wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 05:56 am GMT

PDB ID	:	6GZQ
EMDB ID	:	EMD-0101
Title	:	T. thermophilus hibernating 70S ribosome
Authors	:	Flygaard, R.K.; Jenner, L.B.
Deposited on	:	2018-07-04
Resolution	:	3.28 Å(reported)

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

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

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

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

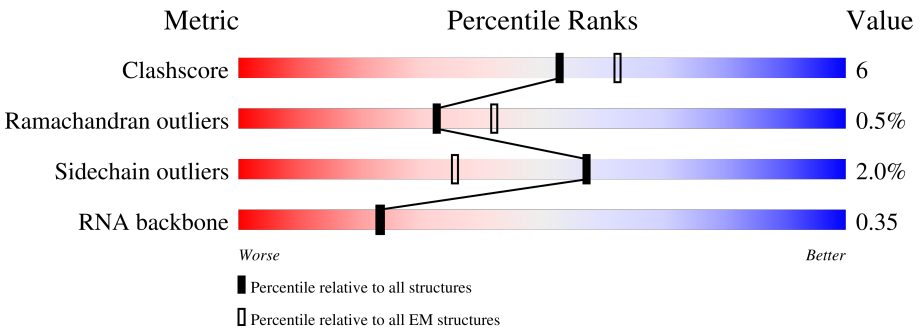
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C1	272	• 89% 11%
2	D1	205	• 88% 10% •
3	E1	208	5% 87% 13%
4	F1	181	• 78% 20% •
5	G1	170	• 73% 24% • •
6	H1	50	16% 90% 10%
7	I1	138	• 91% 9%

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Mol	Chain	Length	Quality of chain
8	J1	122	84% 16%
9	K1	150	81% 17%
10	L1	141	85% 13%
11	M1	117	83% 17%
12	N1	111	7% 77% 23%
13	O1	137	7% 78% 20%
14	P1	117	89% 9%
15	Q1	101	93% 6%
16	R1	113	82% 17%
17	S1	92	92% 8%
18	T1	102	8% 77% 20%
19	U1	179	28% 83% 15%
20	V1	77	5% 88% 12%
21	W1	97	7% 88% 12%
22	X1	69	6% 88% 12%
23	Y1	59	5% 92% 8%
24	Z1	63	21% 65% 32%
25	a1	59	5% 97%
26	b1	45	84% 13%
27	c1	49	8% 96%
28	d1	61	5% 89% 11%
29	A1	2912	48% 37% 14%
30	B1	122	55% 36% 9%
31	e1	36	94% 6%
32	B2	237	13% 81% 17%

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Mol	Chain	Length	Quality of chain
33	C2	206	86% 13%
34	D2	208	87% 12%
35	E2	151	91% 9%
36	F2	101	6% 83% 17%
37	G2	155	8% 77% 23%
38	H2	138	89% 11%
39	I2	127	8% 76% 24%
40	J2	99	77% 22%
41	K2	118	5% 83% 17%
42	L2	125	8% 84% 15%
43	M2	117	13% 74% 24%
44	N2	60	88% 12%
45	O2	88	91% 9%
46	P2	84	92% 8%
47	Q2	100	82% 18%
48	R2	62	6% 79% 21%
49	S2	78	9% 77% 18% 5%
50	T2	99	89% 10%
51	U2	25	72% 28%
52	V2	121	12% 73% 24%
53	A2	1506	42% 40% 15%

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 144138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C1	272	2116	1335	420	358	3	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D1	205	1569	991	300	272	6	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E1	208	1628	1037	304	284	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F1	181	1474	942	268	260	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G1	170	1308	829	245	233	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H1	50	383	245	66	71	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I1	138	1105	712	206	183	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J1	122	933	588	171	170	4	0	0

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K1	150	1145	712	232	198	3	0	0

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L1	141	1122	715	212	188	7	0	0

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	M1	117	960	599	202	159	0	0

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	N1	111	882	556	176	150	0	0

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O1	137	1142	710	234	197	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	P1	117	964	610	202	151	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q1	101	779	501	142	135	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R1	113	900	566	177	155	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	S1	92	726	471	131	124	0	0

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T1	102	786	505	150	126	5	0	0

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U1	179	1429	911	255	260	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V1	77	613	379	129	104	1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W1	97	763	481	150	131	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X1	69	581	358	118	104	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	Y1	59	469	298	90	81	0	0

- Molecule 24 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z1	63	516	326	93	92	5	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a1	59	459	288	90	76	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b1	45	390	241	79	66	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	c1	49	430	263	108	57	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d1	61	489	312	99	76	2	0	0

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	A1	2912	62707	27911	11722	20163	2911	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	156	U	UNK	conflict	GB 55771382
A1	682	A	G	conflict	GB 55771382
A1	686	C	G	conflict	GB 55771382
A1	697	G	C	conflict	GB 55771382
A1	701	A	C	conflict	GB 55771382
A1	1106	U	G	conflict	GB 55771382
A1	1128	A	C	conflict	GB 55771382

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	B1	122	2617	1166	486	844	121	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e1	36	299	183	67	46	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	B2	237	1925	1228	344	348	5	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	C2	206	1613	1016	314	282	1	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	D2	208	1703	1066	339	291	7	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	E2	151	1156	729	218	205	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	F2	101	843	531	155	154	3	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	G2	155	1257	781	252	218	6	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	H2	138	1116	705	215	193	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	I2	127	1010	639	197	174	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	J2	99	802	504	157	140	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	K2	118	879	546	167	163	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	L2	125	976	614	196	165	1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	M2	117	934	577	192	163	2	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	N2	60	492	312	104	72	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	O2	88	734	459	147	126	2	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	P2	84	706	446	140	119	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Q2	100	835	534	155	144	2	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	R2	62	515	328	101	86	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	S2	78	625	398	115	110	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	T2	99	763	470	162	129	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	U2	25	218	134	52	32	0	0

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	V2	121	983	615	185	182	1	0	0

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

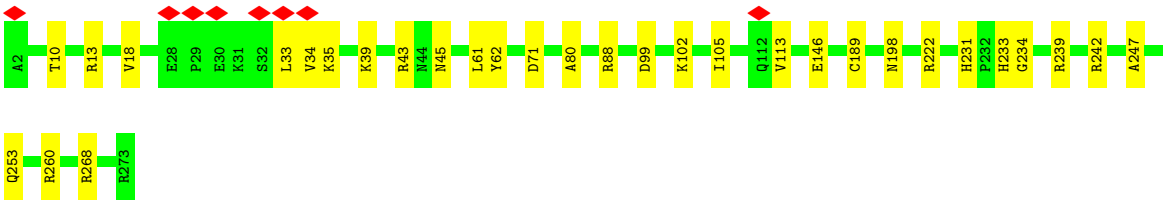
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	A2	1506	32369	14408	5997	10459	1505	0	0

3 Residue-property plots (i)

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

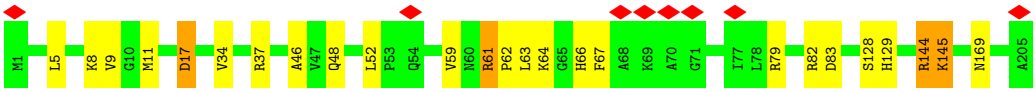
• Molecule 1: 50S ribosomal protein L2

Chain C1:



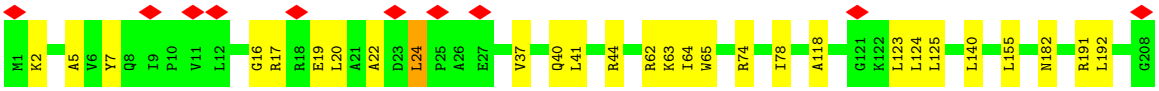
• Molecule 2: 50S ribosomal protein L3

Chain D1:



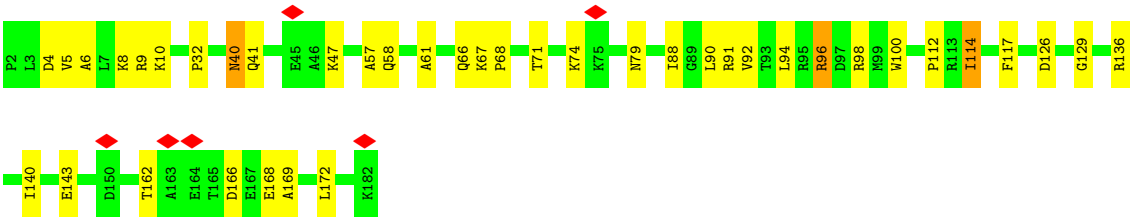
• Molecule 3: 50S ribosomal protein L4

Chain E1:



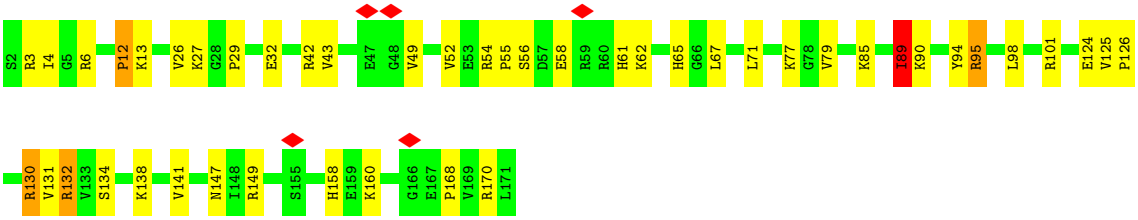
• Molecule 4: 50S ribosomal protein L5

Chain F1:



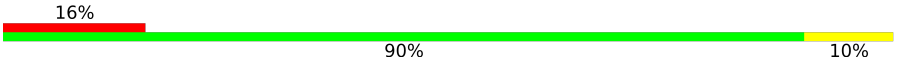
- Molecule 5: 50S ribosomal protein L6

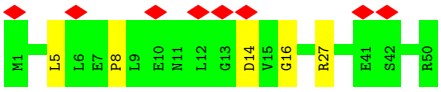
Chain G1:



- Molecule 6: 50S ribosomal protein L9

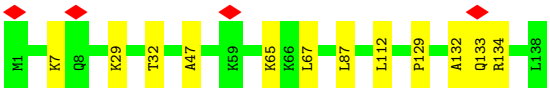
Chain H1:





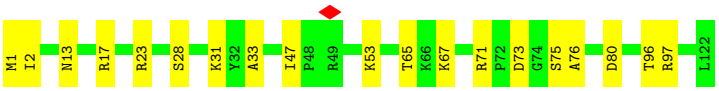
- Molecule 7: 50S ribosomal protein L13

Chain I1:



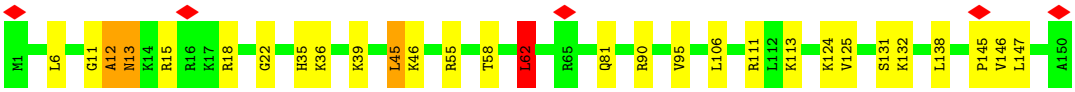
- Molecule 8: 50S ribosomal protein L14

Chain J1:



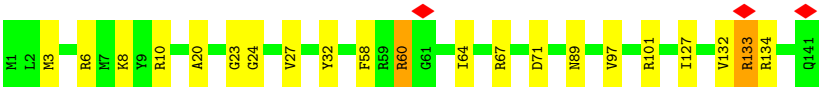
- Molecule 9: 50S ribosomal protein L15

Chain K1:



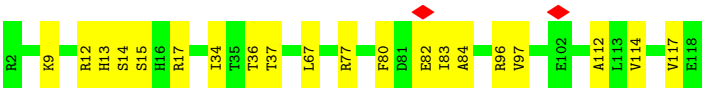
- Molecule 10: 50S ribosomal protein L16

Chain L1:



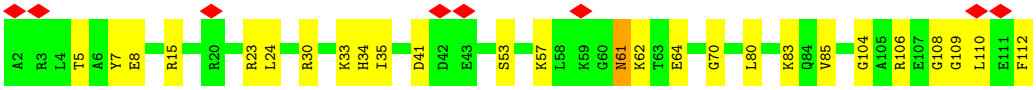
- Molecule 11: 50S ribosomal protein L17

Chain M1:



