



wwPDB EM Validation Summary Report ⓘ

Jan 13, 2025 – 01:30 PM EST

PDB ID : 9E1P
EMDB ID : EMD-47416
Title : Snf2h bound nucleosome complex - ClassB2
Authors : Malik, D.; Deshmukh, A.A.; Bilokapic, S.; Halic, M.
Deposited on : 2024-10-21
Resolution : 3.25 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.40

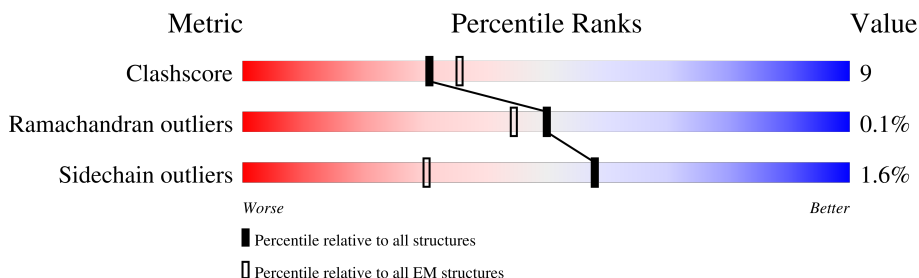
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	126	
4	H	126	

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Mol	Chain	Length	Quality of chain
5	I	152	 43% 57%
6	J	152	 54% 46%
7	W	1052	 5% 31% 11% 58%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16007 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	1	0
			807	510	156	138	3		
1	E	96	Total	C	N	O	S	0	0
			790	499	151	137	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	85	Total	C	N	O	S	0	0
			679	428	135	115	1		
2	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			837	526	165	146		
3	G	109	Total	C	N	O	0	0
			837	526	165	146		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			746	469	134	141	2		
4	H	96	Total	C	N	O	S	0	0
			756	475	138	141	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 DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	152	Total	C	N	O	P	0	0
			3135	1482	591	910	152		

- Molecule 6 is a DNA chain called DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	152	Total	C	N	O	P	0	0
			3096	1470	561	913	152		

- 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	444	Total	C	N	O	S	0	0
			3656	2340	643	650	23		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

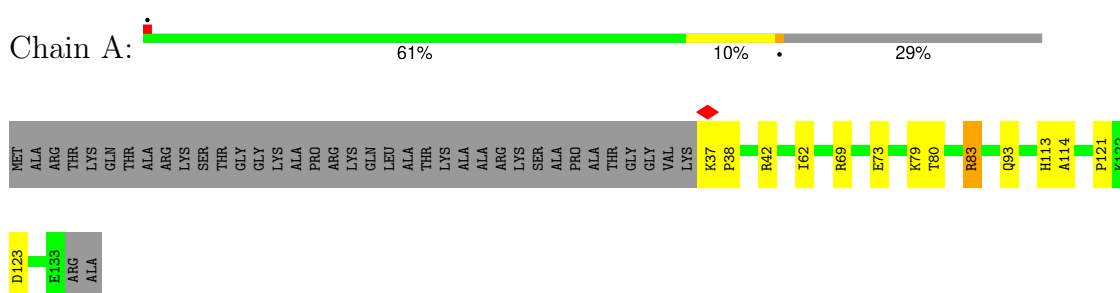


Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	N	O	P	0
			27	10	5	10	2	

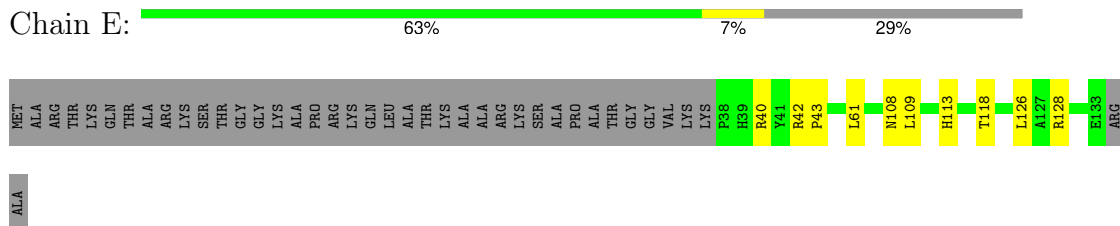
3 Residue-property plots [i](#)

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.

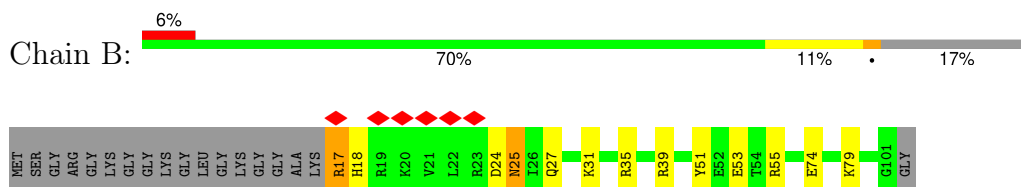
• Molecule 1: Histone H3.2



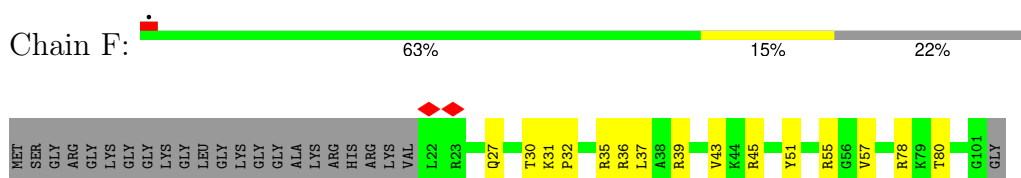
• Molecule 1: Histone H3.2



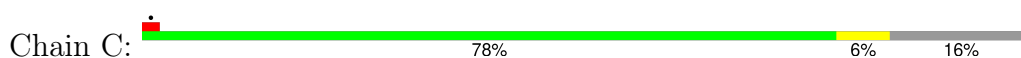
• Molecule 2: Histone H4

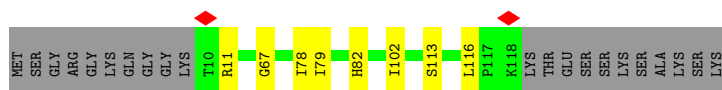


• Molecule 2: Histone H4

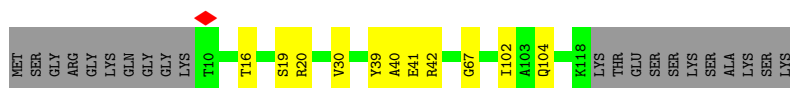
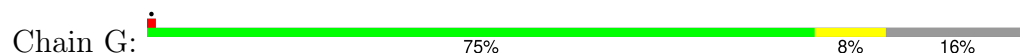


• Molecule 3: Histone H2A type 1

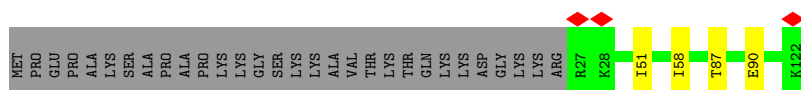




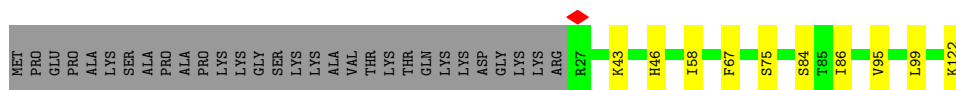
• Molecule 3: Histone H2A type 1



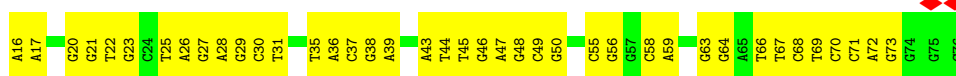
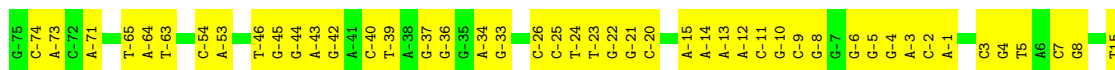
• Molecule 4: Histone H2B 1.1



