wwPDB EM Validation Summary Report

Dec 12, 2022 – 09:15 am GMT

PDB ID	:	6YAN
EMDB ID	:	EMD-10762
Title	:	Mammalian 48S late-stage translation initiation complex with histone 4 mRNA
Authors	:	Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on	:	2020-03-12
Resolution	:	3.48 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:

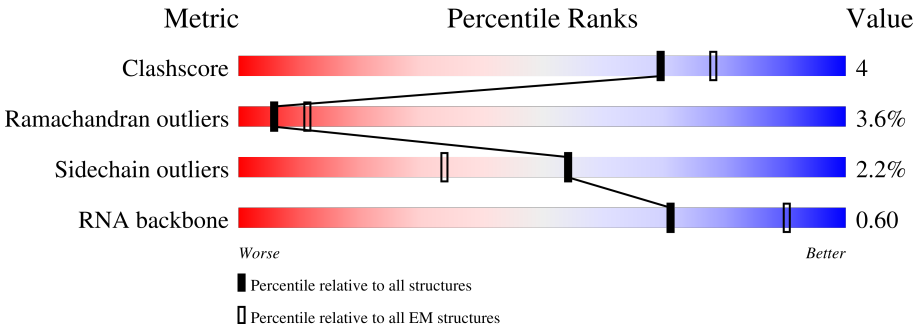
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.48 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	l	25	16% 88% 12%
2	C	208	93% 7%
3	D	215	93% 6%
4	E	226	95% 5%
5	F	227	7% 90% 9%
6	G	263	97%
7	H	191	6% 93% 7%

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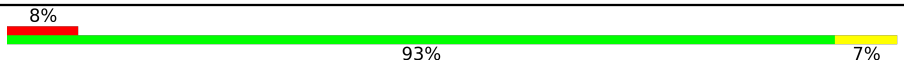
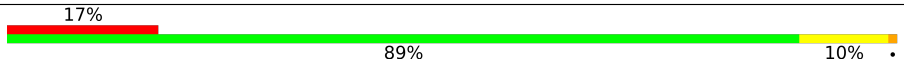
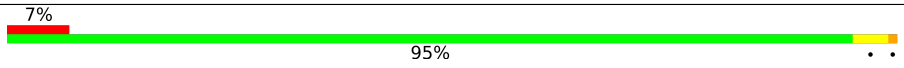
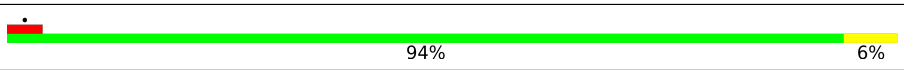
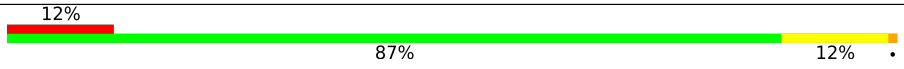
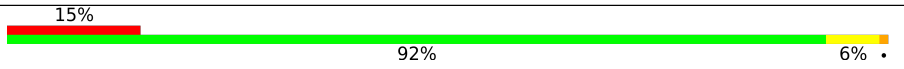
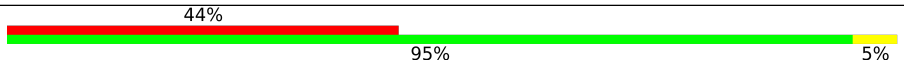
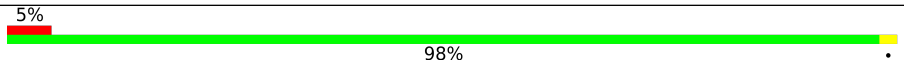
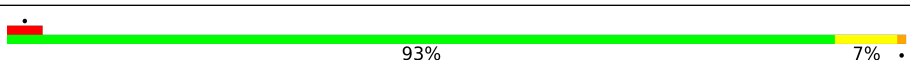
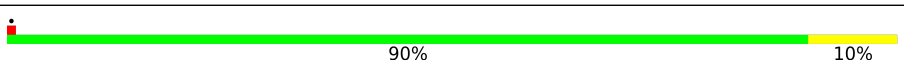
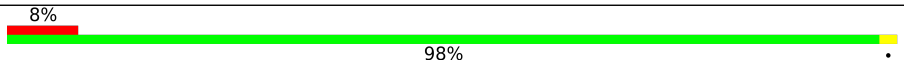
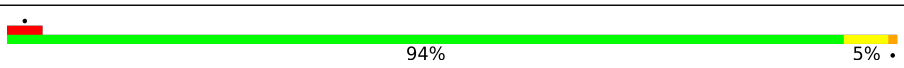
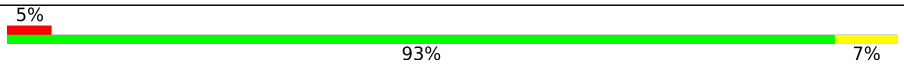
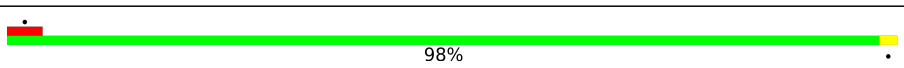
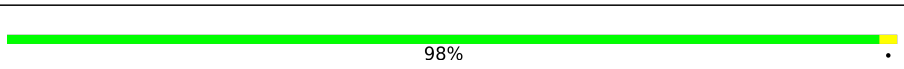
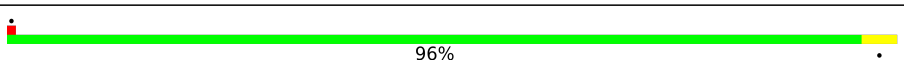
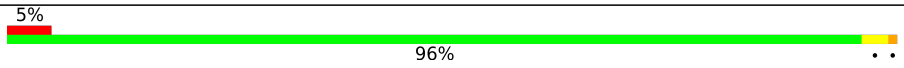
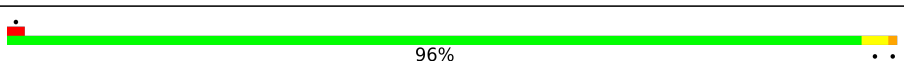
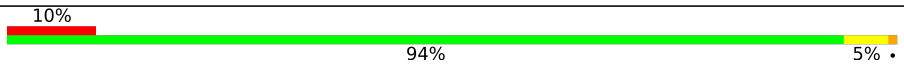
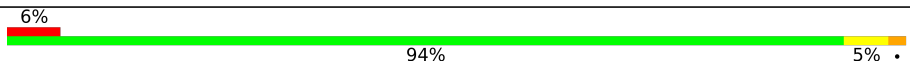
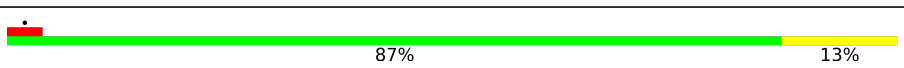
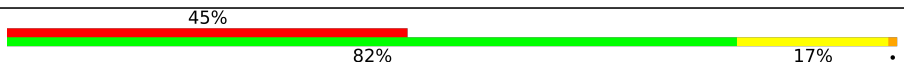
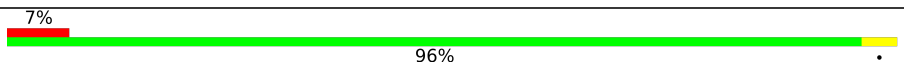
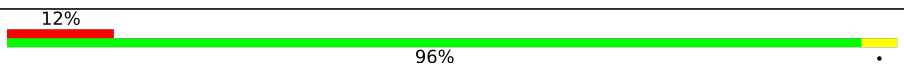
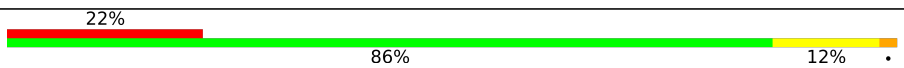
Mol	Chain	Length	Quality of chain
8	I	237	
9	J	190	
10	K	206	
11	L	182	
12	M	98	
13	N	158	
14	O	124	
15	P	150	
16	Q	136	
17	S	141	
18	T	126	
19	V	141	
20	W	104	
21	X	82	
22	Y	129	
23	Z	142	
24	a	126	
25	b	99	
26	c	84	
27	d	64	
28	e	53	
29	f	71	
30	g	313	
31	h	75	
32	i	59	

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Mol	Chain	Length	Quality of chain
33	2	1863	73% 18% 6%
34	3	36	72% 42% 56%
35	A	266	82% 88% 8%
36	B	422	100% 91% 9%
37	U	142	86% 11%
38	R	135	13% 79% 16%
39	1	75	43% 69% 21% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	C4J	2	1244	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 84251 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 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 3 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	215	Total	C	N	O	S	0	0
			1742	1107	309	311	15		

- Molecule 4 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 9 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 12 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	124	Total 958	C 600	N 170	O 179	S 9	0	0

- Molecule 15 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	150	Total 1208	C 773	N 229	O 205	S 1	0	0

- Molecule 16 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	136	Total 1016	C 621	N 199	O 190	S 6	0	0

- Molecule 17 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	141	Total 1123	C 715	N 212	O 193	S 3	0	0

- Molecule 18 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	126	Total 1020	C 639	N 188	O 188	S 5	0	0

- Molecule 19 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	141	Total 1113	C 701	N 213	O 196	S 3	0	0

- Molecule 20 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	104	Total 822	C 514	N 156	O 148	S 4	0	0

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 22 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 23 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	126	Total	C	N	O	S	0	0
			1022	645	198	174	5		

- Molecule 25 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	99	Total	C	N	O	S	0	0
			790	491	162	131	6		

- Molecule 26 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 27 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	64	Total	C	N	O	S	0	0
			507	308	102	95	2		

- Molecule 28 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 29 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 30 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 31 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 33 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	1744	Total	C	N	O	P	0	0
			37202	16613	6663	12186	1740		

- Molecule 34 is a RNA chain called histone 4 (H4) mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	36	Total	C	N	O	P	0	0
			774	346	144	249	35		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 36 is a protein called eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	142	Total	C	N	O	S	0	0
			1172	733	239	199	1		

- Molecule 38 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	135	Total	C	N	O	S	0	0
			1111	704	211	189	7		

- Molecule 39 is a RNA chain called initiator methionylated tRNA.

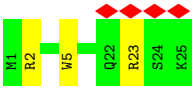
Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

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.