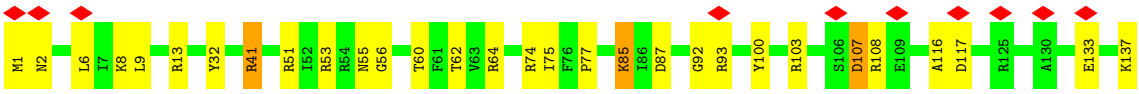
• Molecule 12: 50S ribosomal protein L18

Chain N1:



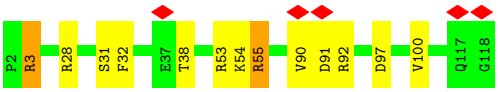
• Molecule 13: 50S ribosomal protein L19

Chain O1:



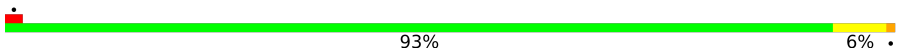
• Molecule 14: 50S ribosomal protein L20

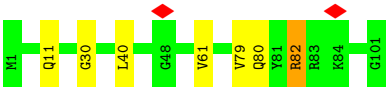
Chain P1:



• Molecule 15: 50S ribosomal protein L21

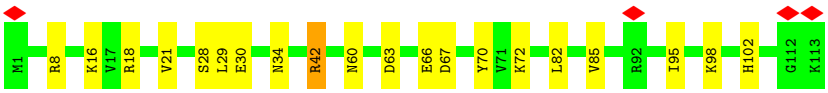
Chain Q1:





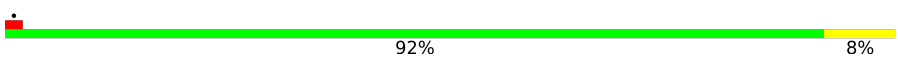
• Molecule 16: 50S ribosomal protein L22

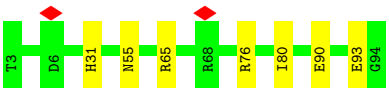
Chain R1:



• Molecule 17: 50S ribosomal protein L23

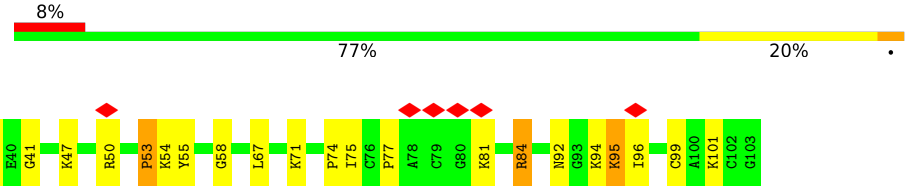
Chain S1:





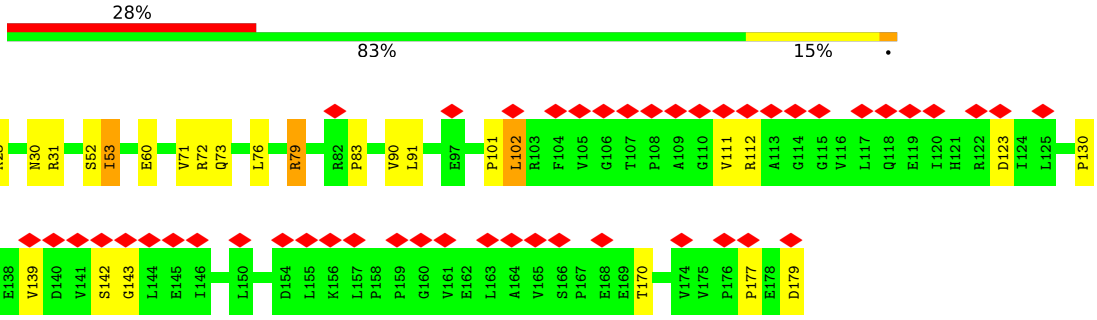
- Molecule 18: 50S ribosomal protein L24

Chain T1:



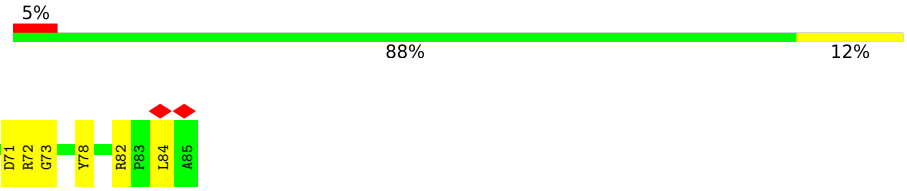
- Molecule 19: 50S ribosomal protein L25

Chain U1:



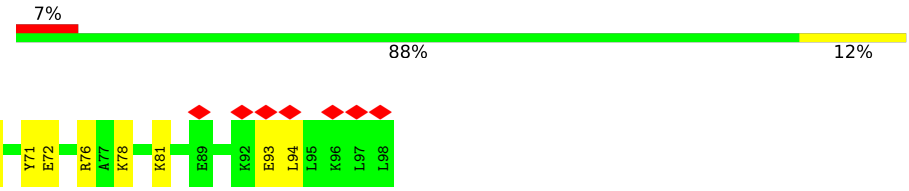
- Molecule 20: 50S ribosomal protein L27

Chain V1:



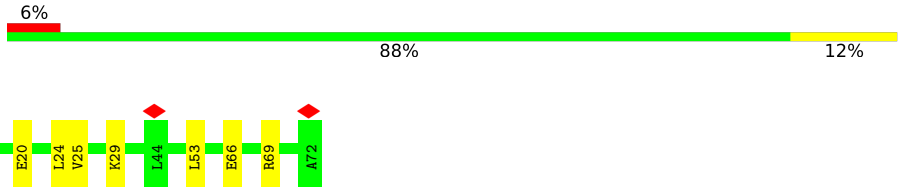
- Molecule 21: 50S ribosomal protein L28

Chain W1:



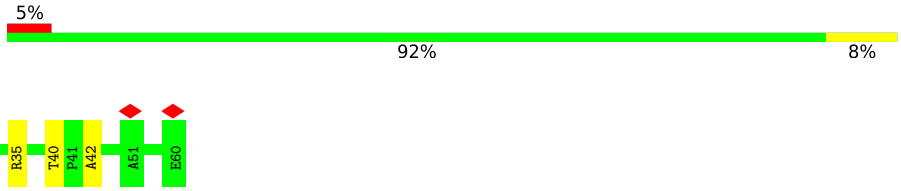
- Molecule 22: 50S ribosomal protein L29

Chain X1:



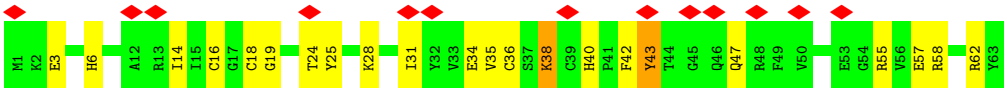
- Molecule 23: 50S ribosomal protein L30

Chain Y1:



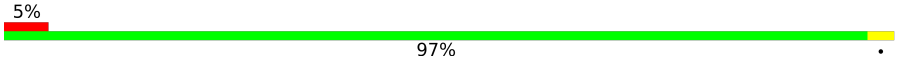
- Molecule 24: 50S ribosomal protein L31

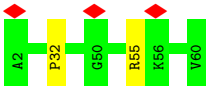
Chain Z1:



- Molecule 25: 50S ribosomal protein L32

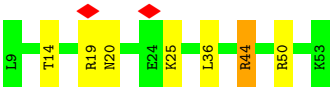
Chain a1:





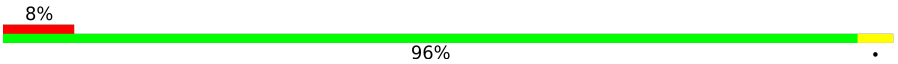
- Molecule 26: 50S ribosomal protein L33

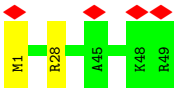
Chain b1:



- Molecule 27: 50S ribosomal protein L34

Chain c1:



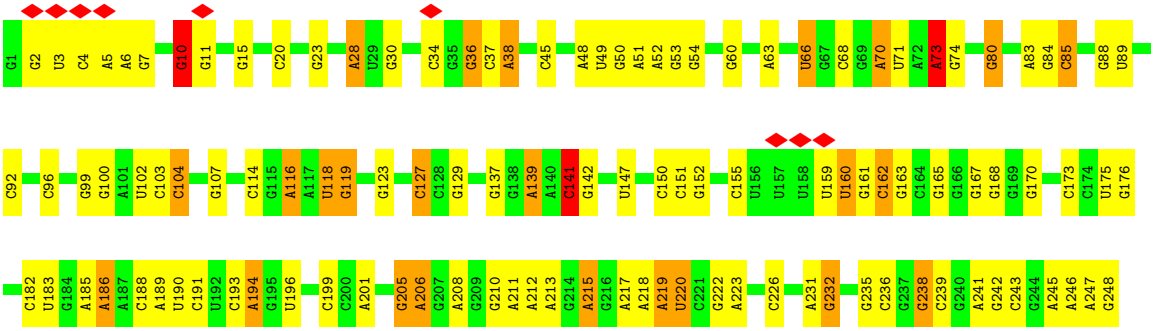


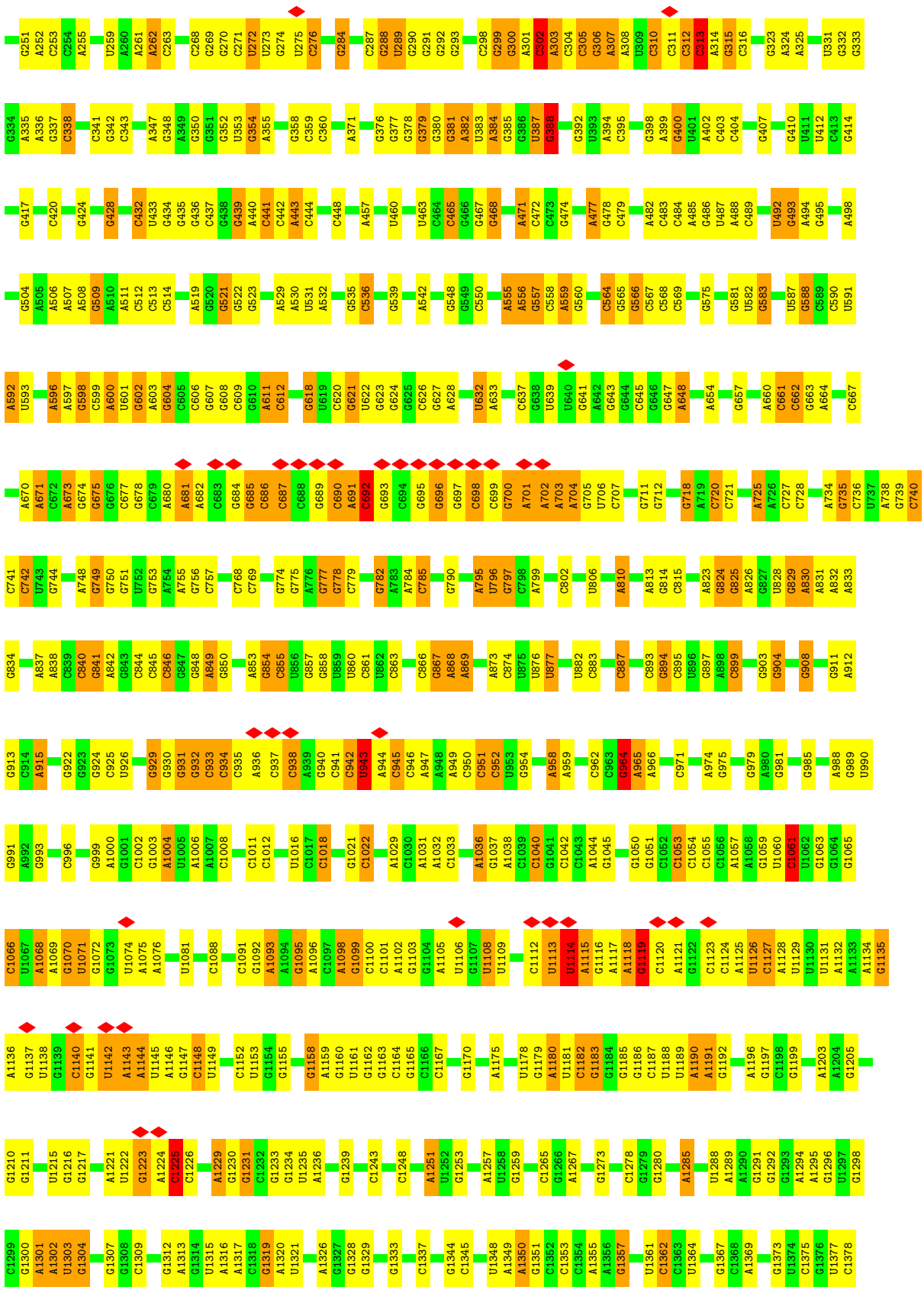
- Molecule 28: 50S ribosomal protein L35

