



# wwPDB EM Validation Summary Report

Oct 3, 2023 – 12:45 PM JST


PDB ID : 8KD3  
EMDB ID : EMD-37123  
Title : Rpd3S in complex with nucleosome with H3K36MLA modification, H3K9Q mutation and 187bp DNA  
Authors : Dong, S.; Li, H.; Wang, M.; Rasheed, N.; Zou, B.; Gao, X.; Guan, J.; Li, W.; Zhang, J.; Wang, C.; Zhou, N.; Shi, X.; Li, M.; Zhou, M.; Huang, J.; Li, H.; Zhang, Y.; Wong, K.H.; Zhang, X.; Chao, W.C.H.; He, J.  
Deposited on : 2023-08-09  
Resolution : 2.90 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](mailto: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>.

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

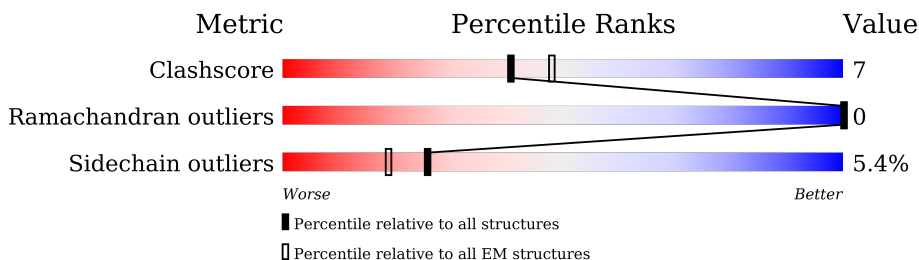
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 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 2.90 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.





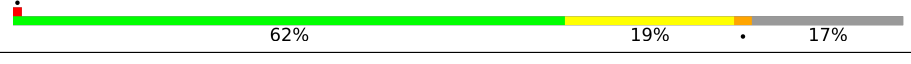
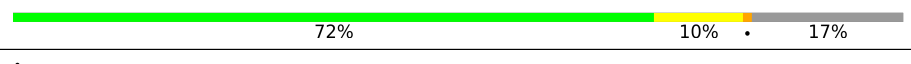
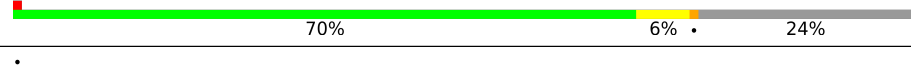

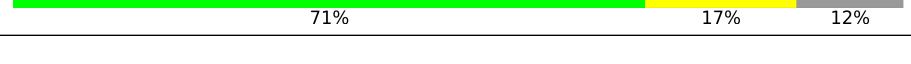
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	433	66% 23% 10%
2	B	1544	27% 7% 65%
3	D	401	8% 35% 11% 42%
3	F	401	35% 39% 10% 50%
4	E	733	6% 32% 11% 57%
4	G	733	13% 13% 83%
5	O	135	59% 15% 27%
5	S	135	59% 17% 24%

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Mol	Chain	Length	Quality of chain
6	P	102	 62% 15% 23%
6	T	102	 58% 19% 23%
7	Q	129	 62% 19% 17%
7	U	129	 72% 10% 17%
8	R	122	 70% 6% 24%
8	V	122	 62% 11% 25%
9	X	187	 7% 65% 22% 12%
10	Y	187	 6% 71% 17% 12%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27576 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 deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	388	3073	1945	521	582	25	0	0

- Molecule 2 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	542	4545	2926	761	843	15	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP P22579
B	-6	HIS	-	expression tag	UNP P22579
B	-5	HIS	-	expression tag	UNP P22579
B	-4	HIS	-	expression tag	UNP P22579
B	-3	HIS	-	expression tag	UNP P22579
B	-2	HIS	-	expression tag	UNP P22579
B	-1	HIS	-	expression tag	UNP P22579
B	0	HIS	-	expression tag	UNP P22579
B	1	HIS	-	expression tag	UNP P22579

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	231	1884	1205	312	355	12	0	0
3	F	200	1647	1061	273	302	11	0	0

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	318	Total	C	N	O	S	0	0
			2620	1666	456	481	17		
4	G	126	Total	C	N	O	S	0	0
			1043	673	174	186	10		

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	685	MET	-	expression tag	UNP Q04779
E	686	HIS	-	expression tag	UNP Q04779
E	687	HIS	-	expression tag	UNP Q04779
E	688	HIS	-	expression tag	UNP Q04779
E	689	HIS	-	expression tag	UNP Q04779
E	690	HIS	-	expression tag	UNP Q04779
E	691	HIS	-	expression tag	UNP Q04779
E	692	HIS	-	expression tag	UNP Q04779
E	693	HIS	-	expression tag	UNP Q04779
E	694	PRO	-	expression tag	UNP Q04779
E	695	GLN	-	expression tag	UNP Q04779
E	696	LEU	-	expression tag	UNP Q04779
E	697	ALA	-	expression tag	UNP Q04779
E	698	MET	-	expression tag	UNP Q04779
E	699	TRP	-	expression tag	UNP Q04779
E	700	SER	-	expression tag	UNP Q04779
E	701	HIS	-	expression tag	UNP Q04779
E	702	PRO	-	expression tag	UNP Q04779
E	703	GLN	-	expression tag	UNP Q04779
E	704	PHE	-	expression tag	UNP Q04779
E	705	GLU	-	expression tag	UNP Q04779
E	706	LYS	-	expression tag	UNP Q04779
E	707	GLY	-	expression tag	UNP Q04779
E	708	GLY	-	expression tag	UNP Q04779
E	709	GLY	-	expression tag	UNP Q04779
E	710	SER	-	expression tag	UNP Q04779
E	711	GLY	-	expression tag	UNP Q04779
E	712	GLY	-	expression tag	UNP Q04779
E	713	GLY	-	expression tag	UNP Q04779
E	714	SER	-	expression tag	UNP Q04779
E	715	GLY	-	expression tag	UNP Q04779
E	716	GLY	-	expression tag	UNP Q04779
E	717	GLY	-	expression tag	UNP Q04779
E	718	SER	-	expression tag	UNP Q04779
E	719	TRP	-	expression tag	UNP Q04779

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Chain	Residue	Modelled	Actual	Comment	Reference
E	720	SER	-	expression tag	UNP Q04779
E	721	HIS	-	expression tag	UNP Q04779
E	722	PRO	-	expression tag	UNP Q04779
E	723	GLN	-	expression tag	UNP Q04779
E	724	PHE	-	expression tag	UNP Q04779
E	725	GLU	-	expression tag	UNP Q04779
E	726	LYS	-	expression tag	UNP Q04779
E	727	GLU	-	expression tag	UNP Q04779
E	728	ASN	-	expression tag	UNP Q04779
E	729	LEU	-	expression tag	UNP Q04779
E	730	TYR	-	expression tag	UNP Q04779
E	731	PHE	-	expression tag	UNP Q04779
E	732	GLN	-	expression tag	UNP Q04779
E	733	SER	-	expression tag	UNP Q04779
G	685	MET	-	expression tag	UNP Q04779
G	686	HIS	-	expression tag	UNP Q04779
G	687	HIS	-	expression tag	UNP Q04779
G	688	HIS	-	expression tag	UNP Q04779
G	689	HIS	-	expression tag	UNP Q04779
G	690	HIS	-	expression tag	UNP Q04779
G	691	HIS	-	expression tag	UNP Q04779
G	692	HIS	-	expression tag	UNP Q04779
G	693	HIS	-	expression tag	UNP Q04779
G	694	PRO	-	expression tag	UNP Q04779
G	695	GLN	-	expression tag	UNP Q04779
G	696	LEU	-	expression tag	UNP Q04779
G	697	ALA	-	expression tag	UNP Q04779
G	698	MET	-	expression tag	UNP Q04779
G	699	TRP	-	expression tag	UNP Q04779
G	700	SER	-	expression tag	UNP Q04779
G	701	HIS	-	expression tag	UNP Q04779
G	702	PRO	-	expression tag	UNP Q04779
G	703	GLN	-	expression tag	UNP Q04779
G	704	PHE	-	expression tag	UNP Q04779
G	705	GLU	-	expression tag	UNP Q04779
G	706	LYS	-	expression tag	UNP Q04779
G	707	GLY	-	expression tag	UNP Q04779
G	708	GLY	-	expression tag	UNP Q04779
G	709	GLY	-	expression tag	UNP Q04779
G	710	SER	-	expression tag	UNP Q04779
G	711	GLY	-	expression tag	UNP Q04779
G	712	GLY	-	expression tag	UNP Q04779

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Chain	Residue	Modelled	Actual	Comment	Reference
G	713	GLY	-	expression tag	UNP Q04779
G	714	SER	-	expression tag	UNP Q04779
G	715	GLY	-	expression tag	UNP Q04779
G	716	GLY	-	expression tag	UNP Q04779
G	717	GLY	-	expression tag	UNP Q04779
G	718	SER	-	expression tag	UNP Q04779
G	719	TRP	-	expression tag	UNP Q04779
G	720	SER	-	expression tag	UNP Q04779
G	721	HIS	-	expression tag	UNP Q04779
G	722	PRO	-	expression tag	UNP Q04779
G	723	GLN	-	expression tag	UNP Q04779
G	724	PHE	-	expression tag	UNP Q04779
G	725	GLU	-	expression tag	UNP Q04779
G	726	LYS	-	expression tag	UNP Q04779
G	727	GLU	-	expression tag	UNP Q04779
G	728	ASN	-	expression tag	UNP Q04779
G	729	LEU	-	expression tag	UNP Q04779
G	730	TYR	-	expression tag	UNP Q04779
G	731	PHE	-	expression tag	UNP Q04779
G	732	GLN	-	expression tag	UNP Q04779
G	733	SER	-	expression tag	UNP Q04779

- Molecule 5 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	99	Total	C	N	O	S	0	0
			822	521	159	140	2		
5	S	103	Total	C	N	O	S	0	0
			848	535	164	147	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	9	GLN	LYS	engineered mutation	UNP A0A310TTQ1
O	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
S	9	GLN	LYS	engineered mutation	UNP A0A310TTQ1
S	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	79	Total	C	N	O	S	0	0
			637	403	124	109	1		
6	T	79	Total	C	N	O	S	0	0
			637	403	124	109	1		

- Molecule 7 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	107	Total	C	N	O		0	0
			825	519	163	143			
7	U	107	Total	C	N	O		0	0
			825	519	163	143			

