



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 03:43 PM UTC

PDB ID : 9LIU / pdb_00009liu
EMDB ID : EMD-63123
Title : Structure of isw1-nucleosome double-bound complex in ATP-ATP state
Authors : Sia, Y.; Pan, H.; Chen, Z.
Deposited on : 2025-01-14
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

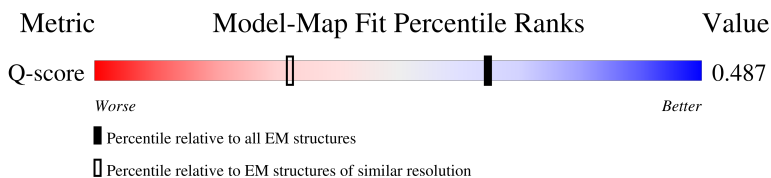
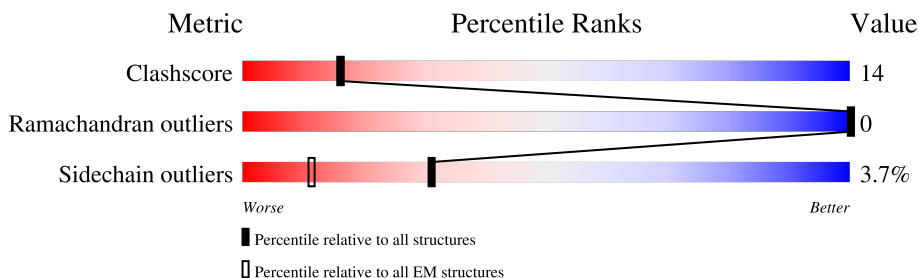
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



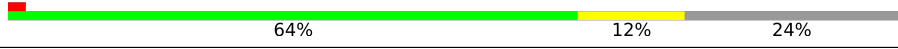
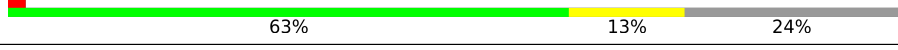
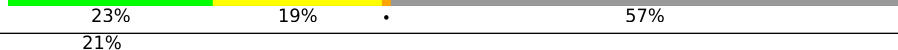
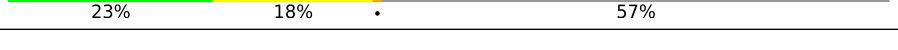
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	A	135	
1	E	135	
2	B	102	
2	F	102	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	122	
4	H	122	
5	I	146	
6	J	146	
7	K	1061	
7	N	1061	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

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

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	F	88	Total	C	N	O	S	0	0
			708	445	143	119	1		

- Molecule 3 is a protein called Histone H2A.

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

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	455	Total	C	N	O	S	0	0
			3738	2397	645	683	13		
7	N	455	Total	C	N	O	S	0	0
			3738	2397	645	683	13		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total	Mg	0
			1	1	
8	N	1	Total	Mg	0
			1	1	

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

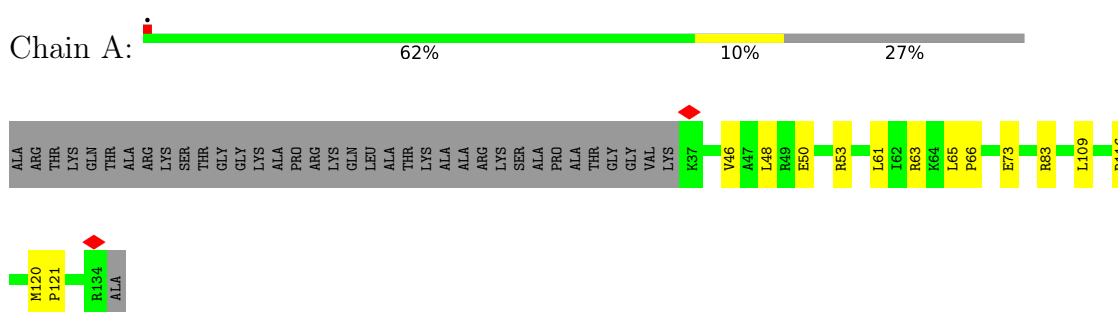


Mol	Chain	Residues	Atoms					AltConf
9	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	N	1	Total	C	N	O	P	0
			31	10	5	13	3	

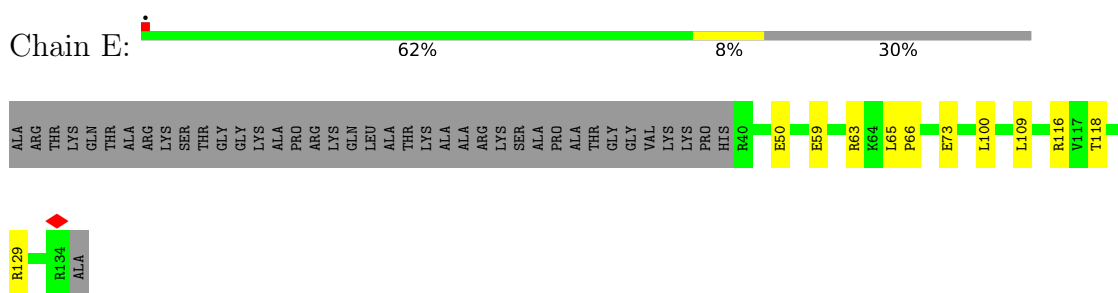
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