Chain d1:

- Molecule 29: 23S ribosomal RNA

Chain A1:

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G334 A335 A336 G337 G338 C341 G342 C343 A347 G348 A349 G350 G351 G352 U353 G354 A355 G358 C359 C360 A371 G376 G377 G378 G379 G380 G381 A382 U383 A384 G385 G386 U387 G388 G392 U393 A394 C395 G398 A399 G400 U401 A402 C403 C404 G407 G410 U411 U412 C413 G414
G417 C420 G424 G428 C432 U433 G434 G435 G436 C437 G438 G439 A440 C441 C442 A443 C444 C448 A457 U460 U463 C464 C465 G466 G467 G468 A471 C472 C473 G474 A477 G478 C479 A482 C483 C484 A485 G486 U487 A488 C489 U492 G493 A494 G495 A498
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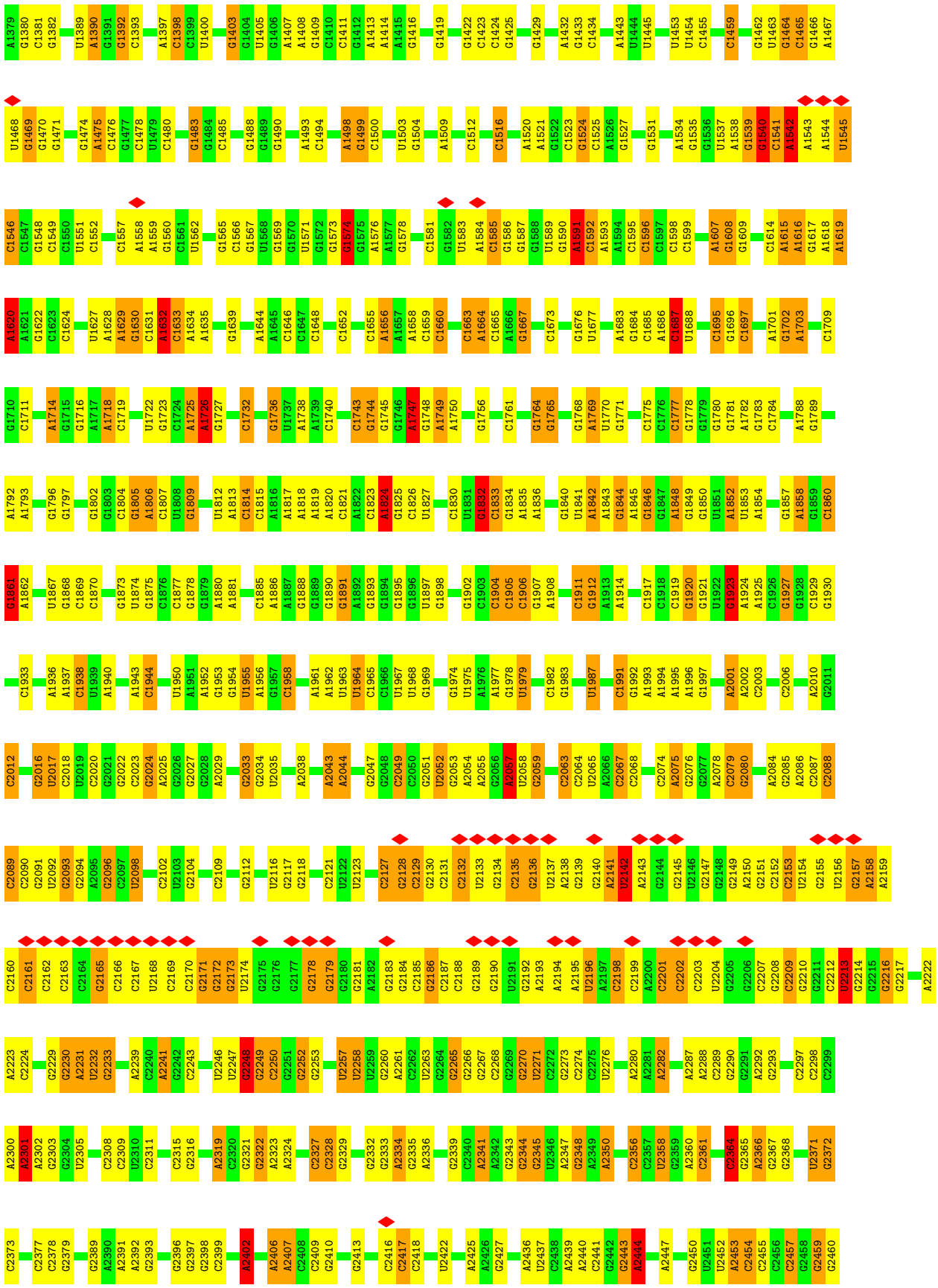
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U1468 G1469 G1470 G1471 G1474 A1475 G1476 G1477 C1478 U1479 C1480 G1483 G1484 C1485 G1488 G1489 G1490 A1493 C1494 A1498 G1499 C1500 U1503 G1504 A1509 C1512 C1516 A1520 A1521 G1522 C1523 G1524 C1525 A1526 G1527 G1531 A1534 G1535 G1536 U1537 A1538 G1539 G1540 C1541 A1542 A1543 A1544 U1545
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G1861 A1862 U1867 G1868 C1869 C1870 G1873 U1874 G1875 C1876 C1877 G1878 G1879 A1880 A1881 C1885 A1886 A1887 G1888 G1889 G1890 G1891 A1892 G1893 G1894 G1895 G1896 U1897 G1898 G1902 C1903 C1904 C1905 C1906 G1907 A1908 C1911 G1912 A1913 A1914 C1917 C1918 C1919 G1920 G1921 U1922 G1923 A1924 A1925 C1926 G1927 G1928 C1929 G1930
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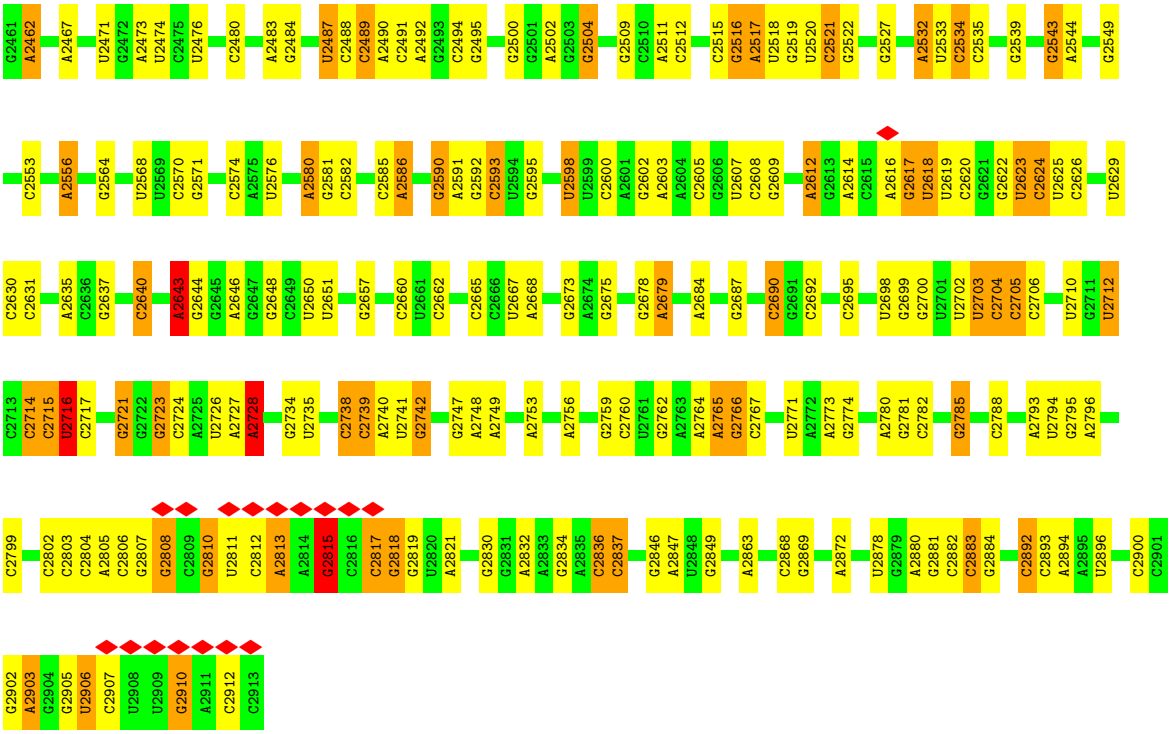
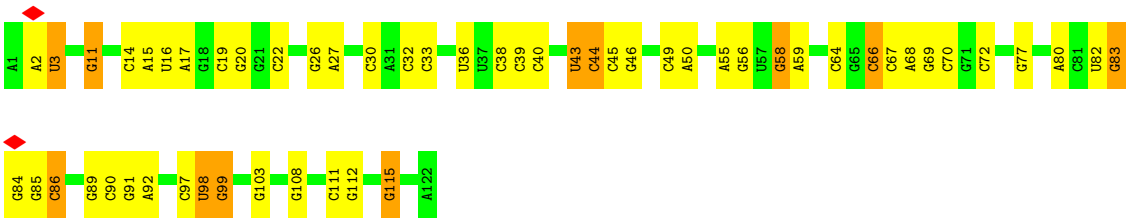


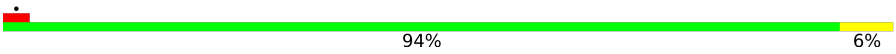
- Molecule 30: 5S ribosomal RNA

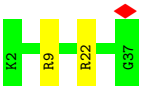
Chain B1:



- Molecule 31: 50S ribosomal protein L36

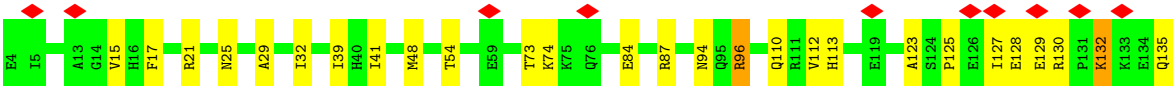
Chain e1:

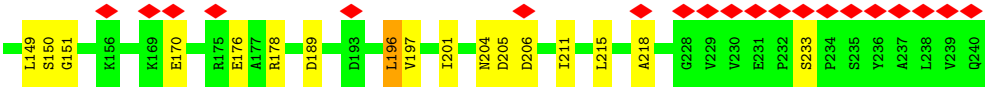




- Molecule 32: 30S ribosomal protein S2

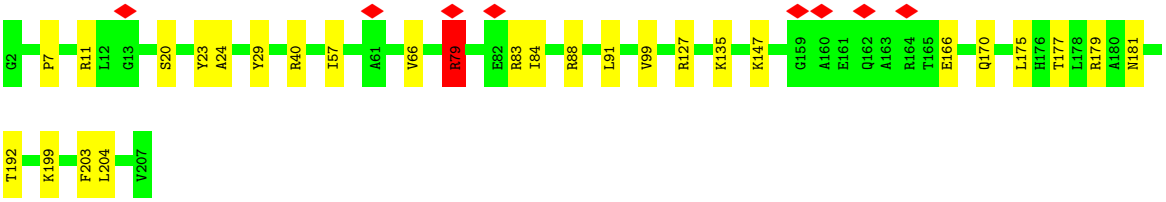
Chain B2:





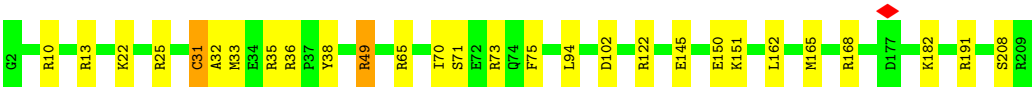
• Molecule 33: 30S ribosomal protein S3

Chain C2:



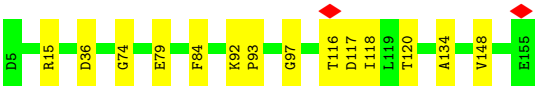
• Molecule 34: 30S ribosomal protein S4

Chain D2:



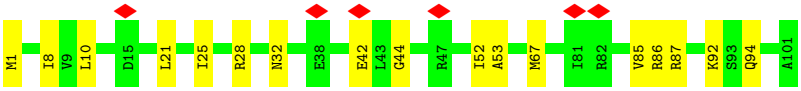
• Molecule 35: 30S ribosomal protein S5

Chain E2:



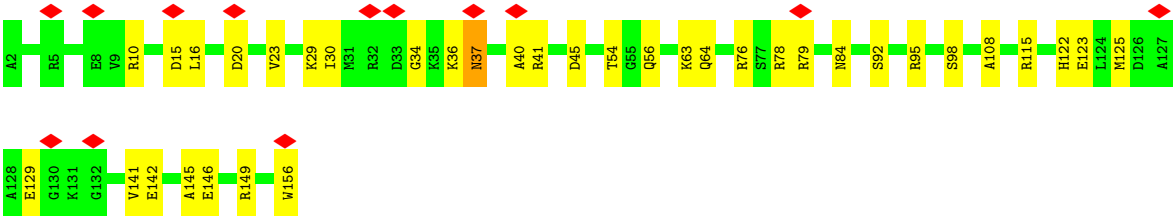
• Molecule 36: 30S ribosomal protein S6

Chain F2:



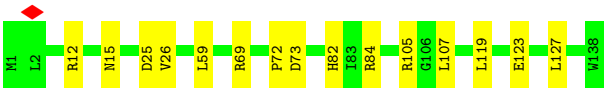
• Molecule 37: 30S ribosomal protein S7

Chain G2:



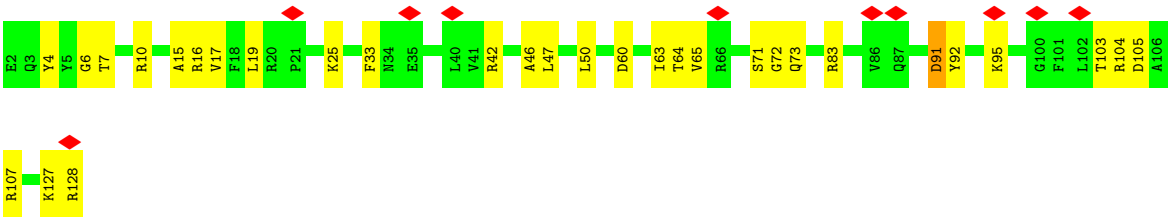
• Molecule 38: 30S ribosomal protein S8

Chain H2:



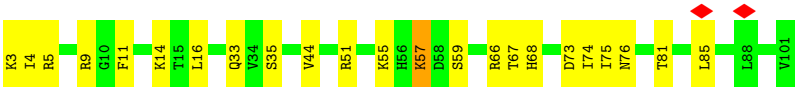
• Molecule 39: 30S ribosomal protein S9

Chain I2:



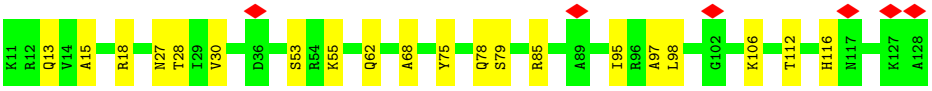
• Molecule 40: 30S ribosomal protein S10

Chain J2:



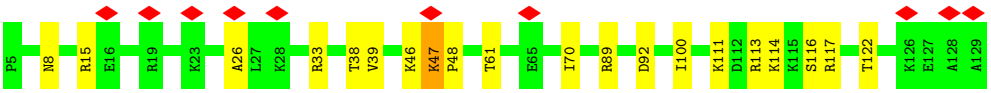
• Molecule 41: 30S ribosomal protein S11

Chain K2:



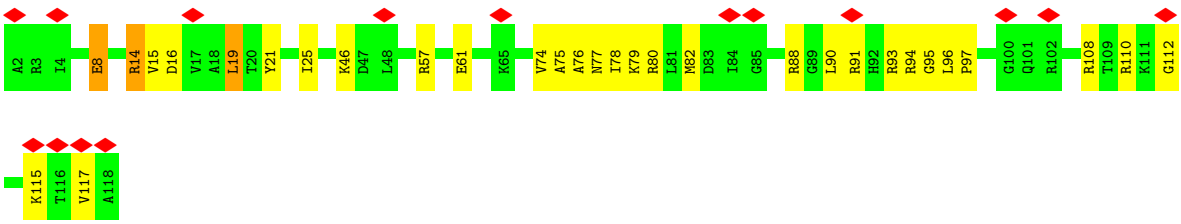
• Molecule 42: 30S ribosomal protein S12

Chain L2:



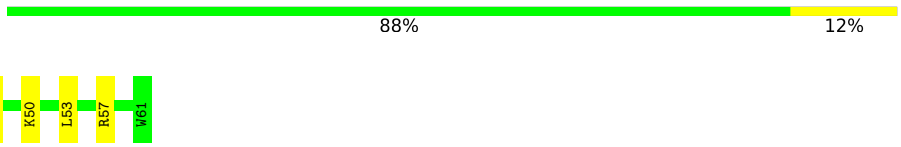
• Molecule 43: 30S ribosomal protein S13

Chain M2:



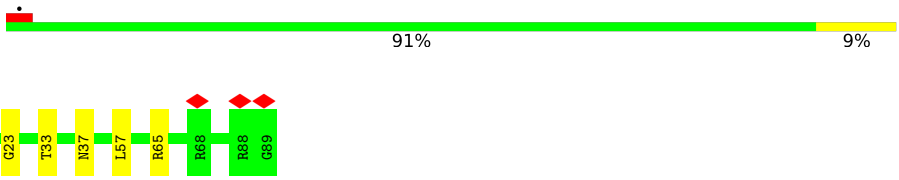
- Molecule 44: 30S ribosomal protein S14 type Z

Chain N2:



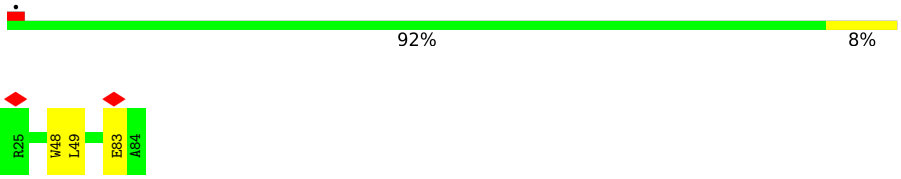
- Molecule 45: 30S ribosomal protein S15

Chain O2:



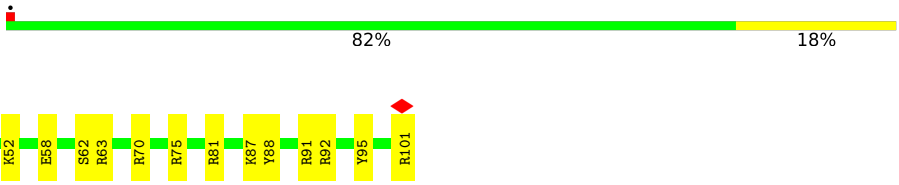
- Molecule 46: 30S ribosomal protein S16

Chain P2:



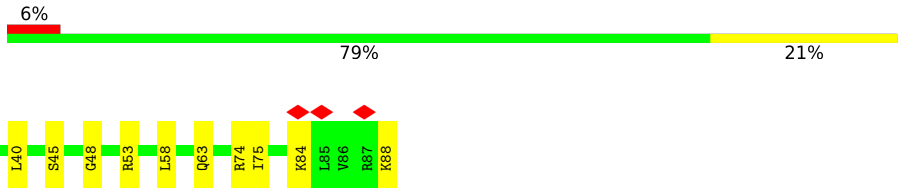
- Molecule 47: 30S ribosomal protein S17

Chain Q2:



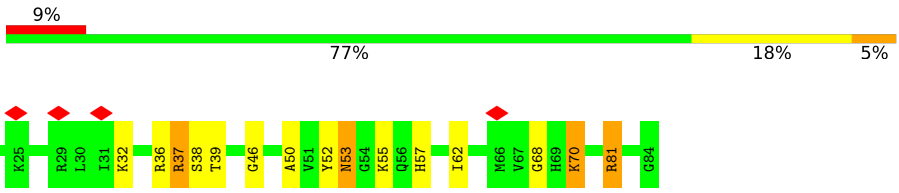
- Molecule 48: 30S ribosomal protein S18

Chain R2:



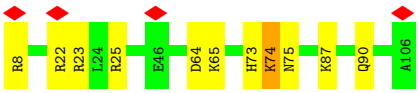
- Molecule 49: 30S ribosomal protein S19

Chain S2:



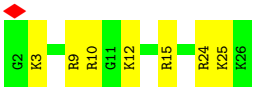
- Molecule 50: 30S ribosomal protein S20

Chain T2:



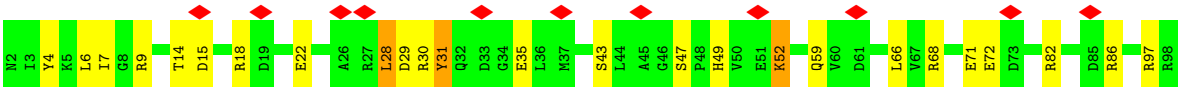
• Molecule 51: 30S ribosomal protein Thx

Chain U2:



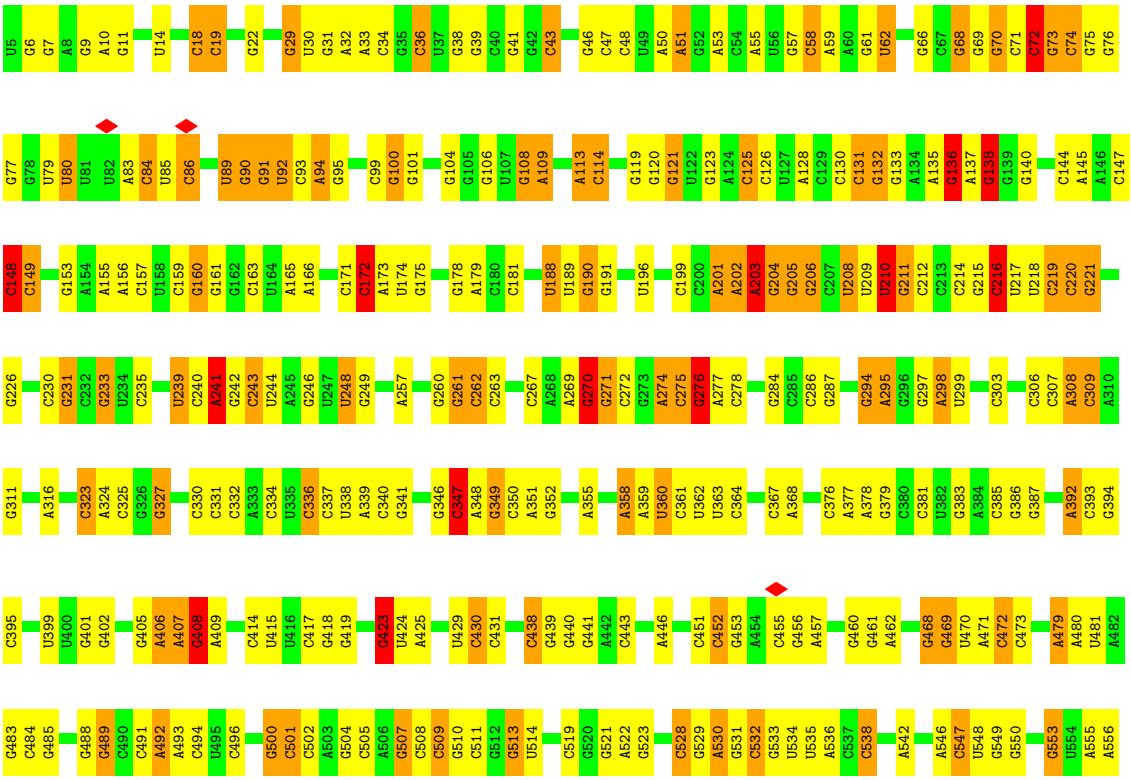
• Molecule 52: Ribosome hibernation promoting factor

