wwPDB EM Validation Summary Report (i)

Nov 6, 2022 – 04:45 PM EST

PDB ID	:	6N7P
EMDB ID	:	EMD-0360
Title	:	S. cerevisiae spliceosomal E complex (UBC4)
Authors	:	Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on	:	2018-11-27
Resolution	:	3.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

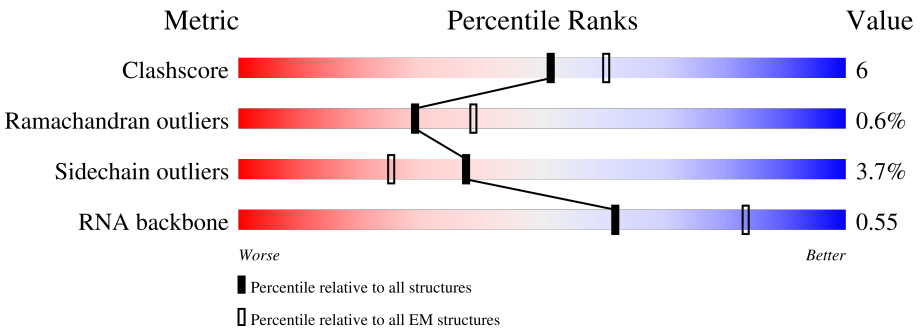
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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	300	33%, 56%, •, •, 38%
2	B	231	10%, 68%, 14%, •, 16%
3	C	350	7%, 29%, 8%, •, 62%
4	D	544	•, 83%, 16%, •
5	E	629	36%, 84%, 7%, 8%
6	F	523	17%, 43%, 7%, •, 49%
7	G	492	•, 40%, 7%, •, 51%

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Mol	Chain	Length	Quality of chain
8	H	105	21% 94% 6%
9	I	261	22% 63% 9% • 26%
10	J	583	34% 33% • 66%
11	K	196	• 58% 5% 37%
12	L	146	• 70% 12% 18%
13	M	110	7% 79% 18% •
14	N	101	• 79% 12% • 8%
15	O	94	70% 9% 21%
16	P	86	67% 16% • 14%
17	Q	77	• 77% 14% • 8%
18	R	568	51% 52% 38% 8% • •
19	r	253	• 6% • 91%
20	X	861	96% 89% 5% • •
21	Y	208	66% 65% • 34%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 41488 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 U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	186	1207	745	228	233	1	0	0

- Molecule 2 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1570	976	301	288	5	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	132	1058	674	193	187	4	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLY	-	expression tag	UNP P32605
C	300	ARG	-	expression tag	UNP P32605
C	301	ARG	-	expression tag	UNP P32605
C	302	ILE	-	expression tag	UNP P32605
C	303	PRO	-	expression tag	UNP P32605
C	304	GLY	-	expression tag	UNP P32605
C	305	LEU	-	expression tag	UNP P32605
C	306	ILE	-	expression tag	UNP P32605
C	307	ASN	-	expression tag	UNP P32605
C	308	PRO	-	expression tag	UNP P32605
C	309	TRP	-	expression tag	UNP P32605
C	310	LYS	-	expression tag	UNP P32605
C	311	ARG	-	expression tag	UNP P32605
C	312	ARG	-	expression tag	UNP P32605
C	313	TRP	-	expression tag	UNP P32605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
C	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
C	320	VAL	-	expression tag	UNP P32605
C	321	SER	-	expression tag	UNP P32605
C	322	ALA	-	expression tag	UNP P32605
C	323	ALA	-	expression tag	UNP P32605
C	324	ASN	-	expression tag	UNP P32605
C	325	ARG	-	expression tag	UNP P32605
C	326	PHE	-	expression tag	UNP P32605
C	327	LYS	-	expression tag	UNP P32605
C	328	LYS	-	expression tag	UNP P32605
C	329	ILE	-	expression tag	UNP P32605
C	330	SER	-	expression tag	UNP P32605
C	331	SER	-	expression tag	UNP P32605
C	332	SER	-	expression tag	UNP P32605
C	333	GLY	-	expression tag	UNP P32605
C	334	ALA	-	expression tag	UNP P32605
C	335	LEU	-	expression tag	UNP P32605
C	336	ASP	-	expression tag	UNP P32605
C	337	TYR	-	expression tag	UNP P32605
C	338	ASP	-	expression tag	UNP P32605
C	339	ILE	-	expression tag	UNP P32605
C	340	PRO	-	expression tag	UNP P32605
C	341	THR	-	expression tag	UNP P32605
C	342	THR	-	expression tag	UNP P32605
C	343	ALA	-	expression tag	UNP P32605
C	344	SER	-	expression tag	UNP P32605
C	345	GLU	-	expression tag	UNP P32605
C	346	ASN	-	expression tag	UNP P32605
C	347	LEU	-	expression tag	UNP P32605
C	348	TYR	-	expression tag	UNP P32605
C	349	PHE	-	expression tag	UNP P32605
C	350	GLN	-	expression tag	UNP P32605

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	544	4561	2990	723	828	20	0	0

- Molecule 5 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	576	3981	2527	693	752	9	0	0

- Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	267	1818	1128	326	353	11	0	0

- Molecule 7 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	239	1954	1267	321	354	12	0	0

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	105	685	425	127	132	1	0	0

- Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	192	1409	878	262	258	11	0	0

- Molecule 10 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	198	984	588	198	198	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	123	1008	636	191	178	3	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	119	921	578	164	176	3	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	107	858	545	159	150	4	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	93	710	450	122	134	4	0	0

- Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	74	563	375	90	95	3	0	0

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	74	584	377	103	103	1	0	0

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	71	543	344	95	103	1	0	0

- Molecule 18 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	R	558	11822	5287	2003	3974	558	0	0

- Molecule 19 is a RNA chain called UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	r	22	471	211	85	153	22	0	0

- Molecule 20 is a protein called Nuclear cap-binding protein complex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	X	826	4101	2449	826	826	0	0

- Molecule 21 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	Y	138	677	401	138	138	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

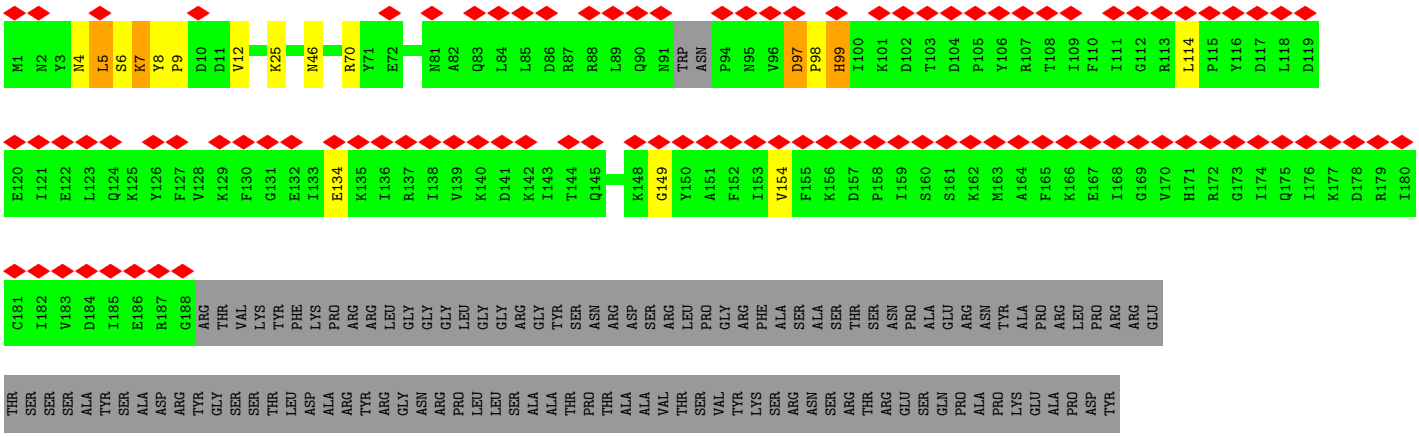
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	B	1	1	1	0
22	I	2	2	2	0

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.

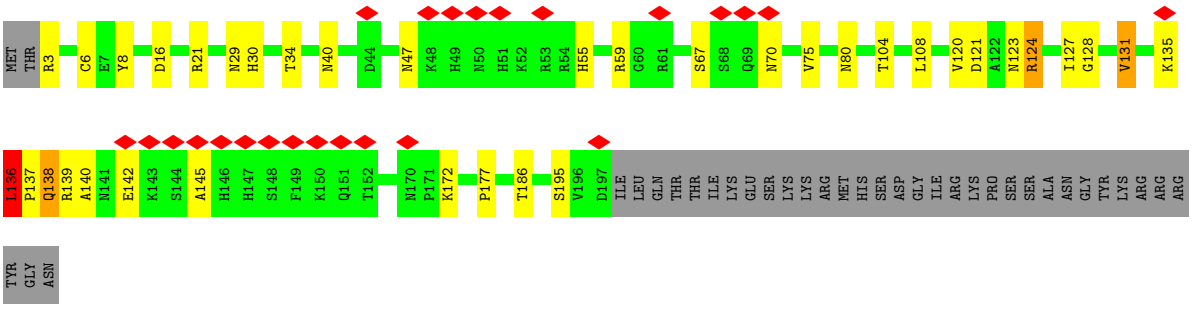
• Molecule 1: U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain A: 33% 56% • • 38%



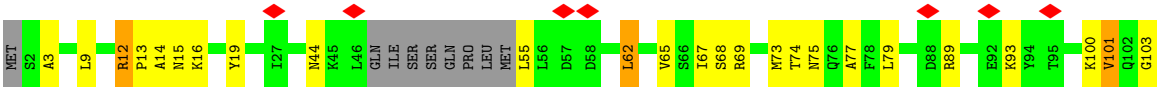
• Molecule 2: U1 small nuclear ribonucleoprotein C

