wwPDB EM Validation Summary Report

Sep 16, 2026 – 11:50 AM EDT

PDB ID	:	7M4W / pdb_00007m4w
EMDB ID	:	EMD-23668
Title	:	A. baumannii Ribosome-Eravacycline complex: Empty 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-03-22
Resolution	:	2.55 Å(reported)

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

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

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

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

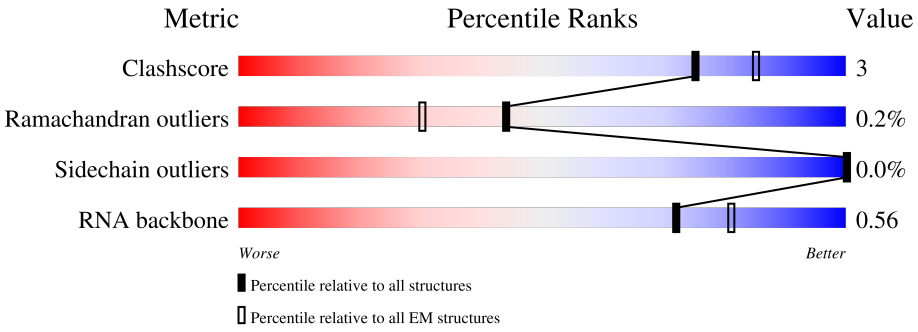
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

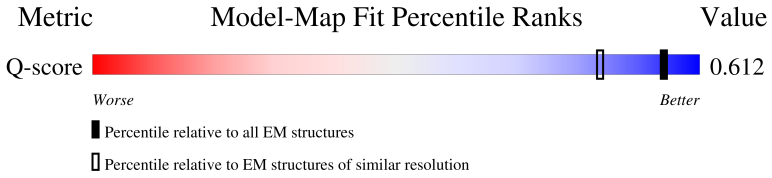
1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 Å.

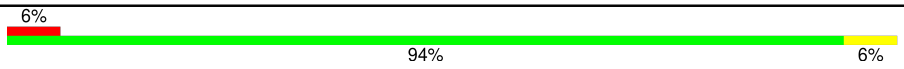
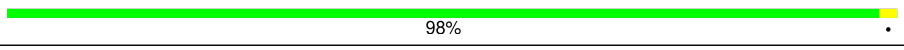
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





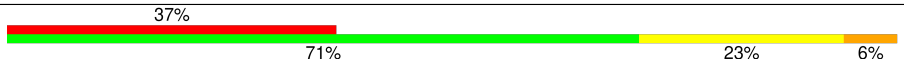
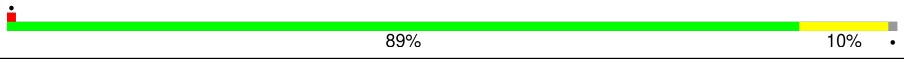
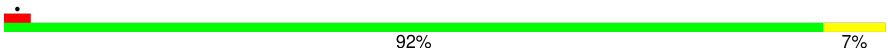
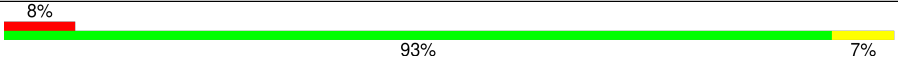
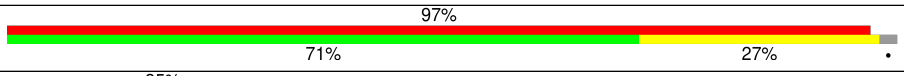
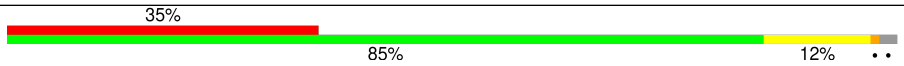
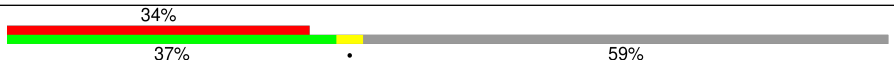
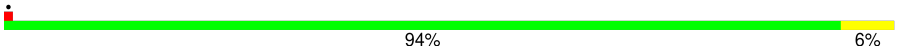
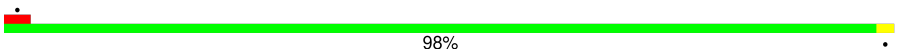
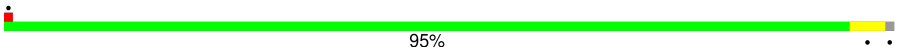
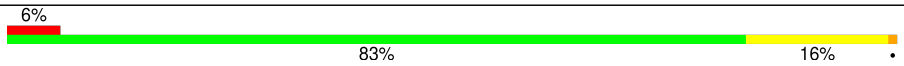
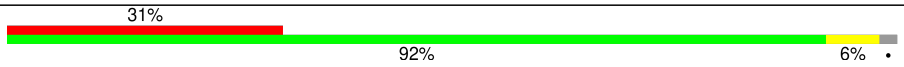
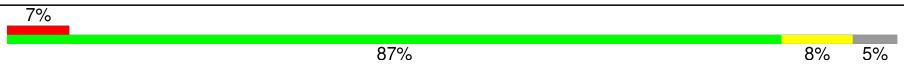
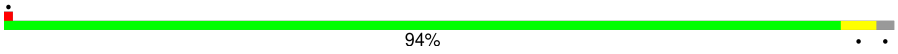
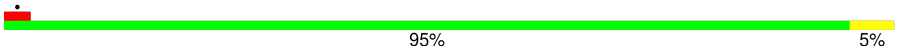
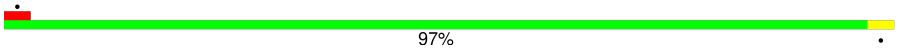
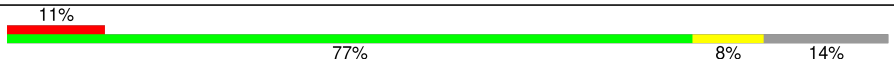
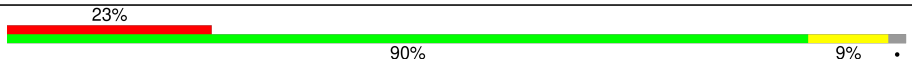
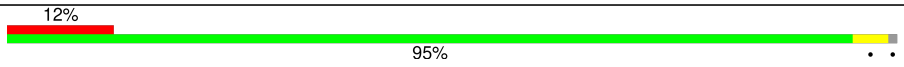
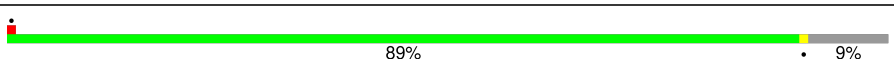
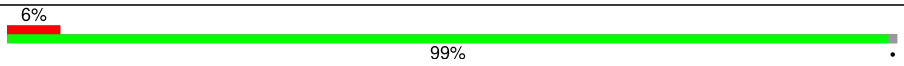
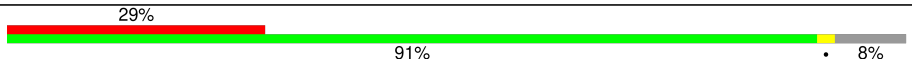
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7475 (2.05 - 3.05)

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	0	51	
2	1	44	
3	2	64	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	

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Mol	Chain	Length	Quality of chain
29	Y	58	90% 9%
30	Z	61	10% 82% 8% 10%
31	a	1544	75% 20%
32	b	250	68% 66% 24% 10%
33	c	250	80% 6% 14%
34	d	208	12% 86% 14%
35	e	165	87% 7% 6%
36	f	127	11% 62% 17% 18%
37	g	156	18% 72% 20% 8%
38	h	131	96%
39	i	128	86% 12%
40	j	103	84% 13%
41	k	128	9% 80% 12% 9%
42	l	124	85% 12%
43	m	118	85% 13%
44	n	101	86% 13%
45	o	89	91% 8%
46	p	101	79% 19%
47	q	85	82% 11% 7%
48	r	75	63% 7% 31%
49	s	91	88% 10%
50	t	88	85% 13%
51	u	71	52% 85% 11%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 137923 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2730	Total	C	N	O	P	0	0
			58566	26143	10721	18972	2730		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	144	Total	C	N	O	0	0
			1071	663	213	195		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	116	Total	C	N	O	0	0
			913	575	176	162		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total 807	C 506	N 155	O 143	S 3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total 826	C 514	N 158	O 150	S 4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total 710	C 452	N 128	O 129	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	103	Total 766	C 476	N 142	O 148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total 760	C 477	N 143	O 139	S 1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	77	Total 585	C 363	N 112	O 108	S 2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total 632	C 395	N 130	O 105	S 2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	143	Total	C	N	O	S	0	0
			1127	706	211	203	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total	C	N	O	0	0
			426	273	74	79		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

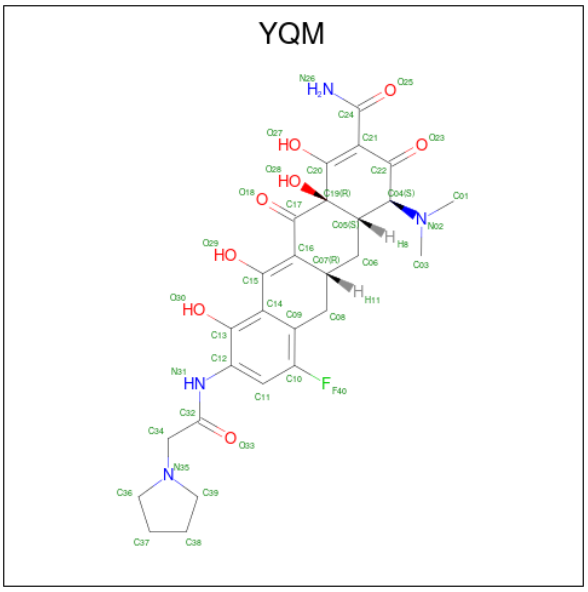
- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	63	Total	C	N	O	S	0	0
			522	327	105	89	1		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total	Zn	0
			1	1	

- Molecule 53 is Eravacycline (CCD ID: YQM) (formula: $C_{27}H_{31}FN_4O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
53	A	1	Total C F N O 40 27 1 4 8	0
53	A	1	Total C F N O 40 27 1 4 8	0
53	a	1	Total C F N O 40 27 1 4 8	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
54	A	136	Total Mg 136 136	0
54	B	1	Total Mg 1 1	0
54	D	1	Total Mg 1 1	0
54	K	1	Total Mg 1 1	0
54	a	52	Total Mg 52 52	0

- Molecule 55 is water.

Mol	Chain	Residues	Atoms	AltConf
55	2	2	Total O 2 2	0

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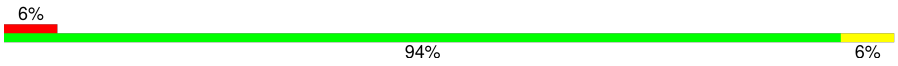
Mol	Chain	Residues	Atoms	AltConf
55	A	597	Total O 597 597	0
55	B	4	Total O 4 4	0
55	C	7	Total O 7 7	0
55	D	4	Total O 4 4	0
55	E	3	Total O 3 3	0
55	K	7	Total O 7 7	0
55	R	1	Total O 1 1	0
55	U	1	Total O 1 1	0
55	Z	2	Total O 2 2	0
55	a	156	Total O 156 156	0
55	i	2	Total O 2 2	0
55	j	3	Total O 3 3	0
55	k	1	Total O 1 1	0
55	m	1	Total O 1 1	0
55	n	3	Total O 3 3	0
55	q	1	Total O 1 1	0
55	s	1	Total O 1 1	0
55	t	1	Total O 1 1	0

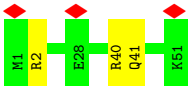
3 Residue-property plots (i)

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 L33

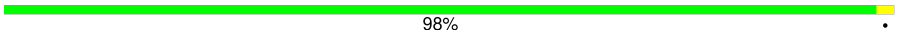
Chain 0:





• Molecule 2: 50S ribosomal protein L34

Chain 1:

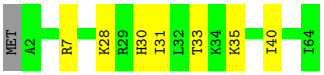




• Molecule 3: 50S ribosomal protein L35

Chain 2:





• Molecule 4: 50S ribosomal protein L36

Chain 3:

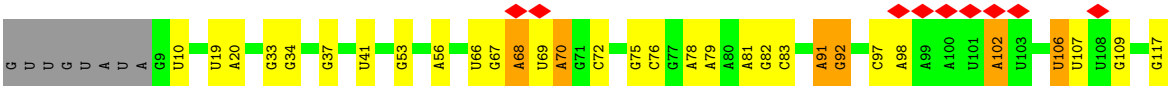


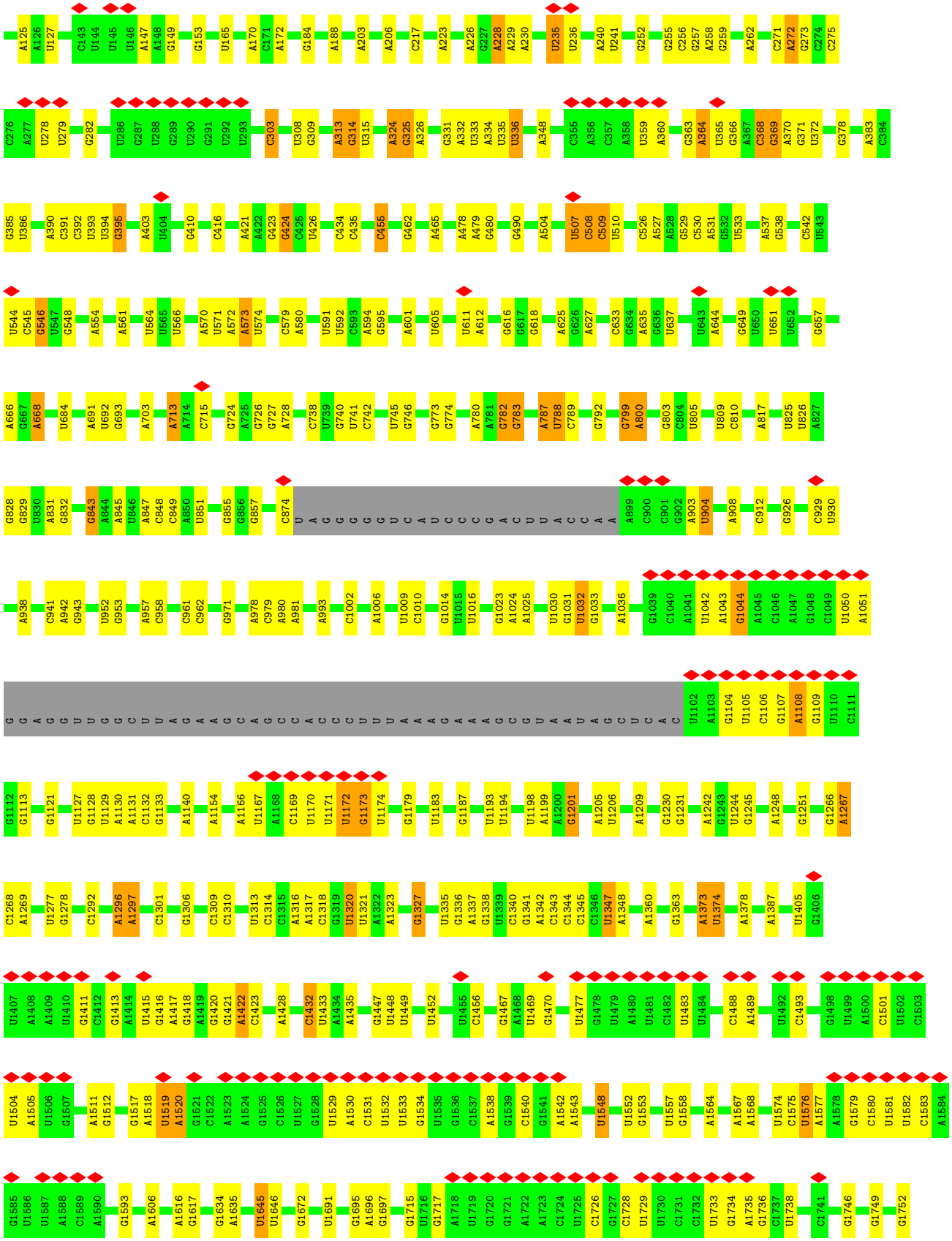


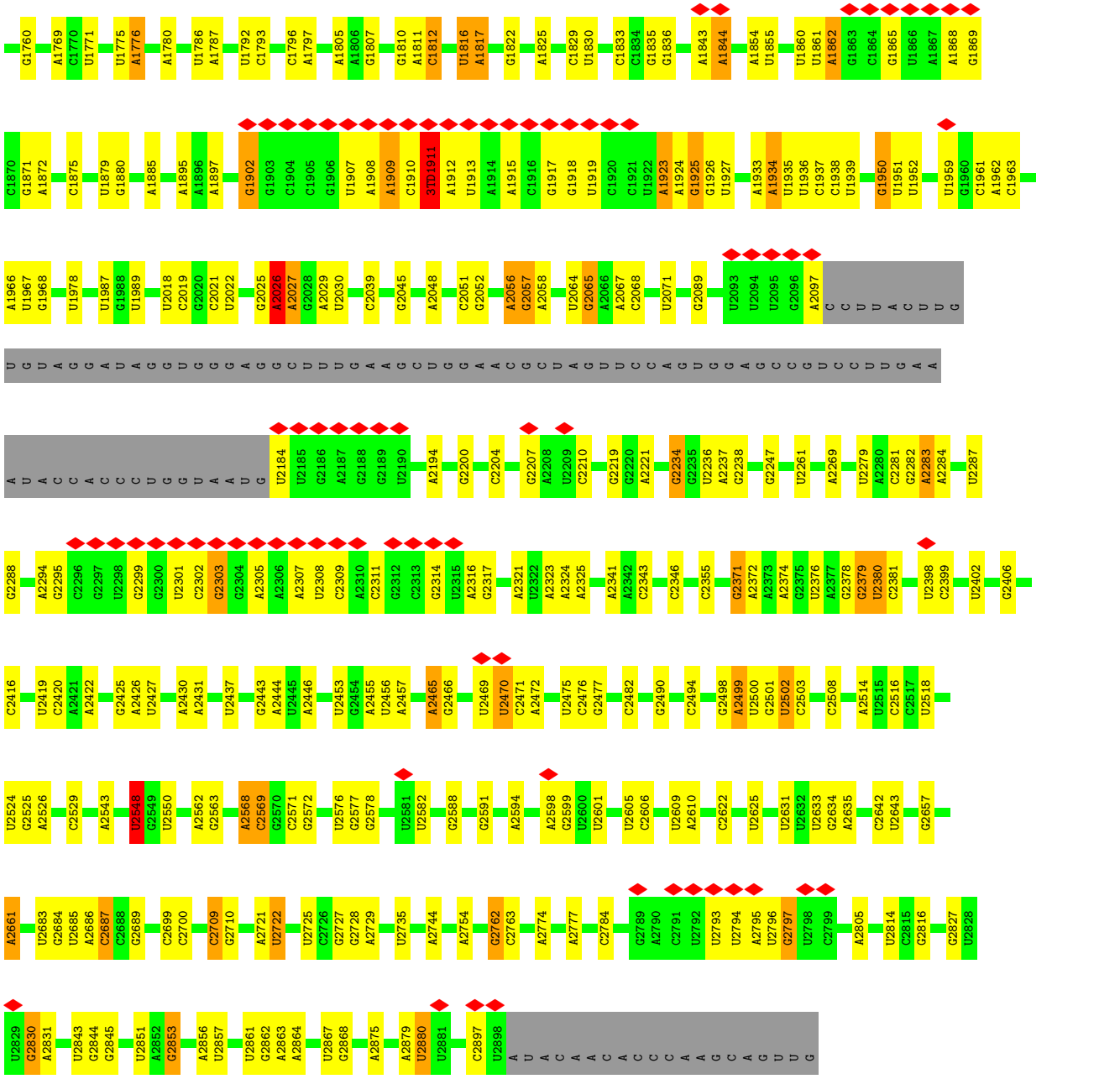
• Molecule 5: 23s ribosomal RNA

Chain A:





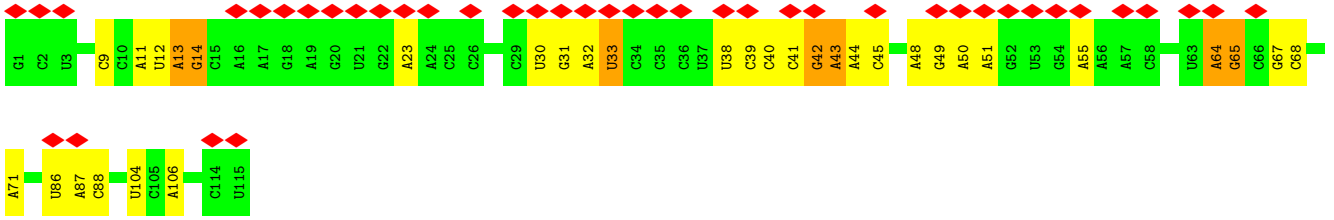




• Molecule 6: 5s ribosomal RNA

Chain B:

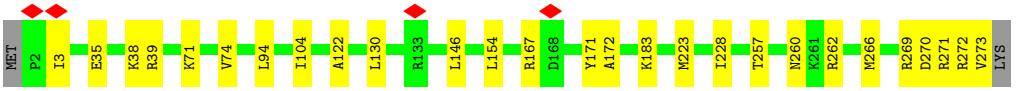




• Molecule 7: 50S ribosomal protein L2

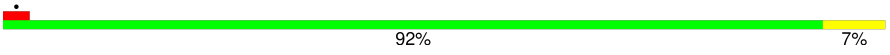
Chain C:

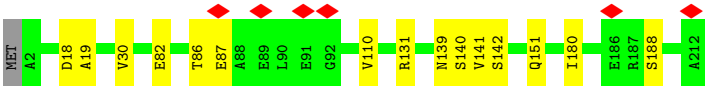




• Molecule 8: 50S ribosomal protein L3

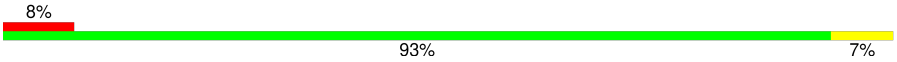
Chain D:

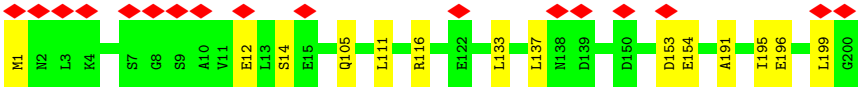




• Molecule 9: 50S ribosomal protein L4

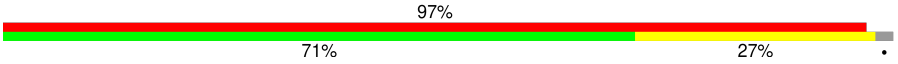
Chain E:

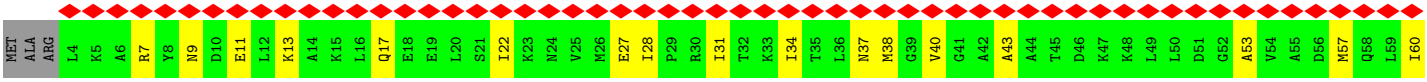


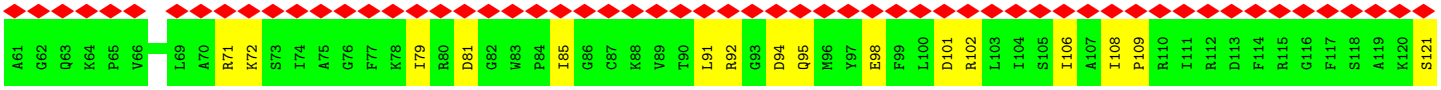


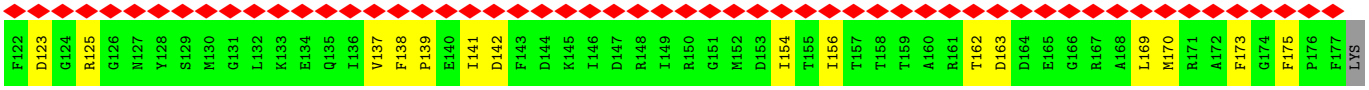
• Molecule 10: 50S ribosomal protein L5

Chain F:





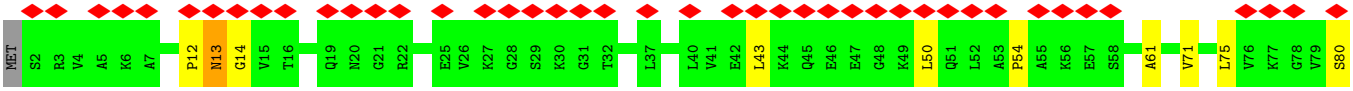


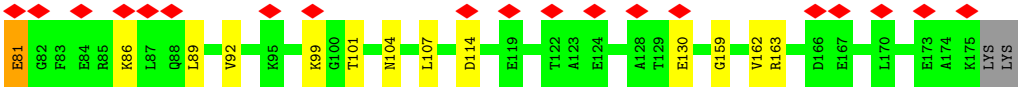


• Molecule 11: 50S ribosomal protein L6

Chain G:



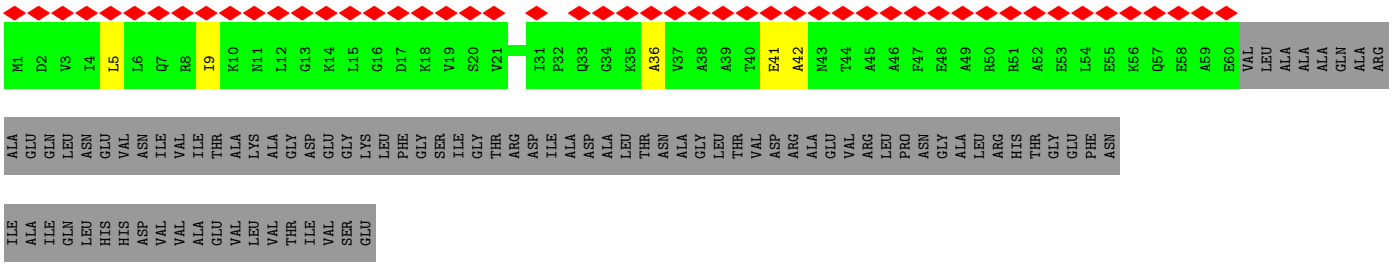




• Molecule 12: 50S ribosomal protein L9

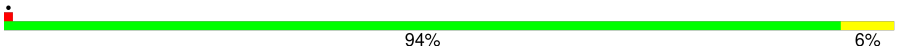
Chain H:

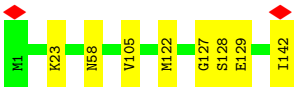




• Molecule 13: 50S ribosomal protein L13

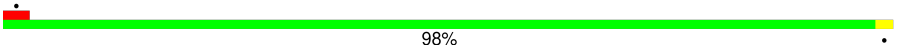
Chain I:

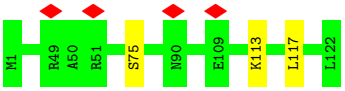




• Molecule 14: 50S ribosomal protein L14

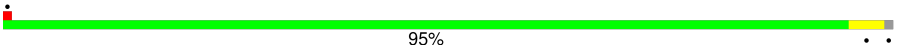
Chain J:

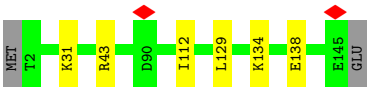




• Molecule 15: 50S ribosomal protein L15

Chain K:

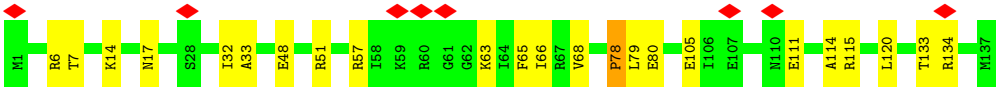




• Molecule 16: 50S ribosomal protein L16

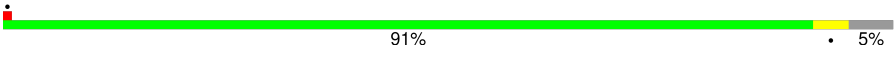
Chain L:

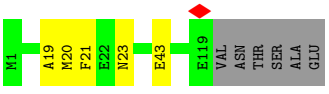




• Molecule 17: 50S ribosomal protein L17

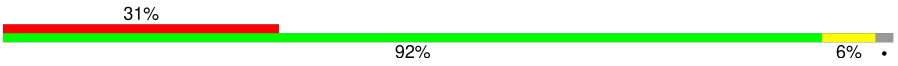
Chain M:

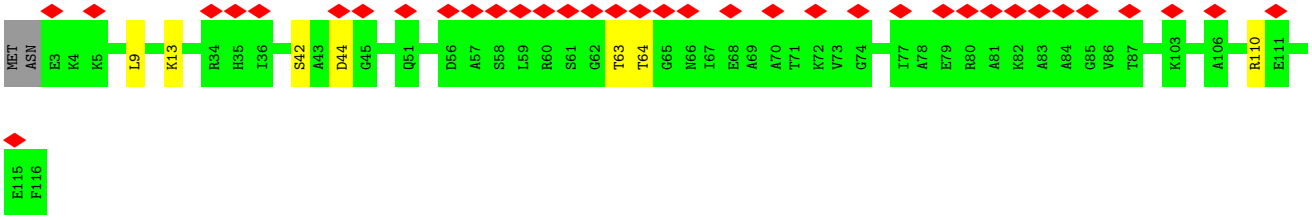




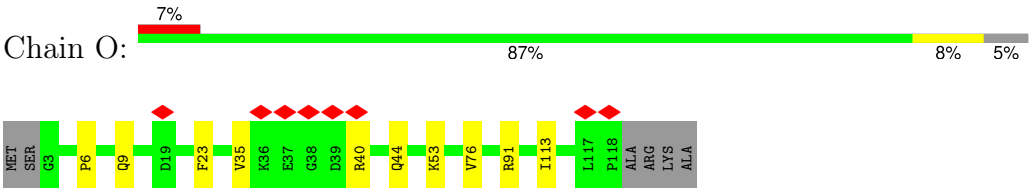
• Molecule 18: 50S ribosomal protein L18

Chain N:

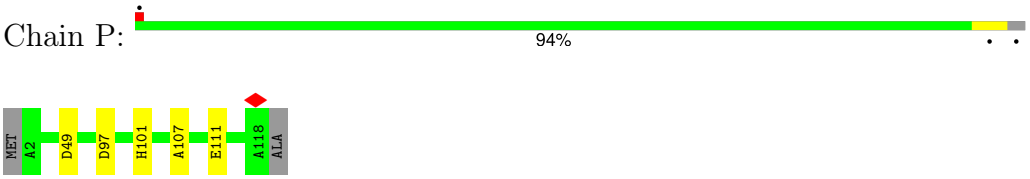




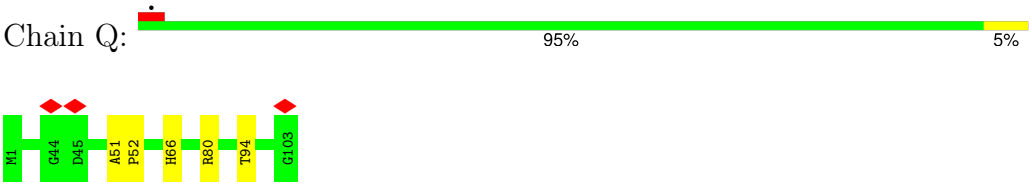
• Molecule 19: 50S ribosomal protein L19



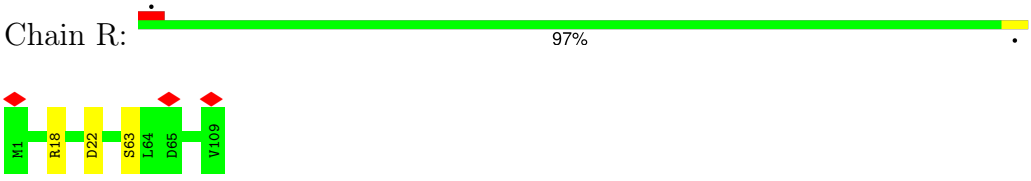
• Molecule 20: 50S ribosomal protein L20



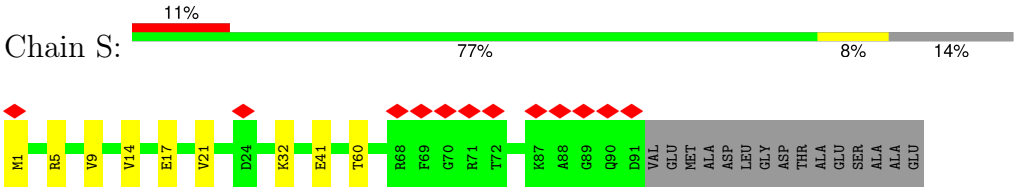
• Molecule 21: 50S ribosomal protein L21



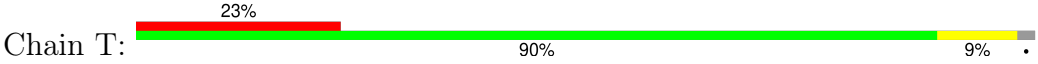
• Molecule 22: 50S ribosomal protein L22

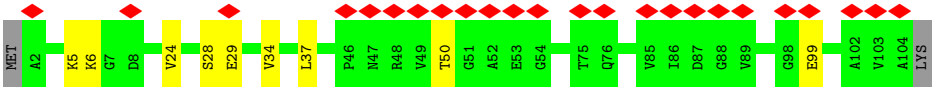


• Molecule 23: 50S ribosomal protein L23



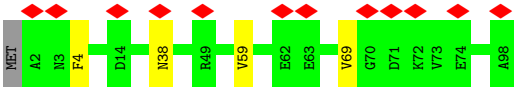
• Molecule 24: 50S ribosomal protein L24



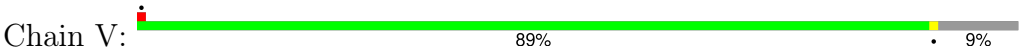


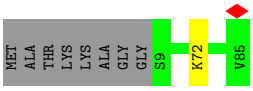
• Molecule 25: 50S ribosomal protein L25





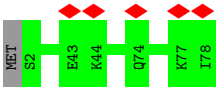
• Molecule 26: 50S ribosomal protein L27



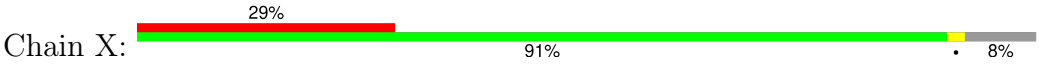


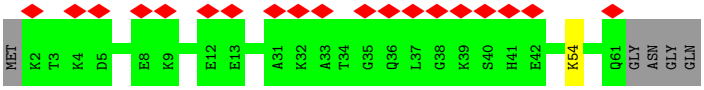
• Molecule 27: 50S ribosomal protein L28



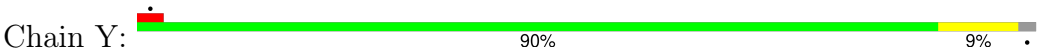


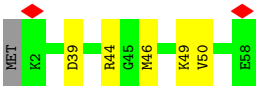
• Molecule 28: 50S ribosomal protein L29



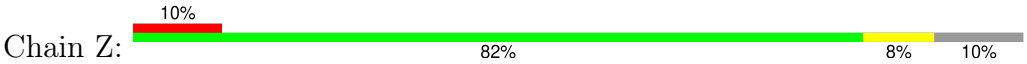


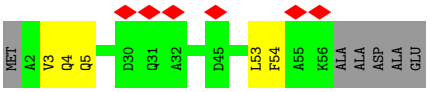
• Molecule 29: 50S ribosomal protein L30





• Molecule 30: 50S ribosomal protein L32

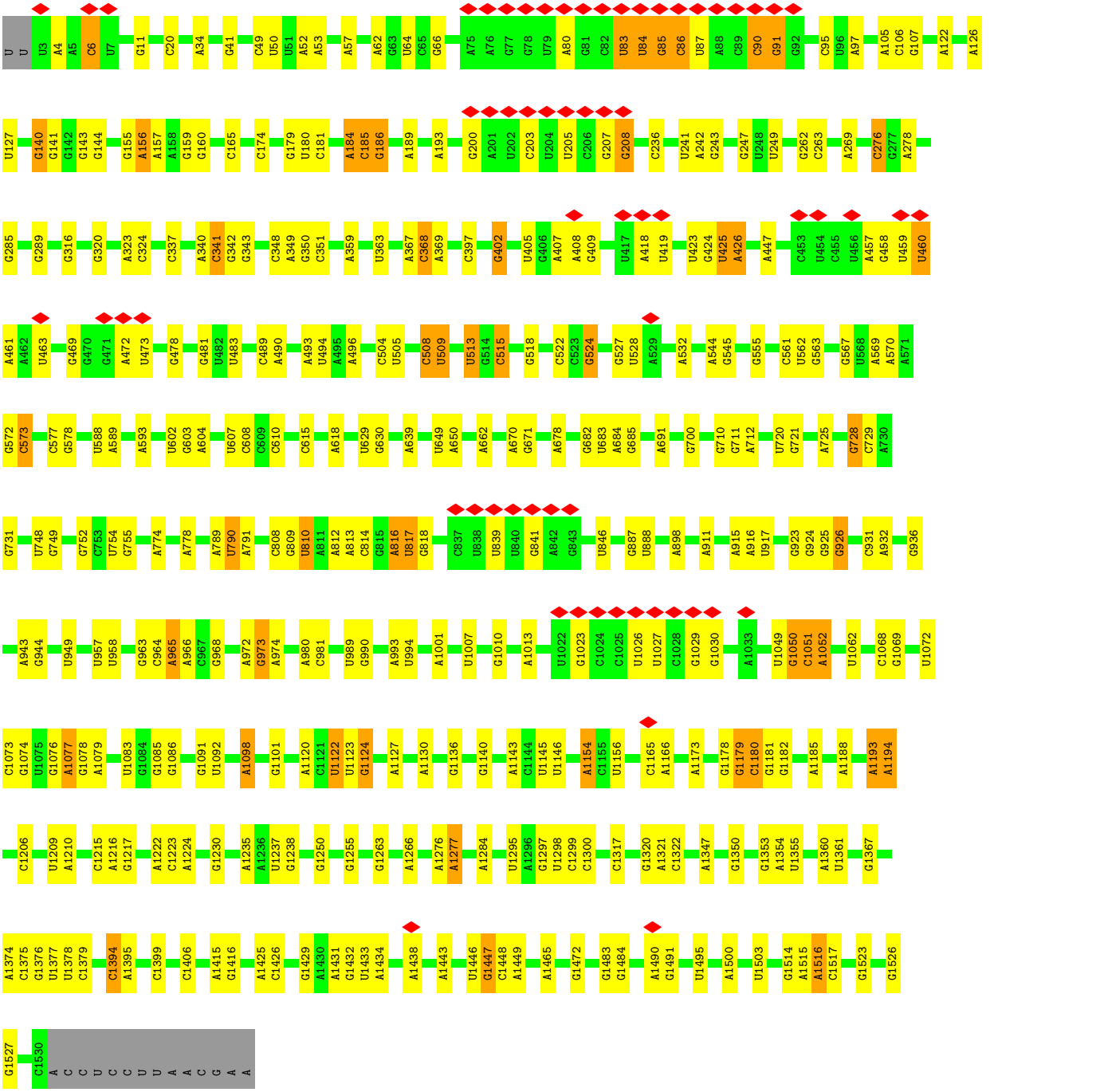




• Molecule 31: 16s Ribosomal RNA

Chain a:

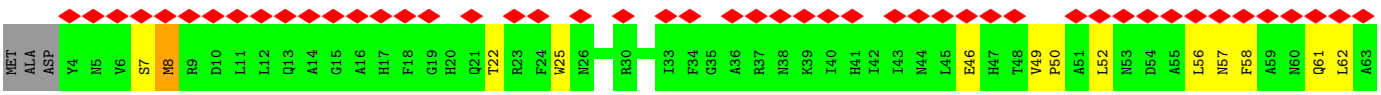


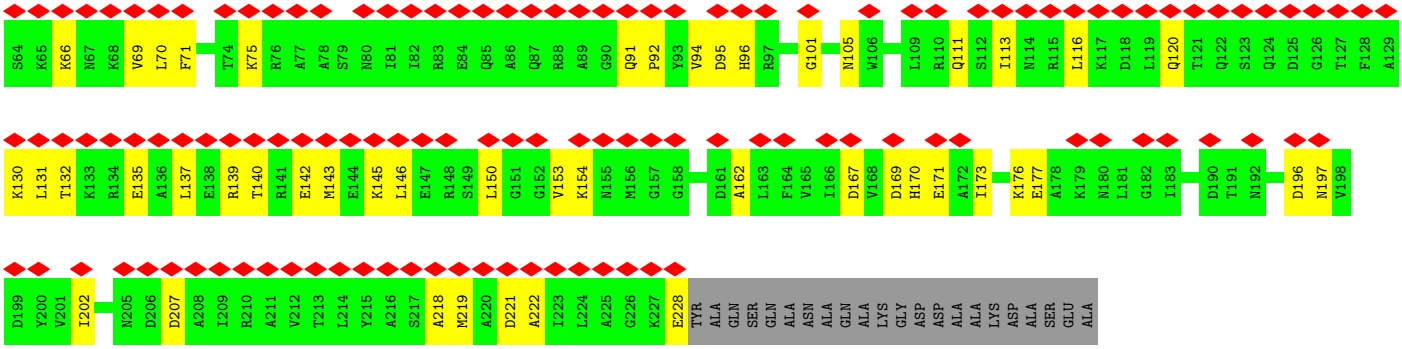


• Molecule 32: 30S ribosomal protein S2

Chain b:



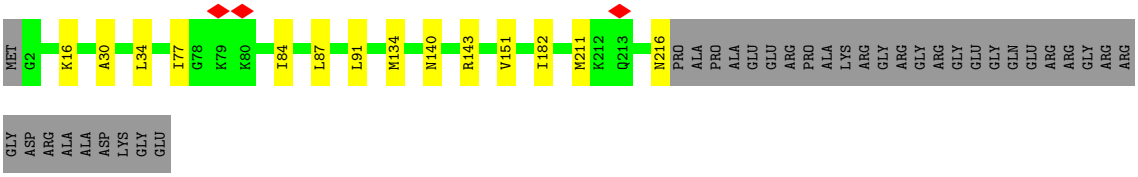




• Molecule 33: 30S ribosomal protein S3

Chain c:

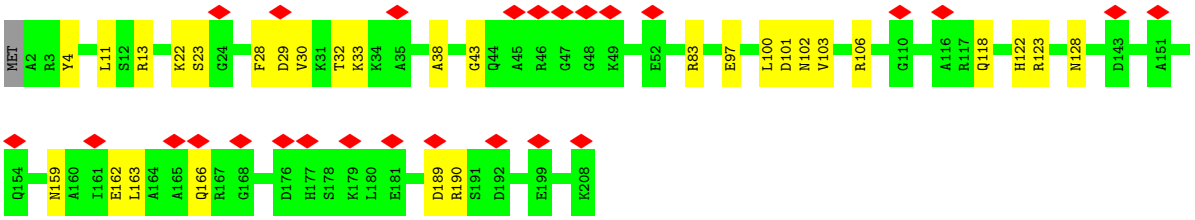




• Molecule 34: 30S ribosomal protein S4

Chain d:

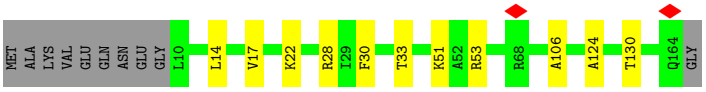




• Molecule 35: 30S ribosomal protein S5

Chain e:

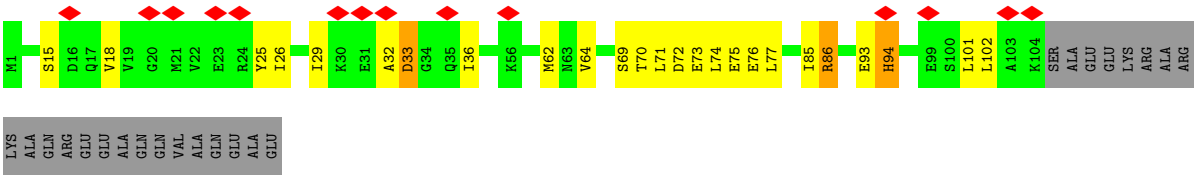




• Molecule 36: 30S ribosomal protein S6

Chain f:

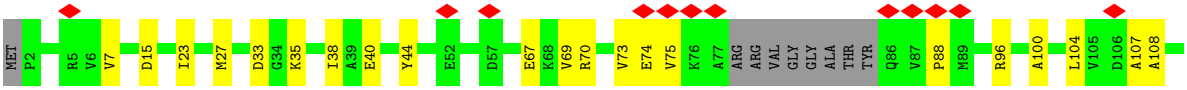


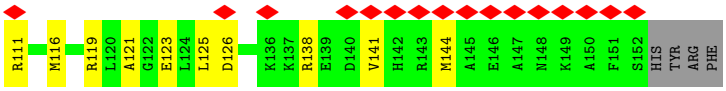


• Molecule 37: 30S ribosomal protein S7

Chain g:

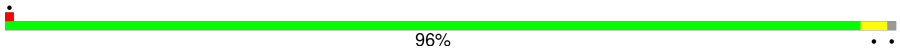


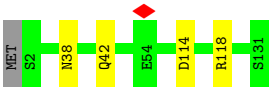




• Molecule 38: 30S ribosomal protein S8

Chain h:

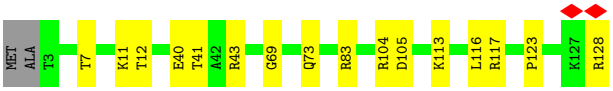




• Molecule 39: 30S ribosomal protein S9

Chain i:

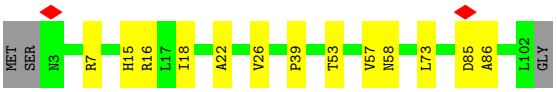




• Molecule 40: 30S ribosomal protein S10

Chain j:

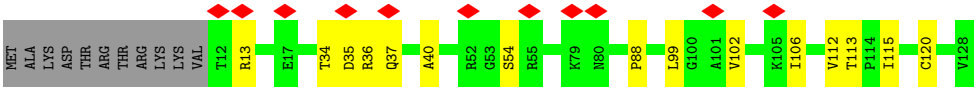




• Molecule 41: 30S ribosomal protein S11

Chain k:

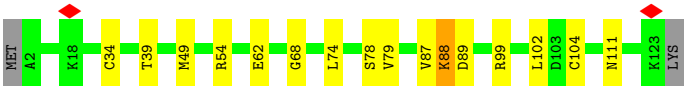




• Molecule 42: 30S ribosomal protein S12

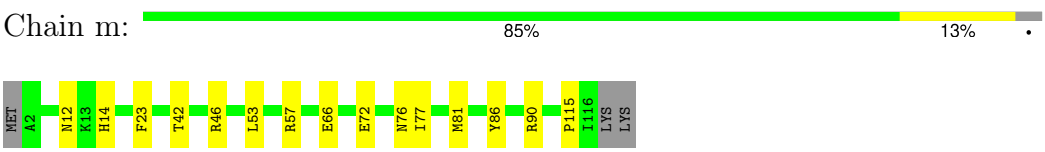
Chain l:





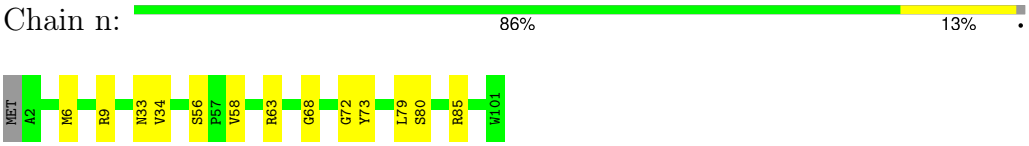
• Molecule 43: 30S ribosomal protein S13

Chain m:



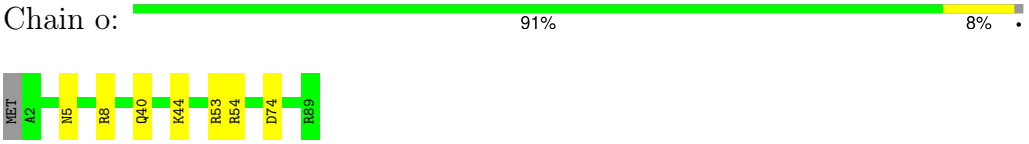
• Molecule 44: 30S ribosomal protein S14

Chain n:



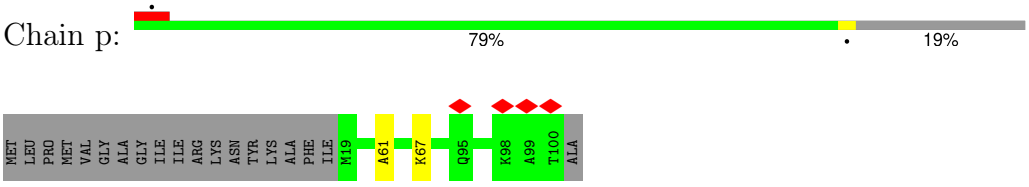
• Molecule 45: 30S ribosomal protein S15

Chain o:



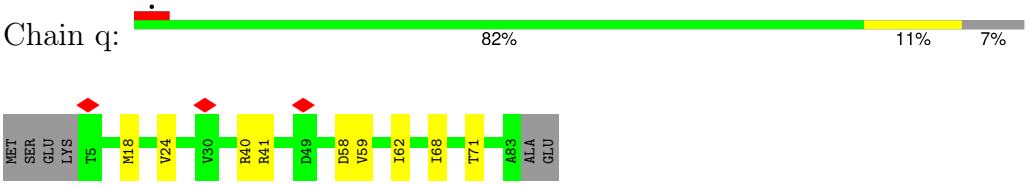
• Molecule 46: 30S ribosomal protein S16

Chain p:



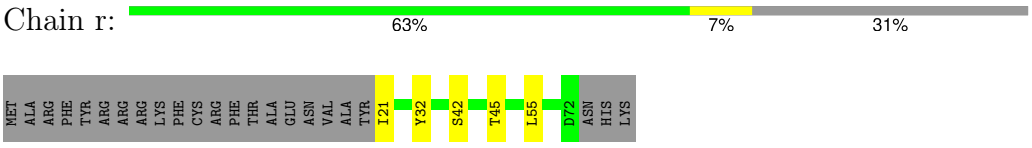
• Molecule 47: 30S ribosomal protein S17

Chain q:



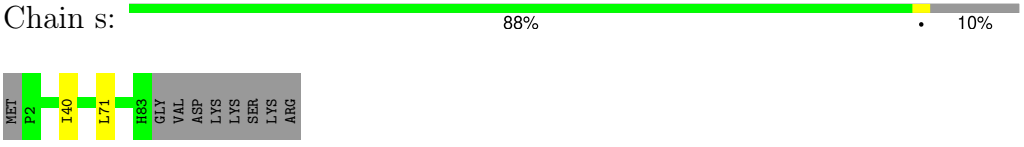
• Molecule 48: 30S ribosomal protein S18

Chain r:



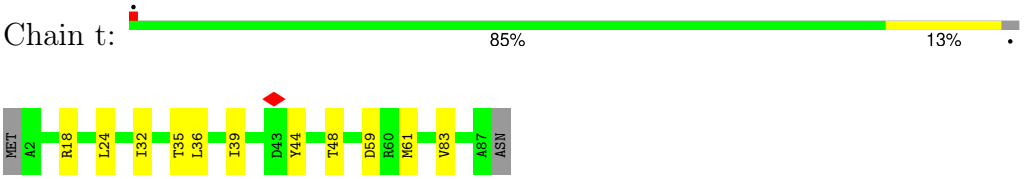
• Molecule 49: 30S ribosomal protein S19

