Full wwPDB EM Validation Report (i)

Jul 18, 2023 – 05:14 pm BST

PDB ID	:	7PAL
EMDB ID	:	EMD-13276
Title	:	70S ribosome with A- and P-site tRNAs in Mycoplasma pneumoniae cells
Authors	:	Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on	:	2021-07-30
Resolution	:	4.70 Å(reported)
Based on initial models	:	3J9W, 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 (i) symbol.

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

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

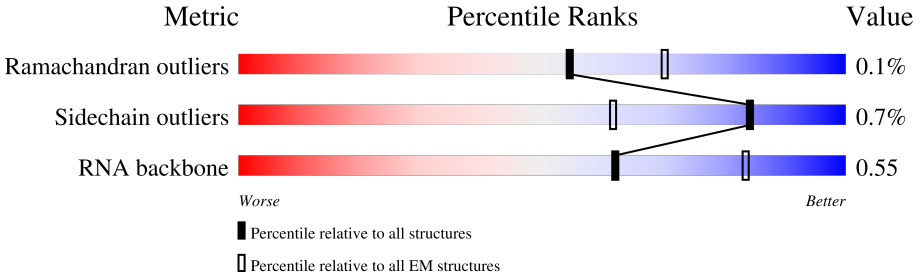
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 4.70 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	100%
3	2	37	100%
4	A	294	27% 82% 18%
5	B	273	19% 78% 21%
6	C	205	33% 98%
7	D	219	14% 69% 30%
8	E	215	36% 78% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	155	43% 99%
10	G	142	25% 99%
11	H	132	36% 96%
12	I	108	34% 94% 6%
13	J	121	24% 94% 6%
14	K	139	15% 96%
15	L	124	49% 95% 5%
16	M	61	13% 98%
17	N	86	23% 97%
18	O	94	26% 83% 15%
19	P	85	32% 98%
20	Q	104	17% 62% 38%
21	R	87	40% 95%
22	S	87	17% 85% 11%
23	T	60	25% 88% 12%
24	Z	5	100%
25	a	287	7% 99%
26	b	287	6% 80% 20%
27	c	212	13% 99%
28	d	180	49% 96%
29	e	184	27% 95%
30	f	149	83% 96%
31	g	161	64% 70% 8% 22%
32	h	137	87% 93% 7%
33	i	146	11% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	j	122	11% 100%
35	k	151	13% 98%
36	l	139	8% 98%
37	m	124	94%
38	n	116	20% 95%
39	o	119	9% 97%
40	p	127	5% 90% 10%
41	q	100	11% 97%
42	r	159	6% 87% 13%
43	s	237	39% 61%
44	t	111	30% 100%
45	u	104	10% 83% 17%
46	v	65	15% 97%
47	w	111	14% 89% 10%
48	x	97	31% 45% 55%
49	y	57	7% 93% 5%
50	z	53	94% 6%
51	3	2907	78% 21%
52	4	108	74% 23%
53	5	1520	80% 19%
54	6	76	5% 75% 24%
54	7	76	43% 75% 24%
55	Y	9	100%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 146334 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
			Total	C	N	O	S		
7	D	153	1173	742	226	202	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	Z	5	31	20	5	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	126	960	612	167	178	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	3	2878	61664	27558	11236	19995	2875	0	0

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	4	105	2239	1003	409	724	103	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	5	1493	31943	14279	5792	10382	1490	0	0

- Molecule 54 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	6	76	1618	723	289	531	75	0	0
54	7	76	1618	723	289	531	75	0	0

- Molecule 55 is a RNA chain called mRNA.

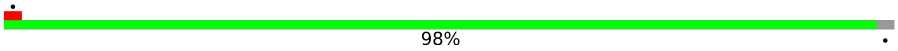
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	Y	9	183	84	29	62	8	0	0

3 Residue-property plots (i)

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

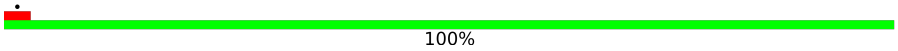
• Molecule 1: 50S ribosomal protein L34

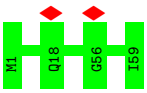
Chain 0:



• Molecule 2: 50S ribosomal protein L35

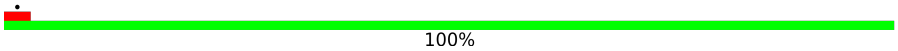
Chain 1:

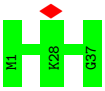




• Molecule 3: 50S ribosomal protein L36

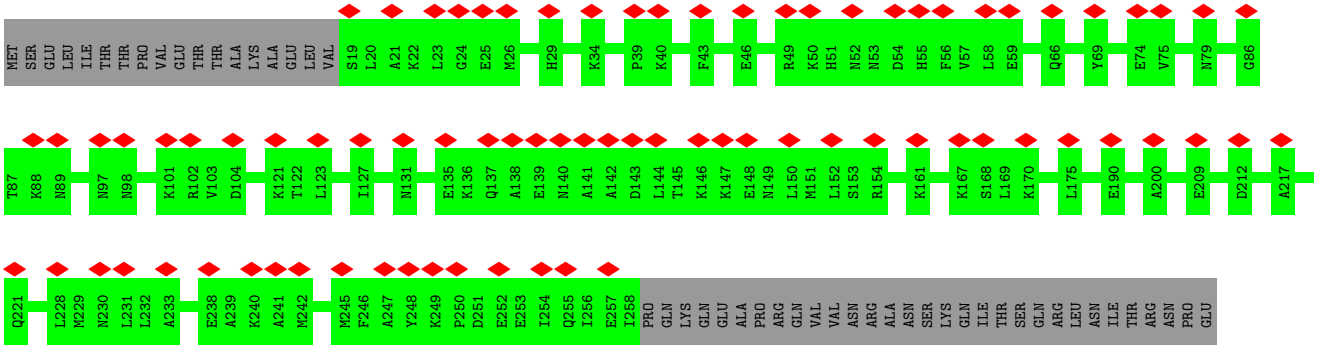
Chain 2:





• Molecule 4: 30S ribosomal protein S2

Chain A:



VAL LEU THR ARG GLU

- Molecule 5: 30S ribosomal protein S3

Chain B:

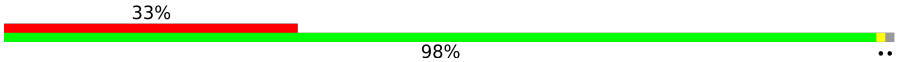
MET GLY Q3 L34 I35 E36 D37 E38 K39 F44 R49 Q52 V53 S54 N55 I58 D66 V67 F68 A72 Q73 P74 A75 F76 L77 I78 G79 S80 E81 N82 K83 N84 I85 Q86 K87 I96 G97 N101 L102 D103 L104 E108 I109 G110 L114 S115 A116 D122

N125 E128 R138 A147 G148 G151 A166 R167 M170 E173 S179 R182 A188 K191 G200 G208 Y211 T212 K213 R217 THR PRO ALA HIS ILE LEU HIS PRO GLN LYS LYS GLN PRO ASN ARG GLN ASN GLN GLN PRO ARG HIS PHE ASN

GLN GLY GLN VAL LEU SER ALA ASN LYS LEU THR GLY SER ASP VAL GLU THR SER SER ILE GLN ALA LEU THR LYS PRO ASN LYS GLU ASP LYS GLN

- Molecule 6: 30S ribosomal protein S4

Chain C:



M1 K2 F8 K9 R10 F16 S17 L18 L19 E20 K23 E24 F25 S26 K27 G28 K29 R41 F42 R43 S44 S45 T46 L54 Q58 Q61 I66 L77 K80 Q81 R82 L85 N88 L89 F90 L93 D98 N99 R103 F106 L124 N125 D126

D130 T131 L136 G139 D140 K141 K145 A146 K147 T148 I149 K150 V154 K155 A156 A157 S158 E159 S160 G161 V162 T169 K172 T173 F174 E175 G176 F181 P182 E183 R184 P188 A189 N192 E193 S194 Y195 K201 R202 L203 VAL LYS

- Molecule 7: 30S ribosomal protein S5

Chain D:

MET THR ASP GLN ASN GLN LYS ALA ASN GLN GLY ASN GLY LEU GLN THR THR ASN LEU GLN ALA HIS ALA GLN ARG LYS HIS ASN LEU ARG PRO SER SER GLU GLY ILE LYS LYS ALA VAL SER LYS LYS GLU GLY GLY GLY HIS ASN ARG ASN ASN GLN ASN ARG ARG PHE GLN LYS PRO

ALA PHE LYS SER GLU F66 E67 E68 S77 R84 K100 N113 H127 E130 I131 G134 S135 I136 Y137 G145 A146 L150 G157 T158 G159 G163 L172 D177 H193 D197 L200 K201 A209 R212 N213 K214 N215 L216 N217 E218 LEU

- Molecule 8: 30S ribosomal protein S6

Chain E:

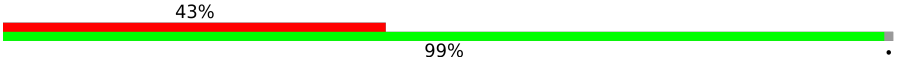
M1 Q2 Y3 I6 L7 L8 V9 D10 G11 S12 L13 S14 L15 E16 Q17 A18 N19 Q20 K24 Q27 T28 L29 T30 N31 V32 E33 G34 L35 Q36 T37 E38 Y39 L40 G41 L42 A55 H56 Y57 K61 F62 S63 G64 D65 N66 K70 D71 F72 K73 N77 I78 N79 K80 Q81

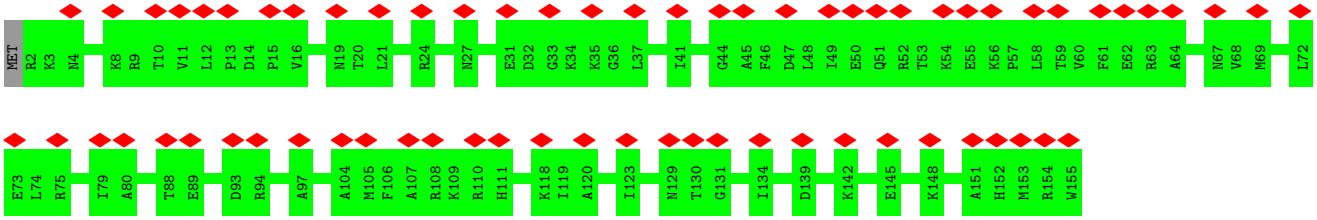
V82 L83 L97 A98 K104 R112 A113 E117 I118 I119 A120 R121 E122 N123 N124 N127 P128 D129 V130 P131 G135 L136 A137 S138 T139 Q140 P141 R142 R145 T146 E147 K148 A149 Q150 K151 P152 K153 E154 E155 L156 G164 N165 F166 D167 SER VAL GLN ALA ASN PRO TYR ARG

PRO ARG PHE LYS ARG PHE ASN ALA GLU HIS VAL ASN GLN ARG GLN GLN GLN ASN ASN ASN ASN ASN ARG PHE ASP ARG ASN ARG ASN ARG GLN HIS ASN ARG PHE LYS ASP LYS GLN

- Molecule 9: 30S ribosomal protein S7

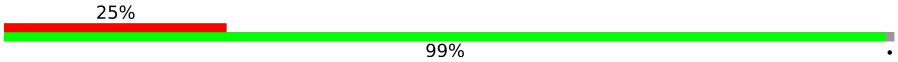
Chain F:

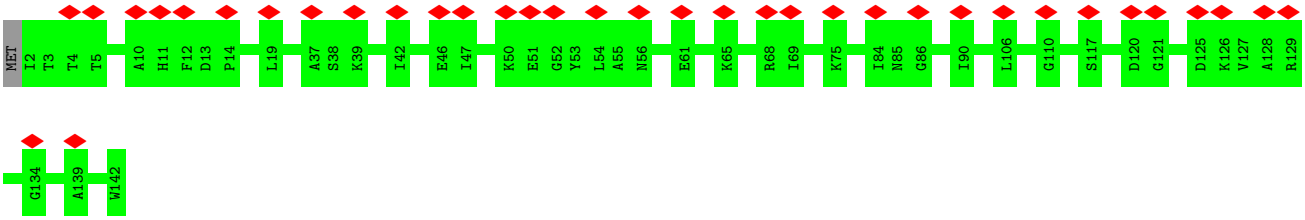




- Molecule 10: 30S ribosomal protein S8

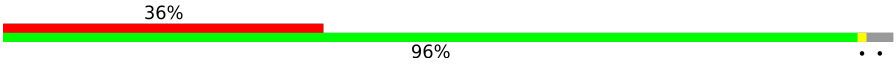
Chain G:

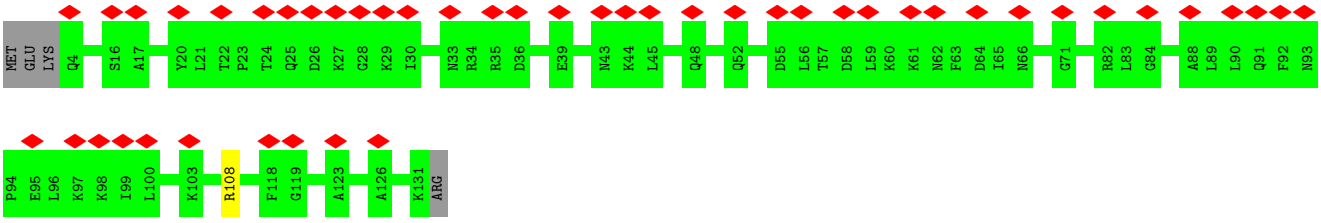




- Molecule 11: 30S ribosomal protein S9

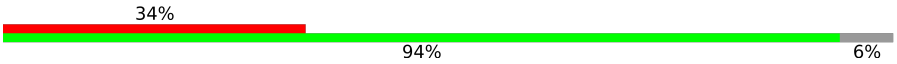
Chain H:

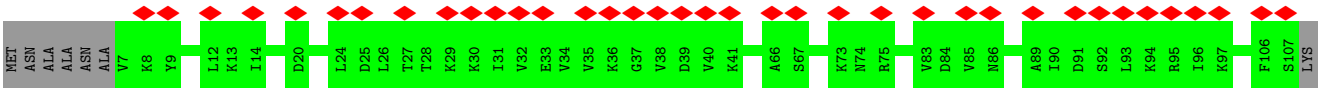




- Molecule 12: 30S ribosomal protein S10

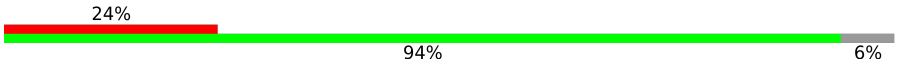
Chain I:

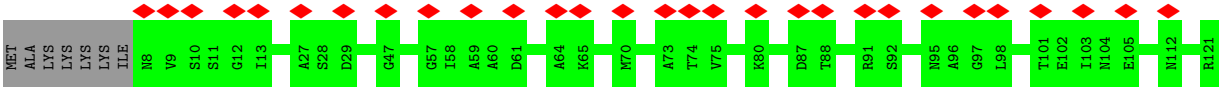




- Molecule 13: 30S ribosomal protein S11

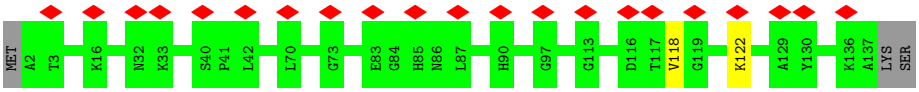
Chain J:





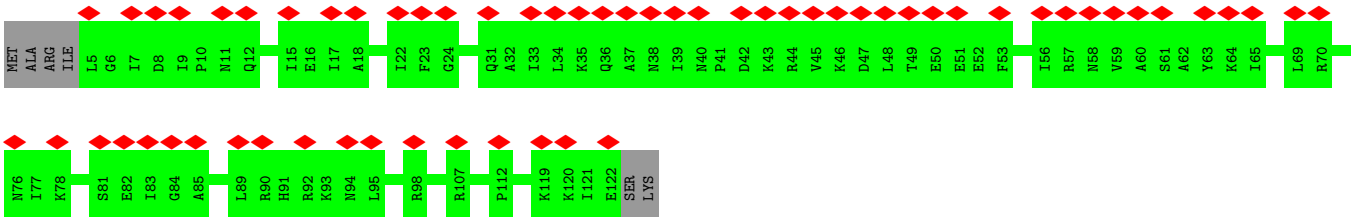
- Molecule 14: 30S ribosomal protein S12

