wwPDB EM Validation Summary Report ⓘ

Mar 24, 2025 – 02:21 PM EDT

PDB ID	:	9NLF
EMDB ID	:	EMD-40924
Title	:	E. coli initiation complex with EQ2-YbiT in Hydrolytic 2/PtIM(a) conformation
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-03-03
Resolution	:	3.20 Å(reported)

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

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

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

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

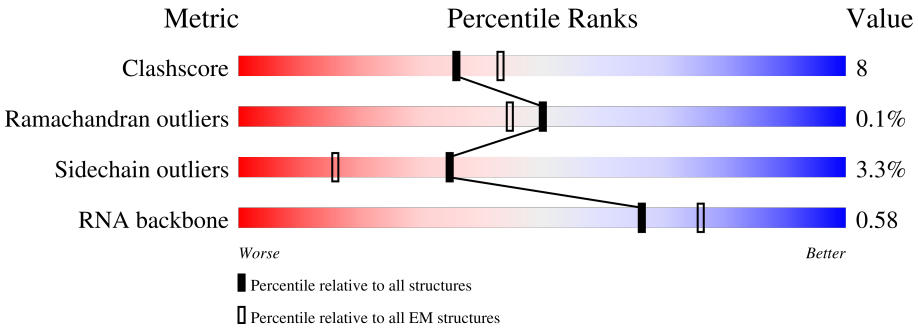
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	220	61%, 85%, 14%
2	13	142	80%, 20%
3	14	122	86%, 13%
4	15	144	78%, 22%
5	16	136	81%, 19%
6	17	120	80%, 20%
7	18	116	76%, 24%

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Mol	Chain	Length	Quality of chain
8	19	114	75% 24%
9	2	271	79% 20%
10	20	117	76% 23%
11	21	103	8% 76% 23%
12	22	110	73% 26%
13	23	93	82% 18%
14	24	102	9% 80% 20%
15	25	94	10% 77% 23%
16	27	77	81% 18%
17	28	77	75% 23%
18	29	63	11% 78% 22%
19	3	209	82% 18%
20	30	58	5% 72% 28%
21	31	66	70% 76% 23%
22	32	56	5% 73% 27%
23	33	50	78% 22%
24	34	46	85% 15%
25	35	64	84% 16%
26	36	38	68% 32%
27	4	201	6% 88% 12%
28	5	177	23% 69% 30%
29	6	176	14% 82% 17%
30	9	149	73% 74% 24%
31	M	9	22% 100%
32	R1	2903	5% 62% 32% 6%

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Mol	Chain	Length	Quality of chain
33	R2	119	63% 34%
34	R3	1539	7% 59% 36% 5%
35	T	77	8% 57% 31% 6% 5%
36	Y	530	22% 68% 30%
37	sb	218	31% 97%
38	sc	206	18% 99%
39	sd	205	20% 99%
40	se	157	96%
41	sf	100	27% 96%
42	sg	151	30% 95% 5%
43	sh	129	5% 97%
44	si	127	19% 94% 6%
45	sj	98	47% 98%
46	sk	116	12% 100%
47	sl	123	7% 97%
48	sm	114	24% 96%
49	sn	100	21% 95% 5%
50	so	88	6% 100%
51	sp	82	12% 98%
52	sq	80	15% 94% 6%
53	sr	65	17% 95% 5%
54	ss	79	25% 94% 6%
55	st	85	8% 98%
56	su	65	45% 89% 11%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	H2U	T	20	X	-	-	-
35	4OC	T	32	X	-	-	-
35	5MU	T	54	X	-	-	-
35	PSU	T	55	X	-	-	-
35	4SU	T	8	X	-	-	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 149993 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	220	1353	804	270	277	2	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	13	142	1129	714	212	199	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	14	122	938	587	180	165	6	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	15	144	1053	654	207	190	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	16	136	1074	686	205	177	6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	17	120	960	593	196	166	5	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	18	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	19	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	271	Total 2082	C 1288	N 423	O 364	S 7	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	20	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	21	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	23	93	Total 738	C 466	N 139	O 131	S 2	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	24	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	25	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	77	Total 588	C 363	N 118	O 106	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	28	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	29	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	209	Total 1565	C 979	N 288	O 294	S 4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- Molecule 33 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 35 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	T	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	8	4SU	G	conflict	GB 932857508

- Molecule 36 is a protein called Probable ATP-binding protein YbiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Y	527	Total	C	N	O	S	0	0
			4170	2636	715	800	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	181	GLN	GLU	conflict	UNP P0A9U3
Y	464	GLN	GLU	conflict	UNP P0A9U3

- Molecule 37 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 38 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	sd	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 40 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	sh	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 44 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	si	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 46 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	sl	123	Total 955	C 590	N 196	O 165	S 4	0	0

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sm	114	Total 883	C 546	N 178	O 156	S 3	0	0

- Molecule 49 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sn	100	Total 805	C 499	N 164	O 139	S 3	0	0

- Molecule 50 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	so	88	Total 714	C 439	N 144	O 130	S 1	0	0

- Molecule 51 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	sp	82	Total 649	C 406	N 128	O 114	S 1	0	0

- Molecule 52 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sq	80	Total 648	C 411	N 121	O 113	S 3	0	0

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sr	65	Total 535	C 339	N 100	O 95	S 1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ss	79	Total 637	C 408	N 120	O 107	S 2	0	0

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	st	85	Total 665	C 411	N 137	O 114	S 3	0	0

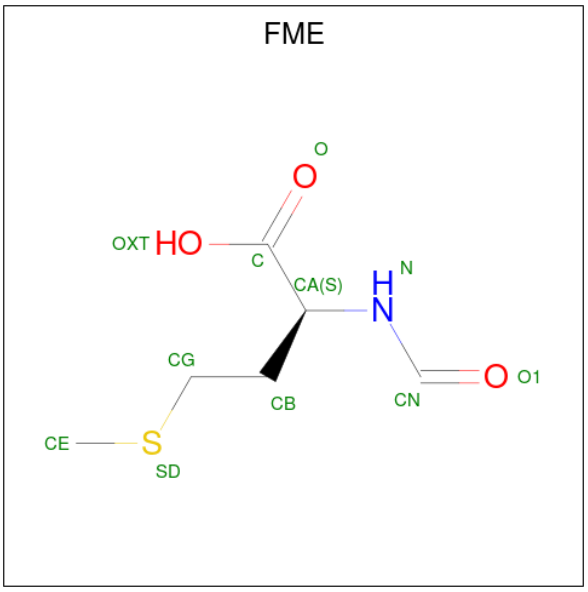
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	su	65	Total 544	C 335	N 117	O 91	S 1	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

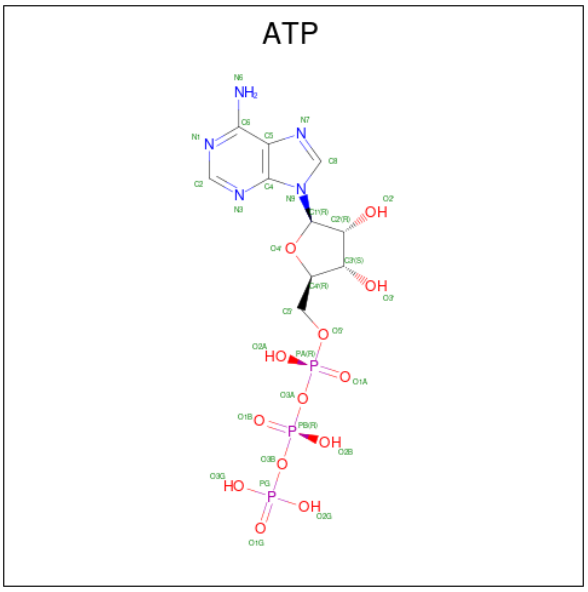
Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total 1	Mg 1	0
57	17	1	Total 1	Mg 1	0
57	32	1	Total 1	Mg 1	0
57	34	1	Total 1	Mg 1	0
57	R1	184	Total 184	Mg 184	0
57	R3	57	Total 57	Mg 57	0

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
59	Y	1	Total	C	N	O	P	0
			31	10	5	13	3	
59	Y	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 60 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
60	Y	2	2	2	0

3 Residue-property plots (i)

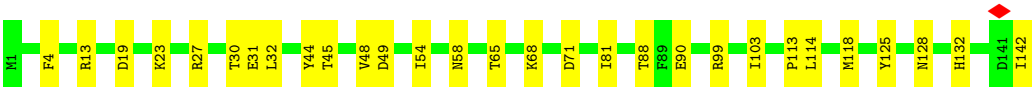
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Large ribosomal subunit protein uL1

Chain 1:

• Molecule 2: Large ribosomal subunit protein uL13

Chain 13:

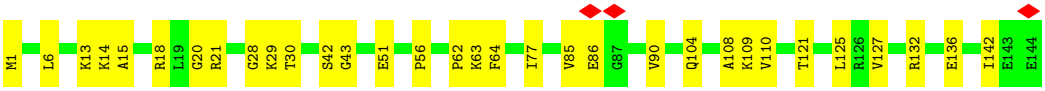


• Molecule 3: 50S ribosomal protein L14

Chain 14:

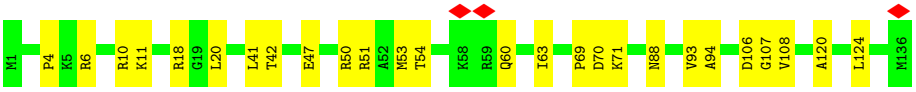
• Molecule 4: Large ribosomal subunit protein uL15

Chain 15:



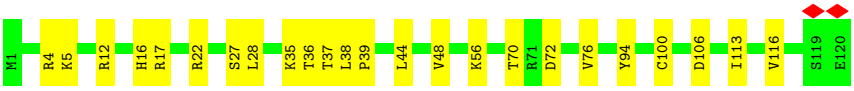
• Molecule 5: 50S ribosomal protein L16

Chain 16:



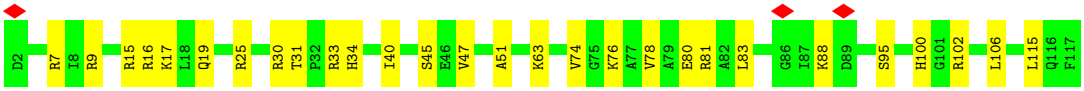
• Molecule 6: Large ribosomal subunit protein bL17

Chain 17:



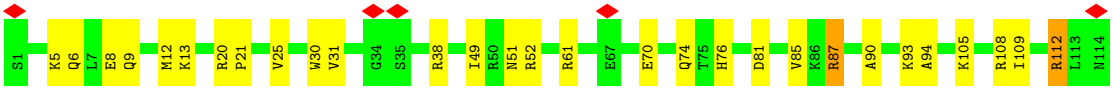
• Molecule 7: Large ribosomal subunit protein uL18

Chain 18:



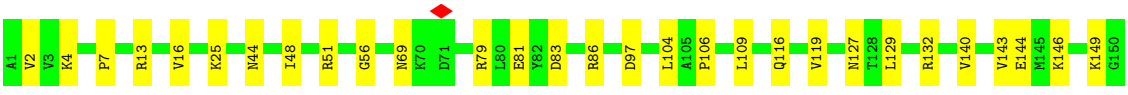
• Molecule 8: 50S ribosomal protein L19

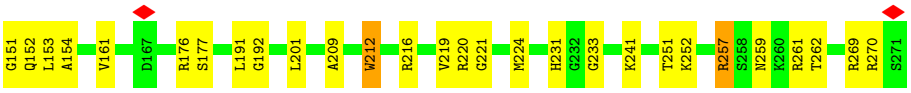
Chain 19:



• Molecule 9: 50S ribosomal protein L2

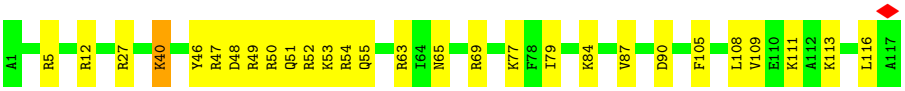
Chain 2:



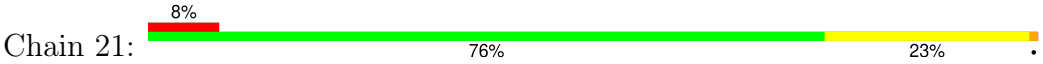


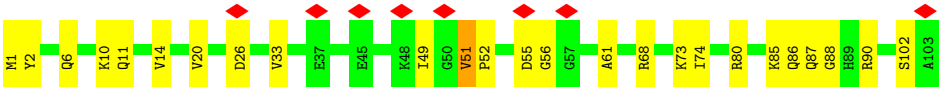
• Molecule 10: Large ribosomal subunit protein bL20

Chain 20:

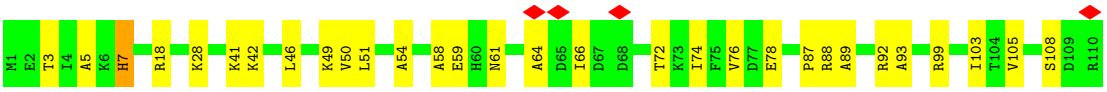


• Molecule 11: Large ribosomal subunit protein bL21

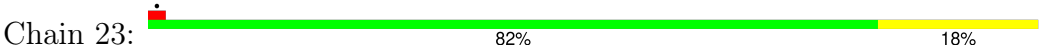


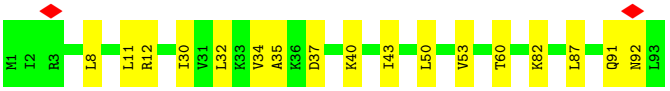


• Molecule 12: Large ribosomal subunit protein uL22

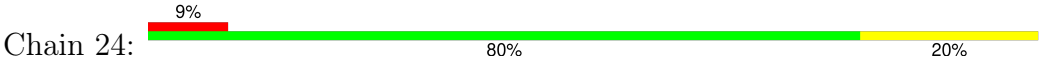


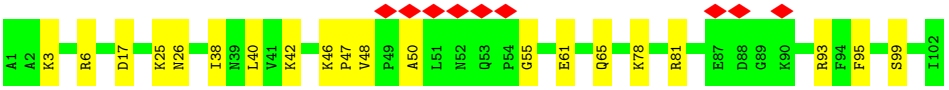
• Molecule 13: Large ribosomal subunit protein uL23



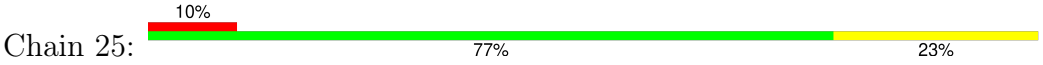


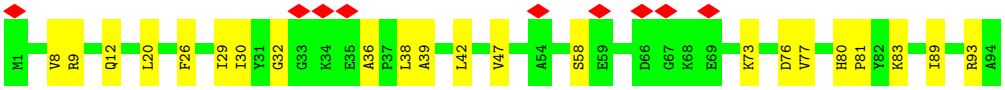
• Molecule 14: Large ribosomal subunit protein uL24



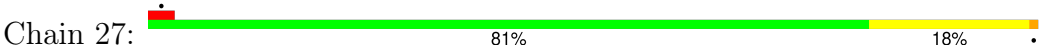


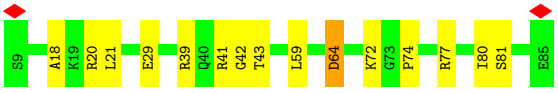
• Molecule 15: Large ribosomal subunit protein bL25





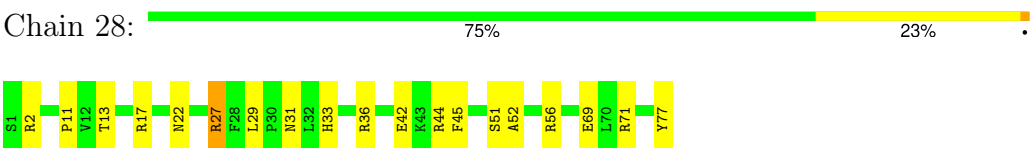
• Molecule 16: Large ribosomal subunit protein bL27