Chain s:



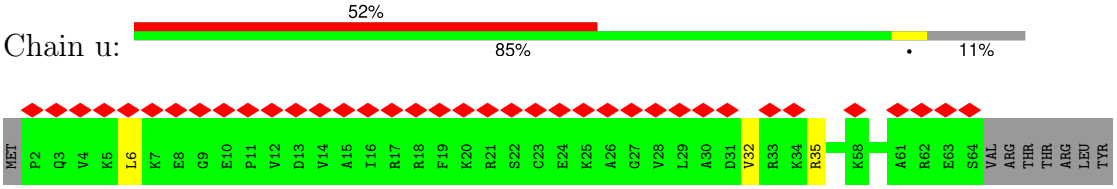
• Molecule 50: 30S ribosomal protein S20

Chain t:



• Molecule 51: 30S ribosomal protein S21

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79574	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 ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.918	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, 2MG, 4OC, PSU, 6MZ, OMU, 2MA, YQM, G7M, MA6, 5MU, 3TD, OMG, ZN, UR3

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	0	0.13	0/434	0.26	0/573
2	1	0.14	0/367	0.28	0/481
3	2	0.15	0/515	0.41	0/678
4	3	0.20	0/296	0.40	0/389
5	A	0.10	0/65229	0.26	0/101736
6	B	0.10	0/2739	0.28	0/4266
7	C	0.13	0/2152	0.35	0/2891
8	D	0.11	0/1590	0.28	0/2142
9	E	0.11	0/1537	0.28	0/2073
10	F	0.17	0/1390	0.45	0/1863
11	G	0.11	0/1337	0.30	0/1807
12	H	0.13	0/461	0.33	0/616
13	I	0.12	0/1151	0.28	0/1551
14	J	0.12	0/956	0.30	0/1286
15	K	0.10	0/1079	0.28	0/1439
16	L	0.13	0/1104	0.29	0/1475
17	M	0.14	0/956	0.33	0/1282
18	N	0.09	0/865	0.24	0/1156
19	O	0.12	0/925	0.32	0/1241
20	P	0.14	0/947	0.30	0/1262
21	Q	0.12	0/818	0.30	0/1094
22	R	0.13	0/831	0.26	0/1113
23	S	0.11	0/716	0.25	0/957
24	T	0.08	0/770	0.24	0/1034
25	U	0.11	0/770	0.29	0/1036
26	V	0.10	0/593	0.28	0/793
27	W	0.09	0/642	0.26	0/856
28	X	0.11	0/487	0.23	0/646
29	Y	0.10	0/460	0.25	0/614
30	Z	0.09	0/462	0.24	0/615
31	a	0.12	0/36476	0.27	0/56895
32	b	0.17	0/1799	0.39	0/2429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.13	0/1714	0.31	0/2304
34	d	0.12	0/1653	0.32	0/2213
35	e	0.13	0/1141	0.32	0/1537
36	f	0.14	0/882	0.38	0/1189
37	g	0.15	0/1142	0.33	0/1528
38	h	0.11	0/993	0.29	0/1331
39	i	0.19	0/1002	0.36	0/1339
40	j	0.14	0/811	0.33	0/1096
41	k	0.13	0/878	0.31	0/1189
42	l	0.14	0/958	0.40	0/1284
43	m	0.29	1/913 (0.1%)	0.55	3/1226 (0.2%)
44	n	0.15	0/803	0.34	0/1071
45	o	0.13	0/715	0.31	0/958
46	p	0.11	0/655	0.33	0/879
47	q	0.12	0/628	0.33	0/847
48	r	0.11	0/432	0.29	0/583
49	s	0.13	0/664	0.30	0/897
50	t	0.16	0/669	0.28	0/892
51	u	0.10	0/528	0.23	0/697
All	All	0.11	1/148035 (0.0%)	0.28	3/221349 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	m	115	PRO	CG-CD	-6.81	1.27	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	m	115	PRO	N-CD-CG	-9.97	88.24	103.20
43	m	115	PRO	CA-N-CD	-7.31	101.77	112.00
43	m	115	PRO	CA-CB-CG	-5.22	94.58	104.50

There are no chirality outliers.

There are no planarity outliers.

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	0	427	0	462	2	0
2	1	363	0	401	1	0
3	2	509	0	566	6	0
4	3	295	0	326	4	0
5	A	58566	0	29451	223	0
6	B	2450	0	1241	16	0
7	C	2111	0	2176	19	0
8	D	1572	0	1610	11	0
9	E	1516	0	1569	9	0
10	F	1370	0	1420	44	0
11	G	1318	0	1373	15	0
12	H	458	0	480	4	0
13	I	1125	0	1148	4	0
14	J	946	0	1007	2	0
15	K	1071	0	1140	3	0
16	L	1087	0	1162	13	0
17	M	942	0	987	3	0
18	N	857	0	899	4	0
19	O	913	0	968	6	0
20	P	934	0	997	3	0
21	Q	807	0	842	5	0
22	R	826	0	894	2	0
23	S	710	0	768	5	0
24	T	766	0	816	7	0
25	U	760	0	783	4	0
26	V	585	0	589	1	0
27	W	632	0	667	0	0
28	X	486	0	528	1	0
29	Y	455	0	476	3	0
30	Z	456	0	448	3	0
31	a	32782	0	16507	135	0
32	b	1769	0	1787	43	0
33	c	1690	0	1774	8	0
34	d	1631	0	1691	19	0
35	e	1129	0	1174	7	0
36	f	867	0	868	21	0
37	g	1127	0	1176	27	0
38	h	985	0	1047	2	0
39	i	991	0	1048	11	0
40	j	801	0	832	10	0
41	k	862	0	877	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	945	0	998	12	0
43	m	903	0	962	7	0
44	n	792	0	833	7	0
45	o	705	0	712	5	0
46	p	644	0	655	1	0
47	q	621	0	665	7	0
48	r	426	0	447	3	0
49	s	646	0	663	1	0
50	t	663	0	715	7	0
51	u	522	0	565	5	0
52	3	1	0	0	0	0
53	A	80	0	0	0	0
53	a	40	0	0	0	0
54	A	136	0	0	0	0
54	B	1	0	0	0	0
54	D	1	0	0	0	0
54	K	1	0	0	0	0
54	a	52	0	0	0	0
55	2	2	0	0	0	0
55	A	597	0	0	25	0
55	B	4	0	0	0	0
55	C	7	0	0	0	0
55	D	4	0	0	0	0
55	E	3	0	0	0	0
55	K	7	0	0	0	0
55	R	1	0	0	0	0
55	U	1	0	0	0	0
55	Z	2	0	0	1	0
55	a	156	0	0	12	0
55	i	2	0	0	0	0
55	j	3	0	0	0	0
55	k	1	0	0	0	0
55	m	1	0	0	0	0
55	n	3	0	0	0	0
55	q	1	0	0	0	0
55	s	1	0	0	0	0
55	t	1	0	0	0	0
All	All	137923	0	92190	706	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 3.

The worst 5 of 706 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)
31:a:85:G:O2'	31:a:86:C:OP2	1.76	1.01
10:F:17:GLN:NE2	10:F:22:ILE:O	1.95	0.99
31:a:789:A:O2'	31:a:790:U:OP2	1.81	0.99
10:F:7:ARG:NH2	10:F:11:GLU:OE1	1.99	0.95
31:a:1490:A:O2'	31:a:1491:G:N7	2.03	0.91

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	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	C	270/274 (98%)	263 (97%)	6 (2%)	1 (0%)	30	39
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	152 (88%)	20 (12%)	0	100	100
11	G	172/177 (97%)	163 (95%)	7 (4%)	2 (1%)	10	13
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
15	K	142/146 (97%)	137 (96%)	4 (3%)	1 (1%)	18	25
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18	25
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	112/116 (97%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	210 (94%)	12 (5%)	1 (0%)	30	39
33	c	213/250 (85%)	206 (97%)	7 (3%)	0	100	100
34	d	205/208 (99%)	198 (97%)	6 (3%)	1 (0%)	24	34
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	102/127 (80%)	94 (92%)	5 (5%)	3 (3%)	3	3
37	g	139/156 (89%)	138 (99%)	1 (1%)	0	100	100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	110 (92%)	9 (8%)	1 (1%)	16	22
43	m	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
44	n	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	u	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
All	All	5420/5872 (92%)	5256 (97%)	153 (3%)	11 (0%)	44	56

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	G	81	GLU
32	b	8	MET
36	f	33	ASP
42	l	88	LYS
11	G	13	ASN

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	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	218 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	144 (100%)	0	100	100
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	77 (100%)	0	100	100
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	184 (100%)	1 (0%)	81	88
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	94 (100%)	0	100	100
37	g	118/128 (92%)	118 (100%)	0	100	100
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	99 (100%)	0	100	100
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	71 (100%)	0	100	100
48	r	46/66 (70%)	46 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	54/62 (87%)	54 (100%)	0	100	100
All	All	4489/4756 (94%)	4488 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	b	111	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
27	W	16	ASN
49	s	56	ASN
32	b	170	HIS
37	g	21	GLN
32	b	85	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	222 (14%)	0
5	A	2726/2918 (93%)	457 (16%)	30 (1%)
6	B	114/115 (99%)	18 (15%)	2 (1%)
All	All	4367/4577 (95%)	697 (15%)	32 (0%)

5 of 697 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	20	A
5	A	41	U
5	A	53	G
5	A	56	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	2419	U

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Mol	Chain	Res	Type
5	A	2568	A
5	A	782	G
5	A	507	U
6	B	13	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PSU	A	2453	5	18,21,22	1.16	1 (5%)	21,30,33	1.98	6 (28%)
5	PSU	A	952	5	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
31	G7M	a	524	31	23,26,27	1.88	2 (8%)	34,39,42	1.05	1 (2%)
31	MA6	a	1516	31	23,26,27	1.37	4 (17%)	33,38,41	3.24	12 (36%)
5	2MG	A	2441	5	23,26,27	0.45	0	33,38,41	0.49	0
31	2MG	a	963	54,31	23,26,27	0.45	0	33,38,41	0.52	0
5	G7M	A	2065	5	23,26,27	1.89	2 (8%)	34,39,42	1.08	1 (2%)
5	OMU	A	2548	5	19,22,23	3.13	8 (42%)	25,31,34	1.79	5 (20%)
31	2MG	a	1204	31	23,26,27	0.47	0	33,38,41	0.51	0
31	5MC	a	964	31	19,22,23	0.52	0	26,32,35	0.57	0
5	5MU	A	1935	5	19,22,23	0.39	0	27,32,35	0.48	0
5	PSU	A	2576	5	18,21,22	1.14	1 (5%)	21,30,33	1.95	6 (28%)
5	OMG	A	2247	5	23,26,27	0.44	0	32,38,41	0.51	0
31	UR3	a	1495	31	19,22,23	2.97	6 (31%)	26,32,35	1.64	4 (15%)
5	PSU	A	1913	5	18,21,22	1.16	1 (5%)	21,30,33	1.90	5 (23%)
31	MA6	a	1515	31	23,26,27	1.38	4 (17%)	33,38,41	3.21	12 (36%)
31	4OC	a	1399	31	20,23,24	3.21	8 (40%)	25,32,35	0.88	1 (4%)
5	2MA	A	2499	5,54	22,25,26	3.99	9 (40%)	32,37,40	2.75	11 (34%)
5	PSU	A	2601	5	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)
31	PSU	a	513	31	18,21,22	1.14	1 (5%)	21,30,33	1.94	6 (28%)
5	PSU	A	1907	5	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	3TD	A	1911	5	19,22,23	4.47	6 (31%)	23,32,35	1.79	3 (13%)
5	PSU	A	2500	5	18,21,22	1.12	1 (5%)	21,30,33	1.97	5 (23%)
5	6MZ	A	2026	5	22,25,26	2.48	4 (18%)	29,36,39	3.32	10 (34%)

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
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	G7M	a	524	31	-	2/7/25/26	0/3/3/3
31	MA6	a	1516	31	-	2/11/29/30	0/3/3/3
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
31	2MG	a	963	54,31	-	2/9/27/28	0/3/3/3
5	G7M	A	2065	5	-	1/7/25/26	0/3/3/3
5	OMU	A	2548	5	-	1/9/27/28	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	0/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	2/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	2MA	A	2499	5,54	-	6/7/25/26	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	2/7/25/26	0/2/2/2
5	PSU	A	1907	5	-	2/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	0/9/27/28	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.46	1.50	1.35
5	A	2499	2MA	C4-N3	12.17	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C2-N1	10.77	1.50	1.37
5	A	2026	6MZ	C6-N6	10.22	1.45	1.34
5	A	2065	G7M	C8-N7	7.54	1.45	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-11.72	102.58	116.86
31	a	1515	MA6	N1-C6-N6	-11.56	102.77	116.86
5	A	2026	6MZ	C1'-N9-C8	8.52	146.00	127.09
5	A	2026	6MZ	C4-N9-C1'	-8.52	106.72	126.63
31	a	1516	MA6	C5-C6-N6	7.85	137.76	125.33

