wwPDB EM Validation Summary Report (i)

Oct 6, 2026 – 10:09 pm BST

PDB ID	:	9R2U / pdb_00009r2u
EMDB ID	:	EMD-53542
Title	:	Drosophila MSL HAT nucleosome complex H4K16ac post-catalytic state
Authors	:	Mueller, M.; Kolesnikova, O.; Doudin, M.; Hoffmann, T.; Becker, P.; Eustermann, S.
Deposited on	:	2025-05-01
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

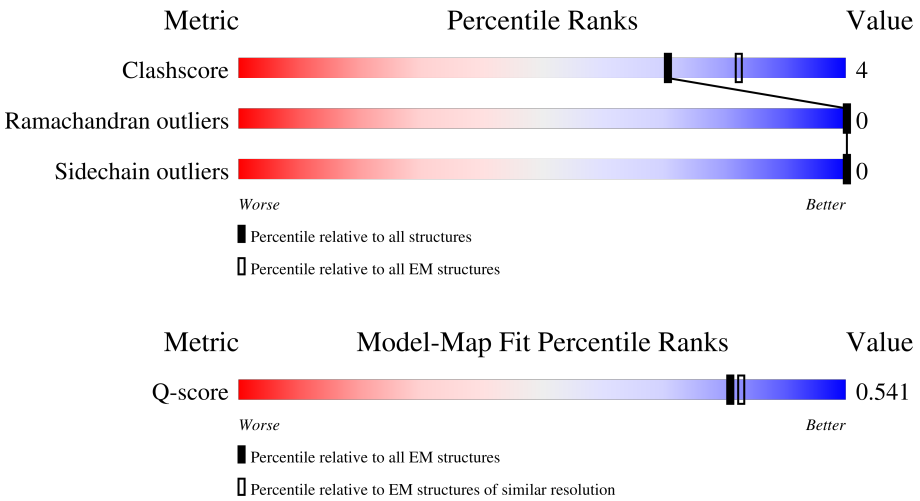
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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 <=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	70% • 27%
1	E	135	67% • 30%
2	B	102	81% 5% • 13%
3	C	129	78% 5% 16%

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Mol	Chain	Length	Quality of chain
3	G	129	79% 17%
4	D	125	75% 24%
4	H	125	71% 25%
5	F	102	72% 9% 20%
6	I	225	45% 16% 35%
7	J	225	40% 23% 35%
8	M	1047	15% 83%
9	N	518	37% 8% 55%
10	O	827	39% 5% 56%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18584 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	98	810	511	157	138	4	0	0
1	E	95	783	494	150	135	4	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	89	715	449	144	121	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	108	833	525	165	143	0	0
3	G	107	826	522	162	142	0	0

- Molecule 4 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	746	467	136	141	2	0	0
4	H	94	735	461	132	140	2	0	0

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	82	653	412	127	113	1	0	0

- Molecule 6 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	147	2996	1423	542	884	147	0	0

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	147	3031	1434	570	880	147	0	0

- Molecule 8 is a protein called Protein male-specific lethal-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	177	1456	911	264	277	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1040	ASP	-	expression tag	UNP P50535
M	1041	TYR	-	expression tag	UNP P50535
M	1042	LYS	-	expression tag	UNP P50535
M	1043	ASP	-	expression tag	UNP P50535
M	1044	ASP	-	expression tag	UNP P50535
M	1045	ASP	-	expression tag	UNP P50535
M	1046	ASP	-	expression tag	UNP P50535
M	1047	LYS	-	expression tag	UNP P50535

- Molecule 9 is a protein called Protein male-specific lethal-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	234	1942	1239	337	352	14	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-5	MET	-	initiating methionine	UNP P50536
N	-4	HIS	-	expression tag	UNP P50536
N	-3	HIS	-	expression tag	UNP P50536
N	-2	HIS	-	expression tag	UNP P50536
N	-1	HIS	-	expression tag	UNP P50536

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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	HIS	-	expression tag	UNP P50536
N	1	HIS	-	expression tag	UNP P50536
N	184	THR	ALA	variant	UNP P50536
N	352	GLY	VAL	variant	UNP P50536

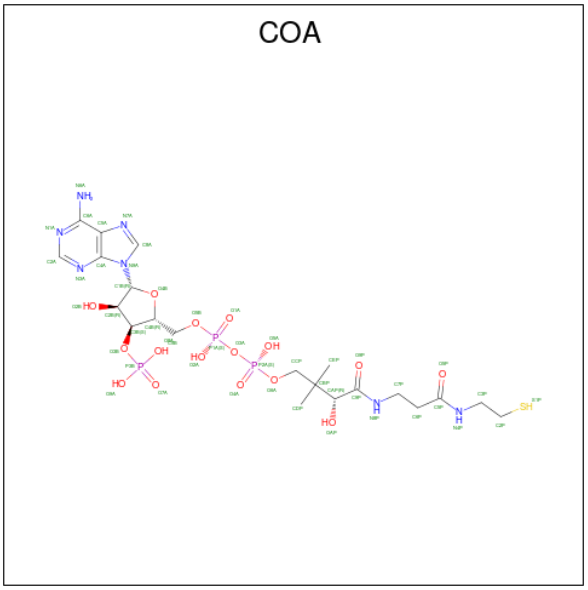
- Molecule 10 is a protein called Histone acetyltransferase MOF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	O	364	3009	1931	507	554	17	0	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	O	1	1	1	0

- Molecule 12 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



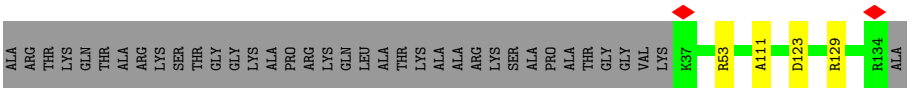
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
12	O	1	48	21	7	16	3	1	0

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.

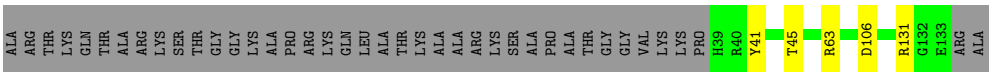
- Molecule 1: Histone H3.1

Chain A:



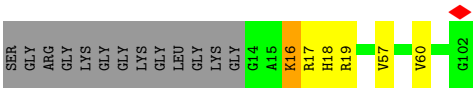
- Molecule 1: Histone H3.1

Chain E:



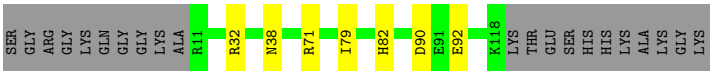
- Molecule 2: Histone H4

Chain B:



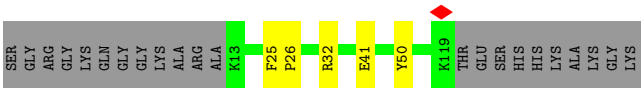
- Molecule 3: Histone H2A type 1-C

Chain C:



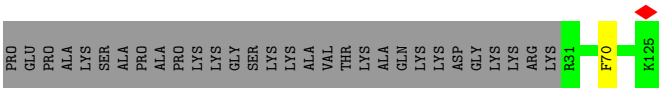
- Molecule 3: Histone H2A type 1-C

Chain G:



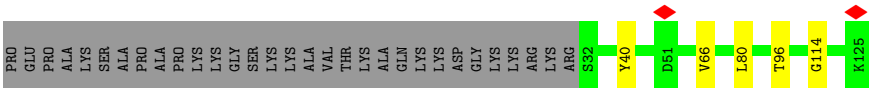
- Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain D:



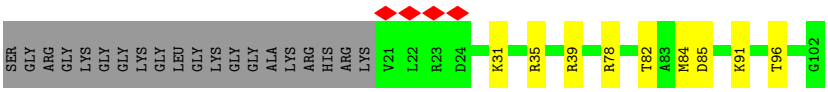
- Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain H:



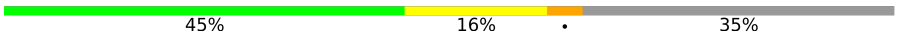
- Molecule 5: Histone H4

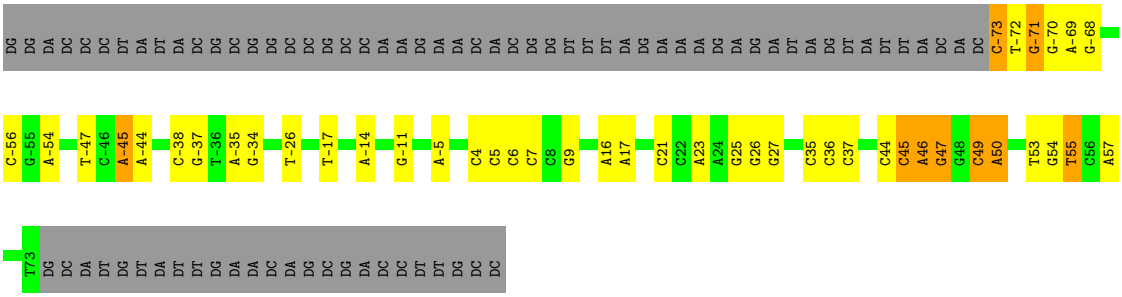
Chain F:



- Molecule 6: DNA

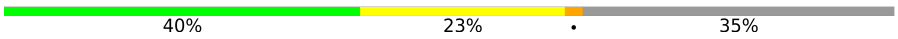
Chain I:

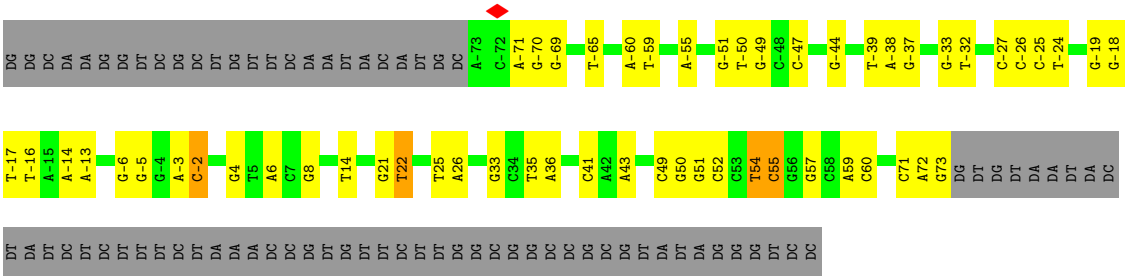




- Molecule 7: DNA

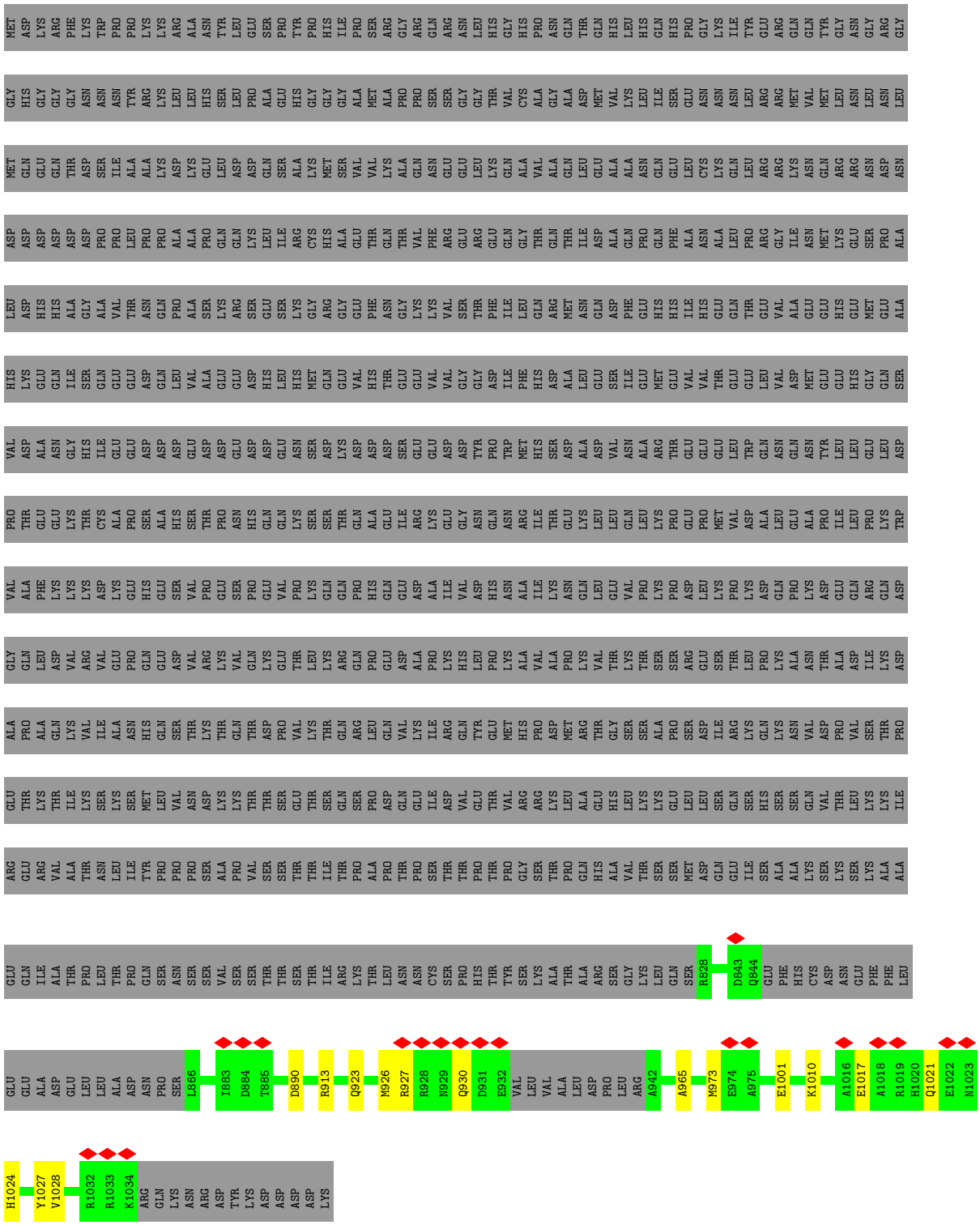
Chain J:





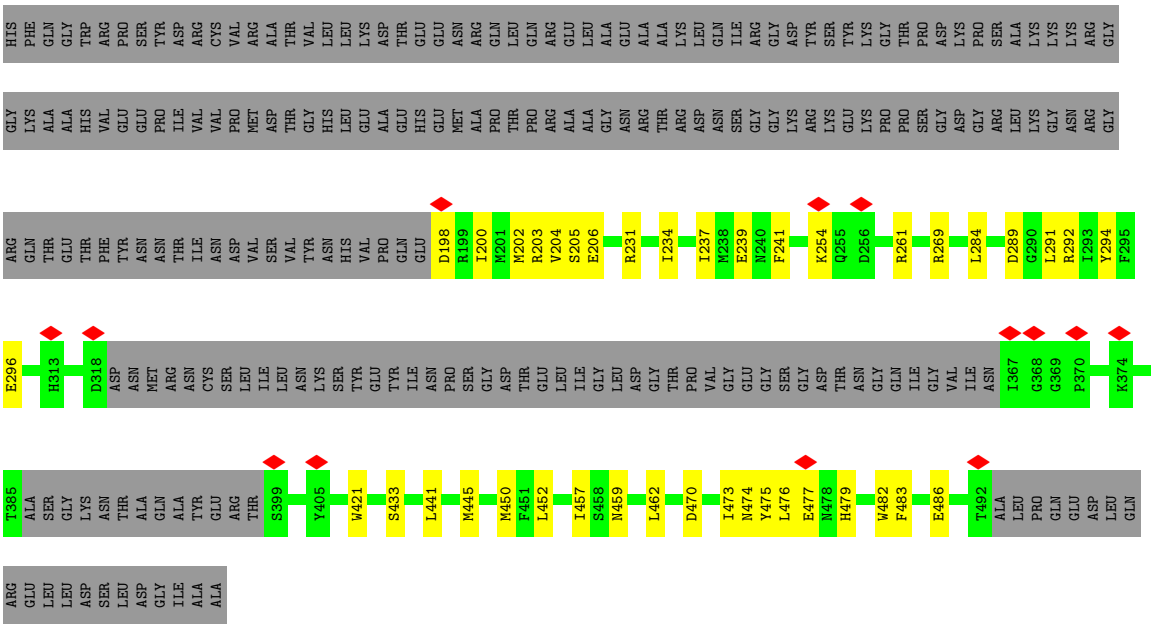
- Molecule 8: Protein male-specific lethal-1

Chain M:



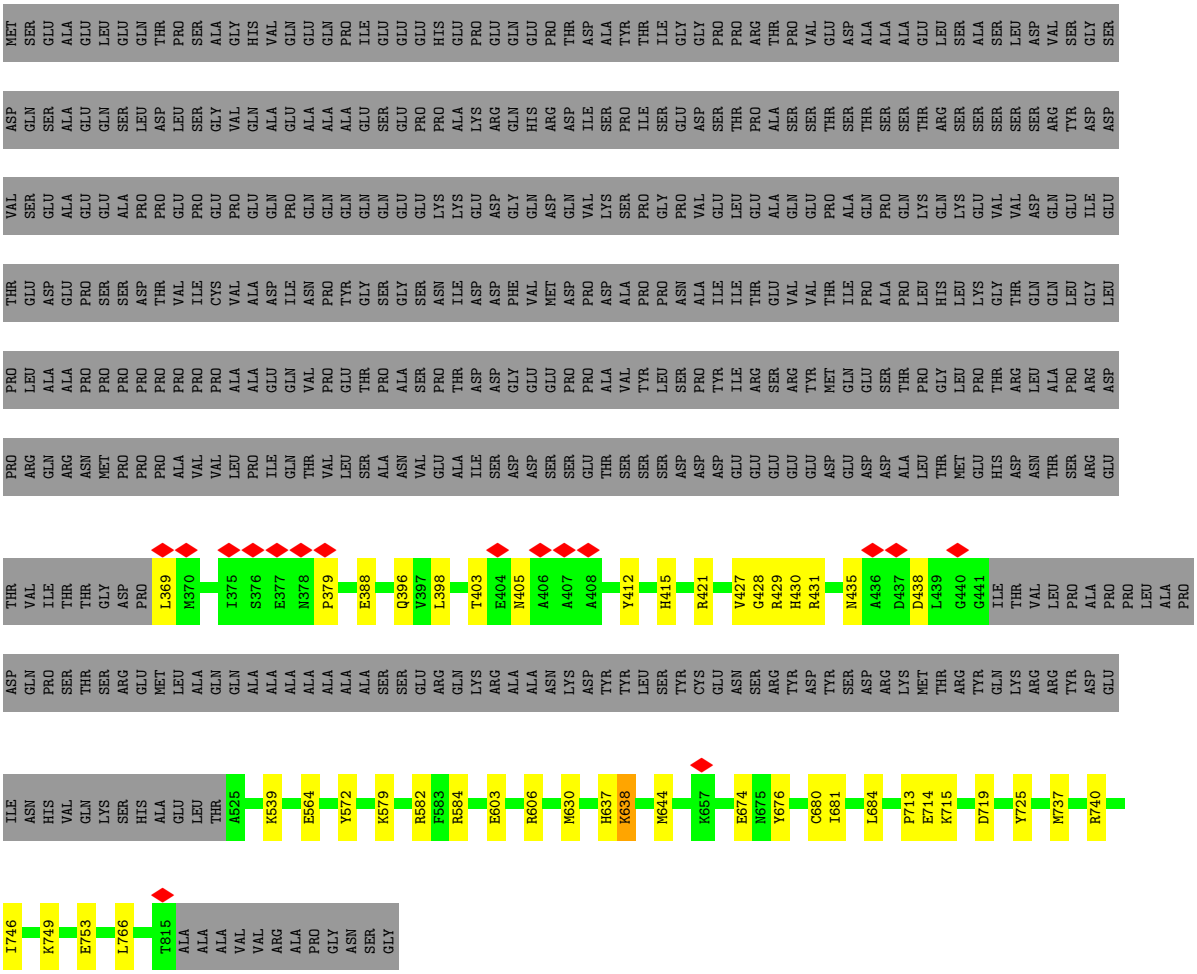
• Molecule 9: Protein male-specific lethal-3

Chain N:



• Molecule 10: Histone acetyltransferase MOF

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92666	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 ($e^-/Å^2$)	48.97	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	8.299	Depositor
Minimum map value	-5.356	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	0.83	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: COA, ZN, ALY

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	0.53	0/822	0.54	0/1102
1	E	0.50	0/794	0.50	0/1065
2	B	0.53	0/710	0.53	0/946
3	C	0.43	0/843	0.44	0/1136
3	G	0.42	0/836	0.50	0/1126
4	D	0.45	0/757	0.46	0/1015
4	H	0.43	0/746	0.50	0/1001
5	F	0.50	0/660	0.51	0/883
6	I	0.99	0/3356	1.39	35/5173 (0.7%)
7	J	0.96	0/3404	1.40	44/5256 (0.8%)
8	M	0.45	0/1487	0.56	0/2011
9	N	0.51	0/1982	0.57	0/2671
10	O	0.58	0/3070	0.60	1/4143 (0.0%)
All	All	0.70	0/19467	0.96	80/27528 (0.3%)

There are no bond length outliers.