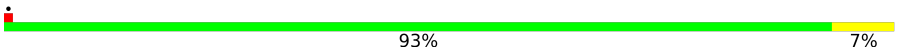
• Molecule 1: 60s ribosomal protein l41

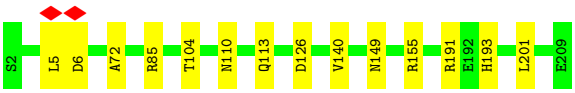
Chain l:



• Molecule 2: 40S ribosomal protein SA

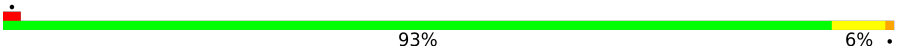
Chain C:

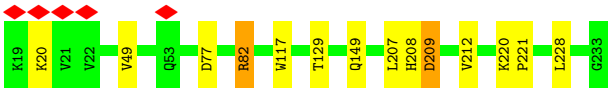




• Molecule 3: ribosomal protein eS1

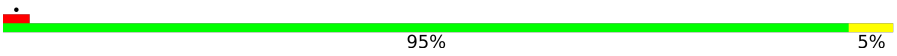
Chain D:

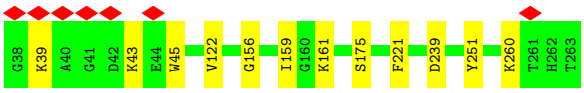




• Molecule 4: 40S ribosomal protein uS5

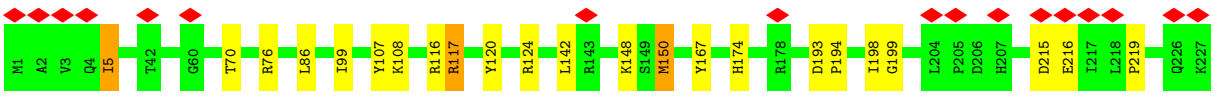
Chain E:





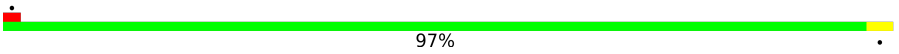
• Molecule 5: Ribosomal protein S3

Chain F:



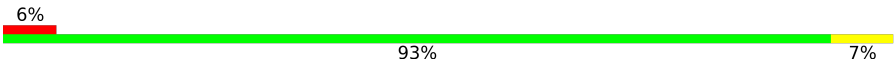
• Molecule 6: 40S ribosomal protein S4

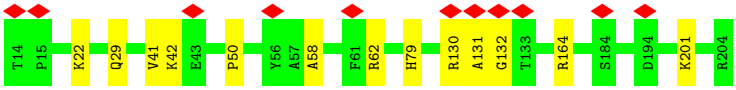
Chain G:



• Molecule 7: Ribosomal protein S5

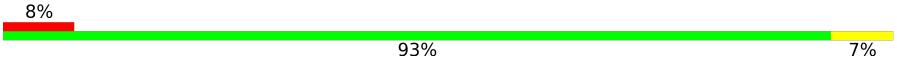
Chain H:

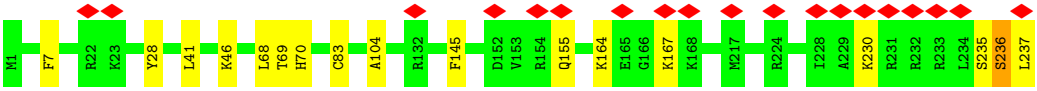




• Molecule 8: 40S ribosomal protein S6

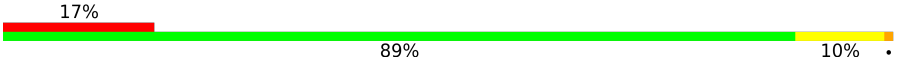
Chain I:

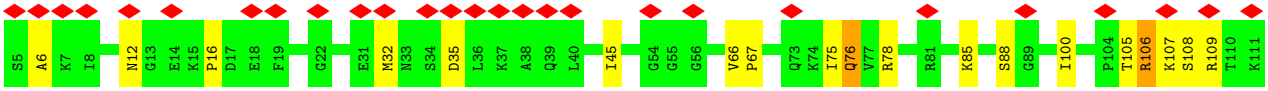


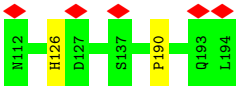


• Molecule 9: ribosomal protein eS7

Chain J:

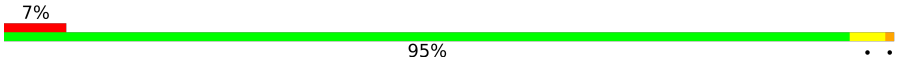


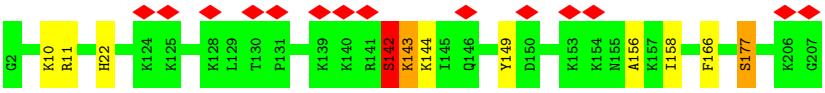




• Molecule 10: 40S ribosomal protein S8

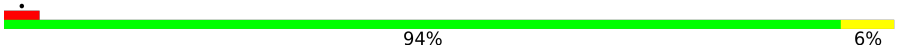
Chain K:





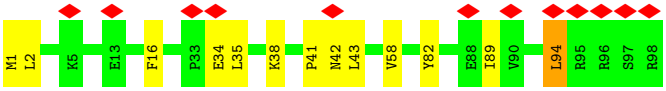
• Molecule 11: Ribosomal protein S9 (Predicted)

Chain L:



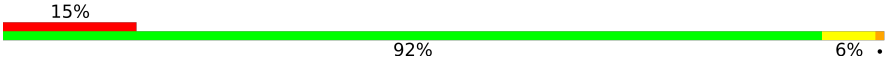
• Molecule 12: 40S ribosomal protein eS10

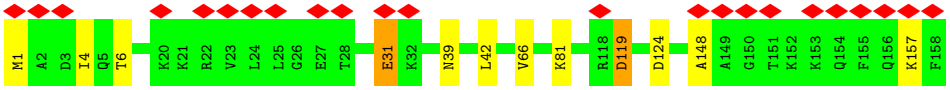
Chain M:



• Molecule 13: Ribosomal protein S11

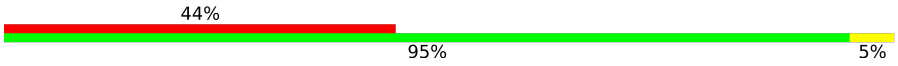
Chain N:

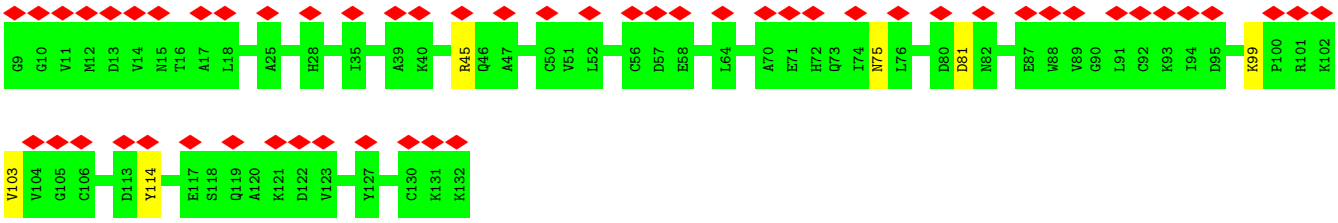




• Molecule 14: 40S ribosomal protein S12

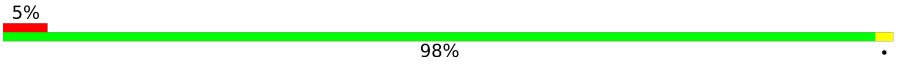
Chain O:

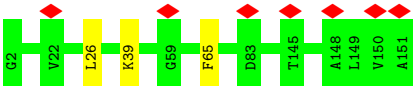




• Molecule 15: ribosomal protein uS15

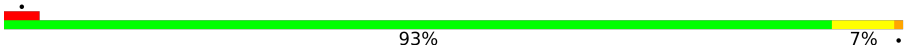
Chain P:

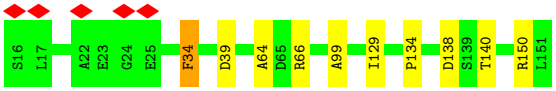




• Molecule 16: 40S ribosomal protein uS11

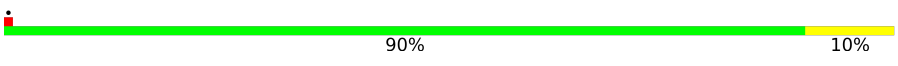
Chain Q:

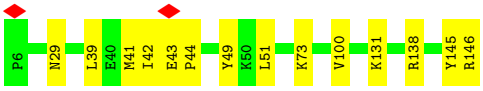




• Molecule 17: ribosomal protein uS9

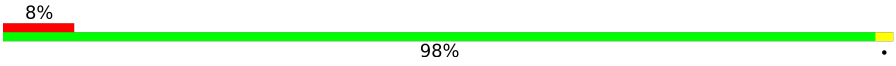
Chain S:

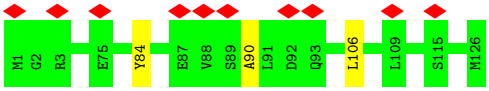




• Molecule 18: ribosomal protein eS17

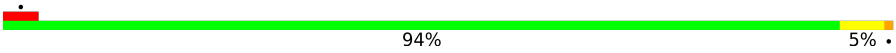
Chain T:

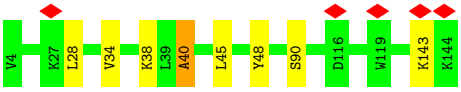




• Molecule 19: 40S ribosomal protein eS19

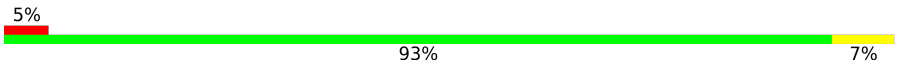
Chain V:

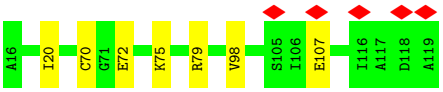




• Molecule 20: Ribosomal_S10 domain-containing protein

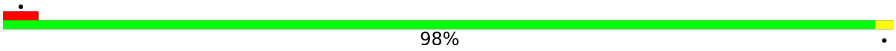
Chain W:

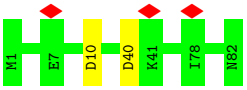




• Molecule 21: 40S ribosomal protein S21

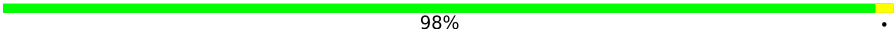
Chain X:

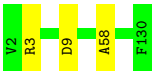




• Molecule 22: Ribosomal protein S15a

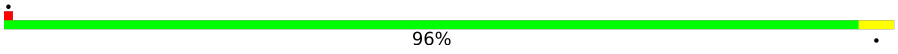
Chain Y:





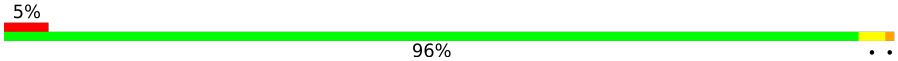
• Molecule 23: 40S ribosomal protein uS12

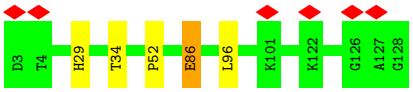
Chain Z:



• Molecule 24: 40S ribosomal protein S24

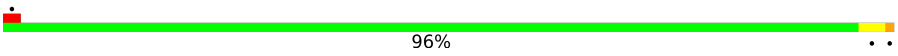
Chain a:

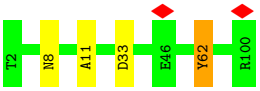




• Molecule 25: 40S ribosomal protein eS26

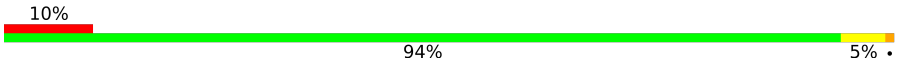
Chain b:

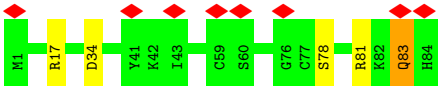




• Molecule 26: 40S ribosomal protein S27

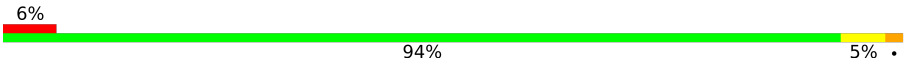
Chain c:

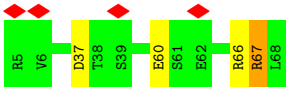




• Molecule 27: ribosomal protein eS28

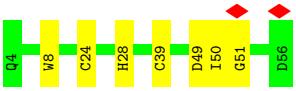
Chain d:





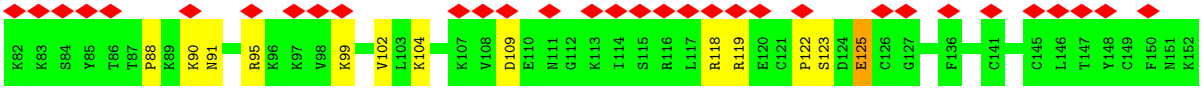
• Molecule 28: ribosomal protein uS14

Chain e:



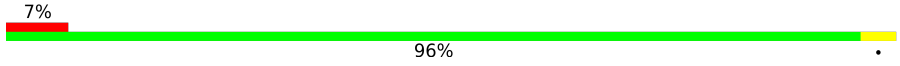
• Molecule 29: ribosomal protein eS31

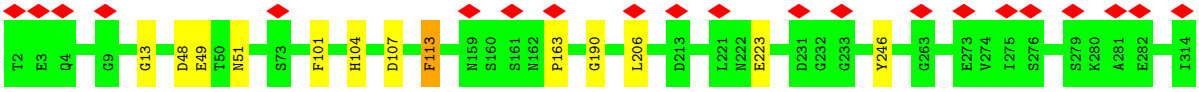
Chain f:



• Molecule 30: ribosomal protein RACK1

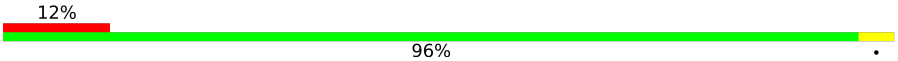
Chain g:

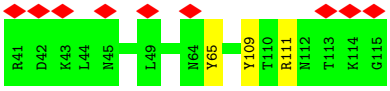




• Molecule 31: ribosomal protein eS25

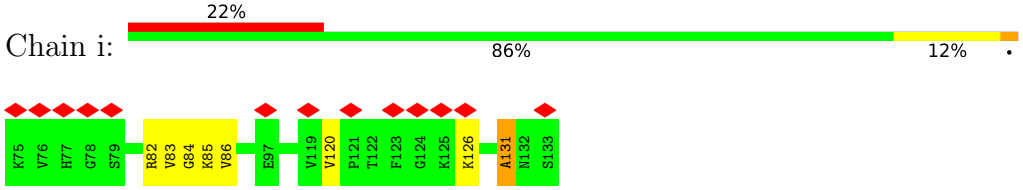
Chain h:





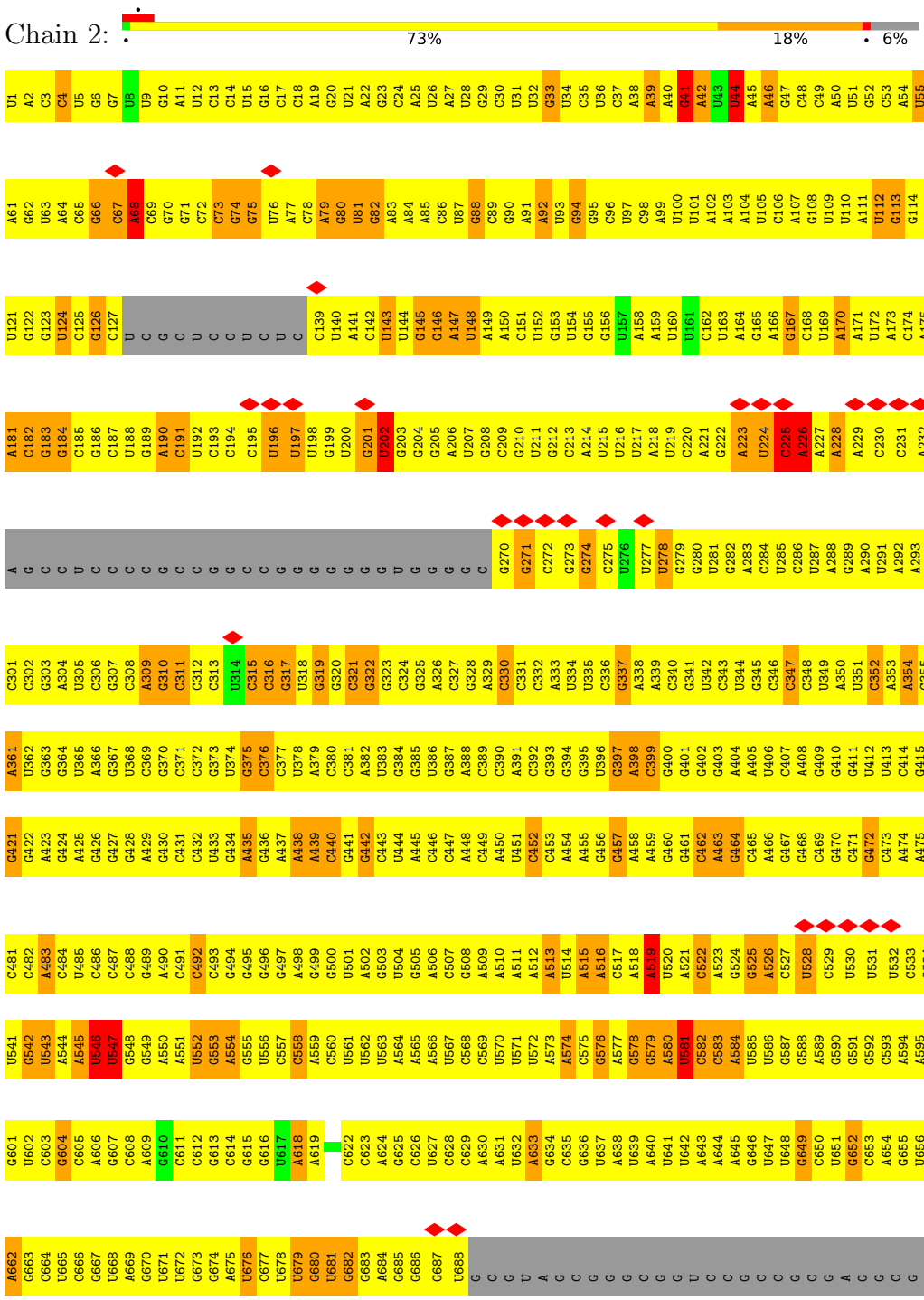
• Molecule 32: 40S ribosomal protein eS30

