Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 07:46 am BST

PDB ID	:	6FYY
EMDB ID	:	EMD-4328
Title	:	Structure of a partial yeast 48S preinitiation complex with eIF5 N-terminal domain (model C2)
Authors	:	Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2018-03-12
Resolution	:	3.02 Å(reported)

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

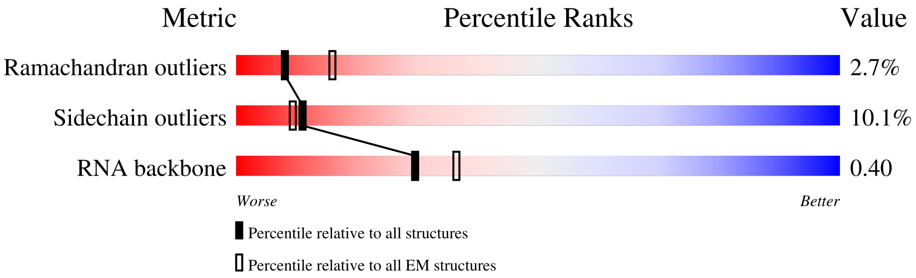
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

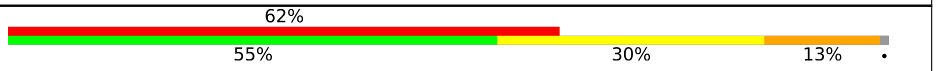
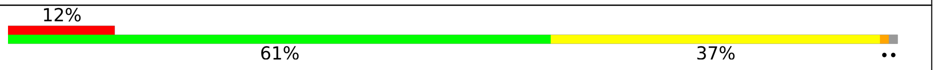
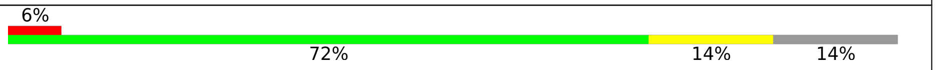
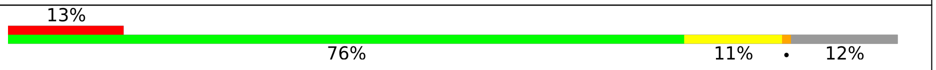
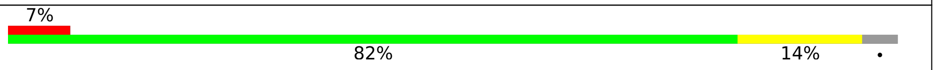
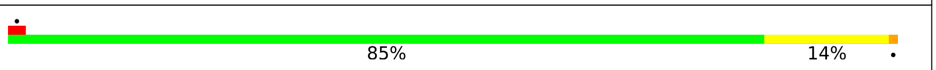
The reported resolution of this entry is 3.02 Å.

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)
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	1	76	
2	2	1798	
3	3	49	
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	

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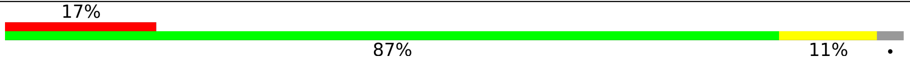
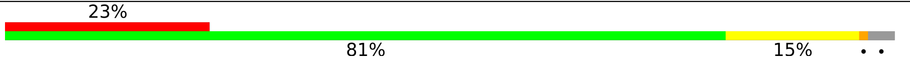
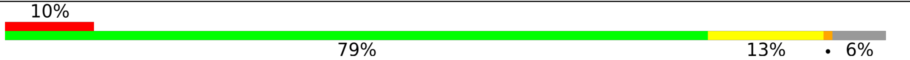
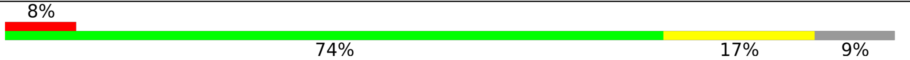
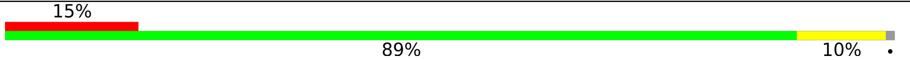
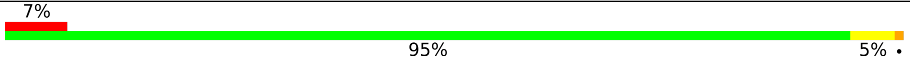
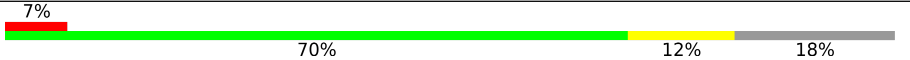
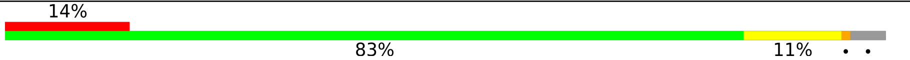
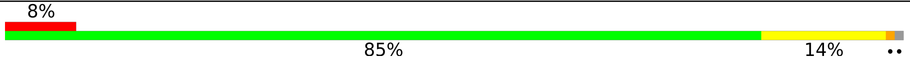
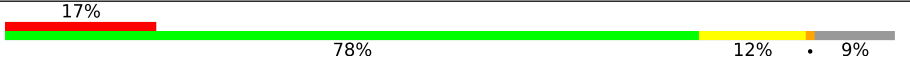
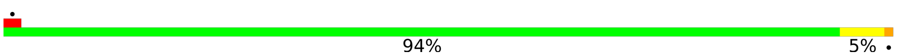
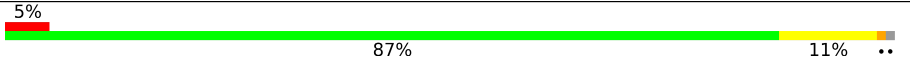
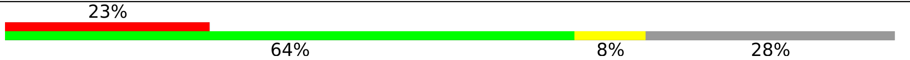
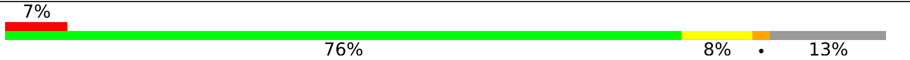
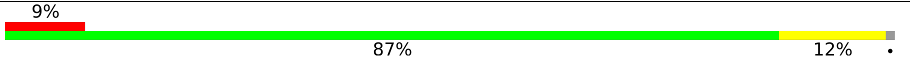
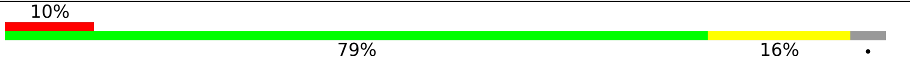
Mol	Chain	Length	Quality of chain
9	F	227	 10% 73% 18% 9%
10	G	236	 17% 87% 11% •
11	H	190	 23% 81% 15% • •
12	I	201	 10% 79% 13% • 6%
13	J	188	 • 81% 15% • •
14	K	106	 8% 74% 17% 9%
15	L	156	 15% 89% 10% •
16	M	134	 56% 72% 15% • 13%
17	N	151	 7% 95% 5% •
18	O	137	 • 81% 12% • 6%
19	P	142	 7% 70% 12% 18%
20	Q	143	 • 85% 14% •
21	R	136	 14% 83% 11% • •
22	S	146	 8% 85% 14% ••
23	T	144	 • 86% 12% ••
24	U	117	 17% 78% 12% • 9%
25	V	87	 • 94% 5% •
26	W	130	 89% 9% ••
27	X	145	 • 88% 11% •
28	Y	135	 5% 87% 11% ••
29	Z	108	 23% 64% 8% 28%
30	a	119	 7% 76% 8% • 13%
31	b	82	 9% 87% 12% •
32	c	67	 10% 79% 16% •
33	d	56	 86% 12% •

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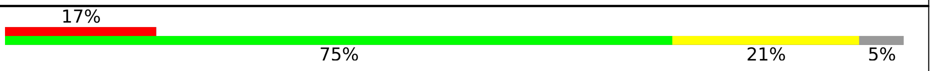
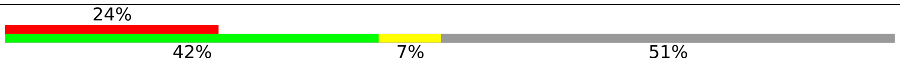
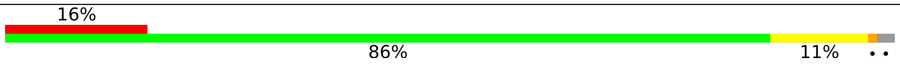
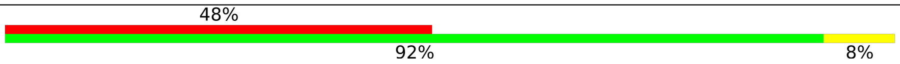
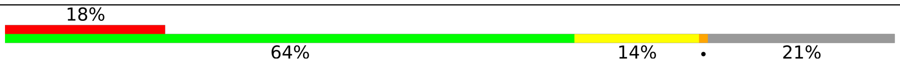
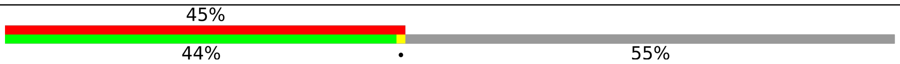
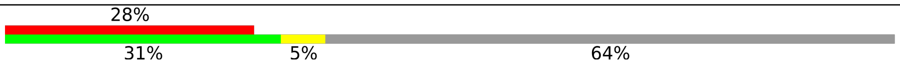
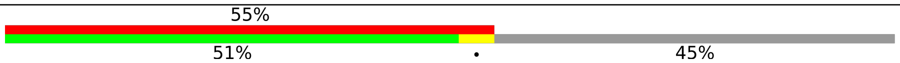
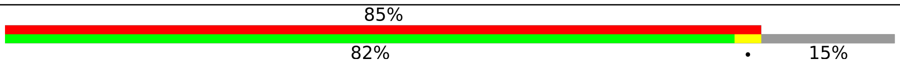
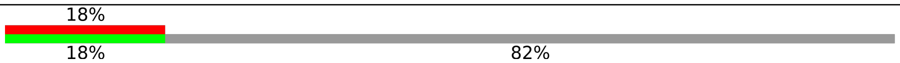
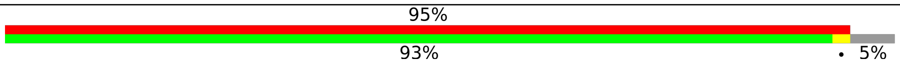
Mol	Chain	Length	Quality of chain
34	e	63	 17% 75% 21% 5%
35	f	150	 24% 42% 7% 51%
36	g	326	 16% 86% 11%
37	h	25	 48% 92% 8%
38	i	153	 18% 64% 14% 21%
39	j	304	 82% 69% 13% 18%
40	k	527	 75% 71% 25%
41	l	285	 45% 44% 55%
42	m	405	 28% 31% 5% 64%
43	o	964	 55% 51% 45%
44	p	763	 85% 82% 15%
45	q	812	 76% 73% 24%
46	r	274	 18% 18% 82%
47	s	347	 95% 93% 5%

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
2	C4J	2	1190	X	-	-	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 104316 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 RNA chain called tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	75	1639	734	298	531	76	0	0

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1780	37812	16904	6659	12469	1780	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208
2	1190	C4J	U	conflict	GB 49642208

- Molecule 3 is a RNA chain called mRNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	31	719	324	108	252	35	4	0

- Molecule 4 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	219	1702	1085	299	316	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	225	1797	1135	330	329	3	0	0

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	220	Total 1648	C 1053	N 291	O 300	S 4	0	0

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	227	Total 1774	C 1126	N 320	O 323	S 5	0	0

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total 2078	C 1322	N 393	O 359	S 4	0	0

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total 1609	C 1008	N 298	O 300	S 3	0	0

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	230	Total 1832	C 1146	N 352	O 330	S 4	0	0

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	184	Total 1483	C 950	N 270	O 263	0	0

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total 1489	C 923	N 300	O 265	S 1	0	0

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	182	1471	929	287	254	1	0	0

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	96	809	533	129	146	1	0	0

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	155	1248	798	237	210	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	M	117	885	553	161	171	0	0

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	151	1195	761	224	207	3	0	0

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	129	955	585	191	176	3	0	0

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	117	923	592	165	161	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	Q	141	1105	709	204	192	0	0

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	R	130	1033	643	194	193	3	0	0

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	145	1189	739	239	209	2	0	0

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	T	143	1110	693	210	207	0	0

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U	106	845	540	152	152	1	0	0

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	V	87	687	424	126	135	2	0	0

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	129	1021	651	187	180	3	0	0

- Molecule 27 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total 1119	C 708	N 218	O 191	S 2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total 1061	C 665	N 207	O 189	0	0

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	78	Total 594	C 376	N 111	O 106	S 1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	103	Total 812	C 500	N 173	O 134	S 5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total 609	C 379	N 112	O 113	S 5	0	0

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total 499	C 308	N 99	O 91	S 1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total 461	C 289	N 93	O 78	S 1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	e	60	472	295	96	80	1	0	0

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	74	584	374	111	95	4	0	0

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	320	2469	1561	432	471	5	0	0

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	25	233	142	63	27	1	0	0

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	121	958	587	183	183	5	0	0

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	j	249	2006	1283	333	382	8	0	0

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	k	396	3034	1932	542	544	16	0	0

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total 1036	C 661	N 186	O 182	S 7	0	0

- Molecule 42 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	147	Total 1140	C 724	N 201	O 208	S 7	0	0

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	529	Total 4070	C 2597	N 697	O 769	S 7	0	0

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	647	Total 5114	C 3274	N 880	O 942	S 18	0	0

- Molecule 45 is a protein called eIF3c,Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	621	Total 4827	C 3076	N 813	O 926	S 12	0	0

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	r	49	Total 392	C 240	N 76	O 76	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	330	Total 2606	C 1661	N 429	O 507	S 9	0	0

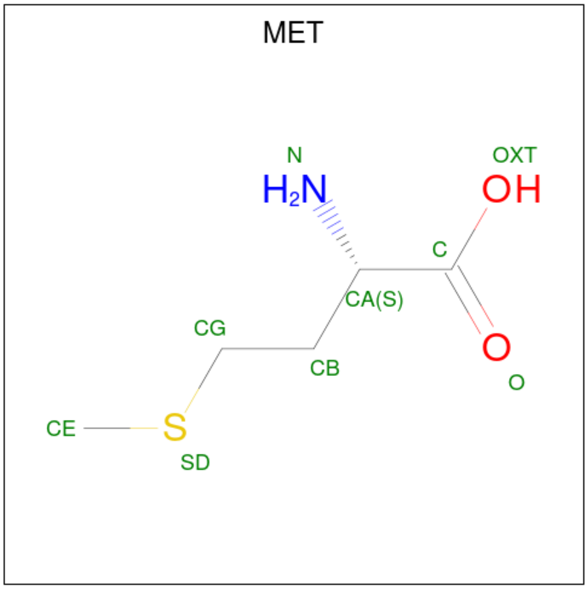
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	2	116	116	116	0
			Total	Mg	
48	k	1	1	1	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

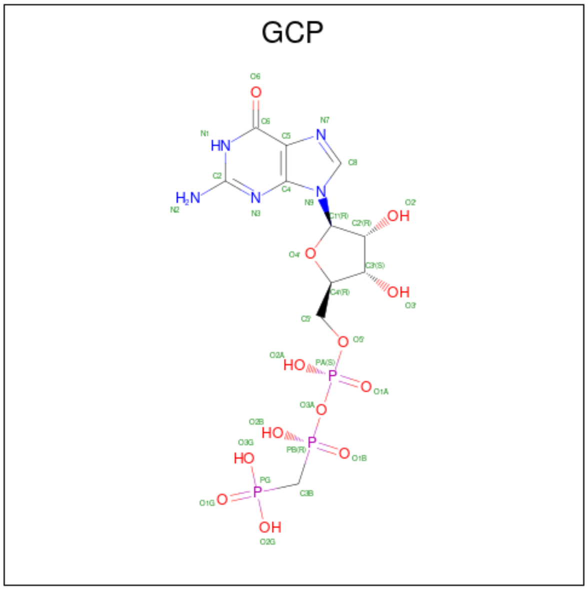
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
49	a	1	1	1	0
			Total	Zn	
49	b	1	1	1	0
			Total	Zn	
49	f	1	1	1	0
			Total	Zn	
49	l	1	1	1	0
			Total	Zn	
49	m	1	1	1	0

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
50	k	1	8	5	1	1	1	0

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



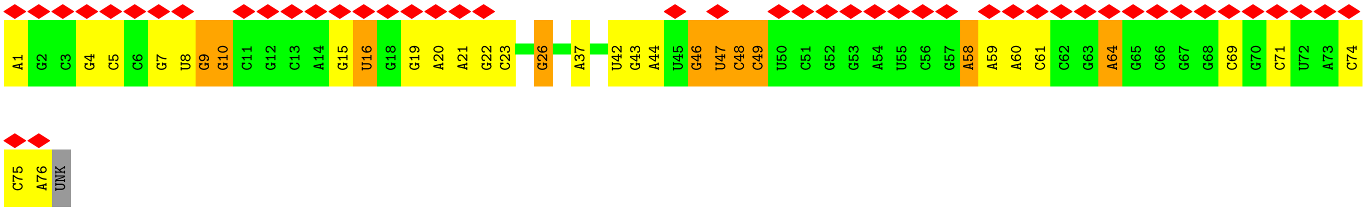
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	k	1	32	11	5	13	3	0

3 Residue-property plots ⓘ

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.

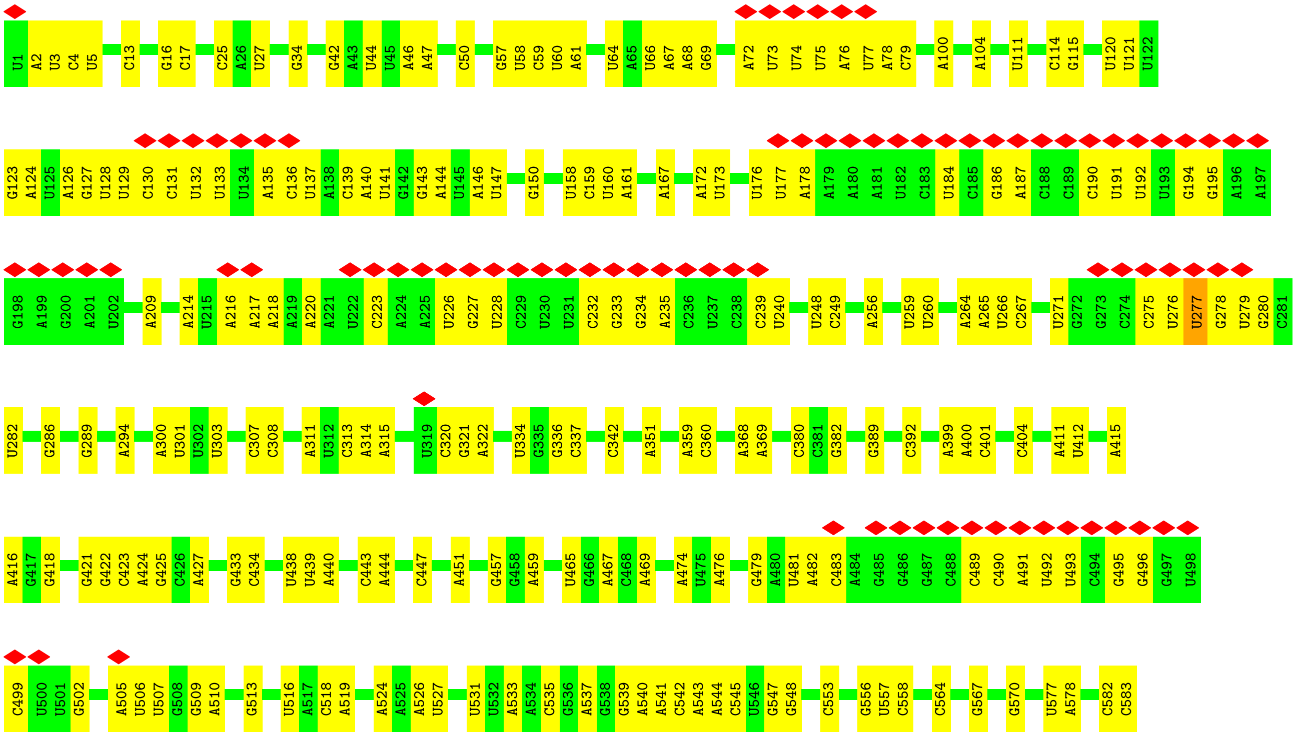
- Molecule 1: tRNAi

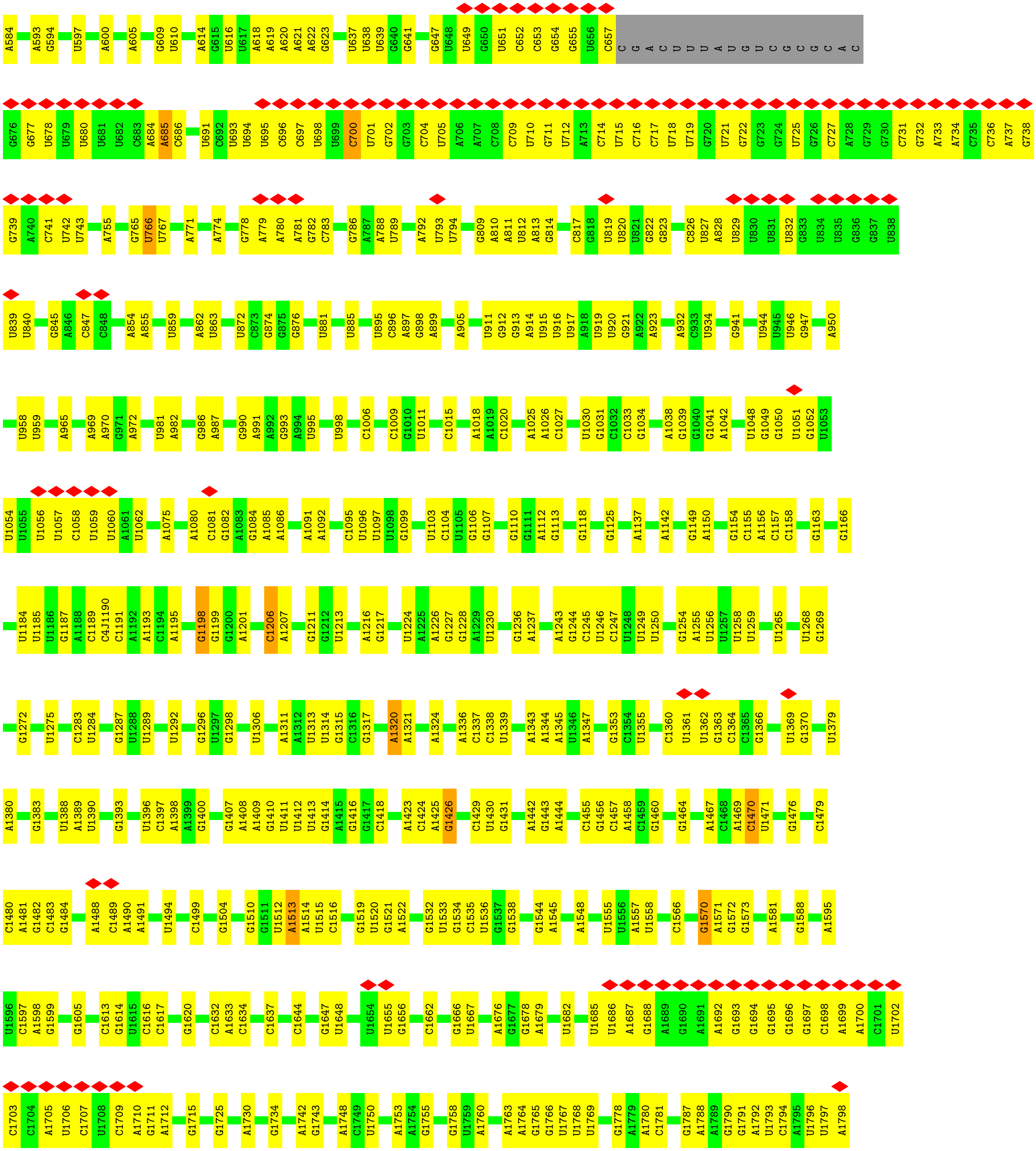
Chain 1:



- Molecule 2: 18S ribosomal RNA

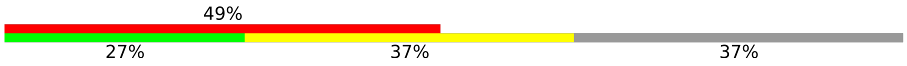
Chain 2:

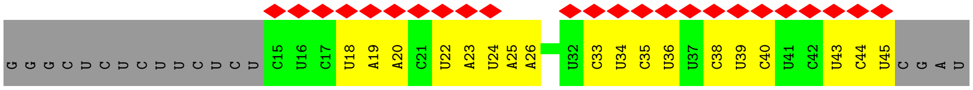




- Molecule 3: mRNA (31-MER)

