



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:01 AM UTC

PDB ID : 8V6V / pdb_00008v6v
EMDB ID : EMD-43002
Title : Cryo-EM structure of doubly-bound SNF2h-nucleosome complex
Authors : Chio, U.S.; Palovcak, E.; Armache, J.P.; Narlikar, G.J.; Cheng, Y.
Deposited on : 2023-12-03
Resolution : 2.80 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:

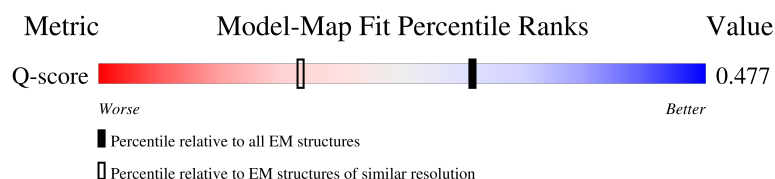
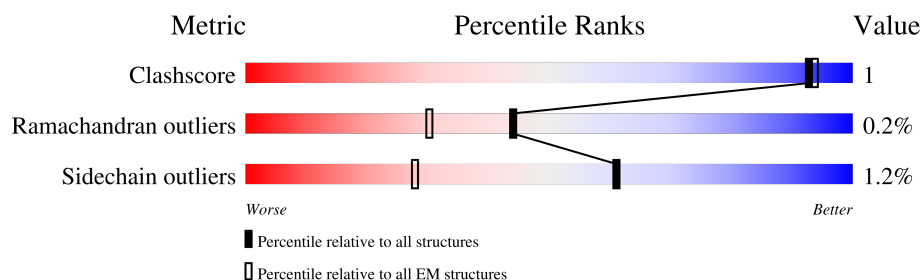
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.



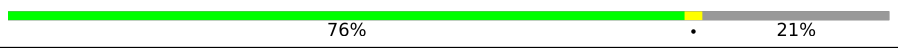
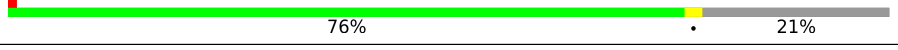
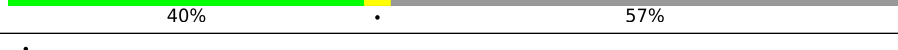
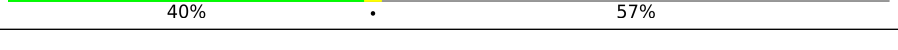
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	

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Mol	Chain	Length	Quality of chain
3	C	129	 81%16%
3	G	129	 82%16%
4	D	122	 76%21%
4	H	122	 76%21%
5	I	207	 67%29%
6	J	207	 65%6%29%
7	W	1052	 40%57%
7	X	1052	 40%57%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 37028 atoms, of which 17386 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 H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	95	Total	C	H	N	O	S	0	0
			1604	495	821	150	136	2		
1	E	95	Total	C	H	N	O	S	0	0
			1604	495	821	150	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
A	110	ALA	CYS	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233
E	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	88	Total	C	H	N	O	S	0	0
			1468	445	761	143	118	1		
2	F	88	Total	C	H	N	O	S	0	0
			1468	445	761	143	118	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	108	Total	C	H	N	O		0	0
			1730	525	896	165	144			
3	G	109	Total	C	H	N	O		0	0
			1752	531	909	167	145			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
C	123	SER	ALA	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897
G	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	96	Total	C	H	N	O	S	0	0
			1542	475	787	138	140	2		
4	H	96	Total	C	H	N	O	S	0	0
			1542	475	787	138	140	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called Widom 601 DNA (147-mer) with 60 base pairs flanking DNA (reverse strand).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	147	Total	C	H	N	O	P	0	0
			4681	1434	1650	570	880	147		

- Molecule 6 is a DNA chain called Widom 601 DNA (147-mer) with 60 base pairs flanking DNA (forward strand).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	147	Total	C	H	N	O	P	0	0
			4647	1423	1651	542	884	147		

- Molecule 7 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	W	449	Total	C	H	N	O	S	0	0
			7455	2368	3759	646	658	24		
7	X	449	Total	C	H	N	O	S	0	0
			7455	2368	3759	646	658	24		

- # ADP

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

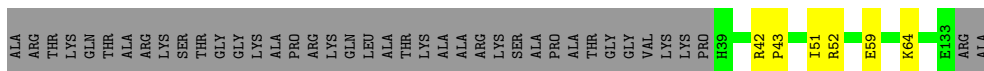
Mol	Chain	Residues	Atoms	AltConf
9	W	1	Total Mg 1 1	0
9	X	1	Total Mg 1 1	0

3 Residue-property plots

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

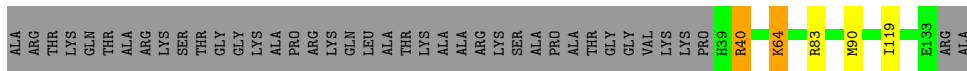
- Molecule 1: Histone H3.2

Chain A: 



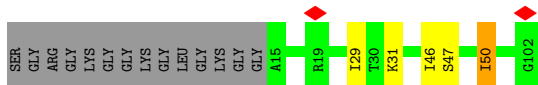
- Molecule 1: Histone H3.2

Chain E: 



- Molecule 2: Histone H4

Chain B: 



- Molecule 2: Histone H4

Chain F: 



- Molecule 3: Histone H2A type 1

Chain C: 



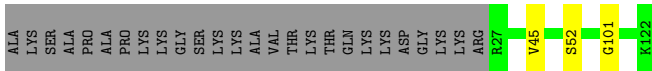
- Molecule 3: Histone H2A type 1

Chain G:  82% 16%

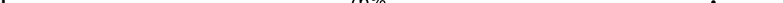


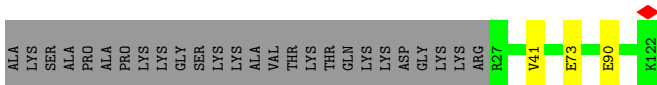
- Molecule 4: Histone H2B

Chain D: 76% . 21%



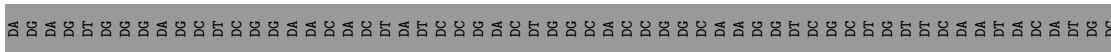
- Molecule 4: Histone H2B

Chain H:  76% 21%

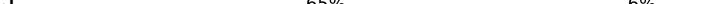


- Molecule 5: Widom 601 DNA (147-mer) with 60 base pairs flanking DNA (reverse strand)

Chain I: 67% . 29%

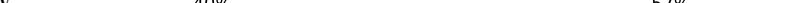


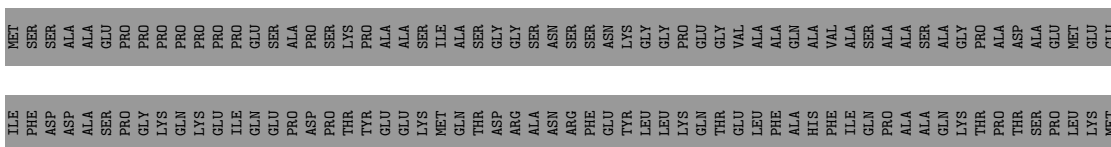
- Molecule 6: Widom 601 DNA (147-mer) with 60 base pairs flanking DNA (forward strand)

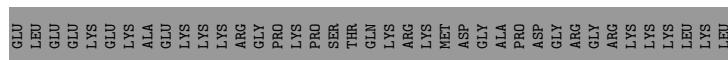
Chain J: 



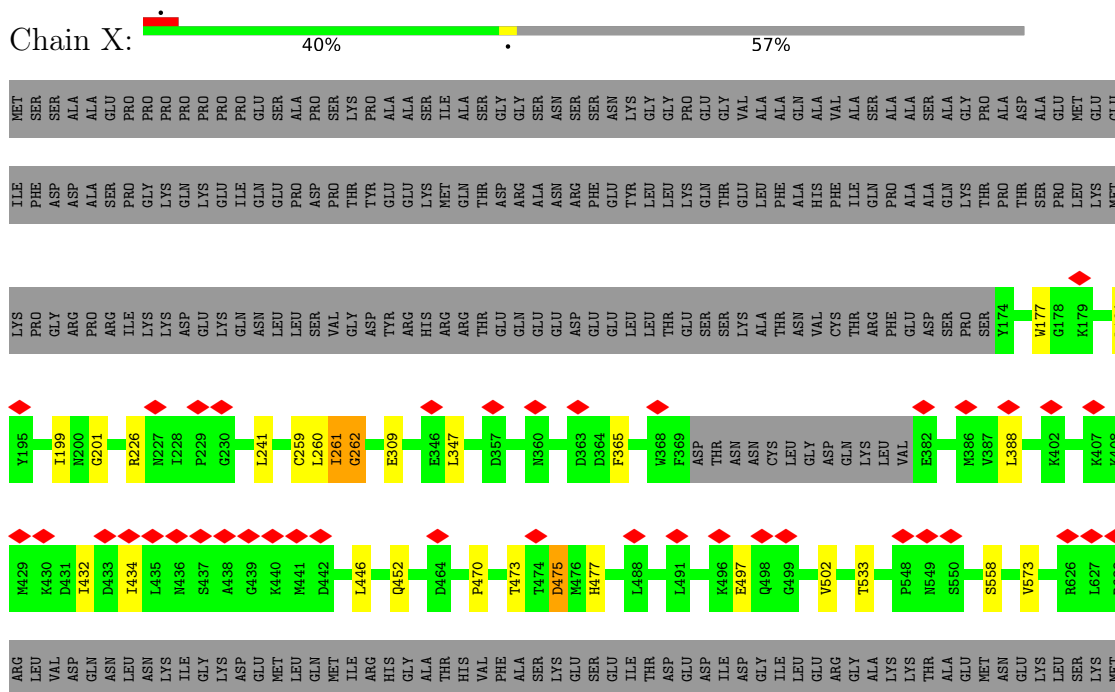
- Molecule 7: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5