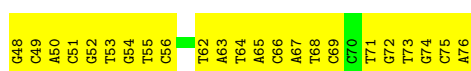
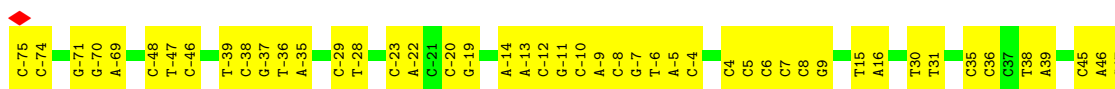
• Molecule 4: Histone H2B 1.1



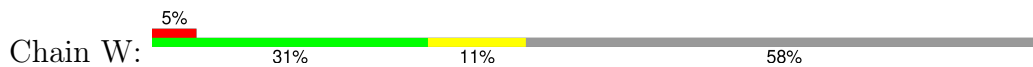
• Molecule 5: DNA (152-MER)



• Molecule 6: DNA (152-MER)



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



MET	ILE	LYS	Q184	F297	F391	L478	T599	LEU	ARG	TYR	GLU	LYS	ARG	LYS	ASP
SER	PHE	PRO	V185	K298	R394	P493	K600	GLY	LYS	LYS	TRP	LYS	LYS	ALA	GLY
ALA	ASP	GLY	R186	W302	R395	K494	R606	ARG	ASN	PRO	ARG	VAL	ALA	ASN	PRO
ALA	ALA	PRO	G187	R303	T396	L495	F607	ALA	TYR	ARG	ASP	ALA	ALA	ASN	ASP
GLU	SER	ARG	L188	Y304	K397	K496	I608	LYS	VAL	PRO	ASP	VAL	ALA	LYS	LYS
PRO	PRO	ILE	N189	L305	A398	E497	T609	THR	ASP	GLU	ILE	ASP	ALA	THR	ILE
PRO	GLY	LYS	I192	T306	D399	S500	D610	ALA	ALA	LEU	ILE	ALA	TYR	GLU	GLY
PRO	LYS	LYS	T202	I307	V400	L515	N611	ALA	TYR	PRO	ILE	ALA	ASP	PRO	PRO
PRO	GLN	ASP	D205	K314	E401	L616	T612	GLN	PHE	ALA	ALA	ALA	ARG	ALA	ALA
PRO	ILE	LYS	E206	R315	K402	M520	I617	GLY	GLU	ALA	ARG	ALA	GLU	GLU	GLY
GLU	GLN	ASN	M207	E316	S403	W521	V618	LEU	ALA	GLN	ARG	ALA	GLU	LYS	LYS
SER	GLU	LEU	G208	V324	L404	R522	D628	SER	LEU	ALA	VAL	LEU	LEU	LEU	LEU
ALA	PRO	LEU	L209	R325	L412	R523	Q634	THR	ARG	LYS	GLY	VAL	VAL	GLN	GLN
PRO	ASP	SER	G210	T329	K418	Y524	G634	MET	SER	GLU	MET	LYS	LYS	LYS	LYS
SER	THR	VAL	G210	T330	M419	E525	Q634	GLY	GLU	GLU	GLY	PRO	PRO	GLU	GLU
LYS	TYR	ASP	L213	T330	N429	L529	Q634	ARG	PRO	GLN	GLY	PRO	PRO	GLU	GLU
PRO	TYR	TYR	G220	T330	K430	D630	G631	LEU	LYS	LEU	GLY	GLU	GLU	GLU	GLU
ALA	GLU	ARG	Y221	T330	ASP	Q631	Q631	SER	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	LYS	ARG	R226	E346	ILE	R534	Q631	THR	ALA	ALA	PHE	ALA	ALA	ALA	ALA
ILE	GLN	ARG	W227	W348	ASP	R538	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	THR	THR	I228	L354	ASP	ILE	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLY	ASP	GLN	M233	L354	ILE	ILE	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	ASP	GLU	V234	D357	ILE	ILE	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ASN	ASN	GLU	L235	D357	ILE	ILE	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	ARG	ASP	K238	S361	ALA	ALA	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	PHE	GLU	L241	D363	GLY	GLY	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
LYS	TYR	LEU	M245	D363	LYS	LYS	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLY	LEU	LEU	K249	ASP	MET	MET	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
PRO	GLY	GLY	M245	PHE	ASP	ASP	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLU	GLN	SER	K249	ASP	ASP	ASP	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLY	THR	SER	L255	TRP	R445	R445	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
VAL	GLU	LYS	R256	PHE	L446	L446	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ALA	LEU	ALA	S257	ASP	L447	L447	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ALA	PHE	THR	VAL	ASN	N448	N448	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLN	HIS	VAL	I261	ASN	Q452	Q452	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
VAL	PHE	CYS	G262	CYS	L453	L453	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ALA	ILE	ALA	D263	LEU	R454	R454	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	GLN	PRO	F167	GLY	K455	K455	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ALA	ALA	ALA	E169	D273	L462	L462	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
SER	ALA	ALA	G170	D273	F463	F463	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLY	GLN	LYS	D281	Q378	D464	D464	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
PRO	THR	PRO	V282	L380	G465	G465	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ALA	THR	ALA	T285	Y391	A466	A466	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
ASP	SER	ASP	E288	R383	E467	E467	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLU	PRO	GLU	K292	L384	P468	P468	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
MET	LEU	LYS	E293	H385	G469	G469	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLU	LYS	LYS	R181	M386	P470	P470	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
GLU	MET	GLY	D182	R389	Y472	Y472	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
			Y183	P390	T473	T473	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA
					D475	D475	Q631	THR	ALA	ALA	THR	ALA	ALA	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	30.600	Depositor
Minimum map value	-0.316	Depositor
Average map value	-0.022	Depositor
Map value standard deviation	0.273	Depositor
Recommended contour level	4	Depositor
Map size (Å)	497.0, 497.0, 497.0	wwPDB
Map dimensions	497, 497, 497	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: 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	0.33	0/822	0.54	0/1102
1	E	0.29	0/802	0.52	0/1076
2	B	0.29	0/687	0.60	0/921
2	F	0.28	0/648	0.56	0/868
3	C	0.27	0/847	0.53	0/1144
3	G	0.26	0/847	0.53	0/1144
4	D	0.28	0/757	0.47	0/1018
4	H	0.28	0/767	0.49	0/1029
5	I	0.63	0/3521	0.89	0/5437
6	J	0.64	0/3468	0.94	0/5345
7	W	0.26	0/3733	0.50	0/5041
All	All	0.46	0/16899	0.72	0/24125

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	807	0	851	11	0
1	E	790	0	826	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	679	0	717	11	0
2	F	641	0	684	11	0
3	C	837	0	891	7	0
3	G	837	0	891	13	0
4	D	746	0	764	3	0
4	H	756	0	786	11	0
5	I	3135	0	1704	68	0
6	J	3096	0	1706	57	0
7	W	3656	0	3730	86	0
8	W	27	0	12	7	0
All	All	16007	0	13562	254	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 9.