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	93	Total	C	N	O	S	0	0
			730	460	131	137	2		
8	V	91	Total	C	N	O	S	0	0
			715	451	128	134	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	THR	SER	engineered mutation	UNP P02281
V	29	THR	SER	engineered mutation	UNP P02281

- Molecule 9 is a DNA chain called 187bp DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	164	Total	C	N	O	P	0	0
			3384	1599	639	982	164		

- Molecule 10 is a DNA chain called 187bp DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	164	Total	C	N	O	P	0	0
			3340	1585	605	986	164		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

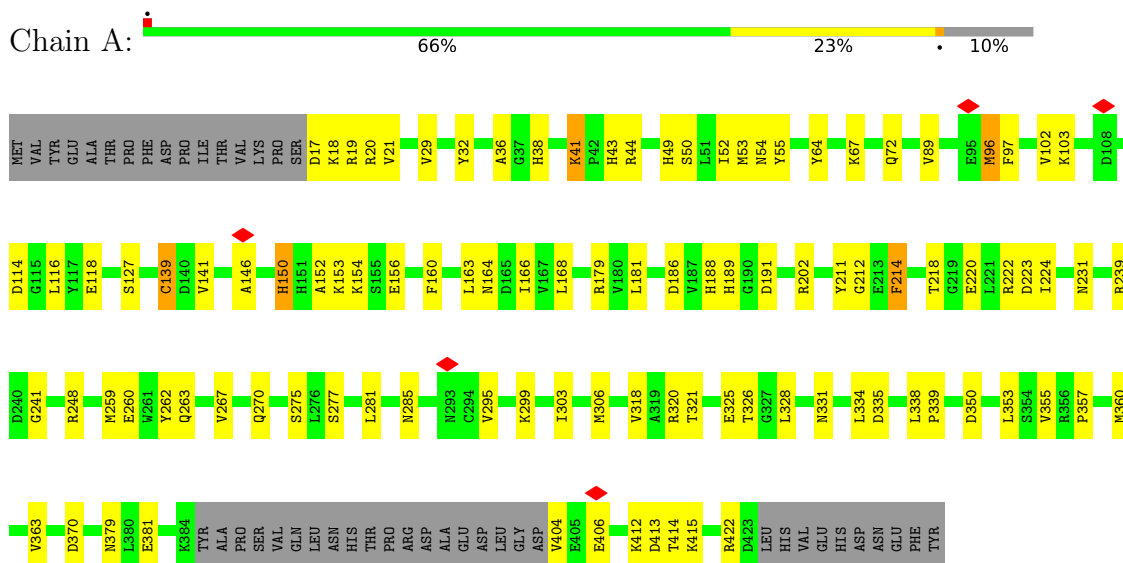


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
11	A	1	Total 1	Zn 1	0

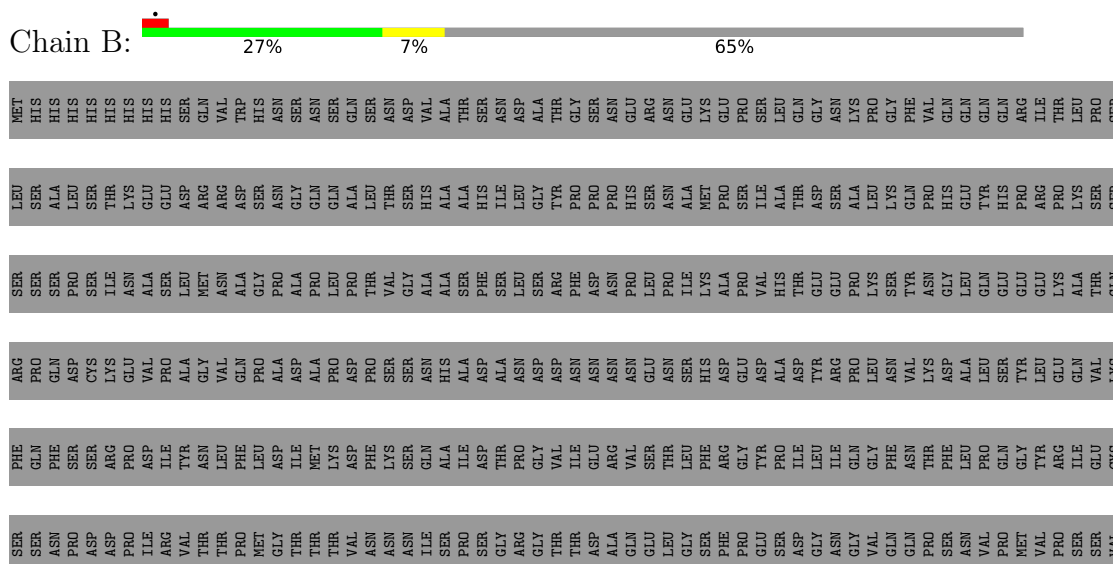
### 3 Residue-property plots [i](#)

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.

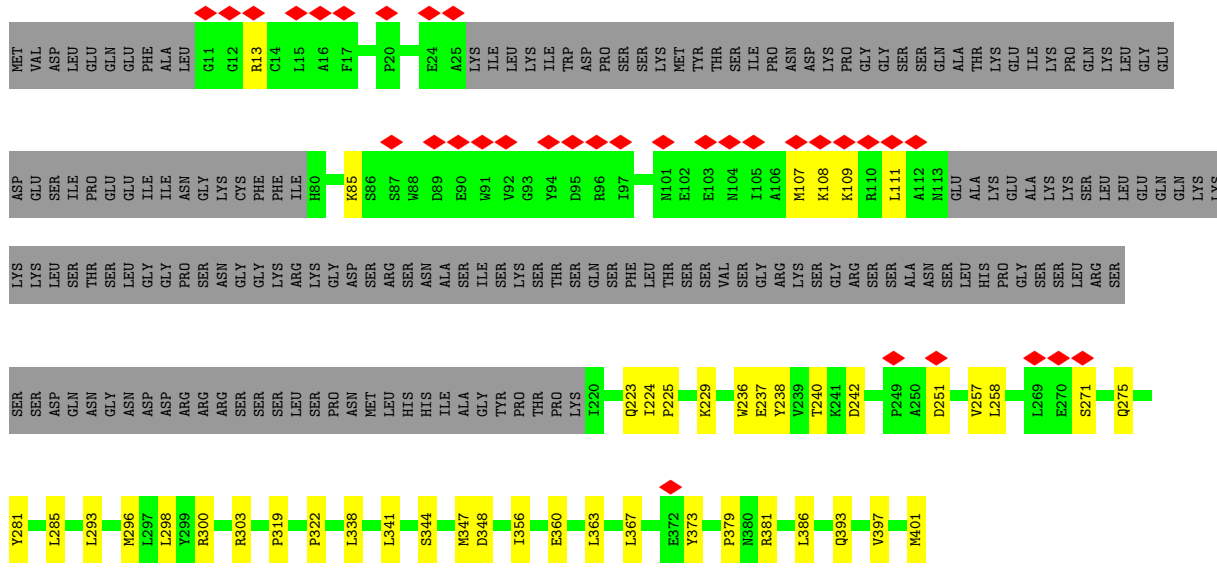
- Molecule 1: Histone deacetylase RPD3



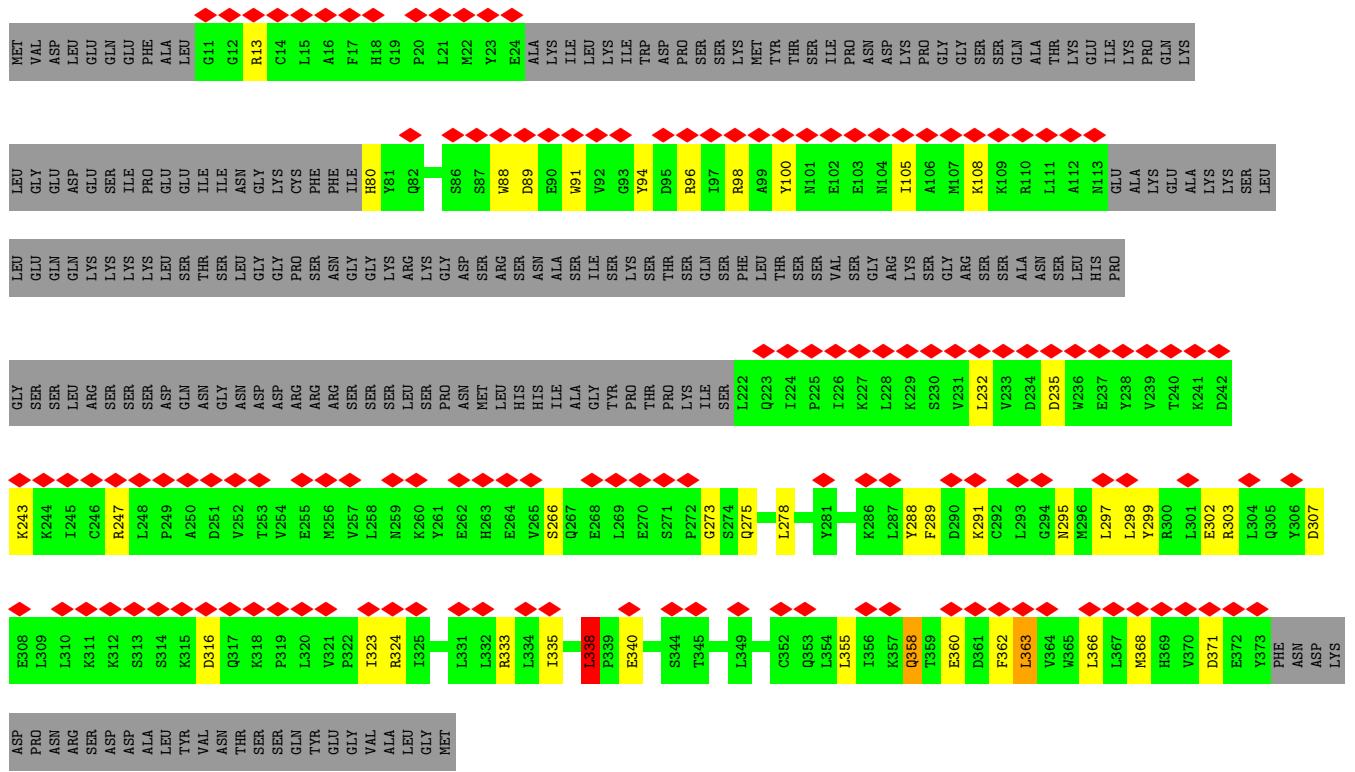
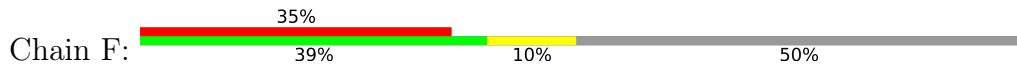
- Molecule 2: Transcriptional regulatory protein SIN3



