



Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 01:27 PM JST

PDB ID : 9JNP / pdb_00009jnp
EMDB ID : EMD-61624
Title : Structure of isw1-nucleosome complex in ATP state
Authors : Sia, Y.; Pan, H.; Chen, Z.
Deposited on : 2024-09-23
Resolution : 2.30 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

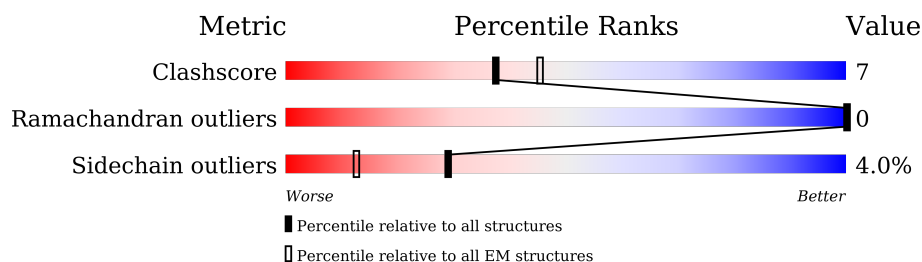
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	A	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	

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Mol	Chain	Length	Quality of chain
5	I	146	<div><div></div><div>68%</div><div>32%</div></div>
6	J	146	<div><div></div><div>68%</div><div>32%</div></div>
7	K	1061	<div><div></div><div>31%</div><div>11%</div><div>57%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15781 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	86	Total	C	N	O	S	0	0
			672	424	130	117	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		

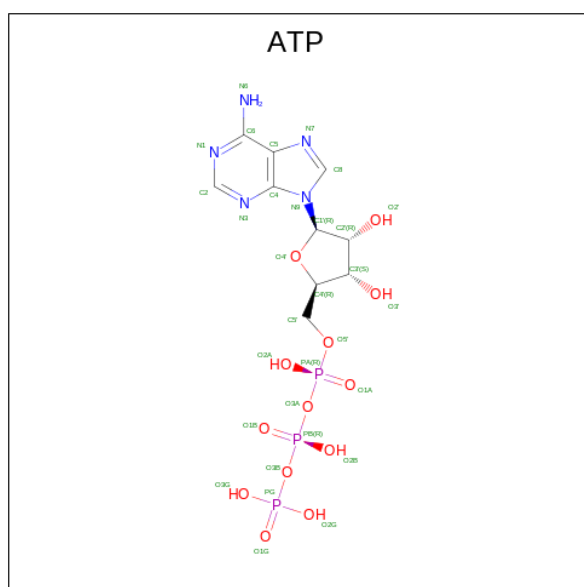
- Molecule 6 is a DNA chain called DNA (146-MER).

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		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

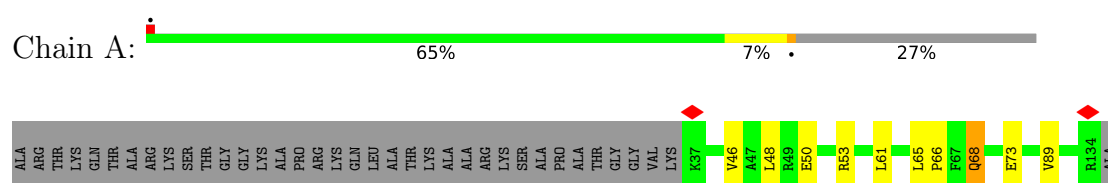
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	K	1	Total	Mg	0
			1	1	

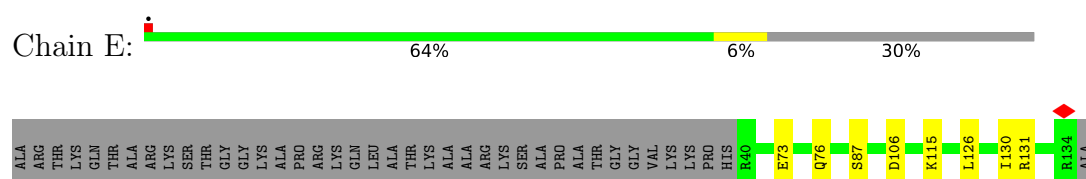
3 Residue-property plots [i](#)

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.

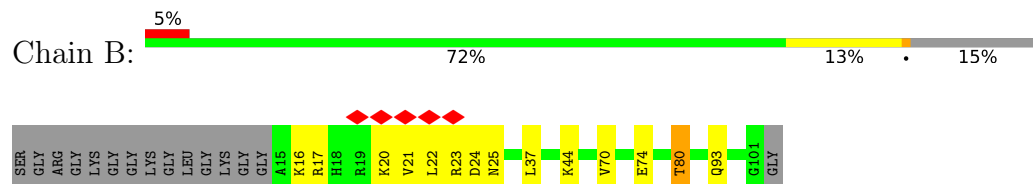
• Molecule 1: Histone H3




• Molecule 1: Histone H3



• Molecule 2: Histone H4



Chain G:  74% 9% 17%



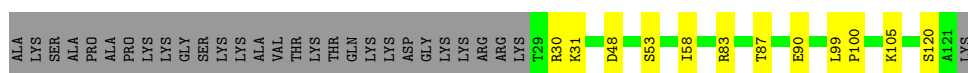
- Molecule 4: Histone H2B

Chain D:  66% 9% 24%



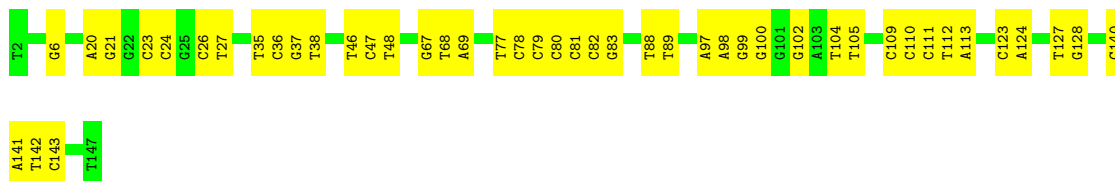
- Molecule 4: Histone H2B

Chain H:  66% 10% 24%



- Molecule 5: DNA (146-MER)

Chain I:  68% 32%



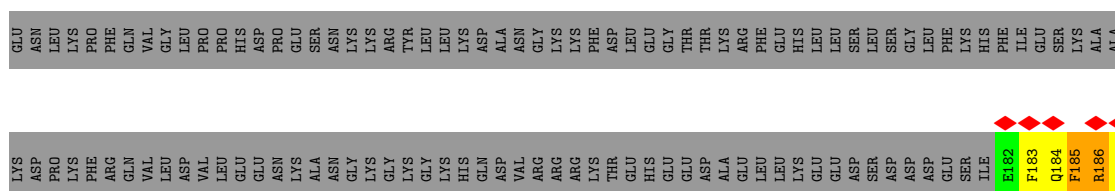
- Molecule 6: DNA (146-MER)

Chain J:  68% 32%



- Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1

Chain K:  31% 11% 57%



ASN	GLY	ASN	LEU	VAL	THR	ASP	ILE	ASN	SER
ARG	ARG	LYS	VAL	LYS	VAL	LYS	ASP	LYS	LEU
ILE	ARG	GLN	MET	GLY	ASN	LYS	ASN	THR	LYS
ARG	GLY	GLN	TYR	TYR	ASP	GLY	ASP	GLU	GLY
GLY	ARG	ALA	GLY	GLY	ASN	LYS	ALA	ASN	ASN
ASP	ASP	LEU	ARG	ARG	VAL	ASP	VAL	E445	E446
PHE	CYS	ARG	ILE	ASN	ILE	ASP	LEU	K425	E426
ALA	PRO	ALA	ASP	ASP	THR	ASP	TYR	L421	L422
GLN	PHE	LEU	LYS	LEU	GLY	SER	THR	E447	D448
THR	GLY	THR	GLN	GLN	GLY	LYS	LEU	ASP	ASP
ALA	ALA	GLU	ILE	ILE	SER	ASP	GLY	L356	L355
ASN	ASN	PHE	TYR	TYR	THR	LYS	LEU	L363	L364
LYS	ASP	ARG	ASN	ARG	THR	ASP	ASP	W364	W363
LYS	TYR	ASN	ASN	ASN	PRO	ASP	SER	D373	D372
GLU	PHE	GLU	PRO	PRO	LYS	ASP	MET	F369	F370
ASN	ARG	ASN	PHE	PHE	LYS	ASP	ILE	L370	L371
VAL	SER	VAL	ASN	ASN	PRO	GLY	GLN	L371	L372
ASP	ARG	ARG	ASP	GLY	GLY	LEU	PHE	F372	F373
THR	THR	THR	VAL	VAL	THR	LYS	GLY	D377	D378
VAL	VAL	VAL	VAL	VAL	THR	GLY	GLY	I374	I375
GLY	GLY	GLY	GLY	GLY	THR	ASP	ASP	D380	D381
LYS	LYS	LYS	LYS	LYS	THR	ASP	GLY	A378	A379
LYS	ALA	ALA	ALA	ALA	THR	LYS	LYS	Q379	Q380
ILE	ILE	ILE	ILE	ILE	SER	THR	GLY	D383	D384
GLY	GLY	GLY	GLY	GLY	ASN	GLY	GLY	F385	F386
THR	THR	THR	THR	THR	ASN	LYS	LYS	S387	S388
GLY	GLY	GLY	GLY	GLY	PRO	ILE	ILE	GLU	GLU
LYS	LYS	LYS	LYS	LYS	GLY	LYS	LYS	THR	THR
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLU	GLU
ALA	ALA	ALA	ALA	ALA	ILE	ILE	ILE	ASP	ASP
GLY	GLY	GLY	GLY	GLY	LYS	LYS	LYS	Q394	Q395
LYS	LYS	LYS	LYS	LYS	PRO	PRO	PRO	D396	D397
ILE	ILE	ILE	ILE	ILE	GLY	GLY	GLY	K396	K397
VAL	VAL	VAL	VAL	VAL	LEU	LEU	LEU	V398	V399
THR	THR	THR	THR	THR	ASN	ASN	ASN	K399	K400
LYS	LYS	LYS	LYS	LYS	THR	THR	THR	Q400	Q401
GLY	GLY	GLY	GLY	GLY	ALA	ALA	ALA	L401	L402
THR	THR	THR	THR	THR	LYS	LYS	LYS	H402	H403
LYS	LYS	LYS	LYS	LYS	THR	THR	THR	T403	T404
ASP	ASP	ASP	ASP	ASP	ARG	ARG	ARG	Y404	Y405
THR	THR	THR	THR	THR	VAL	VAL	VAL	L405	L406
HIS	HIS	HIS	HIS	HIS	PRO	PRO	PRO	D536	D537
					GLU	GLU	GLU	Y537	Y538
					ASN	ASN	ASN	C538	C539
					TYR	TYR	TYR	Y539	Y540
					SER	SER	SER	F540	F541
					GLU	GLU	GLU	R541	R542
					ILE	ILE	ILE	D416	D417
					ARG	ARG	ARG	R412	R413
					THR	THR	THR	I413	I414
					ASP	ASP	ASP	K414	K415
					GLY	GLY	GLY	S415	S416
					LYS	LYS	LYS	D824	D825
					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
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					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
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					THR	THR	THR	R328	R329
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
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					THR	THR	THR	R328	R329
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					GLY	GLY	GLY	W318	W319
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					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
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					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
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					VAL	VAL	VAL	E319	E320
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					ILE	ILE	ILE	Y320	Y321
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
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					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
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					THR	THR	THR	R328	R329
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
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					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
					ASP	ASP	ASP	Y320	Y321
					GLY	GLY	GLY	W318	W319
					VAL	VAL	VAL	E319	E320
					ILE	ILE	ILE	Y320	Y321
					ASP	ASP	ASP	D824	D825
					THR	THR	THR	R328	R329
</									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1080568	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	0.444	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.09	Depositor
Map size (\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 (\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: MG, ATP