Chain V2:



• Molecule 53: 16S ribosomal RNA

Chain A2:



A557 G558 G559 G560 C561 G562 U563 G564 U565 A566 G567 G568 C569 C573 U574 G575 G576 G577 G578 C582 U586 G587 U588 G589 A590 G593 A594 C598 G599 U602 C603 A604 A605 C606 C607 G608 U609 G610 G611 G612 G613 G614 A615 G620 G621 G622 A625 C630 C634 U635

A636 C639 G640 G641 U642 G643 G644 G645 A646 G647 A648 G649 G650 G651 U652 G657 A658 A659 U660 C663 C664 G665 G666 A670 G671 C672 G673 A677 A678 A679 U680 G681 C682 G683 C684 A685 G686 A687 U688 A689 C690 C691 G692 G693 G694 A695 G696 G697 A698 A699 C700 G701 C702 C703 G704

G707 G708 C709 G714 C715 A716 G717 C718 C721 C722 U723 G724 G725 U726 C727 C728 A729 C730 C731 C732 G733 U734 G735 A736 C737 G738 C745 G746 C747 G748 A749 A750 A751 G752 C753 A763 G769 A770 U771 U772 A773 G774 A775 U776 A777 C778 C779 G782 G783 U784 A785 G786

C793 U796 A797 A798 A799 C800 G801 A802 U803 G804 C807 G808 C809 U810 A811 G812 G813 U818 G819 G820 C823 U824 C825 C826 U827 G828 C834 G835 C839 A842 G846 U847 U848 A849 A850 C856 C857 G858 C859 C860 U861 G862 A866 C873 A877 A878 G879 G880

C881 A884 C887 A890 A891 A892 G893 G894 A895 A896 A900 C901 G902 G903 G904 G905 G906 C907 C908 C909 G910 C911 A912 C913 A914 A915 G916 C917 G921 G922 A923 G924 G925 U929 G930 G931 U932 A935 A936 U937 A941 A942 G943 C944 A945 A946 C947 G948 C949 G950 A951 A952

G953 A954 A955 C956 U959 A960 C961 C962 A963 G964 G965 C966 C967 U968 U969 G970 A971 C972 A973 U974 G975 C976 U977 A978 G979 G980 G981 A982 A983 C984 C985 C986 G987 G988 G989 U990 G991 A992 A993 A994 G995 U998 G999 G1000 G1001 G1002 U1003 G1004 C1005 C1006 C1007 C1008 G1009 C1010 G1011 A1012 G1013 G1014

G1015 G1016 A1017 G1018 C1019 C1020 C1021 U1022 A1023 G1024 C1025 G1030 U1031 G1032 C1033 A1037 G1040 C1041 C1042 G1046 A1049 G1050 C1051 U1052 C1053 G1054 U1055 G1056 G1059 U1060 G1061 A1062 G1063 U1068 U1073 G1076 U1077 C1078 C1079 C1080 G1081 C1082 A1083 A1084 A1087 G1088 C1089 G1090 C1091

C1095 C1100 C1101 U1107 U1108 G1109 C1110 C1111 A1112 G1113 C1114 G1115 G1116 U1117 U1118 C1119 G1120 C1121 C1122 C1123 G1124 G1125 G1126 C1127 A1128 A1133 A1134 C1135 G1136 G1137 G1138 A1139 C1140 U1141 G1142 C1143 C1144 C1145 G1146 A1149 A1150 A1151 G1155 G1156 A1157 A1161 G1162 G1163 A1164 G1165 G1166 G1167 G1168 A1169

C1170 G1171 A1172 C1173 G1174 U1175 C1176 U1177 G1178 A1182 G1183 C1184 C1190 C1191 U1192 U1193 A1194 C1195 G1196 G1197 C1198 C1199 U1200 G1201 G1202 G1203 A1206 C1207 A1208 C1209 A1210 C1211 G1212 U1213 G1214 C1215 U1216 A1217 C1218 A1219 A1220 U1221 G1222 C1223 C1224 C1227 U1228 A1229 C1230 A1231 A1232 A1233 G1234 C1235 G1236 A1237

U1238 G1239 C1240 C1243 C1244 G1247 C1248 A1249 A1250 C1251 G1252 G1253 G1254 C1258 U1259 A1260 A1261 U1262 C1263 G1264 C1265 A1266 A1267 A1268 A1269 A1270 G1271 G1272 U1273 G1274 G1275 G1276 C1279 A1280 G1281 U1282 U1283 C1284 G1285 G1286 A1287 U1288 U1289 G1292 G1293 U1294 C1298 A1299 A1300 C1301 C1302 C1303 G1304 A1305

C1306 C1307 G1312 A1313 C1317 G1318 G1319 U1322 C1323 G1324 C1325 U1326 A1327 G1328 U1332 C1333 G1334 C1335 G1336 G1337 A1338 U1339 C1340 A1341 G1342 C1343 C1344 A1345 U1346 G1352 G1353 U1354 G1355 A1356 A1357 U1358 A1359 C1360 G1361 U1362 U1363 C1364 G1367 G1368 C1371 U1372 U1373 G1374 C1377 A1378 C1379 A1380

C1381 C1382 G1383 C1386 G1387 U1388 C1391 G1392 C1393 C1394 A1395 A1400 G1401 G1404 G1405 U1409 A1410 C1411 G1412 C1413 G1414 U1418 C1419 G1420 C1421 C1422 G1423 G1424 G1425 A1426 G1427 A1431 C1432 G1433 G1434 G1435 C1436 A1437 G1438 G1439 C1440 C1443 U1449 A1450 G1451 G1452 C1456 G1457 U1458 G1459

A1460 G1464 G1465 G1466 C1467 G1468 A1469 A1470 G1471 U1472 C1473 G1474 U1475 A1476 A1479 A1480 G1481 G1482 U1483 A1484 G1488 U1489 C1492 G1493 G1494 A1495 A1496 U1499 G1506 G1507 A1508 U1509 C1510

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.06	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	35.207	Depositor
Minimum map value	-15.042	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.439	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	770.0, 770.0, 770.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	C1	0.77	1/2166 (0.0%)	0.76	0/2919
2	D1	0.71	0/1602	0.77	1/2160 (0.0%)
3	E1	0.72	0/1663	0.69	0/2249
4	F1	0.53	0/1499	0.66	0/2016
5	G1	0.52	0/1333	0.73	1/1802 (0.1%)
6	H1	0.49	0/387	0.71	0/523
7	I1	0.68	0/1132	0.68	0/1525
8	J1	0.70	0/943	0.69	0/1269
9	K1	0.61	0/1162	0.84	1/1544 (0.1%)
10	L1	0.65	0/1143	0.70	0/1527
11	M1	0.66	0/974	0.79	0/1302
12	N1	0.58	0/892	0.72	0/1187
13	O1	0.62	0/1156	0.67	0/1542
14	P1	0.77	0/982	0.68	0/1306
15	Q1	0.61	0/790	0.67	0/1057
16	R1	0.64	0/911	0.75	3/1220 (0.2%)
17	S1	0.68	0/740	0.72	0/993
18	T1	0.55	0/799	0.69	0/1064
19	U1	0.52	0/1461	0.66	1/1982 (0.1%)
20	V1	0.69	0/621	0.69	0/827
21	W1	0.66	0/770	0.74	0/1022
22	X1	0.52	0/583	0.69	0/771
23	Y1	0.65	0/474	0.68	0/635
24	Z1	0.48	0/528	0.78	0/709
25	a1	0.75	1/473 (0.2%)	0.71	0/639
26	b1	0.66	0/397	0.95	1/529 (0.2%)
27	c1	0.78	0/438	0.75	0/575
28	d1	0.74	0/495	0.99	3/649 (0.5%)
29	A1	1.64	325/70233 (0.5%)	1.41	861/109643 (0.8%)
30	B1	1.26	2/2928 (0.1%)	1.37	34/4568 (0.7%)
31	e1	0.71	0/302	0.69	0/397
32	B2	0.55	0/1960	0.68	0/2642
33	C2	0.61	0/1637	0.70	0/2205
34	D2	0.67	0/1733	0.76	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	E2	0.66	0/1172	0.71	0/1576
36	F2	0.55	0/856	0.64	0/1154
37	G2	0.51	0/1276	0.66	1/1709 (0.1%)
38	H2	0.70	0/1136	0.68	0/1527
39	I2	0.54	0/1029	0.72	0/1379
40	J2	0.50	0/815	0.65	1/1095 (0.1%)
41	K2	0.58	0/894	0.68	0/1205
42	L2	0.68	0/992	0.72	0/1327
43	M2	0.43	0/944	0.71	0/1265
44	N2	0.62	0/501	0.69	0/664
45	O2	0.59	0/745	0.70	0/992
46	P2	0.71	0/722	0.69	0/970
47	Q2	0.66	0/848	0.66	0/1131
48	R2	0.55	0/520	0.73	0/690
49	S2	0.44	0/639	0.72	0/860
50	T2	0.49	0/765	0.69	0/1007
51	U2	0.54	0/222	0.67	0/288
52	V2	0.59	0/997	0.84	1/1341 (0.1%)
53	A2	3.30	114/36234 (0.3%)	1.91	551/56554 (1.0%)
All	All	1.97	443/156614 (0.3%)	1.41	1460/234050 (0.6%)

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
1	C1	0	1
2	D1	0	1
3	E1	0	1
4	F1	0	1
5	G1	0	1
9	K1	0	2
14	P1	0	1
15	Q1	0	1
17	S1	0	1
18	T1	0	2
19	U1	0	1
24	Z1	0	1
26	b1	0	2
28	d1	0	2
32	B2	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	2
34	D2	0	3
37	G2	0	2
39	I2	0	1
40	J2	0	1
42	L2	0	2
43	M2	0	2
49	S2	0	1
51	U2	0	1
52	V2	0	2
All	All	0	37

The worst 5 of 443 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A2	700	C	N1-C6	189.65	2.50	1.37
53	A2	717	G	C6-N1	170.78	2.59	1.39
53	A2	717	G	N3-C4	146.04	2.37	1.35
53	A2	136	G	C2-N2	143.97	2.78	1.34
53	A2	1121	G	C2-N2	142.36	2.77	1.34

The worst 5 of 1460 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A2	700	C	C4-C5-C6	-192.11	21.34	117.40
53	A2	700	C	N1-C2-N3	-133.89	25.48	119.20
53	A2	700	C	C2-N3-C4	86.94	163.37	119.90
53	A2	700	C	C5-C6-N1	59.60	150.80	121.00
53	A2	700	C	C6-N1-C2	49.66	140.16	120.30

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C1	33	LEU	Peptide
2	D1	61	ARG	Peptide
3	E1	24	LEU	Peptide
4	F1	114	ILE	Peptide
5	G1	89	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	2116	0	2194	20	0
2	D1	1569	0	1634	14	0
3	E1	1628	0	1680	17	0
4	F1	1474	0	1535	30	0
5	G1	1308	0	1382	29	0
6	H1	383	0	410	4	0
7	I1	1105	0	1180	8	0
8	J1	933	0	996	14	0
9	K1	1145	0	1228	17	0
10	L1	1122	0	1179	11	0
11	M1	960	0	1021	12	0
12	N1	882	0	943	17	0
13	O1	1142	0	1202	20	0
14	P1	964	0	1022	8	0
15	Q1	779	0	852	4	0
16	R1	900	0	964	10	0
17	S1	726	0	778	2	0
18	T1	786	0	878	15	0
19	U1	1429	0	1454	18	0
20	V1	613	0	633	6	0
21	W1	763	0	848	6	0
22	X1	581	0	629	5	0
23	Y1	469	0	518	2	0
24	Z1	516	0	514	15	0
25	a1	459	0	479	0	0
26	b1	390	0	404	0	0
27	c1	430	0	480	0	0
28	d1	489	0	560	0	0
29	A1	62707	0	31613	271	0
30	B1	2617	0	1328	12	0
31	e1	299	0	326	0	0
32	B2	1925	0	1975	27	0
33	C2	1613	0	1677	15	0
34	D2	1703	0	1765	19	0
35	E2	1156	0	1213	9	0
36	F2	843	0	857	12	0
37	G2	1257	0	1296	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H2	1116	0	1177	10	0
39	I2	1010	0	1037	24	0
40	J2	802	0	849	13	0
41	K2	879	0	899	13	0
42	L2	976	0	1062	13	0
43	M2	934	0	992	25	0
44	N2	492	0	533	5	0
45	O2	734	0	771	6	0
46	P2	706	0	725	4	0
47	Q2	835	0	904	14	0
48	R2	515	0	568	8	0
49	S2	625	0	636	12	0
50	T2	763	0	861	7	0
51	U2	218	0	234	5	0
52	V2	983	0	1008	27	0
53	A2	32369	0	16339	365	0
All	All	144138	0	98242	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1080 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:1110:C:C5	53:A2:1110:C:C6	1.92	1.57
53:A2:216:C:C6	53:A2:216:C:C5	1.89	1.55
53:A2:216:C:C5	53:A2:216:C:C4	2.03	1.47
53:A2:1110:C:C5	53:A2:1110:C:C4	2.06	1.41
53:A2:136:G:N2	53:A2:216:C:N3	1.78	1.32