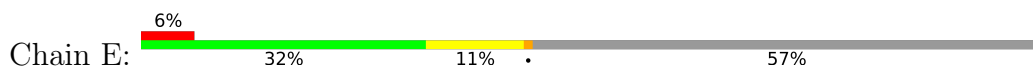


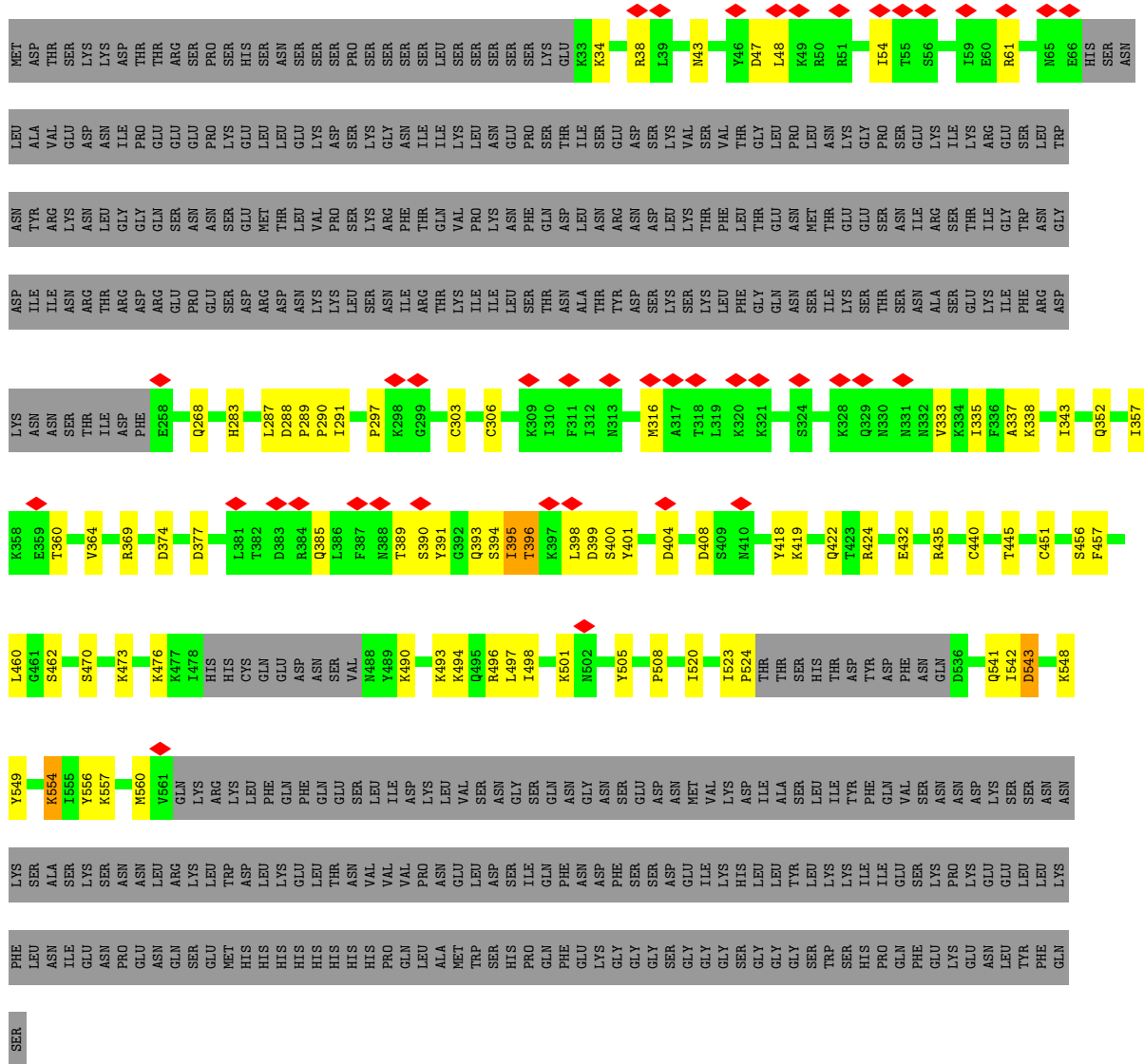


• Molecule 3: Chromatin modification-related protein EAF3

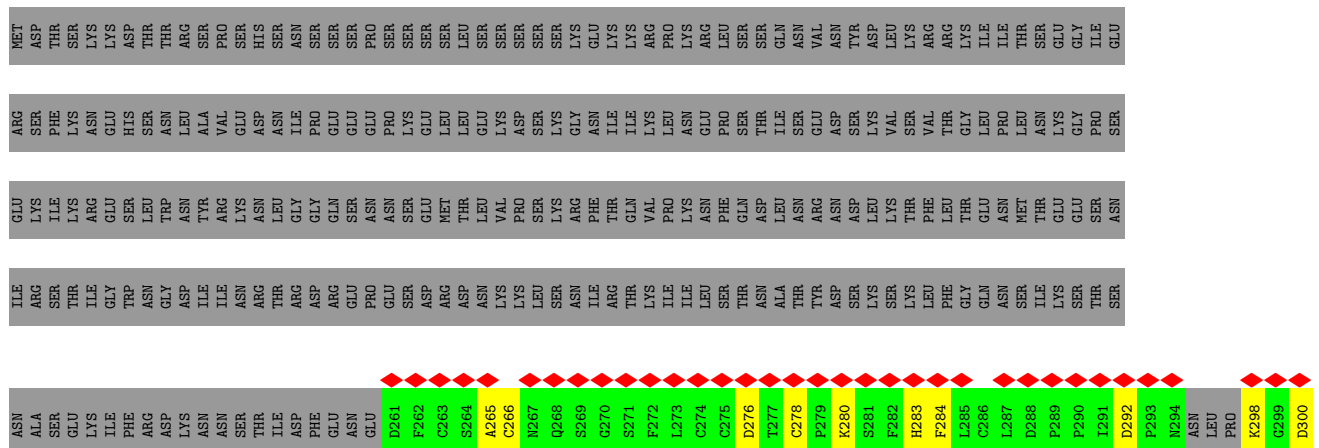


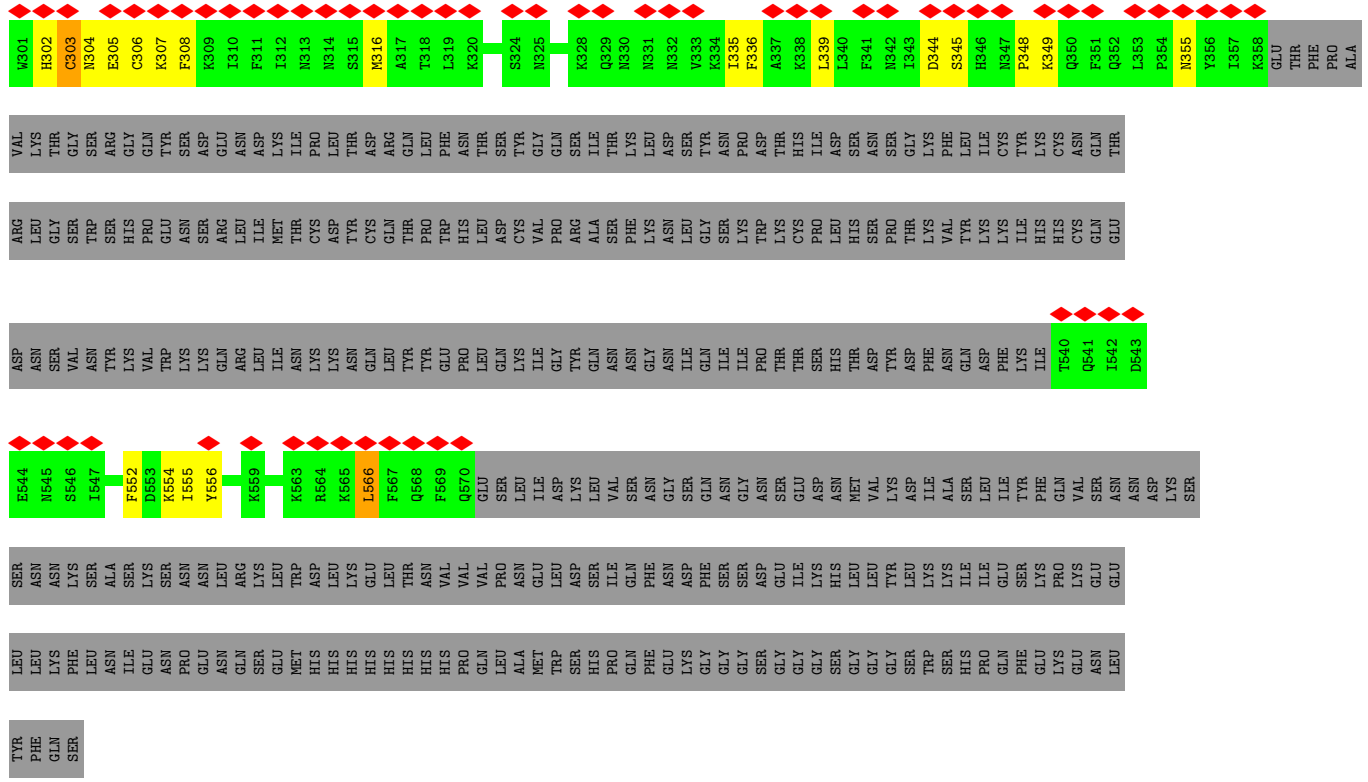
• Molecule 4: Transcriptional regulatory protein RCO1



