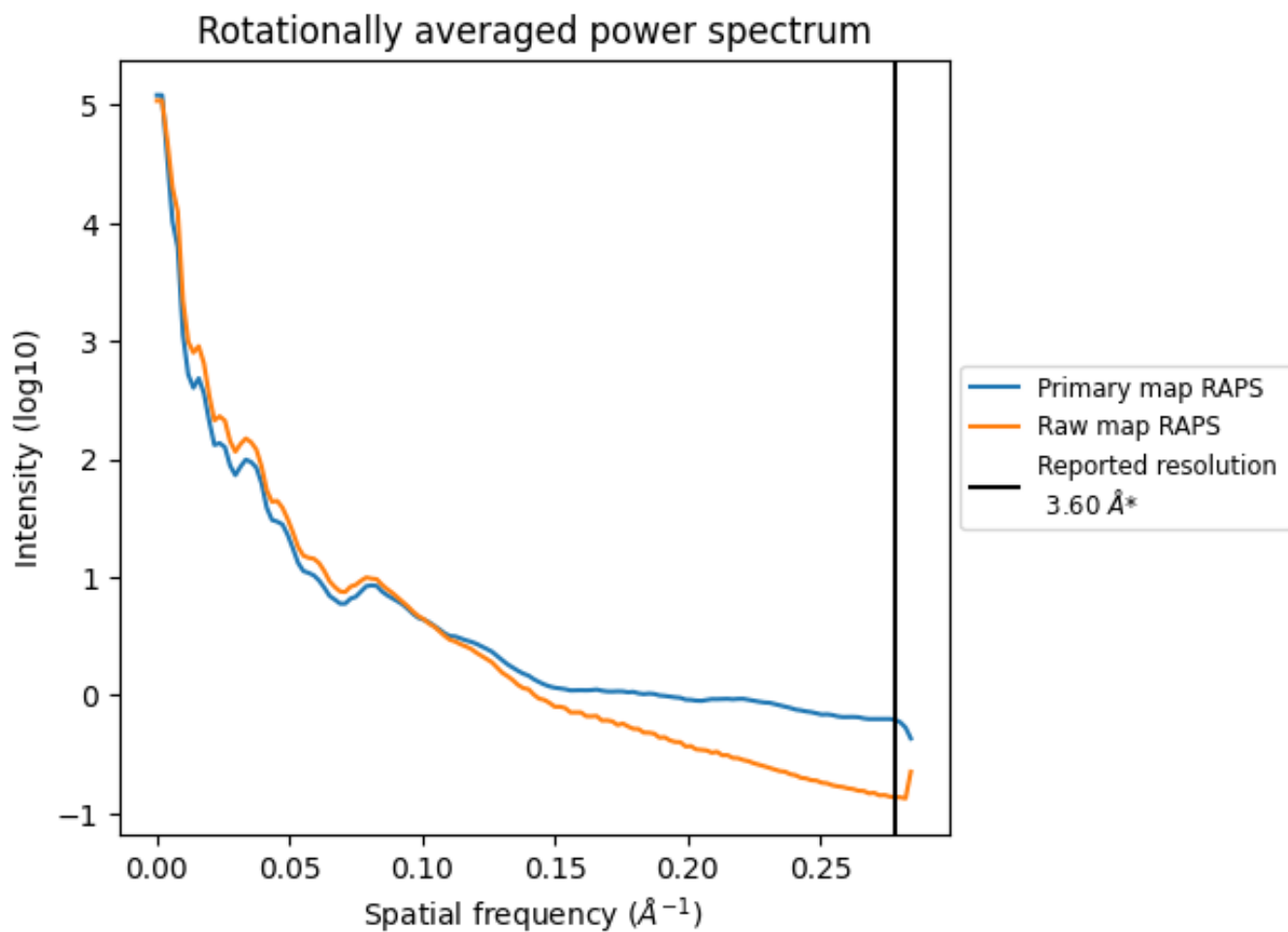
7.2 Volume estimate [i](#)



