Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:27 pm GMT

PDB ID	:	6ENU
EMDB ID	:	EMD-3903
Title	:	Polyproline-stalled ribosome in the presence of elongation-factor P (EF-P)
Authors	:	Huter, P.; Arenz, S.; Wilson, D.N.
Deposited on	:	2017-10-06
Resolution	:	3.10 Å(reported)

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

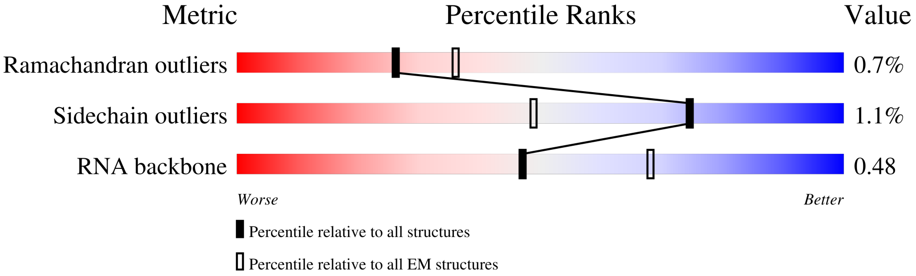
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

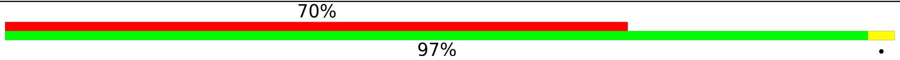
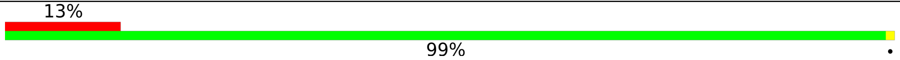
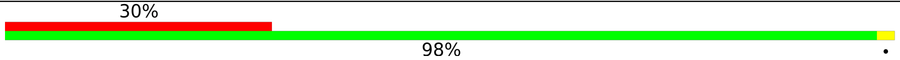
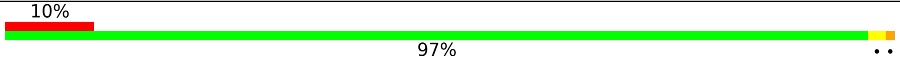
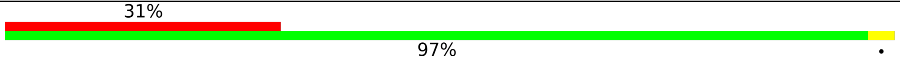
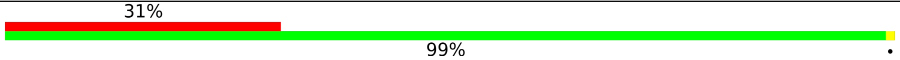
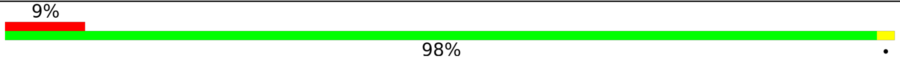
The reported resolution of this entry is 3.10 Å.

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	a	1539	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	

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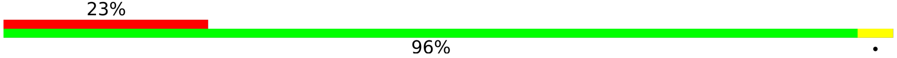
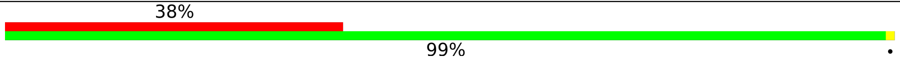
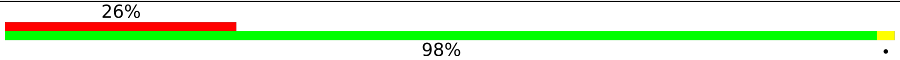
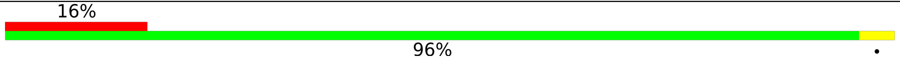
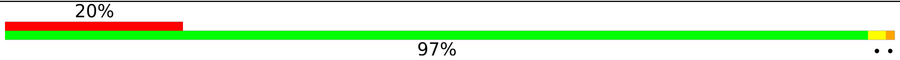
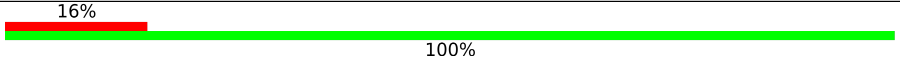
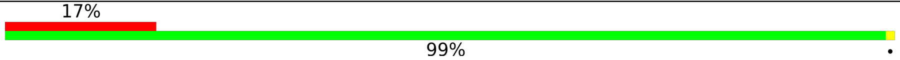
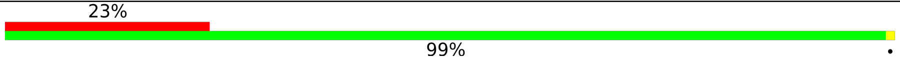
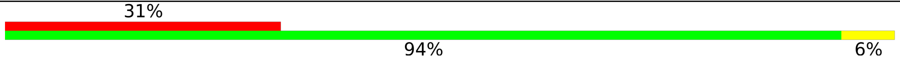
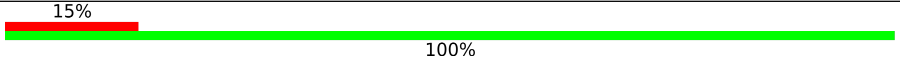
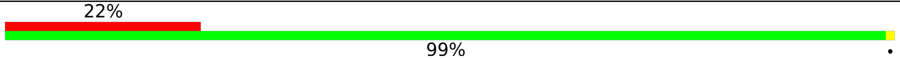
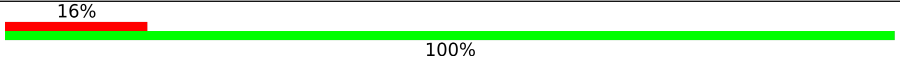
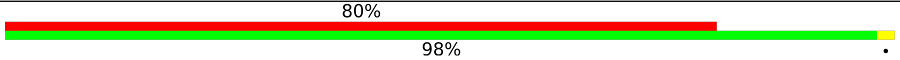
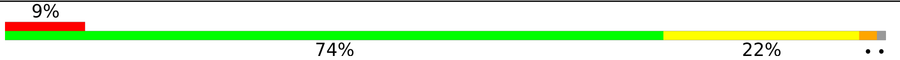
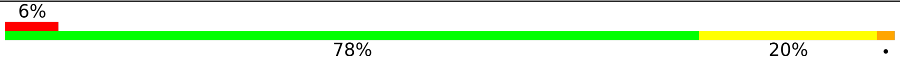
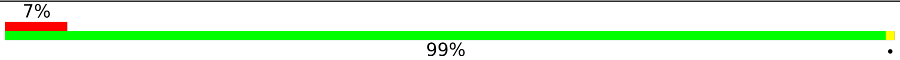
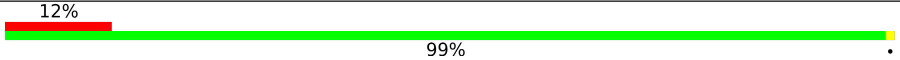
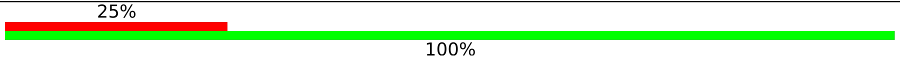
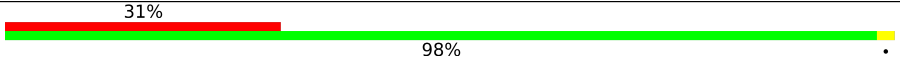
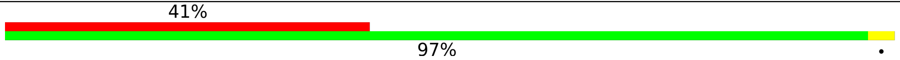
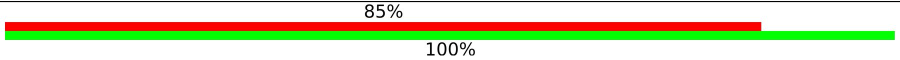
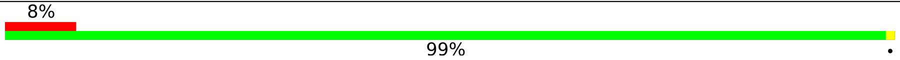
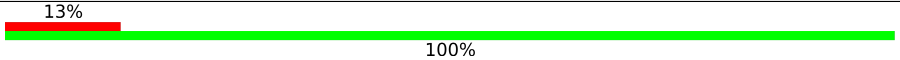
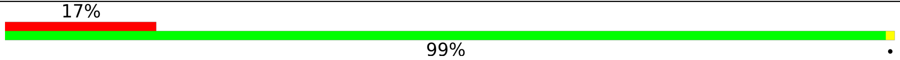
Mol	Chain	Length	Quality of chain
9	i	127	 23% 96%
10	j	98	 38% 99%
11	k	116	 26% 98%
12	l	123	 16% 96%
13	m	114	 20% 97%
14	n	101	 16% 100%
15	o	88	 17% 99%
16	p	82	 23% 99%
17	q	80	 31% 94% 6%
18	r	65	 15% 100%
19	s	79	 22% 99%
20	t	85	 16% 100%
21	u	65	 80% 98%
22	v	6	 50% 50%
23	A	2903	 9% 74% 22%
24	B	120	 6% 78% 20%
25	C	271	 7% 99%
26	D	209	 12% 99%
27	E	201	 25% 100%
28	F	177	 31% 98%
29	G	176	 41% 97%
30	H	149	 85% 100%
31	J	142	 8% 99%
32	K	122	 13% 100%
33	L	143	 17% 99%

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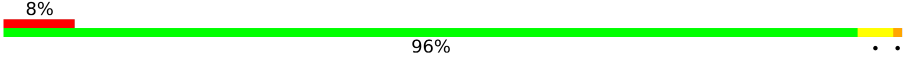
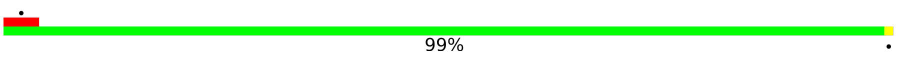
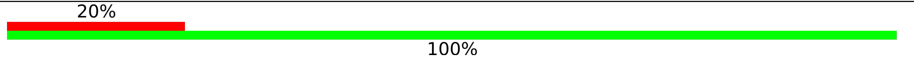
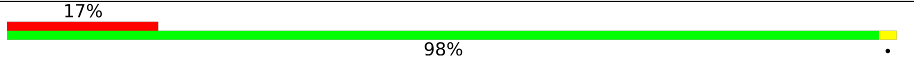
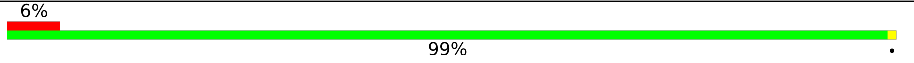
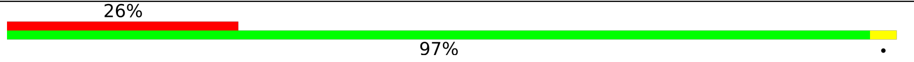
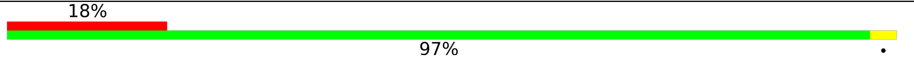
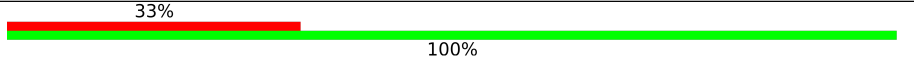
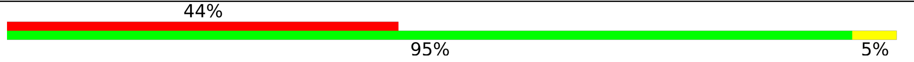
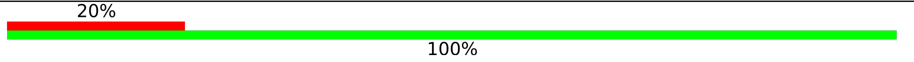
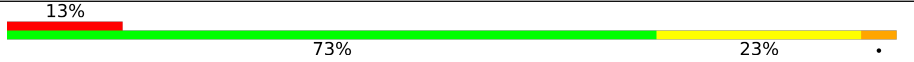
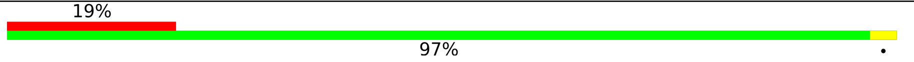
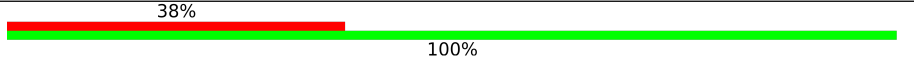
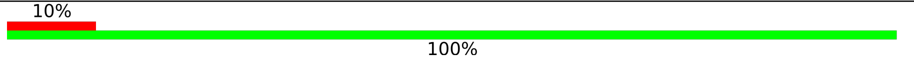
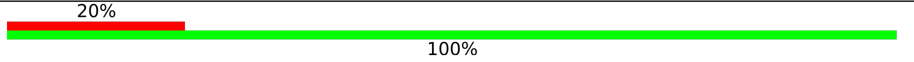
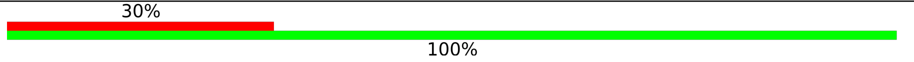
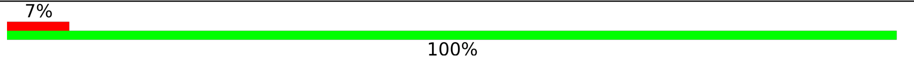
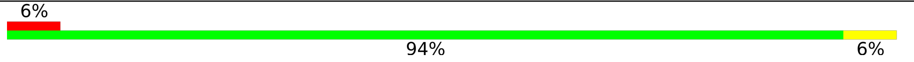
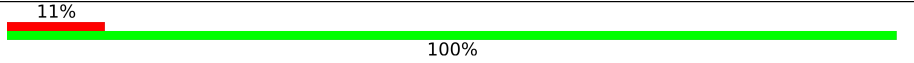
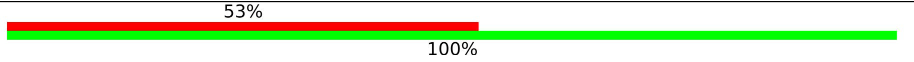
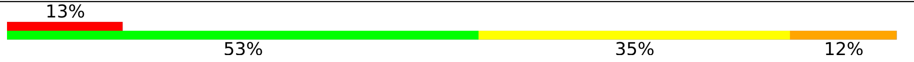
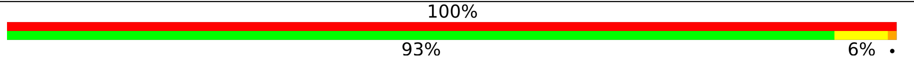
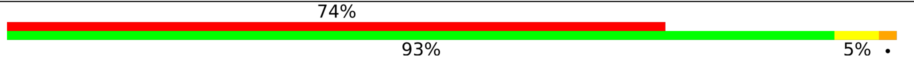
Mol	Chain	Length	Quality of chain
34	M	136	
35	N	120	
36	O	116	
37	P	114	
38	Q	117	
39	R	103	
40	S	110	
41	T	93	
42	U	102	
43	V	94	
44	W	78	
45	X	77	
46	Y	63	
47	Z	58	
48	0	56	
49	1	50	
50	2	46	
51	3	64	
52	4	38	
53	6	66	
54	x	77	
55	7	224	
56	w	188	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146475 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33016	14725	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1141	709	218	208	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	65	504	317	96	91	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	6	Total	C	N	O	P	0	0
			126	56	22	42	6		

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2871	Total	C	N	O	P	0	0
			61641	27498	11350	19922	2871		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627
A	2104	U	C	conflict	GB 802133627

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1213441078

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

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

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	L	143	1045	649	206	189	1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	W	78	592	365	119	107	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	0	56	444	269	94	80	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	1	50	409	263	75	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	2	46	377	228	90	57	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	3	64	504	323	105	74	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	4	38	302	185	65	48	4	0	0

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	6	66	522	323	99	94	6	0	0

- Molecule 54 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	x	77	1646	733	295	541	77	0	0

- Molecule 55 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	7	224	1663	1039	303	315	6	0	0

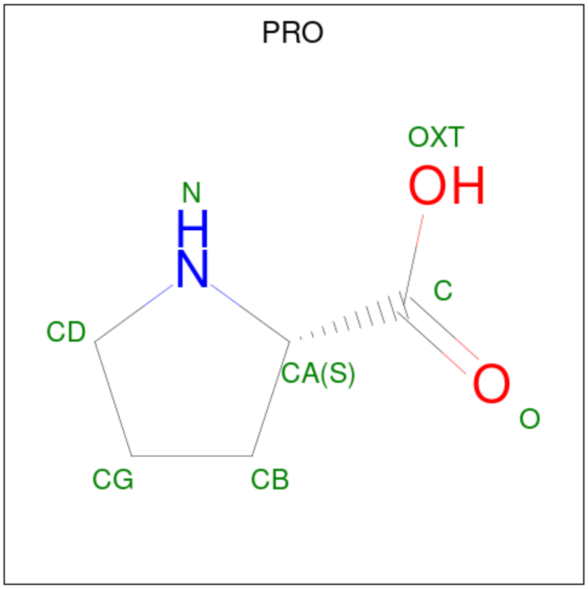
- Molecule 56 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	w	188	1461	928	242	286	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	34	KEO	LYS	engineered mutation	UNP P0A6N4

- Molecule 57 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).

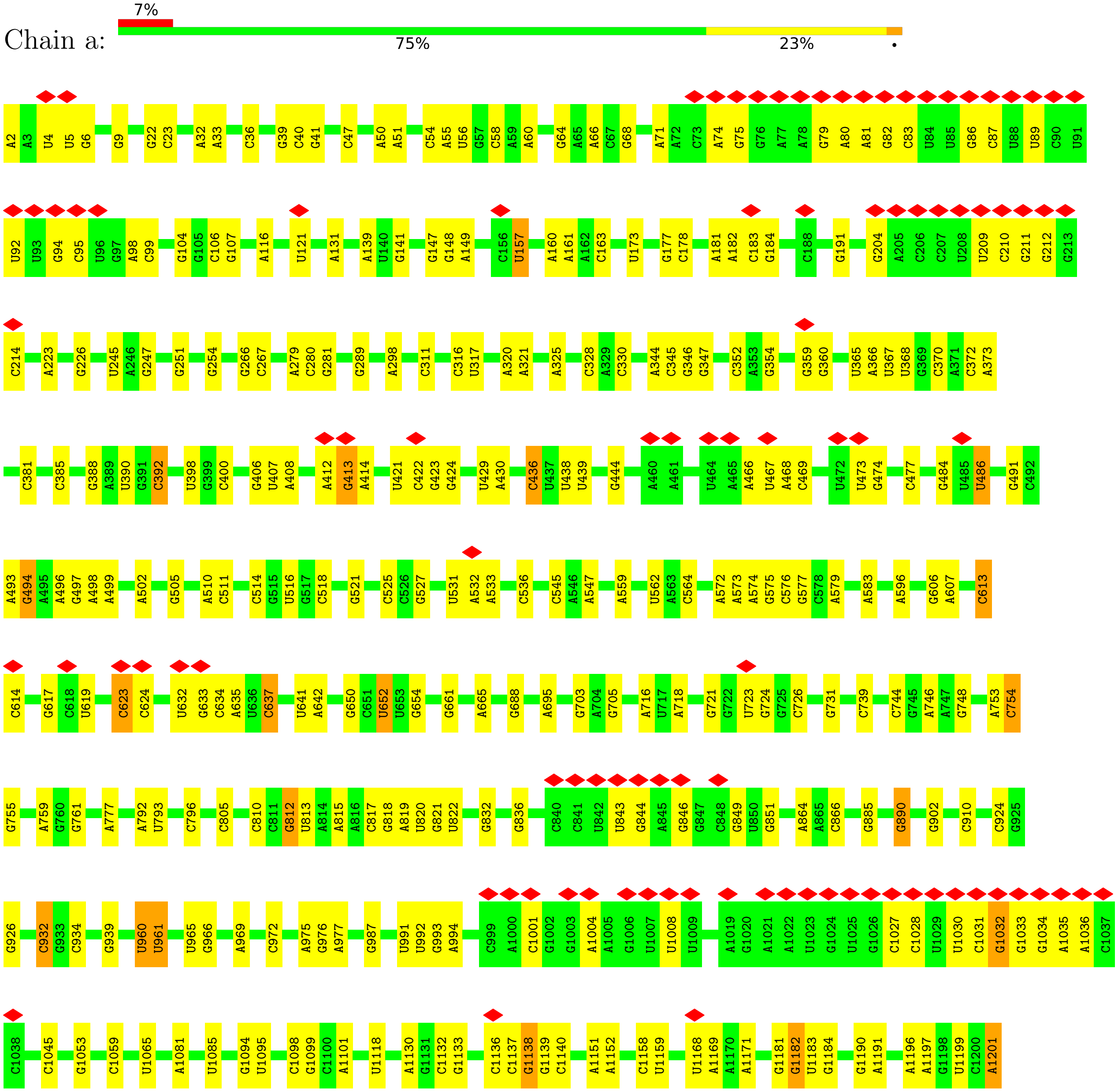


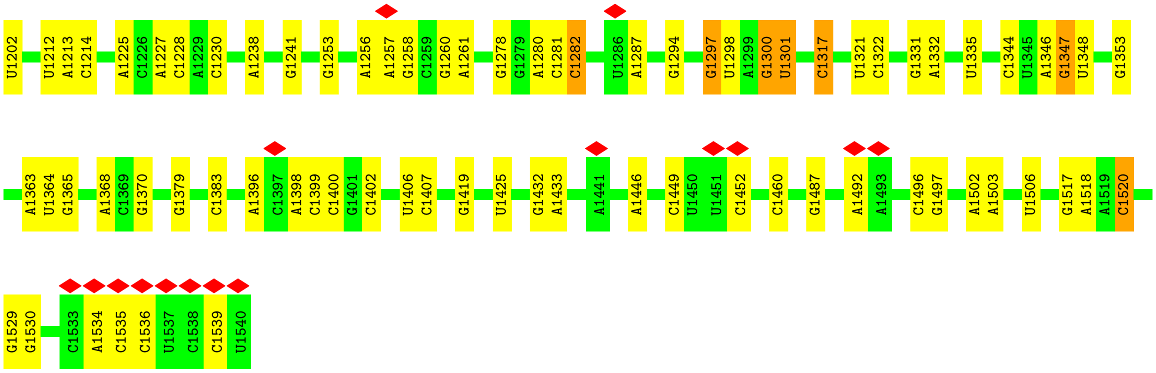
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	A	1	7	5	1	1	0
			Total	C	N	O	
57	x	1	7	5	1	1	0

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.