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	0.43	0/813	0.46	0/1093
1	E	0.44	0/789	0.44	0/1059
2	B	0.44	0/711	0.53	0/950
2	F	0.45	0/680	0.49	0/912
3	C	0.41	0/821	0.46	0/1112
3	G	0.41	0/825	0.45	0/1116
4	D	0.43	0/729	0.47	0/985
4	H	0.43	0/737	0.46	0/993
5	I	0.90	0/3333	0.97	0/5137
6	J	0.92	0/3381	0.94	0/5221
7	K	0.37	0/3811	0.52	2/5146 (0.0%)
All	All	0.66	0/16630	0.73	2/23724 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	189	PRO	CA-N-CD	-11.04	96.04	111.50
7	K	189	PRO	N-CD-CG	-5.55	94.87	103.20

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	8	0
1	E	779	0	815	3	0
2	B	703	0	757	14	0
2	F	672	0	698	6	0
3	C	811	0	849	6	0
3	G	815	0	860	10	0
4	D	718	0	725	8	0
4	H	726	0	747	6	0
5	I	2975	0	1639	35	0
6	J	3011	0	1639	31	0
7	K	3738	0	3796	101	0
8	K	31	0	12	3	0
9	K	1	0	0	0	0
All	All	15781	0	13368	212	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 7.

