Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:37 pm GMT

PDB ID	:	5O61
EMDB ID	:	EMD-3751
Title	:	The complete structure of the Mycobacterium smegmatis 70S ribosome
Authors	:	Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2017-06-03
Resolution	:	3.31 Å(reported)

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

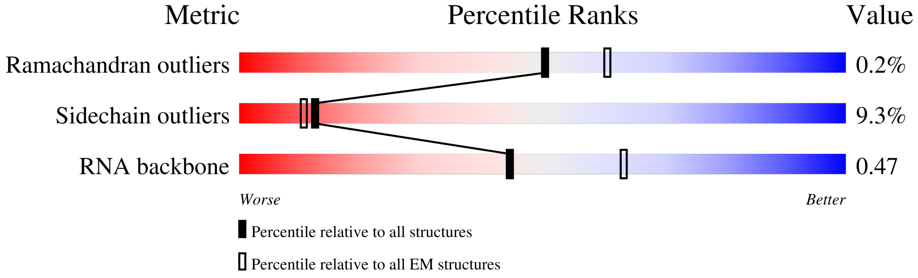
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

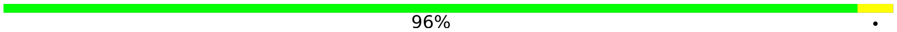
The reported resolution of this entry is 3.31 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	3	24	 92% • •
2	A	3120	 75% 24% •
3	B	118	 79% 21%
4	C	278	 90% 9% •
5	D	217	 89% 9% •
6	E	215	 89% 8% •
7	F	187	 88% 9% • •
8	G	179	 92% 7% •
9	H	151	 96% •

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Mol	Chain	Length	Quality of chain
10	I	175	69% • 28%
11	J	142	85% 8% 6%
12	K	147	94% 5% •
13	L	122	91% 9%
14	M	147	91% 7% •
15	N	138	92% 7% •
16	O	199	55% 5% 41%
17	P	127	93% 6% •
18	Q	113	90% 10%
19	R	129	91% 5% •
20	S	103	90% 7% •
21	T	153	68% 7% 25%
22	U	100	94% • •
23	V	105	88% 5% 8%
24	W	215	80% 10% 11%
25	X	88	85% 5% 10%
26	Y	64	92% 6% •
27	Z	77	79% • 17%
28	a	61	90% 7% •
29	b	57	82% 12% 5%
30	c	55	76% 13% 11%
31	d	47	89% 9% •
32	e	64	89% 9% •
33	f	37	95% 5%
34	g	75	68% 11% 21%

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Mol	Chain	Length	Quality of chain
35	BA	1528	74% 23% • •
36	BB	33	85% 12% •
37	BC	275	70% 6% 24%
38	BD	201	93% 7%
39	BE	214	78% 6% 16%
40	BF	96	92% 8%
41	BG	156	92% 7% •
42	BH	132	94% 5% •
43	BI	150	76% 8% 16%
44	BJ	101	91% 7% •
45	BK	138	77% 7% 17%
46	BL	124	89% 10% •
47	BM	124	82% 11% 6%
48	BN	61	93% 5% •
49	BO	89	92% 7% •
50	BP	156	67% 5% 28%
51	BQ	98	88% 8% •
52	BR	84	76% • 23%
53	BS	93	78% 10% 12%
54	BT	86	87% 12% •
55	BV	277	75% 7% 18%
56	BW	76	74% 24% •
57	BX	6	67% 33%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 151463 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 bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	3	23	189	111	50	28	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	3119	66981	29854	12313	21695	3119	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	118	2522	1126	468	810	118	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	275	2110	1298	438	370	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	214	1587	982	310	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	209	1569	969	295	303	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	182	1445	907	271	261	6	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	176	1348	845	249	253	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	151	1018	635	188	194	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	126	918	580	156	180	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	133	990	625	175	187	3	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	146	1130	722	207	200	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	122	938	586	179	170	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	145	1078	676	205	194	3	0	0

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	136	1092	690	213	187	2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	118	928	583	180	163	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	P	126	956	586	199	171	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	113	907	570	171	165	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	R	124	988	613	203	172	0	0

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	S	100	754	478	137	139	0	0

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	T	114	873	543	171	159	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	U	97	756	479	138	139	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	97	732	456	137	137	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	W	192	1428	881	255	292	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	X	79	586	361	123	102	0	0

- Molecule 26 is a protein called LSU ribosomal protein L28P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	63	470	283	103	80	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	64	531	324	103	103	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	a	59	474	292	95	87	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	54	423	260	93	69	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	49	405	248	82	71	4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	46	377	225	97	54	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	e	63	502	302	115	85	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	37	299	181	66	47	5	0	0

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	59	458	284	84	85	5	0	0

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	BA	1511	32439	14448	5930	10550	1511	0	0

- Molecule 36 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BB	32	280	172	71	36	1	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BC	208	1660	1036	322	298	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	BD	200	1641	1028	316	295	2	0	0

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BE	180	1296	812	245	235	4	0	0

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BF	96	771	486	138	145	2	0	0

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BG	155	1232	768	241	221	2	0	0

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	131	Total 1010	C 633	N 189	O 187	S 1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BI	122	Total 994	C 630	N 194	O 170	0	0

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	99	Total 788	C 495	N 146	O 144	S 3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	115	Total 855	C 528	N 170	O 156	S 1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BL	122	Total 958	C 594	N 197	O 165	S 2	0	0

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	116	Total 935	C 572	N 191	O 169	S 3	0	0

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	60	Total 477	C 302	N 97	O 73	S 5	0	0

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BO	88	Total 720	C 449	N 147	O 124	0	0

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	113	Total 891	C 570	N 162	O 159	0	0

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	94	Total 748	C 469	N 142	O 135	S 2	0	0

- Molecule 52 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	65	Total 513	C 318	N 102	O 90	S 3	0	0

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	82	Total 662	C 425	N 124	O 112	S 1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BT	85	Total 660	C 402	N 139	O 119	0	0

- Molecule 55 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BV	228	Total 1793	C 1132	N 322	O 330	S 9	0	0

- Molecule 56 is a RNA chain called P/P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	BW	76	1619	723	290	531	75	0	0

- Molecule 57 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	BX	6	117	54	13	45	5	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	A	390	390	390	0
58	B	9	9	9	0
58	C	4	4	4	0
58	F	1	1	1	0
58	M	1	1	1	0
58	N	1	1	1	0
58	T	1	1	1	0
58	c	1	1	1	0
58	BA	215	215	215	0
58	BF	1	1	1	0
58	BR	1	1	1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	Y	1	1	1	0
59	c	1	1	1	0

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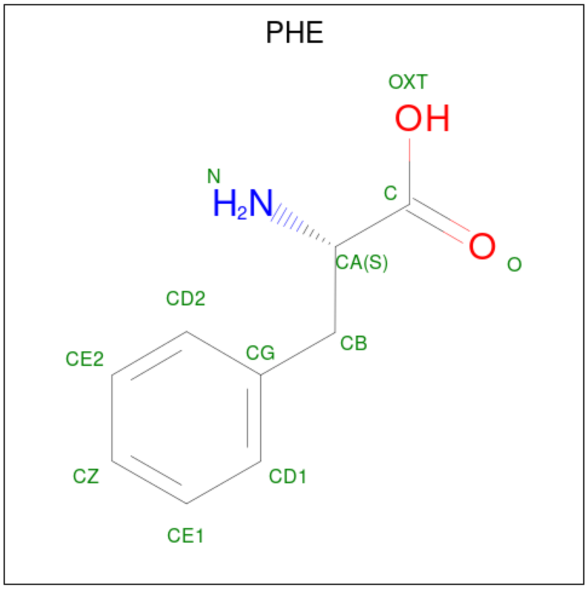
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	f	1	1	1	0
59	g	1	1	1	0
59	BN	1	1	1	0
59	BR	1	1	1	0

- Molecule 60 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



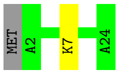
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	BW	1	11	9	1	1	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

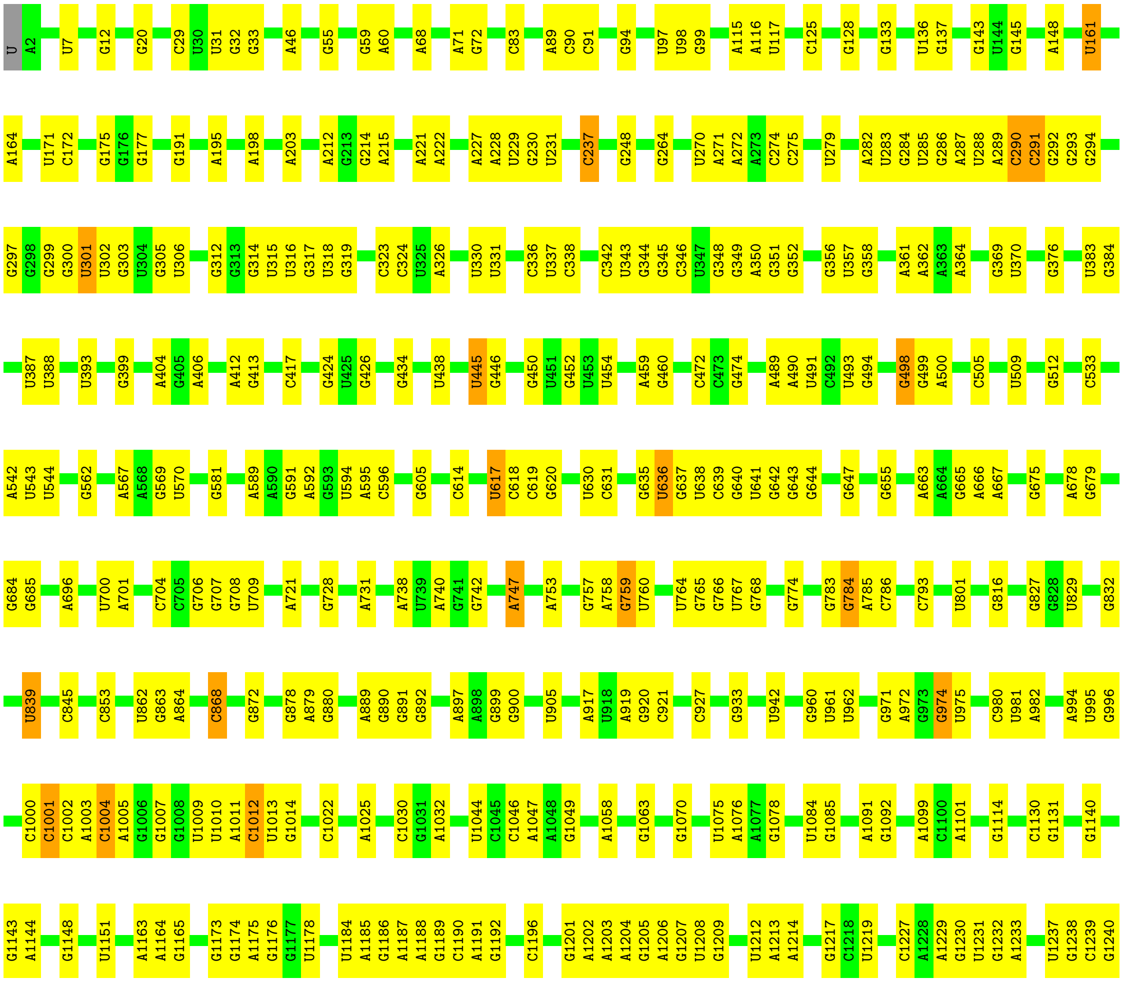
- Molecule 1: 50S ribosomal protein bL37

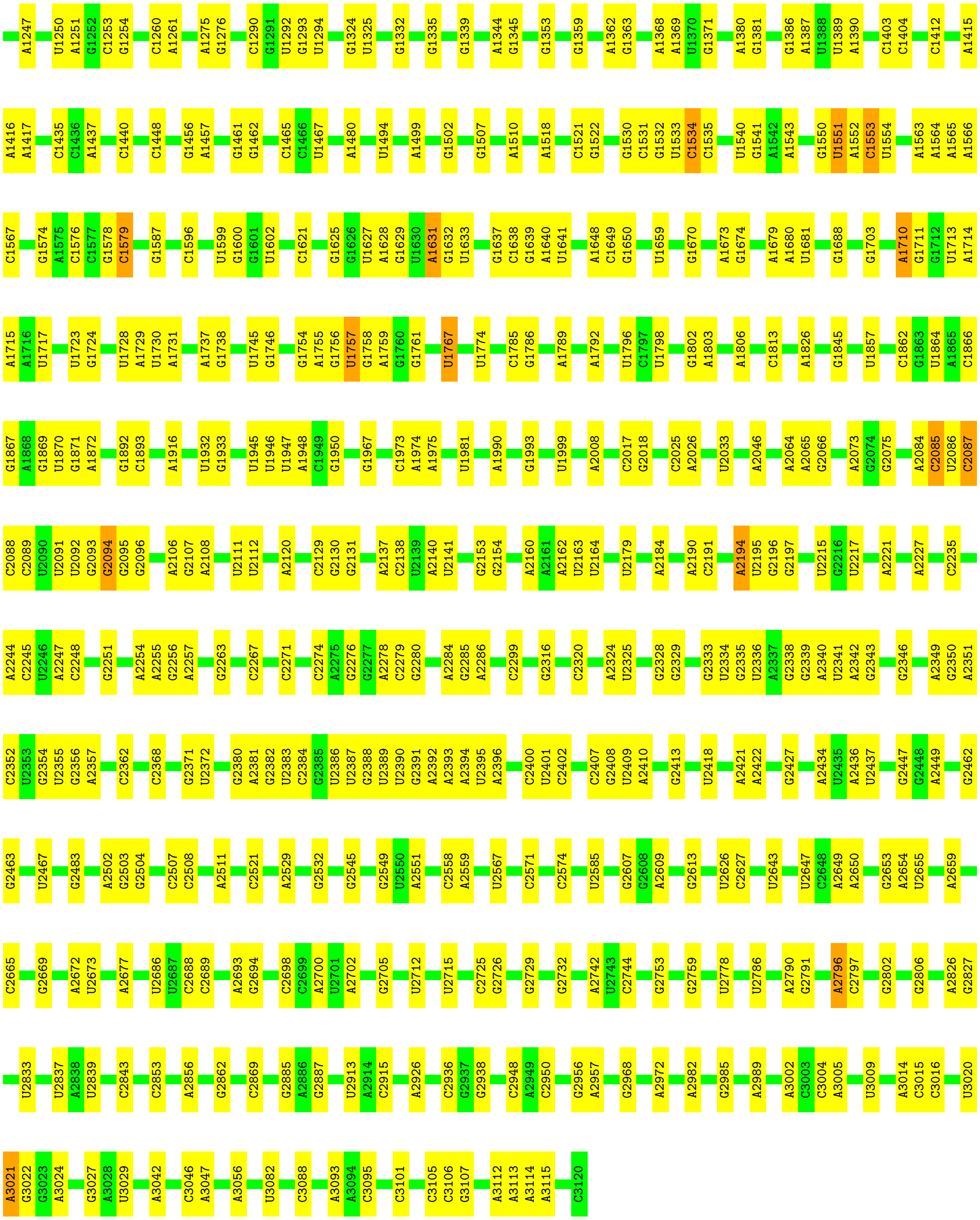
Chain 3:



- Molecule 2: 23S rRNA

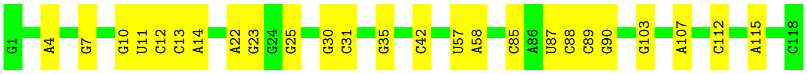
Chain A:





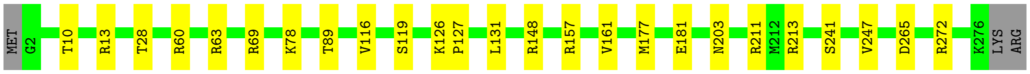
- Molecule 3: 5S rRNA

Chain B:



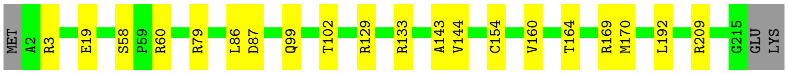
- Molecule 4: 50S ribosomal protein L2

Chain C:



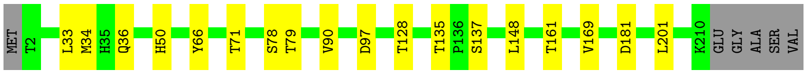
- Molecule 5: 50S ribosomal protein L3

Chain D:



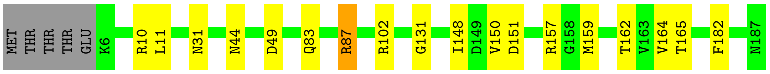
- Molecule 6: 50S ribosomal protein L4

Chain E:



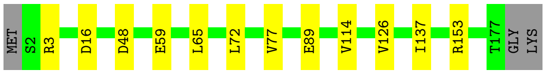
- Molecule 7: 50S ribosomal protein L5

Chain F:



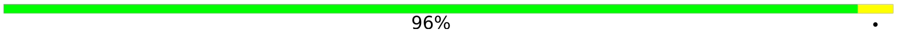
- Molecule 8: 50S ribosomal protein L6

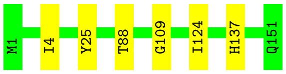
Chain G:



- Molecule 9: 50S ribosomal protein L9

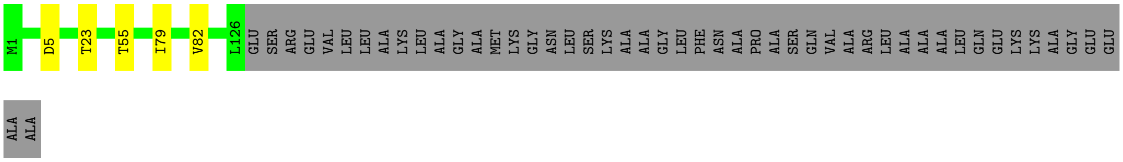
Chain H:





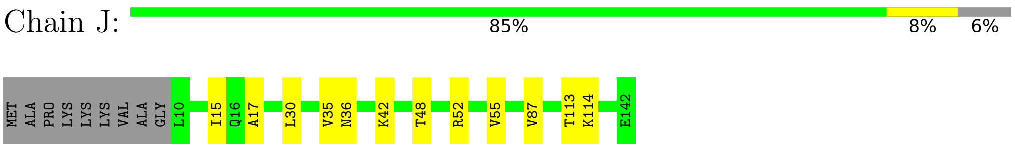
- Molecule 10: 50S ribosomal protein L10

Chain I:



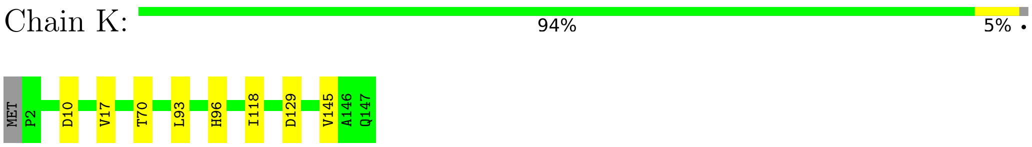
- Molecule 11: 50S ribosomal protein L11

Chain J:



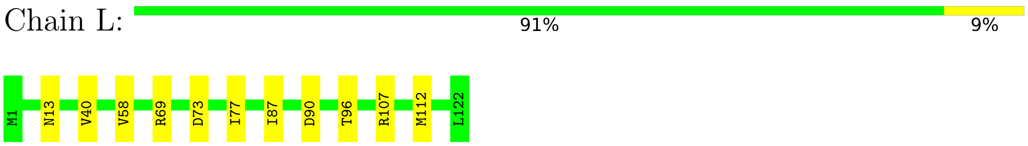
- Molecule 12: 50S ribosomal protein L13

Chain K:



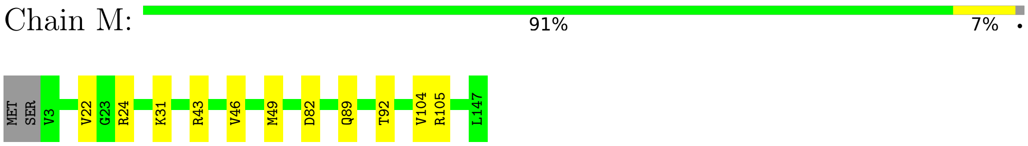
- Molecule 13: 50S ribosomal protein L14

Chain L:



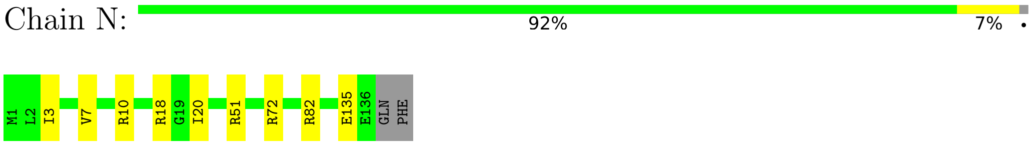
- Molecule 14: 50S ribosomal protein L15

Chain M:



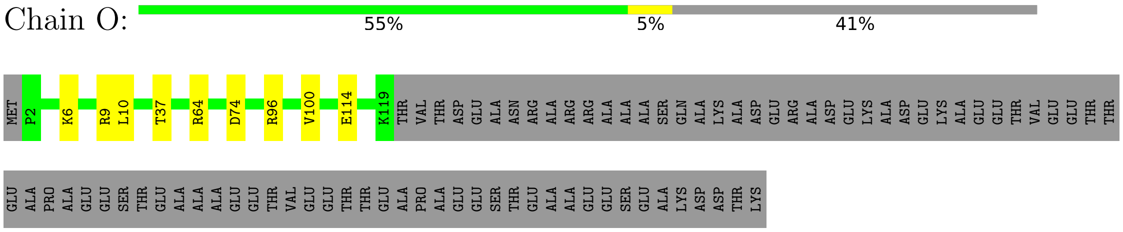
- Molecule 15: 50S ribosomal protein L16

Chain N:



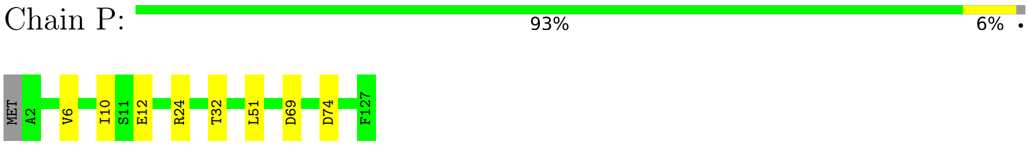
- Molecule 16: 50S ribosomal protein L17

Chain O:



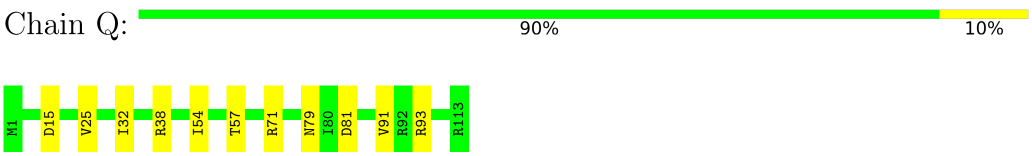
- Molecule 17: 50S ribosomal protein L18

Chain P:



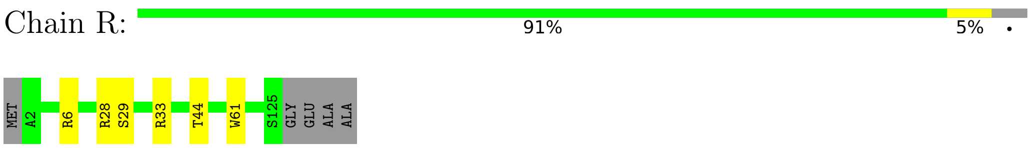
- Molecule 18: 50S ribosomal protein L19

Chain Q:



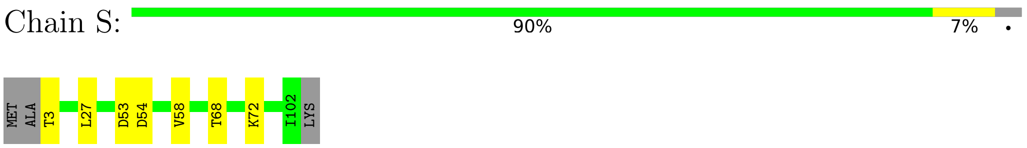
- Molecule 19: 50S ribosomal protein L20

Chain R:



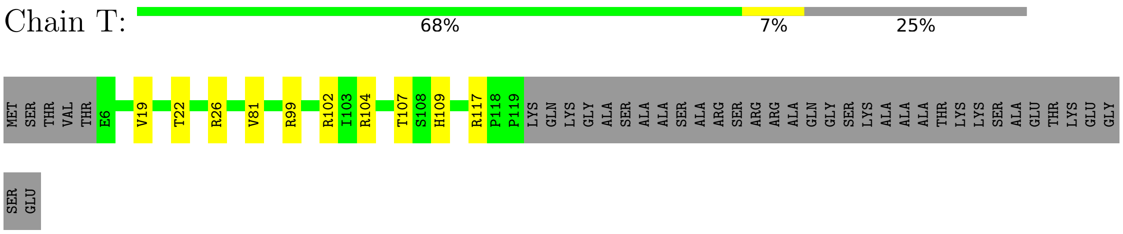
- Molecule 20: 50S ribosomal protein L21

Chain S:



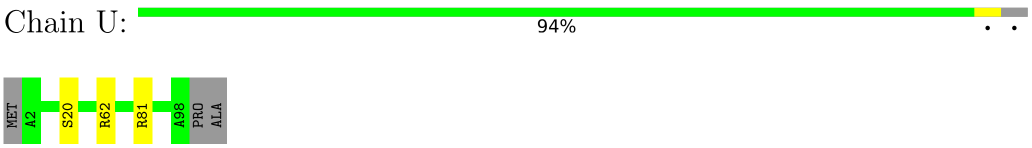
- Molecule 21: 50S ribosomal protein L22

Chain T:



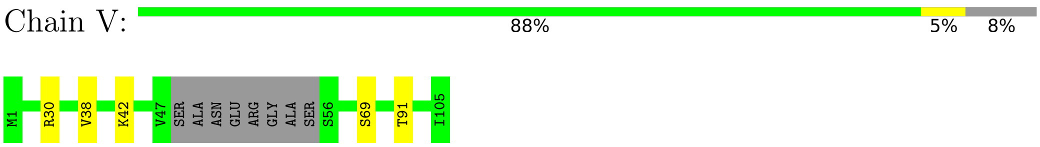
- Molecule 22: 50S ribosomal protein L23

Chain U:



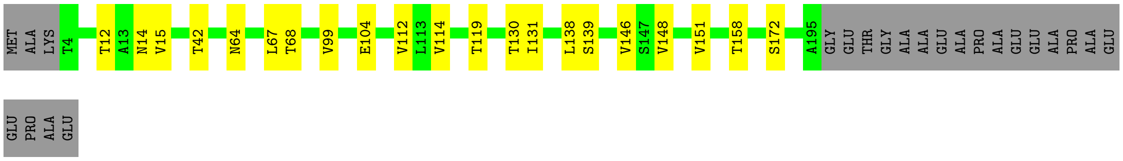
- Molecule 23: 50S ribosomal protein L24

Chain V:



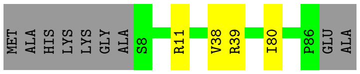
- Molecule 24: 50S ribosomal protein L25

Chain W:



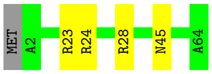
- Molecule 25: 50S ribosomal protein L27

Chain X:



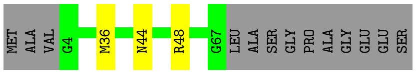
- Molecule 26: LSU ribosomal protein L28P

Chain Y:



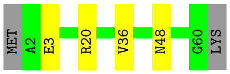
- Molecule 27: 50S ribosomal protein L29

Chain Z:



- Molecule 28: 50S ribosomal protein L30

Chain a:

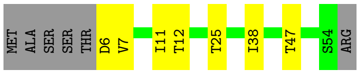


- Molecule 29: 50S ribosomal protein L32

Chain b:

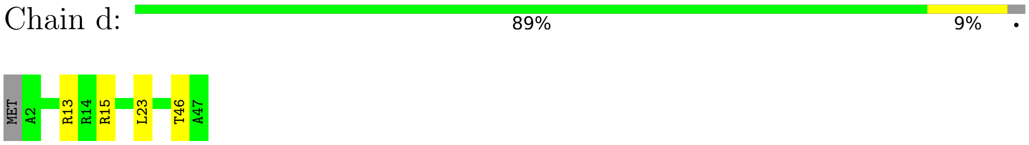
- Molecule 30: 50S ribosomal protein L33 1

Chain c:



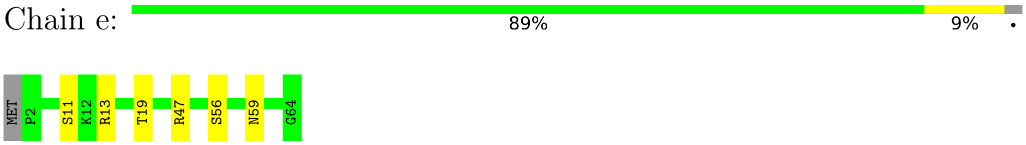
- Molecule 31: 50S ribosomal protein L34

Chain d:



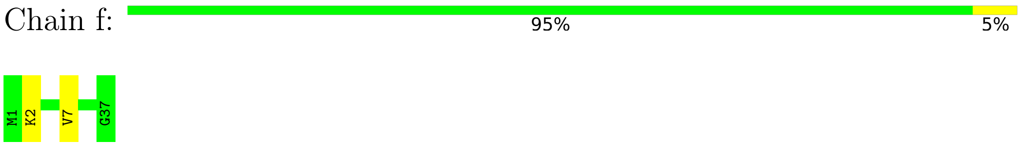
- Molecule 32: 50S ribosomal protein L35

Chain e:



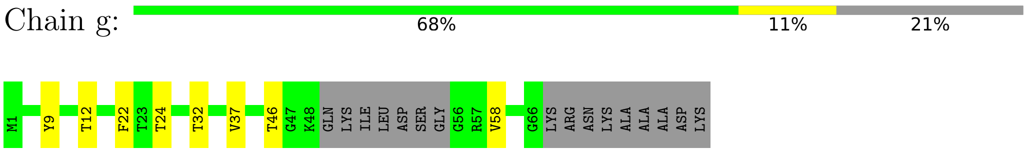
- Molecule 33: 50S ribosomal protein L36

Chain f:



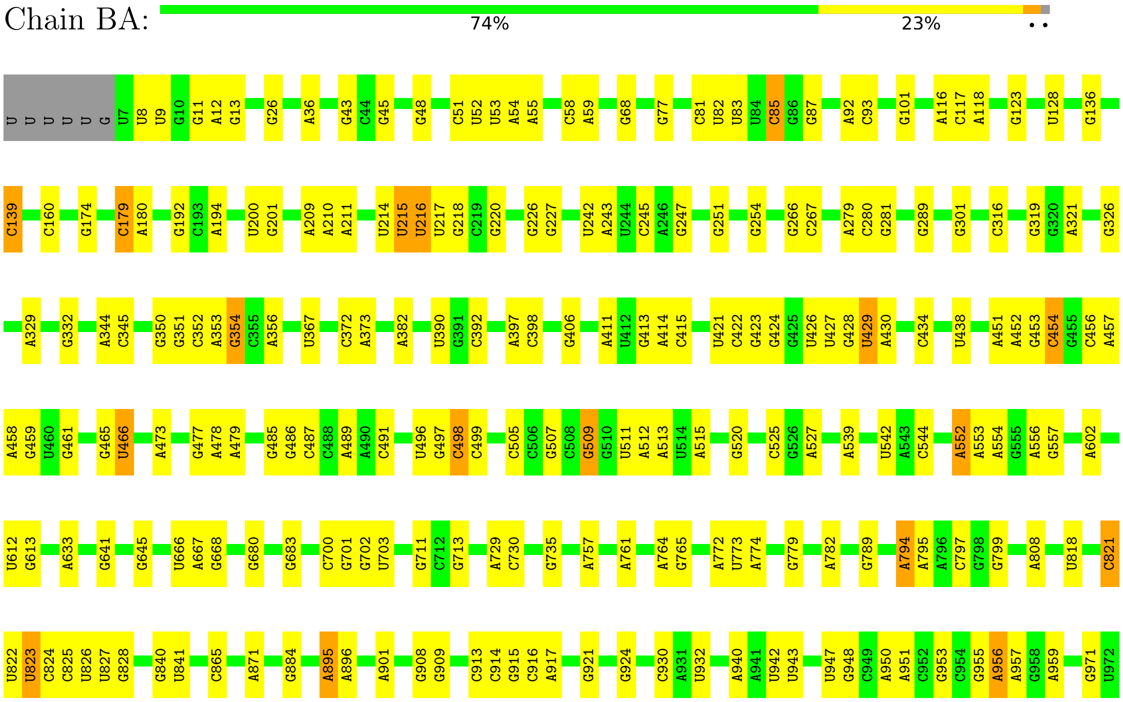
- Molecule 34: 50S ribosomal protein L31

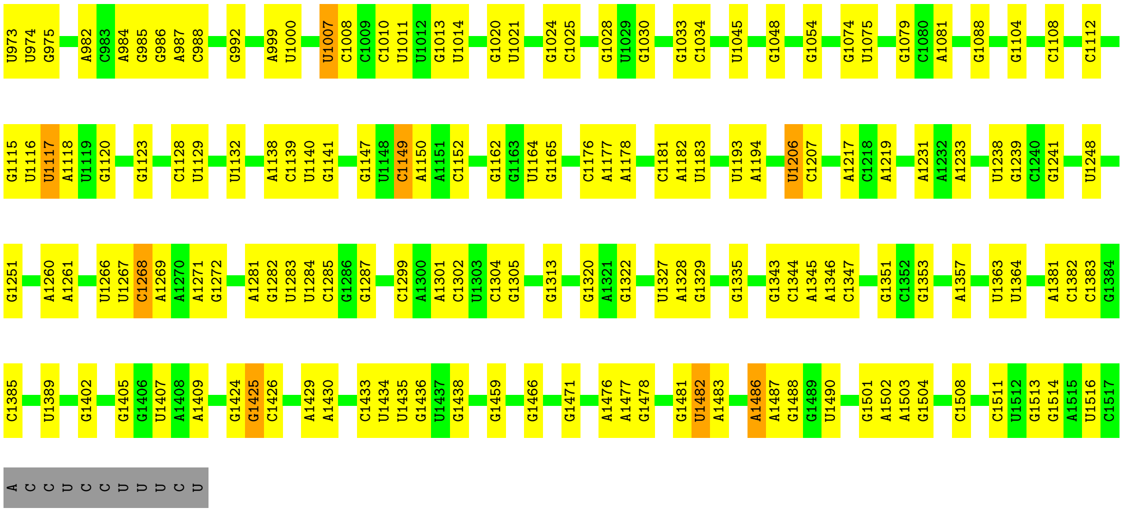
Chain g:



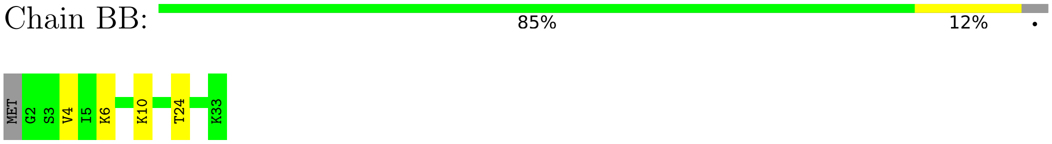
- Molecule 35: 16S rRNA

Chain BA:

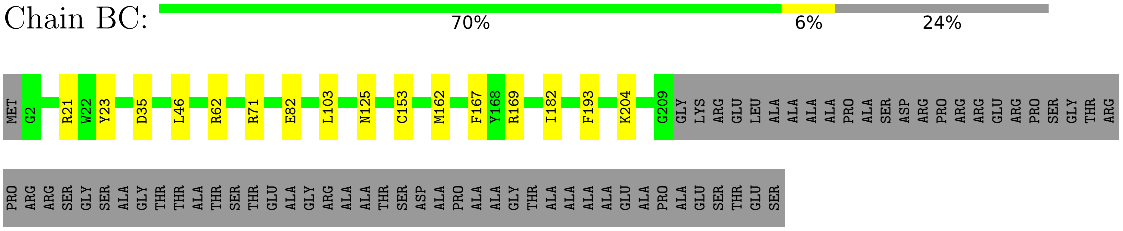




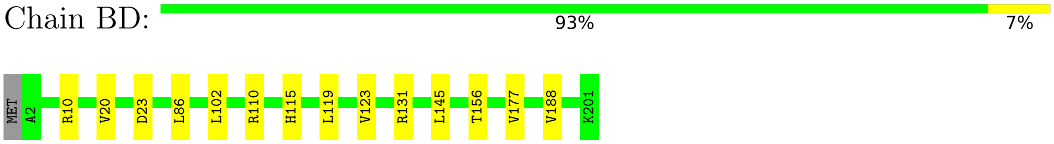
- Molecule 36: Conserved domain protein



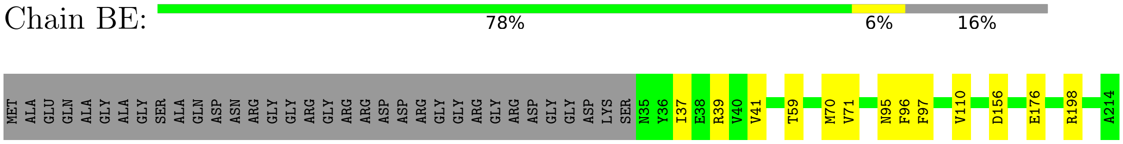
- Molecule 37: 30S ribosomal protein S3



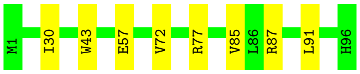
- Molecule 38: 30S ribosomal protein S4



- Molecule 39: 30S ribosomal protein S5

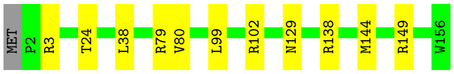


- Molecule 40: 30S ribosomal protein S6



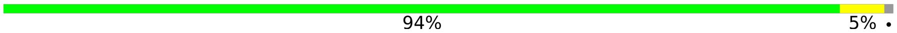
- Molecule 41: 30S ribosomal protein S7

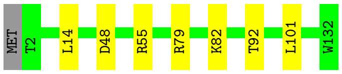
Chain BG:



- Molecule 42: 30S ribosomal protein S8

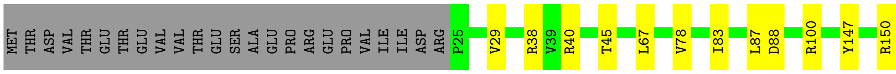
Chain BH:





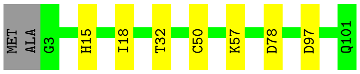
- Molecule 43: 30S ribosomal protein S9

Chain BI:



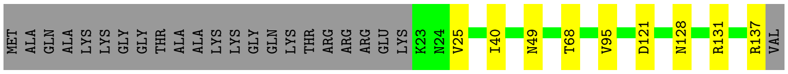
- Molecule 44: 30S ribosomal protein S10

Chain BJ:



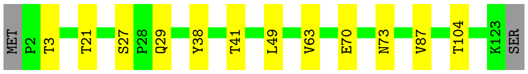
- Molecule 45: 30S ribosomal protein S11

Chain BK:



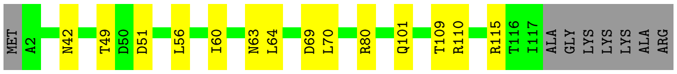
- Molecule 46: 30S ribosomal protein S12

Chain BL:



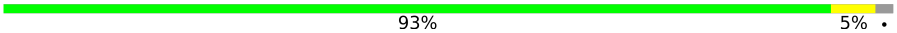
- Molecule 47: 30S ribosomal protein S13

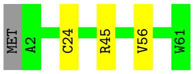
Chain BM:



- Molecule 48: 30S ribosomal protein S14 type Z

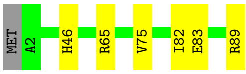
Chain BN:





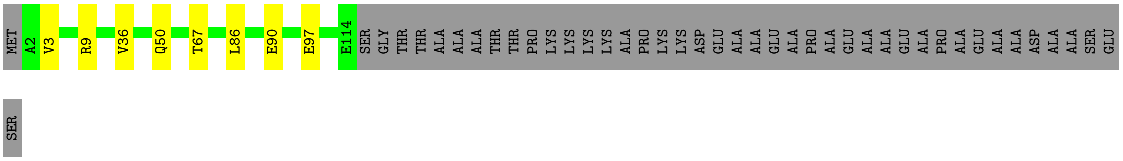
- Molecule 49: 30S ribosomal protein S15

Chain BO:



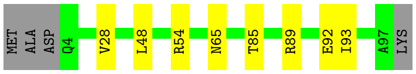
- Molecule 50: 30S ribosomal protein S16

Chain BP:



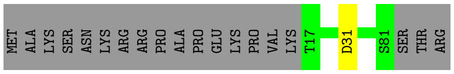
- Molecule 51: 30S ribosomal protein S17

Chain BQ:



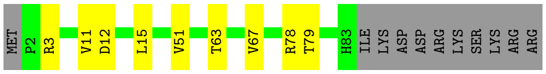
- Molecule 52: 30S ribosomal protein S18 2

Chain BR:



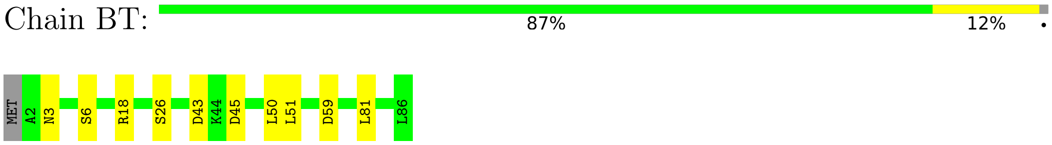
- Molecule 53: 30S ribosomal protein S19

Chain BS:



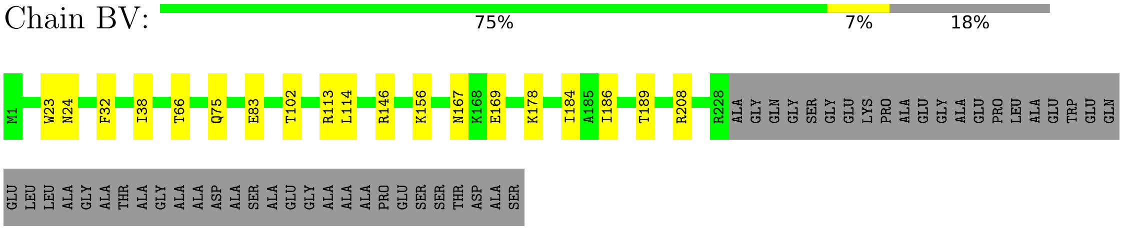
- Molecule 54: 30S ribosomal protein S20

Chain BT:



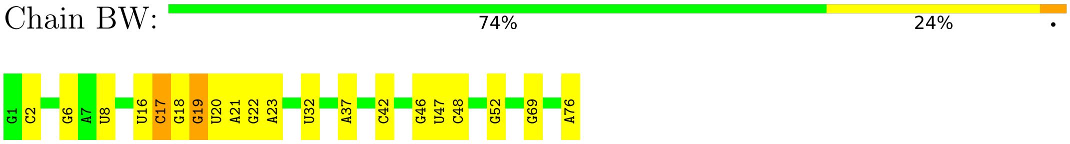
- Molecule 55: 30S ribosomal protein S2

Chain BV:



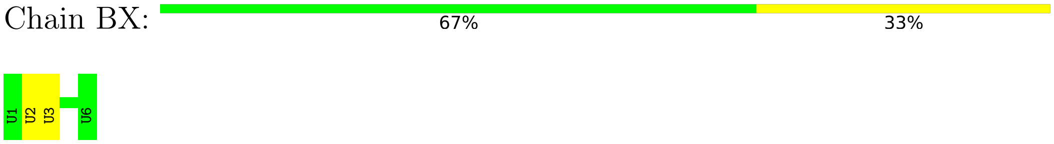
- Molecule 56: P/P-site Phe-tRNA(Phe)

Chain BW:



- Molecule 57: mRNA fragment

Chain BX:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.437	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	3	0.46	0/191	0.52	0/247
2	A	0.78	4/75001 (0.0%)	1.06	101/117027 (0.1%)
3	B	0.48	0/2821	0.93	1/4396 (0.0%)
4	C	0.50	0/2153	0.62	0/2895
5	D	0.49	0/1609	0.62	0/2165
6	E	0.42	0/1592	0.56	0/2153
7	F	0.38	0/1467	0.60	2/1973 (0.1%)
8	G	0.36	0/1369	0.52	0/1848
9	H	0.44	0/1027	0.53	1/1398 (0.1%)
10	I	0.62	0/925	0.61	0/1246
11	J	0.65	0/1006	0.63	0/1364
12	K	0.46	0/1157	0.56	0/1567
13	L	0.48	0/946	0.58	0/1268
14	M	0.46	0/1091	0.66	0/1457
15	N	0.50	0/1118	0.63	0/1506
16	O	0.46	0/945	0.63	0/1267
17	P	0.36	0/966	0.53	0/1298
18	Q	0.47	0/921	0.64	0/1236
19	R	0.64	1/1000 (0.1%)	0.73	4/1341 (0.3%)
20	S	0.43	0/764	0.61	0/1030
21	T	0.58	0/887	0.63	1/1204 (0.1%)
22	U	0.45	0/766	0.54	0/1030
23	V	0.39	0/738	0.55	0/987
24	W	0.38	0/1443	0.56	0/1970
25	X	0.49	0/595	0.57	0/798
26	Y	0.50	0/478	0.62	0/641
27	Z	0.43	0/534	0.52	0/713
28	a	0.47	0/477	0.59	0/640
29	b	0.46	0/427	0.61	0/572
30	c	0.40	0/413	0.56	0/553
31	d	0.49	0/380	0.63	1/500 (0.2%)
32	e	0.44	0/507	0.56	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.50	0/303	0.59	0/401
34	g	0.41	0/467	0.53	0/626
35	BA	0.57	1/36309 (0.0%)	1.02	60/56657 (0.1%)
36	BB	0.42	0/280	0.56	0/359
37	BC	0.39	0/1684	0.54	0/2261
38	BD	0.51	1/1672 (0.1%)	0.59	1/2251 (0.0%)
39	BE	0.40	0/1312	0.54	0/1772
40	BF	0.40	0/782	0.61	0/1059
41	BG	0.41	0/1252	0.50	0/1690
42	BH	0.35	0/1025	0.58	0/1385
43	BI	0.40	0/1012	0.53	0/1362
44	BJ	0.43	0/802	0.54	0/1086
45	BK	0.39	0/873	0.56	0/1180
46	BL	0.40	0/969	0.58	0/1294
47	BM	0.36	0/942	0.53	0/1260
48	BN	0.34	0/488	0.55	0/650
49	BO	0.37	0/729	0.55	0/977
50	BP	0.40	0/908	0.64	0/1226
51	BQ	0.39	0/759	0.57	0/1016
52	BR	0.42	0/518	0.53	0/693
53	BS	0.47	0/680	0.58	0/915
54	BT	0.42	0/663	0.54	0/882
55	BV	0.53	0/1822	0.56	0/2457
56	BW	0.68	0/1809	1.08	2/2819 (0.1%)
57	BX	0.57	0/128	0.95	0/196
All	All	0.65	7/163902 (0.0%)	0.95	174/245436 (0.1%)