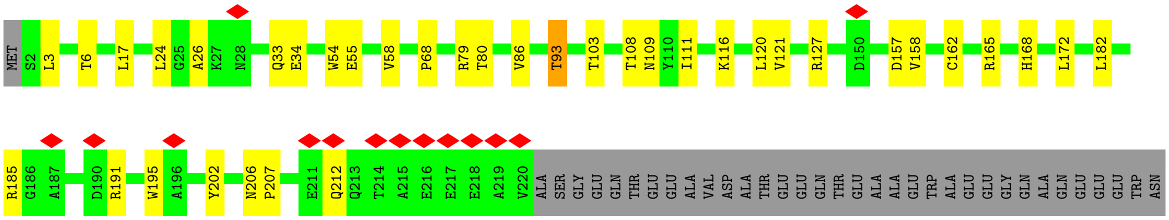
Chain 3:





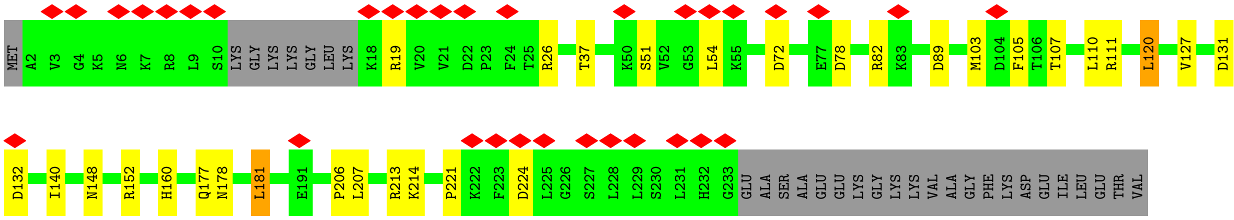
- Molecule 4: 40S ribosomal protein S0

Chain A:



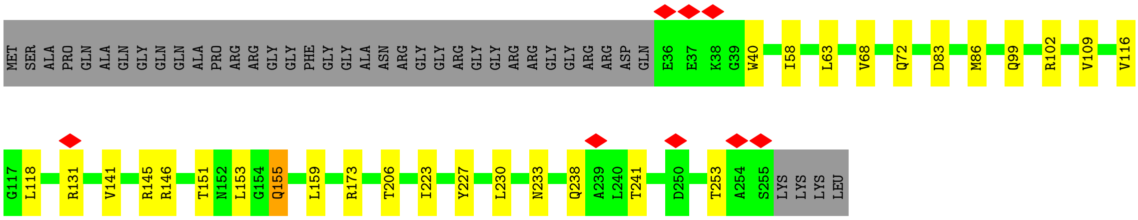
- Molecule 5: 40S ribosomal protein S1

Chain B:



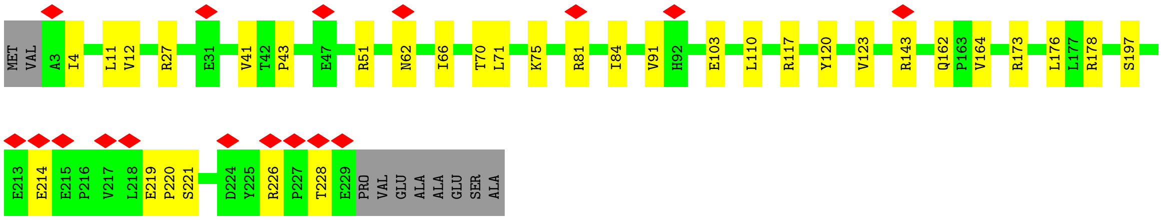
- Molecule 6: KLLA0F09812p

Chain C:

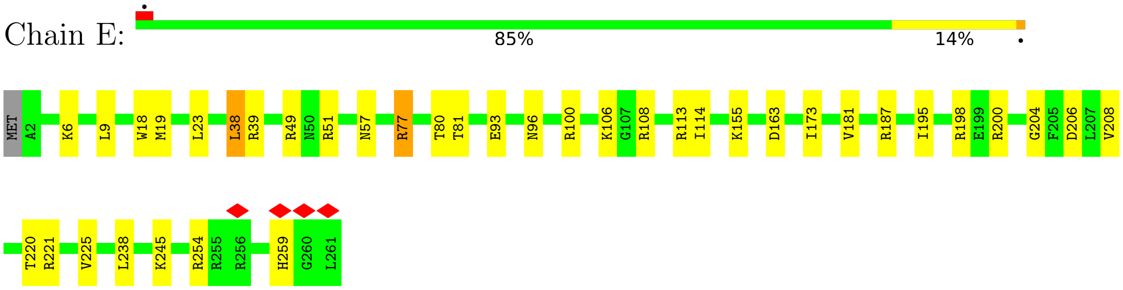


- Molecule 7: KLLA0D08305p

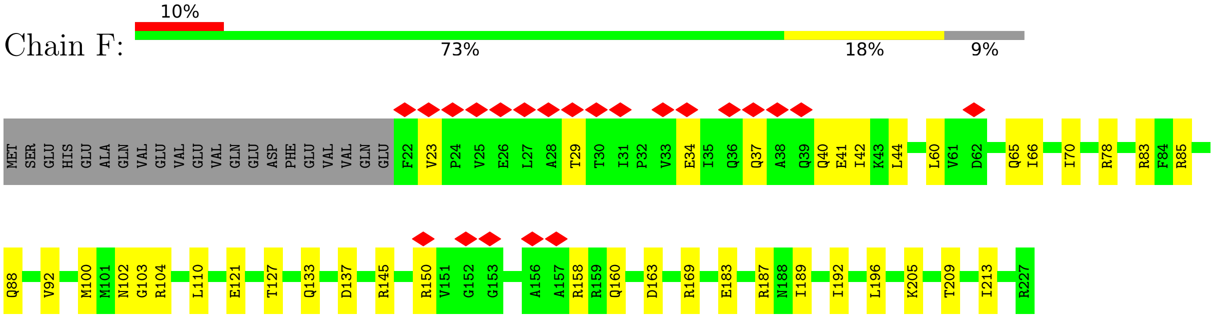
Chain D:



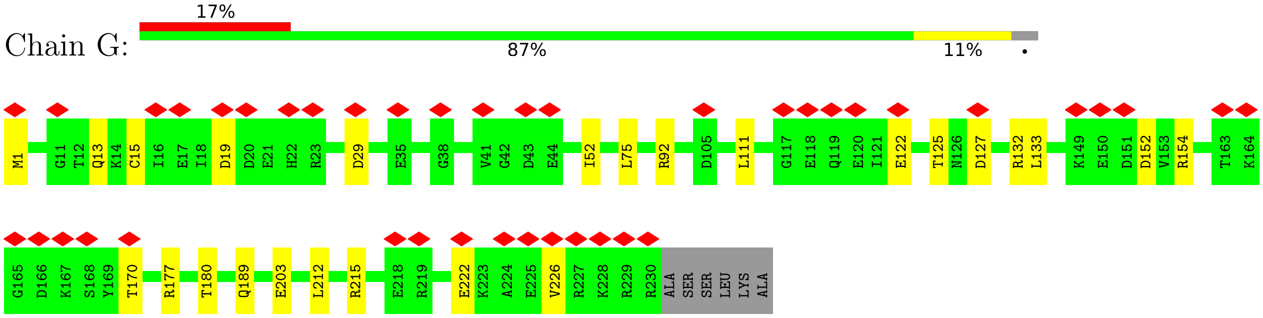
- Molecule 8: 40S ribosomal protein S4



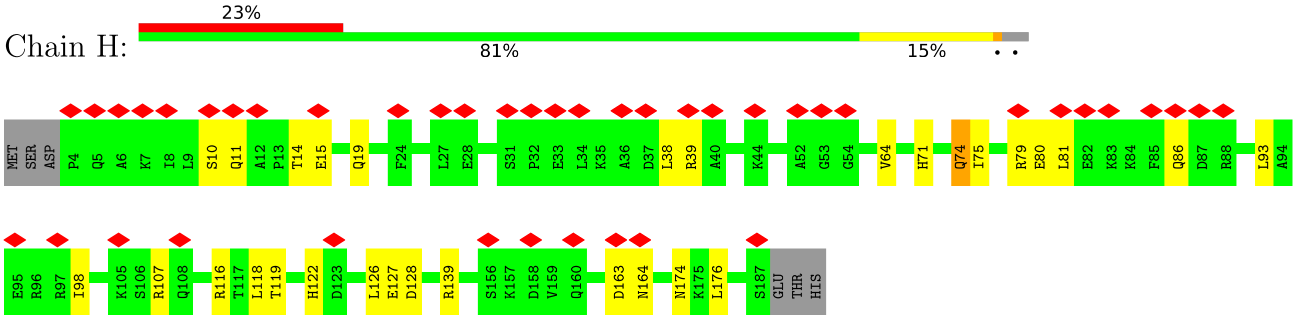
- Molecule 9: KLLA0D10659p



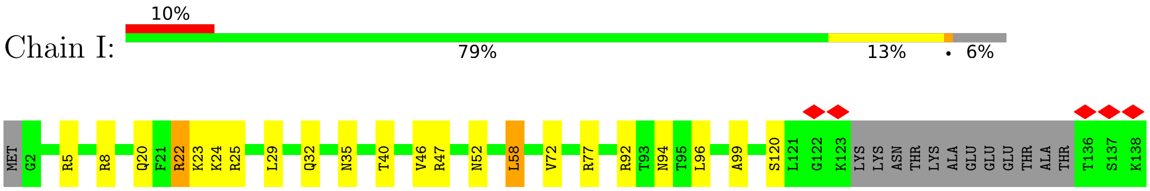
- Molecule 10: 40S ribosomal protein S6

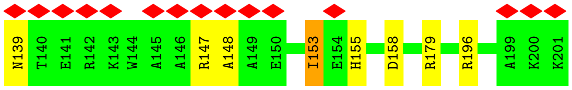


- Molecule 11: 40S ribosomal protein S7



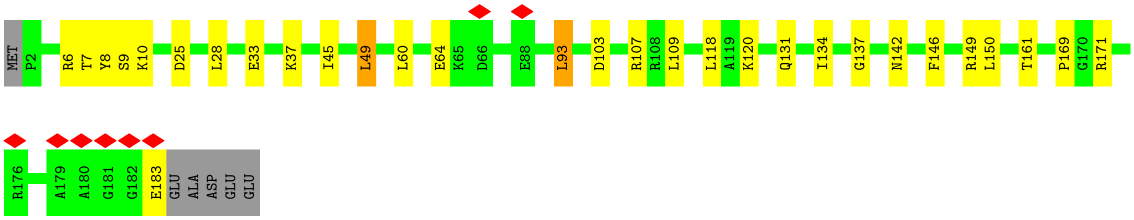
- Molecule 12: 40S ribosomal protein S8





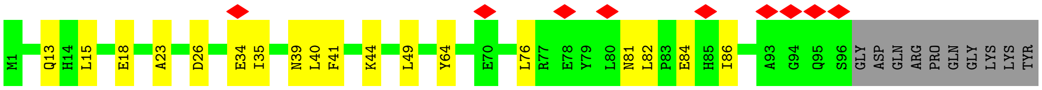
- Molecule 13: KLLA0E23673p

Chain J:



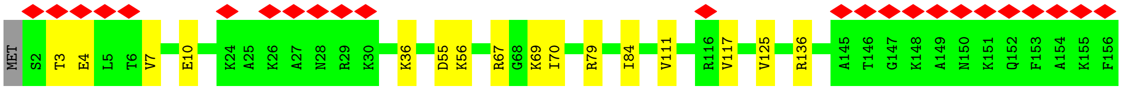
- Molecule 14: KLLA0B08173p

Chain K:



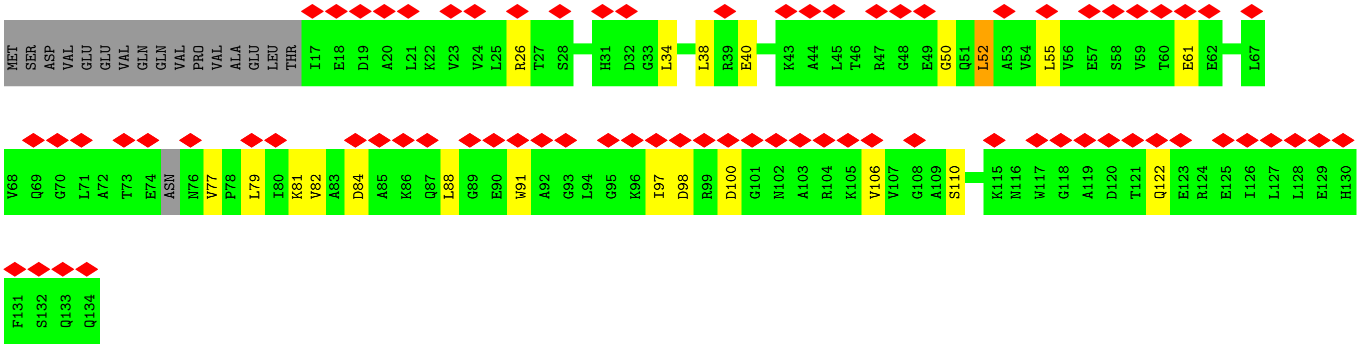
- Molecule 15: KLLA0A10483p

Chain L:



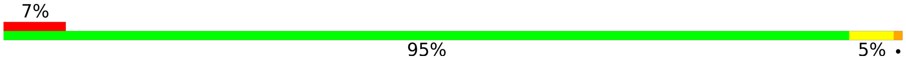
- Molecule 16: 40S ribosomal protein S12

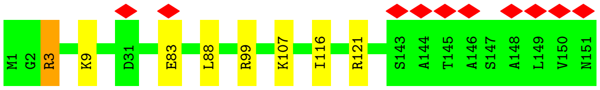
Chain M:



- Molecule 17: KLLA0F18040p

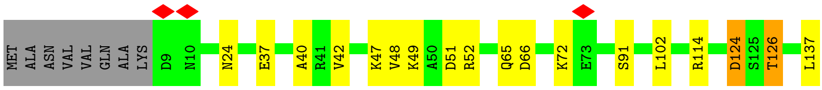
Chain N:





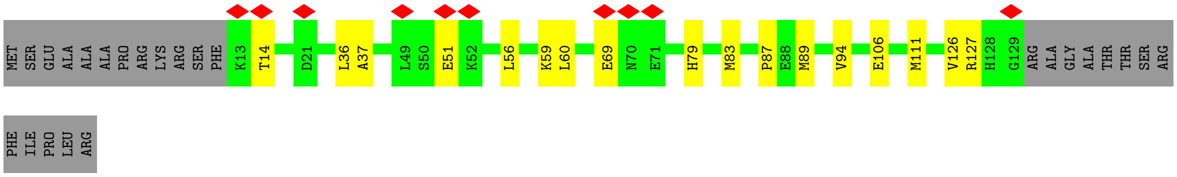
- Molecule 18: 40S ribosomal protein S14

Chain O:



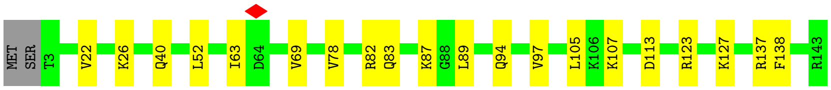
- Molecule 19: KLLA0F07843p

Chain P:



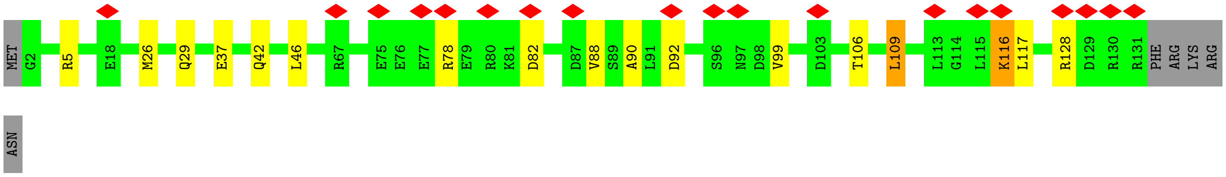
- Molecule 20: 40S ribosomal protein S16

Chain Q:



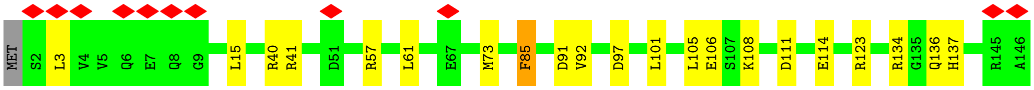
- Molecule 21: KLLA0B01474p

Chain R:



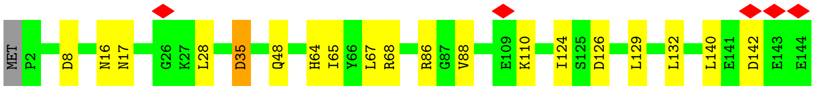
- Molecule 22: KLLA0B01562p

Chain S:



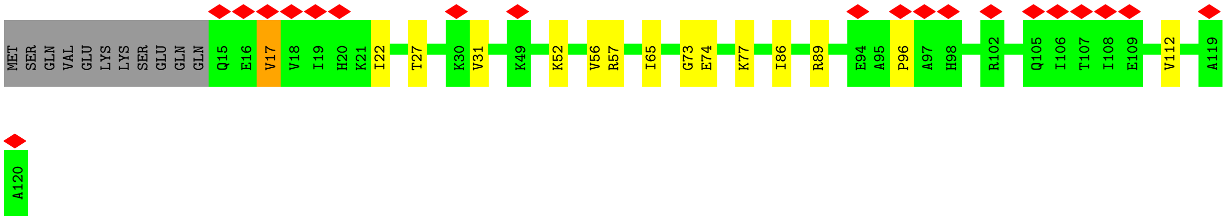
- Molecule 23: KLLA0A07194p

Chain T:



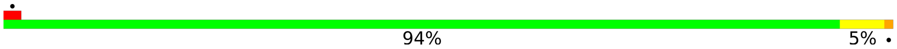
- Molecule 24: KLLA0F25542p

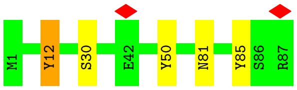
Chain U:



- Molecule 25: 40S ribosomal protein S21

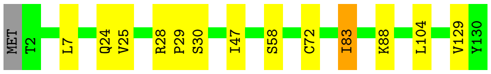
Chain V:





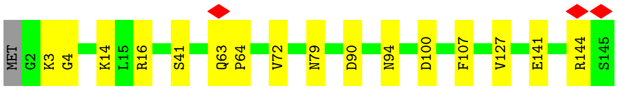
- Molecule 26: 40S ribosomal protein S22

Chain W:



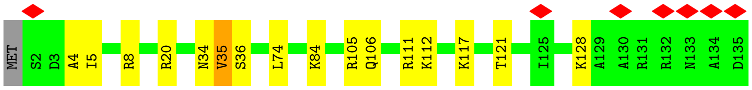
- Molecule 27: KLLA0B11231p

Chain X:



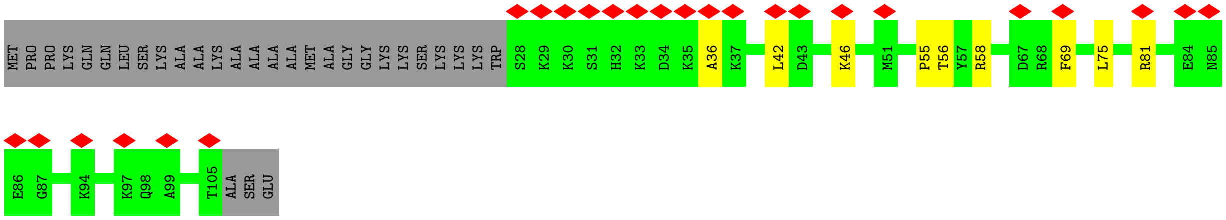
- Molecule 28: 40S ribosomal protein S24

Chain Y:



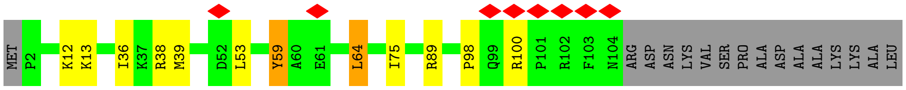
- Molecule 29: KLLA0B06182p

Chain Z:



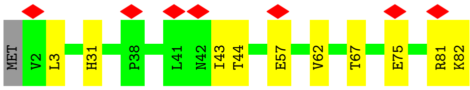
- Molecule 30: 40S ribosomal protein S26

Chain a:



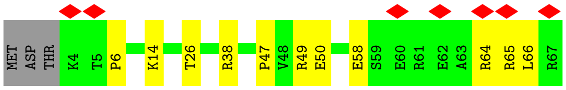
- Molecule 31: 40S ribosomal protein S27

Chain b:



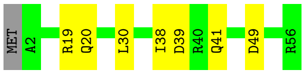
- Molecule 32: 40S ribosomal protein S28

Chain c:



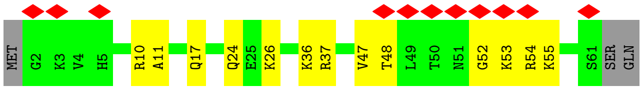
- Molecule 33: 40S ribosomal protein S29

Chain d:



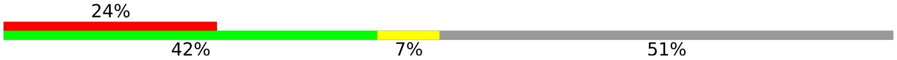
- Molecule 34: 40S ribosomal protein S30

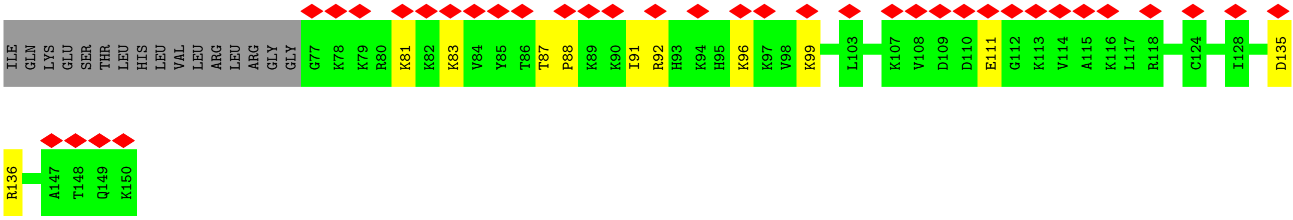
Chain e:



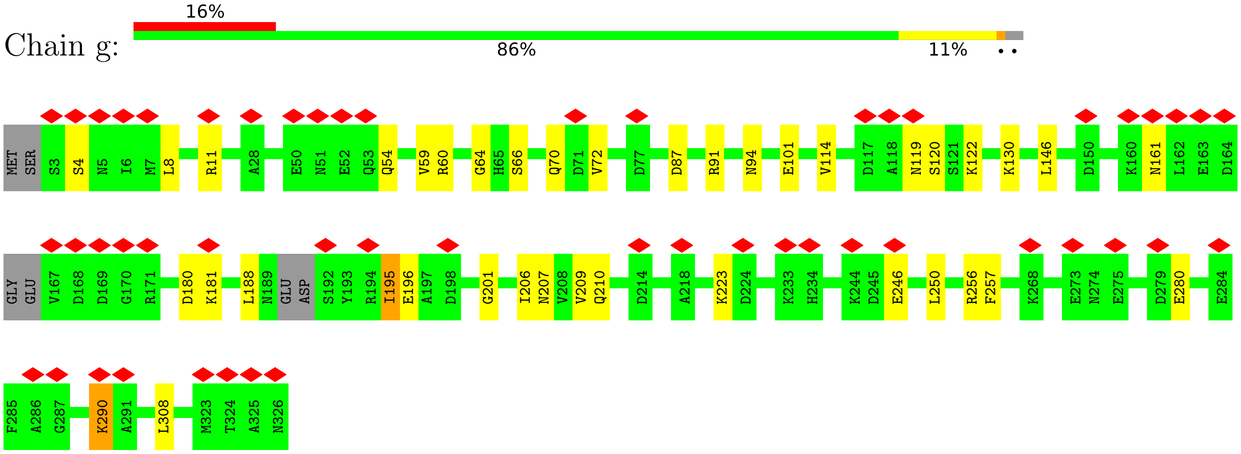
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

Chain f:

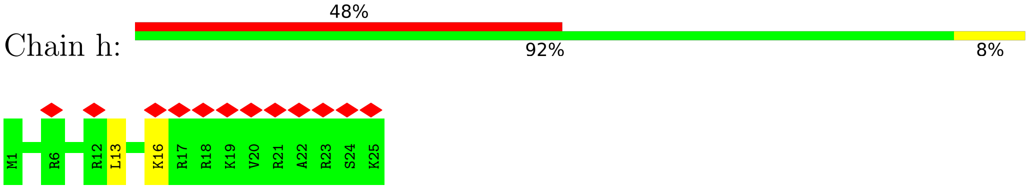




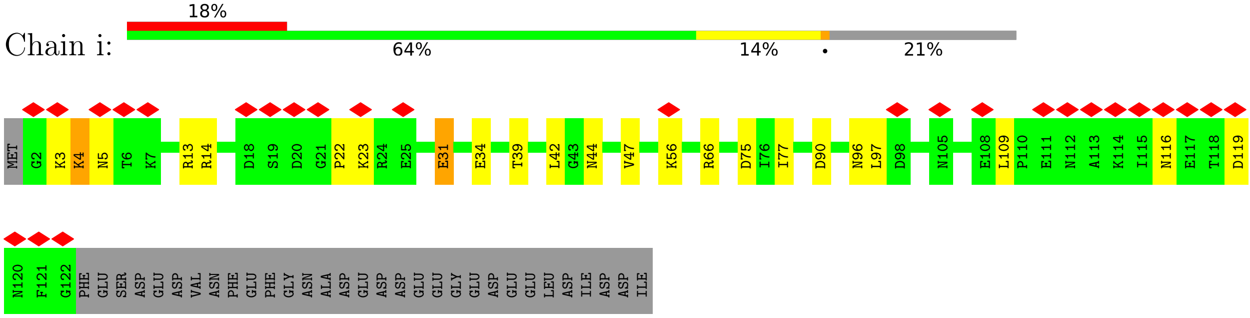
- Molecule 36: KLLA0E12277p



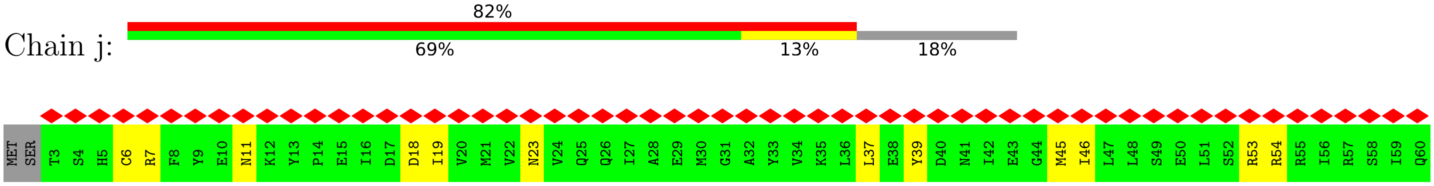
- Molecule 37: 60S ribosomal protein L41-A