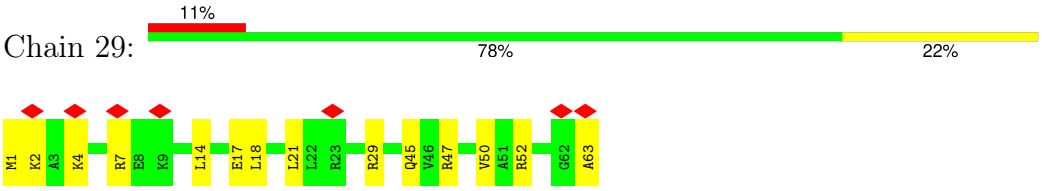
• Molecule 17: 50S ribosomal protein L28

Chain 28:



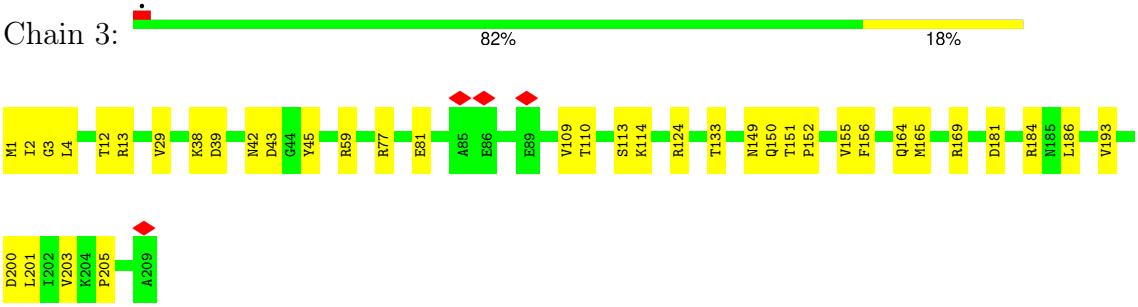
• Molecule 18: Large ribosomal subunit protein uL29

Chain 29:



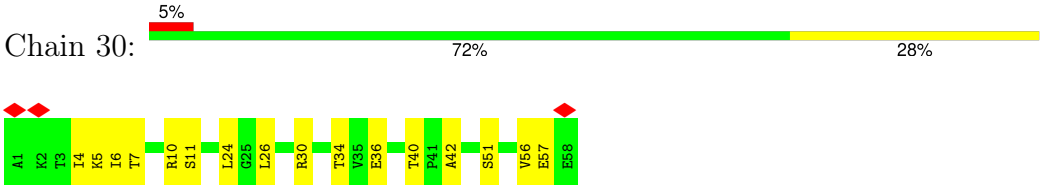
• Molecule 19: 50S ribosomal protein L3

Chain 3:



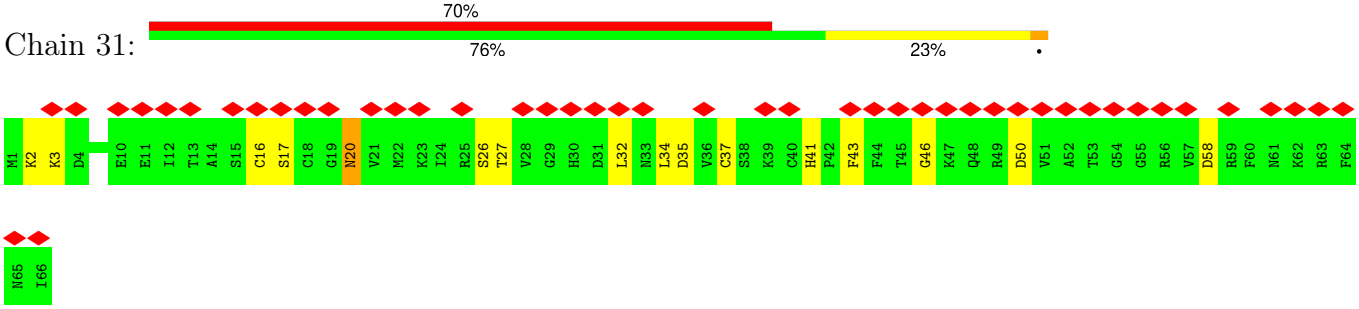
• Molecule 20: 50S ribosomal protein L30

Chain 30:



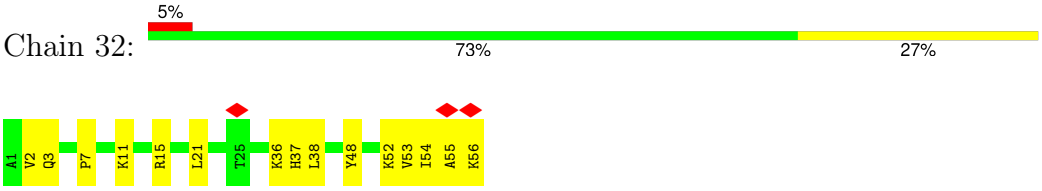
• Molecule 21: Large ribosomal subunit protein bL31

Chain 31:



• Molecule 22: 50S ribosomal protein L32

Chain 32:



• Molecule 23: Large ribosomal subunit protein bL33

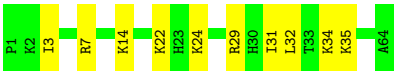
Chain 33:

• Molecule 24: 50S ribosomal protein L34

Chain 34:

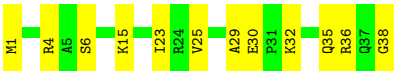
• Molecule 25: Large ribosomal subunit protein bL35

Chain 35:



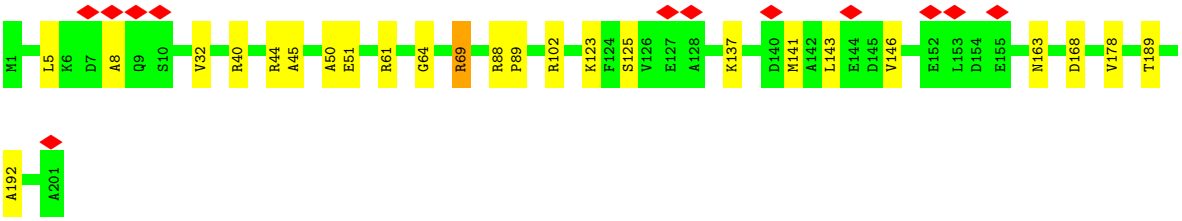
• Molecule 26: 50S ribosomal protein L36

Chain 36:



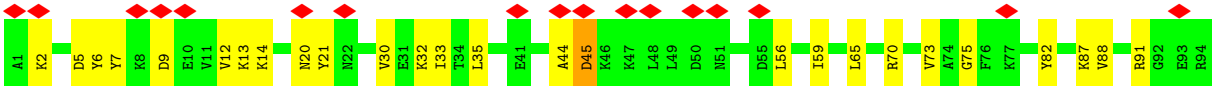
• Molecule 27: Large ribosomal subunit protein uL4

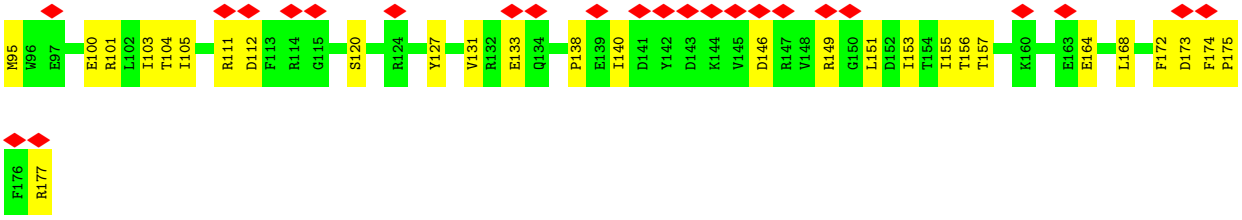
Chain 4:



• Molecule 28: 50S ribosomal protein L5

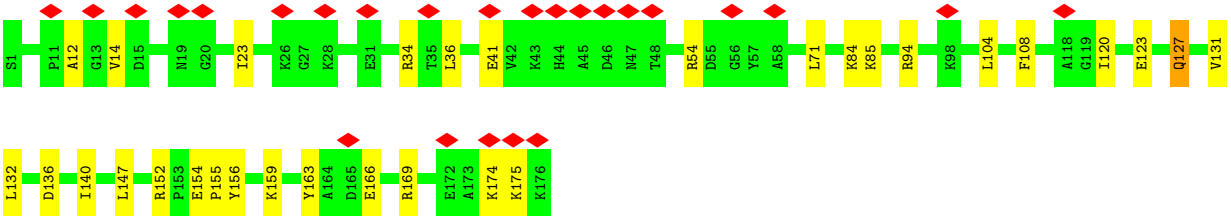
Chain 5:





• Molecule 29: Large ribosomal subunit protein uL6

Chain 6:

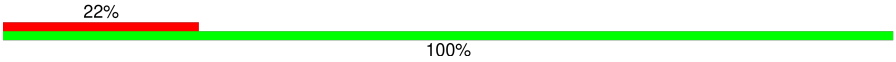


• Molecule 30: Large ribosomal subunit protein bL9

Chain 9:

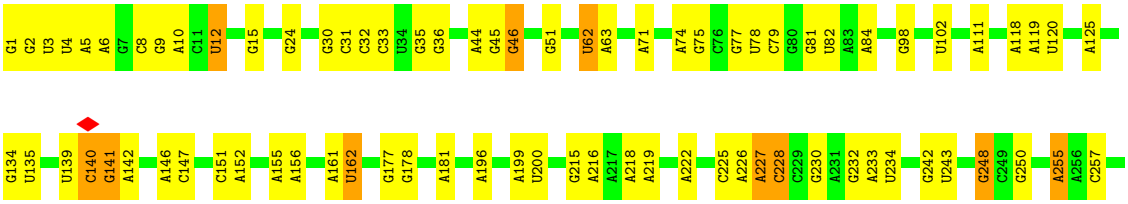
• Molecule 31: mRNA

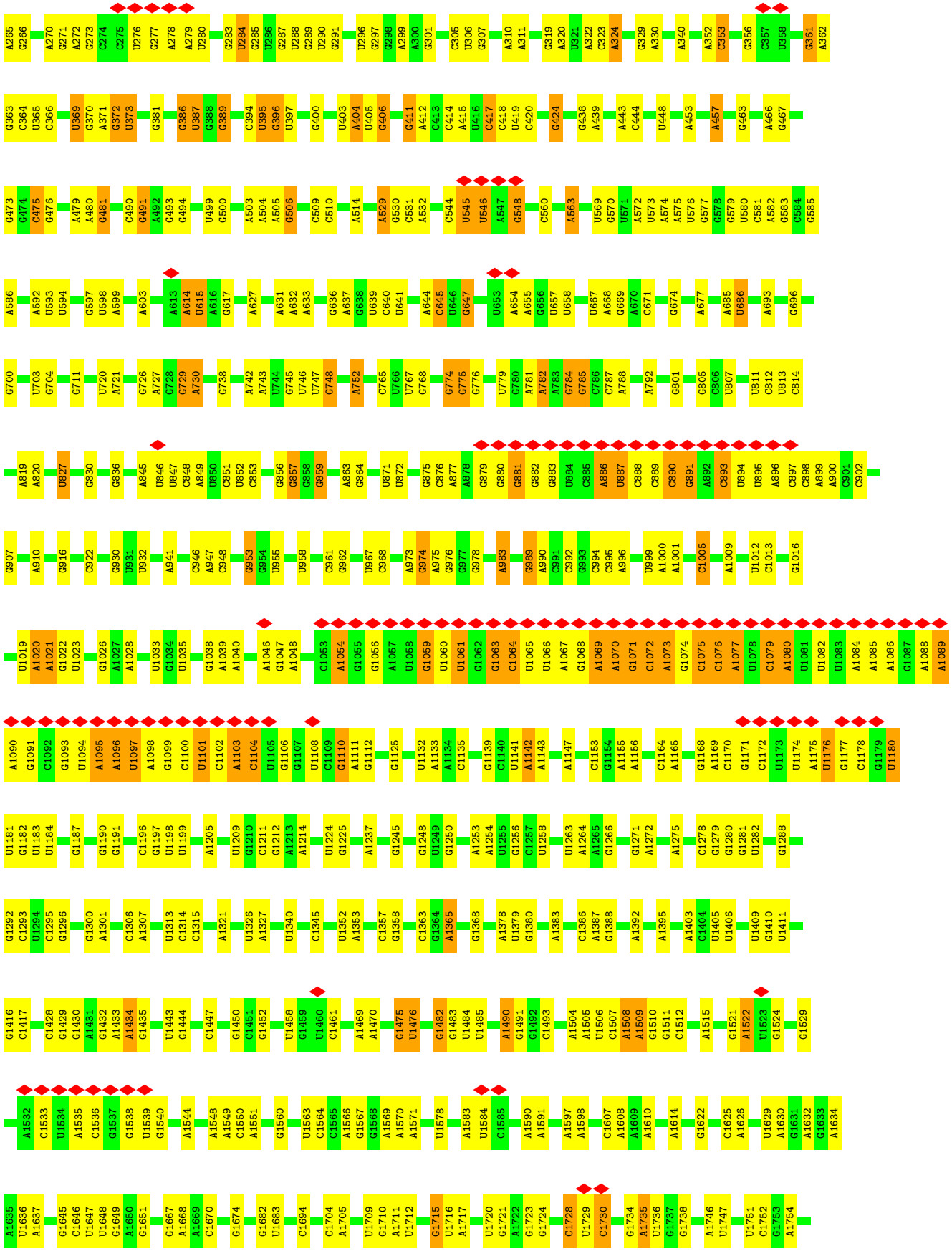
Chain M:

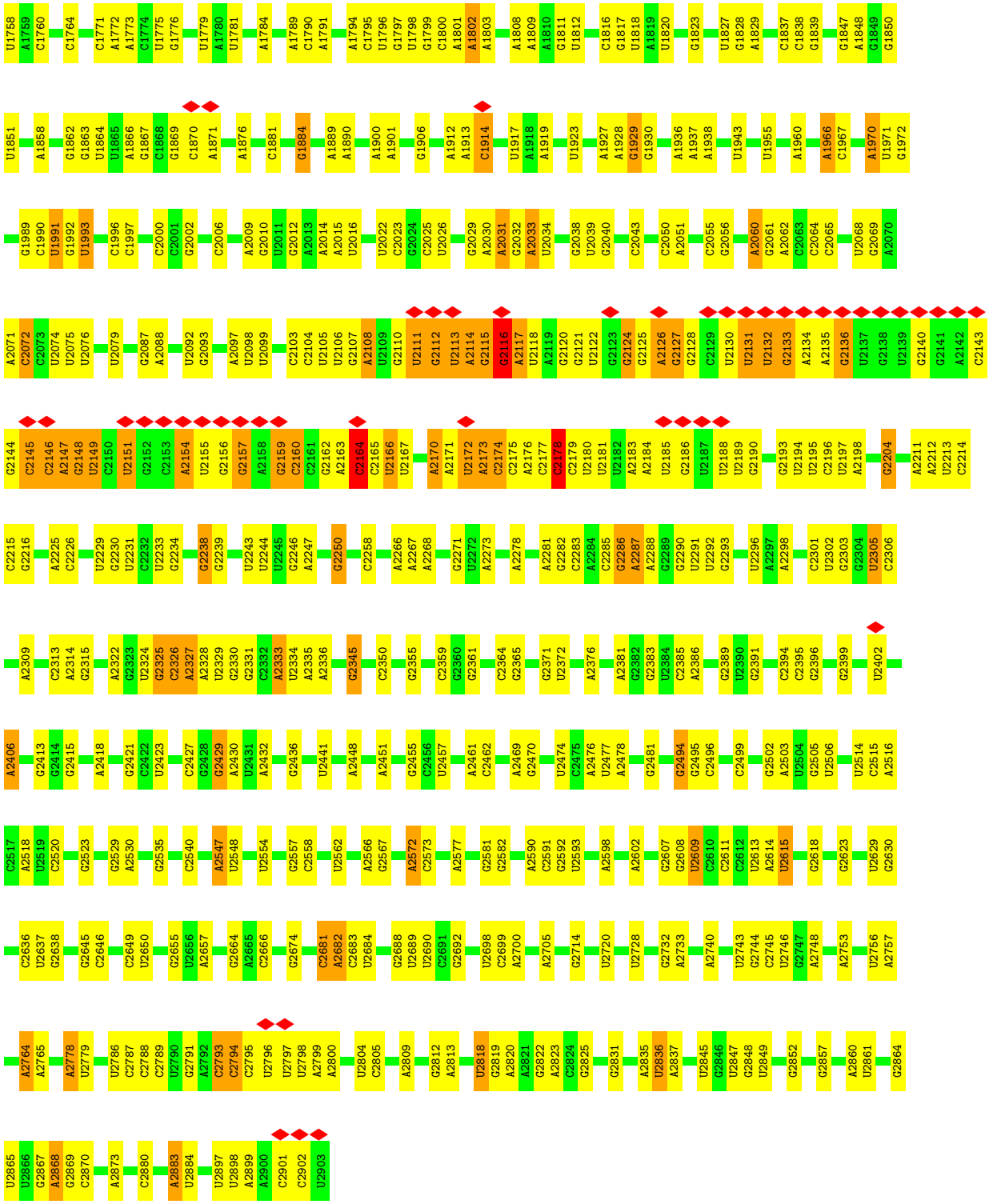


• Molecule 32: 23S ribosomal RNA

Chain R1:

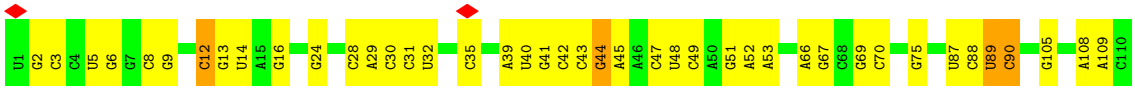



A265 G266 A270 C271 A272 G273 C274 C275 U276 G277 A278 A279 U280 G283 U284 C285 U286 U287 U288 G289 U290 G291 U296 C297 G298 A299 A300 G301 C305 U306 G307 A310 A311 G319 A320 U321 A322 C323 A324 G329 A330 A340 A352 C353 G356 C357 U358 G361 A362
G363 C364 U365 C366 U369 G370 A371 G372 U373 G381 G386 U387 G388 G389 C394 U395 G396 U397 G400 U403 A404 U405 G406 G411 A412 C413 C414 A415 U416 C417 C418 U419 C420 G424 G438 A439 A443 C444 U448 A453 A457 G463 A466 G467
G473 G474 C475 G476 A479 A480 G481 C490 G491 A492 G493 G494 U499 G500 A503 A504 A505 G506 C509 C510 A514 A529 G530 C531 A532 C544 U545 U546 A547 G548 C560 A563 U569 G570 U571 A572 U573 A574 A575 U576 G577 G578 G579 U580 C581 A582 G583 C584 G585
A586 A592 U593 U594 G597 U598 A599 A603 A613 A614 U615 A616 G617 A627 A631 A632 A633 G636 A637 G638 U639 C640 U641 A644 C645 U646 G647 U653 A654 A655 G656 U657 U658 U667 A668 G669 A670 C671 G674 A677 A685 U686 A693 G696
G700 U703 G704 C711 U720 A721 G726 A727 G728 G729 A730 G738 A742 A743 U744 G745 U746 U747 G748 A752 C765 U766 U767 G768 G774 G775 G776 U779 G780 A781 A782 A783 G784 G785 C786 C787 A788 A792 G801 C805 C806 U807 U811 C812 U813 C814
A819 A820 U827 G830 G836 A845 U846 U847 C848 A849 U850 C851 U852 C853 G856 G857 G858 G859 A863 G864 U871 U872 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886 U887 C888 G889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902
G907 A910 G916 C922 G930 U931 U932 A941 C946 A947 C948 G953 G954 U955 U958 C961 G962 U967 C968 A973 G974 A975 G976 G977 G978 A983 G989 A990 C991 C992 G993 C994 C995 A996 U999 A1000 A1001 C1005 A1009 U1012 C1013 G1016
U1019 A1020 A1021 G1022 U1023 G1026 A1027 A1028 U1033 G1034 U1035 G1038 A1039 A1040 A1046 G1047 A1048 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089
A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 G1125 U1132 A1133 A1134 C1135 G1139 C1140 U1141 A1142 A1143 A1147 C1153 G1154 A1155 A1156 C1164 A1165 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180
U1181 G1182 U1183 U1184 G1187 G1190 G1191 C1196 G1197 U1198 U1199 A1205 U1209 G1210 C1211 G1212 A1213 A1214 U1224 G1225 A1237 G1245 G1248 U1249 G1250 A1253 A1254 U1255 G1256 C1257 U1258 U1263 A1264 A1265 G1266 G1271 A1272 A1275 C1278 C1279 G1280 G1281 U1282 G1288
G1292 C1293 U1294 C1295 G1296 G1300 A1301 C1306 A1307 U1313 C1314 C1315 A1321 U1326 A1327 U1340 C1345 U1352 A1353 C1357 G1358 C1363 G1364 A1365 G1368 A1378 U1379 G1380 A1383 C1386 A1387 G1388 A1392 A1395 A1403 C1404 U1405 U1406 U1409 G1410 U1411
G1416 C1417 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 U1443 G1444 C1447 G1450 C1451 G1452 U1458 G1459 U1460 C1461 A1469 A1470 G1475 U1476 G1482 G1483 U1484 U1485 A1490 G1491 G1492 C1493 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1511 C1512 A1515 G1521 A1522 U1523 G1524 G1529
A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 A1544 A1548 A1549 C1550 A1551 G1560 U1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 U1578 A1583 U1584 C1585 A1590 A1591 A1597 A1598 C1607 A1608 A1609 A1610 A1614 G1622 C1625 A1626 U1629 A1630 G1631 A1632 G1633 A1634
A1635 U1636 A1637 G1645 C1646 U1647 U1648 G1649 A1650 G1651 G1667 A1668 A1669 C1670 G1674 G1682 U1683 C1694 C1704 A1705 U1709 G1710 A1711 U1712 G1715 U1716 A1717 U1720 G1721 A1722 G1723 G1724 C1728 U1729 C1730 G1734 A1735 U1736 G1737 G1738 A1746 U1747 U1751 C1752 G1753 A1754



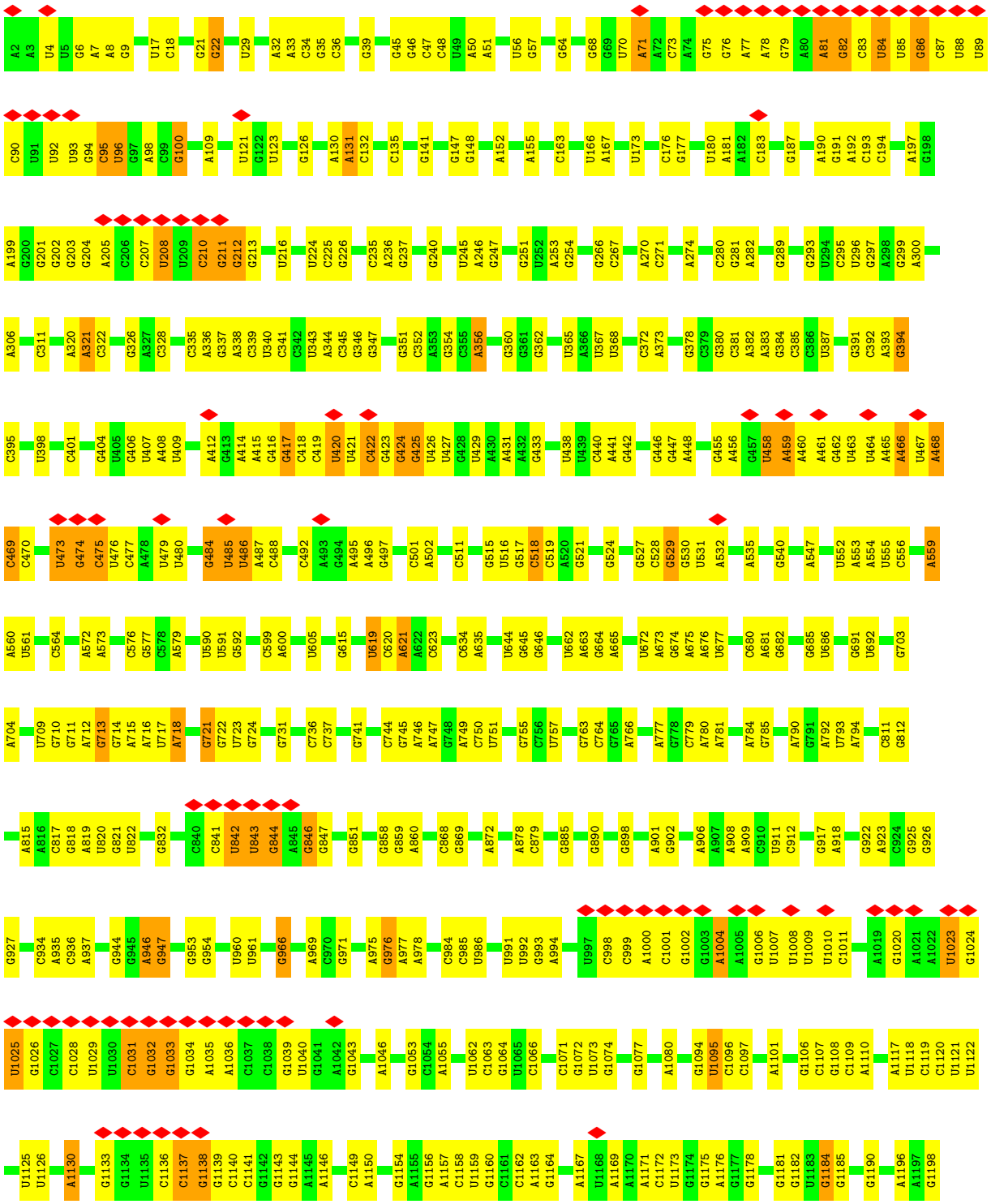
• Molecule 33: 5S ribosomal RNA

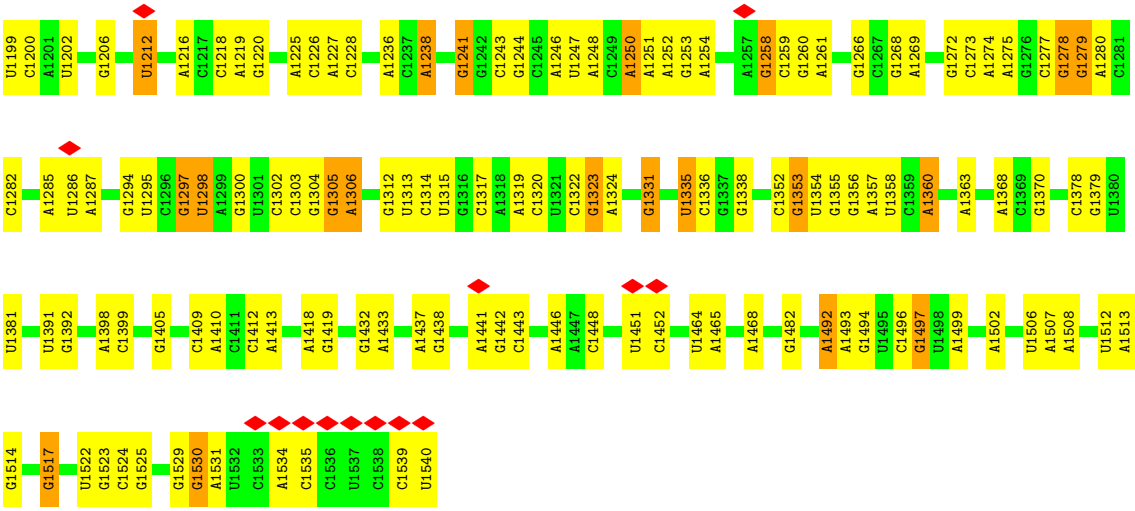
Chain R2:



• Molecule 34: 16S ribosomal RNA

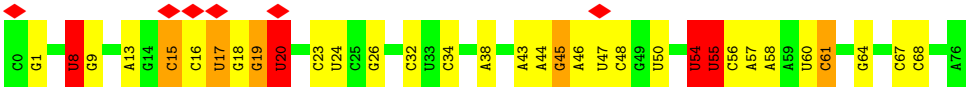
Chain R3:





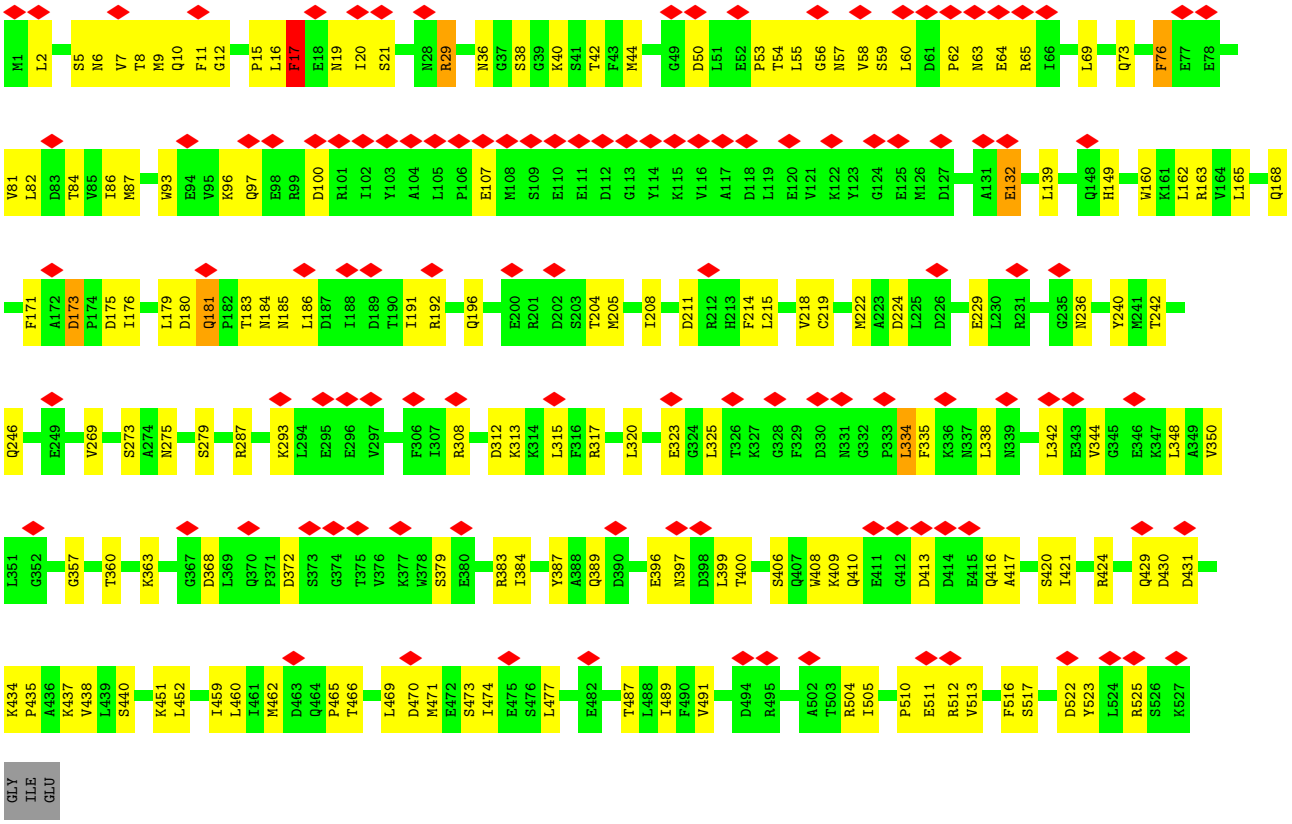
• Molecule 35: tRNA

Chain T:



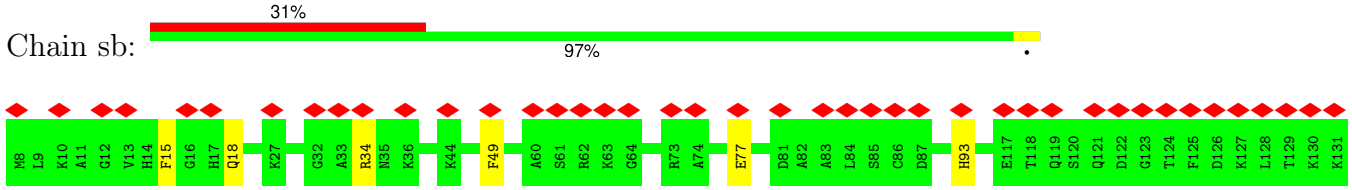
• Molecule 36: Probable ATP-binding protein YbiT

Chain Y:



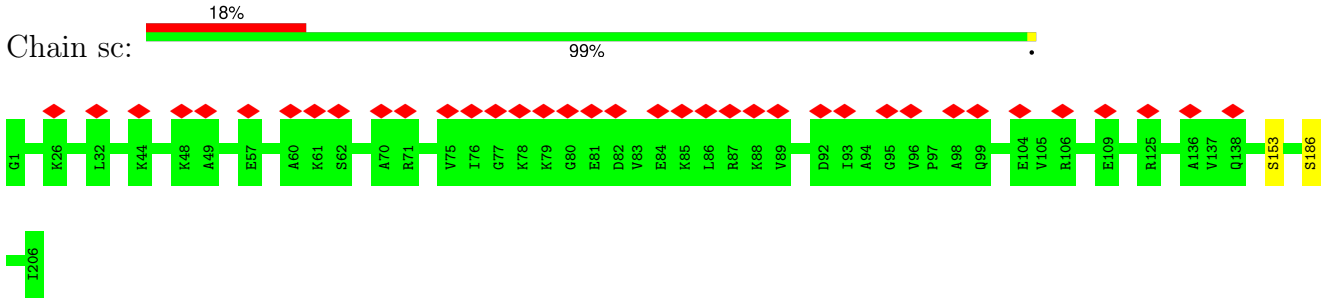
• Molecule 37: Small ribosomal subunit protein uS2

Chain sb:



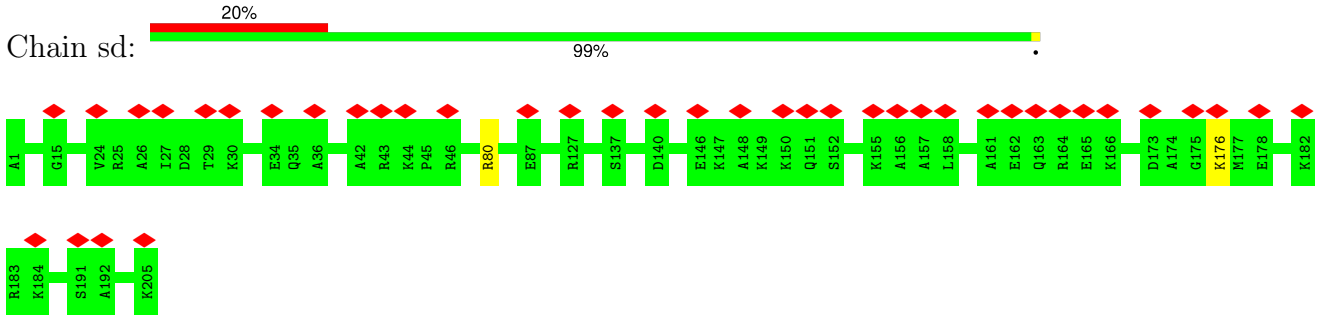
• Molecule 38: Small ribosomal subunit protein uS3

Chain sc:



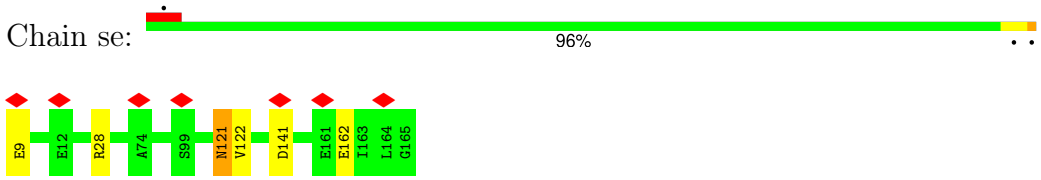
• Molecule 39: 30S ribosomal protein S4

Chain sd:



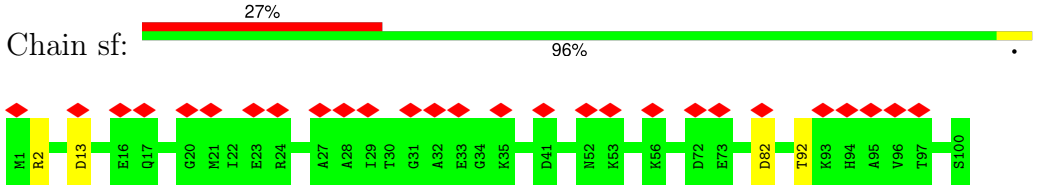
• Molecule 40: Small ribosomal subunit protein uS5

Chain se:



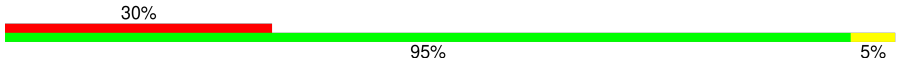
• Molecule 41: 30S ribosomal protein S6, non-modified isoform

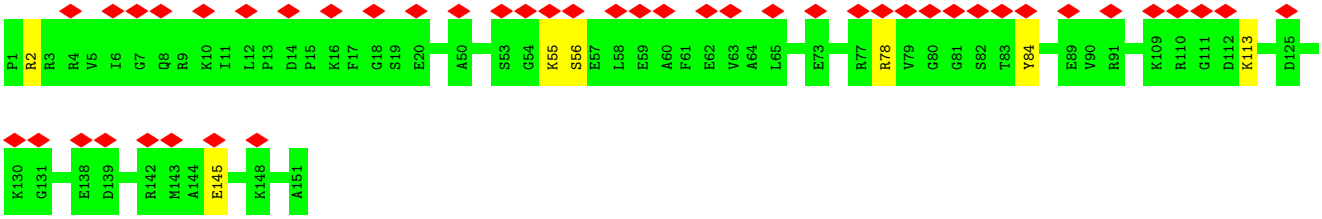
Chain sf:



• Molecule 42: 30S ribosomal protein S7

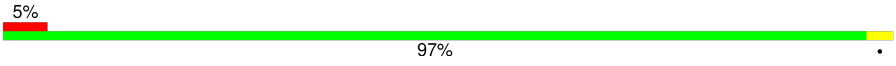
Chain sg:

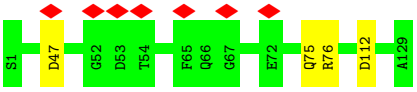




• Molecule 43: 30S ribosomal protein S8

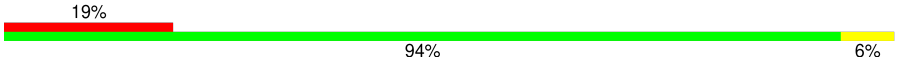
Chain sh:

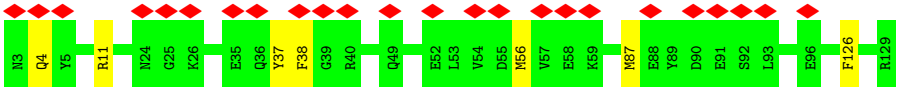




• Molecule 44: Small ribosomal subunit protein uS9

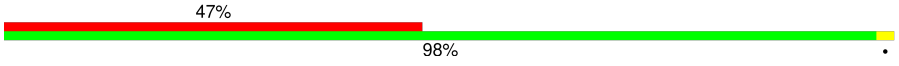
Chain si:

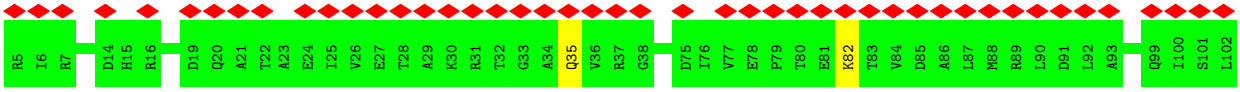




• Molecule 45: 30S ribosomal protein S10

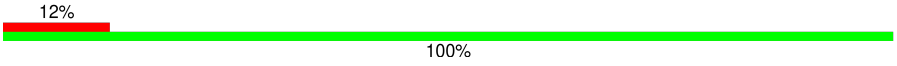
Chain sj:

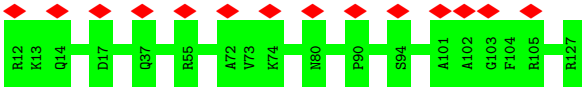




• Molecule 46: Small ribosomal subunit protein uS11

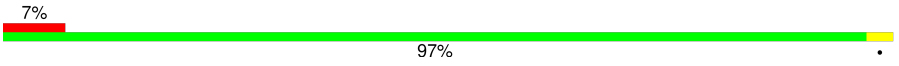
Chain sk:

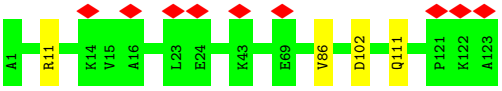




• Molecule 47: Small ribosomal subunit protein uS12

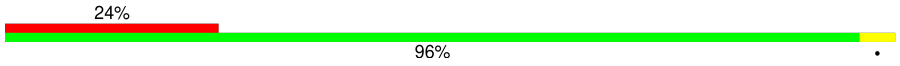
Chain sl:

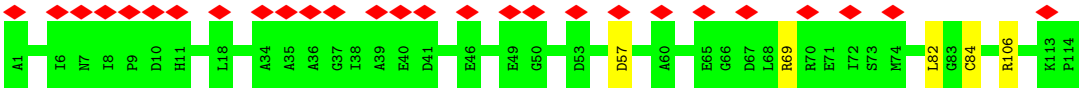




• Molecule 48: 30S ribosomal protein S13

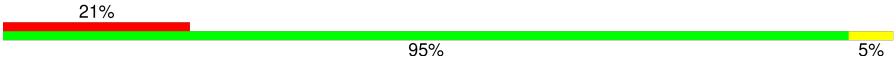
Chain sm:

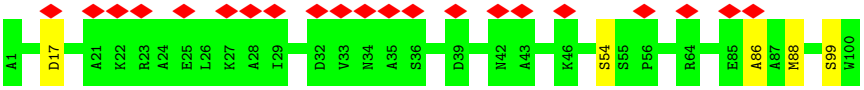




• Molecule 49: Small ribosomal subunit protein uS14

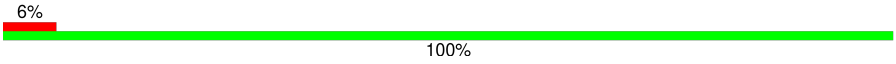
Chain sn:





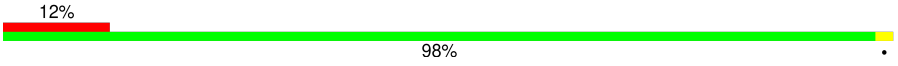
• Molecule 50: Small ribosomal subunit protein uS15

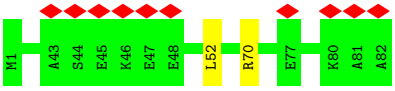
Chain so:



• Molecule 51: Small ribosomal subunit protein bS16

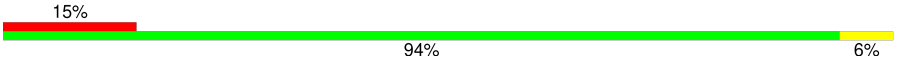
Chain sp:

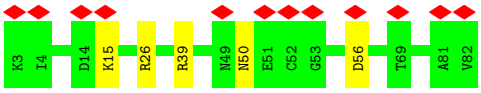




• Molecule 52: Small ribosomal subunit protein uS17

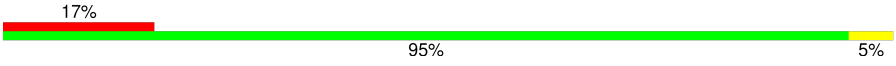
Chain sq:

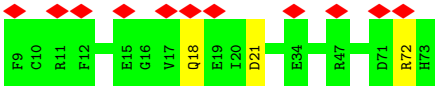




• Molecule 53: 30S ribosomal protein S18

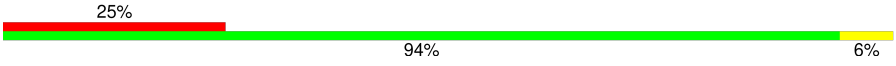
Chain sr:

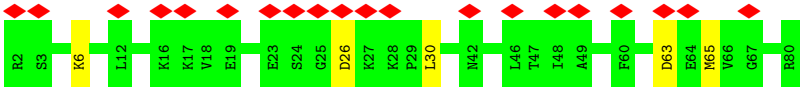




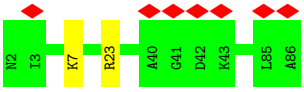
• Molecule 54: 30S ribosomal protein S19

Chain ss:

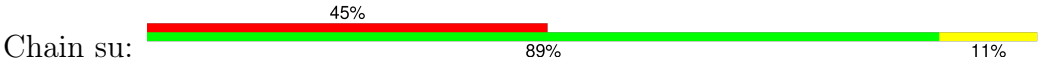


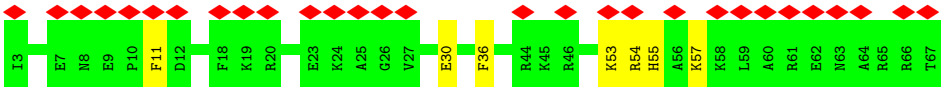


• Molecule 55: 30S ribosomal protein S20



• Molecule 56: Small ribosomal subunit protein bS21





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.850	Depositor
Minimum map value	-3.878	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.250	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, FME, PSU, MG, 4OC, 4SU, H2U, ATP, NA