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	963	2MG	O4'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
31	a	513	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2548	OMU	1	0
31	a	964	5MC	2	0
5	A	1935	5MU	1	0
5	A	2247	OMG	1	0
5	A	1911	3TD	1	0
5	A	2026	6MZ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 195 ligands modelled in this entry, 192 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	YQM	A	3201	54	43,44,44	3.68	23 (53%)	53,69,69	2.81	23 (43%)
53	YQM	A	3202	54	43,44,44	3.73	21 (48%)	53,69,69	2.79	23 (43%)
53	YQM	a	1601	54	43,44,44	3.60	21 (48%)	53,69,69	2.76	22 (41%)

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
53	YQM	A	3201	54	-	0/16/81/81	0/5/5/5
53	YQM	A	3202	54	-	5/16/81/81	0/5/5/5
53	YQM	a	1601	54	-	4/16/81/81	0/5/5/5

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3201	YQM	C19-C20	14.24	1.64	1.52
53	A	3202	YQM	C19-C20	14.18	1.64	1.52
53	a	1601	YQM	C19-C20	14.07	1.64	1.52
53	A	3202	YQM	C19-C17	8.53	1.66	1.55
53	a	1601	YQM	C19-C17	8.35	1.66	1.55

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	3201	YQM	C34-N35-C39	-7.64	103.44	113.34
53	A	3202	YQM	C34-C32-N31	7.45	128.01	114.23
53	a	1601	YQM	C34-C32-N31	6.92	127.05	114.23
53	a	1601	YQM	C34-N35-C39	-6.69	104.67	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	3201	YQM	C34-C32-N31	6.68	126.60	114.23

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

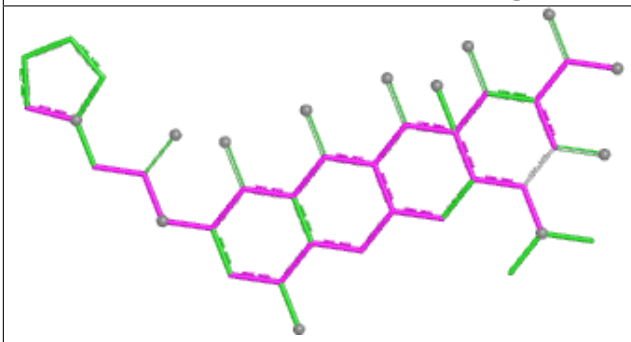
Mol	Chain	Res	Type	Atoms
53	A	3202	YQM	C22-C21-C24-N26
53	a	1601	YQM	C20-C21-C24-N26
53	a	1601	YQM	C20-C21-C24-O25
53	a	1601	YQM	C22-C21-C24-N26
53	a	1601	YQM	C22-C21-C24-O25

There are no ring outliers.

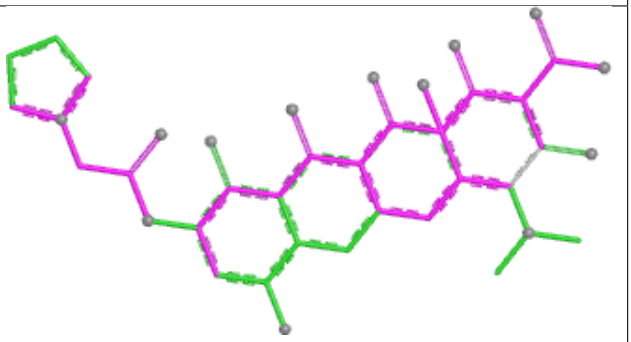
No monomer is involved in short contacts.

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

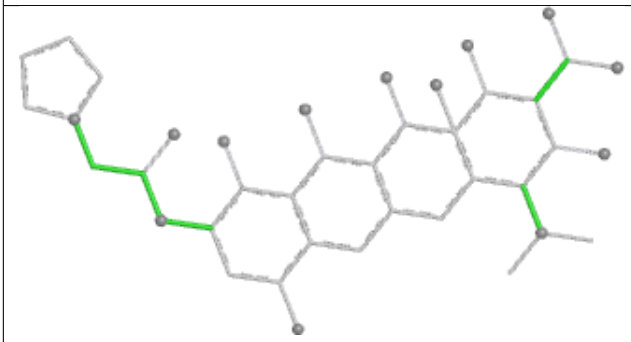
Ligand YQM A 3201



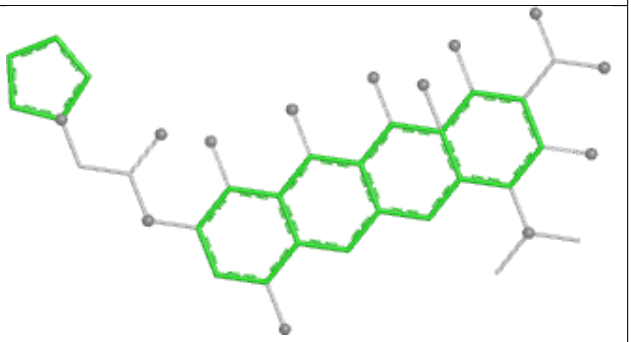
Bond lengths



Bond angles

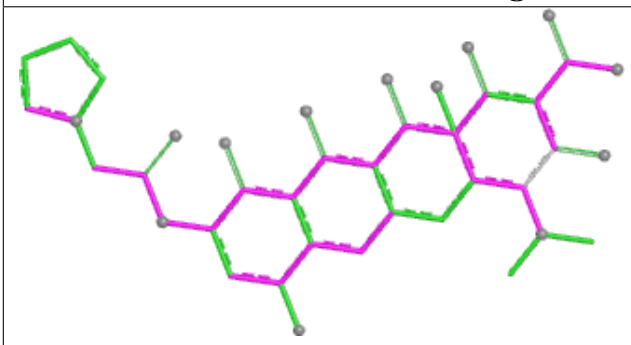


Torsions

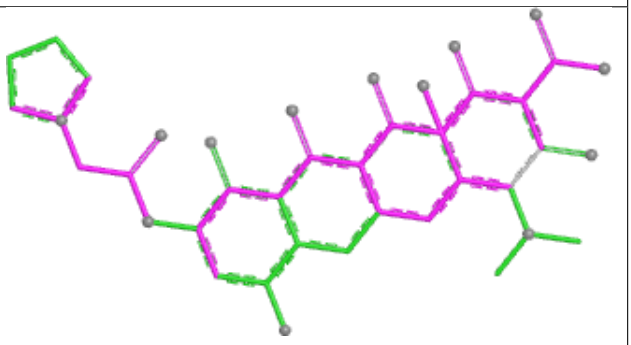


Rings

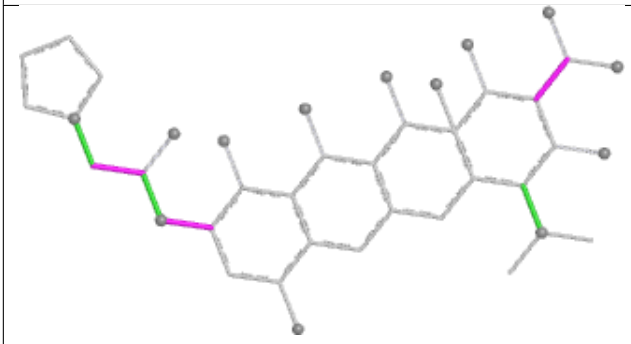
Ligand YQM A 3202



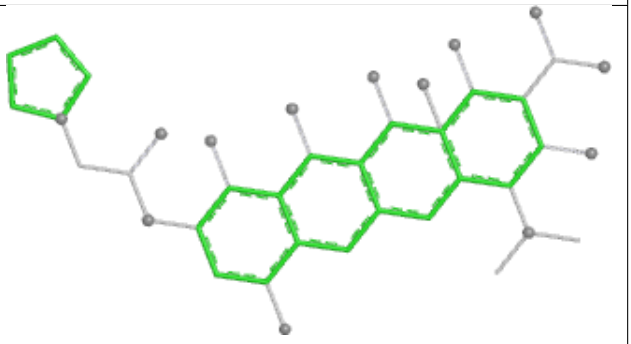
Bond lengths



Bond angles

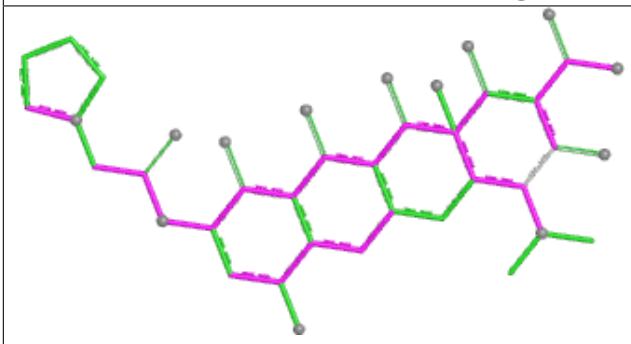


Torsions

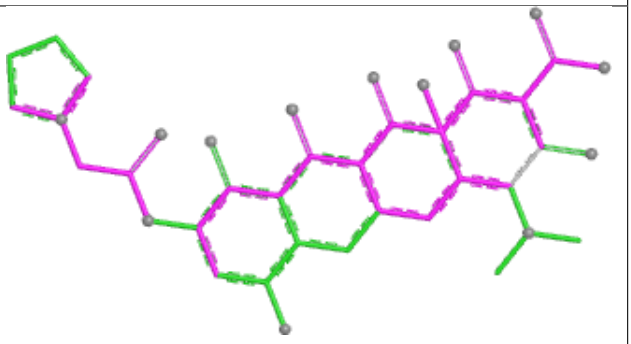


Rings

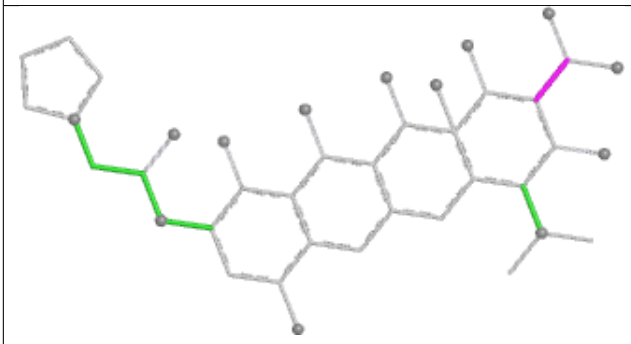
Ligand YQM a 1601



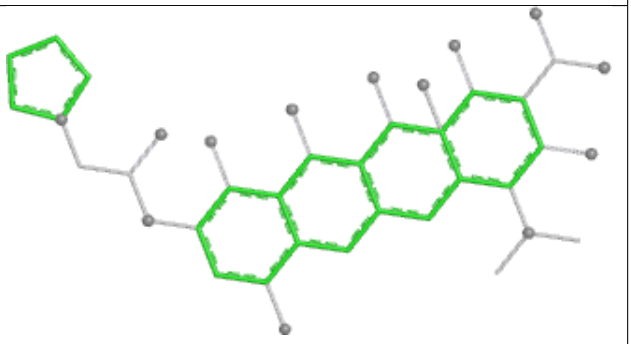
Bond lengths



Bond angles



Torsions



Rings

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.

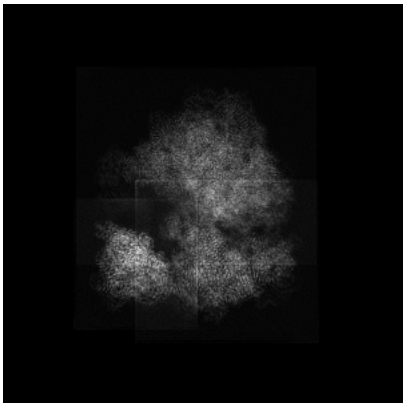
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23668. These allow visual inspection of the internal detail of the map and identification of artifacts.

