Full wwPDB EM Validation Report (i)

May 18, 2024 – 12:07 PM EDT

PDB ID	:	6V4X
EMDB ID	:	EMD-21050
Title	:	Cryo-EM structure of an active human histone pre-mRNA 3'-end processing machinery at 3.2 Angstrom resolution
Authors	:	Sun, Y.; Zhang, Y.; Walz, T.; Tong, L.
Deposited on	:	2019-12-02
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

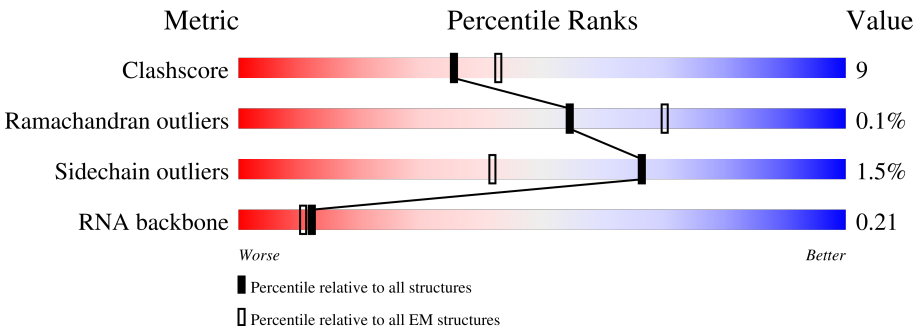
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	146	46% 10% • 43%
2	B	95	68% 12% 20%
3	F	86	69% 17% 14%
4	E	92	76% 12% 12%
5	G	84	76% 14% • 8%
6	C	123	77% 15% 7%
7	D	259	33% 8% 59%

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Mol	Chain	Length	Quality of chain
8	H	684	59% 13% 27%
9	I	782	51% 14% 35%
10	J	1072	5% 26% 71%
11	Z	60	18% 12% 15% 55%
12	Y	52	10% 19% 17% 10% 52%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 16499 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 Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	83	652	409	115	122	6	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P62318
A	-18	GLY	-	expression tag	UNP P62318
A	-17	SER	-	expression tag	UNP P62318
A	-16	SER	-	expression tag	UNP P62318
A	-15	HIS	-	expression tag	UNP P62318
A	-14	HIS	-	expression tag	UNP P62318
A	-13	HIS	-	expression tag	UNP P62318
A	-12	HIS	-	expression tag	UNP P62318
A	-11	HIS	-	expression tag	UNP P62318
A	-10	HIS	-	expression tag	UNP P62318
A	-9	SER	-	expression tag	UNP P62318
A	-8	SER	-	expression tag	UNP P62318
A	-7	GLY	-	expression tag	UNP P62318
A	-6	LEU	-	expression tag	UNP P62318
A	-5	VAL	-	expression tag	UNP P62318
A	-4	PRO	-	expression tag	UNP P62318
A	-3	ARG	-	expression tag	UNP P62318
A	-2	GLY	-	expression tag	UNP P62318
A	-1	SER	-	expression tag	UNP P62318
A	0	HIS	-	expression tag	UNP P62318

- Molecule 2 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	76	612	387	111	107	7	0	0

- Molecule 3 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	74	579	375	95	104	5	0	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	81	670	426	119	120	5	0	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	77	604	381	110	107	6	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	77	LEU	-	expression tag	UNP P62308
G	78	GLU	-	expression tag	UNP P62308
G	79	HIS	-	expression tag	UNP P62308
G	80	HIS	-	expression tag	UNP P62308
G	81	HIS	-	expression tag	UNP P62308
G	82	HIS	-	expression tag	UNP P62308
G	83	HIS	-	expression tag	UNP P62308
G	84	HIS	-	expression tag	UNP P62308

- Molecule 6 is a protein called U7 snRNA-associated Sm-like protein LSm10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	114	911	565	175	169	2	0	0

- Molecule 7 is a protein called U7 snRNA-associated Sm-like protein LSm11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	106	872	556	170	141	5	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	MET	-	expression tag	UNP P83369
D	-9	HIS	-	expression tag	UNP P83369
D	-8	HIS	-	expression tag	UNP P83369
D	-7	HIS	-	expression tag	UNP P83369
D	-6	HIS	-	expression tag	UNP P83369
D	-5	HIS	-	expression tag	UNP P83369
D	-4	HIS	-	expression tag	UNP P83369
D	-3	SER	-	expression tag	UNP P83369
D	-2	GLY	-	expression tag	UNP P83369
D	-1	GLY	-	expression tag	UNP P83369
D	0	SER	-	expression tag	UNP P83369

- Molecule 8 is a protein called Cleavage and polyadenylation specificity factor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	499	3980	2534	682	735	29	0	0

- Molecule 9 is a protein called Cleavage and polyadenylation specificity factor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	510	4055	2580	692	760	23	0	0

- Molecule 10 is a protein called Symplekin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	311	2461	1569	422	457	13	0	0

- Molecule 11 is a RNA chain called U7 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	Z	27	564	253	88	196	27	0	0

- Molecule 12 is a RNA chain called modified H2a pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	Y	25	537	241	102	169	25	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

Interest" by depositor).

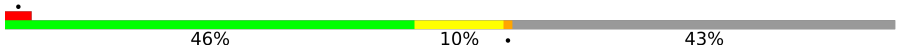
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
13	H	2	2	2	0

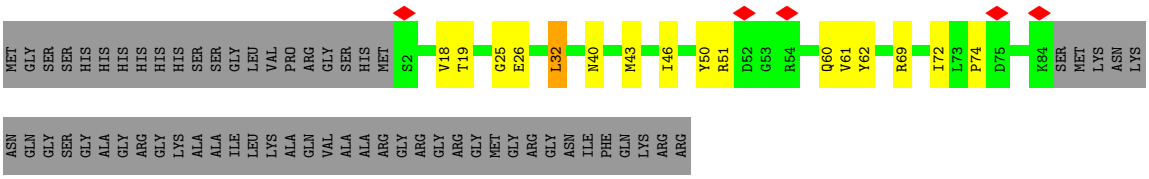
3 Residue-property plots (i)

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: Small nuclear ribonucleoprotein Sm D3

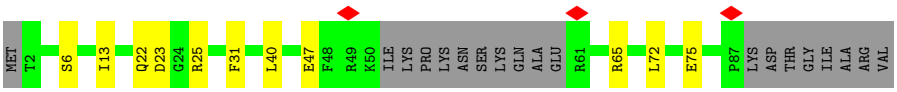
Chain A:





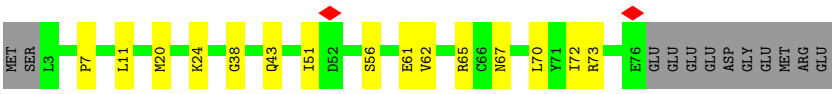
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain B:



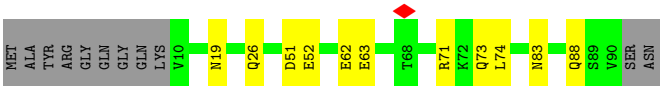
• Molecule 3: Small nuclear ribonucleoprotein F

Chain F:



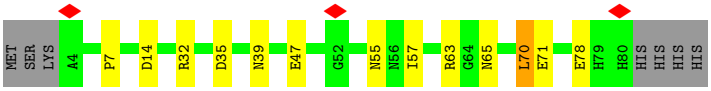
• Molecule 4: Small nuclear ribonucleoprotein E

Chain E:



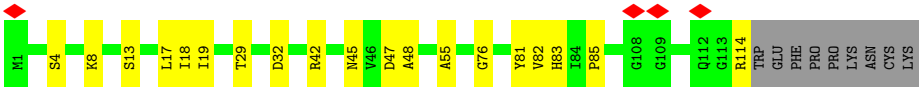
• Molecule 5: Small nuclear ribonucleoprotein G

Chain G:



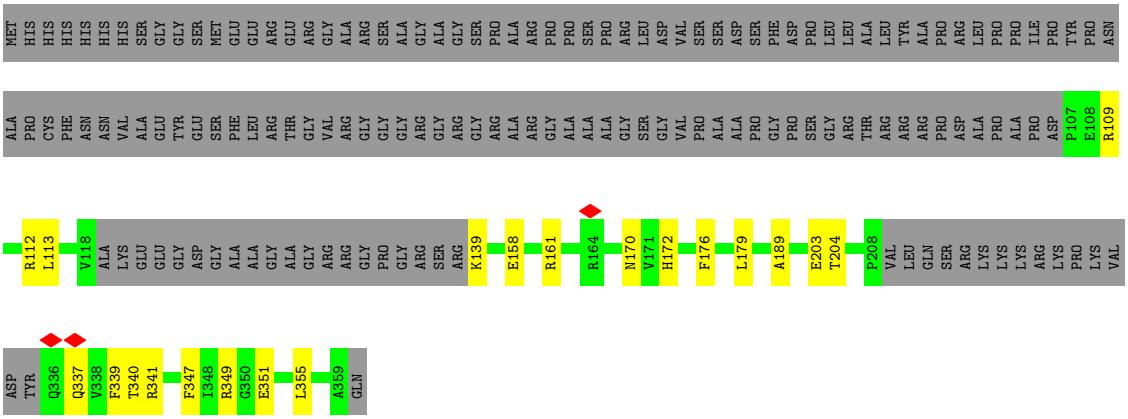
• Molecule 6: U7 snRNA-associated Sm-like protein LSm10