Chain W:  40% 57%





- Molecule 7: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC Patch CTF estimation	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.094	Depositor
Minimum map value	-0.715	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	325.1712, 325.1712, 325.1712	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8468, 0.8468, 0.8468	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.33	0/794	1.23	4/1066 (0.4%)
1	E	1.01	0/794	1.12	3/1066 (0.3%)
2	B	1.09	4/715 (0.6%)	1.12	1/955 (0.1%)
2	F	1.05	2/715 (0.3%)	1.16	2/955 (0.2%)
3	C	1.05	0/844	1.12	2/1138 (0.2%)
3	G	1.00	0/853	1.18	2/1149 (0.2%)
4	D	1.04	0/766	1.20	2/1029 (0.2%)
4	H	0.96	0/766	1.20	1/1029 (0.1%)
5	I	0.26	0/3404	0.51	1/5256 (0.0%)
6	J	0.24	0/3356	0.49	0/5173
7	W	0.82	0/3776	1.12	16/5101 (0.3%)
7	X	0.83	0/3776	1.11	16/5101 (0.3%)
All	All	0.79	6/20559 (0.0%)	0.96	50/29018 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	50	ILE	C-O	-5.89	1.17	1.24
2	B	31	LYS	C-O	-5.63	1.19	1.24
2	F	38	ALA	C-O	-5.53	1.17	1.24
2	B	47	SER	CA-C	-5.48	1.45	1.53
2	B	46	ILE	C-O	-5.40	1.18	1.24
2	F	46	ILE	C-O	-5.09	1.18	1.24

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	502	VAL	N-CA-C	9.42	122.05	108.48
7	W	502	VAL	N-CA-C	9.41	122.03	108.48
7	X	177	TRP	N-CA-C	8.33	121.28	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101	GLY	N-CA-C	8.10	122.44	112.73
7	W	177	TRP	N-CA-C	7.99	122.12	112.38
1	E	83	ARG	N-CA-C	-7.80	98.72	109.95
7	W	201	GLY	N-CA-C	7.55	124.69	112.61
7	X	201	GLY	N-CA-C	7.50	124.61	112.61
7	W	388	LEU	N-CA-C	7.47	119.50	111.36
7	X	388	LEU	N-CA-C	7.46	119.49	111.36
7	X	558	SER	N-CA-C	-6.69	101.52	110.55
1	A	59	GLU	N-CA-C	6.64	119.29	110.53
7	W	347	LEU	N-CA-C	-6.56	104.92	113.12
1	E	64	LYS	N-CA-C	6.51	118.46	111.36
3	G	113	SER	N-CA-C	6.51	118.37	111.28
3	G	105	GLY	N-CA-C	-6.27	101.11	110.71
1	A	64	LYS	N-CA-C	6.23	120.08	112.23
1	A	51	ILE	N-CA-C	-6.14	104.36	110.62
1	A	52	ARG	N-CA-C	6.11	118.02	111.36
7	W	262	GLY	N-CA-C	6.04	119.10	111.85
7	X	262	GLY	N-CA-C	6.02	119.08	111.85
7	W	179	LYS	N-CA-C	5.97	118.68	109.07
3	C	86	ALA	N-CA-C	5.87	117.48	111.14
4	H	41	VAL	N-CA-C	-5.81	105.42	111.58
7	X	259	CYS	N-CA-C	5.69	117.68	108.34
7	W	259	CYS	N-CA-C	5.68	117.66	108.34
4	D	45	VAL	N-CA-C	5.63	116.28	110.82
1	E	40	ARG	N-CA-C	5.62	122.77	110.80
7	W	309	GLU	N-CA-C	-5.59	103.68	111.39
7	X	533	THR	N-CA-C	5.58	116.73	109.64
7	W	533	THR	N-CA-C	5.57	116.71	109.64
7	W	365	PHE	N-CA-C	-5.53	105.40	111.82
7	X	365	PHE	N-CA-C	-5.51	105.43	111.82
7	X	347	LEU	N-CA-C	-5.44	104.89	112.45
7	W	470	PRO	N-CA-C	5.42	117.31	110.70
5	I	113	DG	C2'-C3'-O3'	-5.41	103.39	111.50
7	X	470	PRO	N-CA-C	5.40	117.29	110.70
7	X	309	GLU	N-CA-C	-5.37	103.83	111.24
7	X	261	ILE	CB-CA-C	-5.28	106.77	111.74
7	W	261	ILE	CB-CA-C	-5.28	106.78	111.74
7	X	573	VAL	N-CA-C	5.22	116.89	108.85
7	W	573	VAL	N-CA-C	5.22	116.89	108.85
7	W	250	ARG	N-CA-C	5.20	117.95	111.24
7	X	475	ASP	N-CA-C	5.19	120.08	113.18
2	F	51	TYR	CB-CA-C	5.15	119.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	ILE	N-CA-C	-5.12	100.10	107.37
7	X	262	GLY	CA-C-O	-5.12	117.58	122.13
7	W	262	GLY	CA-C-O	-5.11	117.58	122.13
2	F	29	ILE	N-CA-C	-5.10	100.13	107.37
3	C	109	PRO	CA-C-O	-5.08	115.80	121.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	783	821	820	1	0
1	E	783	821	820	5	0
2	B	707	761	760	0	0
2	F	707	761	760	4	0
3	C	834	896	895	1	0
3	G	843	909	908	0	0
4	D	755	787	786	1	0
4	H	755	787	786	1	0
5	I	3031	1650	1649	5	0
6	J	2996	1651	1651	8	0
7	W	3696	3759	3757	16	0
7	X	3696	3759	3757	15	0
8	W	27	12	12	0	0
8	X	27	12	12	0	0
9	W	1	0	0	0	0
9	X	1	0	0	0	0
All	All	19642	17386	17373	50	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 1.