The worst 5 of 254 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:W:238:LYS:NZ	7:W:261:ILE:HD11	1.63	1.12
7:W:238:LYS:HZ2	7:W:261:ILE:HD11	1.29	0.88
7:W:238:LYS:HZ1	7:W:261:ILE:HD11	1.39	0.84
7:W:455:LYS:HB2	7:W:462:LEU:HD12	1.65	0.78
3:G:20:ARG:HH11	4:H:122:LYS:HB3	1.49	0.76

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	96/136 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	94/136 (69%)	90 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	83/103 (81%)	81 (98%)	2 (2%)	0	100	100
2	F	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
3	G	107/130 (82%)	103 (96%)	4 (4%)	0	100	100
4	D	94/126 (75%)	92 (98%)	2 (2%)	0	100	100
4	H	94/126 (75%)	93 (99%)	1 (1%)	0	100	100
7	W	438/1052 (42%)	405 (92%)	32 (7%)	1 (0%)	44	71
All	All	1191/2042 (58%)	1139 (96%)	51 (4%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	566	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/111 (78%)	83 (96%)	3 (4%)	31	56
1	E	84/111 (76%)	84 (100%)	0	100	100
2	B	69/79 (87%)	66 (96%)	3 (4%)	25	51
2	F	66/79 (84%)	66 (100%)	0	100	100
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	85/102 (83%)	84 (99%)	1 (1%)	67	79
4	D	80/106 (76%)	80 (100%)	0	100	100
4	H	82/106 (77%)	82 (100%)	0	100	100
7	W	409/939 (44%)	398 (97%)	11 (3%)	40	63
All	All	1046/1735 (60%)	1028 (98%)	18 (2%)	58	73

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	W	394	ARG
7	W	591	ASP
7	W	555	PHE
7	W	177	TRP
7	W	391	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
7	W	598	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](#)

1 ligand is modelled in this entry.

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	-	24,29,29	0.88	0	29,45,45	1.15	2 (6%)

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	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	1101	ADP	N3-C2-N1	-3.51	123.91	128.67
8	W	1101	ADP	C4-C5-N7	-2.56	106.63	109.34

There are no chirality outliers.

All (1) torsion outliers are listed below:

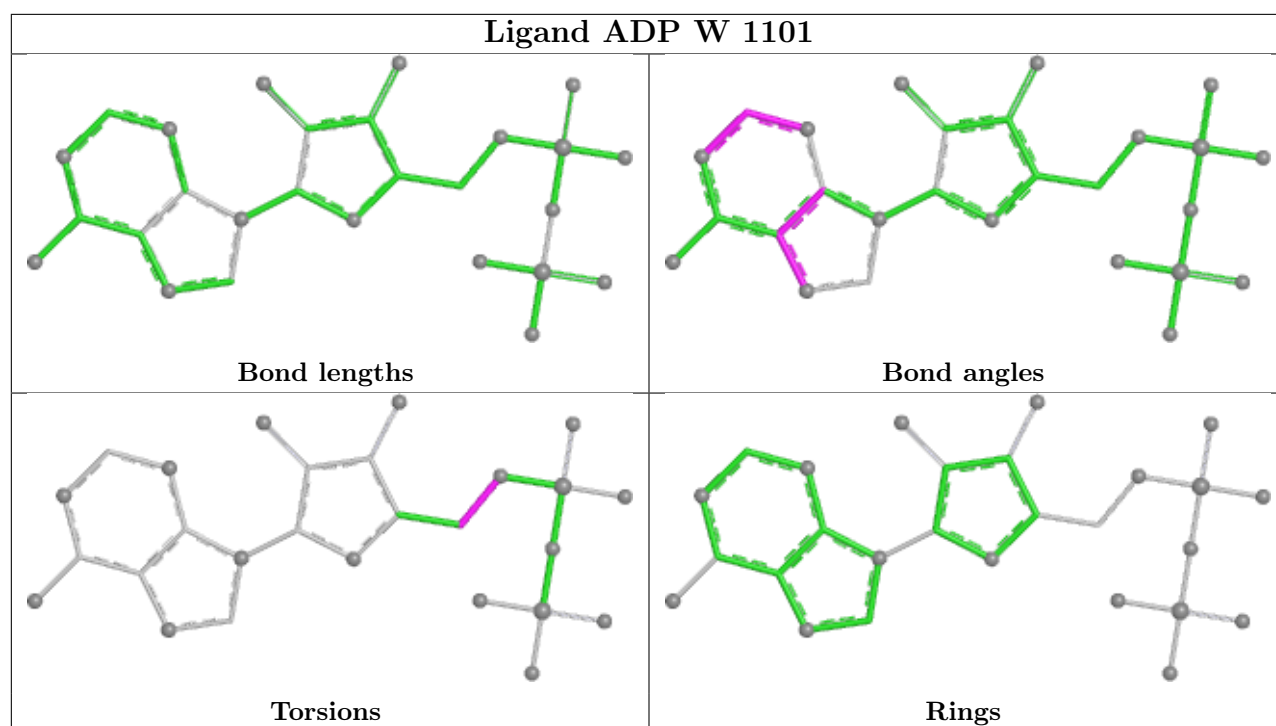
Mol	Chain	Res	Type	Atoms
8	W	1101	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	1101	ADP	7	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.

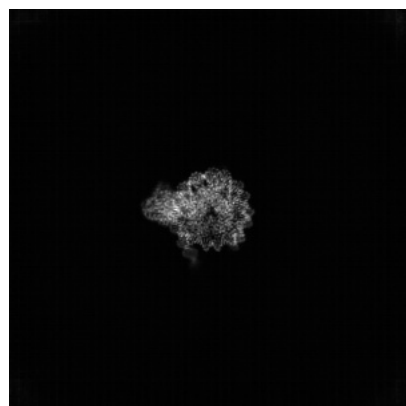
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47416. 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