Chain C:



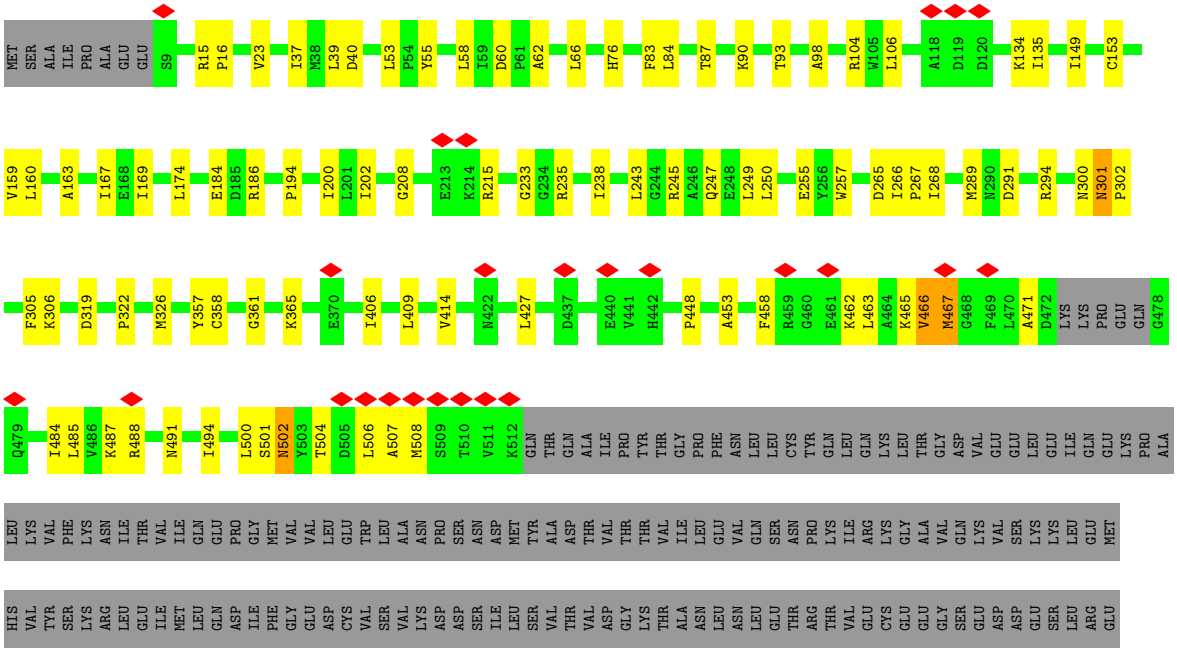
• Molecule 7: U7 snRNA-associated Sm-like protein LSm11

Chain D:



• Molecule 8: Cleavage and polyadenylation specificity factor subunit 3

Chain H:



MET VAL GLU LEU ALA ALA GLN ARG LEU TYR GLU ALA LEU THR PRO VAL HIS

• Molecule 9: Cleavage and polyadenylation specificity factor subunit 2

Chain I: 51% 14% 35%

MET T2 S3 I4 I5 K6 L7 E15 E16 S17 A18 L19 L23 Q24 V25 D26 L31 C34 G35 W36 K50 D56 L60 F63 D64 P65 L68 L71 A86 T87 I88 P89 V90 F97 F123 I126 Q127 Q128 L129 K130 H153 M154 W160 K161

I162 V163 K164 D165 G166 E167 E168 E169 I170 R180 M191 R194 I199 Q209 R215 Q218 N232 Y233 L234 I235 A236 V237 D238 W254 D258 L266 A267 L268 L269 W286 K290 R293 R299 N300 N301 R306 H307 L308 L317 S322 V326

L327 A328 E334 S338 R339 P349 K350 N351 I354 T360 P361 R366 E380 L381 R382 K383 R384 V385 K386 LEU GLU GLY LYS GLU LEU GLU GLU TYR LEU GLU LYS GLU LYS LEU LYS LYS GLU ALA ALA LYS LYS LEU GLU GLN SER LYS GLU ALA ASP ILE ASP SER SER

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

LYS PRO GLU ASP PHE LEU VAL PRO GLU LEU GLN ALA THR GLU GLU GLU LYS SER LYS LEU GLU SER GLY LEU THR ASN GLY ASP GLU PRO MET ASP GLN ASP LEU SER ASP VAL P519 C522 I523 S524 T525 K532 D539 G546 D547 S548 I549 K557 Q560 L561 I562

F581 K584 D585 D598 A599 T600 S601 E602 T603 H604 I605 Y606 Q607 V608 R609 L610 K611 D612 S613 L614 V615 S616 S617 L618 Q619 K622 A623 K624 D625 A626 E627 L628 A629 W630 I631 D632 G633 V634 M637 ARG VAL SER LYS VAL ASP THR GLY VAL ILE LEU GLU GLU GLY GLU LEU LYS

ASP ASP GLY GLU ASP SER GLU MET GLN VAL GLU ALA PRO SER ASP SER SER VAL ILE ALA GLN GLN LYS ALA MET LYS SER LEU PHE GLY ASP ASP GLU LYS GLU THR GLY GLU GLU SER GLU ILE I697 P698 T699 L700 E701 P702 LEU PRO PRO HIS GLU VAL PRO GLY HIS GLN SER VAL

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

LEU TYR GLU GLN TYR ALA ILE VAL

• Molecule 10: Symplekin

Chain J: 5% 26% 71%

M30 V36 N48 V58 Q59 E60 I63 N64 Q81 K84 V92 R102 D103 N113 L117 R148 E152 D159 G166 I169 V192 T193 L194 M198 A199 D200 S201 E202 I203 P204 R205 H209 D210 D214 P217 R218 D219 H220 N226

V227 L228 H245 I251 T254 L260 R267 V274 E279 H282 A283 N284 L285 P286 P287 T288 L289 A290 K291 S292 Q293 S296 V297 R298 K302 L306 S307 K310 H311 S314 L315 E316 F317 Q318 A319 Q320 L324 L325 V326 D327 L328 G329 T330 P331 Q332 A333

E334 I335 A336 R337 N338 M339 P340 SER SER LYS ASP THR ARG LYS ARG PRO ARG ASP ASP SER ASP SER THR LEU LYS LYS MET LYS LEU GLU PRO ASN LEU GLY GLU ASP ASP GLU ASP LYS ASP LEU GLU PRO GLY PRO SER GLY THR SER LYS ALA SER ALA GLN ILE SER GLY GLN SER

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

ALA THR GLN MET THR ALA ALA GLY LEU GLY PRO GLY VAL GLU GLN THR LYS GLN CYS LYS GLU GLU PRO LYS GLU GLU LYS VAL VAL LYS THR GLU SER VAL LEU ILE LYS ARG ARG LEU SER ALA GLN GLY GLN ALA ILE SER VAL VAL GLY SER LEU SER SER MET SER PRO LEU GLU

GLU GLU ALA PRO GLN ALA LYS ARG ARG PRO GLU PRO ILE ILE PRO VAL THR GLN PRO ARG LEU ALA GLY ALA GLY ARG LYS LYS ILE PHE ARG LEU SER ASP VAL LEU LYS PRO LEU THR ASP ALA GLN VAL GLU ALA MET LYS LEU GLY ALA VAL LYS ARG ILE LEU ARG LEU GLU

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

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

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

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

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

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

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

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

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

• Molecule 11: U7 snRNA

Chain Z:

A G U G U6 U7 A8 C12 U16 G20 A21 A22 U23 U24 U25 G26 U27 C28 U29 A30 G31 U32 A G G C U U U C U G G C U U U U A C C G G A A A G C C C

• Molecule 12: modified H2a pre-mRNA

Chain Y:

C C A A A G G C U C U U U U C A G A G C C A C C C25 A26 C27 U28 G29 A30 A31 U32 C33 A34 G35 A36 U37 G41 A42 G46 U47 A48 A49 C A C

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325282	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 ($e^-/Å^2$)	70, 73	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.106	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0243	Depositor
Map size (Å)	357.38, 357.38, 357.38	wwPDB
Map dimensions	334, 334, 334	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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

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	0.30	0/660	0.57	0/889
2	B	0.34	0/620	0.55	0/826
3	F	0.36	0/591	0.64	0/799
4	E	0.34	0/678	0.55	0/910
5	G	0.32	0/613	0.55	0/821
6	C	0.32	0/923	0.61	0/1246
7	D	0.33	0/888	0.63	0/1192
8	H	0.34	0/4068	0.57	0/5498
9	I	0.35	0/4135	0.63	0/5596
10	J	0.26	0/2497	0.50	0/3385
11	Z	0.58	0/627	0.94	0/972
12	Y	0.59	2/602 (0.3%)	1.18	4/936 (0.4%)
All	All	0.35	2/16902 (0.0%)	0.64	4/23070 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Y	46	G	O3'-P	7.30	1.70	1.61
12	Y	48	A	O3'-P	6.75	1.69	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Y	48	A	P-O3'-C3'	16.28	139.23	119.70
12	Y	48	A	OP2-P-O3'	12.11	131.83	105.20
12	Y	48	A	OP1-P-O3'	-10.86	81.30	105.20
12	Y	47	U	P-O3'-C3'	-9.85	107.88	119.70