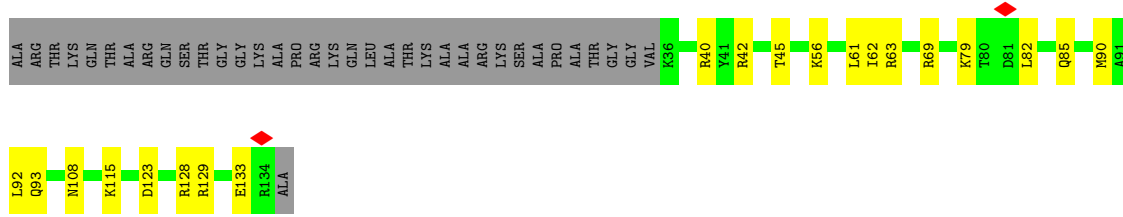


● Molecule 4: Transcriptional regulatory protein RCO1

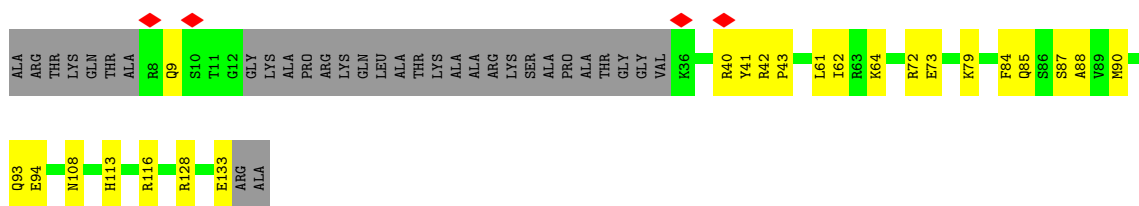




• Molecule 5: Histone H3

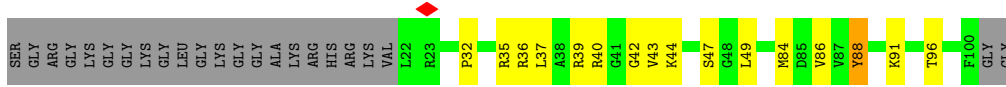


• Molecule 5: Histone H3

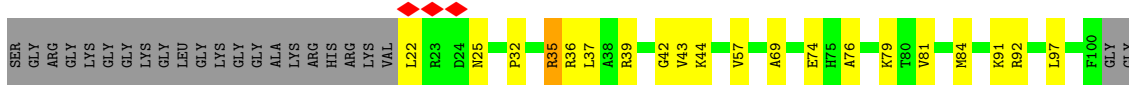


• Molecule 6: Histone H4

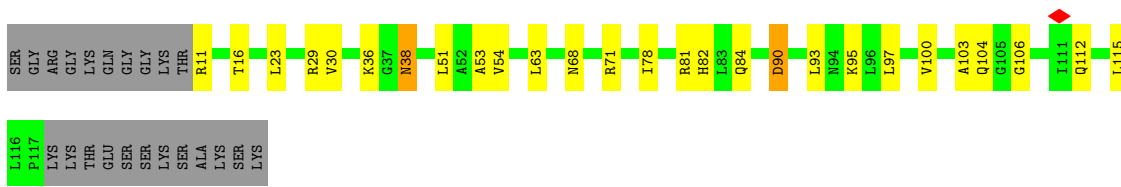




• Molecule 6: Histone H4



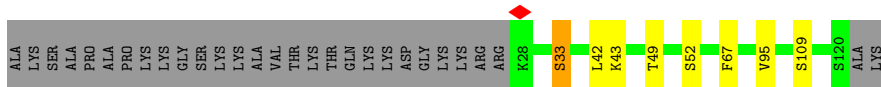
• Molecule 7: Histone H2A



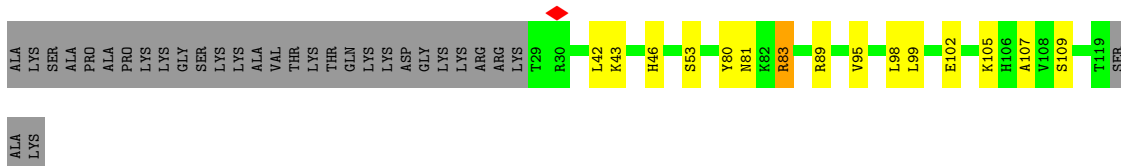
• Molecule 7: Histone H2A



• Molecule 8: Histone H2B 1.1

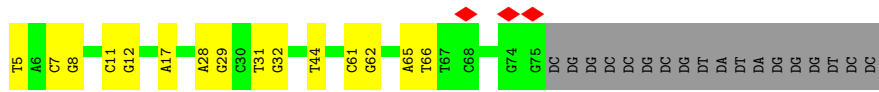
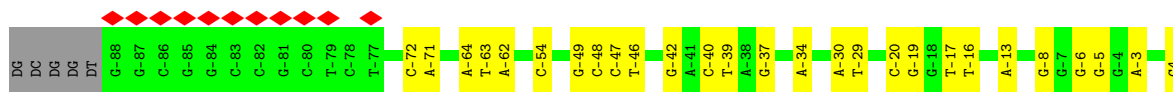


• Molecule 8: Histone H2B 1.1

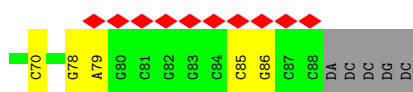
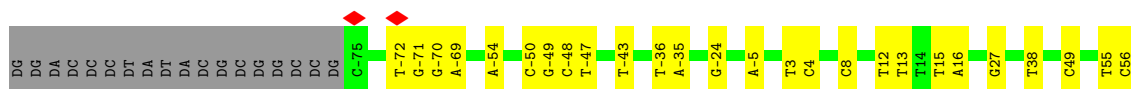


• Molecule 9: 187bp DNA





• Molecule 10: 187bp DNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.570	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0496	Depositor
Map size ( $\text{\AA}$ )	383.4, 383.4, 383.4	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.71, 0.71, 0.71	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: ZN, M3L

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	0.28	0/3147	0.52	1/4250 (0.0%)
2	B	0.27	0/4648	0.53	1/6267 (0.0%)
3	D	0.29	0/1922	0.69	5/2594 (0.2%)
3	F	0.28	0/1681	0.65	2/2268 (0.1%)
4	E	0.30	0/2683	0.59	1/3611 (0.0%)
4	G	0.28	0/1068	0.51	1/1430 (0.1%)
5	O	0.25	0/823	0.58	1/1106 (0.1%)
5	S	0.25	0/848	0.58	1/1138 (0.1%)
6	P	0.25	0/644	0.62	0/863
6	T	0.25	0/644	0.56	0/863
7	Q	0.27	0/835	0.59	0/1127
7	U	0.26	0/835	0.59	0/1127
8	R	0.24	0/741	0.50	0/997
8	V	0.25	0/726	0.50	0/978
9	X	0.55	0/3801	0.90	0/5870
10	Y	0.52	0/3741	0.89	0/5766
All	All	0.36	0/28787	0.68	13/40255 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	319	PRO	CA-N-CD	-10.13	97.32	111.50
3	D	111	LEU	CA-CB-CG	7.81	133.26	115.30
3	D	107	MET	CA-CB-CG	7.05	125.29	113.30
4	G	566	LEU	CA-CB-CG	7.05	131.52	115.30
3	D	386	LEU	CA-CB-CG	6.45	130.13	115.30

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	3073	0	2937	73	0
2	B	4545	0	4507	79	0
3	D	1884	0	1876	39	0
3	F	1647	0	1661	25	0
4	E	2620	0	2593	77	0
4	G	1043	0	1021	21	0
5	O	822	0	874	17	0
5	S	848	0	896	18	0
6	P	637	0	681	12	0
6	T	637	0	681	24	0
7	Q	825	0	882	27	0
7	U	825	0	882	10	0
8	R	730	0	755	12	0
8	V	715	0	737	17	0
9	X	3384	0	1838	30	0
10	Y	3340	0	1840	21	0
11	A	1	0	0	0	0
All	All	27576	0	24661	389	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 389 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)
1:A:36:ALA:CB	4:E:48:LEU:CD2	1.81	1.52
1:A:36:ALA:HB1	4:E:48:LEU:CD2	0.97	1.44
1:A:36:ALA:CB	4:E:48:LEU:HD22	1.47	1.35
1:A:224:ILE:HD12	1:A:231:ASN:OD1	1.35	1.25
2:B:1299:ASN:ND2	2:B:1301:PHE:CZ	2.10	1.18

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	384/433 (89%)	366 (95%)	18 (5%)	0	100	100
2	B	536/1544 (35%)	516 (96%)	20 (4%)	0	100	100
3	D	225/401 (56%)	209 (93%)	16 (7%)	0	100	100
3	F	194/401 (48%)	187 (96%)	7 (4%)	0	100	100
4	E	310/733 (42%)	264 (85%)	46 (15%)	0	100	100
4	G	120/733 (16%)	112 (93%)	8 (7%)	0	100	100
5	O	97/135 (72%)	96 (99%)	1 (1%)	0	100	100
5	S	99/135 (73%)	96 (97%)	3 (3%)	0	100	100
6	P	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
6	T	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
7	Q	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
7	U	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
8	R	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
8	V	89/122 (73%)	89 (100%)	0	0	100	100
All	All	2509/5221 (48%)	2381 (95%)	128 (5%)	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	326/367 (89%)	302 (93%)	24 (7%)	13	38
2	B	504/1399 (36%)	478 (95%)	26 (5%)	23	55
3	D	210/359 (58%)	200 (95%)	10 (5%)	25	58
3	F	184/359 (51%)	166 (90%)	18 (10%)	8	24
4	E	302/692 (44%)	287 (95%)	15 (5%)	24	57
4	G	121/692 (18%)	115 (95%)	6 (5%)	24	57
5	O	85/108 (79%)	84 (99%)	1 (1%)	71	91
5	S	88/108 (82%)	83 (94%)	5 (6%)	20	51
6	P	66/78 (85%)	63 (96%)	3 (4%)	27	61
6	T	66/78 (85%)	64 (97%)	2 (3%)	41	75
7	Q	84/101 (83%)	79 (94%)	5 (6%)	19	49
7	U	84/101 (83%)	81 (96%)	3 (4%)	35	69
8	R	80/102 (78%)	78 (98%)	2 (2%)	47	78
8	V	78/102 (76%)	75 (96%)	3 (4%)	33	67
All	All	2278/4646 (49%)	2155 (95%)	123 (5%)	26	54

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	348	ASP
5	S	41	TYR
4	E	549	TYR
8	R	109	SER
7	U	50	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
7	Q	73	ASN
5	S	108	ASN
8	V	81	ASN
6	T	25	ASN
4	G	302	HIS

### 5.3.3 RNA

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
5	M3L	S	36	5	10,11,12	0.51	0	9,14,16	0.48	0
5	M3L	O	36	5	10,11,12	0.57	0	9,14,16	0.45	0

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
5	M3L	S	36	5	-	1/9/10/12	-
5	M3L	O	36	5	-	5/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	36	M3L	N-CA-CB-CG
5	O	36	M3L	C-CA-CB-CG
5	O	36	M3L	CG-CD-CE-NZ
5	O	36	M3L	CA-CB-CG-CD
5	O	36	M3L	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

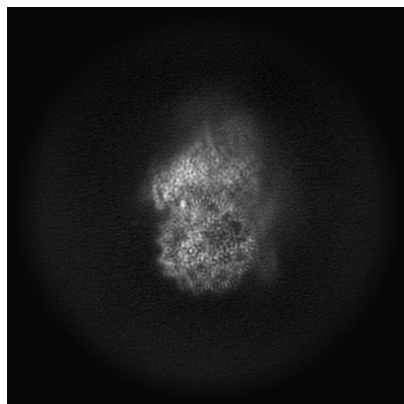
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37123. These allow visual inspection of the internal detail of the map and identification of artifacts.

