Full wwPDB EM Validation Report ⓘ

Oct 13, 2022 – 03:41 am BST

PDB ID	:	7PIR
EMDB ID	:	EMD-13448
Title	:	70S ribosome with A*- and P/E-site tRNAs in pseudouridimycin-treated Mycoplasma pneumoniae cells
Authors	:	Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on	:	2021-08-23
Resolution	:	12.10 Å(reported)
Based on initial models	:	7OOD, 7OOC, 4V7C

This is a Full wwPDB EM Validation 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:

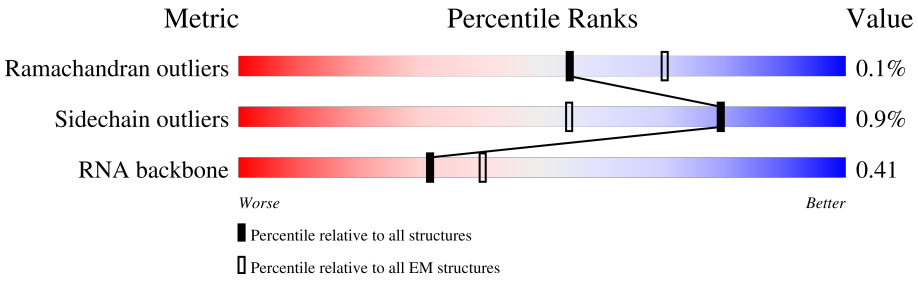
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 12.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	48	98% ·
2	1	59	97% ·
3	2	37	100%
4	A	294	18% 80% · 18%
5	B	273	10% 78% 21%
6	C	205	13% 98% ··
7	D	219	9% 70% 30%
8	E	215	17% 77% 22%

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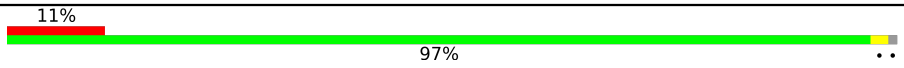
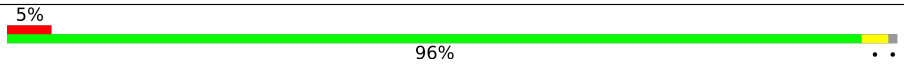
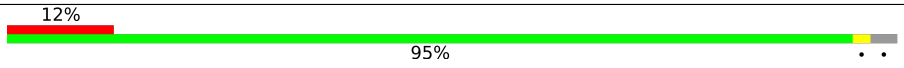
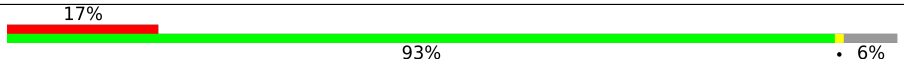
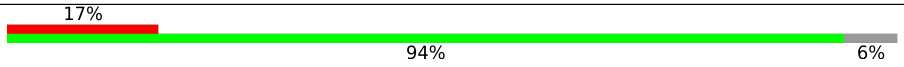
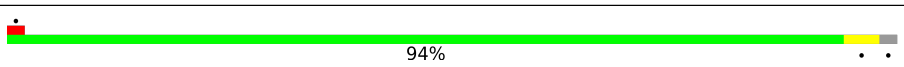
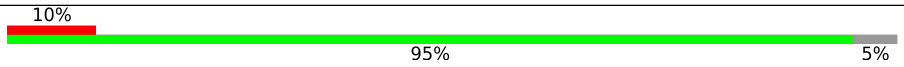
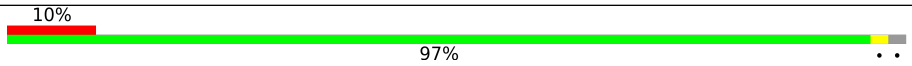
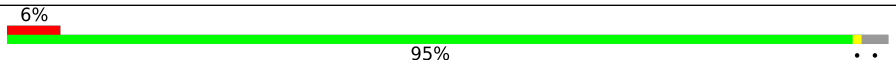
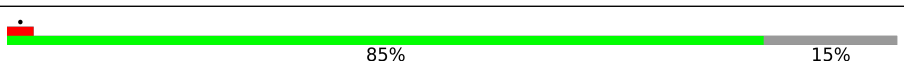
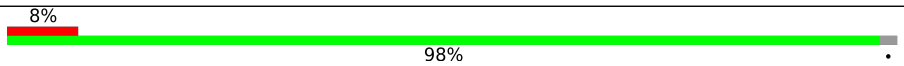
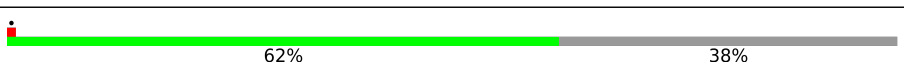
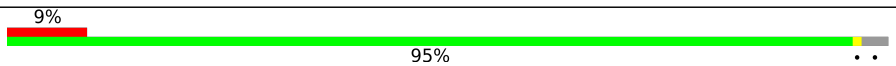
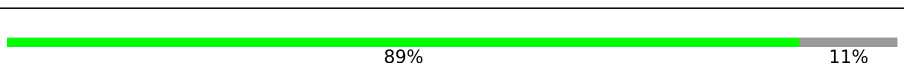
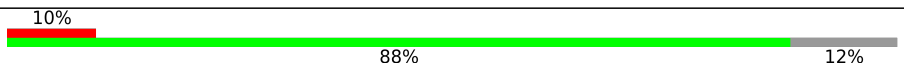
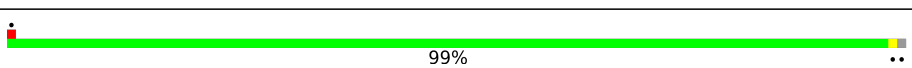
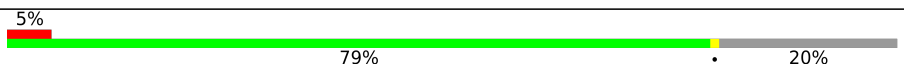
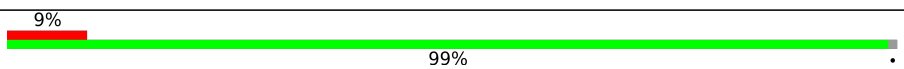
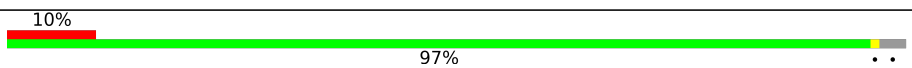
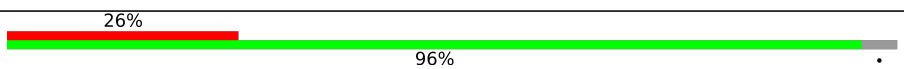
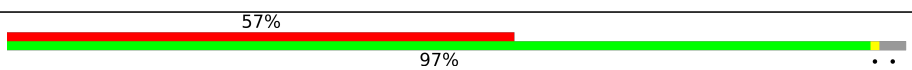
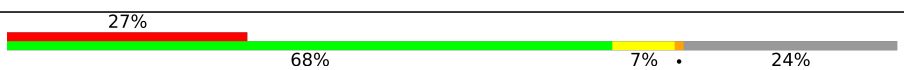
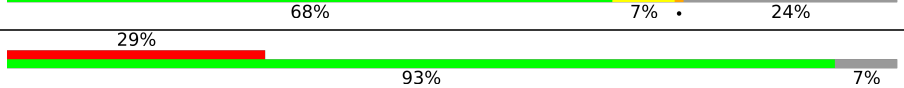
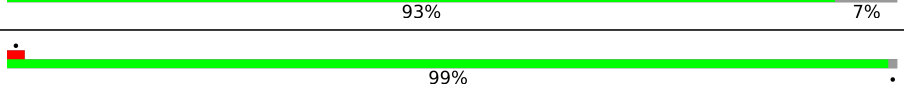
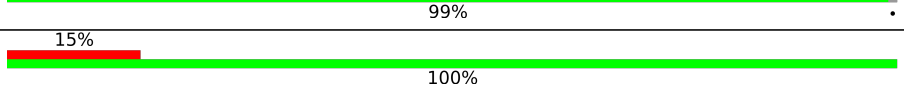
Mol	Chain	Length	Quality of chain
9	F	155	
10	G	142	
11	H	132	
12	I	108	
13	J	121	
14	K	139	
15	L	124	
16	M	61	
17	N	86	
18	O	94	
19	P	85	
20	Q	104	
21	R	87	
22	S	87	
23	T	60	
24	a	287	
25	b	287	
26	c	212	
27	d	180	
28	e	184	
29	f	149	
30	g	161	
31	h	137	
32	i	146	
33	j	122	

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Mol	Chain	Length	Quality of chain
34	k	151	11% 98%
35	l	139	5% 98%
36	m	124	94%
37	n	116	9% 97%
38	o	119	8% 97%
39	p	127	89% 10%
40	q	100	8% 98%
41	r	159	87% 13%
42	s	237	39% 61%
43	t	111	13% 100%
44	u	104	83% 17%
45	v	65	95%
46	w	111	5% 90% 10%
47	x	97	16% 45% 55%
48	y	57	5% 93% 5%
49	z	53	94% 6%
50	3	2907	62% 36%
51	4	108	61% 35%
52	5	1520	64% 34%
53	6	76	59% 39%
53	8	76	59% 39%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 146081 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	47	380	236	81	61	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	477	300	99	77	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	37	304	189	65	46	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	240	1921	1226	334	352	9	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	215	1698	1073	313	307	5	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	203	1660	1051	314	290	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	118	Total	C	N	O	0	0
			951	594	191	166		

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	83	Total	C	N	O	0	0
			673	428	125	120		

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	83	Total	C	N	O	0	0
			675	425	135	115		

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	65	Total	C	N	O	S	0	0
			535	342	103	86	4		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	84	Total	C	N	O	S	0	0
			682	435	127	118	2		

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	77	Total	C	N	O	0	0
			629	383	135	111		

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	53	Total	C	N	O	S	0	0
			471	295	103	72	1		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	145	Total	C	N	O	S	0	0
			1160	746	204	207	3		

- Molecule 30 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	122	Total	C	N	O	S	0	0
			921	586	162	170	3		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	k	148	Total	C	N	O	0	0
			1153	731	226	196		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	112	Total	C	N	O	S	0	0
			889	557	175	155	2		

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	115	Total	C	N	O	S	0	0
			938	592	180	165	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	114	Total	C	N	O	S	0	0
			947	603	188	154	2		

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	92	Total	C	N	O	S	0	0
			720	475	122	122	1		

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	111	Total	C	N	O	S	0	0
			872	550	166	153	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	86	Total	C	N	O	S	0	0
			657	409	130	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	63	Total	C	N	O	S	0	0
			513	317	108	87	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	w	100	Total	C	N	O	0	0
			818	517	153	148		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 49 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 50 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

- Molecule 53 is a RNA chain called tRNA-Phe.

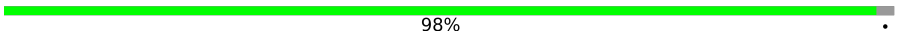
Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		
53	8	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		

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.

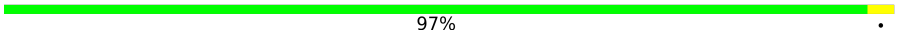
• Molecule 1: 50S ribosomal protein L34

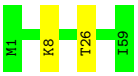
Chain 0:



• Molecule 2: 50S ribosomal protein L35

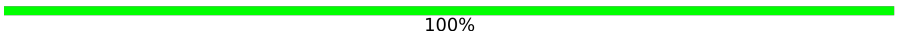
Chain 1:





• Molecule 3: 50S ribosomal protein L36

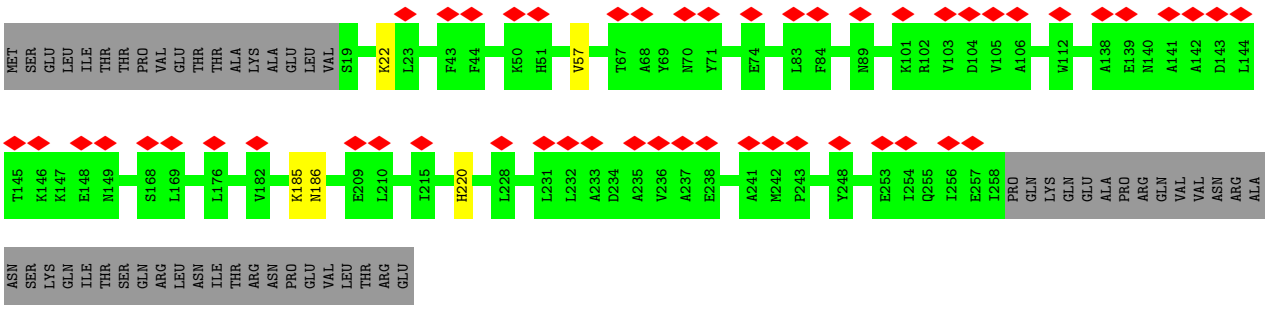
Chain 2:



There are no outlier residues recorded for this chain.

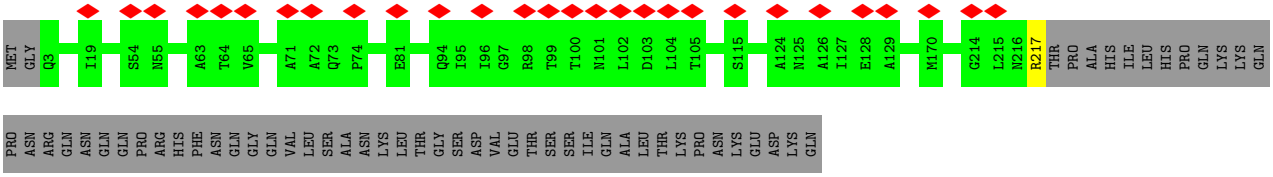
• Molecule 4: 30S ribosomal protein S2

Chain A:

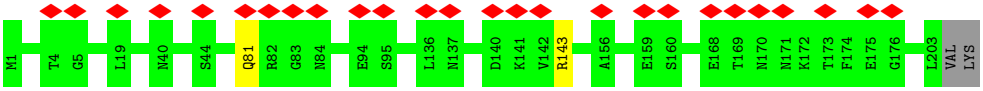


• Molecule 5: 30S ribosomal protein S3

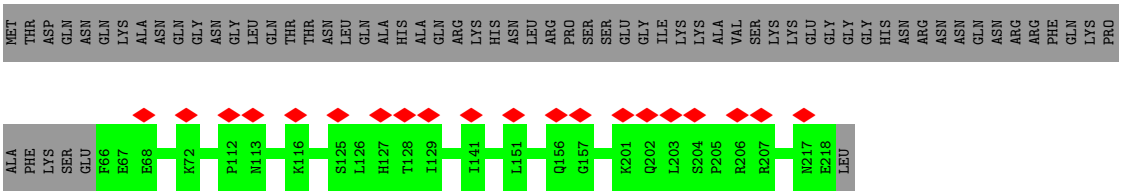
Chain B:



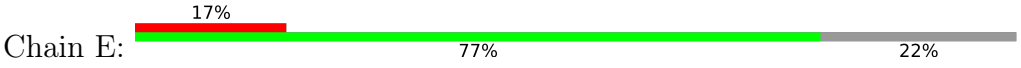
• Molecule 6: 30S ribosomal protein S4

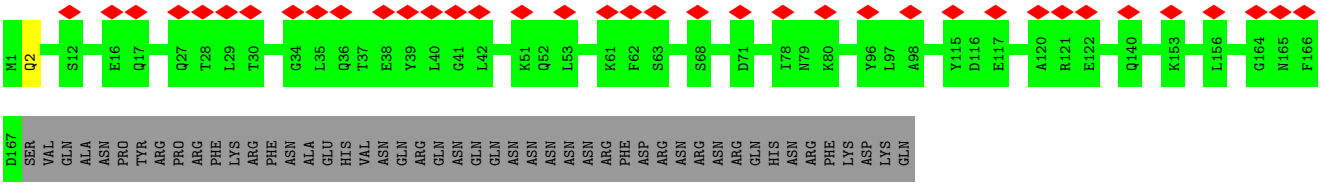


• Molecule 7: 30S ribosomal protein S5

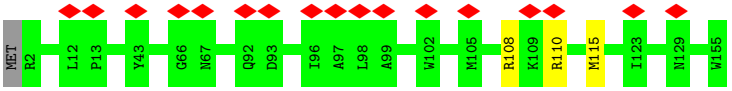


• Molecule 8: 30S ribosomal protein S6

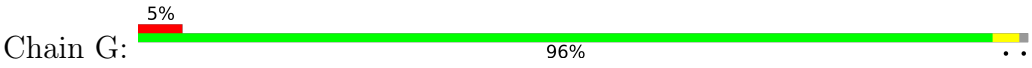


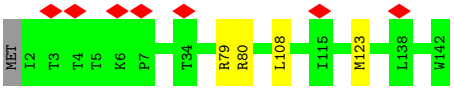


• Molecule 9: 30S ribosomal protein S7



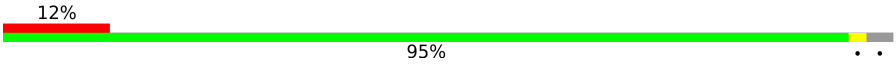
• Molecule 10: 30S ribosomal protein S8

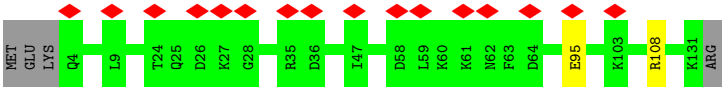




• Molecule 11: 30S ribosomal protein S9

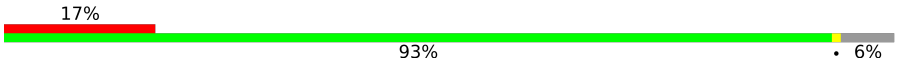
Chain H:

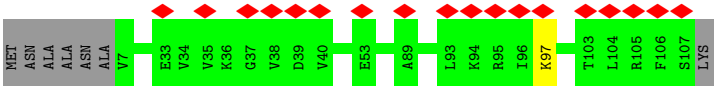




• Molecule 12: 30S ribosomal protein S10

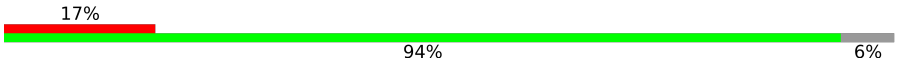
Chain I:

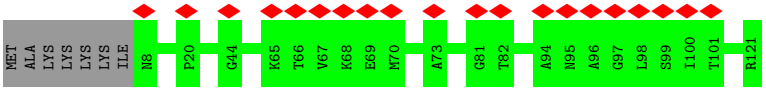




• Molecule 13: 30S ribosomal protein S11

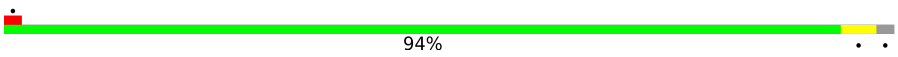
Chain J:





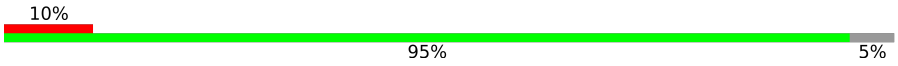
• Molecule 14: 30S ribosomal protein S12

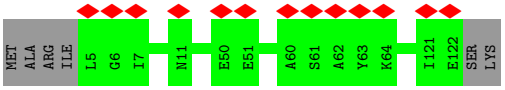
Chain K:



• Molecule 15: 30S ribosomal protein S13

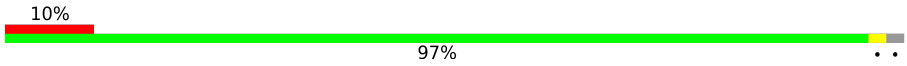
Chain L:

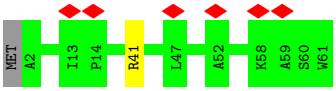




• Molecule 16: 30S ribosomal protein S14 type Z

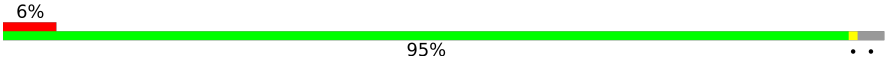
Chain M:

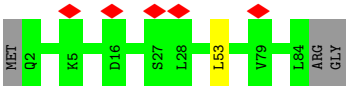




• Molecule 17: 30S ribosomal protein S15

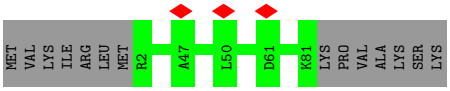
Chain N:





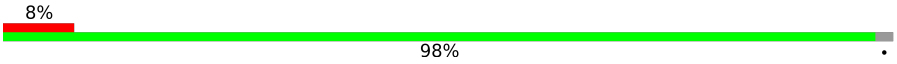
• Molecule 18: 30S ribosomal protein S16

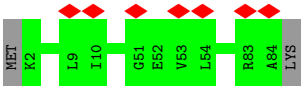
Chain O:



• Molecule 19: 30S ribosomal protein S17

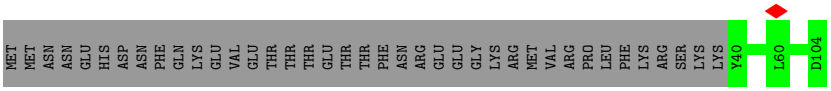
Chain P:





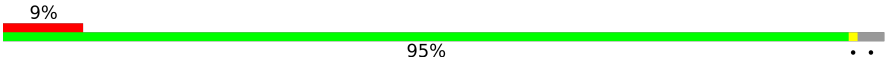
• Molecule 20: 30S ribosomal protein S18

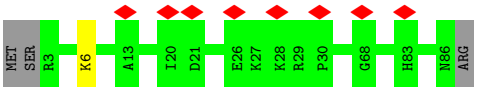
Chain Q:



• Molecule 21: 30S ribosomal protein S19

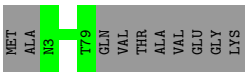
Chain R:





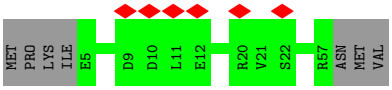
• Molecule 22: 30S ribosomal protein S20

Chain S:



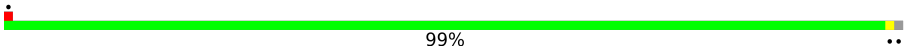
• Molecule 23: 30S ribosomal protein S21

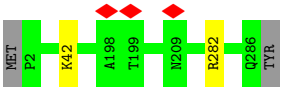
Chain T:



• Molecule 24: 50S ribosomal protein L2

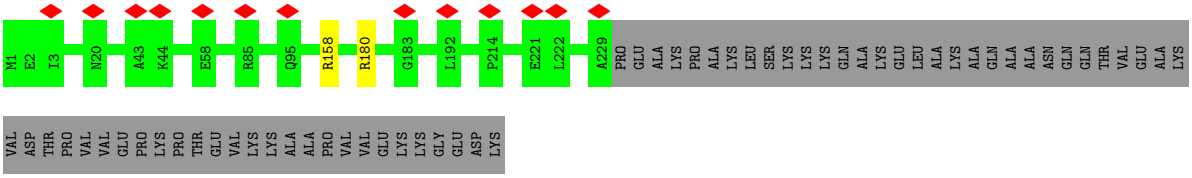
Chain a:





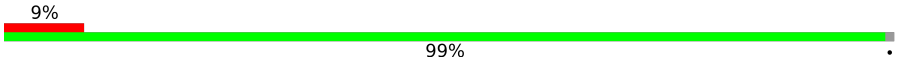
• Molecule 25: 50S ribosomal protein L3

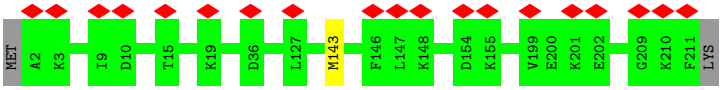
Chain b:



• Molecule 26: 50S ribosomal protein L4

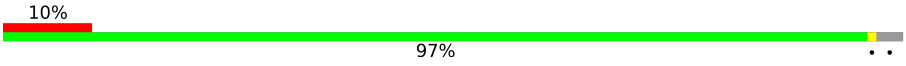
Chain c:

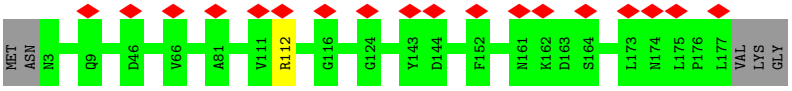




• Molecule 27: 50S ribosomal protein L5

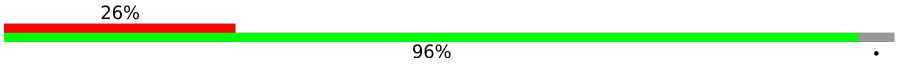
Chain d:

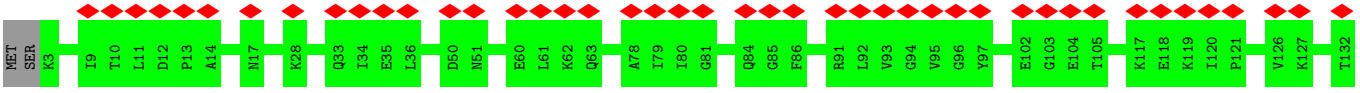


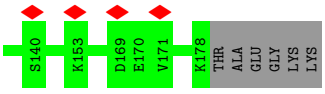


• Molecule 28: 50S ribosomal protein L6

Chain e:

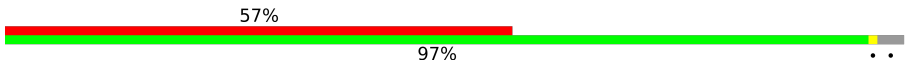


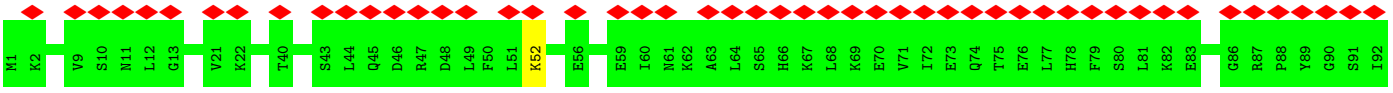


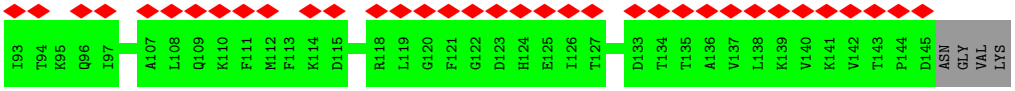


• Molecule 29: 50S ribosomal protein L9

Chain f:

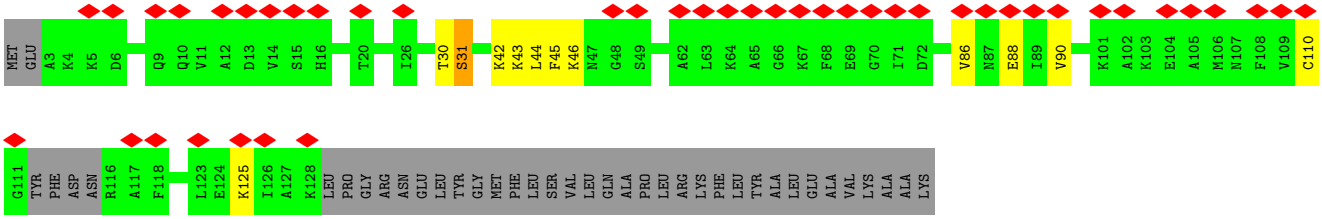






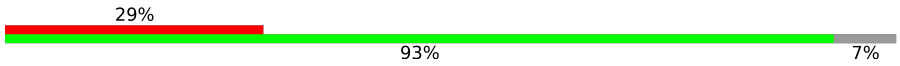
• Molecule 30: 50S ribosomal protein L10

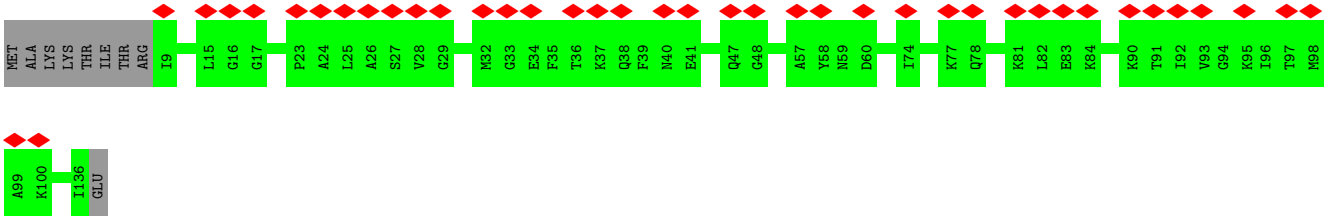
Chain g:



• Molecule 31: 50S ribosomal protein L11

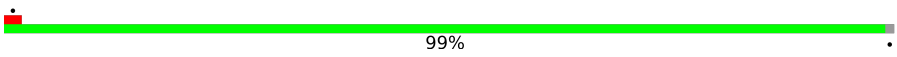
Chain h:

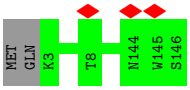




• Molecule 32: 50S ribosomal protein L13

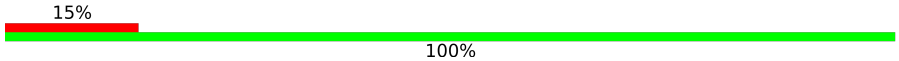
Chain i:

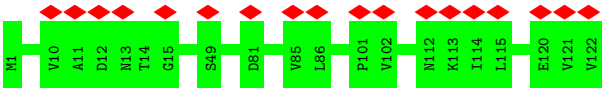




• Molecule 33: 50S ribosomal protein L14

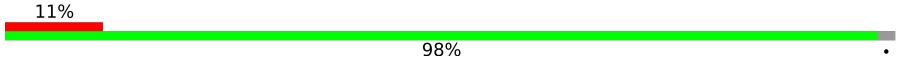
Chain j:

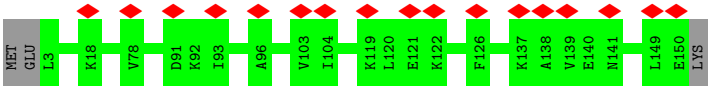




• Molecule 34: 50S ribosomal protein L15

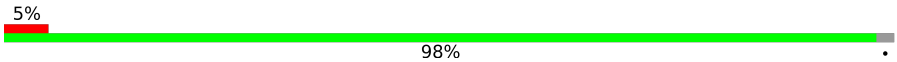
Chain k:

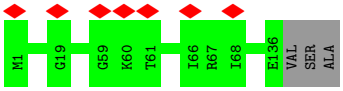




• Molecule 35: 50S ribosomal protein L16

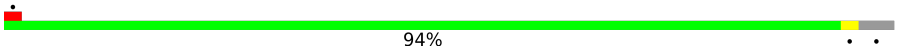
Chain l:

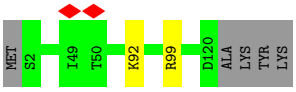




• Molecule 36: 50S ribosomal protein L17

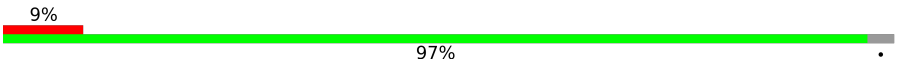
Chain m:

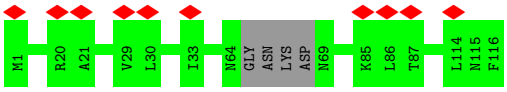




• Molecule 37: 50S ribosomal protein L18

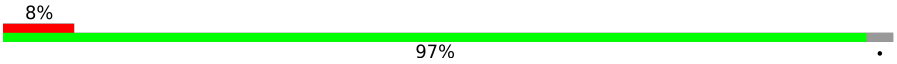
Chain n:

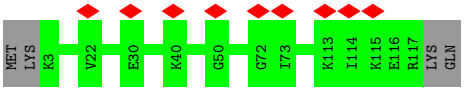




• Molecule 38: 50S ribosomal protein L19

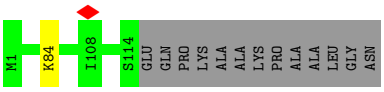
Chain o:





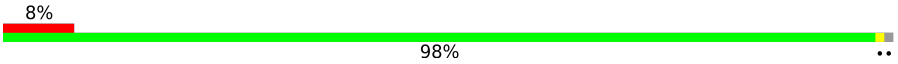
• Molecule 39: 50S ribosomal protein L20

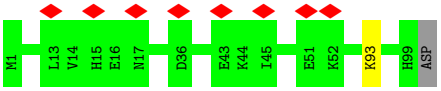
Chain p:



• Molecule 40: 50S ribosomal protein L21

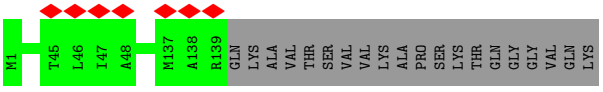
Chain q:





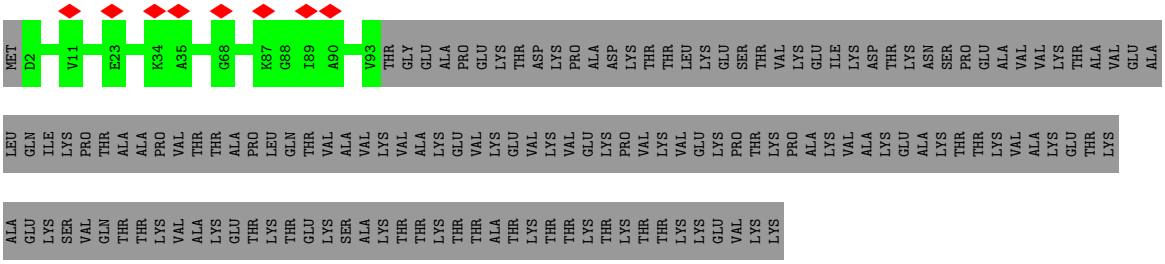
• Molecule 41: 50S ribosomal protein L22

Chain r:



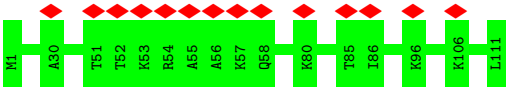
• Molecule 42: 50S ribosomal protein L23

Chain s:



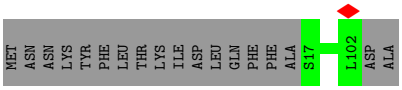
• Molecule 43: 50S ribosomal protein L24

Chain t:



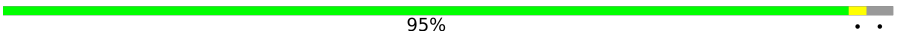
• Molecule 44: 50S ribosomal protein L27

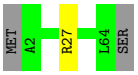
Chain u:



• Molecule 45: 50S ribosomal protein L28

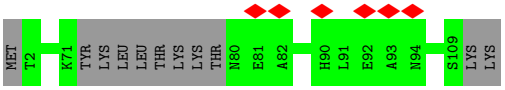
Chain v:





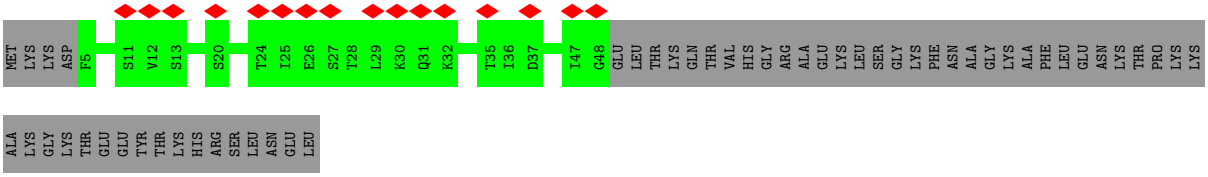
• Molecule 46: 50S ribosomal protein L29

Chain w:



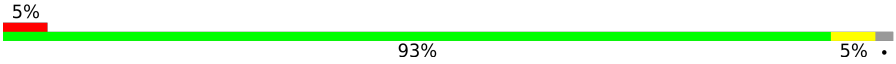
• Molecule 47: 50S ribosomal protein L31

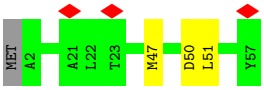
Chain x:



• Molecule 48: 50S ribosomal protein L32

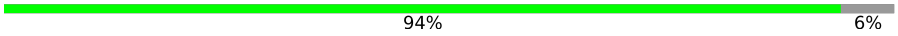
Chain y:

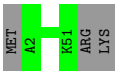




• Molecule 49: 50S ribosomal protein L33 1

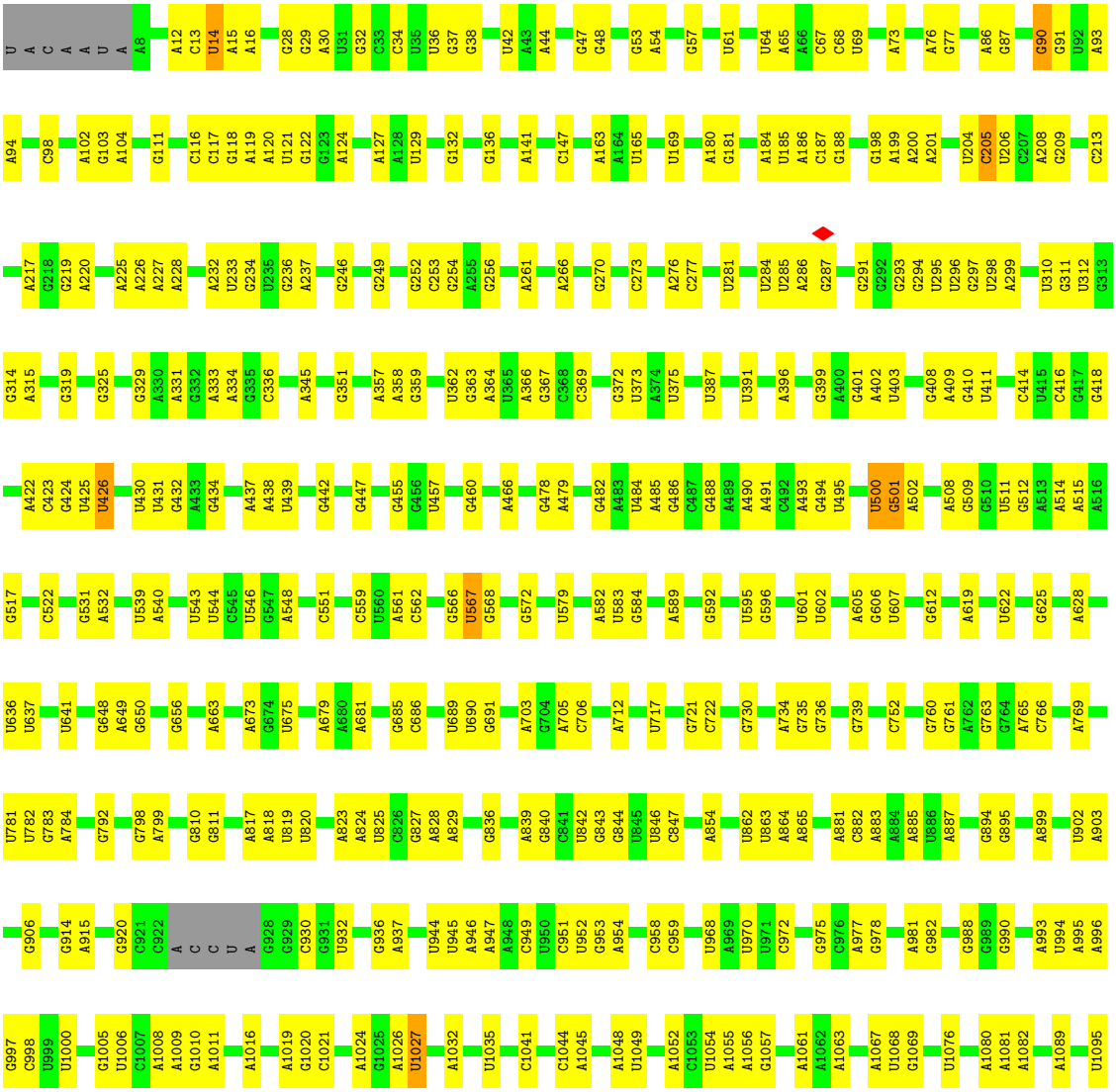
Chain z:

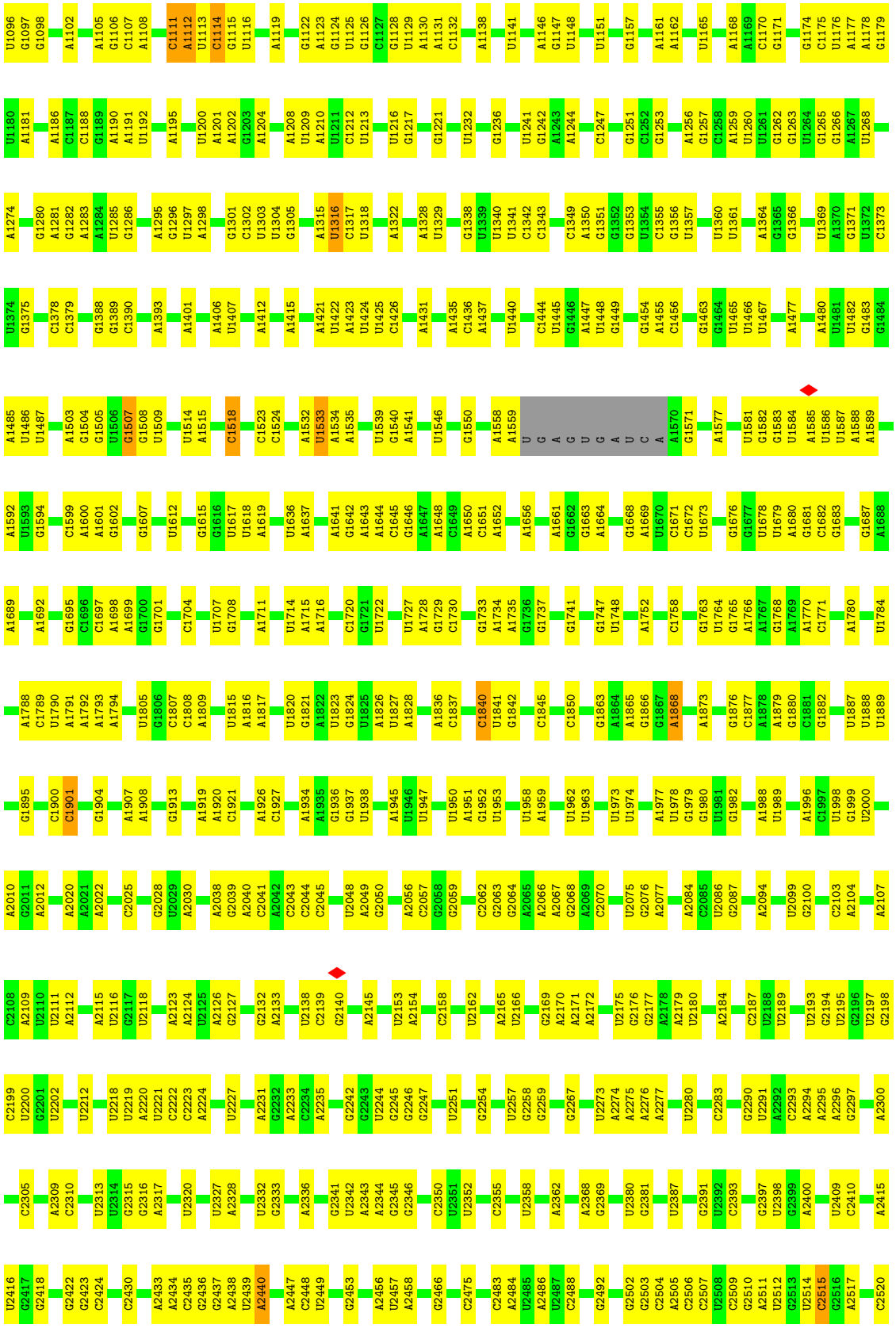


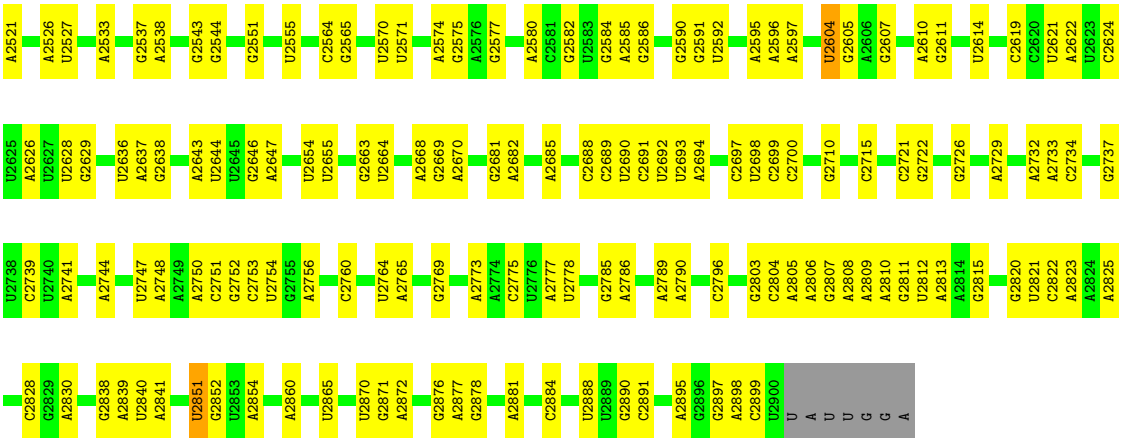


• Molecule 50: 23S ribosomal RNA

Chain 3:

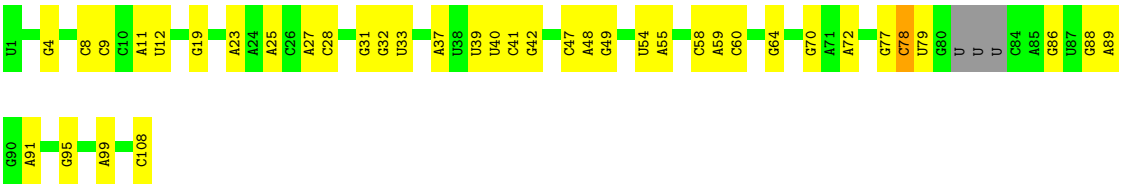






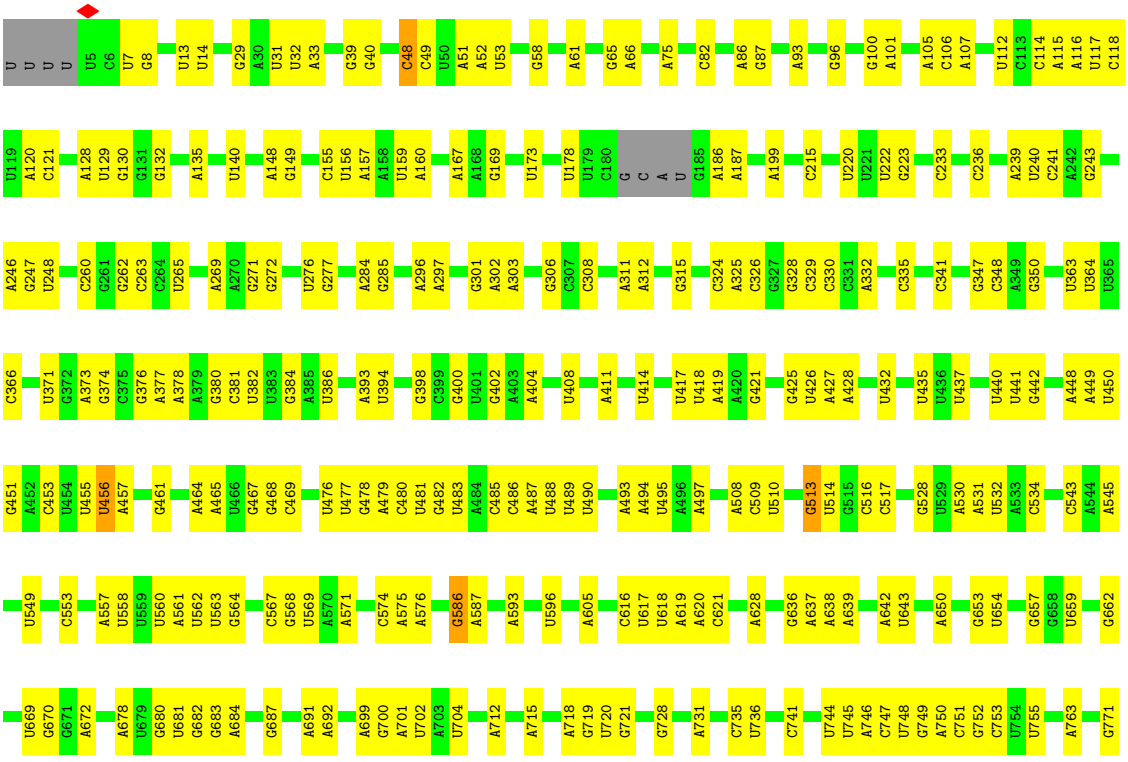
• Molecule 51: 5S ribosomal RNA

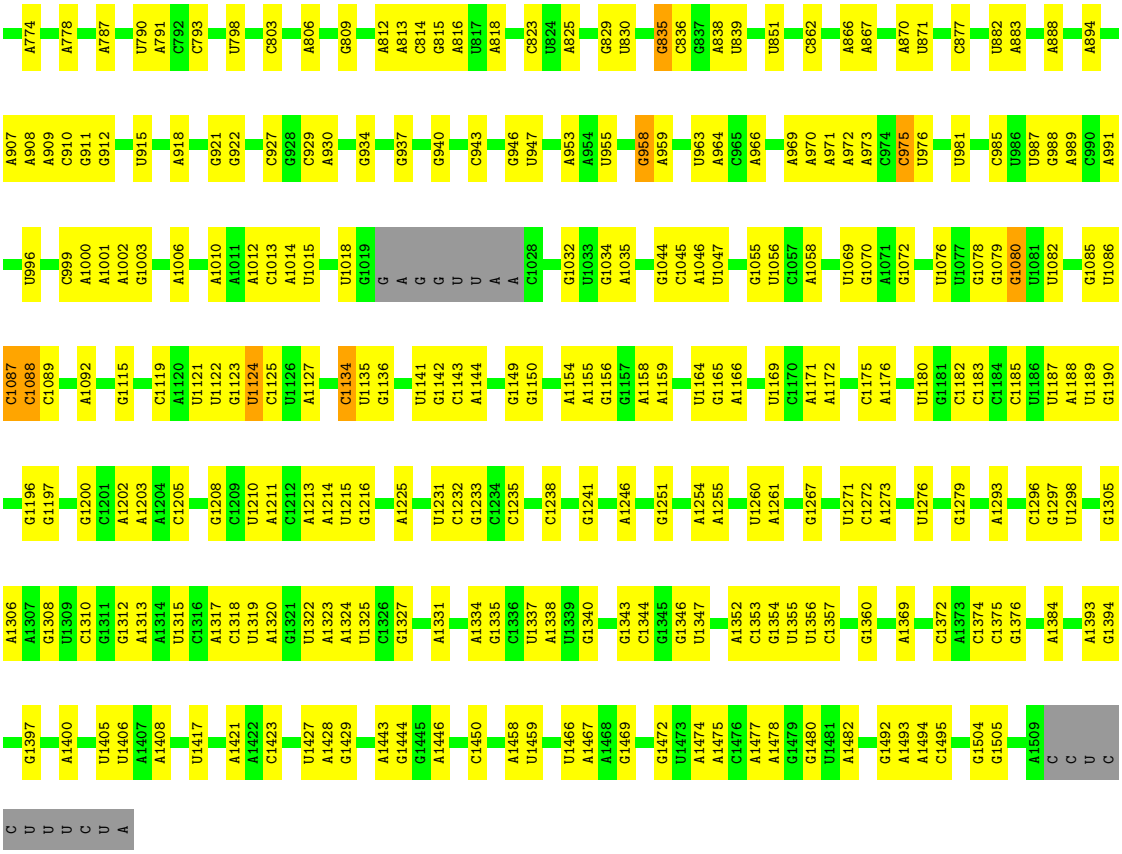
Chain 4:



• Molecule 52: 16S ribosomal RNA

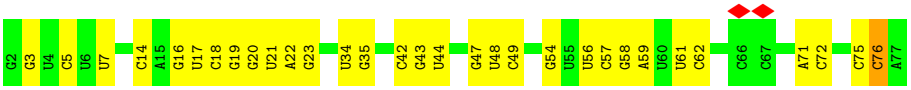
Chain 5:





• Molecule 53: tRNA-Phe

Chain 6:



• Molecule 53: tRNA-Phe

Chain 8:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	940	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 ($e^-/Å^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.996	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

5 Model quality

5.1 Standard geometry

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	0.23	0/383	0.38	0/504
2	1	0.32	0/484	0.64	0/637
3	2	0.22	0/306	0.45	0/401
4	A	0.26	0/1954	0.49	1/2642 (0.0%)
5	B	0.25	0/1721	0.46	0/2323
6	C	0.31	0/1691	0.55	1/2267 (0.0%)
7	D	0.27	0/1188	0.56	0/1593
8	E	0.25	0/1384	0.47	0/1867
9	F	0.29	0/1266	0.70	3/1700 (0.2%)
10	G	0.28	0/1126	0.54	1/1517 (0.1%)
11	H	0.27	0/1044	0.49	0/1395
12	I	0.29	0/820	0.54	0/1103
13	J	0.26	0/844	0.47	0/1136
14	K	0.27	0/1094	0.53	1/1468 (0.1%)
15	L	0.23	0/962	0.45	0/1289
16	M	0.26	0/483	0.51	0/643
17	N	0.28	0/679	0.55	1/907 (0.1%)
18	O	0.23	0/659	0.41	0/885
19	P	0.23	0/684	0.47	0/913
20	Q	0.25	0/545	0.46	0/730
21	R	0.26	0/698	0.49	0/936
22	S	0.24	0/631	0.41	0/838
23	T	0.22	0/475	0.45	0/621
24	a	0.25	0/2267	0.48	0/3044
25	b	0.27	0/1795	0.52	0/2412
26	c	0.29	0/1671	0.50	1/2246 (0.0%)
27	d	0.30	0/1409	0.55	0/1894
28	e	0.26	0/1420	0.50	0/1912
29	f	0.26	0/1183	0.52	0/1587
30	g	0.36	0/927	0.58	0/1236
31	h	0.26	0/968	0.52	0/1298
32	i	0.24	0/1186	0.46	0/1592
33	j	0.24	0/953	0.49	0/1275
34	k	0.24	0/1170	0.47	0/1559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	l	0.28	0/1104	0.50	0/1481
36	m	0.26	0/973	0.50	0/1309
37	n	0.24	0/897	0.46	0/1198
38	o	0.24	0/948	0.49	0/1262
39	p	0.24	0/961	0.42	0/1278
40	q	0.28	0/828	0.53	0/1111
41	r	0.25	0/1077	0.49	0/1441
42	s	0.26	0/732	0.48	0/988
43	t	0.26	0/879	0.53	0/1165
44	u	0.25	0/665	0.47	0/884
45	v	0.23	0/519	0.49	0/695
46	w	0.23	0/826	0.46	0/1104
47	x	0.29	0/353	0.47	0/474
48	y	0.30	0/457	0.50	0/601
49	z	0.25	0/412	0.44	0/547
50	3	0.66	6/69073 (0.0%)	0.89	108/107710 (0.1%)
51	4	0.24	0/2505	0.87	3/3902 (0.1%)
52	5	0.24	1/35768 (0.0%)	0.86	43/55764 (0.1%)
53	6	1.04	5/1808 (0.3%)	2.54	14/2817 (0.5%)
53	8	1.04	5/1808 (0.3%)	2.54	14/2817 (0.5%)
All	All	0.50	17/158663 (0.0%)	0.88	191/236918 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	3	2440	A	N3-C4	84.54	1.85	1.34
50	3	2440	A	C6-N1	73.80	1.87	1.35
50	3	2440	A	C5-C6	61.45	1.96	1.41
50	3	2440	A	C5-C4	59.03	1.80	1.38
50	3	2440	A	C2-N3	56.92	1.84	1.33
50	3	2440	A	N1-C2	52.03	1.81	1.34
53	6	76	C	N1-C6	27.54	1.53	1.37
53	8	76	C	N1-C6	27.30	1.53	1.37
53	6	76	C	C1'-N1	23.73	1.84	1.48
53	8	76	C	C1'-N1	23.71	1.84	1.48
53	6	76	C	N1-C2	20.79	1.60	1.40
53	8	76	C	N1-C2	20.70	1.60	1.40
53	8	76	C	C4-C5	-7.10	1.37	1.43
53	6	76	C	C4-C5	-7.01	1.37	1.43
53	6	76	C	N3-C4	-6.63	1.29	1.33
53	8	76	C	N3-C4	-6.48	1.29	1.33
52	5	736	U	C2-N3	-5.04	1.34	1.37