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C1	270/272 (99%)	237 (88%)	32 (12%)	1 (0%)	34	67
2	D1	203/205 (99%)	164 (81%)	35 (17%)	4 (2%)	7	34
3	E1	206/208 (99%)	180 (87%)	26 (13%)	0	100	100
4	F1	179/181 (99%)	157 (88%)	22 (12%)	0	100	100
5	G1	168/170 (99%)	136 (81%)	28 (17%)	4 (2%)	6	29
6	H1	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
7	I1	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	J1	120/122 (98%)	97 (81%)	23 (19%)	0	100	100
9	K1	148/150 (99%)	107 (72%)	38 (26%)	3 (2%)	7	34
10	L1	139/141 (99%)	117 (84%)	20 (14%)	2 (1%)	11	40
11	M1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
12	N1	109/111 (98%)	94 (86%)	15 (14%)	0	100	100
13	O1	135/137 (98%)	114 (84%)	20 (15%)	1 (1%)	22	56
14	P1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
15	Q1	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
16	R1	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
17	S1	90/92 (98%)	77 (86%)	13 (14%)	0	100	100
18	T1	100/102 (98%)	77 (77%)	22 (22%)	1 (1%)	15	48
19	U1	177/179 (99%)	134 (76%)	42 (24%)	1 (1%)	25	58
20	V1	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
21	W1	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	14	46
22	X1	67/69 (97%)	60 (90%)	7 (10%)	0	100	100
23	Y1	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
24	Z1	61/63 (97%)	41 (67%)	17 (28%)	3 (5%)	2	14
25	a1	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
26	b1	43/45 (96%)	29 (67%)	14 (33%)	0	100	100
27	c1	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
28	d1	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	9	37
31	e1	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
32	B2	235/237 (99%)	197 (84%)	38 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C2	204/206 (99%)	180 (88%)	24 (12%)	0	100	100
34	D2	206/208 (99%)	178 (86%)	27 (13%)	1 (0%)	29	62
35	E2	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
36	F2	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
37	G2	153/155 (99%)	126 (82%)	27 (18%)	0	100	100
38	H2	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	I2	125/127 (98%)	100 (80%)	25 (20%)	0	100	100
40	J2	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
41	K2	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
42	L2	123/125 (98%)	97 (79%)	25 (20%)	1 (1%)	19	52
43	M2	115/117 (98%)	96 (84%)	18 (16%)	1 (1%)	17	50
44	N2	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
45	O2	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
46	P2	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
47	Q2	98/100 (98%)	84 (86%)	14 (14%)	0	100	100
48	R2	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
49	S2	76/78 (97%)	53 (70%)	23 (30%)	0	100	100
50	T2	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15	48
51	U2	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
52	V2	119/121 (98%)	92 (77%)	26 (22%)	1 (1%)	19	52
All	All	5720/5820 (98%)	4828 (84%)	865 (15%)	27 (0%)	32	62

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G1	90	LYS
50	T2	74	LYS
9	K1	58	THR
19	U1	53	ILE
24	Z1	25	TYR

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C1	214/214 (100%)	210 (98%)	4 (2%)	57	77
2	D1	165/165 (100%)	164 (99%)	1 (1%)	86	91
3	E1	165/165 (100%)	163 (99%)	2 (1%)	71	83
4	F1	155/155 (100%)	152 (98%)	3 (2%)	57	77
5	G1	142/142 (100%)	135 (95%)	7 (5%)	25	56
6	H1	41/41 (100%)	41 (100%)	0	100	100
7	I1	117/117 (100%)	117 (100%)	0	100	100
8	J1	100/100 (100%)	99 (99%)	1 (1%)	76	85
9	K1	116/116 (100%)	111 (96%)	5 (4%)	29	59
10	L1	111/111 (100%)	106 (96%)	5 (4%)	27	58
11	M1	100/100 (100%)	98 (98%)	2 (2%)	55	76
12	N1	87/87 (100%)	84 (97%)	3 (3%)	37	65
13	O1	120/120 (100%)	115 (96%)	5 (4%)	30	60
14	P1	93/93 (100%)	90 (97%)	3 (3%)	39	67
15	Q1	82/82 (100%)	81 (99%)	1 (1%)	71	83
16	R1	92/92 (100%)	91 (99%)	1 (1%)	73	85
17	S1	74/74 (100%)	72 (97%)	2 (3%)	44	71
18	T1	85/85 (100%)	84 (99%)	1 (1%)	71	83
19	U1	158/158 (100%)	156 (99%)	2 (1%)	69	82
20	V1	62/62 (100%)	62 (100%)	0	100	100
21	W1	82/82 (100%)	81 (99%)	1 (1%)	71	83
22	X1	64/64 (100%)	63 (98%)	1 (2%)	62	79
23	Y1	51/51 (100%)	50 (98%)	1 (2%)	55	76
24	Z1	57/57 (100%)	55 (96%)	2 (4%)	36	64
25	a1	51/51 (100%)	50 (98%)	1 (2%)	55	76
26	b1	44/44 (100%)	39 (89%)	5 (11%)	5	23
27	c1	42/42 (100%)	40 (95%)	2 (5%)	25	56
28	d1	51/51 (100%)	49 (96%)	2 (4%)	32	62
31	e1	33/33 (100%)	31 (94%)	2 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	B2	205/205 (100%)	201 (98%)	4 (2%)	55	76
33	C2	160/160 (100%)	158 (99%)	2 (1%)	69	82
34	D2	180/180 (100%)	179 (99%)	1 (1%)	86	91
35	E2	116/116 (100%)	115 (99%)	1 (1%)	78	87
36	F2	90/90 (100%)	90 (100%)	0	100	100
37	G2	126/126 (100%)	125 (99%)	1 (1%)	81	89
38	H2	119/119 (100%)	119 (100%)	0	100	100
39	I2	98/98 (100%)	98 (100%)	0	100	100
40	J2	89/89 (100%)	88 (99%)	1 (1%)	73	85
41	K2	89/89 (100%)	88 (99%)	1 (1%)	73	85
42	L2	104/104 (100%)	102 (98%)	2 (2%)	57	77
43	M2	94/94 (100%)	91 (97%)	3 (3%)	39	67
44	N2	49/49 (100%)	47 (96%)	2 (4%)	30	61
45	O2	79/79 (100%)	79 (100%)	0	100	100
46	P2	72/72 (100%)	72 (100%)	0	100	100
47	Q2	95/95 (100%)	94 (99%)	1 (1%)	73	85
48	R2	55/55 (100%)	53 (96%)	2 (4%)	35	63
49	S2	67/67 (100%)	63 (94%)	4 (6%)	19	49
50	T2	76/76 (100%)	75 (99%)	1 (1%)	69	82
51	U2	20/20 (100%)	19 (95%)	1 (5%)	24	55
52	V2	103/103 (100%)	98 (95%)	5 (5%)	25	56
All	All	4840/4840 (100%)	4743 (98%)	97 (2%)	57	76

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	b1	44	ARG
34	D2	49	ARG
27	c1	1	MET
32	B2	25	ASN
41	K2	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
22	X1	47	ASN
52	V2	107	GLN
32	B2	113	HIS
52	V2	2	ASN
48	R2	36	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A1	2911/2912 (99%)	950 (32%)	25 (0%)
30	B1	121/122 (99%)	29 (23%)	0
53	A2	1505/1506 (99%)	522 (34%)	23 (1%)
All	All	4537/4540 (99%)	1501 (33%)	48 (1%)

5 of 1501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A1	2	G
29	A1	3	U
29	A1	4	C
29	A1	10	G
29	A1	15	G

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A2	241	A
53	A2	890	A
53	A2	261	G
53	A2	562	G
53	A2	959	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C1	1
25	a1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C1	239:ARG	C	240:ALA	N	1.18
1	a1	32:PRO	C	33:CYS	N	1.17

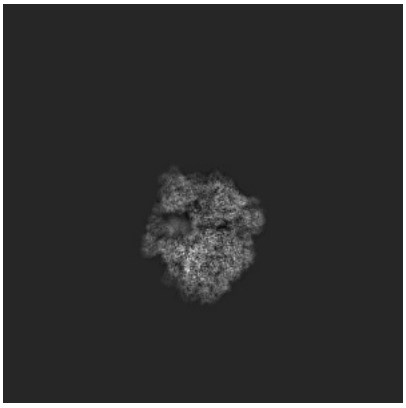
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0101. These allow visual inspection of the internal detail of the map and identification of artifacts.

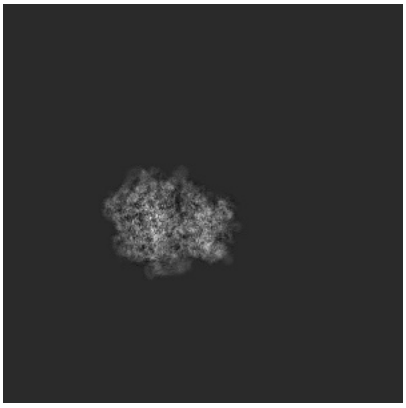
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

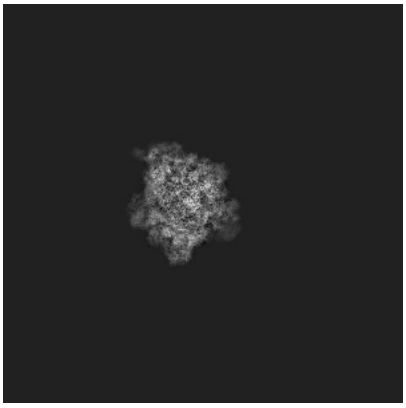
6.1.1 Primary map



X



Y

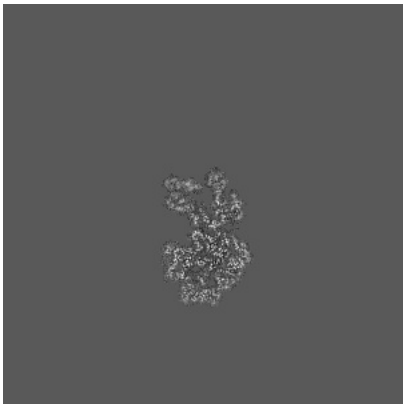


Z

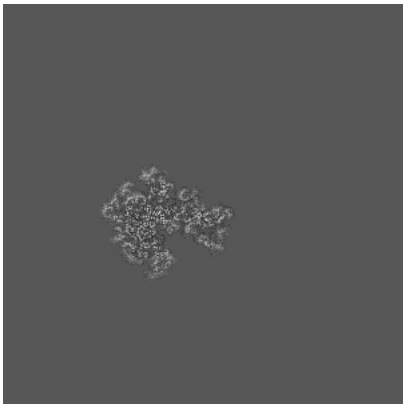
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