All (50) 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:X:241:LEU:HD13	7:X:261:ILE:CD1	1.70	1.22
7:W:241:LEU:HD13	7:W:261:ILE:CD1	1.70	1.19
7:W:241:LEU:HD13	7:W:261:ILE:HD11	1.16	1.12
7:X:241:LEU:HD13	7:X:261:ILE:HD11	1.16	1.07
1:E:64:LYS:HE2	1:E:90:MET:HE1	1.46	0.97
1:E:119:ILE:HG22	2:F:50:ILE:HD11	1.52	0.91
7:X:241:LEU:CD1	7:X:261:ILE:HD11	2.04	0.87
1:E:119:ILE:HG22	2:F:50:ILE:CD1	2.05	0.86
7:W:241:LEU:CD1	7:W:261:ILE:HD11	2.04	0.84
7:W:241:LEU:HD13	7:W:261:ILE:HD13	1.62	0.81
7:X:241:LEU:HD13	7:X:261:ILE:HD13	1.62	0.80
7:X:260:LEU:O	7:X:261:ILE:HG13	1.84	0.77
5:I:118:DT:H2'	5:I:119:DA:C8	2.19	0.77
7:W:194:LEU:HD22	7:W:199:ILE:HD11	1.67	0.76
7:W:260:LEU:O	7:W:261:ILE:HG13	1.84	0.76
7:X:194:LEU:HD22	7:X:199:ILE:HD11	1.67	0.75
7:W:432:ILE:HD12	7:W:446:LEU:HD21	1.76	0.66
7:W:194:LEU:HD22	7:W:199:ILE:CD1	2.27	0.64
7:X:194:LEU:HD22	7:X:199:ILE:CD1	2.27	0.64
1:E:64:LYS:HE2	1:E:90:MET:CE	2.23	0.63
7:X:194:LEU:CD2	7:X:199:ILE:HD11	2.31	0.61
7:W:194:LEU:CD2	7:W:199:ILE:HD11	2.31	0.60
7:X:432:ILE:HD12	7:X:446:LEU:HD21	1.85	0.58
7:X:427:ILE:HG12	7:X:432:ILE:HD11	1.88	0.56
2:F:92:ARG:HD2	4:H:73:GLU:OE2	2.05	0.56
7:W:427:ILE:HG12	7:W:432:ILE:HD11	1.88	0.54
1:E:64:LYS:CE	1:E:90:MET:HE1	2.31	0.52
6:J:69:DA:H2''	6:J:70:DC:C6	2.45	0.51
7:W:446:LEU:HD22	7:W:452:GLN:HG3	1.92	0.51
5:I:157:DG:H2''	5:I:158:DC:O5'	2.12	0.49
5:I:180:DG:C6	6:J:27:DT:H73	2.47	0.49
4:D:52:SER:HB2	6:J:20:DA:OP1	2.13	0.49
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.50	0.46
5:I:152:DG:H2''	5:I:153:DC:C6	2.51	0.46
5:I:197:DG:N2	6:J:12:DC:O2	2.48	0.46
7:X:261:ILE:HG22	7:X:262:GLY:N	2.29	0.46
6:J:41:DA:H2''	6:J:42:DC:O5'	2.15	0.46
6:J:48:DT:C4	6:J:49:DA:C6	3.03	0.46
7:W:261:ILE:HG22	7:W:262:GLY:N	2.30	0.46
7:W:260:LEU:C	7:W:261:ILE:HG13	2.40	0.46
7:X:260:LEU:C	7:X:261:ILE:HG13	2.40	0.45
7:W:595:ARG:O	7:W:596:ILE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:260:LEU:O	7:X:261:ILE:CG1	2.61	0.43
6:J:143:DC:H2'	6:J:144:DC:C6	2.54	0.42
7:X:261:ILE:CG2	7:X:262:GLY:N	2.82	0.42
7:W:261:ILE:CG2	7:W:262:GLY:N	2.82	0.42
6:J:80:DC:H1'	6:J:81:DC:C6	2.55	0.42
7:W:260:LEU:O	7:W:261:ILE:CG1	2.62	0.41
7:X:446:LEU:HD22	7:X:452:GLN:HG3	2.03	0.41
1:A:42:ARG:O	1:A:43:PRO:C	2.62	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	93/135 (69%)	92 (99%)	1 (1%)	0	100	100
1	E	93/135 (69%)	92 (99%)	0	1 (1%)	11	36
2	B	86/102 (84%)	85 (99%)	1 (1%)	0	100	100
2	F	86/102 (84%)	85 (99%)	1 (1%)	0	100	100
3	C	106/129 (82%)	103 (97%)	3 (3%)	0	100	100
3	G	107/129 (83%)	106 (99%)	1 (1%)	0	100	100
4	D	94/122 (77%)	93 (99%)	1 (1%)	0	100	100
4	H	94/122 (77%)	93 (99%)	1 (1%)	0	100	100
7	W	445/1052 (42%)	412 (93%)	31 (7%)	2 (0%)	30	60
7	X	445/1052 (42%)	412 (93%)	32 (7%)	1 (0%)	43	72
All	All	1649/3080 (54%)	1573 (95%)	72 (4%)	4 (0%)	44	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	472	TYR
7	W	434	ILE
7	X	434	ILE
1	E	40	ARG

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	82/109 (75%)	82 (100%)	0	100	100
1	E	82/109 (75%)	82 (100%)	0	100	100
2	B	72/78 (92%)	71 (99%)	1 (1%)	59	85
2	F	72/78 (92%)	71 (99%)	1 (1%)	59	85
3	C	85/101 (84%)	84 (99%)	1 (1%)	63	87
3	G	86/101 (85%)	85 (99%)	1 (1%)	63	87
4	D	82/102 (80%)	82 (100%)	0	100	100
4	H	82/102 (80%)	81 (99%)	1 (1%)	63	87
7	W	412/939 (44%)	406 (98%)	6 (2%)	57	84
7	X	412/939 (44%)	406 (98%)	6 (2%)	57	84
All	All	1467/2658 (55%)	1450 (99%)	17 (1%)	61	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	50	ILE
3	C	43	VAL
2	F	32	PRO
3	G	100	VAL
4	H	90	GLU
7	W	226	ARG
7	W	473	THR
7	W	477	HIS
7	W	497	GLU
7	W	567	ASN

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Mol	Chain	Res	Type
7	W	633	GLN
7	X	226	ARG
7	X	473	THR
7	X	475	ASP
7	X	477	HIS
7	X	497	GLU
7	X	633	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	75	HIS
3	C	82	HIS
4	D	92	GLN
2	F	75	HIS
3	G	89	ASN
4	H	44	GLN
4	H	46	HIS
4	H	81	ASN
4	H	92	GLN
7	W	331	ASN
7	W	343	ASN
7	W	584	GLN
7	X	331	ASN
7	X	584	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
8	ADP	W	1101	9	28,29,29	1.39	5 (17%)	43,45,45	1.79	8 (18%)
8	ADP	X	1101	9	28,29,29	1.38	5 (17%)	43,45,45	1.83	10 (23%)

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	ADP	W	1101	9	-	4/16/32/32	0/3/3/3
8	ADP	X	1101	9	-	1/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1101	ADP	C5-C4	4.55	1.47	1.39
8	X	1101	ADP	C5-C4	4.53	1.47	1.39
8	X	1101	ADP	C5-C6	2.65	1.48	1.41
8	W	1101	ADP	C5-C6	2.59	1.48	1.41
8	X	1101	ADP	C5-N7	-2.42	1.34	1.39
8	W	1101	ADP	C5-N7	-2.38	1.34	1.39
8	X	1101	ADP	C8-N7	2.31	1.36	1.31
8	W	1101	ADP	C8-N7	2.24	1.36	1.31
8	W	1101	ADP	C4-N9	-2.04	1.33	1.37
8	X	1101	ADP	C4-N9	-2.02	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	1101	ADP	C5-C4-N3	-5.76	118.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	1101	ADP	C5-C4-N3	-5.67	118.91	126.72
8	W	1101	ADP	N3-C4-N9	4.56	134.92	127.17
8	X	1101	ADP	N3-C4-N9	4.38	134.61	127.17
8	X	1101	ADP	C4-C5-N7	-3.71	106.34	110.58
8	W	1101	ADP	C2-N3-C4	3.65	120.75	111.83
8	X	1101	ADP	C2-N3-C4	3.53	120.46	111.83
8	W	1101	ADP	C4-C5-N7	-3.49	106.59	110.58
8	W	1101	ADP	N3-C2-N1	-3.22	123.71	128.58
8	X	1101	ADP	N3-C2-N1	-3.02	124.02	128.58
8	X	1101	ADP	C4-N9-C8	2.76	108.64	105.74
8	X	1101	ADP	C5-N7-C8	2.73	107.74	103.45
8	W	1101	ADP	C4-N9-C8	2.70	108.57	105.74
8	W	1101	ADP	C5-N7-C8	2.43	107.26	103.45
8	X	1101	ADP	C3'-C2'-C1'	2.28	105.77	101.46
8	X	1101	ADP	N9-C8-N7	-2.21	110.80	113.94
8	X	1101	ADP	C6-C5-N7	2.16	136.25	132.09
8	W	1101	ADP	C6-C5-N7	2.11	136.15	132.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