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	6	76	C	C6-N1-C2	-96.08	81.87	120.30
53	8	76	C	C6-N1-C2	-95.94	81.93	120.30
53	6	76	C	C5-C6-N1	57.88	149.94	121.00
53	8	76	C	C5-C6-N1	57.74	149.87	121.00
53	8	76	C	N3-C2-O2	-34.59	97.69	121.90
53	6	76	C	N3-C2-O2	-34.48	97.77	121.90
50	3	2440	A	N1-C2-N3	-27.59	115.50	129.30
53	8	76	C	N3-C4-C5	-24.68	112.03	121.90
53	6	76	C	N3-C4-C5	-24.59	112.07	121.90
50	3	2440	A	C2-N3-C4	24.46	122.83	110.60
53	8	76	C	N1-C2-N3	21.89	134.53	119.20
53	6	76	C	N1-C2-N3	21.88	134.51	119.20
53	6	76	C	C2-N1-C1'	19.23	139.95	118.80
53	8	76	C	C2-N1-C1'	19.19	139.91	118.80
50	3	2440	A	N7-C8-N9	17.52	122.56	113.80
53	8	76	C	N1-C2-O2	14.82	127.79	118.90
53	6	76	C	N1-C2-O2	14.70	127.72	118.90
53	6	76	C	C2-N3-C4	14.41	127.10	119.90
53	8	76	C	C2-N3-C4	14.34	127.07	119.90
53	6	76	C	C6-N1-C1'	14.28	137.93	120.80
53	8	76	C	C6-N1-C1'	14.27	137.92	120.80
50	3	2440	A	C4-C5-N7	-13.84	103.78	110.70
9	F	108	ARG	NE-CZ-NH1	-13.29	113.66	120.30
50	3	2440	A	N3-C4-N9	11.59	136.68	127.40
53	8	76	C	O4'-C1'-N1	11.15	117.12	108.20
53	6	76	C	O4'-C1'-N1	11.10	117.08	108.20
50	3	2440	A	N9-C4-C5	-11.09	101.36	105.80
50	3	2440	A	C6-N1-C2	10.96	125.17	118.60
53	8	76	C	N1-C1'-C2'	10.29	127.38	114.00
53	6	76	C	N1-C1'-C2'	10.26	127.34	114.00
50	3	1889	U	N3-C2-O2	-9.46	115.58	122.20
50	3	559	C	N3-C2-O2	-9.11	115.53	121.90
50	3	68	C	N3-C2-O2	-9.04	115.57	121.90
50	3	205	C	C2-N1-C1'	8.91	128.60	118.80
9	F	108	ARG	NE-CZ-NH2	8.84	124.72	120.30
50	3	1868	A	N1-C6-N6	-8.54	113.48	118.60
50	3	2199	C	N3-C2-O2	-8.40	116.02	121.90
52	5	1134	C	N1-C2-O2	8.29	123.88	118.90
50	3	501	G	O5'-P-OP2	-8.24	98.29	105.70
50	3	2440	A	C6-C5-N7	8.18	138.02	132.30
50	3	205	C	N1-C2-O2	7.98	123.69	118.90
50	3	1672	C	N3-C2-O2	-7.95	116.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	5	975	C	N1-C2-O2	7.94	123.67	118.90
50	3	567	U	C2-N1-C1'	7.91	127.19	117.70
50	3	187	C	N3-C2-O2	-7.87	116.39	121.90
50	3	1868	A	N1-C2-N3	-7.75	125.43	129.30
50	3	2440	A	N3-C4-C5	-7.70	121.41	126.80
52	5	1088	C	N3-C2-O2	-7.68	116.52	121.90
50	3	2851	U	C2-N1-C1'	7.63	126.85	117.70
50	3	14	U	C2-N1-C1'	7.60	126.82	117.70
50	3	187	C	N1-C2-O2	7.58	123.45	118.90
50	3	1111	C	N3-C2-O2	-7.56	116.61	121.90
53	8	76	C	C5-C4-N4	7.55	125.48	120.20
53	6	76	C	C5-C4-N4	7.54	125.48	120.20
50	3	1868	A	C6-N1-C2	7.49	123.09	118.60
50	3	67	C	N1-C2-O2	7.49	123.39	118.90
50	3	1247	C	N3-C2-O2	-7.39	116.73	121.90
51	4	58	C	N3-C2-O2	-7.38	116.73	121.90
52	5	751	C	C2-N1-C1'	7.37	126.90	118.80
50	3	68	C	N1-C2-O2	7.37	123.32	118.90
51	4	58	C	N1-C2-O2	7.37	123.32	118.90
52	5	1134	C	N3-C2-O2	-7.36	116.75	121.90
50	3	1868	A	C5-C6-N6	7.25	129.50	123.70
52	5	1134	C	C2-N1-C1'	7.25	126.77	118.80
52	5	975	C	C2-N1-C1'	7.21	126.73	118.80
50	3	567	U	N1-C2-O2	7.15	127.80	122.80
50	3	67	C	N3-C2-O2	-7.07	116.95	121.90
52	5	835	G	N1-C6-O6	-7.02	115.69	119.90
52	5	975	C	N3-C2-O2	-6.88	117.08	121.90
50	3	1901	C	N1-C2-O2	6.86	123.02	118.90
50	3	205	C	C6-N1-C2	-6.86	117.56	120.30
50	3	1341	U	C2-N1-C1'	6.84	125.91	117.70
50	3	2199	C	N1-C2-O2	6.83	123.00	118.90
52	5	248	U	C2-N1-C1'	6.80	125.87	117.70
52	5	681	U	C2-N1-C1'	6.72	125.76	117.70
50	3	90	G	N3-C4-N9	6.71	130.03	126.00
52	5	456	U	N3-C2-O2	-6.71	117.50	122.20
50	3	1262	G	N3-C4-N9	6.65	129.99	126.00
52	5	751	C	N1-C2-O2	6.64	122.88	118.90
50	3	1341	U	N1-C2-O2	6.51	127.36	122.80
50	3	1507	G	C4-N9-C1'	-6.42	118.16	126.50
53	8	76	C	N3-C4-N4	6.41	122.49	118.00
50	3	1316	U	C2-N1-C1'	6.39	125.37	117.70
50	3	559	C	N1-C2-O2	6.38	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	6	76	C	N3-C4-N4	6.36	122.45	118.00
50	3	567	U	N3-C2-O2	-6.29	117.79	122.20
50	3	1524	C	N3-C2-O2	-6.25	117.53	121.90
52	5	975	C	C6-N1-C2	-6.23	117.81	120.30
50	3	205	C	C5-C6-N1	6.22	124.11	121.00
50	3	14	U	N1-C2-O2	6.19	127.13	122.80
50	3	1507	G	C8-N9-C1'	6.19	135.04	127.00
50	3	501	G	O5'-P-OP1	6.18	118.11	110.70
52	5	335	C	N3-C2-O2	-6.16	117.59	121.90
50	3	14	U	N3-C2-O2	-6.08	117.94	122.20
53	6	76	C	C4-C5-C6	-6.04	114.38	117.40
50	3	2350	C	N3-C2-O2	-6.01	117.69	121.90
50	3	1533	U	C2-N1-C1'	6.00	124.90	117.70
50	3	1889	U	N1-C2-O2	5.98	126.98	122.80
50	3	205	C	N3-C2-O2	-5.94	117.74	121.90
50	3	1518	C	C2-N1-C1'	5.91	125.31	118.80
53	8	76	C	C4-C5-C6	-5.88	114.46	117.40
52	5	681	U	N3-C2-O2	-5.87	118.09	122.20
50	3	1599	C	N3-C2-O2	-5.87	117.79	121.90
50	3	1303	U	C2-N1-C1'	5.85	124.72	117.70
50	3	2851	U	N1-C2-O2	5.83	126.88	122.80
52	5	862	C	N1-C2-O2	5.83	122.40	118.90
52	5	1183	C	N3-C2-O2	-5.82	117.82	121.90
50	3	205	C	C6-N1-C1'	-5.82	113.82	120.80
50	3	2590	G	N3-C4-N9	5.79	129.47	126.00
52	5	586	G	C8-N9-C1'	-5.79	119.47	127.00
52	5	586	G	C4-N9-C1'	5.77	134.00	126.50
50	3	1114	C	C2-N1-C1'	5.73	125.11	118.80
50	3	2604	U	P-O3'-C3'	5.69	126.53	119.70
51	4	78	C	O4'-C1'-N1	5.69	112.75	108.20
50	3	1341	U	N3-C2-O2	-5.64	118.25	122.20
50	3	1098	G	N1-C2-N2	-5.63	111.13	116.20
50	3	2624	C	N1-C2-O2	5.63	122.28	118.90
6	C	81	GLN	CA-CB-CG	5.62	125.77	113.40
50	3	736	G	N1-C6-O6	-5.59	116.55	119.90
52	5	1088	C	C6-N1-C2	-5.59	118.06	120.30
50	3	1663	G	C5-C6-O6	5.58	131.95	128.60
52	5	1087	C	N1-C2-O2	5.56	122.23	118.90
50	3	2688	C	C6-N1-C2	-5.54	118.08	120.30
50	3	1507	G	N3-C4-N9	-5.52	122.69	126.00
50	3	500	U	C2-N1-C1'	5.51	124.32	117.70
50	3	1507	G	O4'-C1'-N9	5.51	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	5	751	C	C6-N1-C1'	-5.48	114.23	120.80
50	3	1840	C	N3-C2-O2	-5.47	118.07	121.90
14	K	31	LEU	CA-CB-CG	5.45	127.84	115.30
52	5	1088	C	N1-C2-O2	5.45	122.17	118.90
50	3	1263	G	C8-N9-C4	-5.44	104.22	106.40
50	3	1112	A	O4'-C1'-N9	5.44	112.55	108.20
50	3	91	G	C5-C6-O6	5.43	131.86	128.60
50	3	1262	G	N3-C4-C5	-5.42	125.89	128.60
52	5	835	G	C5-C6-O6	5.41	131.84	128.60
50	3	1671	C	N1-C2-O2	5.40	122.14	118.90
50	3	1901	C	N3-C2-O2	-5.39	118.12	121.90
52	5	736	U	N3-C2-O2	-5.38	118.43	122.20
4	A	220	HIS	C-N-CA	-5.38	108.26	121.70
50	3	2503	G	C4-N9-C1'	5.37	133.48	126.50
50	3	1524	C	C6-N1-C2	-5.36	118.16	120.30
50	3	500	U	C5-C4-O4	-5.36	122.68	125.90
52	5	1134	C	C6-N1-C2	-5.36	118.16	120.30
50	3	1010	G	O4'-C1'-N9	5.35	112.48	108.20
50	3	1116	U	C2-N1-C1'	5.35	124.12	117.70
50	3	1114	C	N1-C2-O2	5.30	122.08	118.90
50	3	198	G	N1-C6-O6	-5.29	116.72	119.90
50	3	500	U	P-O3'-C3'	5.29	126.05	119.70
50	3	1027	U	C2-N1-C1'	5.29	124.05	117.70
50	3	1645	C	C2-N1-C1'	5.28	124.61	118.80
52	5	958	G	C5-C6-O6	5.27	131.76	128.60
50	3	426	U	C2-N1-C1'	5.27	124.02	117.70
52	5	877	C	N3-C2-O2	-5.26	118.21	121.90
26	c	143	MET	CA-CB-CG	5.26	122.24	113.30
50	3	1863	G	N1-C6-O6	-5.25	116.75	119.90
52	5	1087	C	C2-N1-C1'	5.25	124.57	118.80
50	3	426	U	N3-C2-O2	-5.24	118.53	122.20
50	3	567	U	C6-N1-C1'	-5.24	113.87	121.20
52	5	486	C	N3-C2-O2	-5.23	118.24	121.90
50	3	91	G	N1-C2-N2	-5.22	111.51	116.20
52	5	48	C	P-O3'-C3'	5.20	125.94	119.70
52	5	736	U	N1-C2-O2	5.19	126.44	122.80
50	3	1663	G	N1-C6-O6	-5.19	116.79	119.90
50	3	2851	U	C6-N1-C1'	-5.18	113.94	121.20
52	5	586	G	N3-C4-N9	5.16	129.09	126.00
50	3	2590	G	C8-N9-C1'	-5.15	120.31	127.00
50	3	1840	C	N1-C2-O2	5.14	121.99	118.90
52	5	1080	G	N1-C2-N2	-5.14	111.57	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	3	1518	C	N1-C2-O2	5.14	121.98	118.90
50	3	1247	C	N1-C2-O2	5.14	121.98	118.90
50	3	1507	G	C6-C5-N7	5.13	133.48	130.40
52	5	513	G	N3-C4-N9	5.12	129.07	126.00
50	3	2590	G	C4-N9-C1'	5.12	133.15	126.50
50	3	47	G	C5-C6-O6	5.11	131.66	128.60
50	3	1316	U	N1-C2-O2	5.11	126.38	122.80
10	G	123	MET	CG-SD-CE	-5.11	92.03	100.20
50	3	2503	G	C8-N9-C1'	-5.10	120.37	127.00
50	3	2796	C	N3-C2-O2	-5.10	118.33	121.90
50	3	426	U	N1-C2-O2	5.09	126.36	122.80
50	3	1262	G	C4-N9-C1'	5.08	133.10	126.50
52	5	1012	A	O4'-C1'-N9	5.08	112.26	108.20
17	N	53	LEU	CA-CB-CG	5.08	126.97	115.30
52	5	862	C	N3-C2-O2	-5.07	118.35	121.90
52	5	751	C	N3-C2-O2	-5.06	118.36	121.90
52	5	1080	G	N3-C2-N2	5.06	123.44	119.90
50	3	2691	C	C5-C6-N1	5.06	123.53	121.00
9	F	115	MET	CG-SD-CE	5.06	108.29	100.20
50	3	2515	C	N1-C2-O2	5.05	121.93	118.90
52	5	1079	G	N3-C4-N9	5.05	129.03	126.00
52	5	1149	G	N3-C4-N9	5.03	129.02	126.00
52	5	1124	U	C2-N1-C1'	5.03	123.73	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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	45/48 (94%)	42 (93%)	3 (7%)	0	100	100
2	1	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	40
3	2	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
4	A	238/294 (81%)	217 (91%)	21 (9%)	0	100	100
5	B	213/273 (78%)	191 (90%)	22 (10%)	0	100	100
6	C	201/205 (98%)	186 (92%)	15 (8%)	0	100	100
7	D	151/219 (69%)	144 (95%)	7 (5%)	0	100	100
8	E	165/215 (77%)	149 (90%)	16 (10%)	0	100	100
9	F	152/155 (98%)	144 (95%)	8 (5%)	0	100	100
10	G	139/142 (98%)	120 (86%)	19 (14%)	0	100	100
11	H	126/132 (96%)	113 (90%)	13 (10%)	0	100	100
12	I	99/108 (92%)	92 (93%)	7 (7%)	0	100	100
13	J	112/121 (93%)	107 (96%)	5 (4%)	0	100	100
14	K	134/139 (96%)	117 (87%)	17 (13%)	0	100	100
15	L	116/124 (94%)	106 (91%)	10 (9%)	0	100	100
16	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
17	N	81/86 (94%)	72 (89%)	9 (11%)	0	100	100
18	O	78/94 (83%)	71 (91%)	7 (9%)	0	100	100
19	P	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
20	Q	63/104 (61%)	51 (81%)	12 (19%)	0	100	100
21	R	82/87 (94%)	71 (87%)	11 (13%)	0	100	100
22	S	75/87 (86%)	75 (100%)	0	0	100	100
23	T	51/60 (85%)	51 (100%)	0	0	100	100
24	a	283/287 (99%)	252 (89%)	30 (11%)	1 (0%)	34	72
25	b	227/287 (79%)	210 (92%)	17 (8%)	0	100	100
26	c	208/212 (98%)	194 (93%)	14 (7%)	0	100	100
27	d	173/180 (96%)	149 (86%)	24 (14%)	0	100	100
28	e	174/184 (95%)	159 (91%)	15 (9%)	0	100	100
29	f	143/149 (96%)	132 (92%)	11 (8%)	0	100	100
30	g	118/161 (73%)	108 (92%)	9 (8%)	1 (1%)	19	60
31	h	126/137 (92%)	107 (85%)	19 (15%)	0	100	100
32	i	142/146 (97%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	j	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	k	146/151 (97%)	136 (93%)	10 (7%)	0	100	100
35	l	134/139 (96%)	122 (91%)	12 (9%)	0	100	100
36	m	117/124 (94%)	110 (94%)	7 (6%)	0	100	100
37	n	108/116 (93%)	99 (92%)	9 (8%)	0	100	100
38	o	113/119 (95%)	105 (93%)	8 (7%)	0	100	100
39	p	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
40	q	97/100 (97%)	85 (88%)	12 (12%)	0	100	100
41	r	137/159 (86%)	126 (92%)	11 (8%)	0	100	100
42	s	90/237 (38%)	82 (91%)	8 (9%)	0	100	100
43	t	109/111 (98%)	100 (92%)	9 (8%)	0	100	100
44	u	84/104 (81%)	78 (93%)	6 (7%)	0	100	100
45	v	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
46	w	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
47	x	42/97 (43%)	38 (90%)	4 (10%)	0	100	100
48	y	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
49	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	5814/6670 (87%)	5329 (92%)	482 (8%)	3 (0%)	54	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	26	THR
30	g	31	SER
24	a	282	ARG

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	40/41 (98%)	40 (100%)	0	100 100
2	1	51/51 (100%)	50 (98%)	1 (2%)	55 74
3	2	35/35 (100%)	35 (100%)	0	100 100
4	A	212/262 (81%)	208 (98%)	4 (2%)	57 75
5	B	180/232 (78%)	179 (99%)	1 (1%)	86 92
6	C	181/183 (99%)	180 (99%)	1 (1%)	86 92
7	D	123/178 (69%)	123 (100%)	0	100 100
8	E	150/196 (76%)	149 (99%)	1 (1%)	84 90
9	F	131/132 (99%)	130 (99%)	1 (1%)	81 89
10	G	123/124 (99%)	120 (98%)	3 (2%)	49 69
11	H	111/115 (96%)	109 (98%)	2 (2%)	59 77
12	I	95/99 (96%)	94 (99%)	1 (1%)	73 84
13	J	91/97 (94%)	91 (100%)	0	100 100
14	K	117/120 (98%)	113 (97%)	4 (3%)	37 60
15	L	100/105 (95%)	100 (100%)	0	100 100
16	M	47/48 (98%)	46 (98%)	1 (2%)	53 72
17	N	76/78 (97%)	76 (100%)	0	100 100
18	O	69/82 (84%)	69 (100%)	0	100 100
19	P	73/75 (97%)	73 (100%)	0	100 100
20	Q	56/94 (60%)	56 (100%)	0	100 100
21	R	74/77 (96%)	73 (99%)	1 (1%)	67 80
22	S	70/77 (91%)	70 (100%)	0	100 100
23	T	49/56 (88%)	49 (100%)	0	100 100
24	a	241/243 (99%)	240 (100%)	1 (0%)	91 94
25	b	186/233 (80%)	184 (99%)	2 (1%)	73 84
26	c	182/184 (99%)	182 (100%)	0	100 100
27	d	150/154 (97%)	149 (99%)	1 (1%)	84 90
28	e	153/159 (96%)	153 (100%)	0	100 100
29	f	123/134 (92%)	122 (99%)	1 (1%)	81 89
30	g	97/129 (75%)	85 (88%)	12 (12%)	4 19
31	h	102/110 (93%)	102 (100%)	0	100 100
32	i	126/128 (98%)	126 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	j	103/103 (100%)	103 (100%)	0	100 100
34	k	123/126 (98%)	123 (100%)	0	100 100
35	l	113/115 (98%)	113 (100%)	0	100 100
36	m	105/109 (96%)	103 (98%)	2 (2%)	57 75
37	n	96/99 (97%)	96 (100%)	0	100 100
38	o	101/105 (96%)	101 (100%)	0	100 100
39	p	100/108 (93%)	99 (99%)	1 (1%)	76 86
40	q	90/91 (99%)	89 (99%)	1 (1%)	73 84
41	r	116/132 (88%)	116 (100%)	0	100 100
42	s	82/208 (39%)	82 (100%)	0	100 100
43	t	96/96 (100%)	96 (100%)	0	100 100
44	u	69/85 (81%)	69 (100%)	0	100 100
45	v	58/60 (97%)	57 (98%)	1 (2%)	60 78
46	w	87/98 (89%)	87 (100%)	0	100 100
47	x	41/86 (48%)	41 (100%)	0	100 100
48	y	48/49 (98%)	45 (94%)	3 (6%)	18 43
49	z	47/50 (94%)	47 (100%)	0	100 100
All	All	5089/5751 (88%)	5043 (99%)	46 (1%)	79 87

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	8	LYS
4	A	22	LYS
4	A	57	VAL
4	A	185	LYS
4	A	186	ASN
5	B	217	ARG
6	C	143	ARG
8	E	2	GLN
9	F	110	ARG
10	G	79	ARG
10	G	80	ARG
10	G	108	LEU
11	H	95	GLU
11	H	108	ARG

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Mol	Chain	Res	Type
12	I	97	LYS
14	K	118	VAL
14	K	120	VAL
14	K	121	GLU
14	K	122	LYS
16	M	41	ARG
21	R	6	LYS
24	a	42	LYS
25	b	158	ARG
25	b	180	ARG
27	d	112	ARG
29	f	52	LYS
30	g	30	THR
30	g	31	SER
30	g	42	LYS
30	g	43	LYS
30	g	44	LEU
30	g	45	PHE
30	g	46	LYS
30	g	86	VAL
30	g	88	GLU
30	g	90	VAL
30	g	110	CYS
30	g	125	LYS
36	m	92	LYS
36	m	99	ARG
39	p	84	LYS
40	q	93	LYS
45	v	27	ARG
48	y	47	MET
48	y	50	ASP
48	y	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	28	HIS
6	C	115	GLN
6	C	121	HIS
9	F	67	ASN
9	F	129	ASN
9	F	141	HIS