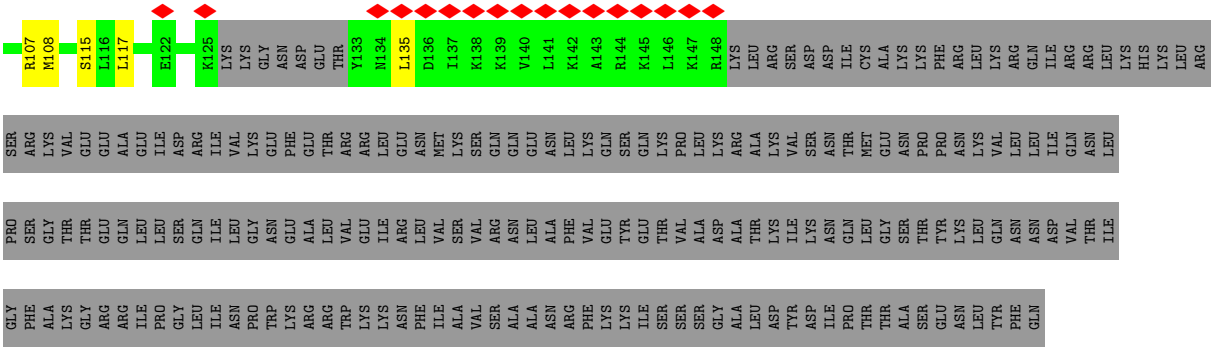
Chain B: 10% 68% 14% • 16%



• Molecule 3: U1 small nuclear ribonucleoprotein A

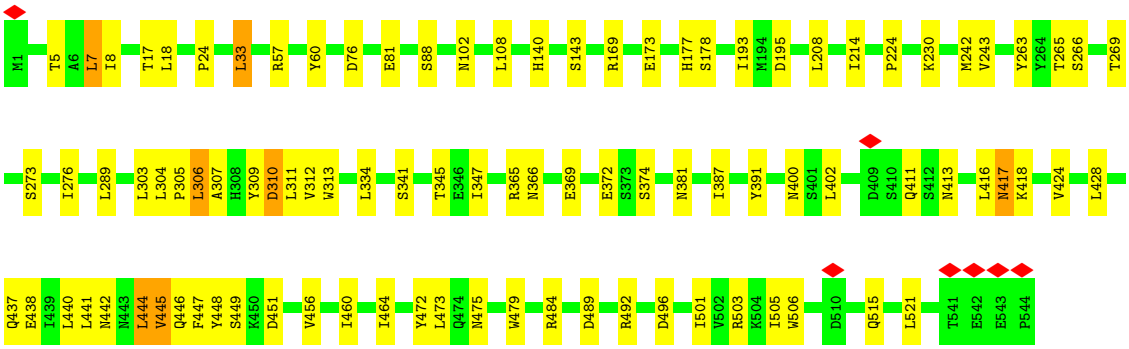
Chain C: 7% 29% 8% • 62%





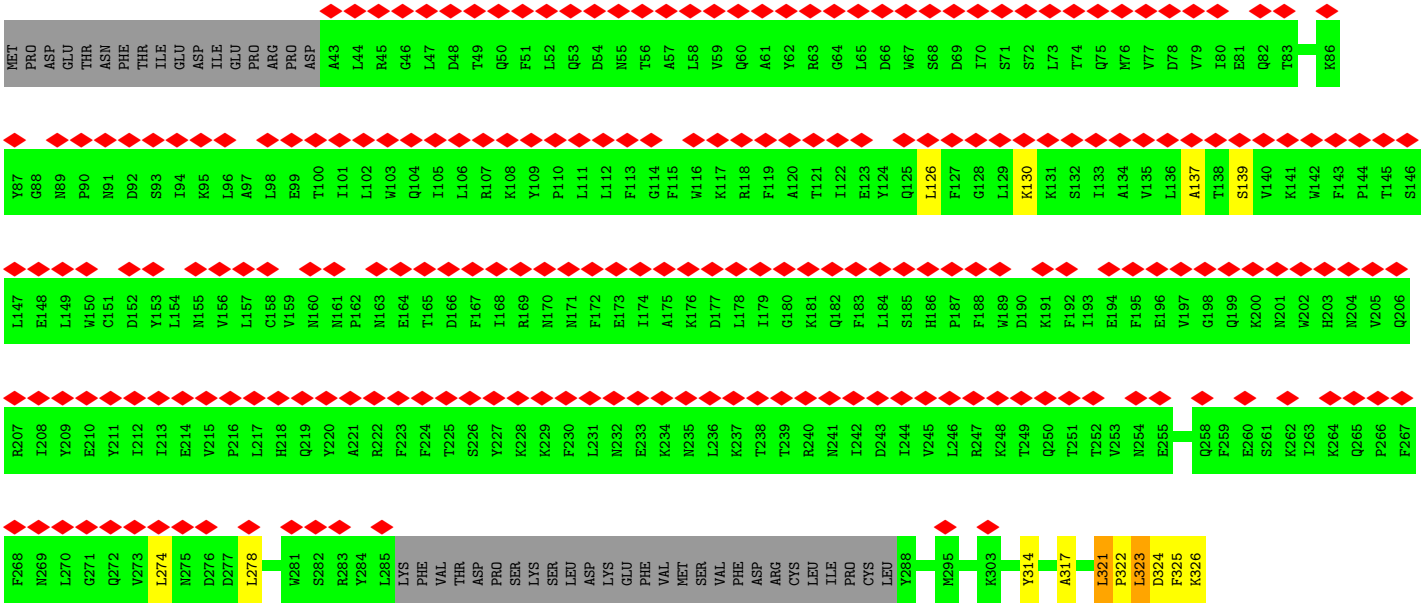
- Molecule 4: U1 small nuclear ribonucleoprotein component PRP42

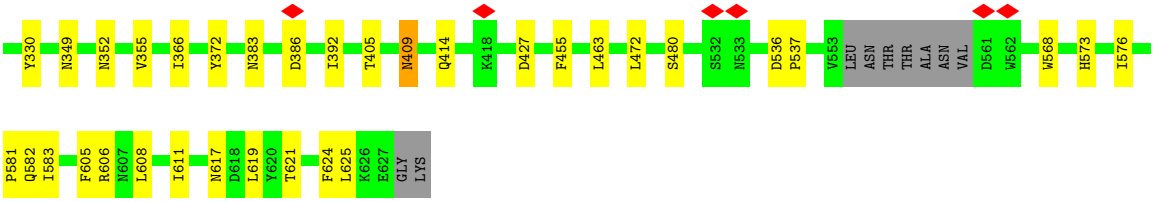
Chain D:



- Molecule 5: Pre-mRNA-processing factor 39

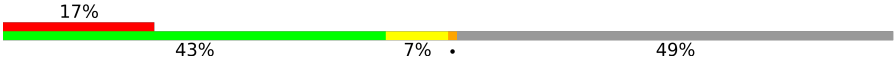
Chain E:

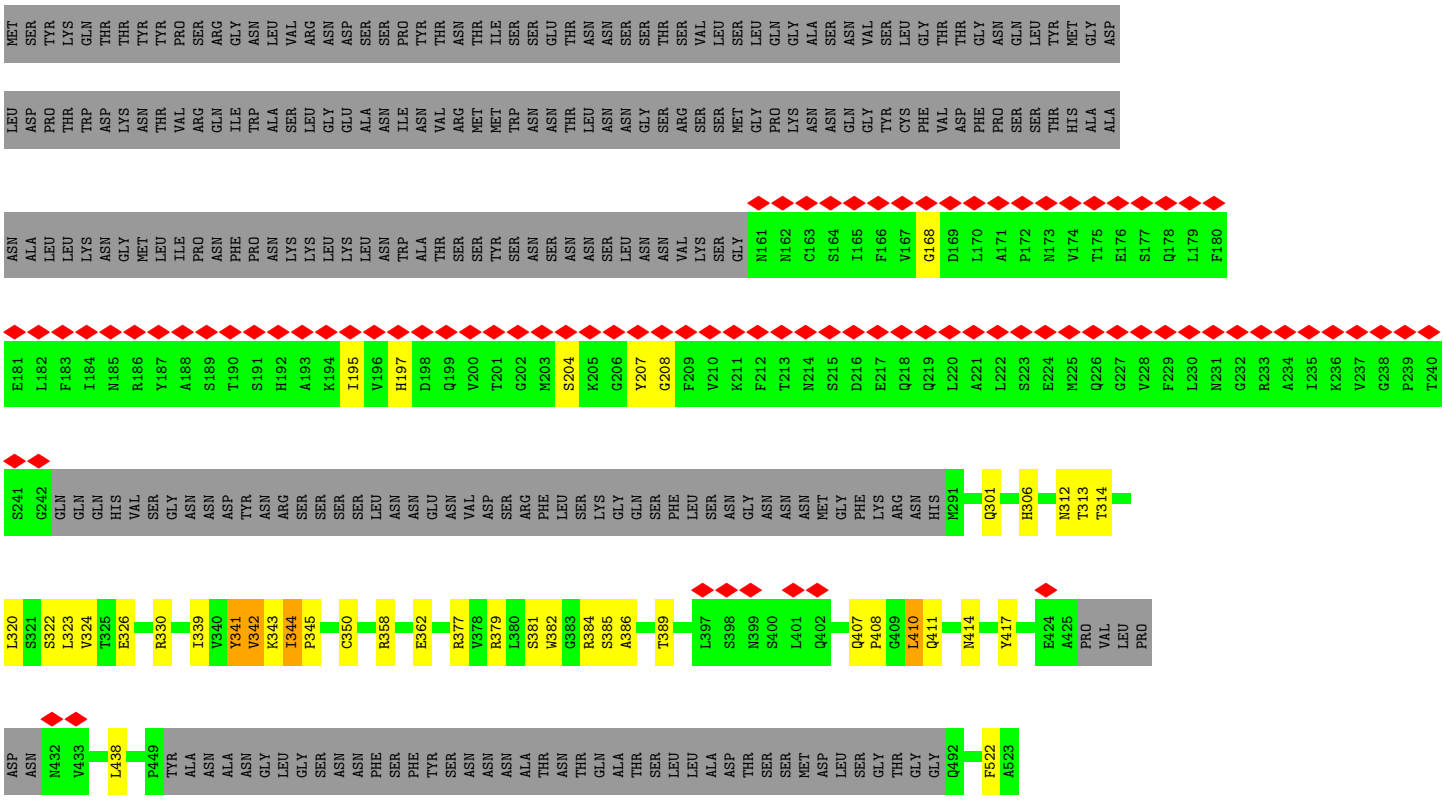




- Molecule 6: Protein NAM8

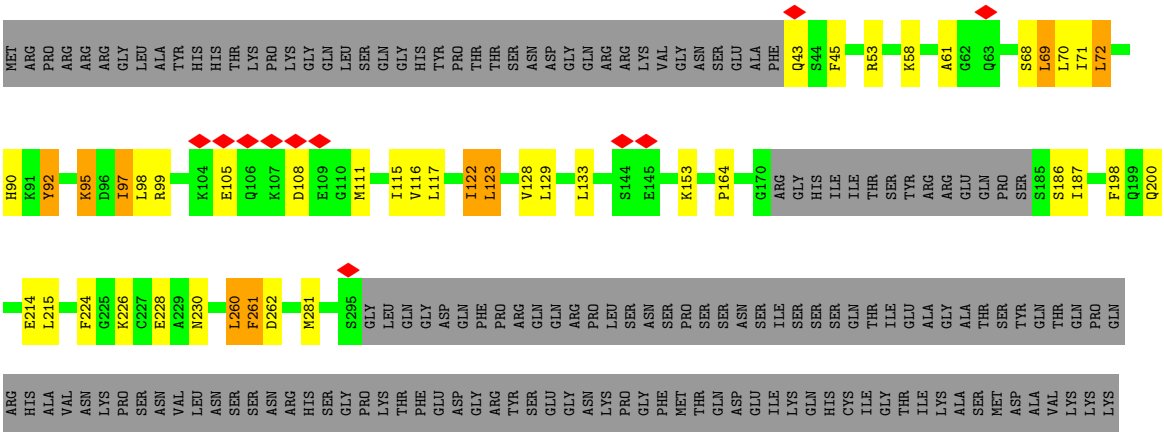
Chain F:

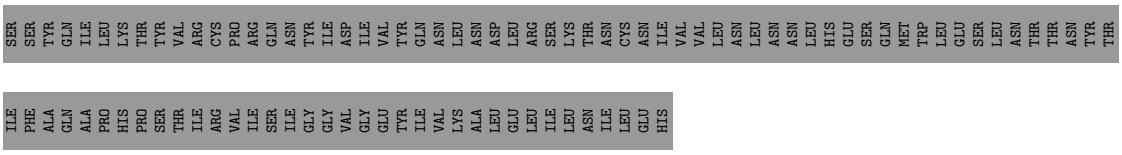




- Molecule 7: 56 kDa U1 small nuclear ribonucleoprotein component

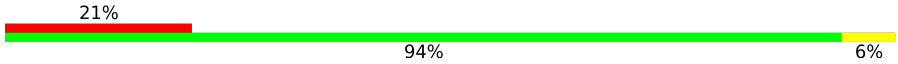
Chain G:

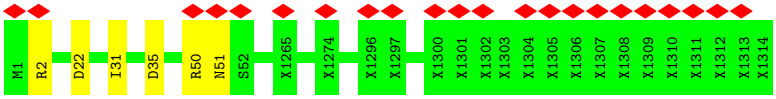




• Molecule 8: U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71

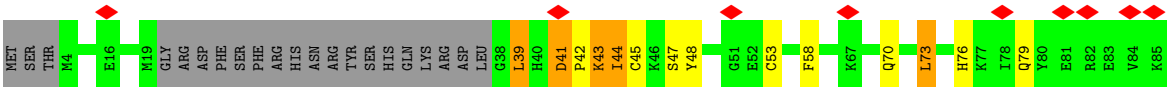
Chain H:

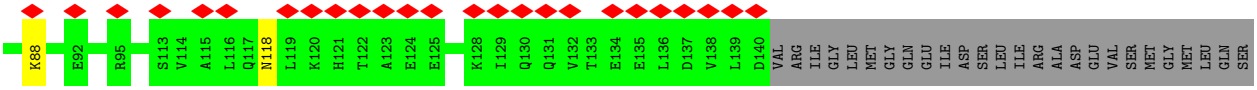


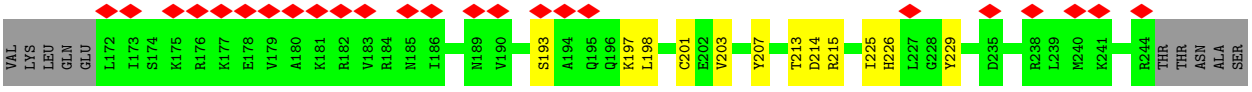


• Molecule 9: Protein LUC7

Chain I:

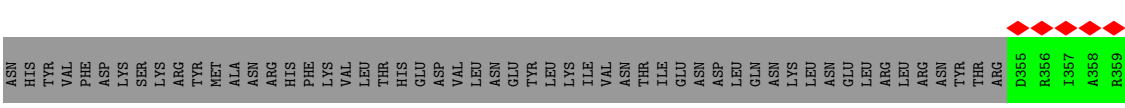


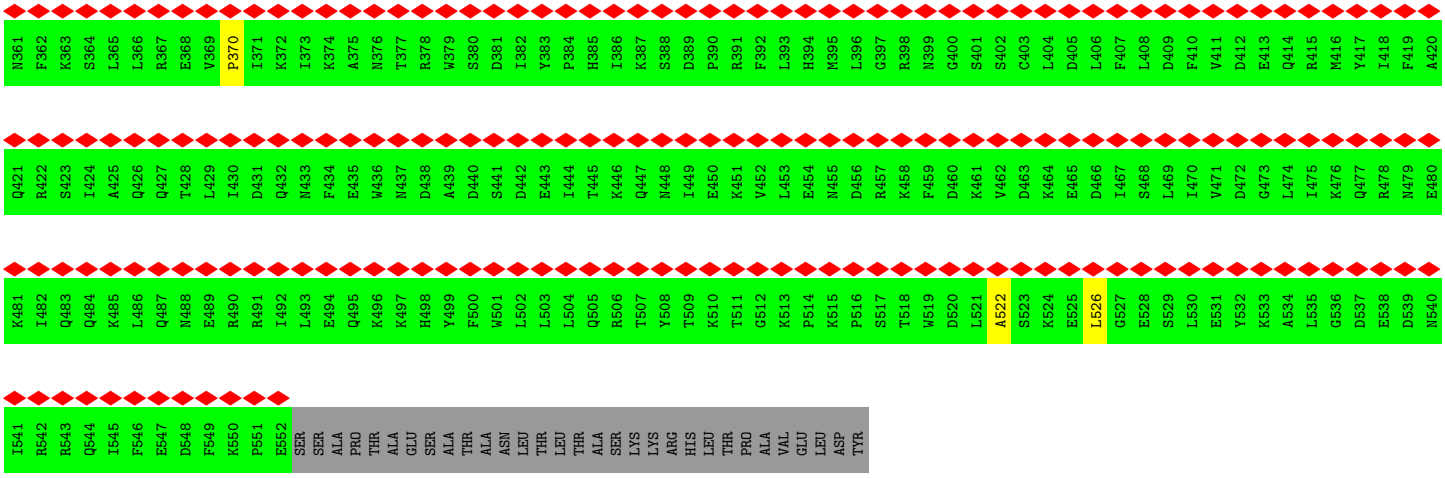




• Molecule 10: Pre-mRNA-processing protein PRP40

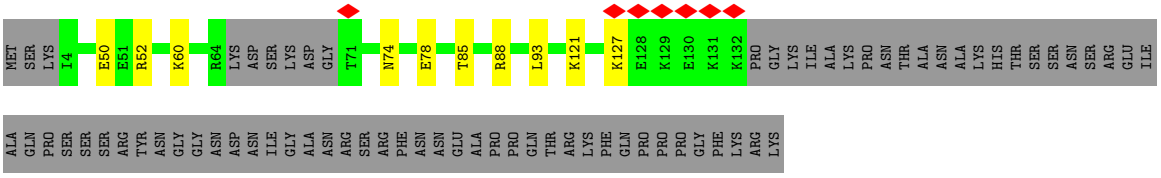
Chain J:





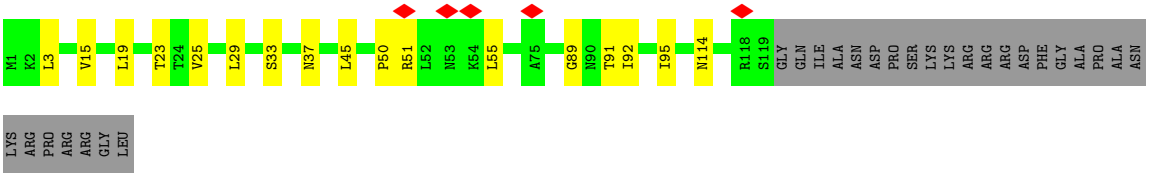
- Molecule 11: Small nuclear ribonucleoprotein-associated protein B

Chain K:



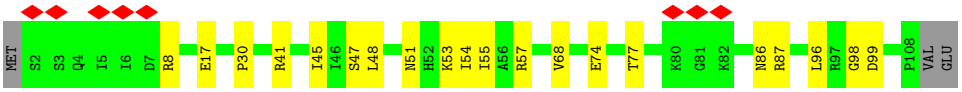
- Molecule 12: Small nuclear ribonucleoprotein Sm D1

Chain L:



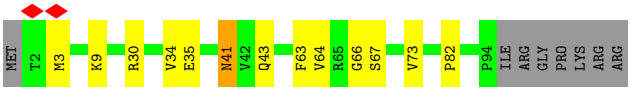
- Molecule 13: Small nuclear ribonucleoprotein Sm D2

Chain M:



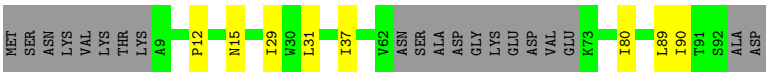
- Molecule 14: Small nuclear ribonucleoprotein Sm D3

Chain N:



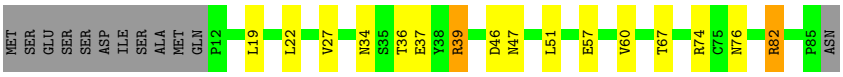
- Molecule 15: Small nuclear ribonucleoprotein E

Chain O: 70% 9% 21%



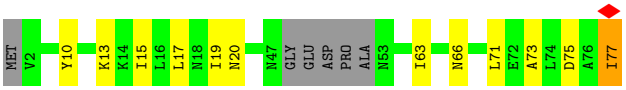
• Molecule 16: Small nuclear ribonucleoprotein F

