wwPDB EM Validation Summary Report ⓘ

Oct 26, 2026 – 06:24 PM EDT

PDB ID	:	37XS / pdb_000037xs
EMDB ID	:	EMD-78606
Title	:	Polynucleotide kinase phosphatase bound to a nucleosome containing a nick with a 3'-phosphate and 5'-OH at SHL-4 (catalytic-FHA, composite)
Authors	:	Boesch, D.J.; Evans, J.J.; Weaver, T.M.
Deposited on	:	2026-08-12
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 ⓘ 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:

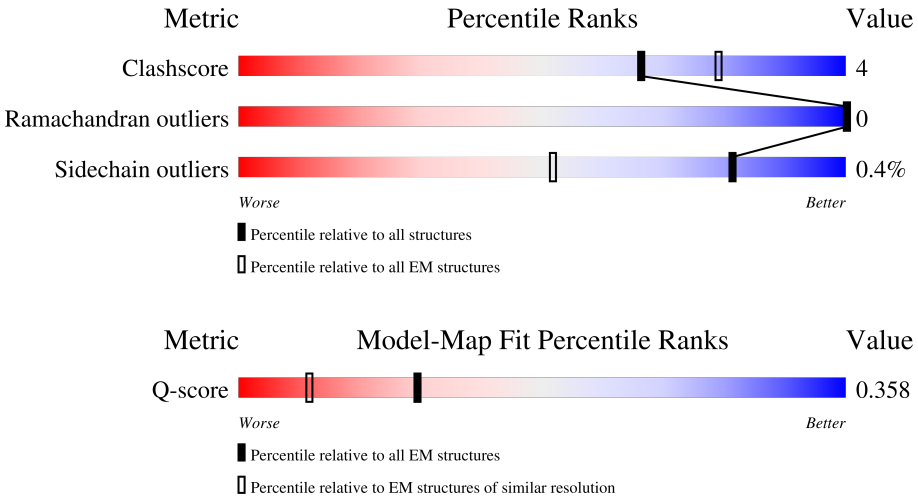
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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.



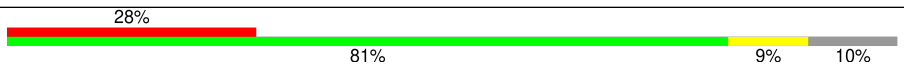
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	66% 5% 29%
1	E	135	68% • 28%
2	B	102	• 78% • 21%
2	F	102	77% • 20%

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	125	
4	H	125	
5	I	147	
6	J	35	
7	K	112	
8	L	528	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15624 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	96	Total	C	N	O	S	0	0
			789	499	151	137	2		
1	E	97	Total	C	N	O	S	0	0
			800	505	155	138	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP Q71DI3
E	110	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	F	82	Total	C	N	O	S	0	0
			657	416	128	112	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			823	520	161	142		
3	G	103	Total	C	N	O	0	0
			793	502	153	138		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			736	461	134	139	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	93	Total	C	N	O	S	0	0
			725	455	130	138	2		

- Molecule 5 is a DNA chain called 601 I strand (non-damaged strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	147	Total	C	N	O	P	0	0
			2996	1423	545	881	147		

- Molecule 6 is a DNA chain called 601 J strand (damaged strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	35	Total	C	N	O	P	0	0
			724	343	131	214	36		

- Molecule 7 is a DNA chain called 601 K strand (damaged strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	112	Total	C	N	O	P	0	0
			2308	1092	435	670	111		

- Molecule 8 is a protein called Bifunctional polynucleotide phosphatase/kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	475	Total	C	N	O	S	0	0
			3625	2314	644	653	14		

There are 9 discrepancies between the modelled and reference sequences:

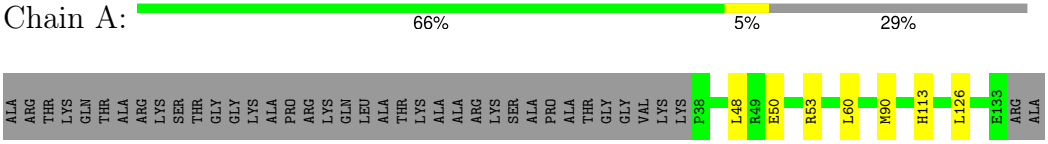
Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	MET	-	initiating methionine	UNP Q96T60
L	-5	HIS	-	expression tag	UNP Q96T60
L	-4	HIS	-	expression tag	UNP Q96T60
L	-3	HIS	-	expression tag	UNP Q96T60
L	-2	HIS	-	expression tag	UNP Q96T60
L	-1	HIS	-	expression tag	UNP Q96T60
L	0	HIS	-	expression tag	UNP Q96T60
L	1	GLY	-	expression tag	UNP Q96T60
L	171	ALA	ASP	engineered mutation	UNP Q96T60

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.

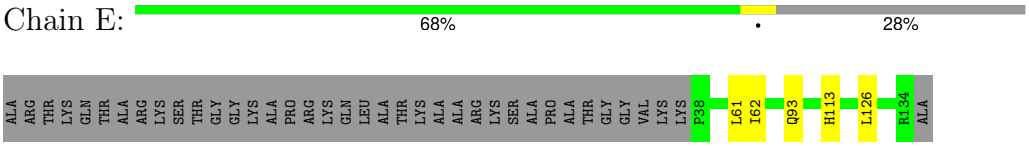
- Molecule 1: Histone H3.2

Chain A:



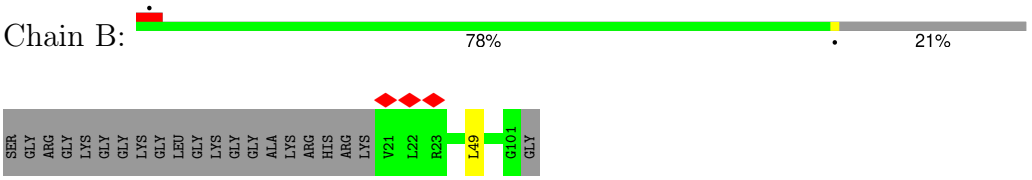
- Molecule 1: Histone H3.2

Chain E:



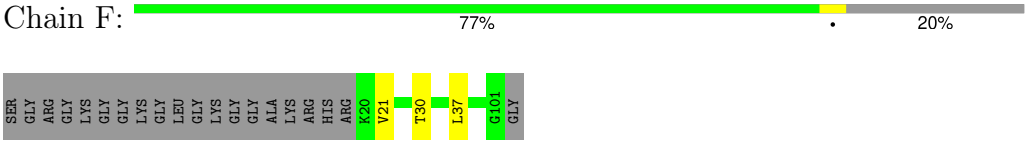
- Molecule 2: Histone H4

Chain B:



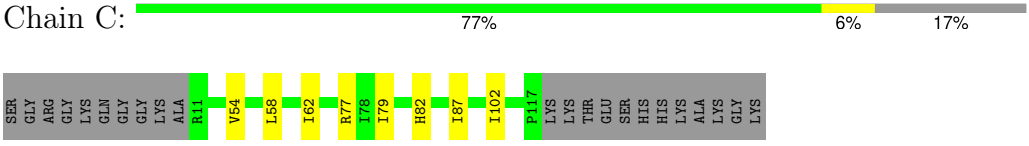
- Molecule 2: Histone H4

Chain F:



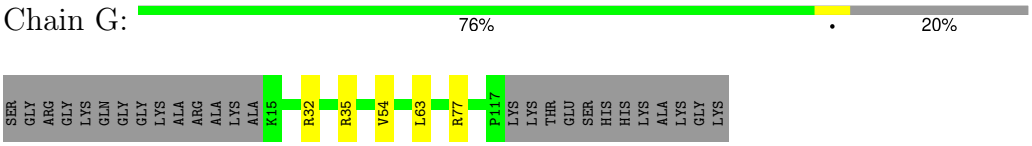
- Molecule 3: Histone H2A type 1

Chain C:



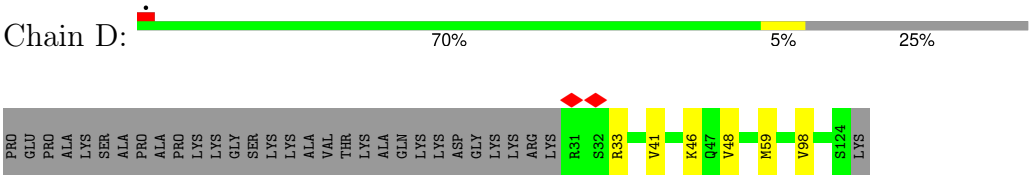
- Molecule 3: Histone H2A type 1

Chain G:



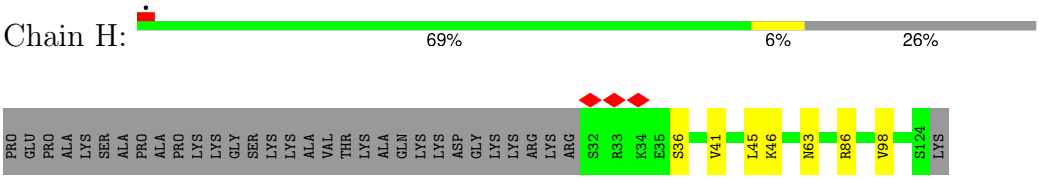
• Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain D:



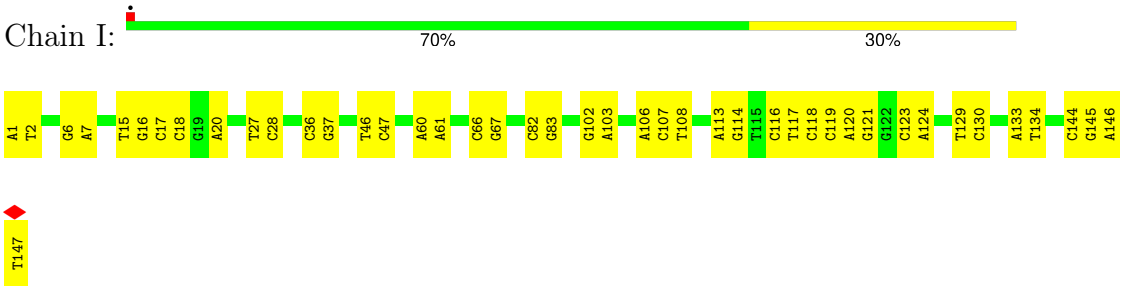
• Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain H:



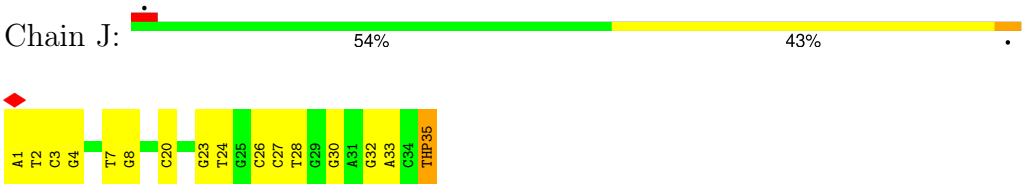
• Molecule 5: 601 I strand (non-damaged strand)

Chain I:



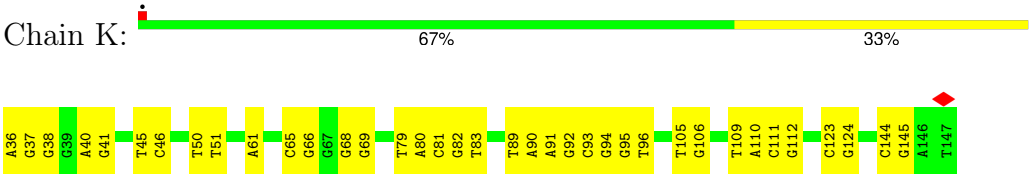
• Molecule 6: 601 J strand (damaged strand)

Chain J:



• Molecule 7: 601 K strand (damaged strand)