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
21	T	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	61	TRP	CD2-CE2	8.39	1.51	1.41
38	BD	115	HIS	ND1-CE1	-6.31	1.19	1.34
35	BA	1476	A	N9-C4	5.55	1.41	1.37
2	A	889	A	N3-C4	-5.52	1.31	1.34

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3021	A	N9-C4	5.24	1.41	1.37
2	A	289	A	N9-C4	5.18	1.41	1.37
2	A	2725	C	N1-C6	-5.13	1.34	1.37

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	R	61	TRP	CG-CD2-CE3	10.37	143.24	133.90
35	BA	1425	G	C8-N9-C4	-9.91	102.44	106.40
35	BA	1425	G	N7-C8-N9	9.13	117.67	113.10
35	BA	85	C	C2-N1-C1'	8.86	128.55	118.80
35	BA	85	C	N1-C2-O2	8.50	124.00	118.90
7	F	87	ARG	NE-CZ-NH2	8.41	124.51	120.30
35	BA	1149	C	C6-N1-C2	-8.38	116.95	120.30
2	A	445	U	C2-N1-C1'	7.64	126.87	117.70
2	A	2245	C	N1-C2-O2	7.51	123.41	118.90
19	R	61	TRP	CD1-CG-CD2	7.34	112.17	106.30
35	BA	1486	A	N7-C8-N9	7.31	117.46	113.80
2	A	2245	C	C2-N1-C1'	7.11	126.62	118.80
35	BA	415	C	C6-N1-C2	-7.06	117.48	120.30
35	BA	1486	A	C8-N9-C4	-7.03	102.99	105.80
35	BA	1425	G	N3-C2-N2	-7.00	115.00	119.90
35	BA	216	U	N3-C2-O2	-6.99	117.31	122.20
35	BA	85	C	C6-N1-C2	-6.95	117.52	120.30
2	A	2025	C	N3-C2-O2	-6.94	117.04	121.90
35	BA	216	U	N1-C2-O2	6.81	127.57	122.80
2	A	868	C	C6-N1-C2	-6.79	117.58	120.30
35	BA	1482	U	P-O3'-C3'	6.75	127.80	119.70
2	A	291	C	C6-N1-C2	-6.71	117.61	120.30
2	A	1579	C	C5-C6-N1	6.70	124.35	121.00
35	BA	85	C	N3-C2-O2	-6.63	117.26	121.90
2	A	1758	G	C5-C6-O6	-6.62	124.63	128.60
2	A	617	U	C2-N1-C1'	6.56	125.57	117.70
2	A	962	U	C2-N1-C1'	6.56	125.57	117.70
35	BA	1268	C	C5-C6-N1	6.55	124.28	121.00
2	A	1758	G	N1-C6-O6	6.54	123.82	119.90
2	A	1553	C	C6-N1-C2	-6.51	117.69	120.30
35	BA	216	U	C2-N1-C1'	6.50	125.50	117.70
35	BA	1149	C	C2-N1-C1'	6.48	125.92	118.80
2	A	161	U	C2-N1-C1'	6.47	125.47	117.70
2	A	1381	G	C5-C6-N1	6.34	114.67	111.50
35	BA	552	A	C8-N9-C4	6.33	108.33	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	BA	1268	C	C2-N1-C1'	6.26	125.69	118.80
35	BA	1425	G	C5-N7-C8	-6.21	101.20	104.30
2	A	1012	C	N1-C2-O2	6.20	122.62	118.90
56	BW	19	G	N7-C8-N9	6.17	116.18	113.10
35	BA	489	A	C8-N9-C4	-6.16	103.34	105.80
2	A	643	G	C4-N9-C1'	6.13	134.47	126.50
35	BA	1149	C	N1-C2-O2	6.12	122.57	118.90
2	A	2245	C	N3-C2-O2	-6.12	117.62	121.90
2	A	445	U	C5-C6-N1	6.11	125.75	122.70
2	A	636	U	C5-C6-N1	6.06	125.73	122.70
2	A	1276	G	C4-N9-C1'	6.05	134.37	126.50
2	A	1403	C	C4-C5-C6	6.04	120.42	117.40
2	A	1621	C	C6-N1-C2	-6.04	117.88	120.30
2	A	445	U	N1-C2-O2	6.00	127.00	122.80
2	A	1276	G	C6-C5-N7	-5.98	126.81	130.40
2	A	2352	C	C5-C6-N1	5.98	123.99	121.00
35	BA	1117	U	O4'-C1'-N1	5.95	112.96	108.20
2	A	445	U	N3-C2-O2	-5.95	118.04	122.20
2	A	2087	C	C5-C6-N1	5.94	123.97	121.00
35	BA	1508	C	C6-N1-C2	-5.93	117.93	120.30
35	BA	1149	C	P-O3'-C3'	5.93	126.81	119.70
2	A	2437	U	C2-N1-C1'	5.91	124.79	117.70
2	A	1534	C	C6-N1-C2	-5.90	117.94	120.30
2	A	2869	C	C6-N1-C2	-5.90	117.94	120.30
2	A	2686	U	N1-C2-O2	5.89	126.93	122.80
2	A	1403	C	N3-C2-O2	-5.89	117.78	121.90
35	BA	415	C	C2-N1-C1'	5.87	125.25	118.80
2	A	1012	C	C2-N1-C1'	5.84	125.23	118.80
35	BA	1149	C	N3-C2-O2	-5.84	117.81	121.90
35	BA	139	C	C6-N1-C2	-5.83	117.97	120.30
35	BA	1117	U	P-O3'-C3'	5.83	126.70	119.70
2	A	1196	C	C6-N1-C2	-5.81	117.98	120.30
2	A	1567	C	C6-N1-C2	-5.79	117.98	120.30
2	A	445	U	P-O3'-C3'	5.78	126.63	119.70
35	BA	413	G	O4'-C1'-N9	5.77	112.81	108.20
2	A	2796	A	O5'-P-OP2	-5.75	100.52	105.70
2	A	2352	C	C6-N1-C2	-5.75	118.00	120.30
2	A	2094	G	P-O3'-C3'	5.75	126.60	119.70
19	R	61	TRP	CE2-CD2-CE3	-5.75	111.81	118.70
2	A	1993	G	C4-N9-C1'	5.73	133.95	126.50
56	BW	17	C	C6-N1-C2	-5.73	118.01	120.30
35	BA	85	C	C6-N1-C1'	-5.72	113.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3046	C	N3-C2-O2	-5.72	117.90	121.90
2	A	1631	A	N1-C6-N6	5.71	122.02	118.60
35	BA	489	A	N7-C8-N9	5.71	116.65	113.80
3	B	88	C	C2-N1-C1'	5.70	125.08	118.80
2	A	237	C	C5-C6-N1	5.69	123.84	121.00
35	BA	429	U	P-O3'-C3'	5.68	126.52	119.70
2	A	2521	C	C6-N1-C2	-5.68	118.03	120.30
2	A	617	U	N1-C2-O2	5.67	126.77	122.80
2	A	1567	C	C5-C6-N1	5.67	123.83	121.00
35	BA	1486	A	C5-N7-C8	-5.67	101.07	103.90
35	BA	215	U	N3-C2-O2	-5.66	118.24	122.20
2	A	291	C	C5-C6-N1	5.65	123.83	121.00
35	BA	1149	C	C5-C6-N1	5.65	123.83	121.00
35	BA	821	C	N1-C2-O2	5.63	122.28	118.90
35	BA	1117	U	OP1-P-O3'	5.63	117.58	105.20
2	A	1757	U	C2-N1-C1'	5.60	124.42	117.70
2	A	2245	C	C6-N1-C1'	-5.60	114.08	120.80
35	BA	498	C	P-O3'-C3'	5.58	126.39	119.70
35	BA	354	G	C4-N9-C1'	5.57	133.74	126.50
38	BD	115	HIS	ND1-CG-CD2	-5.57	98.20	106.00
2	A	747	A	O4'-C1'-N9	5.57	112.65	108.20
35	BA	466	U	C2-N1-C1'	5.56	124.38	117.70
2	A	2094	G	OP1-P-O3'	5.55	117.40	105.20
31	d	23	LEU	CA-CB-CG	-5.54	102.55	115.30
2	A	1535	C	C2-N1-C1'	5.53	124.88	118.80
35	BA	956	A	O4'-C1'-N9	5.51	112.61	108.20
2	A	301	U	N1-C2-O2	5.51	126.65	122.80
2	A	2278	A	N1-C2-N3	5.50	132.05	129.30
35	BA	794	A	N1-C6-N6	5.50	121.90	118.60
2	A	533	C	C6-N1-C2	-5.50	118.10	120.30
2	A	1576	C	C6-N1-C2	-5.50	118.10	120.30
2	A	498	G	C4-N9-C1'	5.49	133.64	126.50
2	A	445	U	C6-N1-C2	-5.48	117.71	121.00
2	A	2248	C	C6-N1-C2	-5.48	118.11	120.30
2	A	2843	C	C6-N1-C2	-5.47	118.11	120.30
2	A	362	A	O4'-C1'-N9	5.45	112.56	108.20
2	A	161	U	O4'-C1'-N1	5.45	112.56	108.20
2	A	2085	C	P-O3'-C3'	5.45	126.24	119.70
2	A	974	G	P-O3'-C3'	5.43	126.22	119.70
35	BA	1511	C	C6-N1-C2	-5.42	118.13	120.30
35	BA	509	G	N7-C8-N9	5.42	115.81	113.10
35	BA	730	C	C6-N1-C2	-5.42	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	905	U	C2-N1-C1'	5.41	124.19	117.70
2	A	1032	A	N1-C2-N3	5.41	132.00	129.30
2	A	1534	C	N1-C2-O2	5.39	122.14	118.90
2	A	617	U	N3-C2-O2	-5.39	118.43	122.20
2	A	1530	G	N3-C4-N9	-5.38	122.77	126.00
2	A	784	G	C4-N9-C1'	5.37	133.48	126.50
2	A	1621	C	C5-C6-N1	5.35	123.68	121.00
2	A	1276	G	C8-N9-C1'	-5.35	120.04	127.00
35	BA	326	G	N3-C4-C5	-5.34	125.93	128.60
2	A	1993	G	C8-N9-C1'	-5.34	120.06	127.00
2	A	2025	C	N1-C2-O2	5.33	122.09	118.90
2	A	759	G	P-O3'-C3'	5.30	126.06	119.70
35	BA	1206	U	C2-N1-C1'	5.29	124.05	117.70
35	BA	1011	U	C2-N1-C1'	5.29	124.05	117.70
2	A	839	U	C2-N1-C1'	5.28	124.04	117.70
2	A	786	C	C6-N1-C2	-5.27	118.19	120.30
2	A	1767	U	C5-C6-N1	5.27	125.33	122.70
2	A	290	C	C2-N1-C1'	5.26	124.58	118.80
35	BA	454	C	C5-C6-N1	5.22	123.61	121.00
2	A	2271	C	C6-N1-C2	-5.22	118.21	120.30
35	BA	85	C	C5-C6-N1	5.22	123.61	121.00
2	A	191	G	O4'-C1'-N9	5.21	112.37	108.20
35	BA	1007	U	P-O3'-C3'	5.21	125.96	119.70
2	A	1759	A	N1-C6-N6	5.21	121.73	118.60
7	F	87	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
2	A	1004	C	C5-C6-N1	5.19	123.59	121.00
35	BA	1011	U	C5-C6-N1	5.18	125.29	122.70
2	A	635	G	N3-C4-C5	-5.18	126.01	128.60
2	A	3046	C	C6-N1-C2	-5.18	118.23	120.30
2	A	1710	A	C2-N3-C4	5.16	113.18	110.60
2	A	1650	G	C4-N9-C1'	5.14	133.19	126.50
2	A	1602	U	C5-C6-N1	5.14	125.27	122.70
2	A	1631	A	C5-C6-N6	-5.14	119.59	123.70
35	BA	487	C	C6-N1-C2	-5.14	118.25	120.30
2	A	1001	C	C6-N1-C2	-5.13	118.25	120.30
2	A	1758	G	C4-C5-N7	5.12	112.85	110.80
35	BA	1486	A	C6-C5-N7	-5.12	128.71	132.30
35	BA	895	A	P-O3'-C3'	5.11	125.83	119.70
2	A	1276	G	C4-C5-N7	5.10	112.84	110.80
2	A	643	G	C8-N9-C1'	-5.09	120.38	127.00
35	BA	179	C	C2-N1-C1'	5.08	124.39	118.80
9	H	109	GLY	N-CA-C	5.07	125.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	T	109	HIS	ND1-CG-CD2	-5.06	98.92	106.00
2	A	853	C	C6-N1-C2	-5.05	118.28	120.30
2	A	1276	G	N3-C4-N9	5.05	129.03	126.00
19	R	61	TRP	CD2-CE3-CZ3	5.05	125.36	118.80
2	A	2712	U	C2-N3-C4	-5.03	123.98	127.00
2	A	1551	U	C5-C6-N1	5.03	125.21	122.70
2	A	1534	C	C2-N1-C1'	5.02	124.33	118.80
2	A	1412	C	C6-N1-C2	-5.02	118.29	120.30
2	A	2194	A	C8-N9-C4	-5.02	103.79	105.80
35	BA	509	G	C8-N9-C4	-5.01	104.39	106.40
35	BA	179	C	N1-C2-O2	5.01	121.91	118.90
35	BA	823	U	C5-C6-N1	5.01	125.20	122.70
2	A	933	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	T	117	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/24 (88%)	21 (100%)	0	0	100	100
4	C	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
5	D	212/217 (98%)	199 (94%)	12 (6%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	29	61
7	F	180/187 (96%)	167 (93%)	12 (7%)	1 (1%)	25	57
8	G	174/179 (97%)	167 (96%)	7 (4%)	0	100	100
9	H	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	55
10	I	124/175 (71%)	115 (93%)	9 (7%)	0	100	100
11	J	131/142 (92%)	124 (95%)	6 (5%)	1 (1%)	19	51
12	K	144/147 (98%)	136 (94%)	8 (6%)	0	100	100
13	L	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
14	M	143/147 (97%)	135 (94%)	7 (5%)	1 (1%)	22	55
15	N	134/138 (97%)	123 (92%)	11 (8%)	0	100	100
16	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100
17	P	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
18	Q	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	R	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
20	S	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
21	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
22	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
23	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
24	W	190/215 (88%)	185 (97%)	5 (3%)	0	100	100
25	X	77/88 (88%)	73 (95%)	4 (5%)	0	100	100
26	Y	61/64 (95%)	61 (100%)	0	0	100	100
27	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
28	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
29	b	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
30	c	47/55 (86%)	45 (96%)	1 (2%)	1 (2%)	7	32
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
32	e	61/64 (95%)	61 (100%)	0	0	100	100
33	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	g	55/75 (73%)	54 (98%)	1 (2%)	0	100	100
36	BB	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
37	BC	206/275 (75%)	190 (92%)	14 (7%)	2 (1%)	15	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BD	198/201 (98%)	186 (94%)	12 (6%)	0	100	100
39	BE	178/214 (83%)	170 (96%)	8 (4%)	0	100	100
40	BF	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
41	BG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
42	BH	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
43	BI	124/150 (83%)	119 (96%)	5 (4%)	0	100	100
44	BJ	97/101 (96%)	90 (93%)	7 (7%)	0	100	100
45	BK	113/138 (82%)	106 (94%)	7 (6%)	0	100	100
46	BL	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
47	BM	114/124 (92%)	106 (93%)	8 (7%)	0	100	100
48	BN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
49	BO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
50	BP	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
51	BQ	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
52	BR	63/84 (75%)	62 (98%)	1 (2%)	0	100	100
53	BS	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
54	BT	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
55	BV	226/277 (82%)	207 (92%)	18 (8%)	1 (0%)	34	66
All	All	5979/6679 (90%)	5688 (95%)	281 (5%)	10 (0%)	50	76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	c	7	VAL
37	BC	125	ASN
5	D	143	ALA
14	M	31	LYS
6	E	90	VAL
11	J	17	ALA
37	BC	162	MET
55	BV	156	LYS
9	H	124	ILE
7	F	131	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	18/19 (95%)	17 (94%)	1 (6%)	21	53
4	C	215/218 (99%)	190 (88%)	25 (12%)	5	22
5	D	160/163 (98%)	141 (88%)	19 (12%)	5	21
6	E	169/173 (98%)	152 (90%)	17 (10%)	7	28
7	F	151/156 (97%)	134 (89%)	17 (11%)	6	23
8	G	148/150 (99%)	136 (92%)	12 (8%)	11	37
9	H	90/116 (78%)	86 (96%)	4 (4%)	28	60
10	I	89/120 (74%)	84 (94%)	5 (6%)	21	53
11	J	102/108 (94%)	91 (89%)	11 (11%)	6	25
12	K	119/120 (99%)	111 (93%)	8 (7%)	16	46
13	L	100/100 (100%)	89 (89%)	11 (11%)	6	24
14	M	112/114 (98%)	102 (91%)	10 (9%)	9	33
15	N	114/116 (98%)	105 (92%)	9 (8%)	12	39
16	O	97/158 (61%)	88 (91%)	9 (9%)	9	31
17	P	93/94 (99%)	85 (91%)	8 (9%)	10	36
18	Q	100/100 (100%)	89 (89%)	11 (11%)	6	24
19	R	97/99 (98%)	92 (95%)	5 (5%)	23	55
20	S	81/83 (98%)	74 (91%)	7 (9%)	10	36
21	T	90/117 (77%)	82 (91%)	8 (9%)	9	33
22	U	83/85 (98%)	80 (96%)	3 (4%)	35	65
23	V	81/86 (94%)	76 (94%)	5 (6%)	18	49
24	W	155/168 (92%)	134 (86%)	21 (14%)	4	17
25	X	58/63 (92%)	54 (93%)	4 (7%)	15	45
26	Y	50/51 (98%)	46 (92%)	4 (8%)	12	38
27	Z	58/66 (88%)	55 (95%)	3 (5%)	23	55
28	a	52/54 (96%)	48 (92%)	4 (8%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	b	43/46 (94%)	36 (84%)	7 (16%)	2	10
30	c	47/52 (90%)	41 (87%)	6 (13%)	4	18
31	d	35/36 (97%)	32 (91%)	3 (9%)	10	36
32	e	53/54 (98%)	47 (89%)	6 (11%)	6	23
33	f	35/35 (100%)	33 (94%)	2 (6%)	20	52
34	g	51/63 (81%)	43 (84%)	8 (16%)	2	12
36	BB	30/31 (97%)	26 (87%)	4 (13%)	4	17
37	BC	170/212 (80%)	156 (92%)	14 (8%)	11	37
38	BD	175/176 (99%)	162 (93%)	13 (7%)	13	41
39	BE	127/147 (86%)	114 (90%)	13 (10%)	7	27
40	BF	85/85 (100%)	77 (91%)	8 (9%)	8	31
41	BG	131/132 (99%)	120 (92%)	11 (8%)	11	36
42	BH	107/108 (99%)	100 (94%)	7 (6%)	17	47
43	BI	102/125 (82%)	90 (88%)	12 (12%)	5	21
44	BJ	89/90 (99%)	82 (92%)	7 (8%)	12	39
45	BK	89/105 (85%)	80 (90%)	9 (10%)	7	28
46	BL	103/105 (98%)	91 (88%)	12 (12%)	5	21
47	BM	99/104 (95%)	85 (86%)	14 (14%)	3	16
48	BN	49/50 (98%)	46 (94%)	3 (6%)	18	49
49	BO	76/77 (99%)	70 (92%)	6 (8%)	12	39
50	BP	92/118 (78%)	84 (91%)	8 (9%)	10	35
51	BQ	80/83 (96%)	72 (90%)	8 (10%)	7	28
52	BR	55/72 (76%)	54 (98%)	1 (2%)	59	79
53	BS	73/84 (87%)	64 (88%)	9 (12%)	4	20
54	BT	69/70 (99%)	59 (86%)	10 (14%)	3	15
55	BV	191/218 (88%)	173 (91%)	18 (9%)	8	31
All	All	4938/5375 (92%)	4478 (91%)	460 (9%)	12	31