Chain K: 15% 96%



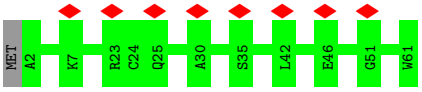
• Molecule 15: 30S ribosomal protein S13

Chain L: 49% 95% 5%



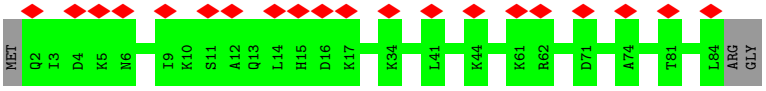
• Molecule 16: 30S ribosomal protein S14 type Z

Chain M: 13% 98%



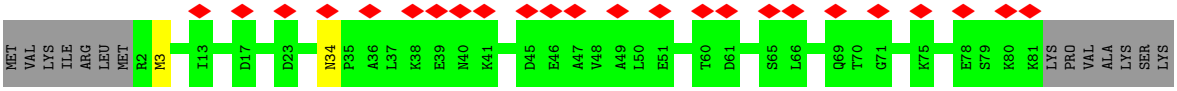
• Molecule 17: 30S ribosomal protein S15

Chain N: 23% 97%



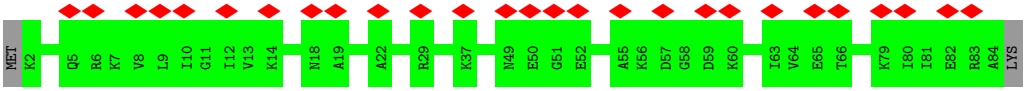
• Molecule 18: 30S ribosomal protein S16

Chain O: 26% 83% 15%



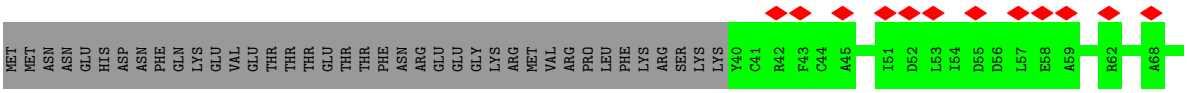
• Molecule 19: 30S ribosomal protein S17

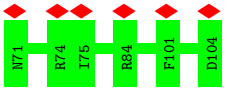
Chain P: 32% 98%



• Molecule 20: 30S ribosomal protein S18

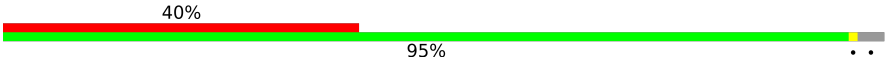
Chain Q: 17% 62% 38%

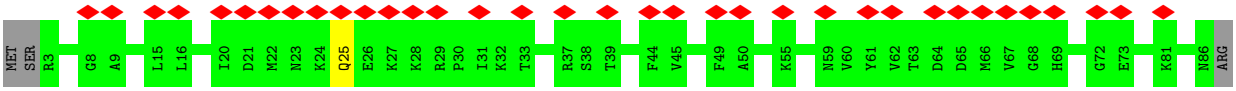




• Molecule 21: 30S ribosomal protein S19

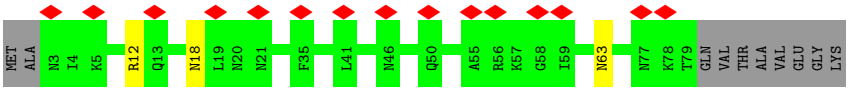
Chain R:





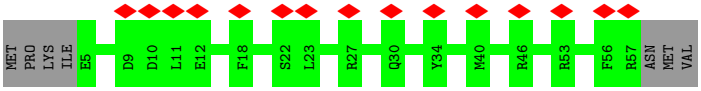
• Molecule 22: 30S ribosomal protein S20

Chain S:



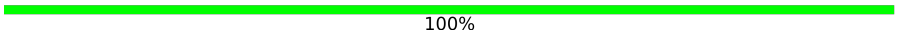
• Molecule 23: 30S ribosomal protein S21

Chain T:



• Molecule 24: nascent peptide

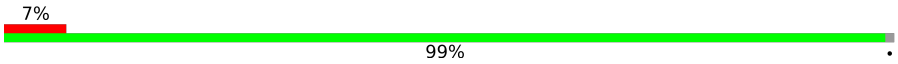
Chain Z:

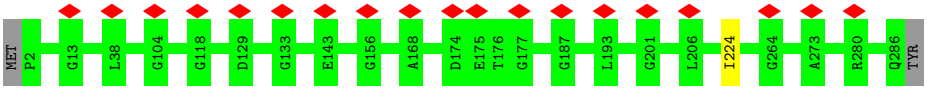


There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L2

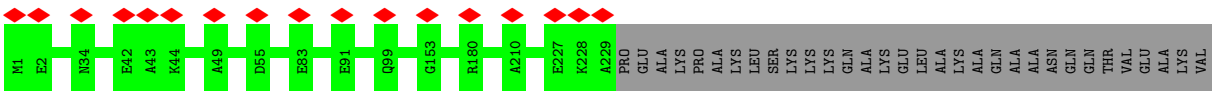
Chain a:

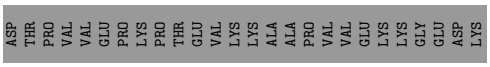




• Molecule 26: 50S ribosomal protein L3

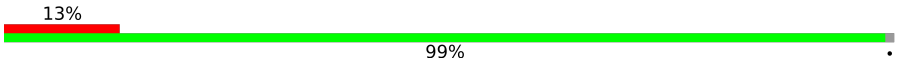
Chain b:

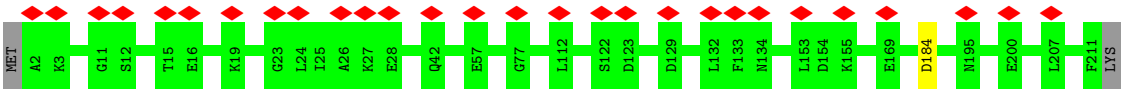




- Molecule 27: 50S ribosomal protein L4

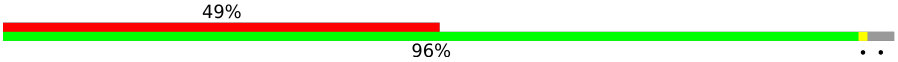
Chain c:

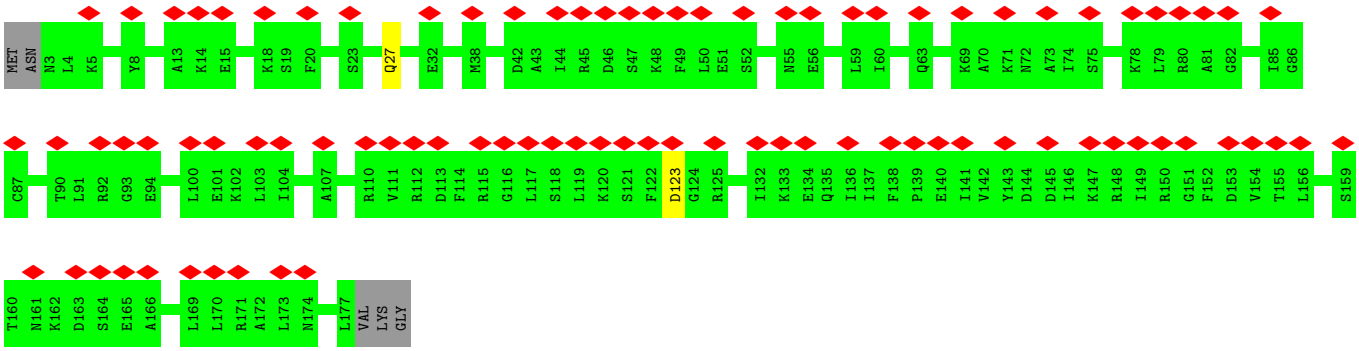




- Molecule 28: 50S ribosomal protein L5

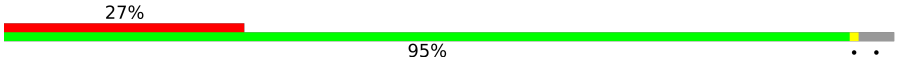
Chain d:

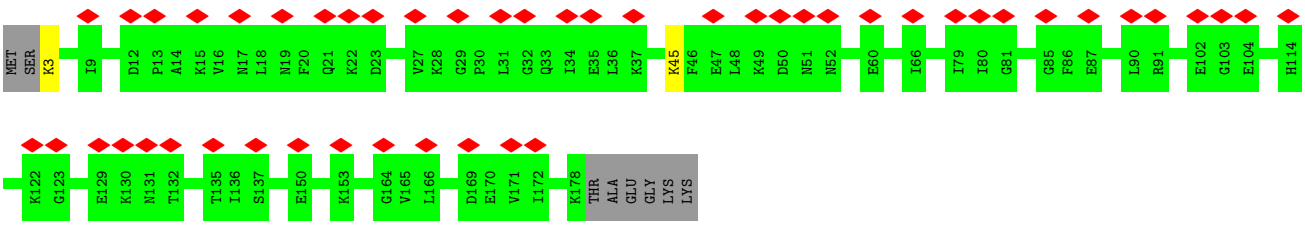




- Molecule 29: 50S ribosomal protein L6

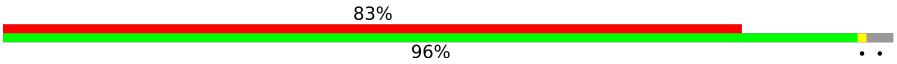
Chain e:

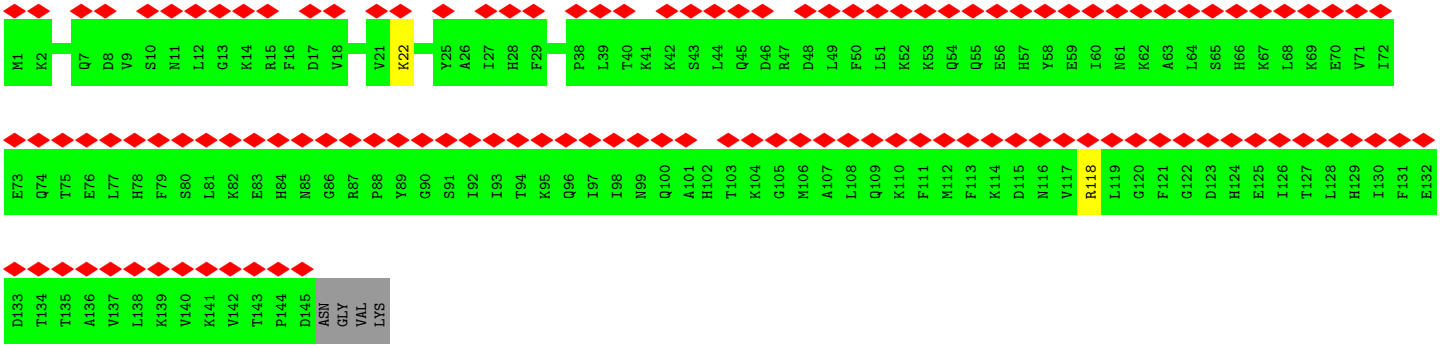




- Molecule 30: 50S ribosomal protein L9

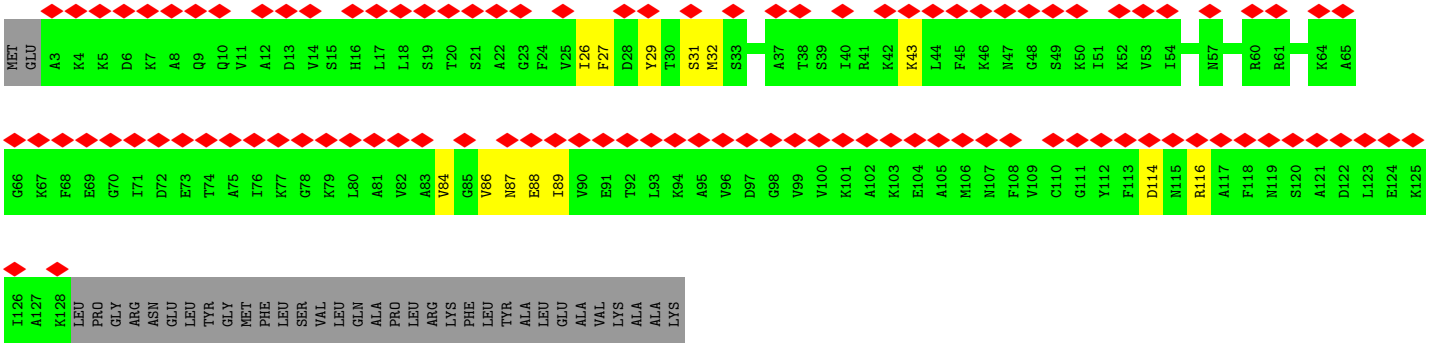
Chain f:





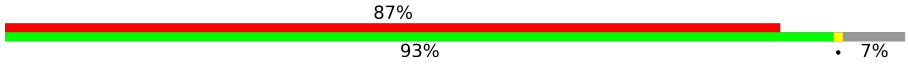
- Molecule 31: 50S ribosomal protein L10

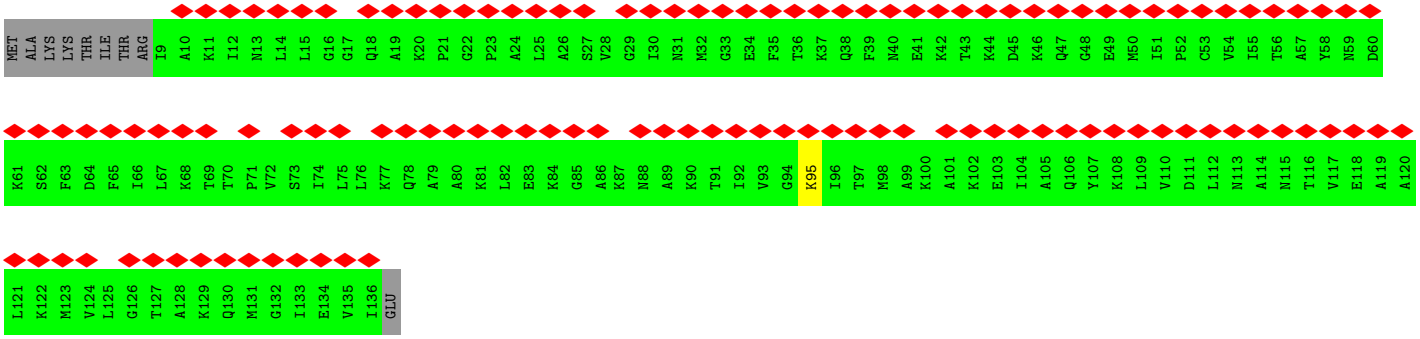
Chain g:



- Molecule 32: 50S ribosomal protein L11

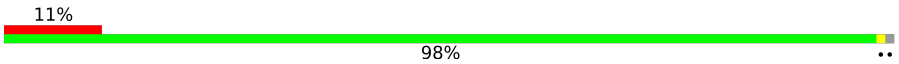
Chain h:

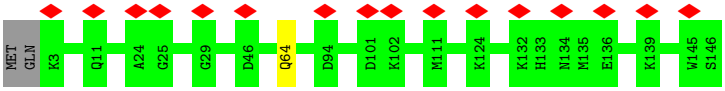




- Molecule 33: 50S ribosomal protein L13

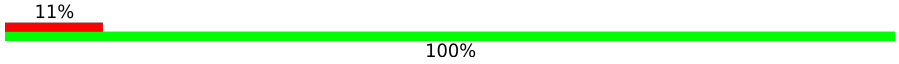
Chain i:

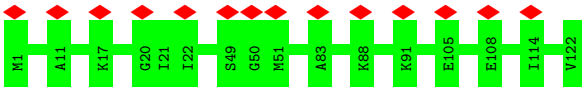




- Molecule 34: 50S ribosomal protein L14

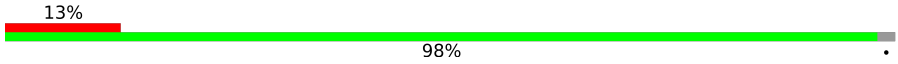
Chain j:

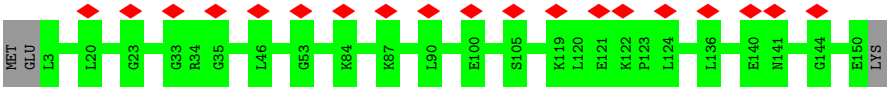




- Molecule 35: 50S ribosomal protein L15

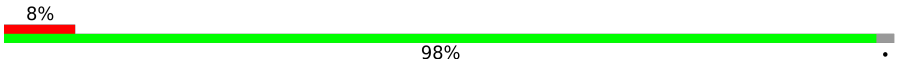
Chain k:

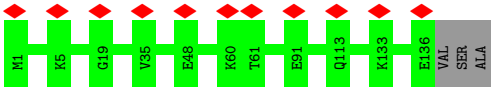




• Molecule 36: 50S ribosomal protein L16

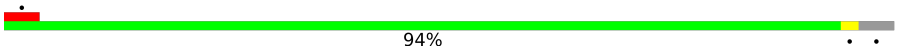
Chain l:

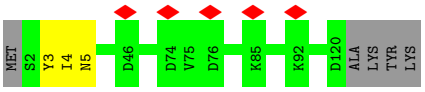




• Molecule 37: 50S ribosomal protein L17

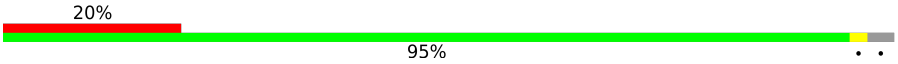
Chain m:

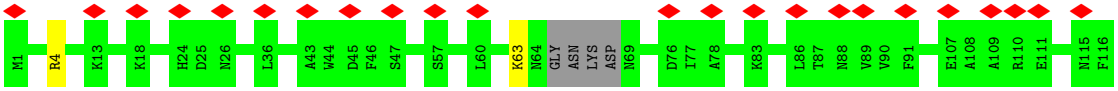




• Molecule 38: 50S ribosomal protein L18

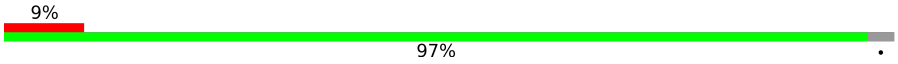
Chain n:

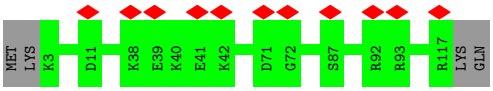




• Molecule 39: 50S ribosomal protein L19

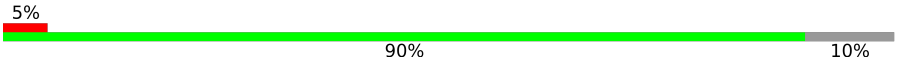
Chain o:

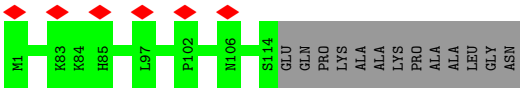




• Molecule 40: 50S ribosomal protein L20

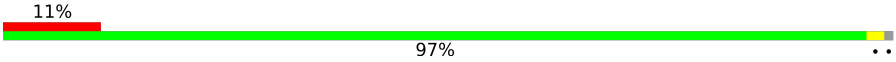
Chain p:

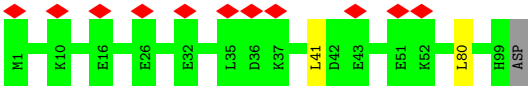




• Molecule 41: 50S ribosomal protein L21

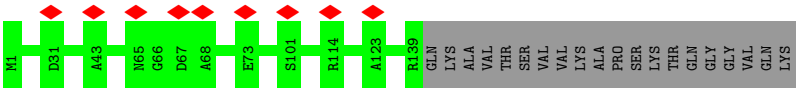
Chain q:





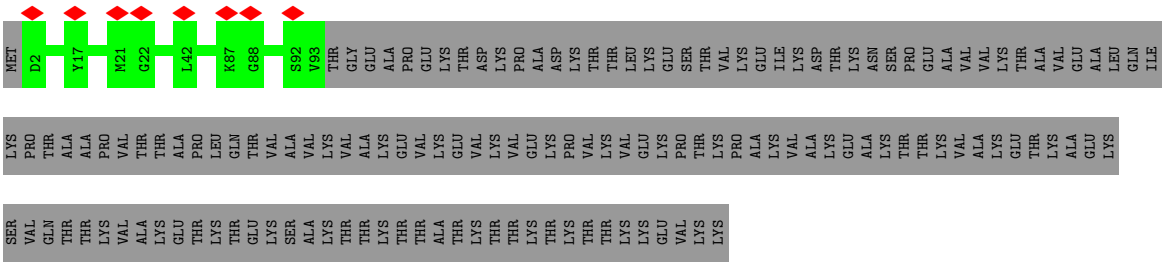
• Molecule 42: 50S ribosomal protein L22

Chain r: 6% 87% 13%



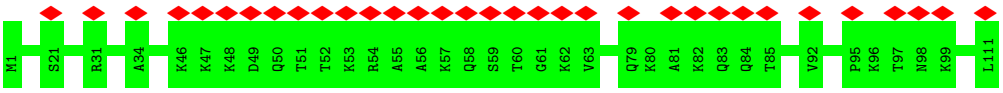
• Molecule 43: 50S ribosomal protein L23

Chain s: 39% 61%



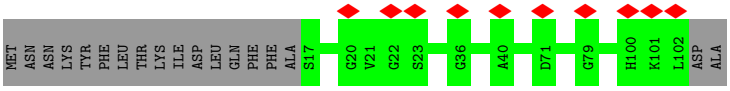
• Molecule 44: 50S ribosomal protein L24

Chain t: 30% 100%



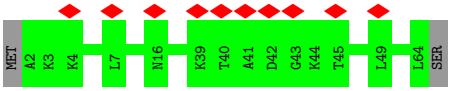
• Molecule 45: 50S ribosomal protein L27

Chain u: 10% 83% 17%



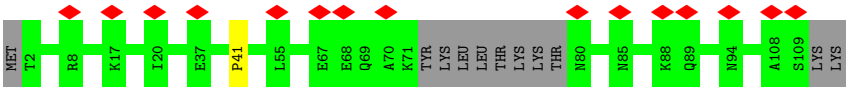
• Molecule 46: 50S ribosomal protein L28

Chain v: 15% 97%



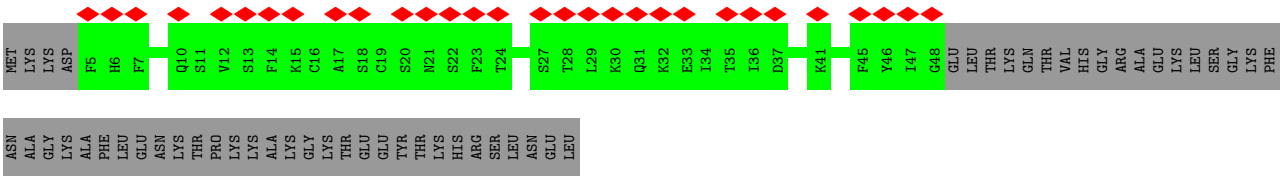
• Molecule 47: 50S ribosomal protein L29

Chain w: 14% 89% 10%



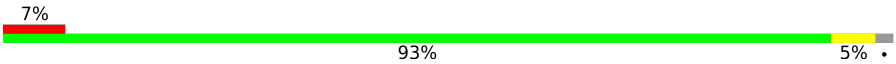
• Molecule 48: 50S ribosomal protein L31

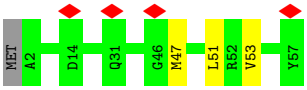
Chain x:



- Molecule 49: 50S ribosomal protein L32

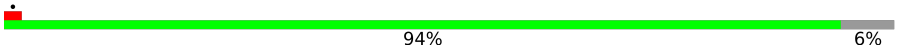
Chain y:

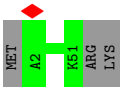




- Molecule 50: 50S ribosomal protein L33 1

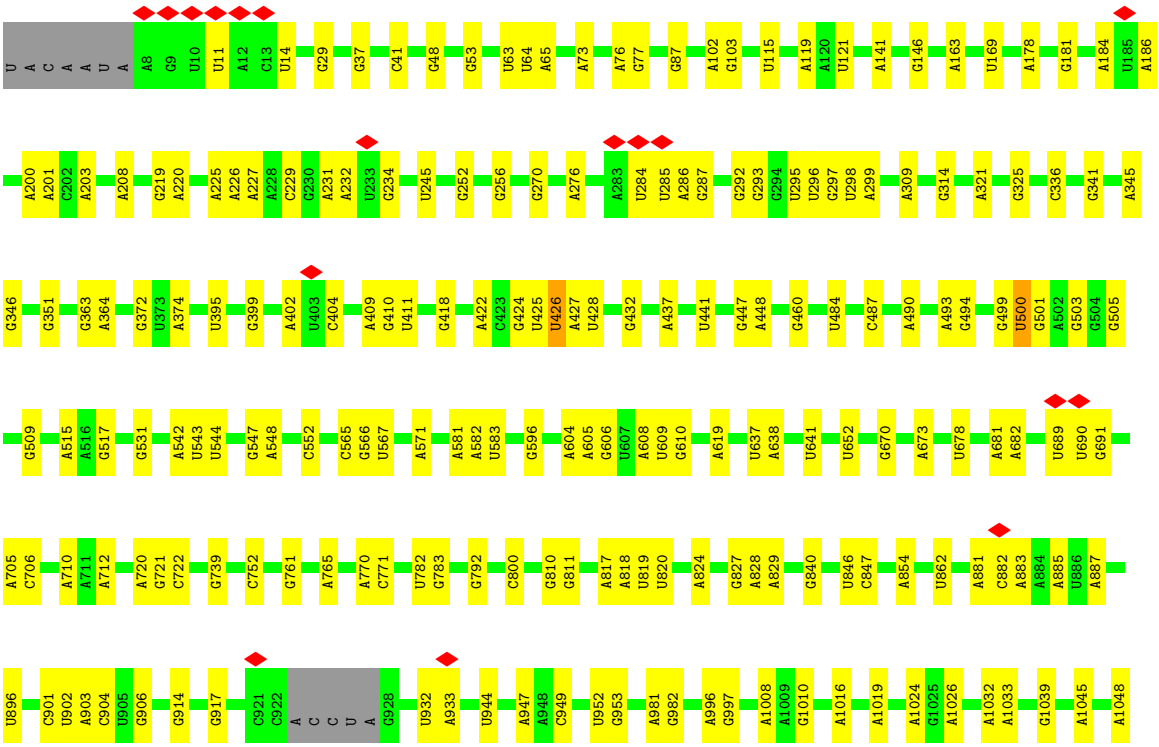
Chain z:

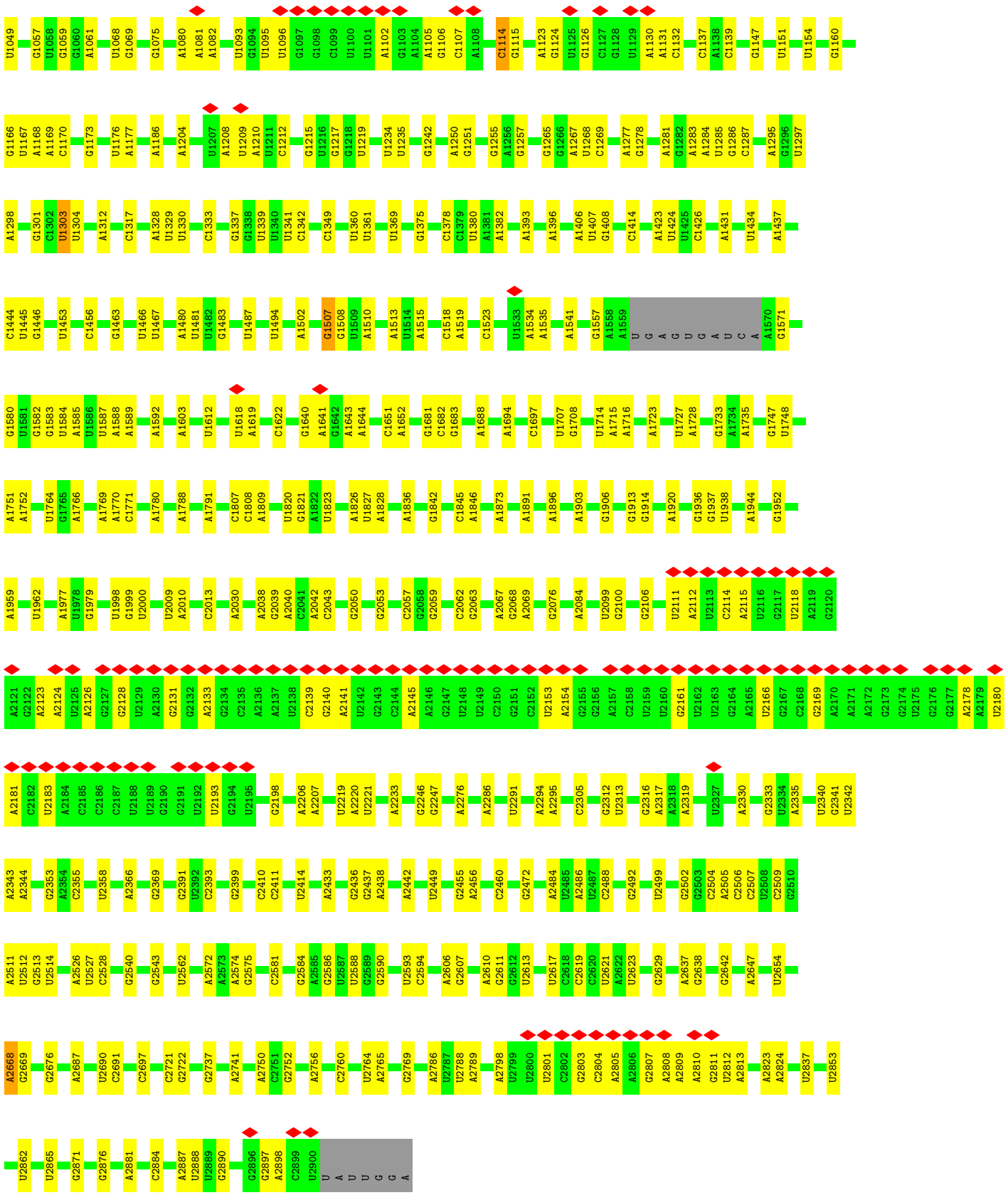




- Molecule 51: 23S ribosomal RNA

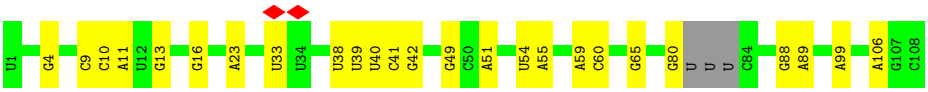
Chain 3:





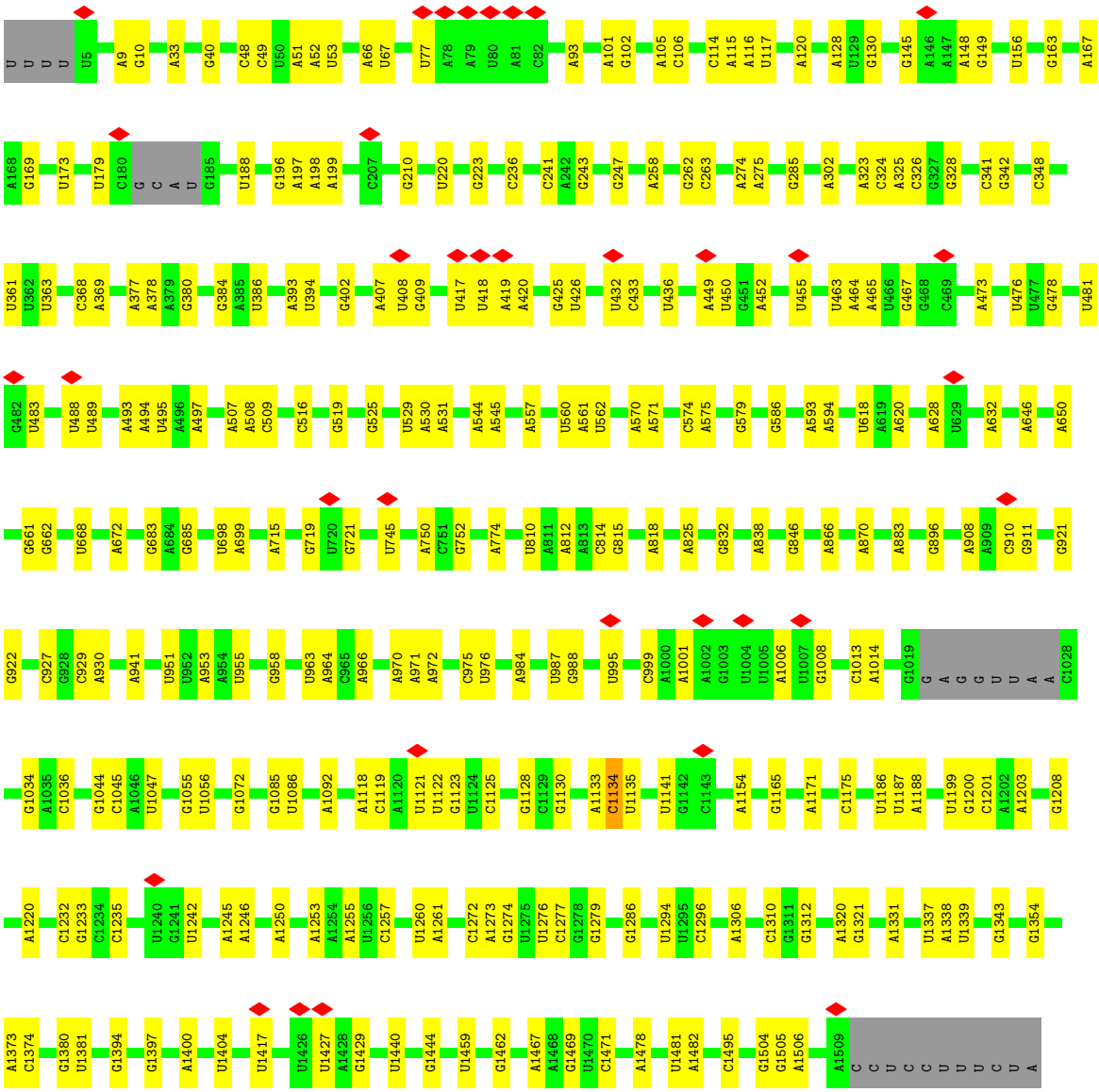
• Molecule 52: 5S ribosomal RNA

Chain 4:



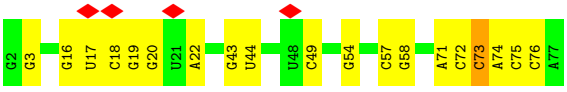
• Molecule 53: 16S ribosomal RNA

Chain 5:

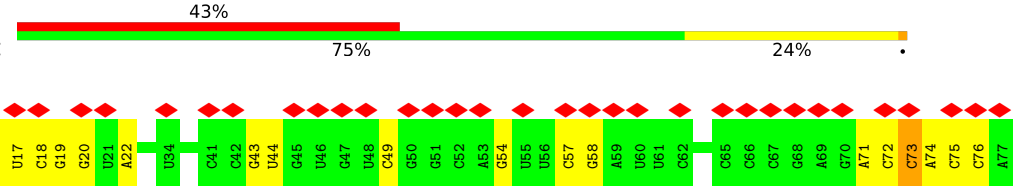


• Molecule 54: tRNA-Phe

Chain 6:



• Molecule 54: tRNA-Phe

Chain 7: 

• Molecule 55: mRNA

Chain Y:

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	32086	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	2.977	Depositor
Minimum map value	-1.334	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.65	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.23	0/383	0.46	0/504
2	1	0.23	0/484	0.48	0/637
3	2	0.23	0/306	0.47	0/401
4	A	0.26	0/1954	0.47	0/2642
5	B	0.26	0/1721	0.52	1/2323 (0.0%)
6	C	0.27	0/1691	0.47	1/2267 (0.0%)
7	D	0.24	0/1188	0.50	0/1593
8	E	0.25	0/1384	0.46	0/1867
9	F	0.27	0/1266	0.49	0/1700
10	G	0.25	0/1126	0.50	0/1517
11	H	0.25	0/1044	0.49	0/1395
12	I	0.25	0/820	0.53	0/1103
13	J	0.25	0/844	0.46	0/1136
14	K	0.27	0/1094	0.54	0/1468
15	L	0.26	0/962	0.49	0/1289
16	M	0.25	0/483	0.43	0/643
17	N	0.23	0/679	0.44	0/907
18	O	0.24	0/659	0.44	0/885
19	P	0.24	0/684	0.46	0/913
20	Q	0.25	0/545	0.46	0/730
21	R	0.27	0/698	0.48	0/936
22	S	0.24	0/631	0.46	0/838
23	T	0.26	0/475	0.43	0/621
24	Z	0.23	0/30	0.69	0/41
25	a	0.24	0/2267	0.47	1/3044 (0.0%)
26	b	0.26	0/1795	0.50	0/2412
27	c	0.25	0/1671	0.48	1/2246 (0.0%)
28	d	0.25	0/1409	0.50	1/1894 (0.1%)
29	e	0.26	0/1420	0.51	0/1912
30	f	0.24	0/1183	0.43	0/1587
31	g	0.35	0/969	0.57	0/1295
32	h	0.25	0/968	0.48	0/1298
33	i	0.28	0/1186	0.51	0/1592
34	j	0.26	0/953	0.48	0/1275

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	k	0.25	0/1170	0.50	0/1559
36	l	0.25	0/1104	0.48	0/1481
37	m	0.29	0/973	0.53	0/1309
38	n	0.25	0/897	0.49	0/1198
39	o	0.24	0/948	0.50	0/1262
40	p	0.27	0/961	0.49	0/1278
41	q	0.26	0/828	0.55	2/1111 (0.2%)
42	r	0.25	0/1077	0.46	0/1441
43	s	0.26	0/732	0.50	0/988
44	t	0.26	0/879	0.51	0/1165
45	u	0.25	0/665	0.48	0/884
46	v	0.23	0/519	0.46	0/695
47	w	0.26	0/826	0.48	1/1104 (0.1%)
48	x	0.26	0/353	0.47	0/474
49	y	0.30	0/457	0.56	0/601
50	z	0.24	0/412	0.51	0/547
51	3	0.19	0/69073	0.77	16/107710 (0.0%)
52	4	0.18	0/2505	0.74	0/3902
53	5	0.18	0/35768	0.75	8/55764 (0.0%)
54	6	0.20	0/1808	0.82	1/2817 (0.0%)
54	7	0.20	0/1808	0.82	1/2817 (0.0%)
55	Y	0.15	0/203	0.69	0/313
All	All	0.21	0/158938	0.70	34/237331 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	C	0	1
21	R	0	1
31	g	0	1
37	m	0	1
All	All	0	4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	3	567	U	C2-N1-C1'	7.90	127.18	117.70
53	5	361	U	C2-N1-C1'	7.84	127.11	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	w	41	PRO	CA-N-CD	-7.65	100.79	111.50
51	3	567	U	N1-C2-O2	7.30	127.91	122.80
51	3	1507	G	O4'-C1'-N9	6.77	113.62	108.20
51	3	14	U	C2-N1-C1'	6.77	125.83	117.70
53	5	544	A	N1-C6-N6	6.74	122.64	118.60
51	3	567	U	N3-C2-O2	-6.53	117.63	122.20
51	3	500	U	C5-C4-O4	-6.28	122.13	125.90
6	C	1	MET	CG-SD-CE	6.15	110.04	100.20
41	q	80	LEU	CA-CB-CG	5.98	129.06	115.30
27	c	184	ASP	CB-CG-OD2	5.95	123.65	118.30
53	5	361	U	N1-C2-O2	5.93	126.95	122.80
51	3	426	U	C2-N1-C1'	5.92	124.81	117.70
51	3	1341	U	C2-N1-C1'	5.72	124.56	117.70
51	3	2691	C	N1-C2-O2	5.71	122.33	118.90
51	3	1173	G	N3-C4-C5	-5.63	125.79	128.60
51	3	2668	A	O4'-C1'-N9	-5.58	103.74	108.20
41	q	41	LEU	CA-CB-CG	5.57	128.11	115.30
51	3	14	U	N3-C2-O2	-5.53	118.33	122.20
51	3	14	U	N1-C2-O2	5.51	126.66	122.80
53	5	361	U	N3-C2-O2	-5.47	118.37	122.20
53	5	1471	C	N1-C2-O2	5.45	122.17	118.90
54	7	73	C	N3-C2-O2	-5.44	118.09	121.90
54	6	73	C	N3-C2-O2	-5.44	118.09	121.90
5	B	74	PRO	CA-N-CD	-5.41	103.92	111.50
25	a	224	ILE	C-N-CA	-5.37	108.27	121.70
53	5	1119	C	C2-N1-C1'	5.27	124.60	118.80
51	3	567	U	C6-N1-C1'	-5.26	113.84	121.20
51	3	1303	U	C2-N1-C1'	5.20	123.94	117.70
53	5	361	U	C6-N1-C1'	-5.19	113.94	121.20
51	3	1114	C	C2-N1-C1'	5.10	124.41	118.80
28	d	123	ASP	CB-CG-OD1	5.04	122.84	118.30
53	5	1134	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	1	MET	Peptide
21	R	25	GLN	Peptide
31	g	114	ASP	Peptide
37	m	3	TYR	Peptide

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%)	43 (96%)	2 (4%)	0	100	100
2	1	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
4	A	238/294 (81%)	214 (90%)	24 (10%)	0	100	100
5	B	213/273 (78%)	196 (92%)	17 (8%)	0	100	100
6	C	201/205 (98%)	187 (93%)	14 (7%)	0	100	100
7	D	151/219 (69%)	145 (96%)	6 (4%)	0	100	100
8	E	165/215 (77%)	144 (87%)	21 (13%)	0	100	100
9	F	152/155 (98%)	143 (94%)	9 (6%)	0	100	100
10	G	139/142 (98%)	126 (91%)	13 (9%)	0	100	100
11	H	126/132 (96%)	111 (88%)	15 (12%)	0	100	100
12	I	99/108 (92%)	89 (90%)	10 (10%)	0	100	100
13	J	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
14	K	134/139 (96%)	119 (89%)	15 (11%)	0	100	100
15	L	116/124 (94%)	104 (90%)	12 (10%)	0	100	100
16	M	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
17	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
18	O	78/94 (83%)	72 (92%)	6 (8%)	0	100	100
19	P	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
20	Q	63/104 (61%)	55 (87%)	8 (13%)	0	100	100
21	R	82/87 (94%)	70 (85%)	12 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	75/87 (86%)	73 (97%)	2 (3%)	0	100	100
23	T	51/60 (85%)	49 (96%)	2 (4%)	0	100	100
24	Z	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
25	a	283/287 (99%)	264 (93%)	19 (7%)	0	100	100
26	b	227/287 (79%)	216 (95%)	11 (5%)	0	100	100
27	c	208/212 (98%)	198 (95%)	10 (5%)	0	100	100
28	d	173/180 (96%)	157 (91%)	16 (9%)	0	100	100
29	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
30	f	143/149 (96%)	131 (92%)	12 (8%)	0	100	100
31	g	124/161 (77%)	112 (90%)	11 (9%)	1 (1%)	19	60
32	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
33	i	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
34	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	k	146/151 (97%)	134 (92%)	12 (8%)	0	100	100
36	l	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
37	m	117/124 (94%)	109 (93%)	7 (6%)	1 (1%)	17	56
38	n	108/116 (93%)	100 (93%)	8 (7%)	0	100	100
39	o	113/119 (95%)	104 (92%)	9 (8%)	0	100	100
40	p	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
41	q	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
42	r	137/159 (86%)	127 (93%)	10 (7%)	0	100	100
43	s	90/237 (38%)	84 (93%)	6 (7%)	0	100	100
44	t	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
45	u	84/104 (81%)	80 (95%)	4 (5%)	0	100	100
46	v	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
47	w	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
48	x	42/97 (43%)	34 (81%)	8 (19%)	0	100	100
49	y	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	8	40
50	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	5823/6675 (87%)	5407 (93%)	413 (7%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	m	4	ILE
49	y	53	VAL
31	g	87	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	35 (100%)	0	100	100
4	A	212/262 (81%)	212 (100%)	0	100	100
5	B	180/232 (78%)	179 (99%)	1 (1%)	86	92
6	C	181/183 (99%)	179 (99%)	2 (1%)	73	85
7	D	123/178 (69%)	122 (99%)	1 (1%)	81	89
8	E	150/196 (76%)	150 (100%)	0	100	100
9	F	131/132 (99%)	131 (100%)	0	100	100
10	G	123/124 (99%)	123 (100%)	0	100	100
11	H	111/115 (96%)	110 (99%)	1 (1%)	78	88
12	I	95/99 (96%)	95 (100%)	0	100	100
13	J	91/97 (94%)	91 (100%)	0	100	100
14	K	117/120 (98%)	115 (98%)	2 (2%)	60	78
15	L	100/105 (95%)	100 (100%)	0	100	100
16	M	47/48 (98%)	47 (100%)	0	100	100
17	N	76/78 (97%)	76 (100%)	0	100	100
18	O	69/82 (84%)	67 (97%)	2 (3%)	42	64
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%)	74 (100%)	0	100	100
22	S	70/77 (91%)	67 (96%)	3 (4%)	29	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	T	49/56 (88%)	49 (100%)	0	100	100
24	Z	3/3 (100%)	3 (100%)	0	100	100
25	a	241/243 (99%)	241 (100%)	0	100	100
26	b	186/233 (80%)	186 (100%)	0	100	100
27	c	182/184 (99%)	182 (100%)	0	100	100
28	d	150/154 (97%)	149 (99%)	1 (1%)	84	90
29	e	153/159 (96%)	151 (99%)	2 (1%)	69	82
30	f	123/134 (92%)	121 (98%)	2 (2%)	62	79
31	g	101/129 (78%)	90 (89%)	11 (11%)	6	25
32	h	102/110 (93%)	101 (99%)	1 (1%)	76	86
33	i	126/128 (98%)	125 (99%)	1 (1%)	81	89
34	j	103/103 (100%)	103 (100%)	0	100	100
35	k	123/126 (98%)	123 (100%)	0	100	100
36	l	113/115 (98%)	113 (100%)	0	100	100
37	m	105/109 (96%)	104 (99%)	1 (1%)	76	86
38	n	96/99 (97%)	94 (98%)	2 (2%)	53	72
39	o	101/105 (96%)	101 (100%)	0	100	100
40	p	100/108 (93%)	100 (100%)	0	100	100
41	q	90/91 (99%)	90 (100%)	0	100	100
42	r	116/132 (88%)	116 (100%)	0	100	100
43	s	82/208 (39%)	82 (100%)	0	100	100
44	t	96/96 (100%)	96 (100%)	0	100	100
45	u	69/85 (81%)	69 (100%)	0	100	100
46	v	58/60 (97%)	58 (100%)	0	100	100
47	w	87/98 (89%)	87 (100%)	0	100	100
48	x	41/86 (48%)	41 (100%)	0	100	100
49	y	48/49 (98%)	46 (96%)	2 (4%)	30	55
50	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5096/5754 (89%)	5061 (99%)	35 (1%)	84	90