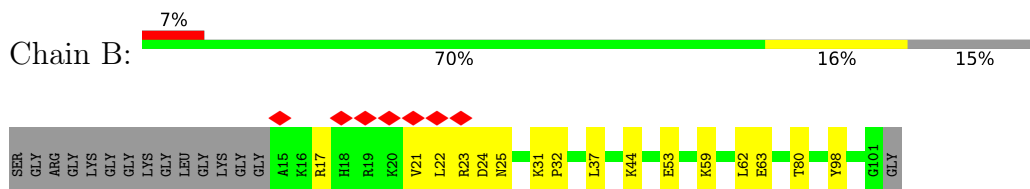
- Molecule 1: Histone H3



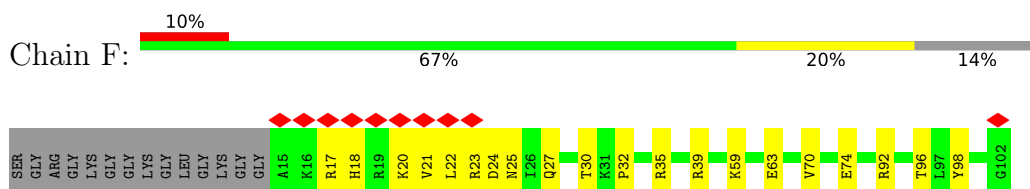
- Molecule 1: Histone H3



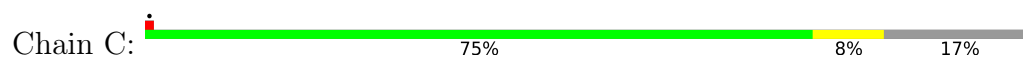
- Molecule 2: Histone H4



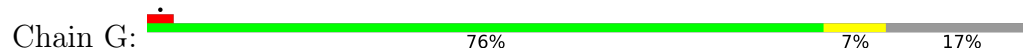
- Molecule 2: Histone H4



- Molecule 3: Histone H2A



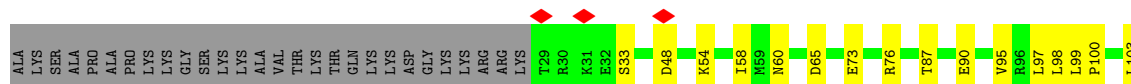
- Molecule 3: Histone H2A



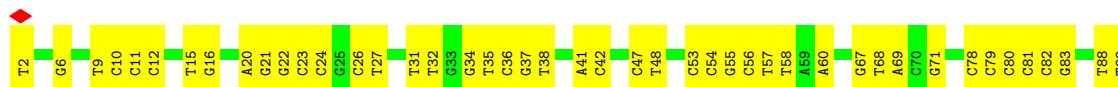
- Molecule 4: Histone H2B



- Molecule 4: Histone H2B

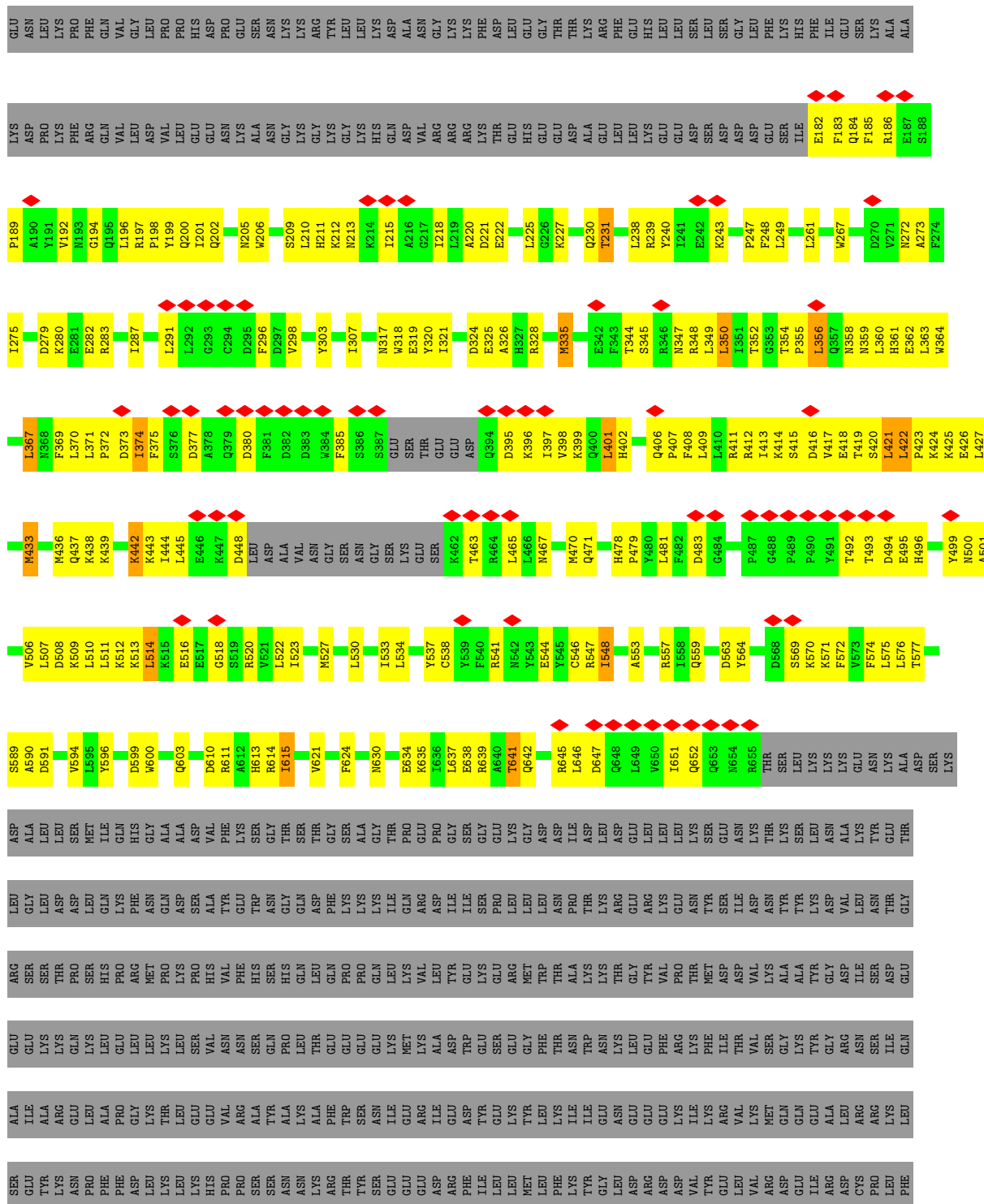


- Molecule 5: DNA (146-MER)



- Molecule 6: DNA (146-MER)





GLU	THR
ASP	ALA
LEU	ASN
GLY	GLY
PHE	LEU
TYR	ASP
GLY	ASP
PHE	LEU
ARG	GLN
SER	ASP
ARG	VAL
THR	GLY
THR	GLY
PRO	VAL
VAL	GLY
VAL	SER
GLU	LEU
LEU	LYS
ALA	LYS
ALA	GLY
ARG	ILE
ARG	GLY
ASN	GLY
ASN	THR
THR	ASP
THR	LEU
LEU	GLY
GLN	SER
GLY	ASN
GLY	VAL
CYS	LYS
LEU	LYS
GLY	ASP
GLU	ALA
LYS	LYS
LEU	GLY
PHE	LEU
GLY	ASN
ALA	VAL
ALA	VAL
ASP	GLY
ASP	THR
ALA	THR
THR	THR
LYS	HIS

● Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1



GLU	LYS	P189	L261	T344	L405	M467	D532	D605	LYS	THR	GLY
ASN	ASP	A190	L265	S345	Q406	M470	L534	M609	ASP	LEU	ARG
LEU	PRO	Y191	R266	R346	P407	Q471	E535	D610	ALA	GLY	SER
LYS	LYS	Y192	R267	N347	F408	L472	D536	D611	LEU	LEU	THR
PRO	PHE	N193	T268	R348	L409	R473	D537	D612	ASP	ASP	PRO
GLN	ARG	G194	P269	L349	R411	M477	C538	H613	SER	LEU	SER
VAL	GLN	Q195	D270	L350	R412	H478	D539	H614	ILE	GLN	HIS
GLY	VAL	L196	V271	T352	I413	P479	F540	H615	GLN	LYS	PRO
LEU	VAL	R197	N272	L351	R414	H480	R541	G616	GLY	PHE	ARG
ASP	GLY	P198	A273	P355	S415	Y480	N542	Q617	ALA	GLN	PRO
PRO	LEU	Y199	D274	L356	D416	L481	E543	H618	ALA	ASP	LYS
HIS	GLY	Q200	F275	Q357	V417	F482	E544	R619	ASP	SER	PRO
ASP	ASN	I201	I276	P358	V418	D483	F645	R620	VAL	ALA	VAL
PRO	LYS	Q202	D279	N359	E418	G484	G646	V621	ASN	VAL	ASN
GLY	ALA	N205	K280	N360	T419	E485	C546	V622	GLY	GLY	ASN
ALA	GLY	W206	E281	H361	S420	A486	R547	R623	SER	THR	SER
SER	ILE	L209	R283	E362	L421	P487	E548	F624	GLY	GLY	GLN
ARG	GLY	S209	T287	W364	P423	G488	A553	H625	THR	GLN	PRO
TYR	LYS	L210	Q288	A365	K424	P489	H554	H626	SER	GLY	LEU
LEU	LYS	H211	K289	L366	K425	P490	E555	V627	GLY	PHE	THR
VAL	LYS	N212	K290	N367	E426	F491	D556	H628	GLY	LYS	GLU
GLY	GLY	N213	L367	L368	L427	T492	E557	D629	ALA	LYS	GLU
THR	THR	K214	L291	F369	N428	T493	E558	M630	THR	ILE	LYS
LYS	ASP	I215	L292	L370	M432	D494	Q559	G631	PRO	ARG	LEU
ALA	ALA	A216	Q293	L371	G432	E495	D562	V632	GLY	ASP	VAL
GLY	LYS	G217	C294	P372	M433	E496	D563	H633	GLY	ILE	ALA
ASN	LYS	L219	D295	D373	S434	L497	N565	E634	GLY	ILE	GLU
ASP	PHE	A220	F296	I374	S435	M436	A566	L637	GLY	THR	LYS
LEU	ASP	E222	D297	F375	M437	Q437	P567	E638	GLY	PRO	GLU
ALA	THR	M223	V298	S376	K438	N500	D568	R639	GLY	ILE	GLY
THR	THR	G224	Y303	D377	K439	A501	S569	T641	ASP	ASN	THR
ARG	LYS	L225	E304	A378	W440	A502	K570	Q642	ASP	PRO	ALA
PHE	GLY	K227	I307	Q379	Y441	K503	K571	L644	LEU	LYS	LYS
LEU	LEU	Q230	R308	F381	K442	Q505	F572	R645	GLY	THR	GLY
HIS	LEU	T231	K315	D382	K443	V506	V573	L646	LEU	ARG	TYR
LEU	LEU	F234	I316	D383	L444	L507	F574	D647	LEU	LYS	VAL
SER	SER	L235	N317	W384	L445	D508	L575	L576	LEU	ASN	ARG
GLY	SER	G236	W318	F385	E446	K509	L577	T577	SER	TYR	THR
ASN	GLY	Y237	E319	S386	K447	L510	L583	Q648	GLY	SER	PHE
LEU	LEU	L238	Y320	S387	D448	L511	G584	L649	ASP	ILE	ALA
PHE	PHE	R239	I321	GLU	LEU	K512	D587	V650	VAL	ASP	ASP
LYS	HIS	Y240	D324	ASP	ASP	K513	G588	T651	VAL	VAL	THR
ILE	ILE	I241	E325	THR	ALA	L514	L587	Q652	LYS	LYS	SER
PHE	PHE	E242	A326	GLY	VAL	R515	T588	Q653	THR	GLY	ALA
GLY	GLY	K243	H327	GLY	ASN	K615	A590	N654	LYS	TYR	LYS
SER	SER	P245	R328	ASP	GLY	E516	D591	R655	LEU	ASP	GLY
LYS	LYS	G246	E332	Q394	ASN	E517	D591	THR	ALA	ILE	ARG
ALA	ALA	P247	M335	D395	GLY	G518	V594	LYS	LYS	ASN	ASN
ASP	ASP	F248	R341	K396	LYS	S519	L595	GLU	GLY	SER	ILE
GLN	GLN	L249	E342	I397	GLY	R520	V596	ASN	ASP	SER	ASP
		N258	F343	V398	SER	L522	D597	GLU	ILE	ASP	
				Q400	K462	T523	S598	ALA	ASP		
				H402	T463	Q526	N600	SER			
				T403	L465						
				V404	L466						

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24645	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.085	Depositor
Map size ($\text{\AA}$)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/813	0.53	0/1093
1	E	0.57	0/789	0.53	0/1059
2	B	0.61	0/711	0.57	0/950
2	F	0.61	0/716	0.63	0/955
3	C	0.57	0/821	0.49	0/1112
3	G	0.56	0/825	0.52	0/1116
4	D	0.57	0/729	0.51	0/985
4	H	0.55	0/737	0.54	0/993
5	I	0.54	0/3333	0.47	0/5137
6	J	0.55	0/3381	0.45	0/5221
7	K	0.37	0/3811	0.51	0/5146
7	N	0.36	0/3811	0.50	0/5146
All	All	0.50	0/20477	0.50	0/28913

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	801	0	831	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	779	0	815	11	0
2	B	703	0	757	18	0
2	F	708	0	760	22	0
3	C	811	0	849	11	0
3	G	815	0	860	8	0
4	D	718	0	725	17	0
4	H	726	0	747	15	0
5	I	2975	0	1639	61	0
6	J	3011	0	1639	61	0
7	K	3738	0	3796	173	0
7	N	3738	0	3796	161	0
8	K	1	0	0	0	0
8	N	1	0	0	0	0
9	K	31	0	12	5	0
9	N	31	0	12	1	0
All	All	19587	0	17238	526	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 14.