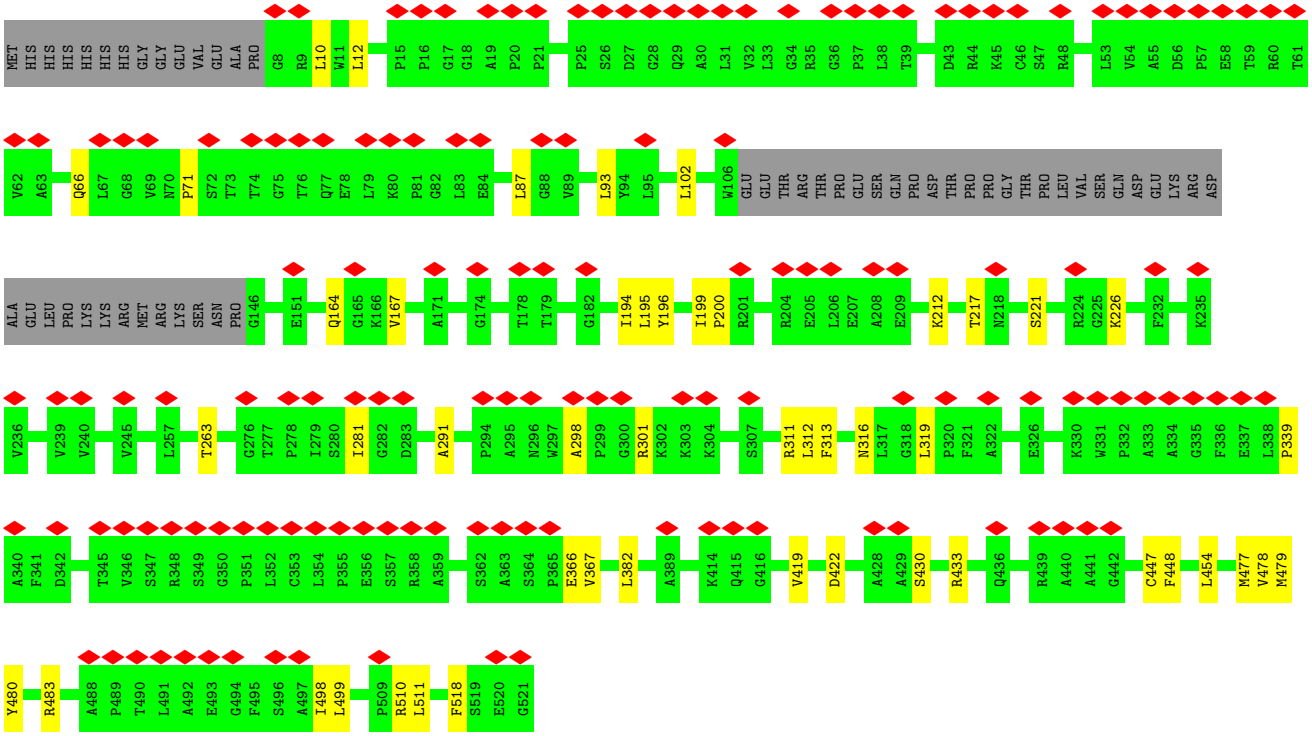
Chain K:



• Molecule 8: Bifunctional polynucleotide phosphatase/kinase

Chain L:




MET HIS HIS HIS HIS HIS GLY GLY GLU VAL GLU ALA PRO G8 R9 L10 W11 L12 P15 P16 G17 G18 A19 P20 P21 P25 S26 D27 G28 Q29 A30 L31 V32 L33 G34 R35 G36 P37 L38 T39 D43 R44 K45 C46 S47 R48 L53 V54 A55 D56 P57 E58 T59 R60 T61
V62 A63 Q66 L67 G68 V69 N70 P71 S72 T73 T74 G75 T76 Q77 E78 L79 K80 P81 G82 L83 E84 L87 G88 V89 L93 Y94 L95 L102 W106 GLU GLU THR ARG THR PRO GLU SER GLN PRO ASP THR PRO PRO GLY THR PRO LEU VAL SER GLN ASP GLU LYS ARG ASP
ALA GLU LEU PRO LYS LYS ARG MET ARG LYS SER ASN PRO G146 E151 Q164 G165 K166 V167 A171 G174 T178 T179 G182 I194 L195 Y196 I199 P200 R201 R204 E205 L206 E207 A208 E209 K212 T217 N218 S221 R224 G225 K226 F232 K235
V236 V239 V240 V245 L257 T263 G276 T277 P278 I279 S280 I281 G282 D283 A291 P294 A295 N296 W297 A298 P299 G300 R301 K302 K303 K304 S307 R311 L312 F313 N316 L317 G318 L319 P320 F321 A322 E326 K330 W331 P332 A333 A334 G335 F336 E337 L338 P339
A340 F341 D342 T345 V346 S347 R348 S349 G350 P351 L352 C353 L354 P355 E356 S357 R358 A359 S362 A363 S364 P365 E366 V367 L382 A389 K414 Q415 G416 V419 D422 A428 A429 S430 R433 Q436 R439 A440 A441 G442 C447 F448 L454 M477 V478 M479
Y480 R483 A488 P489 T490 L491 A492 E493 G494 F495 S496 A497 I498 L499 P509 R510 L511 F518 S519 E520 G521

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42334	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.031	Depositor
Minimum map value	-12.296	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.012	Depositor
Recommended contour level	4.8	Depositor
Map size (Å)	260.80002, 260.80002, 260.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65200007, 0.65200007, 0.65200007	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/801	0.29	0/1075
1	E	0.15	0/812	0.28	0/1089
2	B	0.18	0/655	0.32	0/878
2	F	0.27	0/664	0.39	0/889
3	C	0.15	0/833	0.29	0/1124
3	G	0.13	0/803	0.28	0/1085
4	D	0.17	0/747	0.29	0/1004
4	H	0.14	0/736	0.27	0/990
5	I	0.72	0/3357	0.92	0/5174
6	J	0.67	0/785	0.87	0/1210
7	K	0.74	0/2592	0.90	0/4003
8	L	0.11	0/3717	0.25	0/5054
All	All	0.48	0/16502	0.64	0/23575

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

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	789	0	826	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	800	0	839	4	0
2	B	648	0	693	0	0
2	F	657	0	706	3	0
3	C	823	0	884	5	0
3	G	793	0	848	6	0
4	D	736	0	756	4	0
4	H	725	0	743	7	0
5	I	2996	0	1650	30	0
6	J	724	0	395	12	0
7	K	2308	0	1257	21	0
8	L	3625	0	3612	31	0
All	All	15624	0	13209	112	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 112 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)
5:I:113:DA:H1'	5:I:114:DG:H5'	1.70	0.73
6:J:32:DG:H2"	6:J:33:DA:H5"	1.75	0.69
3:C:54:VAL:HG21	4:D:98:VAL:HG21	1.79	0.65
8:L:291:ALA:HB1	8:L:311:ARG:HH21	1.63	0.64
2:F:30:THR:HG21	7:K:61:DA:H5"	1.81	0.62