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

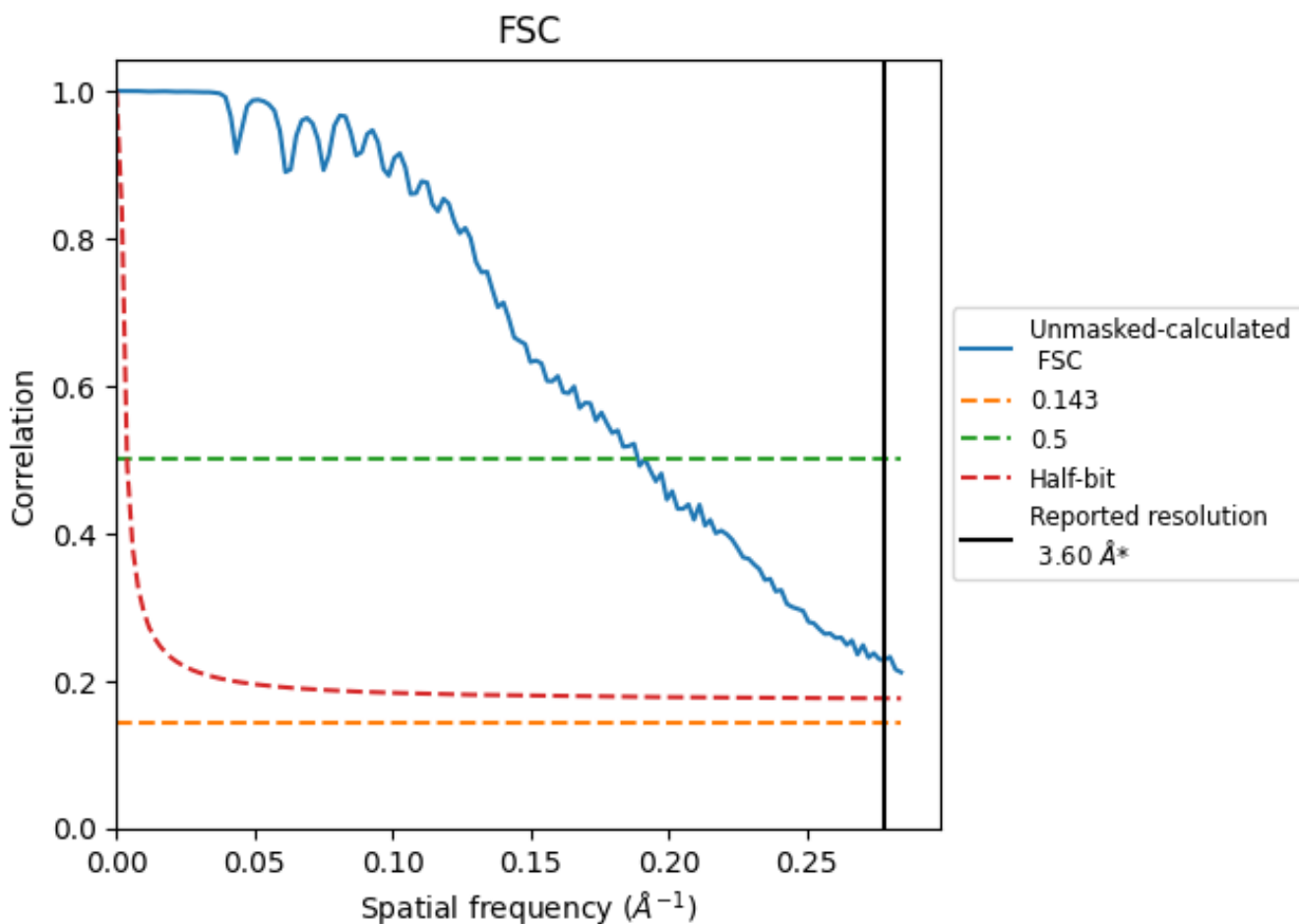


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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\AA^{-1}