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	50	DA	O5'-C5'-C4'	10.35	117.68	109.40
6	I	-45	DA	O5'-C5'-C4'	9.21	116.77	109.40
6	I	-35	DA	O5'-C5'-C4'	8.18	115.94	109.40
6	I	47	DG	O4'-C1'-N9	-7.93	102.45	108.00
6	I	57	DA	O4'-C1'-N9	-7.74	102.58	108.00

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	810	0	851	3	0
1	E	783	0	818	5	0
2	B	715	0	763	7	0
3	C	833	0	895	6	0
3	G	826	0	890	6	0
4	D	746	0	769	1	0
4	H	735	0	756	4	0
5	F	653	0	696	5	0
6	I	2996	0	1651	14	0
7	J	3031	0	1649	15	0
8	M	1456	0	1424	16	0
9	N	1942	0	1947	34	0
10	O	3009	0	2970	30	0
11	O	1	0	0	0	0
12	O	48	0	32	2	0
All	All	18584	0	16111	121	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 4.

The worst 5 of 121 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)
9:N:254:LYS:HB2	9:N:269:ARG:HH22	1.40	0.85
8:M:973:MET:HE2	9:N:450:MET:HE2	1.69	0.71
9:N:470:ASP:O	9:N:474:ASN:ND2	2.23	0.70
9:N:476:LEU:HA	9:N:479:HIS:HB2	1.77	0.67
3:C:32:ARG:NH1	6:I:-44:DA:OP1	2.27	0.66

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%)	93 (100%)	0	0	100	100
2	B	86/102 (84%)	81 (94%)	5 (6%)	0	100	100
3	C	106/129 (82%)	104 (98%)	2 (2%)	0	100	100
3	G	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	D	93/125 (74%)	92 (99%)	1 (1%)	0	100	100
4	H	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
5	F	80/102 (78%)	77 (96%)	3 (4%)	0	100	100
8	M	171/1047 (16%)	163 (95%)	8 (5%)	0	100	100
9	N	228/518 (44%)	218 (96%)	10 (4%)	0	100	100
10	O	359/827 (43%)	343 (96%)	16 (4%)	0	100	100
All	All	1509/3374 (45%)	1456 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/110 (78%)	86 (100%)	0	100	100
1	E	83/110 (76%)	83 (100%)	0	100	100
2	B	71/77 (92%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	84/98 (86%)	84 (100%)	0	100	100
3	G	84/98 (86%)	84 (100%)	0	100	100
4	D	82/105 (78%)	82 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
5	F	67/78 (86%)	67 (100%)	0	100	100
8	M	158/934 (17%)	158 (100%)	0	100	100
9	N	216/457 (47%)	216 (100%)	0	100	100
10	O	328/725 (45%)	328 (100%)	0	100	100
All	All	1340/2897 (46%)	1340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	84	ASN
4	H	95	GLN
9	N	262	ASN
8	M	1021	GLN
9	N	217	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
10	ALY	O	638	10	10,11,12	0.61	0	7,12,14	0.95	1 (14%)
2	ALY	B	16	2	10,11,12	0.53	0	7,12,14	1.92	3 (42%)

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
10	ALY	O	638	10	-	3/9/10/12	-
2	ALY	B	16	2	-	4/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	16	ALY	CE-NZ-CH	3.48	127.90	122.56
2	B	16	ALY	CD-CE-NZ	2.48	119.30	112.21
2	B	16	ALY	OH-CH-CH3	-2.14	118.09	122.06
10	O	638	ALY	CE-NZ-CH	2.11	125.80	122.56

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	16	ALY	C-CA-CB-CG
2	B	16	ALY	OH-CH-NZ-CE
2	B	16	ALY	CH3-CH-NZ-CE
10	O	638	ALY	OH-CH-NZ-CE
10	O	638	ALY	CH3-CH-NZ-CE

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	O	638	ALY	2	0
2	B	16	ALY	4	0

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	$\#\|Z\| > 2$
12	COA	O	1001	-	44,50,50	2.77	13 (29%)	65,75,75	1.89	14 (21%)

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
12	COA	O	1001	-	-	12/48/64/64	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	1001	COA	O4B-C1B	8.18	1.61	1.42
12	O	1001	COA	O4B-C4B	-7.81	1.27	1.45
12	O	1001	COA	C2B-C1B	-7.17	1.30	1.53
12	O	1001	COA	C5P-N4P	5.10	1.45	1.33
12	O	1001	COA	C9P-N8P	4.88	1.44	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	1001	COA	C5A-C4A-N3A	-6.26	118.58	126.75
12	O	1001	COA	C6P-C7P-N8P	-4.68	102.45	111.90
12	O	1001	COA	N3A-C2A-N1A	-4.65	121.32	128.60
12	O	1001	COA	N3A-C4A-N9A	4.39	134.32	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	1001	COA	C2A-N3A-C4A	4.00	121.21	111.75

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

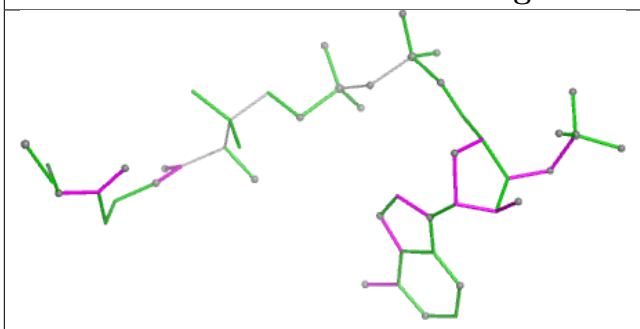
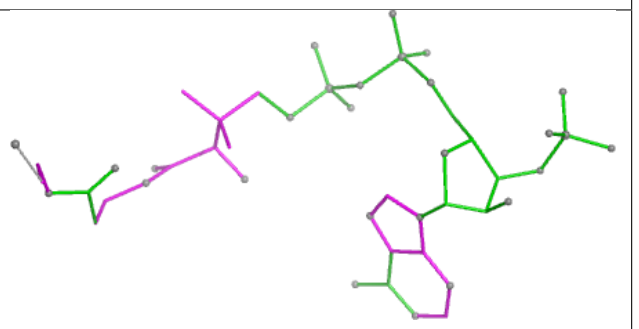
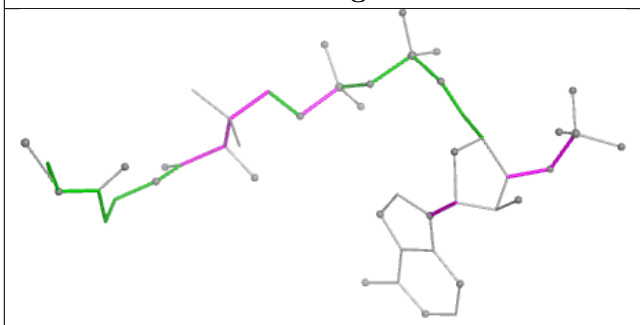
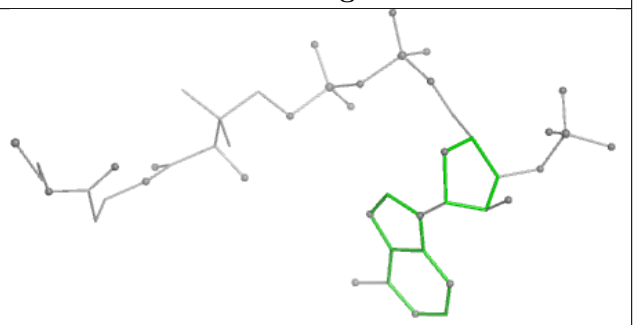
Mol	Chain	Res	Type	Atoms
12	O	1001	COA	C4B-C3B-O3B-P3B
12	O	1001	COA	O9P-C9P-CAP-CBP
12	O	1001	COA	N8P-C9P-CAP-CBP
12	O	1001	COA	O9P-C9P-CAP-OAP
12	O	1001	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	O	1001	COA	2	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 then 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.