The worst 5 of 526 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)
5:I:6:DG:N2	6:J:142:DC:O2	2.01	0.92
2:F:92:ARG:HH12	4:H:97:LEU:HB3	1.35	0.91
7:K:611:ARG:HH11	7:K:614:ARG:HH11	1.19	0.86
7:N:611:ARG:HH11	7:N:614:ARG:HH11	1.19	0.84
7:N:614:ARG:NH1	9:N:1202:ATP:O3G	2.12	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
1	E	93/135 (69%)	88 (95%)	5 (5%)	0	100	100
2	B	85/102 (83%)	78 (92%)	7 (8%)	0	100	100
2	F	86/102 (84%)	79 (92%)	7 (8%)	0	100	100
3	C	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
3	G	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
4	D	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
4	H	91/122 (75%)	87 (96%)	4 (4%)	0	100	100
7	K	449/1061 (42%)	414 (92%)	35 (8%)	0	100	100
7	N	449/1061 (42%)	415 (92%)	34 (8%)	0	100	100
All	All	1650/3098 (53%)	1551 (94%)	99 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	72/78 (92%)	72 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	K	413/958 (43%)	386 (94%)	27 (6%)	15	37
7	N	413/958 (43%)	386 (94%)	27 (6%)	15	37
All	All	1455/2698 (54%)	1401 (96%)	54 (4%)	31	59

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	N	335	MET
7	N	421	LEU
7	N	570	LYS
7	N	350	LEU
7	N	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
7	N	542	ASN
7	N	642	GLN
7	N	586	ASN
7	K	542	ASN
7	N	357	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ATP	K	1202	8	32,33,33	1.27	4 (12%)	48,52,52	1.83	9 (18%)
9	ATP	N	1202	8	32,33,33	1.28	4 (12%)	48,52,52	1.83	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	K	1202	8	-	7/22/38/38	0/3/3/3
9	ATP	N	1202	8	-	7/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	1202	ATP	C5-C4	4.42	1.47	1.39
9	K	1202	ATP	C5-C4	4.39	1.46	1.39
9	K	1202	ATP	C5-N7	-2.53	1.34	1.39
9	N	1202	ATP	C5-N7	-2.53	1.34	1.39
9	K	1202	ATP	C5-C6	2.46	1.47	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	1202	ATP	C5-C4-N3	-5.95	118.52	126.72
9	K	1202	ATP	C5-C4-N3	-5.93	118.55	126.72
9	K	1202	ATP	N3-C4-N9	4.85	135.41	127.17
9	N	1202	ATP	N3-C4-N9	4.83	135.39	127.17
9	K	1202	ATP	C2-N3-C4	3.73	120.95	111.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

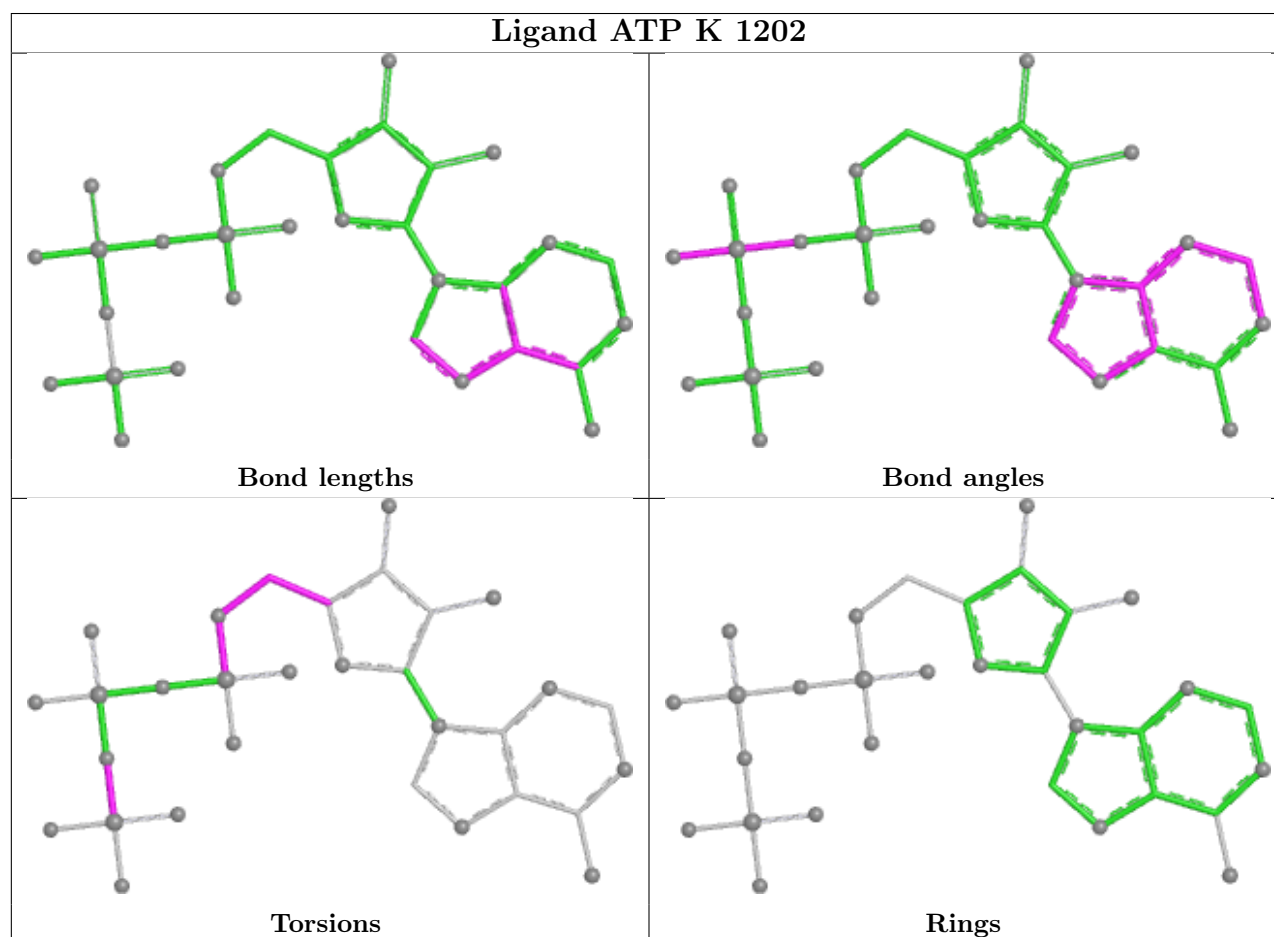
Mol	Chain	Res	Type	Atoms
9	K	1202	ATP	PB-O3B-PG-O2G
9	K	1202	ATP	PB-O3B-PG-O3G
9	K	1202	ATP	C5'-O5'-PA-O2A
9	K	1202	ATP	C5'-O5'-PA-O3A
9	N	1202	ATP	PB-O3B-PG-O2G