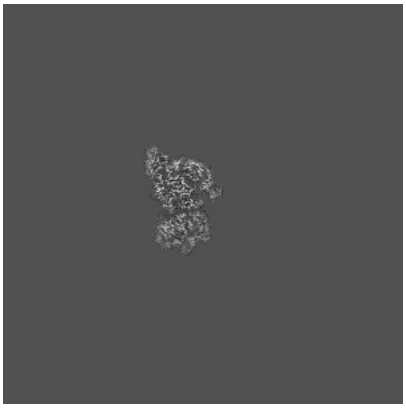
6.2.1 Primary map



X Index: 350



Y Index: 350

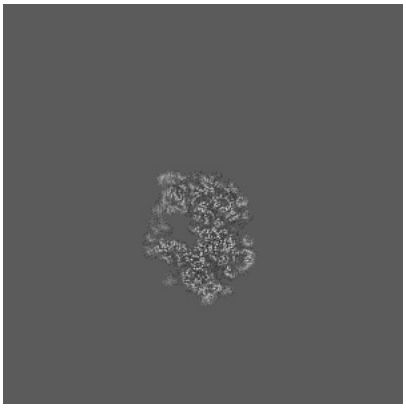


Z Index: 350

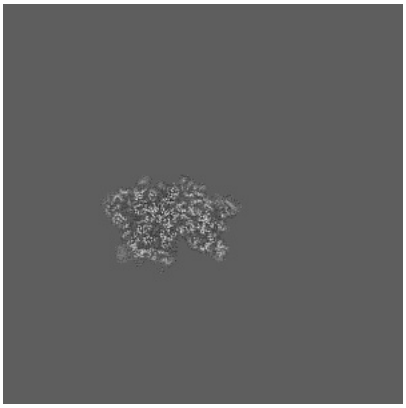
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

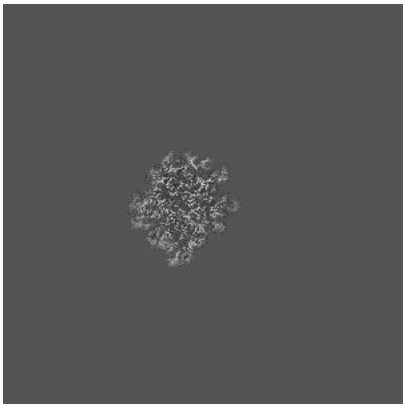
6.3.1 Primary map



X Index: 328



Y Index: 372



Z Index: 268

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

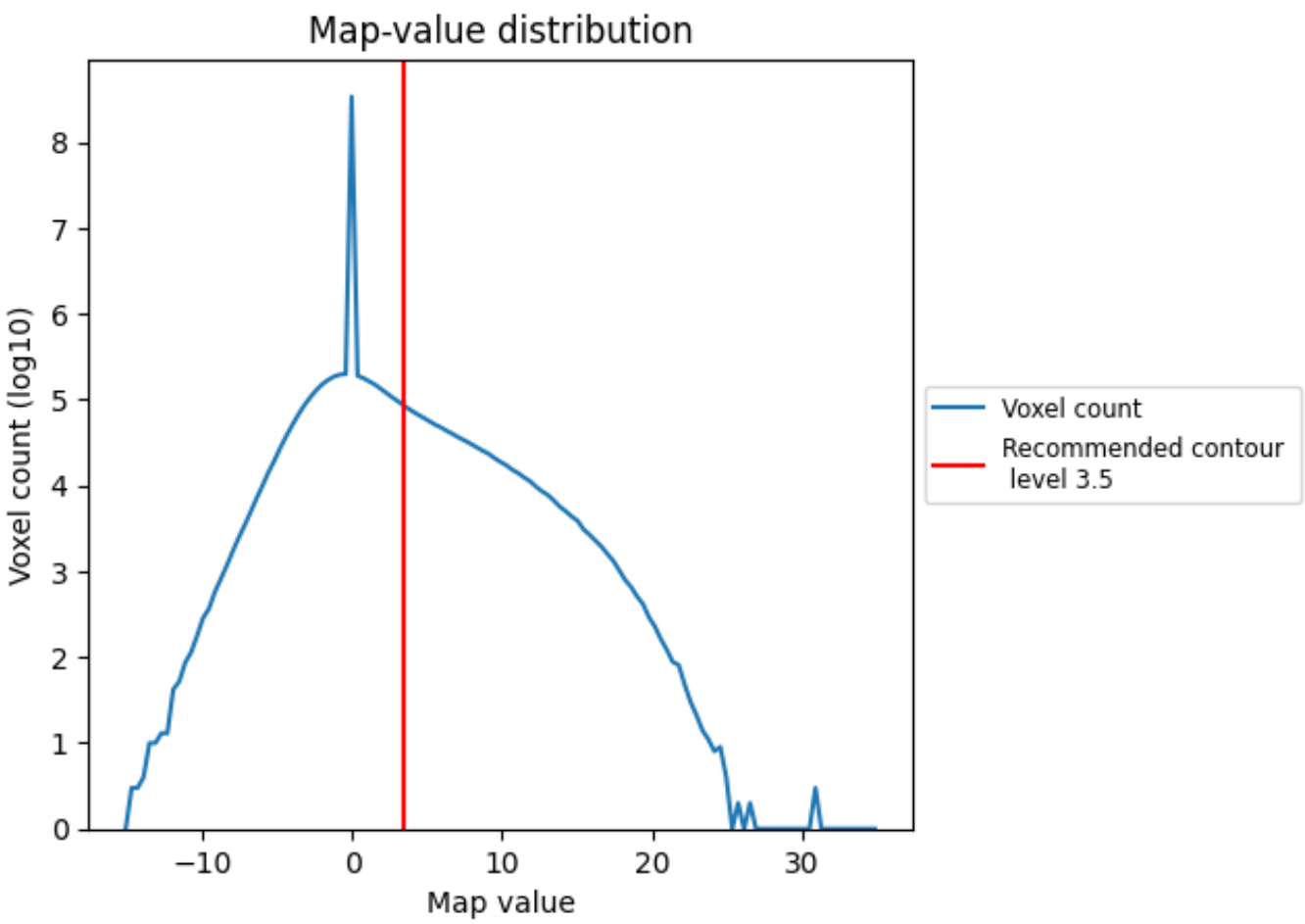
6.5 Mask visualisation (i)

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

7 Map analysis (i)

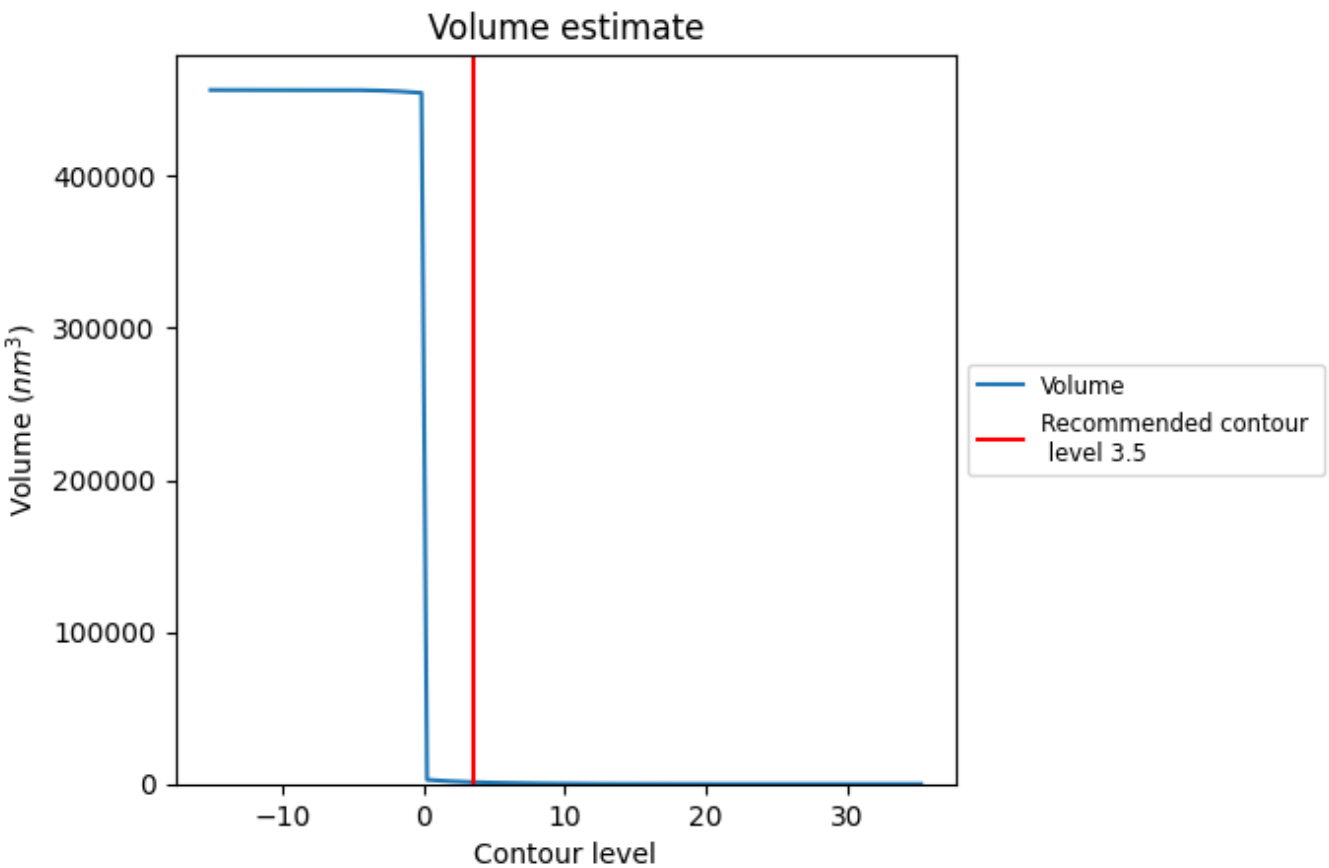
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

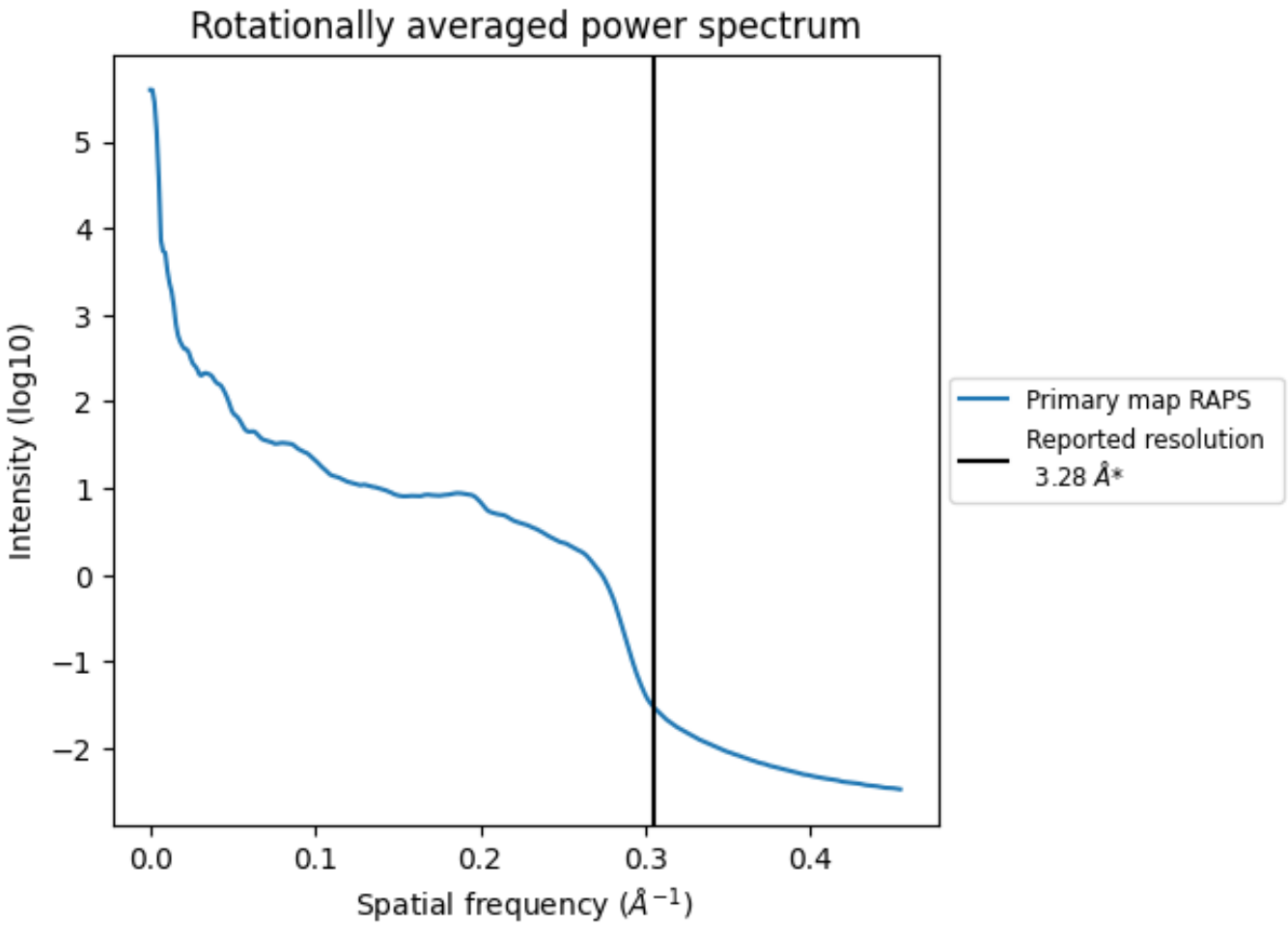
7.2 Volume estimate (i)