All (212) 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)
7:K:396:LYS:HG2	7:K:397:ILE:HG12	1.53	0.88
5:I:6:DG:N2	6:J:142:DC:O2	2.07	0.87
7:K:184:GLN:HB3	7:K:186:ARG:HH12	1.47	0.80
7:K:185:PHE:CE1	7:K:189:PRO:HD3	2.20	0.76
7:K:468:ILE:HD12	7:K:468:ILE:H	1.52	0.75
7:K:648:GLN:NE2	7:K:649:LEU:HD22	2.05	0.71
7:K:532:ASP:OD1	7:K:547:ARG:NH1	2.23	0.71
2:B:20:LYS:NZ	2:B:21:VAL:O	2.22	0.70
7:K:492:THR:O	7:K:496:HIS:NE2	2.23	0.69
7:K:614:ARG:NH1	8:K:1201:ATP:O3G	2.23	0.69
7:K:398:VAL:HG13	7:K:399:LYS:HD2	1.76	0.68
5:I:47:DC:H2"	5:I:48:DT:H72	1.77	0.67
7:K:189:PRO:HB2	7:K:192:VAL:HB	1.77	0.67
5:I:6:DG:N1	6:J:142:DC:N3	2.32	0.66
6:J:58:DT:OP1	7:K:283:ARG:NH2	2.30	0.65
7:K:396:LYS:H	7:K:396:LYS:HD3	1.60	0.65
7:K:520:ARG:NH2	7:K:569:SER:OG	2.30	0.64
7:K:184:GLN:HB3	7:K:186:ARG:NH1	2.13	0.64
7:K:348:ARG:NH2	7:K:369:PHE:O	2.33	0.62
7:K:399:LYS:O	7:K:403:THR:HG23	1.99	0.62
7:K:605:ASP:O	7:K:609:MET:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:421:LEU:HD11	7:K:617:GLN:HB3	1.80	0.62
1:A:68:GLN:HG3	1:A:89:VAL:HG11	1.81	0.61
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.33	0.61
7:K:508:ASP:OD2	7:K:541:ARG:NH1	2.33	0.61
2:B:17:ARG:HH22	7:K:493:THR:HG22	1.64	0.61
5:I:67:DG:H2''	5:I:68:DT:H71	1.82	0.61
7:K:196:LEU:H	7:K:196:LEU:HD23	1.66	0.61
3:G:41:GLU:HG2	3:G:42:ARG:HG3	1.82	0.61
7:K:638:GLU:O	7:K:642:GLN:NE2	2.33	0.61
1:A:46:VAL:O	1:A:50:GLU:HG3	2.02	0.60
2:B:70:VAL:O	2:B:74:GLU:HG3	2.01	0.60
3:G:91:GLU:H	3:G:91:GLU:CD	2.04	0.60
5:I:36:DC:H2''	5:I:37:DG:C8	2.37	0.59
5:I:97:DA:H2'	5:I:98:DA:C8	2.38	0.59
7:K:279:ASP:OD1	7:K:280:LYS:N	2.35	0.59
7:K:483:ASP:OD1	7:K:483:ASP:N	2.34	0.58
5:I:23:DC:H1'	5:I:24:DC:H5'	1.85	0.58
7:K:319:GLU:HG2	7:K:346:ARG:HH21	1.69	0.58
3:G:76:THR:O	3:G:76:THR:OG1	2.21	0.58
6:J:89:DT:H2''	6:J:90:DA:C8	2.39	0.58
2:B:21:VAL:HG13	2:B:23:ARG:H	1.69	0.57
1:E:106:ASP:OD2	1:E:131:ARG:NH1	2.33	0.57
7:K:185:PHE:HE1	7:K:189:PRO:HD3	1.67	0.57
7:K:221:ASP:OD2	7:K:412:ARG:NH2	2.38	0.57
7:K:354:THR:HB	7:K:603:GLN:HG2	1.87	0.56
6:J:94:DG:H2''	6:J:95:DG:O5'	2.05	0.56
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.37	0.56
7:K:477:ASN:ND2	7:K:597:ASP:OD2	2.39	0.56
7:K:611:ARG:HH11	7:K:614:ARG:HH11	1.55	0.55
4:D:87:THR:OG1	4:D:90:GLU:OE2	2.21	0.55
7:K:220:ALA:O	7:K:411:ARG:HG2	2.07	0.55
7:K:239:ARG:HH11	7:K:240:TYR:HE1	1.53	0.55
2:F:89:ALA:O	2:F:93:GLN:HG2	2.07	0.54
7:K:411:ARG:HB2	7:K:655:ARG:HB3	1.89	0.54
5:I:82:DC:H2''	5:I:83:DG:C8	2.42	0.54
7:K:530:LEU:HD21	7:K:596:TYR:CD1	2.43	0.54
5:I:37:DG:H2''	5:I:38:DT:H71	1.88	0.53
5:I:123:DC:H2''	5:I:124:DA:C8	2.43	0.53
7:K:548:ILE:HG22	7:K:574:PHE:HE1	1.74	0.53
6:J:81:DC:H2''	6:J:82:DG:C8	2.43	0.53
1:A:50:GLU:HA	1:A:53:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:364:TRP:NE1	7:K:377:ASP:O	2.42	0.53
7:K:496:HIS:HA	7:K:499:TYR:CE2	2.44	0.53
7:K:196:LEU:HA	8:K:1201:ATP:HN62	1.74	0.53
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.91	0.52
5:I:68:DT:H2''	5:I:69:DA:C8	2.44	0.52
7:K:320:TYR:CE1	7:K:347:ASN:HB3	2.44	0.52
2:B:22:LEU:O	2:B:23:ARG:HG2	2.10	0.52
5:I:104:DT:H2'	5:I:105:DT:H71	1.92	0.52
7:K:328:ARG:HH11	7:K:328:ARG:HB3	1.74	0.52
3:G:91:GLU:OE1	3:G:91:GLU:N	2.29	0.52
7:K:413:ILE:HG23	7:K:415:SER:H	1.74	0.52
5:I:78:DC:H2''	5:I:79:DC:C5	2.44	0.52
5:I:109:DC:H2''	5:I:110:DC:C5	2.44	0.52
7:K:467:ASN:O	7:K:471:GLN:HG2	2.10	0.51
3:C:91:GLU:H	3:C:91:GLU:CD	2.13	0.51
7:K:538:CYS:HB3	7:K:543:TYR:HB2	1.91	0.51
4:D:83:ARG:HG3	4:D:83:ARG:HH11	1.74	0.51
5:I:88:DT:H2''	5:I:89:DT:C7	2.40	0.51
7:K:394:GLN:N	7:K:396:LYS:HZ2	2.08	0.51
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.46	0.51
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.92	0.51
7:K:186:ARG:HA	7:K:186:ARG:HH11	1.75	0.50
5:I:77:DT:H2''	5:I:78:DC:C6	2.47	0.50
7:K:189:PRO:HG2	7:K:196:LEU:HD21	1.93	0.50
7:K:303:TYR:OH	7:K:324:ASP:O	2.29	0.50
7:K:520:ARG:NH2	7:K:571:LYS:O	2.41	0.50
6:J:50:DT:H2'	6:J:51:DT:H71	1.92	0.50
5:I:140:DC:H2''	5:I:141:DA:C8	2.47	0.50
3:C:71:ARG:HG2	3:C:71:ARG:HH11	1.78	0.49
6:J:54:DC:H2''	6:J:55:DG:C8	2.47	0.49
7:K:651:ILE:HD12	7:K:651:ILE:H	1.77	0.49
7:K:223:MET:HE3	7:K:610:ASP:OD2	2.12	0.49
7:K:280:LYS:HB3	7:K:283:ARG:HH21	1.78	0.49
5:I:35:DT:H2''	5:I:36:DC:H5''	1.94	0.49
6:J:15:DT:H2''	6:J:16:DC:O5'	2.11	0.49
6:J:77:DC:H2''	6:J:78:DG:C8	2.47	0.49
7:K:337:SER:OG	7:K:341:ARG:NH1	2.45	0.49
5:I:26:DC:H2''	5:I:27:DT:C6	2.48	0.49
6:J:7:DT:H2''	6:J:8:DG:C8	2.48	0.49
6:J:3:DC:H2''	6:J:4:DG:C8	2.47	0.48
7:K:328:ARG:HB3	7:K:328:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:HD13	4:D:42:LEU:HB2	1.96	0.48
6:J:20:DC:H2''	6:J:21:DA:C8	2.49	0.48
5:I:46:DT:H2''	5:I:47:DC:C6	2.49	0.48
6:J:134:DC:H2''	6:J:135:DC:H5'	1.96	0.48
4:D:83:ARG:HG3	4:D:83:ARG:NH1	2.29	0.48
5:I:127:DT:H2''	5:I:128:DG:C8	2.49	0.48
6:J:1:DA:H1'	6:J:2:DT:H5'	1.95	0.48
7:K:261:LEU:HD22	7:K:275:ILE:HG13	1.96	0.48
6:J:123:DC:H2''	6:J:124:DG:C8	2.49	0.47
7:K:196:LEU:HD12	7:K:200:GLN:HB3	1.95	0.47
3:G:76:THR:HG23	6:J:131:DG:H3'	1.96	0.47
6:J:129:DC:H2''	6:J:130:DG:N7	2.29	0.47
7:K:645:ARG:HG2	7:K:649:LEU:HD23	1.96	0.47
6:J:111:DC:H2''	6:J:112:DG:C8	2.49	0.47
7:K:648:GLN:HA	7:K:652:GLN:HE21	1.79	0.47
7:K:371:LEU:HB3	7:K:374:ILE:HB	1.97	0.47
5:I:47:DC:H2''	5:I:48:DT:C7	2.45	0.46
7:K:385:PHE:HA	7:K:397:ILE:HD12	1.96	0.46
5:I:79:DC:H2''	5:I:80:DC:C5	2.50	0.46
7:K:639:ARG:HE	7:K:639:ARG:HB3	1.57	0.46
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.98	0.46
5:I:112:DT:H2''	5:I:113:DA:C8	2.51	0.46
7:K:647:ASP:OD1	7:K:648:GLN:N	2.48	0.46
4:H:105:LYS:NZ	4:H:105:LYS:HB3	2.31	0.46
7:K:396:LYS:HD3	7:K:396:LYS:N	2.29	0.46
1:A:48:LEU:HD11	2:B:44:LYS:HD2	1.98	0.46
7:K:426:GLU:H	7:K:426:GLU:HG2	1.63	0.46
7:K:508:ASP:OD1	7:K:537:TYR:OH	2.31	0.46
2:B:16:LYS:NZ	2:B:16:LYS:H	2.14	0.46
2:F:91:LYS:HB2	2:F:91:LYS:HE2	1.68	0.46
5:I:88:DT:H2''	5:I:89:DT:H71	1.97	0.45
7:K:199:TYR:HB2	7:K:412:ARG:NH1	2.32	0.45
5:I:142:DT:H2''	5:I:143:DC:C5	2.52	0.45
7:K:611:ARG:HH11	7:K:614:ARG:NH1	2.13	0.45
6:J:56:DG:H4'	7:K:304:GLU:HG3	1.99	0.45
7:K:520:ARG:NH1	7:K:589:SER:OG	2.50	0.45
7:K:492:THR:HG23	7:K:496:HIS:CE1	2.51	0.45
7:K:648:GLN:HE21	7:K:649:LEU:HD22	1.77	0.45
7:K:186:ARG:HB3	7:K:187:GLU:CD	2.37	0.44
2:B:16:LYS:NZ	7:K:536:ASP:OD1	2.43	0.44
7:K:599:ASP:OD1	7:K:600:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:648:GLN:HE22	7:K:649:LEU:HD22	1.81	0.44
5:I:20:DA:H2''	5:I:21:DG:H8	1.82	0.44
5:I:88:DT:H2''	5:I:89:DT:C5	2.52	0.44
7:K:425:LYS:HE3	7:K:620:GLN:HE21	1.82	0.44
7:K:257:LEU:HD22	7:K:300:ILE:HG22	1.99	0.44
4:H:48:ASP:OD1	4:H:48:ASP:N	2.51	0.44
5:I:37:DG:H2''	5:I:38:DT:C7	2.47	0.44
7:K:399:LYS:HD2	7:K:399:LYS:N	2.33	0.44
4:H:83:ARG:HA	4:H:83:ARG:HD3	1.71	0.44
6:J:132:DC:H2''	6:J:133:DA:C8	2.53	0.44
7:K:399:LYS:HD2	7:K:399:LYS:H	1.83	0.44
3:C:15:LYS:NZ	3:C:15:LYS:HB3	2.32	0.43
6:J:119:DT:H2''	6:J:120:DG:C8	2.52	0.43
7:K:564:TYR:O	7:K:569:SER:OG	2.33	0.43
7:K:350:LEU:HD13	7:K:370:LEU:HD21	2.00	0.43
7:K:422:LEU:HD12	7:K:422:LEU:HA	1.74	0.43
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.27	0.43
6:J:129:DC:H2''	6:J:130:DG:C8	2.53	0.43
7:K:238:LEU:HD12	7:K:238:LEU:HA	1.85	0.43
1:A:48:LEU:CD1	2:B:44:LYS:HD2	2.49	0.43
6:J:78:DG:H2''	6:J:79:DT:C6	2.54	0.43
7:K:196:LEU:HA	8:K:1201:ATP:N6	2.34	0.43
7:K:425:LYS:CE	7:K:620:GLN:HE21	2.31	0.43
7:K:210:LEU:HD13	7:K:215:ILE:HG13	1.99	0.43
5:I:80:DC:H2''	5:I:81:DC:C5	2.54	0.43
6:J:94:DG:H4'	6:J:95:DG:OP1	2.19	0.42
7:K:216:ALA:HB1	7:K:370:LEU:HD22	2.00	0.42
7:K:612:ALA:O	7:K:617:GLN:NE2	2.52	0.42
4:D:33:SER:OG	4:D:34:TYR:N	2.52	0.42
6:J:9:DT:H2''	6:J:10:DA:C8	2.54	0.42
4:H:87:THR:OG1	4:H:90:GLU:OE2	2.31	0.42
6:J:27:DC:H2''	6:J:28:DT:C5	2.54	0.42
7:K:396:LYS:O	7:K:400:GLN:HG3	2.20	0.42
5:I:99:DG:H2''	5:I:100:DG:N7	2.35	0.42
6:J:108:DC:H2''	6:J:109:DT:C6	2.55	0.42
7:K:197:ARG:HB2	7:K:199:TYR:CE1	2.54	0.42
2:B:20:LYS:HD2	2:B:20:LYS:HA	1.89	0.42
5:I:20:DA:H2''	5:I:21:DG:C8	2.55	0.42
5:I:110:DC:H2''	5:I:111:DC:C5	2.54	0.42
2:F:24:ASP:OD1	2:F:26:ILE:HG22	2.20	0.41
3:G:68:ASN:OD1	3:G:71:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.01	0.41
2:F:31:LYS:HD2	2:F:51:TYR:CE2	2.55	0.41
7:K:572:PHE:CD2	7:K:573:VAL:HG13	2.55	0.41
7:K:248:PHE:HB2	7:K:298:VAL:HG22	2.02	0.41
1:E:126:LEU:O	1:E:130:ILE:HG12	2.20	0.41
4:H:99:LEU:HA	4:H:100:PRO:HD3	1.89	0.41
7:K:247:PRO:HB2	7:K:318:TRP:CE3	2.56	0.41
7:K:363:LEU:HD12	7:K:363:LEU:HA	1.82	0.41
5:I:67:DG:H2''	5:I:68:DT:C7	2.49	0.41
7:K:642:GLN:O	7:K:645:ARG:NH1	2.54	0.41
2:B:80:THR:HG22	5:I:102:DG:OP1	2.20	0.41
2:B:23:ARG:O	2:B:24:ASP:OD1	2.40	0.40
6:J:54:DC:H2''	6:J:55:DG:H8	1.85	0.40
7:K:370:LEU:HB3	7:K:371:LEU:HD22	2.03	0.40
7:K:445:LEU:HA	7:K:445:LEU:HD23	1.89	0.40
4:D:43:LYS:HD3	4:D:43:LYS:HA	1.89	0.40
3:G:90:ASP:OD1	3:G:93:LEU:HB2	2.21	0.40
7:K:292:LEU:HD23	7:K:292:LEU:HA	1.86	0.40
7:K:544:GLU:OE1	7:K:544:GLU:N	2.54	0.40
3:G:13:LYS:HB3	3:G:13:LYS:NZ	2.36	0.40
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.90	0.40
7:K:397:ILE:HG22	7:K:401:LEU:HD23	2.03	0.40
4:D:48:ASP:OD1	4:D:48:ASP:N	2.52	0.40
6:J:4:DG:C8	6:J:4:DG:H5'	2.57	0.40
6:J:26:DC:H6	6:J:26:DC:H2'	1.77	0.40
7:K:213:ASN:OD1	7:K:213:ASN:N	2.55	0.40
7:K:356:LEU:HD22	7:K:651:ILE:HD13	2.01	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	
1	A	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
1	E	93/135 (69%)	90 (97%)	3 (3%)	0	100	100
2	B	85/102 (83%)	81 (95%)	4 (5%)	0	100	100
2	F	84/102 (82%)	83 (99%)	1 (1%)	0	100	100
3	C	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
3	G	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
4	D	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
4	H	91/122 (75%)	90 (99%)	1 (1%)	0	100	100
7	K	449/1061 (42%)	420 (94%)	29 (6%)	0	100	100
All	All	1199/2037 (59%)	1154 (96%)	45 (4%)	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%)	83 (99%)	1 (1%)	67	81
1	E	82/110 (74%)	79 (96%)	3 (4%)	29	43
2	B	72/78 (92%)	70 (97%)	2 (3%)	38	55
2	F	67/78 (86%)	66 (98%)	1 (2%)	60	76
3	C	81/101 (80%)	78 (96%)	3 (4%)	29	43
3	G	82/101 (81%)	80 (98%)	2 (2%)	44	61
4	D	77/102 (76%)	73 (95%)	4 (5%)	19	28
4	H	79/102 (78%)	75 (95%)	4 (5%)	20	29
7	K	413/958 (43%)	392 (95%)	21 (5%)	20	29
All	All	1037/1740 (60%)	996 (96%)	41 (4%)	29	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
2	B	80	THR
2	B	93	GLN
3	C	35	ARG
3	C	74	LYS
3	C	91	GLU
4	D	48	ASP
4	D	82	LYS
4	D	113	LYS
4	D	117	LYS
1	E	76	GLN
1	E	87	SER
1	E	115	LYS
2	F	77	LYS
3	G	75	LYS
3	G	76	THR
4	H	30	ARG
4	H	31	LYS
4	H	53	SER
4	H	120	SER
7	K	183	PHE
7	K	185	PHE
7	K	186	ARG
7	K	195	GLN
7	K	210	LEU
7	K	223	MET
7	K	320	TYR
7	K	380	ASP
7	K	396	LYS
7	K	412	ARG
7	K	422	LEU
7	K	462	LYS
7	K	492	THR
7	K	496	HIS
7	K	540	PHE
7	K	542	ASN
7	K	570	LYS
7	K	574	PHE
7	K	645	ARG
7	K	647	ASP
7	K	648	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
7	K	642	GLN
7	K	648	GLN
7	K	652	GLN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ATP	K	1201	9	26,33,33	0.92	1 (3%)	31,52,52	1.63	5 (16%)