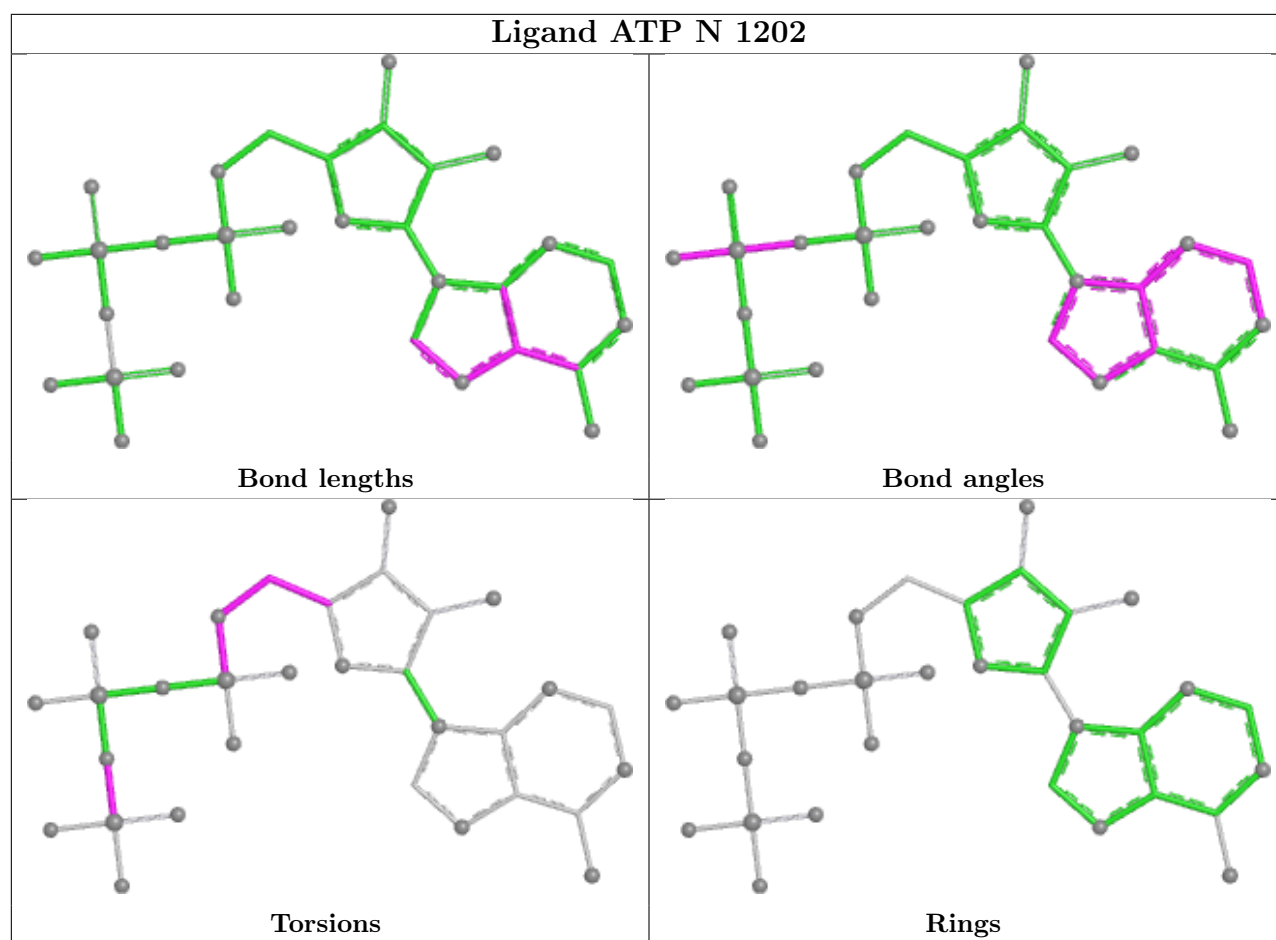
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1202	ATP	5	0
9	N	1202	ATP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

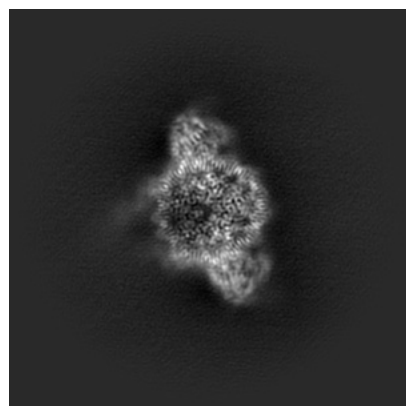
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63123. These allow visual inspection of the internal detail of the map and identification of artifacts.

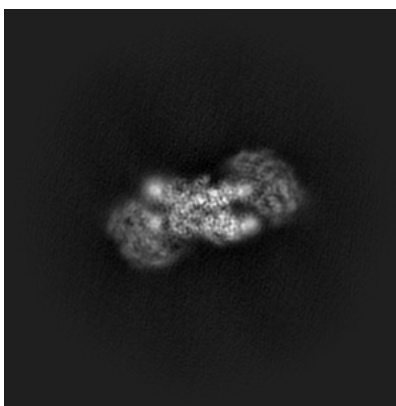
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

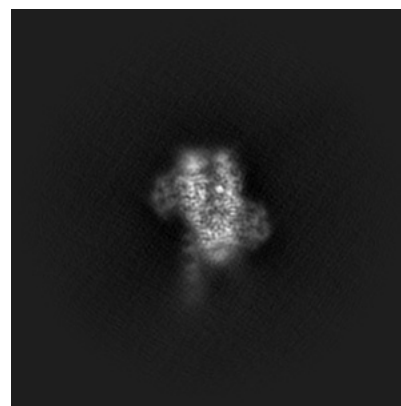
6.1.1 Primary map



X

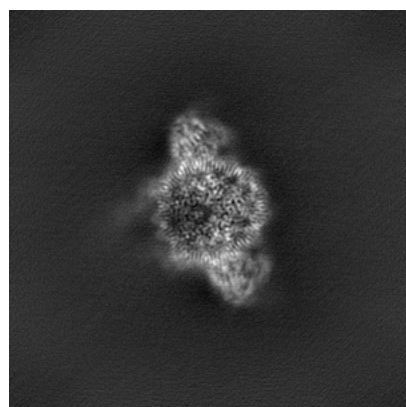


Y

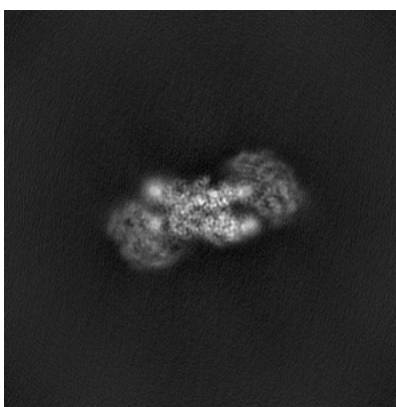


Z

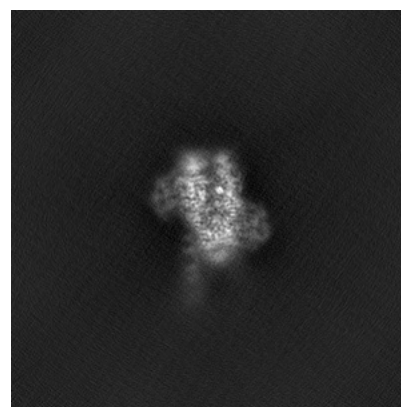
6.1.2 Raw map



X



Y

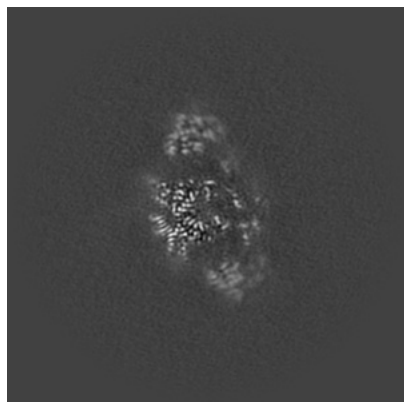


Z

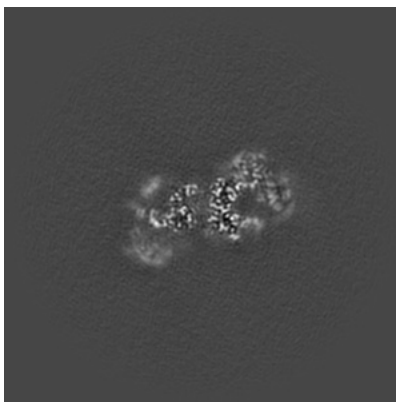
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

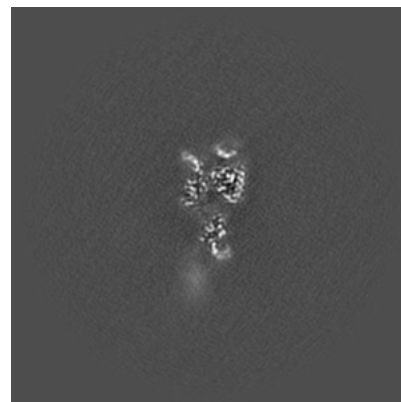
6.2.1 Primary map



X Index: 160

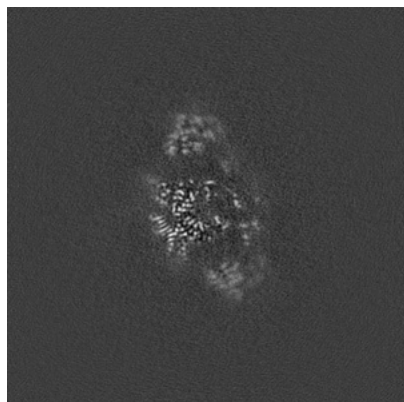


Y Index: 160

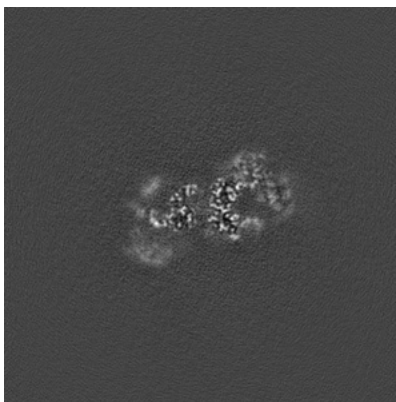


Z Index: 160

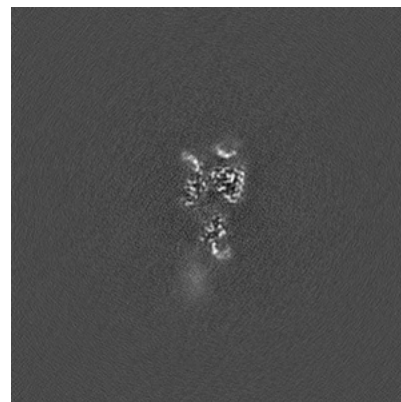
6.2.2 Raw map



X Index: 160



Y Index: 160

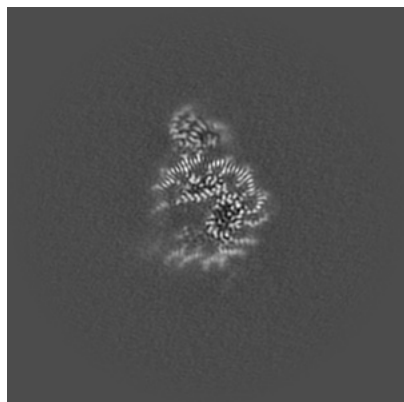


Z Index: 160

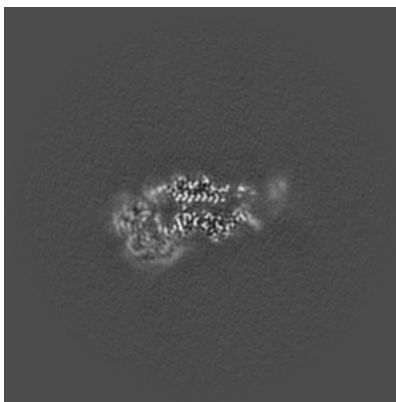
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