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	652	0	670	20	0
2	B	612	0	634	8	0
3	F	579	0	590	11	0
4	E	670	0	696	9	0
5	G	604	0	621	19	0
6	C	911	0	923	17	0
7	D	872	0	907	20	0
8	H	3980	0	3947	76	0
9	I	4055	0	4080	103	0
10	J	2461	0	2566	17	0
11	Z	564	0	285	23	0
12	Y	537	0	271	10	0
13	H	2	0	0	0	0
All	All	16499	0	16190	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (279) 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:62:TYR:HB3	5:G:70:LEU:HD21	1.27	1.10
8:H:471:ALA:HB1	9:I:604:HIS:O	1.59	1.00
9:I:194:ARG:NH2	9:I:557:LYS:HB3	1.79	0.98
1:A:62:TYR:HB3	5:G:70:LEU:CD2	1.93	0.97
8:H:465:LYS:NZ	9:I:166:GLY:HA2	1.90	0.86
9:I:328:ALA:HB1	9:I:338:SER:HB2	1.61	0.83
9:I:194:ARG:NH2	9:I:557:LYS:CB	2.43	0.81
9:I:194:ARG:HG3	9:I:557:LYS:O	1.80	0.81
8:H:501:SER:HB3	8:H:507:ALA:CB	2.11	0.80
8:H:501:SER:HB3	8:H:507:ALA:HB2	1.62	0.79
8:H:500:LEU:HB3	8:H:507:ALA:HA	1.63	0.79
9:I:327:LEU:N	9:I:327:LEU:HD23	1.99	0.77
9:I:5:ILE:H	9:I:600:THR:HG22	1.51	0.76
1:A:62:TYR:CB	5:G:70:LEU:HD21	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:337:GLN:HB2	7:D:339:PHE:CZ	2.23	0.73
11:Z:7:U:H5”	11:Z:7:U:H6	1.54	0.73
9:I:634:VAL:CG1	9:I:701:GLU:HB2	2.18	0.73
8:H:467:MET:CB	9:I:605:ILE:HG12	2.18	0.72
8:H:106:LEU:HD23	8:H:243:LEU:HD12	1.71	0.72
9:I:194:ARG:HH22	9:I:557:LYS:HB3	1.50	0.72
1:A:62:TYR:O	5:G:70:LEU:CD2	2.38	0.71
1:A:62:TYR:O	5:G:70:LEU:HD23	1.88	0.71
9:I:610:LEU:CD2	9:I:700:LEU:HD12	2.20	0.71
9:I:5:ILE:N	9:I:600:THR:HG22	2.06	0.70
9:I:608:VAL:HG22	9:I:698:PRO:HG2	1.74	0.70
8:H:471:ALA:CB	9:I:604:HIS:O	2.38	0.70
1:A:32:LEU:C	1:A:32:LEU:HD12	2.12	0.69
6:C:32:ASP:HB2	6:C:81:TYR:HB2	1.74	0.69
9:I:328:ALA:HB1	9:I:338:SER:CB	2.22	0.69
8:H:500:LEU:CB	8:H:507:ALA:HA	2.23	0.68
8:H:465:LYS:HZ3	9:I:166:GLY:HA2	1.58	0.68
9:I:5:ILE:HG13	9:I:599:ALA:O	1.94	0.67
9:I:17:SER:HB2	9:I:360:THR:HG22	1.76	0.67
11:Z:7:U:H5”	11:Z:7:U:C6	2.30	0.66
6:C:18:ILE:HD13	6:C:48:ALA:HA	1.77	0.66
3:F:7:PRO:HG2	4:E:51:ASP:HB2	1.78	0.65
8:H:465:LYS:HZ2	9:I:166:GLY:HA2	1.60	0.65
8:H:186:ARG:NH1	8:H:255:GLU:OE2	2.30	0.65
8:H:98:ALA:HB1	8:H:160:LEU:CD1	2.27	0.65
9:I:634:VAL:HG12	9:I:701:GLU:O	1.97	0.65
5:G:7:PRO:HG3	11:Z:24:U:O4	1.98	0.64
9:I:269:LEU:HD11	9:I:317:LEU:HD22	1.80	0.64
8:H:200:ILE:HD11	8:H:458:PHE:HE2	1.62	0.64
8:H:194:PRO:HD2	8:H:409:LEU:HD21	1.80	0.64
3:F:20:MET:SD	3:F:73:ARG:NH1	2.71	0.64
8:H:200:ILE:HD11	8:H:458:PHE:CE2	2.33	0.64
9:I:5:ILE:H	9:I:600:THR:CG2	2.11	0.63
8:H:467:MET:HB3	9:I:605:ILE:HG12	1.79	0.63
9:I:618:LEU:HB3	9:I:627:GLU:HB3	1.82	0.62
8:H:500:LEU:HB3	8:H:506:LEU:O	2.00	0.62
9:I:602:GLU:CD	9:I:602:GLU:H	2.02	0.62
9:I:5:ILE:CG1	9:I:600:THR:HG22	2.30	0.61
8:H:500:LEU:HD23	8:H:506:LEU:O	2.00	0.61
1:A:19:THR:HB	1:A:72:ILE:HB	1.82	0.61
11:Z:7:U:H2’	11:Z:8:A:H8	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:ILE:HG12	9:I:600:THR:HG22	1.82	0.60
9:I:634:VAL:HG12	9:I:701:GLU:HB2	1.83	0.60
9:I:23:LEU:HD13	9:I:23:LEU:O	2.01	0.60
9:I:603:THR:HG23	9:I:603:THR:O	2.02	0.60
9:I:5:ILE:N	9:I:600:THR:CG2	2.64	0.60
6:C:76:GLY:O	7:D:349:ARG:NH1	2.35	0.59
8:H:301:ASN:HD22	8:H:302:PRO:HD2	1.67	0.59
6:C:17:LEU:HD11	7:D:189:ALA:O	2.01	0.59
9:I:560:GLN:NE2	9:I:601:SER:HB2	2.16	0.59
9:I:611:LYS:HD3	9:I:701:GLU:HG3	1.83	0.59
11:Z:7:U:H2'	11:Z:8:A:C8	2.37	0.59
8:H:184:GLU:O	8:H:215:ARG:NH1	2.35	0.59
8:H:257:TRP:CE2	8:H:268:ILE:HD11	2.38	0.59
11:Z:7:U:H6	11:Z:7:U:C5'	2.15	0.59
9:I:610:LEU:HD23	9:I:700:LEU:HD12	1.85	0.58
11:Z:26:G:O2'	11:Z:27:U:OP2	2.18	0.58
7:D:158:GLU:OE2	7:D:161:ARG:NH2	2.35	0.58
8:H:501:SER:CB	8:H:507:ALA:HB2	2.32	0.58
9:I:6:LYS:HG2	9:I:598:ASP:HA	1.84	0.58
9:I:234:LEU:HD11	9:I:328:ALA:HB2	1.85	0.58
8:H:153:CYS:HB2	8:H:163:ALA:HB1	1.86	0.58
2:B:31:PHE:HE1	2:B:40:LEU:HD22	1.69	0.58
8:H:500:LEU:O	8:H:504:THR:O	2.22	0.58
3:F:67:ASN:ND2	11:Z:28:C:OP2	2.37	0.57
2:B:47:GLU:OE1	2:B:65:ARG:NH1	2.38	0.57
9:I:560:GLN:HE21	9:I:601:SER:HB2	1.70	0.57
8:H:98:ALA:HB1	8:H:160:LEU:HD13	1.87	0.57
9:I:611:LYS:HB2	9:I:699:THR:HB	1.86	0.57
9:I:60:LEU:O	9:I:160:TRP:NE1	2.36	0.57
8:H:463:LEU:HA	9:I:609:ARG:HA	1.86	0.56
9:I:31:LEU:HD21	9:I:34:CYS:HB3	1.88	0.56
12:Y:49:A:H4'	12:Y:49:A:OP1	2.05	0.56
9:I:164:LYS:HB3	9:I:168:GLU:HB2	1.88	0.56
10:J:260:LEU:HB3	10:J:274:VAL:HG13	1.87	0.55
8:H:265:ASP:OD1	8:H:266:ILE:N	2.38	0.55
8:H:406:ILE:HD11	8:H:414:VAL:HG21	1.88	0.55
9:I:349:PRO:HG3	9:I:532:LYS:HE2	1.87	0.55
9:I:603:THR:O	9:I:605:ILE:HG13	2.06	0.55
12:Y:46:G:H2'	12:Y:47:U:C6	2.41	0.55
9:I:162:ILE:HB	9:I:170:ILE:HB	1.88	0.55
8:H:37:ILE:HD11	8:H:149:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:23:LEU:HD13	9:I:23:LEU:C	2.27	0.55
11:Z:32:U:H2'	11:Z:32:U:O2	2.07	0.55
3:F:24:LYS:NZ	4:E:83:ASN:OD1	2.39	0.54
9:I:88:ILE:HG12	9:I:128:GLN:HB3	1.89	0.54
9:I:4:ILE:HG22	9:I:4:ILE:O	2.06	0.54
4:E:62:GLU:OE1	4:E:73:GLN:NE2	2.40	0.54
8:H:485:LEU:HD12	8:H:494:ILE:HB	1.89	0.54
12:Y:48:A:C2'	12:Y:49:A:OP1	2.56	0.54
5:G:39:ASN:OD1	5:G:63:ARG:HA	2.09	0.53
8:H:467:MET:HB2	9:I:605:ILE:HG12	1.88	0.53
9:I:235:ILE:O	9:I:328:ALA:N	2.31	0.53
8:H:300:ASN:HD21	8:H:306:LYS:NZ	2.05	0.53
8:H:291:ASP:OD1	8:H:294:ARG:NH1	2.41	0.53
10:J:36:VAL:HG13	10:J:58:VAL:HG13	1.91	0.53
4:E:62:GLU:OE2	4:E:71:ARG:NH2	2.40	0.53
9:I:194:ARG:CZ	9:I:557:LYS:HB2	2.40	0.52
11:Z:30:A:C6	11:Z:32:U:H1'	2.44	0.52
9:I:560:GLN:NE2	9:I:601:SER:CB	2.72	0.52
3:F:65:ARG:NH2	11:Z:27:U:O2'	2.42	0.52
3:F:62:VAL:HG13	7:D:355:LEU:HD13	1.92	0.52
2:B:13:ILE:HA	2:B:31:PHE:HD2	1.75	0.52
7:D:172:HIS:HD2	7:D:179:LEU:HD11	1.75	0.52
12:Y:46:G:H2'	12:Y:47:U:H6	1.73	0.51
1:A:26:GLU:HG3	1:A:50:TYR:HA	1.92	0.51
5:G:14:ASP:OD1	5:G:32:ARG:NH1	2.44	0.51
8:H:55:TYR:HB3	8:H:58:LEU:HD23	1.93	0.51
8:H:502:ASN:O	9:I:194:ARG:CD	2.58	0.51
7:D:204:THR:HG22	7:D:340:THR:OG1	2.11	0.51
10:J:203:ILE:HD11	10:J:267:ARG:HH12	1.76	0.51
2:B:40:LEU:HD12	2:B:72:LEU:HD23	1.93	0.51
7:D:337:GLN:HG3	7:D:339:PHE:HE2	1.75	0.51
9:I:290:LYS:NZ	12:Y:46:G:OP1	2.38	0.51
10:J:63:ILE:O	10:J:102:ARG:NH1	2.43	0.51
7:D:176:PHE:CE2	11:Z:30:A:C2	2.98	0.51
9:I:611:LYS:CD	9:I:701:GLU:OE2	2.59	0.51
8:H:500:LEU:HB2	8:H:507:ALA:O	2.12	0.50
1:A:43:MET:HB3	1:A:46:ILE:HD11	1.93	0.50
3:F:51:ILE:HG22	3:F:56:SER:HB2	1.93	0.50
3:F:43:GLN:NE2	3:F:61:GLU:OE2	2.43	0.50
10:J:81:GLN:HB3	10:J:92:VAL:HG11	1.94	0.50
8:H:62:ALA:O	8:H:90:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:PHE:O	8:H:87:THR:OG1	2.29	0.49
9:I:546:GLY:HA2	9:I:549:ILE:HG22	1.94	0.49
8:H:238:ILE:HB	8:H:326:MET:HB3	1.94	0.49
10:J:194:LEU:HD22	10:J:228:LEU:HB3	1.95	0.49
1:A:69:ARG:HH11	2:B:25:ARG:HH22	1.59	0.49