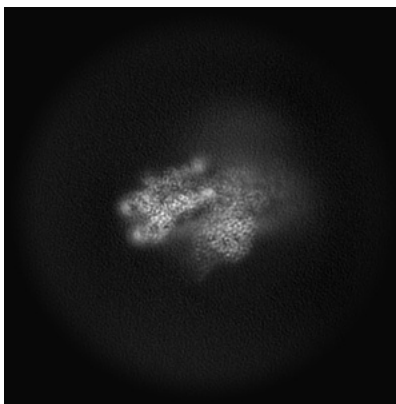
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

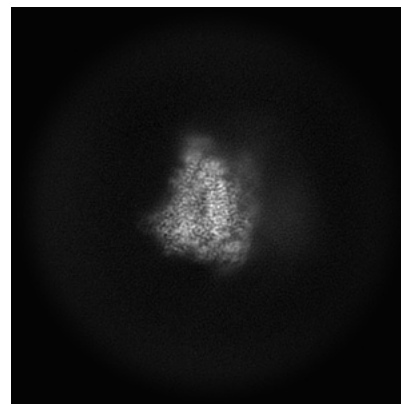
#### 6.1.1 Primary map



X

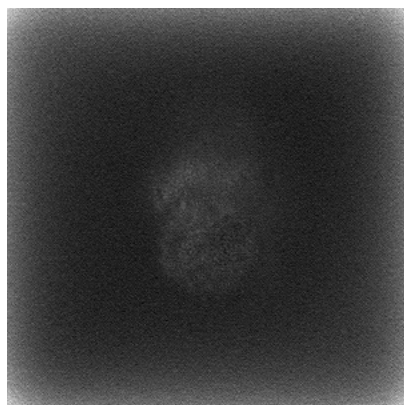


Y



Z

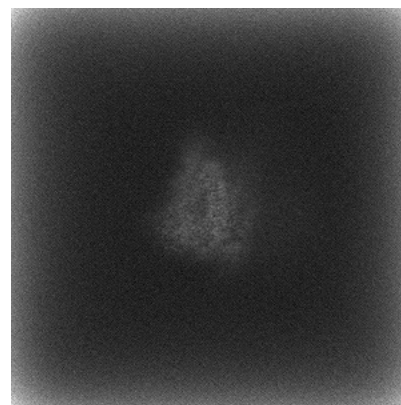
#### 6.1.2 Raw map



X



Y



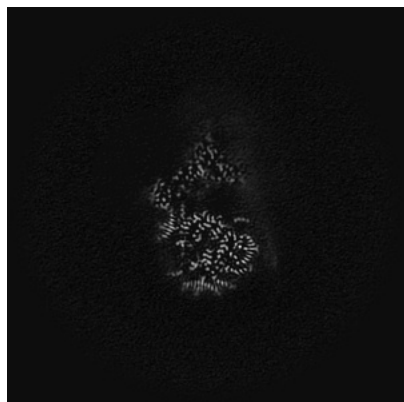
Z

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

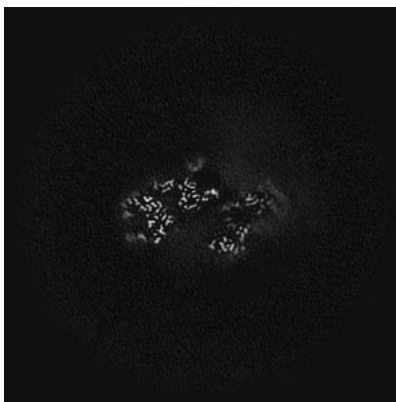


## 6.2 Central slices [i](#)

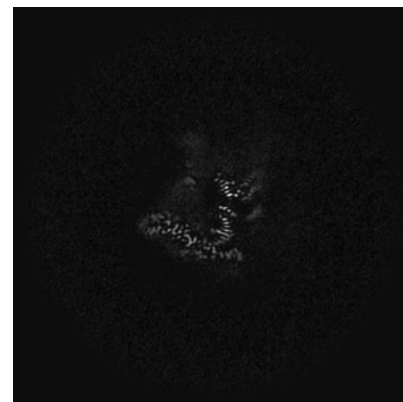
### 6.2.1 Primary map



X Index: 270

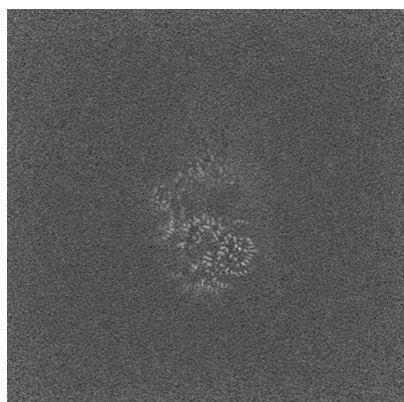


Y Index: 270



Z Index: 270

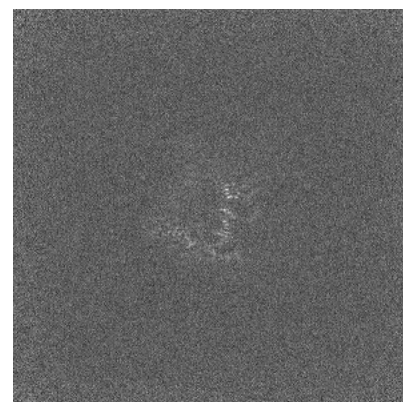
### 6.2.2 Raw map



X Index: 270



Y Index: 270

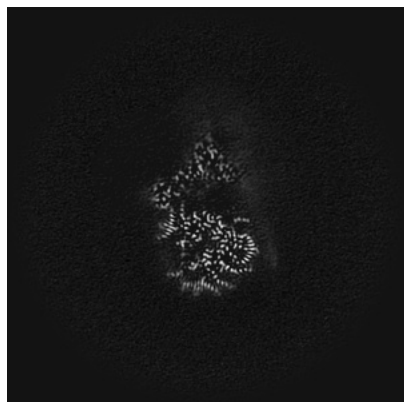


Z Index: 270

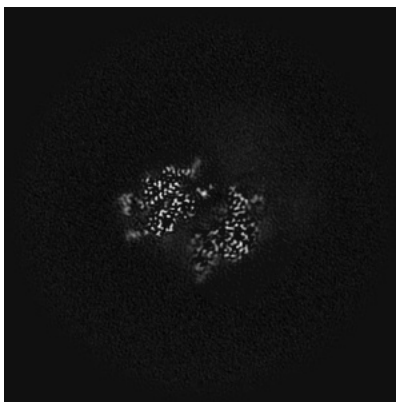
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