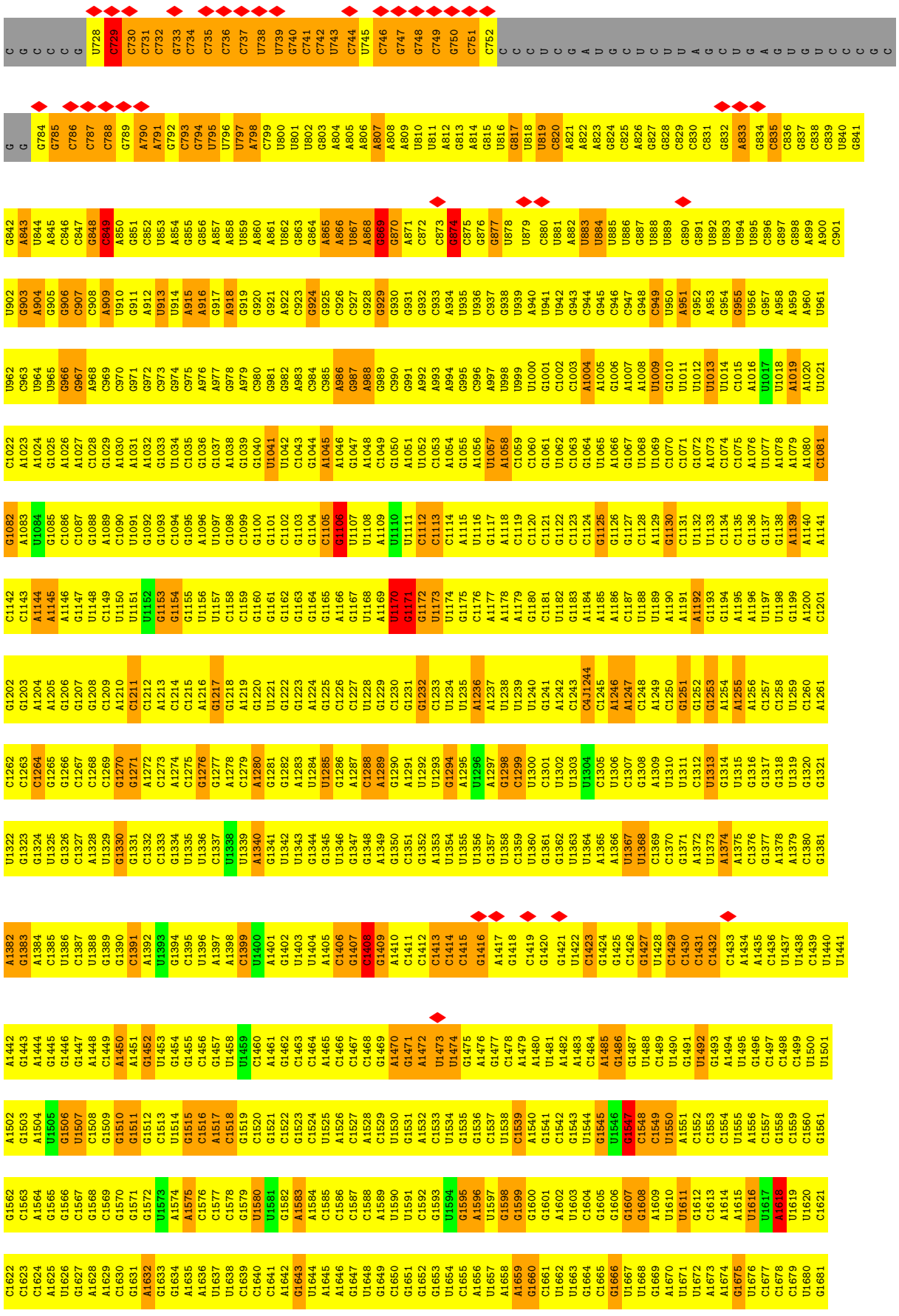
Chain i:

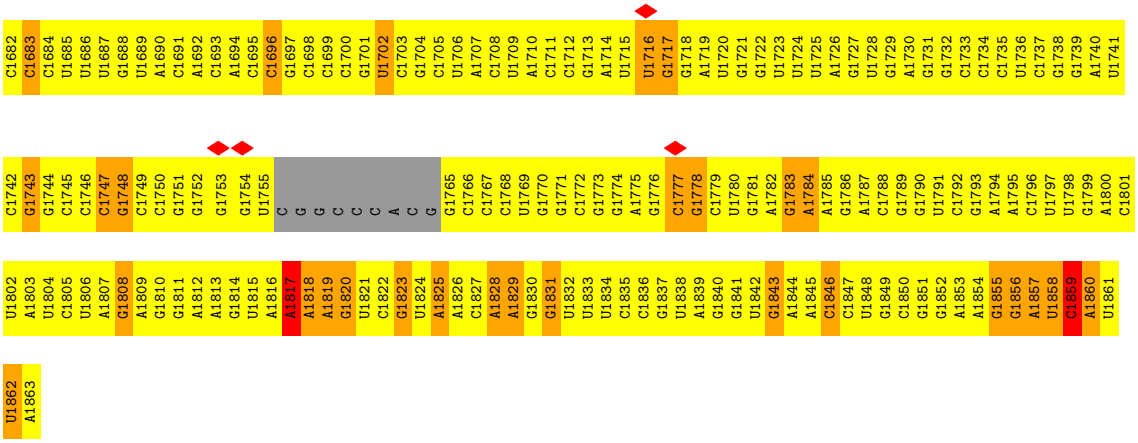


• Molecule 33: 18S ribosomal RNA

Chain 2:

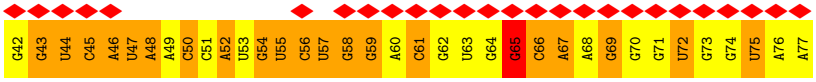






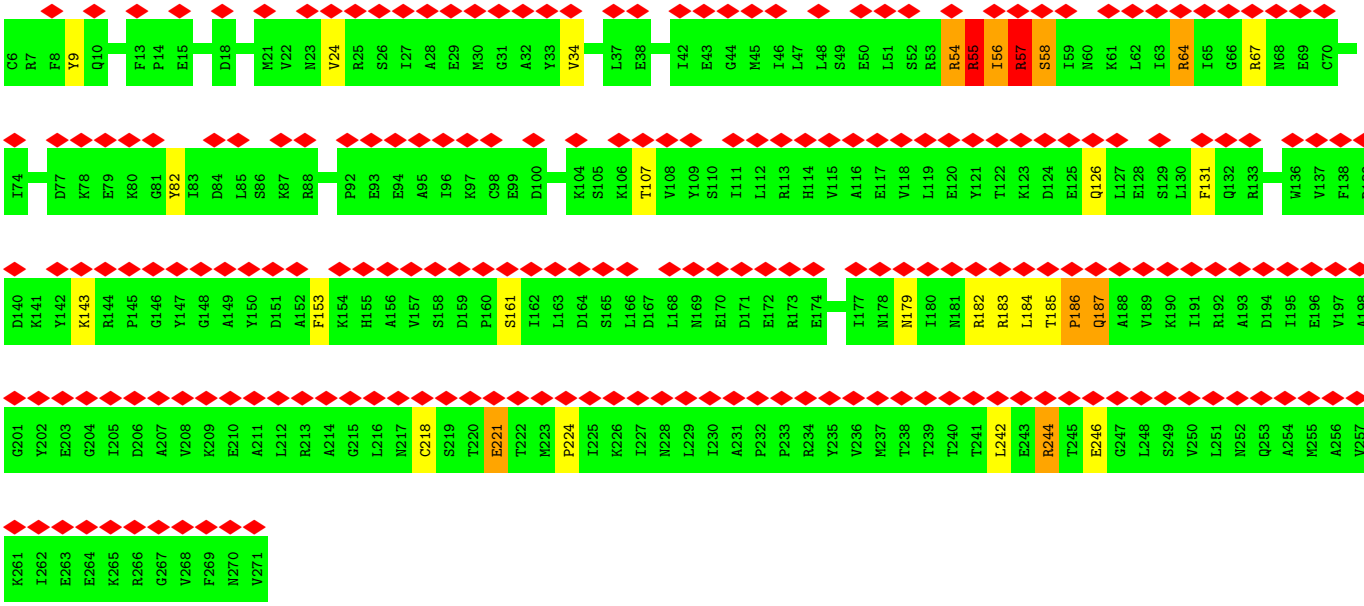
• Molecule 34: histone 4 (H4) mRNA

Chain 3:



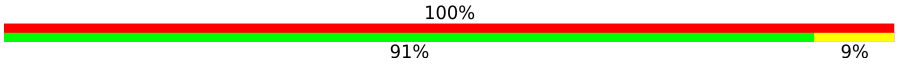
• Molecule 35: Eukaryotic translation initiation factor 2 subunit 1

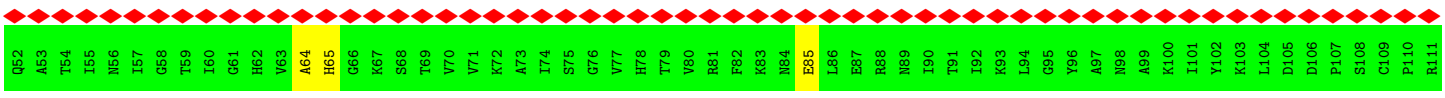
Chain A:



• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma

Chain B:





P112 E113 C114 Y115 R116 S117 C118 G119 S120 S121 T122 P123 D124 E125 F126 P127 T128 D129 I130 P131 G132 T133 K134 G135 N136 F137 K138 L139 V140 R141 H142 V143 S144 F145 V146 D147 C148 P149 G150 H151 D152 I153 L154 M155 A156 T157 M158 L159 N160 G161 A162 A163 V164 M165 D166 A167 A168 L169 L170 L171

I172 A173 G174 N175 E176 S177 C178 P179 Q180 P181 Q182 T183 S184 E185 H186 L187 A188 A189 I190 E191 I192 M193 K194 L195 K196 H197 I198 L199 I200 L201 Q202 N203 K204 I205 D206 L207 V208 K209 E210 S211 Q212 A213 K214 E215 Q216 Y217 E218 Q219 I220 L221 A222 F223 V224 Q225 G226 T227 V228 A229 E230 G231

A232 P233 I234 I235 P236 I237 S238 A239 Q240 L241 K242 Y243 N244 I245 E246 V247 V248 C249 E250 Y251 I252 V253 K254 K255 I256 P257 V258 P259 P260 R261 D262 F263 T264 S265 E266 P267 R268 L269 I270 V271 I272 R273 S274 F275 D276 V277 N278 K279 P280 G281 C282 E283 V284 D285 D286 L287 K288 G289 G290 V291

A292 G293 G294 S295 I296 L297 K298 G299 V300 L301 K302 V303 G304 Q305 E306 I307 E308 V309 R310 P311 G312 I313 V314 S315 K316 D317 S318 E319 G320 K321 L322 M323 C324 K325 P326 I327 F328 S329 K330 I331 V332 S333 L334 F335 A336 E337 H338 N339 D340 L341 Q342 Y343 A344 A345 P346 G347 G348 L349 I350 G351

V352 G353 T354 K355 I356 D357 P358 T359 L360 C361 R362 A363 D364 R365 M366 V367 G368 Q369 V370 L371 G372 A373 V374 G375 A376 L377 P378 E379 I380 F381 T382 E383 L384 E385 I386 S387 Y388 F389 L390 L391 R392 R393 L394 L395 G396 V397 R398 T399 E400 G401 D402 K403 K404 A405 A406 K407 V408 Q409 K410 L411

S412 K413 N414 E415 V416 L417 M418 V419 N420 I421 G422 S423 L424 S425 T426 G427 G428 R429 V430 S431 A432 V433 K434 A435 D436 L437 G438 K439 I440 V441 L442 T443 N444 P445 V446 C447 T448 E449 V450 G451 E452 K453 I454 A455 L456 S457 R458 R459 V460 E461 K462 H463 W464 R465 L466 I467 G468 W469 G470 Q471

I472 R473

- Molecule 37: 40S ribosomal protein uS13

Chain U:

P6 E7 K8 L13 R23 R38 R39 N73 K88 D89 V90 K91 K94 Y95 L99 K116 G133 T139 G140 R141 R142 G143 R144 T145 V146 G147

- Molecule 38: Ribosomal protein S15

Chain R:

V4 E5 Q6 K7 K8 K9 R10 T11 F12 R13 K14 F15 T16 Y17 R18 G19 V20 D21 D27 Y37 S38 R42 L49 R50 R51 M70 E71 K72 P73 E74 K77 M83 I84 G99 K100 E110 V126 K127 H128 G129 R130 P131 G132 I133 G134 A135 T136 H137 S138

- Molecule 39: initiator methionylated tRNA

Chain 1:

A2 G3 C4 A5 G6 A7 G8 U9 G10 G11 C12 G13 C14 A15 G16 C17 G18 G19 A20 A21 G22 C23 G24 U25 G26 C27 U28 G29 G30 G31 C32 C33 C34 A35 U36 A37 A38 C39 C40 C41 A42 G43 A44 G45 G46 U47 C48 G49 A50 U51 G52 G53 A54 U55 C56 G57 A58 A59 A60 C61

C62 A63 U64 C65 C66 U67 C68 U69 G70 C71 U72 A73 C74 C75 A76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	26	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	0.110	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: C4J, T6A

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	l	1.35	0/241	0.96	0/305
2	C	0.97	0/1680	0.99	0/2283
3	D	0.90	0/1770	1.02	2/2367 (0.1%)
4	E	0.91	0/1779	0.99	5/2399 (0.2%)
5	F	0.97	0/1793	1.03	1/2412 (0.0%)
6	G	0.97	0/2125	1.00	0/2856
7	H	0.99	0/1531	0.97	0/2059
8	I	1.07	0/1946	1.03	6/2587 (0.2%)
9	J	0.96	0/1553	1.00	0/2079
10	K	1.03	0/1709	1.05	5/2278 (0.2%)
11	L	1.07	0/1523	0.98	2/2031 (0.1%)
12	M	0.96	0/852	1.01	0/1147
13	N	1.00	0/1319	1.01	0/1761
14	O	0.90	0/968	1.04	2/1296 (0.2%)
15	P	0.97	0/1232	0.92	2/1656 (0.1%)
16	Q	1.02	0/1029	1.05	2/1380 (0.1%)
17	S	1.01	0/1141	1.01	0/1528
18	T	0.99	0/1032	0.99	0/1383
19	V	0.98	0/1133	0.99	3/1517 (0.2%)
20	W	0.96	0/832	1.02	0/1117
21	X	0.99	0/627	1.01	0/839
22	Y	0.99	0/1051	0.98	0/1406
23	Z	0.99	0/1125	0.99	2/1500 (0.1%)
24	a	1.01	0/1038	1.04	1/1377 (0.1%)
25	b	1.06	0/803	1.03	1/1076 (0.1%)
26	c	0.94	0/673	1.00	0/902
27	d	1.13	0/509	1.02	0/680
28	e	1.10	0/455	1.05	0/603
29	f	0.98	0/594	1.07	0/786
30	g	0.92	0/2494	1.10	4/3394 (0.1%)
31	h	0.97	0/605	1.08	2/810 (0.2%)
32	i	1.09	0/478	1.06	1/628 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	2	1.61	115/41562 (0.3%)	2.42	4485/64770 (6.9%)
34	3	1.22	0/867	1.89	54/1352 (4.0%)
35	A	1.00	0/2178	1.08	9/2935 (0.3%)
36	B	0.92	0/3267	1.07	4/4415 (0.1%)
37	U	1.01	0/1190	0.92	0/1592
38	R	0.99	0/1132	0.99	3/1510 (0.2%)
39	1	2.46	8/1770 (0.5%)	2.77	221/2759 (8.0%)
All	All	1.35	123/89606 (0.1%)	1.90	4817/129775 (3.7%)

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
2	C	0	1
3	D	0	1
5	F	0	2
8	I	0	2
9	J	0	2
11	L	0	2
12	M	0	5
17	S	0	2
26	c	0	1
28	e	0	2
29	f	0	1
31	h	0	1
32	i	0	2
33	2	1	64
34	3	1	0
35	A	0	8
36	B	0	11
37	U	0	3
39	1	3	3
All	All	5	113

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	19	G	O3'-P	43.51	2.13	1.61
39	1	16	G	O3'-P	-39.18	1.14	1.61
39	1	17	C	O3'-P	32.10	1.99	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	1815	U	O3'-P	-29.22	1.26	1.61
39	1	17	C	C2'-O2'	-26.05	1.07	1.41

The worst 5 of 4817 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	19	G	O3'-P-O5'	31.90	164.60	104.00
39	1	16	G	P-O3'-C3'	23.25	147.60	119.70
33	2	351	U	P-O3'-C3'	18.59	142.01	119.70
33	2	797	U	O3'-P-O5'	-17.82	70.15	104.00
33	2	676	U	O3'-P-O5'	-17.57	70.62	104.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'
34	3	65	G	C3'
39	1	17	C	C2',C3'
39	1	18	G	C3'

5 of 113 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	193	HIS	Peptide
3	D	208	HIS	Peptide
5	F	107	TYR	Sidechain
5	F	167	TYR	Sidechain
8	I	68	LEU	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	l	240	0	289	0	0
2	C	1643	0	1646	1	0
3	D	1742	0	1815	0	0
4	E	1743	0	1836	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1765	0	1863	23	0
6	G	2083	0	2189	0	0
7	H	1509	0	1563	8	0
8	I	1924	0	2086	12	0
9	J	1530	0	1623	27	0
10	K	1680	0	1762	1	0
11	L	1499	0	1608	0	0
12	M	828	0	854	0	0
13	N	1296	0	1374	0	0
14	O	958	0	993	0	0
15	P	1208	0	1294	1	0
16	Q	1016	0	1039	0	0
17	S	1123	0	1193	2	0
18	T	1020	0	1075	0	0
19	V	1113	0	1149	5	0
20	W	822	0	887	1	0
21	X	620	0	622	0	0
22	Y	1034	0	1080	0	0
23	Z	1107	0	1179	2	0
24	a	1022	0	1084	0	0
25	b	790	0	839	0	0
26	c	659	0	683	0	0
27	d	507	0	536	0	0
28	e	445	0	442	0	0
29	f	582	0	599	0	0
30	g	2437	0	2393	0	0
31	h	599	0	655	0	0
32	i	473	0	524	0	0
33	2	37202	0	18777	310	0
34	3	774	0	390	81	0
35	A	2147	0	2187	26	0
36	B	3214	0	3354	0	0
37	U	1172	0	1226	50	0
38	R	1111	0	1166	58	0
39	1	1614	0	824	60	0
All	All	84251	0	66698	517	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 517 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)
37:U:147:GLY:CA	38:R:131:PRO:HG3	1.22	1.68
37:U:147:GLY:HA3	38:R:131:PRO:CG	1.34	1.55
39:1:16:G:O3'	39:1:17:C:P	1.14	1.52
33:2:1817:A:C2'	33:2:1818:A:H5'	1.47	1.42
5:F:117:ARG:HH12	34:3:67:A:N6	1.14	1.41

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	l	23/25 (92%)	23 (100%)	0	0	100	100
2	C	206/208 (99%)	176 (85%)	21 (10%)	9 (4%)	2	20
3	D	213/215 (99%)	185 (87%)	19 (9%)	9 (4%)	3	22
4	E	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	6	35
5	F	225/227 (99%)	205 (91%)	13 (6%)	7 (3%)	4	28
6	G	261/263 (99%)	229 (88%)	26 (10%)	6 (2%)	6	34
7	H	189/191 (99%)	165 (87%)	16 (8%)	8 (4%)	3	22
8	I	233/237 (98%)	206 (88%)	20 (9%)	7 (3%)	4	28
9	J	188/190 (99%)	162 (86%)	18 (10%)	8 (4%)	2	21
10	K	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	4	29
11	L	180/182 (99%)	167 (93%)	6 (3%)	7 (4%)	3	23
12	M	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	1	13
13	N	156/158 (99%)	130 (83%)	19 (12%)	7 (4%)	2	20
14	O	122/124 (98%)	103 (84%)	15 (12%)	4 (3%)	4	27
15	P	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
16	Q	134/136 (98%)	116 (87%)	11 (8%)	7 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	S	139/141 (99%)	123 (88%)	12 (9%)	4 (3%)	4 29
18	T	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	9 41
19	V	139/141 (99%)	124 (89%)	10 (7%)	5 (4%)	3 25
20	W	102/104 (98%)	95 (93%)	4 (4%)	3 (3%)	4 29
21	X	80/82 (98%)	66 (82%)	13 (16%)	1 (1%)	12 45
22	Y	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9 41
23	Z	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	11 43
24	a	122/126 (97%)	106 (87%)	12 (10%)	4 (3%)	4 27
25	b	97/99 (98%)	81 (84%)	13 (13%)	3 (3%)	4 28
26	c	82/84 (98%)	72 (88%)	8 (10%)	2 (2%)	6 33
27	d	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	2 18
28	e	51/53 (96%)	39 (76%)	8 (16%)	4 (8%)	1 9
29	f	69/71 (97%)	56 (81%)	6 (9%)	7 (10%)	0 6
30	g	311/313 (99%)	273 (88%)	31 (10%)	7 (2%)	6 34
31	h	73/75 (97%)	70 (96%)	2 (3%)	1 (1%)	11 43
32	i	57/59 (97%)	45 (79%)	7 (12%)	5 (9%)	1 7
35	A	264/266 (99%)	225 (85%)	29 (11%)	10 (4%)	3 24
36	B	420/422 (100%)	350 (83%)	48 (11%)	22 (5%)	2 16
37	U	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	3 25
38	R	133/135 (98%)	105 (79%)	18 (14%)	10 (8%)	1 9
All	All	5534/5610 (99%)	4836 (87%)	500 (9%)	198 (4%)	6 25

5 of 198 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	209	ASP
3	D	221	PRO
5	F	193	ASP
5	F	219	PRO
6	G	2	ALA