All (460) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	7	LYS
4	C	10	THR

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Mol	Chain	Res	Type
4	C	13	ARG
4	C	28	THR
4	C	60	ARG
4	C	63	ARG
4	C	69	ARG
4	C	78	LYS
4	C	89	THR
4	C	116	VAL
4	C	119	SER
4	C	126	LYS
4	C	127	PRO
4	C	131	LEU
4	C	148	ARG
4	C	157	ARG
4	C	161	VAL
4	C	177	MET
4	C	181	GLU
4	C	203	ASN
4	C	211	ARG
4	C	213	ARG
4	C	241	SER
4	C	247	VAL
4	C	265	ASP
4	C	272	ARG
5	D	3	ARG
5	D	19	GLU
5	D	58	SER
5	D	60	ARG
5	D	79	ARG
5	D	86	LEU
5	D	87	ASP
5	D	99	GLN
5	D	102	THR
5	D	129	ARG
5	D	133	ARG
5	D	144	VAL
5	D	154	CYS
5	D	160	VAL
5	D	164	THR
5	D	169	ARG
5	D	170	MET
5	D	192	LEU

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Mol	Chain	Res	Type
5	D	209	ARG
6	E	33	LEU
6	E	34	MET
6	E	36	GLN
6	E	50	HIS
6	E	66	TYR
6	E	71	THR
6	E	78	SER
6	E	79	THR
6	E	97	ASP
6	E	128	THR
6	E	135	THR
6	E	137	SER
6	E	148	LEU
6	E	161	THR
6	E	169	VAL
6	E	181	ASP
6	E	201	LEU
7	F	10	ARG
7	F	11	LEU
7	F	31	ASN
7	F	44	ASN
7	F	49	ASP
7	F	83	GLN
7	F	87	ARG
7	F	102	ARG
7	F	148	ILE
7	F	150	VAL
7	F	151	ASP
7	F	157	ARG
7	F	159	MET
7	F	162	THR
7	F	164	VAL
7	F	165	THR
7	F	182	PHE
8	G	3	ARG
8	G	16	ASP
8	G	48	ASP
8	G	59	GLU
8	G	65	LEU
8	G	72	LEU
8	G	77	VAL

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Mol	Chain	Res	Type
8	G	89	GLU
8	G	114	VAL
8	G	126	VAL
8	G	137	ILE
8	G	153	ARG
9	H	4	ILE
9	H	25	TYR
9	H	88	THR
9	H	137	HIS
10	I	5	ASP
10	I	23	THR
10	I	55	THR
10	I	79	ILE
10	I	82	VAL
11	J	15	ILE
11	J	30	LEU
11	J	35	VAL
11	J	36	ASN
11	J	42	LYS
11	J	48	THR
11	J	52	ARG
11	J	55	VAL
11	J	87	VAL
11	J	113	THR
11	J	114	LYS
12	K	10	ASP
12	K	17	VAL
12	K	70	THR
12	K	93	LEU
12	K	96	HIS
12	K	118	ILE
12	K	129	ASP
12	K	145	VAL
13	L	13	ASN
13	L	40	VAL
13	L	58	VAL
13	L	69	ARG
13	L	73	ASP
13	L	77	ILE
13	L	87	ILE
13	L	90	ASP
13	L	96	THR

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Mol	Chain	Res	Type
13	L	107	ARG
13	L	112	MET
14	M	22	VAL
14	M	24	ARG
14	M	43	ARG
14	M	46	VAL
14	M	49	MET
14	M	82	ASP
14	M	89	GLN
14	M	92	THR
14	M	104	VAL
14	M	105	ARG
15	N	3	ILE
15	N	7	VAL
15	N	10	ARG
15	N	18	ARG
15	N	20	ILE
15	N	51	ARG
15	N	72	ARG
15	N	82	ARG
15	N	135	GLU
16	O	6	LYS
16	O	9	ARG
16	O	10	LEU
16	O	37	THR
16	O	64	ARG
16	O	74	ASP
16	O	96	ARG
16	O	100	VAL
16	O	114	GLU
17	P	6	VAL
17	P	10	ILE
17	P	12	GLU
17	P	24	ARG
17	P	32	THR
17	P	51	LEU
17	P	69	ASP
17	P	74	ASP
18	Q	15	ASP
18	Q	25	VAL
18	Q	32	ILE
18	Q	38	ARG

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Mol	Chain	Res	Type
18	Q	54	ILE
18	Q	57	THR
18	Q	71	ARG
18	Q	79	ASN
18	Q	81	ASP
18	Q	91	VAL
18	Q	93	ARG
19	R	6	ARG
19	R	28	ARG
19	R	29	SER
19	R	33	ARG
19	R	44	THR
20	S	3	THR
20	S	27	LEU
20	S	53	ASP
20	S	54	ASP
20	S	58	VAL
20	S	68	THR
20	S	72	LYS
21	T	19	VAL
21	T	22	THR
21	T	26	ARG
21	T	81	VAL
21	T	99	ARG
21	T	102	ARG
21	T	104	ARG
21	T	107	THR
22	U	20	SER
22	U	62	ARG
22	U	81	ARG
23	V	30	ARG
23	V	38	VAL
23	V	42	LYS
23	V	69	SER
23	V	91	THR
24	W	12	THR
24	W	14	ASN
24	W	15	VAL
24	W	42	THR
24	W	64	ASN
24	W	67	LEU
24	W	68	THR

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Mol	Chain	Res	Type
24	W	99	VAL
24	W	104	GLU
24	W	112	VAL
24	W	114	VAL
24	W	119	THR
24	W	130	THR
24	W	131	ILE
24	W	138	LEU
24	W	139	SER
24	W	146	VAL
24	W	148	VAL
24	W	151	VAL
24	W	158	THR
24	W	172	SER
25	X	11	ARG
25	X	38	VAL
25	X	39	ARG
25	X	80	ILE
26	Y	23	ARG
26	Y	24	ARG
26	Y	28	ARG
26	Y	45	ASN
27	Z	36	MET
27	Z	44	ASN
27	Z	48	ARG
28	a	3	GLU
28	a	20	ARG
28	a	36	VAL
28	a	48	ASN
29	b	3	VAL
29	b	6	ARG
29	b	8	MET
29	b	10	ARG
29	b	14	ARG
29	b	35	GLN
29	b	39	VAL
30	c	6	ASP
30	c	11	ILE
30	c	12	THR
30	c	25	THR
30	c	38	ILE
30	c	47	THR

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Mol	Chain	Res	Type
31	d	13	ARG
31	d	15	ARG
31	d	46	THR
32	e	11	SER
32	e	13	ARG
32	e	19	THR
32	e	47	ARG
32	e	56	SER
32	e	59	ASN
33	f	2	LYS
33	f	7	VAL
34	g	9	TYR
34	g	12	THR
34	g	22	PHE
34	g	24	THR
34	g	32	THR
34	g	37	VAL
34	g	46	THR
34	g	58	VAL
36	BB	4	VAL
36	BB	6	LYS
36	BB	10	LYS
36	BB	24	THR
37	BC	21	ARG
37	BC	23	TYR
37	BC	35	ASP
37	BC	46	LEU
37	BC	62	ARG
37	BC	71	ARG
37	BC	82	GLU
37	BC	103	LEU
37	BC	153	CYS
37	BC	167	PHE
37	BC	169	ARG
37	BC	182	ILE
37	BC	193	PHE
37	BC	204	LYS
38	BD	10	ARG
38	BD	20	VAL
38	BD	23	ASP
38	BD	86	LEU
38	BD	102	LEU

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Mol	Chain	Res	Type
38	BD	110	ARG
38	BD	119	LEU
38	BD	123	VAL
38	BD	131	ARG
38	BD	145	LEU
38	BD	156	THR
38	BD	177	VAL
38	BD	188	VAL
39	BE	37	ILE
39	BE	39	ARG
39	BE	41	VAL
39	BE	59	THR
39	BE	70	MET
39	BE	71	VAL
39	BE	95	ASN
39	BE	96	PHE
39	BE	97	PHE
39	BE	110	VAL
39	BE	156	ASP
39	BE	176	GLU
39	BE	198	ARG
40	BF	30	ILE
40	BF	43	TRP
40	BF	57	GLU
40	BF	72	VAL
40	BF	77	ARG
40	BF	85	VAL
40	BF	87	ARG
40	BF	91	LEU
41	BG	3	ARG
41	BG	24	THR
41	BG	38	LEU
41	BG	79	ARG
41	BG	80	VAL
41	BG	99	LEU
41	BG	102	ARG
41	BG	129	ASN
41	BG	138	ARG
41	BG	144	MET
41	BG	149	ARG
42	BH	14	LEU
42	BH	48	ASP

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Mol	Chain	Res	Type
42	BH	55	ARG
42	BH	79	ARG
42	BH	82	LYS
42	BH	92	THR
42	BH	101	LEU
43	BI	29	VAL
43	BI	38	ARG
43	BI	40	ARG
43	BI	45	THR
43	BI	67	LEU
43	BI	78	VAL
43	BI	83	ILE
43	BI	87	LEU
43	BI	88	ASP
43	BI	100	ARG
43	BI	147	TYR
43	BI	150	ARG
44	BJ	15	HIS
44	BJ	18	ILE
44	BJ	32	THR
44	BJ	50	CYS
44	BJ	57	LYS
44	BJ	78	ASP
44	BJ	97	ASP
45	BK	25	VAL
45	BK	40	ILE
45	BK	49	ASN
45	BK	68	THR
45	BK	95	VAL
45	BK	121	ASP
45	BK	128	ASN
45	BK	131	ARG
45	BK	137	ARG
46	BL	3	THR
46	BL	21	THR
46	BL	27	SER
46	BL	29	GLN
46	BL	38	TYR
46	BL	41	THR
46	BL	49	LEU
46	BL	63	VAL
46	BL	70	GLU