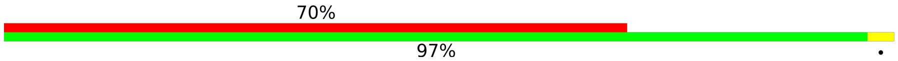
- Molecule 1: 16S ribosomal RNA





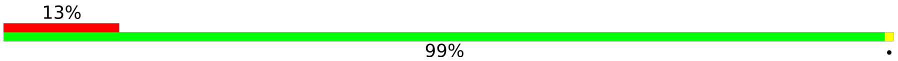
- Molecule 2: 30S ribosomal protein S2

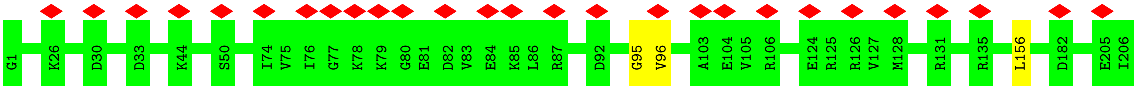
Chain b:



- Molecule 3: 30S ribosomal protein S3

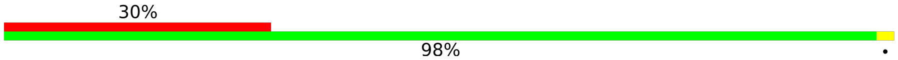
Chain c:

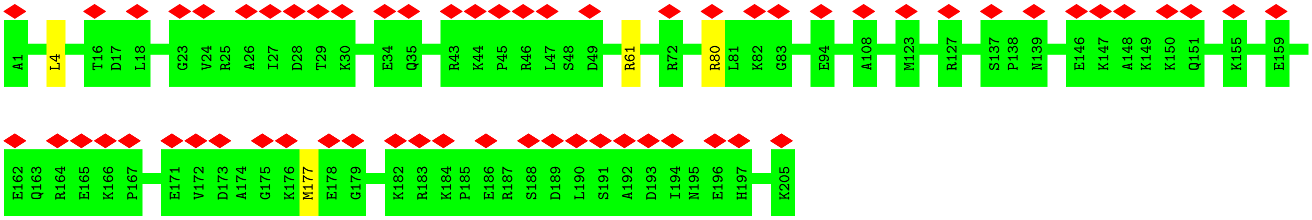




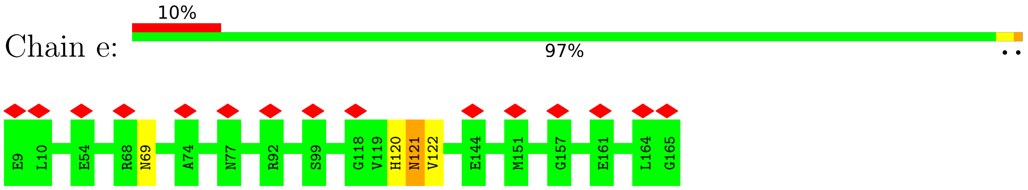
- Molecule 4: 30S ribosomal protein S4

Chain d:

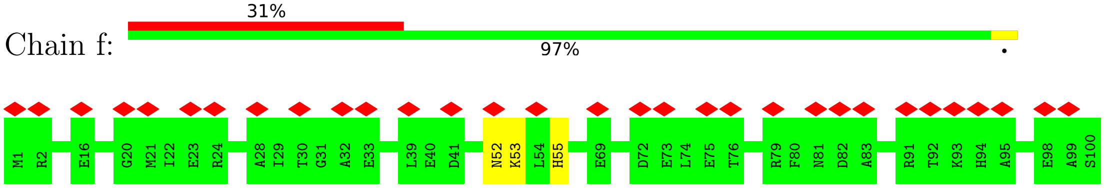




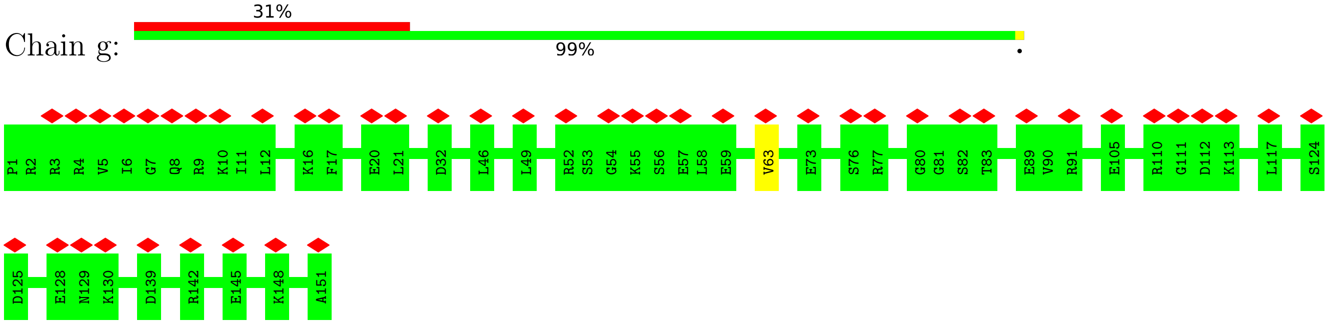
- Molecule 5: 30S ribosomal protein S5



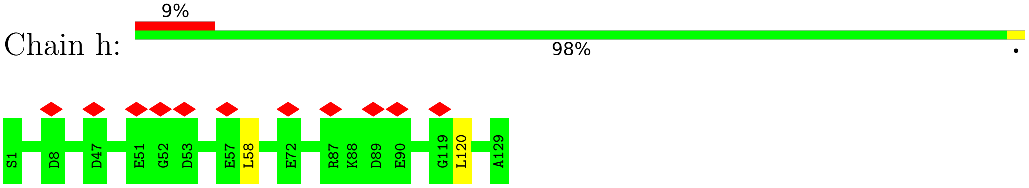
- Molecule 6: 30S ribosomal protein S6



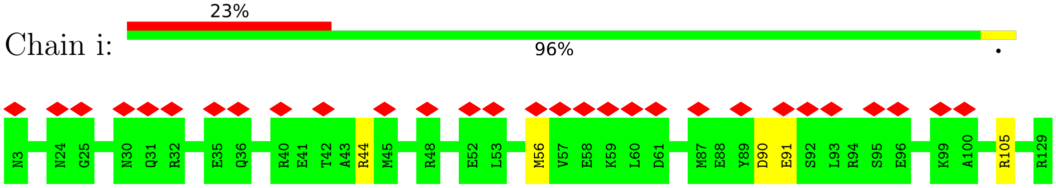
- Molecule 7: 30S ribosomal protein S7



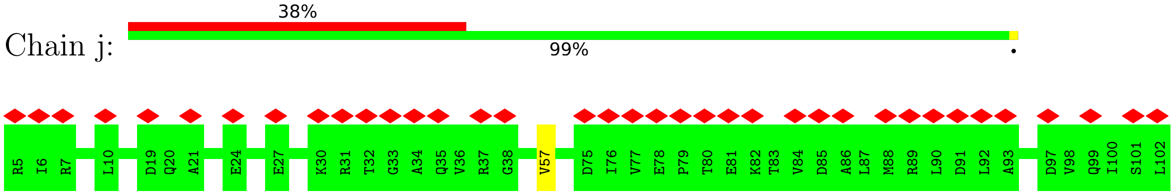
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

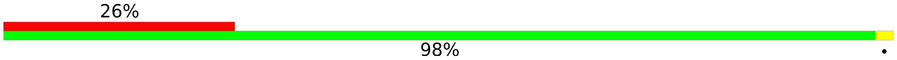


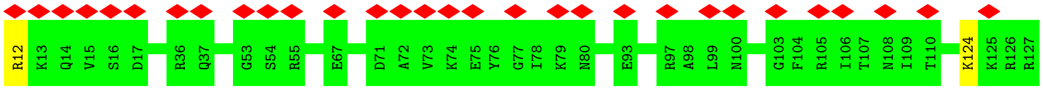
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

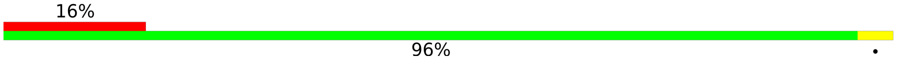
Chain k:

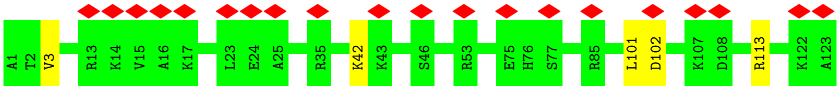




- Molecule 12: 30S ribosomal protein S12

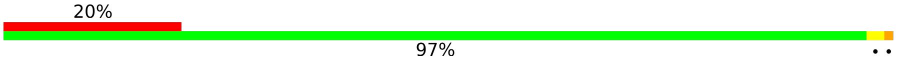
Chain l:

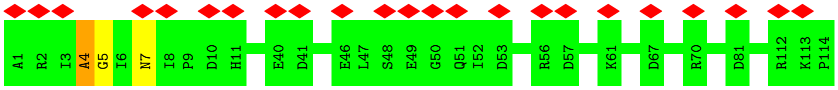




- Molecule 13: 30S ribosomal protein S13

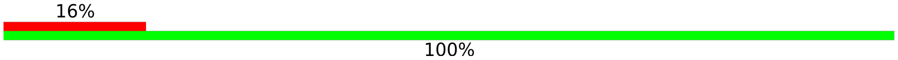
Chain m:

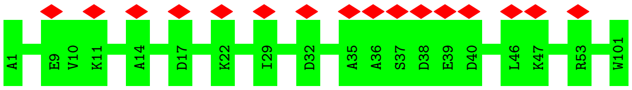




- Molecule 14: 30S ribosomal protein S14

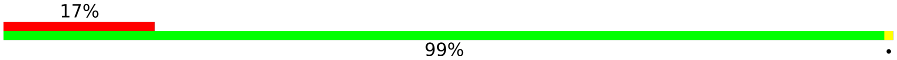
Chain n:

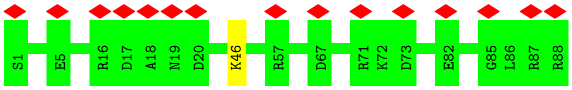




- Molecule 15: 30S ribosomal protein S15

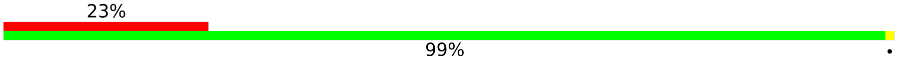
Chain o:

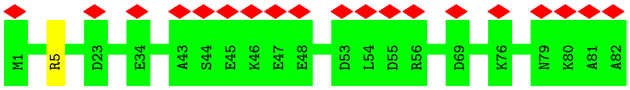




- Molecule 16: 30S ribosomal protein S16

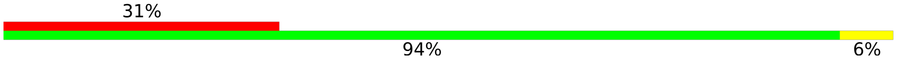
Chain p:

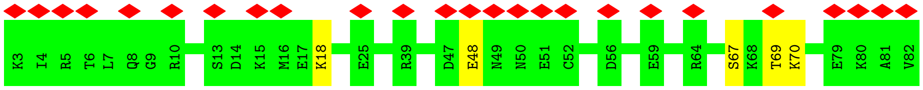




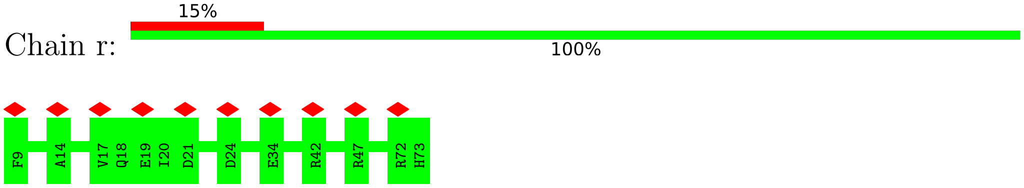
- Molecule 17: 30S ribosomal protein S17

Chain q:

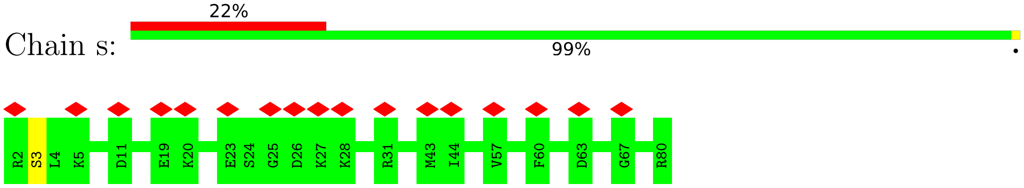




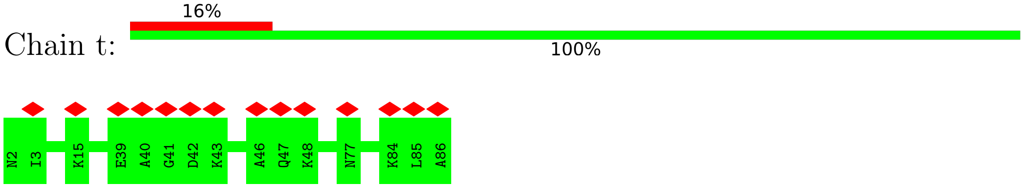
- Molecule 18: 30S ribosomal protein S18



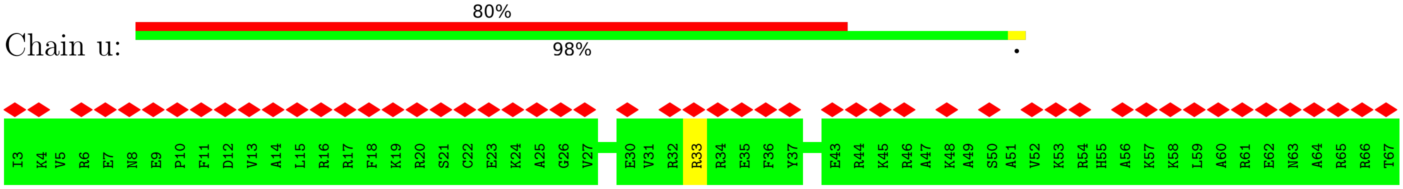
- Molecule 19: 30S ribosomal protein S19



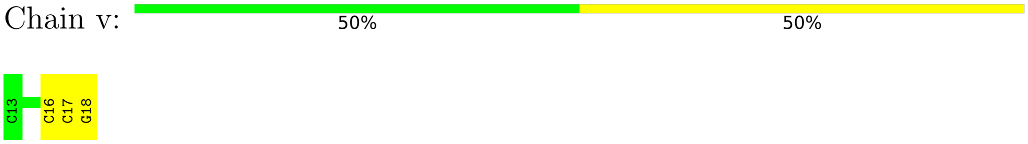
- Molecule 20: 30S ribosomal protein S20



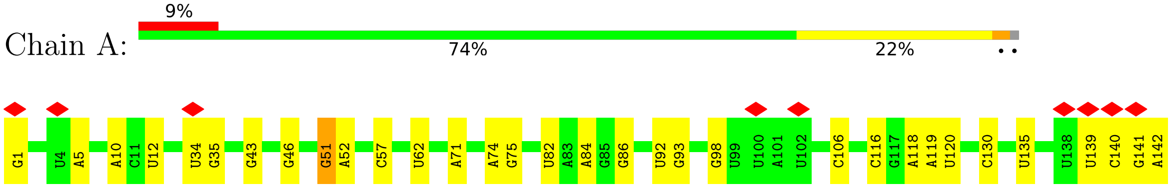
- Molecule 21: 30S ribosomal protein S21