Chain P: 67% 16% • 14%



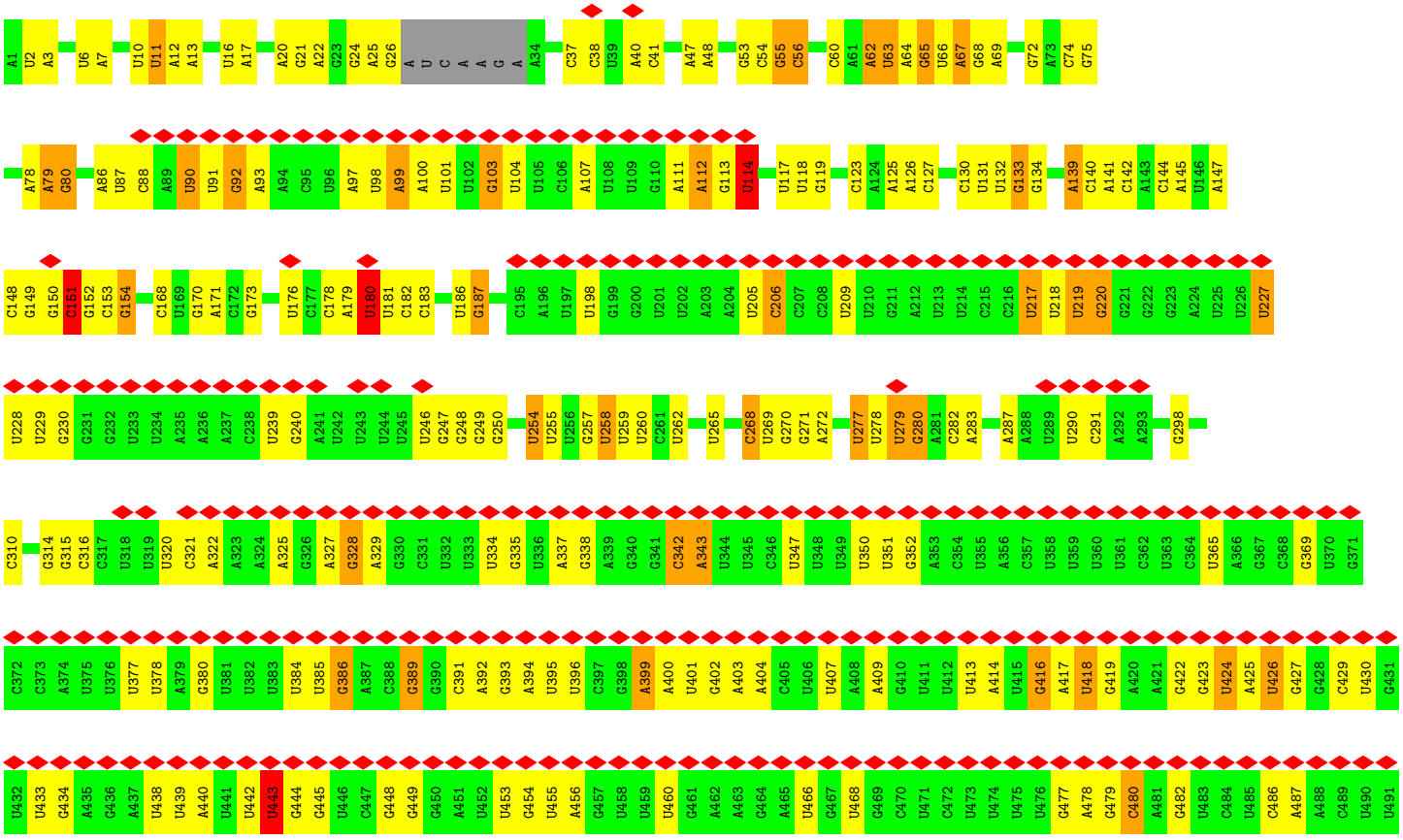
• Molecule 17: Small nuclear ribonucleoprotein G

Chain Q: 77% 14% • 8%



• Molecule 18: U1 snRNA

Chain R: 51% 52% 38% 8% • •



U492 G493 C494 U495 C496 G497 U498 U499 C500 C501 C502 G503 U504 U505 A506 U507 G508 G509 G510 A511 A512 A513 A514 A515 U516 U517 U518 U519 G520 G521 A522 A523 G524 G525 A533 G540 G541 U542 A545 U551 A552 A553 U554 U555 U556 U557 U558 G559 A560 U561 U562 U563 A564 U565 U U

U

- Molecule 19: UBC4 pre-mRNA

Chain r: 6% 91%

G G G A A C U A A G U G A U-9 C-8 U-7 A-6 G-5 A-4 A-3 A-2 G-1 A10 A11 G12 U13 U A U G G C C A C G U U A C U G A A U G C A A G A A C U A U U G A A C A A A U C A A C A U G C U A U U G A A C G G U G A A G G G A G U U A C C A C C A U C C U A

A A U A A A C A U U U A U G C U C C U U A U U U A A C U A A C A A A A U C A A C A U G C U A U U G A A C U A A G A A G U A C G G G A A U C C C A C C U A

C U U C U G G G U A C A C C A U C A G G G G U A C G A C C U G A G U A G A U C U G A U U C A A G U A C C A C C A U C U C U A C G G G A A A U U C

U C U A G

- Molecule 20: Nuclear cap-binding protein complex subunit 1

Chain X: 96% 89% 5%

MET PHE ASN ARG LYS ARG ARG GLY ASP PHE ASP GLU ASP GLU ASN TYR ARG ASP PHE ARG PRO ARG MET PRO LYS ARG GLN ARG ILE PRO PRO VAL VAL GLN LEU C36 K37 E38 M39 M40 P41 D42 I43 R44 T45 I46 G47 E48 S49 V50 K51 A52 F53 E54 D55 D56 I57 K58 F59 L60

S61 E62 A63 I64 M65 N66 E67 Y68 G69 H70 E71 D72 Y73 F74 N75 N76 A77 L78 L79 S80 T81 L82 N83 A84 V85 V86 V87 E88 Q89 P90 Q91 K92 Q93 A94 A95 I96 A97 L98 L99 T100 M101 V102 V103 N104 S105 K106 N107 N108 V109 A110 G111 K112 S113 I114 I115 N116 Y117 F118 F119 E120

E121 L122 Q123 K124 W125 C126 K127 Q128 T129 Y130 N131 D132 E133 F134 K135 S136 T137 S138 N139 E140 T141 G142 P143 W144 N145 K146 I147 K148 L149 I150 L151 R152 F153 L154 S155 I156 L157 S158 P159 M160 F161 L162 V163 D164 E165 L166 I167 N168 I169 Y170 K171 S172 L173 F174 E175 L176 S177 I178 E179 L180

N181 N182 L183 D184 P185 G186 N187 R188 V189 P190 L191 S192 E193 A194 I195 Y196 T197 N198 T199 L200 L201 N202 I203 P204 Y205 L206 F207 F208 F209 N210 R211 N212 N213 D214 G215 L216 R217 T218 K219 V220 E221 E222 L223 L224 A225 Y226 V227 E228 Q229 N230 Y231 L232 V233 K234 T235 T236 D237 I238 N239 L240

L241 R242 E243 Y244 N245 G246 E247 P248 P249 Y250 E251 M252 V253 E254 L255 V256 R257 V258 V259 L260 P261 N262 V263 K264 K265 A266 L267 I268 N269 N270 L271 E272 Q273 L274 N275 E276 L277 F278 P279 D280 W281 N282 H283 L284 L285 T286 P287 Q288 T289 G290 D291 E292 G293 F294 N295 D296 A297 L298 T299 L300

P301 S302 V303 D304 D305 L306 K307 S308 F309 V310 R311 L312 N313 K314 N315 F316 G317 S318 V319 D320 S321 M322 W323 K324 T325 P326 R327 Y328 A329 F330 H331 V332 Y333 L334 P335 N336 S337 A338 G339 N340 F341 E342 T343 V344 V345 P346 I347 S348 T349 Y350 A351 G352 Q353 L354 F355 N356 D357 I358 I359 I360

D361 L362 V363 E364 S365 L366 E367 F368 N369 R370 K371 E372 V373 A374 R375 Q376 V377 I378 T379 L380 D381 L382 F383 F384 K385 A386 G387 I388 F389 T390 E391 P392 G393 E394 S395 I396 A397 Q398 L399 I400 A401 T402 Y403 E404 E405 N406 P407 L408 A409 P410 T411 F412 K413 I414 E415 D416 L417 A418 I419 E420

T421 I422 L423 G424 L425 I426 F427 K428 L429 P430 S431 V432 S433 Q434 P435 F436 A437 Y438 F439 Y440 T441 L442 L443 V444 D445 I446 C447 Q448 N449 S450 P451 K452 A453 I454 A455 P456 V457 F458 G459 R460 A461 F462 R463 F464 F465 Y466 S467 H468 L469 D470 S471 L472 D473 F474 E475 L476 K477 L478 R479 Y480

L481 D482 W483 F484 S485 I486 Q487 M488 S489 N490 F491 N492 F493 S494 W495 K496 W497 N498 E499 W500 E501 D502 D503 S504 I505 K506 F507 G508 K509 Y510 F511 Y512 N513 P514 K515 V516 N517 F518 A519 K520 N521 L522 I523 Q524 K525 E526 L527 R528 L529 T530 S531 N532 F533 S534 E535 V536 E537 D538 S539 L540

P541 Q542 E543 F544 T545 K546 Y547 L548 D549 T550 S551 Y552 I553 P554 R555 D556 Q557 L558 I559 N560 Y561 Y562 Q563 S564 L565 F566 T567 G568 Y569 T570 V571 E572 E573 D574 S575 V576 R577 K578 N579 D580 L581 Y582 F583 R584 Q585 E586 G587 V588 P589 M590 E591 N592 T593 V594 R595 K596 I597 L598 D599 Y600

T601 H602 K603 A604 N605 N606 S607 R608 E609 V610 T611 E612 L613 E614 S615 I616 L617 G618 E619 L620 K621 N622 E623 Y624 G625 S626 I627 I628 S629 D630 F631 N632 R633 F634 V635 I636 I637 L638 L639 V640 Q641 A642 V643 T644 D645 S646 G647 S648 R649 S650 L651 S652 H653 A654 M655 K656 Y657 I658 N659 D660