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Mol	Chain	Res	Type
46	BL	73	ASN
46	BL	87	VAL
46	BL	104	THR
47	BM	42	ASN
47	BM	49	THR
47	BM	51	ASP
47	BM	56	LEU
47	BM	60	ILE
47	BM	63	ASN
47	BM	64	LEU
47	BM	69	ASP
47	BM	70	LEU
47	BM	80	ARG
47	BM	101	GLN
47	BM	109	THR
47	BM	110	ARG
47	BM	115	ARG
48	BN	24	CYS
48	BN	45	ARG
48	BN	56	VAL
49	BO	46	HIS
49	BO	65	ARG
49	BO	75	VAL
49	BO	82	ILE
49	BO	83	GLU
49	BO	89	ARG
50	BP	3	VAL
50	BP	9	ARG
50	BP	36	VAL
50	BP	50	GLN
50	BP	67	THR
50	BP	86	LEU
50	BP	90	GLU
50	BP	97	GLU
51	BQ	28	VAL
51	BQ	48	LEU
51	BQ	54	ARG
51	BQ	65	ASN
51	BQ	85	THR
51	BQ	89	ARG
51	BQ	92	GLU
51	BQ	93	ILE

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Mol	Chain	Res	Type
52	BR	31	ASP
53	BS	3	ARG
53	BS	11	VAL
53	BS	12	ASP
53	BS	15	LEU
53	BS	51	VAL
53	BS	63	THR
53	BS	67	VAL
53	BS	78	ARG
53	BS	79	THR
54	BT	3	ASN
54	BT	6	SER
54	BT	18	ARG
54	BT	26	SER
54	BT	43	ASP
54	BT	45	ASP
54	BT	50	LEU
54	BT	51	LEU
54	BT	59	ASP
54	BT	81	LEU
55	BV	23	TRP
55	BV	24	ASN
55	BV	32	PHE
55	BV	38	ILE
55	BV	66	THR
55	BV	75	GLN
55	BV	83	GLU
55	BV	102	THR
55	BV	113	ARG
55	BV	114	LEU
55	BV	146	ARG
55	BV	167	ASN
55	BV	169	GLU
55	BV	178	LYS
55	BV	184	ILE
55	BV	186	ILE
55	BV	189	THR
55	BV	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
1	3	18	HIS
4	C	76	ASN
4	C	91	ASN
4	C	129	ASN
4	C	130	ASN
4	C	143	HIS
4	C	205	ASN
5	D	34	ASN
5	D	130	HIS
5	D	179	ASN
6	E	100	GLN
6	E	125	HIS
6	E	151	ASN
6	E	202	ASN
7	F	146	HIS
8	G	66	HIS
8	G	86	GLN
9	H	11	HIS
9	H	147	ASN
10	I	100	ASN
11	J	32	GLN
11	J	33	HIS
12	K	77	HIS
12	K	103	ASN
12	K	132	HIS
13	L	3	GLN
14	M	54	GLN
14	M	58	HIS
14	M	76	GLN
14	M	127	ASN
15	N	123	HIS
16	O	17	GLN
17	P	22	HIS
18	Q	26	ASN
18	Q	79	ASN
19	R	11	GLN
19	R	41	HIS
19	R	72	ASN
19	R	94	ASN
19	R	122	ASN
20	S	67	HIS
20	S	76	HIS

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Mol	Chain	Res	Type
20	S	85	HIS
21	T	67	ASN
22	U	41	GLN
22	U	61	ASN
23	V	31	ASN
23	V	67	HIS
23	V	101	ASN
24	W	46	HIS
24	W	93	GLN
24	W	94	HIS
25	X	29	GLN
25	X	44	HIS
26	Y	22	HIS
26	Y	45	ASN
29	b	36	GLN
30	c	22	ASN
30	c	48	HIS
32	e	25	GLN
32	e	31	HIS
37	BC	8	HIS
38	BD	51	GLN
38	BD	77	GLN
38	BD	84	ASN
38	BD	115	HIS
39	BE	146	HIS
39	BE	157	ASN
39	BE	160	ASN
39	BE	163	HIS
40	BF	80	ASN
41	BG	28	ASN
41	BG	106	ASN
43	BI	57	ASN
43	BI	64	HIS
43	BI	146	GLN
45	BK	27	HIS
45	BK	49	ASN
45	BK	128	ASN
46	BL	29	GLN
46	BL	73	ASN
47	BM	101	GLN
48	BN	11	ASN
49	BO	28	GLN

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Mol	Chain	Res	Type
50	BP	41	HIS
50	BP	81	GLN
51	BQ	46	HIS
51	BQ	62	HIS
53	BS	52	HIS
53	BS	57	HIS
54	BT	52	HIS
54	BT	68	HIS
54	BT	70	ASN
54	BT	71	GLN
55	BV	24	ASN
55	BV	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	740 (23%)	29 (0%)
3	B	117/118 (99%)	23 (19%)	1 (0%)
35	BA	1510/1528 (98%)	362 (23%)	13 (0%)
56	BW	75/76 (98%)	20 (26%)	0
57	BX	5/6 (83%)	2 (40%)	0
All	All	4825/4848 (99%)	1147 (23%)	43 (0%)

All (1147) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	33	G
2	A	46	A
2	A	55	G
2	A	59	G
2	A	60	A
2	A	68	A
2	A	71	A
2	A	72	G
2	A	83	C

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Mol	Chain	Res	Type
2	A	89	A
2	A	90	C
2	A	91	C
2	A	94	G
2	A	98	U
2	A	99	G
2	A	115	A
2	A	116	A
2	A	117	U
2	A	125	C
2	A	128	G
2	A	133	G
2	A	136	U
2	A	137	G
2	A	143	G
2	A	145	G
2	A	148	A
2	A	161	U
2	A	164	A
2	A	171	U
2	A	172	C
2	A	175	G
2	A	177	G
2	A	195	A
2	A	198	A
2	A	203	A
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	237	C
2	A	248	G
2	A	264	G
2	A	270	U
2	A	271	A
2	A	272	A

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Mol	Chain	Res	Type
2	A	274	C
2	A	275	C
2	A	279	U
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C
2	A	292	G
2	A	293	G
2	A	294	G
2	A	297	G
2	A	299	G
2	A	300	G
2	A	301	U
2	A	302	U
2	A	303	G
2	A	305	G
2	A	306	U
2	A	312	G
2	A	314	G
2	A	315	U
2	A	316	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	323	C
2	A	324	C
2	A	326	A
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	343	U
2	A	344	G
2	A	345	G
2	A	346	C

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Mol	Chain	Res	Type
2	A	348	G
2	A	349	G
2	A	350	A
2	A	351	G
2	A	352	G
2	A	356	G
2	A	357	U
2	A	358	G
2	A	361	A
2	A	364	A
2	A	369	G
2	A	370	U
2	A	376	G
2	A	383	U
2	A	384	G
2	A	387	U
2	A	388	U
2	A	393	U
2	A	399	G
2	A	404	A
2	A	406	A
2	A	412	A
2	A	413	G
2	A	417	C
2	A	424	G
2	A	426	G
2	A	434	G
2	A	438	U
2	A	445	U
2	A	446	G
2	A	450	G
2	A	452	G
2	A	454	U
2	A	459	A
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	490	A
2	A	491	U
2	A	493	U
2	A	494	G

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Mol	Chain	Res	Type
2	A	498	G
2	A	499	G
2	A	500	A
2	A	505	C
2	A	509	U
2	A	512	G
2	A	542	A
2	A	543	U
2	A	544	U
2	A	562	G
2	A	567	A
2	A	569	G
2	A	570	U
2	A	581	G
2	A	589	A
2	A	591	G
2	A	592	A
2	A	594	U
2	A	595	A
2	A	596	C
2	A	605	G
2	A	614	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	630	U
2	A	631	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	644	G
2	A	647	G
2	A	655	G
2	A	663	A
2	A	665	G
2	A	666	A
2	A	667	A

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Mol	Chain	Res	Type
2	A	675	G
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	700	U
2	A	701	A
2	A	704	C
2	A	706	G
2	A	707	G
2	A	708	G
2	A	709	U
2	A	721	A
2	A	728	G
2	A	731	A
2	A	738	A
2	A	740	A
2	A	742	G
2	A	747	A
2	A	753	A
2	A	757	G
2	A	758	A
2	A	759	G
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	767	U
2	A	768	G
2	A	774	G
2	A	783	G
2	A	784	G
2	A	785	A
2	A	793	C
2	A	801	U
2	A	816	G
2	A	827	G
2	A	829	U
2	A	832	G
2	A	839	U
2	A	845	C

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Mol	Chain	Res	Type
2	A	862	U
2	A	863	G
2	A	864	A
2	A	868	C
2	A	872	G
2	A	878	G
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	892	G
2	A	897	A
2	A	899	G
2	A	900	G
2	A	917	A
2	A	919	A
2	A	920	G
2	A	921	C
2	A	927	C
2	A	942	U
2	A	960	G
2	A	961	U
2	A	971	G
2	A	972	A
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A
2	A	994	A
2	A	995	U
2	A	996	G
2	A	1000	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1005	A
2	A	1007	G
2	A	1009	U
2	A	1010	U
2	A	1011	A
2	A	1012	C
2	A	1013	U

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Mol	Chain	Res	Type
2	A	1014	G
2	A	1022	C
2	A	1025	A
2	A	1030	C
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1058	A
2	A	1063	G
2	A	1070	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G
2	A	1091	A
2	A	1092	G
2	A	1099	A
2	A	1101	A
2	A	1114	G
2	A	1130	C
2	A	1131	G
2	A	1140	G
2	A	1143	G
2	A	1144	A
2	A	1148	G
2	A	1151	U
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1174	G
2	A	1175	A
2	A	1176	G
2	A	1178	U
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G

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Mol	Chain	Res	Type
2	A	1190	C
2	A	1191	A
2	A	1192	G
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1204	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1217	G
2	A	1219	U
2	A	1227	C
2	A	1229	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1237	U
2	A	1238	G
2	A	1239	C
2	A	1240	G
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1275	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1294	U
2	A	1324	G
2	A	1325	U
2	A	1332	G
2	A	1335	G

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Mol	Chain	Res	Type
2	A	1339	G
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1359	G
2	A	1362	A
2	A	1363	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1380	A
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1390	A
2	A	1404	C
2	A	1415	A
2	A	1416	A
2	A	1417	A
2	A	1435	C
2	A	1437	A
2	A	1440	C
2	A	1448	C
2	A	1456	G
2	A	1457	A
2	A	1461	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U
2	A	1499	A
2	A	1502	G
2	A	1507	G
2	A	1510	A
2	A	1518	A
2	A	1521	C
2	A	1522	G
2	A	1531	C
2	A	1532	G
2	A	1533	U
2	A	1534	C

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Mol	Chain	Res	Type
2	A	1540	U
2	A	1541	G
2	A	1543	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1574	G
2	A	1578	G
2	A	1579	C
2	A	1587	G
2	A	1596	C
2	A	1599	U
2	A	1600	G
2	A	1625	G
2	A	1627	U
2	A	1628	A
2	A	1629	G
2	A	1631	A
2	A	1632	G
2	A	1633	U
2	A	1637	G
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1659	U
2	A	1670	G
2	A	1673	A
2	A	1674	G
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1703	G

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Mol	Chain	Res	Type
2	A	1710	A
2	A	1711	G
2	A	1714	A
2	A	1715	A
2	A	1717	U
2	A	1723	U
2	A	1724	G
2	A	1728	U
2	A	1729	A
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1738	G
2	A	1745	U
2	A	1746	G
2	A	1754	G
2	A	1755	A
2	A	1756	G
2	A	1757	U
2	A	1761	G
2	A	1767	U
2	A	1774	U
2	A	1785	C
2	A	1786	G
2	A	1789	A
2	A	1792	A
2	A	1796	U
2	A	1798	U
2	A	1802	G
2	A	1803	A
2	A	1806	A
2	A	1813	C
2	A	1826	A
2	A	1845	G
2	A	1857	U
2	A	1862	C
2	A	1864	U
2	A	1866	C
2	A	1867	G
2	A	1869	G
2	A	1870	U
2	A	1871	G

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Mol	Chain	Res	Type
2	A	1872	A
2	A	1892	G
2	A	1893	C
2	A	1916	A
2	A	1932	U
2	A	1933	G
2	A	1945	U
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1950	G
2	A	1967	G
2	A	1973	C
2	A	1974	A
2	A	1975	A
2	A	1981	U
2	A	1990	A
2	A	1999	U
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2064	A
2	A	2065	A
2	A	2066	G
2	A	2073	A
2	A	2075	G
2	A	2084	A
2	A	2085	C
2	A	2086	U
2	A	2087	C
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A

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Mol	Chain	Res	Type
2	A	2107	G
2	A	2108	A
2	A	2111	U
2	A	2112	U
2	A	2120	A
2	A	2129	C
2	A	2130	G
2	A	2131	G
2	A	2137	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2153	G
2	A	2154	G
2	A	2160	A
2	A	2162	A
2	A	2163	U
2	A	2164	U
2	A	2179	U
2	A	2184	A
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2197	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2227	A
2	A	2235	C
2	A	2244	A
2	A	2247	A
2	A	2251	G
2	A	2254	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2274	C
2	A	2276	G

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Mol	Chain	Res	Type
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2299	C
2	A	2316	G
2	A	2320	C
2	A	2324	A
2	A	2325	U
2	A	2328	G
2	A	2329	G
2	A	2333	G
2	A	2334	U
2	A	2335	G
2	A	2336	U
2	A	2338	G
2	A	2339	G
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2362	C
2	A	2368	C
2	A	2371	G
2	A	2372	U
2	A	2380	G
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2389	U
2	A	2390	U

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Mol	Chain	Res	Type
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2410	A
2	A	2413	G
2	A	2418	U
2	A	2421	A
2	A	2422	A
2	A	2427	G
2	A	2434	A
2	A	2436	A
2	A	2447	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2483	G
2	A	2502	A
2	A	2503	G
2	A	2504	G
2	A	2507	C
2	A	2508	C
2	A	2511	A
2	A	2529	A
2	A	2532	G
2	A	2545	G
2	A	2549	G
2	A	2551	A
2	A	2558	C
2	A	2559	A
2	A	2567	U
2	A	2571	C
2	A	2574	C

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Mol	Chain	Res	Type
2	A	2585	U
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2626	U
2	A	2627	C
2	A	2643	U
2	A	2647	U
2	A	2649	A
2	A	2650	A
2	A	2653	G
2	A	2654	A
2	A	2655	U
2	A	2659	A
2	A	2665	C
2	A	2669	G
2	A	2672	A
2	A	2673	U
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2702	A
2	A	2705	G
2	A	2715	U
2	A	2726	G
2	A	2729	G
2	A	2732	G
2	A	2742	A
2	A	2744	C
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2796	A
2	A	2797	C
2	A	2802	G

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Mol	Chain	Res	Type
2	A	2806	G
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2839	U
2	A	2853	C
2	A	2856	A
2	A	2862	G
2	A	2885	G
2	A	2887	G
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2938	G
2	A	2948	C
2	A	2950	C
2	A	2956	G
2	A	2957	A
2	A	2968	G
2	A	2972	A
2	A	2982	A
2	A	2985	G
2	A	2989	A
2	A	3002	A
2	A	3004	C
2	A	3005	A
2	A	3009	U
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3020	U
2	A	3021	A
2	A	3022	G
2	A	3024	A
2	A	3027	G
2	A	3029	U
2	A	3042	A
2	A	3047	A
2	A	3056	A
2	A	3082	U