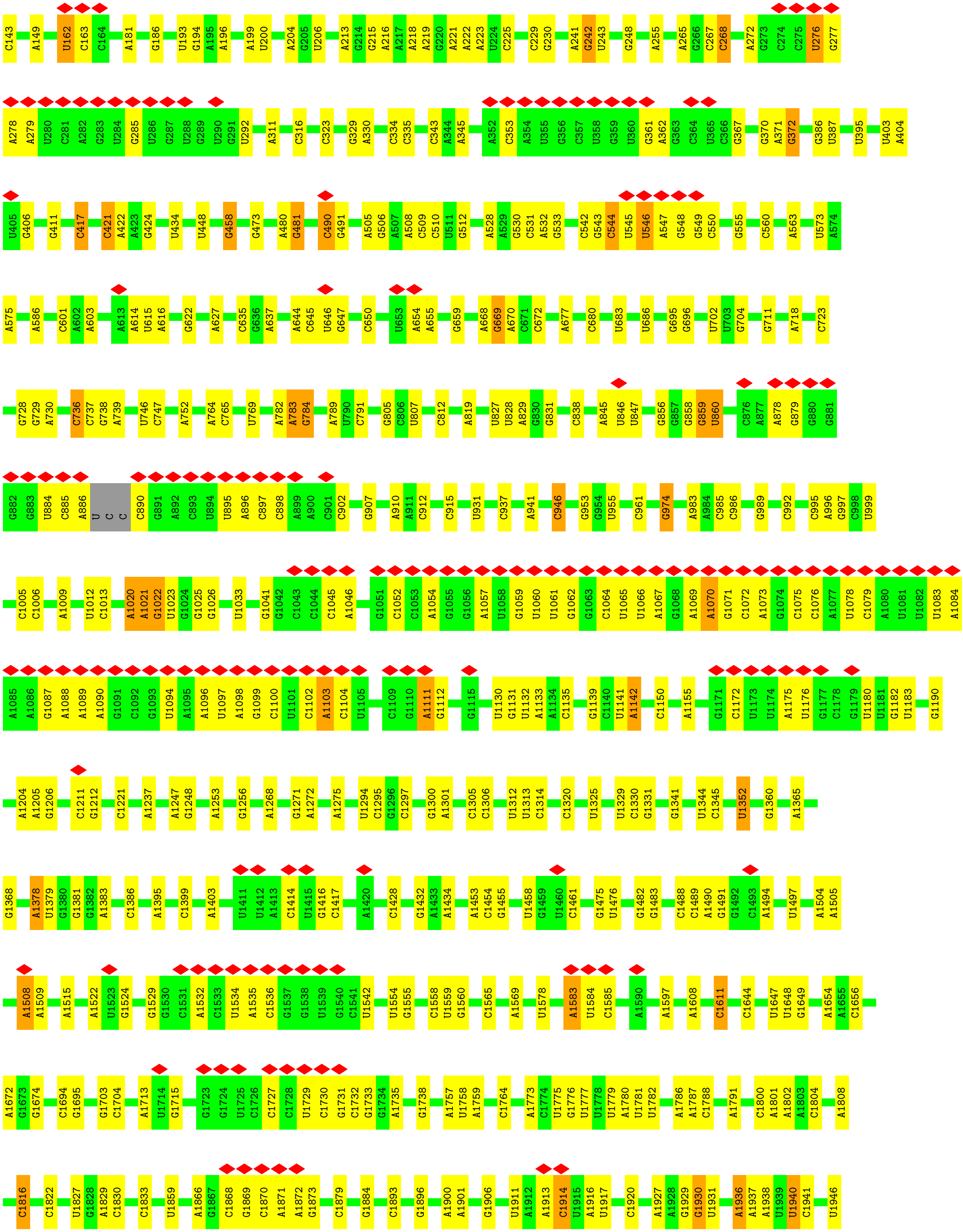


- Molecule 22: mRNA



- Molecule 23: 23S Ribosomal RNA

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A278 A279 U280 C281 A282 G283 U284 G285 U286 G287 U288 G289 U290 G291 U292 A311 C316 C323 G329 A330 C334 C335 C343 A344 A345 A352 C353 A354 U355 G356 C357 U358 G359 U360 G361 A362 G363 C364 U365 C366 G367 G370 A371 G372 G386 U387 U395 U403 A404
U405 G406 G411 C417 C421 A422 A423 G424 U434 U448 G458 G473 A480 G481 C490 G491 A505 G506 A507 A508 C509 C510 U511 G512 A528 A529 G530 C531 A532 G533 C542 G543 C544 U545 U546 A547 G548 G549 C550 G555 C560 A563 U573 A574
A575 A586 C601 A602 A603 A613 A614 U615 A616 G622 A627 C635 G636 A637 A644 C645 U646 G647 C650 U653 A654 A655 G659 A668 G669 A670 C671 C672 A677 C680 U683 U686 G695 G696 U702 U703 G704 G711 A718 C723
G728 G729 A730 C736 C737 G738 A739 U746 C747 A752 A764 C765 U769 A782 A783 G784 A789 U790 C791 G805 C806 U807 C812 A819 U827 U828 A829 G830 G831 C838 A845 U846 U847 G856 G857 G858 G859 U860 C876 A877 A878 G879 G880 G881
G882 G883 U884 C885 A886 U C C C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 G907 A910 A911 C912 C915 U931 C937 A941 C946 G953 G954 U955 C961 G974 A983 A984 C985 C986 G989 C992 C995 A996 G997 C998 U999
C1005 C1006 A1009 U1012 C1013 A1020 A1021 G1022 U1023 G1024 G1025 G1026 U1033 G1041 G1042 C1043 C1044 C1045 A1046 G1051 C1052 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
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A1204 A1205 G1206 C1211 G1212 C1221 A1237 A1247 G1248 A1253 G1256 A1268 G1271 A1272 A1275 U1294 C1295 G1296 C1297 G1300 A1301 C1305 C1306 U1312 U1313 C1314 C1320 U1325 U1329 C1330 G1331 G1341 U1344 C1345 U1352 G1360 A1365
G1368 A1378 U1379 G1380 G1381 G1382 A1383 C1386 A1395 C1399 A1403 U1411 U1412 A1413 C1414 U1415 G1416 C1417 A1420 C1428 G1432 A1433 A1434 A1453 C1454 G1455 U1458 G1459 U1460 C1461 G1475 U1476 G1482 G1483 C1488 C1489 A1490 G1491 G1492 C1493 A1494 U1497 A1504 A1505
A1508 A1509 A1515 A1522 U1523 G1524 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 U1554 G1555 C1558 U1559 G1560 C1565 A1569 U1578 A1583 U1584 C1585 A1590 A1597 A1608 C1611 C1644 U1647 U1648 G1649 A1654 A1655 C1656
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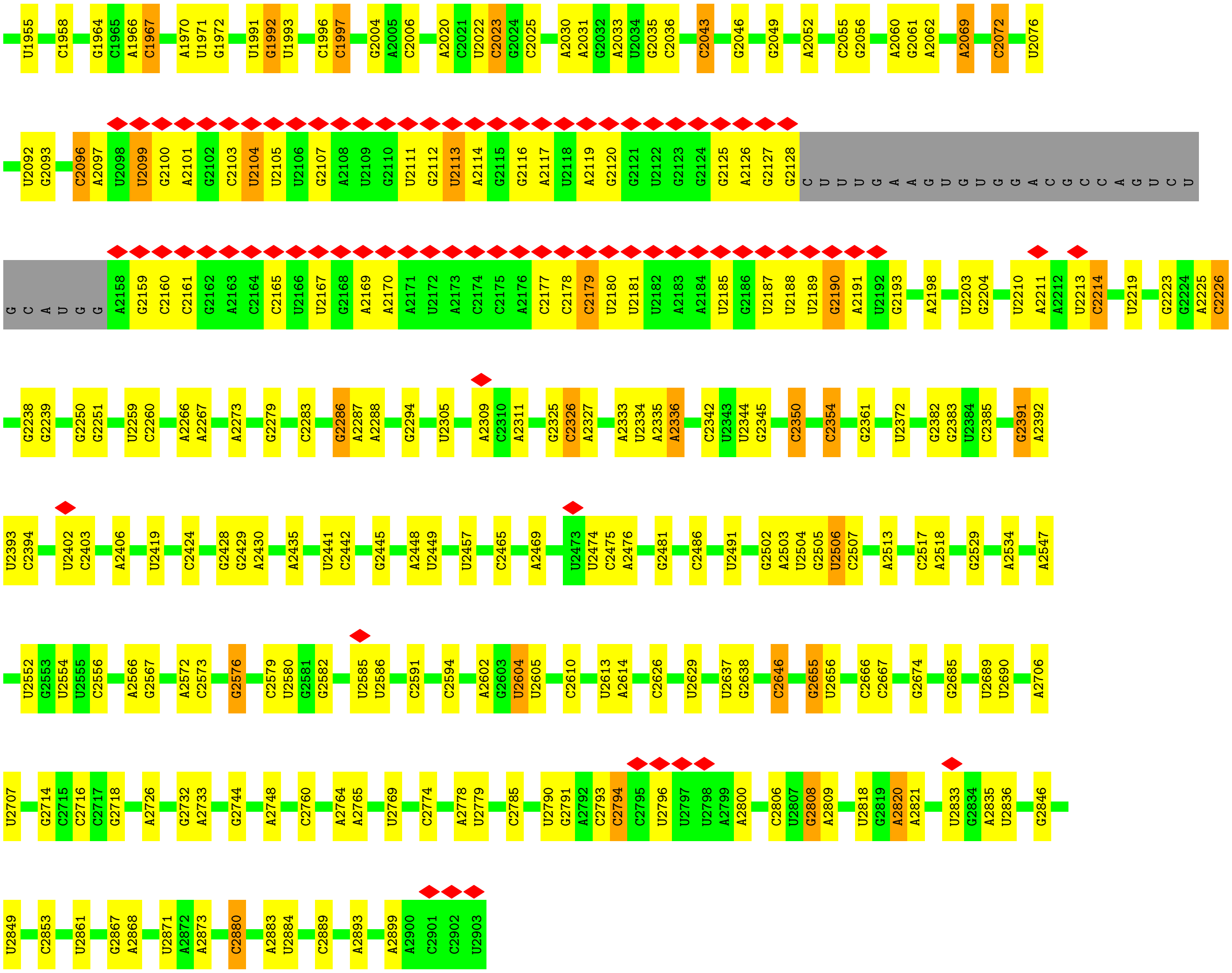
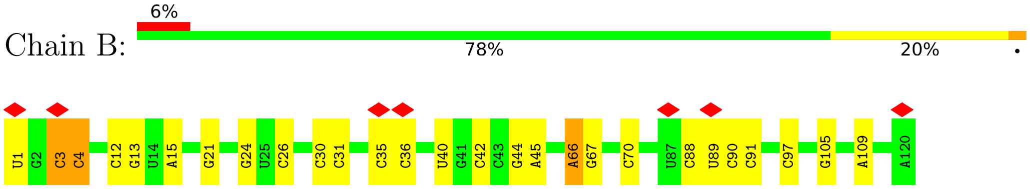
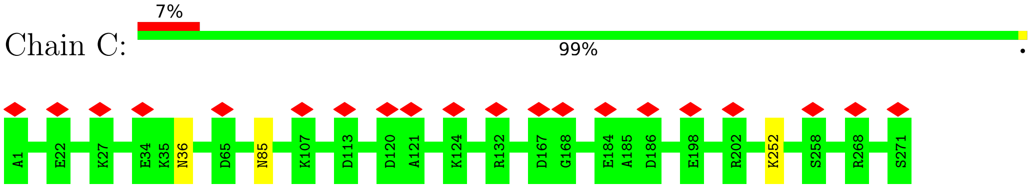


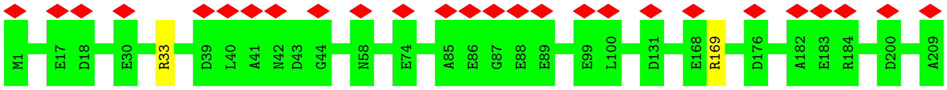
- Molecule 24: 5S Ribosomal RNA



- Molecule 25: 50S ribosomal protein L2

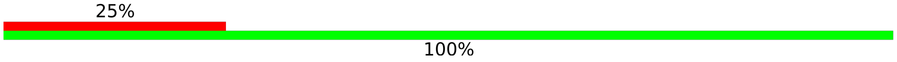


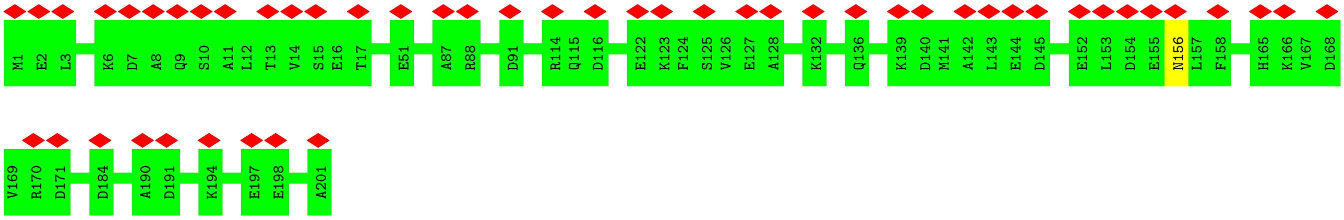
- Molecule 26: 50S ribosomal protein L3



- Molecule 27: 50S ribosomal protein L4

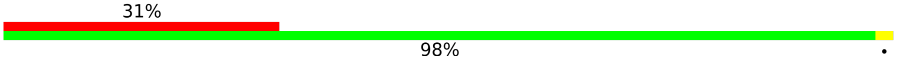
Chain E:

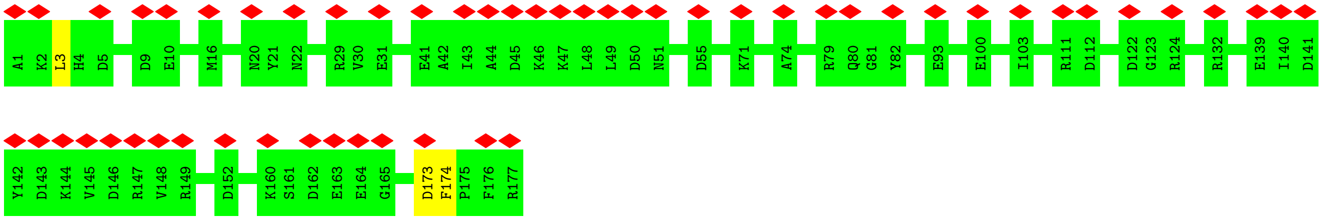




- Molecule 28: 50S ribosomal protein L5

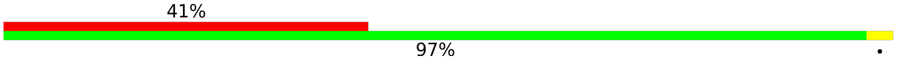
Chain F:

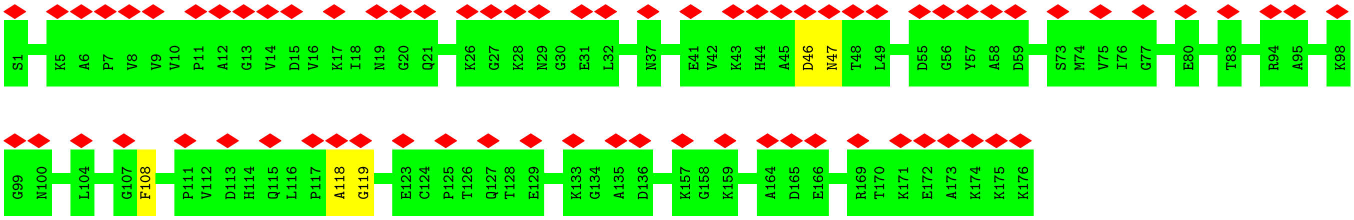




- Molecule 29: 50S ribosomal protein L6

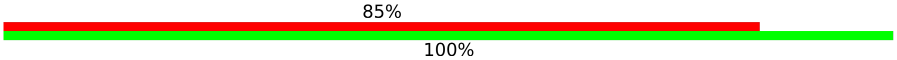
Chain G:

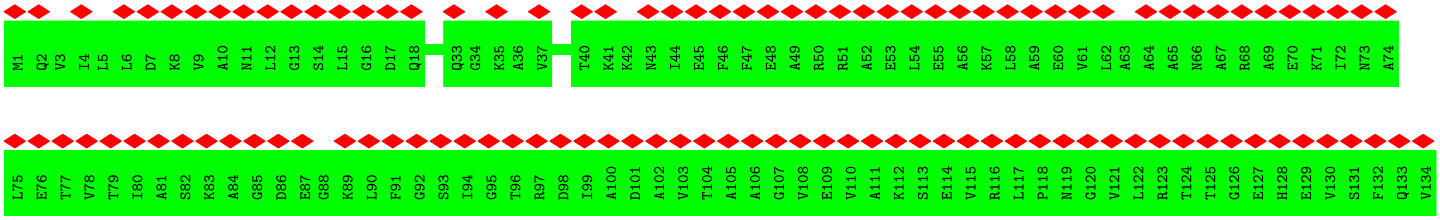


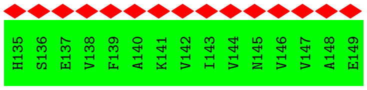


- Molecule 30: 50S ribosomal protein L9

Chain H:

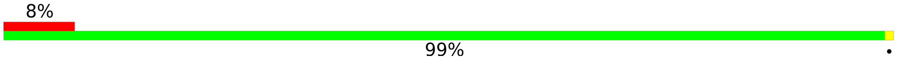


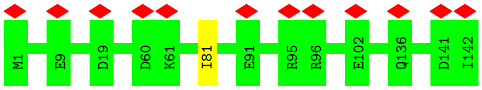




- Molecule 31: 50S ribosomal protein L13

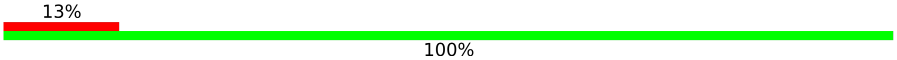
Chain J:

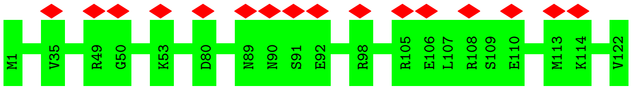




- Molecule 32: 50S ribosomal protein L14

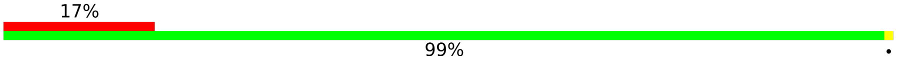
Chain K:

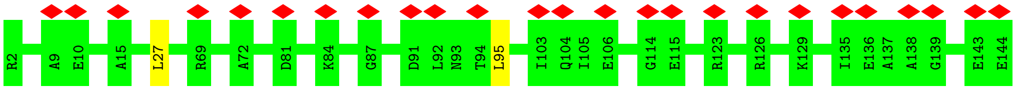




- Molecule 33: 50S ribosomal protein L15

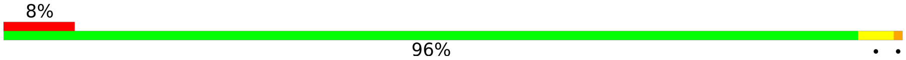
Chain L:

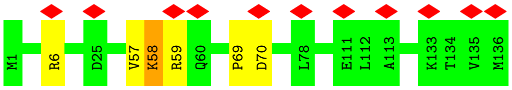




- Molecule 34: 50S ribosomal protein L16

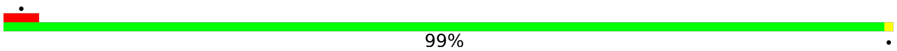
Chain M:

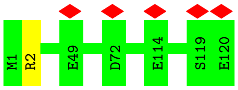




- Molecule 35: 50S ribosomal protein L17

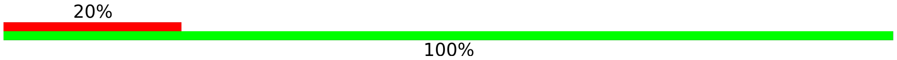
Chain N:

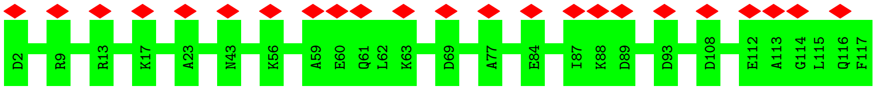




- Molecule 36: 50S ribosomal protein L18

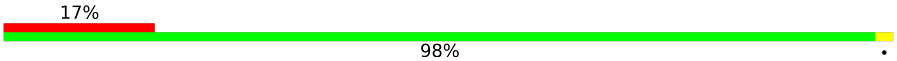
Chain O:

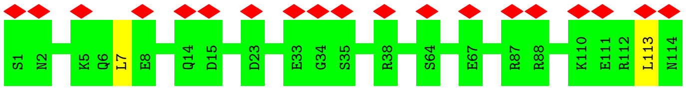




- Molecule 37: 50S ribosomal protein L19

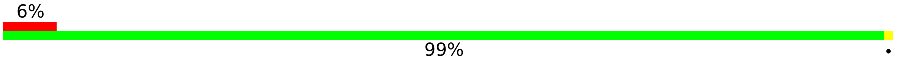
Chain P:

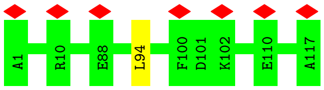




- Molecule 38: 50S ribosomal protein L20

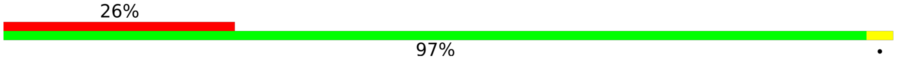
Chain Q:

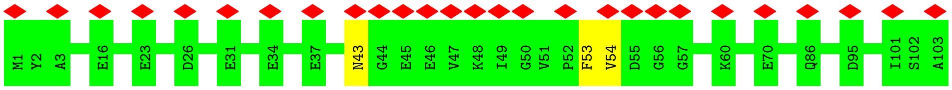




- Molecule 39: 50S ribosomal protein L21

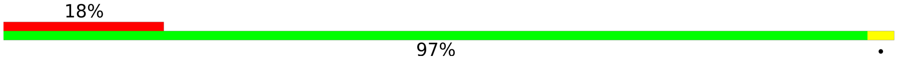
Chain R:

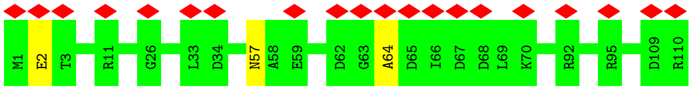




- Molecule 40: 50S ribosomal protein L22

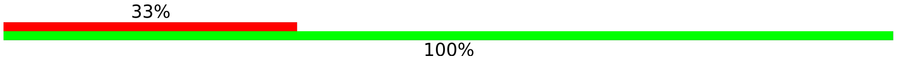
Chain S:

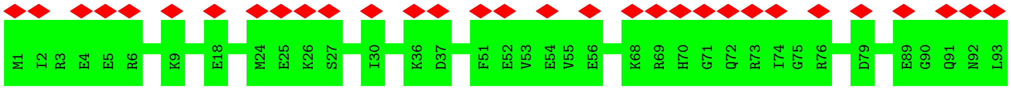




- Molecule 41: 50S ribosomal protein L23

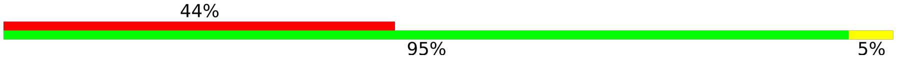
Chain T:

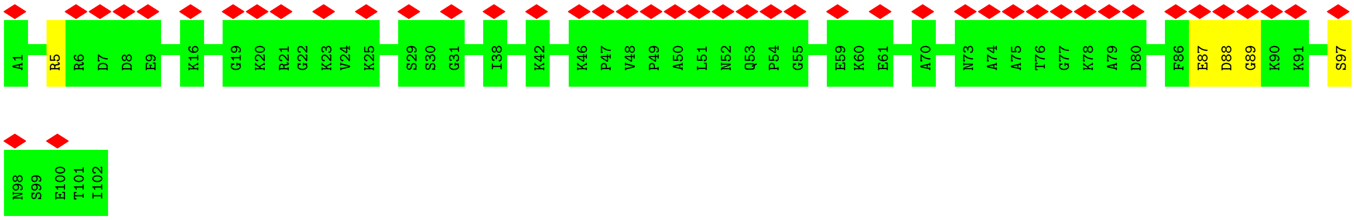




- Molecule 42: 50S ribosomal protein L24

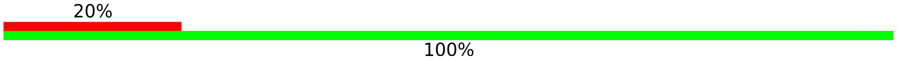
Chain U:

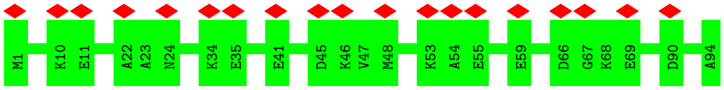




- Molecule 43: 50S ribosomal protein L25

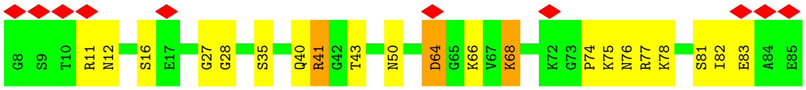
Chain V:





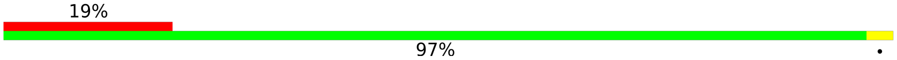
- Molecule 44: 50S ribosomal protein L27

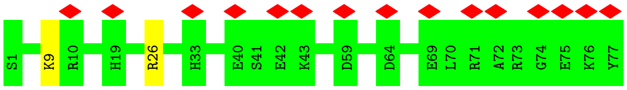
Chain W:



- Molecule 45: 50S ribosomal protein L28

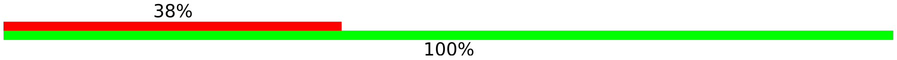
Chain X:

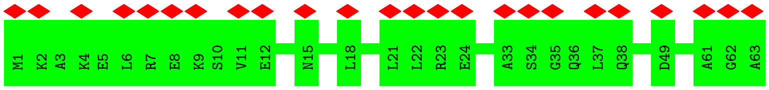




- Molecule 46: 50S ribosomal protein L29

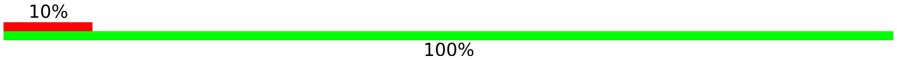
Chain Y:

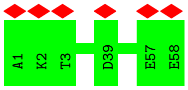




- Molecule 47: 50S ribosomal protein L30

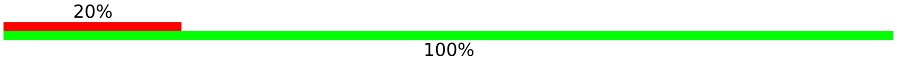
Chain Z:

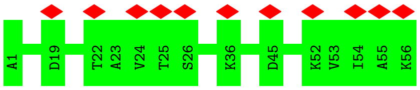




- Molecule 48: 50S ribosomal protein L32

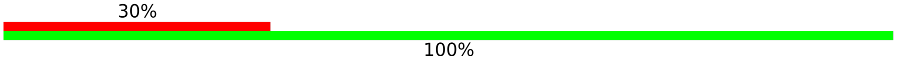
Chain 0:

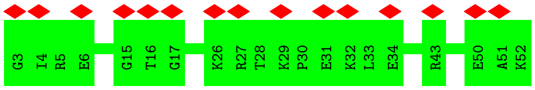




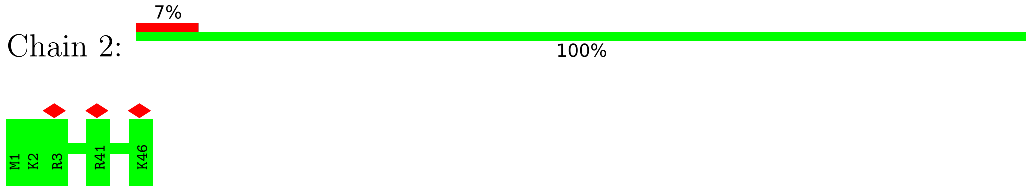
- Molecule 49: 50S ribosomal protein L33

Chain 1:

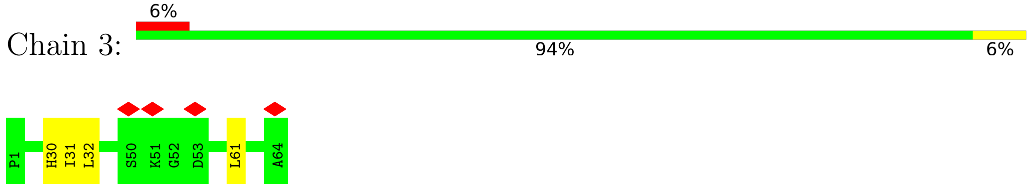




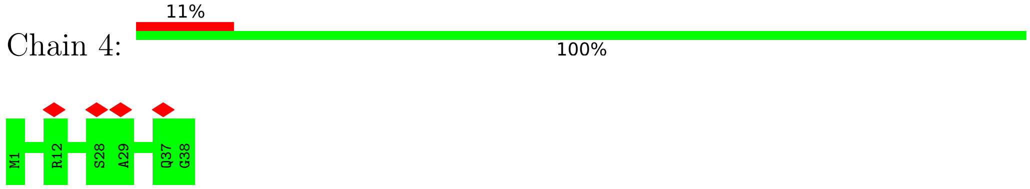
- Molecule 50: 50S ribosomal protein L34



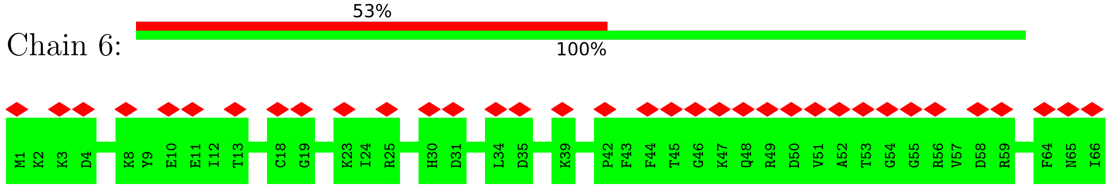
- Molecule 51: 50S ribosomal protein L35



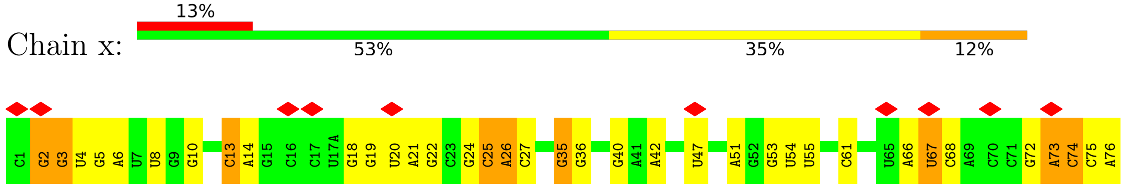
- Molecule 52: 50S ribosomal protein L36



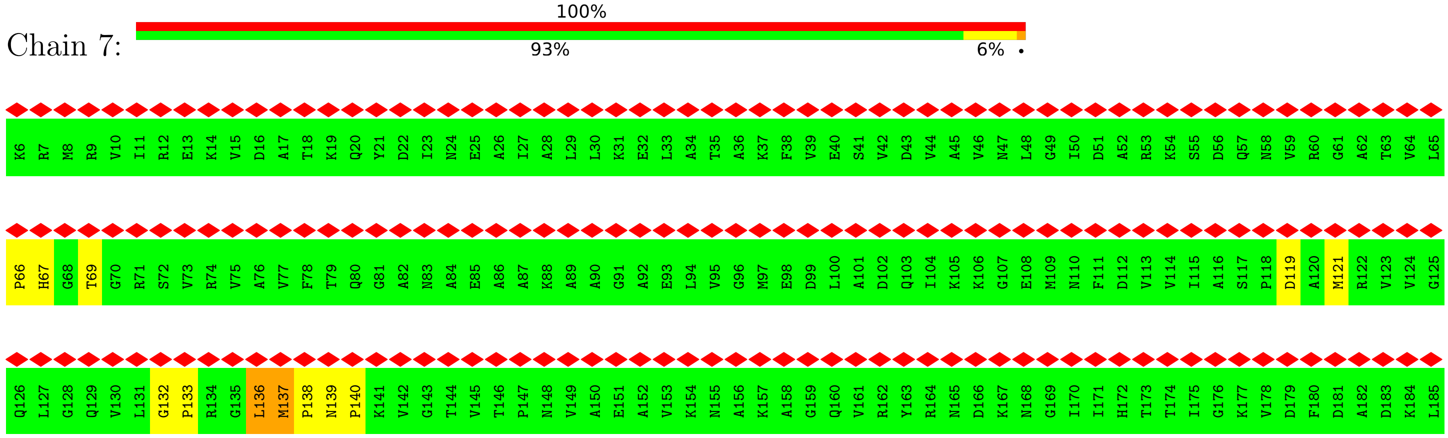
- Molecule 53: 50S ribosomal protein L31

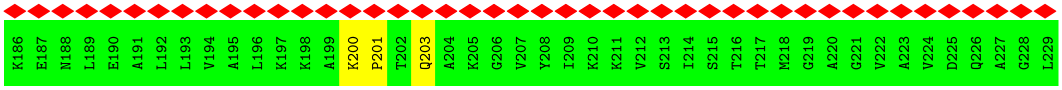


- Molecule 54: Proline tRNA



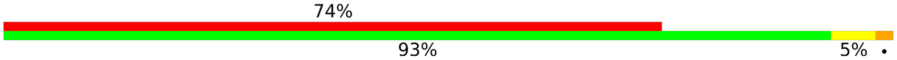
- Molecule 55: 50S ribosomal protein L1

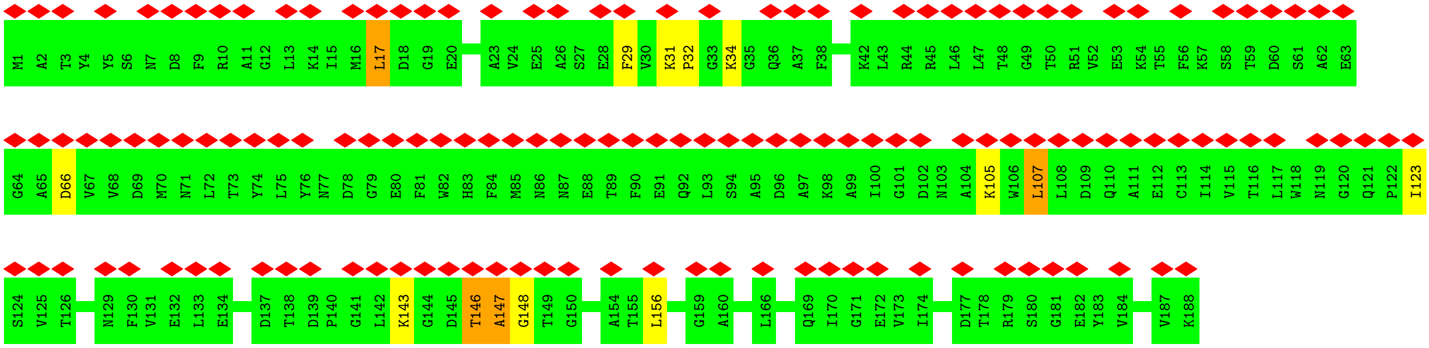




- Molecule 56: Elongation factor P

Chain w:





4 Experimental information (i)

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.669	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KEO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	a	0.81	2/36967 (0.0%)	1.07	146/57666 (0.3%)
2	b	0.34	0/1735	0.61	0/2338
3	c	0.40	0/1651	0.61	0/2225
4	d	0.40	0/1665	0.69	1/2227 (0.0%)
5	e	0.46	0/1154	0.70	1/1554 (0.1%)
6	f	0.40	0/835	0.67	0/1128
7	g	0.36	0/1195	0.64	0/1602
8	h	0.43	0/989	0.67	1/1326 (0.1%)
9	i	0.41	0/1034	0.67	0/1375
10	j	0.38	0/796	0.71	0/1077
11	k	0.40	0/885	0.65	0/1195
12	l	0.47	0/969	0.69	0/1300
13	m	0.37	0/892	0.70	0/1193
14	n	0.40	0/811	0.62	0/1081
15	o	0.36	0/722	0.60	0/964
16	p	0.46	0/659	0.66	0/884
17	q	0.41	0/657	0.65	0/881
18	r	0.41	0/511	0.62	0/689
19	s	0.42	0/652	0.63	0/877
20	t	0.35	0/671	0.57	0/888
21	u	0.37	0/500	0.71	0/668
22	v	0.78	0/139	1.14	1/214 (0.5%)
23	A	0.83	3/69039 (0.0%)	1.07	268/107701 (0.2%)
24	B	0.72	1/2876 (0.0%)	1.08	13/4483 (0.3%)
25	C	0.49	0/2121	0.65	0/2852
26	D	0.44	0/1586	0.62	0/2134
27	E	0.39	0/1571	0.57	0/2113
28	F	0.40	0/1434	0.62	1/1926 (0.1%)
29	G	0.35	0/1343	0.57	0/1816
30	H	0.30	0/1122	0.58	0/1515
31	J	0.41	0/1152	0.57	0/1551
32	K	0.46	0/947	0.64	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	L	0.40	0/1054	0.69	1/1403 (0.1%)
34	M	0.44	0/1093	0.66	1/1460 (0.1%)
35	N	0.39	0/973	0.66	0/1301
36	O	0.39	0/902	0.59	0/1209
37	P	0.43	0/929	0.64	2/1242 (0.2%)
38	Q	0.47	0/960	0.61	1/1278 (0.1%)
39	R	0.41	0/829	0.64	0/1107
40	S	0.41	0/864	0.65	0/1156
41	T	0.36	0/744	0.60	0/994
42	U	0.36	0/787	0.60	0/1051
43	V	0.38	0/766	0.59	0/1025
44	W	0.58	0/599	0.82	0/792
45	X	0.46	1/635 (0.2%)	0.57	0/848
46	Y	0.32	0/510	0.55	0/677
47	Z	0.36	0/453	0.63	0/605
48	0	0.43	0/450	0.57	0/599
49	1	0.40	0/416	0.58	0/554
50	2	0.46	0/380	0.61	0/498
51	3	0.45	0/513	0.76	1/676 (0.1%)
52	4	0.45	0/303	0.66	0/397
53	6	0.31	0/531	0.57	0/709
54	x	0.72	1/1839 (0.1%)	1.34	26/2866 (0.9%)
55	7	0.28	0/1678	0.74	3/2262 (0.1%)
56	w	0.41	1/1470 (0.1%)	0.78	4/1992 (0.2%)
All	All	0.72	9/158958 (0.0%)	0.98	471/237412 (0.2%)

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	b	0	3
3	c	0	2
5	e	0	1
6	f	0	1
7	g	0	1
9	i	0	1
11	k	0	1
12	l	0	2
13	m	0	1
17	q	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	s	0	1
21	u	0	1
28	F	0	2
29	G	0	2
31	J	0	1
34	M	0	2
39	R	0	1
42	U	0	4
51	3	0	1
55	7	0	1
56	w	0	3
All	All	0	35

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	x	74	C	O3'-P	-11.19	1.47	1.61
1	a	2	A	OP3-P	-10.69	1.48	1.61
23	A	1	G	OP3-P	-10.60	1.48	1.61
24	B	1	U	OP3-P	-10.53	1.48	1.61
23	A	528	A	N9-C4	-6.63	1.33	1.37
45	X	9	LYS	C-N	-5.84	1.20	1.34
23	A	1142	A	N9-C4	-5.69	1.34	1.37
56	w	147	ALA	N-CA	5.16	1.56	1.46
1	a	493	A	N9-C4	5.12	1.41	1.37