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
8	ATP	K	1201	9	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1201	ATP	C5-C4	2.12	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1201	ATP	PA-O3A-PB	-4.43	117.61	132.83
8	K	1201	ATP	N3-C2-N1	-3.26	123.59	128.68
8	K	1201	ATP	PB-O3B-PG	-3.11	122.17	132.83
8	K	1201	ATP	C3'-C2'-C1'	2.82	105.22	100.98
8	K	1201	ATP	C4-C5-N7	-2.52	106.77	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

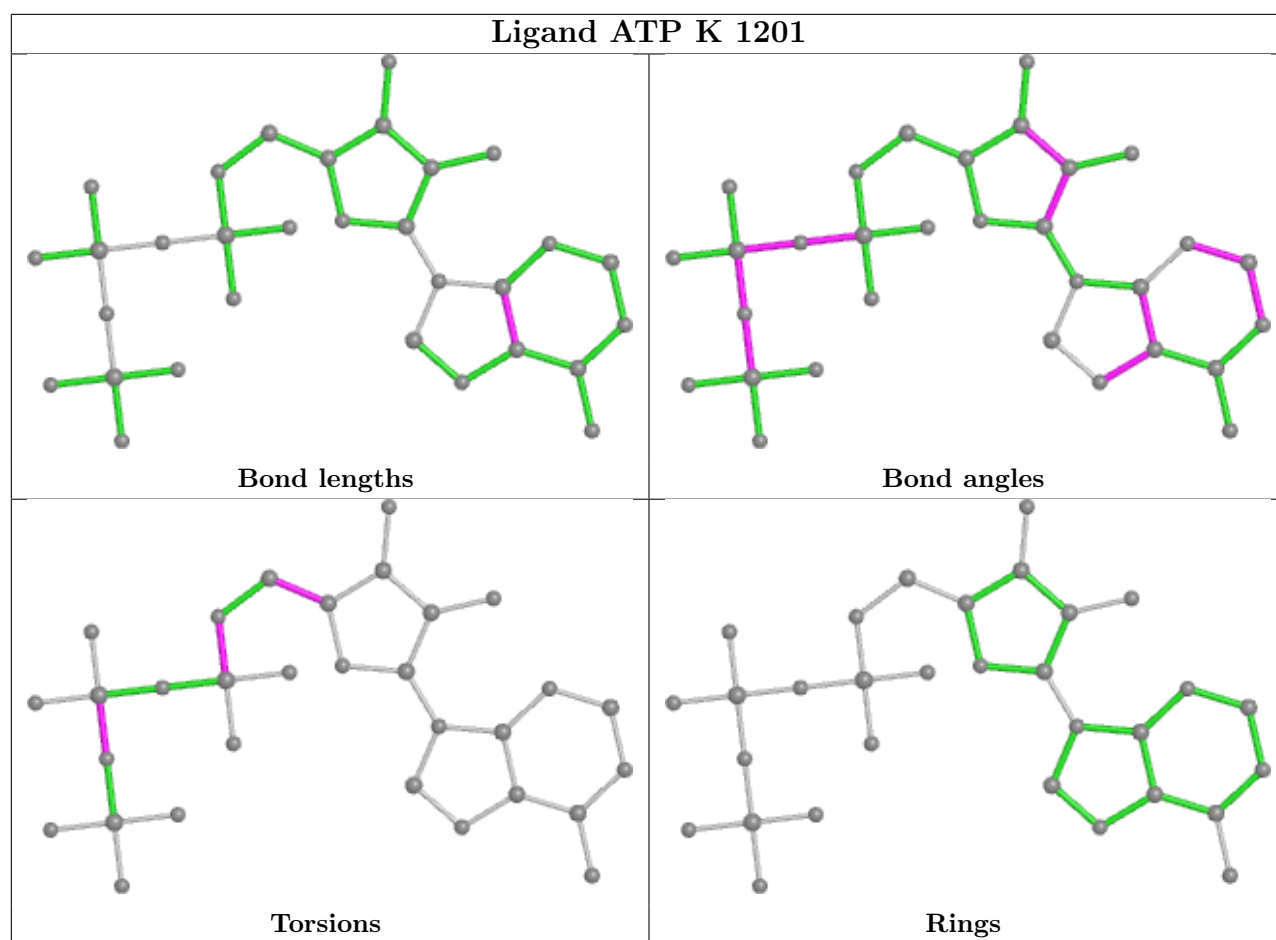
Mol	Chain	Res	Type	Atoms
8	K	1201	ATP	C5'-O5'-PA-O2A
8	K	1201	ATP	C5'-O5'-PA-O3A
8	K	1201	ATP	PG-O3B-PB-O2B
8	K	1201	ATP	C3'-C4'-C5'-O5'
8	K	1201	ATP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1201	ATP	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

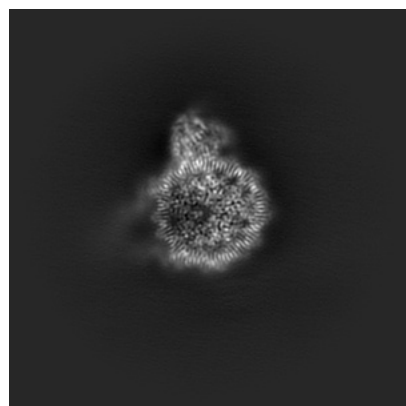
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61624. These allow visual inspection of the internal detail of the map and identification of artifacts.

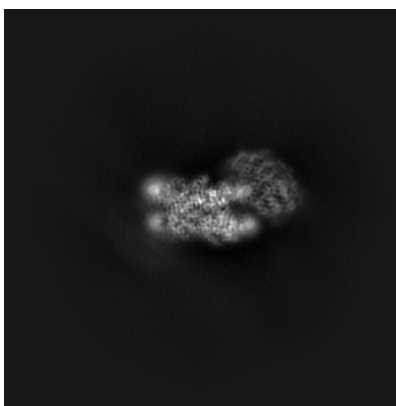
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