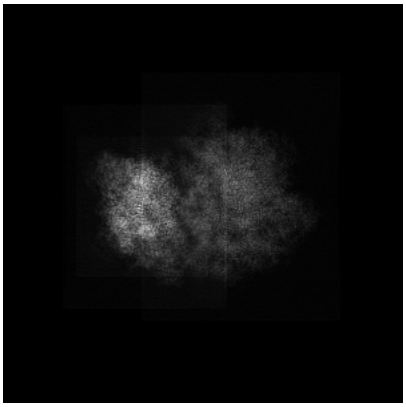
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

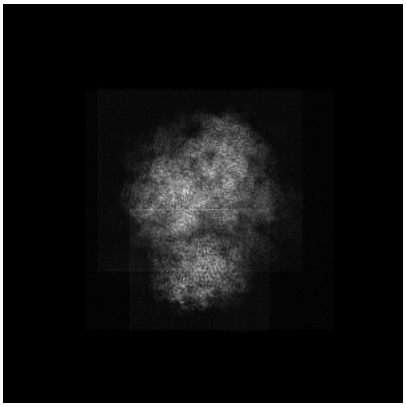
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

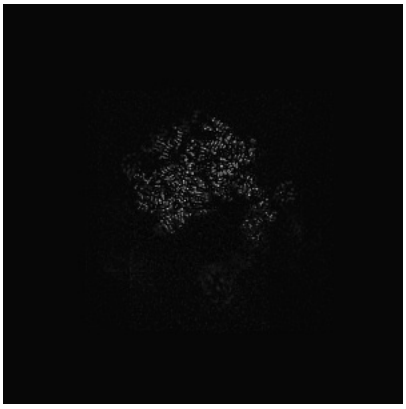
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

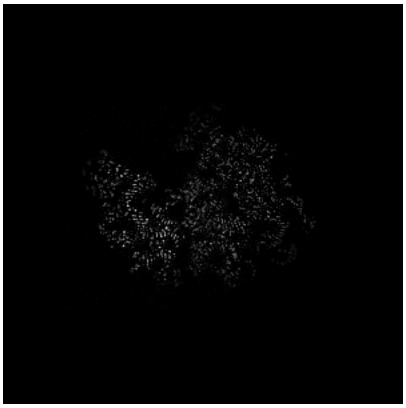
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

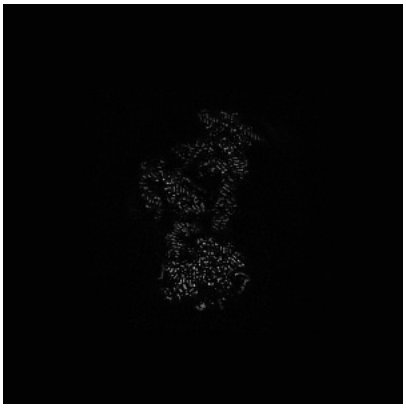
6.3.1 Primary map



X Index: 231



Y Index: 271

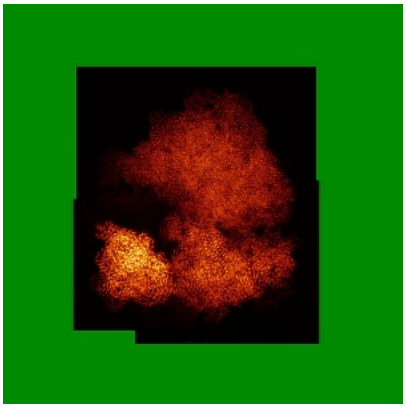


Z Index: 178

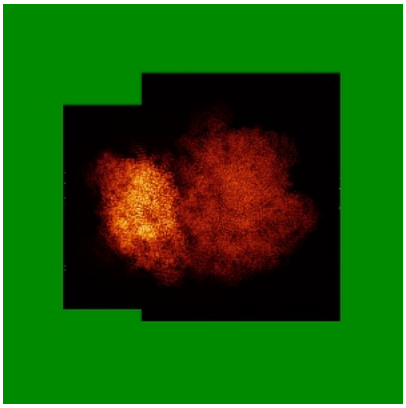
The images above show the largest variance slices of the map in three orthogonal directions.

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

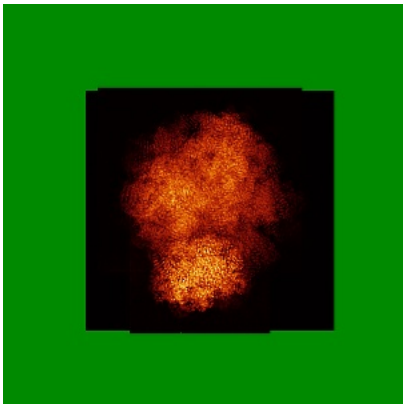
6.4.1 Primary map



X



Y

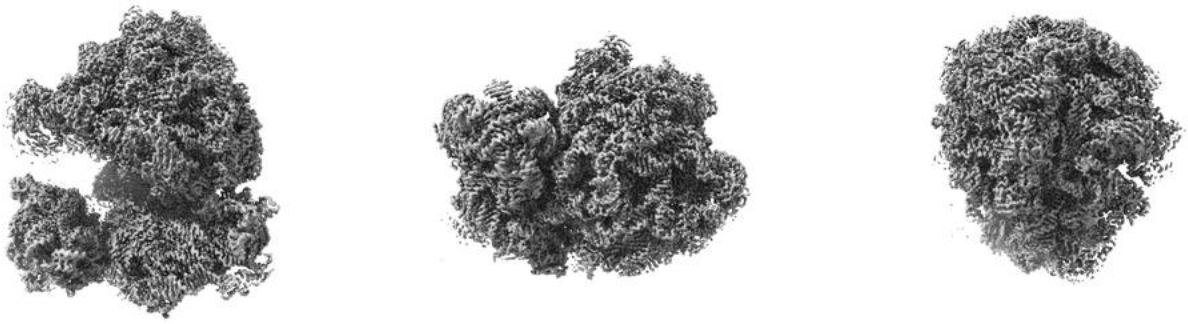


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

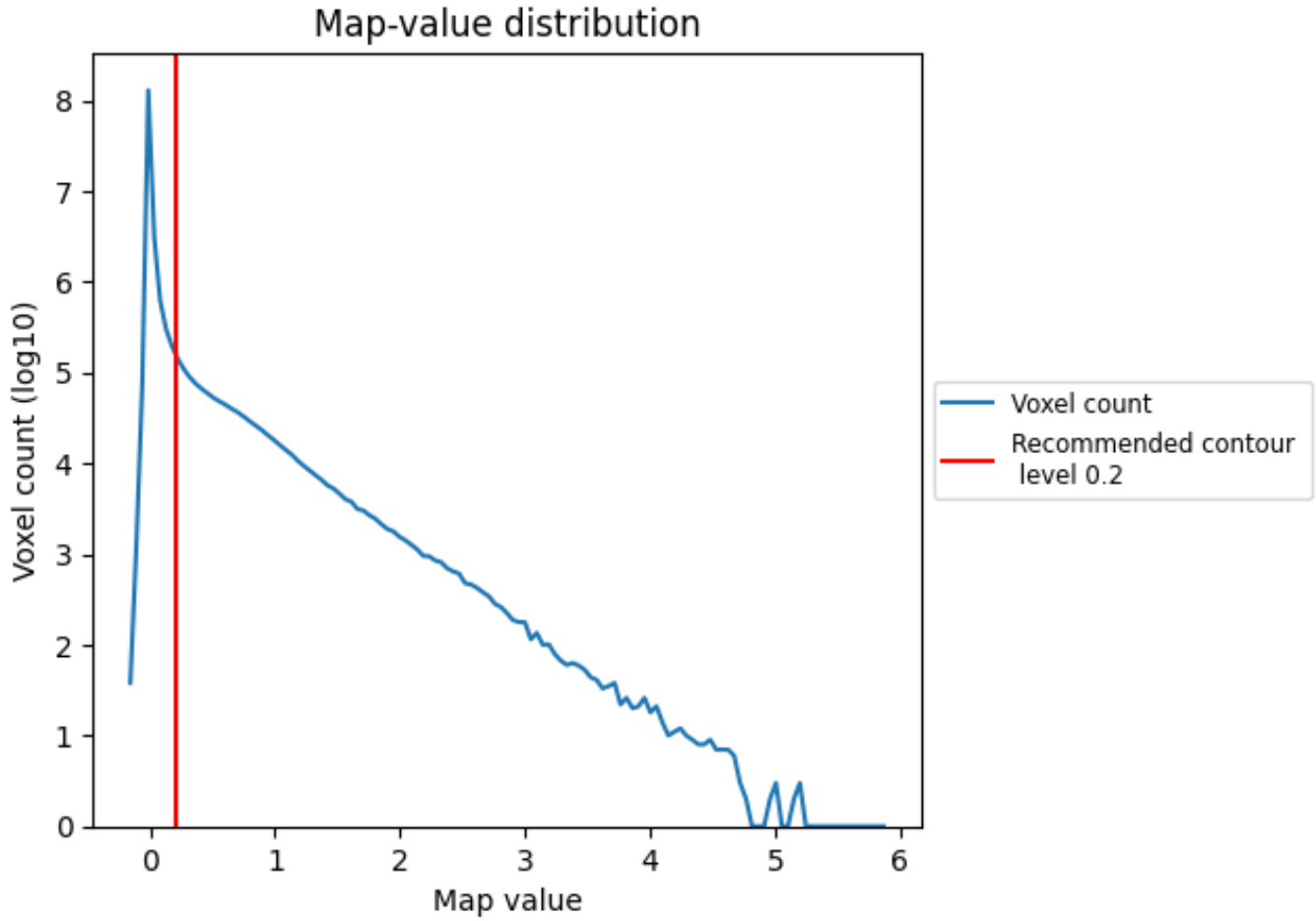
6.6 Mask visualisation (i)

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

7 Map analysis

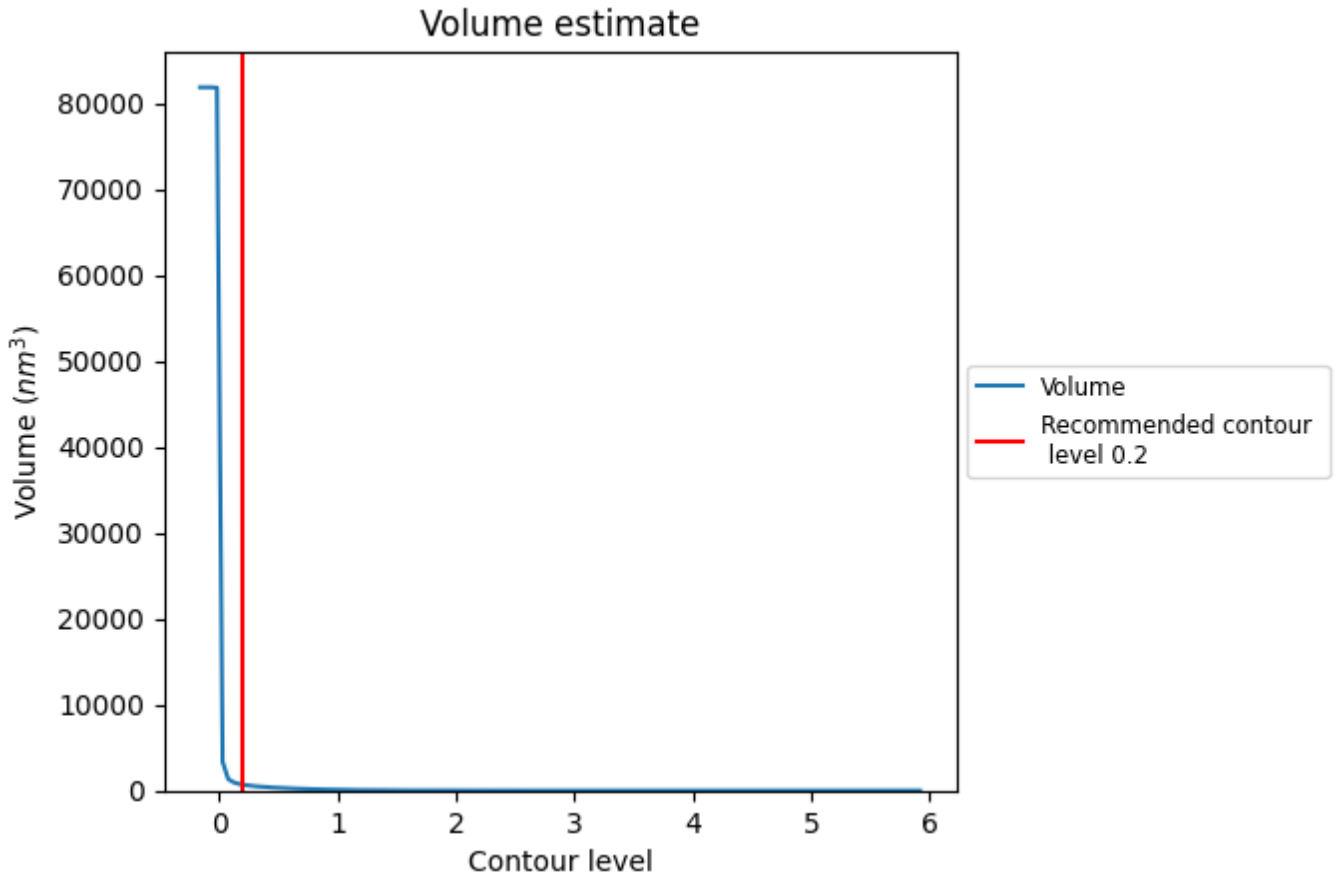
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