L661 K662 E663 D664 L665 K666 T667 I668 F669 A670 K671 I672 E673 L674 D675 I676 E677 T678 K679 E680 Y681 I682 I683 I684 E685 A686 V687 L688 T689 F690 W691 N692 A693 N694 P695 Q696 T697 G698 F699 L700 V701 A702 D703 A704 F705 K706 Y707 A708 G709 L710 L711 T712 S713 R714 T715 I716 F717 T718 F719 I720

F721 N722 E723 T724 G725 L726 K727 N728 N729 G730 L731 I732 E733 A734 T735 A736 I737 E738 A739 V740 F741 R742 N743 L744 S745 Q746 Q747 I748 S749 E750 E751 N752 E753 S754 G755 N756 N757 F758 E759 F760 V761 F762 E763 R764 L765 C766 T767 I768 A769 N770 S771 T772 I773 D774 L775 L776 D777 V778 N779 A780

D781 E782 D783 I784 E785 I786 P787 K788 V789 N790 G791 E792 M793 D794 I795 D796 D797 I798 E799 D800 D801 K802 L803 D804 L805 K806 W807 K808 Y809 F810 T811 V812 I813 G814 F815 I816 K817 S818 I819 L820 R821 R822 Y823 S824 H825 E826 Y827 R828 E829 L830 A831 D832 K833 F834 I835 A836 N837 I838 D839 N840

A841 I842 P843 H844 E845 S846 T847 R848 R849 T850 I851 S852 N853 W854 I855 Q856 E857 T858 K859 E860 V861

- Molecule 21: Nuclear cap-binding protein subunit 2

Chain Y: 66% 65% 34%

MET SER LEU GLU GLU PHE ASP GLU VAL LYS TYR ASP HIS SER THR LYS ARG LEU D19 T20 P21 S22 R23 Y24 L25 L26 R27 K28 A29 R30 R31 N32 P33 N34 G35 L36 Q37 E38 L39 R40 E41 S42 M43 K44 S45 S46 T47 I48 Y49 V50 G51 N52 L53 S54 F55 Y56 T57 S58 E59 E60

Q61 I62 Y63 E64 L65 F66 S67 K68 C69 G70 T71 I72 K73 R74 I75 I76 M77 G78 L79 D80 R81 F82 K83 F84 T85 P86 C87 G88 F89 C90 F91 I92 I93 Y94 S95 C96 P97 D98 E99 A100 L101 N102 A103 L104 K105 Y106 L107 S108 D109 T110 K111 L112 D113 E114 K115 T116 I117 T118 I119 D120

L121 D122 P123 G124 F125 E126 D127 G128 R129 Q130 F131 G132 R133 G134 K135 S136 G137 G138 G139 Q139 V140 S141 D142 E143 L144 R145 F146 D147 F148 D149 A150 S151 R152 G153 G154 F155 A156 ILE PRO PHE ALA GLU ARG VAL GLY VAL PRO HIS SER ARG PHE ASP ASN SER SER SER GLN SER ASN THR ASN

ASN TYR ILE PRO PRO PRO ASP ALA MET GLY THR PHE ARG PRO GLY PHE ASP GLU GLU ARG GLU ASP ASP ASN TYR VAL PRO GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124825	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.206	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	522.24, 522.24, 522.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.46	0/1224	0.59	0/1675
2	B	0.54	0/1601	0.65	0/2154
3	C	0.44	0/1072	0.68	0/1437
4	D	0.76	0/4676	0.72	0/6320
5	E	0.55	0/4046	0.60	0/5539
6	F	0.60	0/1844	0.68	0/2511
7	G	0.61	0/1996	0.68	0/2682
8	H	0.49	0/428	0.55	0/575
9	I	0.38	0/1428	0.60	0/1924
10	J	0.37	0/983	0.49	0/1371
11	K	0.66	0/1014	0.73	0/1350
12	L	0.57	0/930	0.73	0/1261
13	M	0.53	0/872	0.63	0/1174
14	N	0.71	0/722	0.72	0/979
15	O	0.55	0/573	0.68	0/778
16	P	0.65	0/597	0.74	0/809
17	Q	0.64	0/546	0.69	0/735
18	R	0.66	0/13201	1.19	79/20553 (0.4%)
19	r	0.52	0/527	1.05	0/819
20	X	0.26	0/4100	0.59	4/5721 (0.1%)
21	Y	0.26	0/676	0.55	0/937
All	All	0.59	0/43056	0.87	83/61304 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
20	X	0	24

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	26

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	227	U	N1-C2-O2	12.02	131.22	122.80
18	R	227	U	C2-N1-C1'	11.79	131.85	117.70
18	R	227	U	N3-C2-O2	-11.14	114.40	122.20
18	R	442	U	OP2-P-O3'	-10.46	82.18	105.20
18	R	442	U	OP1-P-O3'	-10.46	82.20	105.20

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	12	ARG	Peptide,Sidechain
20	X	281	TRP	Peptide
20	X	284	LEU	Peptide
20	X	69	GLY	Peptide
20	X	70	HIS	Peptide

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	1207	0	927	14	0
2	B	1570	0	1553	33	0
3	C	1058	0	1118	26	0
4	D	4561	0	4549	72	0
5	E	3981	0	3282	35	0
6	F	1818	0	1567	29	0
7	G	1954	0	1961	44	0
8	H	685	0	477	4	0
9	I	1409	0	1285	24	0
10	J	984	0	416	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1008	0	1109	9	0
12	L	921	0	972	10	0
13	M	858	0	882	13	0
14	N	710	0	730	16	0
15	O	563	0	594	5	0
16	P	584	0	586	11	0
17	Q	543	0	560	7	0
18	R	11822	0	5939	99	0
19	r	471	0	236	0	0
20	X	4101	0	1779	14	0
21	Y	677	0	298	1	0
22	B	1	0	0	0	0
22	I	2	0	0	0	0
All	All	41488	0	30820	413	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 6.

The worst 5 of 413 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)
4:D:303:LEU:CD1	4:D:312:VAL:HG11	1.70	1.21
2:B:8:TYR:CE1	14:N:82:PRO:HG3	1.80	1.15
3:C:13:PRO:HD2	3:C:19:TYR:CD1	1.82	1.14
2:B:136:LEU:HD23	2:B:137:PRO:HD2	1.11	1.09
2:B:8:TYR:HE1	14:N:82:PRO:CG	1.64	1.09

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	182/300 (61%)	162 (89%)	17 (9%)	3 (2%)	9	46
2	B	193/231 (84%)	180 (93%)	10 (5%)	3 (2%)	9	46
3	C	126/350 (36%)	120 (95%)	6 (5%)	0	100	100
4	D	542/544 (100%)	515 (95%)	27 (5%)	0	100	100
5	E	570/629 (91%)	532 (93%)	38 (7%)	0	100	100
6	F	259/523 (50%)	240 (93%)	19 (7%)	0	100	100
7	G	235/492 (48%)	218 (93%)	17 (7%)	0	100	100
8	H	50/105 (48%)	47 (94%)	3 (6%)	0	100	100
9	I	186/261 (71%)	174 (94%)	11 (6%)	1 (0%)	29	68
10	J	196/583 (34%)	185 (94%)	10 (5%)	1 (0%)	29	68
11	K	119/196 (61%)	111 (93%)	8 (7%)	0	100	100
12	L	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
13	M	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
14	N	91/101 (90%)	84 (92%)	7 (8%)	0	100	100
15	O	70/94 (74%)	68 (97%)	2 (3%)	0	100	100
16	P	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
17	Q	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
20	X	824/861 (96%)	727 (88%)	80 (10%)	17 (2%)	7	40
21	Y	136/208 (65%)	120 (88%)	15 (11%)	1 (1%)	22	61
All	All	4140/5897 (70%)	3827 (92%)	287 (7%)	26 (1%)	29	64

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
2	B	139	ARG
10	J	370	PRO
20	X	71	GLU
20	X	284	LEU

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	82/265 (31%)	78 (95%)	4 (5%)	25	59
2	B	171/214 (80%)	161 (94%)	10 (6%)	20	55
3	C	117/317 (37%)	112 (96%)	5 (4%)	29	63
4	D	508/519 (98%)	491 (97%)	17 (3%)	38	69
5	E	316/603 (52%)	307 (97%)	9 (3%)	43	72
6	F	157/451 (35%)	149 (95%)	8 (5%)	24	58
7	G	218/448 (49%)	207 (95%)	11 (5%)	24	59
8	H	48/48 (100%)	46 (96%)	2 (4%)	30	63
9	I	130/234 (56%)	124 (95%)	6 (5%)	27	61
11	K	114/176 (65%)	114 (100%)	0	100	100
12	L	107/129 (83%)	106 (99%)	1 (1%)	78	90
13	M	95/103 (92%)	94 (99%)	1 (1%)	73	88
14	N	81/89 (91%)	78 (96%)	3 (4%)	34	66
15	O	62/83 (75%)	62 (100%)	0	100	100
16	P	64/77 (83%)	59 (92%)	5 (8%)	12	44
17	Q	59/66 (89%)	55 (93%)	4 (7%)	16	50
All	All	2329/3822 (61%)	2243 (96%)	86 (4%)	37	66

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	95	LYS
9	I	118	ASN
7	G	122	ILE
8	H	51	ASN
14	N	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	407	GLN
9	I	40	HIS
6	F	411	GLN
7	G	90	HIS
9	I	118	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	556/568 (97%)	134 (24%)	18 (3%)
19	r	21/253 (8%)	6 (28%)	0
All	All	577/821 (70%)	140 (24%)	18 (3%)

5 of 140 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	10	U
18	R	11	U
18	R	12	A
18	R	13	A
18	R	17	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	277	U
18	R	505	U
18	R	399	A
18	R	133	G
18	R	268	C

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 3 ligands modelled in this entry, 3 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	52:SER	C	1262:UNK	N	64.87

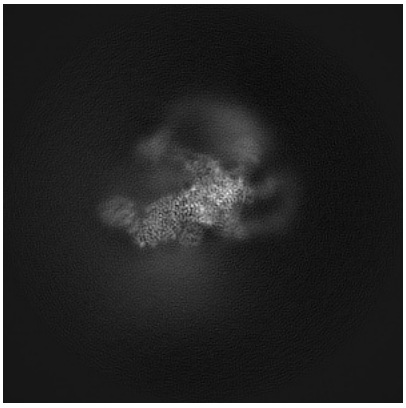
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0360. These allow visual inspection of the internal detail of the map and identification of artifacts.