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	182	ARG
6	C	10	ARG
6	C	61	GLN
7	D	213	ASN
11	H	108	ARG
14	K	118	VAL
14	K	122	LYS
18	O	3	MET
18	O	34	ASN
22	S	12	ARG
22	S	18	ASN
22	S	63	ASN
28	d	27	GLN
29	e	3	LYS
29	e	45	LYS
30	f	22	LYS
30	f	118	ARG
31	g	26	ILE
31	g	27	PHE
31	g	29	TYR
31	g	31	SER
31	g	32	MET
31	g	43	LYS
31	g	84	VAL
31	g	86	VAL
31	g	88	GLU
31	g	89	ILE
31	g	116	ARG
32	h	95	LYS
33	i	64	GLN
37	m	5	ASN
38	n	4	ARG
38	n	63	LYS
49	y	47	MET
49	y	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	220	HIS
6	C	61	GLN
7	D	213	ASN
9	F	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	23	ASN
10	G	62	ASN
23	T	8	ASN
23	T	35	HIS
26	b	34	ASN
26	b	144	GLN
26	b	148	GLN
26	b	225	GLN
28	d	83	GLN
33	i	82	GLN
35	k	36	GLN
35	k	117	HIS
36	l	99	GLN
40	p	36	GLN
41	q	87	GLN
42	r	33	GLN
42	r	38	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	3	2875/2907 (98%)	587 (20%)	25 (0%)
52	4	103/108 (95%)	24 (23%)	2 (1%)
53	5	1490/1520 (98%)	279 (18%)	5 (0%)
54	6	75/76 (98%)	18 (24%)	1 (1%)
54	7	75/76 (98%)	18 (24%)	1 (1%)
55	Y	8/9 (88%)	0	0
All	All	4626/4696 (98%)	926 (20%)	34 (0%)

All (926) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	3	11	U
51	3	29	G
51	3	37	G
51	3	41	C
51	3	48	G
51	3	53	G
51	3	63	U
51	3	64	U
51	3	65	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	73	A
51	3	76	A
51	3	77	G
51	3	87	G
51	3	102	A
51	3	103	G
51	3	115	U
51	3	119	A
51	3	121	U
51	3	141	A
51	3	146	G
51	3	163	A
51	3	169	U
51	3	178	A
51	3	181	G
51	3	184	A
51	3	186	A
51	3	200	A
51	3	201	A
51	3	203	A
51	3	208	A
51	3	219	G
51	3	220	A
51	3	225	A
51	3	226	A
51	3	227	A
51	3	229	C
51	3	231	A
51	3	232	A
51	3	234	G
51	3	245	U
51	3	252	G
51	3	256	G
51	3	270	G
51	3	276	A
51	3	284	U
51	3	285	U
51	3	286	A
51	3	287	G
51	3	292	G
51	3	293	G
51	3	295	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	296	U
51	3	297	G
51	3	298	U
51	3	299	A
51	3	309	A
51	3	314	G
51	3	321	A
51	3	325	G
51	3	336	C
51	3	341	G
51	3	345	A
51	3	346	G
51	3	351	G
51	3	363	G
51	3	364	A
51	3	372	G
51	3	374	A
51	3	395	U
51	3	399	G
51	3	402	A
51	3	404	C
51	3	409	A
51	3	410	G
51	3	411	U
51	3	418	G
51	3	422	A
51	3	424	G
51	3	425	U
51	3	426	U
51	3	427	A
51	3	428	U
51	3	432	G
51	3	437	A
51	3	441	U
51	3	447	G
51	3	448	A
51	3	460	G
51	3	484	U
51	3	487	C
51	3	490	A
51	3	493	A
51	3	494	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	499	G
51	3	501	G
51	3	503	G
51	3	505	G
51	3	509	G
51	3	515	A
51	3	517	G
51	3	531	G
51	3	542	A
51	3	543	U
51	3	544	U
51	3	547	G
51	3	548	A
51	3	552	C
51	3	565	C
51	3	566	G
51	3	571	A
51	3	581	A
51	3	582	A
51	3	583	U
51	3	596	G
51	3	604	A
51	3	605	A
51	3	606	G
51	3	608	A
51	3	609	U
51	3	610	G
51	3	619	A
51	3	637	U
51	3	638	A
51	3	641	U
51	3	652	U
51	3	670	G
51	3	673	A
51	3	678	U
51	3	681	A
51	3	682	A
51	3	689	U
51	3	690	U
51	3	691	G
51	3	705	A
51	3	706	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	710	A
51	3	712	A
51	3	720	A
51	3	721	G
51	3	722	C
51	3	739	G
51	3	752	C
51	3	761	G
51	3	765	A
51	3	771	C
51	3	782	U
51	3	783	G
51	3	792	G
51	3	800	C
51	3	810	G
51	3	811	G
51	3	817	A
51	3	818	A
51	3	819	U
51	3	820	U
51	3	824	A
51	3	827	G
51	3	828	A
51	3	829	A
51	3	840	G
51	3	846	U
51	3	847	C
51	3	854	A
51	3	862	U
51	3	881	A
51	3	882	C
51	3	883	A
51	3	885	A
51	3	887	A
51	3	896	U
51	3	902	U
51	3	904	C
51	3	906	G
51	3	914	G
51	3	917	G
51	3	932	U
51	3	933	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	944	U
51	3	947	A
51	3	949	C
51	3	952	U
51	3	953	G
51	3	981	A
51	3	982	G
51	3	997	G
51	3	1008	A
51	3	1010	G
51	3	1016	A
51	3	1019	A
51	3	1024	A
51	3	1026	A
51	3	1032	A
51	3	1033	A
51	3	1039	G
51	3	1045	A
51	3	1048	A
51	3	1049	U
51	3	1057	G
51	3	1059	G
51	3	1061	A
51	3	1068	U
51	3	1069	G
51	3	1075	G
51	3	1080	A
51	3	1081	A
51	3	1082	A
51	3	1093	U
51	3	1095	U
51	3	1096	U
51	3	1102	A
51	3	1105	A
51	3	1106	G
51	3	1107	C
51	3	1114	C
51	3	1115	G
51	3	1123	A
51	3	1124	G
51	3	1126	G
51	3	1130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	1131	A
51	3	1132	C
51	3	1137	C
51	3	1139	C
51	3	1147	G
51	3	1151	U
51	3	1154	U
51	3	1160	G
51	3	1166	G
51	3	1167	U
51	3	1168	A
51	3	1169	A
51	3	1170	C
51	3	1176	U
51	3	1177	A
51	3	1186	A
51	3	1204	A
51	3	1208	A
51	3	1209	U
51	3	1210	A
51	3	1212	C
51	3	1215	G
51	3	1217	G
51	3	1219	U
51	3	1234	U
51	3	1235	U
51	3	1242	G
51	3	1250	A
51	3	1251	G
51	3	1255	G
51	3	1257	G
51	3	1265	G
51	3	1267	A
51	3	1268	U
51	3	1269	C
51	3	1277	A
51	3	1278	G
51	3	1281	A
51	3	1283	A
51	3	1284	A
51	3	1285	U
51	3	1286	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	1287	C
51	3	1295	A
51	3	1298	A
51	3	1301	G
51	3	1303	U
51	3	1304	U
51	3	1312	A
51	3	1317	C
51	3	1328	A
51	3	1329	U
51	3	1330	U
51	3	1333	C
51	3	1337	G
51	3	1339	U
51	3	1342	C
51	3	1349	C
51	3	1360	U
51	3	1361	U
51	3	1369	U
51	3	1375	G
51	3	1378	C
51	3	1380	U
51	3	1382	A
51	3	1393	A
51	3	1396	A
51	3	1406	A
51	3	1407	U
51	3	1408	G
51	3	1414	C
51	3	1423	A
51	3	1424	U
51	3	1426	C
51	3	1431	A
51	3	1434	U
51	3	1437	A
51	3	1444	C
51	3	1445	U
51	3	1446	G
51	3	1453	U
51	3	1456	C
51	3	1463	G
51	3	1466	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	1467	U
51	3	1480	A
51	3	1481	U
51	3	1483	G
51	3	1487	U
51	3	1494	U
51	3	1502	A
51	3	1507	G
51	3	1508	G
51	3	1510	A
51	3	1513	A
51	3	1515	A
51	3	1518	C
51	3	1519	A
51	3	1523	C
51	3	1534	A
51	3	1535	A
51	3	1541	A
51	3	1557	G
51	3	1571	G
51	3	1580	G
51	3	1582	G
51	3	1584	U
51	3	1585	A
51	3	1588	A
51	3	1589	A
51	3	1592	A
51	3	1603	A
51	3	1612	U
51	3	1618	U
51	3	1619	A
51	3	1622	C
51	3	1640	G
51	3	1641	A
51	3	1643	A
51	3	1644	A
51	3	1651	C
51	3	1652	A
51	3	1681	G
51	3	1682	C
51	3	1683	G
51	3	1688	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	1694	A
51	3	1697	C
51	3	1707	U
51	3	1708	G
51	3	1714	U
51	3	1715	A
51	3	1716	A
51	3	1723	A
51	3	1727	U
51	3	1728	A
51	3	1733	G
51	3	1735	A
51	3	1747	G
51	3	1748	U
51	3	1751	A
51	3	1752	A
51	3	1764	U
51	3	1766	A
51	3	1769	A
51	3	1770	A
51	3	1771	C
51	3	1780	A
51	3	1788	A
51	3	1791	A
51	3	1807	C
51	3	1808	C
51	3	1809	A
51	3	1821	G
51	3	1823	U
51	3	1826	A
51	3	1827	U
51	3	1828	A
51	3	1836	A
51	3	1842	G
51	3	1845	C
51	3	1846	A
51	3	1873	A
51	3	1891	A
51	3	1896	A
51	3	1903	A
51	3	1906	G
51	3	1913	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	1914	G
51	3	1920	A
51	3	1936	G
51	3	1937	G
51	3	1938	U
51	3	1944	A
51	3	1952	G
51	3	1959	A
51	3	1962	U
51	3	1977	A
51	3	1979	G
51	3	1998	U
51	3	1999	G
51	3	2000	U
51	3	2009	U
51	3	2010	A
51	3	2013	C
51	3	2030	A
51	3	2038	A
51	3	2039	G
51	3	2040	A
51	3	2042	A
51	3	2043	C
51	3	2050	G
51	3	2053	G
51	3	2057	C
51	3	2059	G
51	3	2062	C
51	3	2063	G
51	3	2067	A
51	3	2068	G
51	3	2069	A
51	3	2076	G
51	3	2084	A
51	3	2099	U
51	3	2100	G
51	3	2106	G
51	3	2111	U
51	3	2112	A
51	3	2114	C
51	3	2115	A
51	3	2118	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	2123	A
51	3	2124	A
51	3	2126	A
51	3	2128	G
51	3	2131	G
51	3	2133	A
51	3	2139	C
51	3	2140	G
51	3	2141	A
51	3	2145	A
51	3	2153	U
51	3	2154	A
51	3	2161	G
51	3	2166	U
51	3	2169	G
51	3	2178	A
51	3	2180	U
51	3	2181	A
51	3	2183	U
51	3	2193	U
51	3	2198	G
51	3	2206	A
51	3	2207	A
51	3	2219	U
51	3	2220	A
51	3	2221	U
51	3	2233	A
51	3	2246	G
51	3	2247	G
51	3	2276	A
51	3	2286	A
51	3	2291	U
51	3	2294	A
51	3	2295	A
51	3	2305	C
51	3	2312	G
51	3	2313	U
51	3	2316	G
51	3	2317	A
51	3	2319	A
51	3	2330	A
51	3	2333	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	2335	A
51	3	2340	U
51	3	2341	G
51	3	2342	U
51	3	2343	A
51	3	2344	A
51	3	2353	G
51	3	2355	C
51	3	2358	U
51	3	2366	A
51	3	2369	G
51	3	2391	G
51	3	2393	C
51	3	2399	G
51	3	2410	C
51	3	2411	C
51	3	2414	U
51	3	2433	A
51	3	2436	G
51	3	2437	G
51	3	2438	A
51	3	2442	A
51	3	2449	U
51	3	2455	G
51	3	2456	A
51	3	2460	C
51	3	2472	G
51	3	2484	A
51	3	2486	A
51	3	2488	C
51	3	2492	G
51	3	2499	U
51	3	2502	G
51	3	2505	A
51	3	2507	C
51	3	2509	C
51	3	2511	A
51	3	2512	U
51	3	2513	G
51	3	2514	U
51	3	2526	A
51	3	2527	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	2528	C
51	3	2540	G
51	3	2543	G
51	3	2562	U
51	3	2572	A
51	3	2574	A
51	3	2575	G
51	3	2581	C
51	3	2584	G
51	3	2586	G
51	3	2588	U
51	3	2590	G
51	3	2593	U
51	3	2594	C
51	3	2606	A
51	3	2607	G
51	3	2610	A
51	3	2611	G
51	3	2613	U
51	3	2617	U
51	3	2619	C
51	3	2621	U
51	3	2623	U
51	3	2629	G
51	3	2637	A
51	3	2638	G
51	3	2642	G
51	3	2647	A
51	3	2654	U
51	3	2669	G
51	3	2676	G
51	3	2687	A
51	3	2690	U
51	3	2697	C
51	3	2721	C
51	3	2722	G
51	3	2737	G
51	3	2741	A
51	3	2750	A
51	3	2752	G
51	3	2756	A
51	3	2760	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	2764	U
51	3	2765	A
51	3	2769	G
51	3	2786	A
51	3	2788	U
51	3	2789	A
51	3	2798	A
51	3	2801	U
51	3	2803	G
51	3	2804	C
51	3	2805	A
51	3	2807	G
51	3	2808	A
51	3	2809	A
51	3	2810	A
51	3	2811	G
51	3	2812	U
51	3	2813	A
51	3	2824	A
51	3	2837	U
51	3	2853	U
51	3	2862	U
51	3	2865	U
51	3	2871	G
51	3	2876	G
51	3	2881	A
51	3	2884	C
51	3	2887	A
51	3	2888	U
51	3	2890	G
51	3	2897	G
51	3	2898	A
52	4	4	G
52	4	9	C
52	4	10	C
52	4	11	A
52	4	13	G
52	4	16	G
52	4	23	A
52	4	33	U
52	4	38	U
52	4	39	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	4	40	U
52	4	41	C
52	4	42	G
52	4	49	G
52	4	51	A
52	4	54	U
52	4	55	A
52	4	60	C
52	4	65	G
52	4	80	G
52	4	88	G
52	4	89	A
52	4	99	A
52	4	106	A
53	5	9	A
53	5	10	G
53	5	33	A
53	5	40	G
53	5	48	C
53	5	49	C
53	5	51	A
53	5	52	A
53	5	53	U
53	5	66	A
53	5	67	U
53	5	77	U
53	5	93	A
53	5	101	A
53	5	102	G
53	5	105	A
53	5	106	C
53	5	114	C
53	5	115	A
53	5	116	A
53	5	117	U
53	5	120	A
53	5	128	A
53	5	130	G
53	5	145	G
53	5	148	A
53	5	149	G
53	5	156	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	163	G
53	5	167	A
53	5	169	G
53	5	173	U
53	5	179	U
53	5	188	U
53	5	196	G
53	5	197	A
53	5	198	A
53	5	199	A
53	5	210	G
53	5	220	U
53	5	223	G
53	5	236	C
53	5	241	C
53	5	243	G
53	5	247	G
53	5	258	A
53	5	262	G
53	5	263	C
53	5	274	A
53	5	275	A
53	5	285	G
53	5	302	A
53	5	323	A
53	5	324	C
53	5	325	A
53	5	326	C
53	5	328	G
53	5	341	C
53	5	342	G
53	5	348	C
53	5	363	U
53	5	368	C
53	5	369	A
53	5	377	A
53	5	378	A
53	5	380	G
53	5	384	G
53	5	386	U
53	5	393	A
53	5	394	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	402	G
53	5	407	A
53	5	408	U
53	5	409	G
53	5	417	U
53	5	418	U
53	5	419	A
53	5	420	A
53	5	425	G
53	5	426	U
53	5	432	U
53	5	433	C
53	5	436	U
53	5	449	A
53	5	450	U
53	5	452	A
53	5	455	U
53	5	463	U
53	5	464	A
53	5	465	A
53	5	467	G
53	5	473	A
53	5	476	U
53	5	478	G
53	5	481	U
53	5	483	U
53	5	488	U
53	5	489	U
53	5	493	A
53	5	494	A
53	5	495	U
53	5	497	A
53	5	507	A
53	5	508	A
53	5	509	C
53	5	516	C
53	5	519	G
53	5	525	G
53	5	529	U
53	5	530	A
53	5	531	A
53	5	545	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	557	A
53	5	560	U
53	5	561	A
53	5	562	U
53	5	570	A
53	5	571	A
53	5	574	C
53	5	575	A
53	5	579	G
53	5	586	G
53	5	593	A
53	5	594	A
53	5	618	U
53	5	620	A
53	5	628	A
53	5	632	A
53	5	646	A
53	5	650	A
53	5	661	G
53	5	662	G
53	5	668	U
53	5	672	A
53	5	683	G
53	5	685	G
53	5	698	U
53	5	699	A
53	5	715	A
53	5	719	G
53	5	721	G
53	5	745	U
53	5	750	A
53	5	752	G
53	5	774	A
53	5	810	U
53	5	812	A
53	5	814	C
53	5	815	G
53	5	818	A
53	5	825	A
53	5	832	G
53	5	838	A
53	5	846	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	866	A
53	5	870	A
53	5	883	A
53	5	896	G
53	5	908	A
53	5	910	C
53	5	911	G
53	5	921	G
53	5	922	G
53	5	927	C
53	5	929	C
53	5	930	A
53	5	941	A
53	5	951	U
53	5	953	A
53	5	955	U
53	5	958	G
53	5	963	U
53	5	964	A
53	5	966	A
53	5	970	A
53	5	971	A
53	5	972	A
53	5	975	C
53	5	976	U
53	5	984	A
53	5	987	U
53	5	988	G
53	5	995	U
53	5	999	C
53	5	1001	A
53	5	1006	A
53	5	1008	G
53	5	1013	C
53	5	1014	A
53	5	1034	G
53	5	1036	C
53	5	1044	G
53	5	1045	C
53	5	1047	U
53	5	1055	G
53	5	1056	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	1072	G
53	5	1085	G
53	5	1086	U
53	5	1092	A
53	5	1118	A
53	5	1121	U
53	5	1122	U
53	5	1123	G
53	5	1125	C
53	5	1128	G
53	5	1130	G
53	5	1133	A
53	5	1134	C
53	5	1135	U
53	5	1141	U
53	5	1154	A
53	5	1165	G
53	5	1171	A
53	5	1175	C
53	5	1187	U
53	5	1188	A
53	5	1199	U
53	5	1200	G
53	5	1201	C
53	5	1203	A
53	5	1208	G
53	5	1220	A
53	5	1232	C
53	5	1233	G
53	5	1235	C
53	5	1242	U
53	5	1245	A
53	5	1246	A
53	5	1250	A
53	5	1253	A
53	5	1255	A
53	5	1257	C
53	5	1260	U
53	5	1261	A
53	5	1272	C
53	5	1273	A
53	5	1274	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	1276	U
53	5	1277	C
53	5	1279	G
53	5	1286	G
53	5	1294	U
53	5	1296	C
53	5	1306	A
53	5	1310	C
53	5	1312	G
53	5	1320	A
53	5	1321	G
53	5	1331	A
53	5	1337	U
53	5	1338	A
53	5	1339	U
53	5	1343	G
53	5	1354	G
53	5	1373	A
53	5	1374	C
53	5	1380	G
53	5	1381	U
53	5	1394	G
53	5	1397	G
53	5	1400	A
53	5	1404	U
53	5	1417	U
53	5	1427	U
53	5	1429	G
53	5	1440	U
53	5	1444	G
53	5	1459	U
53	5	1462	G
53	5	1467	A
53	5	1469	G
53	5	1478	A
53	5	1481	U
53	5	1482	A
53	5	1495	C
53	5	1504	G
53	5	1505	G
53	5	1506	A
54	6	3	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	6	17	U
54	6	18	C
54	6	19	G
54	6	20	G
54	6	22	A
54	6	43	G
54	6	44	U
54	6	49	C
54	6	54	G
54	6	57	C
54	6	58	G
54	6	71	A
54	6	72	C
54	6	73	C
54	6	74	A
54	6	75	C
54	6	76	C
54	7	3	G
54	7	17	U
54	7	18	C
54	7	19	G
54	7	20	G
54	7	22	A
54	7	43	G
54	7	44	U
54	7	49	C
54	7	54	G
54	7	57	C
54	7	58	G
54	7	71	A
54	7	72	C
54	7	73	C
54	7	74	A
54	7	75	C
54	7	76	C