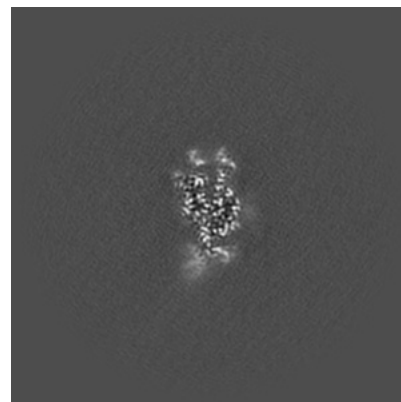
6.3.1 Primary map



X Index: 173

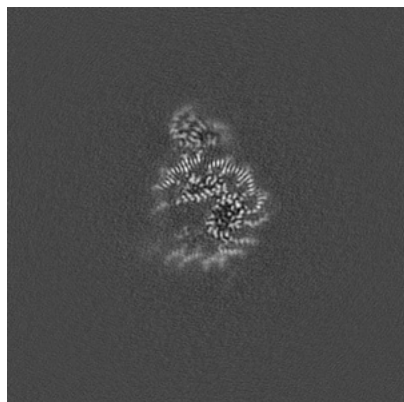


Y Index: 174

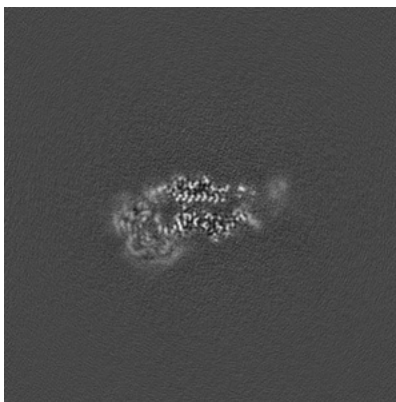


Z Index: 175

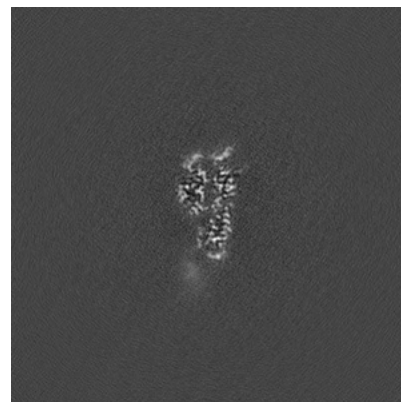
6.3.2 Raw map



X Index: 173



Y Index: 174

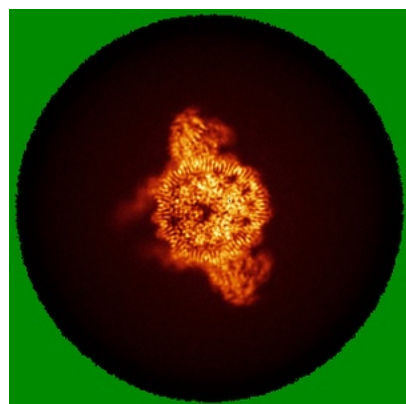


Z Index: 166

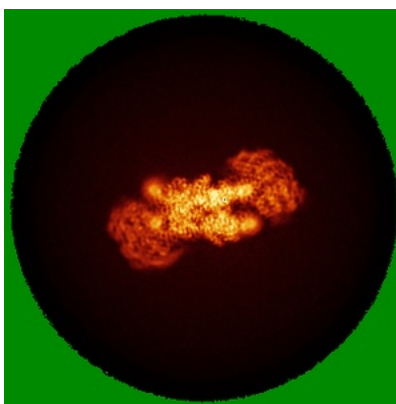
The images above show the largest variance slices of the map in three orthogonal directions.

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

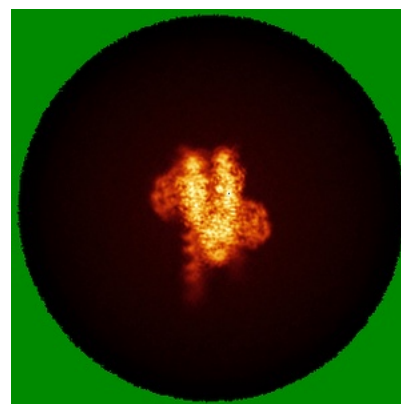
6.4.1 Primary map



X

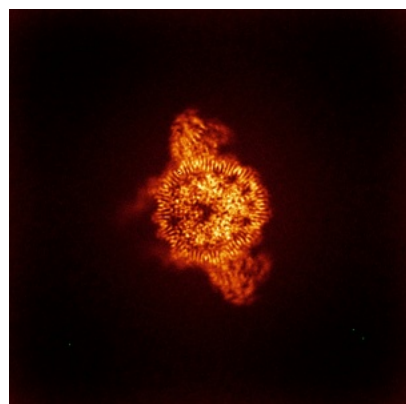


Y

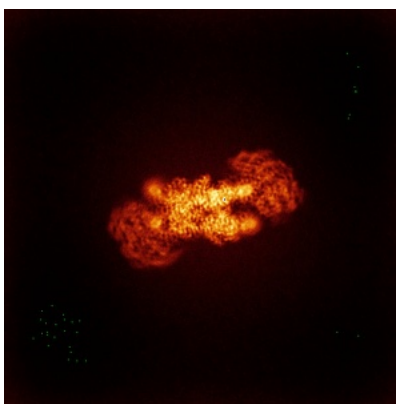


Z

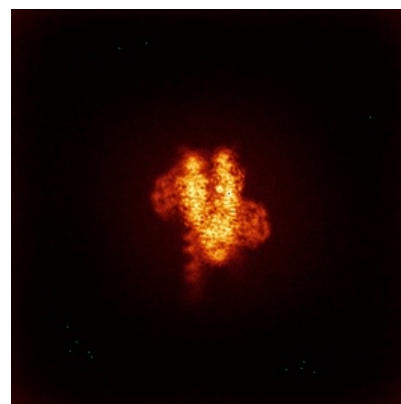
6.4.2 Raw map



X



Y

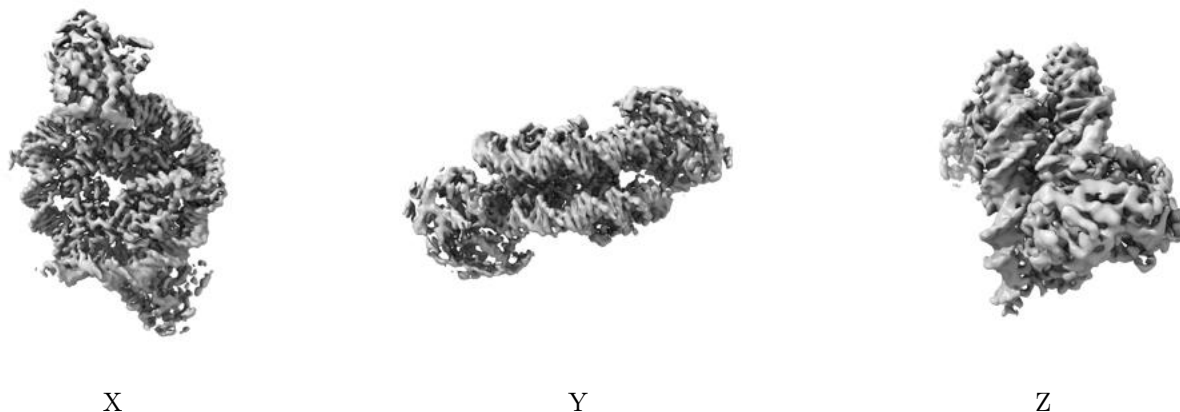


Z

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.