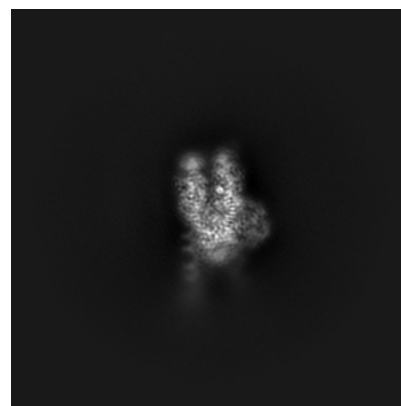
6.1.1 Primary map



X

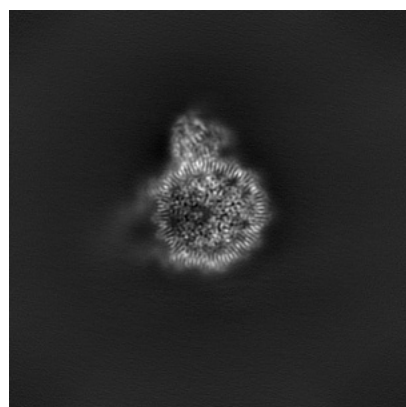


Y

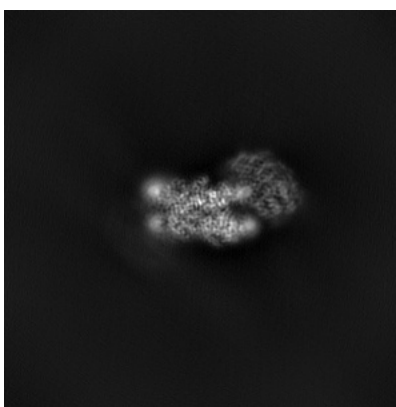


Z

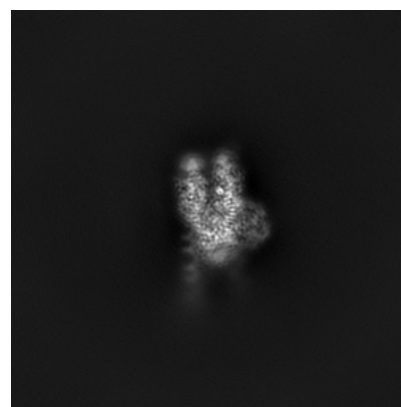
6.1.2 Raw map



X



Y

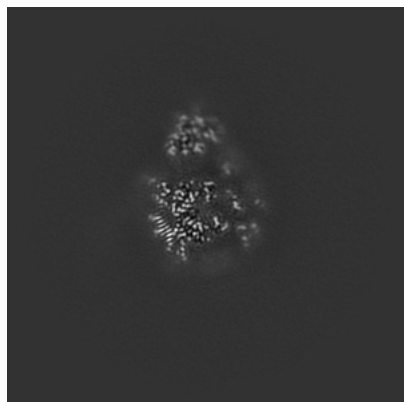


Z

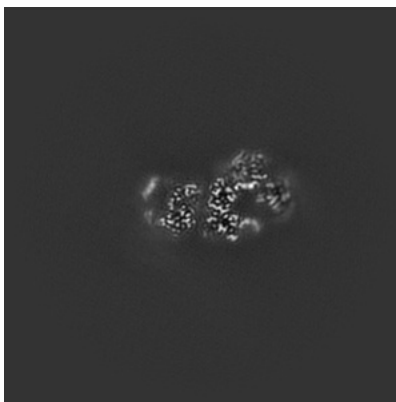
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

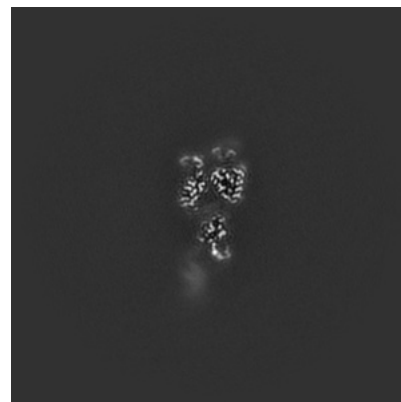
6.2.1 Primary map



X Index: 160

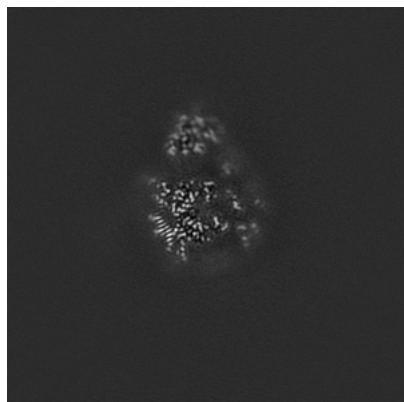


Y Index: 160

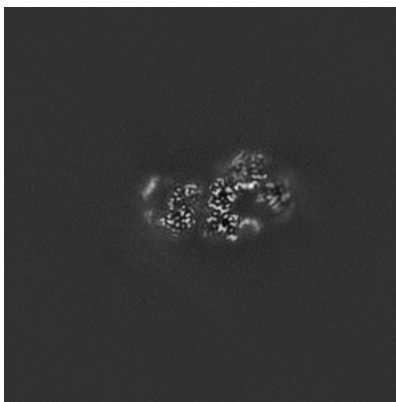


Z Index: 160

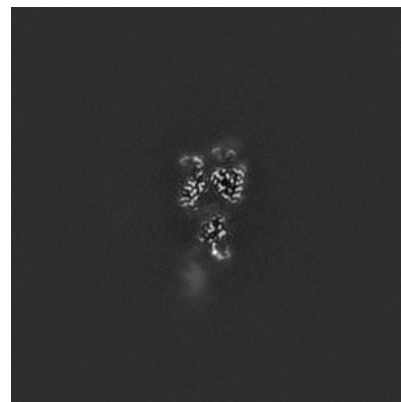
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

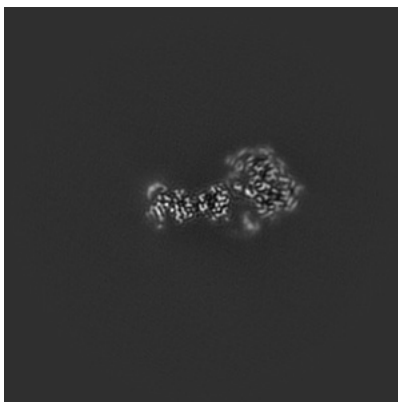
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

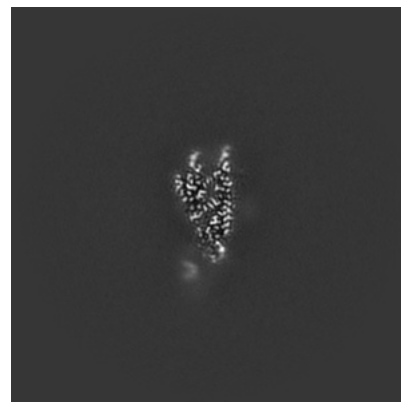
6.3.1 Primary map



X Index: 172

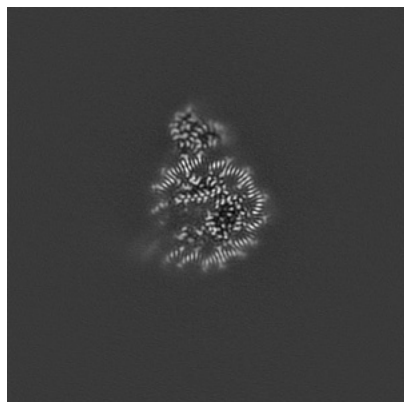


Y Index: 141

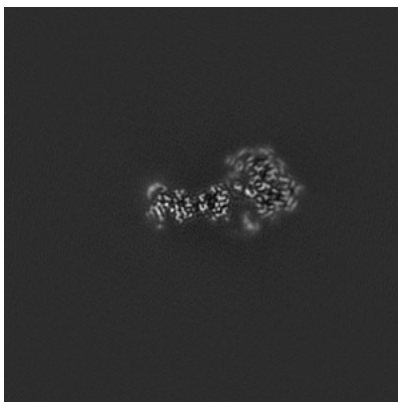


Z Index: 168

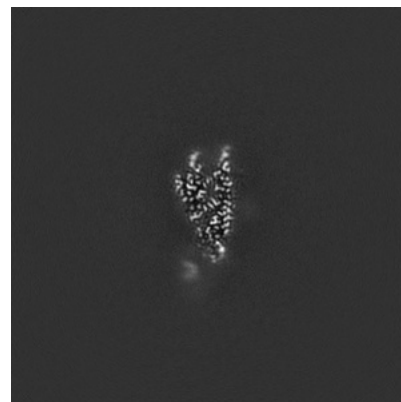
6.3.2 Raw map



X Index: 172



Y Index: 141

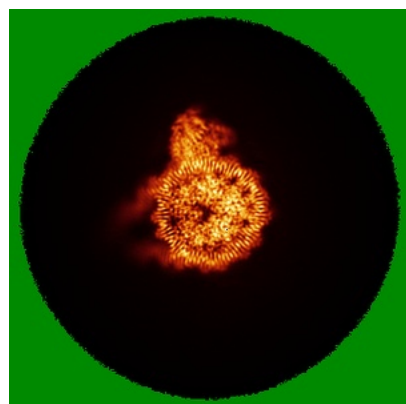


Z Index: 168

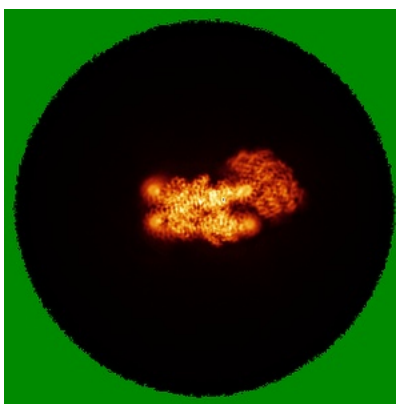
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X

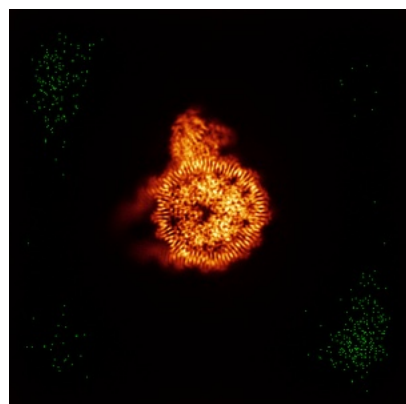


Y

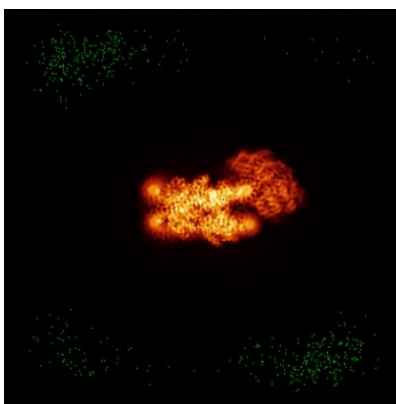


Z

6.4.2 Raw map



X



Y

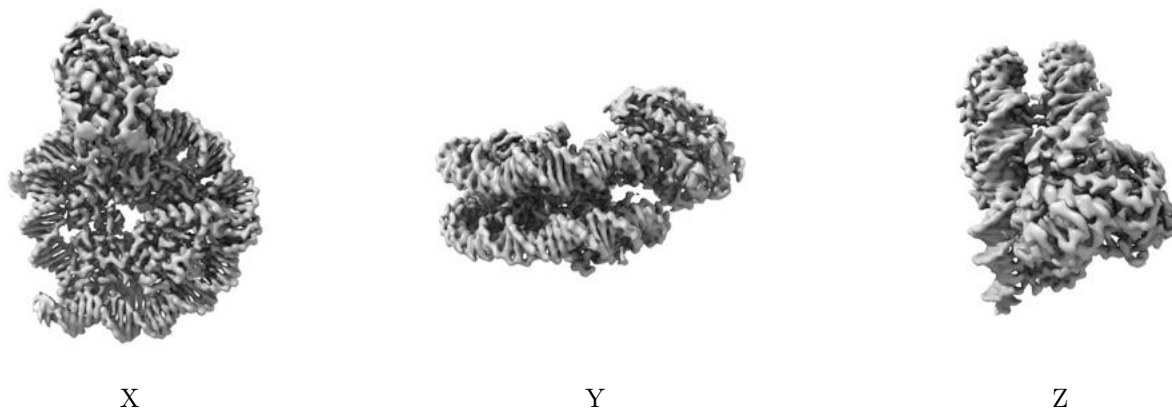


Z

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.