Ligand COA O 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

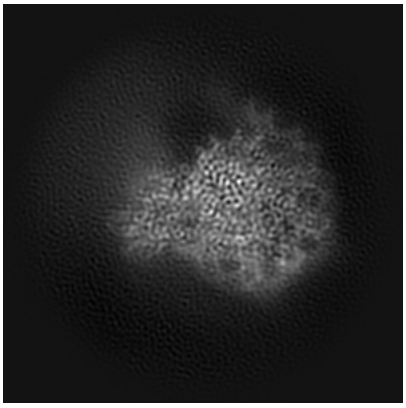
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-53542. These allow visual inspection of the internal detail of the map and identification of artifacts.

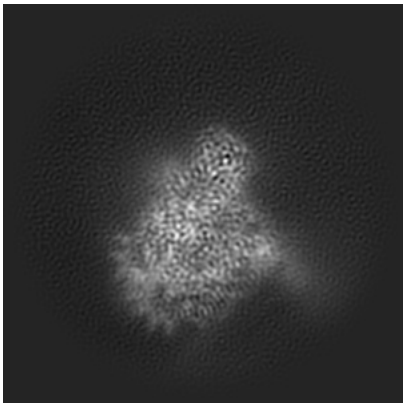
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

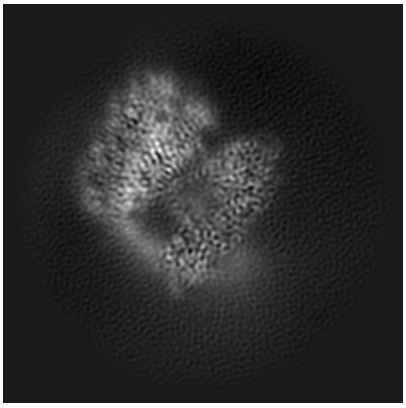
6.1.1 Primary map



X



Y

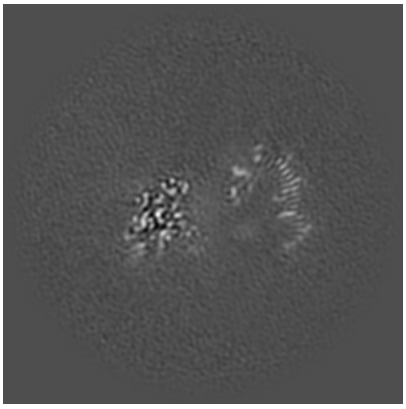


Z

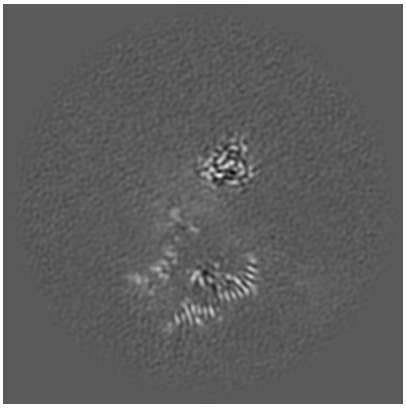
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

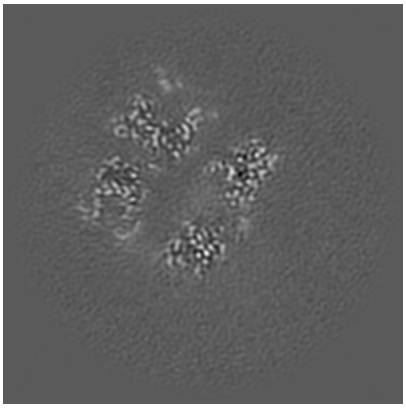
6.2.1 Primary map



X Index: 128



Y Index: 128

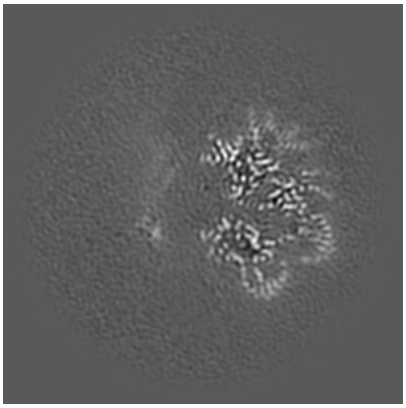


Z Index: 128

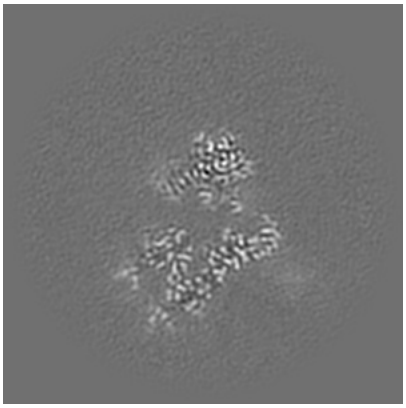
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

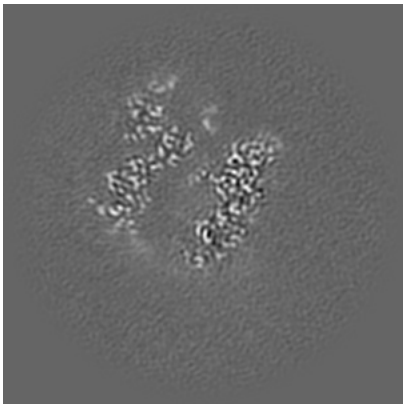
6.3.1 Primary map



X Index: 95



Y Index: 150

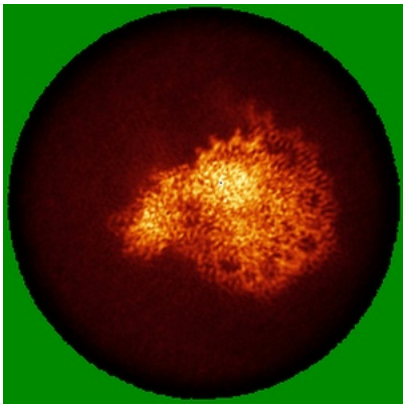


Z Index: 135

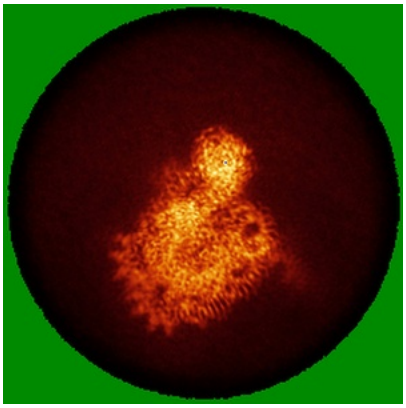
The images above show the largest variance slices of the map in three orthogonal directions.