9:I:7:LEU:HD21	9:I:562:ILE:HD13	1.95	0.49
9:I:130:LYS:HA	9:I:286:TRP:HH2	1.77	0.49
9:I:327:LEU:N	9:I:327:LEU:CD2	2.73	0.49
9:I:19:LEU:O	9:I:35:GLY:N	2.45	0.49
9:I:209:GLN:HE21	9:I:215:ARG:HH22	1.60	0.49
6:C:82:VAL:HB	7:D:347:PHE:HB3	1.93	0.49
9:I:23:LEU:CD1	9:I:25:VAL:HG23	2.43	0.49
1:A:62:TYR:CD2	5:G:70:LEU:HD21	2.48	0.49
8:H:501:SER:HB3	8:H:507:ALA:HB1	1.90	0.49
9:I:384:ARG:HD3	9:I:523:ILE:HD11	1.95	0.49
8:H:233:GLY:HA2	8:H:322:PRO:HG3	1.95	0.48
5:G:70:LEU:HD23	5:G:70:LEU:H	1.78	0.48
9:I:634:VAL:O	9:I:700:LEU:HD23	2.12	0.48
7:D:170:ASN:OD1	7:D:170:ASN:N	2.47	0.48
8:H:98:ALA:HB1	8:H:160:LEU:HD11	1.95	0.48
5:G:63:ARG:NH2	11:Z:23:U:C6	2.82	0.48
9:I:232:ASN:N	9:I:351:ASN:OD1	2.46	0.48
12:Y:46:G:H2'	12:Y:47:U:O4'	2.13	0.48
7:D:337:GLN:HG3	7:D:339:PHE:CE2	2.48	0.48
9:I:611:LYS:HD3	9:I:701:GLU:CG	2.43	0.48
8:H:289:MET:O	8:H:294:ARG:NH2	2.46	0.48
5:G:35:ASP:OD1	5:G:39:ASN:N	2.45	0.47
1:A:18:VAL:HG12	1:A:74:PRO:HD3	1.95	0.47
8:H:208:GLY:HA2	8:H:427:LEU:HB2	1.96	0.47
9:I:180:ARG:NH2	9:I:290:LYS:HD2	2.29	0.47
1:A:61:VAL:HA	5:G:71:GLU:HA	1.96	0.47
3:F:24:LYS:HA	3:F:70:LEU:HD12	1.95	0.47
5:G:65:ASN:HB2	11:Z:23:U:O2	2.14	0.47
9:I:63:PRO:HD3	9:I:90:VAL:HG22	1.97	0.47
9:I:215:ARG:NH2	9:I:539:ASP:O	2.48	0.47
11:Z:20:G:H5'	11:Z:21:A:H5"	1.96	0.47
8:H:300:ASN:ND2	8:H:306:LYS:CE	2.78	0.47
9:I:215:ARG:HA	9:I:218:GLN:HG2	1.97	0.47
8:H:245:ARG:O	8:H:249:LEU:HG	2.15	0.47
7:D:113:LEU:HD13	8:H:53:LEU:HD12	1.97	0.47
8:H:487:LYS:NZ	9:I:619:GLN:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:ARG:HB2	8:H:361:GLY:HA2	1.97	0.46
9:I:68:LEU:HD13	9:I:123:PHE:HZ	1.79	0.46
9:I:266:LEU:HB3	9:I:308:LEU:HD13	1.97	0.46
10:J:217:PRO:HG2	10:J:220:HIS:HB2	1.96	0.46
2:B:6:SER:HG	6:C:4:SER:HG	1.60	0.46
6:C:83:HIS:CE1	7:D:341:ARG:HH12	2.33	0.46
8:H:160:LEU:HD13	8:H:160:LEU:O	2.15	0.46
9:I:267:ALA:HB3	9:I:326:VAL:HG22	1.97	0.46
9:I:180:ARG:HH22	9:I:290:LYS:HD2	1.81	0.46
9:I:5:ILE:O	9:I:600:THR:CG2	2.63	0.46
10:J:166:GLY:HA2	10:J:169:ILE:HD12	1.97	0.46
9:I:199:ILE:HG23	9:I:562:ILE:HD11	1.96	0.46
8:H:235:ARG:NH2	8:H:319:ASP:O	2.42	0.46
8:H:463:LEU:HD13	9:I:607:GLN:HE21	1.81	0.46
1:A:40:ASN:HD21	11:Z:24:U:H3	1.63	0.45
6:C:17:LEU:HD23	6:C:17:LEU:HA	1.67	0.45
6:C:18:ILE:CD1	6:C:47:ASP:O	2.65	0.45
8:H:23:VAL:HG11	12:Y:26:A:H5'	1.97	0.45
8:H:84:LEU:O	8:H:134:LYS:NZ	2.40	0.45
10:J:289:LEU:HD12	10:J:293:GLN:HG3	1.98	0.45
1:A:60:GLN:NE2	5:G:78:GLU:OE2	2.50	0.45
8:H:93:THR:HG23	8:H:135:ILE:HA	1.98	0.45
8:H:174:LEU:HD21	8:H:202:ILE:HD12	1.98	0.45
9:I:611:LYS:HB3	9:I:700:LEU:O	2.16	0.45
2:B:23:ASP:O	11:Z:32:U:OP1	2.35	0.45
10:J:48:ASN:ND2	12:Y:36:A:N7	2.64	0.45
3:F:11:LEU:HD21	3:F:72:ILE:HG21	1.99	0.44
8:H:16:PRO:HG2	8:H:448:PRO:HG2	1.99	0.44
8:H:160:LEU:HD13	8:H:160:LEU:C	2.37	0.44
9:I:65:PRO:HD3	9:I:97:PHE:CD1	2.52	0.44
8:H:149:ILE:HG12	8:H:169:ILE:HG12	2.00	0.44
9:I:232:ASN:ND2	9:I:322:SER:O	2.41	0.44
9:I:611:LYS:HD2	9:I:699:THR:OG1	2.17	0.44
7:D:203:GLU:O	7:D:340:THR:HG23	2.17	0.44
1:A:62:TYR:HB3	5:G:70:LEU:HD23	1.92	0.44
8:H:37:ILE:HG12	8:H:66:LEU:HB2	1.98	0.44
8:H:39:LEU:HD21	8:H:167:ILE:HD11	1.99	0.44
8:H:40:ASP:OD2	8:H:76:HIS:ND1	2.35	0.44
6:C:18:ILE:HD13	6:C:47:ASP:O	2.18	0.44
7:D:351:GLU:HG3	11:Z:28:C:H5"	1.99	0.44
8:H:484:ILE:HG21	8:H:500:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:194:ARG:CZ	9:I:557:LYS:CB	2.94	0.44
6:C:13:SER:HA	6:C:18:ILE:HG22	2.00	0.44
8:H:60:ASP:OD1	8:H:60:ASP:N	2.50	0.44
11:Z:26:G:N2	12:Y:33:C:O2	2.47	0.44
6:C:42:ARG:HB3	6:C:55:ALA:HB3	1.99	0.43
8:H:358:CYS:HB3	8:H:365:LYS:HB2	2.00	0.43
4:E:63:GLU:HG3	4:E:74:LEU:HD11	2.00	0.43
10:J:60:GLU:HG2	10:J:64:ASN:HD22	1.83	0.43
6:C:8:LYS:CE	11:Z:26:G:O6	2.67	0.43
9:I:5:ILE:O	9:I:600:THR:HG22	2.18	0.43
9:I:56:ASP:N	9:I:56:ASP:OD1	2.50	0.43
9:I:383:LYS:HA	9:I:522:CYS:HA	2.01	0.43
4:E:52:GLU:HG3	10:J:84:LYS:HG2	2.01	0.42
4:E:88:GLN:HG3	5:G:57:ILE:HB	1.99	0.42
7:D:337:GLN:O	7:D:339:PHE:CD2	2.72	0.42
5:G:47:GLU:HB3	5:G:55:ASN:HB2	2.01	0.42
9:I:60:LEU:HD21	9:I:71:LEU:HD22	2.01	0.42
1:A:32:LEU:C	1:A:32:LEU:CD1	2.85	0.42
8:H:462:LYS:HD2	9:I:614:LEU:HD13	2.01	0.42
5:G:70:LEU:HD23	5:G:70:LEU:O	2.20	0.42
6:C:29:THR:HG22	6:C:85:PRO:HD3	2.01	0.42
11:Z:26:G:O2'	11:Z:27:U:P	2.78	0.42
3:F:38:GLY:O	11:Z:22:A:N6	2.53	0.42
9:I:209:GLN:HE21	9:I:215:ARG:NH2	2.18	0.42
9:I:235:ILE:HG22	9:I:237:VAL:HG13	2.02	0.42
8:H:466:VAL:HG13	8:H:494:ILE:HG23	2.02	0.42
9:I:235:ILE:HG12	9:I:354:ILE:HB	2.02	0.42
9:I:697:ILE:N	9:I:698:PRO:HD2	2.35	0.42
1:A:32:LEU:HD12	1:A:32:LEU:O	2.20	0.41
12:Y:46:G:C5	12:Y:47:U:C5	3.08	0.41
6:C:32:ASP:OD2	6:C:83:HIS:NE2	2.42	0.41
8:H:250:LEU:HD13	8:H:305:PHE:CE2	2.54	0.41
6:C:18:ILE:CG2	6:C:19:ILE:N	2.82	0.41
8:H:15:ARG:HE	8:H:453:ALA:HB2	1.86	0.41
9:I:4:ILE:N	9:I:26:ASP:OD1	2.33	0.41
10:J:251:ILE:HA	10:J:254:THR:HG22	2.03	0.41
10:J:81:GLN:HB2	10:J:117:LEU:HD21	2.02	0.41
1:A:25:GLY:HA3	1:A:51:ARG:HD3	2.03	0.41
1:A:32:LEU:HA	1:A:43:MET:HA	2.02	0.41
8:H:243:LEU:HA	8:H:247:GLN:HE22	1.85	0.41
9:I:86:ALA:HB3	9:I:126:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:30:A:N1	11:Z:32:U:H1'	2.35	0.41
8:H:488:ARG:HA	9:I:622:LYS:HB2	2.03	0.41
9:I:194:ARG:HH22	9:I:557:LYS:CB	2.19	0.41
8:H:300:ASN:ND2	8:H:306:LYS:HE3	2.35	0.41
9:I:361:PRO:HA	9:I:366:ARG:HG3	2.03	0.41
9:I:380:GLU:N	9:I:525:THR:O	2.48	0.41
7:D:109:ARG:HA	7:D:112:ARG:HE	1.84	0.41
9:I:334:GLU:HA	9:I:339:ARG:HH11	1.86	0.41
4:E:26:GLN:NE2	10:J:113:ASN:HD21	2.19	0.40
8:H:485:LEU:HD13	9:I:631:ILE:HD12	2.03	0.40
9:I:97:PHE:CZ	9:I:238:ASP:HB3	2.56	0.40
9:I:153:HIS:CD2	9:I:154:MET:HG3	2.57	0.40
8:H:501:SER:CA	8:H:507:ALA:HB2	2.50	0.40
10:J:192:VAL:O	10:J:267:ARG:NH2	2.53	0.40
2:B:22:GLN:NE2	2:B:75:GLU:O	2.55	0.40
4:E:26:GLN:HE21	10:J:113:ASN:HD21	1.70	0.40
7:D:337:GLN:CG	7:D:339:PHE:CE2	3.05	0.40
8:H:235:ARG:NE	8:H:319:ASP:OD1	2.40	0.40
7:D:337:GLN:O	7:D:339:PHE:CE2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	81/146 (56%)	78 (96%)	3 (4%)	0	100	100
2	B	72/95 (76%)	68 (94%)	4 (6%)	0	100	100
3	F	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
4	E	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
5	G	75/84 (89%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	112/123 (91%)	100 (89%)	12 (11%)	0	100	100
7	D	100/259 (39%)	93 (93%)	7 (7%)	0	100	100
8	H	495/684 (72%)	469 (95%)	25 (5%)	1 (0%)	47	79
9	I	504/782 (64%)	457 (91%)	47 (9%)	0	100	100
10	J	309/1072 (29%)	303 (98%)	6 (2%)	0	100	100
All	All	1899/3423 (56%)	1790 (94%)	108 (6%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	267	PRO