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	94/135 (70%)	93 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
2	F	80/102 (78%)	77 (96%)	3 (4%)	0	100	100
3	C	105/129 (81%)	105 (100%)	0	0	100	100
3	G	101/129 (78%)	101 (100%)	0	0	100	100
4	D	92/125 (74%)	92 (100%)	0	0	100	100
4	H	91/125 (73%)	88 (97%)	3 (3%)	0	100	100
8	L	471/528 (89%)	465 (99%)	6 (1%)	0	100	100
All	All	1208/1510 (80%)	1193 (99%)	15 (1%)	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	83/109 (76%)	83 (100%)	0	100	100
1	E	84/109 (77%)	84 (100%)	0	100	100
2	B	67/78 (86%)	66 (98%)	1 (2%)	57	76
2	F	68/78 (87%)	68 (100%)	0	100	100
3	C	83/98 (85%)	82 (99%)	1 (1%)	63	79
3	G	81/98 (83%)	81 (100%)	0	100	100
4	D	81/105 (77%)	80 (99%)	1 (1%)	63	79
4	H	80/105 (76%)	80 (100%)	0	100	100
8	L	377/435 (87%)	376 (100%)	1 (0%)	86	88
All	All	1004/1215 (83%)	1000 (100%)	4 (0%)	81	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	49	LEU
3	C	62	ILE
4	D	48	VAL
8	L	366	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	73	ASN
4	H	63	ASN
8	L	66	GLN
8	L	248	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
6	THP	J	35	6	22,25,26	0.76	0	32,37,40	0.87	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
6	THP	J	35	6	-	7/12/26/27	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	35	THP	O4-C4-C5	-2.13	122.48	124.92
6	J	35	THP	O2P-P1-O1P	2.06	118.86	110.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	35	THP	O4'-C1'-N1-C2
6	J	35	THP	O4'-C1'-N1-C6
6	J	35	THP	C3'-C4'-C5'-O5'
6	J	35	THP	O4'-C4'-C5'-O5'
6	J	35	THP	C2'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	35	THP	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

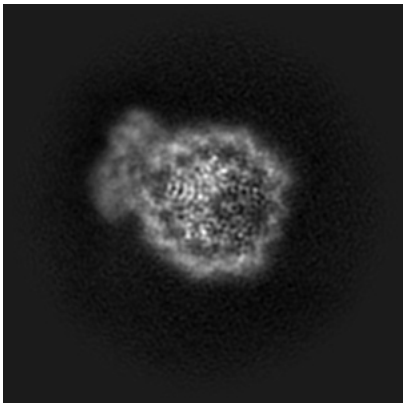
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78606. These allow visual inspection of the internal detail of the map and identification of artifacts.

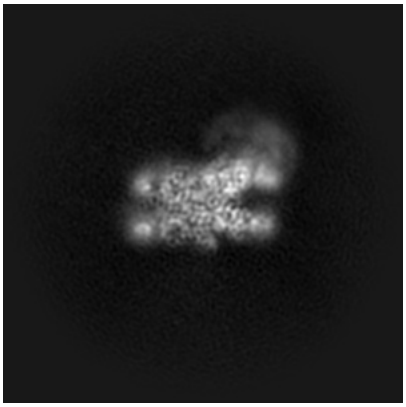
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

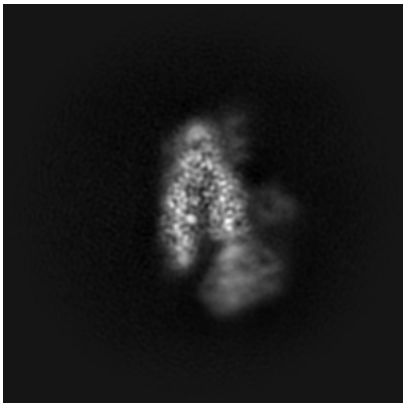
6.1.1 Primary map



X



Y

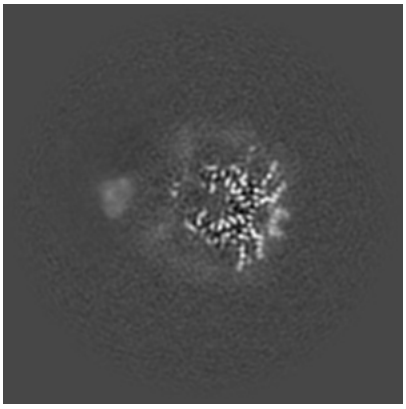


Z

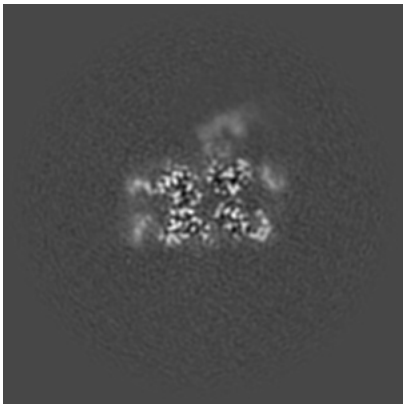
The images above show the map projected in three orthogonal directions.

6.2 Central slices

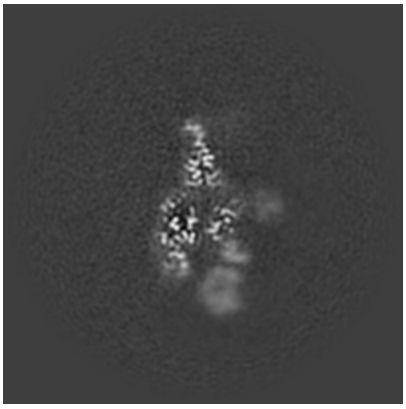
6.2.1 Primary map



X Index: 200



Y Index: 200

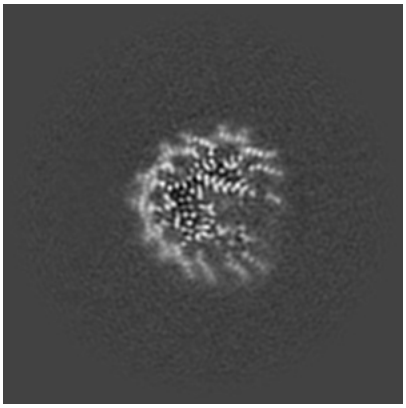


Z Index: 200

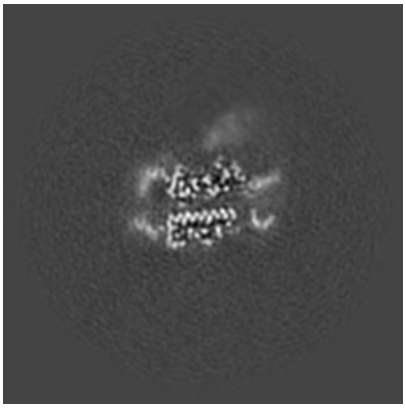
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