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

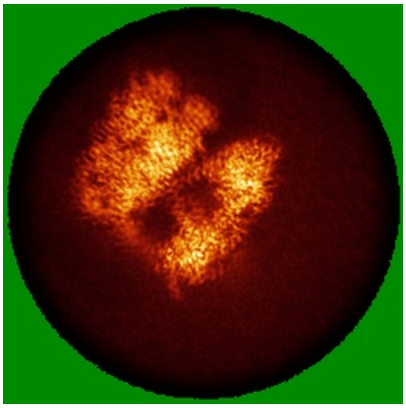
6.4.1 Primary map



X



Y

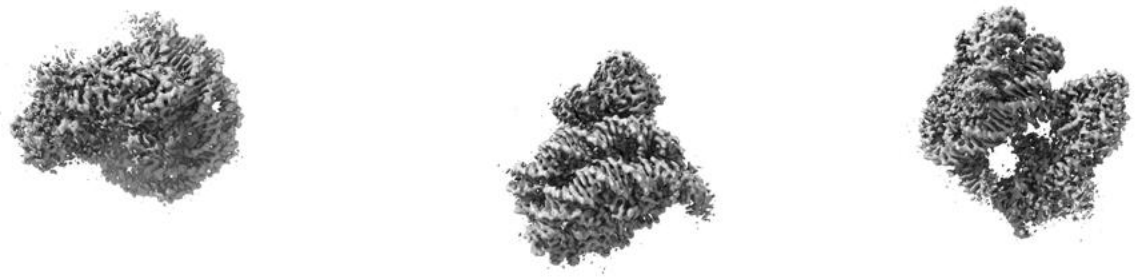


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.83. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

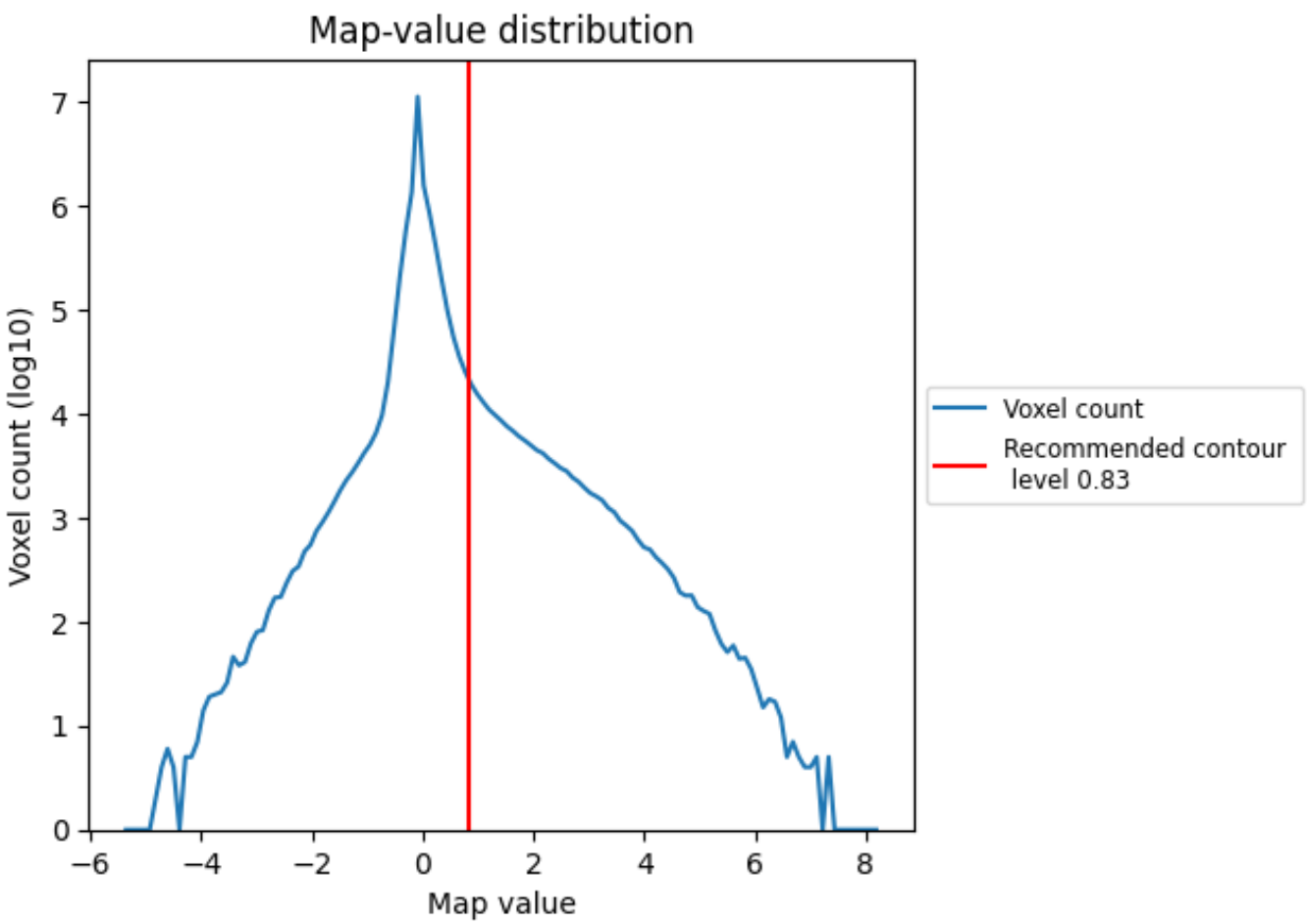
6.6 Mask visualisation (i)

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

7 Map analysis (i)

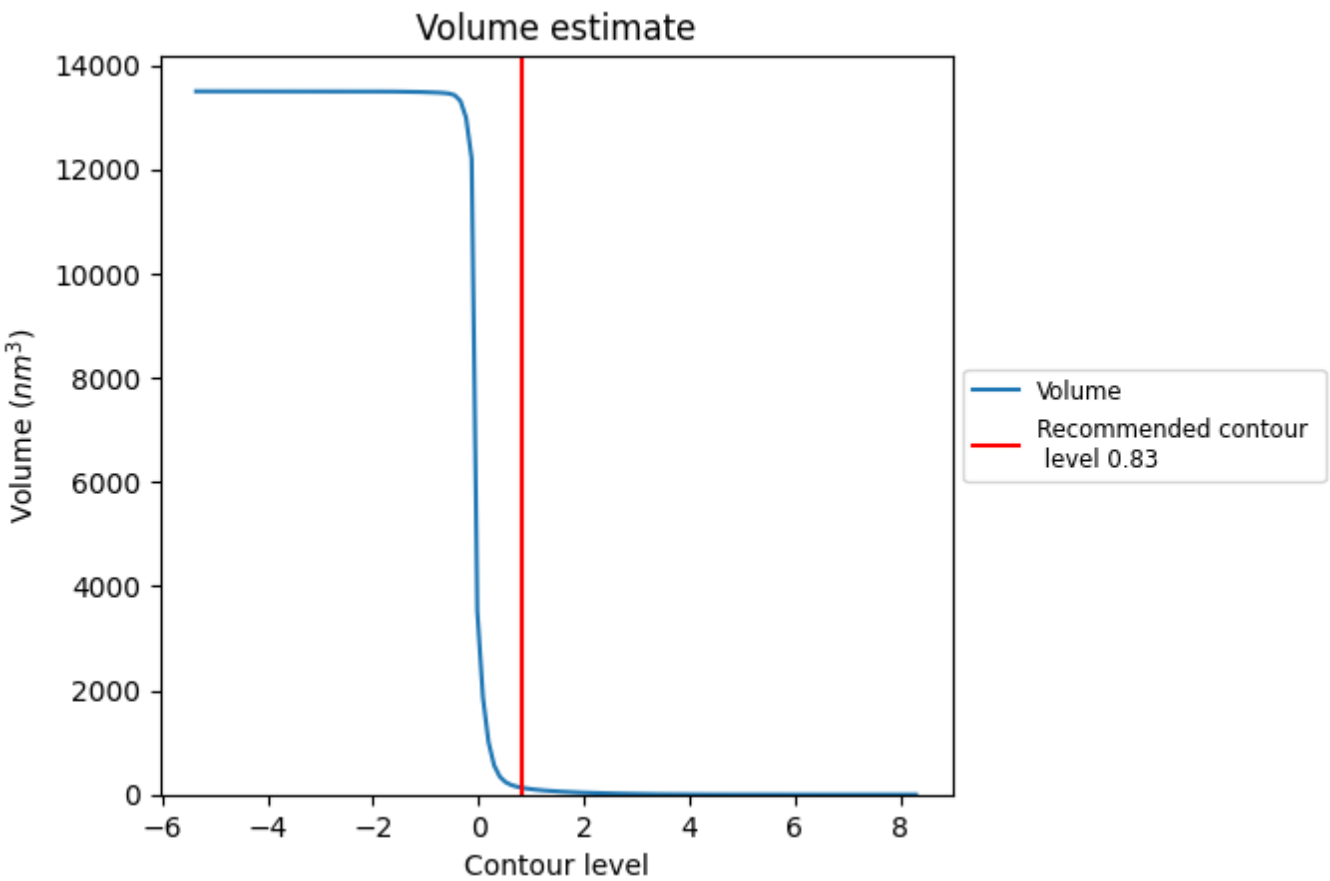
This section contains the results of statistical analysis of the map.