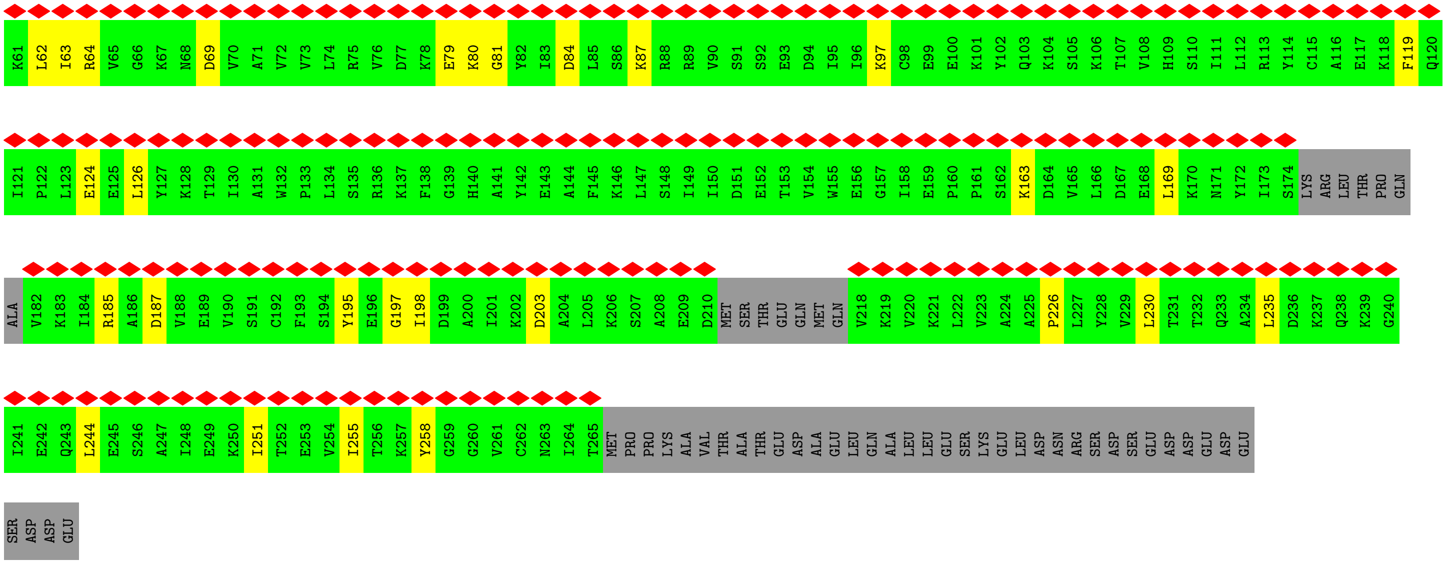


- Molecule 38: Eukaryotic translation initiation factor 1A

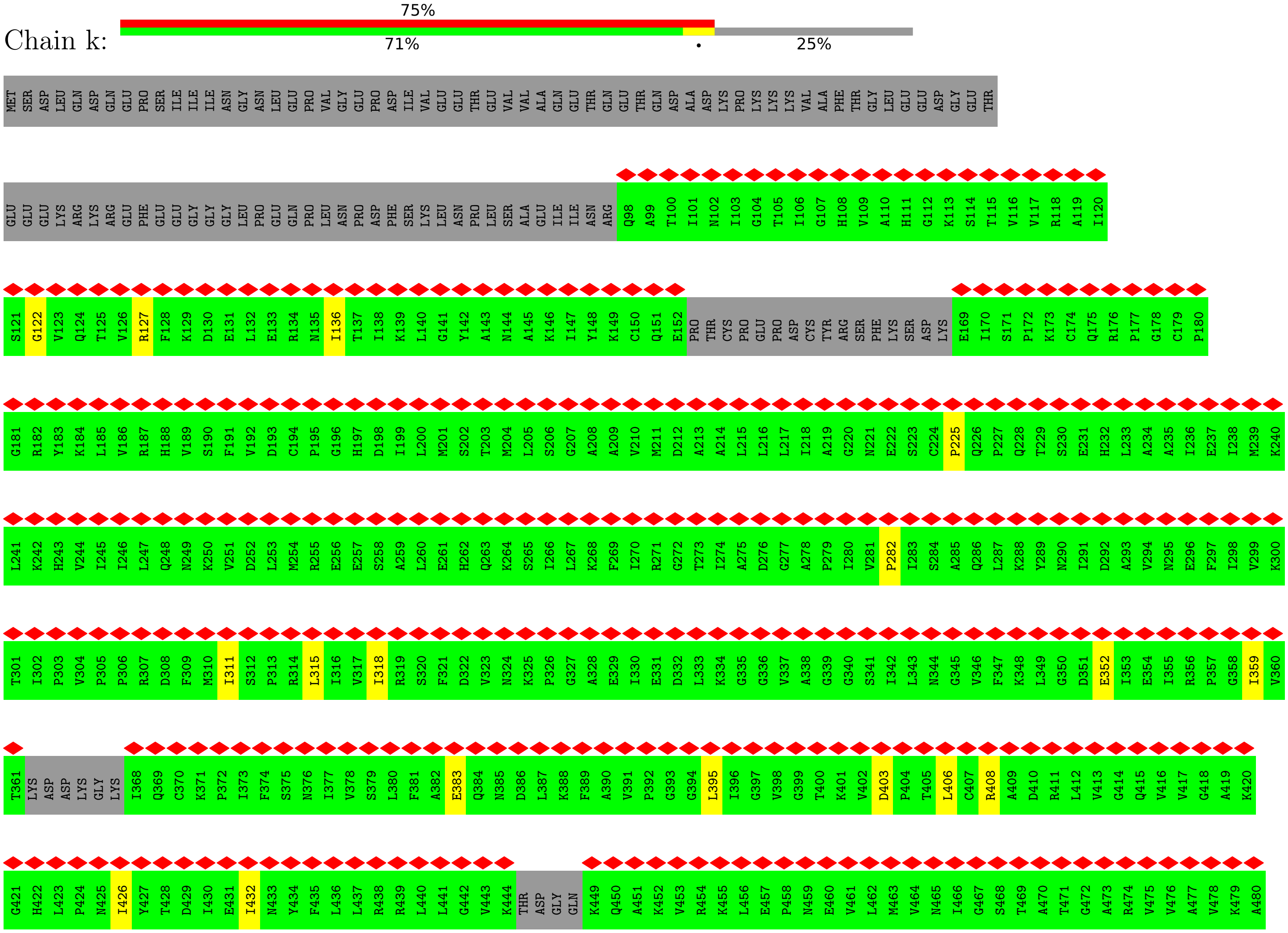


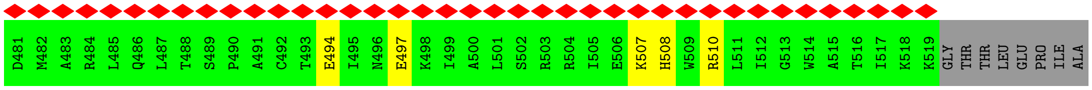
- Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha





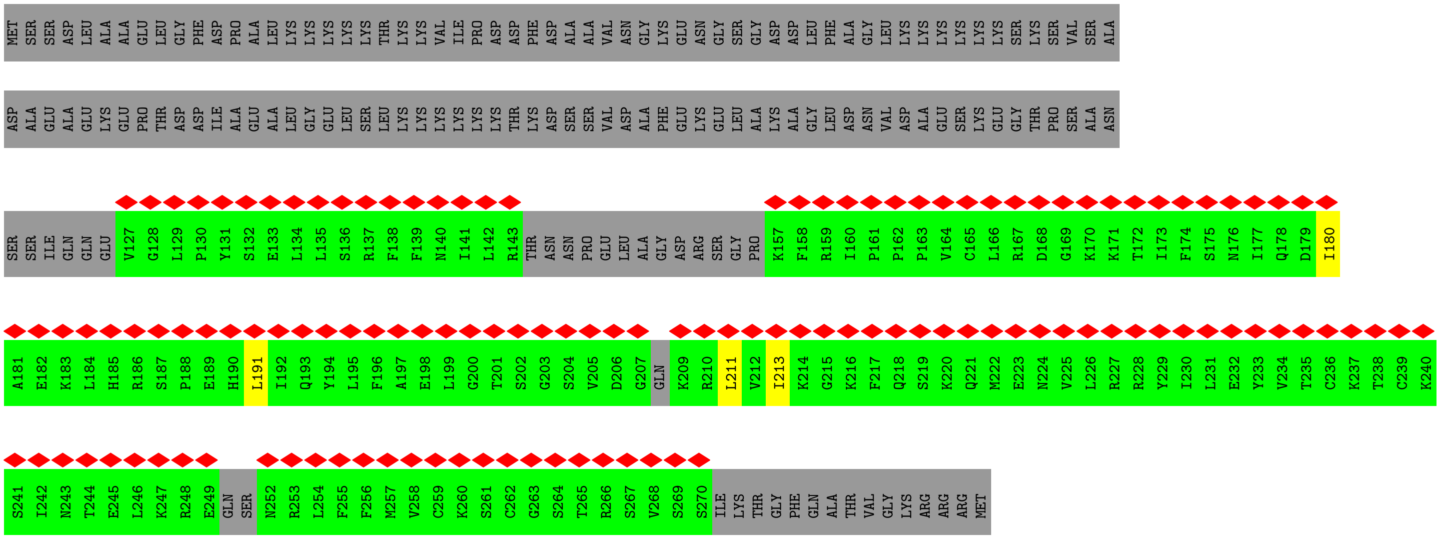
- Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma





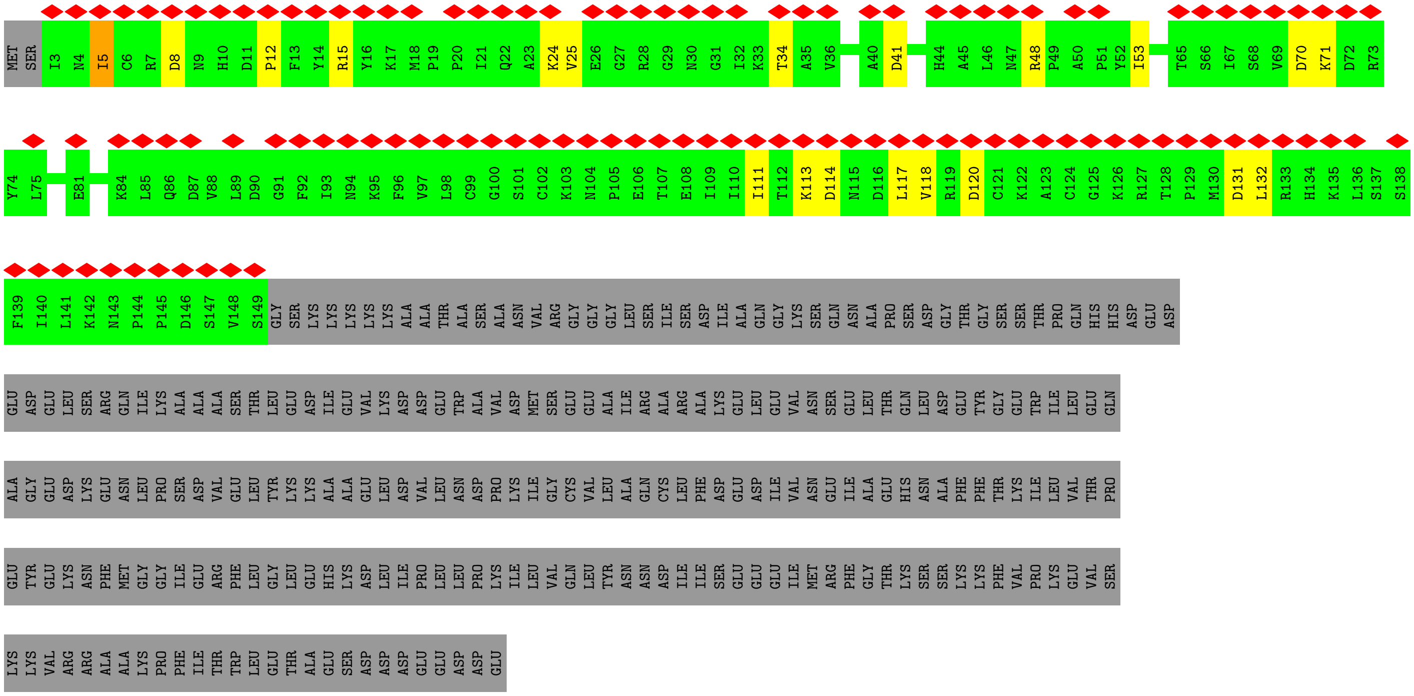
- Molecule 41: Eukaryotic translation initiation factor 2 subunit beta

Chain l:



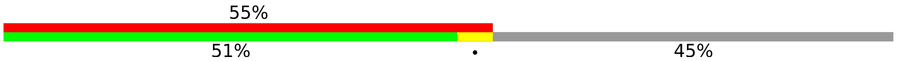
- Molecule 42: Eukaryotic translation initiation factor 5

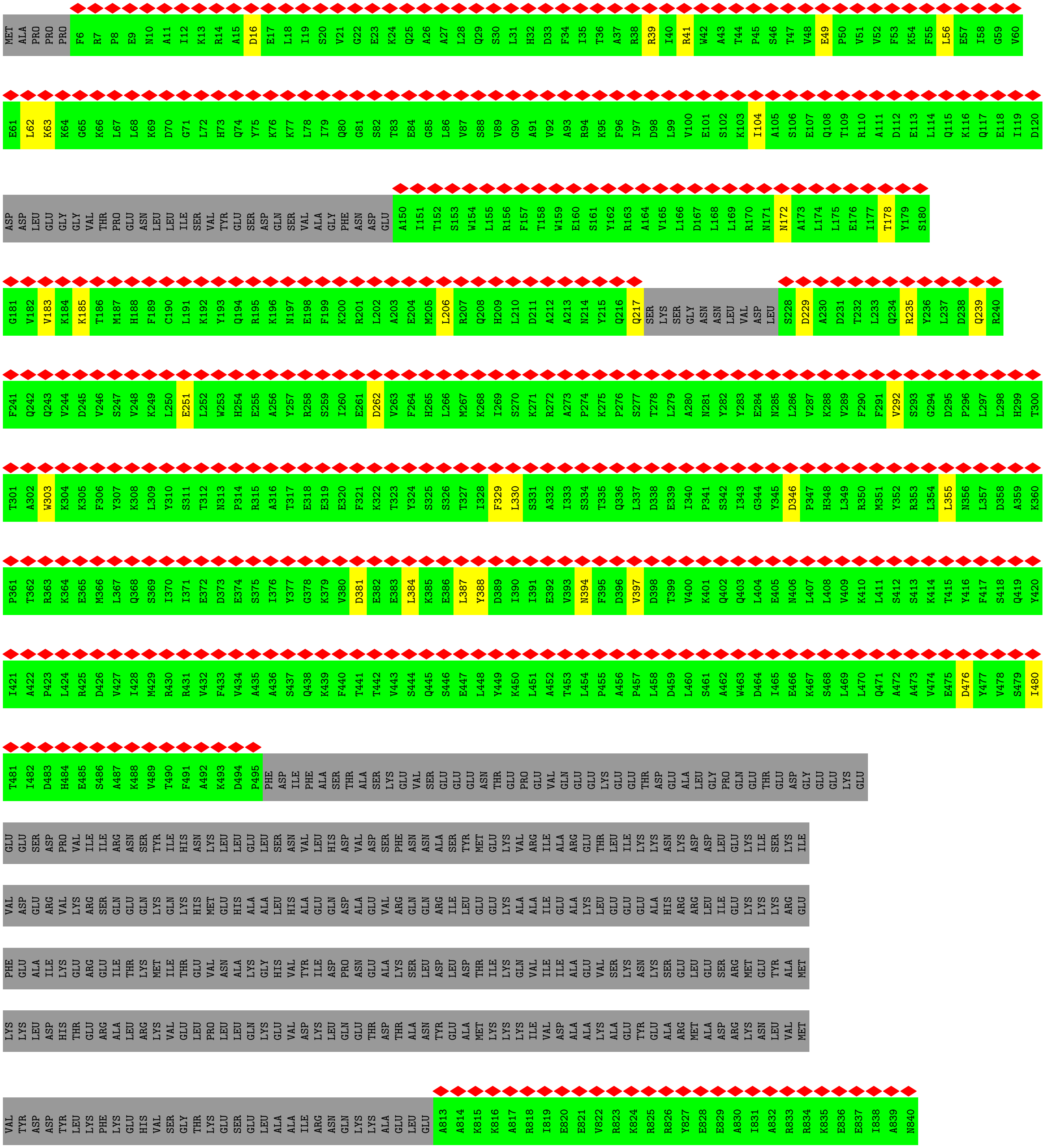
Chain m:

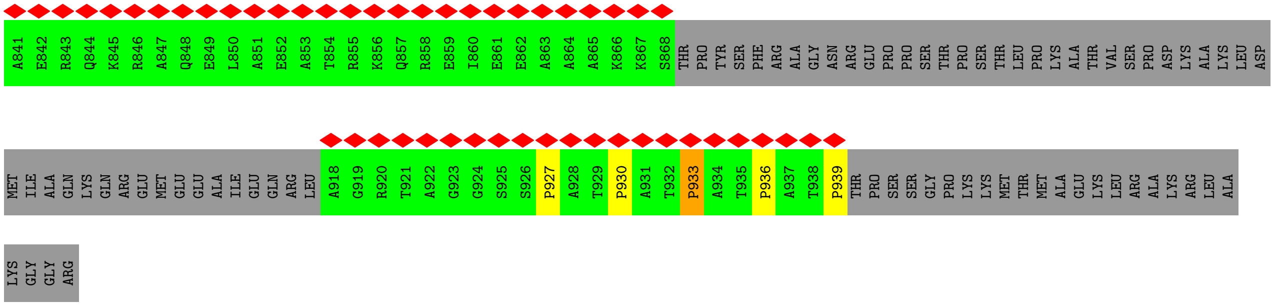


- Molecule 43: Eukaryotic translation initiation factor 3 subunit A

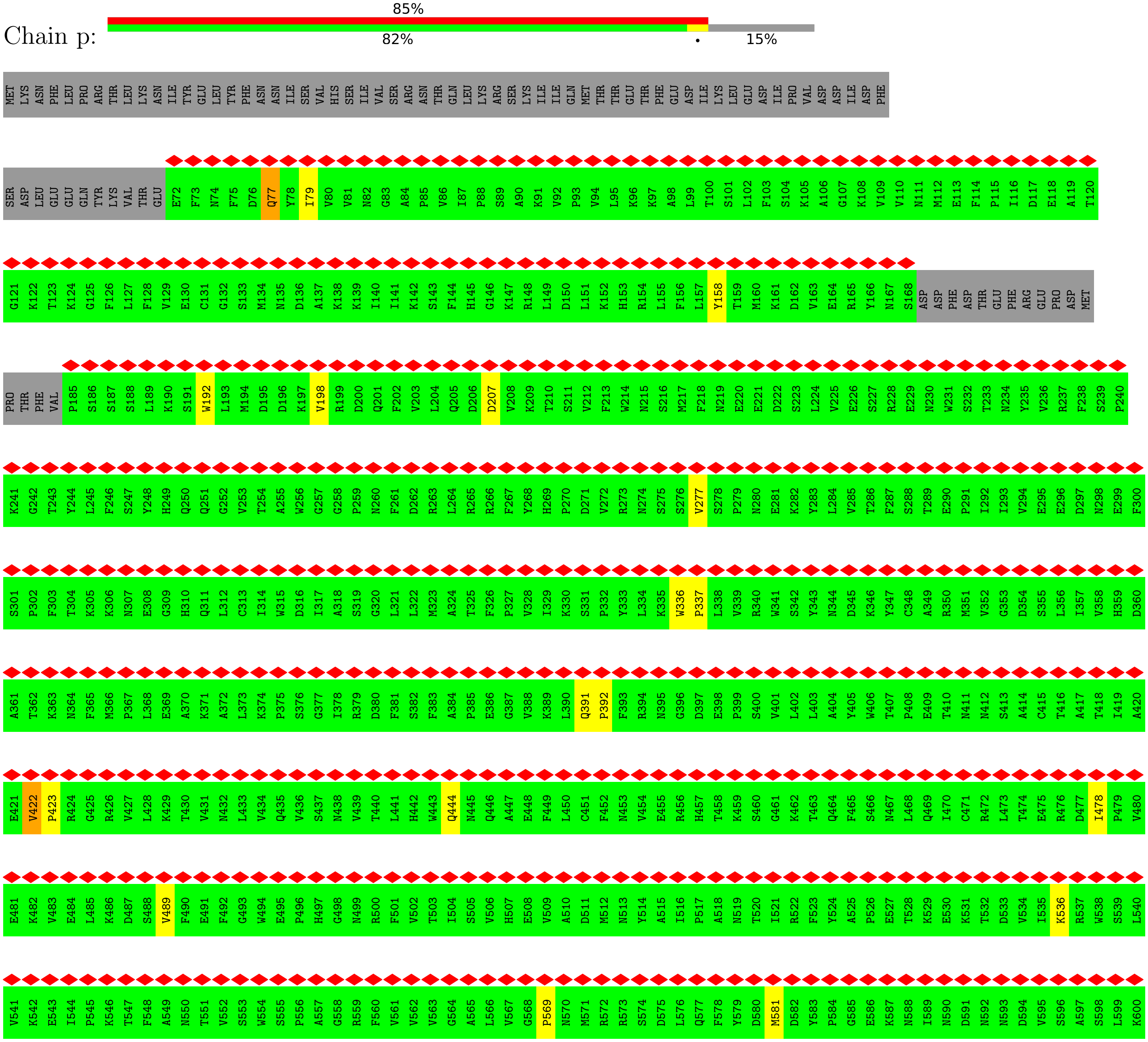
Chain o:

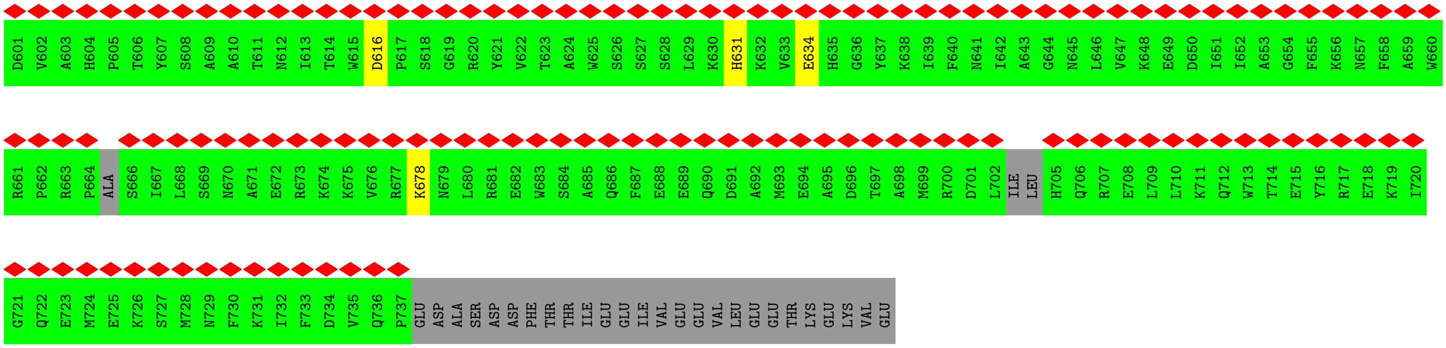

55%
51%
•
45%


MET ALA PRO PRO PRO F6 R7 P8 E9 N10 A11 I12 K13 R14 A15 D16 E17 L18 I19 S20 V21 G22 E23 K24 Q25 A26 A27 L28 Q29 S30 L31 H32 D33 F34 I35 T36 A37 R38 R39 I40 R41 W42 A43 T44 P45 S46 T47 V48 E49 P50 V51 V52 F53 K54 F55 L56 E57 I58 G59 V60
E61 L62 K63 K64 G65 K66 L67 L68 K69 D70 G71 L72 H73 Q74 Y75 K76 K77 L78 I79 Q80 G81 S82 T83 E84 G85 L86 V87 S88 V89 G90 A91 V92 A93 R94 K95 F96 I97 D98 L99 V100 E101 S102 K103 I104 A105 S106 E107 Q108 T109 R110 A111 D112 E113 L114 Q115 K116 Q117 E118 I119 D120
ASP ASP LEU GLU GLY GLY VAL THR PRO GLU ASN LEU LEU ILE SER VAL TYR GLU SER ASP GLN SER VAL ALA GLY PHE ASN ASP GLU A150 I151 T152 S153 W154 L155 R156 F157 T158 W159 E160 S161 Y162 R163 A164 V165 L166 D167 L168 L169 R170 N171 N172 A173 L174 L175 E176 I177 T178 Y179 S180
G181 V182 V183 K184 K185 T186 M187 H188 F189 C190 L191 K192 Y193 Q194 R195 K196 N197 E198 F199 K200 R201 L202 A203 E204 M205 L206 R207 Q208 H209 L210 D211 A212 A213 N214 Y215 Q216 Q217 SER LYS SER GLY ASN ASN LEU VAL ASP LEU S228 D229 A230 D231 T232 L233 Q234 R235 Y236 L237 D238 Q239 R240
F241 Q242 Q243 V244 D245 V246 S247 V248 K249 L250 E251 L252 W253 H254 E255 A256 Y257 R258 S259 I260 E261 D262 V263 F264 H265 L266 M267 K268 I269 S270 K271 R272 A273 P274 K275 P276 S277 T278 L279 A280 N281 Y282 Y283 E284 N285 L286 V287 K288 V289 F290 F291 V292 S293 G294 D295 P296 L297 L298 H299 T300
T301 A302 W303 K304 K305 F306 Y307 K308 L309 Y310 S311 T312 N313 P314 R315 A316 T317 E318 E319 E320 F321 K322 T323 Y324 S325 S326 T327 I328 F329 L330 S331 A332 I333 S334 T335 Q336 L337 D338 E339 I340 P341 S342 I343 G344 Y345 D346 P347 H348 L349 R350 M351 Y352 R353 L354 L355 N356 L357 D358 A359 K360
P361 T362 R363 K364 E365 M366 L367 Q368 S369 I370 I371 E372 D373 E374 S375 I376 Y377 G378 K379 V380 D381 E382 E383 L384 K385 E386 L387 Y388 D389 I390 I391 E392 V393 N394 F395 D396 V397 D398 T399 V400 K401 Q402 Q403 L404 E405 N406 L407 L408 V409 K410 L411 S412 S413 K414 T415 Y416 F417 S418 Q419 Y420
I421 A422 P423 L424 R425 D426 V427 I428 M429 R430 R431 V432 F433 V434 A435 A436 S437 Q438 K439 F440 T441 T442 V443 S444 Q445 S446 E447 L448 Y449 K450 L451 A452 T453 L454 P455 A456 P457 L458 D459 L460 S461 A462 W463 D464 I465 E466 K467 S468 L469 L470 Q471 A472 A473 V474 E475 D476 Y477 V478 S479 I480
T481 I482 D483 H484 E485 S486 A487 K488 V489 T490 F491 A492 K493 D494 P495 PHE ASP ILE PHE ALA SER THR ALA SER LYS GLU VAL SER GLU GLU ASN THR GLU PRO GLU VAL GLN GLU LYS GLU GLU THR ASP GLU ALA LEU GLY PRO GLN GLU THR GLU ASP GLY GLU GLU LYS GLU
GLU GLU SER ASP PRO VAL ILE ILE ARG ASN SER TYR ILE HIS ASN LYS LEU LEU GLU LEU SER ASN VAL LEU HIS ASP VAL ASP SER PHE ASN ASN ALA SER TYR MET GLU LYS VAL ARG ILE ALA ARG GLU THR LEU ILE LYS LYS ASN LYS ASP ASP LEU GLU LYS ILE SER LYS ILE
VAL ASP GLU ARG VAL LYS ARG SER GLN GLU GLN LYS GLN LYS HIS MET GLU HIS ALA ALA LEU HIS ALA GLU GLN ASP ALA GLU VAL ARG GLN GLN ARG ILE LEU GLU GLU LYS ALA ALA ILE GLU ALA LYS LEU GLU GLU GLU ALA HIS ARG LEU ILE GLU LYS LYS LYS ARG GLU
PHE GLU ALA ILE LYS GLU ARG GLU ILE THR LYS MET ILE THR GLU VAL ASN ALA LYS GLY HIS VAL TYR ILE ASP PRO ASN GLU ALA LYS SER LEU ASP LEU ASP THR ILE LYS GLN VAL ILE ILE ALA GLU VAL SER LYS ASN LYS SER GLU LEU GLU SER ARG MET GLU TYR ALA MET
LYS LYS LEU ASP HIS THR GLU ARG ALA LEU ARG LYS VAL GLU LEU PRO LEU LEU GLN LYS GLU VAL ASP LYS LEU GLN GLU THR ASP THR ALA ASN TYR GLU ALA MET LYS LYS ILE VAL ASP ALA ALA LYS ALA GLU TYR GLU ALA ARG MET ALA ASP ARG LYS ASN LEU VAL MET
VAL TYR ASP ASP TYR LEU LYS PHE LYS GLU HIS VAL SER GLY THR LYS GLU SER GLU LEU ALA ALA ILE ARG ASN GLN LYS LYS ALA GLU LEU GLU A813 A814 K815 K816 A817 R818 I819 E820 E821 V822 R823 K824 R825 R826 Y827 E828 E829 A830 I831 A832 R833 R834 K835 E836 E837 I838 A839 N840



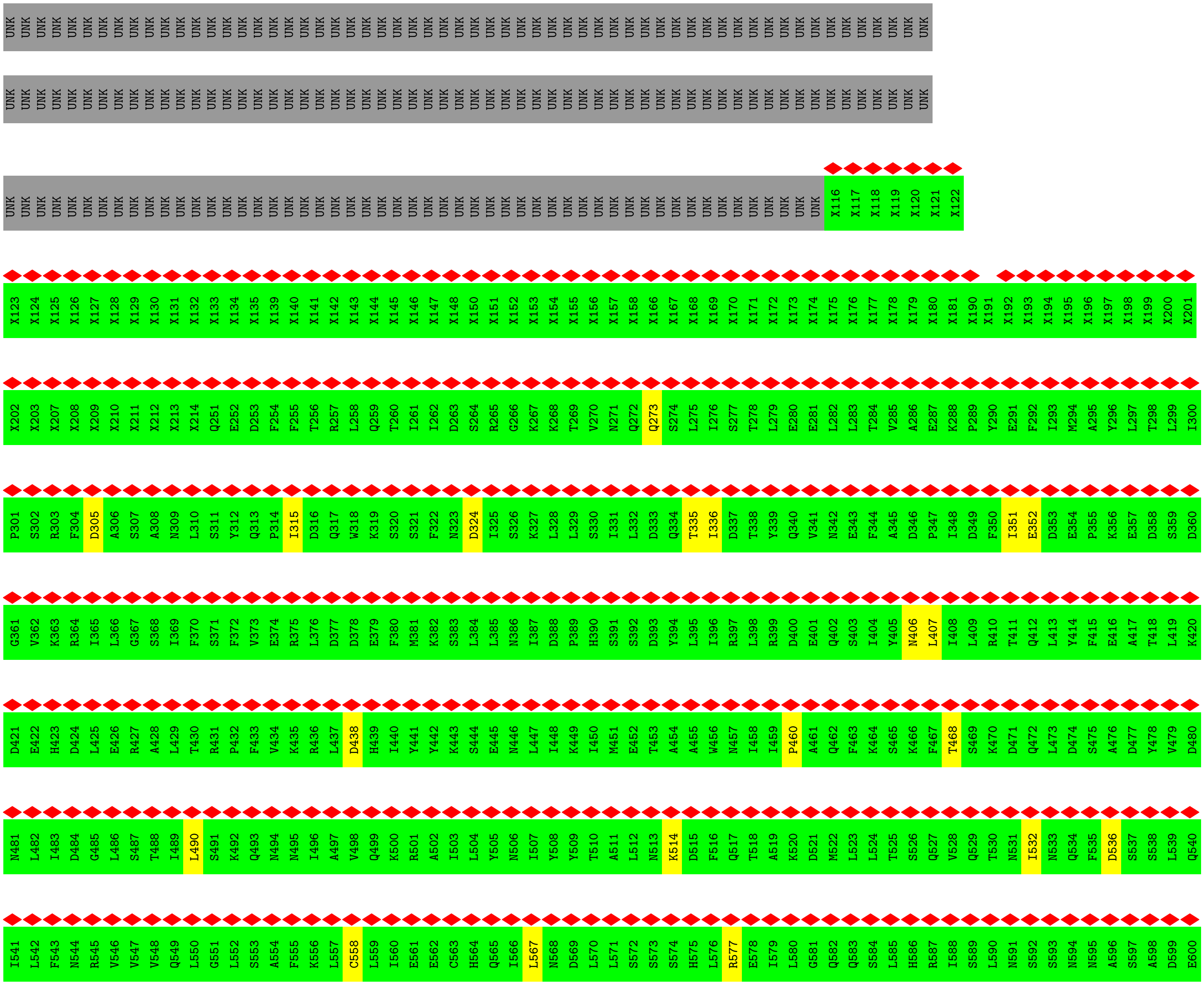
- Molecule 44: Eukaryotic translation initiation factor 3 subunit B

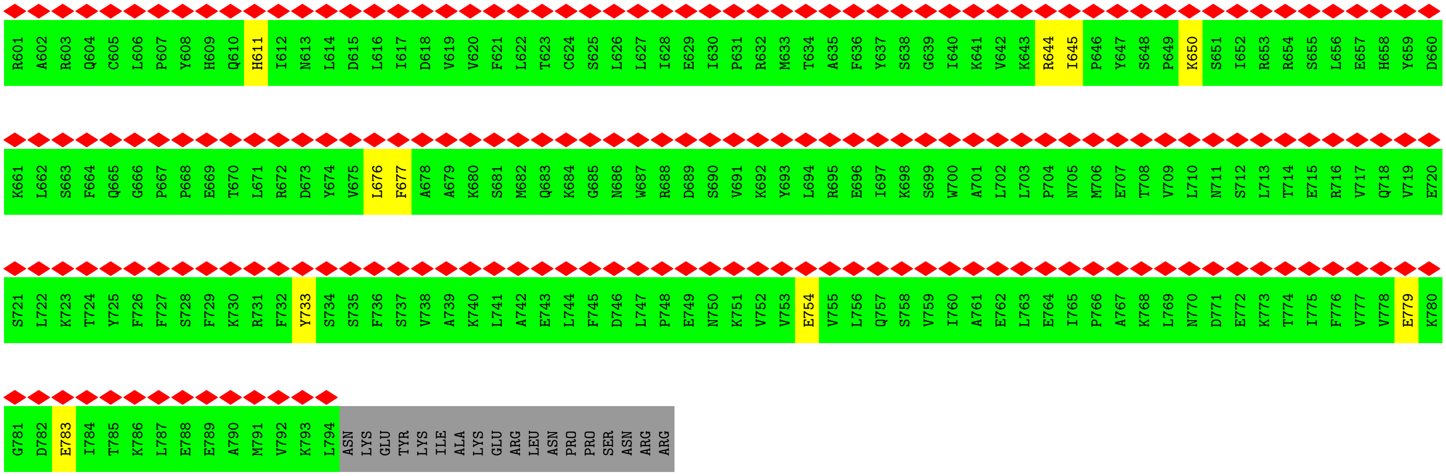




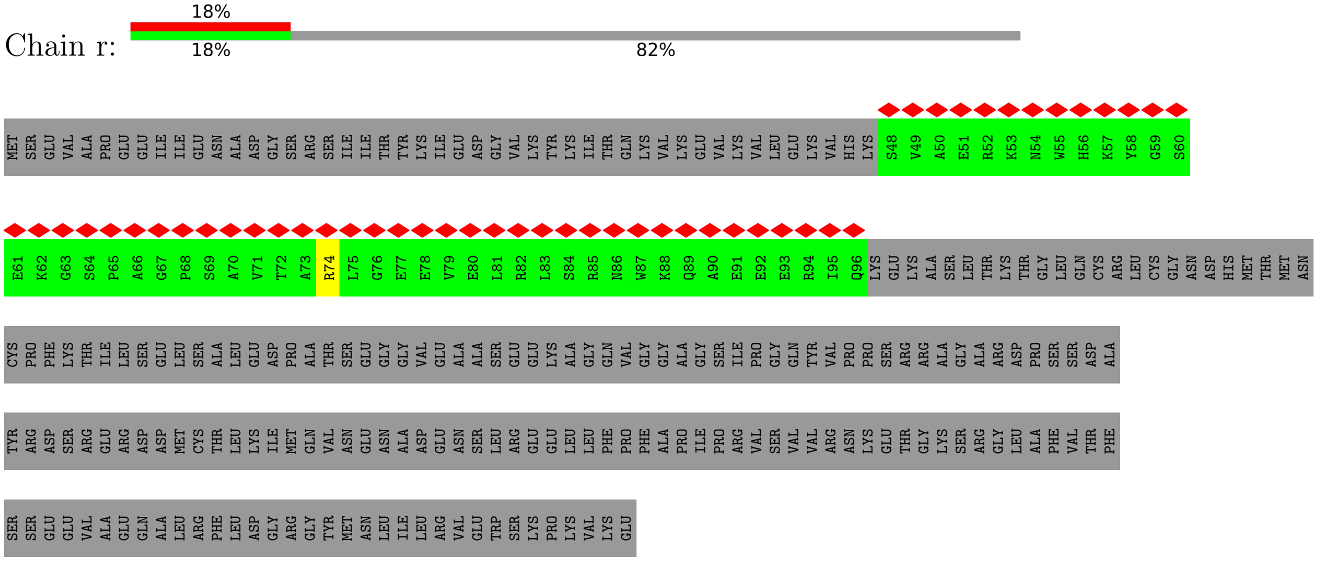
- Molecule 45: eIF3c,Eukaryotic translation initiation factor 3 subunit C

Chain q:

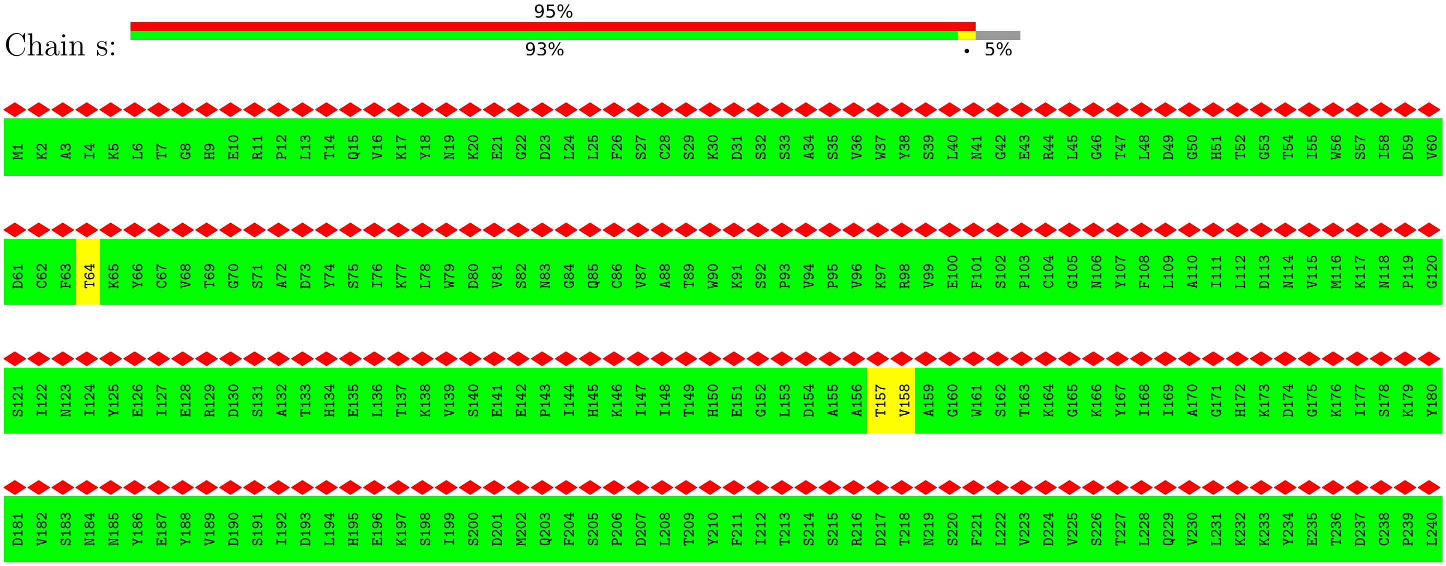


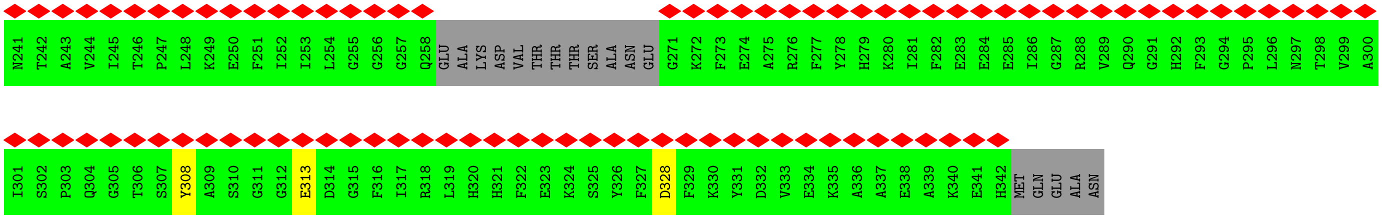


- Molecule 46: Eukaryotic translation initiation factor 3 subunit G



- Molecule 47: Eukaryotic translation initiation factor 3 subunit I




N241
T242
A243
V244
I245
T246
P247
L248
K249
E250
F251
I252
I253
L254
G255
G256
G257
Q258
GLU
ALA
LYS
ASP
VAL
THR
THR
THR
SER
ALA
ASN
GLU
G271
K272
F273
E274
A275
R276
F277
Y278
H279
K280
I281
F282
E283
E284
E285
I286
G287
R288
V289
Q290
G291
H292
F293
G294
P295
L296
N297
T298
V299
A300
I301
S302
P303
Q304
G305
T306
S307
Y308
A309
S310
G311
G312
E313
D314
G315
F316
I317
R318
L319
H320
H321
F322
E323
K324
S325
Y326
F327
D328
F329
K330
Y331
D332
V333
E334
K335
A336
A337
E338
A339
K340
E341
H342
MET
GLN
GLU
ALA
ASN

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.157	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, RIA, GCP, AYA, 1MA, 1MG, ZN, C4J, MA6, T6A, PSU, MG, H2U, M2G, 7MG, 5MC

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	1	0.36	1/1529 (0.1%)	0.71	0/2376
2	2	0.29	0/41987	0.70	9/65416 (0.0%)
3	3	0.39	0/797	0.81	2/1233 (0.2%)
4	A	0.40	0/1742	0.72	1/2383 (0.0%)
5	B	0.37	0/1813	0.73	2/2438 (0.1%)
6	C	0.39	0/1678	0.71	0/2277
7	D	0.40	0/1800	0.73	0/2421
8	E	0.38	0/2122	0.71	1/2861 (0.0%)
9	F	0.39	0/1628	0.75	0/2198
10	G	0.38	0/1855	0.70	0/2479
11	H	0.40	0/1507	0.73	1/2028 (0.0%)
12	I	0.38	0/1515	0.72	0/2029
13	J	0.40	0/1495	0.78	1/2001 (0.0%)
14	K	0.46	0/831	0.76	1/1123 (0.1%)
15	L	0.40	0/1276	0.64	0/1718
16	M	0.42	0/891	0.75	1/1201 (0.1%)
17	N	0.40	0/1218	0.72	0/1638
18	O	0.39	0/966	0.74	0/1297
19	P	0.38	0/942	0.67	0/1269
20	Q	0.39	0/1125	0.73	0/1510
21	R	0.42	0/1044	0.78	1/1402 (0.1%)
22	S	0.39	0/1208	0.74	0/1624
23	T	0.39	0/1129	0.72	0/1520
24	U	0.38	0/857	0.72	0/1158
25	V	0.37	0/696	0.68	0/938
26	W	0.39	0/1039	0.74	0/1399
27	X	0.41	0/1137	0.71	0/1516
28	Y	0.38	0/1075	0.65	0/1433
29	Z	0.38	0/603	0.68	1/814 (0.1%)
30	a	0.37	0/825	0.68	0/1106
31	b	0.36	0/619	0.63	0/837
32	c	0.35	0/501	0.70	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.38	0/473	0.66	0/629
34	e	0.39	0/480	0.69	0/640
35	f	0.41	0/597	0.61	0/795
36	g	0.37	0/2523	0.65	0/3434
37	h	0.33	0/234	0.70	0/300
38	i	0.38	0/969	0.68	0/1287
39	j	0.42	0/2034	0.63	0/2737
40	k	0.39	0/3079	0.60	0/4157
41	l	0.42	0/1051	0.59	0/1402
42	m	0.40	0/1164	0.64	0/1575
43	o	0.42	0/4140	0.64	6/5608 (0.1%)
44	p	0.43	0/5245	0.59	0/7115
45	q	0.44	0/4523	0.61	0/6114
46	r	0.40	0/399	0.54	0/535
47	s	0.43	0/2669	0.59	0/3611
All	All	0.36	1/109030 (0.0%)	0.69	27/156255 (0.0%)

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	2	1	0
20	Q	0	1
44	p	0	2
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-10.07	1.49	1.61

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	18[A]	U	P-O3'-C3'	8.96	130.45	119.70
3	3	18[B]	U	P-O3'-C3'	8.96	130.45	119.70
2	2	685	A	C2'-C3'-O3'	7.20	125.34	109.50
5	B	181	LEU	CA-CB-CG	6.82	130.97	115.30
2	2	616	U	N1-C1'-C2'	6.17	122.03	114.00
43	o	933	PRO	N-CA-CB	6.06	110.58	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	o	939	PRO	N-CA-CB	6.05	110.56	103.30
2	2	700	C	C2'-C3'-O3'	6.03	123.35	113.70
2	2	1470	C	C2'-C3'-O3'	6.02	123.33	113.70
43	o	930	PRO	N-CA-CB	5.99	110.49	103.30
21	R	109	LEU	CA-CB-CG	5.87	128.79	115.30
43	o	936	PRO	N-CA-CB	5.85	110.32	103.30
2	2	1206	C	C2'-C3'-O3'	5.80	122.98	113.70
16	M	52	LEU	CA-CB-CG	5.70	128.41	115.30
43	o	927	PRO	N-CA-CB	5.63	110.06	103.30
29	Z	42	LEU	CA-CB-CG	5.59	128.15	115.30
4	A	120	LEU	CA-CB-CG	5.47	127.89	115.30
5	B	120	LEU	CA-CB-CG	5.43	127.79	115.30
2	2	1198	G	C2'-C3'-O3'	5.43	122.38	113.70
8	E	38	LEU	CA-CB-CG	5.42	127.78	115.30
14	K	41	PHE	N-CA-CB	5.24	120.04	110.60
2	2	277	U	C2'-C3'-O3'	5.19	122.01	113.70
2	2	1320	A	N9-C1'-C2'	5.15	120.70	114.00
11	H	118	LEU	CA-CB-CG	5.12	127.07	115.30
13	J	49	LEU	CA-CB-CG	5.10	127.02	115.30
2	2	1513	A	C2'-C3'-O3'	5.03	121.75	113.70
43	o	387	LEU	CA-CB-CG	5.02	126.84	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	Q	40	GLN	Peptide
44	p	336	TRP	Peptide
44	p	391	GLN	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	A	217/254 (85%)	192 (88%)	16 (7%)	9 (4%)	3	15
5	B	220/255 (86%)	191 (87%)	19 (9%)	10 (4%)	2	13
6	C	218/259 (84%)	197 (90%)	16 (7%)	5 (2%)	6	29
7	D	225/237 (95%)	211 (94%)	8 (4%)	6 (3%)	5	25
8	E	258/261 (99%)	233 (90%)	21 (8%)	4 (2%)	9	38
9	F	204/227 (90%)	173 (85%)	21 (10%)	10 (5%)	2	12
10	G	228/236 (97%)	211 (92%)	15 (7%)	2 (1%)	17	53
11	H	182/190 (96%)	161 (88%)	14 (8%)	7 (4%)	3	17
12	I	184/201 (92%)	162 (88%)	12 (6%)	10 (5%)	2	10
13	J	180/188 (96%)	152 (84%)	20 (11%)	8 (4%)	2	14
14	K	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	21
15	L	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	5	26
16	M	113/134 (84%)	85 (75%)	20 (18%)	8 (7%)	1	5
17	N	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	59
18	O	127/137 (93%)	107 (84%)	13 (10%)	7 (6%)	2	10
19	P	115/142 (81%)	98 (85%)	11 (10%)	6 (5%)	2	11
20	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	6	30
21	R	128/136 (94%)	110 (86%)	11 (9%)	7 (6%)	2	10
22	S	143/146 (98%)	127 (89%)	13 (9%)	3 (2%)	7	31
23	T	141/144 (98%)	132 (94%)	7 (5%)	2 (1%)	11	41
24	U	104/117 (89%)	90 (86%)	9 (9%)	5 (5%)	2	13
25	V	85/87 (98%)	80 (94%)	2 (2%)	3 (4%)	3	18
26	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	3	16
27	X	142/145 (98%)	126 (89%)	12 (8%)	4 (3%)	5	24
28	Y	132/135 (98%)	123 (93%)	5 (4%)	4 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	76/108 (70%)	62 (82%)	10 (13%)	4 (5%)	2	11
30	a	101/119 (85%)	84 (83%)	11 (11%)	6 (6%)	1	8
31	b	79/82 (96%)	68 (86%)	9 (11%)	2 (2%)	5	26
32	c	62/67 (92%)	55 (89%)	5 (8%)	2 (3%)	4	21
33	d	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
34	e	58/63 (92%)	44 (76%)	9 (16%)	5 (9%)	1	3
35	f	72/150 (48%)	57 (79%)	13 (18%)	2 (3%)	5	24
36	g	314/326 (96%)	276 (88%)	29 (9%)	9 (3%)	4	23
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	119/153 (78%)	102 (86%)	11 (9%)	6 (5%)	2	12
39	j	243/304 (80%)	213 (88%)	25 (10%)	5 (2%)	7	31
40	k	388/527 (74%)	333 (86%)	47 (12%)	8 (2%)	7	31
41	l	120/285 (42%)	109 (91%)	11 (9%)	0	100	100
42	m	145/405 (36%)	126 (87%)	17 (12%)	2 (1%)	11	41
43	o	519/964 (54%)	483 (93%)	30 (6%)	6 (1%)	13	46
44	p	637/763 (84%)	583 (92%)	43 (7%)	11 (2%)	9	37
45	q	538/812 (66%)	490 (91%)	39 (7%)	9 (2%)	9	37
46	r	47/274 (17%)	43 (92%)	4 (8%)	0	100	100
47	s	326/347 (94%)	311 (95%)	15 (5%)	0	100	100
All	All	7928/10147 (78%)	7065 (89%)	650 (8%)	213 (3%)	8	25