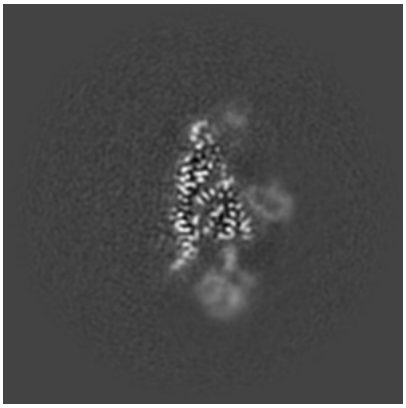
6.3.1 Primary map



X Index: 181



Y Index: 185

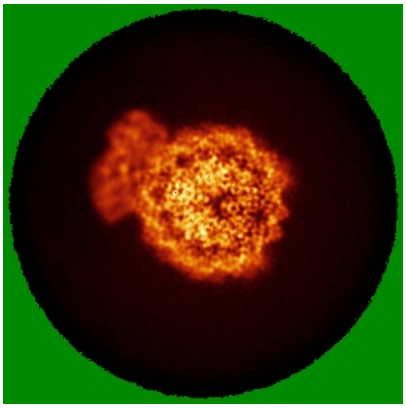


Z Index: 218

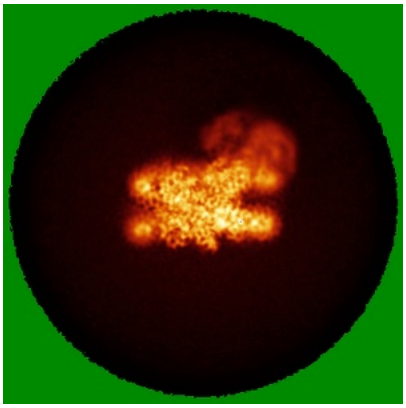
The images above show the largest variance slices of the map in three orthogonal directions.

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

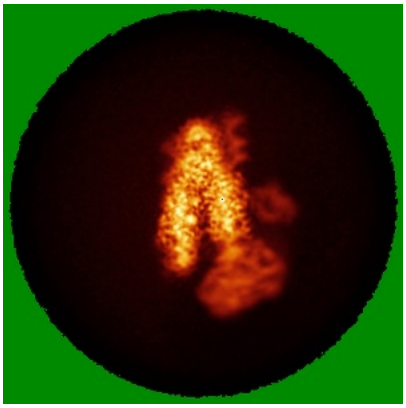
6.4.1 Primary map



X



Y

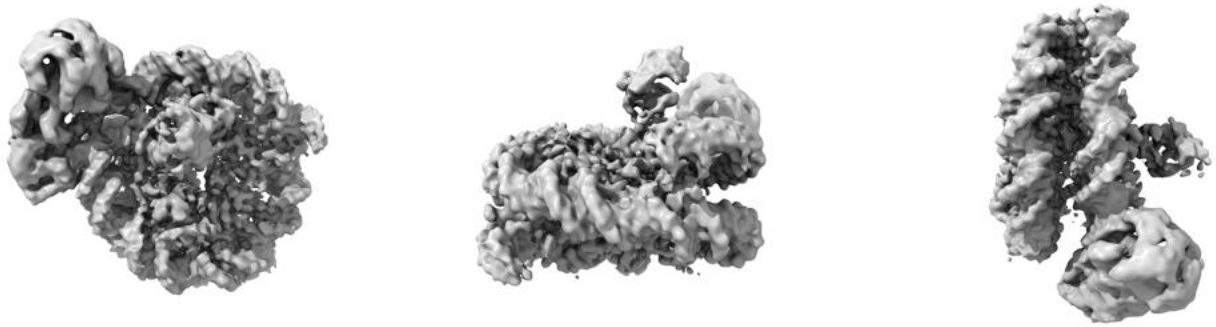


Z

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 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

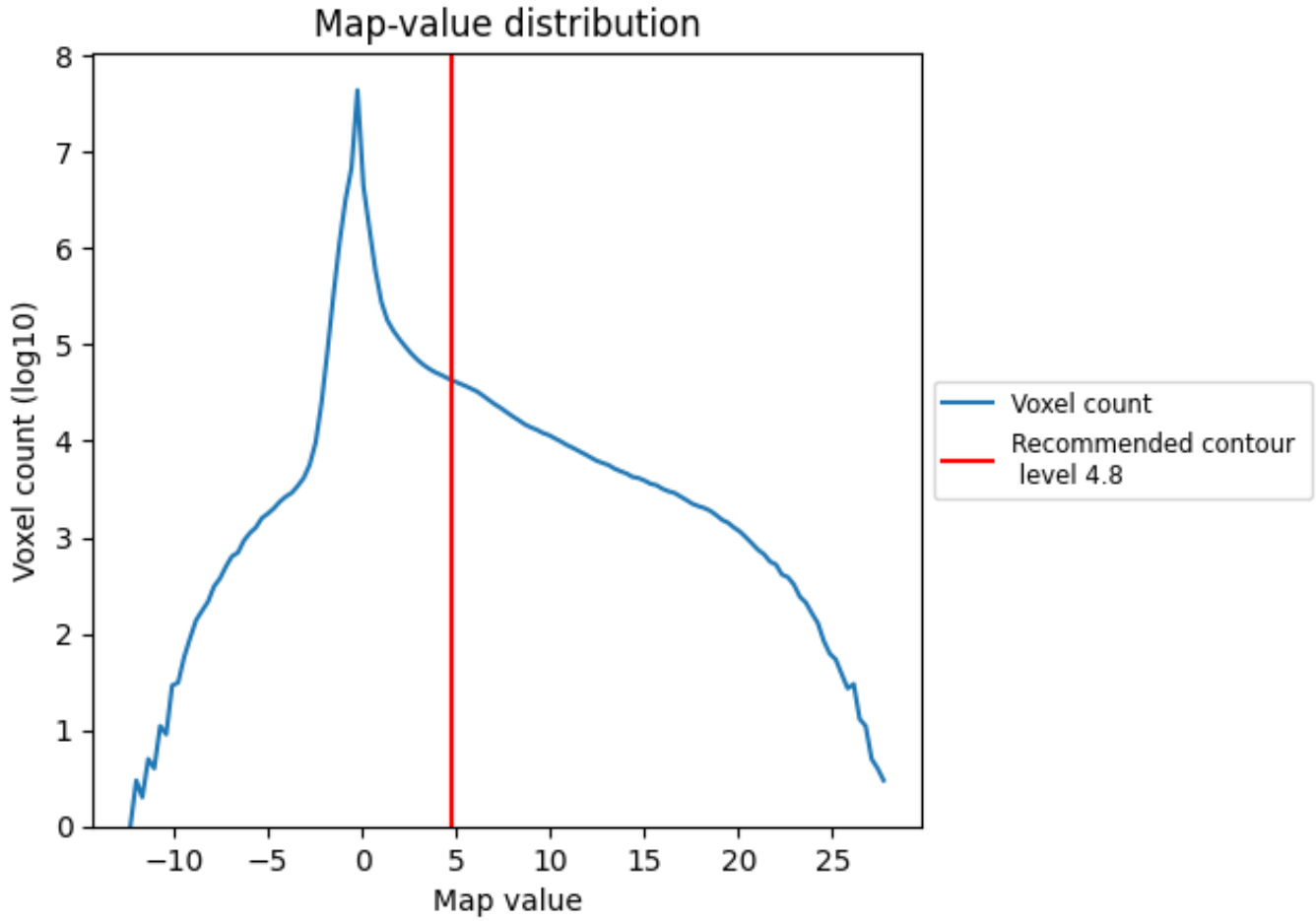
6.6 Mask visualisation (i)