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.

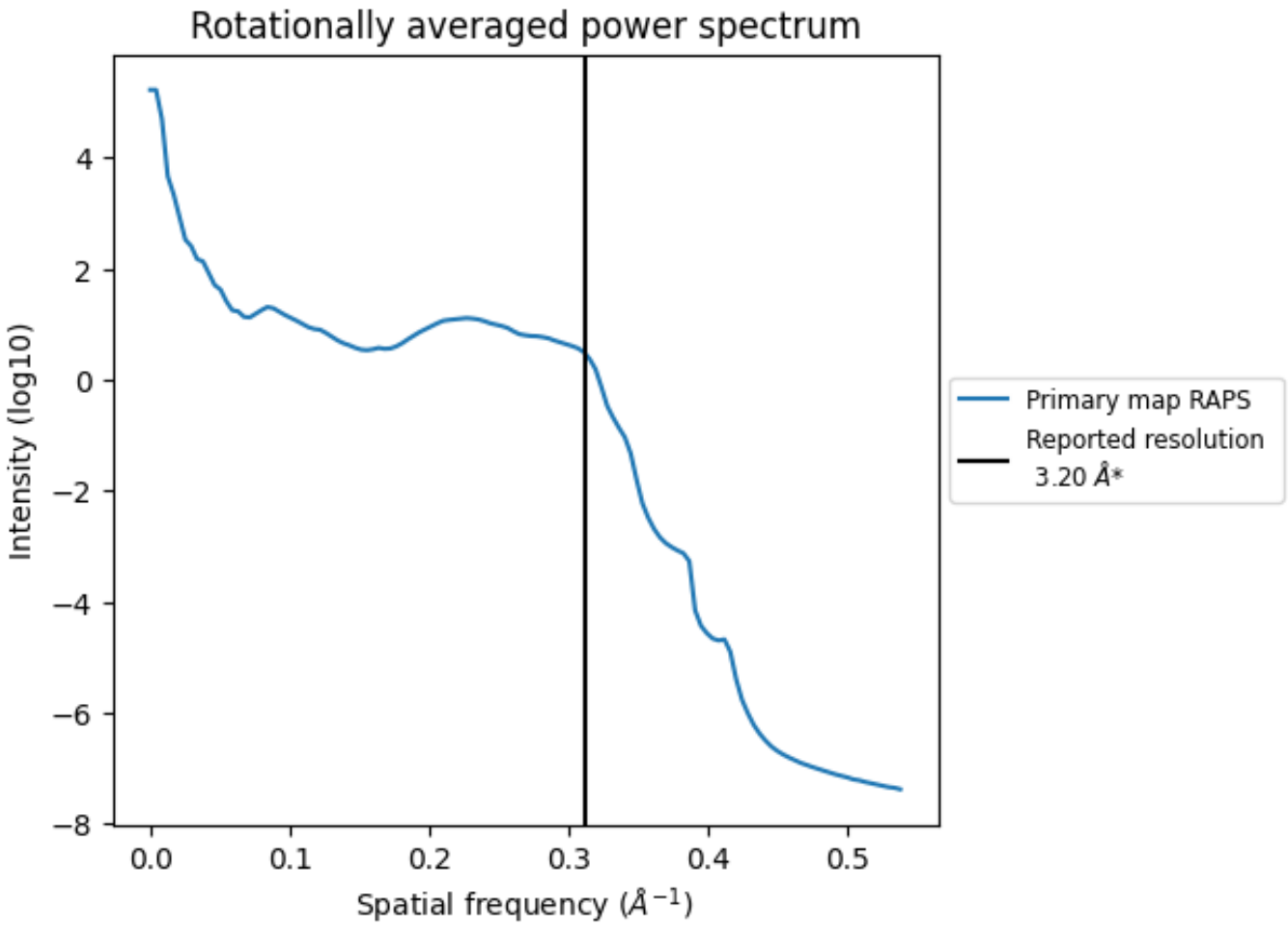
7.2 Volume estimate (i)



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 116 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

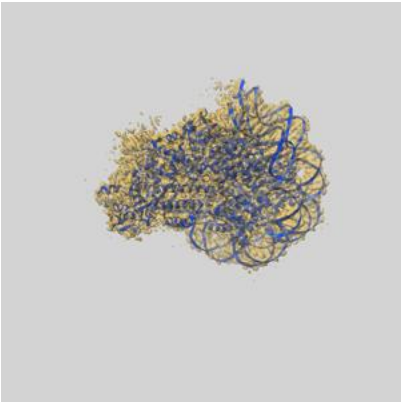
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

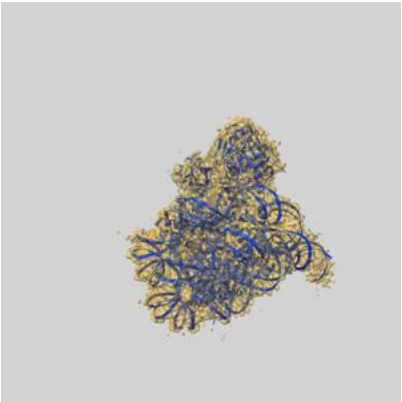
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-53542 and PDB model 9R2U. Per-residue inclusion information can be found in section 3 on page 7.