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Mol	Chain	Res	Type
10	G	73	ASN
11	H	52	GLN
17	N	23	GLN
17	N	32	GLN
17	N	43	ASN
19	P	25	GLN
23	T	35	HIS
24	a	48	ASN
24	a	50	GLN
24	a	238	HIS
25	b	21	ASN
25	b	67	GLN
25	b	135	HIS
26	c	165	ASN
26	c	174	ASN
28	e	72	ASN
29	f	116	ASN
30	g	10	GLN
31	h	115	ASN
32	i	51	GLN
35	l	13	HIS
37	n	64	ASN
38	o	85	ASN
39	p	36	GLN
49	z	24	ASN
49	z	28	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	2875/2907 (98%)	1032 (35%)	34 (1%)
51	4	103/108 (95%)	38 (36%)	2 (1%)
52	5	1490/1520 (98%)	509 (34%)	13 (0%)
53	6	75/76 (98%)	30 (40%)	6 (8%)
53	8	75/76 (98%)	30 (40%)	6 (8%)
All	All	4618/4687 (98%)	1639 (35%)	61 (1%)

All (1639) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	12	A

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Mol	Chain	Res	Type
50	3	13	C
50	3	14	U
50	3	15	A
50	3	16	A
50	3	28	G
50	3	29	G
50	3	30	A
50	3	32	G
50	3	34	C
50	3	36	U
50	3	37	G
50	3	38	G
50	3	42	U
50	3	44	A
50	3	48	G
50	3	53	G
50	3	54	A
50	3	57	G
50	3	61	U
50	3	64	U
50	3	65	A
50	3	69	U
50	3	73	A
50	3	76	A
50	3	77	G
50	3	86	A
50	3	87	G
50	3	90	G
50	3	93	A
50	3	94	A
50	3	98	C
50	3	102	A
50	3	103	G
50	3	104	A
50	3	111	G
50	3	116	C
50	3	117	C
50	3	118	G
50	3	119	A
50	3	120	A
50	3	121	U
50	3	122	G

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Mol	Chain	Res	Type
50	3	124	A
50	3	127	A
50	3	129	U
50	3	132	G
50	3	136	G
50	3	141	A
50	3	147	C
50	3	163	A
50	3	165	U
50	3	169	U
50	3	180	A
50	3	181	G
50	3	184	A
50	3	185	U
50	3	186	A
50	3	188	G
50	3	199	A
50	3	200	A
50	3	201	A
50	3	204	U
50	3	205	C
50	3	206	U
50	3	208	A
50	3	209	G
50	3	213	C
50	3	217	A
50	3	219	G
50	3	220	A
50	3	225	A
50	3	226	A
50	3	227	A
50	3	228	A
50	3	232	A
50	3	233	U
50	3	234	G
50	3	236	G
50	3	237	A
50	3	246	G
50	3	249	G
50	3	252	G
50	3	253	C
50	3	254	G

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Mol	Chain	Res	Type
50	3	256	G
50	3	261	A
50	3	266	A
50	3	270	G
50	3	273	C
50	3	276	A
50	3	277	C
50	3	281	U
50	3	284	U
50	3	285	U
50	3	286	A
50	3	287	G
50	3	291	G
50	3	293	G
50	3	294	G
50	3	295	U
50	3	296	U
50	3	297	G
50	3	298	U
50	3	299	A
50	3	310	U
50	3	311	G
50	3	312	U
50	3	314	G
50	3	315	A
50	3	319	G
50	3	325	G
50	3	329	G
50	3	331	A
50	3	333	A
50	3	334	A
50	3	336	C
50	3	345	A
50	3	351	G
50	3	357	A
50	3	358	A
50	3	359	G
50	3	362	U
50	3	363	G
50	3	364	A
50	3	367	G
50	3	369	C

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Mol	Chain	Res	Type
50	3	372	G
50	3	373	U
50	3	375	U
50	3	387	U
50	3	391	U
50	3	396	A
50	3	399	G
50	3	401	G
50	3	402	A
50	3	403	U
50	3	408	G
50	3	409	A
50	3	410	G
50	3	411	U
50	3	414	C
50	3	416	C
50	3	418	G
50	3	422	A
50	3	423	C
50	3	424	G
50	3	425	U
50	3	426	U
50	3	430	U
50	3	431	U
50	3	432	G
50	3	434	G
50	3	437	A
50	3	438	A
50	3	439	U
50	3	442	G
50	3	447	G
50	3	455	G
50	3	457	U
50	3	460	G
50	3	466	A
50	3	478	G
50	3	479	A
50	3	482	G
50	3	484	U
50	3	485	A
50	3	486	G
50	3	488	G

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Mol	Chain	Res	Type
50	3	490	A
50	3	491	A
50	3	493	A
50	3	494	G
50	3	495	U
50	3	500	U
50	3	501	G
50	3	502	A
50	3	509	G
50	3	511	U
50	3	512	G
50	3	514	A
50	3	515	A
50	3	517	G
50	3	522	C
50	3	531	G
50	3	532	A
50	3	539	U
50	3	540	A
50	3	543	U
50	3	544	U
50	3	546	U
50	3	548	A
50	3	551	C
50	3	561	A
50	3	562	C
50	3	566	G
50	3	567	U
50	3	568	G
50	3	572	G
50	3	579	U
50	3	582	A
50	3	583	U
50	3	584	G
50	3	589	A
50	3	592	G
50	3	595	U
50	3	596	G
50	3	601	U
50	3	602	U
50	3	605	A
50	3	606	G

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Mol	Chain	Res	Type
50	3	607	U
50	3	612	G
50	3	619	A
50	3	622	U
50	3	625	G
50	3	628	A
50	3	636	U
50	3	637	U
50	3	641	U
50	3	648	G
50	3	649	A
50	3	650	G
50	3	656	G
50	3	663	A
50	3	673	A
50	3	675	U
50	3	679	A
50	3	681	A
50	3	685	G
50	3	686	C
50	3	689	U
50	3	690	U
50	3	691	G
50	3	703	A
50	3	705	A
50	3	706	C
50	3	712	A
50	3	717	U
50	3	721	G
50	3	722	C
50	3	730	G
50	3	734	A
50	3	735	G
50	3	739	G
50	3	752	C
50	3	760	G
50	3	761	G
50	3	763	G
50	3	765	A
50	3	766	C
50	3	769	A
50	3	781	U

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Mol	Chain	Res	Type
50	3	782	U
50	3	783	G
50	3	784	A
50	3	792	G
50	3	798	G
50	3	799	A
50	3	810	G
50	3	811	G
50	3	817	A
50	3	818	A
50	3	819	U
50	3	820	U
50	3	823	A
50	3	824	A
50	3	825	U
50	3	827	G
50	3	828	A
50	3	829	A
50	3	836	G
50	3	839	A
50	3	840	G
50	3	842	U
50	3	843	G
50	3	844	G
50	3	846	U
50	3	847	C
50	3	854	A
50	3	862	U
50	3	863	U
50	3	864	A
50	3	865	A
50	3	882	C
50	3	883	A
50	3	885	A
50	3	887	A
50	3	894	G
50	3	895	G
50	3	899	A
50	3	902	U
50	3	903	A
50	3	906	G
50	3	914	G

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Mol	Chain	Res	Type
50	3	915	A
50	3	920	G
50	3	930	C
50	3	932	U
50	3	936	G
50	3	937	A
50	3	944	U
50	3	945	U
50	3	946	A
50	3	947	A
50	3	949	C
50	3	951	C
50	3	952	U
50	3	953	G
50	3	954	A
50	3	958	C
50	3	959	C
50	3	968	U
50	3	970	U
50	3	972	C
50	3	975	G
50	3	977	A
50	3	978	G
50	3	981	A
50	3	982	G
50	3	988	G
50	3	990	G
50	3	993	A
50	3	994	U
50	3	995	A
50	3	997	G
50	3	998	C
50	3	1000	U
50	3	1005	G
50	3	1006	U
50	3	1008	A
50	3	1009	A
50	3	1011	A
50	3	1016	A
50	3	1019	A
50	3	1020	G
50	3	1021	C

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Mol	Chain	Res	Type
50	3	1024	A
50	3	1026	A
50	3	1027	U
50	3	1032	A
50	3	1035	U
50	3	1041	C
50	3	1044	C
50	3	1045	A
50	3	1049	U
50	3	1052	A
50	3	1055	A
50	3	1056	A
50	3	1057	G
50	3	1061	A
50	3	1063	A
50	3	1067	A
50	3	1068	U
50	3	1069	G
50	3	1076	U
50	3	1080	A
50	3	1081	A
50	3	1082	A
50	3	1089	A
50	3	1095	U
50	3	1096	U
50	3	1097	G
50	3	1102	A
50	3	1105	A
50	3	1106	G
50	3	1107	C
50	3	1108	A
50	3	1111	C
50	3	1112	A
50	3	1113	U
50	3	1114	C
50	3	1115	G
50	3	1119	A
50	3	1122	G
50	3	1123	A
50	3	1124	G
50	3	1125	U
50	3	1126	G

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Mol	Chain	Res	Type
50	3	1128	G
50	3	1129	U
50	3	1130	A
50	3	1131	A
50	3	1132	C
50	3	1138	A
50	3	1141	U
50	3	1146	A
50	3	1147	G
50	3	1148	U
50	3	1151	U
50	3	1157	G
50	3	1161	A
50	3	1162	A
50	3	1165	U
50	3	1168	A
50	3	1170	C
50	3	1171	G
50	3	1174	G
50	3	1175	C
50	3	1176	U
50	3	1177	A
50	3	1178	A
50	3	1179	G
50	3	1181	A
50	3	1186	A
50	3	1188	C
50	3	1190	A
50	3	1191	A
50	3	1192	U
50	3	1195	A
50	3	1200	U
50	3	1201	A
50	3	1202	A
50	3	1204	A
50	3	1208	A
50	3	1209	U
50	3	1210	A
50	3	1212	C
50	3	1213	U
50	3	1216	U
50	3	1217	G

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Mol	Chain	Res	Type
50	3	1221	G
50	3	1232	U
50	3	1236	G
50	3	1241	U
50	3	1242	G
50	3	1244	A
50	3	1251	G
50	3	1253	G
50	3	1256	A
50	3	1257	G
50	3	1259	A
50	3	1260	U
50	3	1265	G
50	3	1266	G
50	3	1268	U
50	3	1274	A
50	3	1280	G
50	3	1281	A
50	3	1282	G
50	3	1283	A
50	3	1285	U
50	3	1286	G
50	3	1295	A
50	3	1296	G
50	3	1297	U
50	3	1298	A
50	3	1301	G
50	3	1302	C
50	3	1304	U
50	3	1305	G
50	3	1315	A
50	3	1316	U
50	3	1317	C
50	3	1318	U
50	3	1322	A
50	3	1328	A
50	3	1329	U
50	3	1338	G
50	3	1340	U
50	3	1342	C
50	3	1343	C
50	3	1349	C

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Mol	Chain	Res	Type
50	3	1350	A
50	3	1351	G
50	3	1353	G
50	3	1356	G
50	3	1357	U
50	3	1360	U
50	3	1361	U
50	3	1364	A
50	3	1366	G
50	3	1369	U
50	3	1371	G
50	3	1373	C
50	3	1375	G
50	3	1378	C
50	3	1379	C
50	3	1388	G
50	3	1389	G
50	3	1390	C
50	3	1393	A
50	3	1401	A
50	3	1406	A
50	3	1407	U
50	3	1412	A
50	3	1415	A
50	3	1421	A
50	3	1422	U
50	3	1423	A
50	3	1424	U
50	3	1425	U
50	3	1426	C
50	3	1431	A
50	3	1435	A
50	3	1436	C
50	3	1437	A
50	3	1440	U
50	3	1444	C
50	3	1445	U
50	3	1447	A
50	3	1448	U
50	3	1449	G
50	3	1454	G
50	3	1455	A

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Mol	Chain	Res	Type
50	3	1456	C
50	3	1463	G
50	3	1466	U
50	3	1467	U
50	3	1477	A
50	3	1480	A
50	3	1482	U
50	3	1483	G
50	3	1485	A
50	3	1486	U
50	3	1487	U
50	3	1503	A
50	3	1504	G
50	3	1505	G
50	3	1507	G
50	3	1508	G
50	3	1509	U
50	3	1514	U
50	3	1515	A
50	3	1518	C
50	3	1523	C
50	3	1532	A
50	3	1533	U
50	3	1534	A
50	3	1535	A
50	3	1539	U
50	3	1540	G
50	3	1541	A
50	3	1546	U
50	3	1550	G
50	3	1558	A
50	3	1559	A
50	3	1571	G
50	3	1577	A
50	3	1581	U
50	3	1582	G
50	3	1584	U
50	3	1585	A
50	3	1586	U
50	3	1587	U
50	3	1588	A
50	3	1589	A

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Mol	Chain	Res	Type
50	3	1592	A
50	3	1594	G
50	3	1600	A
50	3	1601	A
50	3	1602	G
50	3	1607	G
50	3	1612	U
50	3	1615	G
50	3	1617	U
50	3	1618	U
50	3	1619	A
50	3	1636	U
50	3	1637	A
50	3	1641	A
50	3	1642	G
50	3	1643	A
50	3	1644	A
50	3	1646	G
50	3	1648	A
50	3	1650	A
50	3	1651	C
50	3	1652	A
50	3	1656	A
50	3	1661	A
50	3	1664	A
50	3	1668	G
50	3	1669	A
50	3	1673	U
50	3	1676	G
50	3	1678	U
50	3	1679	U
50	3	1680	A
50	3	1681	G
50	3	1682	C
50	3	1683	G
50	3	1687	G
50	3	1689	A
50	3	1692	A
50	3	1695	G
50	3	1697	C
50	3	1698	A
50	3	1699	A

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Mol	Chain	Res	Type
50	3	1701	G
50	3	1704	C
50	3	1707	U
50	3	1708	G
50	3	1711	A
50	3	1714	U
50	3	1715	A
50	3	1716	A
50	3	1720	C
50	3	1722	U
50	3	1727	U
50	3	1728	A
50	3	1729	G
50	3	1730	C
50	3	1733	G
50	3	1734	A
50	3	1735	A
50	3	1737	G
50	3	1741	G
50	3	1747	G
50	3	1748	U
50	3	1752	A
50	3	1758	C
50	3	1763	G
50	3	1764	U
50	3	1765	G
50	3	1766	A
50	3	1768	G
50	3	1770	A
50	3	1771	C
50	3	1780	A
50	3	1784	U
50	3	1788	A
50	3	1789	C
50	3	1790	U
50	3	1791	A
50	3	1792	A
50	3	1793	A
50	3	1794	A
50	3	1805	U
50	3	1807	C
50	3	1808	C

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Mol	Chain	Res	Type
50	3	1809	A
50	3	1815	U
50	3	1816	A
50	3	1817	A
50	3	1821	G
50	3	1823	U
50	3	1824	G
50	3	1826	A
50	3	1827	U
50	3	1828	A
50	3	1836	A
50	3	1837	C
50	3	1840	C
50	3	1841	U
50	3	1842	G
50	3	1845	C
50	3	1850	C
50	3	1865	A
50	3	1866	G
50	3	1868	A
50	3	1873	A
50	3	1876	G
50	3	1877	C
50	3	1879	A
50	3	1880	G
50	3	1882	G
50	3	1887	U
50	3	1888	U
50	3	1895	G
50	3	1900	C
50	3	1901	C
50	3	1904	G
50	3	1907	A
50	3	1908	A
50	3	1913	G
50	3	1919	A
50	3	1920	A
50	3	1921	C
50	3	1926	A
50	3	1927	C
50	3	1934	A
50	3	1936	G

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Mol	Chain	Res	Type
50	3	1937	G
50	3	1938	U
50	3	1945	A
50	3	1947	U
50	3	1950	U
50	3	1951	A
50	3	1952	G
50	3	1953	U
50	3	1958	U
50	3	1959	A
50	3	1962	U
50	3	1963	U
50	3	1973	U
50	3	1974	U
50	3	1977	A
50	3	1978	U
50	3	1979	G
50	3	1980	G
50	3	1982	G
50	3	1988	A
50	3	1989	U
50	3	1996	A
50	3	1998	U
50	3	1999	G
50	3	2000	U
50	3	2010	A
50	3	2012	A
50	3	2020	A
50	3	2022	A
50	3	2025	C
50	3	2028	G
50	3	2030	A
50	3	2038	A
50	3	2039	G
50	3	2040	A
50	3	2041	C
50	3	2043	C
50	3	2044	C
50	3	2045	C
50	3	2048	U
50	3	2049	A
50	3	2050	G

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Mol	Chain	Res	Type
50	3	2056	A
50	3	2057	C
50	3	2059	G
50	3	2062	C
50	3	2063	G
50	3	2064	G
50	3	2066	A
50	3	2067	A
50	3	2068	G
50	3	2070	C
50	3	2075	U
50	3	2076	G
50	3	2077	A
50	3	2084	A
50	3	2086	U
50	3	2087	G
50	3	2094	A
50	3	2099	U
50	3	2100	G
50	3	2103	C
50	3	2104	A
50	3	2107	A
50	3	2109	A
50	3	2111	U
50	3	2112	A
50	3	2115	A
50	3	2116	U
50	3	2118	U
50	3	2123	A
50	3	2124	A
50	3	2126	A
50	3	2127	G
50	3	2132	G
50	3	2133	A
50	3	2138	U
50	3	2139	C
50	3	2140	G
50	3	2145	A
50	3	2153	U
50	3	2154	A
50	3	2158	C
50	3	2162	U

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Mol	Chain	Res	Type
50	3	2165	A
50	3	2166	U
50	3	2169	G
50	3	2170	A
50	3	2171	A
50	3	2172	A
50	3	2175	U
50	3	2176	G
50	3	2177	G
50	3	2179	A
50	3	2180	U
50	3	2184	A
50	3	2187	C
50	3	2189	U
50	3	2193	U
50	3	2194	G
50	3	2195	U
50	3	2197	U
50	3	2198	G
50	3	2200	U
50	3	2202	U
50	3	2212	U
50	3	2218	U
50	3	2219	U
50	3	2220	A
50	3	2221	U
50	3	2222	C
50	3	2223	C
50	3	2224	A
50	3	2227	U
50	3	2231	A
50	3	2233	A
50	3	2235	A
50	3	2242	G
50	3	2244	U
50	3	2245	G
50	3	2246	G
50	3	2247	G
50	3	2251	U
50	3	2254	G
50	3	2257	U
50	3	2258	G

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Mol	Chain	Res	Type
50	3	2259	G
50	3	2267	G
50	3	2273	U
50	3	2274	A
50	3	2275	A
50	3	2276	A
50	3	2277	A
50	3	2280	U
50	3	2283	C
50	3	2290	G
50	3	2291	U
50	3	2293	C
50	3	2294	A
50	3	2295	A
50	3	2296	A
50	3	2297	G
50	3	2300	A
50	3	2305	C
50	3	2309	A
50	3	2310	C
50	3	2313	U
50	3	2315	G
50	3	2316	G
50	3	2317	A
50	3	2320	U
50	3	2327	U
50	3	2328	A
50	3	2333	G
50	3	2336	A
50	3	2341	G
50	3	2342	U
50	3	2343	A
50	3	2344	A
50	3	2345	G
50	3	2346	G
50	3	2352	U
50	3	2355	C
50	3	2358	U
50	3	2362	A
50	3	2368	A
50	3	2369	G
50	3	2380	U