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	73/118 (62%)	72 (99%)	1 (1%)	67	86
2	B	69/85 (81%)	69 (100%)	0	100	100
3	F	63/74 (85%)	63 (100%)	0	100	100
4	E	76/84 (90%)	75 (99%)	1 (1%)	69	87
5	G	67/74 (90%)	66 (98%)	1 (2%)	65	85
6	C	101/110 (92%)	100 (99%)	1 (1%)	76	90
7	D	95/206 (46%)	94 (99%)	1 (1%)	73	88
8	H	435/602 (72%)	426 (98%)	9 (2%)	53	79
9	I	455/695 (66%)	447 (98%)	8 (2%)	59	82
10	J	278/946 (29%)	275 (99%)	3 (1%)	73	88
All	All	1712/2994 (57%)	1687 (98%)	25 (2%)	66	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
4	E	19	ASN
5	G	70	LEU
6	C	45	ASN
7	D	139	LYS
8	H	104	ARG
8	H	159	VAL
8	H	301	ASN
8	H	357	TYR
8	H	466	VAL
8	H	467	MET
8	H	491	ASN
8	H	502	ASN
8	H	508	MET
9	I	36	TRP
9	I	50	LYS
9	I	191	MET
9	I	254	TRP
9	I	299	ARG
9	I	301	ASN
9	I	327	LEU
9	I	602	GLU
10	J	205	ARG
10	J	337	ARG
10	J	338	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
3	F	41	ASN
4	E	19	ASN
6	C	45	ASN
6	C	78	ASN
7	D	160	HIS
7	D	172	HIS
7	D	352	ASN
8	H	85	GLN
8	H	97	HIS
8	H	187	HIS
8	H	247	GLN
8	H	296	GLN
8	H	300	ASN