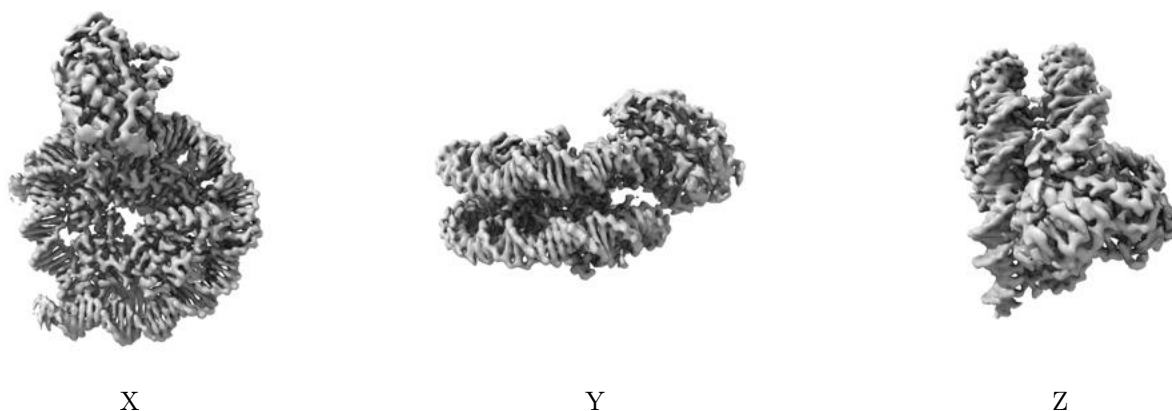
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

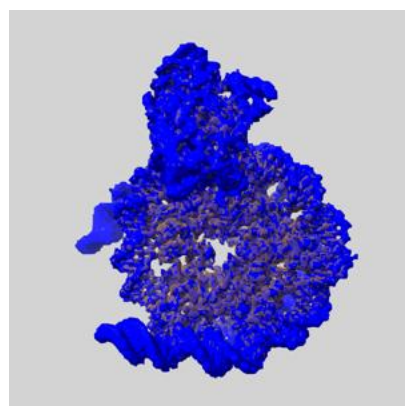
6.6 Mask visualisation [i](#)

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

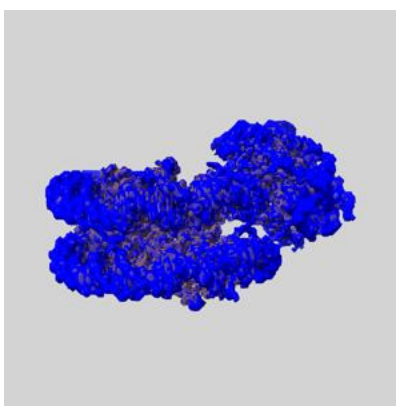
A mask typically either:

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

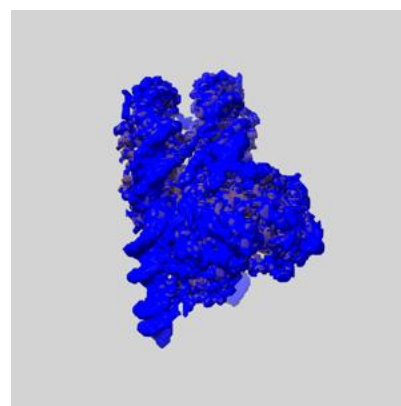
6.6.1 emd_61624_msk_1.map [i](#)