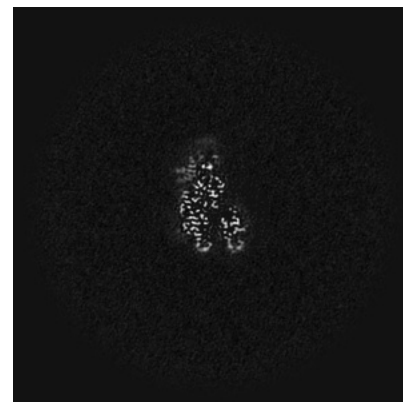
### 6.3.1 Primary map



X Index: 271

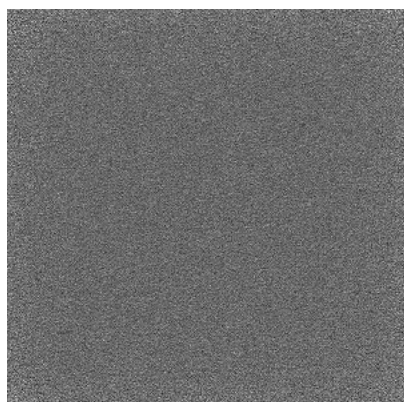


Y Index: 248

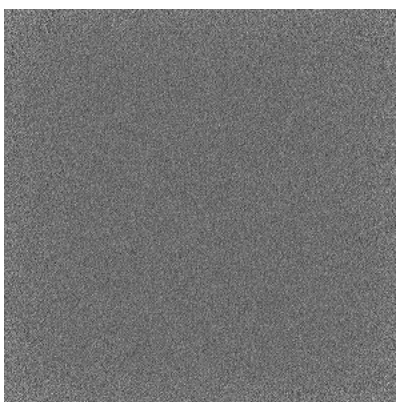


Z Index: 210

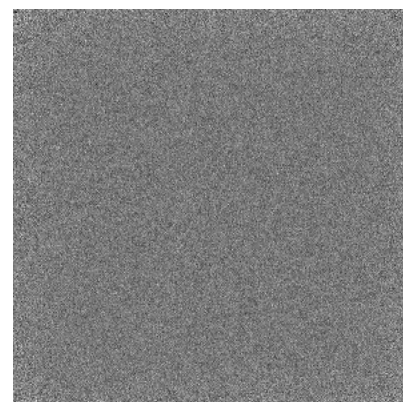
### 6.3.2 Raw map



X Index: 0



Y Index: 0

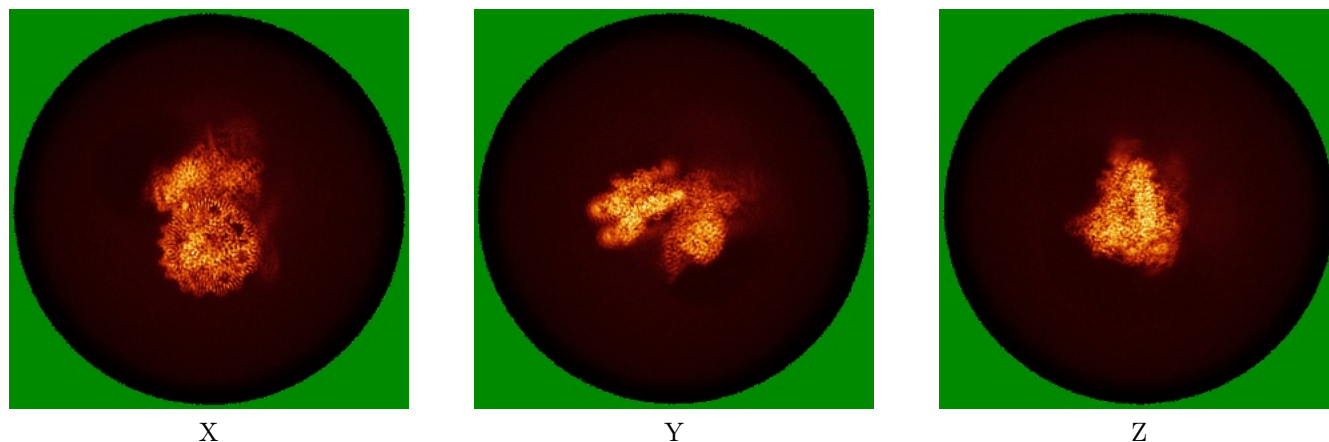


Z Index: 539

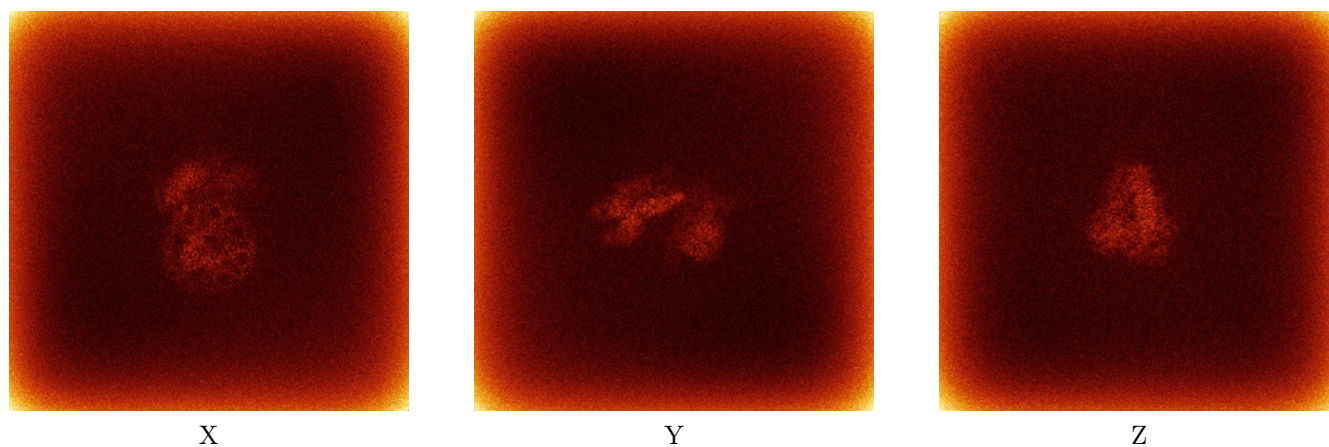
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



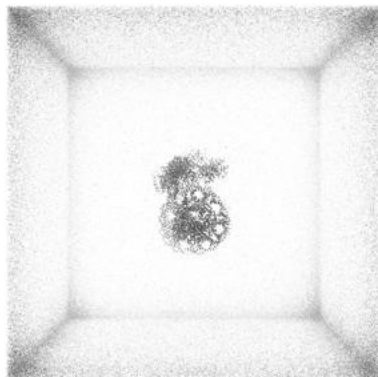
Y



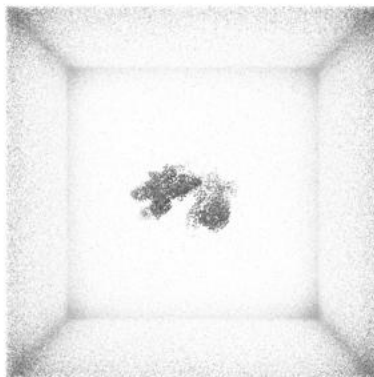
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0496. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

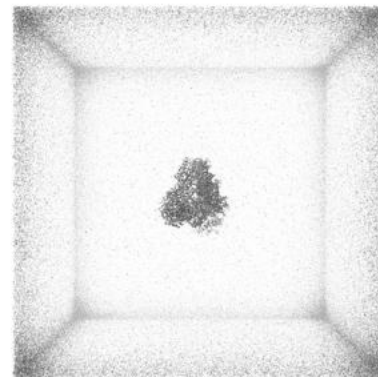
### 6.5.2 Raw map



X



Y



Z

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

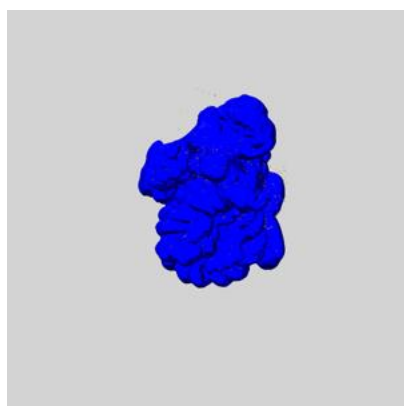
## 6.6 Mask visualisation [i](#)

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

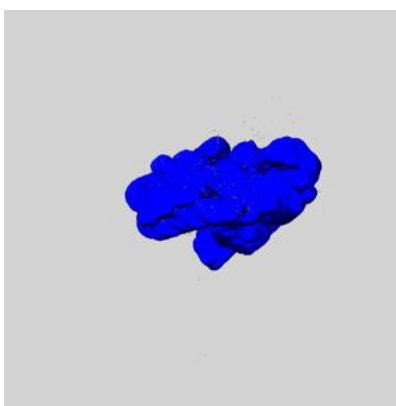
A mask typically either:

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

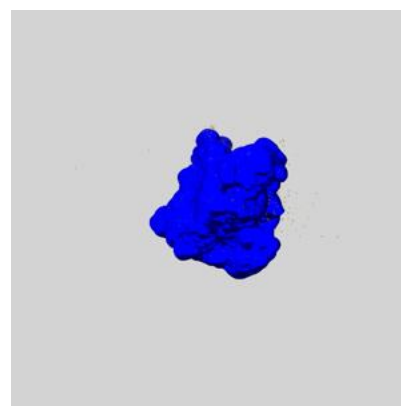
### 6.6.1 emd\_37123\_msk\_1.map [i](#)