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	0.24	0/1361	0.51	0/1796
2	13	0.28	0/1152	0.50	0/1551
3	14	0.29	0/947	0.58	0/1268
4	15	0.27	0/1062	0.59	0/1413
5	16	0.28	0/1093	0.59	0/1460
6	17	0.26	0/973	0.58	0/1301
7	18	0.25	0/902	0.54	0/1209
8	19	0.28	0/929	0.56	0/1242
9	2	0.28	0/2121	0.57	0/2852
10	20	0.30	0/960	0.52	0/1278
11	21	0.29	0/829	0.57	0/1107
12	22	0.27	0/864	0.54	0/1156
13	23	0.27	0/744	0.54	0/994
14	24	0.27	0/787	0.51	0/1051
15	25	0.26	0/766	0.48	0/1025
16	27	0.28	0/595	0.54	0/787
17	28	0.26	0/635	0.56	0/848
18	29	0.24	0/510	0.55	0/677
19	3	0.28	0/1586	0.52	0/2134
20	30	0.25	0/453	0.55	0/605
21	31	0.25	0/531	0.51	0/709
22	32	0.28	0/450	0.58	0/599
23	33	0.28	0/416	0.51	0/554
24	34	0.26	0/380	0.64	0/498
25	35	0.27	0/513	0.53	0/676
26	36	0.27	0/303	0.58	0/397
27	4	0.26	0/1571	0.50	0/2113
28	5	0.26	0/1434	0.51	0/1926
29	6	0.26	0/1343	0.50	0/1816
30	9	0.26	0/1122	0.55	0/1515
31	M	0.21	0/219	0.72	0/339
32	R1	0.35	2/69796 (0.0%)	0.81	22/108886 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	R2	0.29	0/2847	0.82	0/4440
34	R3	0.27	0/36963	0.78	4/57662 (0.0%)
35	T	0.26	0/1716	0.79	2/2672 (0.1%)
36	Y	0.25	0/4245	0.50	0/5723
37	sb	0.25	0/1735	0.50	0/2338
38	sc	0.25	0/1651	0.53	0/2225
39	sd	0.25	0/1665	0.54	0/2227
40	se	0.27	0/1169	0.59	1/1573 (0.1%)
41	sf	0.25	0/835	0.56	0/1128
42	sg	0.25	0/1195	0.54	0/1602
43	sh	0.26	0/989	0.50	0/1326
44	si	0.26	0/1034	0.61	0/1375
45	sj	0.25	0/796	0.57	0/1077
46	sk	0.26	0/885	0.56	0/1195
47	sl	0.27	0/969	0.64	0/1300
48	sm	0.24	0/892	0.57	0/1193
49	sn	0.24	0/817	0.58	0/1088
50	so	0.23	0/722	0.53	0/964
51	sp	0.25	0/659	0.56	0/884
52	sq	0.25	0/657	0.54	0/881
53	sr	0.26	0/544	0.53	0/731
54	ss	0.25	0/652	0.56	0/877
55	st	0.24	0/671	0.46	0/888
56	su	0.28	0/550	0.69	0/728
All	All	0.31	2/162205 (0.0%)	0.74	29/241879 (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
13	23	0	1
30	9	0	1
35	T	7	0
36	Y	0	1
40	se	0	1
41	sf	0	1
47	sl	0	1
49	sn	0	1
All	All	7	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	R1	2116	G	C6-N1	-6.73	1.34	1.39
32	R1	2164	C	N3-C4	-5.71	1.29	1.33

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R1	2116	G	N1-C6-O6	-29.81	102.01	119.90
32	R1	2164	C	N3-C4-N4	-27.42	98.80	118.00
32	R1	2116	G	C5-C6-O6	26.48	144.49	128.60
32	R1	2164	C	C5-C4-N4	22.76	136.13	120.20
32	R1	2164	C	C4-C5-C6	-11.14	111.83	117.40

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	8	4SU	C2',C1'
35	T	20	H2U	C2'
35	T	32	4OC	C2'
35	T	54	5MU	C4',C3'
35	T	55	PSU	C4'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	23	37	ASP	Peptide
30	9	8	LYS	Peptide
36	Y	17	PHE	Peptide
40	se	121	ASN	Peptide
41	sf	92	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	26	0
2	13	1129	0	1162	19	0
3	14	938	0	1012	10	0
4	15	1053	0	1129	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	16	1074	0	1157	17	0
6	17	960	0	1000	15	0
7	18	892	0	923	19	0
8	19	917	0	965	18	0
9	2	2082	0	2157	44	0
10	20	947	0	1022	23	0
11	21	816	0	839	16	0
12	22	857	0	922	26	0
13	23	738	0	807	11	0
14	24	779	0	834	13	0
15	25	753	0	780	13	0
16	27	588	0	604	15	0
17	28	625	0	655	11	0
18	29	509	0	543	10	0
19	3	1565	0	1616	28	0
20	30	449	0	491	10	0
21	31	522	0	524	8	0
22	32	444	0	461	14	0
23	33	409	0	440	7	0
24	34	377	0	418	5	0
25	35	504	0	574	7	0
26	36	302	0	343	9	0
27	4	1552	0	1619	18	0
28	5	1410	0	1447	34	0
29	6	1323	0	1374	19	0
30	9	1111	0	1148	26	0
31	M	195	0	99	0	0
32	R1	62318	0	31346	635	0
33	R2	2546	0	1292	34	0
34	R3	33012	0	16617	317	0
35	T	1639	0	843	14	0
36	Y	4170	0	4132	112	0
37	sb	1704	0	1732	0	0
38	sc	1624	0	1699	0	0
39	sd	1643	0	1710	0	0
40	se	1156	0	1199	0	0
41	sf	817	0	808	0	0
42	sg	1181	0	1240	0	0
43	sh	979	0	1034	0	0
44	si	1022	0	1070	0	0
45	sj	786	0	828	0	0
46	sk	869	0	878	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	sl	955	0	1019	0	0
48	sm	883	0	944	0	0
49	sn	805	0	847	0	0
50	so	714	0	737	0	0
51	sp	649	0	666	0	0
52	sq	648	0	691	0	0
53	sr	535	0	552	0	0
54	ss	637	0	665	0	0
55	st	665	0	714	0	0
56	su	544	0	579	0	0
57	15	1	0	0	0	0
57	17	1	0	0	0	0
57	32	1	0	0	0	0
57	34	1	0	0	0	0
57	R1	184	0	0	0	0
57	R3	57	0	0	0	0
58	T	10	0	10	3	0
59	Y	62	0	24	3	0
60	Y	2	0	0	0	0
All	All	149993	0	102100	1456	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1456 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:284:U:H3	32:R1:356:G:H1	1.14	0.93
32:R1:2116:G:H1	32:R1:2164:C:H42	1.19	0.90
32:R1:1091:G:N2	32:R1:1100:C:O2	2.06	0.87
34:R3:673:A:H2'	34:R3:674:G:C8	2.18	0.79
32:R1:2391:G:O2'	32:R1:2429:G:N2	2.16	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	218/220 (99%)	204 (94%)	14 (6%)	0	100	100
2	13	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
3	14	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
4	15	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
5	16	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
6	17	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
7	18	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
8	19	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
9	2	269/271 (99%)	252 (94%)	17 (6%)	0	100	100
10	20	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
11	21	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	13	47
12	22	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
13	23	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
14	24	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
15	25	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
16	27	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
17	28	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
18	29	61/63 (97%)	61 (100%)	0	0	100	100
19	3	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
20	30	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
21	31	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
22	32	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	33	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
24	34	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
25	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
27	4	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
28	5	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
29	6	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
30	9	147/149 (99%)	131 (89%)	14 (10%)	2 (1%)	9	40
36	Y	525/530 (99%)	458 (87%)	65 (12%)	2 (0%)	30	64
37	sb	216/218 (99%)	198 (92%)	17 (8%)	1 (0%)	25	60
38	sc	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
39	sd	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
40	se	155/157 (99%)	130 (84%)	23 (15%)	2 (1%)	10	41
41	sf	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
42	sg	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
43	sh	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
44	si	125/127 (98%)	105 (84%)	20 (16%)	0	100	100
45	sj	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
46	sk	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
47	sl	121/123 (98%)	99 (82%)	22 (18%)	0	100	100
48	sm	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
49	sn	98/100 (98%)	77 (79%)	21 (21%)	0	100	100
50	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
51	sp	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
52	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
53	sr	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
54	ss	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
55	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
56	su	63/65 (97%)	43 (68%)	20 (32%)	0	100	100
All	All	6324/6429 (98%)	5776 (91%)	540 (8%)	8 (0%)	50	80

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	21	51	VAL
36	Y	58	VAL

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Mol	Chain	Res	Type
37	sb	18	GLN
40	se	122	VAL
30	9	9	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	106/171 (62%)	100 (94%)	6 (6%)	17	50
2	13	116/116 (100%)	114 (98%)	2 (2%)	56	78
3	14	103/103 (100%)	99 (96%)	4 (4%)	27	60
4	15	103/103 (100%)	101 (98%)	2 (2%)	52	76
5	16	109/109 (100%)	108 (99%)	1 (1%)	75	89
6	17	100/100 (100%)	99 (99%)	1 (1%)	73	87
7	18	86/86 (100%)	83 (96%)	3 (4%)	31	63
8	19	99/99 (100%)	96 (97%)	3 (3%)	36	66
9	2	216/216 (100%)	209 (97%)	7 (3%)	34	65
10	20	89/89 (100%)	85 (96%)	4 (4%)	23	56
11	21	84/84 (100%)	80 (95%)	4 (5%)	21	55
12	22	93/93 (100%)	91 (98%)	2 (2%)	47	73
13	23	80/80 (100%)	80 (100%)	0	100	100
14	24	83/83 (100%)	81 (98%)	2 (2%)	44	71
15	25	78/78 (100%)	77 (99%)	1 (1%)	65	83
16	27	59/59 (100%)	57 (97%)	2 (3%)	32	63
17	28	67/67 (100%)	65 (97%)	2 (3%)	36	66
18	29	55/55 (100%)	53 (96%)	2 (4%)	30	62
19	3	164/164 (100%)	163 (99%)	1 (1%)	84	92
20	30	48/48 (100%)	46 (96%)	2 (4%)	25	58
21	31	59/59 (100%)	56 (95%)	3 (5%)	20	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	32	47/47 (100%)	47 (100%)	0	100 100
23	33	45/45 (100%)	44 (98%)	1 (2%)	47 73
24	34	38/38 (100%)	38 (100%)	0	100 100
25	35	51/51 (100%)	49 (96%)	2 (4%)	27 60
26	36	34/34 (100%)	34 (100%)	0	100 100
27	4	165/165 (100%)	162 (98%)	3 (2%)	54 77
28	5	148/148 (100%)	140 (95%)	8 (5%)	18 51
29	6	137/137 (100%)	134 (98%)	3 (2%)	47 73
30	9	114/114 (100%)	107 (94%)	7 (6%)	15 47
36	Y	449/456 (98%)	427 (95%)	22 (5%)	21 54
37	sb	180/180 (100%)	175 (97%)	5 (3%)	38 68
38	sc	170/170 (100%)	168 (99%)	2 (1%)	67 85
39	sd	172/172 (100%)	170 (99%)	2 (1%)	67 85
40	se	119/119 (100%)	116 (98%)	3 (2%)	42 71
41	sf	87/87 (100%)	84 (97%)	3 (3%)	32 63
42	sg	124/124 (100%)	117 (94%)	7 (6%)	17 50
43	sh	104/104 (100%)	100 (96%)	4 (4%)	28 60
44	si	105/105 (100%)	98 (93%)	7 (7%)	13 44
45	sj	86/86 (100%)	84 (98%)	2 (2%)	45 72
46	sk	89/89 (100%)	89 (100%)	0	100 100
47	sl	103/103 (100%)	100 (97%)	3 (3%)	37 67
48	sm	92/92 (100%)	87 (95%)	5 (5%)	18 51
49	sn	83/83 (100%)	79 (95%)	4 (5%)	21 55
50	so	76/76 (100%)	76 (100%)	0	100 100
51	sp	65/65 (100%)	63 (97%)	2 (3%)	35 66
52	sq	74/74 (100%)	69 (93%)	5 (7%)	13 43
53	sr	56/56 (100%)	53 (95%)	3 (5%)	18 51
54	ss	70/70 (100%)	65 (93%)	5 (7%)	12 42
55	st	65/65 (100%)	63 (97%)	2 (3%)	35 66
56	su	55/55 (100%)	48 (87%)	7 (13%)	3 17
All	All	5200/5272 (99%)	5029 (97%)	171 (3%)	35 64

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	sg	2	ARG
49	sn	17	ASP
42	sg	84	TYR
44	si	56	MET
52	sq	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
19	3	42	ASN
42	sg	85	GLN
36	Y	63	ASN
42	sg	147	ASN
38	sc	184	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	M	8/9 (88%)	0	0
32	R1	2901/2903 (99%)	454 (15%)	11 (0%)
33	R2	118/119 (99%)	15 (12%)	1 (0%)
34	R3	1538/1539 (99%)	277 (18%)	4 (0%)
35	T	75/77 (97%)	17 (22%)	4 (5%)
All	All	4640/4647 (99%)	763 (16%)	20 (0%)

5 of 763 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	R1	10	A
32	R1	15	G
32	R1	35	G
32	R1	36	G
32	R1	46	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	R3	1305	G
35	T	17	U

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Mol	Chain	Res	Type
35	T	55	PSU
35	T	19	G
32	R1	1475	G

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

5 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	$\#\|Z\| > 2$
35	PSU	T	55	35	18,21,22	2.35	9 (50%)	21,30,33	2.00	5 (23%)
35	4SU	T	8	35	18,21,22	3.51	7 (38%)	25,30,33	2.30	6 (24%)
35	4OC	T	32	35	20,23,24	3.06	3 (15%)	25,32,35	1.00	2 (8%)
35	5MU	T	54	35	19,22,23	1.94	8 (42%)	27,32,35	2.21	8 (29%)
35	H2U	T	20	35	18,21,22	4.37	5 (27%)	19,30,33	3.98	6 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	T	55	35	1/1/5/5	1/7/25/26	0/2/2/2
35	4SU	T	8	35	2/2/5/5	2/7/25/26	0/2/2/2
35	4OC	T	32	35	1/1/5/6	0/9/29/30	0/2/2/2
35	5MU	T	54	35	2/2/5/5	4/7/25/26	0/2/2/2
35	H2U	T	20	35	1/1/8/9	5/7/38/39	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	32	4OC	O2-C2	11.75	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	20	H2U	O4-C4	10.32	1.43	1.23
35	T	8	4SU	O2-C2	9.84	1.40	1.23
35	T	20	H2U	C2-N1	9.34	1.48	1.35
35	T	20	H2U	O2-C2	8.48	1.38	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	20	H2U	O2-C2-N1	-10.89	110.01	123.10
35	T	20	H2U	O4-C4-N3	-7.43	108.85	120.30
35	T	8	4SU	C4-N3-C2	-6.56	121.02	127.31
35	T	20	H2U	O4-C4-C5	-6.55	108.79	122.20
35	T	20	H2U	O2-C2-N3	-6.34	109.79	121.49

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	20	H2U	C2'
35	T	32	4OC	C2'
35	T	54	5MU	C4'
35	T	54	5MU	C3'
35	T	55	PSU	C4'

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	T	20	H2U	O4'-C4'-C5'-O5'
35	T	20	H2U	C3'-C4'-C5'-O5'
35	T	20	H2U	O4'-C1'-N1-C2
35	T	20	H2U	O4'-C1'-N1-C6
35	T	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	T	55	PSU	1	0
35	T	20	H2U	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 250 ligands modelled in this entry, 247 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
58	FME	T	101	35	8,9,10	1.01	0	8,9,11	0.84	0
59	ATP	Y	602	60	28,33,33	0.67	0	34,52,52	0.59	1 (2%)
59	ATP	Y	601	60	28,33,33	0.67	0	34,52,52	0.61	1 (2%)

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
58	FME	T	101	35	-	3/7/9/11	-
59	ATP	Y	602	60	-	7/18/38/38	0/3/3/3
59	ATP	Y	601	60	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	Y	602	ATP	C5-C6-N6	2.32	123.84	120.31
59	Y	601	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	Y	602	ATP	C5'-O5'-PA-O3A
59	Y	602	ATP	O4'-C4'-C5'-O5'
59	Y	602	ATP	C3'-C4'-C5'-O5'
58	T	101	FME	N-CA-CB-CG
59	Y	602	ATP	PB-O3A-PA-O5'

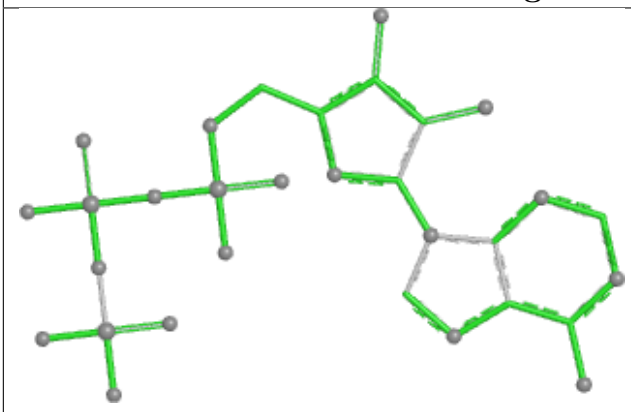
There are no ring outliers.