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Mol	Chain	Res	Type
50	3	2381	G
50	3	2387	U
50	3	2391	G
50	3	2393	C
50	3	2397	G
50	3	2398	U
50	3	2400	A
50	3	2409	U
50	3	2410	C
50	3	2415	A
50	3	2416	U
50	3	2418	G
50	3	2422	G
50	3	2423	G
50	3	2424	C
50	3	2430	C
50	3	2433	A
50	3	2434	A
50	3	2435	C
50	3	2436	G
50	3	2437	G
50	3	2438	A
50	3	2439	U
50	3	2440	A
50	3	2447	A
50	3	2448	C
50	3	2449	U
50	3	2453	G
50	3	2456	A
50	3	2457	U
50	3	2458	A
50	3	2466	G
50	3	2475	C
50	3	2483	C
50	3	2484	A
50	3	2486	A
50	3	2488	C
50	3	2492	G
50	3	2502	G
50	3	2504	C
50	3	2505	A
50	3	2506	C

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Mol	Chain	Res	Type
50	3	2507	C
50	3	2509	C
50	3	2510	G
50	3	2511	A
50	3	2512	U
50	3	2514	U
50	3	2515	C
50	3	2517	A
50	3	2520	C
50	3	2521	A
50	3	2526	A
50	3	2527	U
50	3	2533	A
50	3	2537	G
50	3	2538	A
50	3	2543	G
50	3	2544	G
50	3	2551	G
50	3	2555	U
50	3	2564	C
50	3	2565	G
50	3	2570	U
50	3	2571	U
50	3	2574	A
50	3	2575	G
50	3	2577	G
50	3	2580	A
50	3	2582	G
50	3	2584	G
50	3	2585	A
50	3	2586	G
50	3	2591	G
50	3	2592	U
50	3	2595	A
50	3	2596	A
50	3	2597	A
50	3	2604	U
50	3	2605	G
50	3	2607	G
50	3	2610	A
50	3	2611	G
50	3	2614	U

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Mol	Chain	Res	Type
50	3	2619	C
50	3	2621	U
50	3	2622	A
50	3	2626	A
50	3	2628	U
50	3	2629	G
50	3	2636	U
50	3	2637	A
50	3	2638	G
50	3	2643	A
50	3	2644	U
50	3	2646	G
50	3	2647	A
50	3	2654	U
50	3	2655	U
50	3	2663	G
50	3	2664	U
50	3	2668	A
50	3	2669	G
50	3	2670	A
50	3	2681	G
50	3	2682	A
50	3	2685	A
50	3	2689	C
50	3	2690	U
50	3	2692	U
50	3	2693	U
50	3	2694	A
50	3	2697	C
50	3	2698	U
50	3	2699	C
50	3	2700	C
50	3	2710	G
50	3	2715	C
50	3	2721	C
50	3	2722	G
50	3	2726	G
50	3	2729	A
50	3	2732	A
50	3	2733	A
50	3	2734	C
50	3	2737	G

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Mol	Chain	Res	Type
50	3	2739	C
50	3	2741	A
50	3	2744	A
50	3	2747	U
50	3	2748	A
50	3	2750	A
50	3	2751	C
50	3	2752	G
50	3	2753	C
50	3	2754	U
50	3	2756	A
50	3	2760	C
50	3	2765	A
50	3	2769	G
50	3	2773	A
50	3	2775	C
50	3	2777	A
50	3	2778	U
50	3	2785	G
50	3	2786	A
50	3	2789	A
50	3	2790	A
50	3	2803	G
50	3	2804	C
50	3	2805	A
50	3	2806	A
50	3	2807	G
50	3	2808	A
50	3	2809	A
50	3	2810	A
50	3	2811	G
50	3	2812	U
50	3	2813	A
50	3	2815	G
50	3	2820	G
50	3	2821	U
50	3	2822	C
50	3	2823	A
50	3	2825	A
50	3	2828	C
50	3	2830	A
50	3	2838	G

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Mol	Chain	Res	Type
50	3	2839	A
50	3	2840	U
50	3	2841	A
50	3	2851	U
50	3	2852	G
50	3	2854	A
50	3	2860	A
50	3	2865	U
50	3	2870	U
50	3	2871	G
50	3	2872	A
50	3	2876	G
50	3	2877	A
50	3	2878	G
50	3	2881	A
50	3	2884	C
50	3	2888	U
50	3	2890	G
50	3	2891	C
50	3	2895	A
50	3	2897	G
50	3	2898	A
50	3	2899	C
51	4	4	G
51	4	8	C
51	4	9	C
51	4	11	A
51	4	12	U
51	4	19	G
51	4	23	A
51	4	25	A
51	4	27	A
51	4	28	C
51	4	31	G
51	4	32	G
51	4	33	U
51	4	37	A
51	4	39	U
51	4	40	U
51	4	41	C
51	4	42	G
51	4	47	C

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Mol	Chain	Res	Type
51	4	48	A
51	4	49	G
51	4	54	U
51	4	55	A
51	4	59	A
51	4	60	C
51	4	64	G
51	4	70	G
51	4	72	A
51	4	77	G
51	4	78	C
51	4	79	U
51	4	86	G
51	4	88	G
51	4	89	A
51	4	91	A
51	4	95	G
51	4	99	A
51	4	108	C
52	5	7	U
52	5	8	G
52	5	13	U
52	5	14	U
52	5	29	G
52	5	31	U
52	5	32	U
52	5	33	A
52	5	40	G
52	5	48	C
52	5	49	C
52	5	51	A
52	5	52	A
52	5	53	U
52	5	58	G
52	5	61	A
52	5	65	G
52	5	66	A
52	5	75	A
52	5	82	C
52	5	86	A
52	5	87	G
52	5	93	A

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Mol	Chain	Res	Type
52	5	96	G
52	5	100	G
52	5	101	A
52	5	105	A
52	5	106	C
52	5	107	A
52	5	112	U
52	5	114	C
52	5	115	A
52	5	116	A
52	5	117	U
52	5	118	C
52	5	120	A
52	5	121	C
52	5	128	A
52	5	129	U
52	5	130	G
52	5	132	G
52	5	135	A
52	5	140	U
52	5	148	A
52	5	149	G
52	5	155	C
52	5	156	U
52	5	157	A
52	5	159	U
52	5	160	A
52	5	167	A
52	5	169	G
52	5	173	U
52	5	178	U
52	5	186	A
52	5	187	A
52	5	199	A
52	5	215	C
52	5	220	U
52	5	222	U
52	5	223	G
52	5	233	C
52	5	236	C
52	5	239	A
52	5	240	U

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Mol	Chain	Res	Type
52	5	241	C
52	5	243	G
52	5	246	A
52	5	247	G
52	5	260	C
52	5	262	G
52	5	263	C
52	5	265	U
52	5	269	A
52	5	271	G
52	5	272	G
52	5	276	U
52	5	277	G
52	5	284	A
52	5	285	G
52	5	296	A
52	5	297	A
52	5	301	G
52	5	302	A
52	5	303	A
52	5	306	G
52	5	308	C
52	5	311	A
52	5	312	A
52	5	315	G
52	5	324	C
52	5	325	A
52	5	326	C
52	5	328	G
52	5	329	C
52	5	330	C
52	5	332	A
52	5	341	C
52	5	347	G
52	5	348	C
52	5	350	G
52	5	363	U
52	5	364	U
52	5	366	C
52	5	371	U
52	5	373	A
52	5	374	G

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Mol	Chain	Res	Type
52	5	376	G
52	5	377	A
52	5	378	A
52	5	380	G
52	5	381	C
52	5	382	U
52	5	384	G
52	5	386	U
52	5	393	A
52	5	394	U
52	5	398	G
52	5	400	G
52	5	402	G
52	5	404	A
52	5	408	U
52	5	411	A
52	5	414	U
52	5	417	U
52	5	418	U
52	5	419	A
52	5	421	G
52	5	425	G
52	5	426	U
52	5	427	A
52	5	428	A
52	5	432	U
52	5	435	U
52	5	437	U
52	5	440	U
52	5	441	U
52	5	442	G
52	5	449	A
52	5	450	U
52	5	451	G
52	5	453	C
52	5	455	U
52	5	456	U
52	5	457	A
52	5	461	G
52	5	464	A
52	5	465	A
52	5	467	G

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Mol	Chain	Res	Type
52	5	468	G
52	5	469	C
52	5	476	U
52	5	477	U
52	5	478	G
52	5	479	A
52	5	480	C
52	5	481	U
52	5	482	G
52	5	483	U
52	5	485	C
52	5	487	A
52	5	488	U
52	5	489	U
52	5	490	U
52	5	493	A
52	5	494	A
52	5	495	U
52	5	497	A
52	5	508	A
52	5	509	C
52	5	510	U
52	5	513	G
52	5	514	U
52	5	516	C
52	5	517	C
52	5	528	G
52	5	530	A
52	5	531	A
52	5	532	U
52	5	534	C
52	5	543	C
52	5	545	A
52	5	549	U
52	5	553	C
52	5	557	A
52	5	558	U
52	5	560	U
52	5	561	A
52	5	562	U
52	5	563	U
52	5	564	G

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Mol	Chain	Res	Type
52	5	567	C
52	5	568	G
52	5	569	U
52	5	571	A
52	5	574	C
52	5	575	A
52	5	576	A
52	5	586	G
52	5	587	A
52	5	593	A
52	5	596	U
52	5	605	A
52	5	616	C
52	5	617	U
52	5	618	U
52	5	619	A
52	5	620	A
52	5	621	C
52	5	628	A
52	5	636	G
52	5	637	A
52	5	638	A
52	5	639	A
52	5	642	A
52	5	643	U
52	5	650	A
52	5	653	G
52	5	654	U
52	5	657	G
52	5	659	U
52	5	662	G
52	5	669	U
52	5	670	G
52	5	672	A
52	5	678	A
52	5	680	G
52	5	682	G
52	5	683	G
52	5	684	A
52	5	687	G
52	5	691	A
52	5	692	A

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Mol	Chain	Res	Type
52	5	699	A
52	5	700	G
52	5	701	A
52	5	702	U
52	5	704	U
52	5	712	A
52	5	715	A
52	5	718	A
52	5	719	G
52	5	720	U
52	5	721	G
52	5	728	G
52	5	731	A
52	5	735	C
52	5	741	C
52	5	744	U
52	5	745	U
52	5	746	A
52	5	747	C
52	5	749	G
52	5	750	A
52	5	752	G
52	5	753	C
52	5	755	U
52	5	763	A
52	5	771	G
52	5	774	A
52	5	778	A
52	5	787	A
52	5	790	U
52	5	791	A
52	5	793	C
52	5	798	U
52	5	803	C
52	5	806	A
52	5	809	G
52	5	812	A
52	5	813	A
52	5	814	C
52	5	815	G
52	5	816	A
52	5	818	A

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Mol	Chain	Res	Type
52	5	823	C
52	5	825	A
52	5	829	G
52	5	830	U
52	5	835	G
52	5	836	C
52	5	838	A
52	5	839	U
52	5	851	U
52	5	866	A
52	5	867	A
52	5	870	A
52	5	871	U
52	5	882	U
52	5	883	A
52	5	888	A
52	5	894	A
52	5	907	A
52	5	908	A
52	5	909	A
52	5	910	C
52	5	911	G
52	5	912	G
52	5	915	U
52	5	918	A
52	5	921	G
52	5	922	G
52	5	927	C
52	5	929	C
52	5	930	A
52	5	934	G
52	5	937	G
52	5	940	G
52	5	943	C
52	5	946	G
52	5	947	U
52	5	953	A
52	5	955	U
52	5	958	G
52	5	959	A
52	5	963	U
52	5	964	A

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Mol	Chain	Res	Type
52	5	966	A
52	5	969	A
52	5	970	A
52	5	971	A
52	5	972	A
52	5	973	A
52	5	975	C
52	5	976	U
52	5	981	U
52	5	985	C
52	5	987	U
52	5	988	G
52	5	989	A
52	5	991	A
52	5	996	U
52	5	999	C
52	5	1000	A
52	5	1001	A
52	5	1002	A
52	5	1003	G
52	5	1006	A
52	5	1010	A
52	5	1013	C
52	5	1014	A
52	5	1015	U
52	5	1018	U
52	5	1032	G
52	5	1034	G
52	5	1035	A
52	5	1044	G
52	5	1045	C
52	5	1046	A
52	5	1047	U
52	5	1055	G
52	5	1056	U
52	5	1058	A
52	5	1069	U
52	5	1070	G
52	5	1072	G
52	5	1076	U
52	5	1078	G
52	5	1080	G

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Mol	Chain	Res	Type
52	5	1082	U
52	5	1085	G
52	5	1086	U
52	5	1087	C
52	5	1088	C
52	5	1089	C
52	5	1092	A
52	5	1115	G
52	5	1119	C
52	5	1121	U
52	5	1122	U
52	5	1123	G
52	5	1124	U
52	5	1125	C
52	5	1127	A
52	5	1134	C
52	5	1135	U
52	5	1136	G
52	5	1141	U
52	5	1142	G
52	5	1144	A
52	5	1150	G
52	5	1154	A
52	5	1155	A
52	5	1156	G
52	5	1158	A
52	5	1159	A
52	5	1164	U
52	5	1165	G
52	5	1166	A
52	5	1169	U
52	5	1171	A
52	5	1172	A
52	5	1175	C
52	5	1176	A
52	5	1180	U
52	5	1182	C
52	5	1185	C
52	5	1187	U
52	5	1188	A
52	5	1189	U
52	5	1190	G

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Mol	Chain	Res	Type
52	5	1196	G
52	5	1197	G
52	5	1200	G
52	5	1202	A
52	5	1203	A
52	5	1205	C
52	5	1208	G
52	5	1210	U
52	5	1211	A
52	5	1213	A
52	5	1214	A
52	5	1215	U
52	5	1216	G
52	5	1225	A
52	5	1231	U
52	5	1232	C
52	5	1233	G
52	5	1235	C
52	5	1238	C
52	5	1241	G
52	5	1246	A
52	5	1251	G
52	5	1254	A
52	5	1255	A
52	5	1260	U
52	5	1261	A
52	5	1267	G
52	5	1271	U
52	5	1272	C
52	5	1273	A
52	5	1276	U
52	5	1279	G
52	5	1293	A
52	5	1296	C
52	5	1297	G
52	5	1298	U
52	5	1305	G
52	5	1306	A
52	5	1308	G
52	5	1310	C
52	5	1312	G
52	5	1313	A

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Mol	Chain	Res	Type
52	5	1315	U
52	5	1317	A
52	5	1318	C
52	5	1319	U
52	5	1320	A
52	5	1322	U
52	5	1324	A
52	5	1325	U
52	5	1327	G
52	5	1331	A
52	5	1334	A
52	5	1335	G
52	5	1337	U
52	5	1338	A
52	5	1340	G
52	5	1343	G
52	5	1344	C
52	5	1346	G
52	5	1347	U
52	5	1352	A
52	5	1353	C
52	5	1354	G
52	5	1356	U
52	5	1357	C
52	5	1360	G
52	5	1369	A
52	5	1372	C
52	5	1374	C
52	5	1375	C
52	5	1376	G
52	5	1384	A
52	5	1393	A
52	5	1394	G
52	5	1397	G
52	5	1400	A
52	5	1405	U
52	5	1406	U
52	5	1408	A
52	5	1417	U
52	5	1421	A
52	5	1423	C
52	5	1427	U

Continued on next page...

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Mol	Chain	Res	Type
52	5	1428	A
52	5	1429	G
52	5	1443	A
52	5	1444	G
52	5	1446	A
52	5	1450	C
52	5	1458	A
52	5	1459	U
52	5	1466	U
52	5	1467	A
52	5	1469	G
52	5	1472	G
52	5	1474	A
52	5	1475	A
52	5	1477	A
52	5	1478	A
52	5	1480	G
52	5	1482	A
52	5	1492	G
52	5	1493	A
52	5	1494	A
52	5	1495	C
52	5	1504	G
52	5	1505	G
53	6	3	G
53	6	5	C
53	6	7	U
53	6	14	C
53	6	17	U
53	6	18	C
53	6	19	G
53	6	20	G
53	6	21	U
53	6	22	A
53	6	23	G
53	6	34	U
53	6	35	G
53	6	42	C
53	6	43	G
53	6	44	U
53	6	47	G
53	6	48	U

Continued on next page...

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Mol	Chain	Res	Type
53	6	49	C
53	6	54	G
53	6	56	U
53	6	57	C
53	6	58	G
53	6	59	A
53	6	61	U
53	6	62	C
53	6	71	A
53	6	72	C
53	6	75	C
53	6	76	C
53	8	3	G
53	8	5	C
53	8	7	U
53	8	14	C
53	8	17	U
53	8	18	C
53	8	19	G
53	8	20	G
53	8	21	U
53	8	22	A
53	8	23	G
53	8	34	U
53	8	35	G
53	8	42	C
53	8	43	G
53	8	44	U
53	8	47	G
53	8	48	U
53	8	49	C
53	8	54	G
53	8	56	U
53	8	57	C
53	8	58	G
53	8	59	A
53	8	61	U
53	8	62	C
53	8	71	A
53	8	72	C
53	8	75	C
53	8	76	C

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	3	76	A
50	3	296	U
50	3	311	G
50	3	366	A
50	3	410	G
50	3	425	U
50	3	500	U
50	3	508	A
50	3	514	A
50	3	881	A
50	3	996	A
50	3	1048	A
50	3	1054	U
50	3	1096	U
50	3	1209	U
50	3	1297	U
50	3	1355	C
50	3	1454	G
50	3	1465	U
50	3	1507	G
50	3	1583	G
50	3	1588	A
50	3	1747	G
50	3	1820	U
50	3	1936	G
50	3	2139	C
50	3	2332	U
50	3	2397	G
50	3	2504	C
50	3	2506	C
50	3	2604	U
50	3	2668	A
50	3	2764	U
50	3	2897	G
51	4	54	U
51	4	59	A
52	5	31	U
52	5	39	G
52	5	48	C
52	5	448	A
52	5	619	A
52	5	683	G

Continued on next page...

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Mol	Chain	Res	Type
52	5	748	U
52	5	1135	U
52	5	1143	C
52	5	1158	A
52	5	1188	A
52	5	1323	A
52	5	1355	U
53	6	16	G
53	6	18	C
53	6	34	U
53	6	43	G
53	6	56	U
53	6	58	G
53	8	16	G
53	8	18	C
53	8	34	U
53	8	43	G
53	8	56	U
53	8	58	G

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

There are no ligands in this entry.

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.

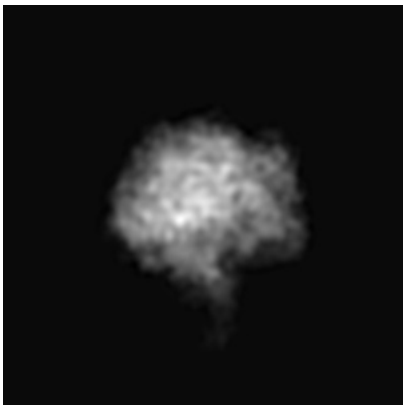
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13448. These allow visual inspection of the internal detail of the map and identification of artifacts.