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	l	24/24 (100%)	21 (88%)	3 (12%)	4 21
2	C	174/174 (100%)	171 (98%)	3 (2%)	60 82
3	D	196/196 (100%)	192 (98%)	4 (2%)	55 79
4	E	187/187 (100%)	183 (98%)	4 (2%)	53 78
5	F	190/190 (100%)	182 (96%)	8 (4%)	30 61
6	G	225/225 (100%)	223 (99%)	2 (1%)	78 91
7	H	161/161 (100%)	159 (99%)	2 (1%)	71 87
8	I	207/207 (100%)	205 (99%)	2 (1%)	76 89
9	J	170/170 (100%)	164 (96%)	6 (4%)	36 66
10	K	177/177 (100%)	174 (98%)	3 (2%)	60 82
11	L	157/157 (100%)	156 (99%)	1 (1%)	86 94
12	M	89/89 (100%)	86 (97%)	3 (3%)	37 67
13	N	142/142 (100%)	135 (95%)	7 (5%)	25 57
14	O	104/104 (100%)	103 (99%)	1 (1%)	76 89
15	P	130/130 (100%)	129 (99%)	1 (1%)	81 92
16	Q	106/106 (100%)	103 (97%)	3 (3%)	43 72
17	S	117/117 (100%)	112 (96%)	5 (4%)	29 61
18	T	114/114 (100%)	113 (99%)	1 (1%)	78 91
19	V	113/113 (100%)	113 (100%)	0	100 100
20	W	94/94 (100%)	92 (98%)	2 (2%)	53 78
21	X	67/67 (100%)	66 (98%)	1 (2%)	65 84
22	Y	112/112 (100%)	111 (99%)	1 (1%)	78 91
23	Z	114/114 (100%)	112 (98%)	2 (2%)	59 81
24	a	108/108 (100%)	107 (99%)	1 (1%)	78 91
25	b	87/87 (100%)	86 (99%)	1 (1%)	73 88
26	c	76/76 (100%)	73 (96%)	3 (4%)	32 63
27	d	57/57 (100%)	55 (96%)	2 (4%)	36 66
28	e	47/47 (100%)	46 (98%)	1 (2%)	53 78
29	f	64/64 (100%)	58 (91%)	6 (9%)	8 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	g	272/272 (100%)	267 (98%)	5 (2%)	59 81
31	h	66/66 (100%)	66 (100%)	0	100 100
32	i	49/49 (100%)	48 (98%)	1 (2%)	55 79
35	A	238/238 (100%)	230 (97%)	8 (3%)	37 67
36	B	354/354 (100%)	350 (99%)	4 (1%)	73 88
37	U	122/122 (100%)	118 (97%)	4 (3%)	38 68
38	R	121/121 (100%)	114 (94%)	7 (6%)	20 52
All	All	4831/4831 (100%)	4723 (98%)	108 (2%)	54 77

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	S	131	LYS
27	d	67	ARG
37	U	141	ARG
20	W	75	LYS
24	a	29	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
36	B	160	ASN
36	B	305	GLN
36	B	203	ASN
25	b	17	HIS
36	B	65	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1732/1863 (92%)	263 (15%)	11 (0%)
34	3	35/36 (97%)	20 (57%)	5 (14%)
39	1	74/75 (98%)	15 (20%)	5 (6%)
All	All	1841/1974 (93%)	298 (16%)	21 (1%)

5 of 298 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	4	C
33	2	33	G
33	2	41	G
33	2	42	A
33	2	44	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	3	58	G
39	1	16	G
39	1	74	C
39	1	17	C
39	1	8	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	C4J	2	1244	33	24,29,30	0.79	1 (4%)	29,42,45	1.03	1 (3%)
39	T6A	1	37	39	27,34,35	1.04	2 (7%)	29,49,52	2.64	9 (31%)

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
33	C4J	2	1244	33	1/1/7/7	9/16/34/35	0/2/2/2
39	T6A	1	37	39	-	6/19/41/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	37	T6A	C5-C4	2.51	1.47	1.40
39	1	37	T6A	O4'-C1'	2.21	1.44	1.41
33	2	1244	C4J	C1'-C5	-2.07	1.45	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	37	T6A	C12-N11-C10	8.56	136.20	121.94
39	1	37	T6A	C2-N1-C6	7.01	122.61	116.59
39	1	37	T6A	C14-C12-C13	3.68	116.47	110.19
39	1	37	T6A	N3-C2-N1	-3.57	123.09	128.68
33	2	1244	C4J	C4-N3-C2	-3.41	121.15	125.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	2	1244	C4J	C31-C3-N3-C2
33	2	1244	C4J	C31-C3-N3-C4
33	2	1244	C4J	C3-C31-C32-C34
33	2	1244	C4J	C3-C31-C32-N33
33	2	1244	C4J	N33-C32-C34-O36

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	1244	C4J	3	0
39	1	37	T6A	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	2	6
39	1	5
8	I	1
24	a	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	I	217:MET	C	218:LYS	N	3.94
1	a	9:THR	C	10:ARG	N	3.27
1	1	19:G	O3'	20:A	P	2.13
1	1	17:C	O3'	18:G	P	1.99

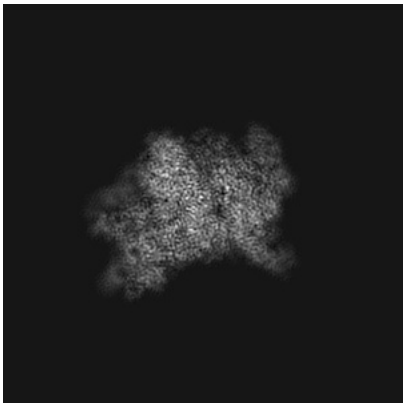
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10762. These allow visual inspection of the internal detail of the map and identification of artifacts.

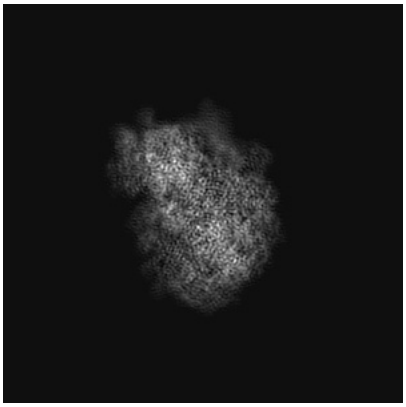
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

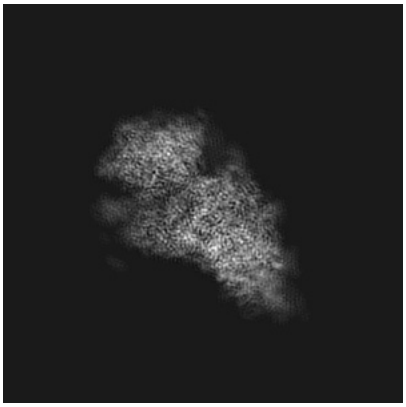
6.1.1 Primary map



X



Y



Z

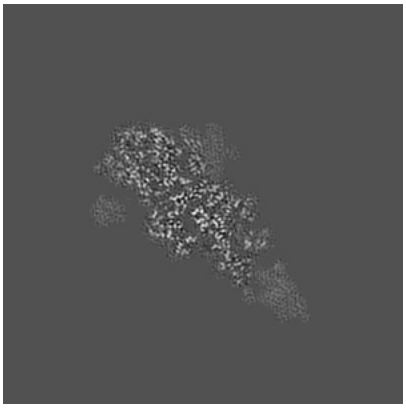
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192

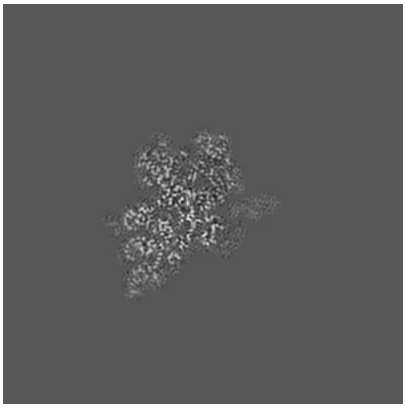


Z Index: 192

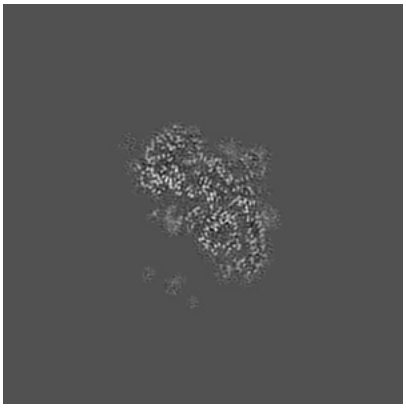
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

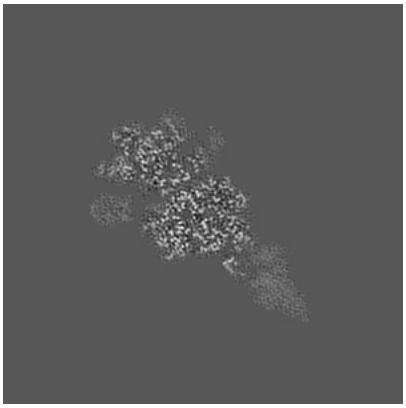
6.3.1 Primary map



X Index: 208



Y Index: 160

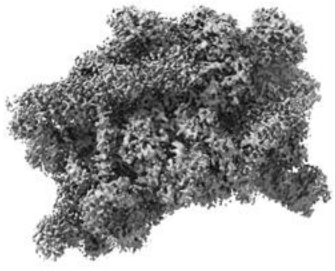


Z Index: 199

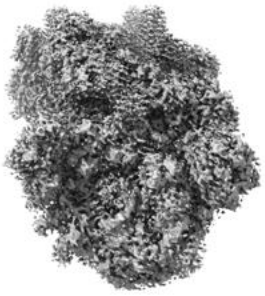
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