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	7	132	GLY	C-N-CD	-15.98	85.44	120.60
55	7	139	ASN	C-N-CD	-15.65	86.17	120.60
54	x	74	C	OP1-P-OP2	14.87	141.90	119.60
54	x	73	A	OP1-P-O3'	-14.14	74.09	105.20
54	x	73	A	OP2-P-O3'	-13.31	75.92	105.20
1	a	614	C	N1-C2-O2	11.85	126.01	118.90
1	a	624	C	C6-N1-C2	-10.20	116.22	120.30
1	a	1301	U	C2-N1-C1'	9.67	129.31	117.70
1	a	614	C	N3-C2-O2	-9.51	115.24	121.90
23	A	62	U	C2-N1-C1'	9.36	128.93	117.70
1	a	1158	C	C2-N1-C1'	9.31	129.04	118.80
23	A	2457	U	N3-C2-O2	-9.20	115.76	122.20
23	A	62	U	N1-C2-O2	9.17	129.22	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1911	U	N3-C2-O2	-9.07	115.85	122.20
1	a	1301	U	N1-C2-O2	8.82	128.97	122.80
54	x	25	C	C6-N1-C2	-8.60	116.86	120.30
23	A	2580	U	C2-N1-C1’	8.52	127.92	117.70
23	A	955	U	C2-N1-C1’	8.36	127.73	117.70
55	7	137	MET	C-N-CD	-8.27	102.41	120.60
23	A	62	U	N3-C2-O2	-8.18	116.47	122.20
23	A	2504	U	N1-C2-O2	8.17	128.52	122.80
24	B	12	C	C2-N1-C1’	8.12	127.74	118.80
23	A	955	U	N3-C2-O2	-8.12	116.52	122.20
1	a	1158	C	N1-C2-O2	8.12	123.77	118.90
54	x	25	C	C5-C6-N1	8.11	125.05	121.00
1	a	614	C	C2-N1-C1’	8.01	127.61	118.80
4	d	4	LEU	CA-CB-CG	7.99	133.67	115.30
23	A	2580	U	N3-C2-O2	-7.98	116.61	122.20
23	A	2504	U	N3-C2-O2	-7.98	116.61	122.20
23	A	2457	U	C2-N1-C1’	7.93	127.21	117.70
23	A	1313	U	N3-C2-O2	-7.92	116.66	122.20
54	x	73	A	P-O3’-C3’	7.88	129.16	119.70
1	a	813	U	N1-C2-O2	7.80	128.26	122.80
1	a	754	C	C2-N1-C1’	7.76	127.34	118.80
24	B	12	C	N1-C2-O2	7.76	123.56	118.90
23	A	2604	U	C2-N1-C1’	7.74	126.99	117.70
1	a	493	A	C2-N3-C4	7.71	114.46	110.60
23	A	2604	U	N1-C2-O2	7.68	128.18	122.80
23	A	2604	U	N3-C2-O2	-7.68	116.82	122.20
1	a	311	C	C6-N1-C2	-7.63	117.25	120.30
23	A	2605	U	C2-N1-C1’	7.63	126.85	117.70
23	A	2457	U	N1-C2-O2	7.62	128.13	122.80
23	A	1313	U	N1-C2-O2	7.56	128.09	122.80
1	a	813	U	N3-C2-O2	-7.39	117.03	122.20
23	A	1313	U	C2-N1-C1’	7.34	126.50	117.70
1	a	1301	U	N3-C2-O2	-7.30	117.09	122.20
1	a	623	C	C6-N1-C1’	7.25	129.50	120.80
23	A	1378	A	P-O3’-C3’	7.25	128.39	119.70
1	a	792	A	O4’-C1’-N9	7.23	113.98	108.20
23	A	2580	U	N1-C2-O2	7.21	127.85	122.80
23	A	1917	U	N3-C2-O2	-7.17	117.18	122.20
1	a	413	G	N3-C4-C5	-7.15	125.03	128.60
23	A	2099	U	N1-C2-O2	7.14	127.80	122.80
1	a	624	C	O4’-C1’-N1	7.13	113.90	108.20
23	A	884	U	N3-C2-O2	-7.12	117.22	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1138	G	C4-N9-C1'	7.12	135.75	126.50
23	A	512	G	O4'-C1'-N9	7.11	113.89	108.20
23	A	1911	U	N1-C2-O2	7.11	127.78	122.80
54	x	24	G	P-O3'-C3'	7.10	128.22	119.70
23	A	417	C	N1-C2-O2	7.09	123.16	118.90
23	A	1920	C	C6-N1-C2	-7.09	117.46	120.30
1	a	1301	U	C6-N1-C1'	-7.09	111.28	121.20
23	A	1911	U	C2-N1-C1'	7.08	126.20	117.70
1	a	1158	C	N3-C2-O2	-7.08	116.94	121.90
1	a	1496	C	C6-N1-C2	-7.08	117.47	120.30
23	A	1914	C	C6-N1-C2	-7.05	117.48	120.30
23	A	544	C	N1-C2-O2	7.03	123.12	118.90
23	A	783	A	C8-N9-C4	-7.03	102.99	105.80
23	A	542	C	N1-C2-O2	7.02	123.11	118.90
51	3	61	LEU	CA-CB-CG	7.01	131.43	115.30
23	A	1297	C	C6-N1-C2	-6.99	117.50	120.30
1	a	413	G	N3-C4-N9	6.97	130.18	126.00
23	A	1930	G	P-O3'-C3'	6.97	128.06	119.70
23	A	783	A	N7-C8-N9	6.94	117.27	113.80
1	a	726	C	C6-N1-C2	-6.94	117.52	120.30
56	w	17	LEU	CA-CB-CG	6.92	131.23	115.30
1	a	516	U	C2-N1-C1'	6.92	126.00	117.70
1	a	613	C	N1-C2-O2	6.90	123.04	118.90
54	x	3	G	P-O3'-C3'	6.86	127.94	119.70
1	a	1027	C	N1-C2-O2	6.86	123.02	118.90
23	A	162	U	N3-C2-O2	-6.84	117.41	122.20
23	A	528	A	C2-N3-C4	-6.84	107.18	110.60
1	a	972	C	C6-N1-C2	-6.79	117.58	120.30
54	x	55	U	C2-N1-C1'	6.79	125.85	117.70
23	A	242	G	P-O3'-C3'	6.79	127.84	119.70
23	A	1070	A	OP2-P-O3'	6.79	120.13	105.20
23	A	2486	C	N1-C2-O2	6.77	122.96	118.90
54	x	55	U	N3-C2-O2	-6.77	117.46	122.20
23	A	1022	G	P-O3'-C3'	6.76	127.81	119.70
1	a	932	C	N1-C2-O2	6.75	122.95	118.90
1	a	1027	C	C6-N1-C2	-6.72	117.61	120.30
23	A	2666	C	N1-C2-O2	6.71	122.93	118.90
23	A	1917	U	C2-N1-C1'	6.70	125.74	117.70
1	a	613	C	C6-N1-C2	-6.70	117.62	120.30
23	A	2655	G	P-O3'-C3'	6.69	127.73	119.70
54	x	67	U	P-O3'-C3'	6.68	127.72	119.70
1	a	1347	G	P-O3'-C3'	6.66	127.69	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	729	G	C8-N9-C1'	-6.63	118.38	127.00
54	x	2	G	P-O3'-C3'	6.63	127.66	119.70
1	a	960	U	N1-C2-O2	6.63	127.44	122.80
1	a	516	U	N3-C2-O2	-6.60	117.58	122.20
56	w	156	LEU	CA-CB-CG	6.60	130.48	115.30
23	A	2475	C	C6-N1-C2	-6.60	117.66	120.30
23	A	1020	A	P-O3'-C3'	6.59	127.61	119.70
23	A	1920	C	C5-C6-N1	6.58	124.29	121.00
23	A	955	U	N1-C2-O2	6.58	127.41	122.80
24	B	12	C	N3-C2-O2	-6.55	117.32	121.90
23	A	490	C	OP2-P-O3'	6.54	119.58	105.20
23	A	974	G	C4-N9-C1'	6.53	134.99	126.50
1	a	754	C	N1-C2-O2	6.50	122.80	118.90
23	A	2326	C	C6-N1-C2	-6.50	117.70	120.30
23	A	1779	U	C5-C6-N1	-6.50	119.45	122.70
1	a	1297	G	P-O3'-C3'	6.47	127.47	119.70
23	A	1993	U	C2-N1-C1'	6.47	125.47	117.70
23	A	1070	A	P-O3'-C3'	6.47	127.46	119.70
23	A	946	C	C6-N1-C2	-6.46	117.71	120.30
1	a	1432	G	P-O3'-C3'	6.45	127.44	119.70
1	a	1407	C	C6-N1-C2	-6.44	117.72	120.30
23	A	2667	C	C6-N1-C2	-6.44	117.72	120.30
24	B	97	C	C6-N1-C2	-6.44	117.73	120.30
23	A	2504	U	C2-N1-C1'	6.42	125.41	117.70
8	h	58	LEU	CA-CB-CG	6.41	130.04	115.30
1	a	1158	C	C6-N1-C1'	-6.40	113.12	120.80
1	a	1059	C	C6-N1-C2	-6.39	117.74	120.30
1	a	739	C	N1-C2-O2	6.39	122.73	118.90
1	a	924	C	C6-N1-C2	-6.38	117.75	120.30
23	A	143	C	N1-C2-O2	6.38	122.73	118.90
1	a	1138	G	N3-C4-N9	6.37	129.82	126.00
23	A	859	G	P-O3'-C3'	6.34	127.31	119.70
23	A	57	C	C6-N1-C2	-6.34	117.77	120.30
23	A	1006	C	C6-N1-C2	-6.32	117.77	120.30
23	A	992	C	C6-N1-C2	-6.32	117.77	120.30
1	a	439	U	C5-C6-N1	6.30	125.85	122.70
1	a	1230	C	C6-N1-C2	-6.29	117.78	120.30
23	A	1111	A	P-O3'-C3'	6.29	127.24	119.70
1	a	1138	G	C8-N9-C1'	-6.28	118.83	127.00
23	A	2403	C	N1-C2-O2	6.28	122.67	118.90
1	a	1201	A	P-O3'-C3'	6.27	127.23	119.70
23	A	729	G	C4-N9-C1'	6.27	134.66	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	2626	C	C6-N1-C2	-6.27	117.79	120.30
1	a	436	C	C6-N1-C2	-6.27	117.79	120.30
1	a	545	C	C6-N1-C2	-6.27	117.79	120.30
23	A	860	U	N1-C2-O2	6.26	127.18	122.80
23	A	51	G	P-O3'-C3'	6.25	127.20	119.70
24	B	70	C	C6-N1-C2	-6.24	117.80	120.30
23	A	162	U	C2-N1-C1'	6.24	125.18	117.70
1	a	178	C	N1-C2-O2	6.22	122.63	118.90
23	A	1914	C	N3-C2-O2	-6.22	117.55	121.90
24	B	12	C	O4'-C1'-N1	6.21	113.17	108.20
23	A	276	U	N1-C2-O2	6.21	127.15	122.80
23	A	2820	A	OP1-P-O3'	6.21	118.86	105.20
23	A	162	U	N1-C2-O2	6.20	127.14	122.80
1	a	961	U	N1-C2-O2	6.20	127.14	122.80
23	A	2342	C	C5-C6-N1	6.19	124.10	121.00
23	A	2774	C	C6-N1-C2	-6.19	117.82	120.30
1	a	890	G	O4'-C1'-N9	6.19	113.15	108.20
1	a	960	U	P-O3'-C3'	6.18	127.12	119.70
1	a	1158	C	C6-N1-C2	-6.17	117.83	120.30
23	A	2099	U	C2-N1-C1'	6.17	125.10	117.70
23	A	2336	A	C5-C6-N6	-6.16	118.77	123.70
1	a	1027	C	C5-C6-N1	6.15	124.08	121.00
23	A	2023	C	N1-C2-O2	6.14	122.58	118.90
1	a	624	C	N3-C4-C5	-6.11	119.45	121.90
23	A	1997	C	N1-C2-O2	6.11	122.57	118.90
1	a	812	G	O4'-C1'-N9	6.11	113.09	108.20
1	a	469	C	N1-C2-O2	6.10	122.56	118.90
54	x	74	C	N1-C2-O2	6.09	122.56	118.90
23	A	62	U	C6-N1-C1'	-6.09	112.68	121.20
23	A	1508	A	O4'-C1'-N9	6.09	113.07	108.20
1	a	606	G	N3-C4-N9	6.09	129.65	126.00
23	A	2808	G	P-O3'-C3'	6.08	127.00	119.70
23	A	2580	U	C6-N1-C1'	-6.08	112.69	121.20
23	A	2605	U	N3-C2-O2	-6.08	117.94	122.20
23	A	2591	C	C6-N1-C2	-6.07	117.87	120.30
23	A	2190	G	P-O3'-C3'	6.06	126.97	119.70
1	a	106	C	C6-N1-C2	-6.05	117.88	120.30
24	B	12	C	C6-N1-C1'	-6.05	113.54	120.80
23	A	2871	U	N1-C2-O2	6.03	127.02	122.80
23	A	1656	C	C6-N1-C2	-6.03	117.89	120.30
1	a	739	C	N3-C2-O2	-6.03	117.68	121.90
23	A	528	A	N3-C4-N9	-6.03	122.58	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	417	C	N3-C2-O2	-6.03	117.68	121.90
23	A	2226	C	C6-N1-C2	-6.01	117.89	120.30
23	A	546	U	C2-N1-C1'	6.01	124.91	117.70
23	A	898	C	C6-N1-C2	-6.00	117.90	120.30
1	a	613	C	N3-C2-O2	-6.00	117.70	121.90
23	A	1917	U	N1-C2-O2	5.99	126.99	122.80
23	A	1378	A	OP1-P-O3'	5.99	118.37	105.20
23	A	1914	C	N1-C2-O2	5.98	122.49	118.90
23	A	601	C	C6-N1-C2	-5.97	117.91	120.30
24	B	3	C	OP1-P-O3'	5.95	118.30	105.20
1	a	1518	A	O4'-C1'-N9	5.95	112.96	108.20
23	A	2104	U	C2-N1-C1'	5.95	124.84	117.70
54	x	24	G	OP1-P-O3'	5.94	118.27	105.20
23	A	2350	C	N1-C2-O2	5.93	122.46	118.90
37	P	113	LEU	CA-CB-CG	5.93	128.95	115.30
1	a	637	C	N1-C2-O2	5.93	122.46	118.90
54	x	13	C	C6-N1-C2	-5.92	117.93	120.30
1	a	739	C	C6-N1-C2	-5.91	117.94	120.30
23	A	2646	C	C6-N1-C2	-5.90	117.94	120.30
23	A	546	U	N1-C2-O2	5.89	126.92	122.80
1	a	606	G	C4-N9-C1'	5.88	134.15	126.50
23	A	736	C	C6-N1-C2	-5.88	117.95	120.30
23	A	2342	C	C6-N1-C2	-5.87	117.95	120.30
1	a	1008	U	N1-C2-O2	5.86	126.91	122.80
1	a	810	C	N1-C2-O2	5.86	122.41	118.90
23	A	1305	C	C6-N1-C2	-5.85	117.96	120.30
1	a	1190	G	P-O3'-C3'	5.85	126.72	119.70
23	A	2043	C	C5-C6-N1	5.84	123.92	121.00
24	B	3	C	N1-C2-O2	5.84	122.41	118.90
23	A	1893	C	N3-C2-O2	-5.83	117.82	121.90
23	A	2354	C	N1-C2-O2	5.83	122.40	118.90
23	A	343	C	C6-N1-C2	-5.83	117.97	120.30
23	A	458	G	O4'-C1'-N9	5.83	112.86	108.20
23	A	2486	C	N3-C2-O2	-5.82	117.83	121.90
23	A	702	U	N1-C2-O2	5.82	126.87	122.80
1	a	1331	G	P-O3'-C3'	5.82	126.68	119.70
1	a	1460	C	C6-N1-C2	-5.81	117.98	120.30
23	A	2072	C	C5-C6-N1	5.81	123.90	121.00
1	a	961	U	C5-C6-N1	5.80	125.60	122.70
23	A	884	U	N1-C2-O2	5.80	126.86	122.80
23	A	915	C	N1-C2-O2	5.79	122.38	118.90
1	a	1138	G	N3-C4-C5	-5.79	125.71	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1300	G	P-O3'-C3'	5.79	126.64	119.70
23	A	783	A	C5-N7-C8	-5.78	101.01	103.90
1	a	960	U	C2-N1-C1'	5.78	124.63	117.70
1	a	493	A	N1-C6-N6	-5.78	115.13	118.60
23	A	1993	U	C5-C6-N1	5.78	125.59	122.70
23	A	1103	A	C2-N3-C4	5.77	113.48	110.60
23	A	1294	U	N3-C2-O2	-5.77	118.16	122.20
1	a	623	C	C2-N1-C1'	-5.76	112.46	118.80
23	A	2579	C	C6-N1-C2	-5.76	117.99	120.30
24	B	31	C	C6-N1-C2	-5.75	118.00	120.30
1	a	1182	G	P-O3'-C3'	5.75	126.60	119.70
23	A	2666	C	C2-N1-C1'	5.75	125.12	118.80
1	a	813	U	C2-N1-C1'	5.75	124.60	117.70
1	a	961	U	N3-C2-O2	-5.75	118.18	122.20
23	A	268	C	C6-N1-C2	-5.75	118.00	120.30
23	A	62	U	C5-C6-N1	5.74	125.57	122.70
23	A	1314	C	N1-C2-O2	5.74	122.34	118.90
23	A	421	C	N1-C2-O2	5.73	122.34	118.90
23	A	2594	C	C6-N1-C2	-5.72	118.01	120.30
23	A	458	G	C4-N9-C1'	-5.71	119.07	126.50
23	A	729	G	N3-C4-N9	5.71	129.43	126.00
23	A	937	C	C6-N1-C2	-5.71	118.02	120.30
23	A	1930	G	OP2-P-O3'	5.71	117.76	105.20
23	A	1816	C	N1-C2-O2	5.71	122.32	118.90
1	a	1045	C	C6-N1-C2	-5.70	118.02	120.30
23	A	1611	C	N1-C2-O2	5.69	122.31	118.90
23	A	1936	A	C2-N3-C4	-5.68	107.76	110.60
23	A	2069	A	N1-C2-N3	-5.68	126.46	129.30
23	A	2286	G	P-O3'-C3'	5.68	126.52	119.70
23	A	1305	C	C5-C6-N1	5.68	123.84	121.00
1	a	494	G	N7-C8-N9	5.67	115.94	113.10
1	a	1520	C	N1-C2-O2	5.67	122.30	118.90
23	A	784	G	OP1-P-O3'	5.67	117.67	105.20
1	a	1520	C	C5-C6-N1	5.67	123.83	121.00
1	a	1520	C	C6-N1-C2	-5.67	118.03	120.30
1	a	1317	C	N1-C2-O2	5.66	122.30	118.90
23	A	1297	C	C5-C6-N1	5.66	123.83	121.00
1	a	623	C	C6-N1-C2	-5.65	118.04	120.30
1	a	965	U	P-O3'-C3'	5.65	126.48	119.70
1	a	1399	C	P-O3'-C3'	5.65	126.48	119.70
1	a	1402	C	N3-C2-O2	-5.65	117.94	121.90
1	a	54	C	N1-C2-O2	5.64	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	617	G	N3-C4-N9	-5.63	122.62	126.00
23	A	490	C	P-O3'-C3'	5.62	126.45	119.70
23	A	1320	C	P-O3'-C3'	5.62	126.45	119.70
23	A	1958	C	C6-N1-C2	-5.61	118.06	120.30
23	A	2179	C	N1-C2-O2	5.61	122.26	118.90
23	A	702	U	N3-C2-O2	-5.60	118.28	122.20
23	A	2354	C	C6-N1-C2	-5.59	118.07	120.30
23	A	135	U	N1-C2-O2	5.58	126.71	122.80
54	x	55	U	N1-C2-O2	5.58	126.71	122.80
23	A	2871	U	N3-C2-O2	-5.57	118.30	122.20
54	x	73	A	C2'-C3'-O3'	5.57	122.61	113.70
23	A	2646	C	N1-C2-O2	5.56	122.24	118.90
1	a	614	C	C6-N1-C2	-5.55	118.08	120.30
23	A	683	U	C5-C6-N1	5.55	125.48	122.70
23	A	1804	C	C6-N1-C2	-5.55	118.08	120.30
23	A	421	C	C2-N1-C1'	5.55	124.91	118.80
23	A	480	A	OP1-P-O3'	5.55	117.42	105.20
23	A	1940	U	P-O3'-C3'	5.55	126.36	119.70
1	a	413	G	C4-N9-C1'	5.54	133.71	126.50
23	A	860	U	C2-N1-C1'	5.53	124.33	117.70
23	A	1656	C	C5-C6-N1	5.52	123.76	121.00
23	A	890	C	N1-C2-O2	5.52	122.21	118.90
23	A	2336	A	N1-C6-N6	5.52	121.91	118.60
1	a	754	C	C6-N1-C1'	-5.52	114.18	120.80
1	a	810	C	N3-C2-O2	-5.52	118.04	121.90
56	w	107	LEU	CA-CB-CG	5.51	127.97	115.30
23	A	1103	A	OP1-P-O3'	5.51	117.32	105.20
24	B	3	C	P-O3'-C3'	5.50	126.30	119.70
23	A	2099	U	N3-C2-O2	-5.50	118.35	122.20
23	A	528	A	N3-C4-C5	5.50	130.65	126.80
23	A	1788	C	C6-N1-C2	-5.50	118.10	120.30
38	Q	94	LEU	CA-CB-CG	5.50	127.94	115.30
23	A	2655	G	OP2-P-O3'	5.49	117.28	105.20
23	A	723	C	C6-N1-C2	-5.49	118.11	120.30
1	a	1301	U	C5-C6-N1	5.48	125.44	122.70
1	a	1449	C	N1-C2-O2	5.48	122.19	118.90
23	A	143	C	N3-C2-O2	-5.48	118.07	121.90
56	w	146	THR	O-C-N	-5.48	113.94	122.70
1	a	965	U	OP1-P-O3'	5.47	117.23	105.20
23	A	546	U	N3-C2-O2	-5.47	118.37	122.20
1	a	516	U	N1-C2-O2	5.47	126.63	122.80
23	A	2552	U	C2-N1-C1'	5.46	124.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	x	3	G	OP1-P-O3’	5.45	117.20	105.20
24	B	4	C	C6-N1-C2	-5.45	118.12	120.30
23	A	2043	C	C6-N1-C2	-5.45	118.12	120.30
28	F	3	LEU	CA-CB-CG	5.45	127.83	115.30
23	A	2785	C	N1-C2-O2	5.44	122.17	118.90
23	A	1827	U	C5-C6-N1	5.44	125.42	122.70
23	A	912	C	N1-C2-O2	5.43	122.16	118.90
23	A	2637	U	C2-N1-C1’	5.43	124.21	117.70
23	A	2880	C	N3-C2-O2	-5.42	118.10	121.90
1	a	1098	C	N3-C2-O2	-5.42	118.10	121.90
1	a	614	C	C6-N1-C1’	-5.42	114.30	120.80
54	x	26	A	C3’-C2’-C1’	5.42	105.83	101.50
5	e	121	ASN	C-N-CA	5.41	135.22	121.70
54	x	35	G	C2’-C3’-O3’	5.41	122.35	113.70
1	a	23	C	C6-N1-C2	-5.41	118.14	120.30
23	A	506	G	N3-C4-N9	-5.41	122.76	126.00
23	A	860	U	N3-C2-O2	-5.40	118.42	122.20
23	A	672	C	C6-N1-C2	-5.40	118.14	120.30
23	A	2889	C	N1-C2-O2	5.39	122.14	118.90
1	a	1032	G	C4-N9-C1’	5.38	133.50	126.50
54	x	75	C	C6-N1-C2	-5.38	118.15	120.30
1	a	107	G	N1-C6-O6	-5.37	116.68	119.90
23	A	884	U	C6-N1-C2	-5.37	117.78	121.00
23	A	130	C	C6-N1-C2	-5.36	118.16	120.30
23	A	2666	C	N3-C2-O2	-5.36	118.15	121.90
23	A	635	C	C6-N1-C2	-5.36	118.16	120.30
23	A	276	U	N3-C2-O2	-5.35	118.45	122.20
23	A	1777	U	C5-C6-N1	5.35	125.38	122.70
1	a	494	G	C6-C5-N7	-5.34	127.19	130.40
1	a	1225	A	C2-N3-C4	5.34	113.27	110.60
1	a	1008	U	N3-C2-O2	-5.34	118.46	122.20
23	A	1911	U	C6-N1-C2	-5.34	117.80	121.00
23	A	372	G	C4-N9-C1’	-5.34	119.56	126.50
23	A	680	C	C6-N1-C2	-5.34	118.17	120.30
23	A	2806	C	C6-N1-C2	-5.34	118.17	120.30
1	a	311	C	N3-C2-O2	-5.33	118.17	121.90
23	A	1005	C	N1-C2-O2	5.33	122.10	118.90
34	M	70	ASP	CB-CG-OD1	5.33	123.10	118.30
54	x	75	C	OP2-P-O3’	5.33	116.92	105.20
23	A	510	C	N1-C2-O2	5.32	122.09	118.90
23	A	1314	C	C2-N1-C1’	5.32	124.65	118.80
1	a	178	C	N3-C2-O2	-5.31	118.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	784	G	P-O3'-C3'	5.31	126.08	119.70
23	A	1314	C	C6-N1-C2	-5.30	118.18	120.30
1	a	36	C	C6-N1-C2	-5.30	118.18	120.30
23	A	1489	C	N1-C2-O2	5.30	122.08	118.90
23	A	2506	U	C2-N1-C1'	5.30	124.06	117.70
23	A	481	G	O4'-C1'-N9	5.30	112.44	108.20
23	A	1320	C	OP1-P-O3'	5.30	116.85	105.20
1	a	866	C	C6-N1-C2	-5.29	118.18	120.30
23	A	985	C	N1-C2-O2	5.29	122.07	118.90
1	a	652	U	N3-C2-O2	-5.28	118.50	122.20
23	A	1868	C	C6-N1-C2	-5.28	118.19	120.30
23	A	1893	C	N1-C2-O2	5.28	122.07	118.90
23	A	2226	C	N1-C2-O2	5.28	122.07	118.90
23	A	2113	U	N3-C2-O2	-5.27	118.51	122.20
23	A	746	U	C2-N1-C1'	5.27	124.03	117.70
1	a	1407	C	C5-C6-N1	5.27	123.64	121.00
23	A	560	C	C5-C6-N1	5.27	123.63	121.00
1	a	494	G	C8-N9-C4	-5.26	104.29	106.40
23	A	560	C	C6-N1-C2	-5.26	118.20	120.30
23	A	106	C	C6-N1-C2	-5.26	118.20	120.30
23	A	955	U	C6-N1-C1'	-5.26	113.84	121.20
23	A	2666	C	C6-N1-C2	-5.25	118.20	120.30
23	A	974	G	C8-N9-C1'	-5.25	120.17	127.00
23	A	2391	G	P-O3'-C3'	5.24	125.99	119.70
23	A	82	U	N1-C2-O2	5.24	126.47	122.80
54	x	13	C	P-O3'-C3'	5.24	125.99	119.70
23	A	1221	C	N1-C2-O2	5.24	122.04	118.90
23	A	2442	C	N1-C2-O2	5.24	122.04	118.90
1	a	960	U	N3-C2-O2	-5.23	118.54	122.20
23	A	1295	C	N1-C2-O2	5.23	122.04	118.90
1	a	960	U	OP2-P-O3'	5.23	116.71	105.20
23	A	12	U	N3-C2-O2	-5.22	118.54	122.20
23	A	242	G	OP2-P-O3'	5.22	116.69	105.20
23	A	1830	C	C6-N1-C2	-5.22	118.21	120.30
1	a	400	C	C6-N1-C2	-5.22	118.21	120.30
23	A	143	C	C6-N1-C2	-5.22	118.21	120.30
23	A	1644	C	N1-C2-O2	5.22	122.03	118.90
1	a	716	A	C2-N3-C4	5.21	113.21	110.60
23	A	986	C	C6-N1-C2	-5.21	118.22	120.30
23	A	1021	A	C2-N3-C4	5.21	113.21	110.60
24	B	66	A	P-O3'-C3'	5.21	125.96	119.70
23	A	1879	C	C6-N1-C2	-5.21	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	486	U	N1-C2-O2	5.21	126.45	122.80
1	a	606	G	C8-N9-C1’	-5.21	120.23	127.00
23	A	1775	U	N1-C2-O2	5.20	126.44	122.80
54	x	67	U	OP1-P-O3’	5.20	116.64	105.20
1	a	1402	C	C6-N1-C2	-5.20	118.22	120.30
23	A	650	C	C6-N1-C2	-5.20	118.22	120.30
23	A	2605	U	C6-N1-C1’	-5.19	113.93	121.20
23	A	2646	C	C5-C6-N1	5.19	123.59	121.00
23	A	1221	C	C6-N1-C2	-5.19	118.22	120.30
23	A	737	C	C6-N1-C2	-5.19	118.22	120.30
23	A	1993	U	N3-C2-O2	-5.19	118.57	122.20
23	A	2023	C	N3-C2-O2	-5.19	118.27	121.90
1	a	1027	C	N3-C2-O2	-5.18	118.27	121.90
23	A	1822	C	C6-N1-C2	-5.18	118.23	120.30
1	a	613	C	C5-C6-N1	5.18	123.59	121.00
1	a	439	U	C2-N1-C1’	5.18	123.92	117.70
1	a	910	C	C6-N1-C2	-5.18	118.23	120.30
23	A	1142	A	N3-C4-C5	5.18	130.42	126.80
23	A	2260	C	N1-C2-O2	5.18	122.01	118.90
1	a	1449	C	N3-C2-O2	-5.17	118.28	121.90
1	a	1059	C	C5-C6-N1	5.17	123.59	121.00
23	A	955	U	O4’-C1’-N1	5.17	112.34	108.20
1	a	177	G	C4-N9-C1’	5.17	133.22	126.50
23	A	421	C	P-O3’-C3’	5.17	125.90	119.70
23	A	974	G	C6-C5-N7	-5.16	127.30	130.40
23	A	2096	C	C2-N1-C1’	5.16	124.48	118.80
54	x	2	G	OP1-P-O3’	5.16	116.55	105.20
1	a	438	U	N3-C2-O2	-5.15	118.59	122.20
23	A	2165	C	C6-N1-C2	-5.15	118.24	120.30
23	A	2025	C	C6-N1-C2	-5.15	118.24	120.30
23	A	1005	C	C6-N1-C2	-5.14	118.24	120.30
23	A	1221	C	N3-C2-O2	-5.14	118.30	121.90
23	A	1993	U	C6-N1-C2	-5.14	117.91	121.00
1	a	157	U	C5-C6-N1	5.14	125.27	122.70
1	a	1098	C	C6-N1-C2	-5.14	118.24	120.30
23	A	838	C	N3-C2-O2	-5.14	118.30	121.90
1	a	726	C	C5-C6-N1	5.13	123.57	121.00
1	a	796	C	C6-N1-C2	-5.13	118.25	120.30
1	a	392	C	N1-C2-O2	5.13	121.98	118.90
23	A	669	G	C4-N9-C1’	5.13	133.16	126.50
23	A	1967	C	C2-N1-C1’	5.13	124.44	118.80
23	A	2023	C	C6-N1-C2	-5.12	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	2099	U	C5-C6-N1	5.12	125.26	122.70
23	A	1992	G	O4'-C1'-N9	-5.12	104.10	108.20
23	A	2853	C	C6-N1-C2	-5.12	118.25	120.30
1	a	545	C	C5-C6-N1	5.12	123.56	121.00
37	P	7	LEU	CA-CB-CG	5.11	127.06	115.30
23	A	2604	U	C6-N1-C1'	-5.11	114.05	121.20
23	A	2475	C	C5-C6-N1	5.11	123.55	121.00
1	a	1098	C	N1-C2-O2	5.11	121.96	118.90
23	A	116	C	N1-C2-O2	5.11	121.96	118.90
23	A	2214	C	N1-C2-O2	5.11	121.96	118.90
23	A	542	C	N3-C2-O2	-5.09	118.33	121.90
23	A	769	U	N3-C2-O2	-5.09	118.64	122.20
23	A	2226	C	N3-C2-O2	-5.09	118.34	121.90
23	A	2605	U	N1-C2-O2	5.09	126.36	122.80
54	x	10	G	C5-C6-O6	-5.08	125.55	128.60
1	a	385	C	C6-N1-C2	-5.08	118.27	120.30
1	a	1282	C	N1-C2-O2	5.07	121.94	118.90
23	A	2626	C	C5-C6-N1	5.07	123.54	121.00
1	a	436	C	C2-N1-C1'	5.06	124.37	118.80
22	v	16	C	N1-C2-O2	5.06	121.94	118.90
1	a	1344	C	C5-C6-N1	5.06	123.53	121.00
23	A	2442	C	C6-N1-C2	-5.06	118.28	120.30
23	A	116	C	N3-C2-O2	-5.05	118.36	121.90
1	a	606	G	N3-C4-C5	-5.05	126.07	128.60
1	a	1317	C	N3-C2-O2	-5.05	118.36	121.90
1	a	624	C	C6-N1-C1'	5.05	126.86	120.80
23	A	2104	U	N3-C2-O2	-5.04	118.67	122.20
23	A	1583	A	O4'-C1'-N9	5.04	112.23	108.20
23	A	2076	U	C2-N1-C1'	5.04	123.74	117.70
23	A	2576	G	C4-N9-C1'	5.04	133.05	126.50
23	A	1816	C	N3-C2-O2	-5.04	118.38	121.90
23	A	1779	U	C2-N1-C1'	-5.03	111.66	117.70
1	a	493	A	N3-C4-C5	-5.03	123.28	126.80
23	A	1993	U	N1-C2-O2	5.02	126.31	122.80
23	A	1352	U	N3-C2-O2	-5.01	118.69	122.20
23	A	2794	C	N1-C2-O2	5.01	121.91	118.90
1	a	932	C	N3-C2-O2	-5.01	118.39	121.90
33	L	95	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	3	30	HIS	Peptide
55	7	66	PRO	Peptide
28	F	173	ASP	Peptide
28	F	174	PHE	Peptide
29	G	118	ALA	Peptide
29	G	46	ASP	Peptide
31	J	81	ILE	Peptide
34	M	57	VAL	Peptide
34	M	58	LYS	Peptide
39	R	53	PHE	Peptide
42	U	5	ARG	Peptide
42	U	87	GLU	Peptide
42	U	88	ASP	Peptide
42	U	97	SER	Peptide
2	b	15	PHE	Peptide
2	b	18	GLN	Peptide
2	b	30	ILE	Peptide
3	c	95	GLY	Peptide
3	c	96	VAL	Peptide
5	e	120	HIS	Peptide
6	f	52	ASN	Peptide
7	g	63	VAL	Peptide
9	i	56	MET	Peptide
11	k	124	LYS	Peptide
12	l	101	LEU	Peptide
12	l	42	LYS	Peptide
13	m	4	ALA	Peptide
17	q	48	GLU	Peptide
17	q	67	SER	Peptide
17	q	69	THR	Peptide
19	s	3	SER	Peptide
21	u	33	ARG	Peptide
56	w	105	LYS	Peptide
56	w	123	ILE	Peptide
56	w	66	ASP	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	
2	b	216/218 (99%)	191 (88%)	25 (12%)	0	100	100
3	c	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
4	d	203/205 (99%)	176 (87%)	27 (13%)	0	100	100
5	e	155/157 (99%)	132 (85%)	21 (14%)	2 (1%)	12	42
6	f	98/100 (98%)	82 (84%)	14 (14%)	2 (2%)	7	31
7	g	149/151 (99%)	130 (87%)	19 (13%)	0	100	100
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
9	i	125/127 (98%)	101 (81%)	22 (18%)	2 (2%)	9	37
10	j	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	15	49
11	k	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
12	l	121/123 (98%)	90 (74%)	29 (24%)	2 (2%)	9	36
13	m	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	8	34
14	n	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
15	o	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	44
16	p	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	q	78/80 (98%)	65 (83%)	12 (15%)	1 (1%)	12	42
18	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
19	s	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
20	t	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
21	u	63/65 (97%)	47 (75%)	16 (25%)	0	100	100
25	C	269/271 (99%)	250 (93%)	19 (7%)	0	100	100
26	D	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
27	E	199/201 (99%)	180 (90%)	19 (10%)	0	100	100
28	F	175/177 (99%)	157 (90%)	18 (10%)	0	100	100
29	G	174/176 (99%)	155 (89%)	16 (9%)	3 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
31	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
32	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
33	L	141/143 (99%)	120 (85%)	21 (15%)	0	100	100
34	M	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	6	29
35	N	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
36	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
37	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
38	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
39	R	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15	49
40	S	108/110 (98%)	99 (92%)	7 (6%)	2 (2%)	8	33
41	T	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
42	U	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	15	49
43	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	W	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	3
45	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
46	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
47	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
48	0	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
49	1	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
50	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	4	22
52	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
53	6	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
55	7	222/224 (99%)	181 (82%)	34 (15%)	7 (3%)	4	22
56	w	185/188 (98%)	153 (83%)	28 (15%)	4 (2%)	6	29
All	All	5989/6092 (98%)	5301 (88%)	644 (11%)	44 (1%)	26	57