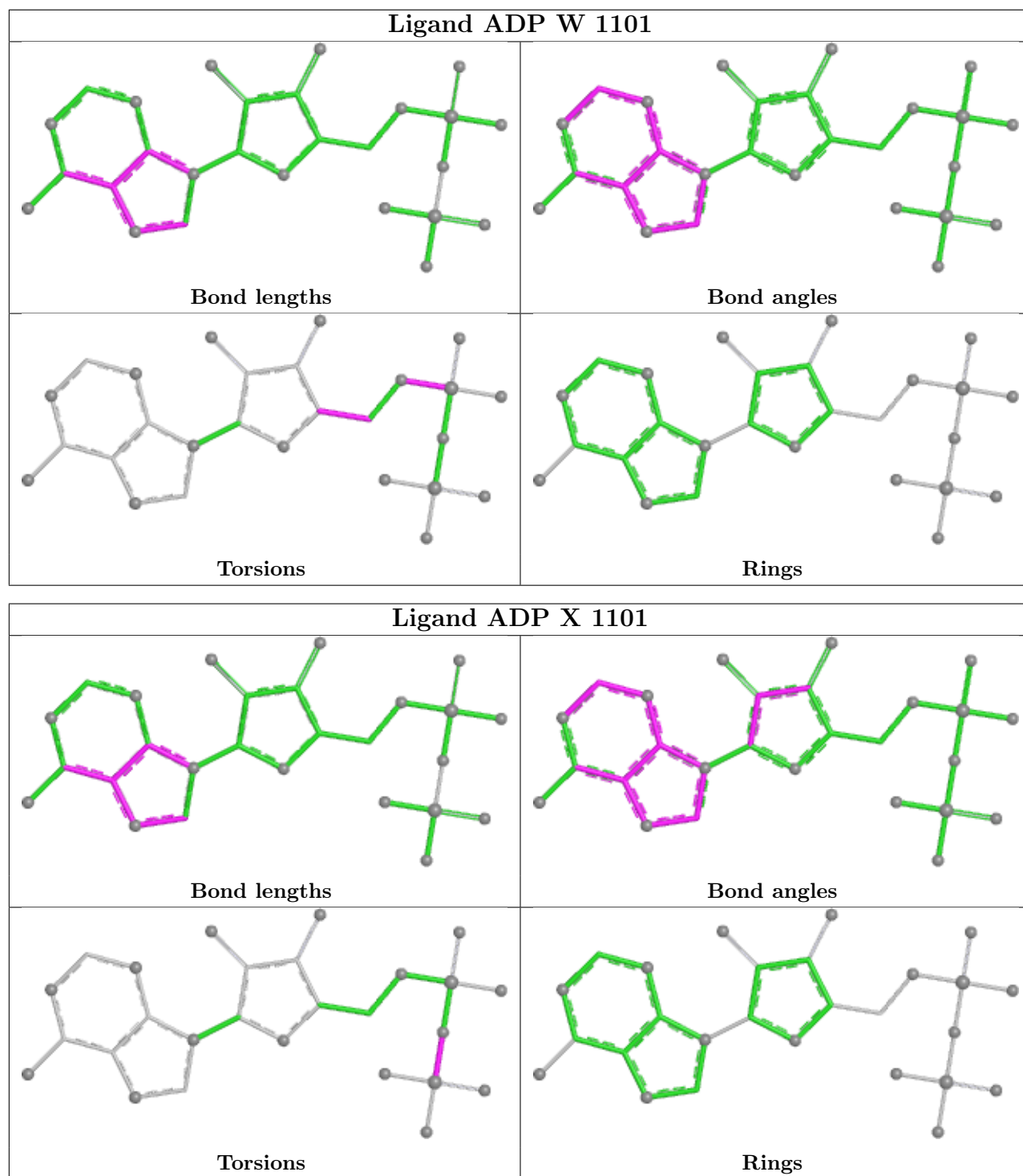
Mol	Chain	Res	Type	Atoms
8	W	1101	ADP	C5'-O5'-PA-O3A
8	W	1101	ADP	O4'-C4'-C5'-O5'
8	W	1101	ADP	C3'-C4'-C5'-O5'
8	W	1101	ADP	C5'-O5'-PA-O1A
8	X	1101	ADP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

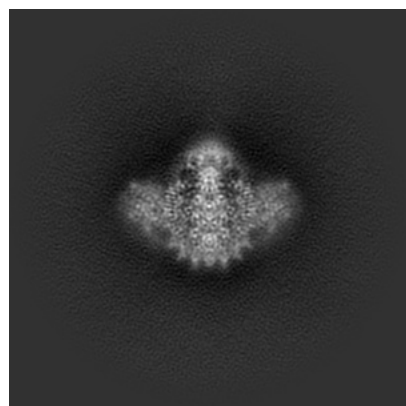
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43002. These allow visual inspection of the internal detail of the map and identification of artifacts.

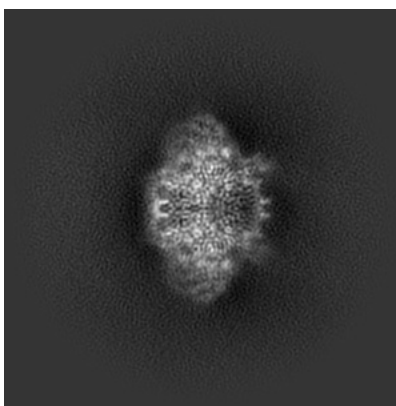
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

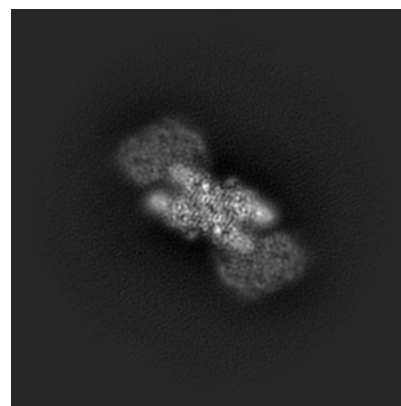
6.1.1 Primary map



X

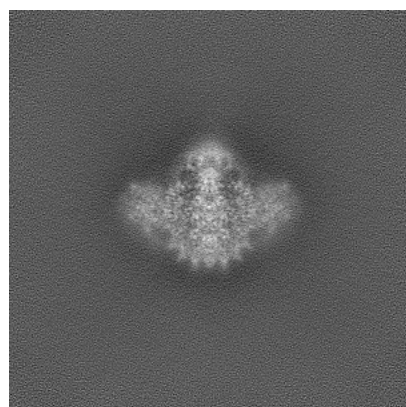


Y

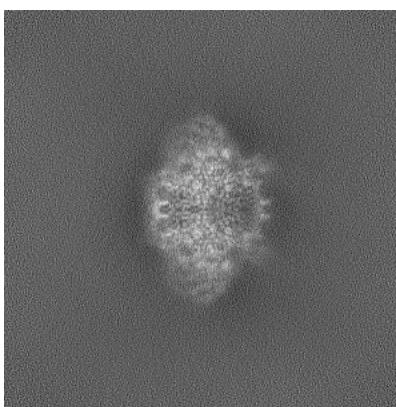


Z

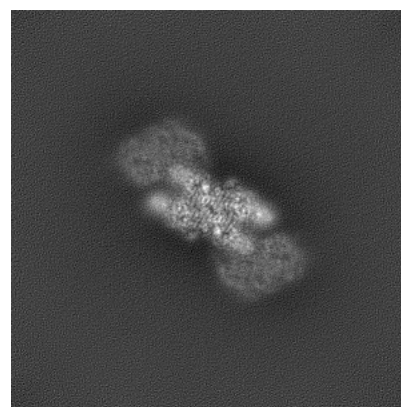
6.1.2 Raw map



X



Y

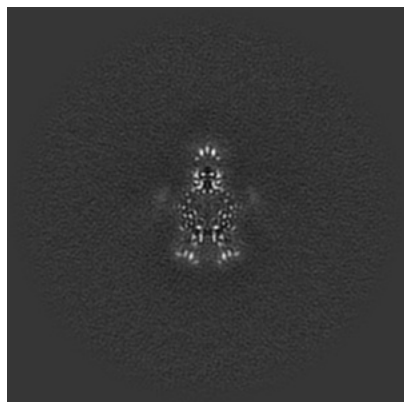


Z

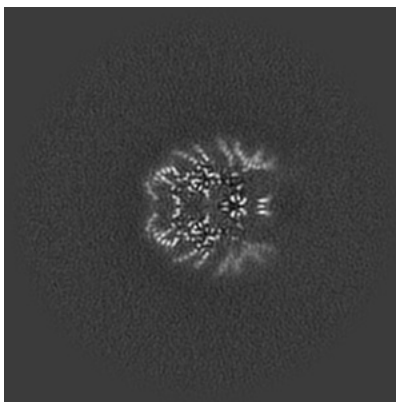
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