X



Y

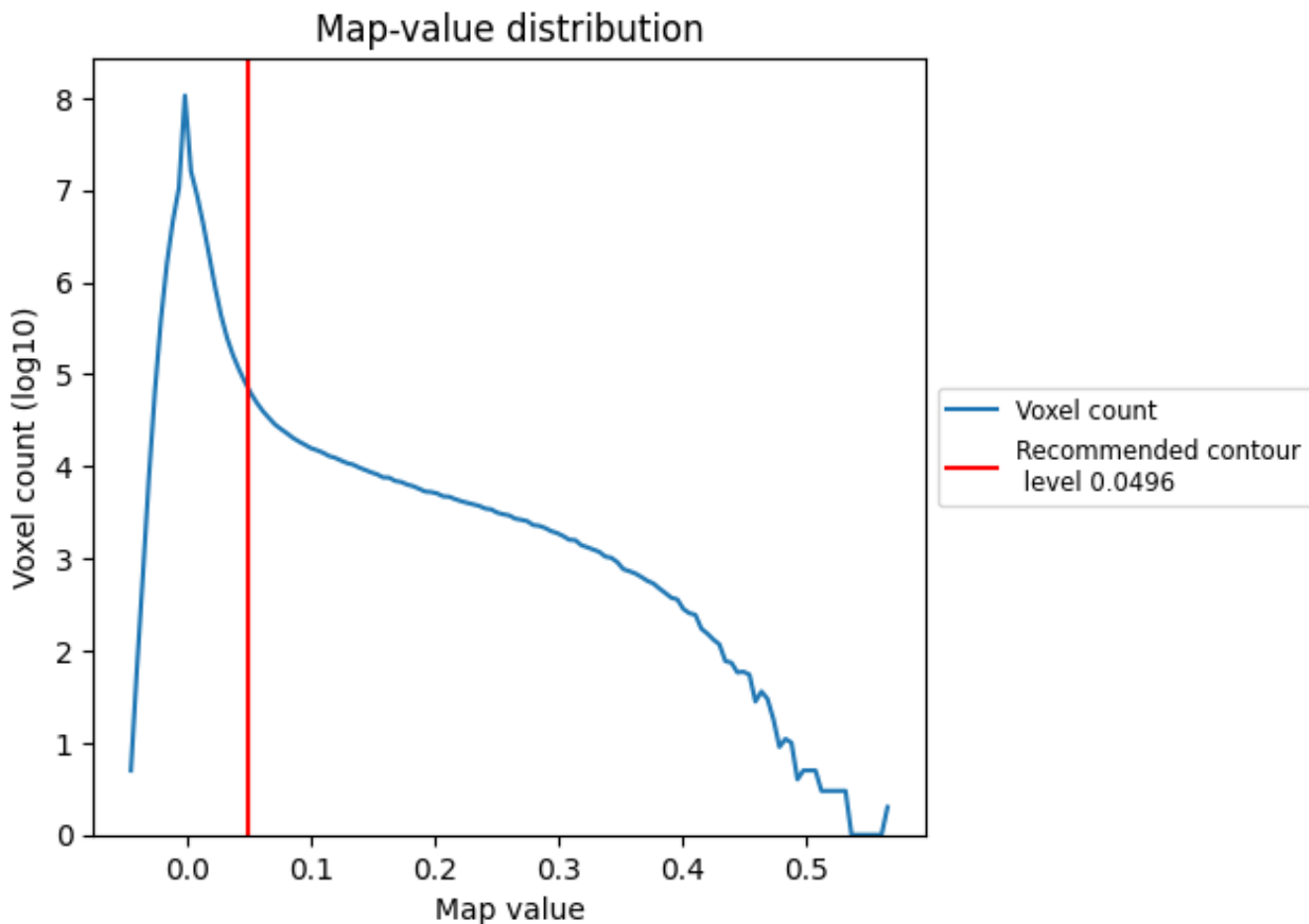


Z

## 7 Map analysis [i](#)

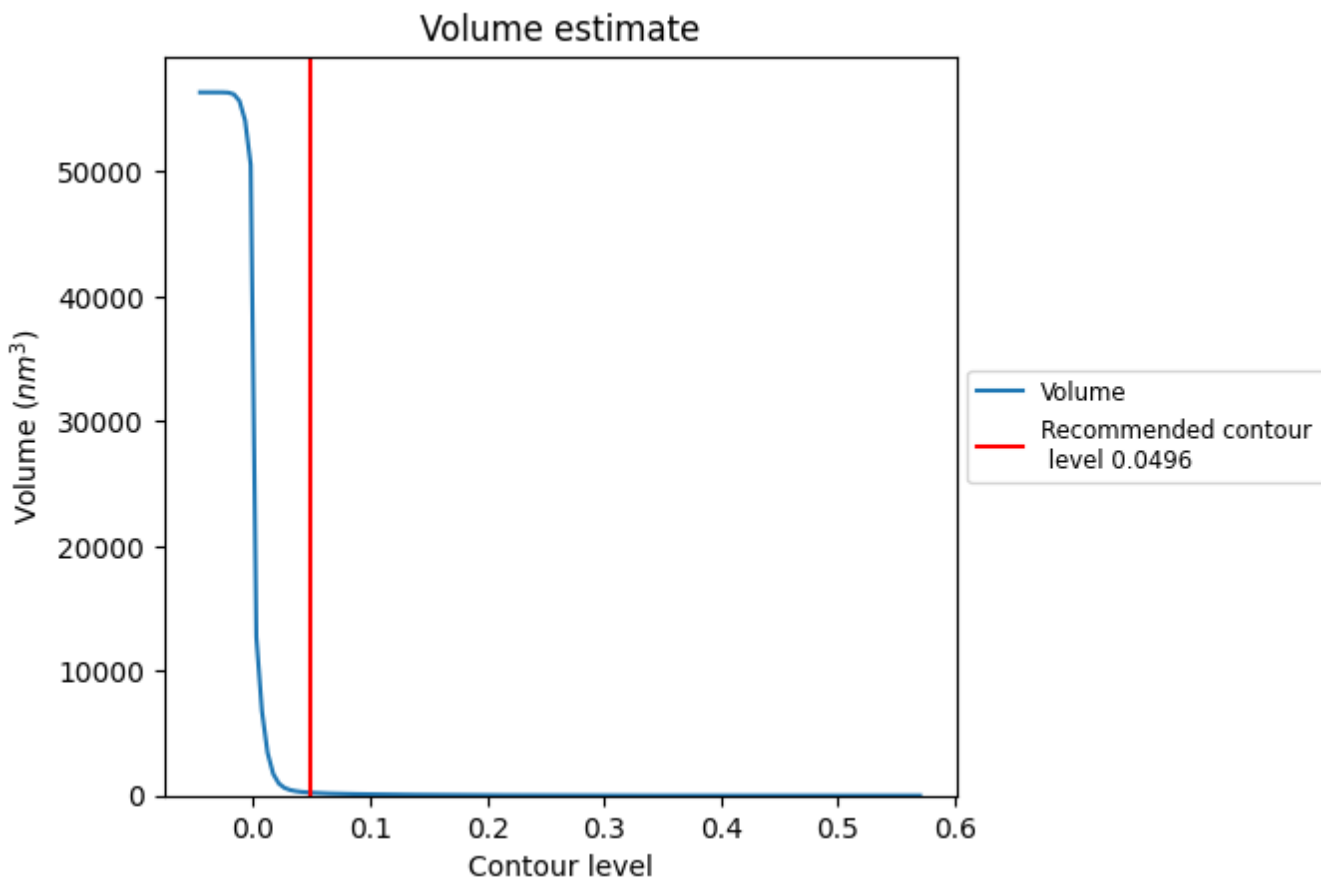
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

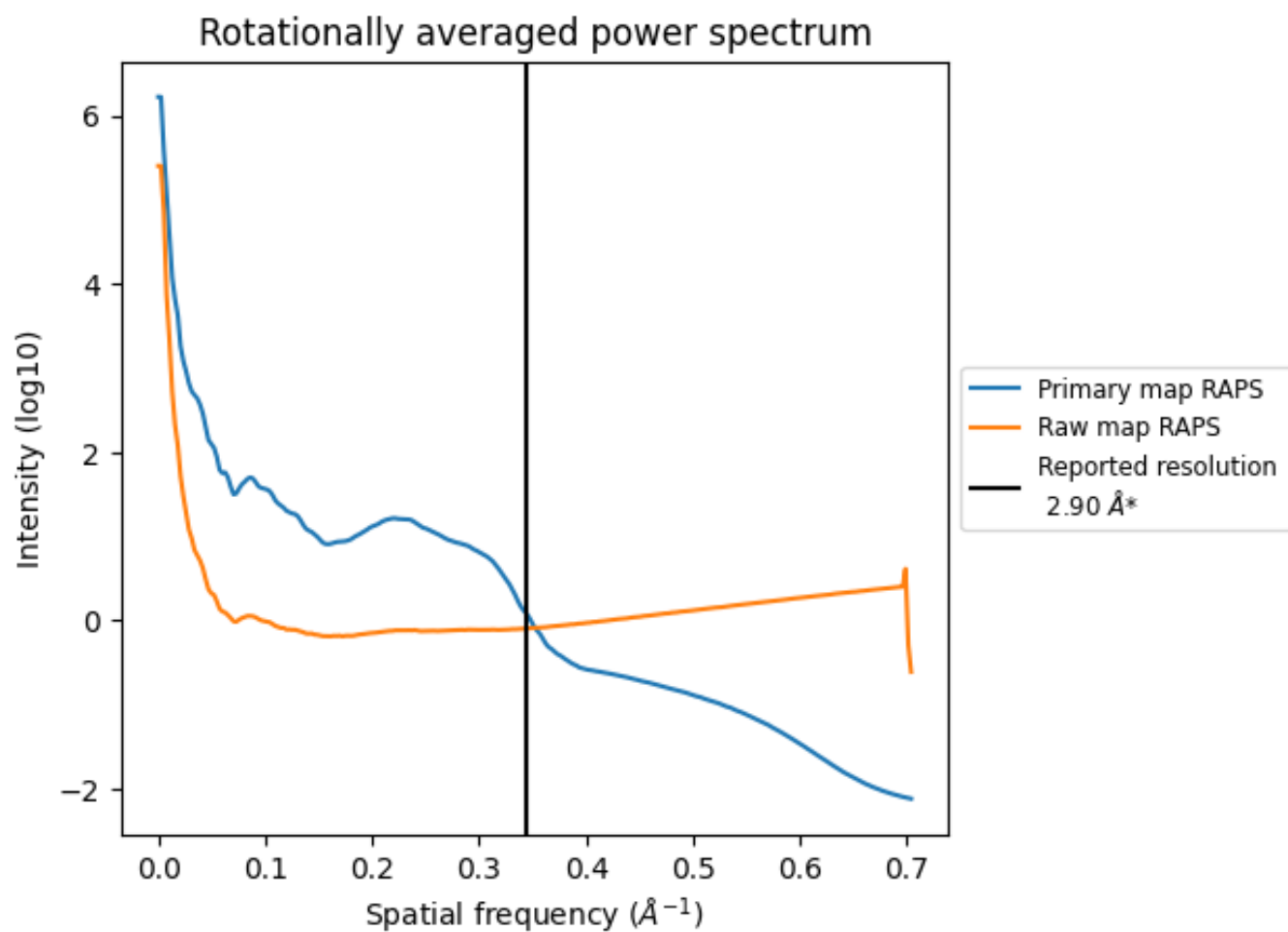
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227  $\text{nm}^3$ ; this corresponds to an approximate mass of 205 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](#)



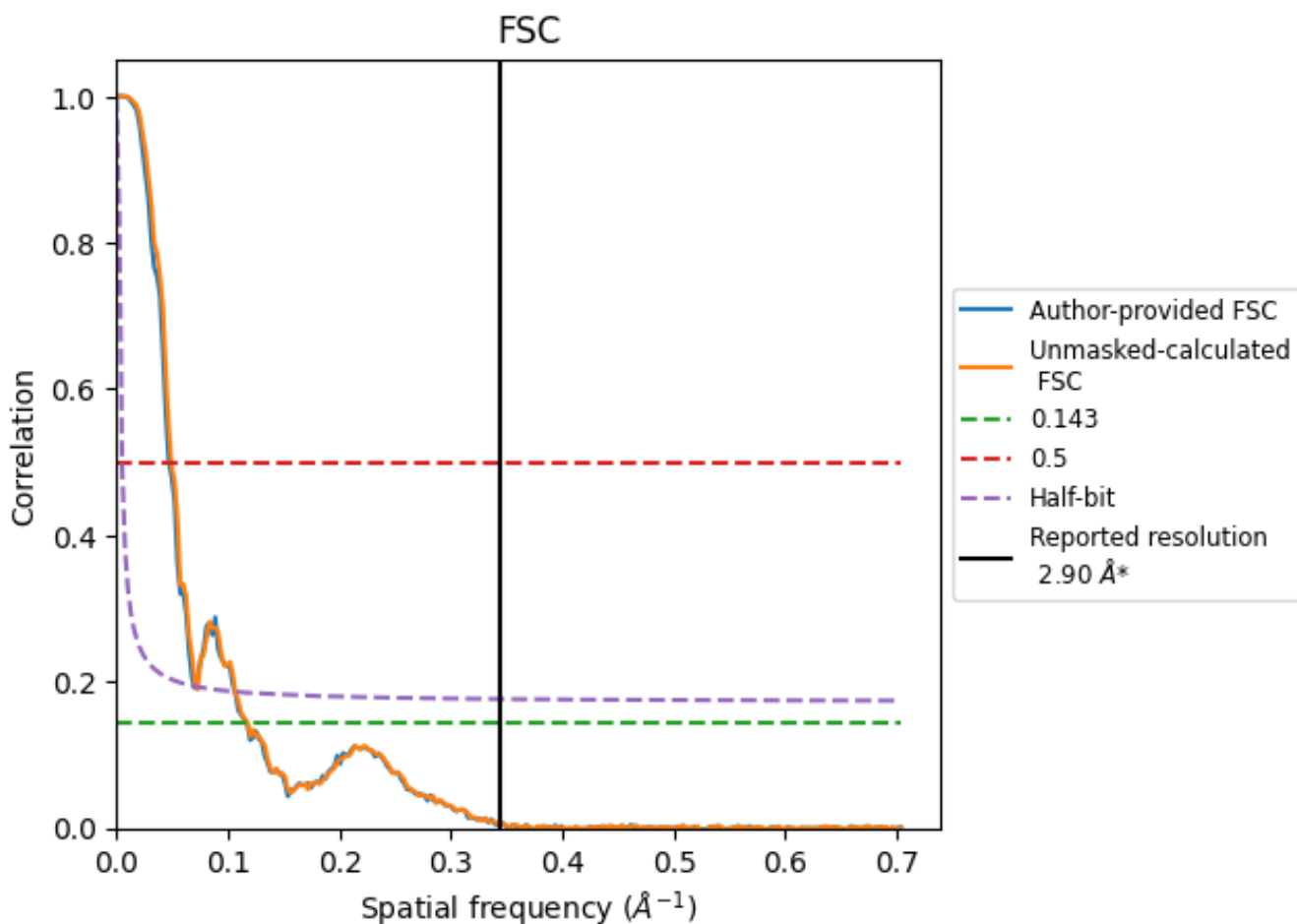
\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>



## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	8.55	21.19	14.27
Unmasked-calculated*	8.50	20.28	13.89

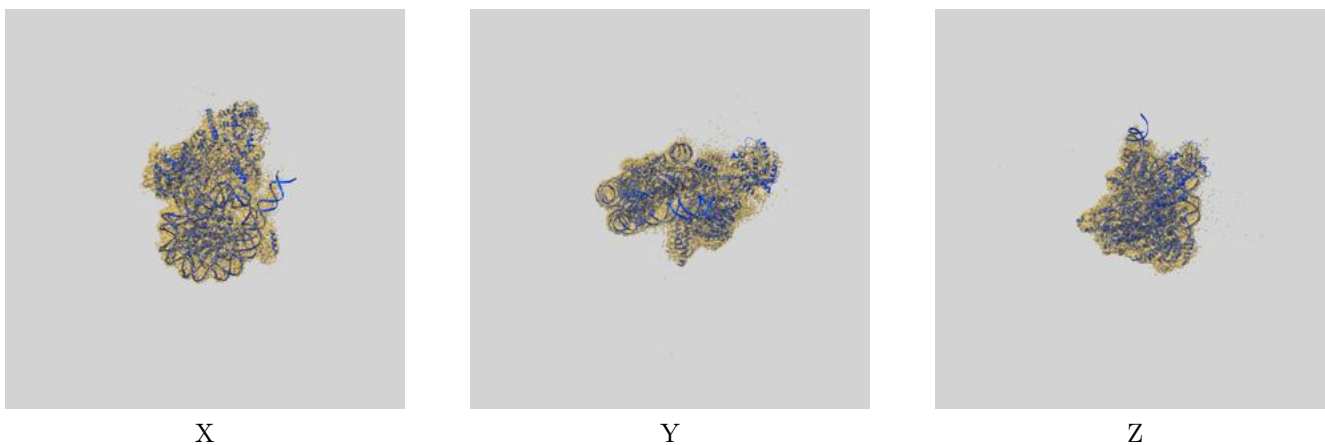
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.55 differs from the reported value 2.9 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.50 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

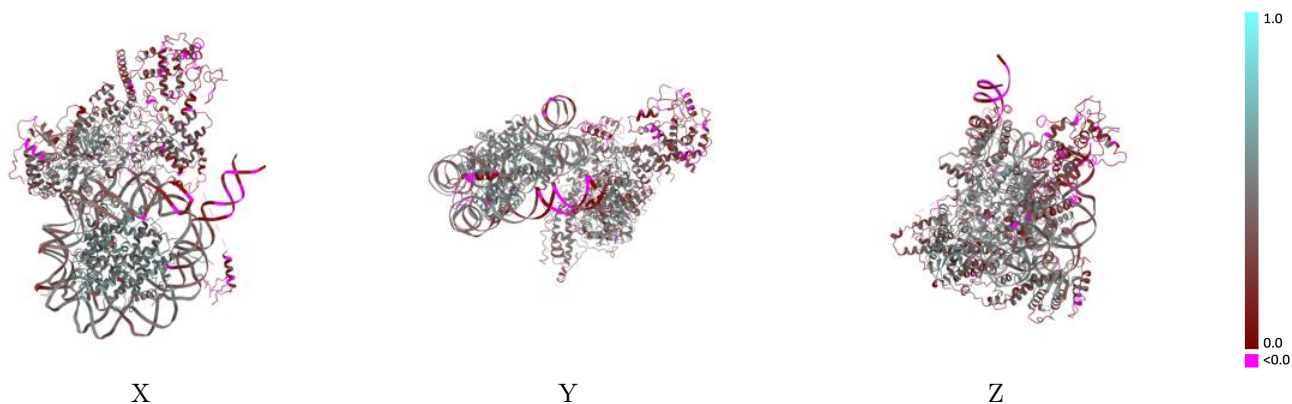
This section contains information regarding the fit between EMDB map EMD-37123 and PDB model 8KD3. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



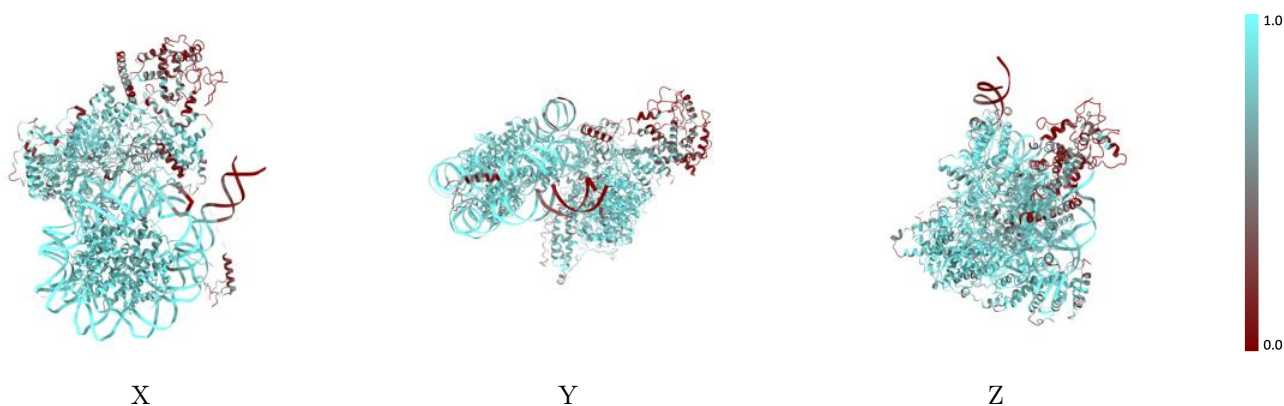
The images above show the 3D surface view of the map at the recommended contour level 0.0496 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



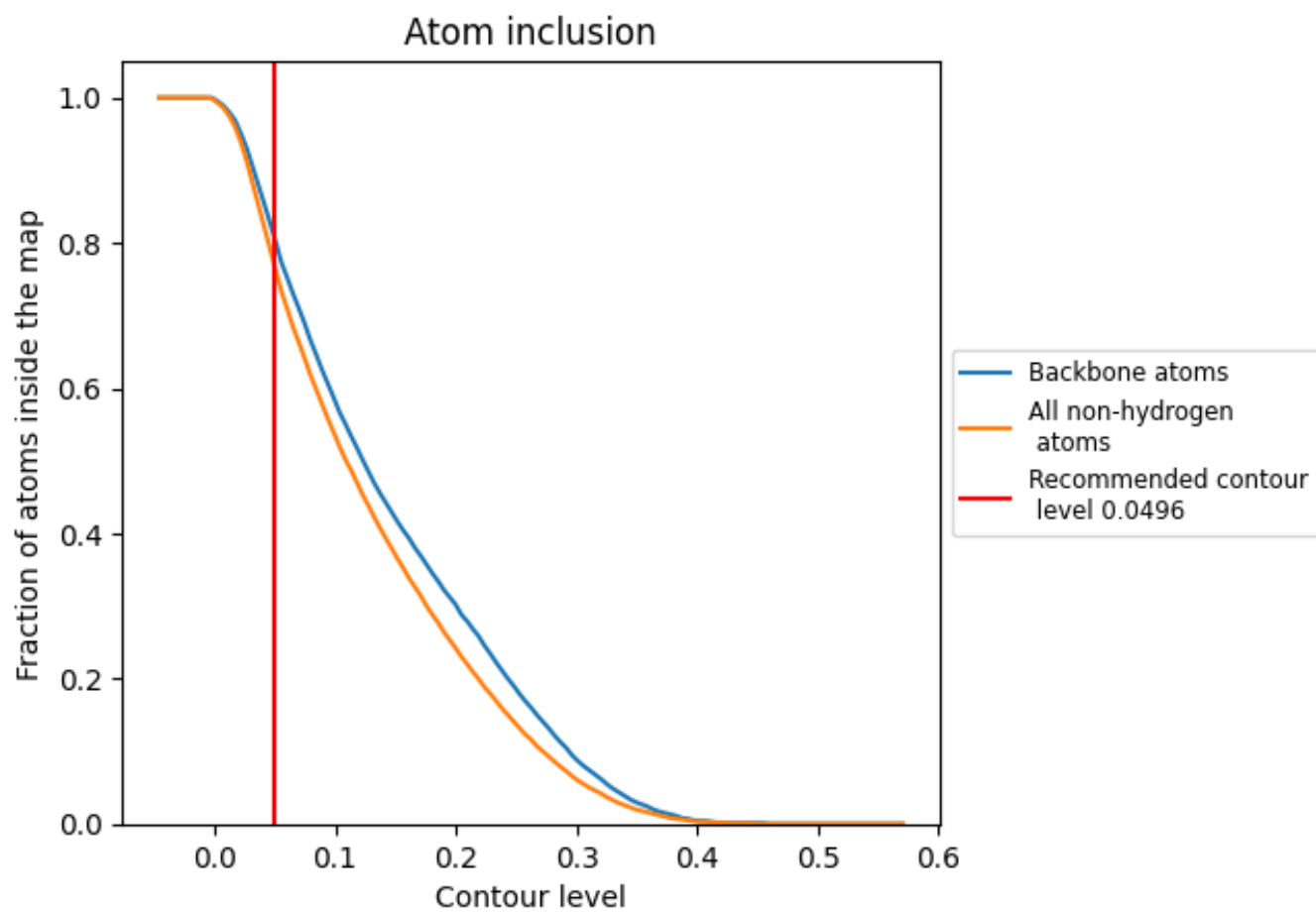
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0496).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.0496) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.3760
A	 0.8740	 0.4180
B	 0.7730	 0.3650
D	 0.7370	 0.3390
E	 0.7290	 0.3350
F	 0.2770	 0.1630
G	 0.2030	 0.1560
O	 0.8910	 0.5040
P	 0.9300	 0.5330
Q	 0.9110	 0.5030
R	 0.9260	 0.5060
S	 0.8650	 0.4690
T	 0.8950	 0.5230
U	 0.8960	 0.4820
V	 0.8970	 0.4870
X	 0.8350	 0.3630
Y	 0.8390	 0.3680