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

7 Map analysis

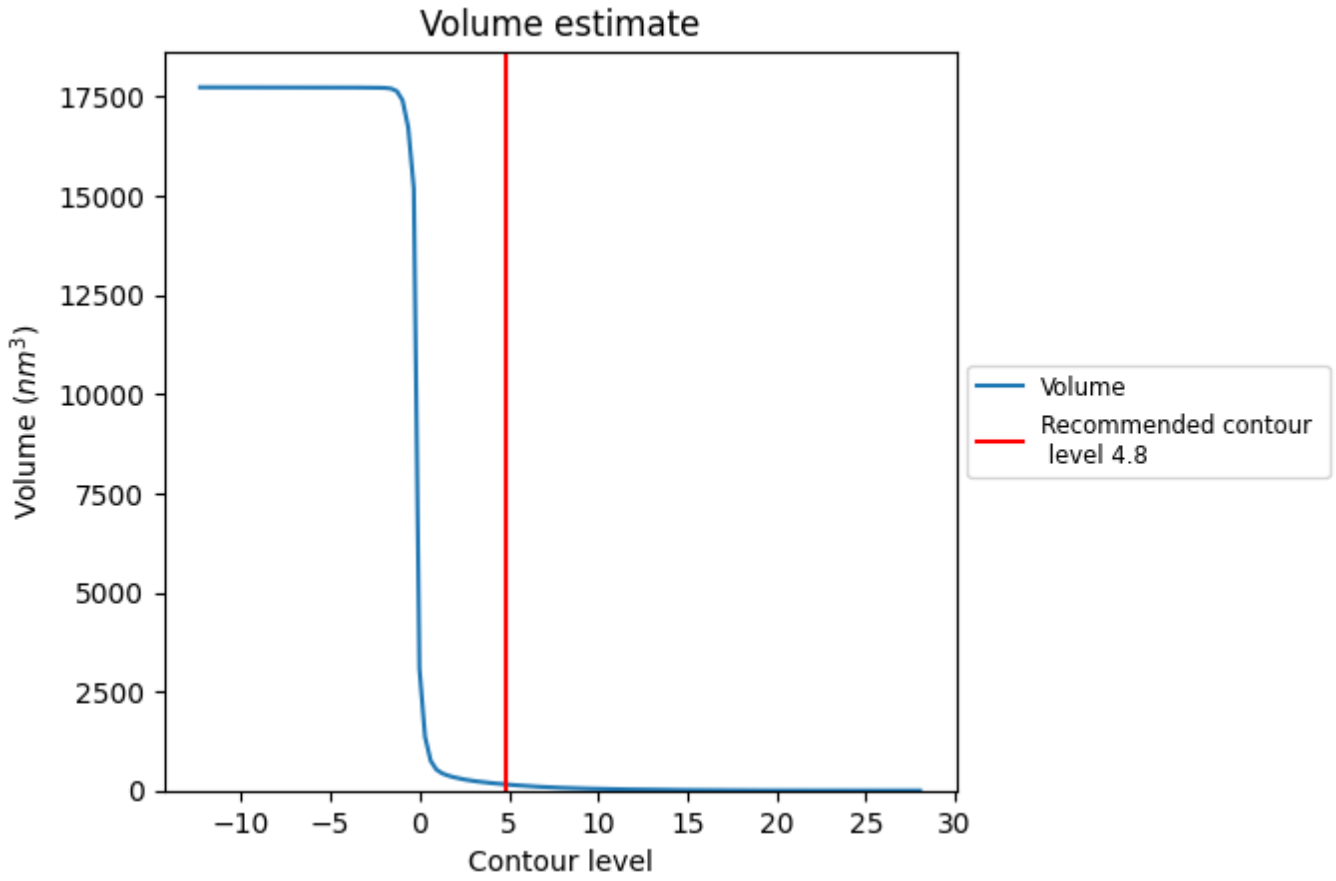
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