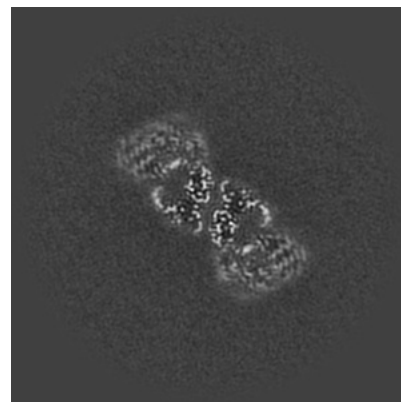
6.2.1 Primary map



X Index: 192

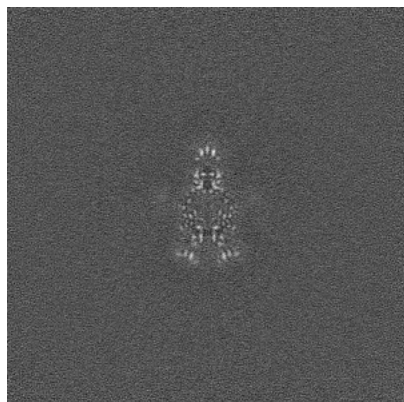


Y Index: 192

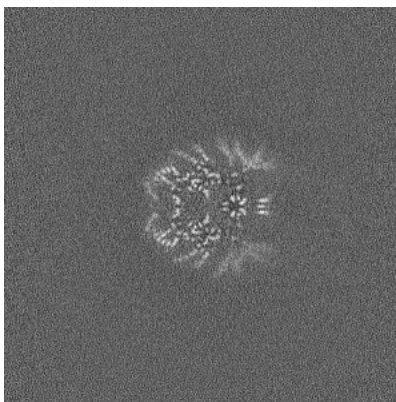


Z Index: 192

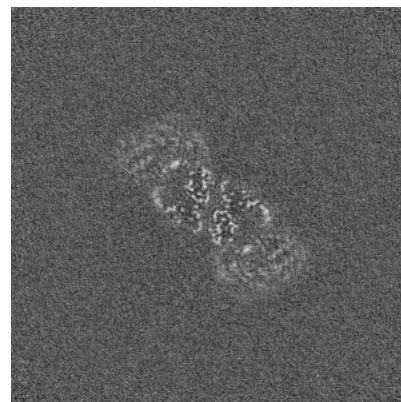
6.2.2 Raw map



X Index: 192



Y Index: 192

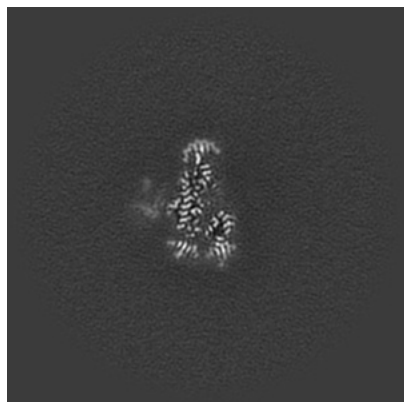


Z Index: 192

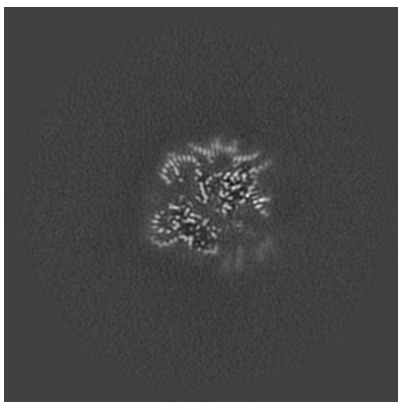
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

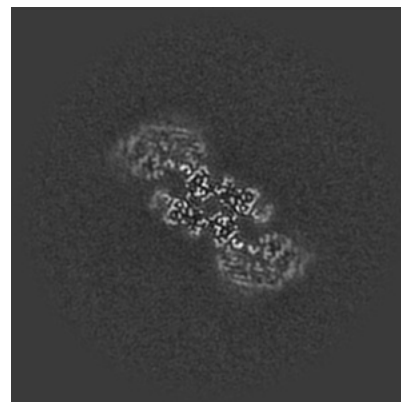
6.3.1 Primary map



X Index: 199

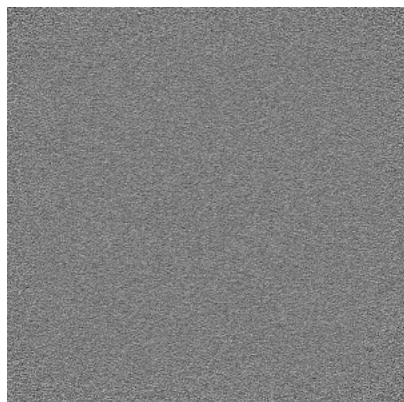


Y Index: 186

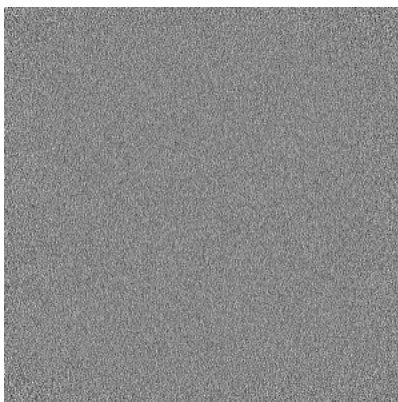


Z Index: 186

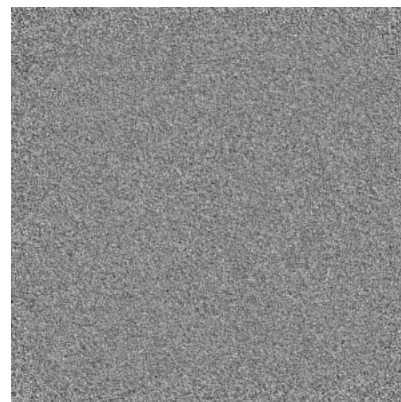
6.3.2 Raw map



X Index: 0



Y Index: 0

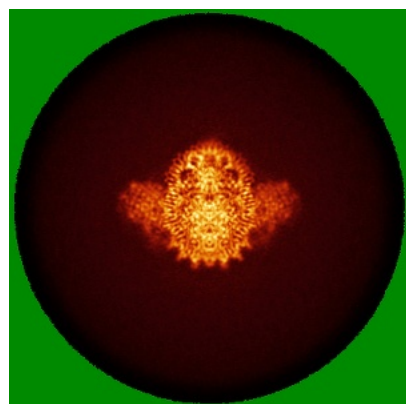


Z Index: 0

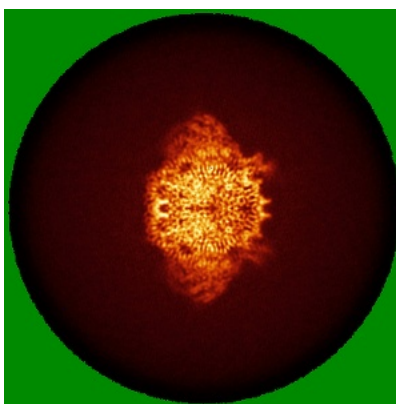
The images above show the largest variance slices of the map in three orthogonal directions.

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

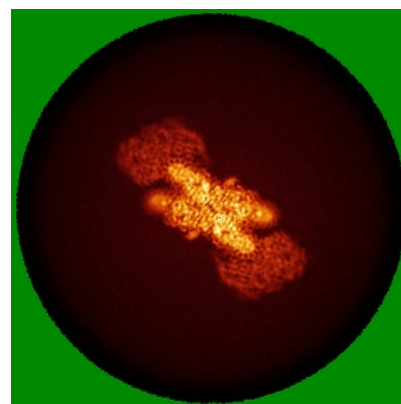
6.4.1 Primary map



X

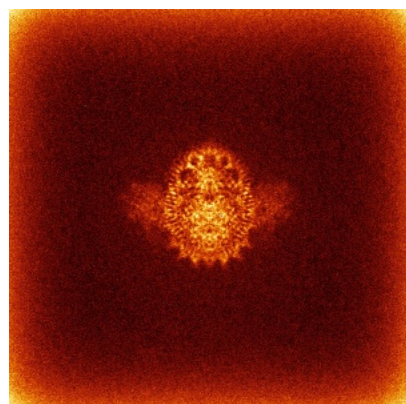


Y

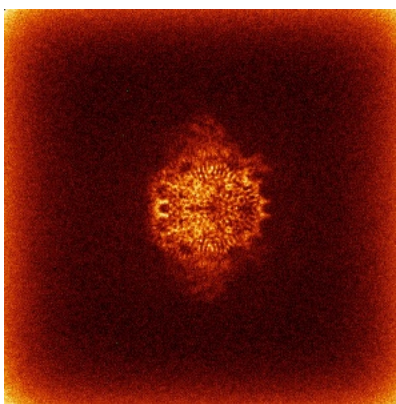


Z

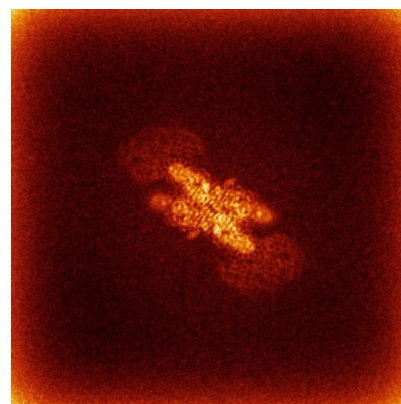
6.4.2 Raw map



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.