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	141	VAL
7	D	220	PRO
9	F	104	ARG
11	H	64	VAL
11	H	74	GLN
12	I	22	ARG
12	I	153	ILE
13	J	169	PRO
16	M	82	VAL
16	M	84	ASP
18	O	91	SER

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Mol	Chain	Res	Type
18	O	124	ASP
19	P	36	LEU
24	U	17	VAL
24	U	96	PRO
25	V	30	SER
26	W	58	SER
27	X	63	GLN
30	a	36	ILE
34	e	54	ARG
38	i	31	GLU
38	i	66	ARG
38	i	116	ASN
44	p	337	PRO
44	p	392	PRO
4	A	206	ASN
5	B	19	ARG
5	B	214	LYS
7	D	221	SER
9	F	44	LEU
9	F	103	GLY
10	G	122	GLU
11	H	163	ASP
12	I	40	THR
12	I	147	ARG
13	J	118	LEU
15	L	3	THR
15	L	55	ASP
16	M	110	SER
17	N	3	ARG
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
20	Q	138	PHE
21	R	99	VAL
21	R	117	LEU
22	S	85	PHE
25	V	12	TYR
27	X	3	LYS
28	Y	4	ALA
29	Z	55	PRO
29	Z	56	THR
34	e	47	VAL

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Mol	Chain	Res	Type
34	e	48	THR
36	g	4	SER
36	g	195	ILE
38	i	4	LYS
39	j	81	GLY
40	k	122	GLY
42	m	12	PRO
44	p	423	PRO
4	A	26	ALA
4	A	202	TYR
5	B	51	SER
5	B	131	ASP
5	B	148	ASN
7	D	197	SER
9	F	37	GLN
9	F	127	THR
11	H	10	SER
12	I	94	ASN
13	J	146	PHE
13	J	171	ARG
14	K	64	TYR
16	M	50	GLY
16	M	98	ASP
18	O	40	ALA
18	O	126	THR
19	P	69	GLU
20	Q	97	VAL
21	R	5	ARG
21	R	92	ASP
26	W	29	PRO
26	W	72	CYS
30	a	13	LYS
30	a	59	TYR
32	c	6	PRO
36	g	64	GLY
36	g	119	ASN
36	g	146	LEU
38	i	22	PRO
39	j	64	ARG
40	k	127	ARG
40	k	497	GLU
40	k	507	LYS

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Mol	Chain	Res	Type
43	o	62	LEU
43	o	63	LYS
43	o	251	GLU
44	p	77	GLN
45	q	460	PRO
45	q	468	THR
45	q	536	ASP
45	q	558	CYS
4	A	158	VAL
4	A	195	TRP
4	A	207	PRO
6	C	151	THR
6	C	253	THR
8	E	77	ARG
8	E	245	LYS
9	F	205	LYS
11	H	14	THR
11	H	98	ILE
12	I	99	ALA
12	I	120	SER
13	J	93	LEU
14	K	23	ALA
16	M	77	VAL
16	M	81	LYS
16	M	122	GLN
19	P	87	PRO
20	Q	113	ASP
21	R	90	ALA
21	R	116	LYS
23	T	28	LEU
23	T	35	ASP
24	U	77	LYS
25	V	81	ASN
27	X	41	SER
30	a	100	ARG
31	b	75	GLU
34	e	11	ALA
34	e	52	GLY
36	g	120	SER
36	g	161	ASN
36	g	290	LYS
38	i	97	LEU

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Mol	Chain	Res	Type
44	p	634	GLU
45	q	645	ILE
45	q	650	LYS
4	A	93	THR
5	B	54	LEU
5	B	221	PRO
5	B	224	ASP
6	C	40	TRP
8	E	195	ILE
10	G	152	ASP
12	I	52	ASN
12	I	148	ALA
13	J	134	ILE
14	K	26	ASP
15	L	4	GLU
15	L	7	VAL
18	O	42	VAL
21	R	88	VAL
22	S	91	ASP
24	U	73	GLY
24	U	89	ARG
26	W	30	SER
28	Y	36	SER
29	Z	36	ALA
30	a	64	LEU
35	f	111	GLU
40	k	383	GLU
40	k	408	ARG
42	m	5	ILE
43	o	49	GLU
43	o	394	ASN
44	p	207	ASP
44	p	569	PRO
45	q	514	LYS
45	q	779	GLU
4	A	68	PRO
5	B	207	LEU
6	C	155	GLN
7	D	219	GLU
9	F	42	ILE
9	F	66	ILE
9	F	102	ASN

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Mol	Chain	Res	Type
12	I	58	LEU
13	J	120	LYS
13	J	137	GLY
19	P	14	THR
28	Y	5	ILE
29	Z	69	PHE
31	b	62	VAL
39	j	6	CYS
39	j	197	GLY
44	p	198	VAL
44	p	536	LYS
45	q	351	ILE
5	B	206	PRO
27	X	4	GLY
36	g	201	GLY
40	k	225	PRO
43	o	933	PRO
44	p	422	VAL
4	A	103	THR
9	F	23	VAL
22	S	92	VAL
30	a	98	PRO
32	c	47	PRO
35	f	88	PRO
7	D	43	PRO
44	p	478	ILE
7	D	4	ILE
19	P	37	ALA
26	W	83	ILE
39	j	226	PRO
8	E	204	GLY
11	H	75	ILE
28	Y	35	VAL
40	k	282	PRO

5.3.2 Protein sidechains ⓘ

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	
4	A	180/211 (85%)	152 (84%)	28 (16%)	2	12
5	B	201/228 (88%)	180 (90%)	21 (10%)	7	26
6	C	177/203 (87%)	152 (86%)	25 (14%)	3	15
7	D	188/196 (96%)	161 (86%)	27 (14%)	3	14
8	E	223/224 (100%)	188 (84%)	35 (16%)	2	12
9	F	174/194 (90%)	144 (83%)	30 (17%)	2	9
10	G	192/200 (96%)	169 (88%)	23 (12%)	5	21
11	H	164/170 (96%)	141 (86%)	23 (14%)	3	15
12	I	147/159 (92%)	124 (84%)	23 (16%)	2	12
13	J	153/158 (97%)	130 (85%)	23 (15%)	3	13
14	K	88/96 (92%)	74 (84%)	14 (16%)	2	11
15	L	136/137 (99%)	124 (91%)	12 (9%)	10	34
16	M	93/109 (85%)	80 (86%)	13 (14%)	3	15
17	N	128/128 (100%)	120 (94%)	8 (6%)	18	49
18	O	97/104 (93%)	84 (87%)	13 (13%)	4	16
19	P	99/119 (83%)	88 (89%)	11 (11%)	6	23
20	Q	117/119 (98%)	101 (86%)	16 (14%)	3	16
21	R	116/124 (94%)	105 (90%)	11 (10%)	8	31
22	S	127/129 (98%)	108 (85%)	19 (15%)	3	13
23	T	117/118 (99%)	99 (85%)	18 (15%)	2	12
24	U	96/107 (90%)	85 (88%)	11 (12%)	5	22
25	V	73/73 (100%)	70 (96%)	3 (4%)	30	66
26	W	110/111 (99%)	101 (92%)	9 (8%)	11	38
27	X	119/120 (99%)	107 (90%)	12 (10%)	7	27
28	Y	108/109 (99%)	95 (88%)	13 (12%)	5	21
29	Z	59/88 (67%)	55 (93%)	4 (7%)	16	46
30	a	85/100 (85%)	77 (91%)	8 (9%)	8	31
31	b	71/72 (99%)	63 (89%)	8 (11%)	6	23
32	c	55/59 (93%)	46 (84%)	9 (16%)	2	11
33	d	47/48 (98%)	40 (85%)	7 (15%)	3	13
34	e	51/55 (93%)	43 (84%)	8 (16%)	2	12
35	f	60/133 (45%)	51 (85%)	9 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	g	264/272 (97%)	232 (88%)	32 (12%)	5	20
37	h	23/23 (100%)	21 (91%)	2 (9%)	10	35
38	i	100/130 (77%)	81 (81%)	19 (19%)	1	7
39	j	224/274 (82%)	189 (84%)	35 (16%)	2	12
40	k	332/449 (74%)	318 (96%)	14 (4%)	30	65
41	l	119/246 (48%)	115 (97%)	4 (3%)	37	72
42	m	125/352 (36%)	106 (85%)	19 (15%)	3	13
43	o	406/846 (48%)	379 (93%)	27 (7%)	16	47
44	p	544/693 (78%)	532 (98%)	12 (2%)	52	80
45	q	506/523 (97%)	485 (96%)	21 (4%)	30	65
46	r	40/232 (17%)	39 (98%)	1 (2%)	47	78
47	s	287/301 (95%)	281 (98%)	6 (2%)	53	81
All	All	6821/8542 (80%)	6135 (90%)	686 (10%)	11	27

All (686) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	LEU
4	A	6	THR
4	A	17	LEU
4	A	24	LEU
4	A	33	GLN
4	A	34	GLU
4	A	54	TRP
4	A	55	GLU
4	A	58	VAL
4	A	79	ARG
4	A	80	THR
4	A	86	VAL
4	A	93	THR
4	A	108	THR
4	A	109	ASN
4	A	111	ILE
4	A	116	LYS
4	A	121	VAL
4	A	127	ARG
4	A	157	ASP
4	A	162	CYS

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Mol	Chain	Res	Type
4	A	165	ARG
4	A	168	HIS
4	A	172	LEU
4	A	182	LEU
4	A	185	ARG
4	A	191	ARG
4	A	212	GLN
5	B	26	ARG
5	B	37	THR
5	B	72	ASP
5	B	78	ASP
5	B	82	ARG
5	B	89	ASP
5	B	103	MET
5	B	105	PHE
5	B	107	THR
5	B	110	LEU
5	B	111	ARG
5	B	120	LEU
5	B	127	VAL
5	B	132	ASP
5	B	140	ILE
5	B	152	ARG
5	B	160	HIS
5	B	177	GLN
5	B	178	ASN
5	B	181	LEU
5	B	213	ARG
6	C	58	ILE
6	C	63	LEU
6	C	68	VAL
6	C	72	GLN
6	C	83	ASP
6	C	86	MET
6	C	99	GLN
6	C	102	ARG
6	C	109	VAL
6	C	116	VAL
6	C	118	LEU
6	C	131	ARG
6	C	145	ARG
6	C	146	ARG

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Mol	Chain	Res	Type
6	C	153	LEU
6	C	155	GLN
6	C	159	LEU
6	C	173	ARG
6	C	206	THR
6	C	223	ILE
6	C	227	TYR
6	C	230	LEU
6	C	233	ASN
6	C	238	GLN
6	C	241	THR
7	D	11	LEU
7	D	12	VAL
7	D	27	ARG
7	D	41	VAL
7	D	51	ARG
7	D	62	ASN
7	D	66	ILE
7	D	70	THR
7	D	71	LEU
7	D	75	LYS
7	D	81	ARG
7	D	84	ILE
7	D	91	VAL
7	D	103	GLU
7	D	110	LEU
7	D	117	ARG
7	D	120	TYR
7	D	123	VAL
7	D	143	ARG
7	D	162	GLN
7	D	164	VAL
7	D	173	ARG
7	D	176	LEU
7	D	178	ARG
7	D	214	GLU
7	D	226	ARG
7	D	228	THR
8	E	6	LYS
8	E	9	LEU
8	E	18	TRP
8	E	19	MET

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Mol	Chain	Res	Type
8	E	23	LEU
8	E	38	LEU
8	E	39	ARG
8	E	49	ARG
8	E	51	ARG
8	E	57	ASN
8	E	77	ARG
8	E	80	THR
8	E	81	THR
8	E	93	GLU
8	E	96	ASN
8	E	100	ARG
8	E	106	LYS
8	E	108	ARG
8	E	113	ARG
8	E	114	ILE
8	E	155	LYS
8	E	163	ASP
8	E	173	ILE
8	E	181	VAL
8	E	187	ARG
8	E	198	ARG
8	E	200	ARG
8	E	206	ASP
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	238	LEU
8	E	254	ARG
8	E	259	HIS
9	F	29	THR
9	F	34	GLU
9	F	40	GLN
9	F	41	GLU
9	F	60	LEU
9	F	65	GLN
9	F	70	ILE
9	F	78	ARG
9	F	83	ARG
9	F	85	ARG
9	F	88	GLN

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Mol	Chain	Res	Type
9	F	92	VAL
9	F	100	MET
9	F	110	LEU
9	F	121	GLU
9	F	133	GLN
9	F	137	ASP
9	F	145	ARG
9	F	150	ARG
9	F	158	ARG
9	F	160	GLN
9	F	163	ASP
9	F	169	ARG
9	F	183	GLU
9	F	187	ARG
9	F	189	ILE
9	F	192	ILE
9	F	196	LEU
9	F	209	THR
9	F	213	ILE
10	G	1	MET
10	G	13	GLN
10	G	15	CYS
10	G	19	ASP
10	G	29	ASP
10	G	52	ILE
10	G	75	LEU
10	G	92	ARG
10	G	111	LEU
10	G	125	THR
10	G	127	ASP
10	G	132	ARG
10	G	133	LEU
10	G	154	ARG
10	G	170	THR
10	G	177	ARG
10	G	180	THR
10	G	189	GLN
10	G	203	GLU
10	G	212	LEU
10	G	215	ARG
10	G	222	GLU
10	G	226	VAL

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Mol	Chain	Res	Type
11	H	11	GLN
11	H	15	GLU
11	H	19	GLN
11	H	38	LEU
11	H	39	ARG
11	H	71	HIS
11	H	74	GLN
11	H	79	ARG
11	H	80	GLU
11	H	81	LEU
11	H	86	GLN
11	H	93	LEU
11	H	107	ARG
11	H	116	ARG
11	H	119	THR
11	H	122	HIS
11	H	126	LEU
11	H	127	GLU
11	H	128	ASP
11	H	139	ARG
11	H	164	ASN
11	H	174	ASN
11	H	176	LEU
12	I	5	ARG
12	I	8	ARG
12	I	20	GLN
12	I	22	ARG
12	I	23	LYS
12	I	24	LYS
12	I	25	ARG
12	I	29	LEU
12	I	32	GLN
12	I	35	ASN
12	I	46	VAL
12	I	47	ARG
12	I	58	LEU
12	I	72	VAL
12	I	77	ARG
12	I	92	ARG
12	I	96	LEU
12	I	139	ASN
12	I	153	ILE

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Mol	Chain	Res	Type
12	I	155	HIS
12	I	158	ASP
12	I	179	ARG
12	I	196	ARG
13	J	6	ARG
13	J	7	THR
13	J	8	TYR
13	J	9	SER
13	J	10	LYS
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	45	ILE
13	J	49	LEU
13	J	60	LEU
13	J	64	GLU
13	J	93	LEU
13	J	103	ASP
13	J	107	ARG
13	J	109	LEU
13	J	131	GLN
13	J	142	ASN
13	J	149	ARG
13	J	150	LEU
13	J	161	THR
13	J	183	GLU
14	K	13	GLN
14	K	15	LEU
14	K	18	GLU
14	K	34	GLU
14	K	35	ILE
14	K	39	ASN
14	K	40	LEU
14	K	44	LYS
14	K	49	LEU
14	K	76	LEU
14	K	81	ASN
14	K	82	LEU
14	K	84	GLU
14	K	86	ILE
15	L	10	GLU

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Mol	Chain	Res	Type
15	L	36	LYS
15	L	56	LYS
15	L	67	ARG
15	L	69	LYS
15	L	70	ILE
15	L	79	ARG
15	L	84	ILE
15	L	111	VAL
15	L	117	VAL
15	L	125	VAL
15	L	136	ARG
16	M	26	ARG
16	M	34	LEU
16	M	38	LEU
16	M	40	GLU
16	M	52	LEU
16	M	55	LEU
16	M	61	GLU
16	M	79	LEU
16	M	88	LEU
16	M	91	TRP
16	M	97	ILE
16	M	100	ASP
16	M	106	VAL
17	N	3	ARG
17	N	9	LYS
17	N	83	GLU
17	N	88	LEU
17	N	99	ARG
17	N	107	LYS
17	N	116	ILE
17	N	121	ARG
18	O	24	ASN
18	O	37	GLU
18	O	47	LYS
18	O	48	VAL
18	O	49	LYS
18	O	52	ARG
18	O	65	GLN
18	O	66	ASP
18	O	72	LYS
18	O	102	LEU

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Mol	Chain	Res	Type
18	O	124	ASP
18	O	126	THR
18	O	137	LEU
19	P	51	GLU
19	P	56	LEU
19	P	59	LYS
19	P	60	LEU
19	P	79	HIS
19	P	83	MET
19	P	94	VAL
19	P	106	GLU
19	P	111	MET
19	P	126	VAL
19	P	127	ARG
20	Q	22	VAL
20	Q	26	LYS
20	Q	52	LEU
20	Q	63	ILE
20	Q	69	VAL
20	Q	78	VAL
20	Q	82	ARG
20	Q	83	GLN
20	Q	87	LYS
20	Q	89	LEU
20	Q	94	GLN
20	Q	105	LEU
20	Q	107	LYS
20	Q	123	ARG
20	Q	127	LYS
20	Q	137	ARG
21	R	26	MET
21	R	29	GLN
21	R	37	GLU
21	R	42	GLN
21	R	46	LEU
21	R	78	ARG
21	R	82	ASP
21	R	106	THR
21	R	109	LEU
21	R	116	LYS
21	R	128	ARG
22	S	3	LEU

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Mol	Chain	Res	Type
22	S	15	LEU
22	S	40	ARG
22	S	41	ARG
22	S	57	ARG
22	S	61	LEU
22	S	73	MET
22	S	85	PHE
22	S	97	ASP
22	S	101	LEU
22	S	105	LEU
22	S	106	GLU
22	S	108	LYS
22	S	111	ASP
22	S	114	GLU
22	S	123	ARG
22	S	134	ARG
22	S	136	GLN
22	S	137	HIS
23	T	8	ASP
23	T	16	ASN
23	T	17	ASN
23	T	35	ASP
23	T	48	GLN
23	T	64	HIS
23	T	65	ILE
23	T	67	LEU
23	T	68	ARG
23	T	86	ARG
23	T	88	VAL
23	T	110	LYS
23	T	124	ILE
23	T	126	ASP
23	T	129	LEU
23	T	132	LEU
23	T	140	LEU
23	T	142	ASP
24	U	17	VAL
24	U	22	ILE
24	U	27	THR
24	U	31	VAL
24	U	52	LYS
24	U	56	VAL

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Mol	Chain	Res	Type
24	U	57	ARG
24	U	65	ILE
24	U	74	GLU
24	U	86	ILE
24	U	112	VAL
25	V	12	TYR
25	V	50	TYR
25	V	85	TYR
26	W	7	LEU
26	W	24	GLN
26	W	25	VAL
26	W	28	ARG
26	W	47	ILE
26	W	83	ILE
26	W	88	LYS
26	W	104	LEU
26	W	129	VAL
27	X	14	LYS
27	X	16	ARG
27	X	64	PRO
27	X	72	VAL
27	X	79	ASN
27	X	90	ASP
27	X	94	ASN
27	X	100	ASP
27	X	107	PHE
27	X	127	VAL
27	X	141	GLU
27	X	144	ARG
28	Y	8	ARG
28	Y	20	ARG
28	Y	34	ASN
28	Y	35	VAL
28	Y	74	LEU
28	Y	84	LYS
28	Y	105	ARG
28	Y	106	GLN
28	Y	111	ARG
28	Y	112	LYS
28	Y	117	LYS
28	Y	121	THR
28	Y	128	LYS

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Mol	Chain	Res	Type
29	Z	46	LYS
29	Z	58	ARG
29	Z	75	LEU
29	Z	81	ARG
30	a	12	LYS
30	a	38	ARG
30	a	39	MET
30	a	53	LEU
30	a	59	TYR
30	a	64	LEU
30	a	75	ILE
30	a	89	ARG
31	b	3	LEU
31	b	31	HIS
31	b	43	ILE
31	b	44	THR
31	b	57	GLU
31	b	67	THR
31	b	81	ARG
31	b	82	LYS
32	c	14	LYS
32	c	26	THR
32	c	38	ARG
32	c	49	ARG
32	c	50	GLU
32	c	58	GLU
32	c	64	ARG
32	c	65	ARG
32	c	66	LEU
33	d	19	ARG
33	d	20	GLN
33	d	30	LEU
33	d	38	ILE
33	d	39	ASP
33	d	41	GLN
33	d	49	ASP
34	e	10	ARG
34	e	17	GLN
34	e	24	GLN
34	e	26	LYS
34	e	36	LYS
34	e	37	ARG

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Mol	Chain	Res	Type
34	e	53	LYS
34	e	55	LYS
35	f	81	LYS
35	f	83	LYS
35	f	87	THR
35	f	91	ILE
35	f	92	ARG
35	f	96	LYS
35	f	99	LYS
35	f	135	ASP
35	f	136	ARG
36	g	8	LEU
36	g	11	ARG
36	g	54	GLN
36	g	59	VAL
36	g	60	ARG
36	g	66	SER
36	g	70	GLN
36	g	72	VAL
36	g	87	ASP
36	g	91	ARG
36	g	94	ASN
36	g	101	GLU
36	g	114	VAL
36	g	122	LYS
36	g	130	LYS
36	g	180	ASP
36	g	181	LYS
36	g	188	LEU
36	g	195	ILE
36	g	196	GLU
36	g	206	ILE
36	g	207	ASN
36	g	209	VAL
36	g	210	GLN
36	g	223	LYS
36	g	246	GLU
36	g	250	LEU
36	g	256	ARG
36	g	257	PHE
36	g	280	GLU
36	g	290	LYS

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Mol	Chain	Res	Type
36	g	308	LEU
37	h	13	LEU
37	h	16	LYS
38	i	3	LYS
38	i	4	LYS
38	i	5	ASN
38	i	13	ARG
38	i	14	ARG
38	i	23	LYS
38	i	31	GLU
38	i	34	GLU
38	i	39	THR
38	i	42	LEU
38	i	44	ASN
38	i	47	VAL
38	i	56	LYS
38	i	75	ASP
38	i	77	ILE
38	i	90	ASP
38	i	96	ASN
38	i	109	LEU
38	i	119	ASP
39	j	7	ARG
39	j	11	ASN
39	j	18	ASP
39	j	19	ILE
39	j	23	ASN
39	j	37	LEU
39	j	39	TYR
39	j	45	MET
39	j	46	ILE
39	j	53	ARG
39	j	54	ARG
39	j	62	LEU
39	j	63	ILE
39	j	69	ASP
39	j	79	GLU
39	j	80	LYS
39	j	84	ASP
39	j	87	LYS
39	j	97	LYS
39	j	119	PHE

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Mol	Chain	Res	Type
39	j	124	GLU
39	j	126	LEU
39	j	163	LYS
39	j	169	LEU
39	j	185	ARG
39	j	187	ASP
39	j	195	TYR
39	j	198	ILE
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	244	LEU
39	j	251	ILE
39	j	255	ILE
39	j	258	TYR
40	k	136	ILE
40	k	311	ILE
40	k	315	LEU
40	k	318	ILE
40	k	352	GLU
40	k	359	ILE
40	k	395	LEU
40	k	403	ASP
40	k	406	LEU
40	k	426	ILE
40	k	432	ILE
40	k	494	GLU
40	k	508	HIS
40	k	510	ARG
41	l	180	ILE
41	l	191	LEU
41	l	211	LEU
41	l	213	ILE
42	m	5	ILE
42	m	8	ASP
42	m	15	ARG
42	m	24	LYS
42	m	25	VAL
42	m	34	THR
42	m	41	ASP
42	m	48	ARG
42	m	53	ILE