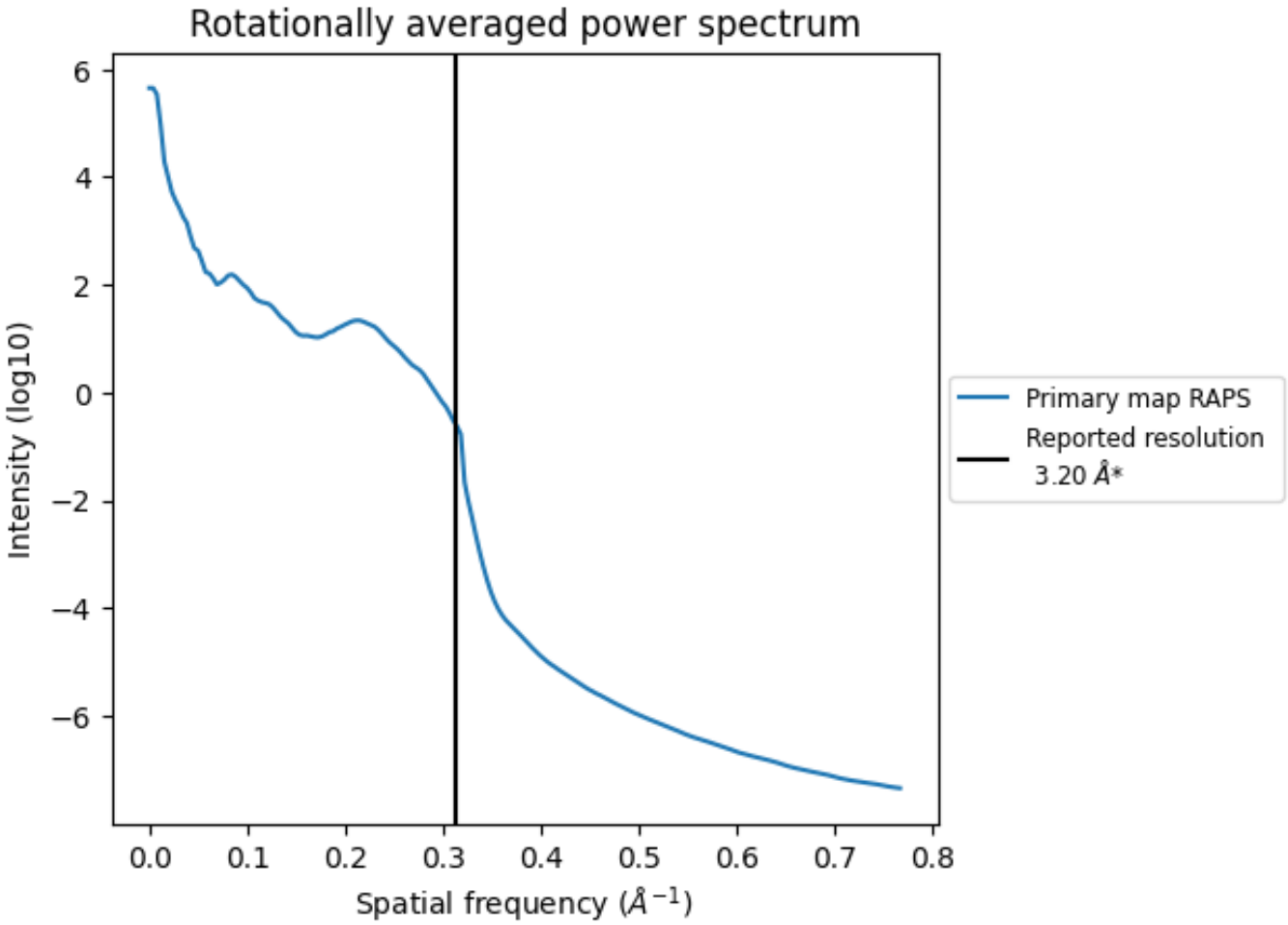
7.2 Volume estimate (i)



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 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}

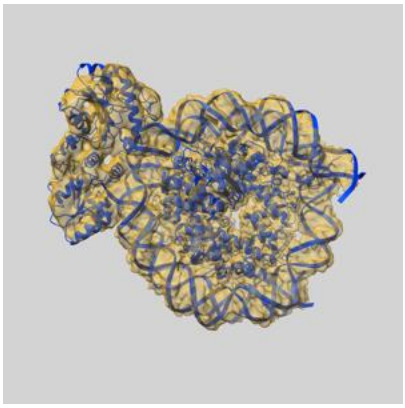
8 Fourier-Shell correlation (i)

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

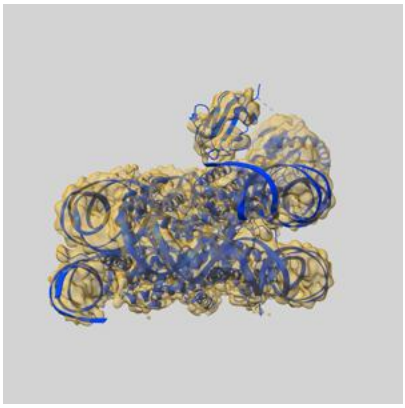
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78606 and PDB model 37XS. Per-residue inclusion information can be found in section 3 on page 6.

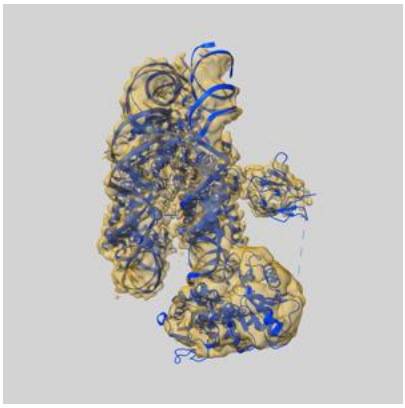
9.1 Map-model overlay



X



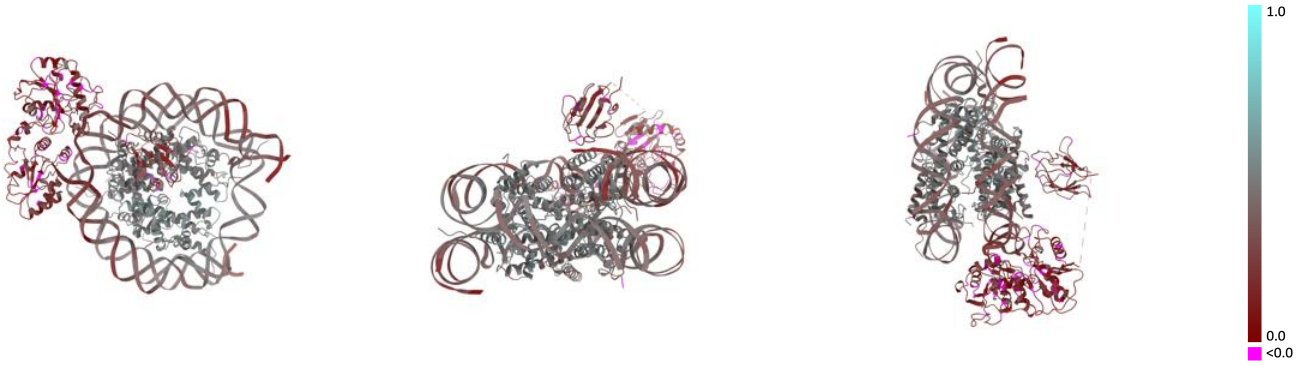
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.8 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.