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Mol	Chain	Res	Type
2	A	3088	C
2	A	3093	A
2	A	3095	C
2	A	3101	C
2	A	3105	C
2	A	3106	C
2	A	3107	G
2	A	3112	A
2	A	3113	A
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	7	G
3	B	11	U
3	B	12	C
3	B	13	C
3	B	14	A
3	B	22	A
3	B	23	G
3	B	25	G
3	B	30	G
3	B	31	C
3	B	35	G
3	B	42	C
3	B	57	U
3	B	58	A
3	B	85	C
3	B	87	U
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	112	C
3	B	115	A
35	BA	8	U
35	BA	9	U
35	BA	11	G
35	BA	12	A
35	BA	13	G
35	BA	26	G
35	BA	36	A
35	BA	43	G

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Mol	Chain	Res	Type
35	BA	45	G
35	BA	48	G
35	BA	51	C
35	BA	52	U
35	BA	53	U
35	BA	54	A
35	BA	55	A
35	BA	58	C
35	BA	59	A
35	BA	68	G
35	BA	77	G
35	BA	81	C
35	BA	82	U
35	BA	83	U
35	BA	85	C
35	BA	87	G
35	BA	92	A
35	BA	93	C
35	BA	101	G
35	BA	116	A
35	BA	117	C
35	BA	118	A
35	BA	123	G
35	BA	128	U
35	BA	136	G
35	BA	139	C
35	BA	160	C
35	BA	174	G
35	BA	179	C
35	BA	180	A
35	BA	192	G
35	BA	194	A
35	BA	200	U
35	BA	201	G
35	BA	209	A
35	BA	210	A
35	BA	211	A
35	BA	214	U
35	BA	215	U
35	BA	216	U
35	BA	217	U
35	BA	218	G

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Mol	Chain	Res	Type
35	BA	220	G
35	BA	226	G
35	BA	227	G
35	BA	242	U
35	BA	243	A
35	BA	245	C
35	BA	247	G
35	BA	251	G
35	BA	254	G
35	BA	266	G
35	BA	267	C
35	BA	279	A
35	BA	280	C
35	BA	281	G
35	BA	289	G
35	BA	301	G
35	BA	316	C
35	BA	319	G
35	BA	321	A
35	BA	329	A
35	BA	332	G
35	BA	344	A
35	BA	345	C
35	BA	350	G
35	BA	351	G
35	BA	352	C
35	BA	353	A
35	BA	354	G
35	BA	356	A
35	BA	367	U
35	BA	372	C
35	BA	373	A
35	BA	382	A
35	BA	390	U
35	BA	392	C
35	BA	397	A
35	BA	398	C
35	BA	406	G
35	BA	411	A
35	BA	414	A
35	BA	421	U
35	BA	422	C

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Mol	Chain	Res	Type
35	BA	423	G
35	BA	424	G
35	BA	426	U
35	BA	427	U
35	BA	428	G
35	BA	429	U
35	BA	430	A
35	BA	434	C
35	BA	438	U
35	BA	451	A
35	BA	452	A
35	BA	453	G
35	BA	454	C
35	BA	456	C
35	BA	457	A
35	BA	458	A
35	BA	459	G
35	BA	461	G
35	BA	465	G
35	BA	466	U
35	BA	473	A
35	BA	477	G
35	BA	478	A
35	BA	479	A
35	BA	485	G
35	BA	486	G
35	BA	491	C
35	BA	496	U
35	BA	497	G
35	BA	498	C
35	BA	499	C
35	BA	505	C
35	BA	507	G
35	BA	509	G
35	BA	511	U
35	BA	512	A
35	BA	513	A
35	BA	515	A
35	BA	520	G
35	BA	525	C
35	BA	527	A
35	BA	539	A

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Mol	Chain	Res	Type
35	BA	542	U
35	BA	544	C
35	BA	552	A
35	BA	553	A
35	BA	554	A
35	BA	556	A
35	BA	557	G
35	BA	602	A
35	BA	612	U
35	BA	613	G
35	BA	633	A
35	BA	641	G
35	BA	645	G
35	BA	666	U
35	BA	667	A
35	BA	668	G
35	BA	680	G
35	BA	683	G
35	BA	700	C
35	BA	701	G
35	BA	702	G
35	BA	703	U
35	BA	711	G
35	BA	713	G
35	BA	729	A
35	BA	735	G
35	BA	757	A
35	BA	761	A
35	BA	764	A
35	BA	765	G
35	BA	772	A
35	BA	773	U
35	BA	774	A
35	BA	779	G
35	BA	782	A
35	BA	789	G
35	BA	794	A
35	BA	795	A
35	BA	797	C
35	BA	799	G
35	BA	808	A
35	BA	818	U

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Mol	Chain	Res	Type
35	BA	821	C
35	BA	822	U
35	BA	823	U
35	BA	824	C
35	BA	825	C
35	BA	826	U
35	BA	827	U
35	BA	828	G
35	BA	840	G
35	BA	841	U
35	BA	865	C
35	BA	871	A
35	BA	884	G
35	BA	896	A
35	BA	901	A
35	BA	908	G
35	BA	909	G
35	BA	913	C
35	BA	914	C
35	BA	915	G
35	BA	916	C
35	BA	917	A
35	BA	921	G
35	BA	924	G
35	BA	930	C
35	BA	932	U
35	BA	940	A
35	BA	942	U
35	BA	943	U
35	BA	947	U
35	BA	948	G
35	BA	950	A
35	BA	951	A
35	BA	953	G
35	BA	955	G
35	BA	956	A
35	BA	957	A
35	BA	959	A
35	BA	971	G
35	BA	973	U
35	BA	974	U
35	BA	975	G

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Mol	Chain	Res	Type
35	BA	982	A
35	BA	984	A
35	BA	985	G
35	BA	986	G
35	BA	987	A
35	BA	988	C
35	BA	992	G
35	BA	999	A
35	BA	1000	U
35	BA	1007	U
35	BA	1008	C
35	BA	1010	C
35	BA	1013	G
35	BA	1014	U
35	BA	1020	G
35	BA	1021	U
35	BA	1024	G
35	BA	1025	C
35	BA	1028	G
35	BA	1030	G
35	BA	1033	G
35	BA	1034	C
35	BA	1045	U
35	BA	1048	G
35	BA	1054	G
35	BA	1074	G
35	BA	1075	U
35	BA	1079	G
35	BA	1081	A
35	BA	1088	G
35	BA	1104	G
35	BA	1108	C
35	BA	1112	C
35	BA	1115	G
35	BA	1116	U
35	BA	1117	U
35	BA	1118	A
35	BA	1120	G
35	BA	1123	G
35	BA	1128	C
35	BA	1129	U
35	BA	1132	U

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Mol	Chain	Res	Type
35	BA	1138	A
35	BA	1139	C
35	BA	1140	U
35	BA	1141	G
35	BA	1147	G
35	BA	1149	C
35	BA	1150	A
35	BA	1152	C
35	BA	1162	G
35	BA	1164	U
35	BA	1165	G
35	BA	1176	C
35	BA	1177	A
35	BA	1178	A
35	BA	1181	C
35	BA	1182	A
35	BA	1183	U
35	BA	1193	U
35	BA	1194	A
35	BA	1206	U
35	BA	1207	C
35	BA	1217	A
35	BA	1219	A
35	BA	1231	A
35	BA	1233	A
35	BA	1238	U
35	BA	1239	G
35	BA	1241	G
35	BA	1248	U
35	BA	1251	G
35	BA	1260	A
35	BA	1261	A
35	BA	1266	U
35	BA	1267	U
35	BA	1268	C
35	BA	1269	A
35	BA	1271	A
35	BA	1272	G
35	BA	1281	A
35	BA	1282	G
35	BA	1283	U
35	BA	1284	U

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Mol	Chain	Res	Type
35	BA	1285	C
35	BA	1287	G
35	BA	1299	C
35	BA	1301	A
35	BA	1302	C
35	BA	1304	C
35	BA	1305	G
35	BA	1313	G
35	BA	1320	G
35	BA	1322	G
35	BA	1327	U
35	BA	1328	A
35	BA	1329	G
35	BA	1335	G
35	BA	1343	G
35	BA	1344	C
35	BA	1345	A
35	BA	1346	A
35	BA	1347	C
35	BA	1351	G
35	BA	1353	G
35	BA	1357	A
35	BA	1363	U
35	BA	1364	U
35	BA	1381	A
35	BA	1382	C
35	BA	1383	C
35	BA	1385	C
35	BA	1389	U
35	BA	1402	G
35	BA	1405	G
35	BA	1407	U
35	BA	1409	A
35	BA	1424	G
35	BA	1425	G
35	BA	1426	C
35	BA	1429	A
35	BA	1430	A
35	BA	1433	C
35	BA	1434	U
35	BA	1435	U
35	BA	1436	G

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Mol	Chain	Res	Type
35	BA	1438	G
35	BA	1459	G
35	BA	1466	G
35	BA	1471	G
35	BA	1478	G
35	BA	1481	G
35	BA	1483	A
35	BA	1486	A
35	BA	1487	A
35	BA	1488	G
35	BA	1490	U
35	BA	1501	G
35	BA	1502	A
35	BA	1503	A
35	BA	1504	G
35	BA	1513	G
35	BA	1514	G
35	BA	1516	U
56	BW	2	C
56	BW	6	G
56	BW	8	U
56	BW	16	U
56	BW	17	C
56	BW	18	G
56	BW	19	G
56	BW	20	U
56	BW	21	A
56	BW	22	G
56	BW	23	A
56	BW	32	U
56	BW	37	A
56	BW	42	C
56	BW	46	G
56	BW	47	U
56	BW	48	C
56	BW	52	G
56	BW	69	G
56	BW	76	A
57	BX	2	U
57	BX	3	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	284	G
2	A	287	A
2	A	316	U
2	A	357	U
2	A	445	U
2	A	759	G
2	A	919	A
2	A	974	G
2	A	980	C
2	A	981	U
2	A	1004	C
2	A	1010	U
2	A	1046	C
2	A	1084	U
2	A	1186	G
2	A	1231	U
2	A	1368	A
2	A	1713	U
2	A	1730	U
2	A	1947	U
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2350	G
2	A	2381	A
2	A	2626	U
2	A	3113	A
3	B	10	G
35	BA	422	C
35	BA	429	U
35	BA	456	C
35	BA	485	G
35	BA	498	C
35	BA	895	A
35	BA	1007	U
35	BA	1116	U
35	BA	1117	U
35	BA	1149	C
35	BA	1266	U
35	BA	1477	A
35	BA	1482	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 632 ligands modelled in this entry, 631 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
60	PHE	BW	101	-	10,11,12	0.78	0	10,13,15	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PHE	BW	101	-	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

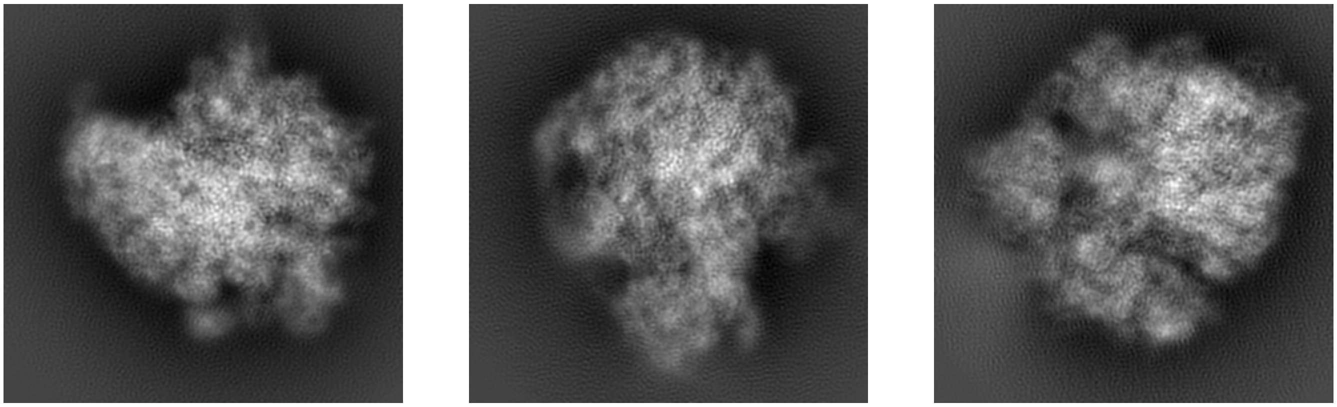
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3751. 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

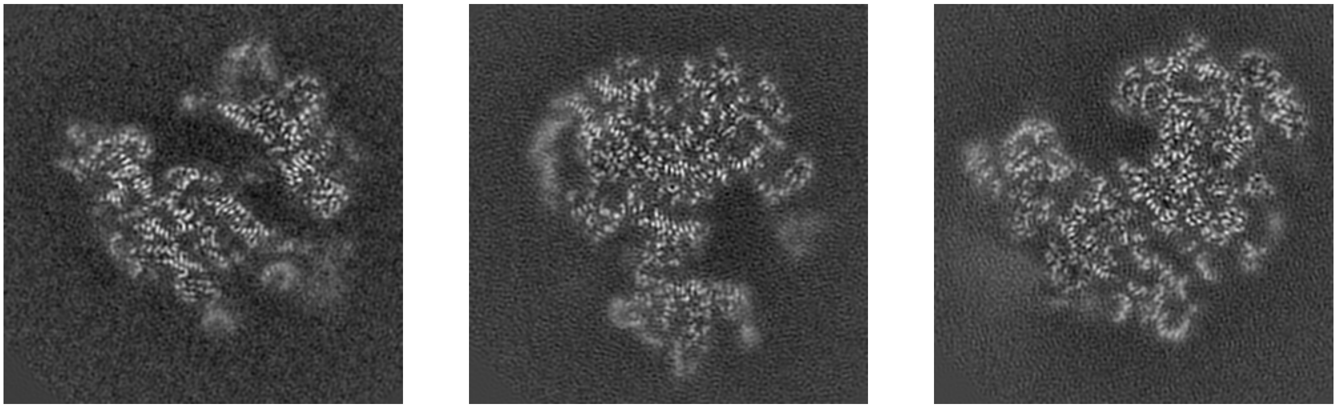


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

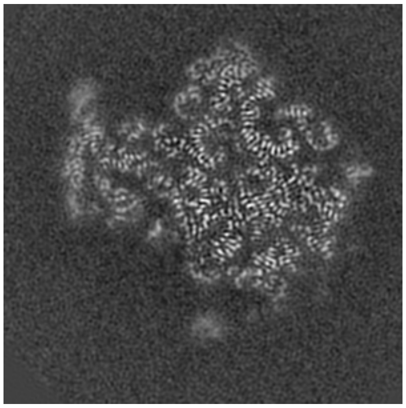


X Index: 108 Y Index: 108 Z Index: 108

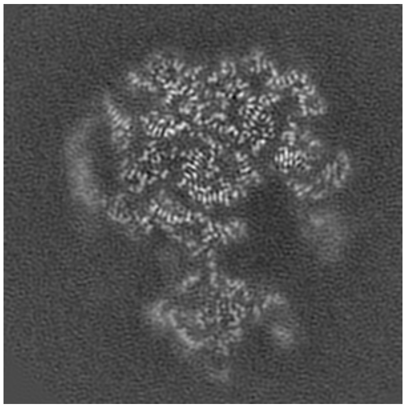
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

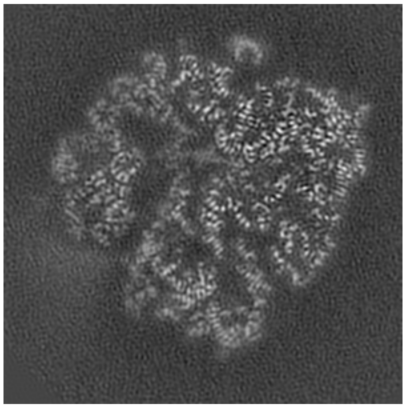
6.3.1 Primary map



X Index: 126



Y Index: 112



Z Index: 123

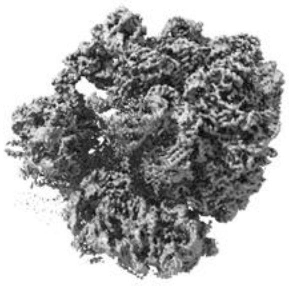
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