8.2 Resolution estimates [i](#)

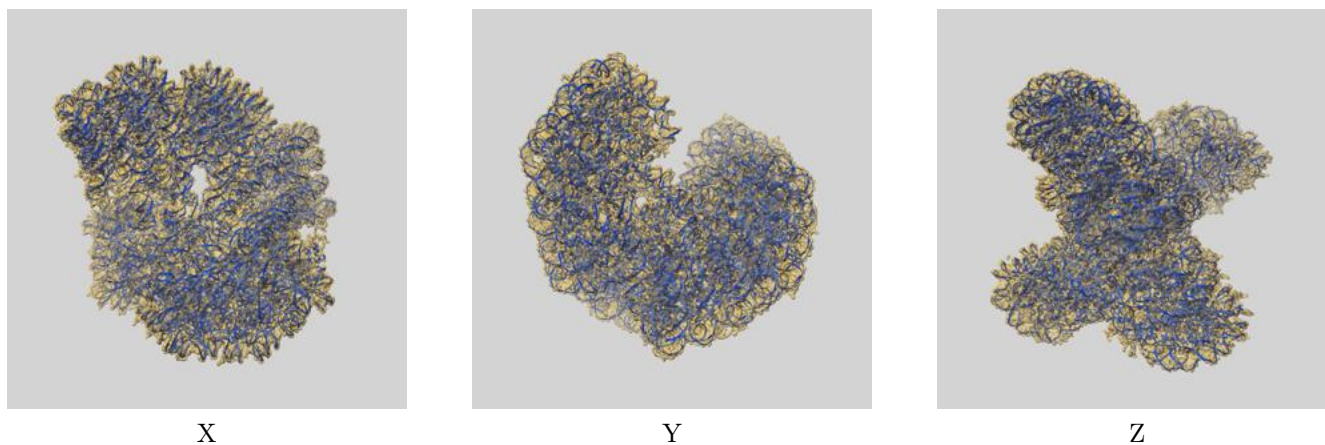
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	5.30	-

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

9 Map-model fit [i](#)

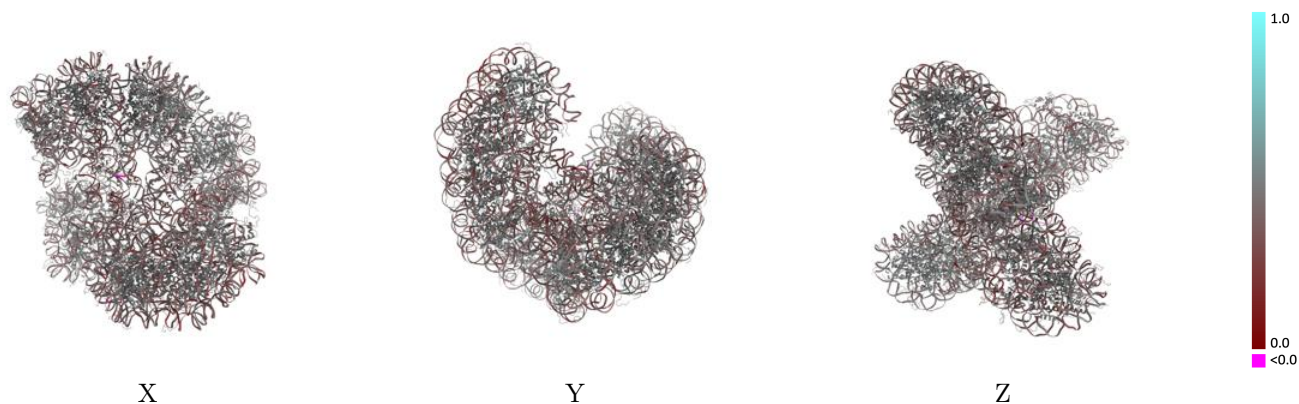
This section contains information regarding the fit between EMDB map EMD-38407 and PDB model 8XJV. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



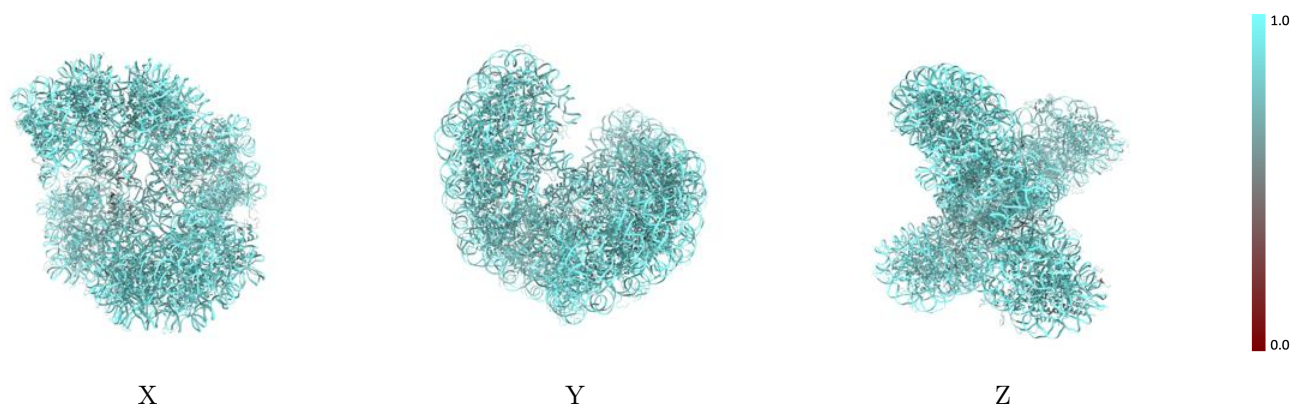
The images above show the 3D surface view of the map at the recommended contour level 0.0293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