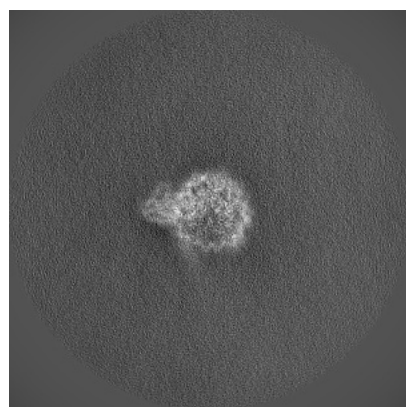


Y

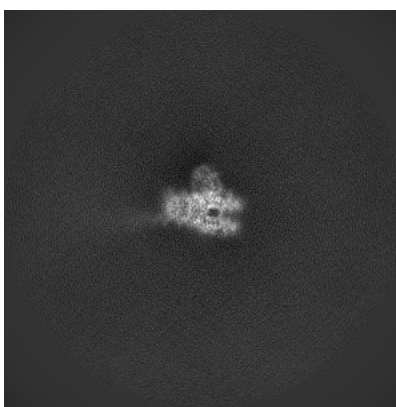


Z

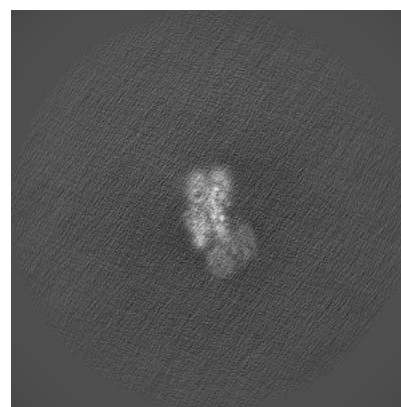
6.1.2 Raw map



X



Y

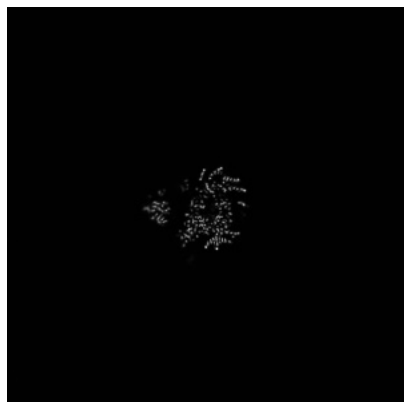


Z

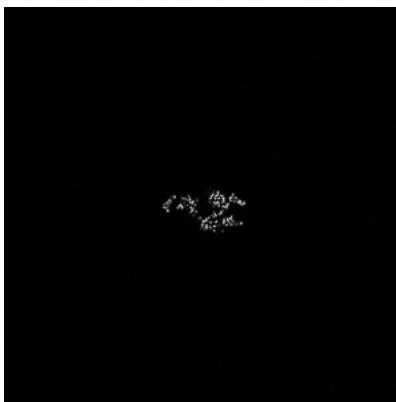
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

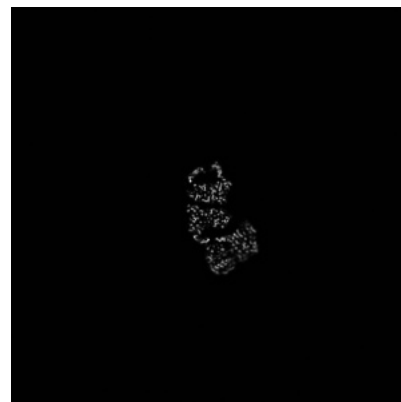
6.2.1 Primary map



X Index: 248

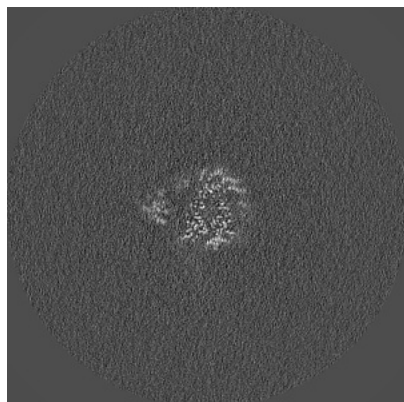


Y Index: 248

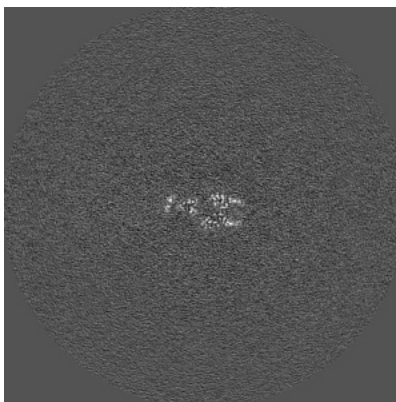


Z Index: 248

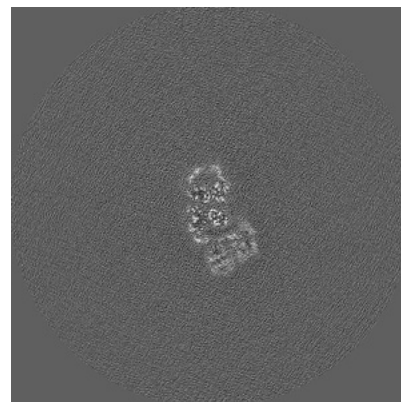
6.2.2 Raw map



X Index: 192



Y Index: 192

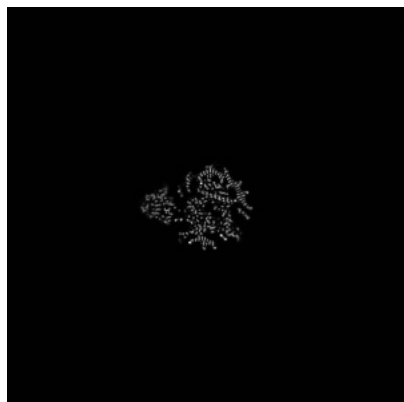


Z Index: 192

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

6.3 Largest variance slices [i](#)

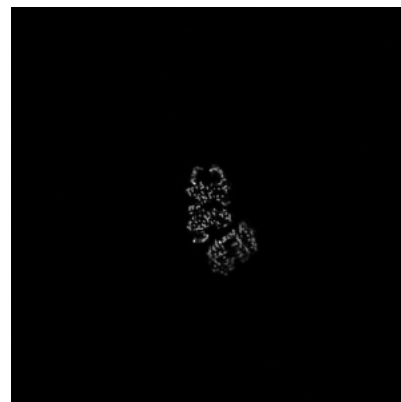
6.3.1 Primary map



X Index: 254

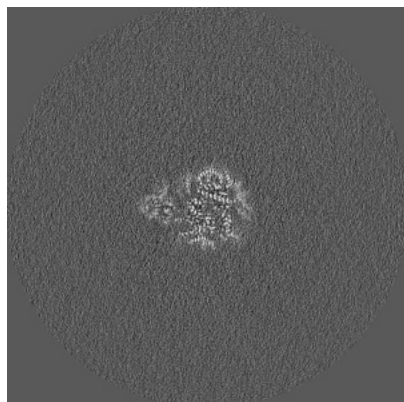


Y Index: 274

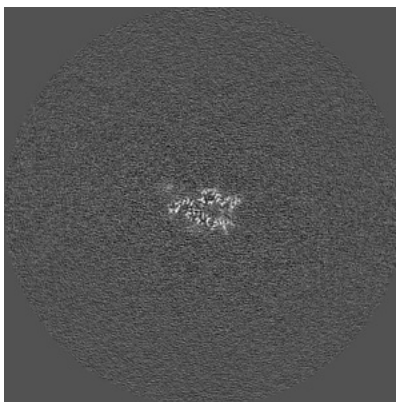


Z Index: 251

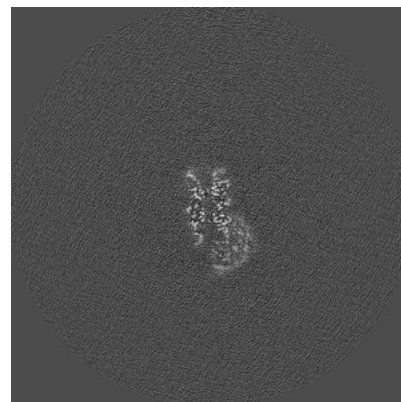
6.3.2 Raw map



X Index: 196



Y Index: 211



Z Index: 198

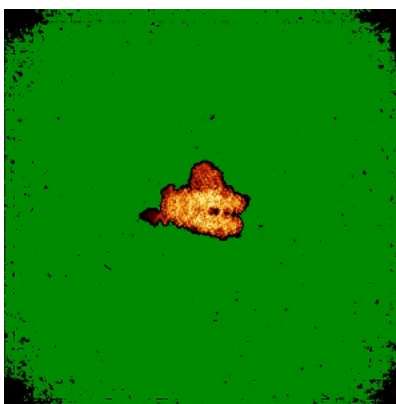
The images above show the largest variance slices of the map in three orthogonal directions.