2 monomers are involved in 6 short contacts:

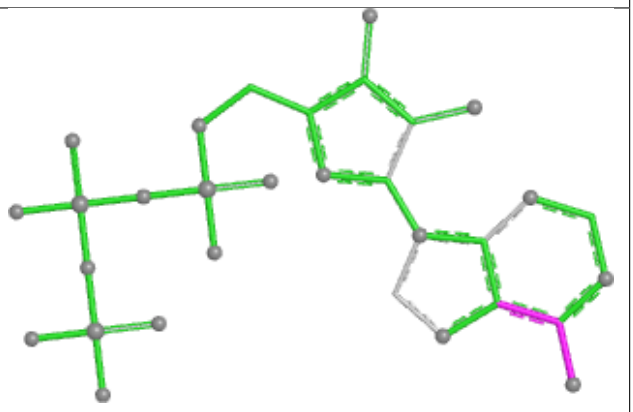
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	T	101	FME	3	0
59	Y	601	ATP	3	0

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.

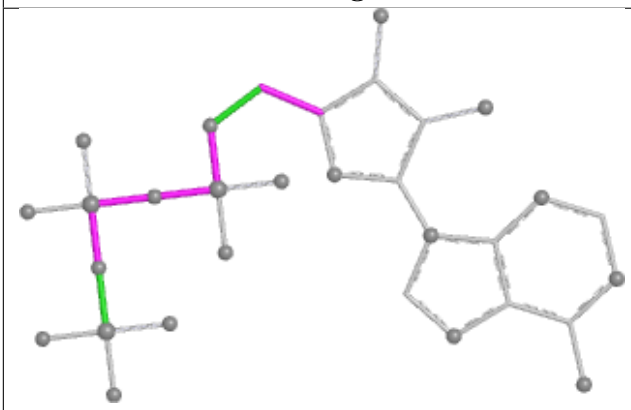
Ligand ATP Y 602



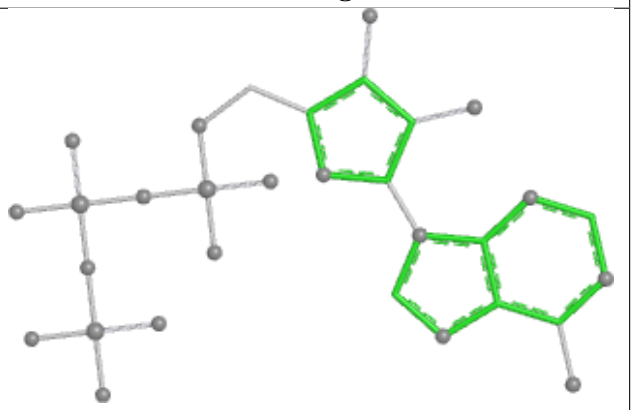
Bond lengths



Bond angles

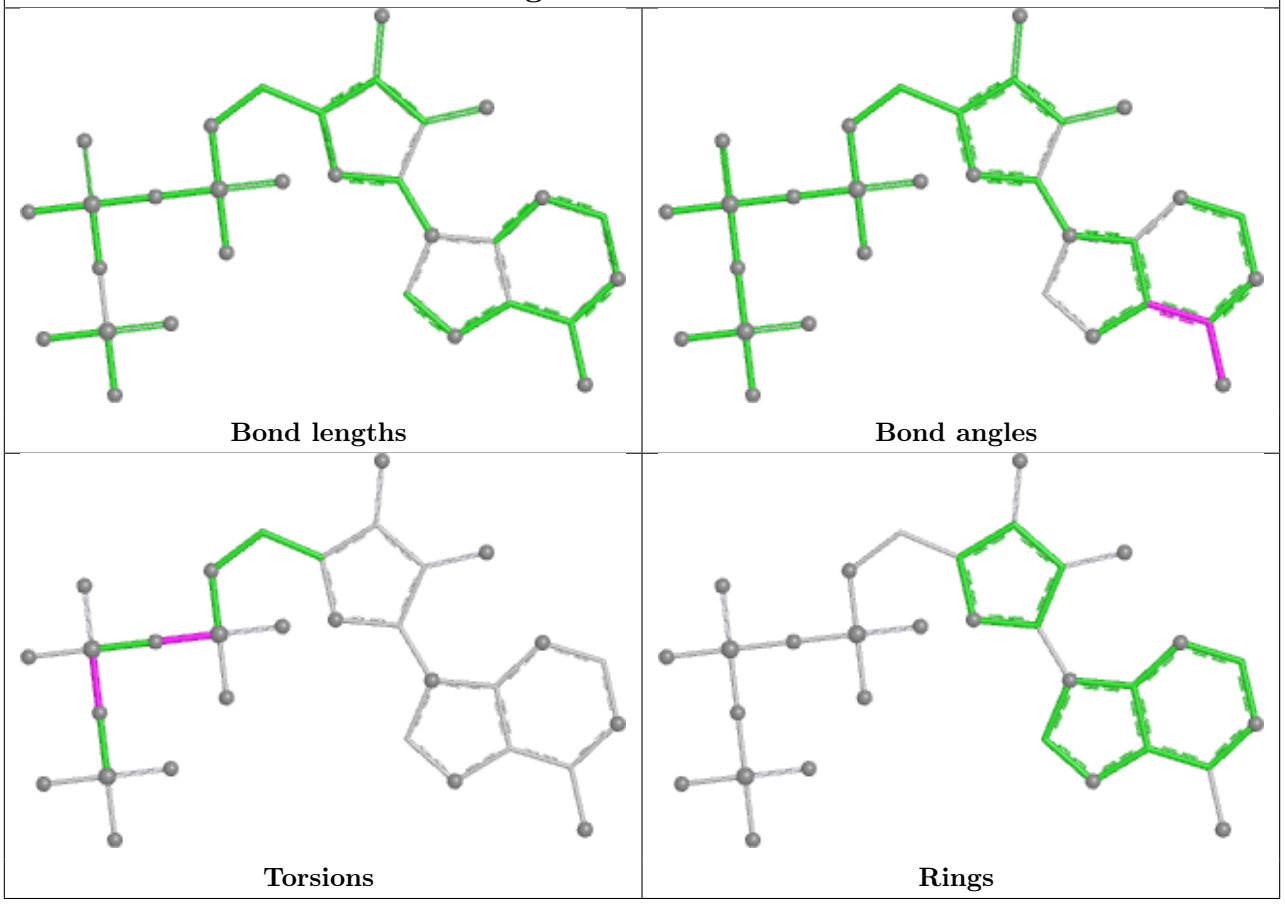


Torsions



Rings

Ligand ATP Y 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	R1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R1	2095:A	O3'	2096:C	P	3.16

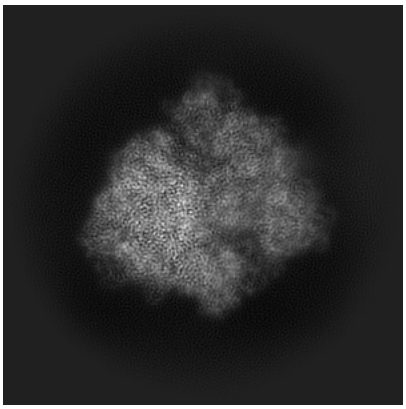
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40924. These allow visual inspection of the internal detail of the map and identification of artifacts.

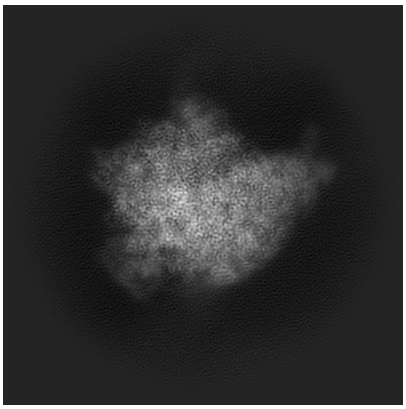
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

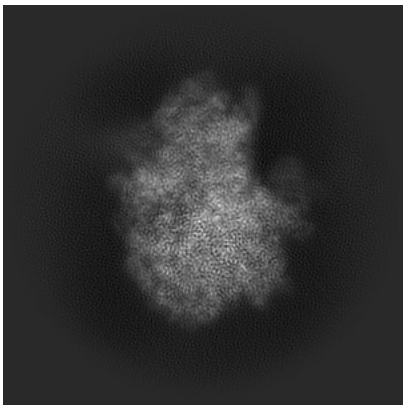
6.1.1 Primary map



X

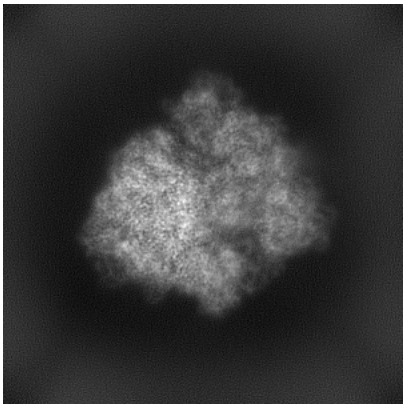


Y

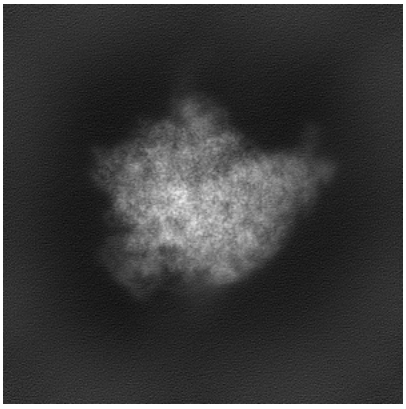


Z

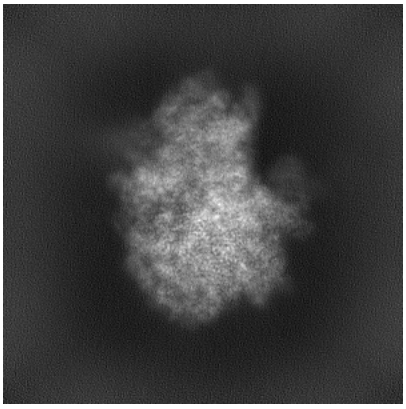
6.1.2 Raw map



X



Y

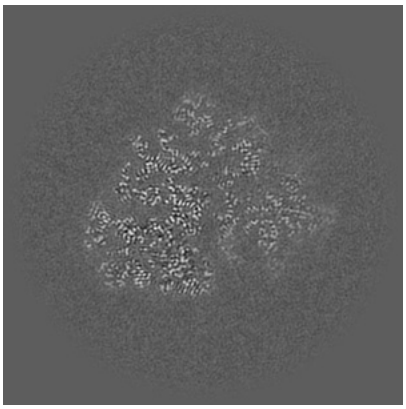


Z

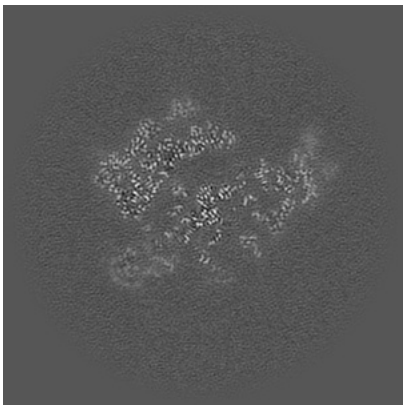
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

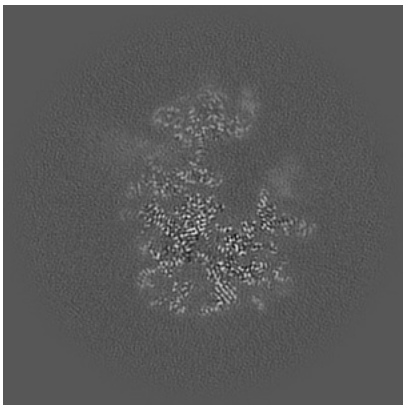
6.2.1 Primary map



X Index: 200

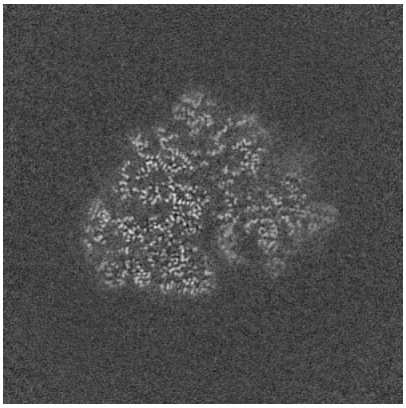


Y Index: 200

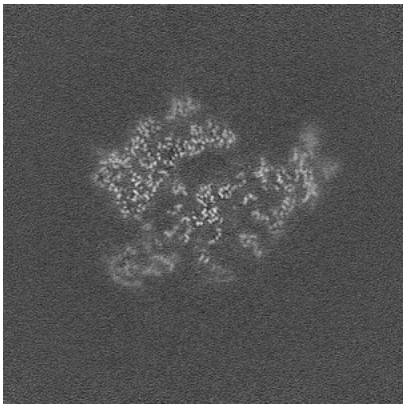


Z Index: 200

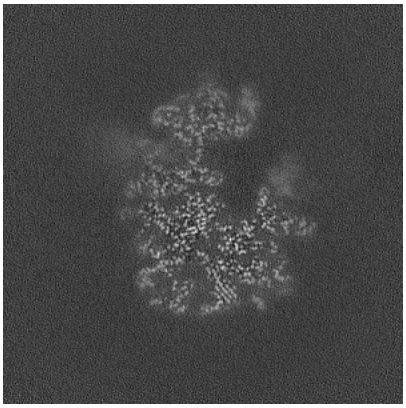
6.2.2 Raw map



X Index: 200



Y Index: 200

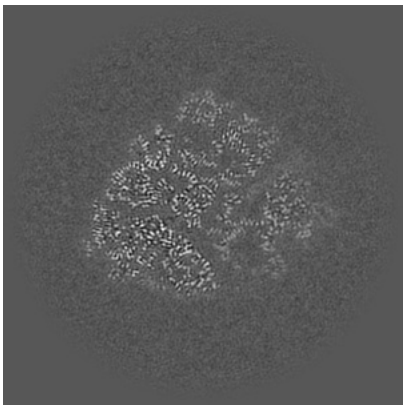


Z Index: 200

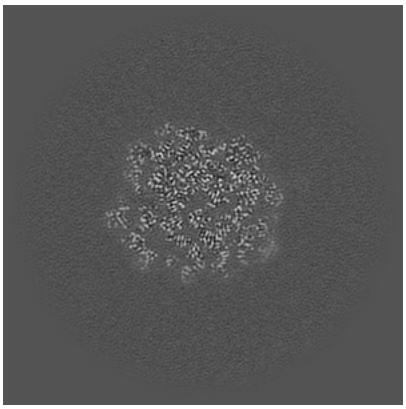
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