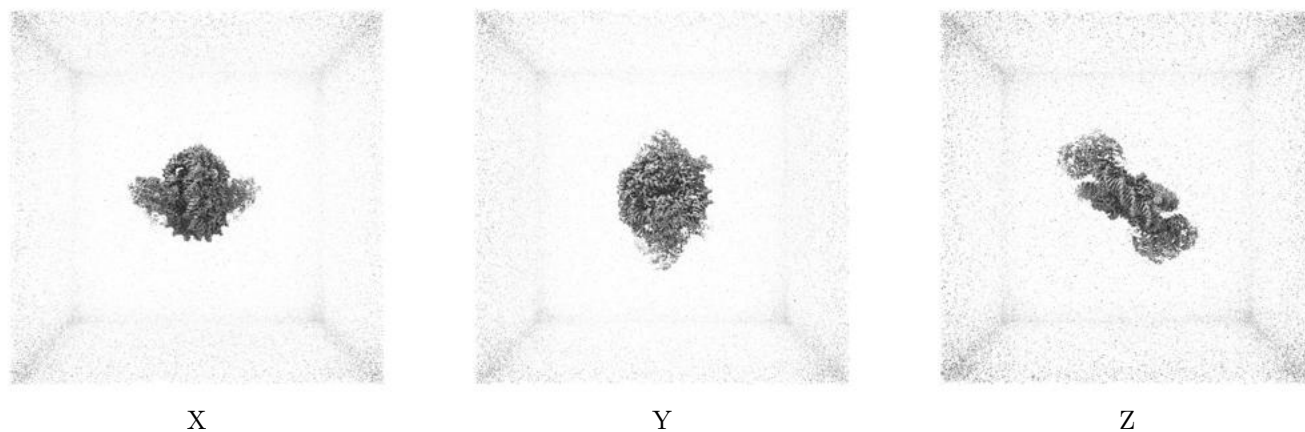
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

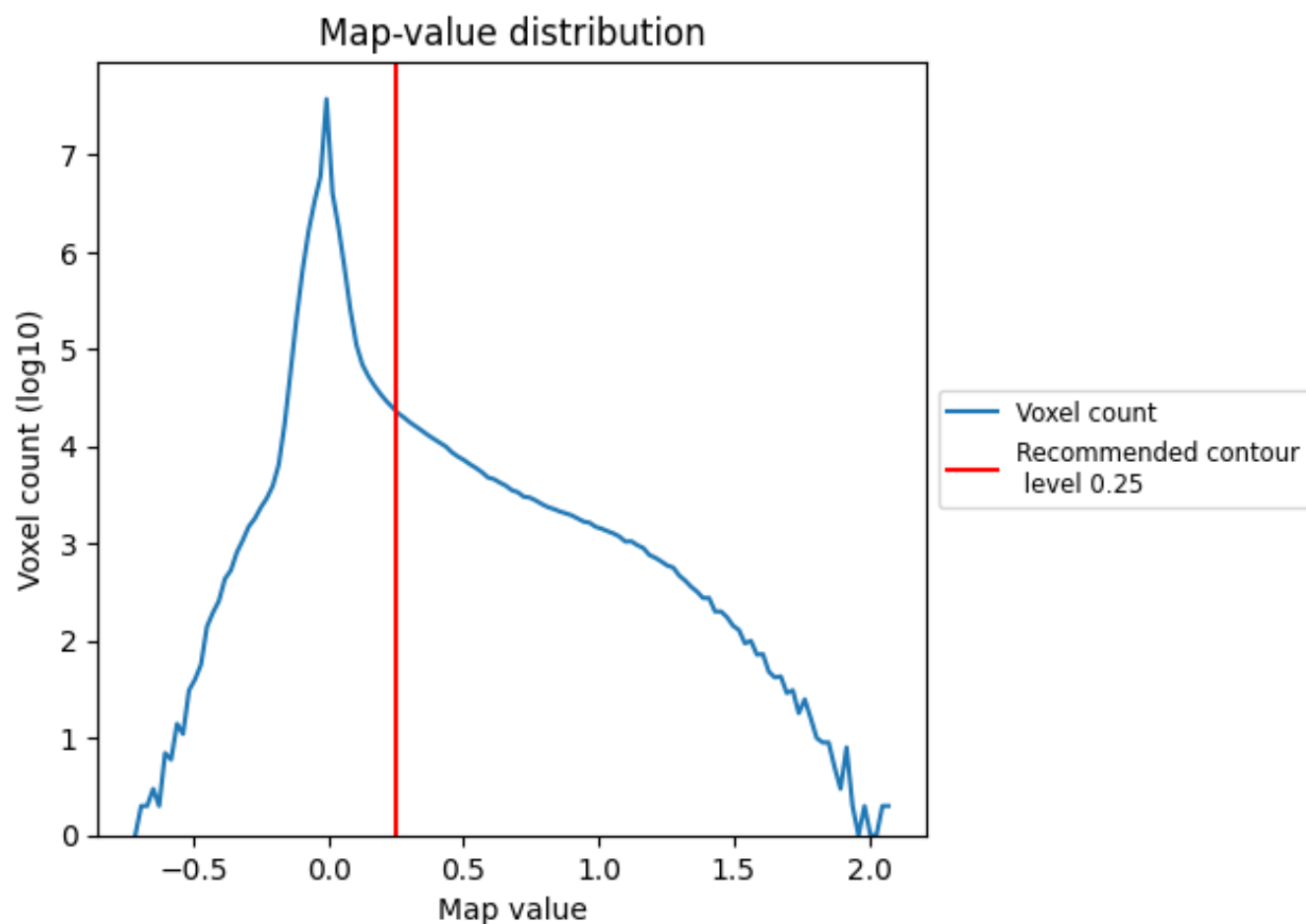
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

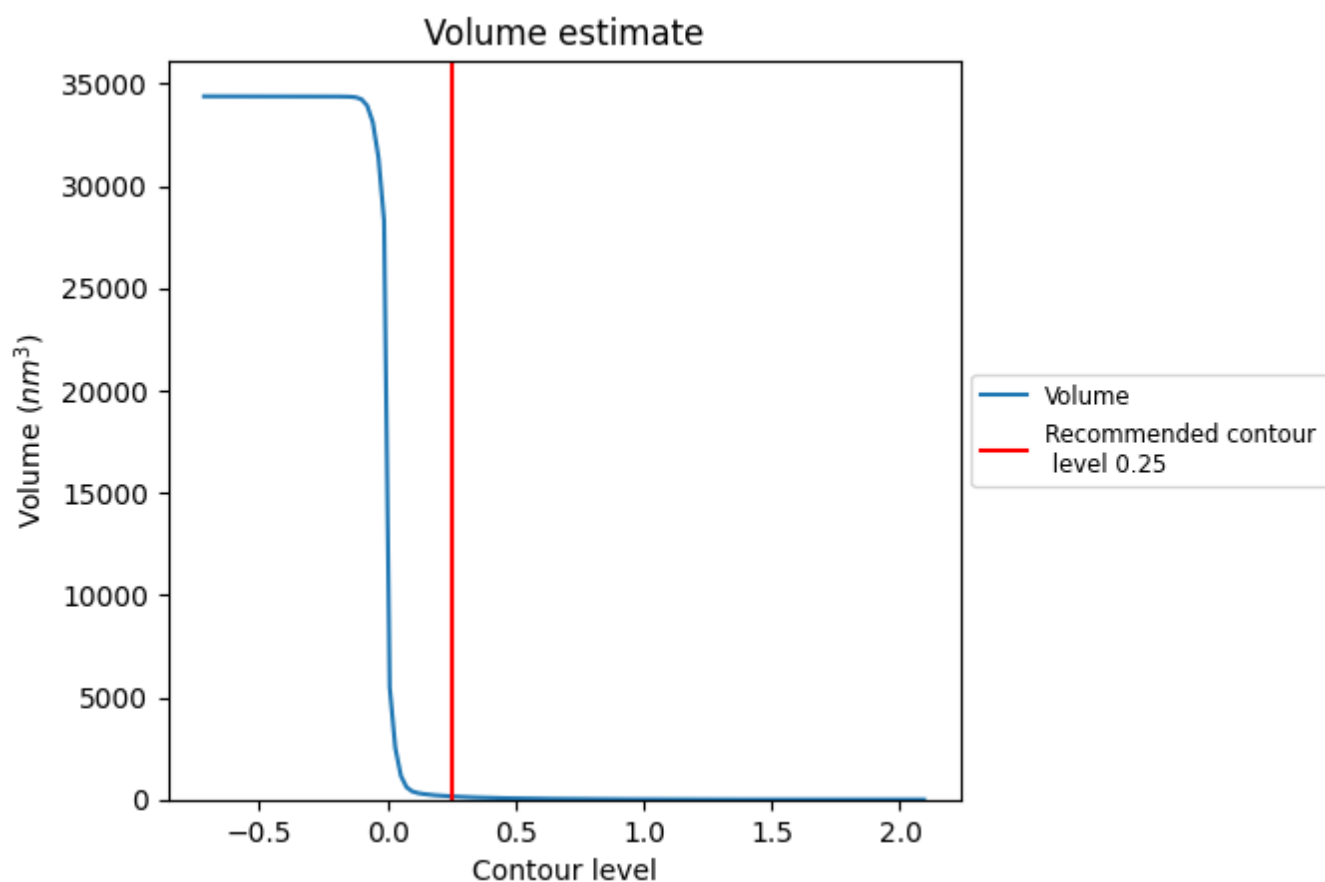
This section contains the results of statistical analysis of the map.