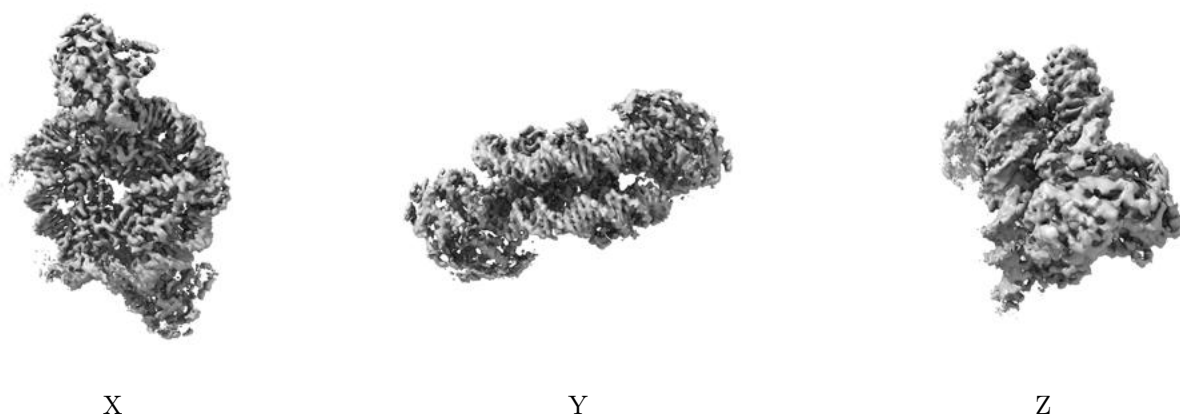
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

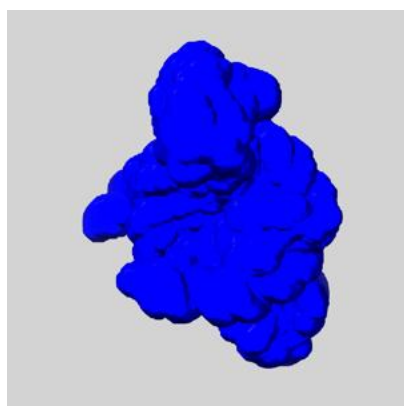
6.6 Mask visualisation [i](#)

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

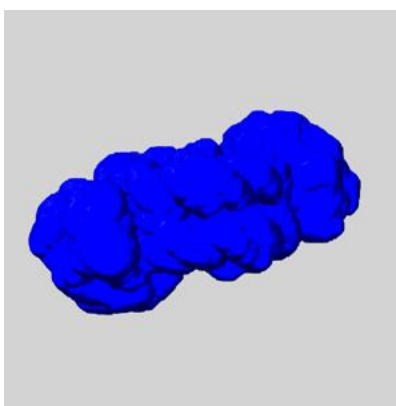
A mask typically either:

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

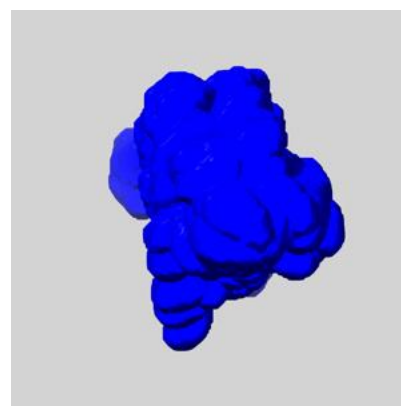
6.6.1 emd_63123_msk_1.map [i](#)



X



Y

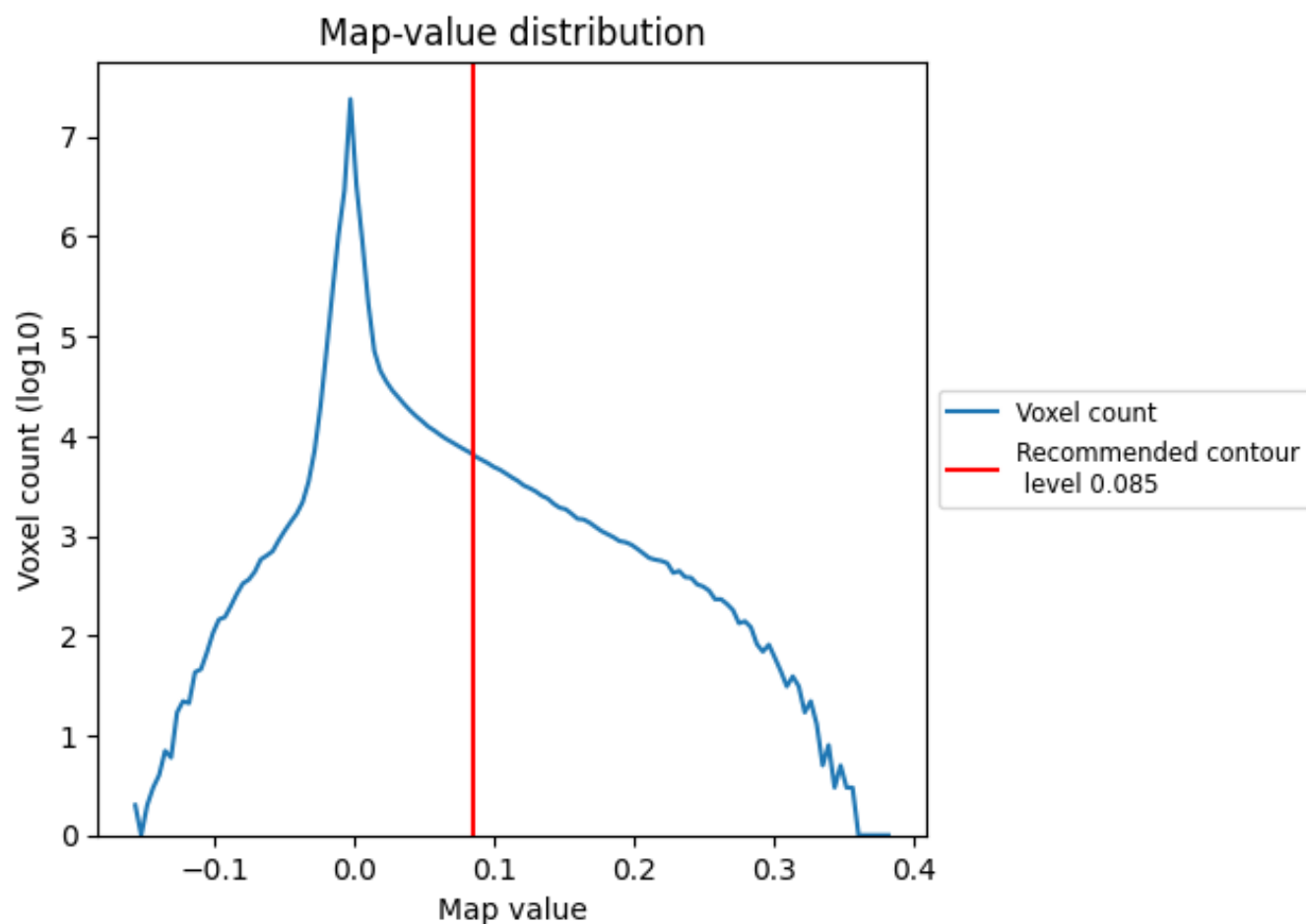


Z

7 Map analysis [i](#)

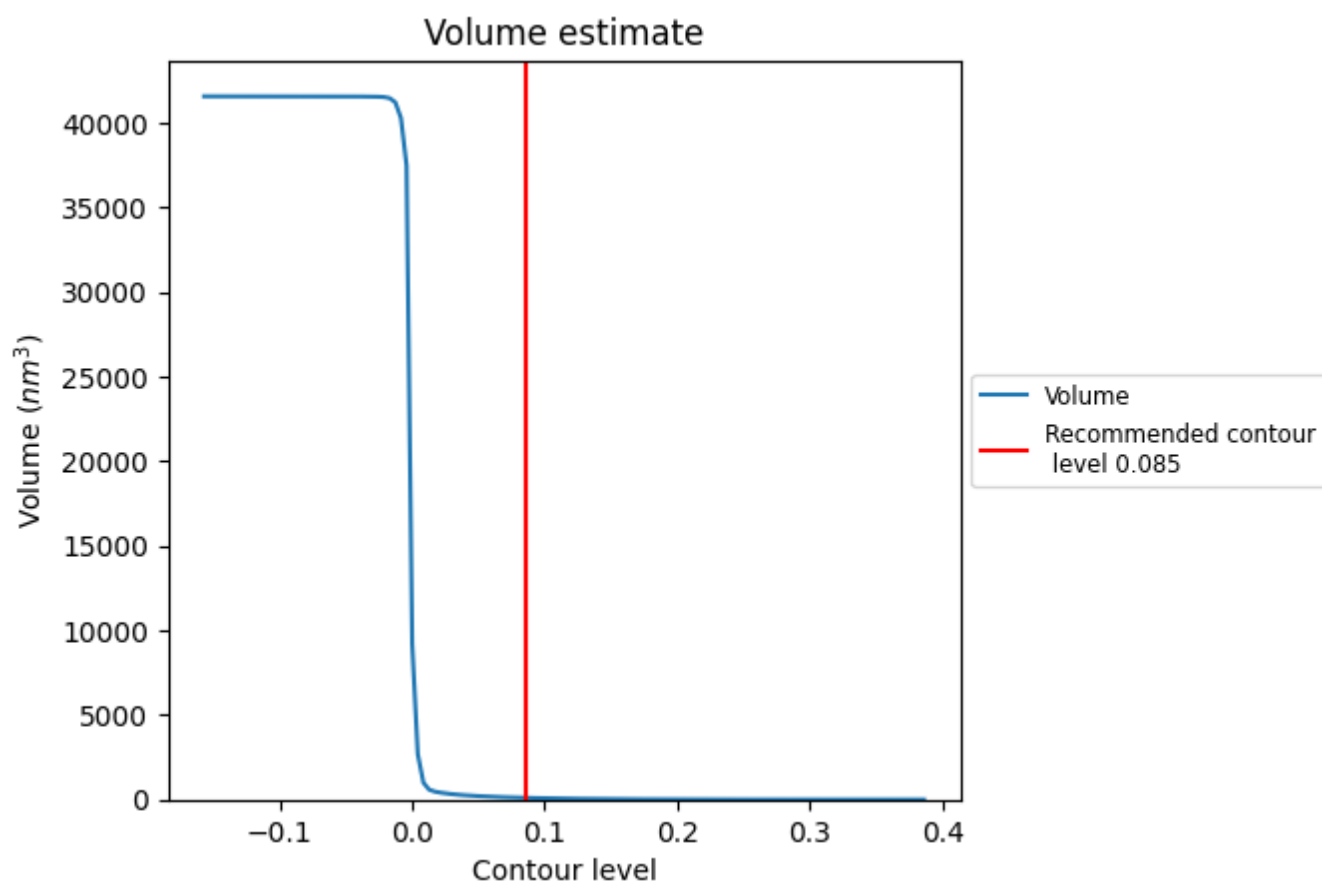
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