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Mol	Chain	Res	Type
42	m	70	ASP
42	m	71	LYS
42	m	111	ILE
42	m	113	LYS
42	m	114	ASP
42	m	117	LEU
42	m	118	VAL
42	m	120	ASP
42	m	131	ASP
42	m	132	LEU
43	o	16	ASP
43	o	39	ARG
43	o	41	ARG
43	o	56	LEU
43	o	104	ILE
43	o	172	ASN
43	o	178	THR
43	o	183	VAL
43	o	185	LYS
43	o	206	LEU
43	o	217	GLN
43	o	229	ASP
43	o	235	ARG
43	o	239	GLN
43	o	262	ASP
43	o	292	VAL
43	o	303	TRP
43	o	329	PHE
43	o	330	LEU
43	o	346	ASP
43	o	355	LEU
43	o	381	ASP
43	o	384	LEU
43	o	388	TYR
43	o	397	VAL
43	o	476	ASP
43	o	480	ILE
44	p	77	GLN
44	p	79	ILE
44	p	158	TYR
44	p	192	TRP
44	p	277	VAL

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Mol	Chain	Res	Type
44	p	422	VAL
44	p	444	GLN
44	p	489	VAL
44	p	581	MET
44	p	616	ASP
44	p	631	HIS
44	p	678	LYS
45	q	273	GLN
45	q	305	ASP
45	q	315	ILE
45	q	324	ASP
45	q	335	THR
45	q	336	ILE
45	q	352	GLU
45	q	406	ASN
45	q	407	LEU
45	q	438	ASP
45	q	490	LEU
45	q	532	ILE
45	q	567	LEU
45	q	577	ARG
45	q	611	HIS
45	q	644	ARG
45	q	676	LEU
45	q	677	PHE
45	q	733	TYR
45	q	754	GLU
45	q	783	GLU
46	r	74	ARG
47	s	64	THR
47	s	157	THR
47	s	158	VAL
47	s	308	TYR
47	s	313	GLU
47	s	328	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	83	GLN
4	A	109	ASN
5	B	101	HIS

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Mol	Chain	Res	Type
5	B	124	ASN
6	C	64	HIS
6	C	99	GLN
6	C	152	ASN
6	C	233	ASN
7	D	159	HIS
7	D	179	GLN
8	E	50	ASN
8	E	57	ASN
8	E	112	HIS
8	E	130	GLN
8	E	216	ASN
9	F	65	GLN
9	F	102	ASN
9	F	188	ASN
10	G	10	ASN
10	G	13	GLN
10	G	139	ASN
11	H	29	ASN
11	H	74	GLN
11	H	110	GLN
11	H	150	GLN
11	H	170	GLN
12	I	64	ASN
13	J	38	ASN
13	J	110	GLN
13	J	142	ASN
13	J	155	HIS
14	K	39	ASN
14	K	81	ASN
14	K	85	HIS
15	L	8	GLN
15	L	138	ASN
17	N	49	GLN
17	N	62	GLN
17	N	105	ASN
18	O	99	GLN
19	P	104	GLN
20	Q	83	GLN
21	R	105	GLN
22	S	87	ASN
22	S	99	HIS

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Mol	Chain	Res	Type
22	S	136	GLN
23	T	12	GLN
23	T	43	ASN
23	T	64	HIS
25	V	21	ASN
25	V	33	GLN
26	W	24	GLN
26	W	80	ASN
26	W	92	ASN
27	X	79	ASN
28	Y	15	ASN
28	Y	22	GLN
28	Y	29	HIS
30	a	17	HIS
30	a	80	HIS
31	b	26	GLN
31	b	42	ASN
32	c	43	ASN
33	d	37	ASN
33	d	41	GLN
34	e	46	ASN
35	f	95	HIS
36	g	51	ASN
36	g	94	ASN
36	g	203	ASN
36	g	321	GLN
38	i	5	ASN
38	i	85	GLN
39	j	60	GLN
39	j	103	GLN
39	j	109	HIS
40	k	124	GLN
40	k	344	ASN
40	k	415	GLN
40	k	465	ASN
42	m	64	GLN
42	m	94	ASN
42	m	134	HIS
43	o	194	GLN
43	o	216	GLN
43	o	243	GLN
43	o	299	HIS

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Mol	Chain	Res	Type
43	o	394	ASN
43	o	403	GLN
44	p	467	ASN
44	p	592	ASN
44	p	712	GLN
45	q	340	GLN
45	q	386	ASN
45	q	406	ASN
45	q	495	ASN
45	q	540	GLN
45	q	582	GLN
45	q	610	GLN
47	s	145	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	72/76 (94%)	29 (40%)	8 (11%)
2	2	1775/1798 (98%)	654 (36%)	72 (4%)
3	3	27/49 (55%)	16 (59%)	4 (14%)
All	All	1874/1923 (97%)	699 (37%)	84 (4%)

All (699) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	5	C
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	15	G
1	1	16	H2U
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	26	M2G
1	1	42	U
1	1	44	A
1	1	46	7MG

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Mol	Chain	Res	Type
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	58	1MA
1	1	59	A
1	1	60	A
1	1	61	C
1	1	64	RIA
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	3	U
2	2	4	C
2	2	5	U
2	2	13	C
2	2	16	G
2	2	17	C
2	2	25	C
2	2	27	U
2	2	34	G
2	2	42	G
2	2	46	A
2	2	47	A
2	2	50	C
2	2	57	G
2	2	58	U
2	2	59	C
2	2	60	U
2	2	61	A
2	2	64	U
2	2	66	U
2	2	67	A
2	2	68	A
2	2	69	G
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A

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Mol	Chain	Res	Type
2	2	77	U
2	2	78	A
2	2	79	C
2	2	100	A
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	121	U
2	2	123	G
2	2	124	A
2	2	126	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	135	A
2	2	136	C
2	2	137	U
2	2	139	C
2	2	140	A
2	2	141	U
2	2	143	G
2	2	144	A
2	2	146	A
2	2	147	U
2	2	150	G
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	172	A
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	184	U
2	2	186	G

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Mol	Chain	Res	Type
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	194	G
2	2	195	G
2	2	209	A
2	2	214	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	223	C
2	2	226	U
2	2	227	G
2	2	228	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	235	A
2	2	239	C
2	2	240	U
2	2	248	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	260	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	267	C
2	2	271	U
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	289	G
2	2	294	A
2	2	300	A

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Mol	Chain	Res	Type
2	2	301	U
2	2	303	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	313	C
2	2	314	A
2	2	315	A
2	2	320	C
2	2	321	G
2	2	322	A
2	2	334	U
2	2	336	G
2	2	337	C
2	2	342	C
2	2	351	A
2	2	359	A
2	2	360	C
2	2	368	A
2	2	369	A
2	2	380	C
2	2	382	G
2	2	389	G
2	2	392	C
2	2	399	A
2	2	400	A
2	2	401	C
2	2	404	C
2	2	411	A
2	2	412	U
2	2	415	A
2	2	416	A
2	2	418	G
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	427	A
2	2	433	G
2	2	434	C
2	2	438	U

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Mol	Chain	Res	Type
2	2	439	U
2	2	440	A
2	2	443	C
2	2	444	A
2	2	447	C
2	2	457	G
2	2	459	A
2	2	469	A
2	2	474	A
2	2	476	A
2	2	479	G
2	2	481	U
2	2	482	A
2	2	483	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	499	C
2	2	502	G
2	2	505	A
2	2	506	U
2	2	507	U
2	2	509	G
2	2	510	A
2	2	513	G
2	2	516	U
2	2	518	C
2	2	519	A
2	2	524	A
2	2	526	A
2	2	527	U
2	2	531	U
2	2	533	A
2	2	535	C
2	2	537	A
2	2	539	G
2	2	540	A
2	2	541	A

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Mol	Chain	Res	Type
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	548	G
2	2	553	C
2	2	556	G
2	2	557	U
2	2	558	C
2	2	564	C
2	2	567	G
2	2	570	G
2	2	577	U
2	2	578	A
2	2	582	C
2	2	583	C
2	2	584	A
2	2	593	A
2	2	594	G
2	2	597	U
2	2	600	A
2	2	605	A
2	2	609	G
2	2	610	U
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	621	A
2	2	622	A
2	2	623	G
2	2	637	U
2	2	638	U
2	2	639	U
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G

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Mol	Chain	Res	Type
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	684	A
2	2	686	C
2	2	691	U
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	701	U
2	2	702	G
2	2	704	C
2	2	705	U
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	714	C
2	2	715	U
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	725	U
2	2	727	C
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	736	C
2	2	737	A
2	2	738	G
2	2	739	G
2	2	741	C
2	2	742	U

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Mol	Chain	Res	Type
2	2	743	U
2	2	755	A
2	2	765	G
2	2	766	PSU
2	2	767	U
2	2	771	A
2	2	774	A
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	786	G
2	2	788	A
2	2	789	U
2	2	792	A
2	2	793	U
2	2	794	U
2	2	809	G
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	832	U
2	2	839	U
2	2	840	U
2	2	845	G
2	2	847	C
2	2	854	A
2	2	855	A
2	2	859	U
2	2	862	A

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Mol	Chain	Res	Type
2	2	863	U
2	2	872	U
2	2	874	G
2	2	876	G
2	2	881	U
2	2	885	U
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	899	A
2	2	905	A
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	916	U
2	2	917	U
2	2	919	U
2	2	920	U
2	2	921	G
2	2	923	A
2	2	932	A
2	2	934	U
2	2	941	G
2	2	944	U
2	2	947	G
2	2	950	A
2	2	958	U
2	2	959	U
2	2	965	A
2	2	969	A
2	2	970	A
2	2	972	A
2	2	981	U
2	2	982	A
2	2	986	G
2	2	987	A
2	2	990	G
2	2	991	A
2	2	993	G

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Mol	Chain	Res	Type
2	2	995	U
2	2	1009	C
2	2	1011	U
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1033	C
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1042	A
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1075	A
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1085	A
2	2	1086	A
2	2	1091	A
2	2	1092	A
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1103	U

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Mol	Chain	Res	Type
2	2	1104	C
2	2	1106	G
2	2	1110	G
2	2	1112	A
2	2	1113	G
2	2	1118	G
2	2	1125	G
2	2	1137	A
2	2	1142	A
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1156	A
2	2	1157	C
2	2	1158	C
2	2	1163	G
2	2	1166	G
2	2	1184	U
2	2	1185	U
2	2	1187	G
2	2	1189	C
2	2	1191	C
2	2	1193	A
2	2	1195	A
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1224	U
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1230	U
2	2	1236	G
2	2	1237	A
2	2	1243	A

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Mol	Chain	Res	Type
2	2	1244	G
2	2	1245	C
2	2	1246	U
2	2	1247	C
2	2	1249	U
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1265	U
2	2	1268	U
2	2	1269	G
2	2	1272	G
2	2	1275	U
2	2	1283	C
2	2	1284	U
2	2	1287	G
2	2	1292	U
2	2	1296	G
2	2	1298	G
2	2	1306	U
2	2	1311	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1347	A
2	2	1353	G
2	2	1355	U
2	2	1360	C

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Mol	Chain	Res	Type
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1379	U
2	2	1380	A
2	2	1383	G
2	2	1388	U
2	2	1389	A
2	2	1390	U
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1407	G
2	2	1408	A
2	2	1409	A
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1418	C
2	2	1423	A
2	2	1424	C
2	2	1425	A
2	2	1426	2MG
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1442	A
2	2	1443	G
2	2	1444	A
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A

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Mol	Chain	Res	Type
2	2	1460	G
2	2	1464	G
2	2	1467	A
2	2	1469	A
2	2	1471	U
2	2	1476	G
2	2	1480	C
2	2	1481	A
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1494	U
2	2	1499	C
2	2	1504	G
2	2	1510	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G
2	2	1544	G
2	2	1548	A
2	2	1555	U
2	2	1557	A
2	2	1558	U
2	2	1566	C
2	2	1570	2MG
2	2	1571	A

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Mol	Chain	Res	Type
2	2	1572	G
2	2	1581	A
2	2	1588	G
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1605	G
2	2	1614	G
2	2	1616	C
2	2	1617	C
2	2	1620	G
2	2	1632	C
2	2	1633	A
2	2	1634	C
2	2	1644	C
2	2	1647	G
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1666	G
2	2	1667	U
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1702	U
2	2	1703	C

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Mol	Chain	Res	Type
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1715	G
2	2	1725	G
2	2	1730	A
2	2	1734	G
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U
2	2	1753	A
2	2	1755	G
2	2	1758	G
2	2	1760	A
2	2	1763	A
2	2	1764	A
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1769	U
2	2	1778	G
2	2	1781	C
2	2	1787	G
2	2	1788	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1796	U
2	2	1797	U
2	2	1798	A
3	3	19	A
3	3	20	A
3	3	22	U
3	3	23	A
3	3	24	U

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Mol	Chain	Res	Type
3	3	25	A
3	3	26	A
3	3	33	C
3	3	34	U
3	3	36	U
3	3	38	C
3	3	39	U
3	3	40	C
3	3	43	U
3	3	44	C
3	3	45	U

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	8	U
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	58	1MA
1	1	74	C
2	2	3	U
2	2	16	G
2	2	44	U
2	2	66	U
2	2	74	U
2	2	126	A
2	2	128	U
2	2	130	C
2	2	131	C
2	2	176	U
2	2	190	C
2	2	216	A
2	2	217	A
2	2	239	C
2	2	275	C
2	2	277	U
2	2	279	U
2	2	321	G
2	2	336	G

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Mol	Chain	Res	Type
2	2	399	A
2	2	451	A
2	2	467	A
2	2	542	C
2	2	544	A
2	2	597	U
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	710	U
2	2	721	U
2	2	780	A
2	2	781	A
2	2	810	A
2	2	826	C
2	2	828	A
2	2	854	A
2	2	896	C
2	2	912	G
2	2	914	A
2	2	946	U
2	2	1057	U
2	2	1058	C
2	2	1080	A
2	2	1107	G
2	2	1198	G
2	2	1206	C
2	2	1226	A
2	2	1284	U
2	2	1320	A
2	2	1338	C
2	2	1343	A
2	2	1430	U
2	2	1455	C
2	2	1456	G
2	2	1470	C
2	2	1479	C
2	2	1513	A
2	2	1515	U
2	2	1533	U
2	2	1545	A

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Mol	Chain	Res	Type
2	2	1570	2MG
2	2	1571	A
2	2	1599	G
2	2	1613	C
2	2	1648	U
2	2	1655	U
2	2	1678	G
2	2	1765	G
2	2	1766	G
2	2	1796	U
2	2	1797	U
3	3	22	U
3	3	33	C
3	3	35	C
3	3	38	C

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

24 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	$\#\|Z\| > 2$
2	PSU	2	1289	2	18,21,22	1.48	3 (16%)	22,30,33	1.89	3 (13%)
2	2MG	2	1426	48,2	18,26,27	0.95	0	16,38,41	1.40	4 (25%)
1	5MC	1	49	1	18,22,23	1.10	1 (5%)	26,32,35	1.34	4 (15%)
1	RIA	1	64	1	31,38,39	0.51	0	39,57,60	0.71	1 (2%)
2	PSU	2	465	2	18,21,22	1.51	3 (16%)	22,30,33	1.89	5 (22%)
2	MA6	2	1780	2	18,26,27	1.13	2 (11%)	19,38,41	1.73	4 (21%)
1	H2U	1	47	1	18,21,22	0.85	0	21,30,33	1.38	3 (14%)
2	PSU	2	998	2	18,21,22	1.41	3 (16%)	22,30,33	1.92	4 (18%)
1	H2U	1	16	1	18,21,22	0.83	0	21,30,33	1.67	4 (19%)
2	PSU	2	120	2	18,21,22	1.40	2 (11%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	1MG	1	9	1	18,26,27	1.02	0	19,39,42	1.58	4 (21%)
1	M2G	1	26	1	20,27,28	1.74	3 (15%)	22,40,43	1.34	4 (18%)
1	2MG	1	10	1	18,26,27	0.98	1 (5%)	16,38,41	1.08	2 (12%)
2	5MC	2	1006	2	18,22,23	0.96	1 (5%)	26,32,35	1.66	6 (23%)
1	1MA	1	58	1	16,25,26	1.86	4 (25%)	18,37,40	1.48	3 (16%)
1	7MG	1	46	1	22,26,27	1.44	4 (18%)	29,39,42	2.62	10 (34%)
2	2MG	2	1570	2	18,26,27	0.94	0	16,38,41	1.42	3 (18%)
2	7MG	2	1573	1,2	22,26,27	1.55	7 (31%)	29,39,42	2.63	6 (20%)
2	C4J	2	1190	2	24,29,30	0.52	0	29,42,45	1.00	1 (3%)
2	PSU	2	766	2	18,21,22	1.37	2 (11%)	22,30,33	2.12	5 (22%)
1	5MC	1	48	1	18,22,23	1.03	1 (5%)	26,32,35	1.26	3 (11%)
5	AYA	B	2	-	6,7,8	0.65	0	5,8,10	0.72	0
1	T6A	1	37	1	27,34,35	1.04	2 (7%)	29,49,52	2.71	10 (34%)
2	5MC	2	1637	2	18,22,23	1.03	1 (5%)	26,32,35	1.36	6 (23%)

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
2	PSU	2	1289	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1426	48,2	-	3/5/27/28	0/3/3/3
1	5MC	1	49	1	-	2/7/25/26	0/2/2/2
1	RIA	1	64	1	-	3/13/51/52	0/4/4/4
2	PSU	2	465	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1780	2	-	5/7/29/30	0/3/3/3
2	PSU	2	998	2	-	0/7/25/26	0/2/2/2
1	H2U	1	47	1	-	4/7/38/39	0/2/2/2
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
2	PSU	2	120	2	-	0/7/25/26	0/2/2/2
1	1MG	1	9	1	-	3/3/25/26	0/3/3/3
1	M2G	1	26	1	-	2/7/29/30	0/3/3/3
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
2	5MC	2	1006	2	-	0/7/25/26	0/2/2/2
1	1MA	1	58	1	-	0/3/25/26	0/3/3/3
1	7MG	1	46	1	-	1/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	2	1570	2	-	0/5/27/28	0/3/3/3
2	7MG	2	1573	1,2	-	2/7/37/38	0/3/3/3
2	C4J	2	1190	2	1/1/7/7	0/16/34/35	0/2/2/2
2	PSU	2	766	2	-	1/7/25/26	0/2/2/2
1	5MC	1	48	1	-	3/7/25/26	0/2/2/2
5	AYA	B	2	-	-	0/4/6/8	-
1	T6A	1	37	1	-	5/19/41/42	0/3/3/3
2	5MC	2	1637	2	-	1/7/25/26	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	1MA	C2-N3	5.71	1.35	1.29
1	1	26	M2G	C2-N3	5.61	1.37	1.30
2	2	465	PSU	C6-C5	4.22	1.40	1.35
2	2	1289	PSU	C6-C5	4.21	1.40	1.35
2	2	120	PSU	C6-C5	3.89	1.39	1.35
2	2	998	PSU	C6-C5	3.88	1.39	1.35
2	2	766	PSU	C6-C5	3.74	1.39	1.35
1	1	26	M2G	C2-N2	3.74	1.42	1.35
1	1	58	1MA	C6-N6	3.44	1.36	1.27
1	1	49	5MC	C6-C5	3.32	1.40	1.34
2	2	1637	5MC	C6-C5	3.29	1.40	1.34
1	1	46	7MG	C5-C4	3.21	1.48	1.38
1	1	48	5MC	C6-C5	3.07	1.39	1.34
2	2	1573	7MG	C5-C4	3.04	1.48	1.38
2	2	1573	7MG	C8-N9	2.98	1.47	1.46
2	2	1573	7MG	C4-N9	-2.77	1.34	1.37
2	2	465	PSU	C4-N3	-2.74	1.33	1.38
1	1	46	7MG	C8-N9	2.68	1.47	1.46
2	2	1289	PSU	C4-N3	-2.65	1.33	1.38
1	1	46	7MG	C4-N9	-2.63	1.34	1.37
2	2	766	PSU	C4-N3	-2.61	1.34	1.38
2	2	1780	MA6	C5-C4	2.55	1.47	1.40
2	2	1006	5MC	C6-N1	-2.54	1.33	1.38
1	1	37	T6A	C5-C4	2.49	1.47	1.40
2	2	998	PSU	C4-N3	-2.31	1.34	1.38
2	2	465	PSU	C2-N3	-2.29	1.33	1.37
2	2	1573	7MG	C5-N7	-2.28	1.33	1.35
2	2	1573	7MG	C6-N1	-2.22	1.34	1.38
1	1	46	7MG	C5-C6	2.22	1.49	1.43
2	2	120	PSU	C4-N3	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1573	7MG	C1'-N9	2.17	1.50	1.46
2	2	998	PSU	C4-C5	2.14	1.50	1.44
1	1	58	1MA	C5-C4	2.13	1.48	1.43
1	1	10	2MG	O4'-C1'	2.12	1.44	1.41
1	1	37	T6A	O4'-C1'	2.11	1.44	1.41
2	2	1780	MA6	C6-N1	2.08	1.36	1.33
1	1	26	M2G	O4'-C1'	2.08	1.44	1.41
2	2	1573	7MG	C5-C6	2.06	1.48	1.43
1	1	58	1MA	O4'-C1'	2.05	1.43	1.41
2	2	1289	PSU	C4-C5	2.04	1.50	1.44