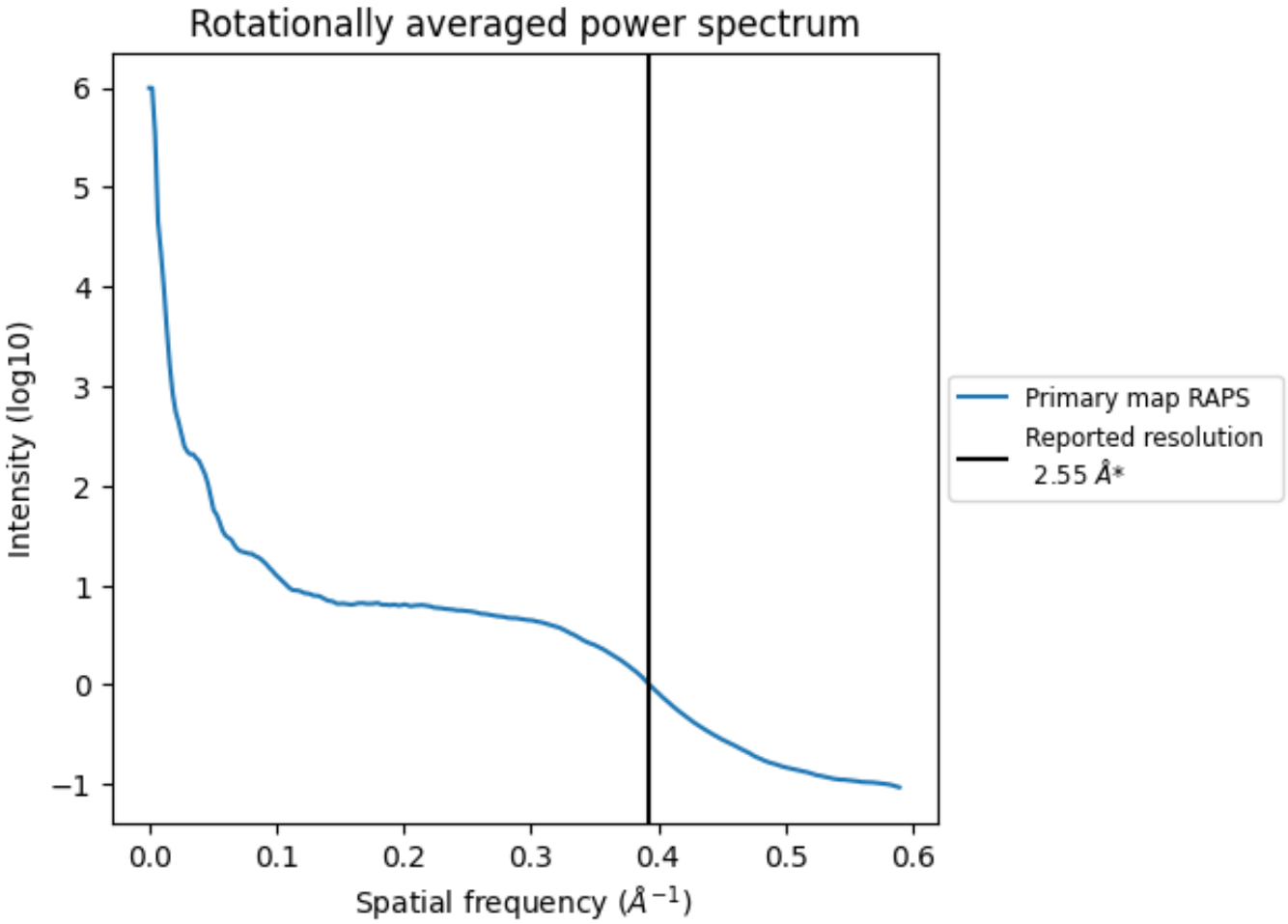
7.2 Volume estimate (i)



The volume at the recommended contour level is 696 nm^3; this corresponds to an approximate mass of 629 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 0.392 Å^{-1}

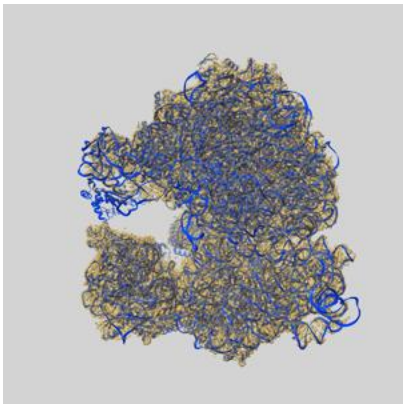
8 Fourier-Shell correlation

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

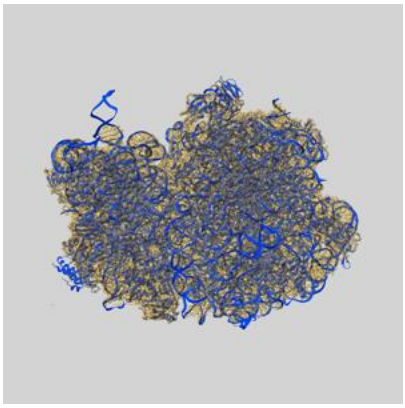
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23668 and PDB model 7M4W. Per-residue inclusion information can be found in section 3 on page 15.

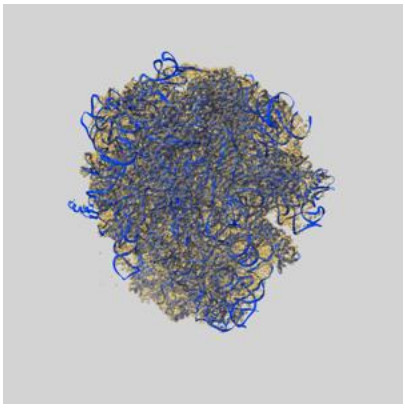
9.1 Map-model overlay



X



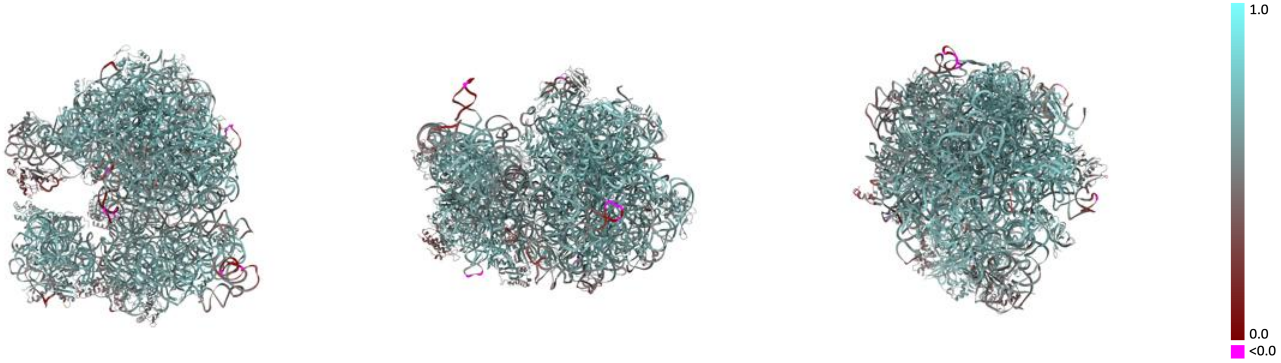
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

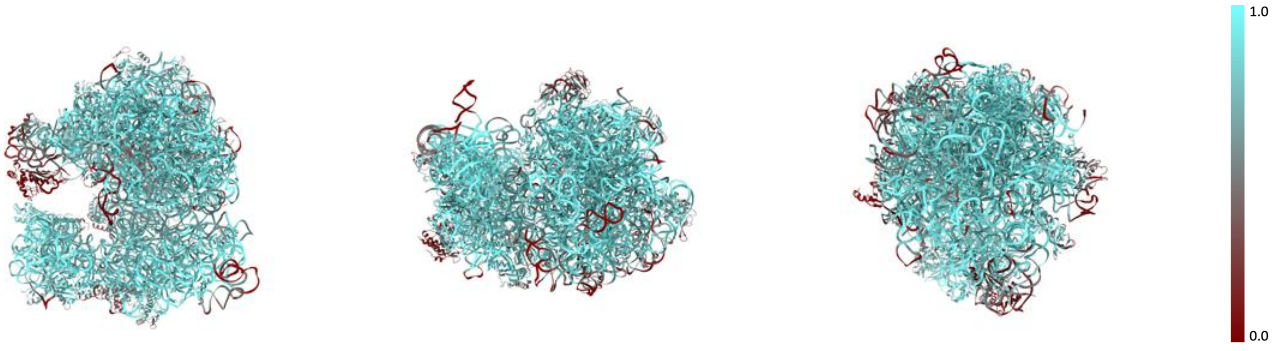
9.2 Q-score mapped to coordinate model



X Y Z

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

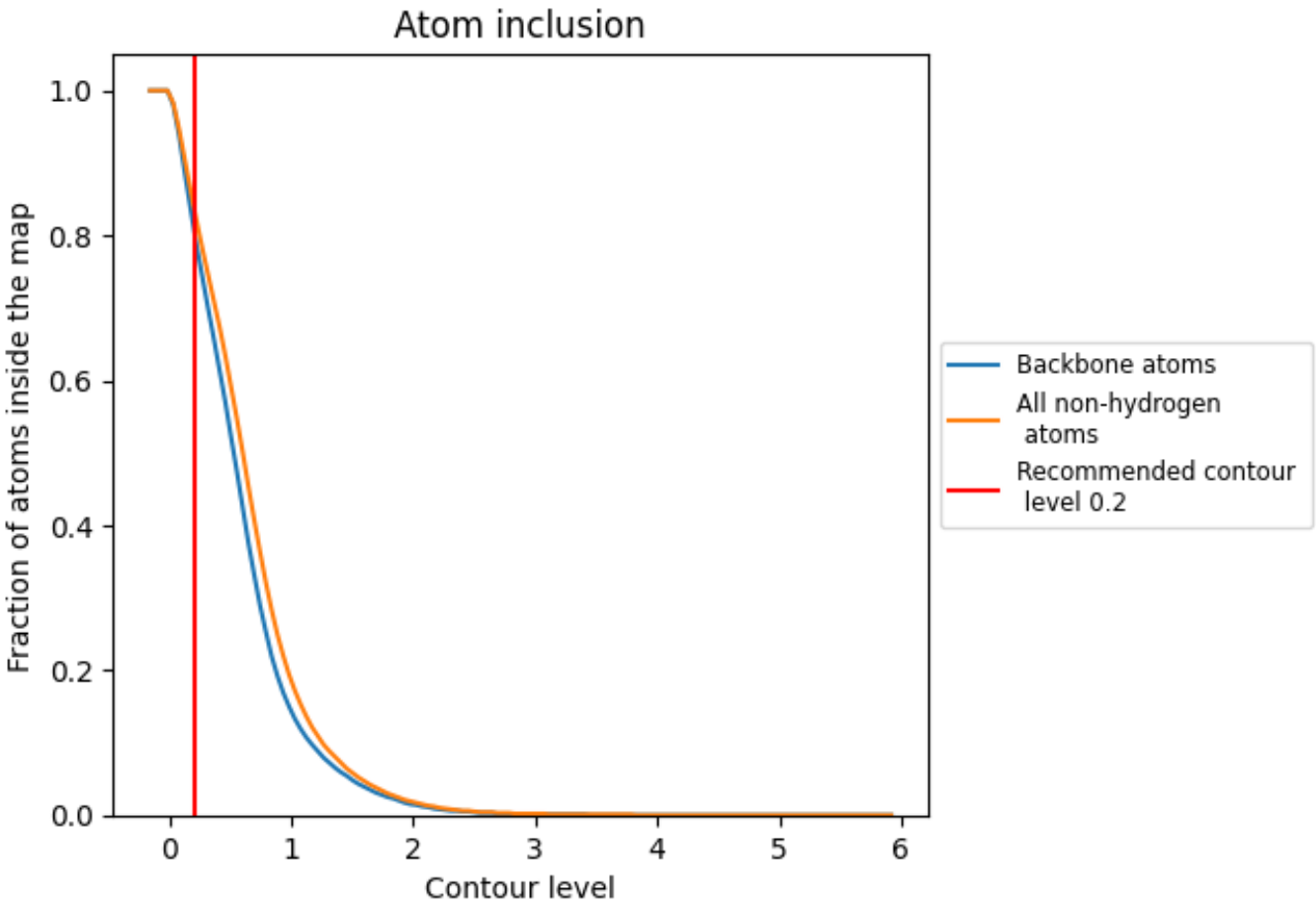
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.6120
0	0.7910	0.6360
1	0.9530	0.7180
2	0.9800	0.7220
3	0.8530	0.6230
A	0.8640	0.6240
B	0.5830	0.5320
C	0.9160	0.6660
D	0.9110	0.6870
E	0.7970	0.6550
F	0.0580	0.3350
G	0.4850	0.5100
H	0.1630	0.4040
I	0.9180	0.7000
J	0.8930	0.6550
K	0.8990	0.6880
L	0.8360	0.6310
M	0.9550	0.7030
N	0.5400	0.5400
O	0.8370	0.6400
P	0.9410	0.7070
Q	0.8380	0.6690
R	0.9110	0.6980
S	0.7340	0.6250
T	0.5490	0.5460
U	0.7110	0.5970
V	0.9120	0.7000
W	0.8500	0.6680
X	0.5100	0.5290
Y	0.8670	0.6710
Z	0.8090	0.6510
a	0.9090	0.6070
b	0.2300	0.3680
c	0.8960	0.6110
d	0.6970	0.5310



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.8820	0.6250
f	0.6980	0.5220
g	0.6750	0.4630
h	0.9300	0.6690
i	0.9180	0.6300
j	0.8700	0.6240
k	0.6960	0.5080
l	0.8580	0.6090
m	0.9230	0.6230
n	0.9320	0.6660
o	0.9280	0.6510
p	0.9020	0.6660
q	0.7610	0.5510
r	0.8890	0.6160
s	0.9570	0.6770
t	0.9060	0.6250
u	0.4080	0.4460