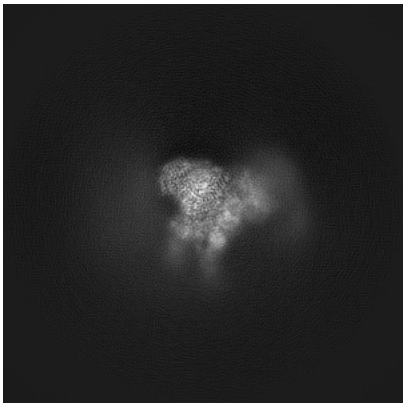
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

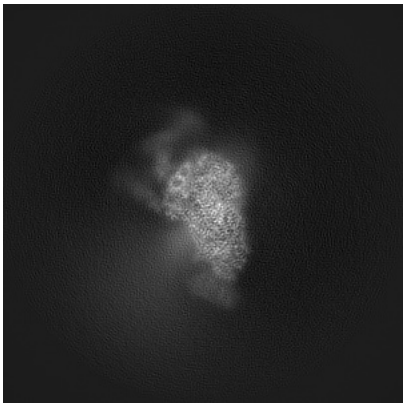
6.1.1 Primary map



X



Y

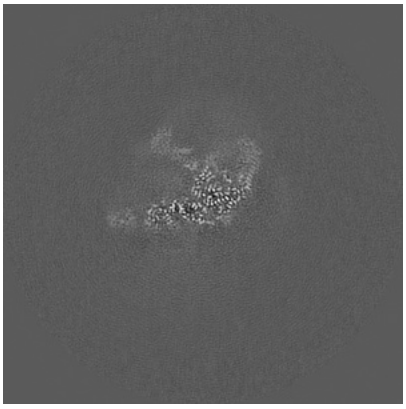


Z

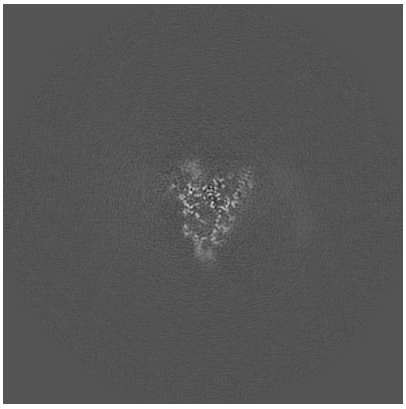
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

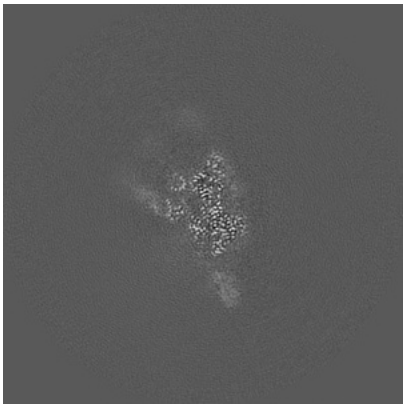
6.2.1 Primary map



X Index: 192



Y Index: 192

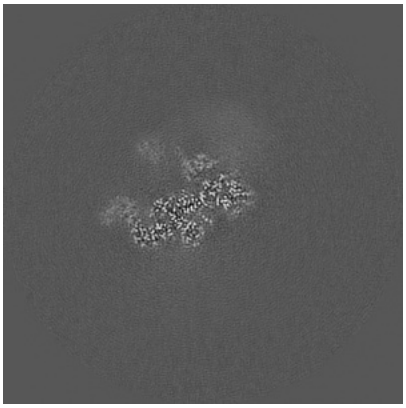


Z Index: 192

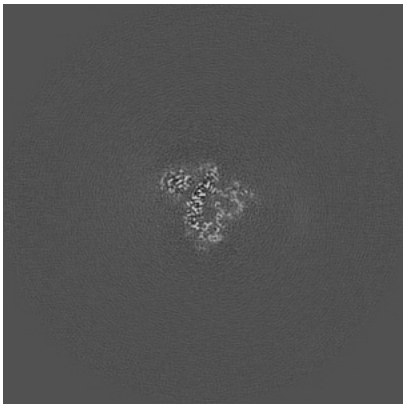
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

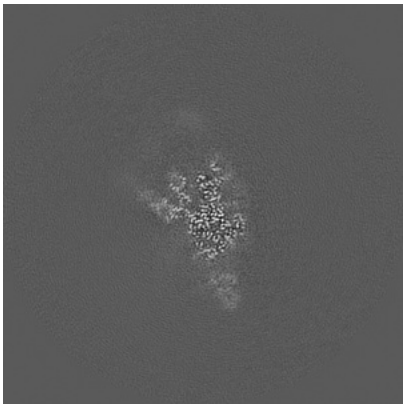
6.3.1 Primary map



X Index: 208



Y Index: 182

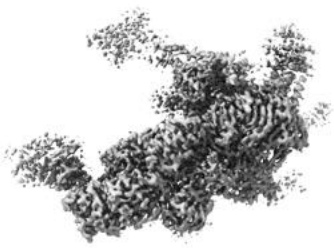


Z Index: 189

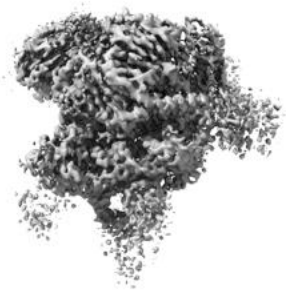
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

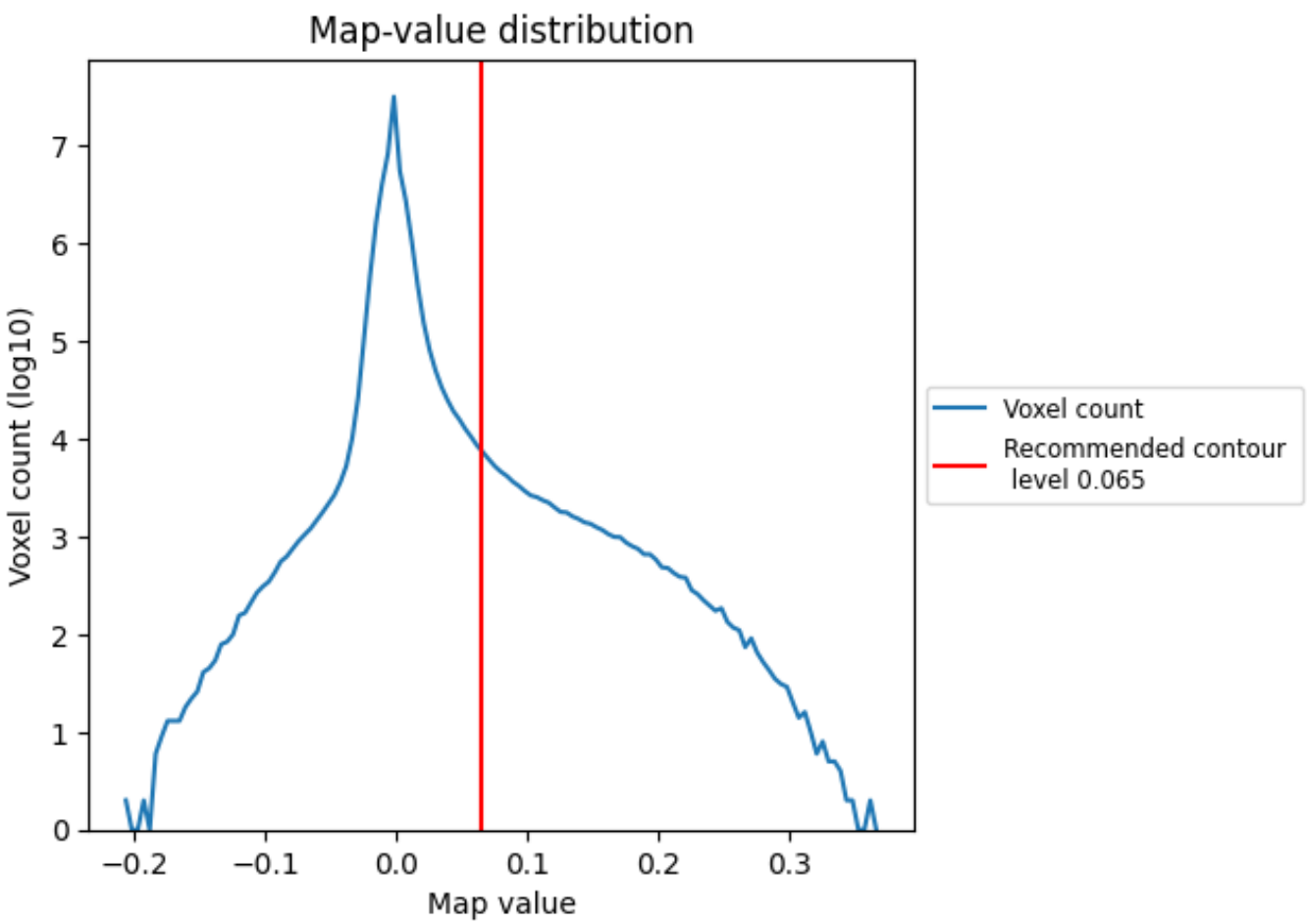
6.5 Mask visualisation (i)