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1573	7MG	N9-C4-N3	8.85	138.71	125.47
1	1	46	7MG	N9-C4-N3	8.73	138.53	125.47
1	1	37	T6A	C12-N11-C10	8.59	136.24	121.94
1	1	37	T6A	C2-N1-C6	7.43	122.96	116.59
2	2	1289	PSU	N1-C2-N3	6.10	122.04	115.13
2	2	465	PSU	N1-C2-N3	5.93	121.85	115.13
2	2	998	PSU	N1-C2-N3	5.93	121.85	115.13
2	2	766	PSU	N1-C2-N3	5.92	121.84	115.13
2	2	1573	7MG	C5-C4-N3	-5.77	117.14	128.13
2	2	120	PSU	N1-C2-N3	5.56	121.42	115.13
1	1	46	7MG	C5-C4-N3	-5.39	117.85	128.13
1	1	16	H2U	O4'-C1'-N1	5.03	116.15	109.30
1	1	37	T6A	C14-C12-C13	5.00	118.72	110.19
2	2	1573	7MG	N9-C8-N7	-4.99	96.24	103.38
1	1	46	7MG	N9-C8-N7	-4.91	96.35	103.38
1	1	46	7MG	C2-N3-C4	4.68	120.64	112.30
2	2	1573	7MG	C2-N3-C4	4.63	120.55	112.30
2	2	766	PSU	C4-N3-C2	-4.07	120.47	126.34
2	2	1780	MA6	C4-C5-N7	-4.07	105.16	109.40
1	1	58	1MA	C3'-C2'-C1'	3.84	106.76	100.98
1	1	37	T6A	N3-C2-N1	-3.78	122.77	128.68
2	2	120	PSU	C4-N3-C2	-3.77	120.91	126.34
2	2	1289	PSU	C4-N3-C2	-3.75	120.94	126.34
2	2	1006	5MC	C5-C4-N3	-3.75	117.63	121.67
2	2	1573	7MG	O4'-C1'-N9	3.73	114.38	109.30
2	2	998	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	1006	5MC	CM5-C5-C6	-3.64	117.99	122.85
2	2	120	PSU	O2-C2-N1	-3.53	118.91	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1780	MA6	N3-C2-N1	-3.46	123.27	128.68
2	2	465	PSU	C4-N3-C2	-3.43	121.40	126.34
2	2	766	PSU	O2-C2-N1	-3.40	119.05	122.79
2	2	1190	C4J	C4-N3-C2	-3.39	121.17	125.46
2	2	998	PSU	O2-C2-N1	-3.34	119.12	122.79
1	1	47	H2U	C3'-C2'-C1'	3.23	107.56	101.43
1	1	9	1MG	O6-C6-C5	-3.17	118.58	124.19
2	2	1780	MA6	C10-N6-C6	-3.15	109.98	119.51
1	1	9	1MG	C5-C6-N1	3.11	118.58	113.90
1	1	26	M2G	N1-C2-N2	3.06	120.65	118.04
1	1	49	5MC	O2-C2-N3	-3.06	117.36	122.33
2	2	465	PSU	C6-C5-C4	-3.05	116.06	118.20
1	1	46	7MG	C5-C6-N1	2.99	116.26	110.99
1	1	48	5MC	O2-C2-N3	-2.91	117.60	122.33
1	1	37	T6A	N6-C6-N1	2.90	122.61	118.72
2	2	766	PSU	C3'-C2'-C1'	2.89	105.01	101.64
1	1	49	5MC	C5-C4-N3	-2.89	118.56	121.67
2	2	1637	5MC	C5-C4-N3	-2.88	118.57	121.67
2	2	1780	MA6	C10-N6-C9	-2.82	107.03	116.12
2	2	1426	2MG	C5-C6-N1	2.78	118.86	113.95
2	2	1573	7MG	C5-C6-N1	2.77	115.88	110.99
2	2	1570	2MG	C3'-C2'-C1'	2.75	105.11	100.98
1	1	46	7MG	O4'-C1'-N9	2.74	113.03	109.30
2	2	1289	PSU	O2-C2-N1	-2.74	119.78	122.79
1	1	48	5MC	C5-C6-N1	-2.73	120.53	123.34
1	1	26	M2G	C5-C6-N1	2.68	118.69	113.95
2	2	1637	5MC	O4'-C1'-N1	2.67	114.47	108.36
1	1	26	M2G	O6-C6-C5	-2.67	119.16	124.37
2	2	1006	5MC	O2-C2-N3	-2.66	118.01	122.33
2	2	1006	5MC	C5-C6-N1	-2.63	120.63	123.34
1	1	16	H2U	C5-C4-N3	2.62	119.59	116.65
2	2	1637	5MC	C5-C6-N1	-2.62	120.65	123.34
1	1	37	T6A	C4-C5-N7	-2.59	106.70	109.40
2	2	1426	2MG	C8-N7-C5	2.57	107.89	102.99
2	2	766	PSU	C6-C5-C4	-2.56	116.41	118.20
2	2	998	PSU	C6-C5-C4	-2.56	116.41	118.20
2	2	1637	5MC	O2-C2-N3	-2.53	118.21	122.33
1	1	48	5MC	O4'-C1'-N1	2.49	114.07	108.36
1	1	16	H2U	C4-N3-C2	-2.47	123.74	125.79
2	2	1570	2MG	C5-C6-N1	2.45	118.28	113.95
1	1	49	5MC	O4'-C1'-N1	2.41	113.87	108.36
2	2	465	PSU	O2-C2-N1	-2.41	120.14	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1426	2MG	O6-C6-C5	-2.39	119.70	124.37
1	1	37	T6A	O10-C10-N6	-2.36	119.62	123.62
1	1	47	H2U	C4-N3-C2	-2.36	123.84	125.79
2	2	120	PSU	C6-C5-C4	-2.33	116.57	118.20
2	2	1006	5MC	N4-C4-N3	2.33	122.73	118.48
1	1	58	1MA	C8-N7-C5	2.32	107.42	102.99
1	1	9	1MG	C3'-C2'-C1'	2.31	104.46	100.98
2	2	1426	2MG	CM2-N2-C2	2.31	128.97	123.86
1	1	37	T6A	C14-C12-N11	2.30	117.60	111.72
1	1	9	1MG	C8-N7-C5	2.27	107.32	102.99
2	2	1570	2MG	C8-N7-C5	2.26	107.29	102.99
2	2	1006	5MC	C2'-C1'-N1	-2.23	106.89	113.22
1	1	46	7MG	CM7-N7-C5	2.22	132.13	126.40
1	1	47	H2U	C5-C4-N3	2.22	119.14	116.65
2	2	1637	5MC	CM5-C5-C6	-2.20	119.91	122.85
1	1	10	2MG	C8-N7-C5	2.17	107.13	102.99
1	1	26	M2G	C8-N7-C5	2.17	107.13	102.99
2	2	1637	5MC	N1-C2-N3	2.13	122.68	118.81
1	1	10	2MG	C5-C6-N1	2.11	117.68	113.95
1	1	46	7MG	C5-C4-N9	-2.10	103.62	106.35
1	1	16	H2U	C4'-O4'-C1'	-2.09	104.85	109.47
1	1	37	T6A	C3'-C2'-C1'	2.07	104.10	100.98
1	1	58	1MA	C5-C6-N1	2.05	116.95	113.90
1	1	37	T6A	C15-C14-C12	2.04	116.41	112.29
1	1	46	7MG	O3'-C3'-C4'	-2.03	105.17	111.05
1	1	64	RIA	C5-C6-N6	2.03	123.44	120.35
1	1	49	5MC	C3'-C2'-C1'	2.02	105.27	101.43
2	2	465	PSU	O2-C2-N3	-2.02	118.00	121.82
1	1	46	7MG	O6-C6-C5	-2.02	122.59	127.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	1780	MA6	O4'-C4'-C5'-O5'
2	2	1780	MA6	C5-C6-N6-C10
2	2	1780	MA6	N1-C6-N6-C10
1	1	9	1MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	9	1MG	C3'-C4'-C5'-O5'
1	1	10	2MG	O4'-C4'-C5'-O5'
1	1	16	H2U	C4'-C5'-O5'-P
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	37	T6A	C14-C12-N11-C10
1	1	37	T6A	N11-C12-C14-O14
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	48	5MC	C4'-C5'-O5'-P
1	1	64	RIA	C3'-C4'-C5'-O5'
2	2	1780	MA6	C3'-C4'-C5'-O5'
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	48	5MC	O4'-C4'-C5'-O5'
1	1	48	5MC	C3'-C4'-C5'-O5'
1	1	47	H2U	C2'-C1'-N1-C2
2	2	1426	2MG	O4'-C4'-C5'-O5'
1	1	26	M2G	O4'-C4'-C5'-O5'
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	47	H2U	C2'-C1'-N1-C6
1	1	37	T6A	N11-C12-C14-C15
1	1	37	T6A	N11-C12-C13-ODA
2	2	1573	7MG	O4'-C4'-C5'-O5'
2	2	1573	7MG	C3'-C4'-C5'-O5'
1	1	49	5MC	O4'-C4'-C5'-O5'
1	1	37	T6A	N11-C12-C13-ODB
1	1	46	7MG	C4'-C5'-O5'-P
1	1	64	RIA	C4A-C5A-O5A-P
1	1	9	1MG	C4'-C5'-O5'-P
2	2	1426	2MG	C4'-C5'-O5'-P
2	2	1780	MA6	C4'-C5'-O5'-P
2	2	766	PSU	C3'-C4'-C5'-O5'
2	2	1426	2MG	C3'-C4'-C5'-O5'
1	1	49	5MC	C3'-C4'-C5'-O5'
2	2	1637	5MC	O4'-C4'-C5'-O5'
1	1	16	H2U	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 124 ligands modelled in this entry, 122 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
51	GCP	k	603	-	27,34,34	1.91	7 (25%)	34,54,54	1.94	8 (23%)
50	MET	k	601	-	6,7,8	0.47	0	2,7,9	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	GCP	k	603	-	-	1/15/38/38	0/3/3/3
50	MET	k	601	-	-	1/5/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.35	1.61	1.50
51	k	603	GCP	C5-C6	4.61	1.49	1.41
51	k	603	GCP	PB-O3A	2.98	1.61	1.58
51	k	603	GCP	PG-O3G	-2.84	1.48	1.54
51	k	603	GCP	PG-O2G	2.83	1.61	1.54
51	k	603	GCP	C5-C4	2.77	1.48	1.40
51	k	603	GCP	PB-O2B	2.18	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	k	603	GCP	C2-N3-C4	5.27	121.38	115.36
51	k	603	GCP	C2-N1-C6	4.05	122.36	115.93
51	k	603	GCP	C5-C6-N1	-3.83	118.19	123.43
51	k	603	GCP	C4-C5-C6	-3.77	117.20	120.80
51	k	603	GCP	N3-C2-N1	-3.51	122.55	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	k	603	GCP	C3'-C2'-C1'	3.13	105.69	100.98
51	k	603	GCP	PB-O3A-PA	-3.04	122.93	132.56
51	k	603	GCP	C4-C5-N7	-2.69	106.60	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

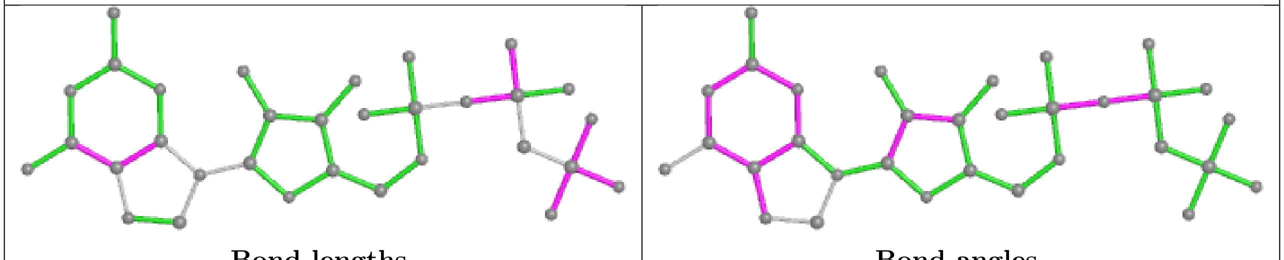
Mol	Chain	Res	Type	Atoms
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	PB-O3A-PA-O1A

There are no ring outliers.

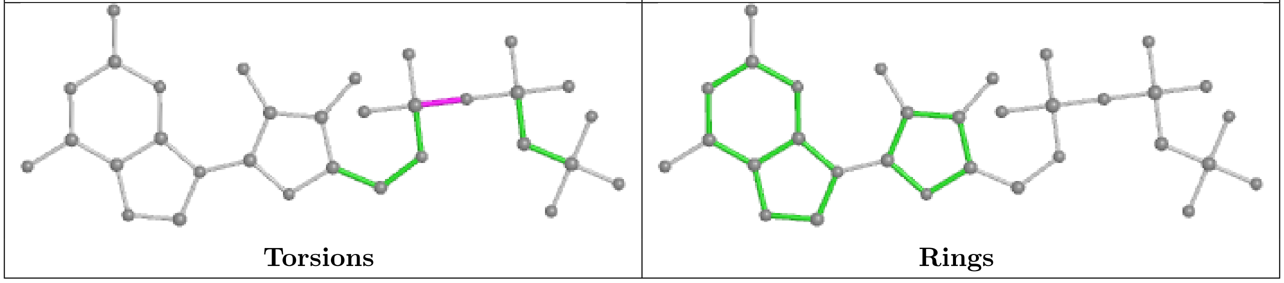
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GCP k 603



Bond lengths **Bond angles**



Torsions **Rings**

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
45	q	8
2	2	1
1	1	1
44	p	1
5	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	214:UNK	C	251:GLN	N	50.55
1	q	158:UNK	C	166:UNK	N	17.71
1	q	181:UNK	C	190:UNK	N	14.31
1	q	135:UNK	C	139:UNK	N	7.79
1	q	203:UNK	C	207:UNK	N	6.84
1	2	224:A	O3’	225:A	P	4.58
1	1	16:H2U	O3’	18:G	P	4.54
1	q	582:GLN	C	583:GLN	N	3.87
1	q	148:UNK	C	150:UNK	N	3.60
1	q	605:CYS	C	606:LEU	N	3.34
1	p	688:GLU	C	689:GLU	N	3.29
1	B	2:AYA	C	3:VAL	N	3.09

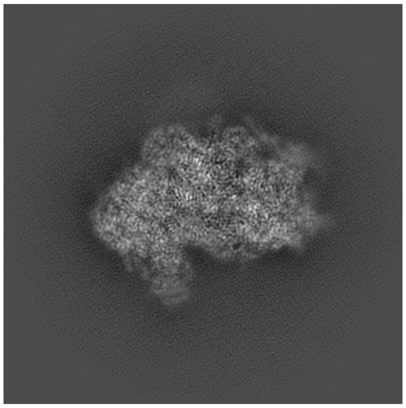
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4328. These allow visual inspection of the internal detail of the map and identification of artifacts.

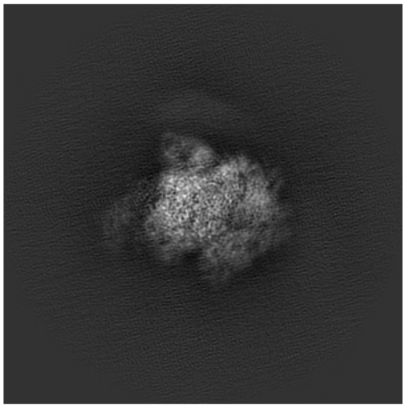
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

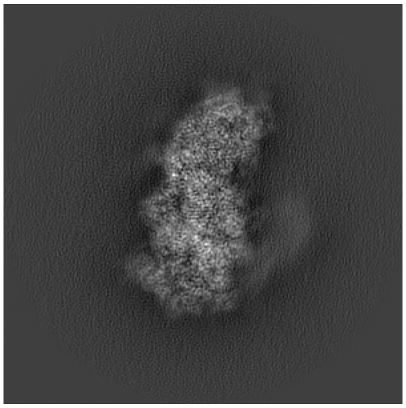
6.1.1 Primary map



X

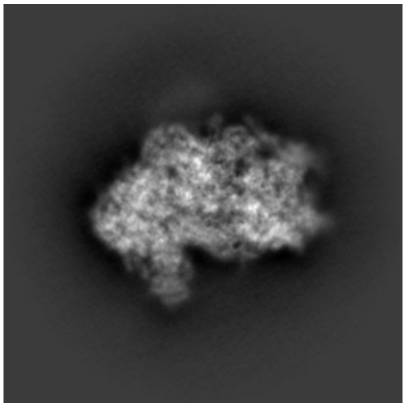


Y

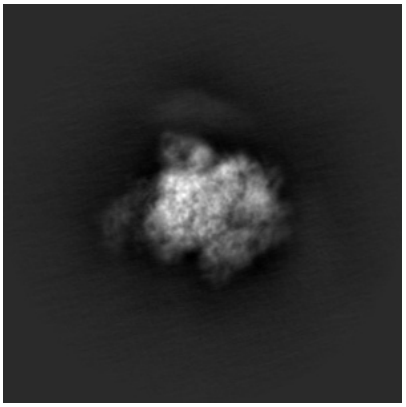


Z

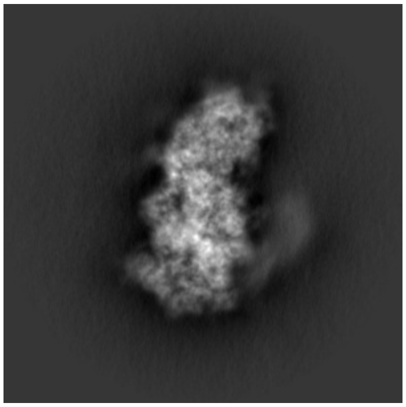
6.1.2 Raw map



X



Y

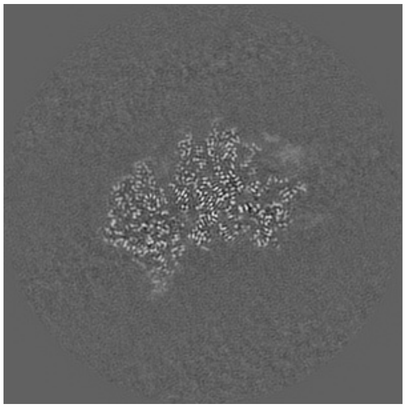


Z

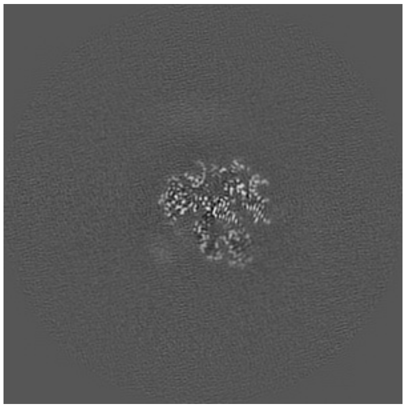
The images above show the map projected in three orthogonal directions.

6.2 Central slices

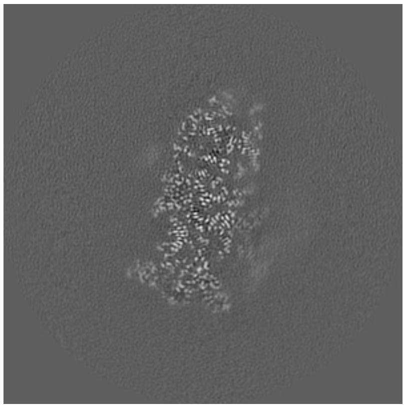
6.2.1 Primary map



X Index: 150

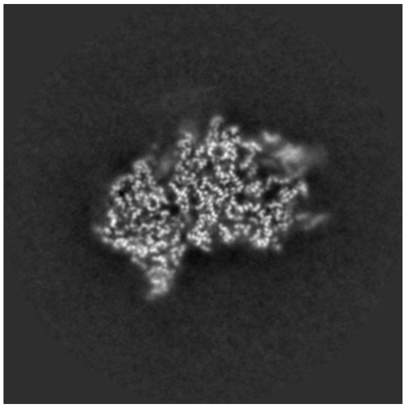


Y Index: 150

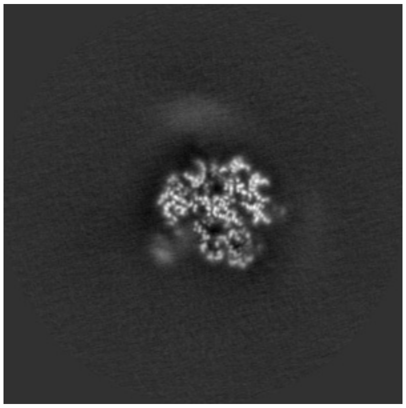


Z Index: 150

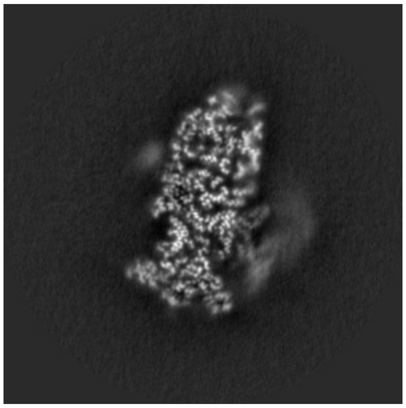
6.2.2 Raw map



X Index: 150



Y Index: 150

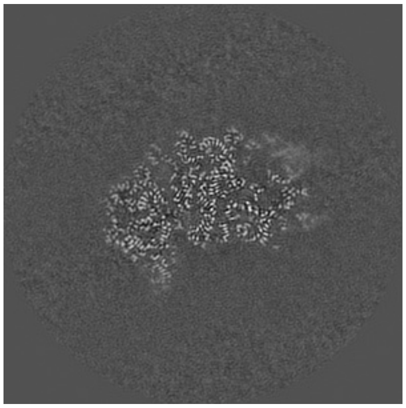


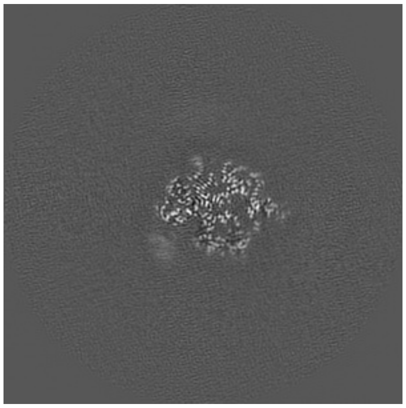
Z Index: 150

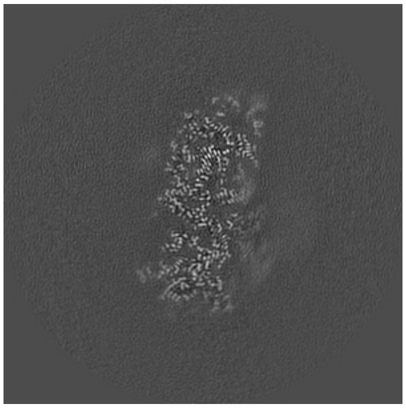
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

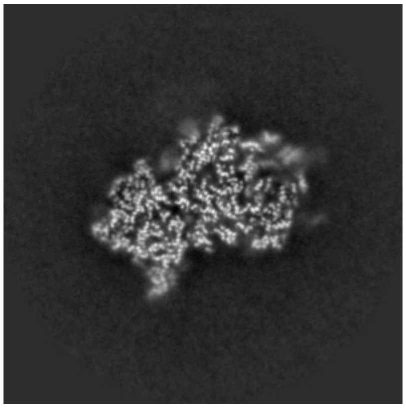
6.3.1 Primary map

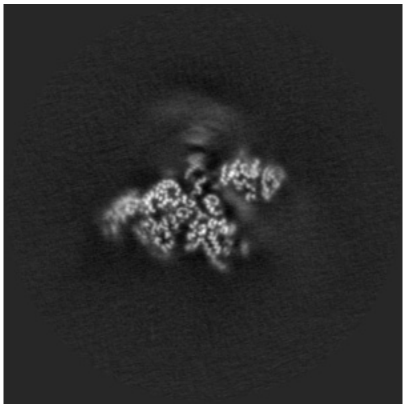

X Index: 152

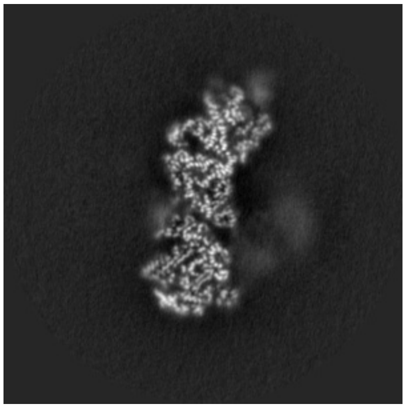

Y Index: 155


Z Index: 147

6.3.2 Raw map


X Index: 148

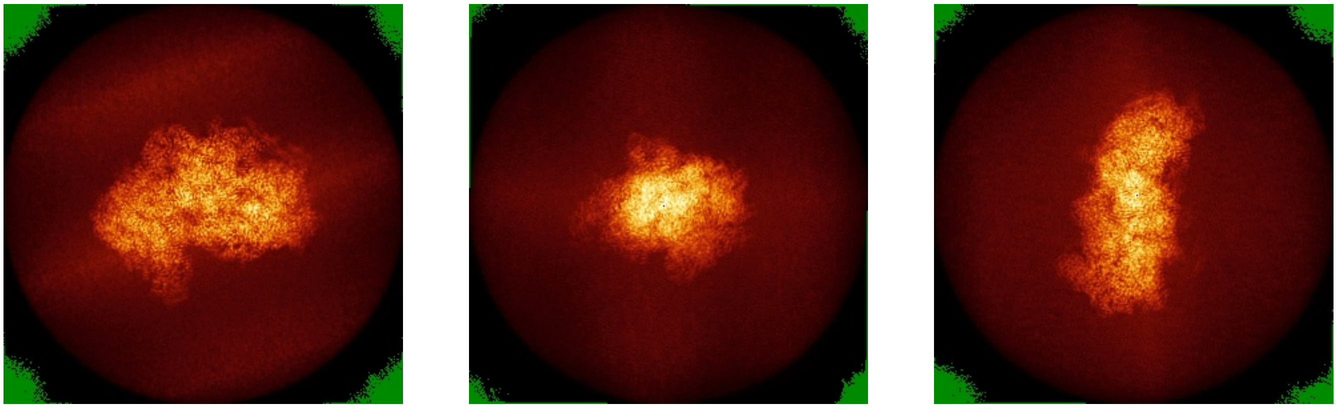

Y Index: 119


Z Index: 132

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

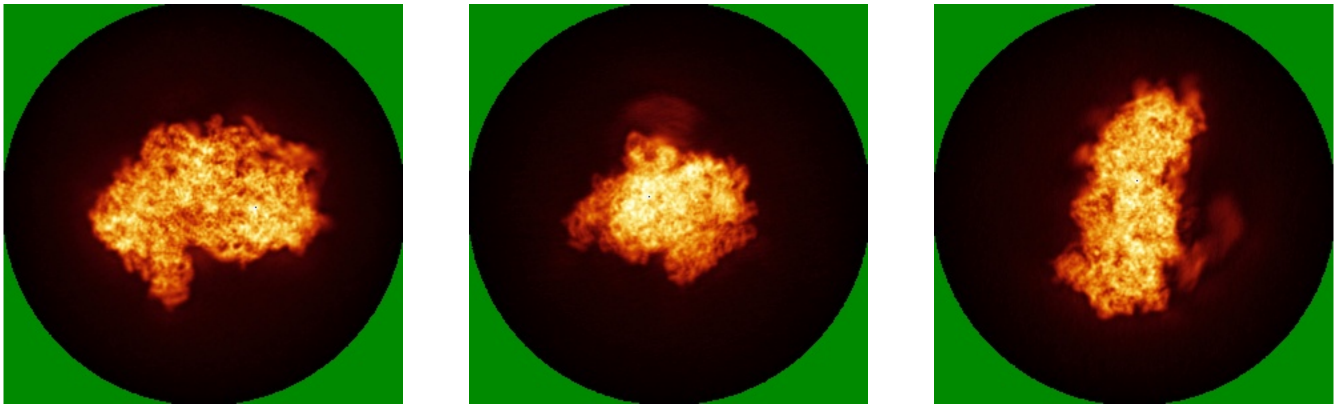
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map



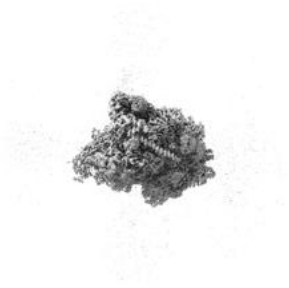
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map