X



Y

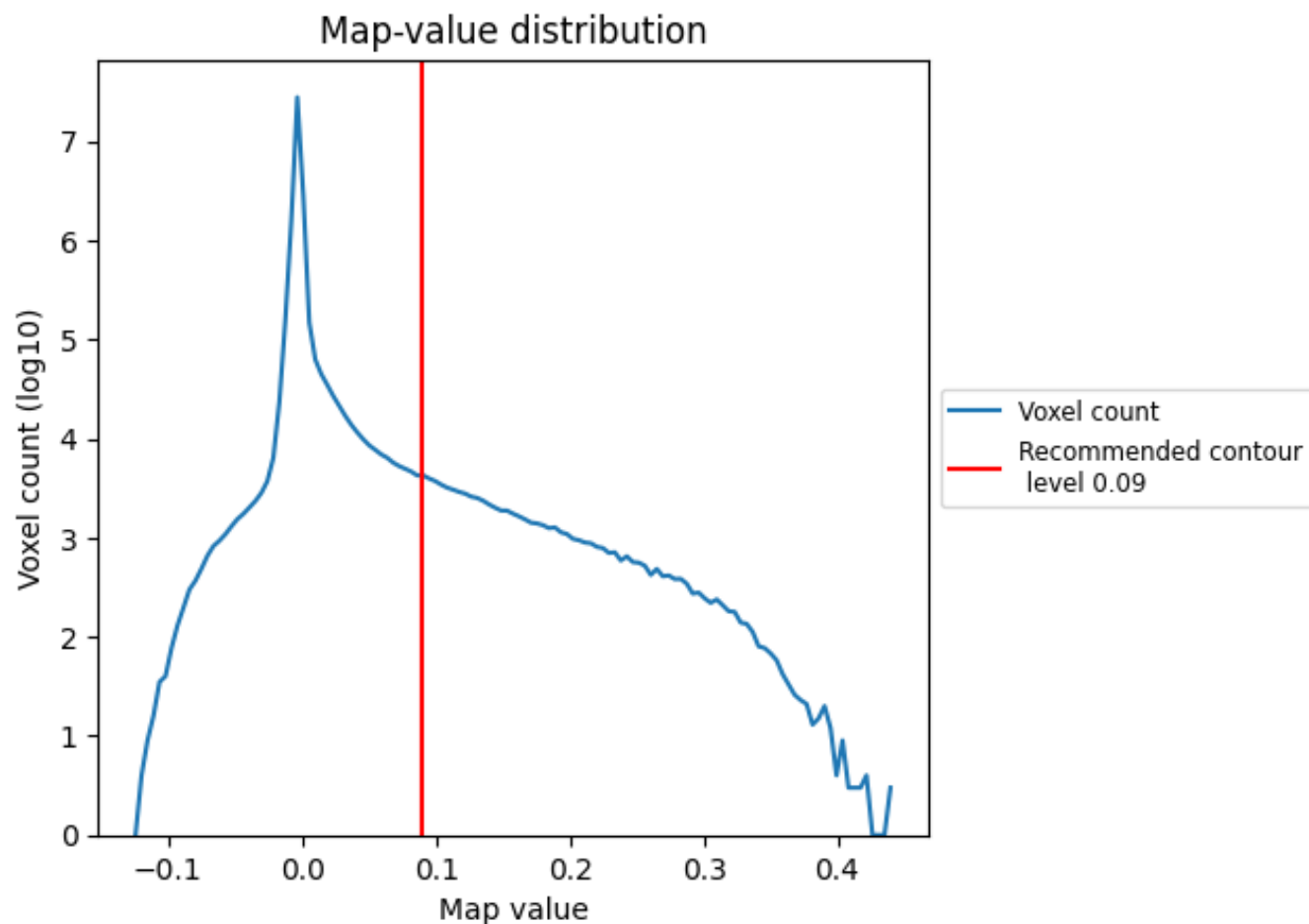


Z

7 Map analysis [i](#)

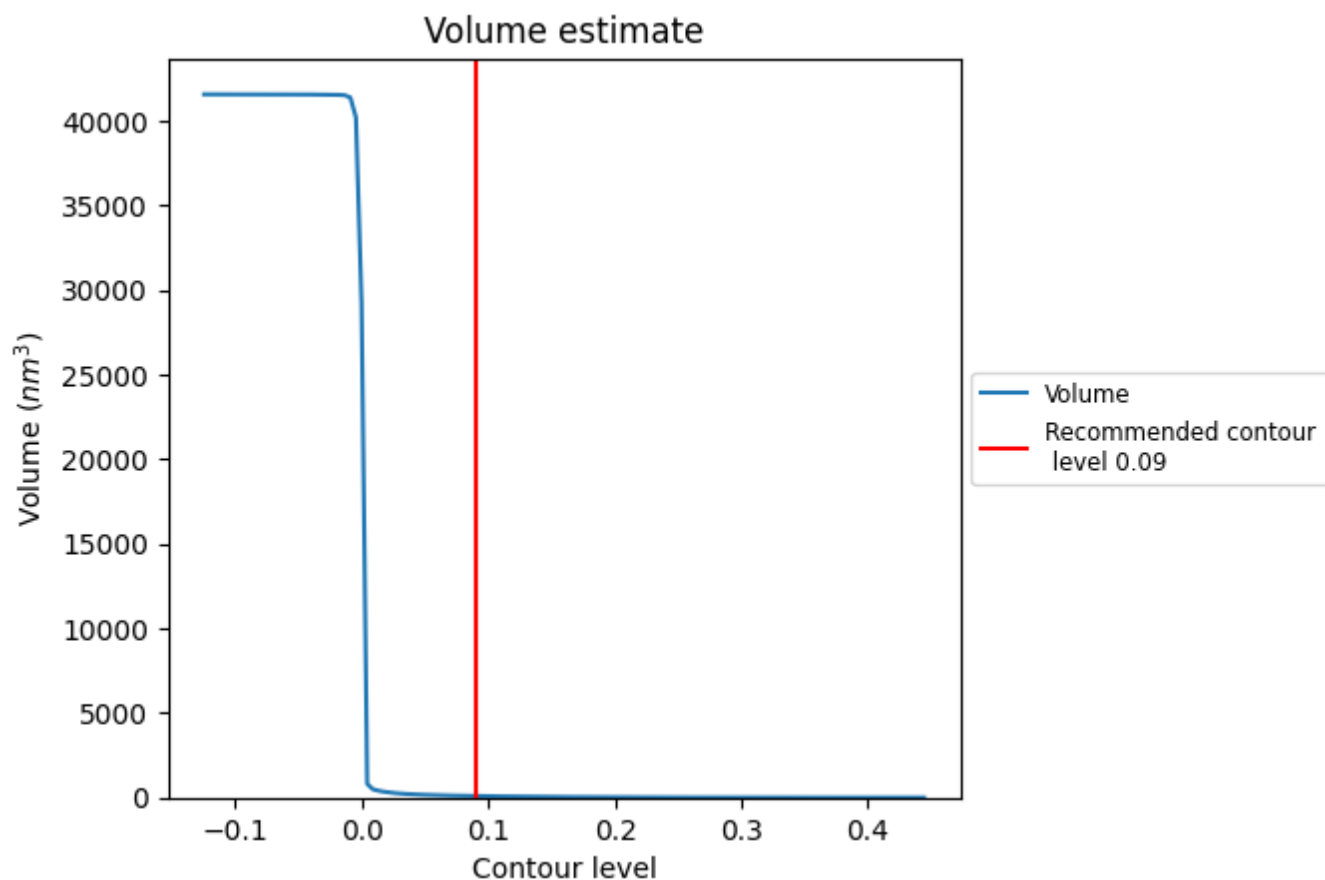
This section contains the results of statistical analysis of the map.

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.

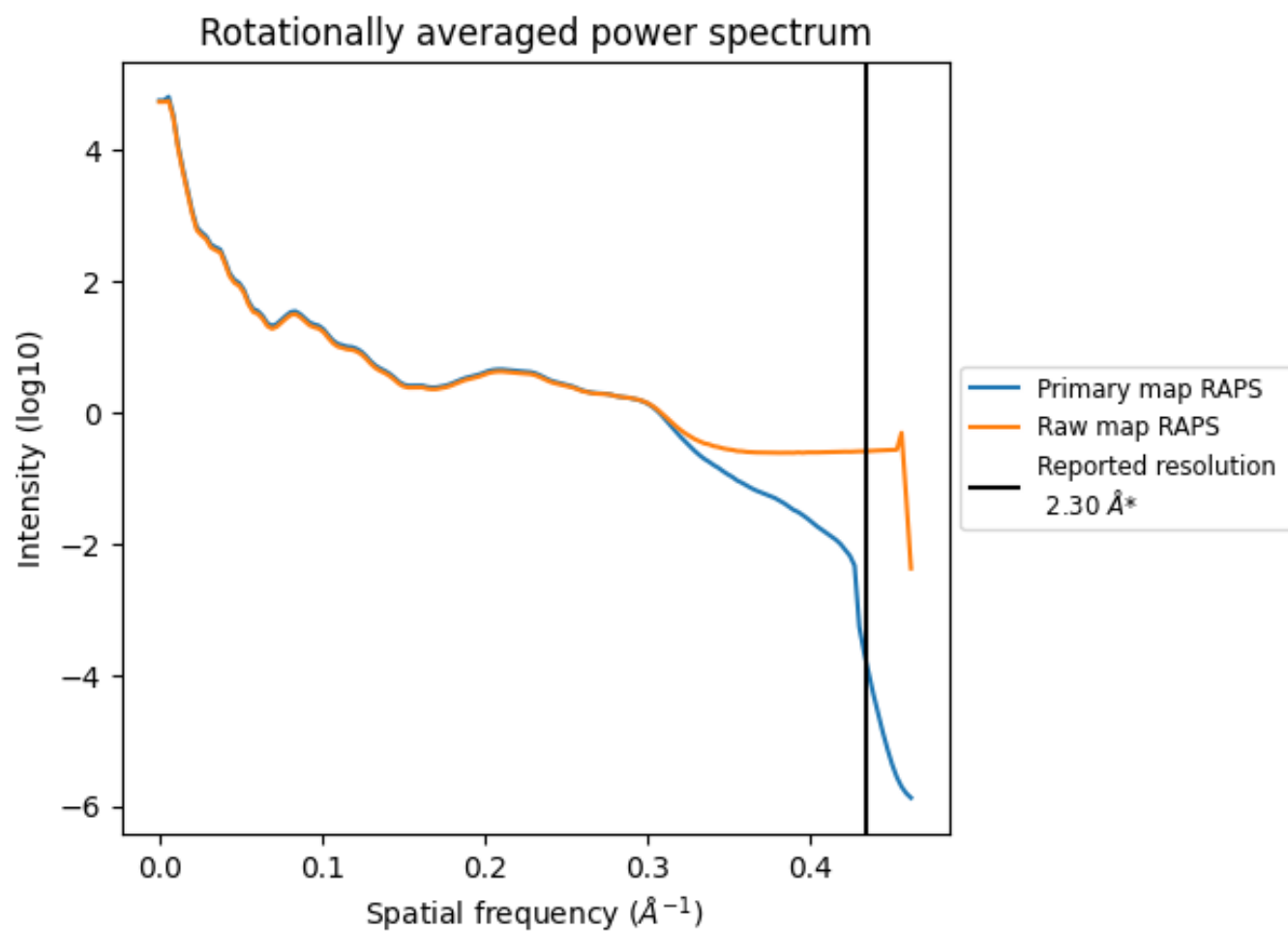
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 83 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 ⓘ

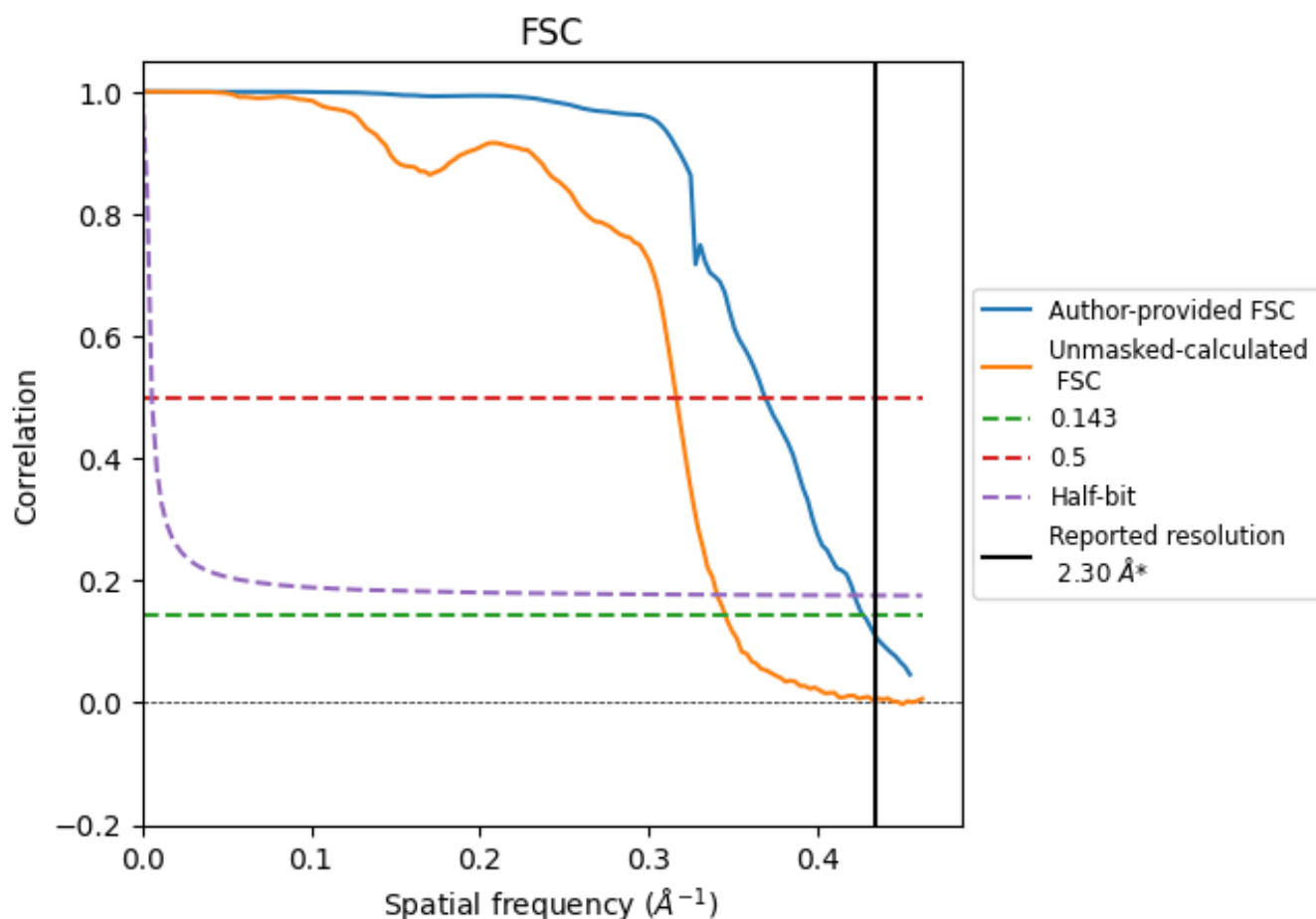


*Reported resolution corresponds to spatial frequency of 0.435 \AA^{-1}

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 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