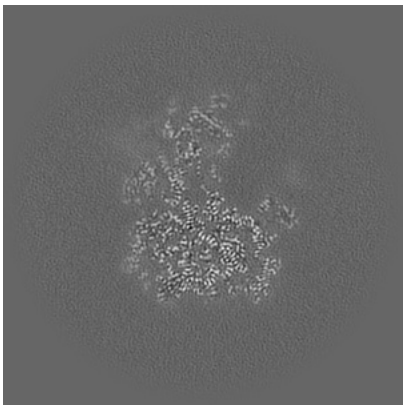
6.3.1 Primary map



X Index: 206

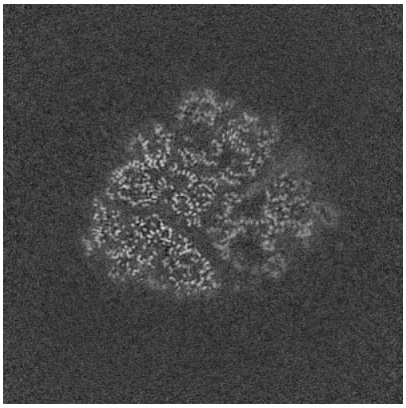


Y Index: 156

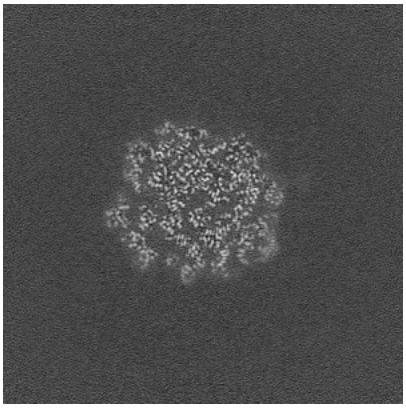


Z Index: 217

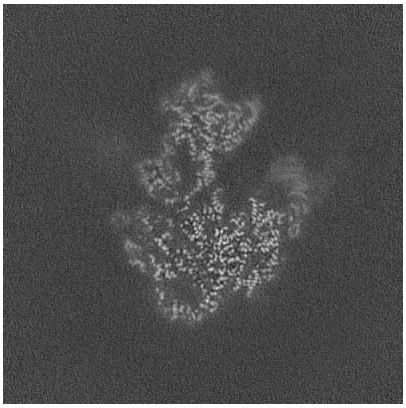
6.3.2 Raw map



X Index: 206



Y Index: 156

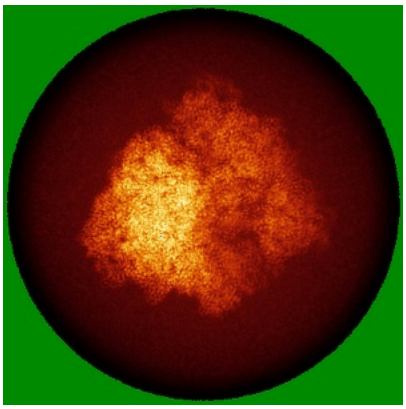


Z Index: 181

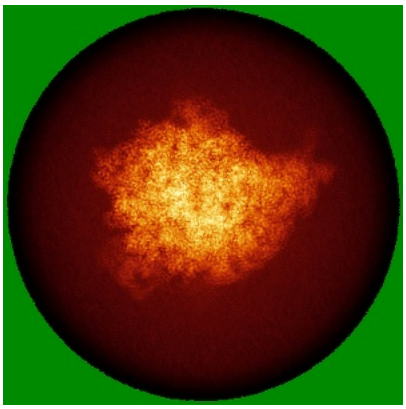
The images above show the largest variance slices of the map in three orthogonal directions.

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

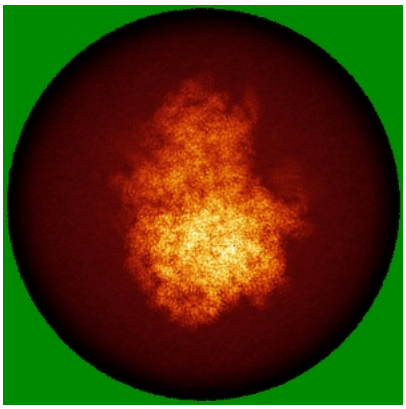
6.4.1 Primary map



X

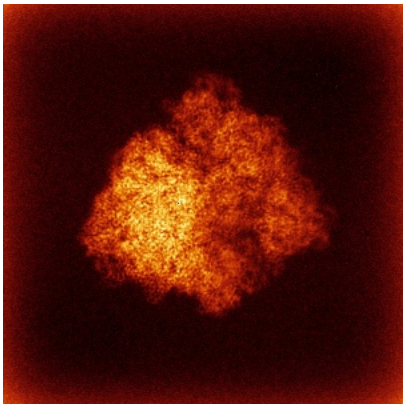


Y

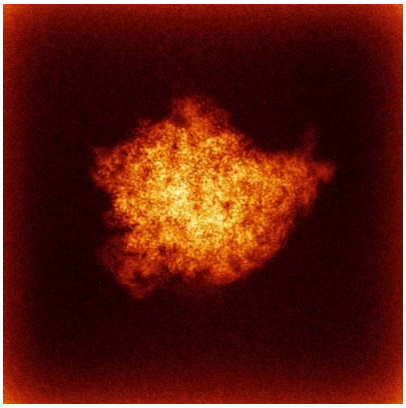


Z

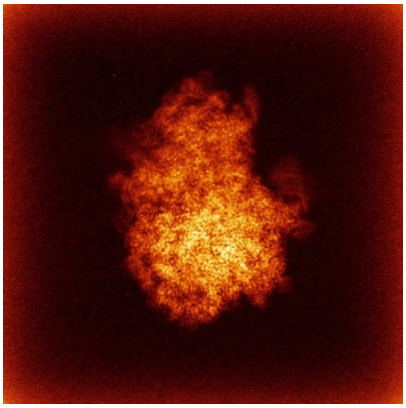
6.4.2 Raw map



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 0.9. 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.

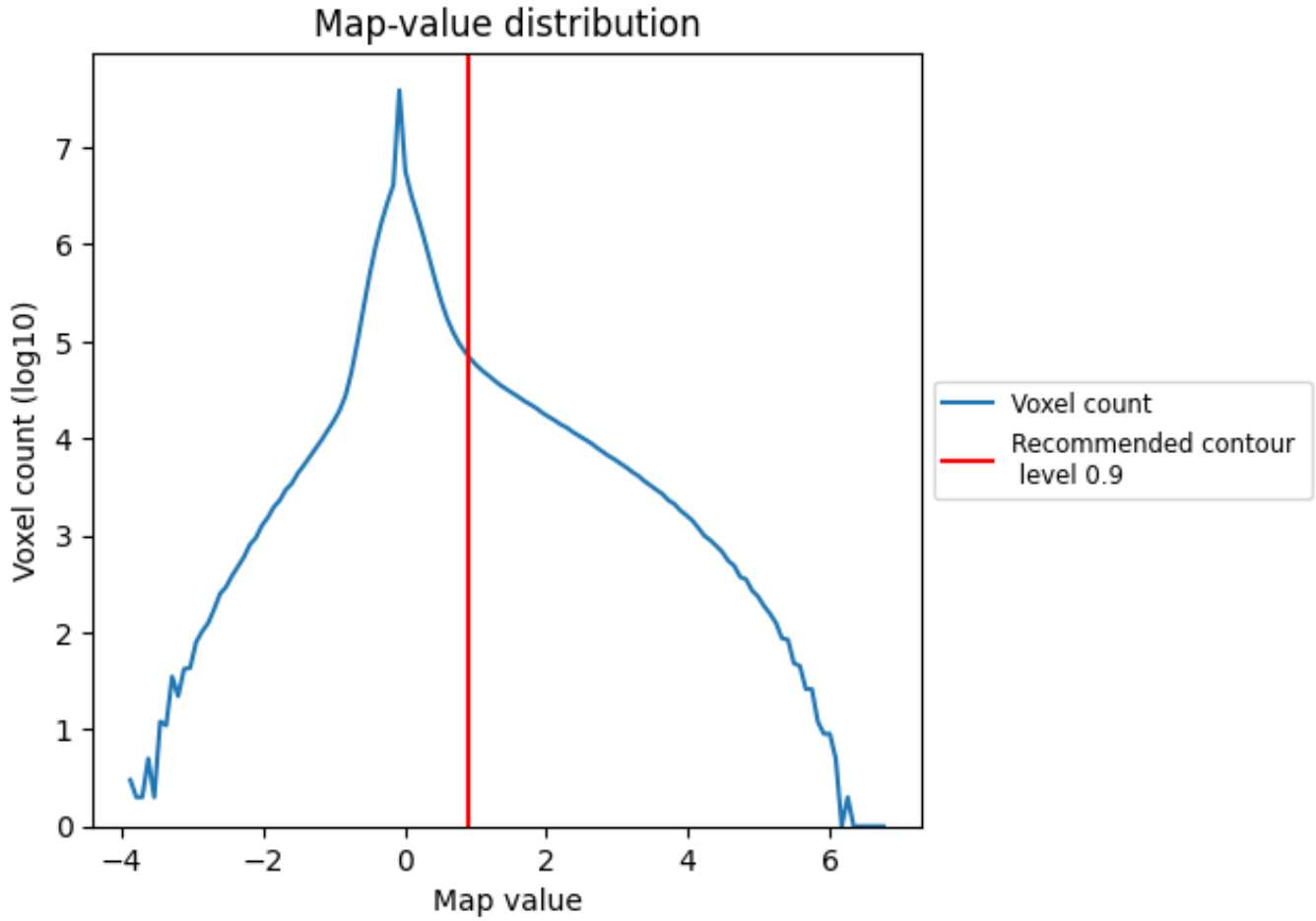
6.6 Mask visualisation (i)

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

7 Map analysis

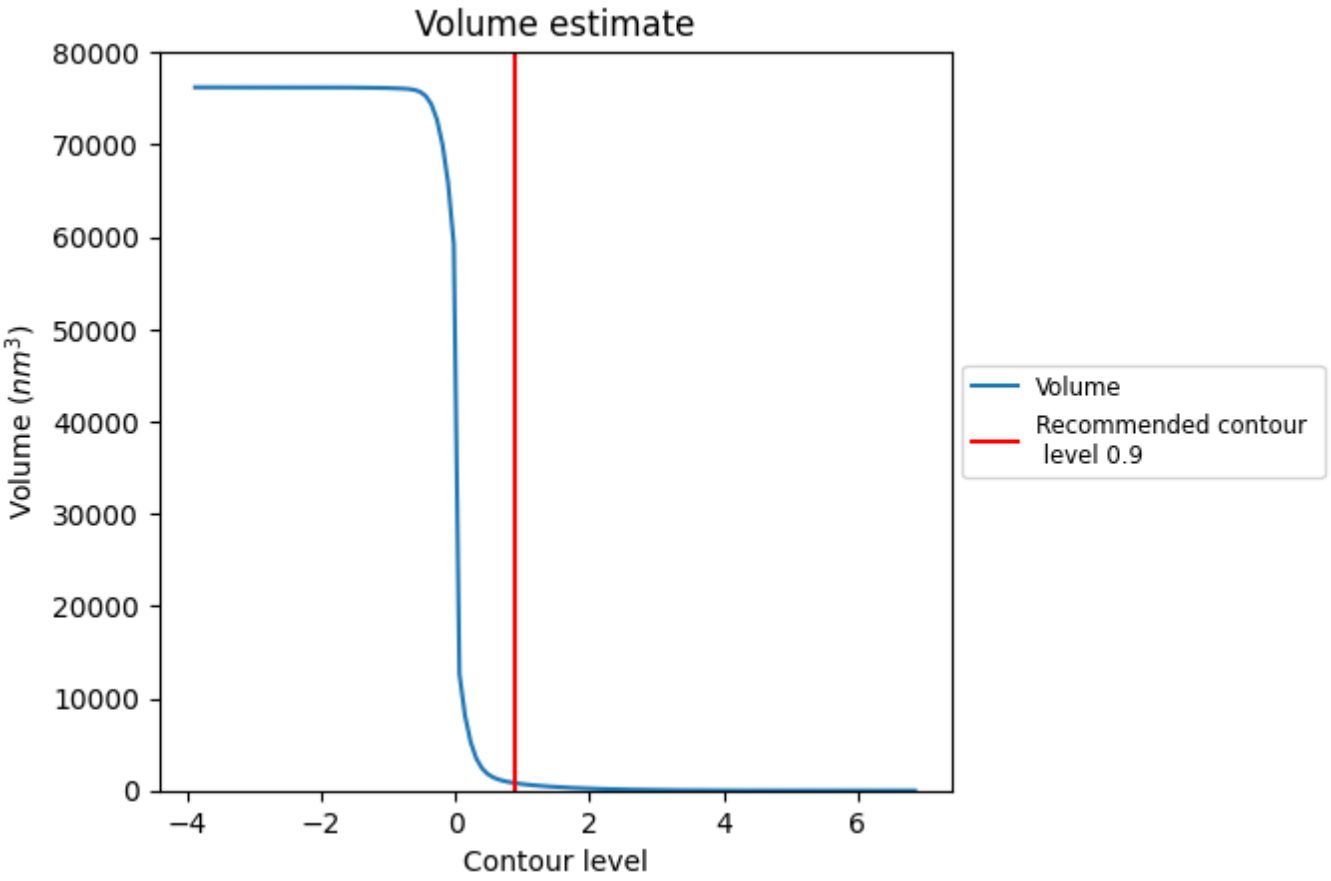
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

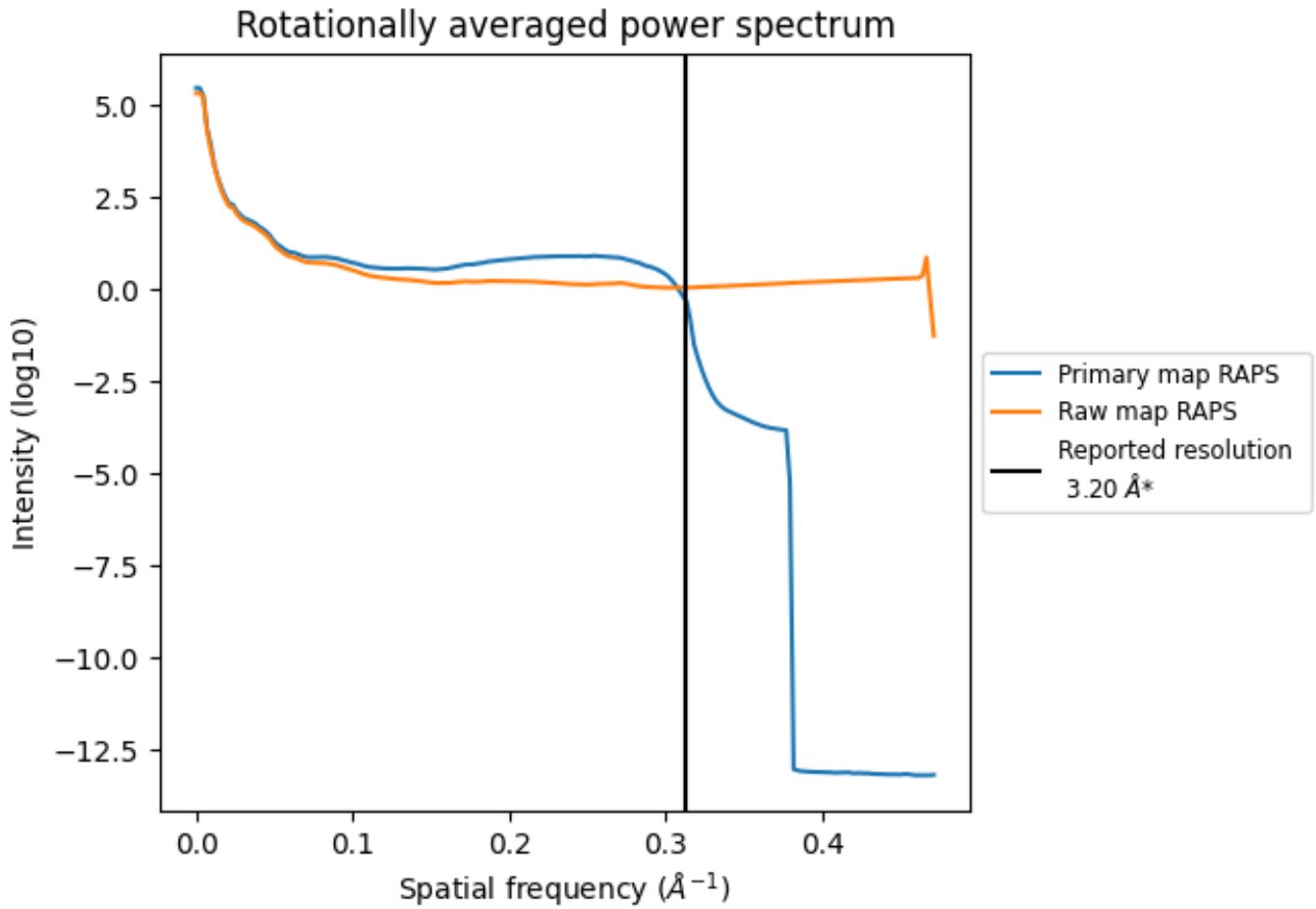
7.2 Volume estimate (i)