The volume at the recommended contour level is 1192 nm^3; this corresponds to an approximate mass of 1077 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

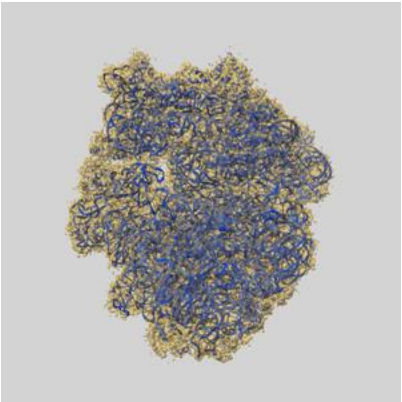
8 Fourier-Shell correlation (i)

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

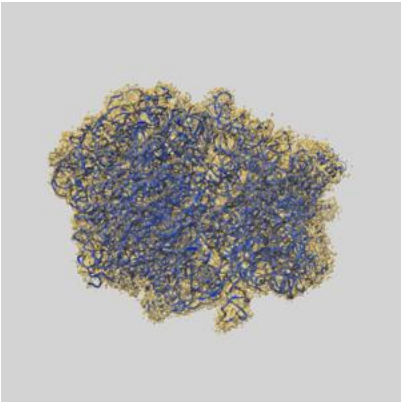
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0101 and PDB model 6GZQ. Per-residue inclusion information can be found in section 3 on page 13.

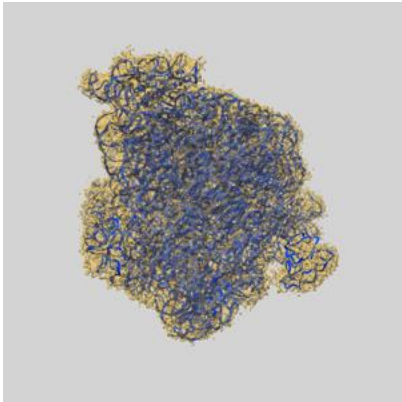
9.1 Map-model overlay (i)



X



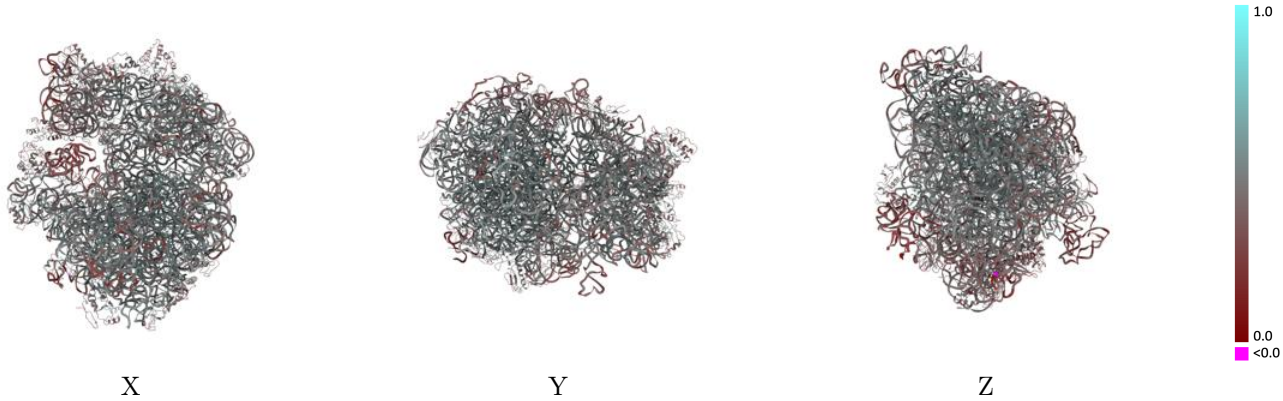
Y



Z

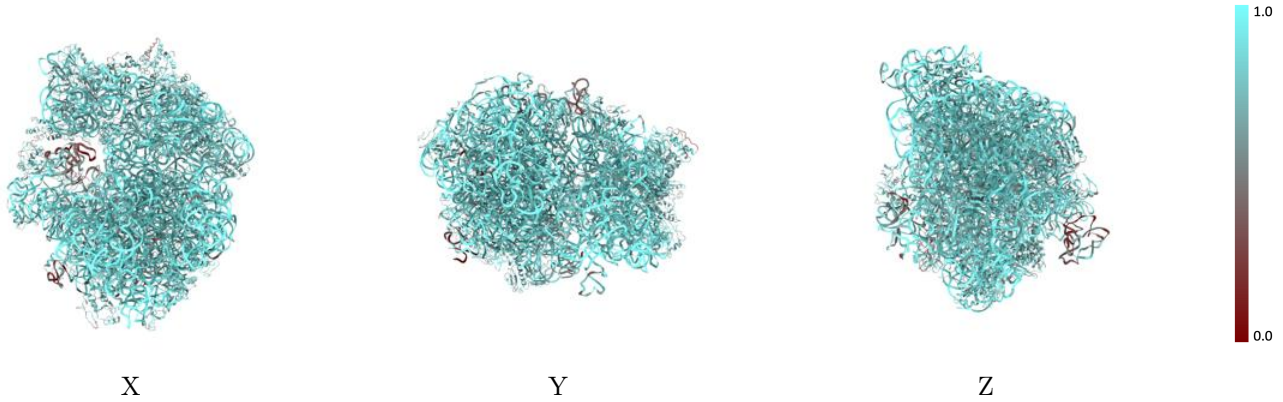
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



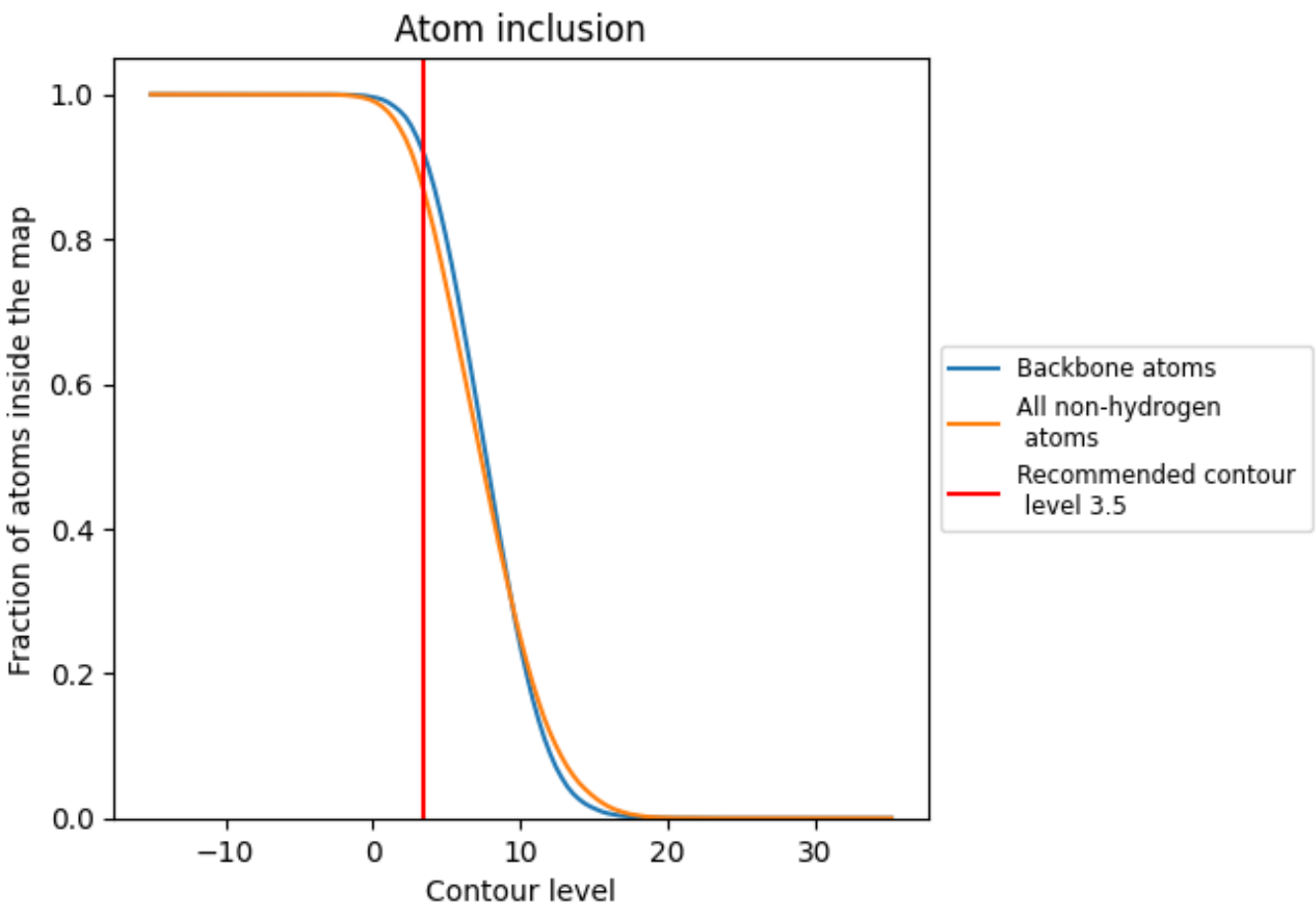
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8646	0.4640
A1	0.9052	0.4790
A2	0.9268	0.4550
B1	0.9297	0.4520
B2	0.6967	0.4040
C1	0.8137	0.5040
C2	0.7503	0.4450
D1	0.8051	0.4980
D2	0.8103	0.4570
E1	0.7647	0.4720
E2	0.7788	0.4800
F1	0.7491	0.4030
F2	0.7380	0.4110
G1	0.7463	0.4010
G2	0.7119	0.3950
H1	0.6587	0.4060
H2	0.8223	0.4730
I1	0.7816	0.4870
I2	0.6852	0.3770
J1	0.7684	0.4970
J2	0.7198	0.4080
K1	0.7656	0.4600
K2	0.7970	0.4540
L1	0.7770	0.4840
L2	0.7709	0.4770
M1	0.8107	0.5090
M2	0.6891	0.3530
N1	0.8208	0.4530
N2	0.7773	0.4590
O1	0.7546	0.4570
O2	0.7952	0.4560
P1	0.8308	0.4940
P2	0.8321	0.4910
Q1	0.7795	0.4640
Q2	0.7908	0.4740

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Chain	Atom inclusion	Q-score
R1	0.7820	0.4920
R2	0.7389	0.4300
S1	0.8073	0.4910
S2	0.7234	0.3600
T1	0.7464	0.4220
T2	0.7591	0.4450
U1	0.5794	0.4000
U2	0.7463	0.3720
V1	0.8256	0.5000
V2	0.6811	0.4230
W1	0.7368	0.4740
X1	0.7629	0.4220
Y1	0.7675	0.4790
Z1	0.6420	0.3110
a1	0.7852	0.4540
b1	0.7520	0.3760
c1	0.7789	0.5200
d1	0.7552	0.4690
e1	0.8182	0.5080