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.

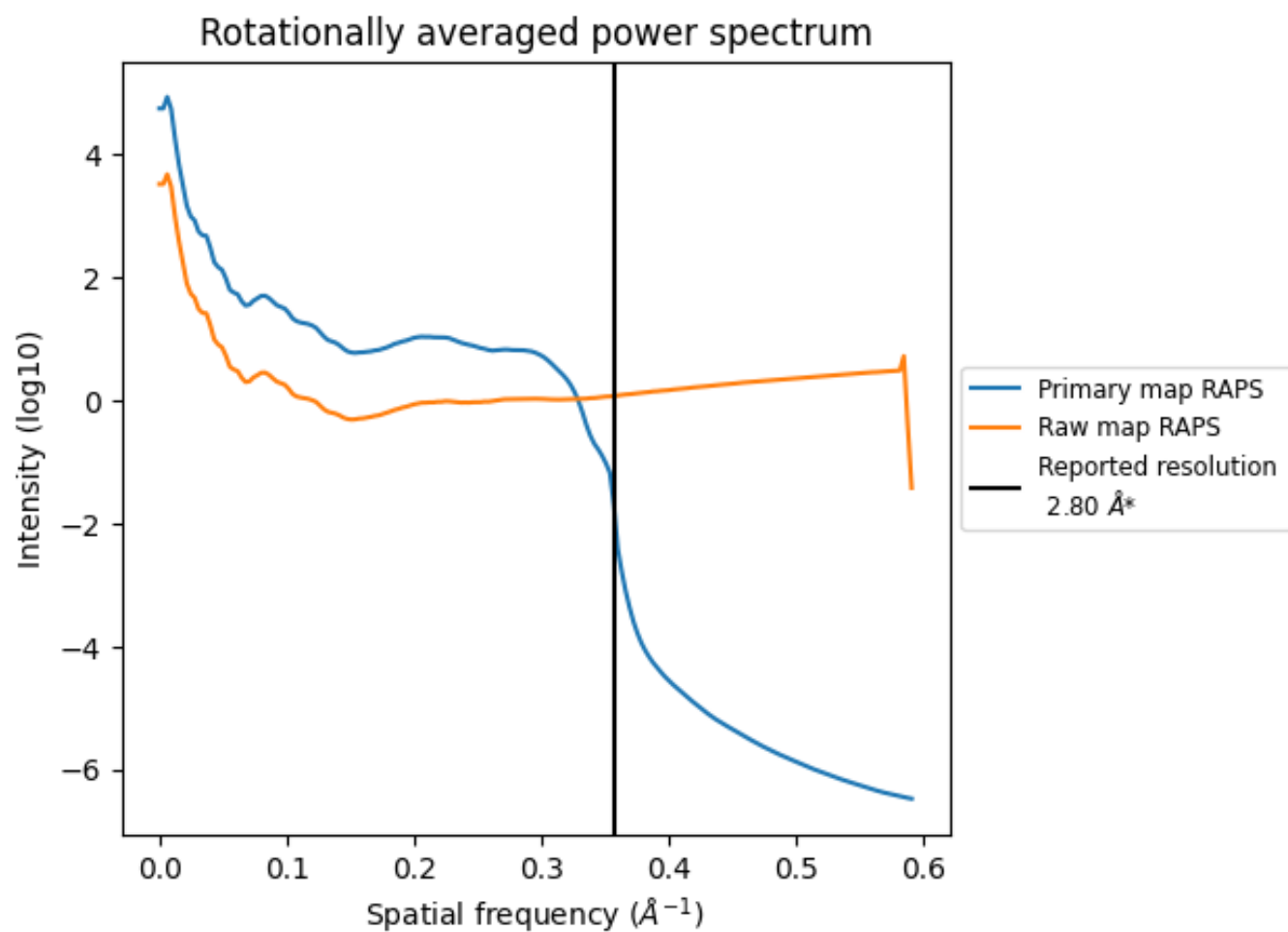
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

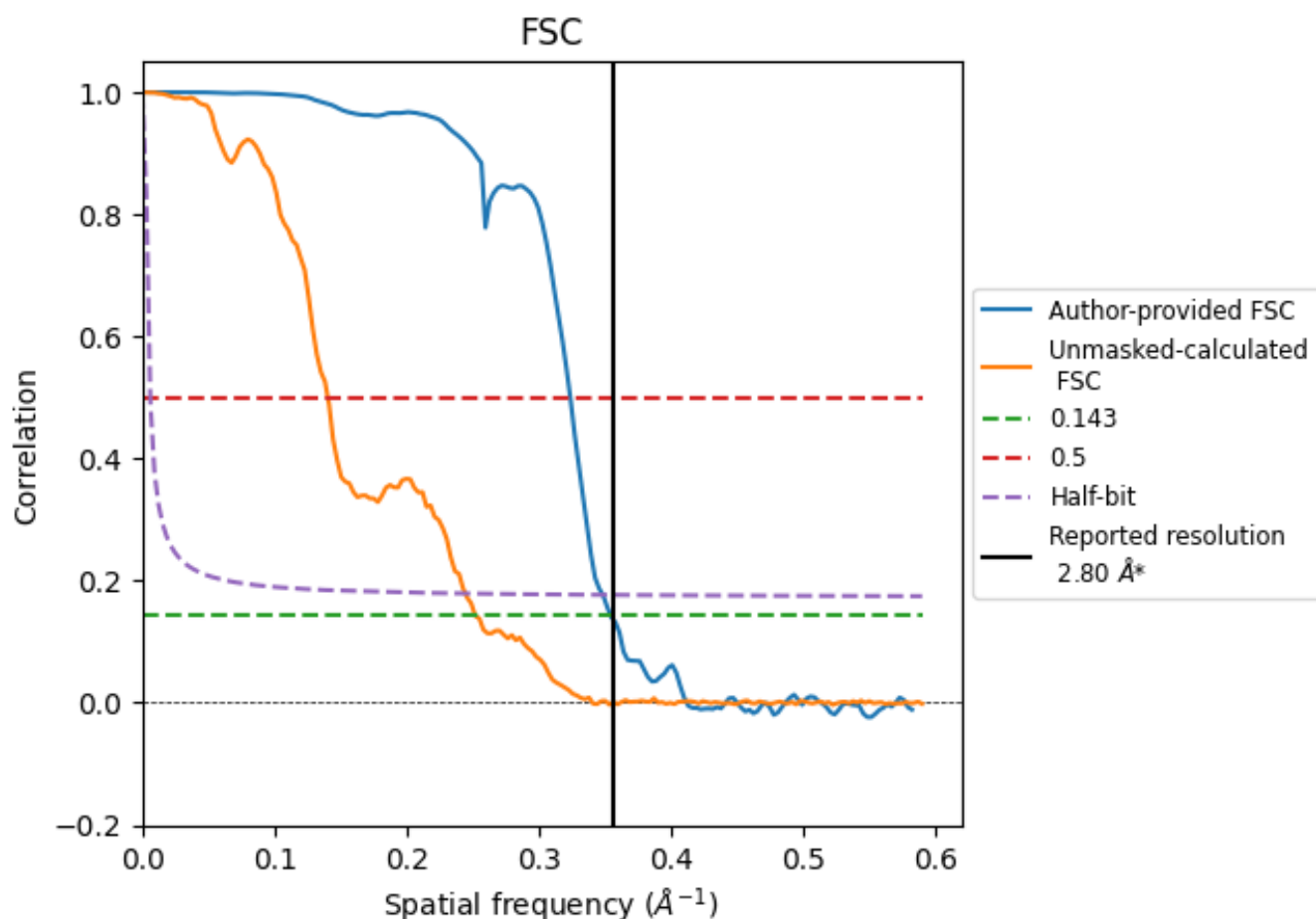


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

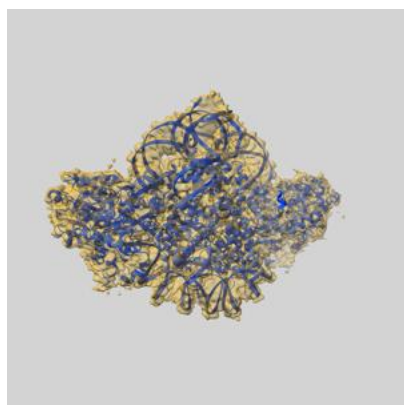
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.09	2.87
Unmasked-calculated*	3.97	7.12	4.09

*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 3.97 differs from the reported value 2.8 by more than 10 %