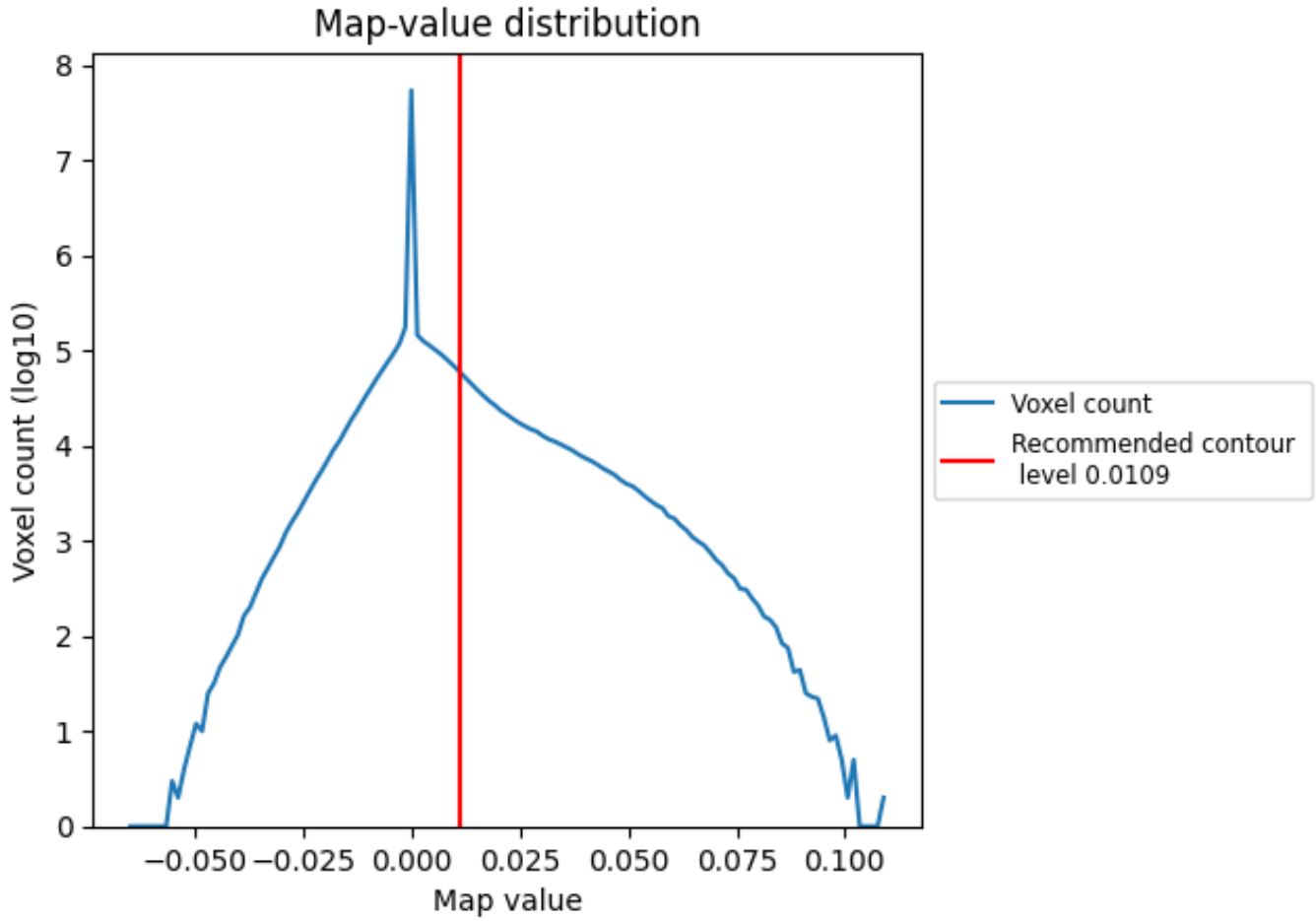
6.5 Mask visualisation (i)

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

7 Map analysis

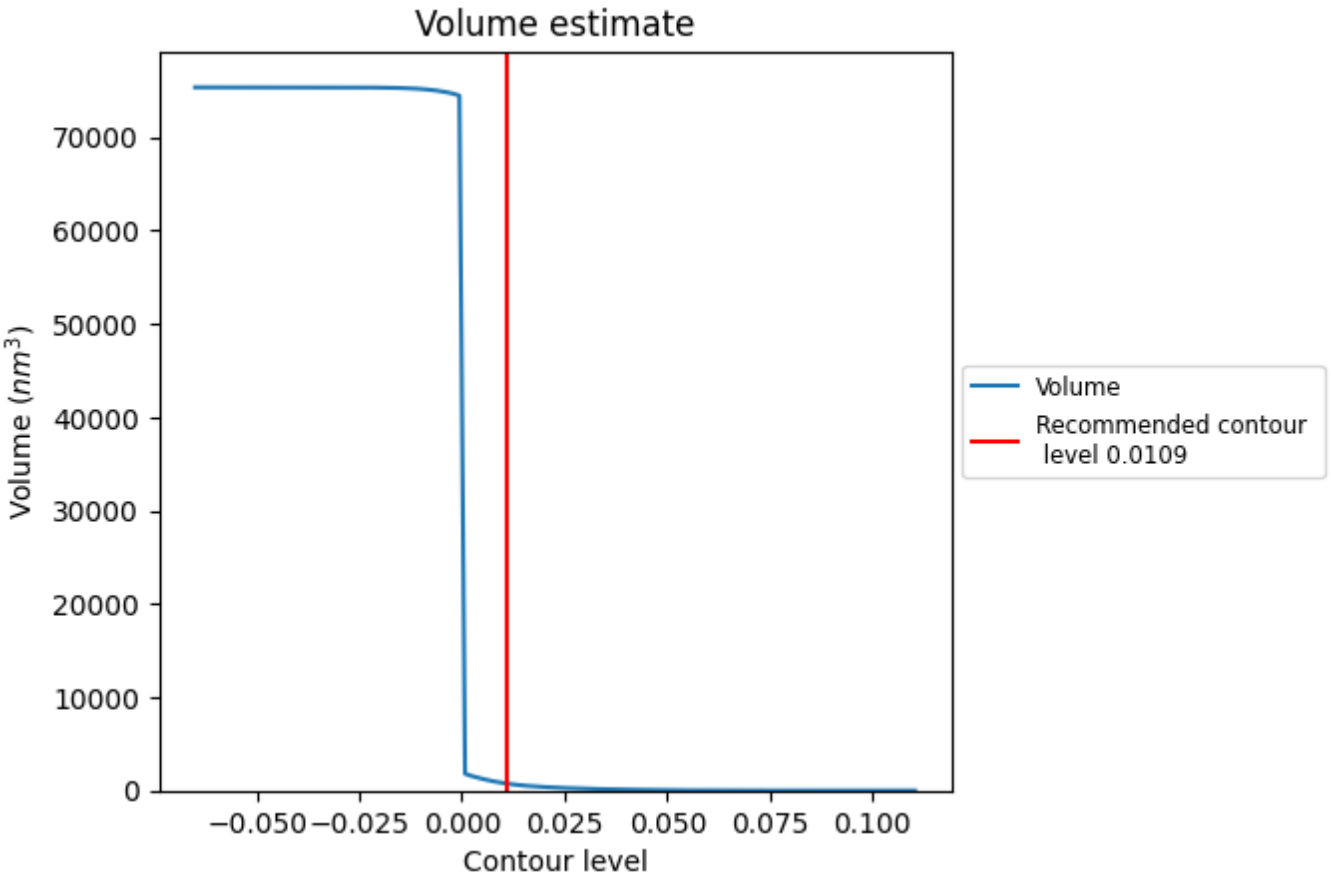
This section contains the results of statistical analysis of the map.

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.

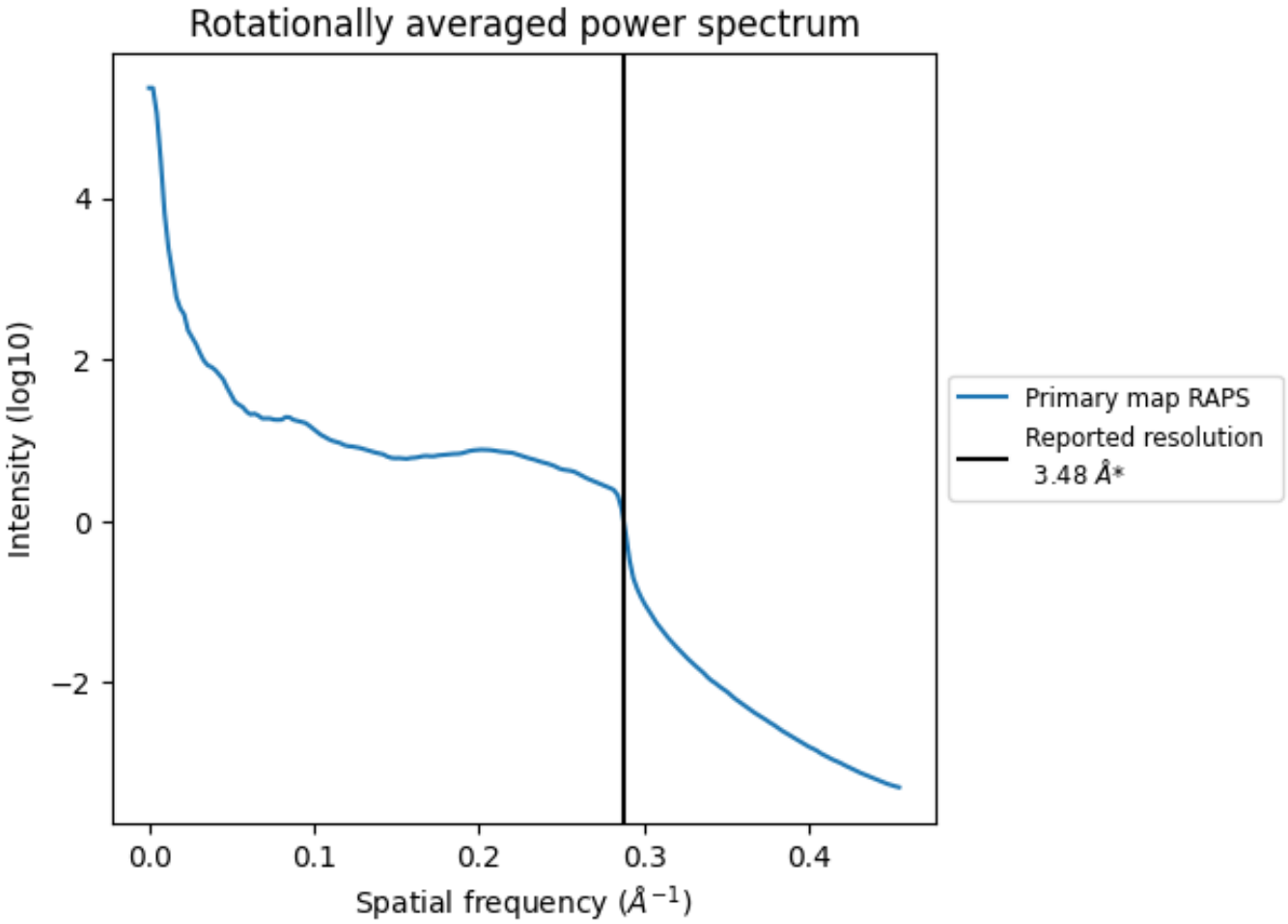
7.2 Volume estimate (i)



The volume at the recommended contour level is 753 nm^3; this corresponds to an approximate mass of 680 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 0.287 $Å^{-1}$

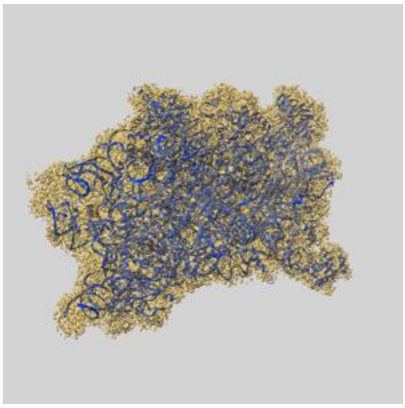
8 Fourier-Shell correlation (i)

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

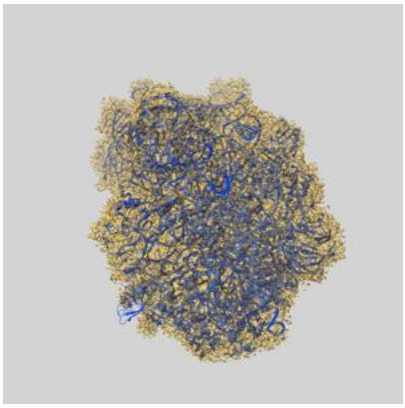
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10762 and PDB model 6YAN. Per-residue inclusion information can be found in section 3 on page 11.