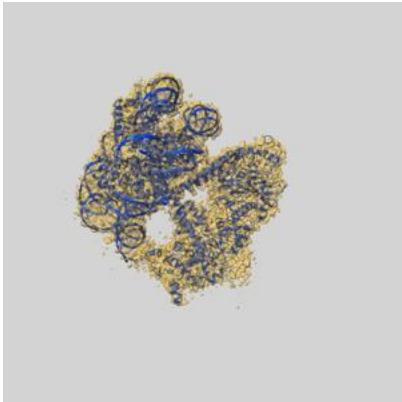
9.1 Map-model overlay (i)



X



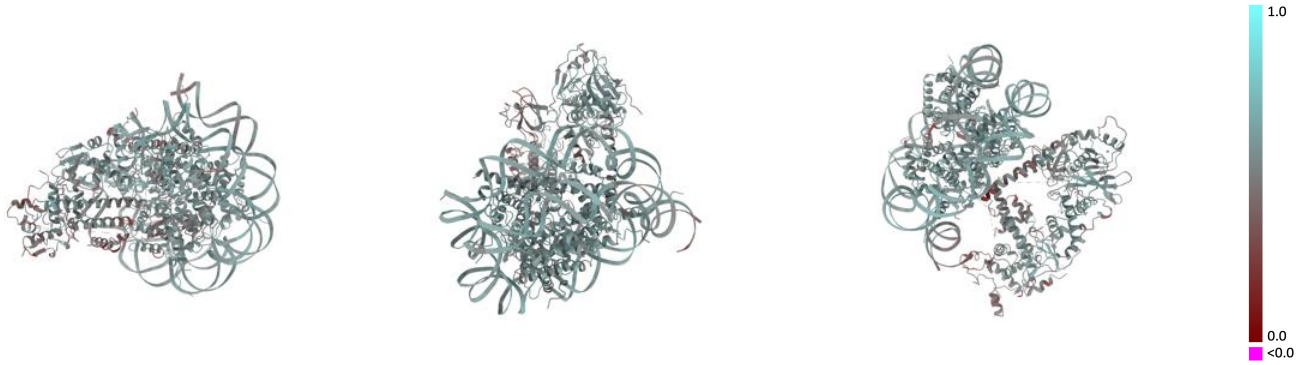
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.83 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.

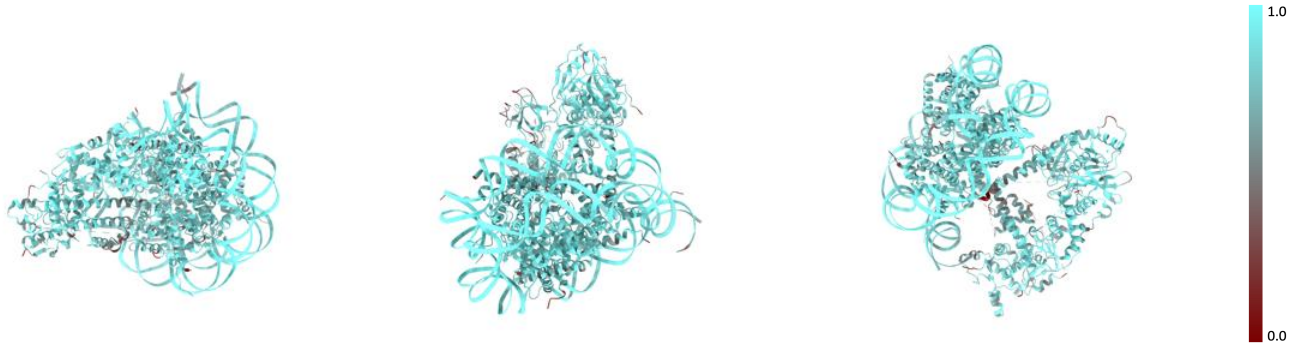
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

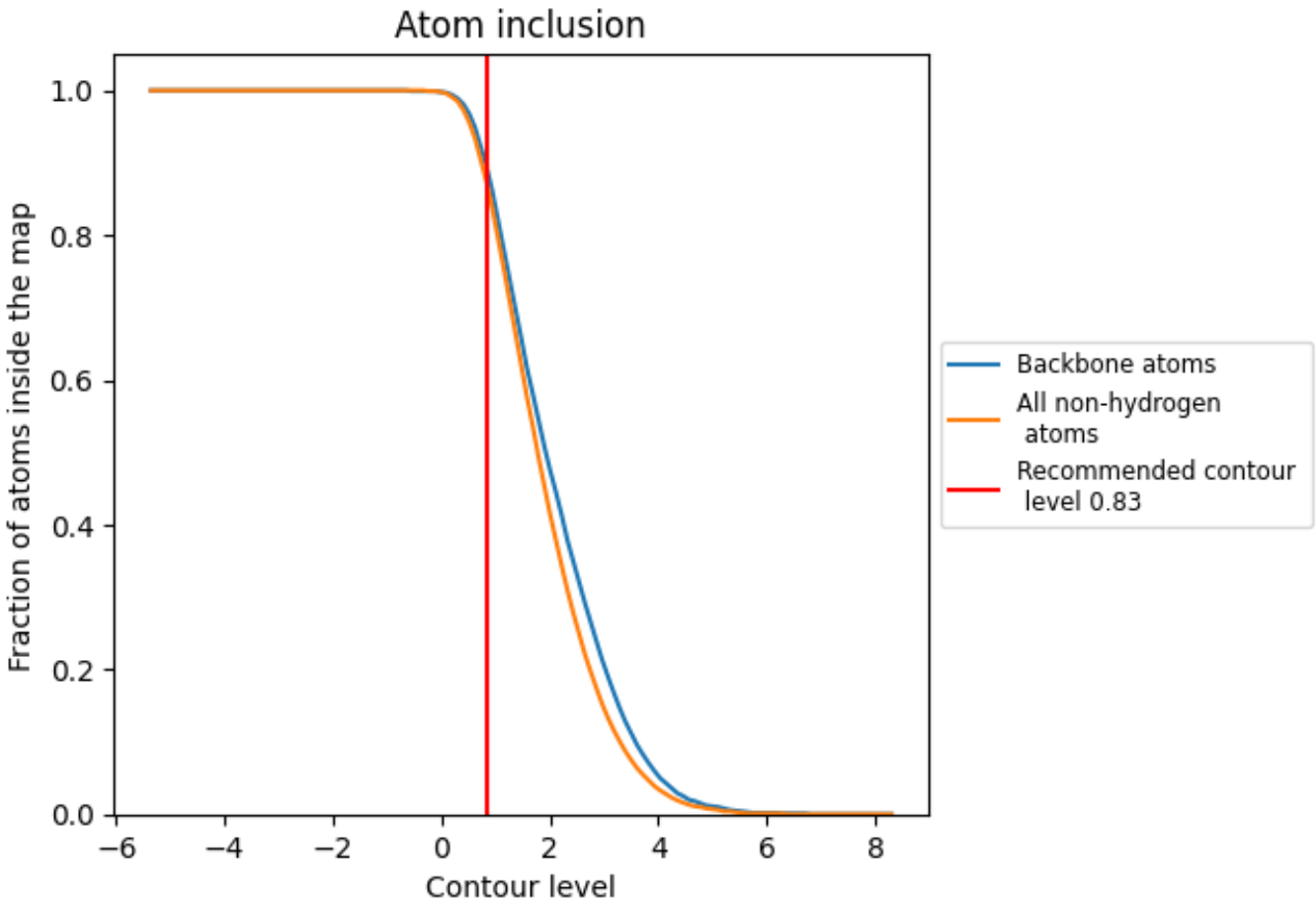
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.83).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.83) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5410
A	0.8880	0.5730
B	0.9080	0.5830
C	0.9080	0.5790
D	0.8760	0.5680
E	0.8910	0.5860
F	0.8600	0.5700
G	0.8660	0.5730
H	0.8610	0.5640
I	0.9210	0.5550
J	0.9350	0.5590
M	0.7560	0.4540
N	0.7980	0.4810
O	0.8540	0.5200