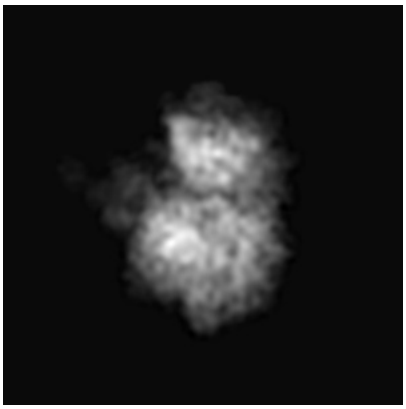
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

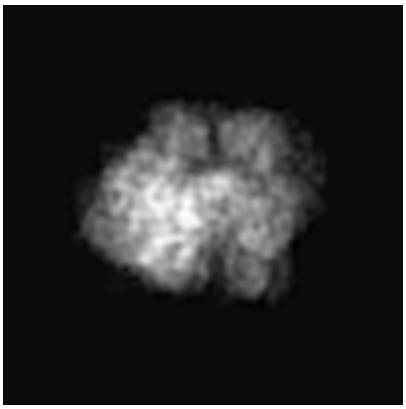
6.1.1 Primary map



X

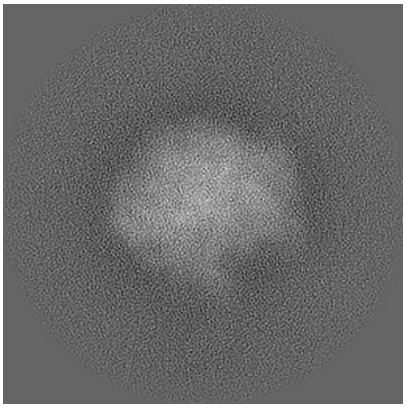


Y

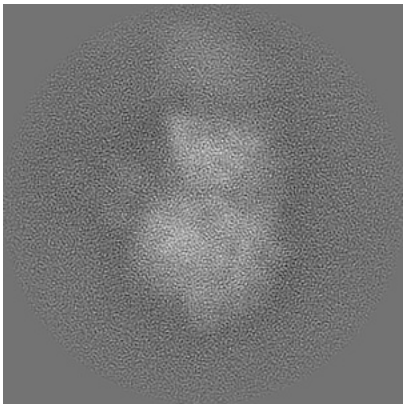


Z

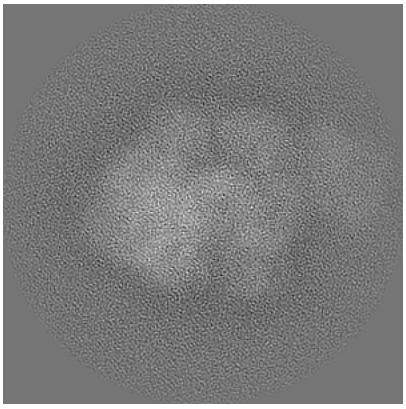
6.1.2 Raw map



X



Y

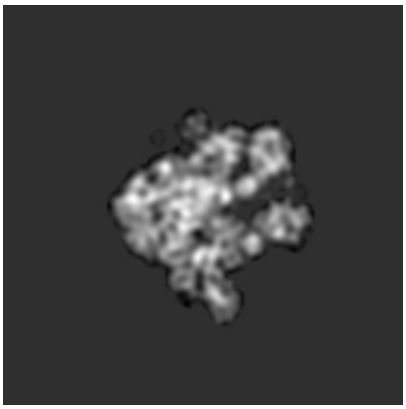


Z

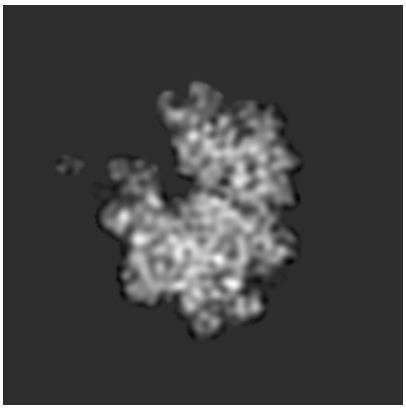
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

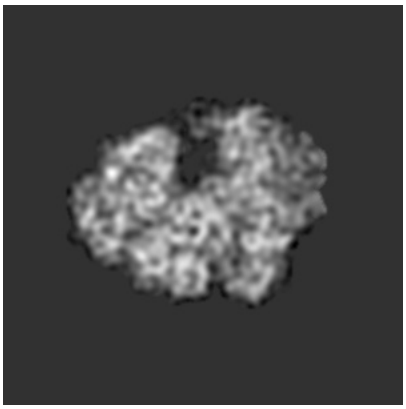
6.2.1 Primary map



X Index: 128

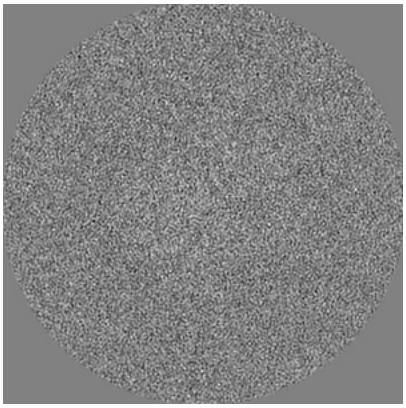


Y Index: 128

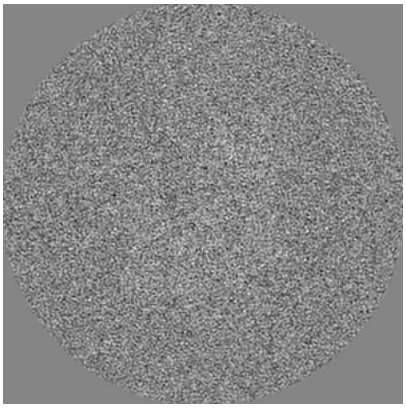


Z Index: 128

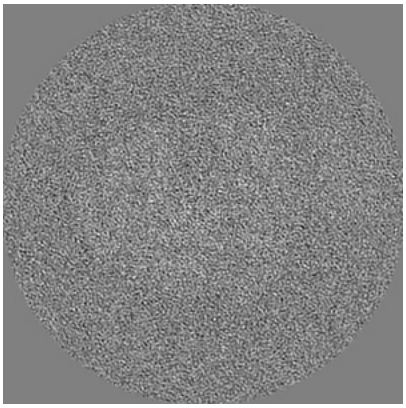
6.2.2 Raw map



X Index: 128



Y Index: 128

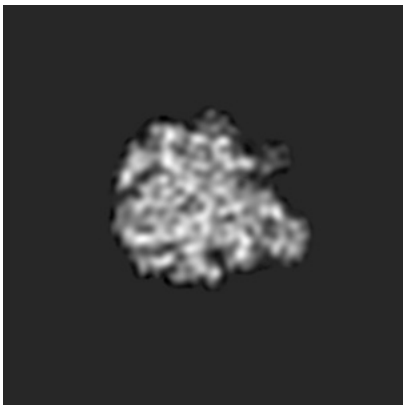


Z Index: 128

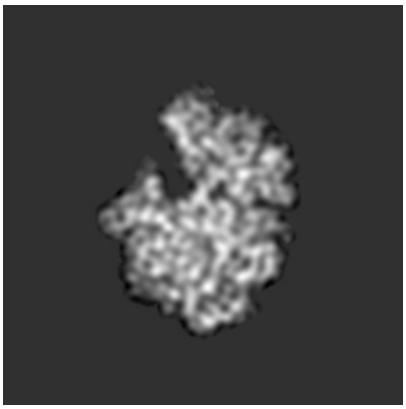
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

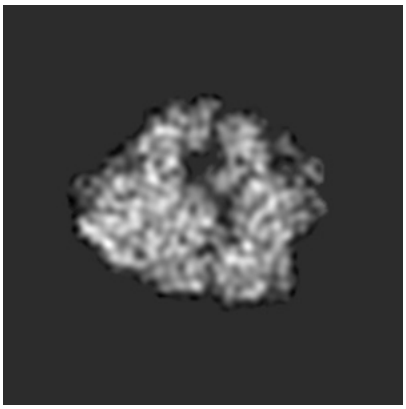
6.3.1 Primary map



X Index: 102

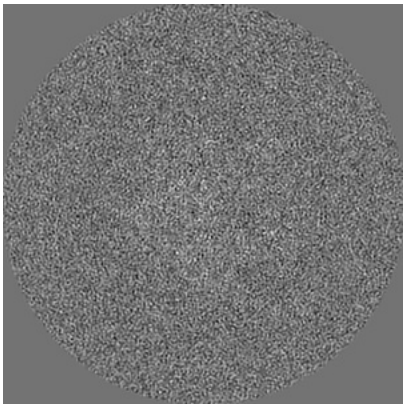


Y Index: 120

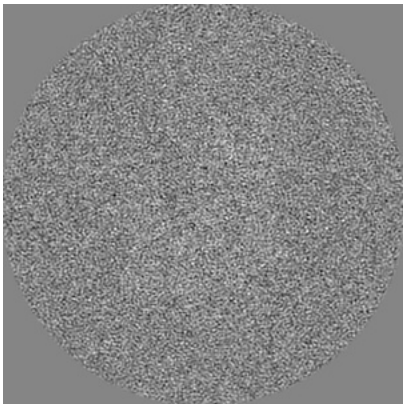


Z Index: 121

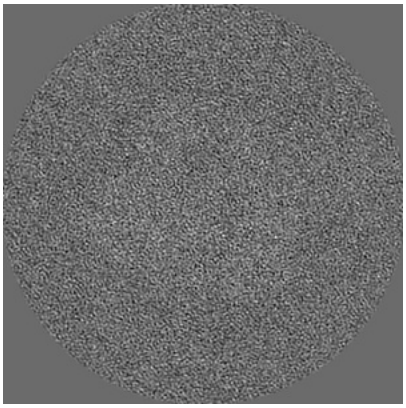
6.3.2 Raw map



X Index: 119



Y Index: 128

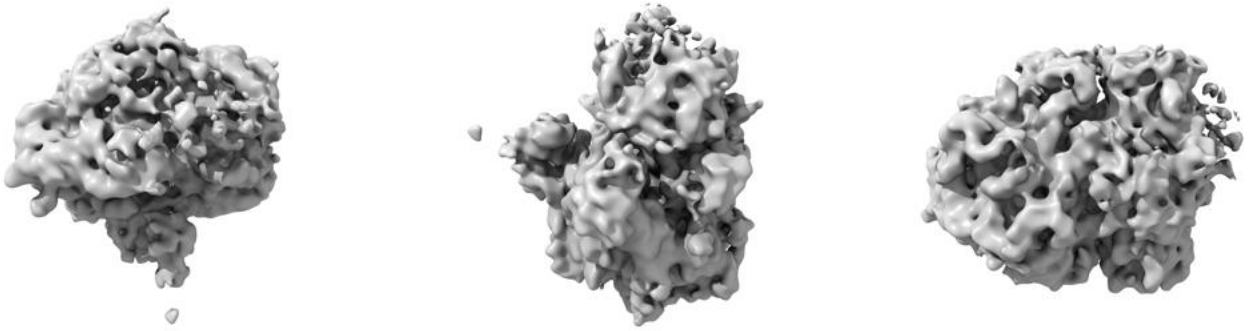


Z Index: 119

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

6.4 Orthogonal surface views (i)

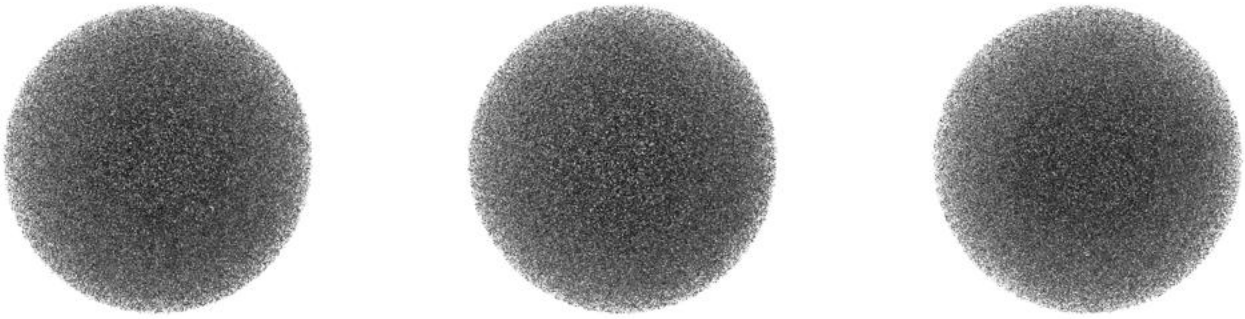
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

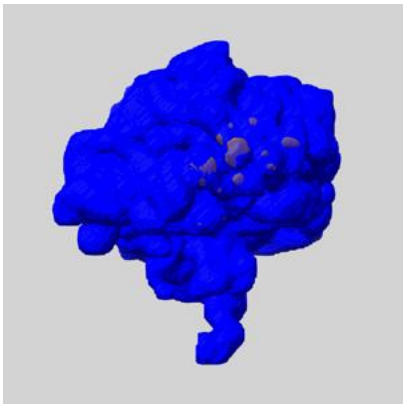
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

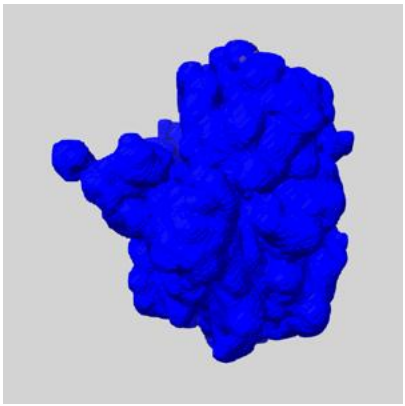
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

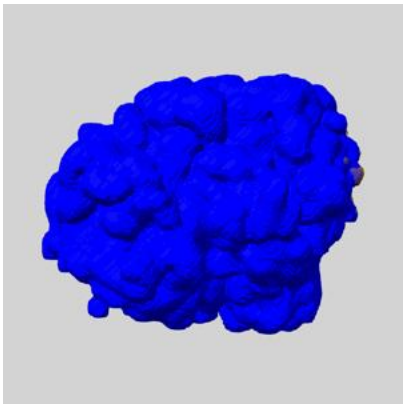
6.5.1 emd_13448_msk_1.map (i)



X



Y

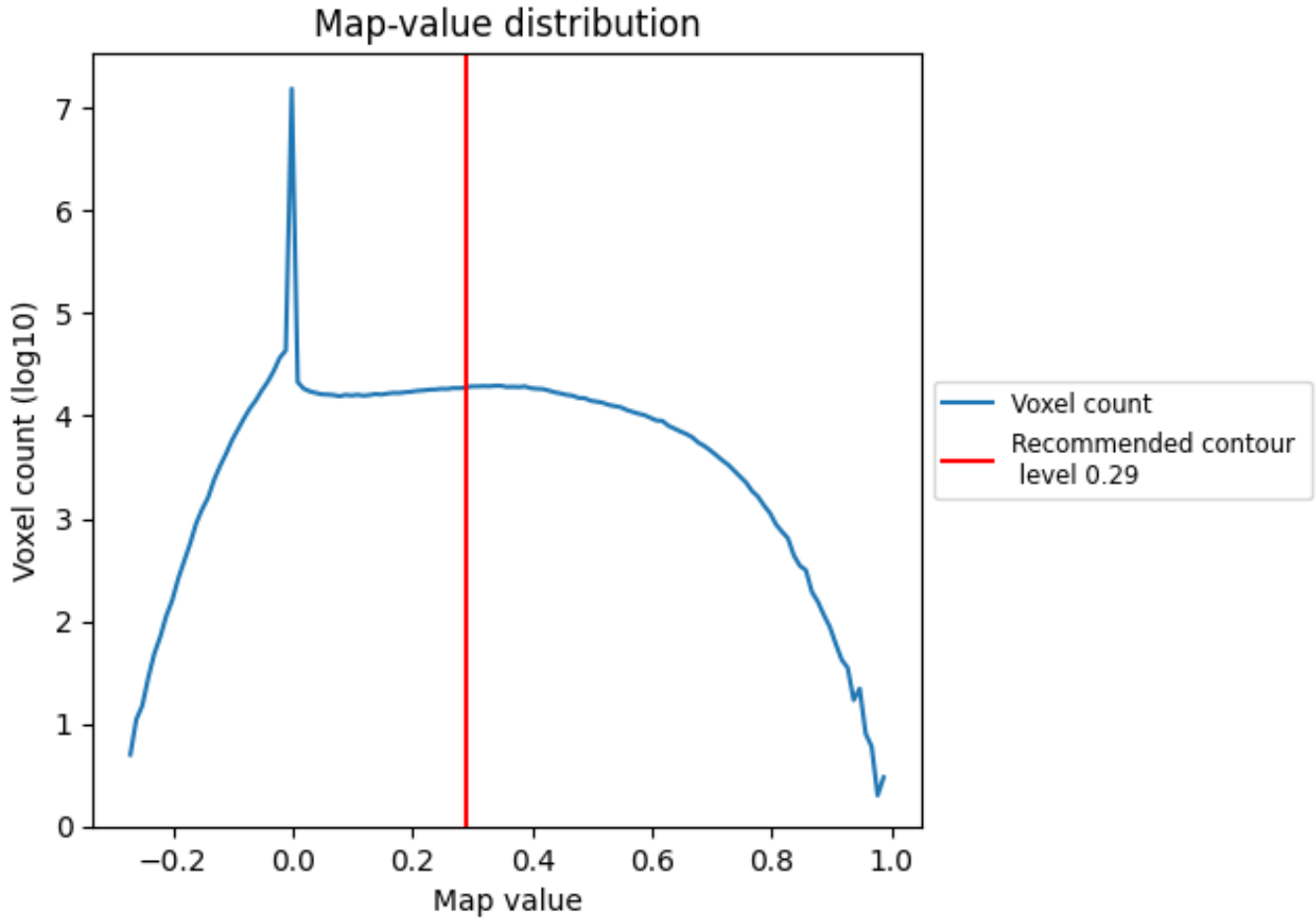


Z

7 Map analysis

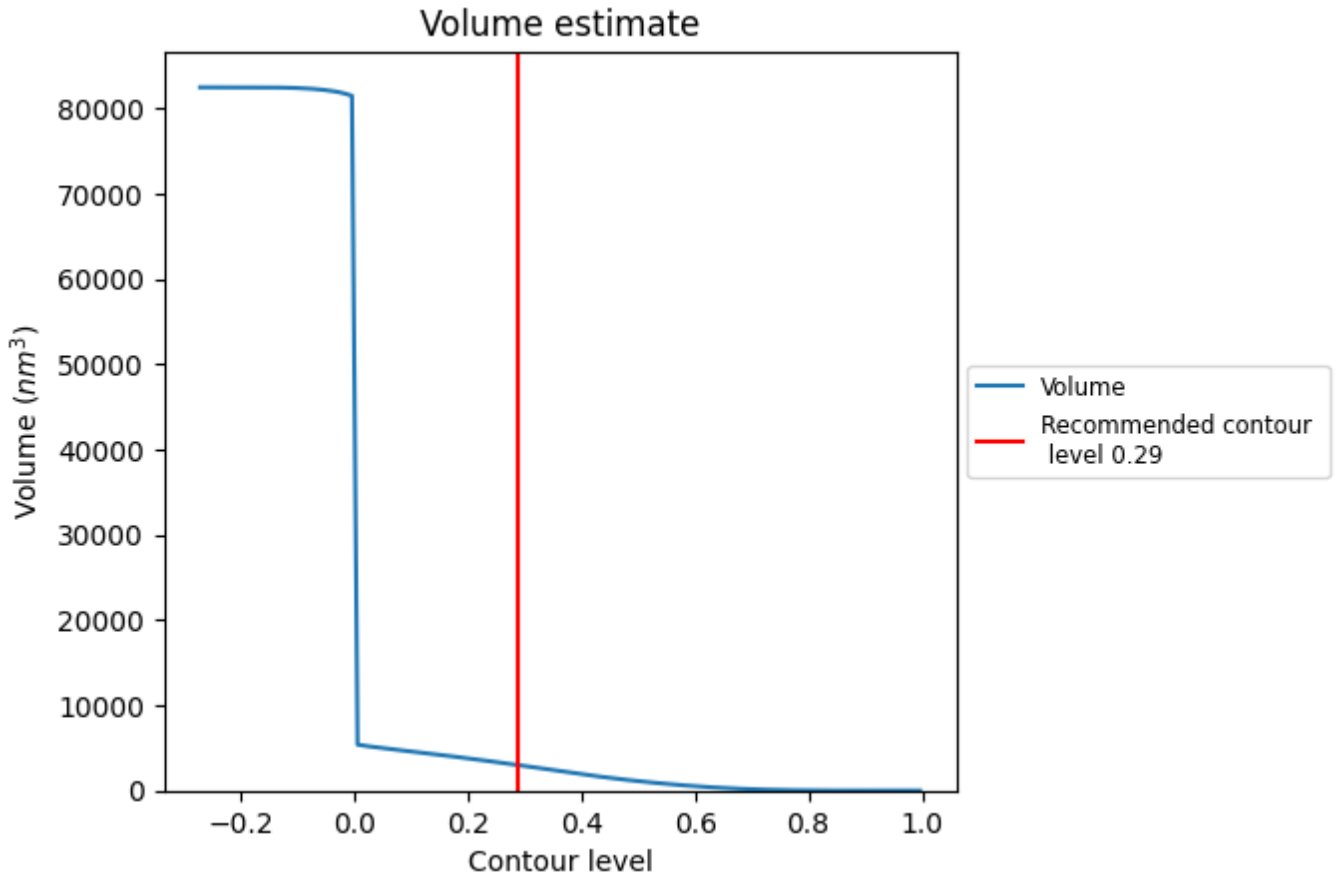
This section contains the results of statistical analysis of the map.