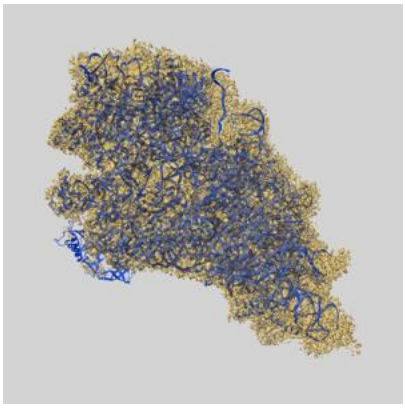
9.1 Map-model overlay



X



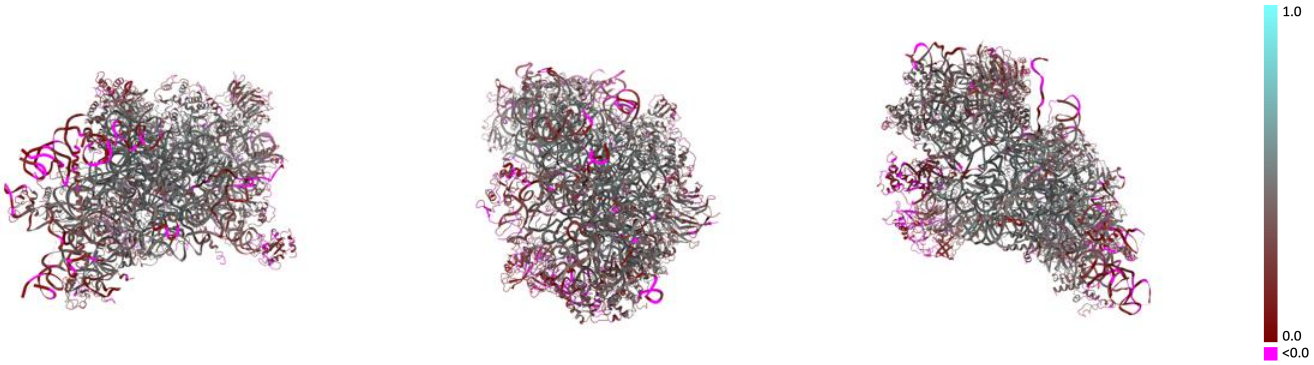
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0109 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.

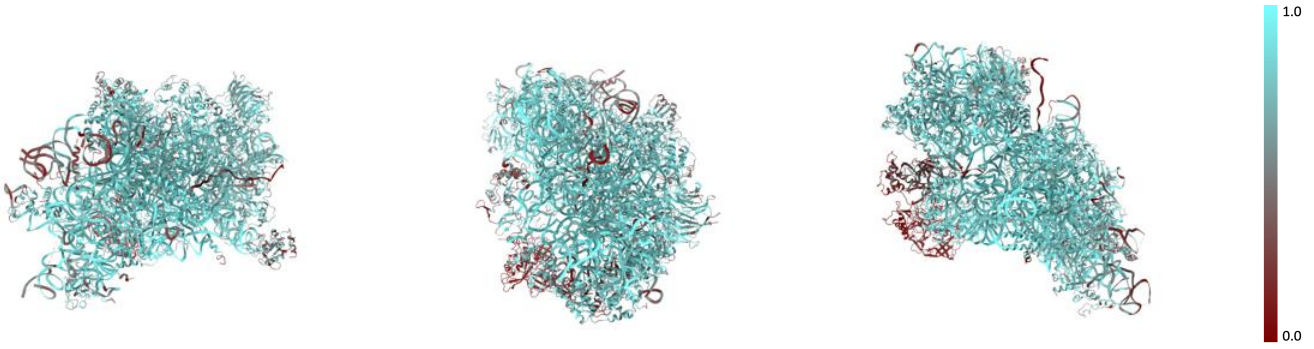
9.2 Q-score mapped to coordinate model (i)



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.

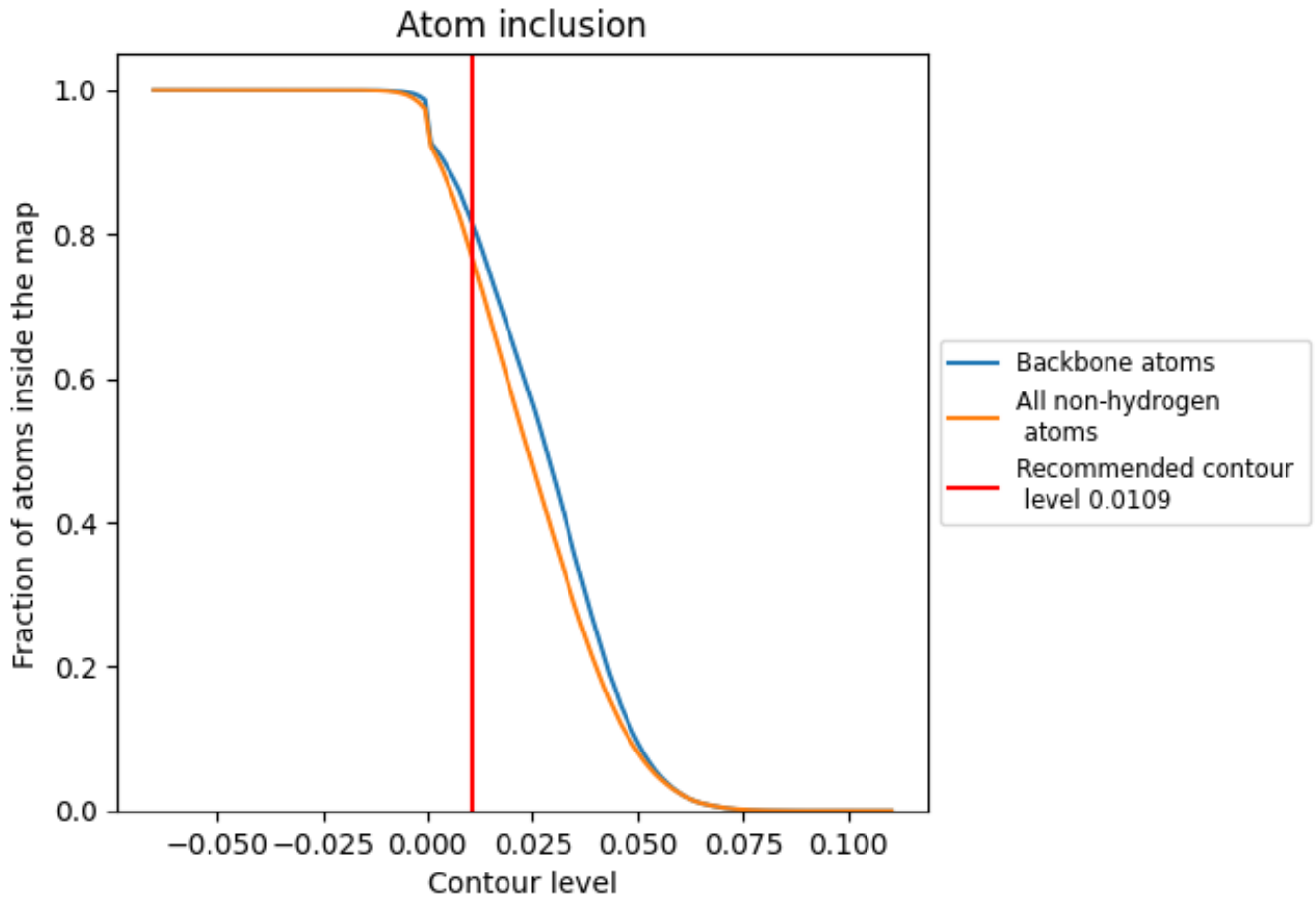
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0109).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7631	0.3510
1	0.5062	0.1520
2	0.8838	0.4010
3	0.3269	0.1390
A	0.1818	0.0510
B	0.0079	-0.0120
C	0.8302	0.4210
D	0.7890	0.4010
E	0.8249	0.4440
F	0.7364	0.3530
G	0.8137	0.4160
H	0.7841	0.3830
I	0.7258	0.2980
J	0.6342	0.2810
K	0.7708	0.3630
L	0.8230	0.4160
M	0.7419	0.3150
N	0.7486	0.3830
O	0.4364	0.1240
P	0.8055	0.3960
Q	0.8065	0.4090
R	0.7001	0.3020
S	0.8142	0.4180
T	0.7288	0.3300
U	0.7693	0.3430
V	0.7773	0.3790
W	0.7503	0.3450
X	0.7921	0.3780
Y	0.8683	0.4780
Z	0.8509	0.4510
a	0.7968	0.3730
b	0.8331	0.4320
c	0.7403	0.3230
d	0.7536	0.3660
e	0.8103	0.3800

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Chain	Atom inclusion	Q-score
f	0.4427	0.0750
g	0.7391	0.3250
h	0.7055	0.3110
i	0.6228	0.2840
l	0.7671	0.3910