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

7 Map analysis (i)

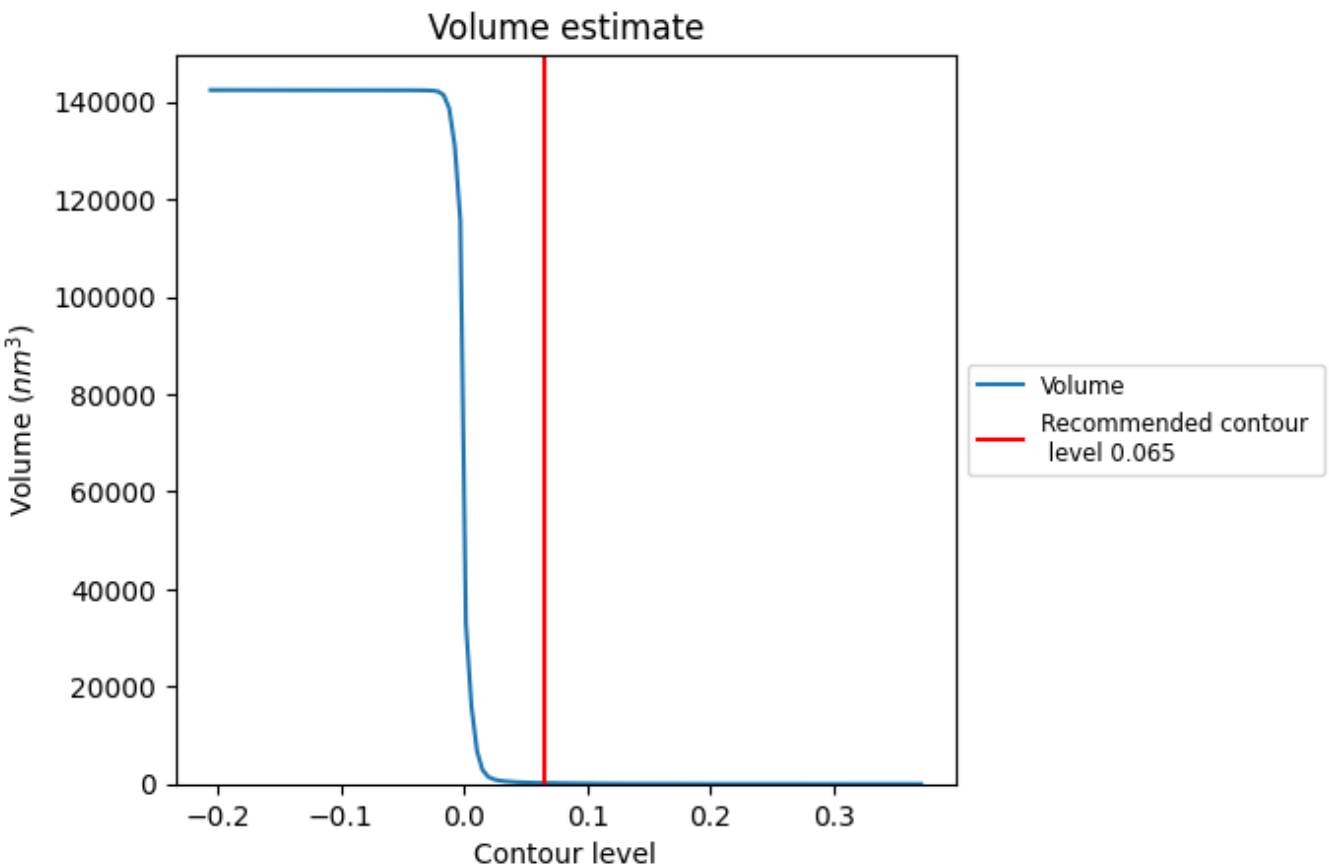
This section contains the results of statistical analysis of the map.

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.

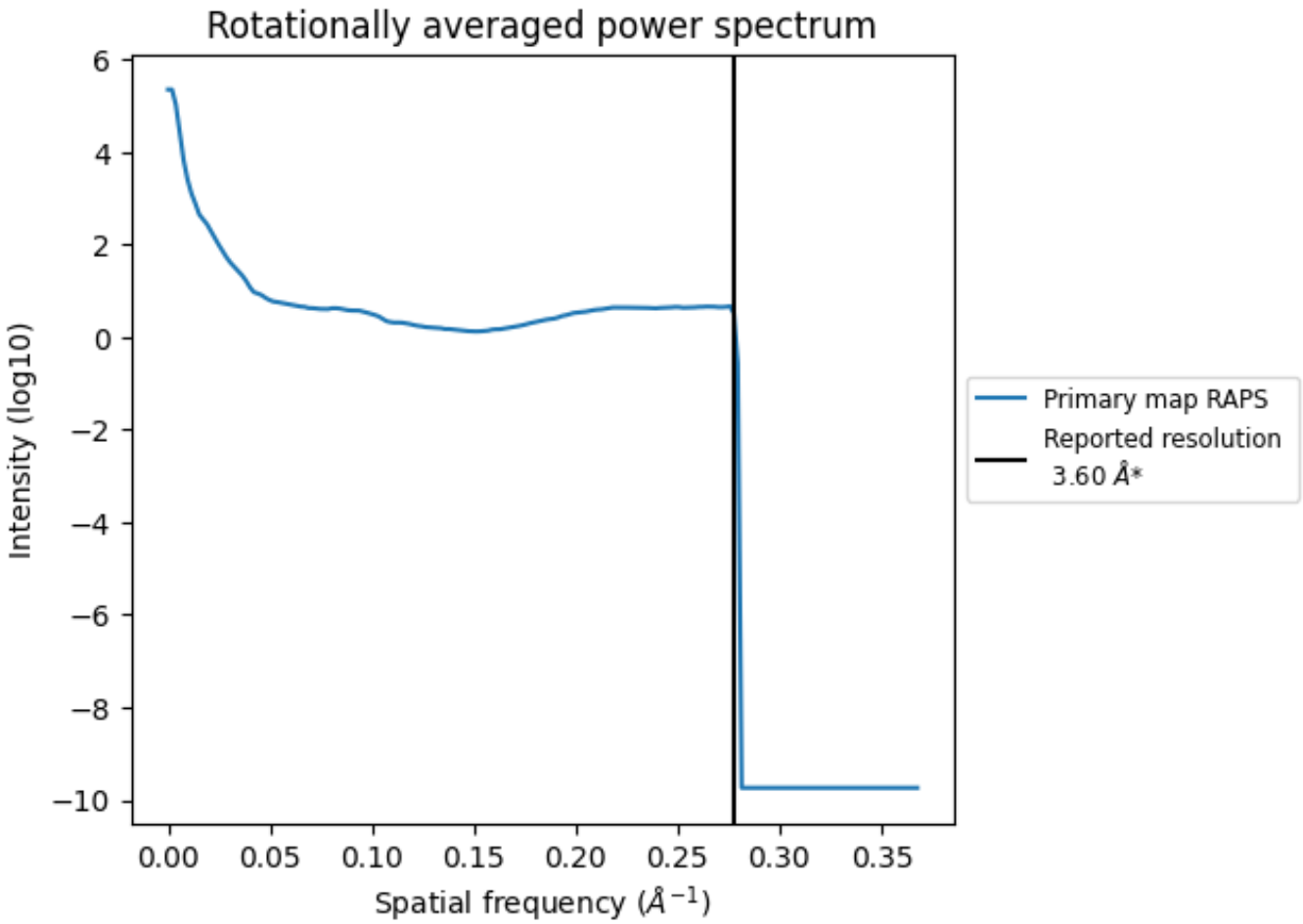
7.2 Volume estimate (i)



The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 171 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)

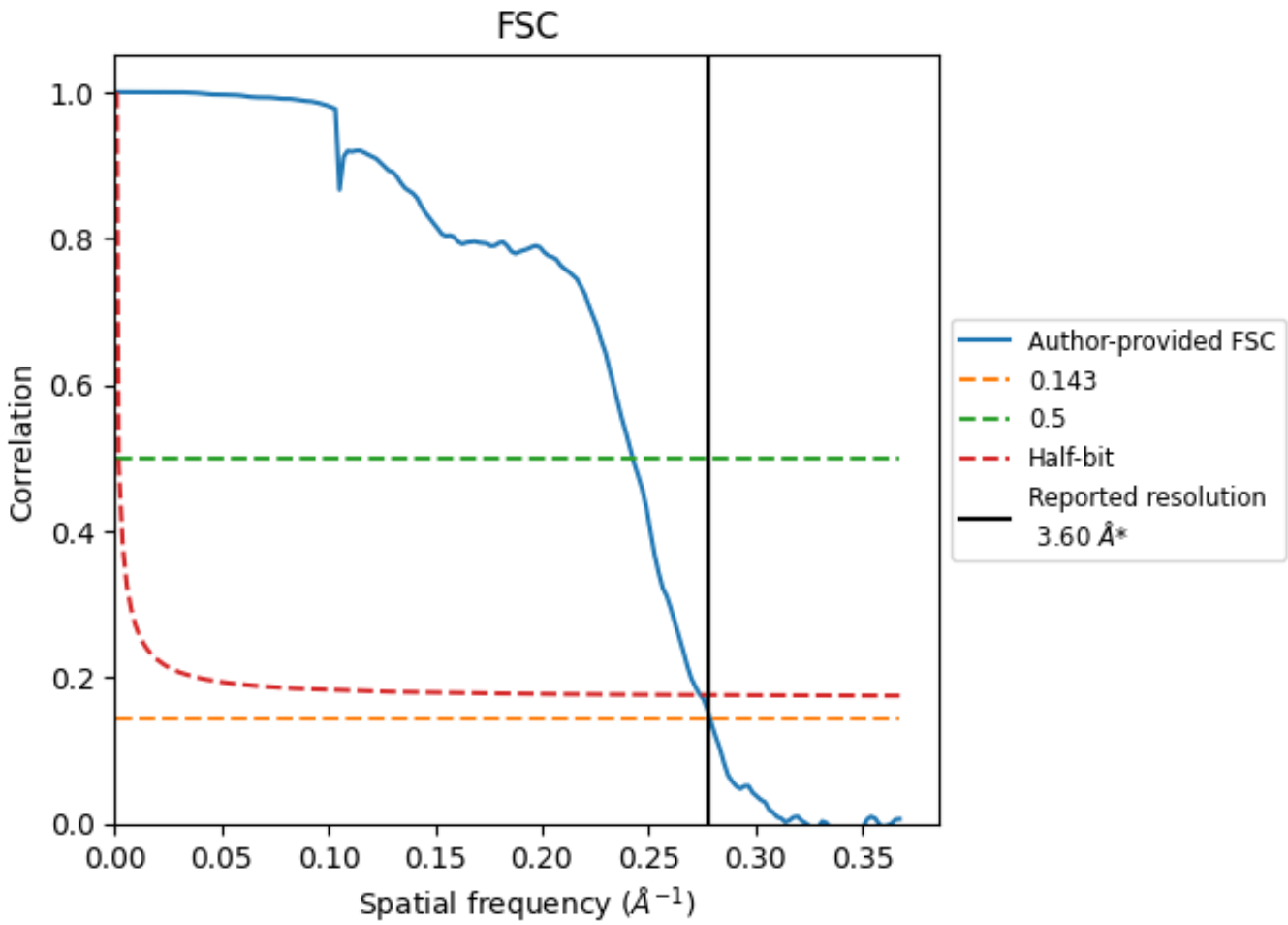


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

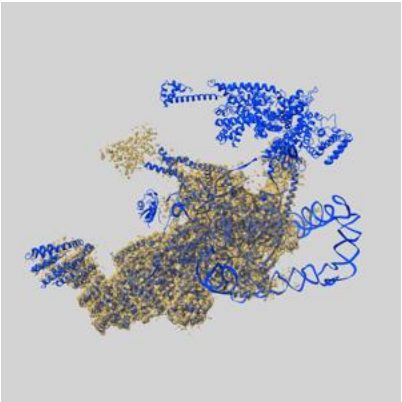
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.12	3.65
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