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

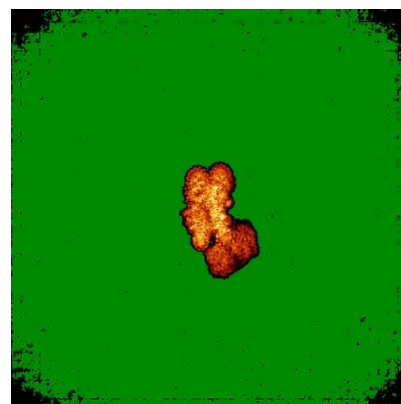
6.4.1 Primary map



X

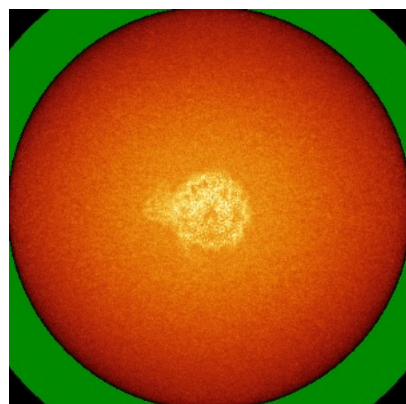


Y

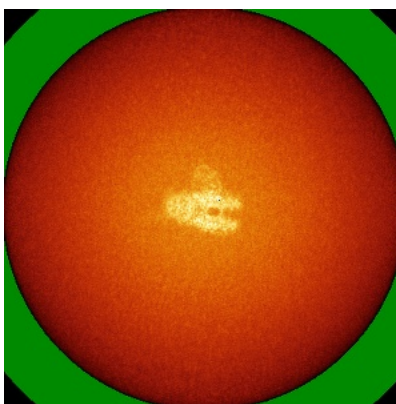


Z

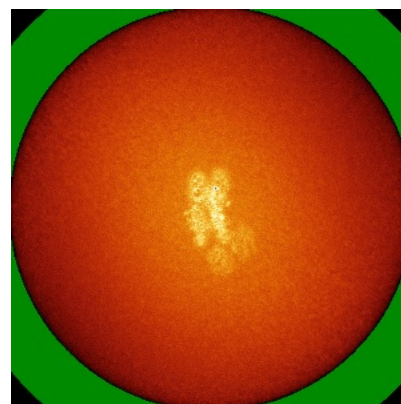
6.4.2 Raw map



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.

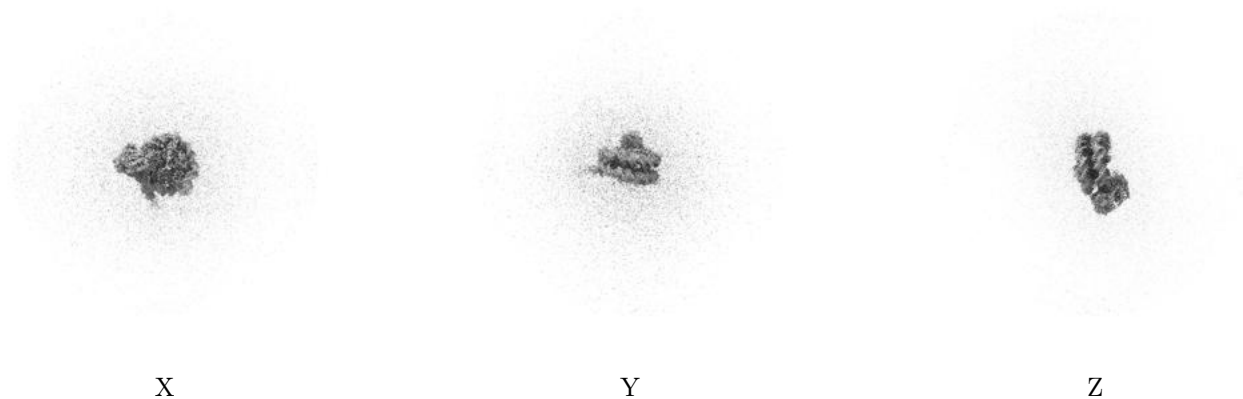
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

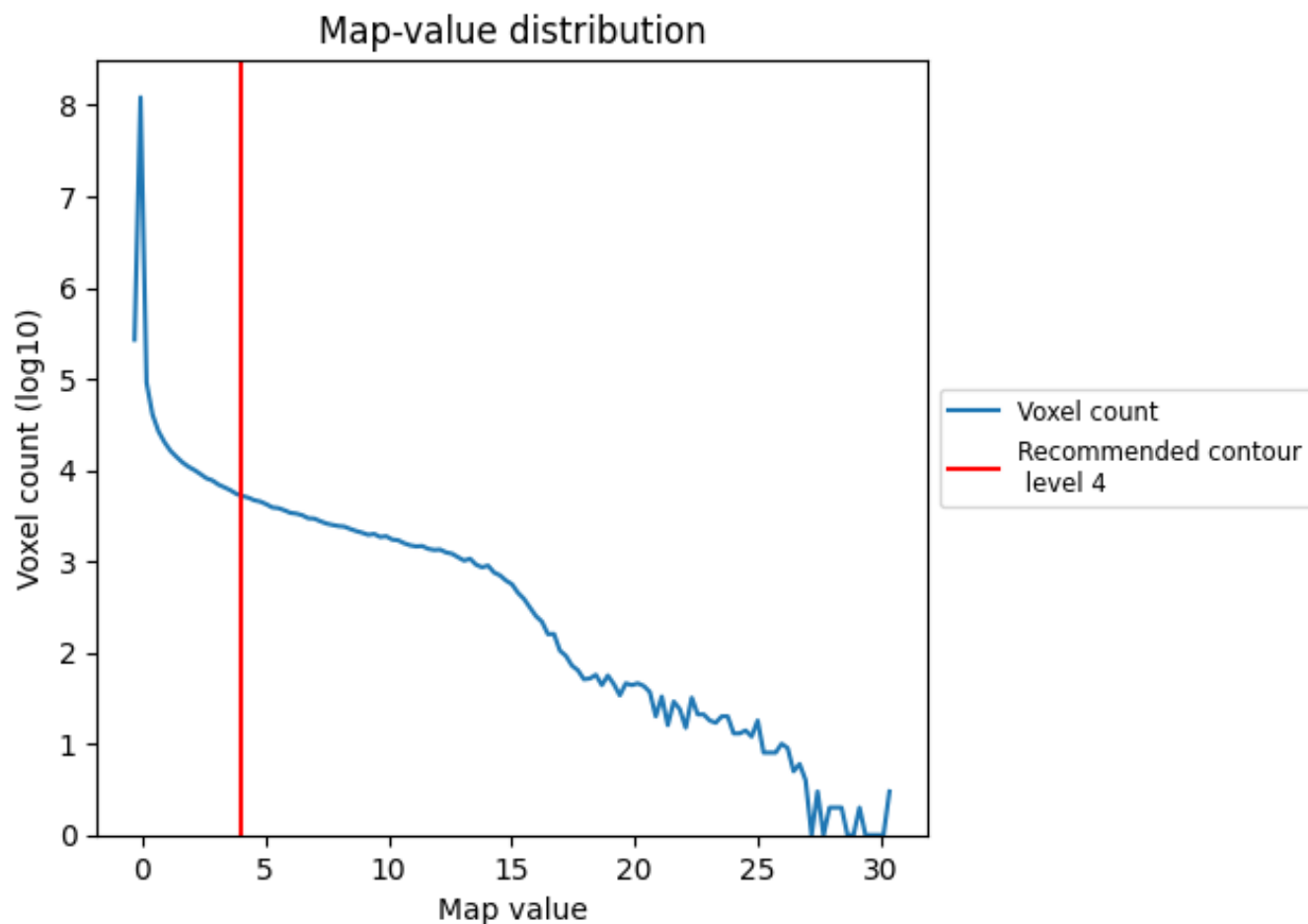
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