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	53	LYS
17	q	70	LYS

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Mol	Chain	Res	Type
29	G	47	ASN
42	U	89	GLY
44	W	27	GLY
51	3	31	ILE
55	7	69	THR
55	7	140	PRO
56	w	147	ALA
6	f	55	HIS
12	l	102	ASP
13	m	5	GLY
15	o	46	LYS
34	M	59	ARG
44	W	28	GLY
44	W	50	ASN
44	W	64	ASP
44	W	74	PRO
44	W	78	LYS
51	3	32	LEU
55	7	133	PRO
55	7	201	PRO
29	G	108	PHE
56	w	32	PRO
56	w	148	GLY
5	e	122	VAL
9	i	90	ASP
9	i	91	GLU
34	M	58	LYS
39	R	54	VAL
40	S	2	GLU
40	S	64	ALA
44	W	41	ARG
44	W	68	LYS
5	e	121	ASN
13	m	4	ALA
29	G	119	GLY
55	7	67	HIS
55	7	138	PRO
12	l	3	VAL
55	7	136	LEU
56	w	146	THR
34	M	69	PRO
10	j	57	VAL

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	
2	b	180/180 (100%)	176 (98%)	4 (2%)	52	78
3	c	170/170 (100%)	169 (99%)	1 (1%)	86	94
4	d	172/172 (100%)	169 (98%)	3 (2%)	60	83
5	e	114/119 (96%)	113 (99%)	1 (1%)	78	91
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	103 (99%)	1 (1%)	76	90
9	i	105/105 (100%)	103 (98%)	2 (2%)	57	81
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	73	89
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	90
13	m	92/92 (100%)	91 (99%)	1 (1%)	73	89
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	64 (98%)	1 (2%)	65	85
17	q	74/74 (100%)	73 (99%)	1 (1%)	67	86
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	C	216/216 (100%)	213 (99%)	3 (1%)	67	86
26	D	164/164 (100%)	162 (99%)	2 (1%)	71	88
27	E	165/165 (100%)	164 (99%)	1 (1%)	86	94
28	F	148/148 (100%)	148 (100%)	0	100	100
29	G	137/137 (100%)	137 (100%)	0	100	100
30	H	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	J	116/116 (100%)	116 (100%)	0	100	100
32	K	103/103 (100%)	103 (100%)	0	100	100
33	L	102/102 (100%)	101 (99%)	1 (1%)	76	90
34	M	109/109 (100%)	108 (99%)	1 (1%)	78	91
35	N	100/100 (100%)	99 (99%)	1 (1%)	76	90
36	O	86/86 (100%)	86 (100%)	0	100	100
37	P	99/99 (100%)	99 (100%)	0	100	100
38	Q	89/89 (100%)	89 (100%)	0	100	100
39	R	84/84 (100%)	83 (99%)	1 (1%)	71	88
40	S	93/93 (100%)	92 (99%)	1 (1%)	73	89
41	T	80/80 (100%)	80 (100%)	0	100	100
42	U	83/83 (100%)	83 (100%)	0	100	100
43	V	78/78 (100%)	78 (100%)	0	100	100
44	W	59/59 (100%)	43 (73%)	16 (27%)	0	1
45	X	67/67 (100%)	66 (98%)	1 (2%)	65	85
46	Y	55/55 (100%)	55 (100%)	0	100	100
47	Z	48/48 (100%)	48 (100%)	0	100	100
48	0	47/47 (100%)	47 (100%)	0	100	100
49	1	45/45 (100%)	45 (100%)	0	100	100
50	2	38/38 (100%)	38 (100%)	0	100	100
51	3	51/51 (100%)	51 (100%)	0	100	100
52	4	34/34 (100%)	34 (100%)	0	100	100
53	6	59/59 (100%)	59 (100%)	0	100	100
55	7	173/173 (100%)	167 (96%)	6 (4%)	36	68
56	w	154/154 (100%)	149 (97%)	5 (3%)	39	69
All	All	4943/4971 (99%)	4887 (99%)	56 (1%)	74	89

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	20	ARG
2	b	23	ASN
2	b	35	ASN

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Mol	Chain	Res	Type
2	b	202	ASN
3	c	156	LEU
4	d	61	ARG
4	d	80	ARG
4	d	177	MET
5	e	69	ASN
8	h	120	LEU
9	i	44	ARG
9	i	105	ARG
11	k	12	ARG
12	l	113	ARG
13	m	7	ASN
16	p	5	ARG
17	q	18	LYS
25	C	36	ASN
25	C	85	ASN
25	C	252	LYS
26	D	33	ARG
26	D	169	ARG
27	E	156	ASN
33	L	27	LEU
34	M	6	ARG
35	N	2	ARG
39	R	43	ASN
40	S	57	ASN
44	W	11	ARG
44	W	12	ASN
44	W	16	SER
44	W	35	SER
44	W	40	GLN
44	W	41	ARG
44	W	43	THR
44	W	64	ASP
44	W	66	LYS
44	W	68	LYS
44	W	75	LYS
44	W	76	ASN
44	W	77	ARG
44	W	81	SER
44	W	82	ILE
44	W	83	GLU
45	X	26	ARG

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Mol	Chain	Res	Type
55	7	119	ASP
55	7	121	MET
55	7	136	LEU
55	7	137	MET
55	7	200	LYS
55	7	203	GLN
56	w	17	LEU
56	w	29	PHE
56	w	31	LYS
56	w	107	LEU
56	w	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	35	ASN
2	b	202	ASN
4	d	115	GLN
4	d	151	GLN
4	d	197	HIS
5	e	69	ASN
6	f	55	HIS
6	f	63	ASN
9	i	36	GLN
12	l	45	ASN
15	o	34	GLN
16	p	63	GLN
16	p	79	ASN
17	q	30	HIS
19	s	13	HIS
19	s	51	HIS
19	s	68	HIS
20	t	19	HIS
20	t	60	GLN
25	C	36	ASN
25	C	114	GLN
25	C	259	ASN
26	D	32	ASN
26	D	49	GLN
26	D	150	GLN
26	D	164	GLN

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Mol	Chain	Res	Type
27	E	156	ASN
29	G	63	GLN
29	G	138	GLN
30	H	66	ASN
31	J	40	HIS
31	J	58	ASN
39	R	18	GLN
39	R	43	ASN
39	R	91	GLN
40	S	57	ASN
41	T	15	HIS
42	U	68	ASN
44	W	40	GLN
45	X	33	HIS
46	Y	58	ASN
51	3	42	HIS
52	4	35	GLN
53	6	20	ASN
55	7	155	ASN
56	w	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	331 (21%)	0
22	v	5/6 (83%)	2 (40%)	0
23	A	2868/2903 (98%)	605 (21%)	27 (0%)
24	B	119/120 (99%)	21 (17%)	1 (0%)
54	x	76/77 (98%)	32 (42%)	0
All	All	4606/4645 (99%)	991 (21%)	28 (0%)

All (991) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	33	A

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Mol	Chain	Res	Type
1	a	39	G
1	a	40	C
1	a	41	G
1	a	47	C
1	a	50	A
1	a	51	A
1	a	55	A
1	a	56	U
1	a	58	C
1	a	60	A
1	a	64	G
1	a	66	A
1	a	68	G
1	a	71	A
1	a	74	A
1	a	75	G
1	a	79	G
1	a	80	A
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	87	C
1	a	89	U
1	a	92	U
1	a	94	G
1	a	95	C
1	a	98	A
1	a	99	C
1	a	104	G
1	a	116	A
1	a	121	U
1	a	131	A
1	a	139	A
1	a	141	G
1	a	147	G
1	a	148	G
1	a	149	A
1	a	157	U
1	a	160	A
1	a	161	A
1	a	163	C

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Mol	Chain	Res	Type
1	a	173	U
1	a	181	A
1	a	182	A
1	a	183	C
1	a	184	G
1	a	191	G
1	a	204	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	214	C
1	a	223	A
1	a	226	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	254	G
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G
1	a	298	A
1	a	316	C
1	a	317	U
1	a	320	A
1	a	321	A
1	a	325	A
1	a	328	C
1	a	330	C
1	a	344	A
1	a	345	C
1	a	346	G
1	a	347	G
1	a	352	C
1	a	354	G
1	a	359	G
1	a	360	G
1	a	365	U
1	a	366	A

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Mol	Chain	Res	Type
1	a	367	U
1	a	368	U
1	a	370	C
1	a	372	C
1	a	373	A
1	a	381	C
1	a	388	G
1	a	390	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	407	U
1	a	408	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	436	C
1	a	444	G
1	a	466	A
1	a	467	U
1	a	468	A
1	a	473	U
1	a	474	G
1	a	477	C
1	a	484	G
1	a	486	U
1	a	491	G
1	a	494	G
1	a	496	A
1	a	497	G
1	a	498	A
1	a	499	A
1	a	502	A
1	a	505	G
1	a	510	A
1	a	511	C

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Mol	Chain	Res	Type
1	a	514	C
1	a	518	C
1	a	521	G
1	a	525	C
1	a	527	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	583	A
1	a	596	A
1	a	607	A
1	a	613	C
1	a	619	U
1	a	623	C
1	a	632	U
1	a	633	G
1	a	634	C
1	a	635	A
1	a	637	C
1	a	641	U
1	a	642	A
1	a	650	G
1	a	652	U
1	a	654	G
1	a	661	G
1	a	665	A
1	a	688	G
1	a	695	A
1	a	703	G
1	a	705	G

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Mol	Chain	Res	Type
1	a	718	A
1	a	721	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	744	C
1	a	746	A
1	a	748	G
1	a	753	A
1	a	754	C
1	a	755	G
1	a	759	A
1	a	761	G
1	a	777	A
1	a	793	U
1	a	805	C
1	a	812	G
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	821	G
1	a	822	U
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	849	G
1	a	851	G
1	a	864	A
1	a	885	G
1	a	890	G
1	a	902	G
1	a	926	G
1	a	932	C
1	a	934	C
1	a	939	G
1	a	960	U
1	a	961	U
1	a	966	G

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Mol	Chain	Res	Type
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	987	G
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1001	C
1	a	1004	A
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1036	A
1	a	1053	G
1	a	1065	U
1	a	1081	A
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1099	G
1	a	1101	A
1	a	1118	U
1	a	1130	A
1	a	1132	C
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1151	A
1	a	1152	A
1	a	1159	U
1	a	1168	U
1	a	1169	A
1	a	1171	A

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Mol	Chain	Res	Type
1	a	1181	G
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1199	U
1	a	1201	A
1	a	1202	U
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1241	G
1	a	1253	G
1	a	1256	A
1	a	1257	A
1	a	1258	G
1	a	1260	G
1	a	1261	A
1	a	1278	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1287	A
1	a	1294	G
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1317	C
1	a	1321	U
1	a	1322	C
1	a	1332	A
1	a	1335	U
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G

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Mol	Chain	Res	Type
1	a	1363	A
1	a	1364	U
1	a	1365	G
1	a	1368	A
1	a	1370	G
1	a	1379	G
1	a	1383	C
1	a	1396	A
1	a	1398	A
1	a	1400	C
1	a	1406	U
1	a	1419	G
1	a	1425	U
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1487	G
1	a	1492	A
1	a	1497	G
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	17	C
22	v	18	G
23	A	5	A
23	A	10	A
23	A	34	U
23	A	35	G
23	A	43	G
23	A	46	G
23	A	51	G
23	A	52	A
23	A	71	A
23	A	74	A

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Mol	Chain	Res	Type
23	A	75	G
23	A	84	A
23	A	86	G
23	A	92	U
23	A	93	G
23	A	98	G
23	A	118	A
23	A	119	A
23	A	120	U
23	A	139	U
23	A	140	C
23	A	141	G
23	A	142	A
23	A	149	A
23	A	162	U
23	A	163	C
23	A	181	A
23	A	186	G
23	A	193	U
23	A	194	G
23	A	196	A
23	A	199	A
23	A	200	U
23	A	204	A
23	A	206	U
23	A	213	A
23	A	215	G
23	A	216	A
23	A	218	A
23	A	219	A
23	A	221	A
23	A	222	A
23	A	223	A
23	A	225	C
23	A	229	C
23	A	230	G
23	A	241	A
23	A	242	G
23	A	243	U
23	A	248	G
23	A	255	A
23	A	265	A

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Mol	Chain	Res	Type
23	A	267	C
23	A	268	C
23	A	272	A
23	A	276	U
23	A	277	G
23	A	278	A
23	A	279	A
23	A	285	G
23	A	292	U
23	A	311	A
23	A	316	C
23	A	323	C
23	A	329	G
23	A	330	A
23	A	334	C
23	A	335	C
23	A	345	A
23	A	353	C
23	A	361	G
23	A	362	A
23	A	367	G
23	A	370	G
23	A	371	A
23	A	372	G
23	A	386	G
23	A	387	U
23	A	395	U
23	A	403	U
23	A	404	A
23	A	406	G
23	A	411	G
23	A	417	C
23	A	421	C
23	A	422	A
23	A	424	G
23	A	434	U
23	A	448	U
23	A	458	G
23	A	473	G
23	A	481	G
23	A	491	G
23	A	505	A