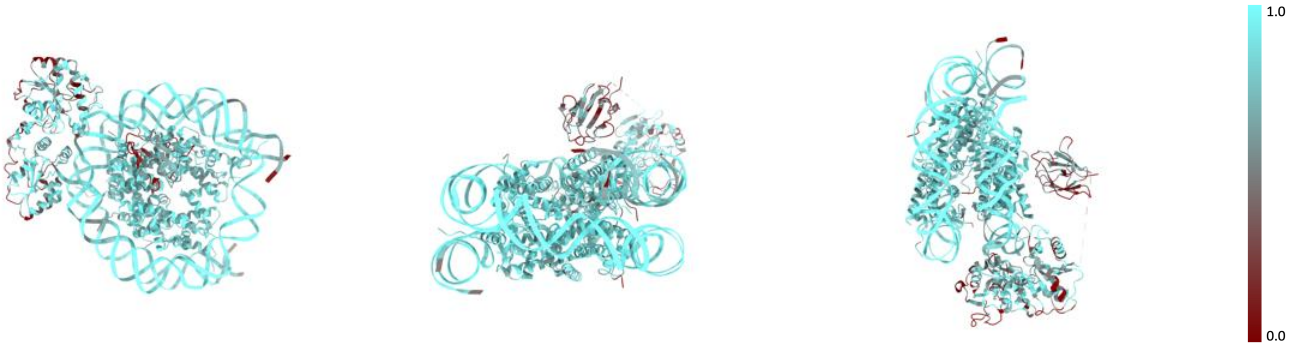
9.2 Q-score mapped to coordinate model (i)



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.

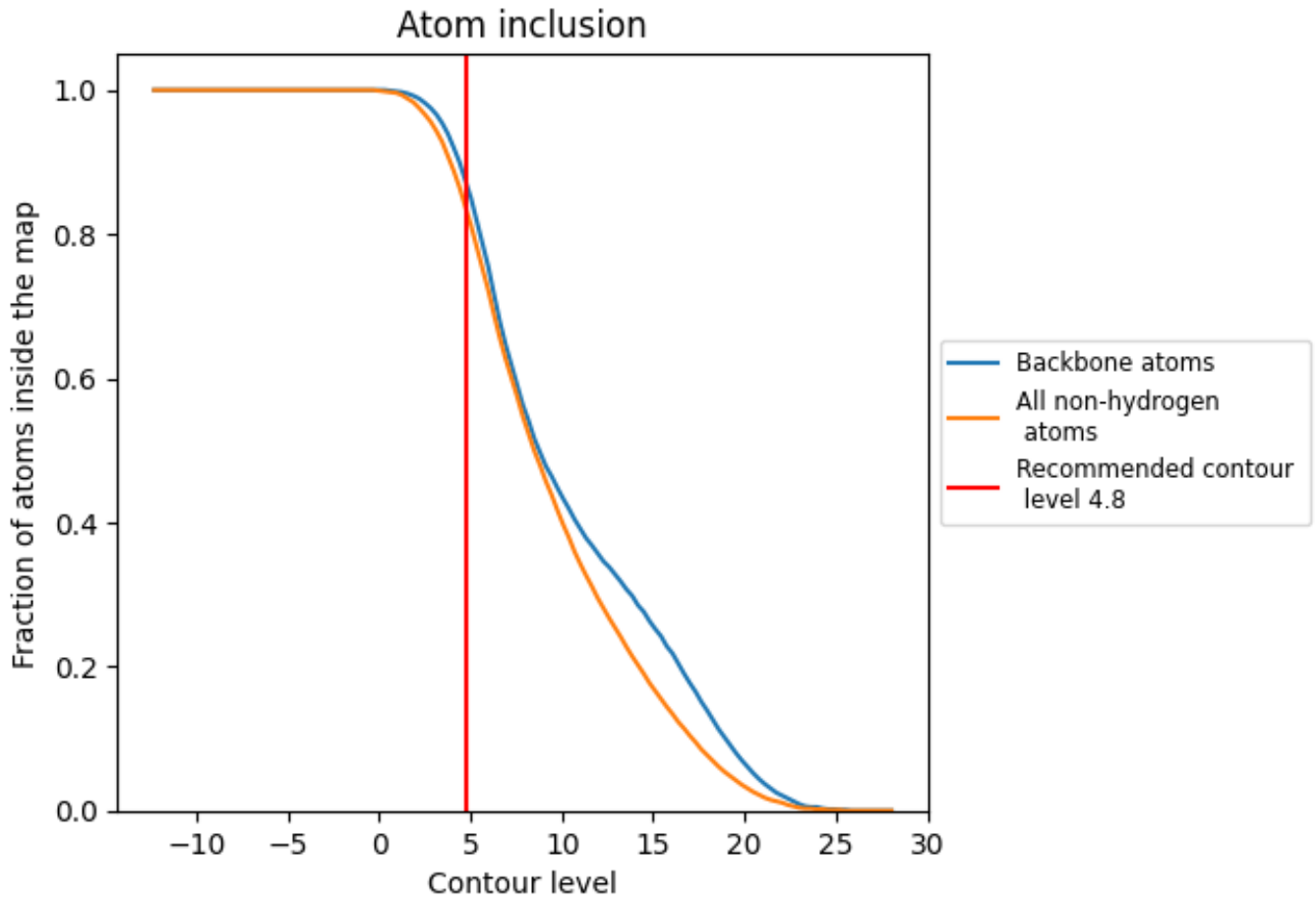
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.8).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.3580
A	0.8780	0.4770
B	0.8990	0.4790
C	0.8860	0.4750
D	0.8830	0.4630
E	0.9220	0.5120
F	0.9220	0.5140
G	0.8820	0.4780
H	0.8740	0.4700
I	0.9030	0.3560
J	0.8190	0.3100
K	0.9550	0.3710
L	0.5940	0.1550