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.

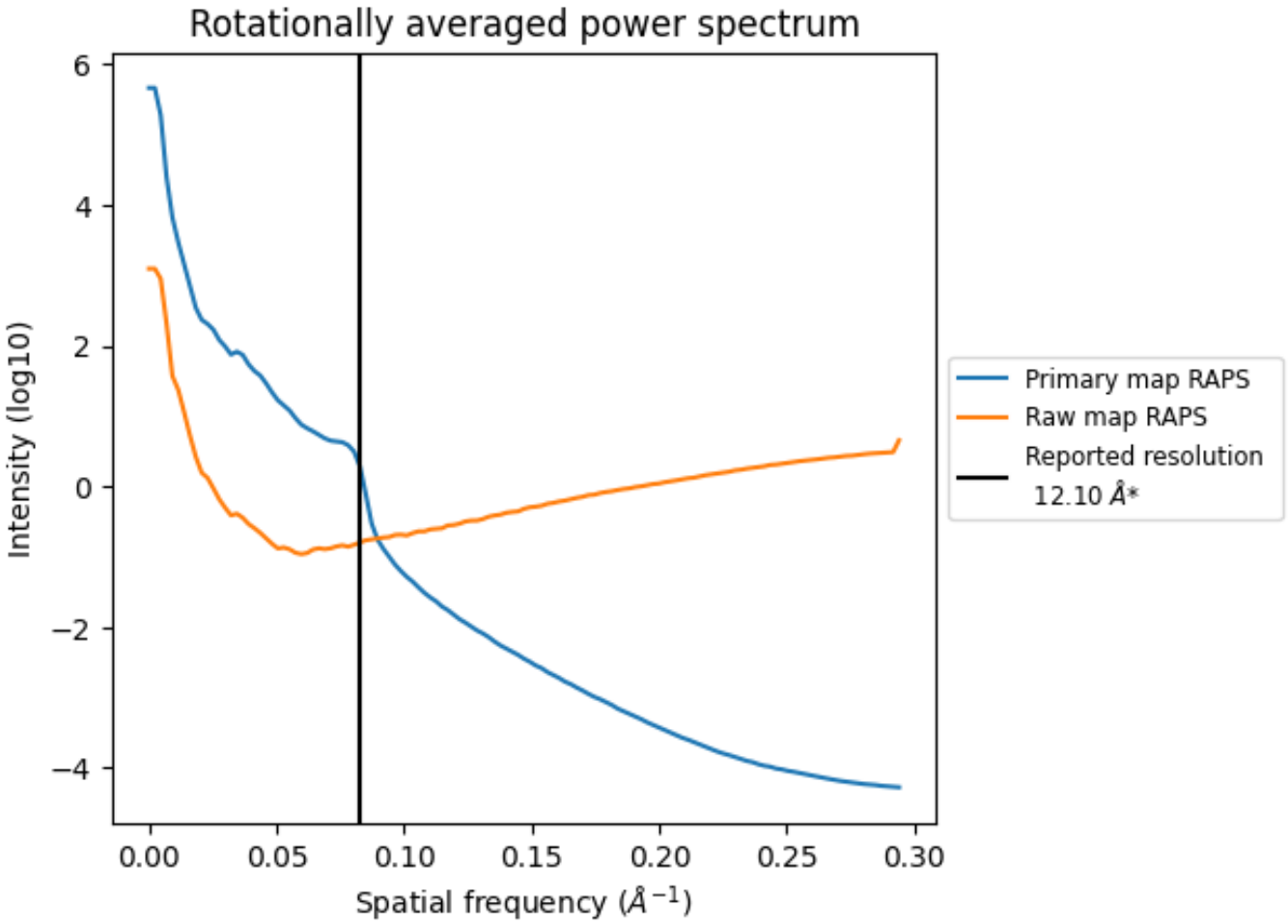
7.2 Volume estimate



The volume at the recommended contour level is 2982 nm^3; this corresponds to an approximate mass of 2693 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)

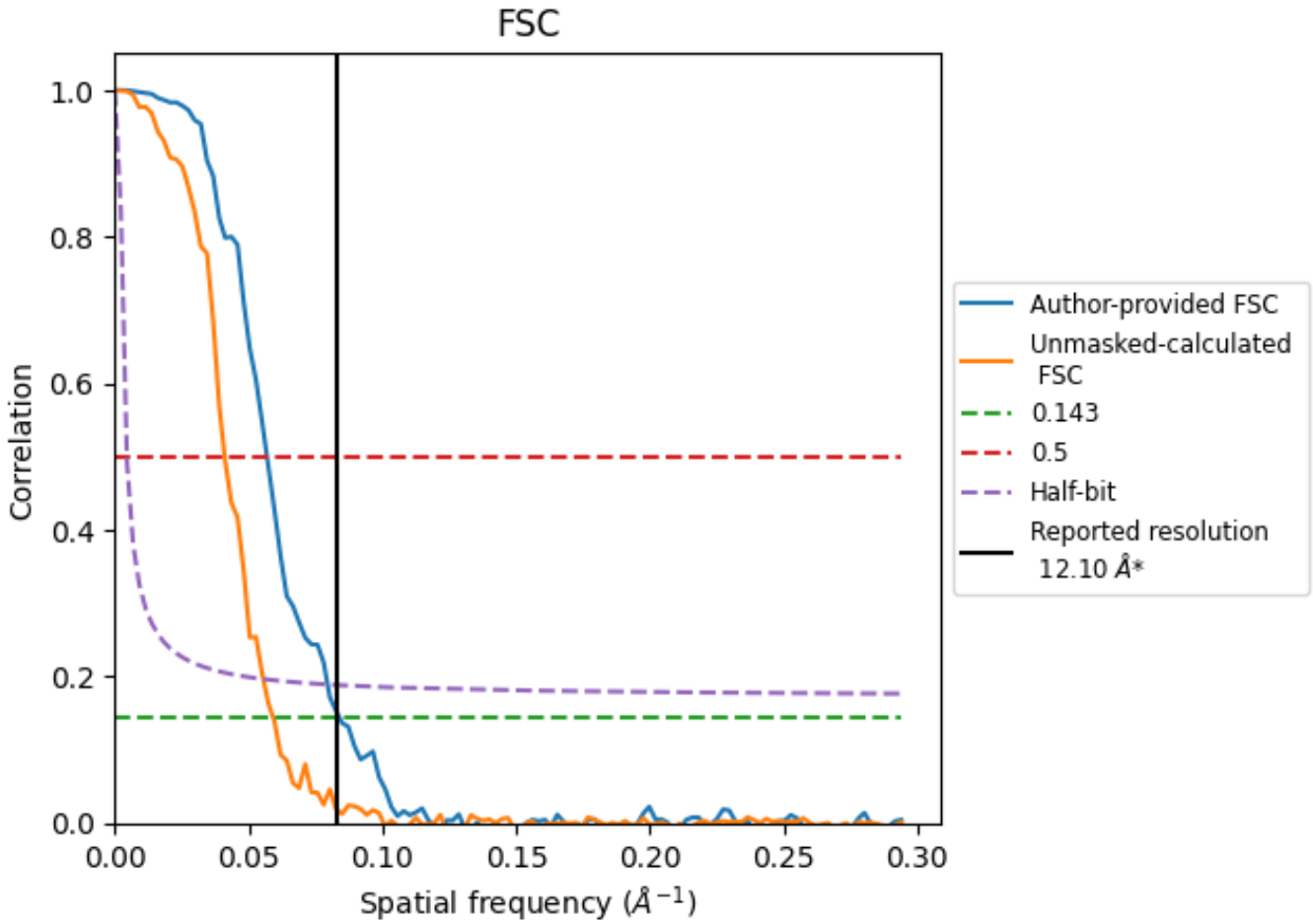


*Reported resolution corresponds to spatial frequency of 0.083 Å^{-1}

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 0.083 Å^{-1}

8.2 Resolution estimates (i)

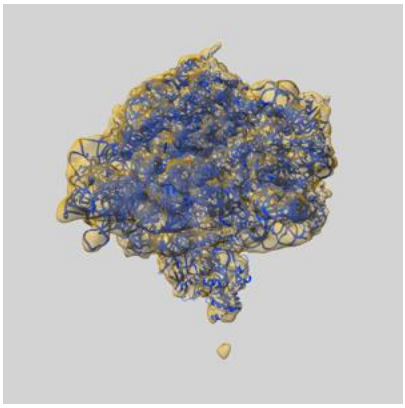
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.10	-	-
Author-provided FSC curve	11.90	17.57	12.56
Unmasked-calculated*	16.86	24.33	17.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 16.86 differs from the reported value 12.1 by more than 10 %

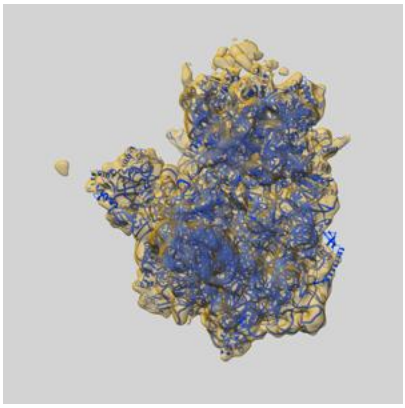
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13448 and PDB model 7PIR. Per-residue inclusion information can be found in section 3 on page 13.

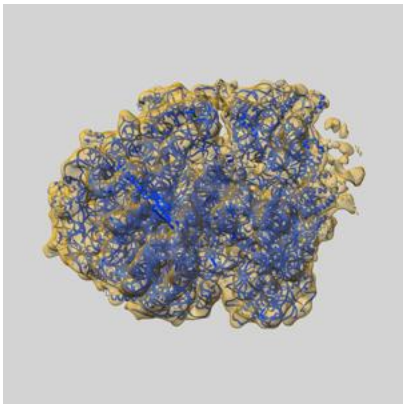
9.1 Map-model overlay



X



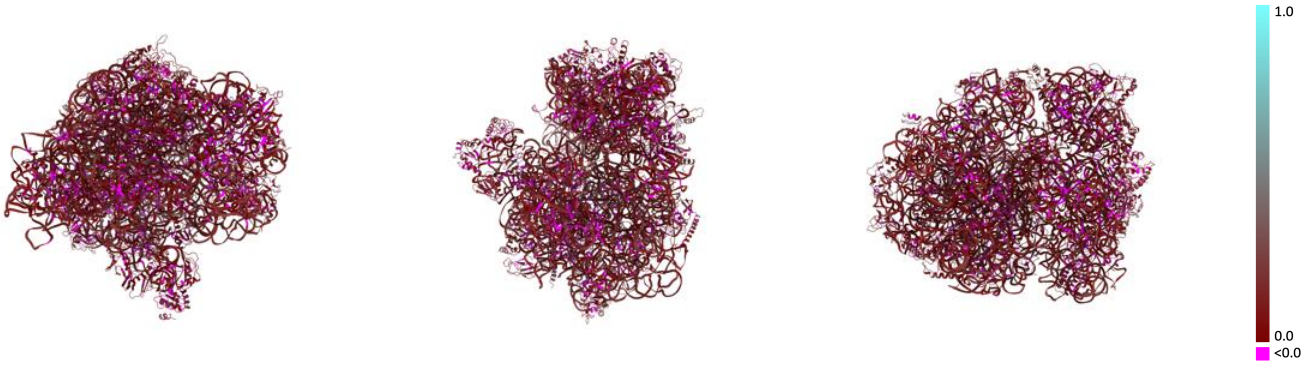
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

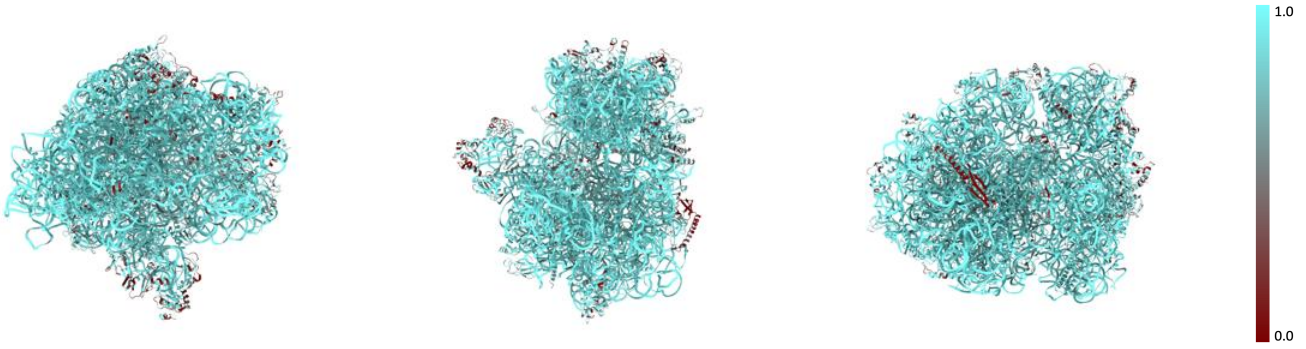
9.2 Q-score mapped to coordinate model (i)



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.

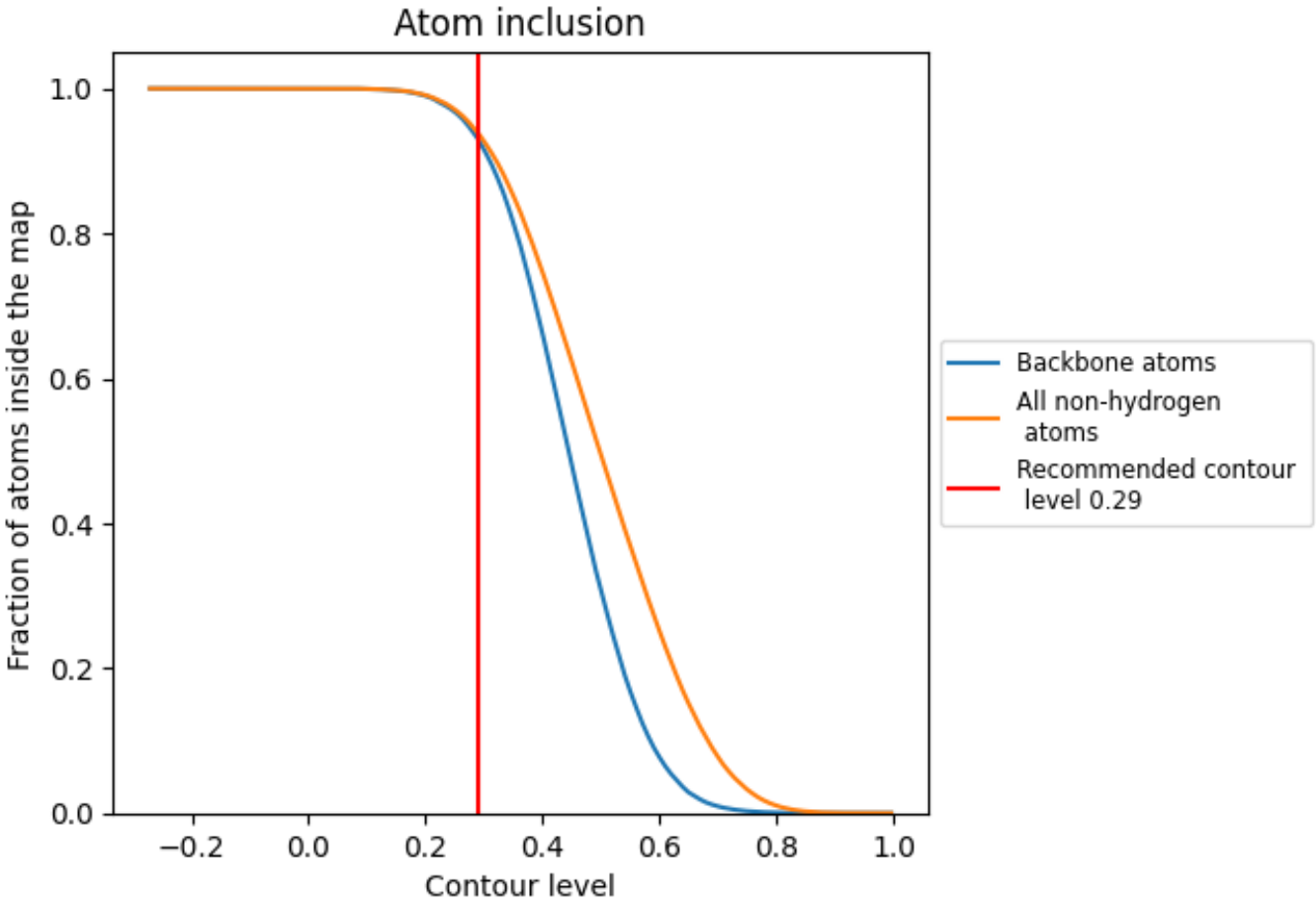
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.29).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9385	0.1040
0	0.9973	0.0760
1	0.9936	0.0650
2	0.9730	0.0330
3	0.9882	0.1150
4	0.9929	0.1240
5	0.9872	0.1150
6	0.8282	0.0820
8	0.9728	0.1300
A	0.7068	0.0950
B	0.7874	0.1110
C	0.8426	0.0710
D	0.8192	0.0700
E	0.7081	0.1080
F	0.8140	0.0850
G	0.8854	0.0850
H	0.8292	0.0670
I	0.7509	0.0790
J	0.7772	0.0670
K	0.9492	0.0650
L	0.8192	0.1010
M	0.8659	0.0000
N	0.8852	0.0830
O	0.9523	0.0750
P	0.8721	0.0900
Q	0.9477	0.0820
R	0.8731	0.0450
S	0.9672	0.0810
T	0.8326	0.1340
a	0.9640	0.0590
b	0.9055	0.0570
c	0.8679	0.0860
d	0.8181	0.0980
e	0.6751	0.0810
f	0.3768	0.0870

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Chain	Atom inclusion	Q-score
g	0.5866	0.0770
h	0.6364	0.0830
i	0.9518	0.0890
j	0.8163	0.0710
k	0.8473	0.0660
l	0.9308	0.0650
m	0.9744	0.0550
n	0.8639	0.0760
o	0.8672	0.0860
p	0.9650	0.0720
q	0.8561	0.0730
r	0.9323	0.0880
s	0.8773	0.0840
t	0.8211	0.0900
u	0.9656	0.0550
v	0.9899	0.0910
w	0.8926	0.1320
x	0.5598	0.1150
y	0.9078	0.0450
z	0.9849	0.0550