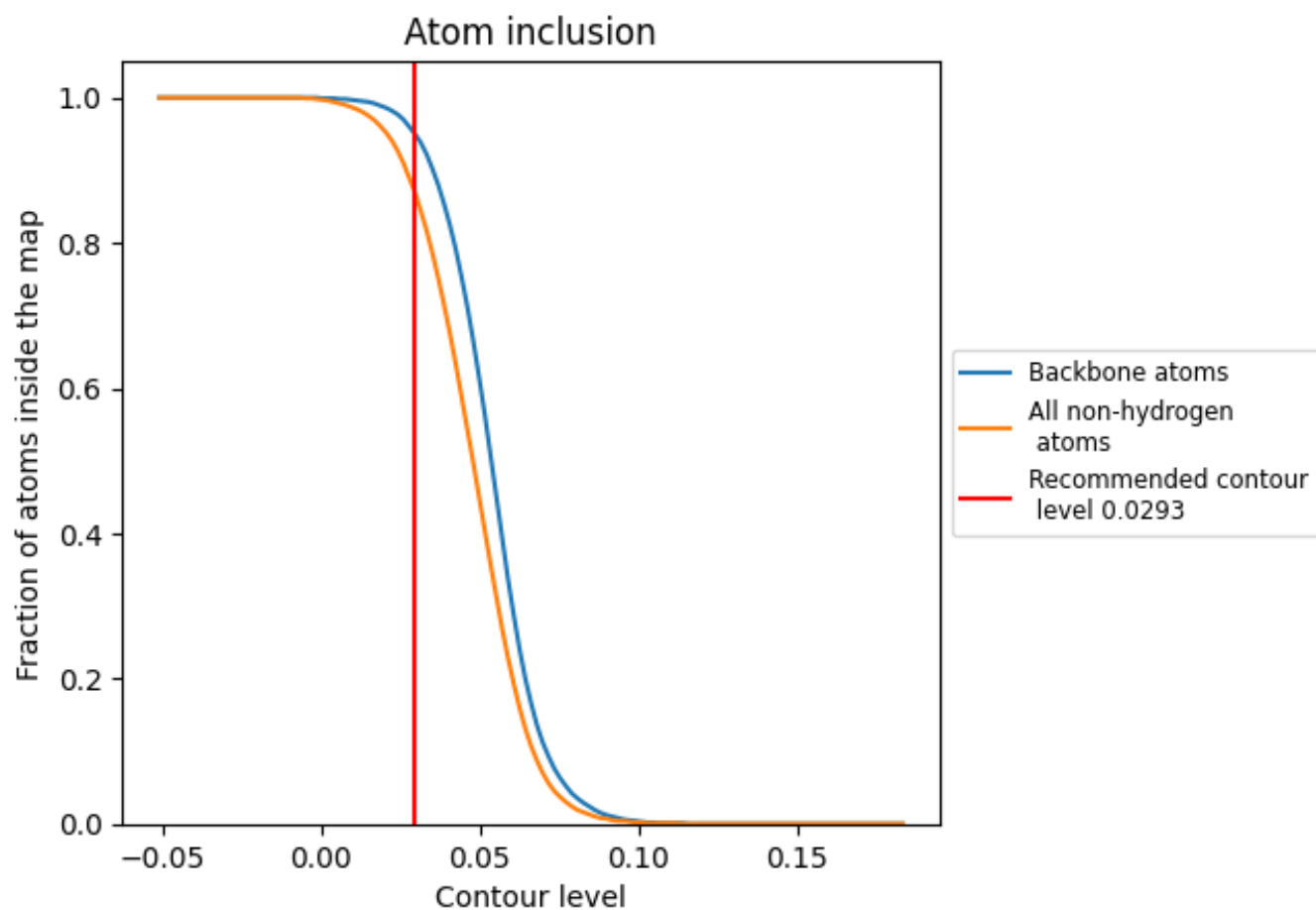
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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