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Mol	Chain	Res	Type
23	A	508	A
23	A	509	C
23	A	530	G
23	A	531	C
23	A	532	A
23	A	533	G
23	A	543	G
23	A	544	C
23	A	545	U
23	A	546	U
23	A	547	A
23	A	548	G
23	A	549	G
23	A	550	C
23	A	555	G
23	A	563	A
23	A	573	U
23	A	575	A
23	A	586	A
23	A	603	A
23	A	614	A
23	A	615	U
23	A	616	A
23	A	622	G
23	A	627	A
23	A	637	A
23	A	644	A
23	A	645	C
23	A	646	U
23	A	647	G
23	A	654	A
23	A	655	A
23	A	659	G
23	A	668	A
23	A	669	G
23	A	670	A
23	A	677	A
23	A	686	U
23	A	695	G
23	A	696	G
23	A	704	G
23	A	711	G

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Mol	Chain	Res	Type
23	A	718	A
23	A	728	G
23	A	730	A
23	A	736	C
23	A	738	G
23	A	739	A
23	A	747	C
23	A	752	A
23	A	764	A
23	A	765	C
23	A	782	A
23	A	783	A
23	A	784	G
23	A	789	A
23	A	791	C
23	A	805	G
23	A	807	U
23	A	812	C
23	A	819	A
23	A	827	U
23	A	828	U
23	A	829	A
23	A	831	G
23	A	845	A
23	A	846	U
23	A	847	U
23	A	856	G
23	A	858	G
23	A	860	U
23	A	878	A
23	A	879	G
23	A	885	C
23	A	886	A
23	A	895	U
23	A	896	A
23	A	897	C
23	A	902	C
23	A	907	G
23	A	910	A
23	A	931	U
23	A	941	A
23	A	946	C

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Mol	Chain	Res	Type
23	A	953	G
23	A	961	C
23	A	974	G
23	A	983	A
23	A	989	G
23	A	995	C
23	A	996	A
23	A	997	G
23	A	999	U
23	A	1009	A
23	A	1012	U
23	A	1013	C
23	A	1021	A
23	A	1023	U
23	A	1025	G
23	A	1026	G
23	A	1033	U
23	A	1041	G
23	A	1045	C
23	A	1046	A
23	A	1052	C
23	A	1054	A
23	A	1057	A
23	A	1059	G
23	A	1060	U
23	A	1061	U
23	A	1062	G
23	A	1064	C
23	A	1065	U
23	A	1066	U
23	A	1067	A
23	A	1069	A
23	A	1070	A
23	A	1071	G
23	A	1072	C
23	A	1073	A
23	A	1075	C
23	A	1076	C
23	A	1078	U
23	A	1079	C
23	A	1083	U
23	A	1084	A

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Mol	Chain	Res	Type
23	A	1087	G
23	A	1088	A
23	A	1089	A
23	A	1090	A
23	A	1094	U
23	A	1096	A
23	A	1097	U
23	A	1098	A
23	A	1099	G
23	A	1100	C
23	A	1102	C
23	A	1103	A
23	A	1104	C
23	A	1111	A
23	A	1112	G
23	A	1130	U
23	A	1131	G
23	A	1132	U
23	A	1133	A
23	A	1135	C
23	A	1139	G
23	A	1142	A
23	A	1150	C
23	A	1155	A
23	A	1172	C
23	A	1175	A
23	A	1176	U
23	A	1180	U
23	A	1183	U
23	A	1204	A
23	A	1205	A
23	A	1206	G
23	A	1211	C
23	A	1212	G
23	A	1237	A
23	A	1247	A
23	A	1248	G
23	A	1253	A
23	A	1256	G
23	A	1268	A
23	A	1271	G
23	A	1272	A

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Mol	Chain	Res	Type
23	A	1275	A
23	A	1300	G
23	A	1301	A
23	A	1306	C
23	A	1312	U
23	A	1325	U
23	A	1329	U
23	A	1330	C
23	A	1341	G
23	A	1344	U
23	A	1345	C
23	A	1352	U
23	A	1360	G
23	A	1365	A
23	A	1368	G
23	A	1378	A
23	A	1379	U
23	A	1381	G
23	A	1383	A
23	A	1386	C
23	A	1395	A
23	A	1403	A
23	A	1414	C
23	A	1416	G
23	A	1417	C
23	A	1428	C
23	A	1434	A
23	A	1453	A
23	A	1454	C
23	A	1455	G
23	A	1458	U
23	A	1461	C
23	A	1475	G
23	A	1476	U
23	A	1482	G
23	A	1483	G
23	A	1488	C
23	A	1490	A
23	A	1491	G
23	A	1494	A
23	A	1497	U
23	A	1504	A

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Mol	Chain	Res	Type
23	A	1505	A
23	A	1508	A
23	A	1509	A
23	A	1515	A
23	A	1522	A
23	A	1524	G
23	A	1529	G
23	A	1532	A
23	A	1534	U
23	A	1535	A
23	A	1536	C
23	A	1542	U
23	A	1554	U
23	A	1555	G
23	A	1558	C
23	A	1559	U
23	A	1560	G
23	A	1565	C
23	A	1569	A
23	A	1578	U
23	A	1583	A
23	A	1584	U
23	A	1585	C
23	A	1597	A
23	A	1608	A
23	A	1611	C
23	A	1647	U
23	A	1648	U
23	A	1649	G
23	A	1654	A
23	A	1672	A
23	A	1674	G
23	A	1694	C
23	A	1695	G
23	A	1703	G
23	A	1704	C
23	A	1713	A
23	A	1715	G
23	A	1727	C
23	A	1729	U
23	A	1730	C
23	A	1731	G

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Mol	Chain	Res	Type
23	A	1732	C
23	A	1733	G
23	A	1735	A
23	A	1738	G
23	A	1757	A
23	A	1758	U
23	A	1759	A
23	A	1764	C
23	A	1773	A
23	A	1776	G
23	A	1780	A
23	A	1781	U
23	A	1782	U
23	A	1786	A
23	A	1787	A
23	A	1791	A
23	A	1800	C
23	A	1801	A
23	A	1802	A
23	A	1808	A
23	A	1816	C
23	A	1829	A
23	A	1833	C
23	A	1859	U
23	A	1866	A
23	A	1869	G
23	A	1870	C
23	A	1871	A
23	A	1872	A
23	A	1873	G
23	A	1884	G
23	A	1896	G
23	A	1900	A
23	A	1901	A
23	A	1906	G
23	A	1913	A
23	A	1914	C
23	A	1916	A
23	A	1927	A
23	A	1929	G
23	A	1930	G
23	A	1931	U

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Mol	Chain	Res	Type
23	A	1936	A
23	A	1937	A
23	A	1938	A
23	A	1941	C
23	A	1946	U
23	A	1955	U
23	A	1964	G
23	A	1966	A
23	A	1967	C
23	A	1970	A
23	A	1971	U
23	A	1972	G
23	A	1991	U
23	A	1992	G
23	A	1996	C
23	A	1997	C
23	A	2004	G
23	A	2006	C
23	A	2020	A
23	A	2022	U
23	A	2023	C
23	A	2030	A
23	A	2031	A
23	A	2033	A
23	A	2035	G
23	A	2036	C
23	A	2043	C
23	A	2046	G
23	A	2049	G
23	A	2052	A
23	A	2055	C
23	A	2056	G
23	A	2060	A
23	A	2061	G
23	A	2062	A
23	A	2069	A
23	A	2072	C
23	A	2092	U
23	A	2093	G
23	A	2096	C
23	A	2097	A
23	A	2099	U

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Mol	Chain	Res	Type
23	A	2100	G
23	A	2101	A
23	A	2103	C
23	A	2104	U
23	A	2105	U
23	A	2107	G
23	A	2111	U
23	A	2112	G
23	A	2113	U
23	A	2114	A
23	A	2116	G
23	A	2117	A
23	A	2119	A
23	A	2120	G
23	A	2125	G
23	A	2126	A
23	A	2127	G
23	A	2128	G
23	A	2159	G
23	A	2160	C
23	A	2161	C
23	A	2167	U
23	A	2169	A
23	A	2170	A
23	A	2177	C
23	A	2178	C
23	A	2179	C
23	A	2180	U
23	A	2181	U
23	A	2185	U
23	A	2187	U
23	A	2188	U
23	A	2189	U
23	A	2190	G
23	A	2191	A
23	A	2193	G
23	A	2198	A
23	A	2203	U
23	A	2204	G
23	A	2210	U
23	A	2211	A
23	A	2213	U

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Mol	Chain	Res	Type
23	A	2214	C
23	A	2219	U
23	A	2223	G
23	A	2225	A
23	A	2226	C
23	A	2238	G
23	A	2239	G
23	A	2250	G
23	A	2251	G
23	A	2259	U
23	A	2266	A
23	A	2267	A
23	A	2273	A
23	A	2279	G
23	A	2283	C
23	A	2287	A
23	A	2288	A
23	A	2294	G
23	A	2305	U
23	A	2309	A
23	A	2311	A
23	A	2325	G
23	A	2327	A
23	A	2333	A
23	A	2334	U
23	A	2335	A
23	A	2336	A
23	A	2344	U
23	A	2345	G
23	A	2350	C
23	A	2354	C
23	A	2361	G
23	A	2372	U
23	A	2382	G
23	A	2383	G
23	A	2385	C
23	A	2392	A
23	A	2393	U
23	A	2394	C
23	A	2402	U
23	A	2406	A
23	A	2419	U

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Mol	Chain	Res	Type
23	A	2424	C
23	A	2428	G
23	A	2429	G
23	A	2430	A
23	A	2435	A
23	A	2441	U
23	A	2445	G
23	A	2448	A
23	A	2449	U
23	A	2465	C
23	A	2469	A
23	A	2474	U
23	A	2476	A
23	A	2481	G
23	A	2491	U
23	A	2502	G
23	A	2503	A
23	A	2505	G
23	A	2506	U
23	A	2507	C
23	A	2513	A
23	A	2517	C
23	A	2518	A
23	A	2529	G
23	A	2534	A
23	A	2547	A
23	A	2554	U
23	A	2556	C
23	A	2566	A
23	A	2567	G
23	A	2572	A
23	A	2573	C
23	A	2576	G
23	A	2582	G
23	A	2585	U
23	A	2586	U
23	A	2602	A
23	A	2604	U
23	A	2610	C
23	A	2613	U
23	A	2614	A
23	A	2629	U

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Mol	Chain	Res	Type
23	A	2638	G
23	A	2646	C
23	A	2655	G
23	A	2656	U
23	A	2674	G
23	A	2685	G
23	A	2689	U
23	A	2690	U
23	A	2706	A
23	A	2707	U
23	A	2714	G
23	A	2716	C
23	A	2718	G
23	A	2726	A
23	A	2732	G
23	A	2733	A
23	A	2744	G
23	A	2748	A
23	A	2760	C
23	A	2764	A
23	A	2765	A
23	A	2769	U
23	A	2778	A
23	A	2779	U
23	A	2790	U
23	A	2791	G
23	A	2793	C
23	A	2794	C
23	A	2796	U
23	A	2800	A
23	A	2808	G
23	A	2809	A
23	A	2818	U
23	A	2820	A
23	A	2821	A
23	A	2833	U
23	A	2835	A
23	A	2836	U
23	A	2846	G
23	A	2849	U
23	A	2861	U
23	A	2867	G

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Mol	Chain	Res	Type
23	A	2868	A
23	A	2873	A
23	A	2880	C
23	A	2883	A
23	A	2884	U
23	A	2893	A
23	A	2899	A
24	B	3	C
24	B	4	C
24	B	13	G
24	B	15	A
24	B	21	G
24	B	24	G
24	B	26	C
24	B	30	C
24	B	35	C
24	B	36	C
24	B	40	U
24	B	42	C
24	B	44	G
24	B	45	A
24	B	67	G
24	B	88	C
24	B	89	U
24	B	90	C
24	B	91	C
24	B	105	G
24	B	109	A
54	x	2	G
54	x	3	G
54	x	4	U
54	x	5	G
54	x	6	A
54	x	8	U
54	x	13	C
54	x	14	A
54	x	18	G
54	x	19	G
54	x	20	U
54	x	21	A
54	x	22	G
54	x	25	C

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Mol	Chain	Res	Type
54	x	26	A
54	x	27	C
54	x	35	G
54	x	36	G
54	x	40	G
54	x	42	A
54	x	47	U
54	x	51	A
54	x	53	G
54	x	54	U
54	x	61	C
54	x	66	A
54	x	67	U
54	x	68	C
54	x	72	G
54	x	73	A
54	x	74	C
54	x	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	51	G
23	A	242	G
23	A	421	C
23	A	490	C
23	A	615	U
23	A	859	G
23	A	1020	A
23	A	1022	G
23	A	1070	A
23	A	1111	A
23	A	1141	U
23	A	1182	G
23	A	1190	G
23	A	1300	G
23	A	1331	G
23	A	1378	A
23	A	1399	C
23	A	1432	G
23	A	1730	C
23	A	1930	G

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Mol	Chain	Res	Type
23	A	1940	U
23	A	2190	G
23	A	2286	G
23	A	2326	C
23	A	2391	G
23	A	2655	G
23	A	2808	G
24	B	66	A

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
56	KEO	w	34	-	16,18,19	1.50	2 (12%)	14,21,23	1.47	3 (21%)

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
56	KEO	w	34	-	-	10/19/20/22	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	34	KEO	C05-NZ	5.12	1.45	1.33
56	w	34	KEO	O02-C05	-2.28	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	34	KEO	C06-C05-NZ	2.93	120.02	115.97
56	w	34	KEO	CE-NZ-C05	-2.85	117.55	122.84
56	w	34	KEO	CB-CG-CD	-2.42	107.31	112.51

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	34	KEO	O-C-CA-CB
56	w	34	KEO	N-CA-CB-CG
56	w	34	KEO	C-CA-CB-CG
56	w	34	KEO	CA-CB-CG-O01
56	w	34	KEO	C05-C06-C07-C08
56	w	34	KEO	C05-C06-C07-N02
56	w	34	KEO	C06-C05-NZ-CE
56	w	34	KEO	O02-C05-NZ-CE
56	w	34	KEO	CA-CB-CG-CD
56	w	34	KEO	C06-C07-C08-C09

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
57	PRO	A	3001	-	5,7,8	0.54	0	7,8,10	1.23	1 (14%)
57	PRO	x	101	-	5,7,8	0.60	0	7,8,10	1.27	1 (14%)

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
57	PRO	A	3001	-	-	0/0/9/11	0/1/1/1
57	PRO	x	101	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A	3001	PRO	O-C-CA	-2.31	118.73	124.78
57	x	101	PRO	O-C-CA	-2.22	118.97	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

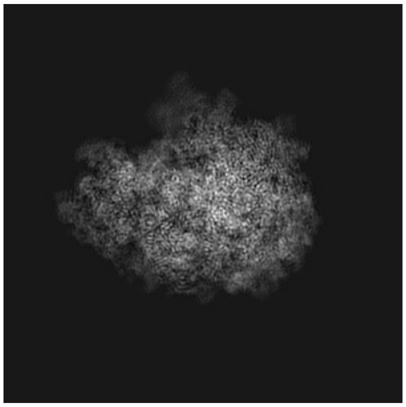
6 Map visualisation ⓘ

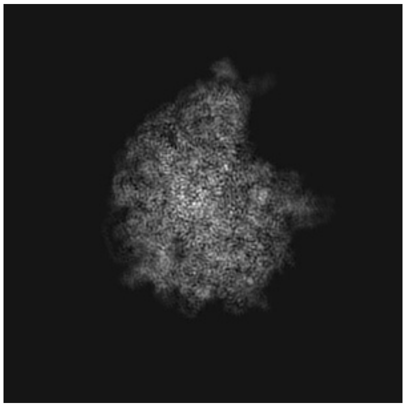
This section contains visualisations of the EMDB entry EMD-3903. These allow visual inspection of the internal detail of the map and identification of artifacts.

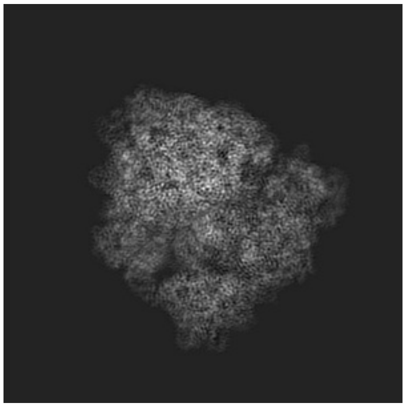
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map


X

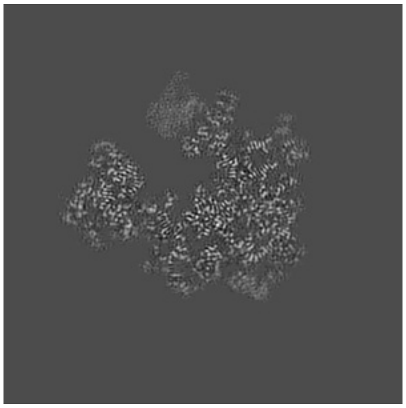

Y

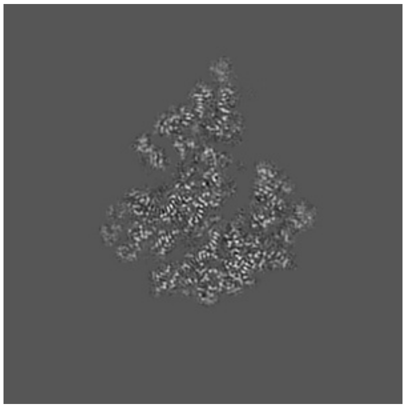

Z

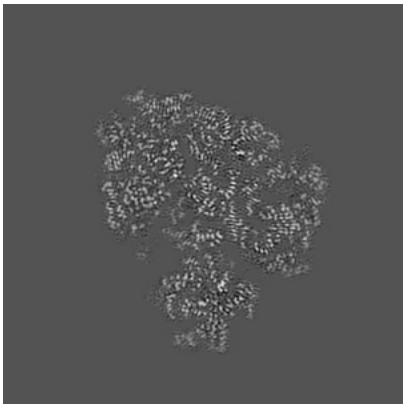
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map


X Index: 180

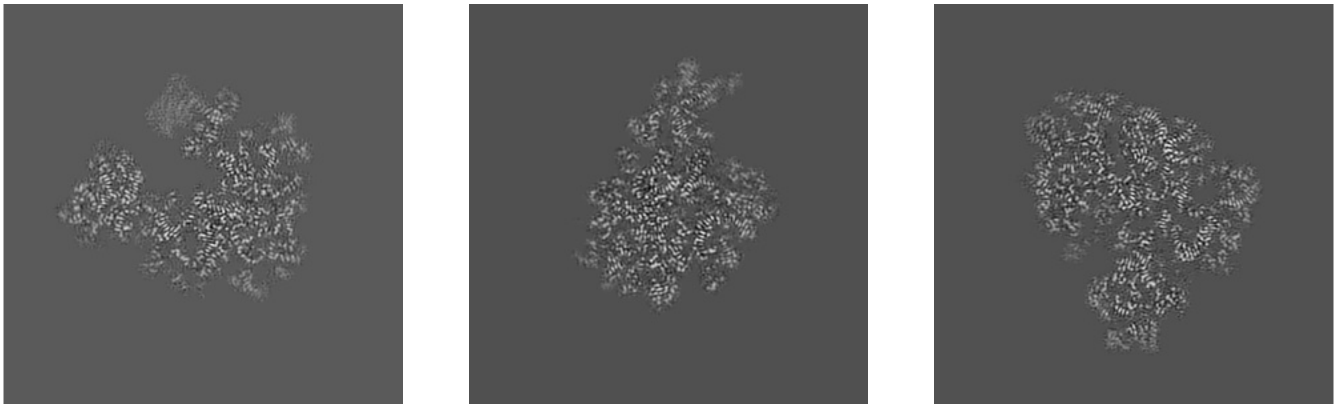

Y Index: 180


Z Index: 180

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

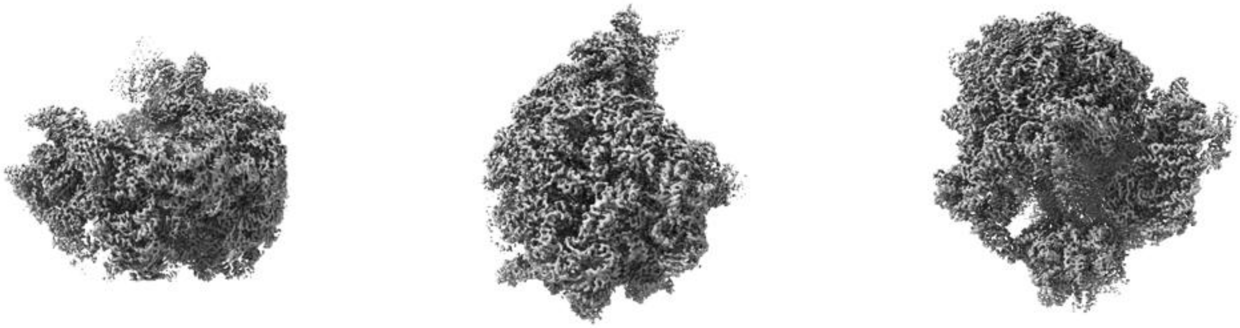


X Index: 177 Y Index: 191 Z Index: 177

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

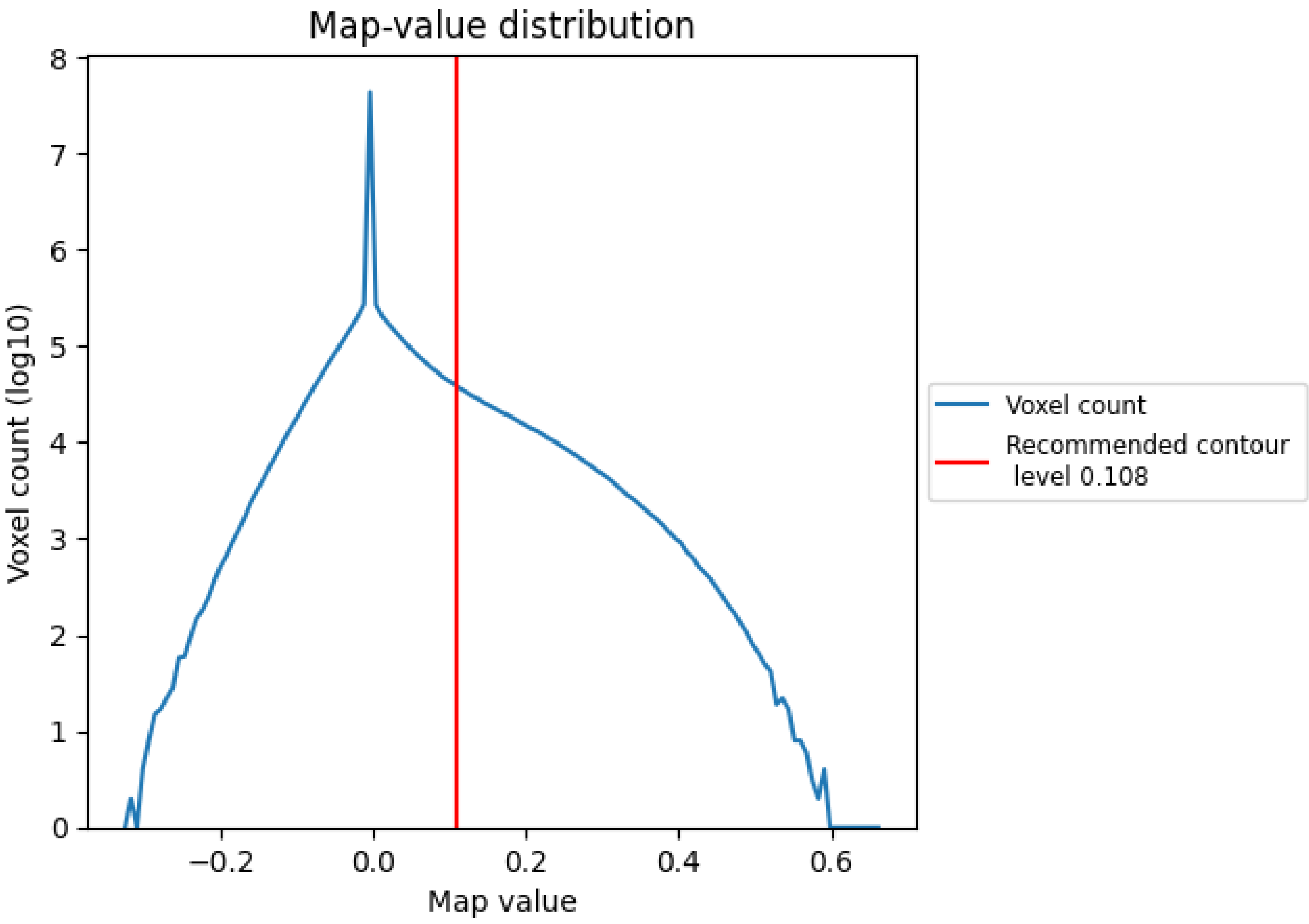
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