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Mol	Chain	Res	Type
8	H	301	ASN
8	H	307	HIS
8	H	491	ASN
8	H	502	ASN
9	I	62	HIS
9	I	301	ASN
9	I	607	GLN
10	J	64	ASN
10	J	113	ASN
10	J	207	GLN
10	J	220	HIS
10	J	338	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Z	26/60 (43%)	12 (46%)	2 (7%)
12	Y	24/52 (46%)	11 (45%)	1 (4%)
All	All	50/112 (44%)	23 (46%)	3 (6%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	Z	7	U
11	Z	12	C
11	Z	16	U
11	Z	20	G
11	Z	21	A
11	Z	22	A
11	Z	24	U
11	Z	27	U
11	Z	28	C
11	Z	29	U
11	Z	31	G
11	Z	32	U
12	Y	26	A
12	Y	27	C
12	Y	28	U
12	Y	29	G
12	Y	31	A
12	Y	35	G

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Mol	Chain	Res	Type
12	Y	36	A
12	Y	37	U
12	Y	41	G
12	Y	42	A
12	Y	49	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	Z	7	U
11	Z	26	G
12	Y	48	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are 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.

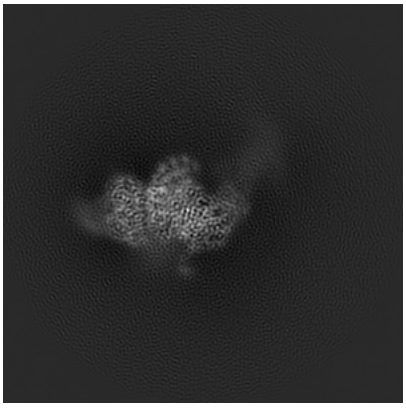
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21050. These allow visual inspection of the internal detail of the map and identification of artifacts.

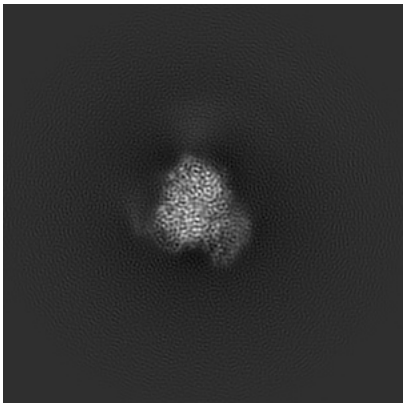
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

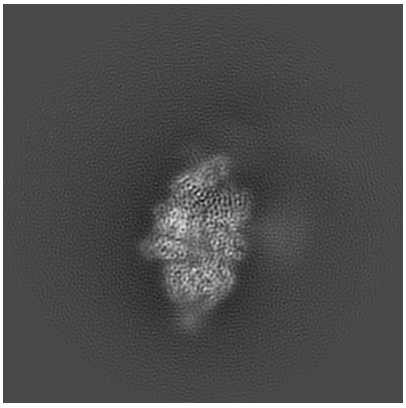
6.1.1 Primary map



X



Y

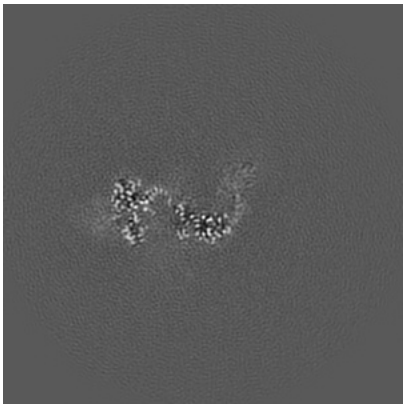


Z

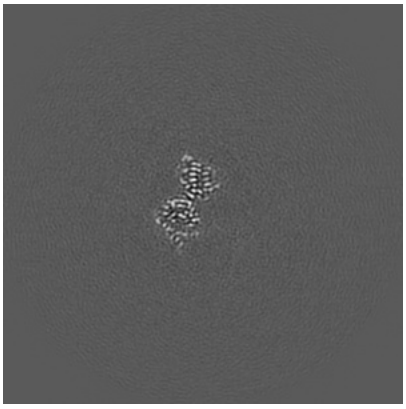
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

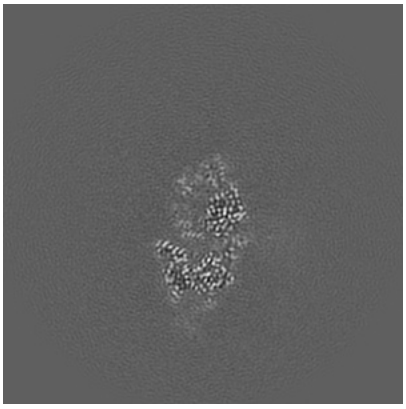
6.2.1 Primary map



X Index: 167



Y Index: 167

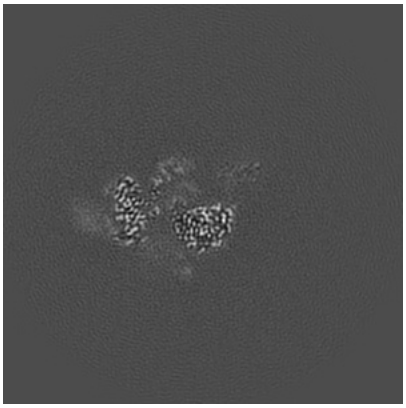


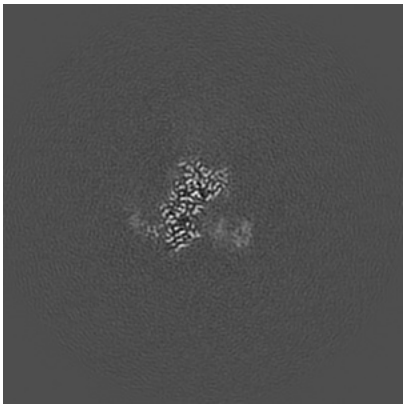
Z Index: 167

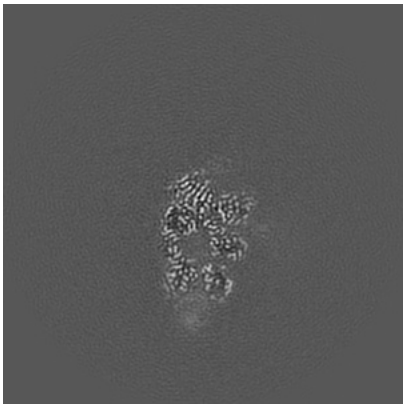
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 153

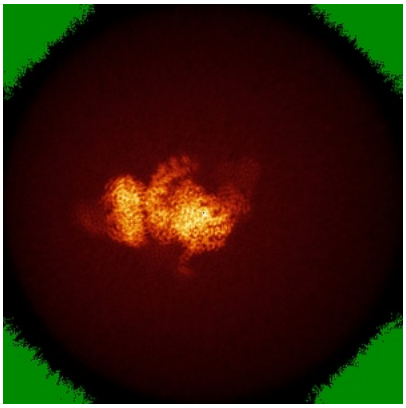

Y Index: 153

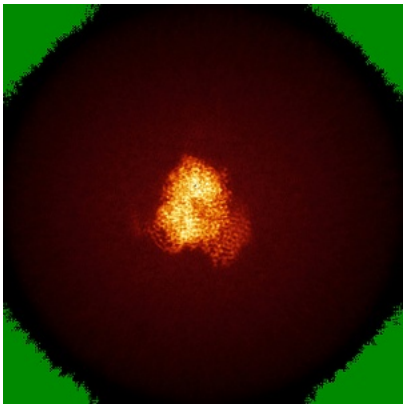

Z Index: 153

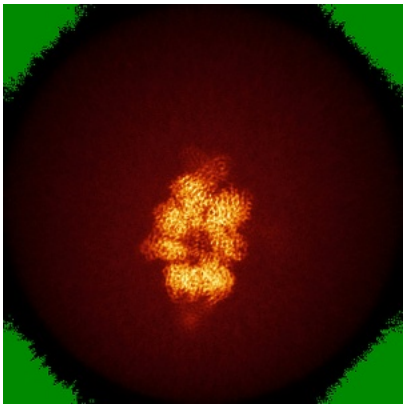
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

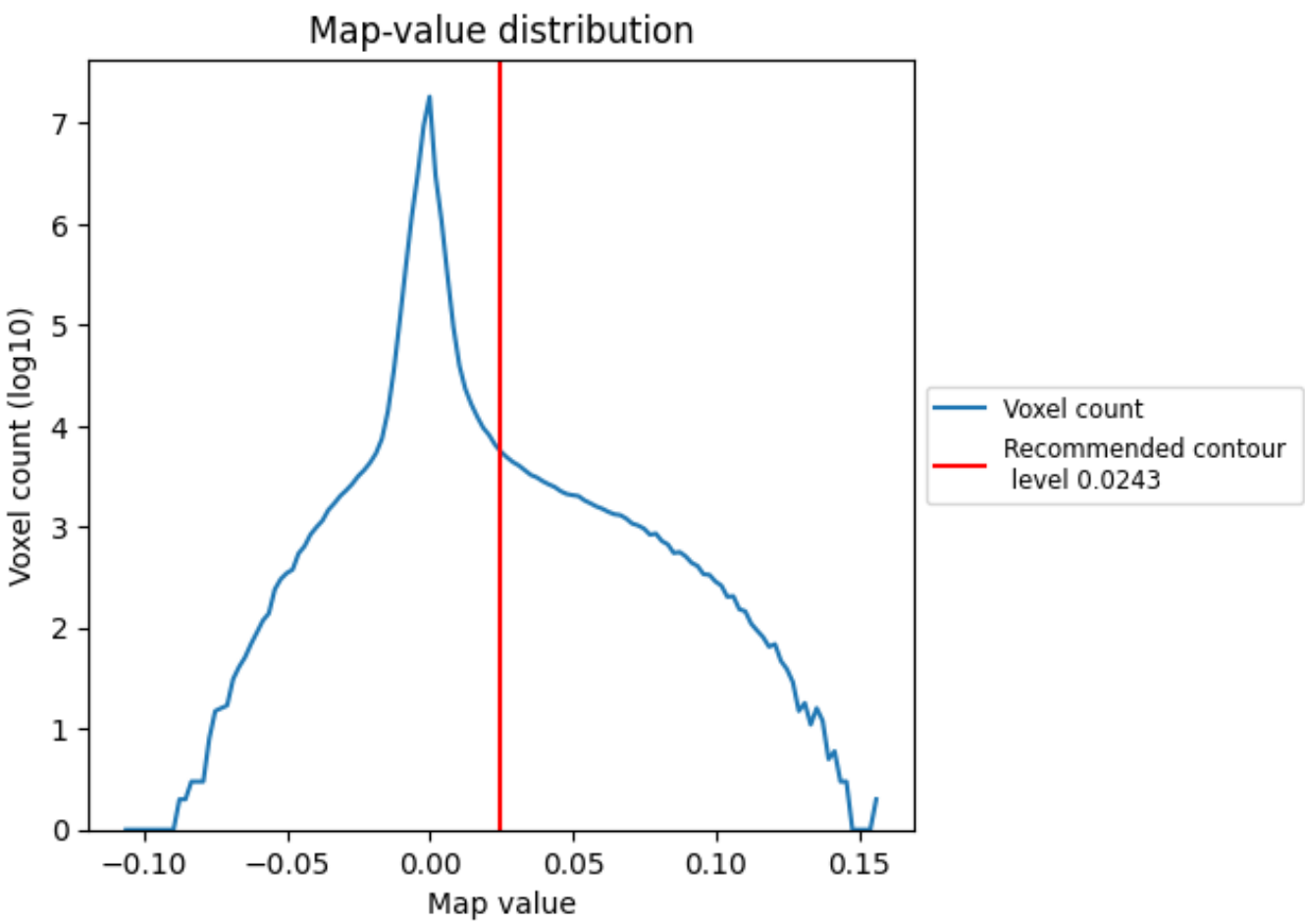
6.6 Mask visualisation (i)