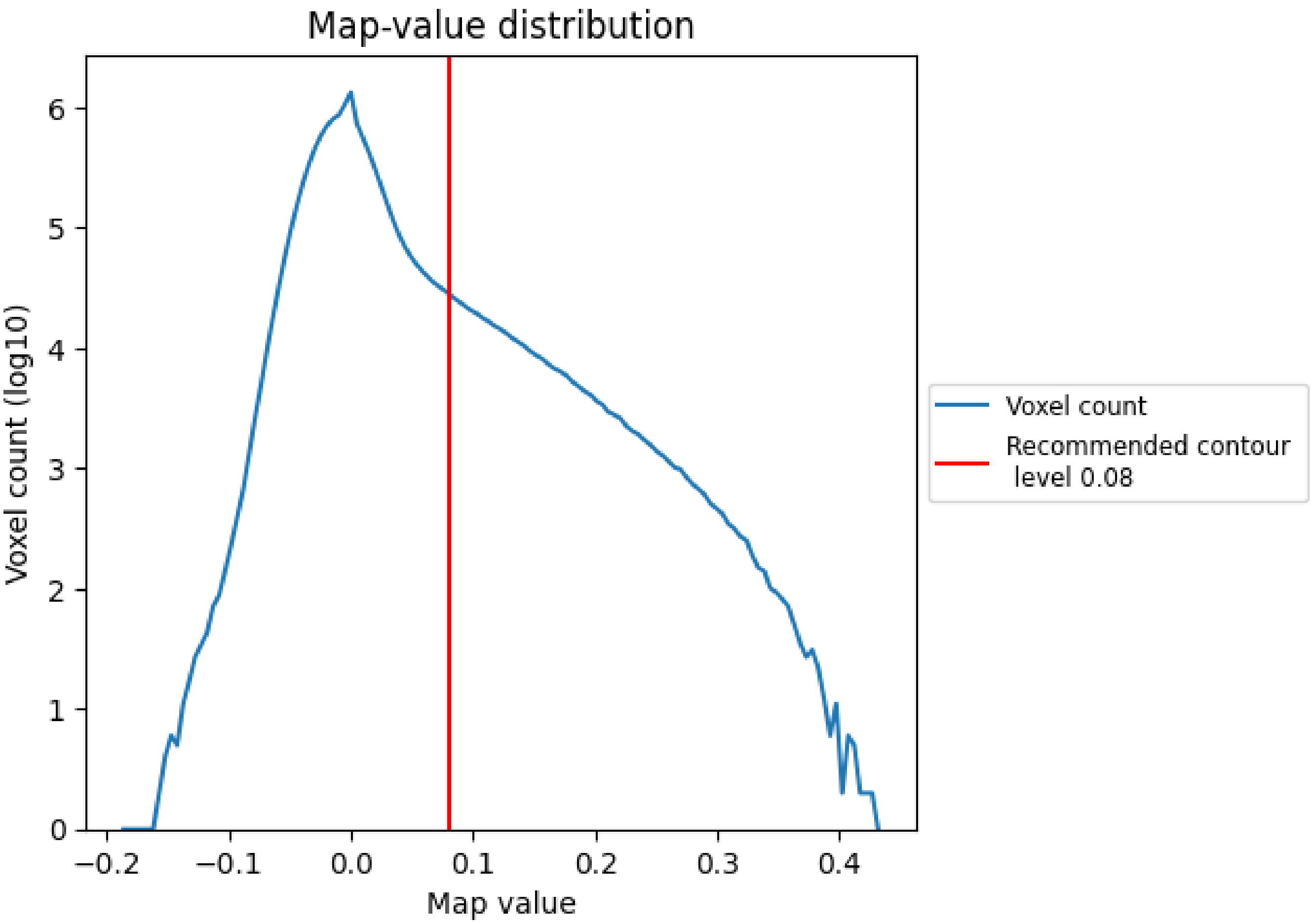
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

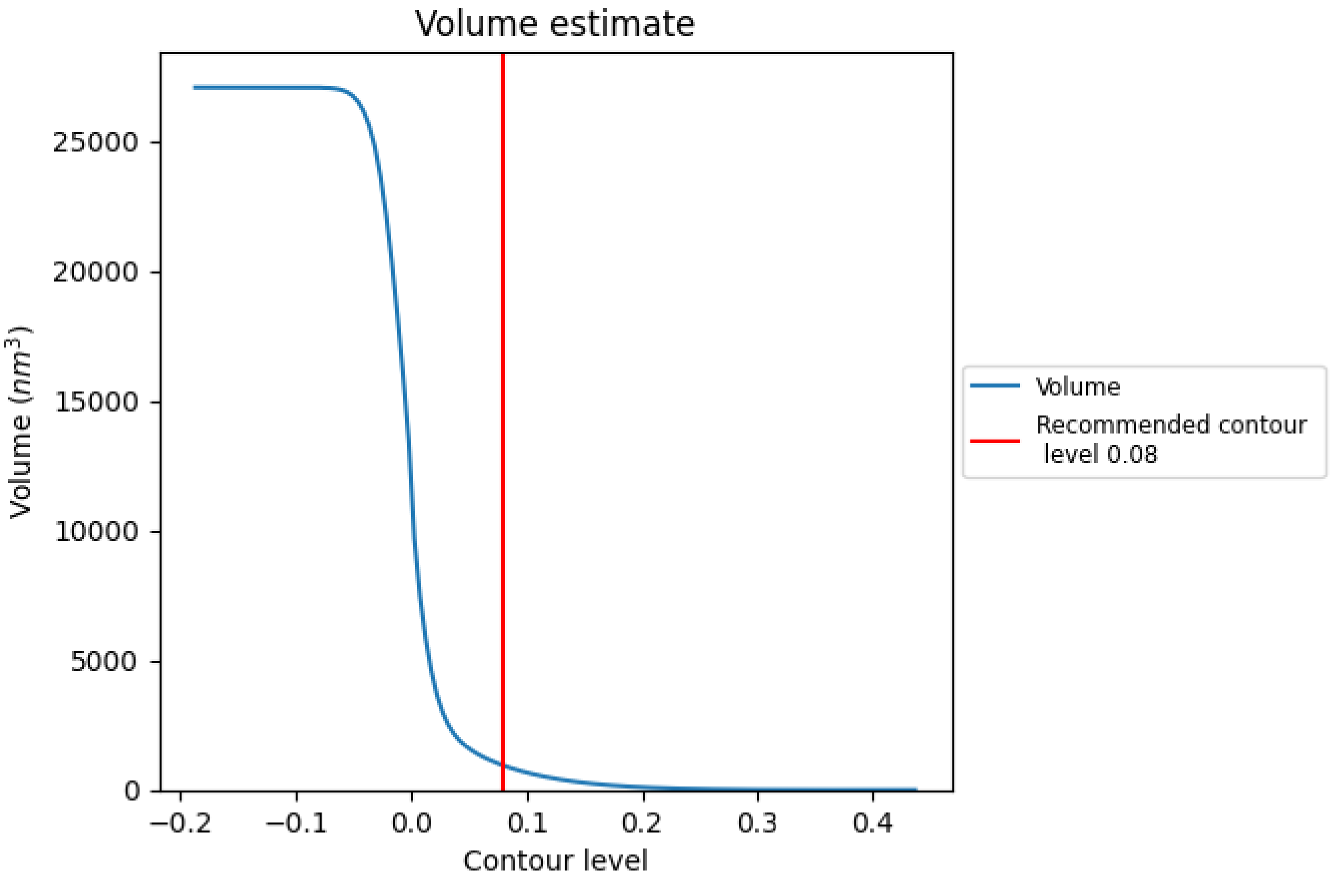
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

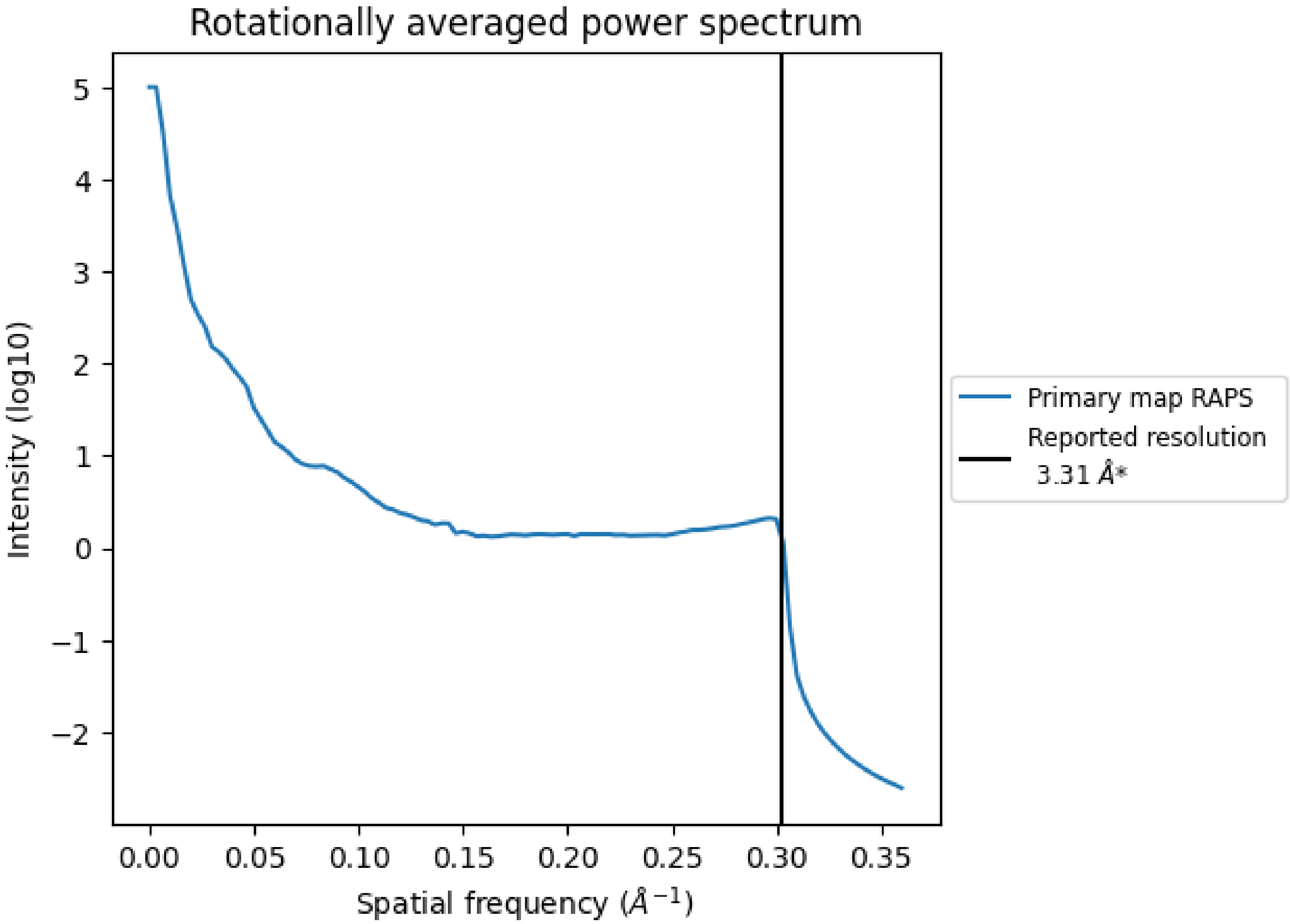
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 945 nm^3; this corresponds to an approximate mass of 853 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)

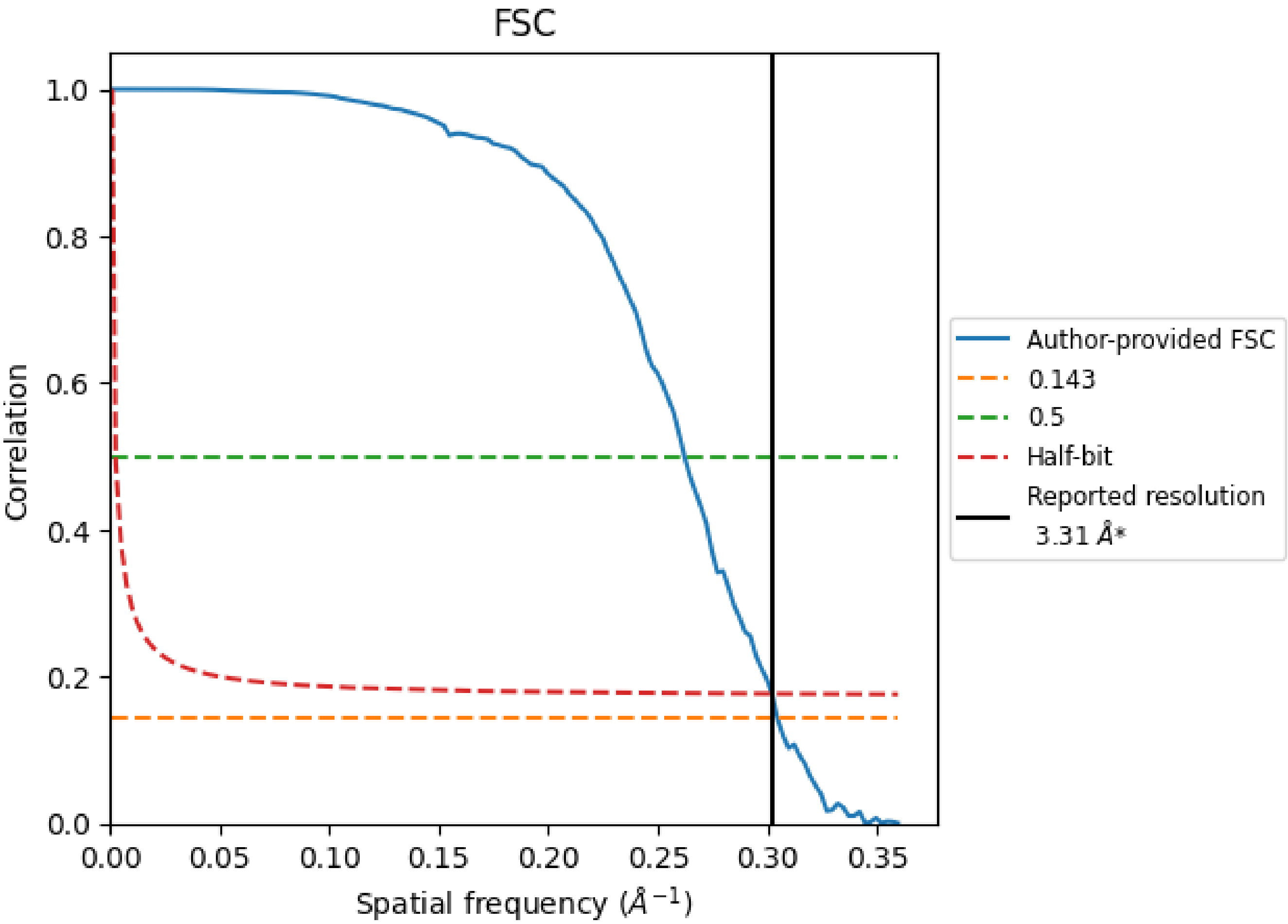


*Reported resolution corresponds to spatial frequency of 0.302 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.302 $Å^{-1}$

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.28	3.81	3.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

This section was not generated.