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	3	410	G
51	3	426	U
51	3	500	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	605	A
51	3	770	A
51	3	881	A
51	3	901	C
51	3	903	A
51	3	996	A
51	3	1048	A
51	3	1209	U
51	3	1297	U
51	3	1507	G
51	3	1583	G
51	3	1587	U
51	3	1588	A
51	3	1820	U
51	3	2342	U
51	3	2504	C
51	3	2506	C
51	3	2668	A
51	3	2764	U
51	3	2808	A
51	3	2823	A
51	3	2897	G
52	4	54	U
52	4	59	A
53	5	393	A
53	5	419	A
53	5	1186	U
53	5	1338	A
53	5	1505	G
54	6	16	G
54	7	16	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

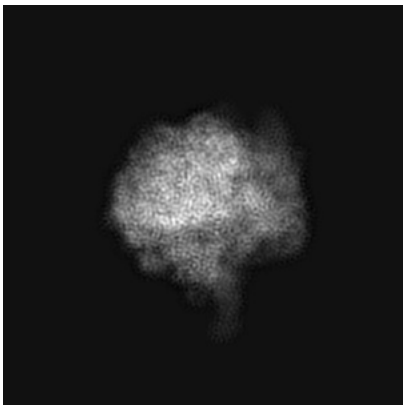
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13276. These allow visual inspection of the internal detail of the map and identification of artifacts.

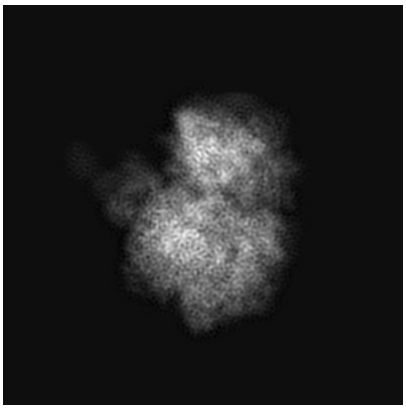
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

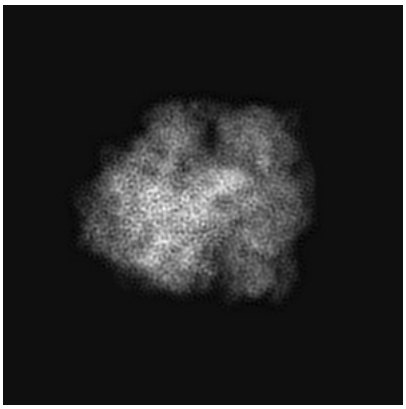
6.1.1 Primary map



X

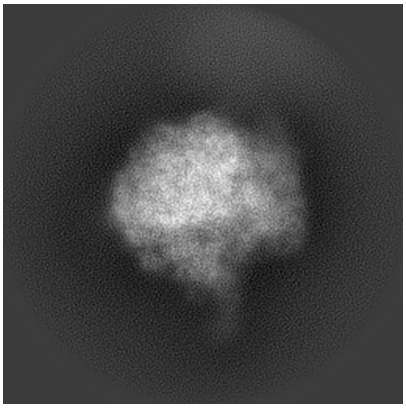


Y

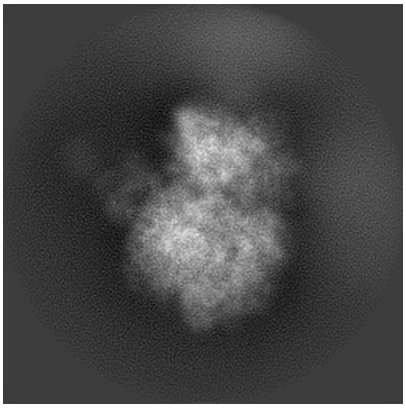


Z

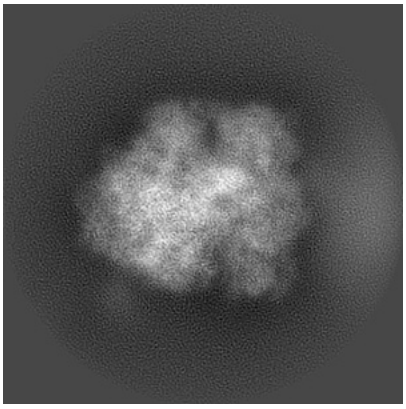
6.1.2 Raw map



X



Y

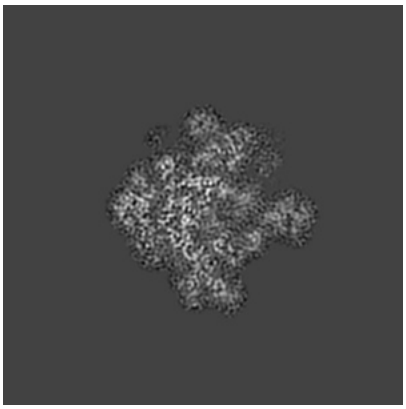


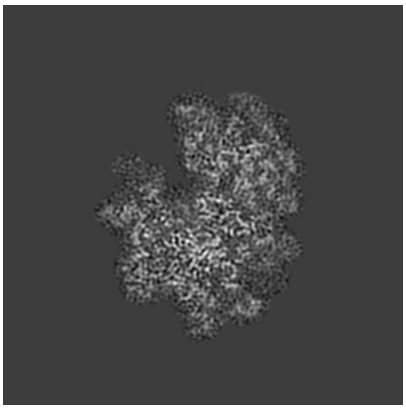
Z

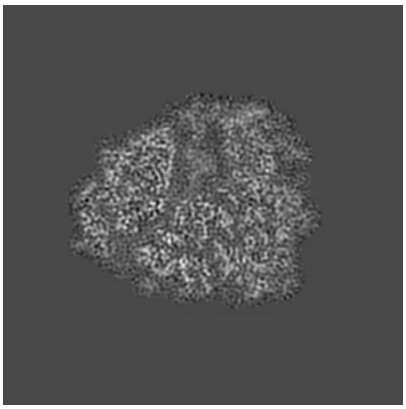
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

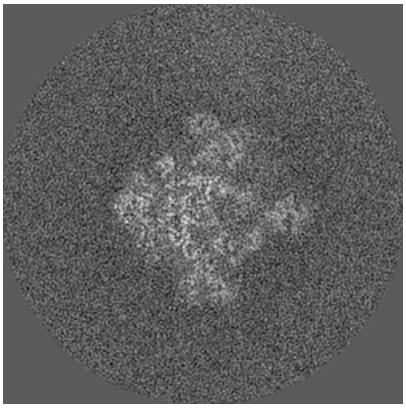
6.2.1 Primary map

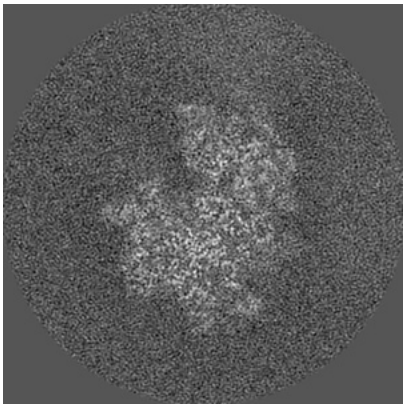

X Index: 128

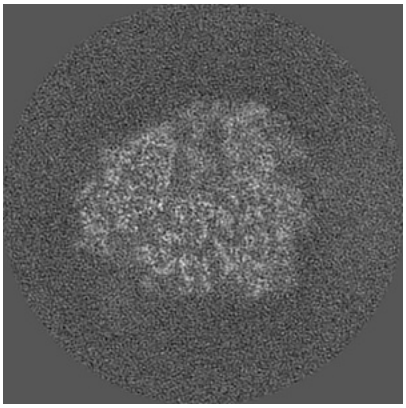

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

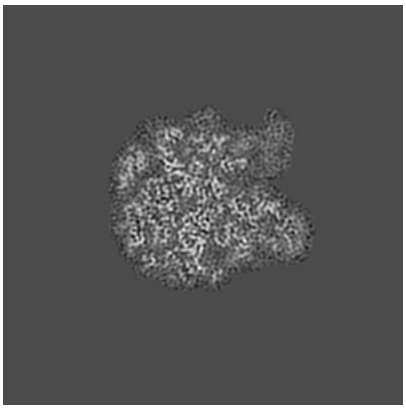

Y Index: 128


Z Index: 128

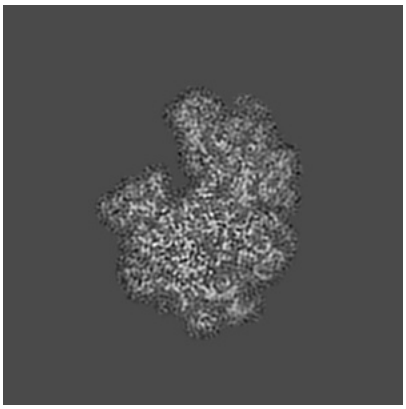
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

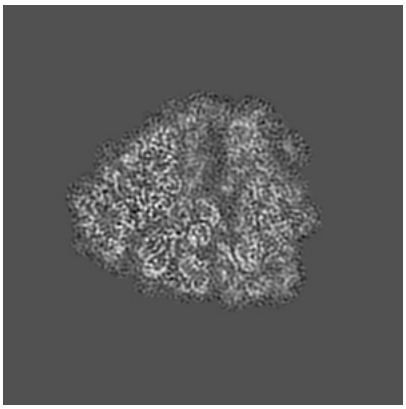
6.3.1 Primary map



X Index: 103

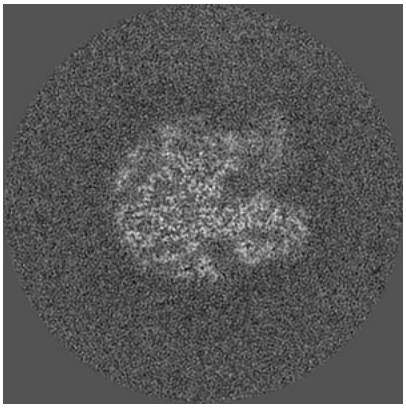


Y Index: 122

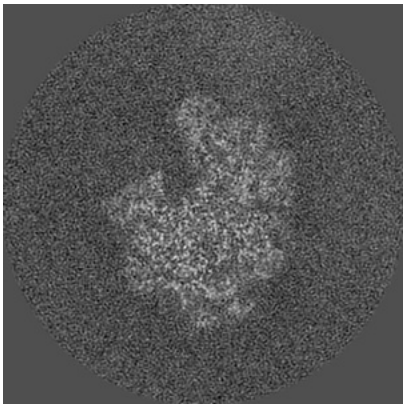


Z Index: 125

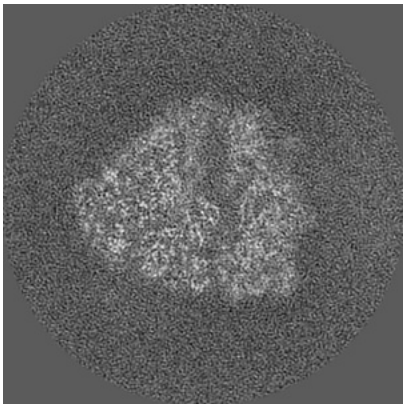
6.3.2 Raw map



X Index: 108



Y Index: 122

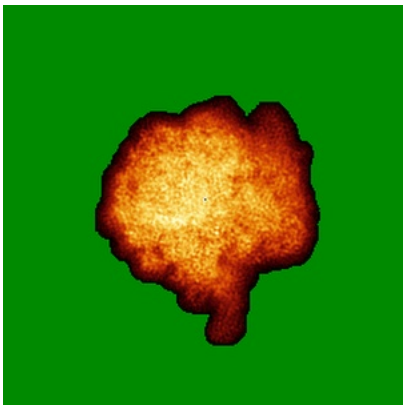


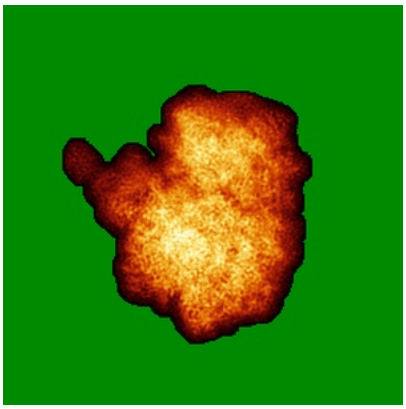
Z Index: 124

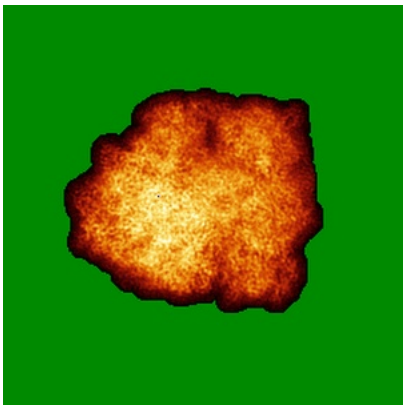
The images above show the largest variance slices of the map in three orthogonal directions.