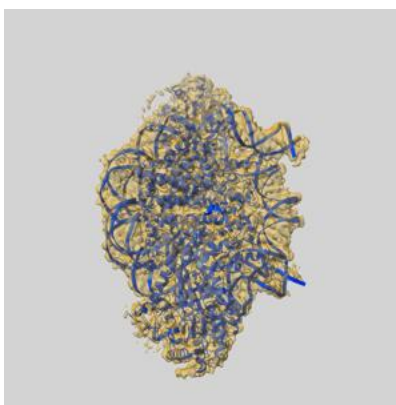
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43002 and PDB model 8V6V. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

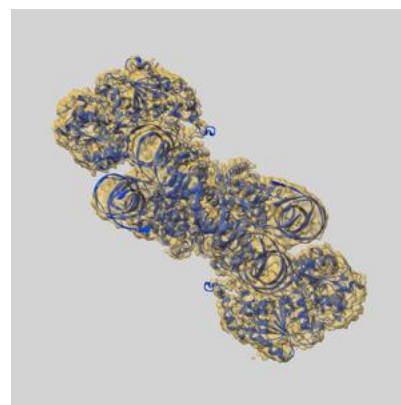
9.1 Map-model overlay [i](#)



X



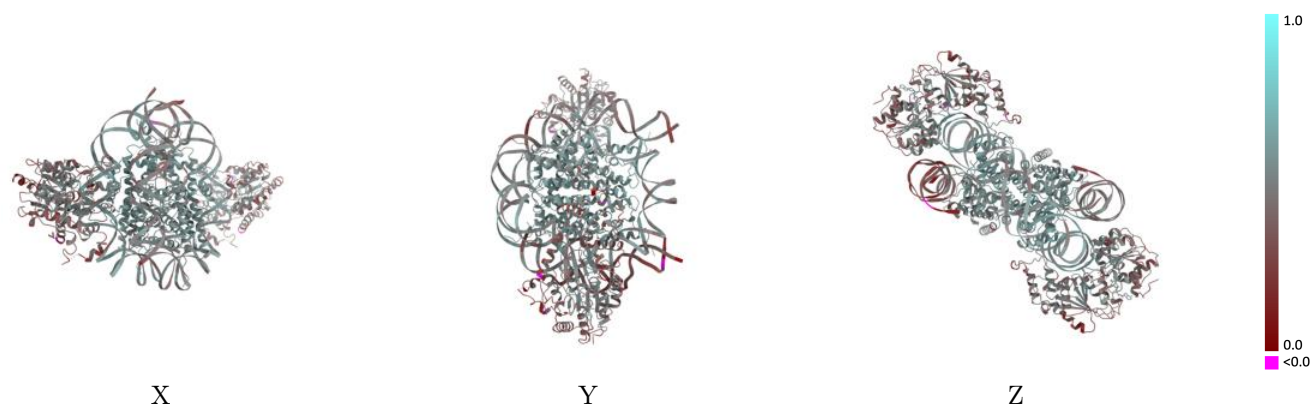
Y



Z

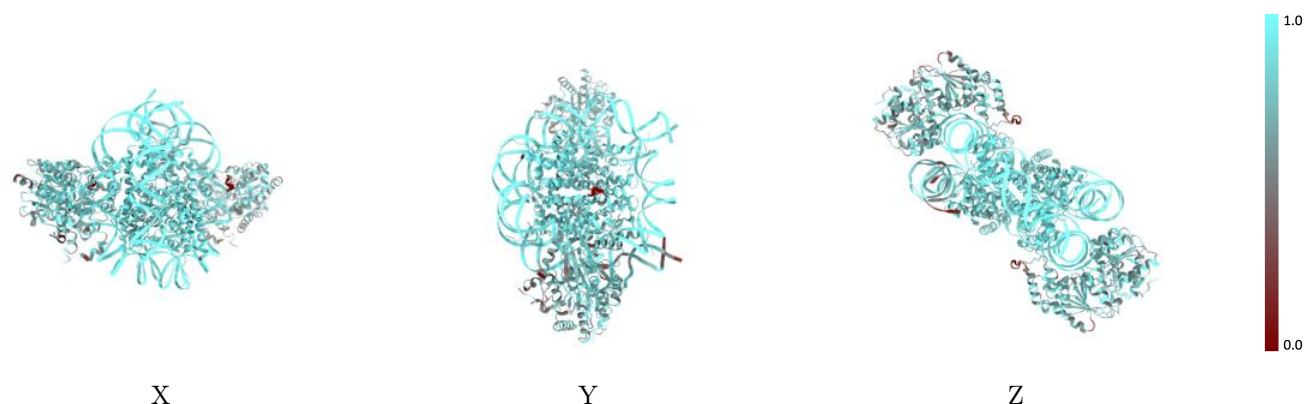
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



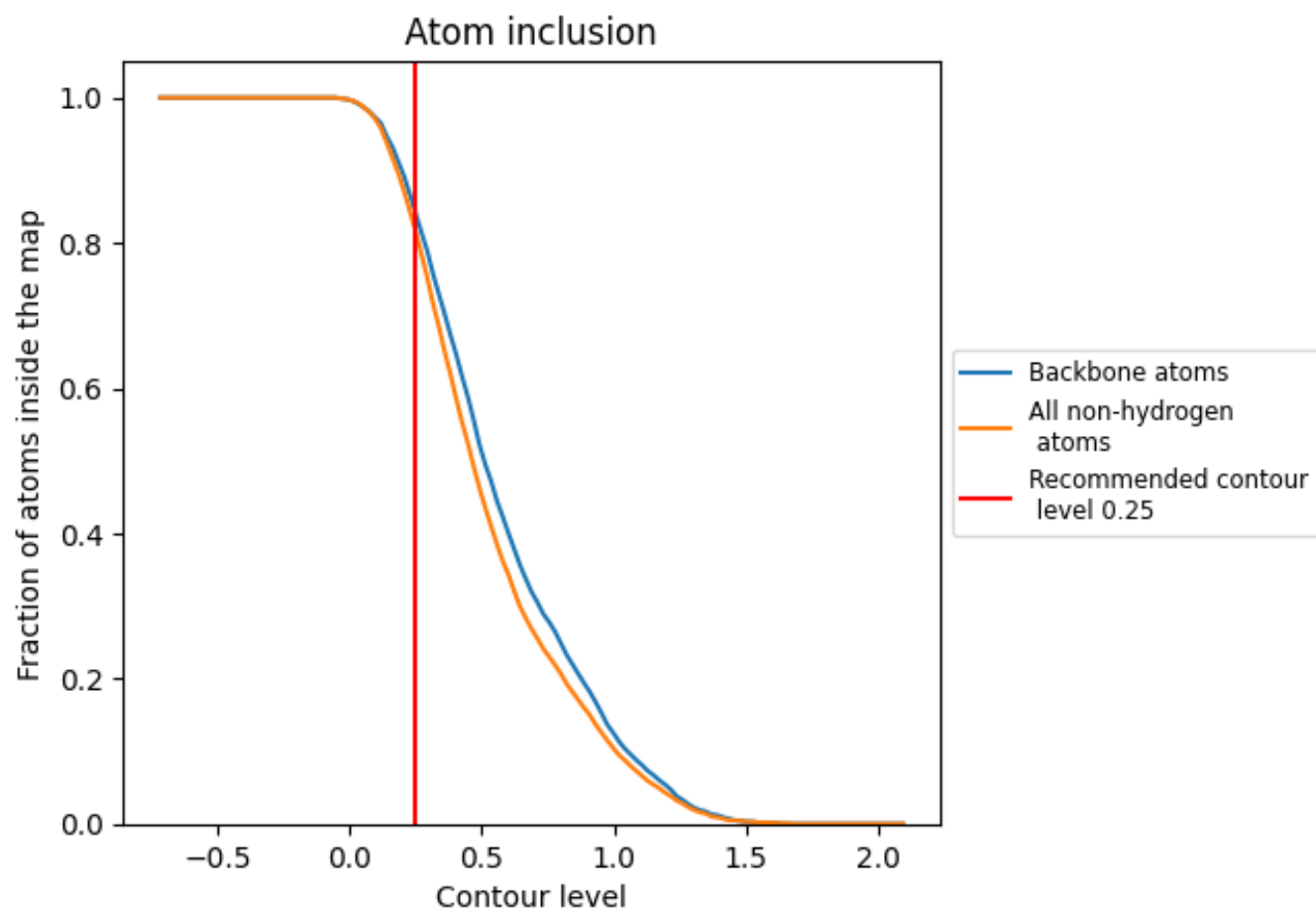
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.4770
A	0.9590	0.6000
B	0.9280	0.5720
C	0.8880	0.5320
D	0.9100	0.5360
E	0.9460	0.5780
F	0.9250	0.5710
G	0.9170	0.5560
H	0.9160	0.5420
I	0.9290	0.4740
J	0.9280	0.4740
W	0.7410	0.4130
X	0.6850	0.4050

1.0

0.0

<0.0