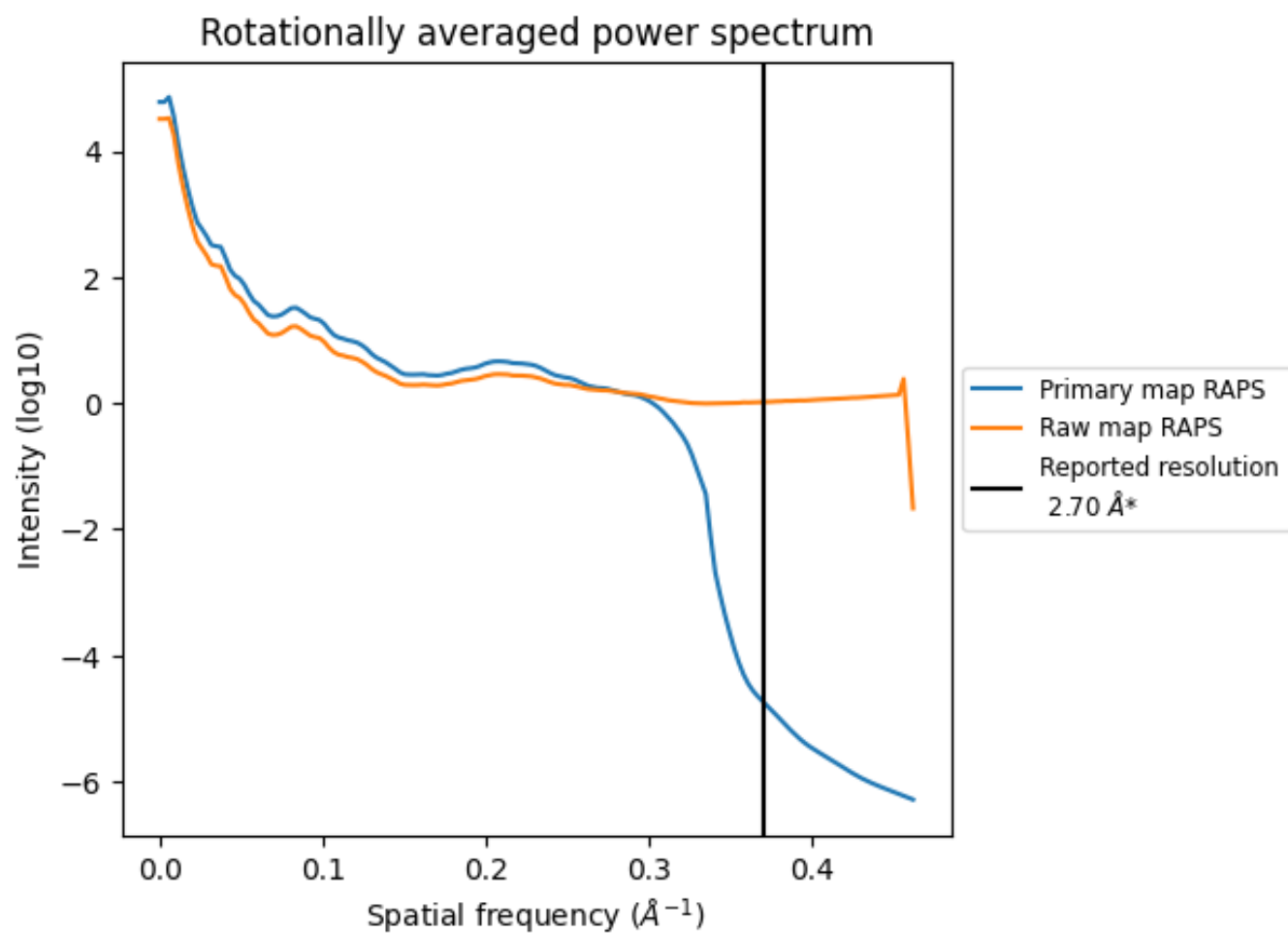
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm³; this corresponds to an approximate mass of 94 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

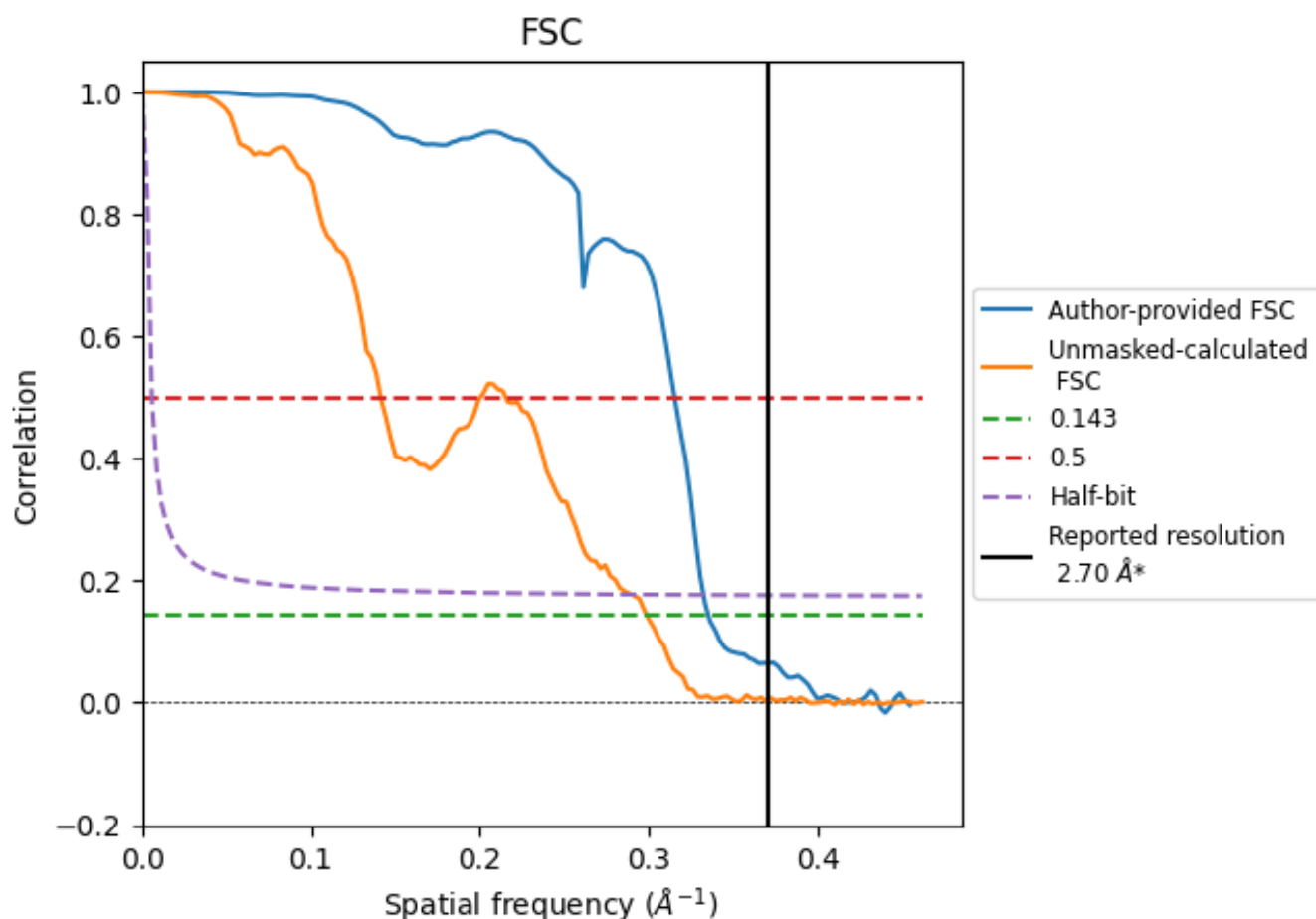


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.98	3.17	3.01
Unmasked-calculated*	3.35	7.08	3.45