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

7 Map analysis (i)

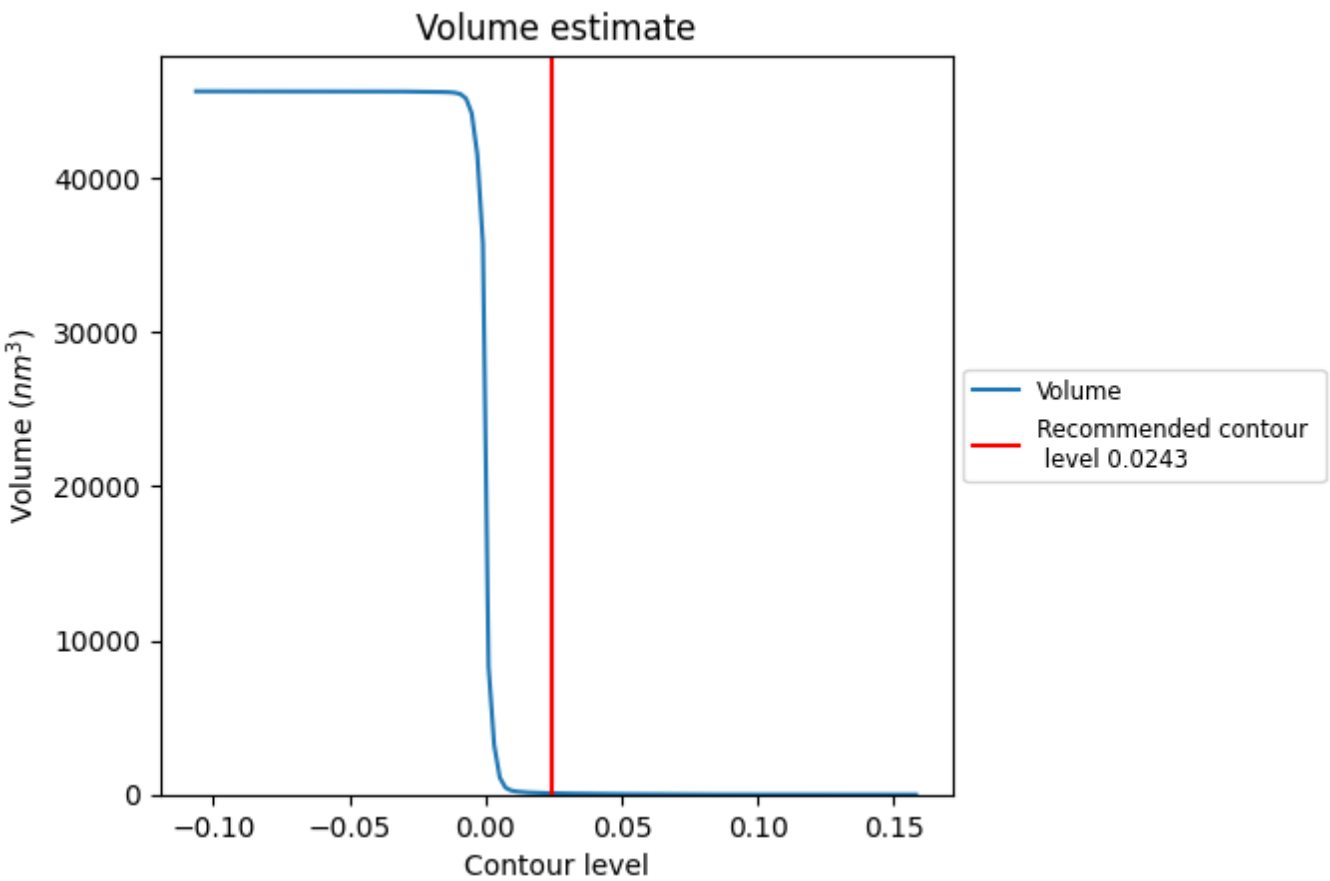
This section contains the results of statistical analysis of the map.

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.

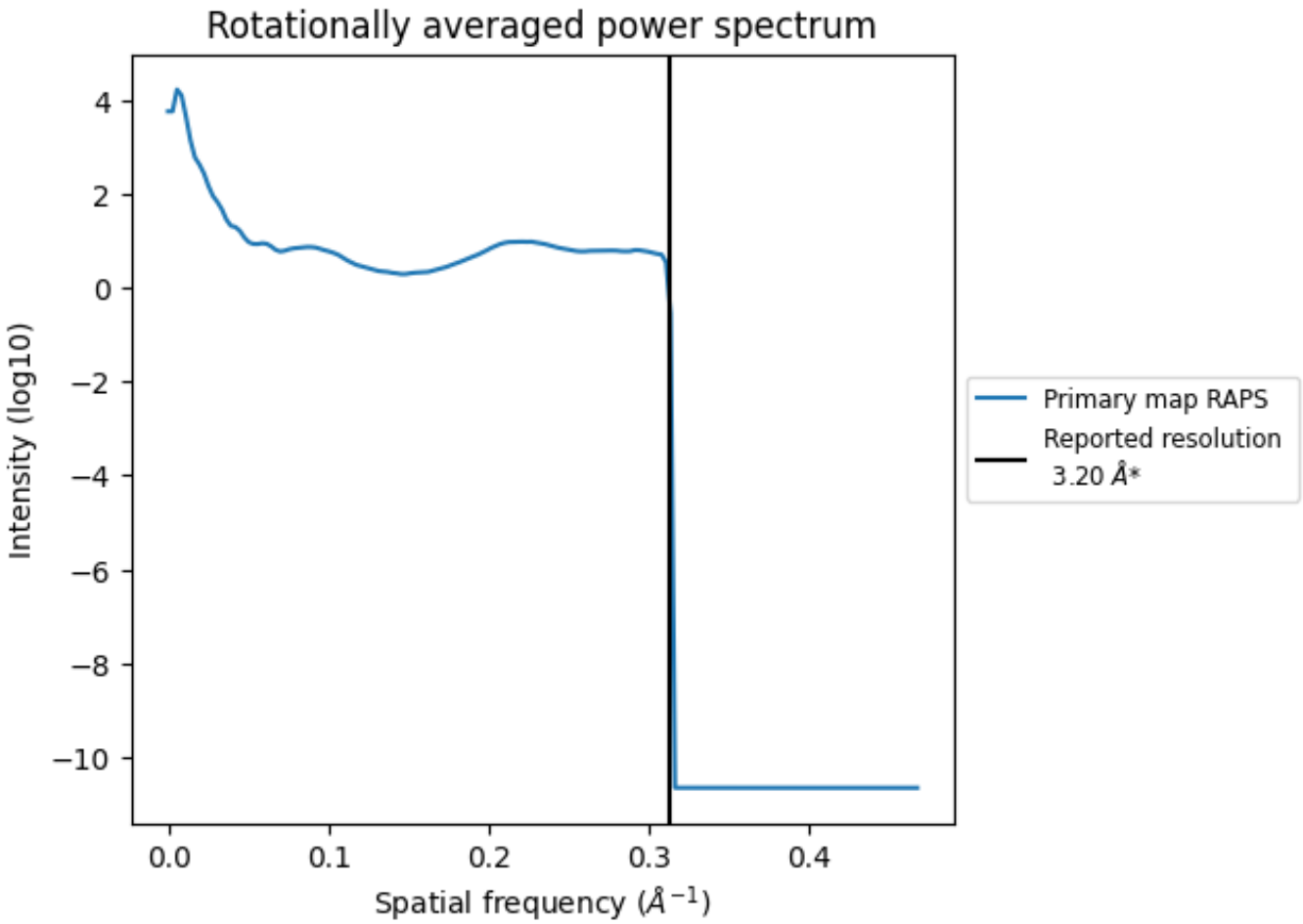
7.2 Volume estimate (i)



The volume at the recommended contour level is 86 nm^3; this corresponds to an approximate mass of 78 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}

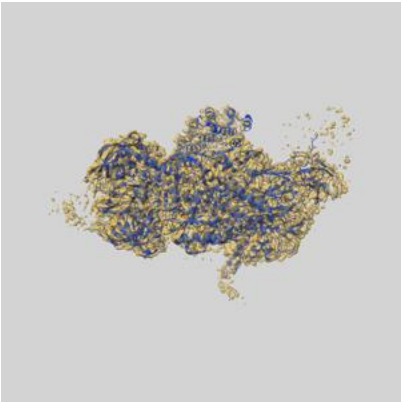
8 Fourier-Shell correlation (i)

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

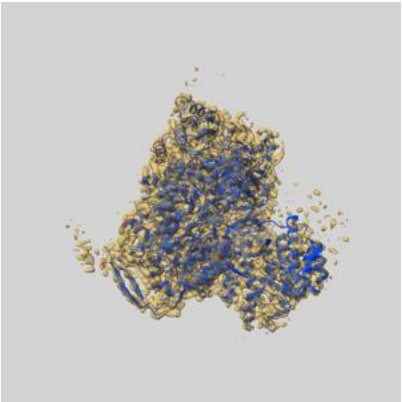
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21050 and PDB model 6V4X. Per-residue inclusion information can be found in section 3 on page 8.