The volume at the recommended contour level is 798 nm^3; this corresponds to an approximate mass of 721 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

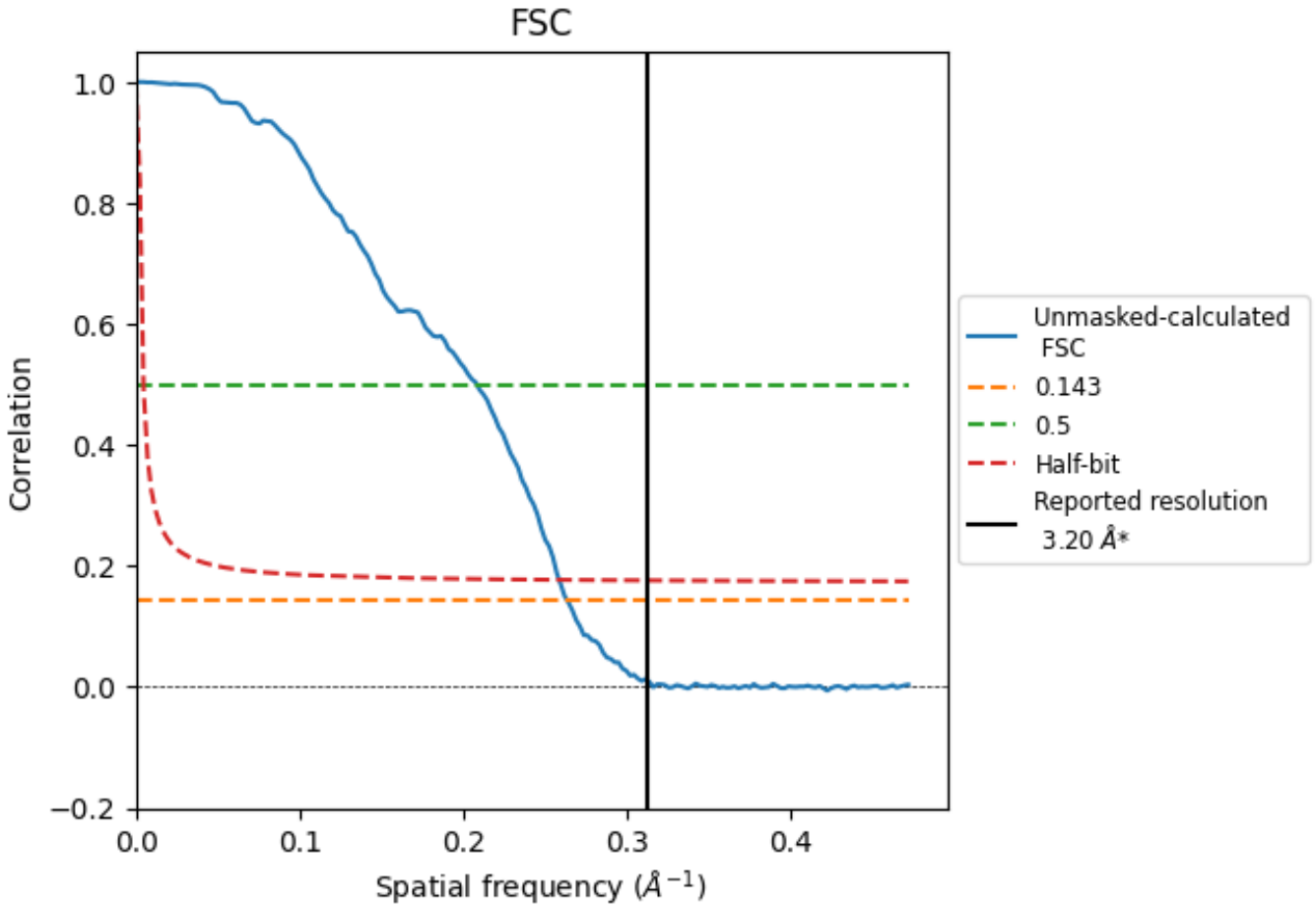


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

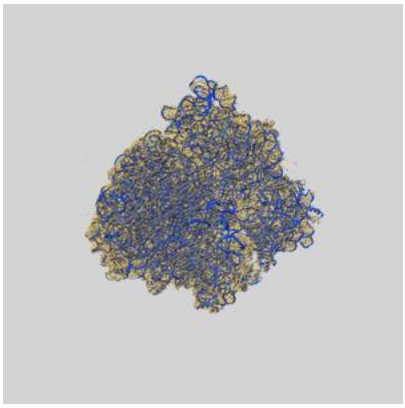
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.80	3.87

*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 3.80 differs from the reported value 3.2 by more than 10 %

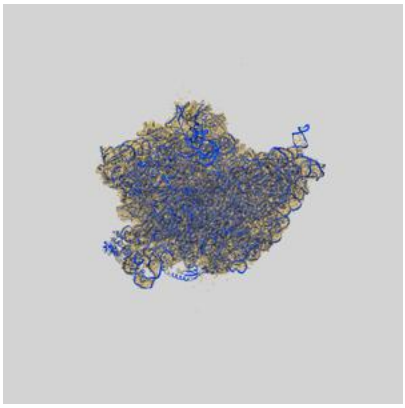
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40924 and PDB model 9NLF. Per-residue inclusion information can be found in section 3 on page 17.

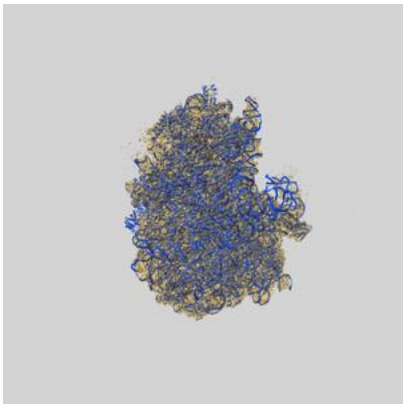
9.1 Map-model overlay



X



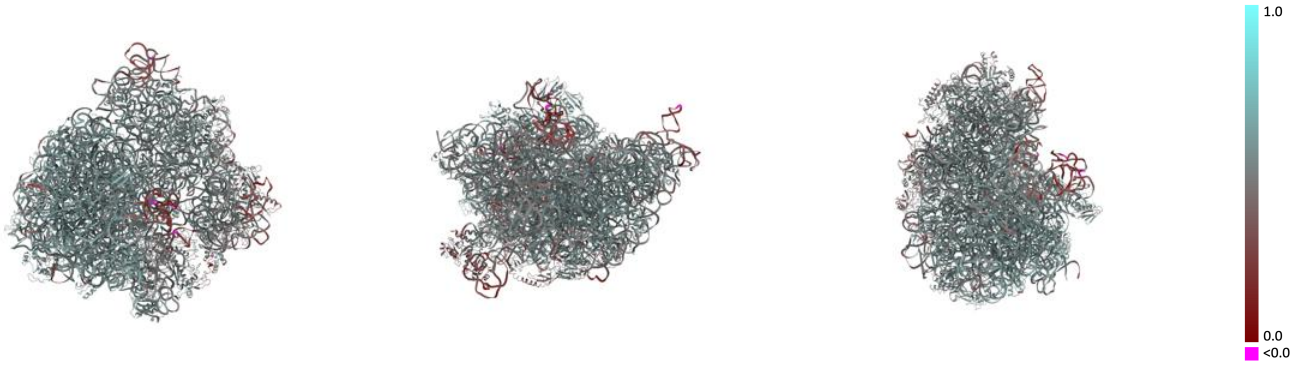
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

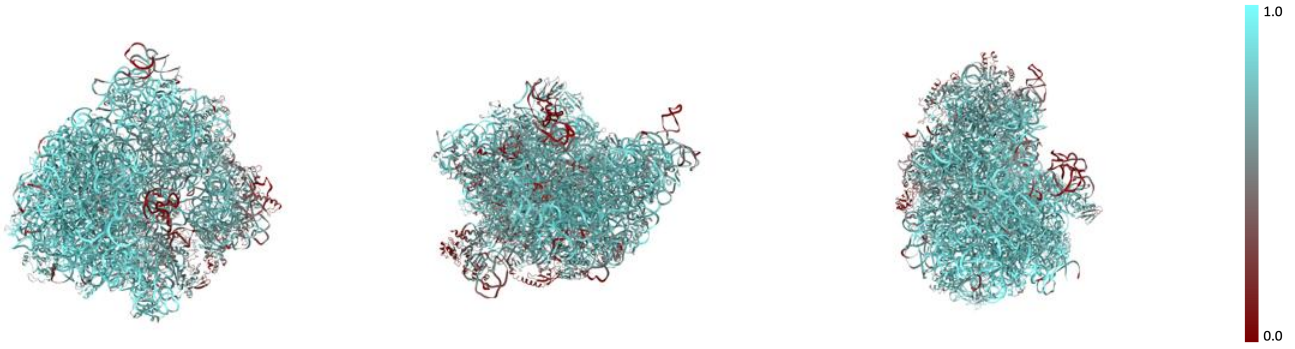
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

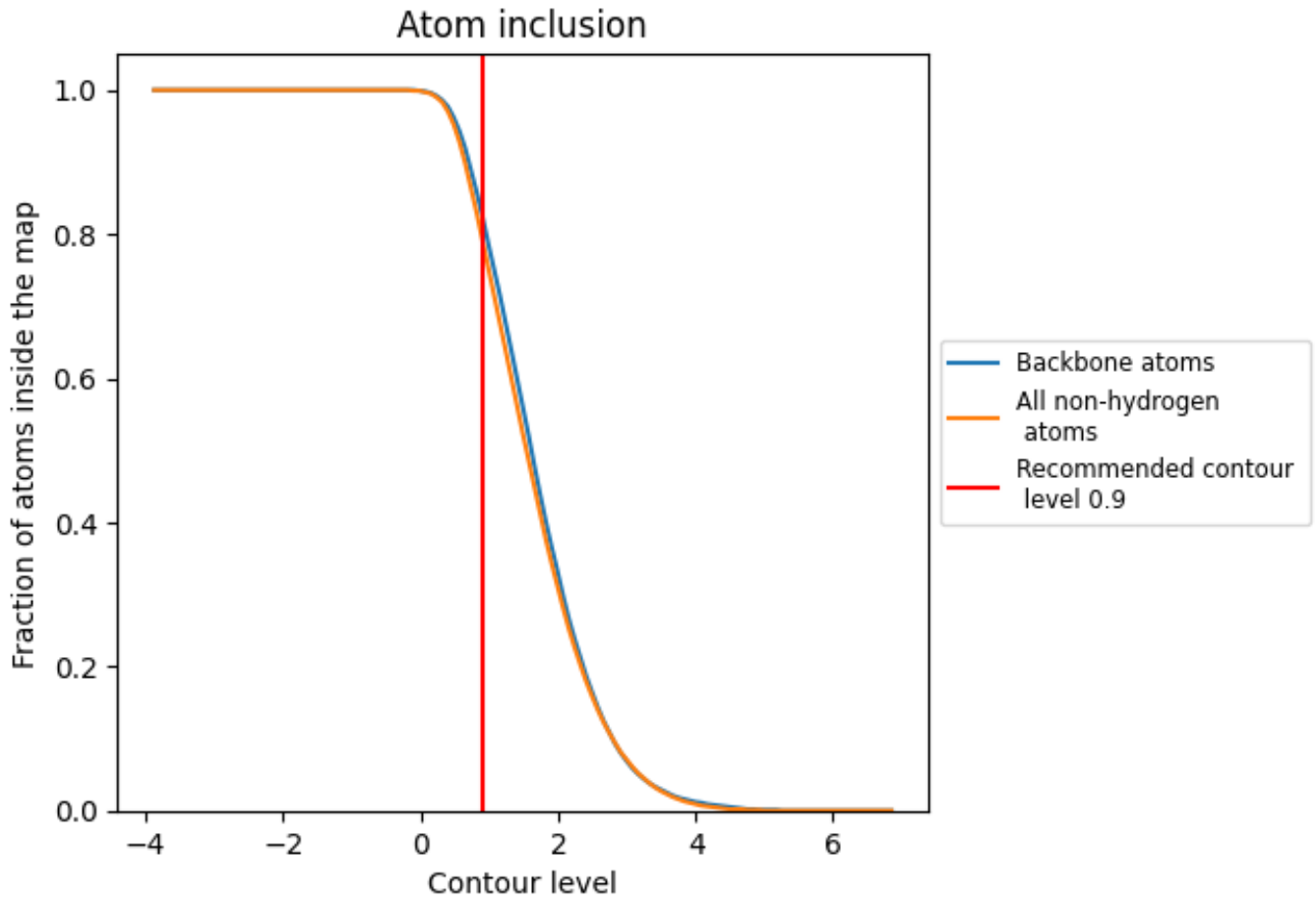
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.5260
1	0.3260	0.4090
13	0.8620	0.5890
14	0.8230	0.5770
15	0.8370	0.5740
16	0.8160	0.5750
17	0.8610	0.5860
18	0.7740	0.5590
19	0.8280	0.5780
2	0.8560	0.5830
20	0.8830	0.5870
21	0.7900	0.5590
22	0.8550	0.5760
23	0.8010	0.5590
24	0.7120	0.5480
25	0.7570	0.5630
27	0.8370	0.5880
28	0.8470	0.5830
29	0.6920	0.5410
3	0.8410	0.5760
30	0.8100	0.5800
31	0.3010	0.4010
32	0.8370	0.5740
33	0.7800	0.5670
34	0.8740	0.5960
35	0.9080	0.6010
36	0.8530	0.5870
4	0.7820	0.5710
5	0.5620	0.5010
6	0.6470	0.5320
9	0.2630	0.4150
M	0.6100	0.5020
R1	0.8680	0.5370
R2	0.8520	0.5180
R3	0.8050	0.5030

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Chain	Atom inclusion	Q-score
T	0.7500	0.4840
Y	0.5920	0.5010
sb	0.5220	0.4730
sc	0.6070	0.5200
sd	0.6350	0.5160
se	0.7210	0.5370
sf	0.5790	0.5000
sg	0.5370	0.4860
sh	0.6980	0.5410
si	0.6320	0.4880
sj	0.4730	0.4560
sk	0.6530	0.5290
sl	0.7090	0.5360
sm	0.5780	0.5000
sn	0.6110	0.4920
so	0.7060	0.5430
sp	0.7210	0.5370
sq	0.6690	0.5330
sr	0.6560	0.5250
ss	0.5640	0.4850
st	0.7320	0.5500
su	0.4270	0.3990