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

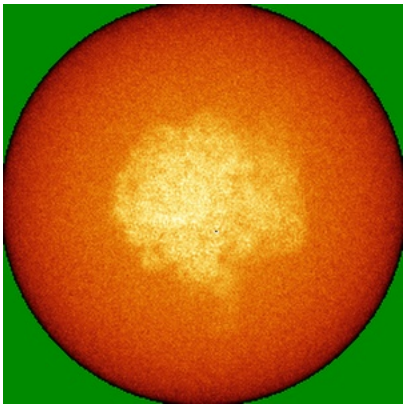
6.4.1 Primary map

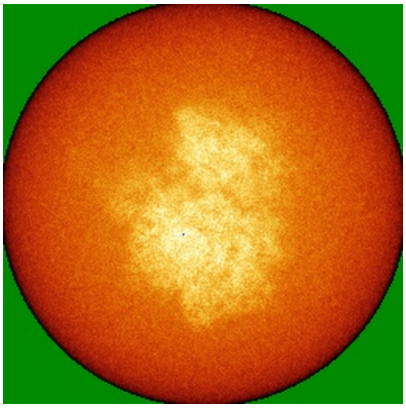

X

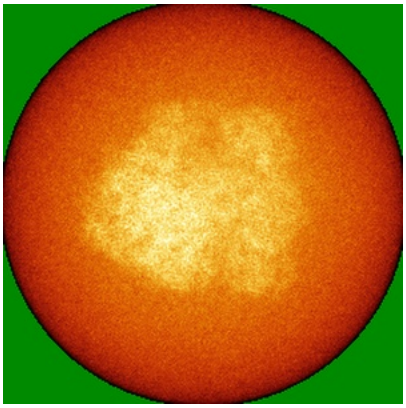

Y


Z

6.4.2 Raw map


X

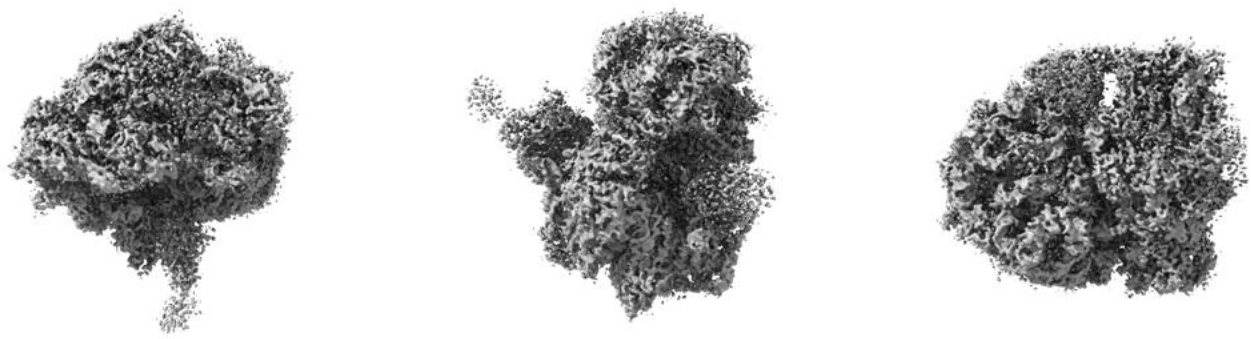

Y


Z

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

6.5 Orthogonal surface views (i)

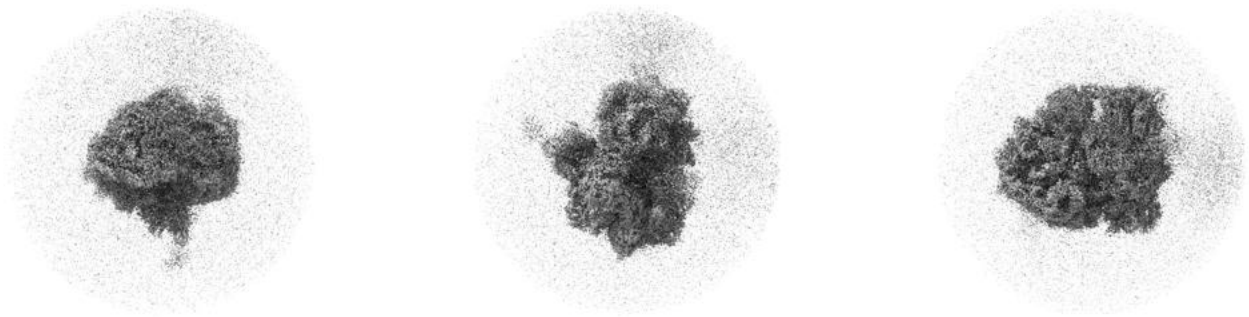
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

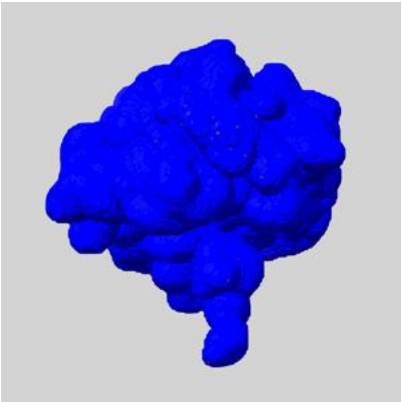
6.6 Mask visualisation (i)

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

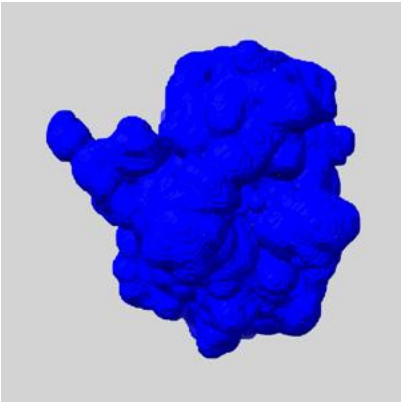
A mask typically either:

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

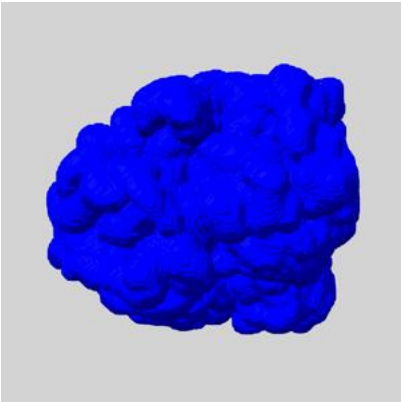
6.6.1 emd_13276_msk_1.map (i)



X



Y

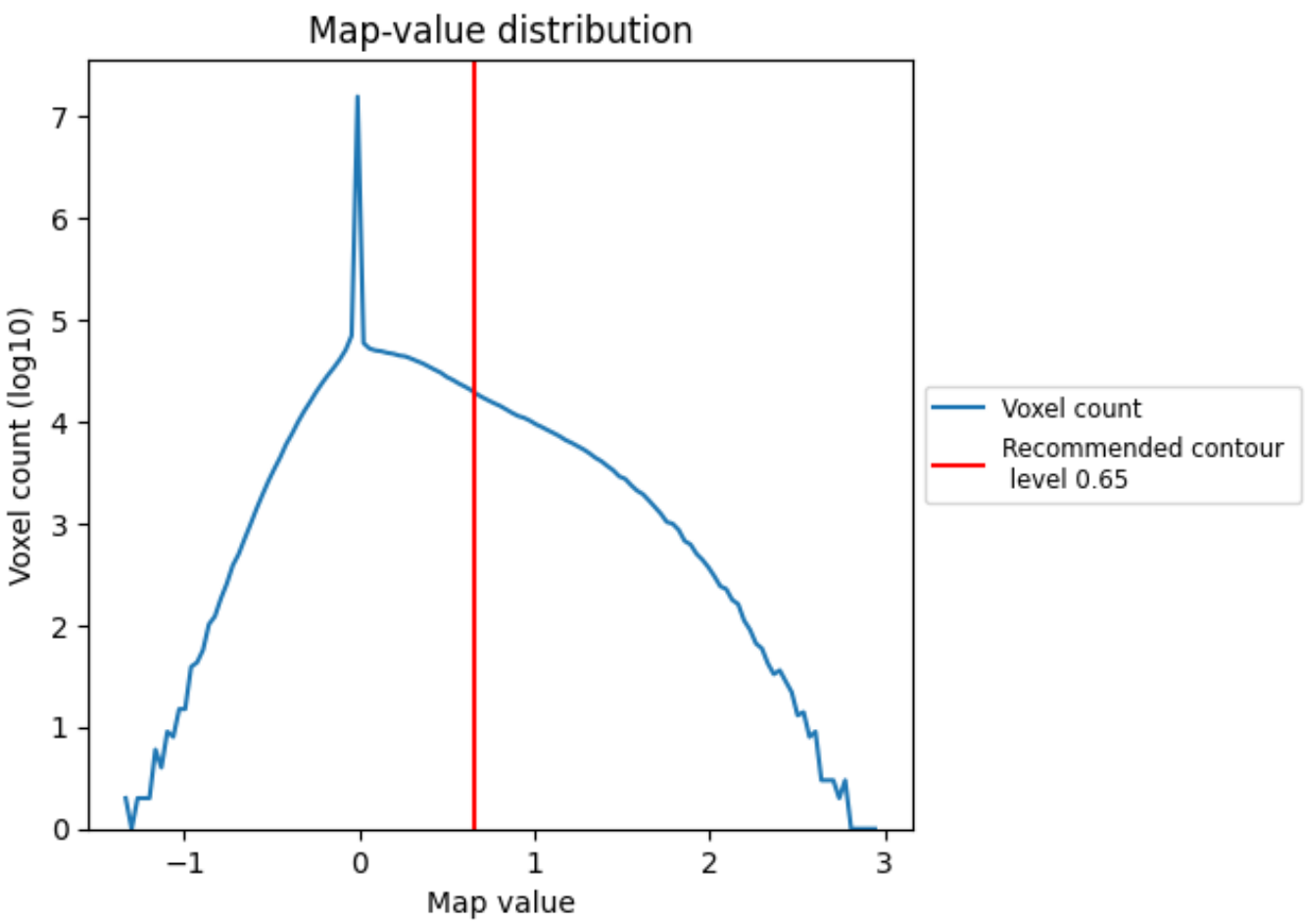


Z

7 Map analysis (i)

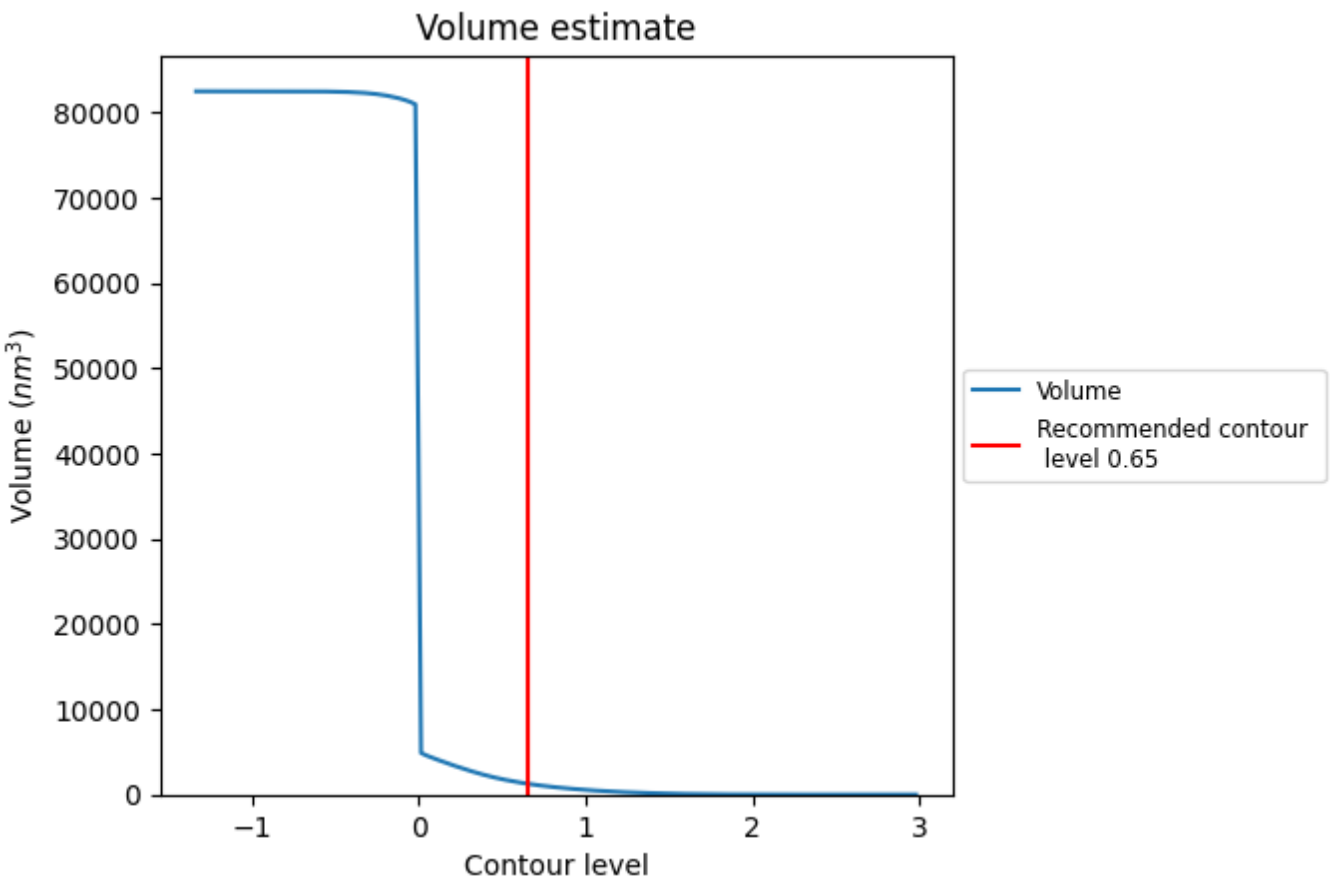
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

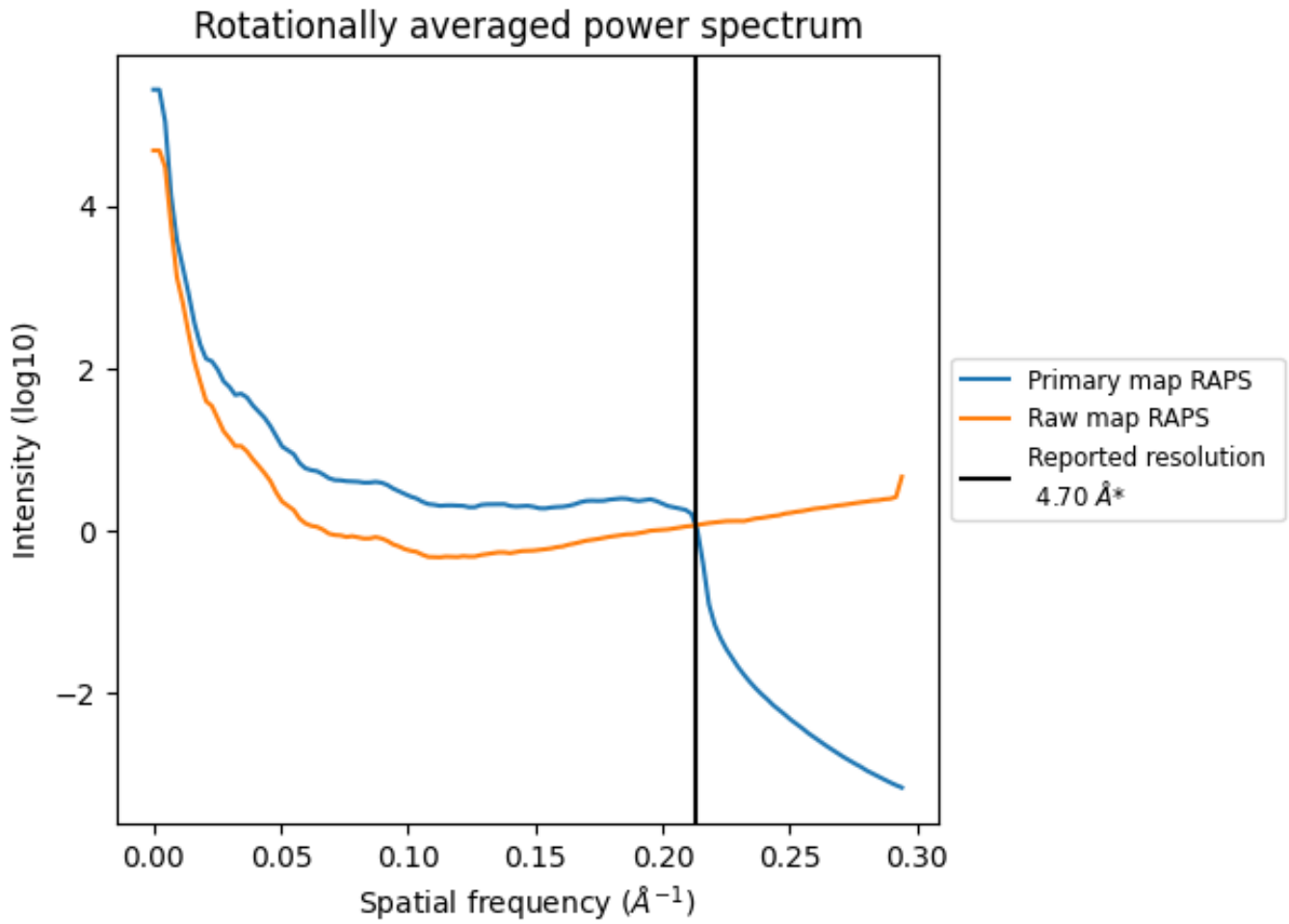
7.2 Volume estimate (i)