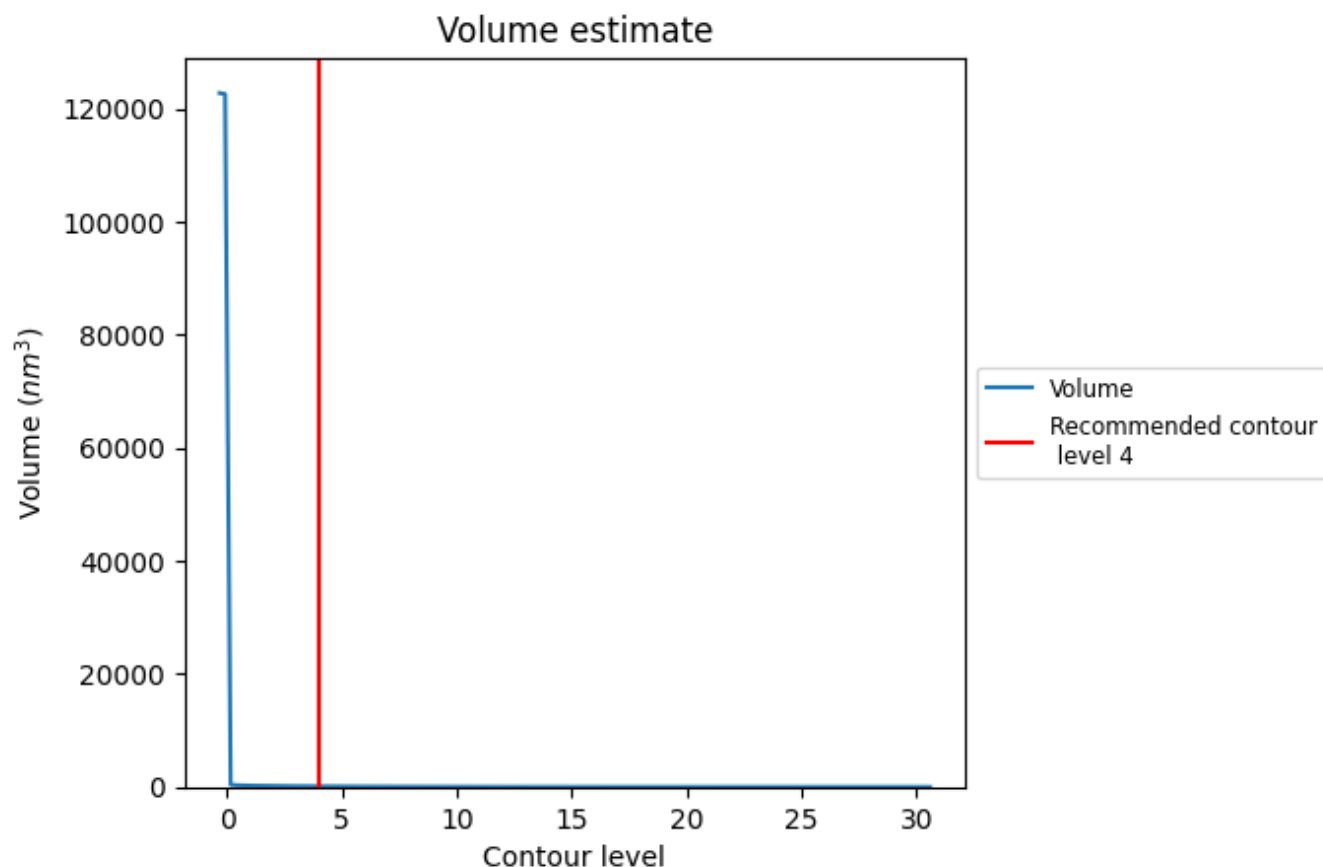
This section contains the results of statistical analysis of the map.

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.

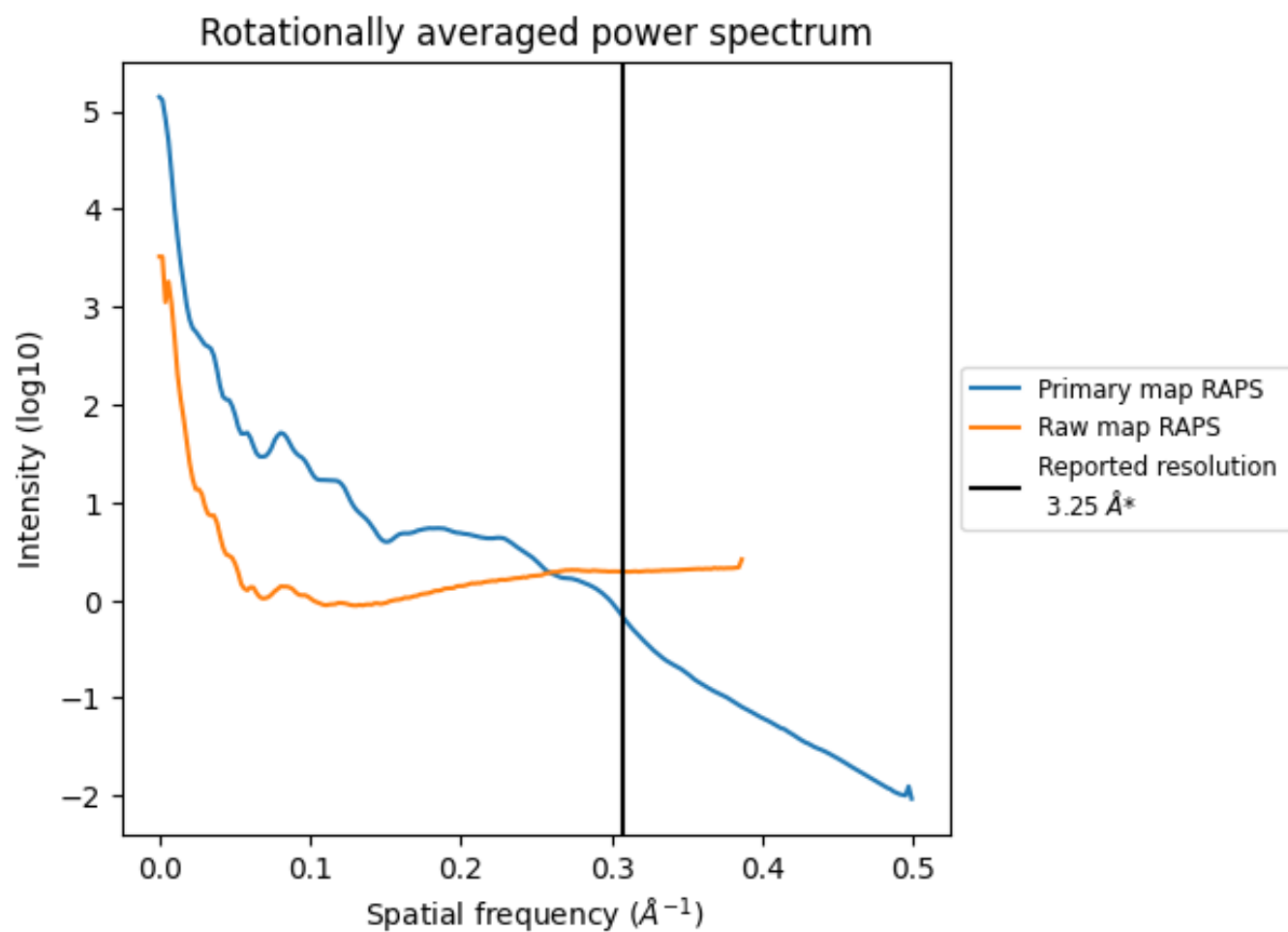
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ

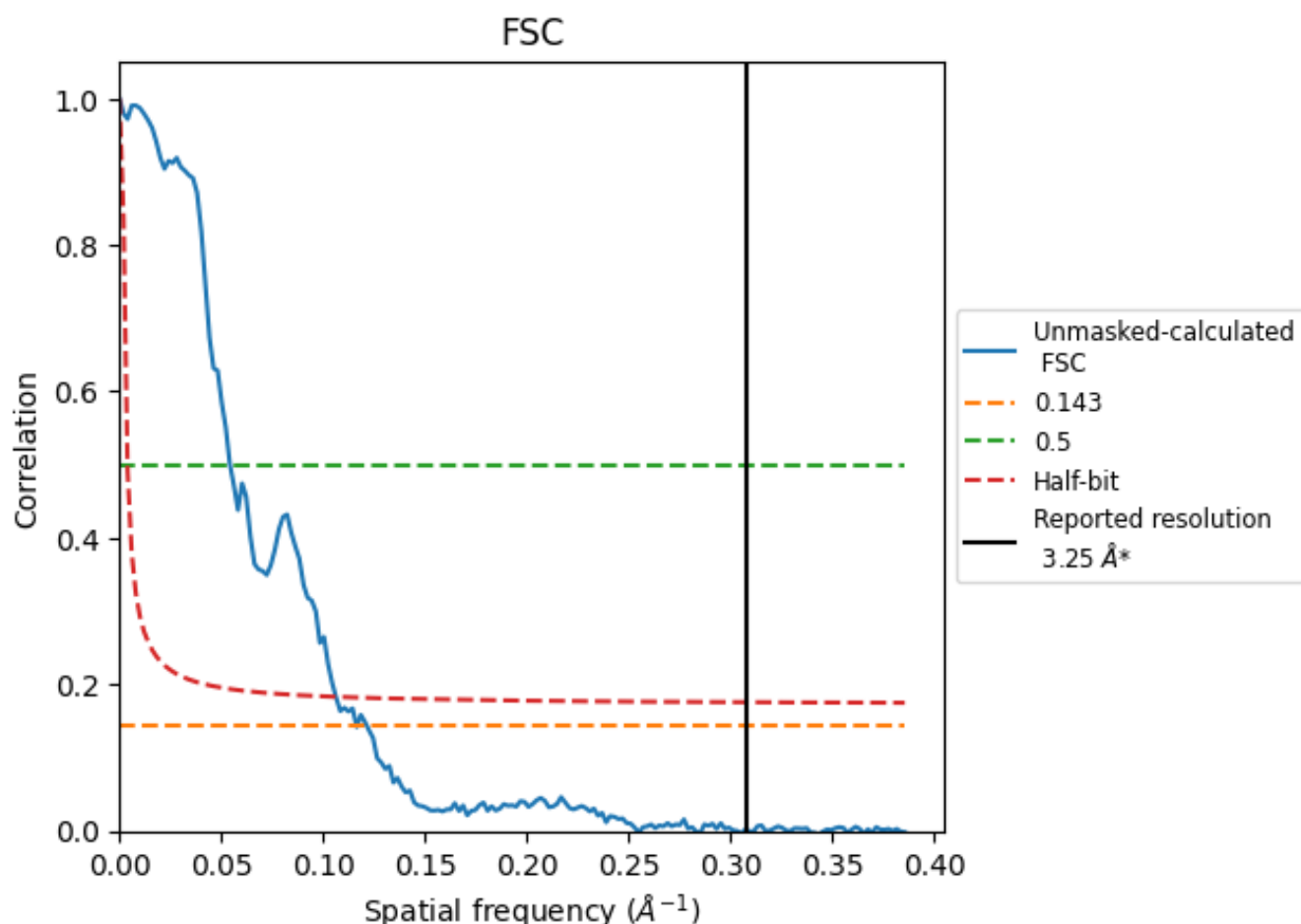


*Reported resolution corresponds to spatial frequency of 0.308 \AA^{-1}

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

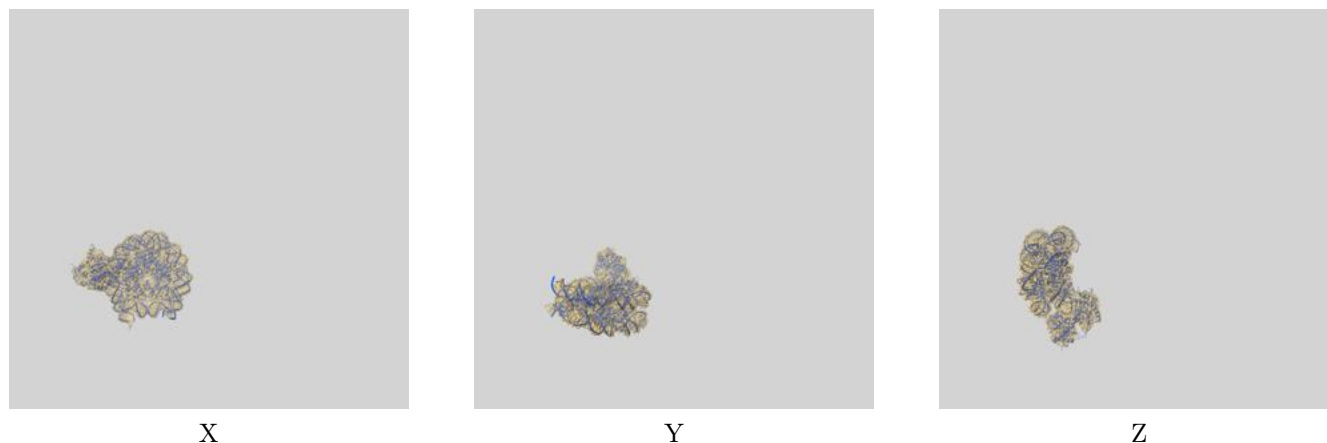
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.60	18.45	9.41

*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 8.60 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

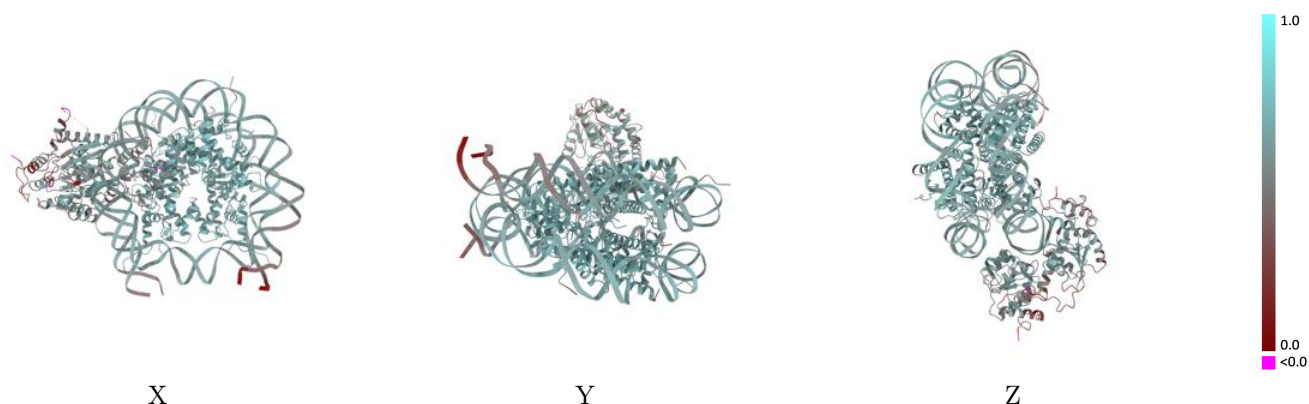
This section contains information regarding the fit between EMDB map EMD-47416 and PDB model 9E1P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