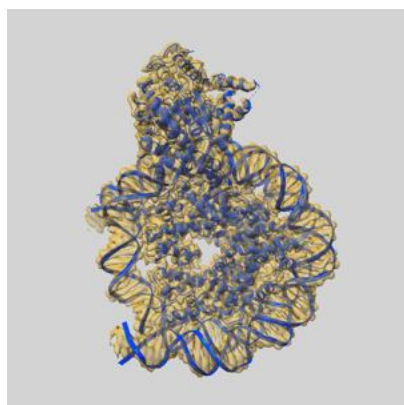
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.34	2.71	2.37
Unmasked-calculated*	2.90	3.16	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.90 differs from the reported value 2.3 by more than 10 %

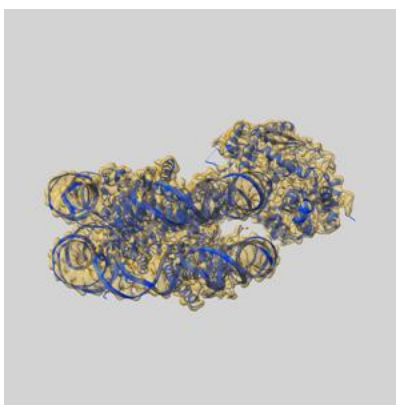
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61624 and PDB model 9JNP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

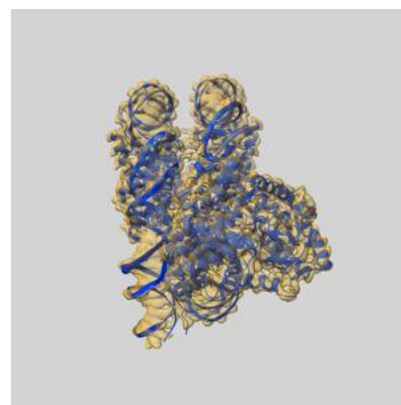
9.1 Map-model overlay [i](#)



X



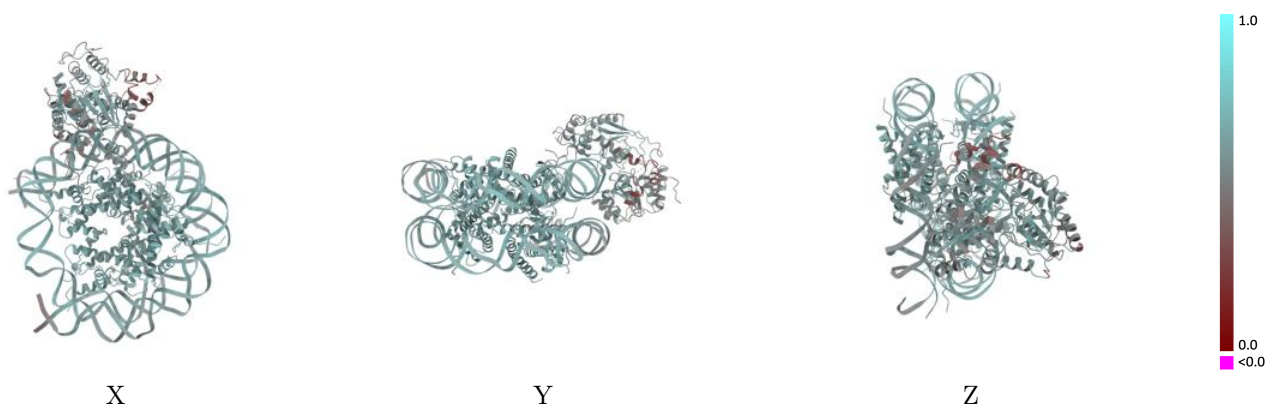
Y



Z

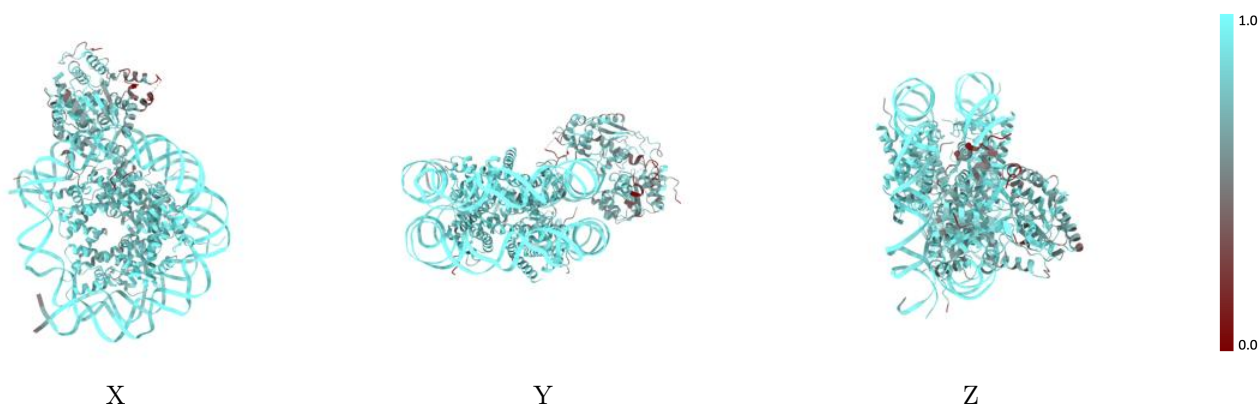
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



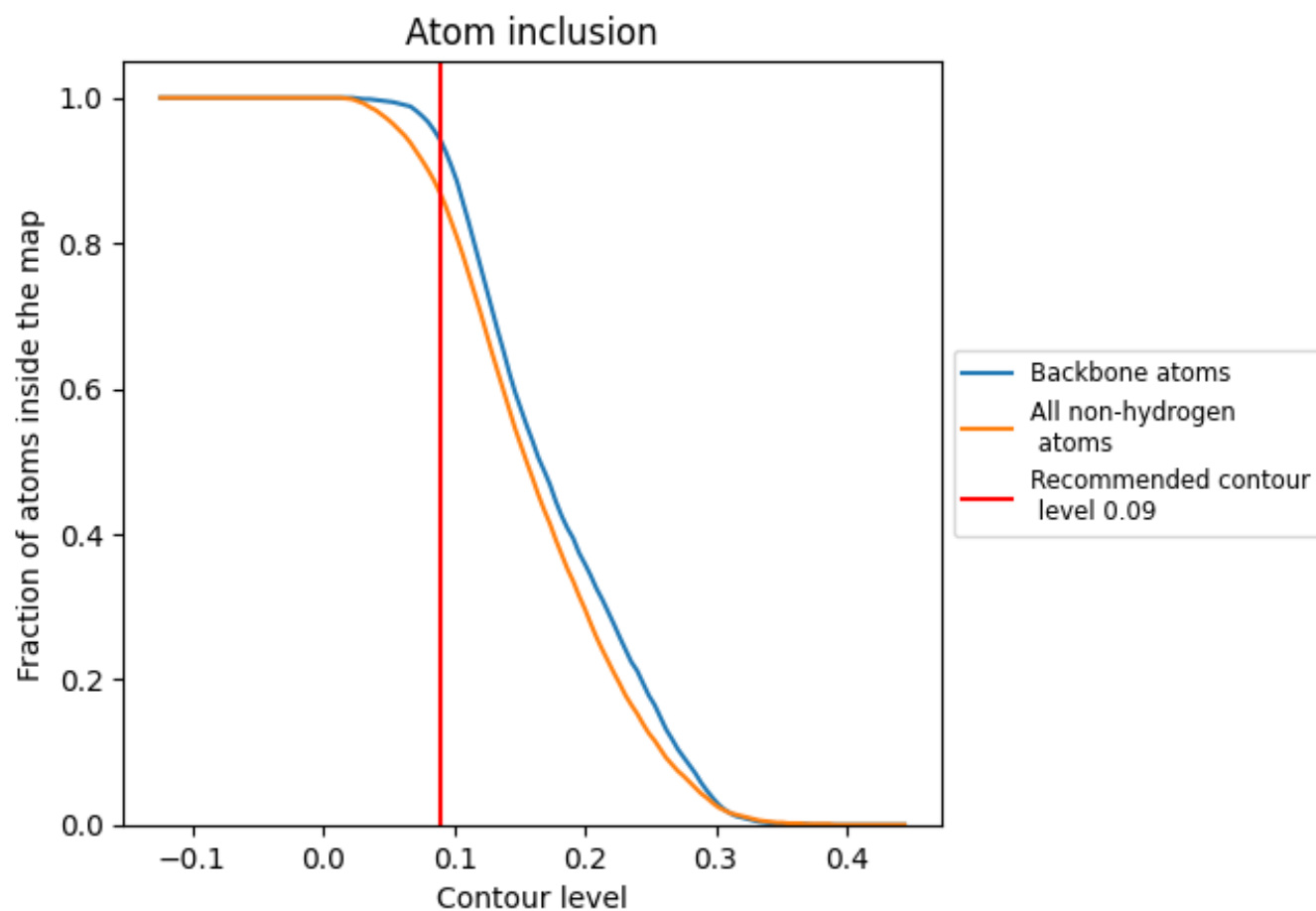
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8660</div>	<div><div></div>0.5870</div>
A	<div><div></div>0.8960</div>	<div><div></div>0.6280</div>
B	<div><div></div>0.8800</div>	<div><div></div>0.6080</div>
C	<div><div></div>0.9170</div>	<div><div></div>0.6320</div>
D	<div><div></div>0.9240</div>	<div><div></div>0.6210</div>
E	<div><div></div>0.9110</div>	<div><div></div>0.6300</div>
F	<div><div></div>0.8640</div>	<div><div></div>0.6130</div>
G	<div><div></div>0.9060</div>	<div><div></div>0.6270</div>
H	<div><div></div>0.9050</div>	<div><div></div>0.6210</div>
I	<div><div></div>0.9410</div>	<div><div></div>0.5940</div>
J	<div><div></div>0.9290</div>	<div><div></div>0.5940</div>
K	<div><div></div>0.6970</div>	<div><div></div>0.5170</div>

1.0

0.0

<0.0