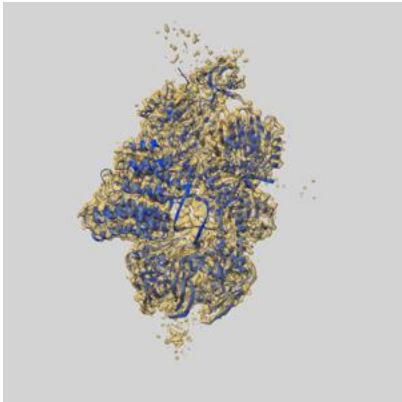
9.1 Map-model overlay (i)



X



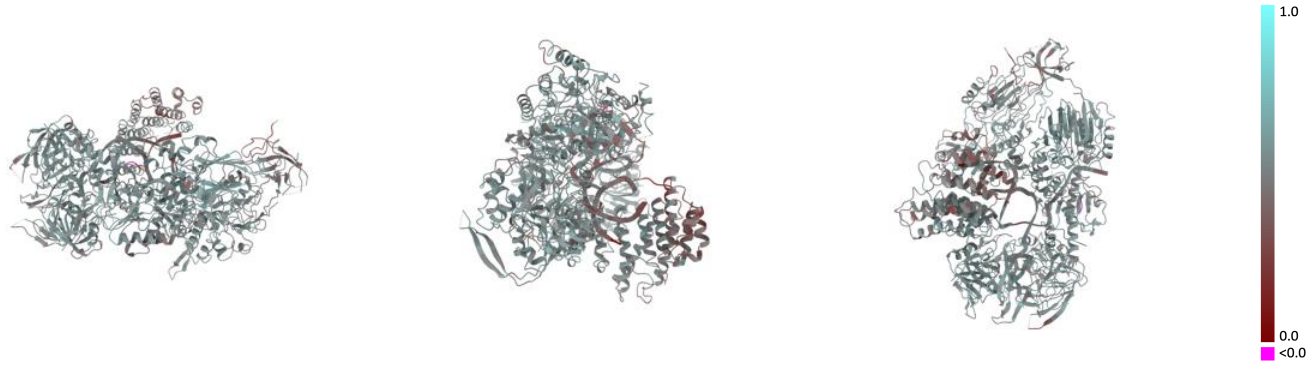
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0243 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.

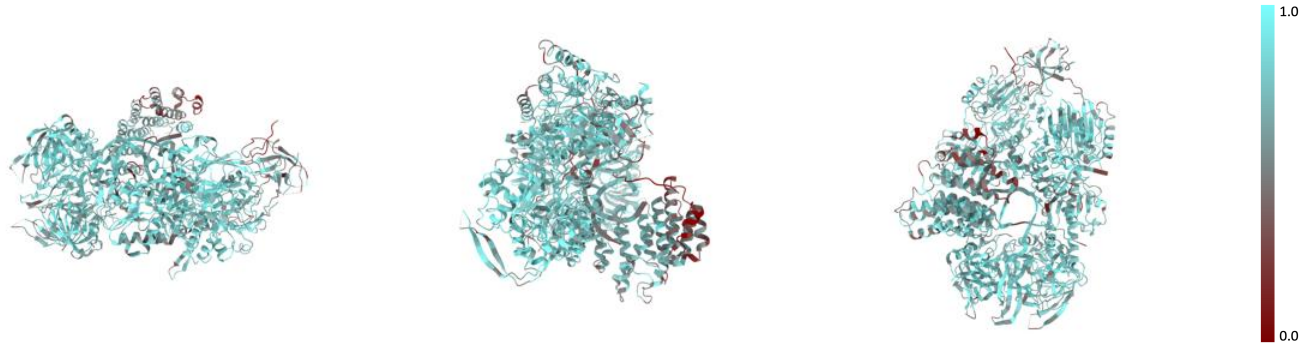
9.2 Q-score mapped to coordinate model (i)



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.

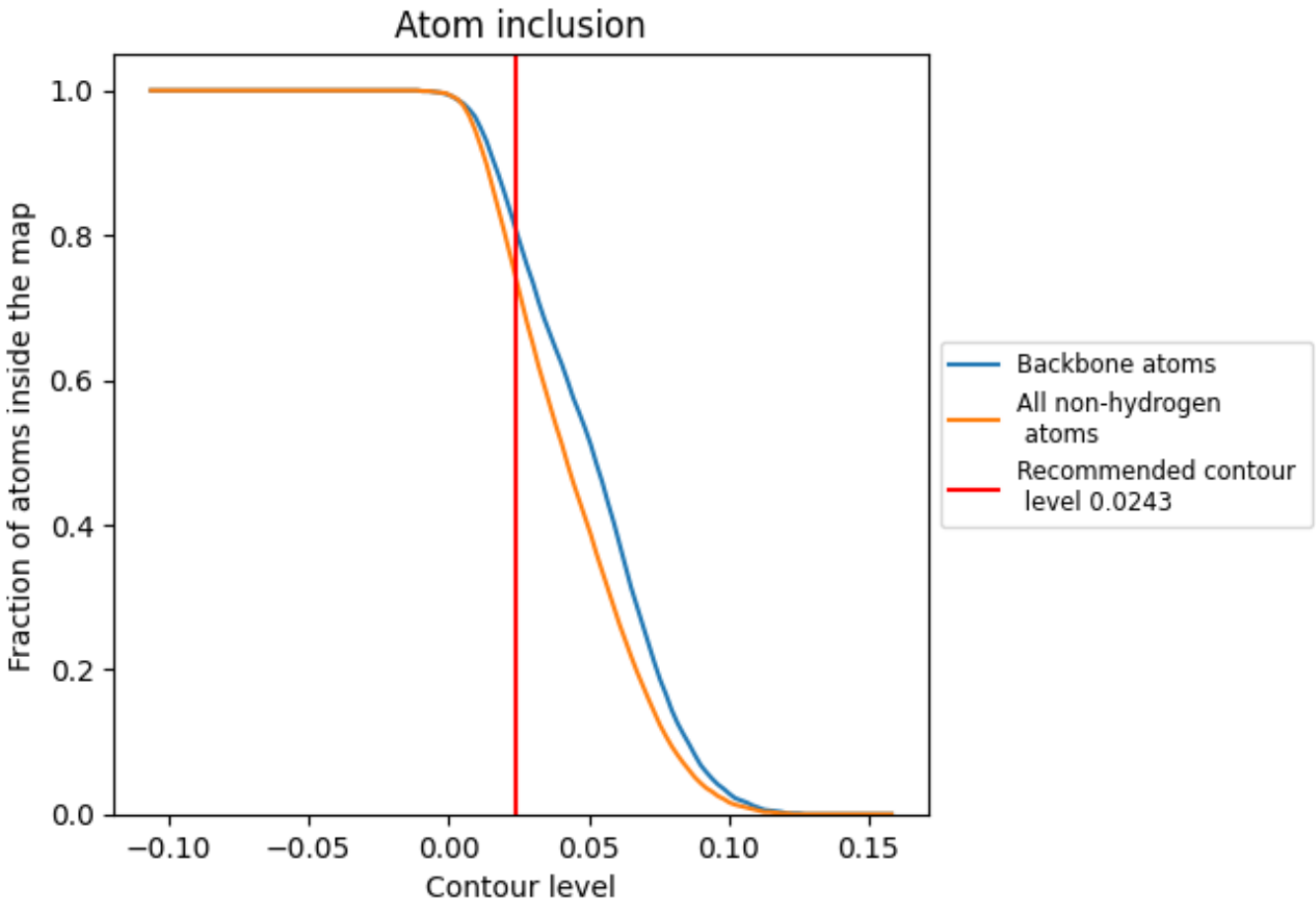
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0243).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5160
A	0.7420	0.5300
B	0.7520	0.5350
C	0.7760	0.5310
D	0.7800	0.5130
E	0.7720	0.5430
F	0.7840	0.5400
G	0.7420	0.5410
H	0.7520	0.5290
I	0.7520	0.5200
J	0.6370	0.4800
Y	0.6630	0.4560
Z	0.7470	0.4820