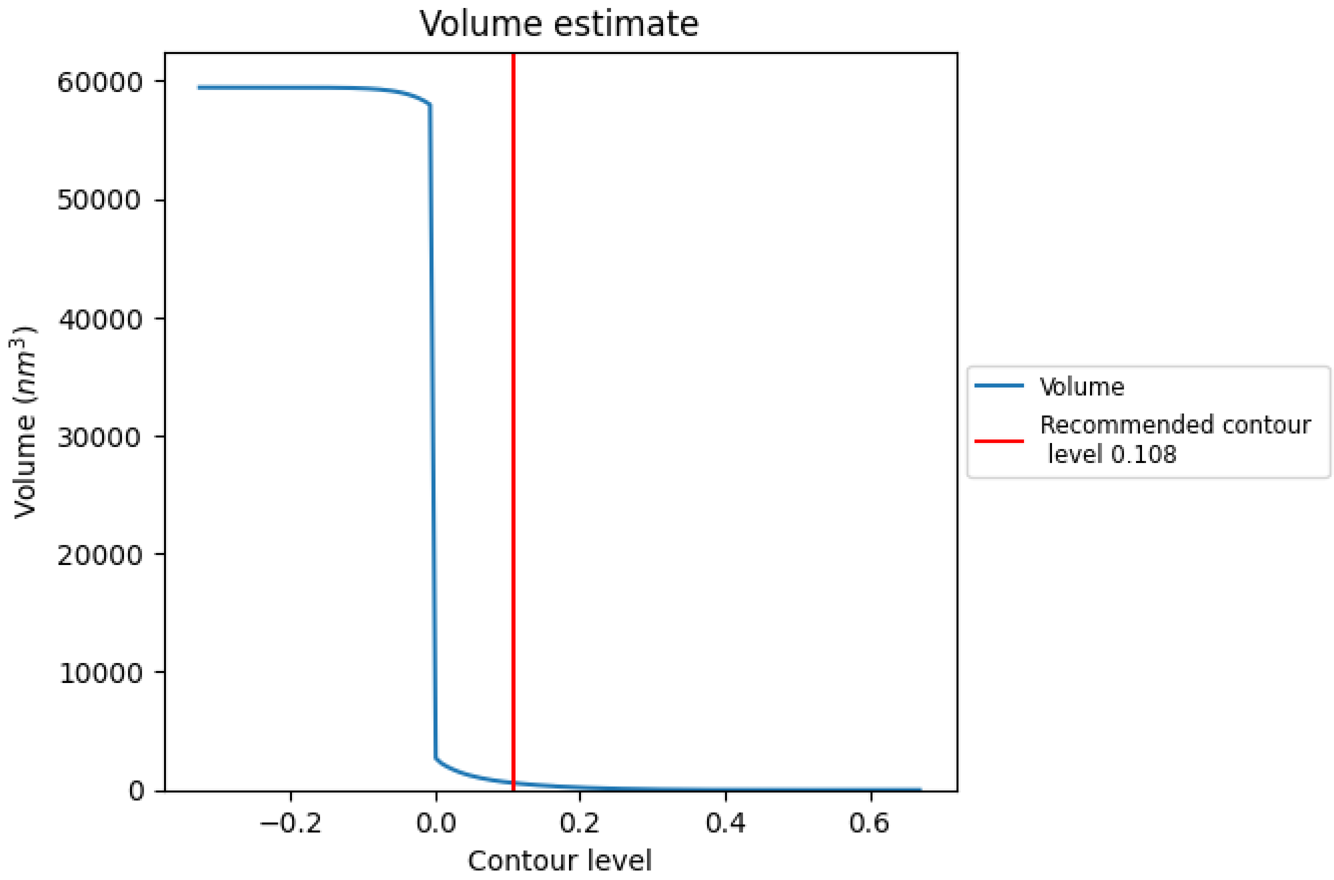
This section contains the results of statistical analysis of the map.

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.

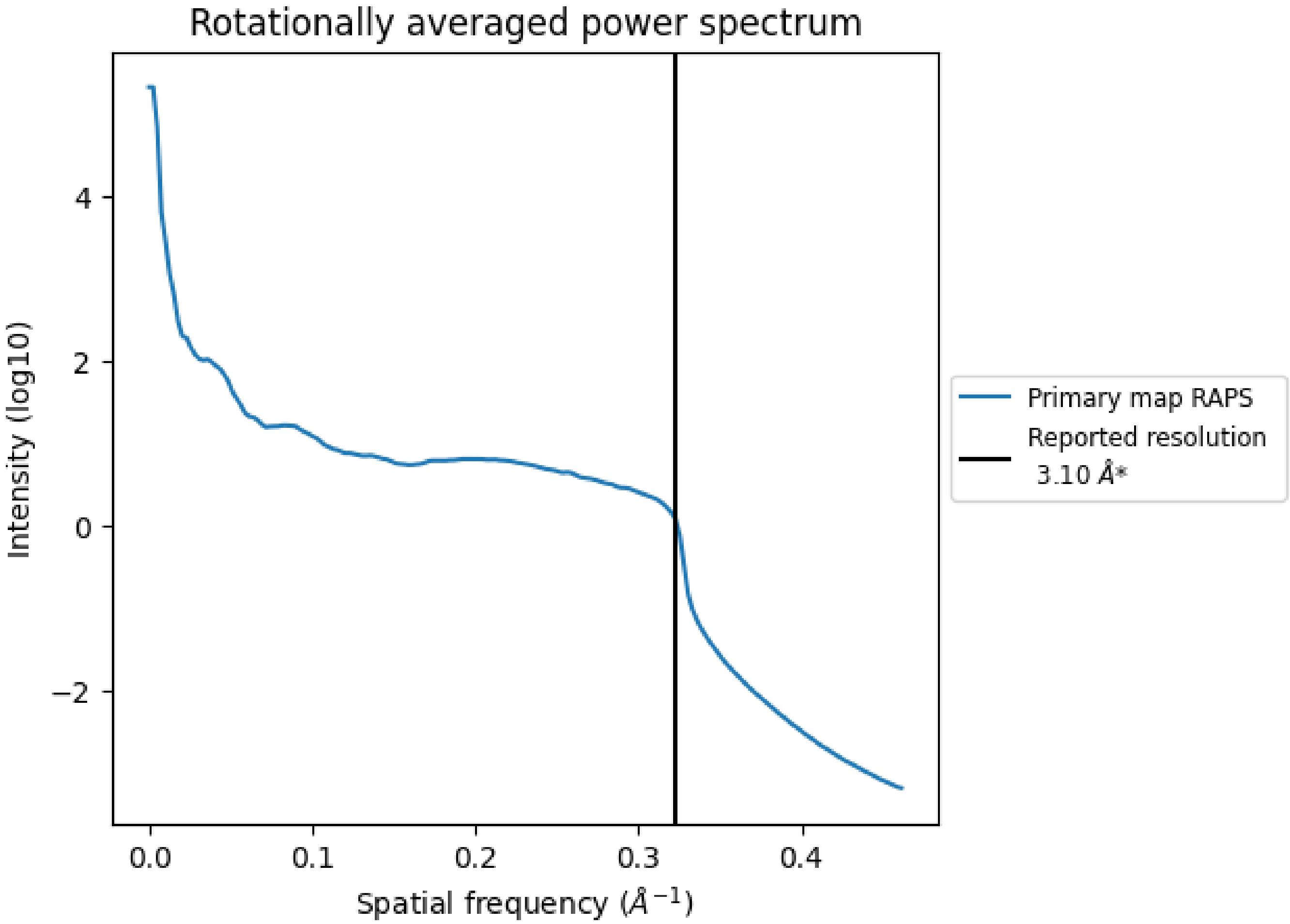
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 532 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 0.323 $Å^{-1}$

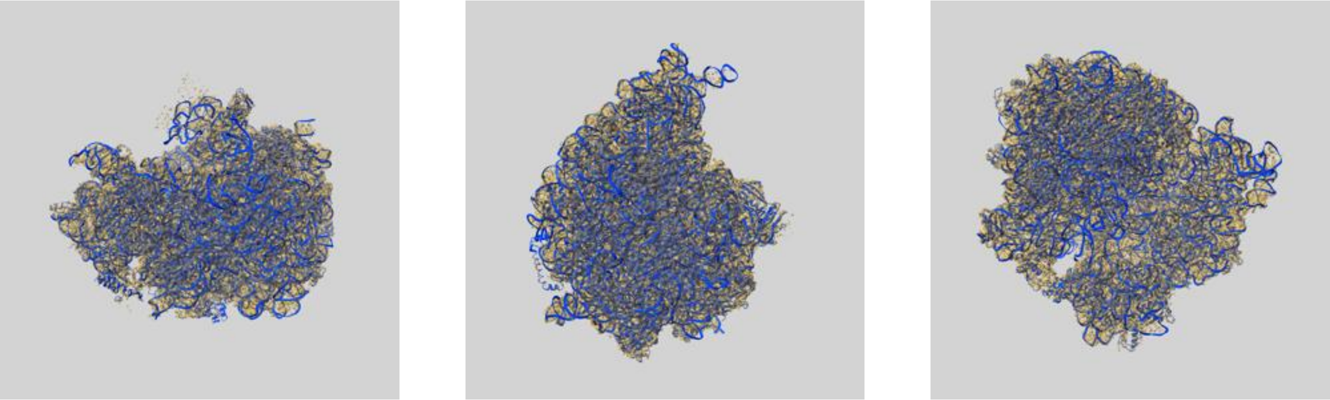
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3903 and PDB model 6ENU. Per-residue inclusion information can be found in section 3 on page 15.

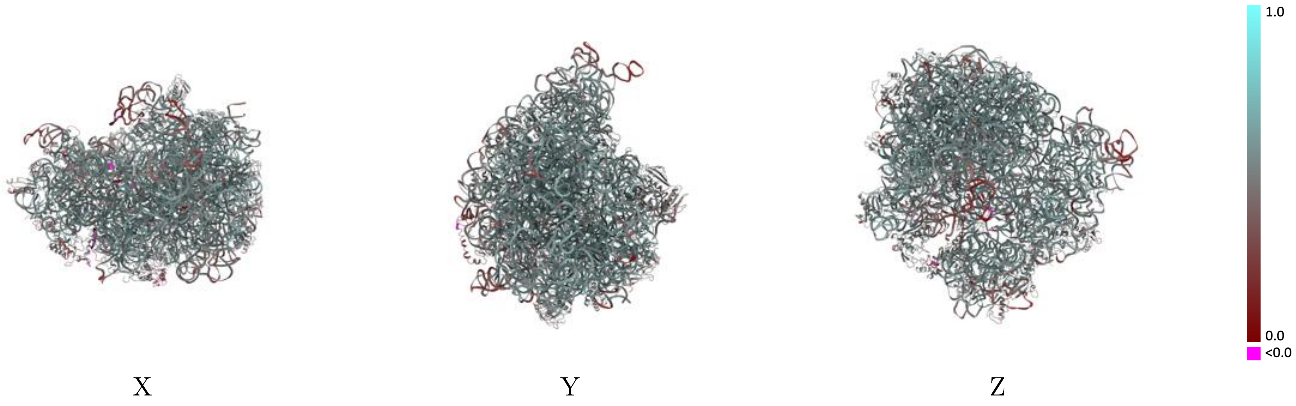
9.1 Map-model overlay



X Y Z

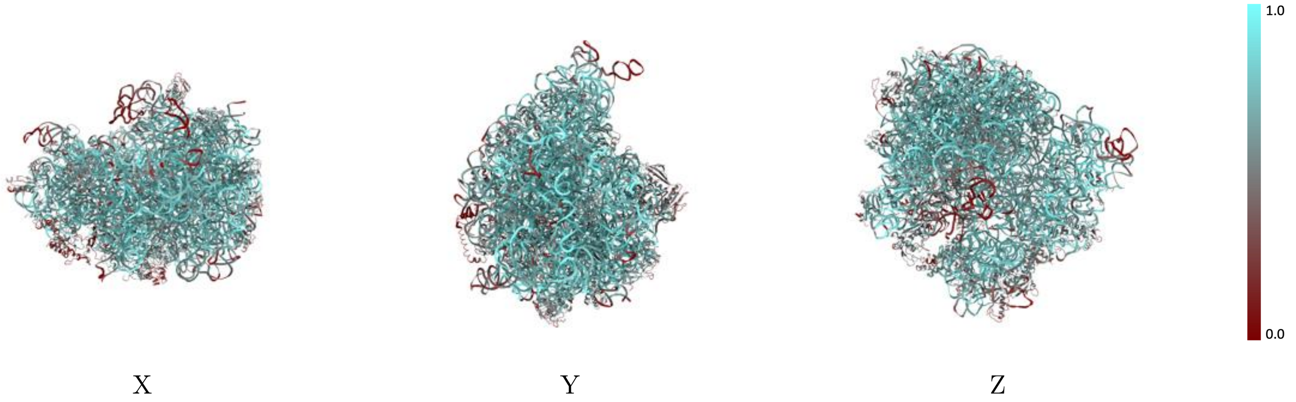
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



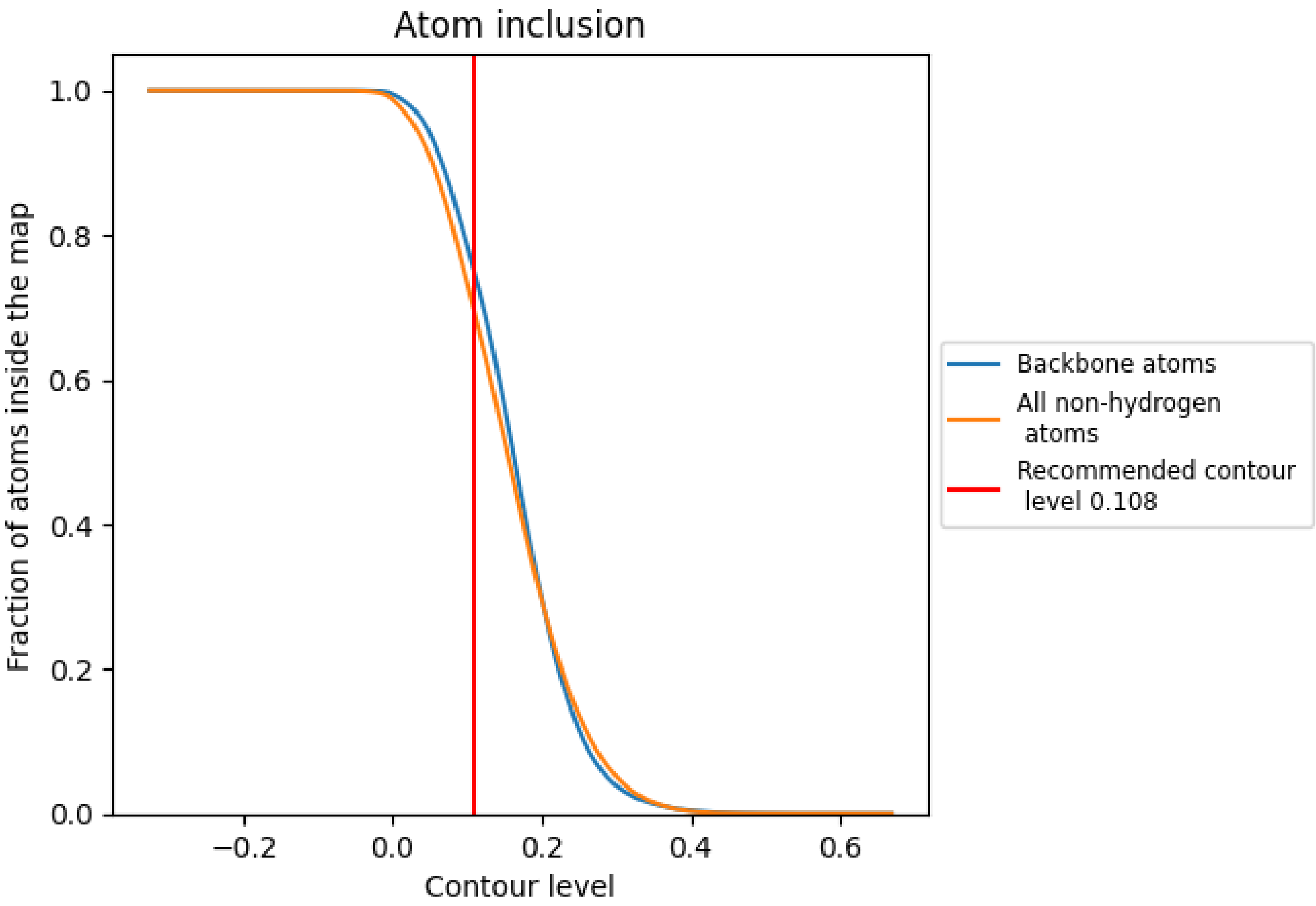
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.108).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7008	0.5240
0	0.6449	0.5110
1	0.5411	0.5120
2	0.7099	0.5260
3	0.6945	0.5630
4	0.6507	0.5380
6	0.3640	0.4000
7	0.0153	0.2330
A	0.7811	0.5460
B	0.7640	0.5450
C	0.6682	0.5470
D	0.6606	0.5420
E	0.5520	0.5010
F	0.5076	0.4750
G	0.4287	0.4500
H	0.1515	0.2990
J	0.6700	0.5310
K	0.6364	0.5190
L	0.6053	0.5170
M	0.6526	0.5410
N	0.6920	0.5360
O	0.6014	0.5110
P	0.5912	0.5220
Q	0.6949	0.5470
R	0.5659	0.5040
S	0.5957	0.5150
T	0.4945	0.4830
U	0.4302	0.4670
V	0.5799	0.5120
W	0.7014	0.5680
X	0.5907	0.5160
Y	0.4588	0.4430
Z	0.6270	0.5260
a	0.7860	0.5430
b	0.2913	0.4060

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Chain	Atom inclusion	Q-score
c	0.6280	0.5090
d	0.5195	0.4650
e	0.6425	0.5080
f	0.5000	0.4660
g	0.5052	0.4770
h	0.6490	0.5250
i	0.5495	0.4680
j	0.4993	0.4560
k	0.5231	0.4900
l	0.6221	0.5050
m	0.5699	0.4820
n	0.6341	0.4950
o	0.5899	0.4970
p	0.5694	0.4690
q	0.5222	0.4810
r	0.5959	0.5030
s	0.5733	0.4790
t	0.5831	0.4880
u	0.2584	0.3250
v	0.7778	0.5620
w	0.2768	0.4440
x	0.6407	0.5170