X

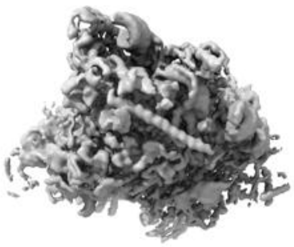

Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map


X


Y


Z

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

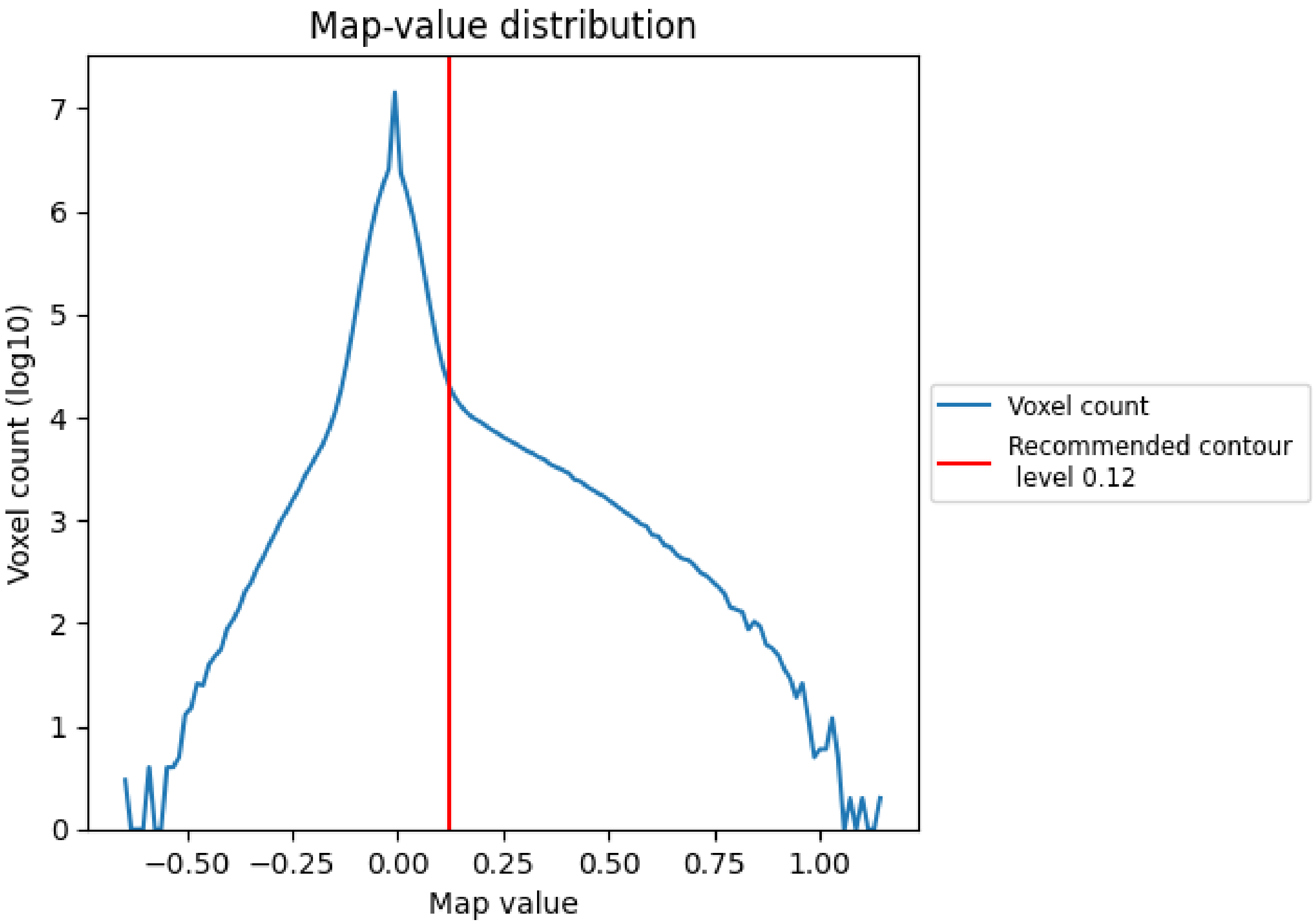
6.6 Mask visualisation (i)

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

7 Map analysis (i)

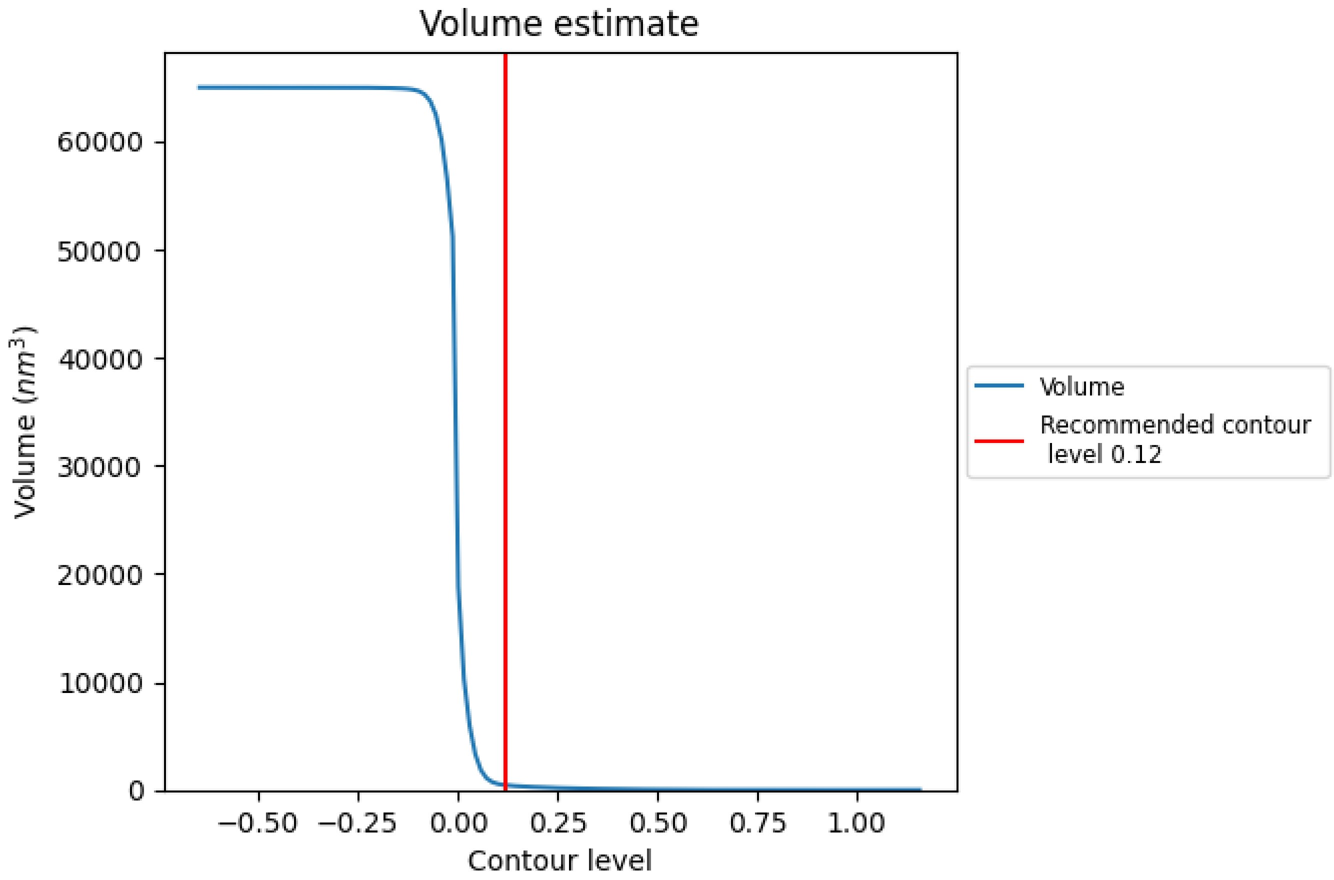
This section contains the results of statistical analysis of the map.

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.

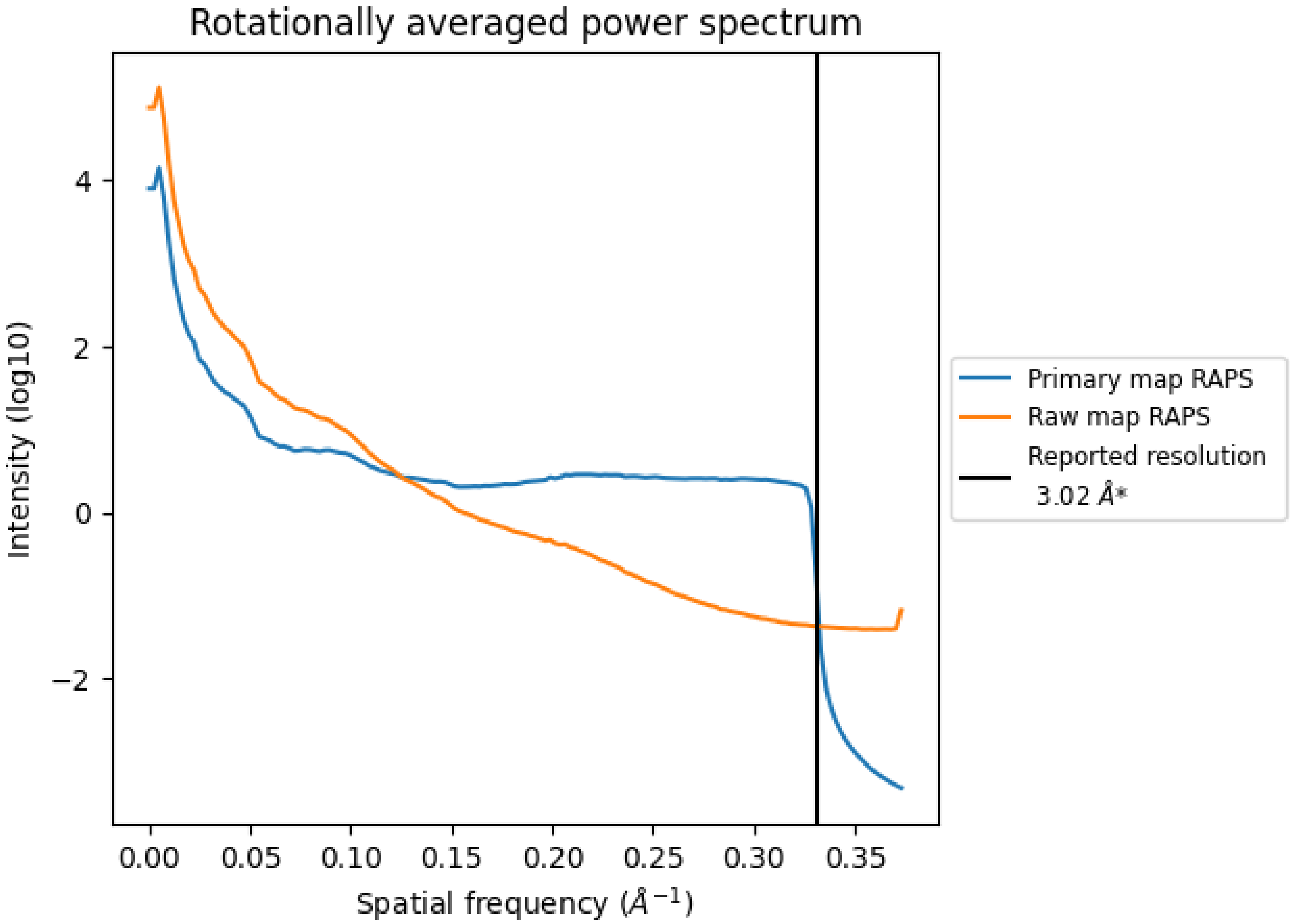
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 447 nm^3; this corresponds to an approximate mass of 404 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 ⓘ

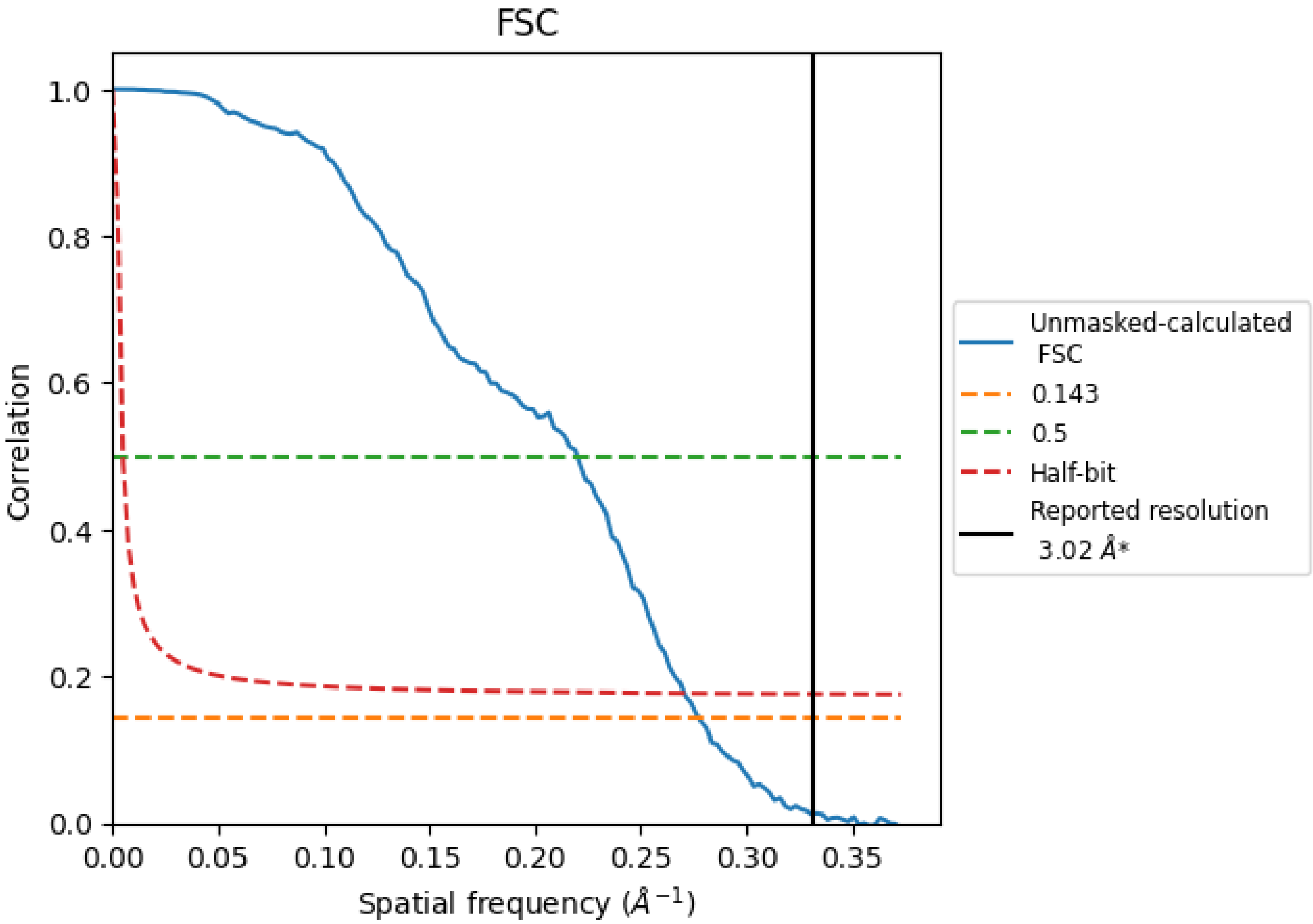


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.331 $Å^{-1}$

8.2 Resolution estimates ⓘ

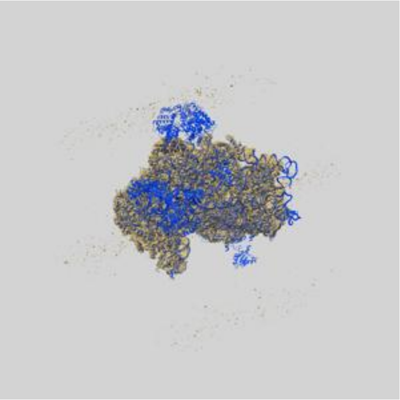
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	4.55	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.02 by more than 10 %

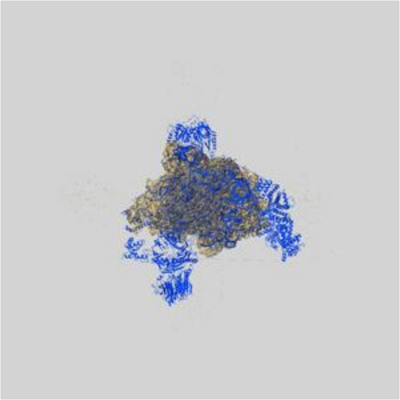
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4328 and PDB model 6FYY. Per-residue inclusion information can be found in section 3 on page 14.

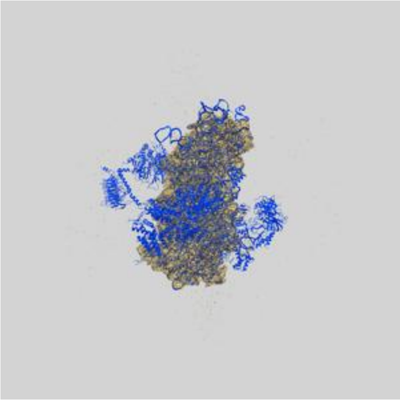
9.1 Map-model overlay ⓘ



X



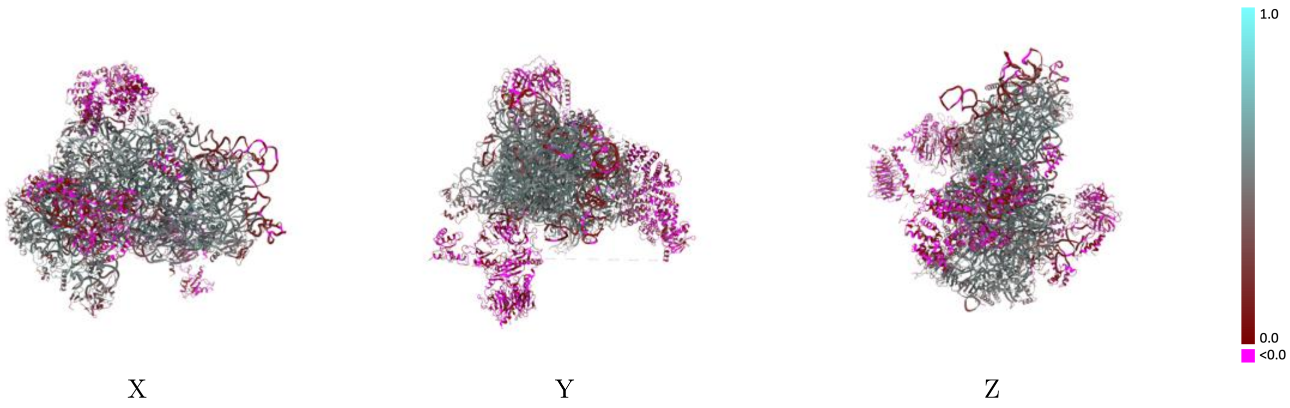
Y



Z

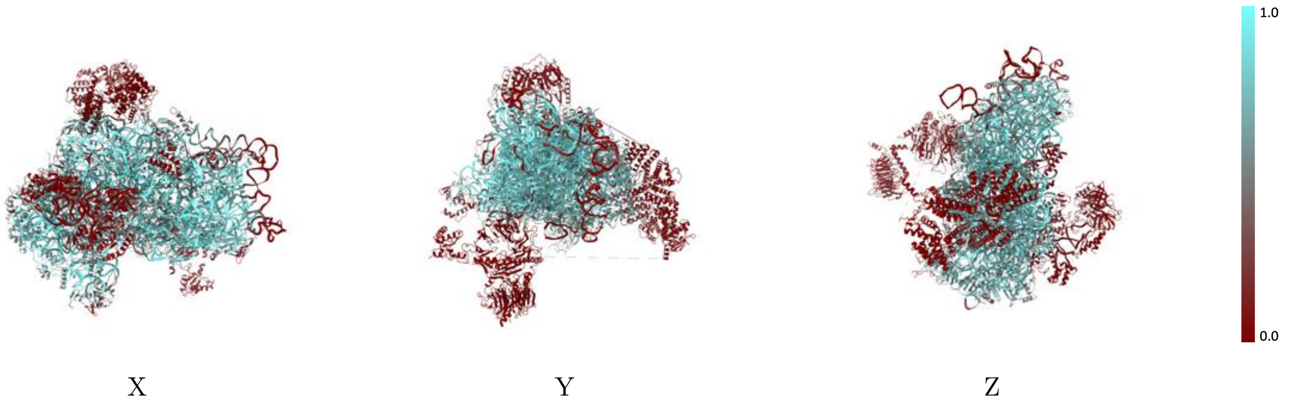
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



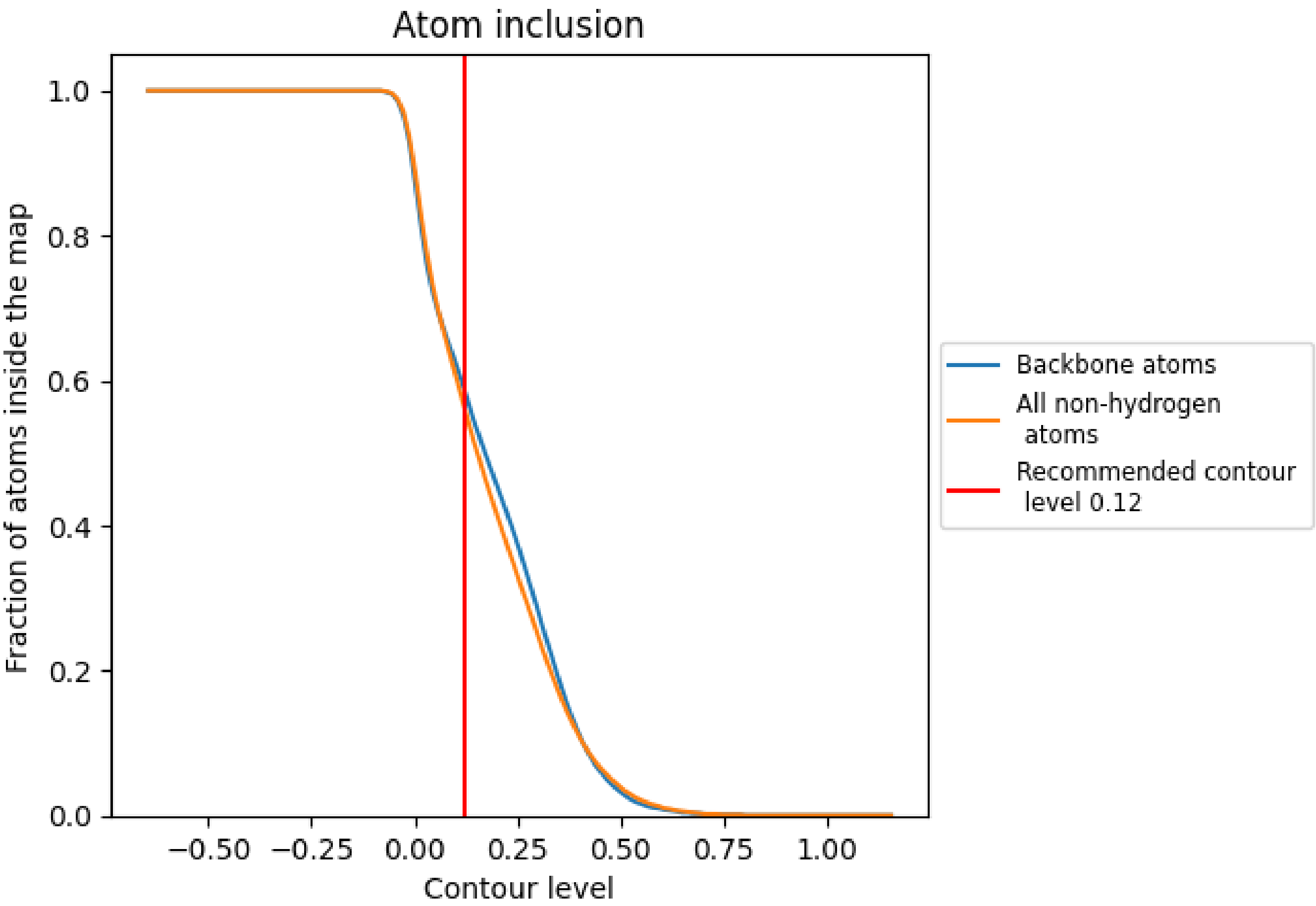
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 59% of all backbone atoms, 57% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5660	0.3780
1	0.3120	0.2600
2	0.8100	0.4820
3	0.2570	0.2510
A	0.7070	0.4840
B	0.6630	0.4590
C	0.7640	0.5220
D	0.6750	0.4700
E	0.7960	0.5310
F	0.6620	0.4770
G	0.6330	0.4360
H	0.5630	0.4250
I	0.7200	0.4870
J	0.7650	0.5110
K	0.6910	0.4620
L	0.6960	0.4930
M	0.2850	0.2570
N	0.7520	0.5110
O	0.7400	0.5100
P	0.7040	0.4800
Q	0.7480	0.5120
R	0.6330	0.4600
S	0.7000	0.4680
T	0.7690	0.5010
U	0.5920	0.4170
V	0.7360	0.5000
W	0.8000	0.5420
X	0.8050	0.5470
Y	0.7550	0.5010
Z	0.4990	0.3820
a	0.7570	0.5150
b	0.6890	0.4940
c	0.6620	0.4980
d	0.8580	0.5620
e	0.6790	0.4730

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Chain	Atom inclusion	Q-score
f	■ 0.4190	■ 0.3750
g	■ 0.6160	■ 0.4590
h	■ 0.4720	■ 0.4180
i	■ 0.6140	■ 0.4750
j	■ 0.0030	■ 0.1410
k	■ 0.0010	■ 0.0430
l	■ 0.0010	■ 0.0530
m	■ 0.2220	■ 0.3860
o	■ 0.0000	■ 0.0240
p	■ 0.0000	■ 0.0450
q	■ 0.0010	■ 0.0430
r	■ 0.0000	■ 0.0090
s	■ 0.0000	■ 0.0250