The volume at the recommended contour level is 1271 nm^3; this corresponds to an approximate mass of 1148 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)

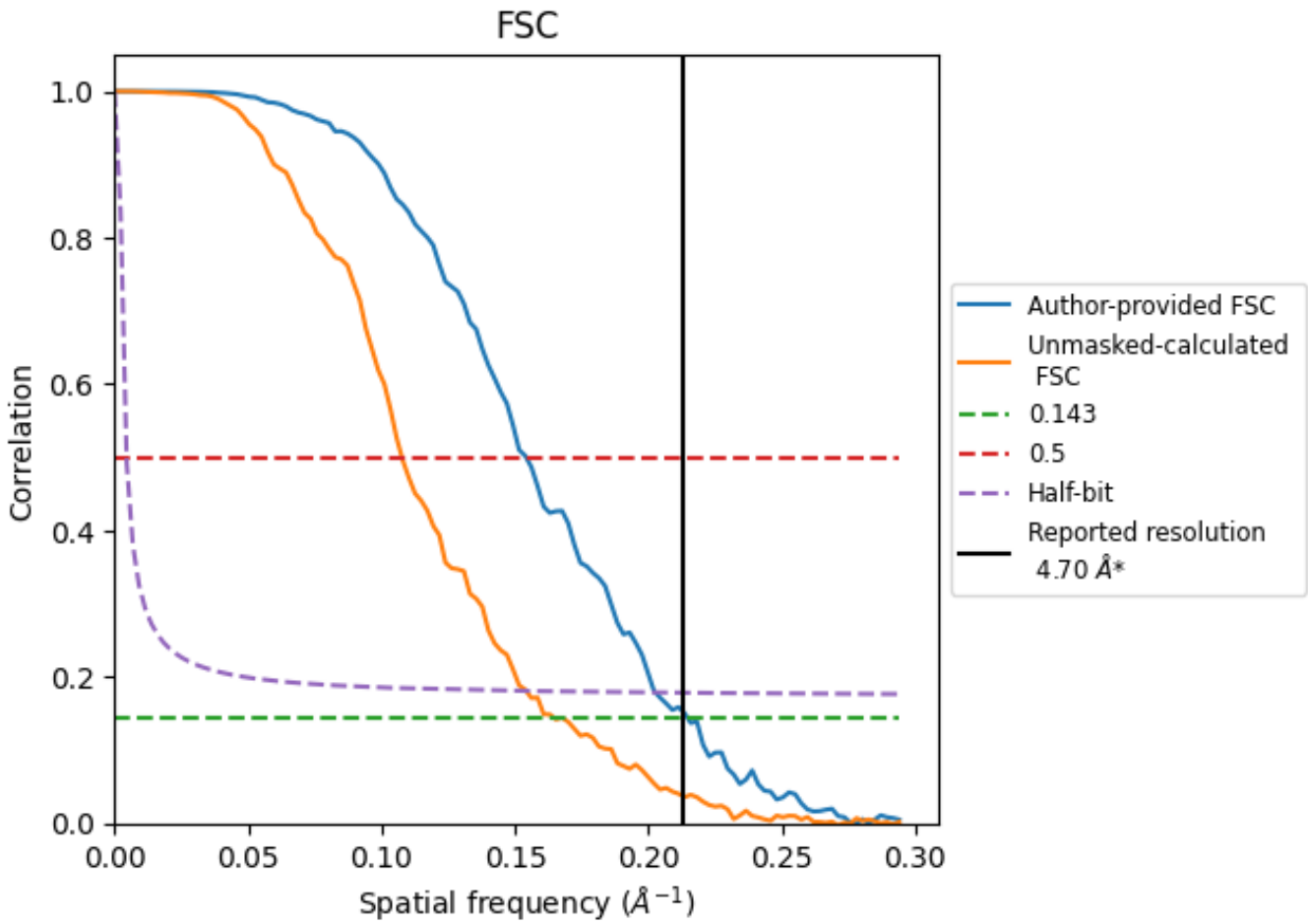


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

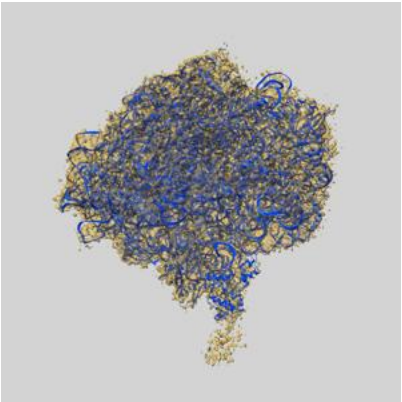
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	6.49	4.93
Unmasked-calculated*	6.06	9.29	6.48

*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 6.06 differs from the reported value 4.7 by more than 10 %

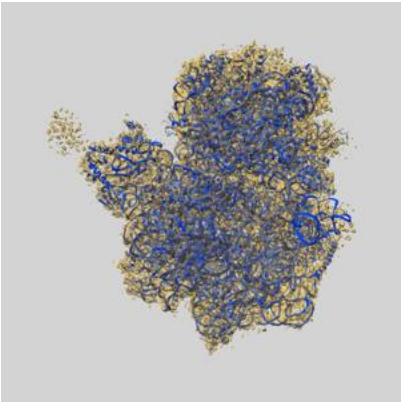
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13276 and PDB model 7PAL. Per-residue inclusion information can be found in section 3 on page 13.

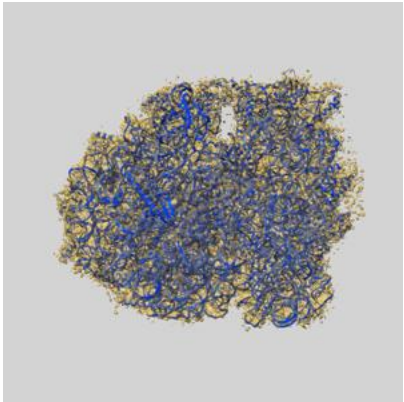
9.1 Map-model overlay (i)



X



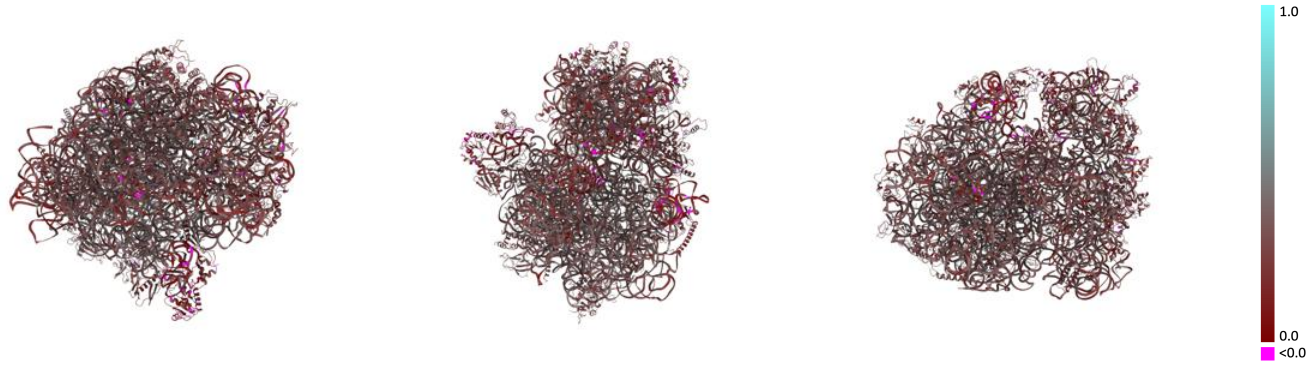
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65 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.

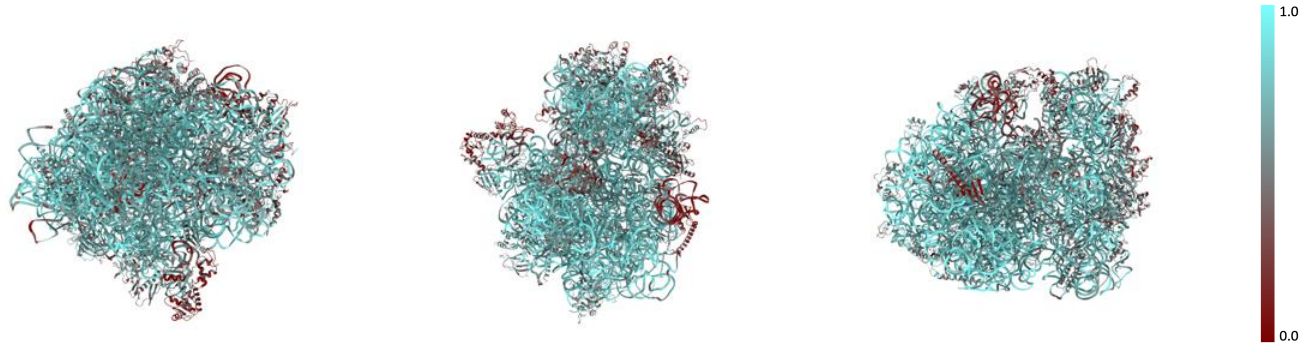
9.2 Q-score mapped to coordinate model (i)



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.

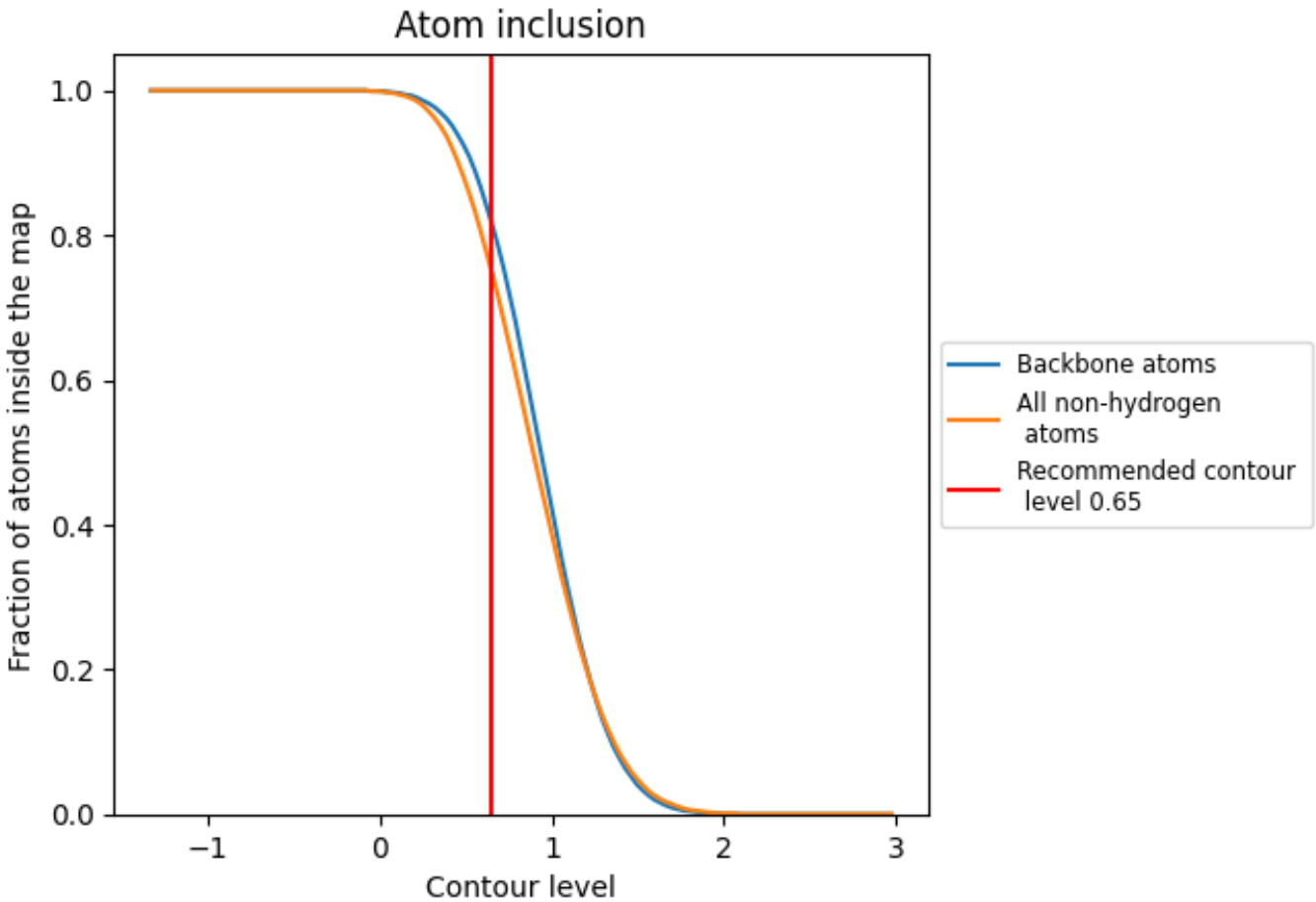
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.65).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.3240
0	0.7810	0.3900
1	0.7210	0.3840
2	0.7570	0.3980
3	0.8500	0.3360
4	0.8490	0.3230
5	0.8350	0.3140
6	0.7460	0.2760
7	0.4730	0.1370
A	0.4840	0.2990
B	0.5330	0.3190
C	0.5170	0.2990
D	0.5850	0.3400
E	0.4360	0.3010
F	0.4250	0.2600
G	0.5520	0.3180
H	0.4800	0.2820
I	0.5030	0.3110
J	0.5500	0.3210
K	0.6310	0.3660
L	0.3930	0.2640
M	0.6260	0.3170
N	0.5260	0.2950
O	0.5800	0.3300
P	0.5450	0.3290
Q	0.5430	0.3020
R	0.4550	0.2820
S	0.5820	0.2880
T	0.5220	0.3260
Y	0.8740	0.3590
Z	0.6770	0.3370
a	0.6940	0.3750
b	0.6780	0.3660
c	0.6310	0.3570
d	0.4230	0.2450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.5340	0.3210
f	0.1870	0.2380
g	0.2460	0.1980
h	0.1330	0.2190
i	0.6580	0.3570
j	0.6510	0.3830
k	0.6730	0.3660
l	0.6870	0.3700
m	0.6860	0.3480
n	0.5960	0.3230
o	0.6440	0.3610
p	0.6940	0.3200
q	0.6520	0.3790
r	0.7230	0.3710
s	0.6600	0.3730
t	0.5120	0.3540
u	0.6780	0.3620
v	0.6830	0.3710
w	0.5870	0.3380
x	0.3410	0.2780
y	0.6750	0.3620
z	0.7080	0.3670