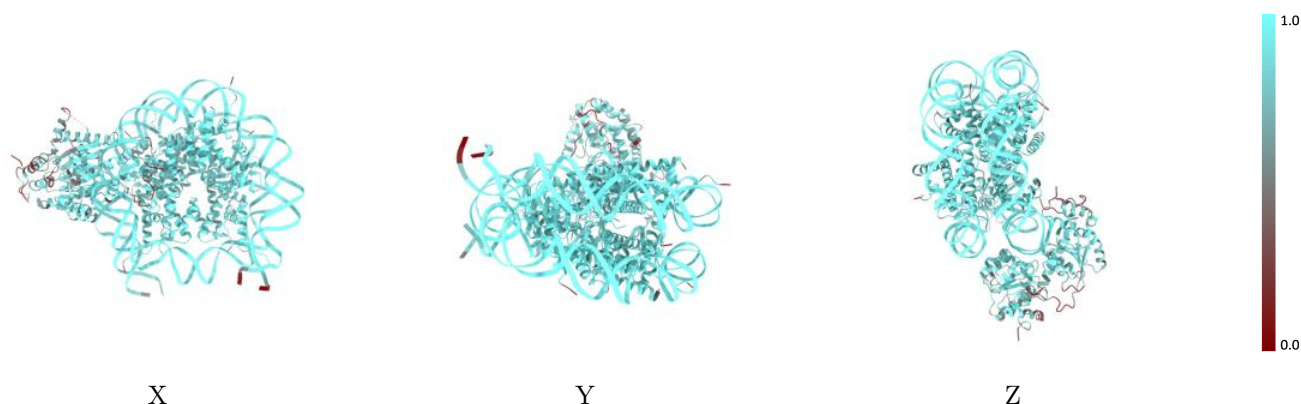
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



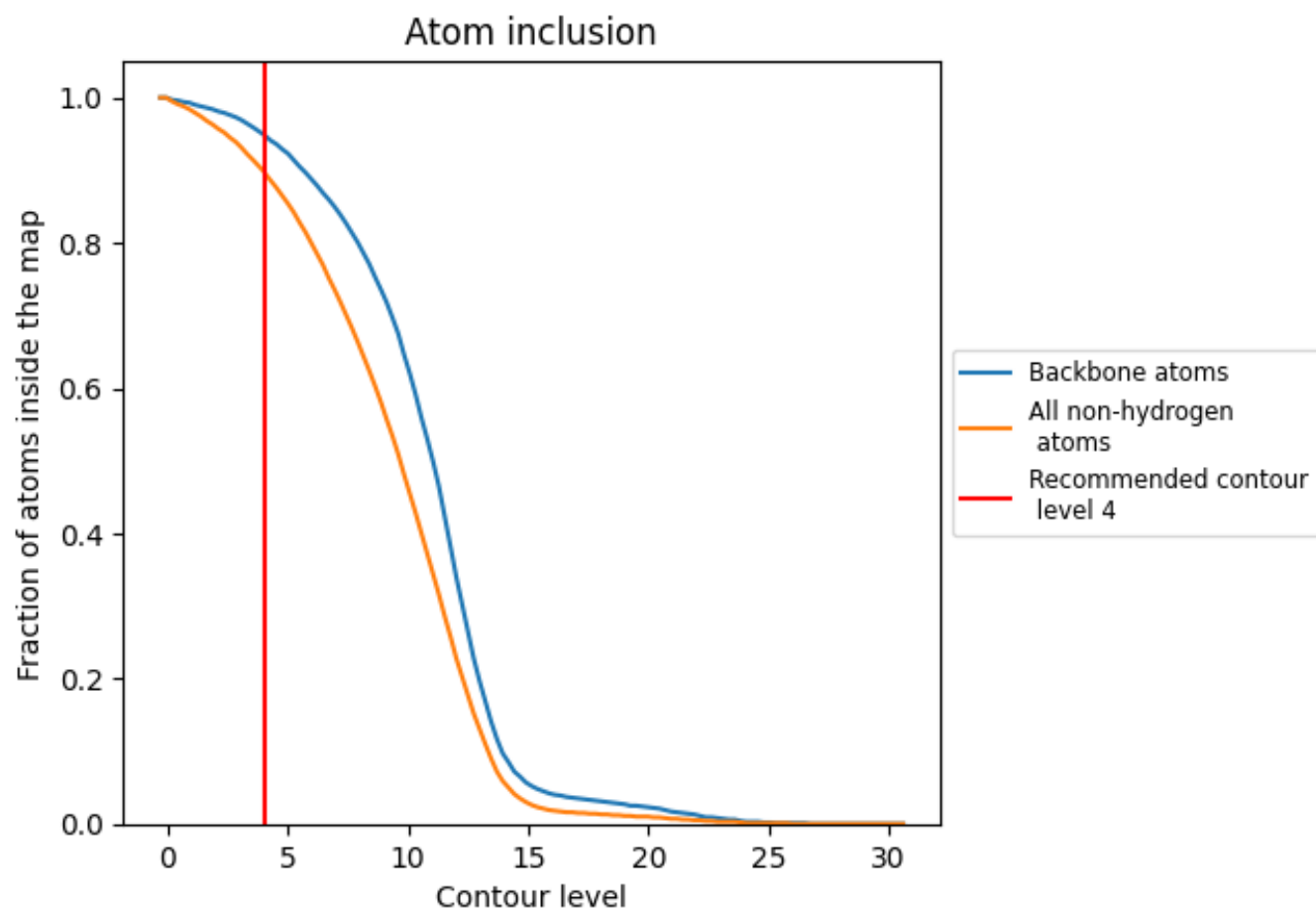
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8980</div>	<div><div></div>0.5760</div>
A	<div><div></div>0.9420</div>	<div><div></div>0.6420</div>
B	<div><div></div>0.9020</div>	<div><div></div>0.6300</div>
C	<div><div></div>0.9420</div>	<div><div></div>0.6430</div>
D	<div><div></div>0.9340</div>	<div><div></div>0.6390</div>
E	<div><div></div>0.9590</div>	<div><div></div>0.6530</div>
F	<div><div></div>0.9530</div>	<div><div></div>0.6560</div>
G	<div><div></div>0.9400</div>	<div><div></div>0.6470</div>
H	<div><div></div>0.9290</div>	<div><div></div>0.6390</div>
I	<div><div></div>0.9510</div>	<div><div></div>0.5670</div>
J	<div><div></div>0.9560</div>	<div><div></div>0.5740</div>
W	<div><div></div>0.7350</div>	<div><div></div>0.4730</div>

1.0

0.0

<0.0