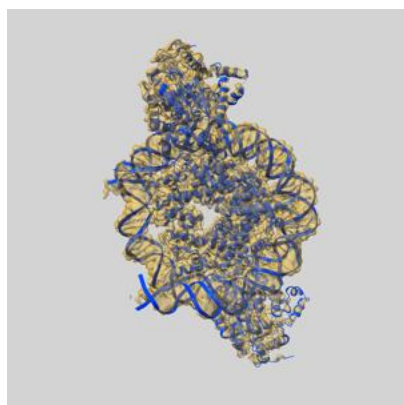
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.98 differs from the reported value 2.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.7 by more than 10 %

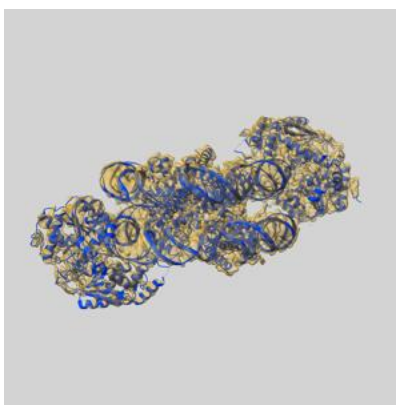
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63123 and PDB model 9LIU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

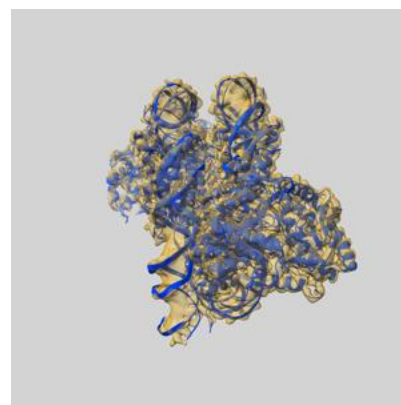
9.1 Map-model overlay [i](#)



X



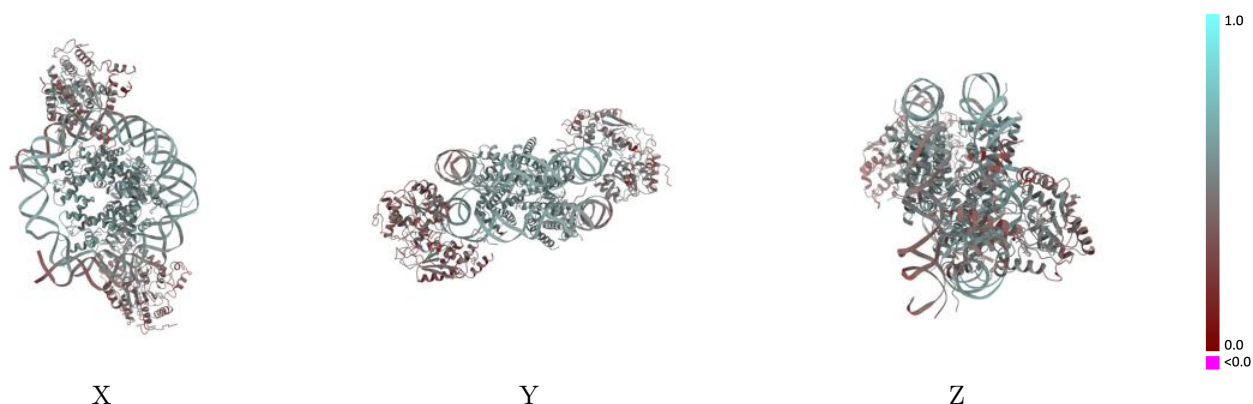
Y



Z

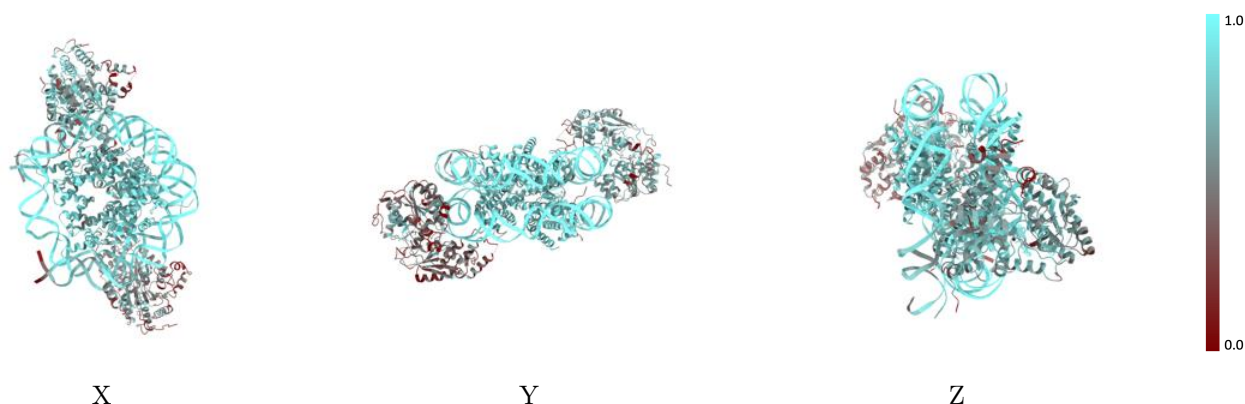
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



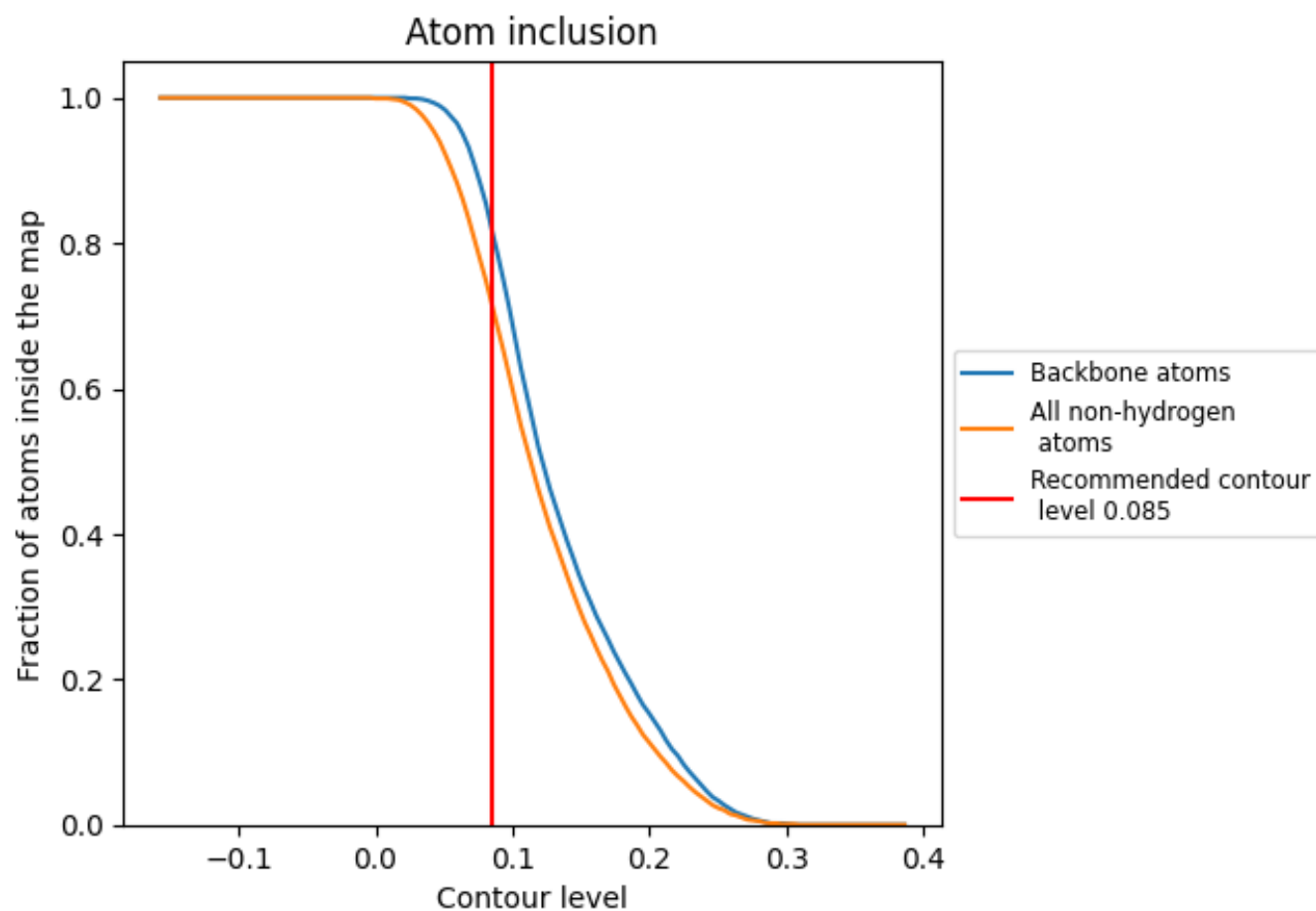
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.4870
A	0.8190	0.5750
B	0.7950	0.5570
C	0.8410	0.5660
D	0.8430	0.5570
E	0.8330	0.5670
F	0.7740	0.5460
G	0.8200	0.5600
H	0.8140	0.5410
I	0.8850	0.5230
J	0.8790	0.5230
K	0.5970	0.4350
N	0.3980	0.3670

1.0

0.0

<0.0