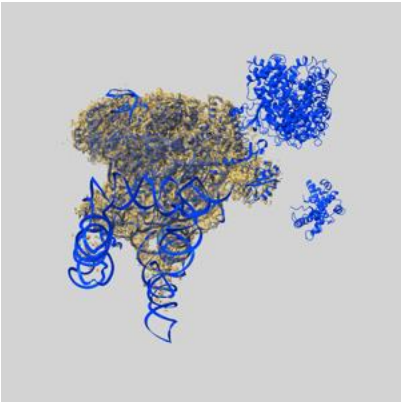
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0360 and PDB model 6N7P. Per-residue inclusion information can be found in section 3 on page 9.

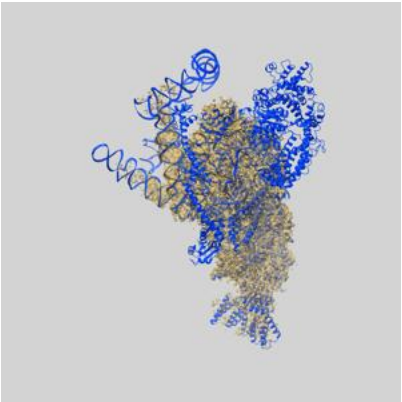
9.1 Map-model overlay (i)



X



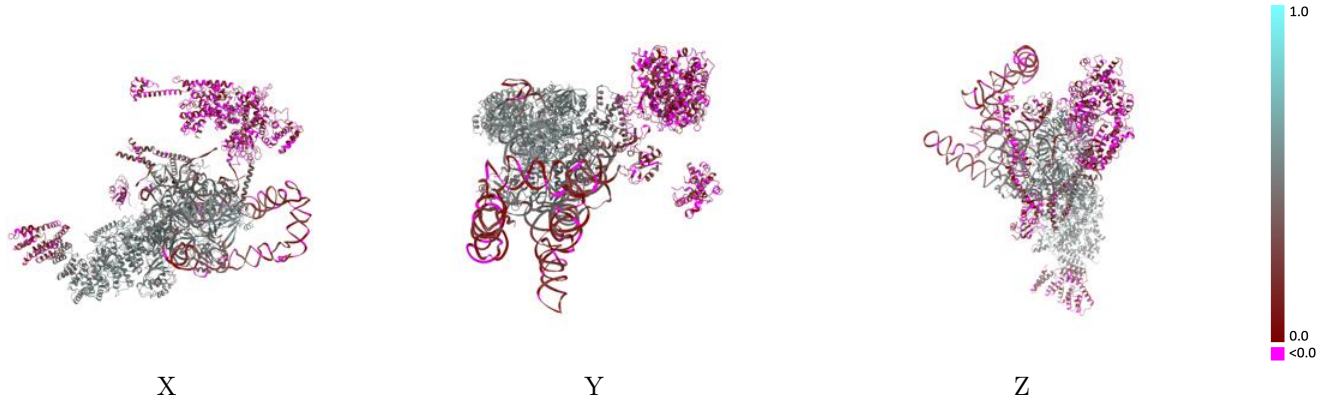
Y



Z

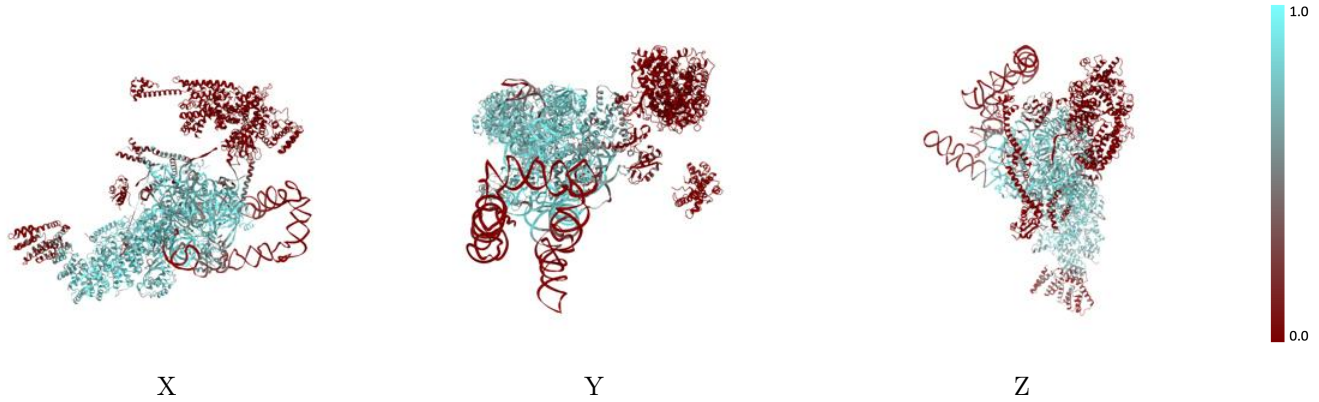
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



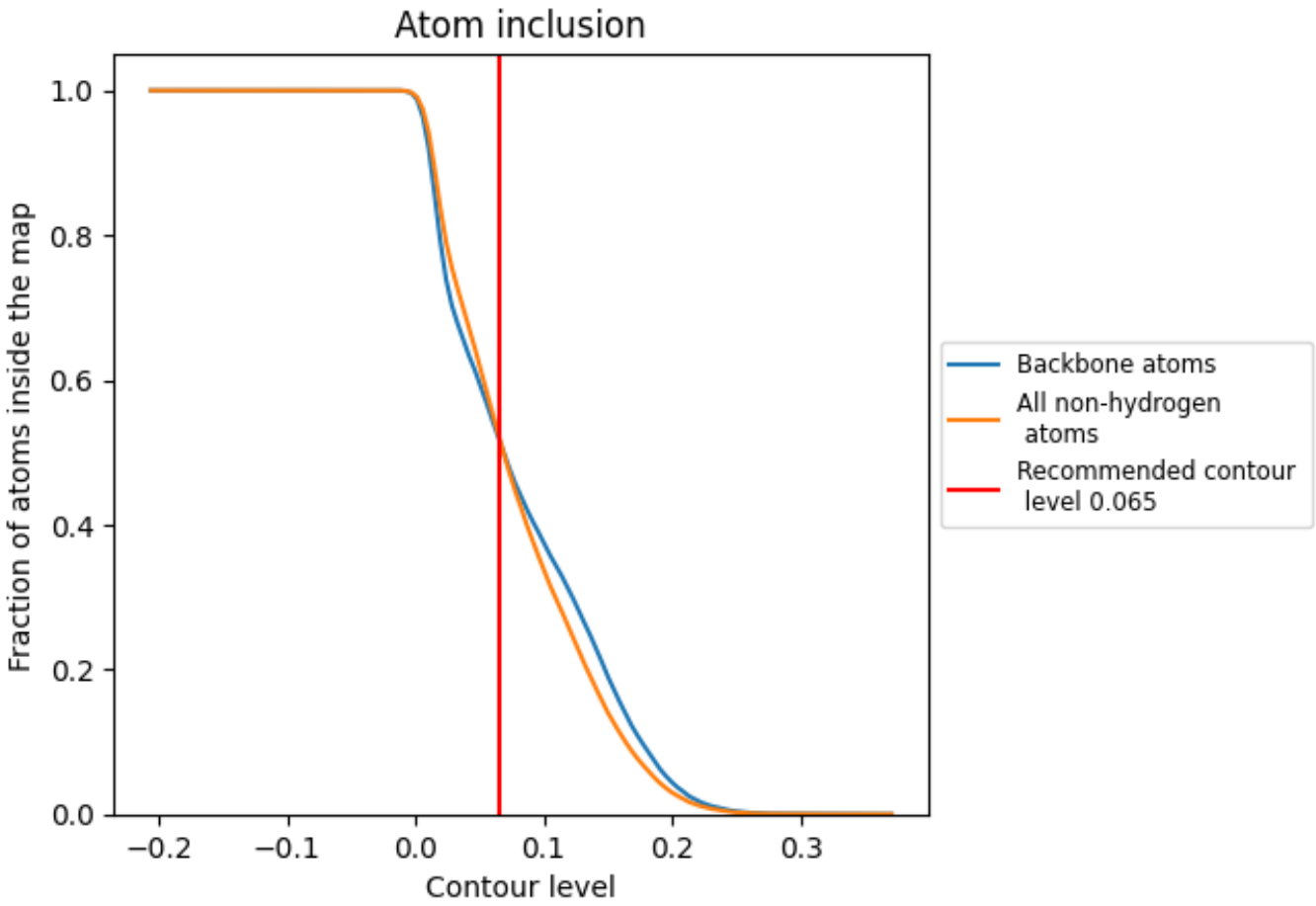
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5232	0.3520
A	0.4786	0.3590
B	0.7207	0.4940
C	0.6145	0.4190
D	0.8349	0.5290
E	0.5893	0.3960
F	0.6129	0.4260
G	0.7566	0.5030
H	0.6721	0.4630
I	0.5690	0.4080
J	0.0000	0.0480
K	0.7591	0.5120
L	0.7974	0.5130
M	0.7628	0.5140
N	0.7881	0.5370
O	0.8071	0.5180
P	0.8307	0.5250
Q	0.8019	0.5270
R	0.4331	0.2710
X	0.0000	0.0480
Y	0.0000	0.0440
r	0.4310	0.2910